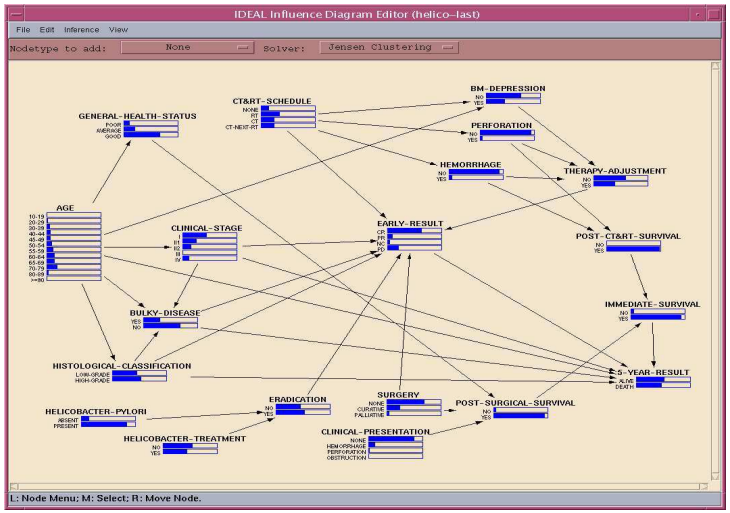
Bayesian networks

Principles and Definitions

Example of a Bayesian network



Why Bayesian networks?

Probabilistic graphical models, such as Bayesian networks, are now the most popular uncertainty formalisms because:

- Handle noise, missing information and probabilistic relations
- Learn from data and can incorporate domain knowledge
- Offer flexible reasoning
- Have compact graphical representation (interface)
- Founded principles: probability theory
- Engineering principles: knowledge acquisition, machine learning and statistics

Popular applications

- Hardware trouble shooting: Microsoft, Boeing, HP
- Biological modelling: gene expressions
- Medical diagnosis and therapy selection: BNs are now the most popular paradigm for medical intelligent systems
- Art: orchestral music accompaniment
- and more . . .

General notation

- Stochastic (= statistical = random) variable: upper-case letter, e.g. X, or upper-case string, e.g. FEVER
- Values: variables can take on values, e.g. $X = x$, FEVER = *yes*
- Binary variables: take one of *two* values, e.g. X = *true* and X = *false*
- Discrete variables: take only one of a finite set of possible values, e.g. $\mathrm{TEMP} = \{$*low, medium, high*$\}$
- Continuous variables: take any value in some interval or intervals of real numbers $\mathcal{R}$, e.g. $\mathrm{TEMP} \in [-50, 50]$

Abbreviated notation

- *Binary* variables: X = *true* as x, and X = *false* as $\neg\mathrm{x}$
- *Non-binary* variables: $X = x$ as x or CITY = *tokyo* as *tokyo*
- *Sets* of variables: analogous to variables
  - Example:

$$\begin{array}{lcl} X_1 = x_1 & & \\ X_2 = x_2 & \qquad X & = (X_1, X_2, \ldots X_n) \\ \quad . \quad \Longrightarrow & x & = (x_1, x_2, \ldots x_n) \\ \quad . & X & = x \\ X_n = x_n & & \end{array}$$

Abreviated notation (cont.)

- Conjunctions: $(X = x) \wedge (Y = y)$ as $(X = x, Y = y)$
- Templates: (X, Y) means $(X = x, Y = y)$, for *any* value x, y, i.e. the choice of the values x and y does not really matter
- Examples:
  - $P(X = x, Y = y) \Leftrightarrow P(X = x \wedge Y = y)$
  - $P(X, Y) \Leftrightarrow P(X = x, Y = y)$, for *any* value x, y
  - $P(X \mid Y) \Leftrightarrow P(X = x \mid Y = y)$, for *any* value x, y
- $\sum_X P(X) = P(\mathrm{x}) + P(\neg\mathrm{x})$, where X is binary

Probability theory

- Probability distribution P: attaches a number in (closed) interval $[0, 1]$ to *Boolean expressions*
- Boolean algebra $\mathbb{B}$ (for two variables RAIN and HAPPY):

  $\top$ (*true*),
  rain, $\neg$*rain*,
  happy, $\neg$*happy*,
  rain $\wedge$ *happy*,..., *rain* $\wedge$ *happy* $\wedge \neg$*happy*, ...,
  $\neg$*rain* $\wedge$ *happy*,..., *rain* $\vee$ *happy*,
  $\bot$ (*false*)

  such that:
  - $\bot \leq$ *rain*, *rain* $\leq$ (*rain* $\vee$ *happy*), ... (in general $\bot \leq x$ for each Boolean expression $x \in \mathbb{B}$);
  - $x \leq \top$ for each Boolean expression $x \in \mathbb{B}$

Probability distribution

- A probability distribution P is defined as a function $P : \mathbb{B} \rightarrow [0, 1]$, such that:
  - $P(\bot) = 0$
  - $P(\top) = 1$
  - $P(x \vee y) = P(x) + P(y)$, if $x \wedge y = \bot$ with $x, y \in \mathbb{B}$
- Examples:
  - $P(\textit{rain} \vee \textit{happy}) = P(\textit{rain}) + P(\textit{happy})$, as $\textit{rain} \wedge \textit{happy} = \bot$ (why? Because I define it that way)
  - $P(\textit{rain} \wedge \textit{happy}) = P(\bot) = 0$
  - $P(\neg\textit{rain} \vee \textit{rain}) = P(\neg\textit{rain}) + P(\textit{rain}) = P(\top) = 1 \Rightarrow P(\neg\textit{rain}) = 1 - P(\textit{rain})$
  - $0 \leq P(\textit{rain}) \leq 1$

Probability distribution (cont.)

- Boolean algebras $\Leftrightarrow$ sets:
  - $\top \Leftrightarrow \Omega$
  - $\bot \Leftrightarrow \varnothing$
  - $x \Leftrightarrow X$
  - $\neg x \Leftrightarrow \bar{X}$
  - $(x \vee y) \Leftrightarrow (X \cup Y)$
  - $(x \wedge y) \Leftrightarrow (X \cap Y)$
  - $x \leq (x \vee y) \Leftrightarrow X \subseteq (X \cup Y)$

with $\Leftrightarrow$ 1-1 correspondence, e.g.

$$P(\overline{\text{Rain}}) = 1 - P(\text{Rain})$$

Joint probability distribution

Let X and Y be random variables with $\{X\} = \{x_1, x_2, \ldots, x_n\}$ and $\{Y\} = \{y_1, y_2, \ldots, y_m\}$.

The product set

$$\{X\} \times \{Y\} = \{x_1, x_2, \ldots, x_n\} \times \{y_1, y_2, \ldots, y_m\}$$

is made into a probability space by defining

$$P(X = x_i \wedge Y = y_j) = P(x_i, y_j)$$

where P is a joint probability function

Marginalisation

Suppose the joint probability distribution of two variables X and Y is given; then

$$\begin{aligned} P(x) = P(X = x) &= P(x \wedge \top) \\ &= P(x \wedge (y \vee \bar{y})) \\ &= P((x \wedge y) \vee (x \wedge \bar{y})) \\ &= P(x \wedge y) + P(x \wedge \bar{y}) \end{aligned}$$

since $P(a \vee b) = P(a) + P(b)$, if $a \wedge b = \bot$

$$\Longrightarrow P(x) = \sum_Y P(x, Y)$$

also known as marginal probability function of X.

Example

- Assume that X_1, X_2, X_3 and X_4 are binary variables. Then $P(X1, X_2, X_3, X_4)$:

$P(x_1, x_2, x_3, x_4)$	=	**0.1**	$P(x_1, \neg x_2, \neg x_3, x_4)$	=	**0.015**
$P(x_1, \neg x_2, x_3, x_4)$	=	**0.04**	$P(x_1, \neg x_2, x_3, \neg x_4)$	=	0.1
$P(x_1, x_2, \neg x_3, x_4)$	=	**0.03**	$P(x_1, x_2, \neg x_3, \neg x_4)$	=	0.004
$P(x_1, x_2, x_3, \neg x_4)$	=	0.1	$P(\neg x_1, \neg x_2, \neg x_3, x_4)$	=	**0.005**
$P(\neg x_1, x_2, x_3, x_4)$	=	**0.0**	$P(\neg x_1, \neg x_2, x_3, \neg x_4)$	=	0.01
$P(\neg x_1, \neg x_2, x_3, x_4)$	=	**0.2**	$P(\neg x_1, x_2, \neg x_3, \neg x_4)$	=	0.01
$P(\neg x_1, x_2, \neg x_3, x_4)$	=	**0.08**	$P(x_1, \neg x_2, \neg x_3, \neg x_4)$	=	0.006
$P(\neg x_1, x_2, x_3, \neg x_4)$	=	0.1	$P(\neg x_1, \neg x_2, \neg x_3, \neg x_4)$	=	0.2

- $\sum_{X1,X2,X3,X4} P(X_1, X_2, X_3, X_4) = 1$
- Marginalisation:

$$P(x_4) = \sum_{X1,X2,X3} P(X_1, X_2, X_3, x_4) = 0.47$$

Conditional probability

(Example: *flu* and *fever*)

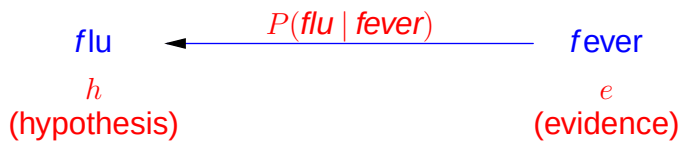
- $P(\textit{flu} \wedge \textit{fever})$: chance of *flu* and *fever* at the same time
- $P(\textit{flu} \mid \textit{fever})$: chance of *flu* knowing that the person already has *fever* (conditional probability)
- Definition:

$$P(\textit{flu} \mid \textit{fever}) = \frac{P(\textit{flu} \wedge \textit{fever})}{P(\textit{fever})}$$

↗ adjust $P(\textit{flu} \wedge \textit{fever})$, so that uncertainty in 'fever' is removed

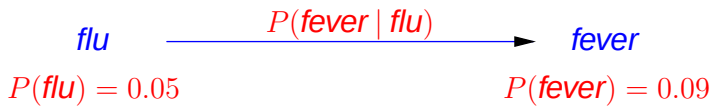
Reversal of chances

- $P(\textit{flu} \mid \textit{fever})$ is usually unknown:



- Known is:

$P(\textit{fever} \mid \textit{flu}) = 0.9$
$P(\textit{flu}) = 0.05$
$P(\textit{fever}) = 0.09$



Bayes' rule

"*I now send you an essay which I have found among the papers of our deceased friend Mr Bayes, and which, in my opinion, has great merit... In an introduction which he has writ to this Essay, he says, that his design at first in thinking on the subject of it was, to find out a method by which we might judge concerning the probability that an event has to happen, in given circumstances, upon supposition that we know nothing concerning it but that, under the same circumstances, it has happened a certain number of times, and failed a certain other number of times.*"

Richard Price
Introducing "Essay towards solving a problem in the doctrine of chances" by Thomas Bayes to the Royal Society of London in 1764

Bayes' rule - Example

- Bayes' rule – reversal of chances:

  $P(e \mid h)$ $P(\textit{fever} \mid \textit{flu}) = 0.9$
  $P(h)$ $P(\textit{flu}) = 0.05$
  $P(e)$ $P(\textit{fever}) = 0.09$

$$\begin{aligned} P(\textit{flu} \mid \textit{fever}) &= \frac{P(\textit{fever} \mid \textit{flu})P(\textit{flu})}{P(\textit{fever})} \\ &= 0.9 \cdot 0.05/0.09 = 0.5 \end{aligned}$$

- Definition of Bayes' rule (the 'chance reverter'):

$$P(h \mid e) = \frac{P(e \mid h)P(h)}{P(e)}$$

Chain rule (derivation)

Definition of conditional probability:

$$P(X_1 \mid X_2, \ldots, X_n) = \frac{P(X_1, X_2, \ldots, X_n)}{P(X_2, \ldots, X_n)}$$

$$\Rightarrow P(X_1, X_2, \ldots, X_n) = P(X_1 \mid X_2, \ldots, X_n)P(X_2, \ldots, X_n)$$

Furthermore,

$$\begin{aligned} P(X_2, \ldots, X_n) &= P(X_2 \mid X_3, \ldots, X_n)P(X_3, \ldots, X_n) \\ &\vdots \quad \vdots \quad \vdots \\ P(X_{n-1}, X_n) &= P(X_{n-1} \mid X_n)P(X_n) \\ P(X_n) &= P(X_n) \end{aligned}$$

Chain rule (definition)

$$\begin{aligned} P(X_1, X_2, \ldots, X_n) &= P(X_1 \mid X_2, \ldots, X_n) \cdot \\ &\quad P(X_2 \mid X_3, \ldots, X_n) \cdot \\ &\quad P(X_3 \mid X_4, \ldots, X_n) \cdot \\ &\quad \vdots \\ &\quad P(X_{n-1} \mid X_n) \cdot \\ &\quad P(X_n) \\ &= \prod_{i=1}^{n-1} P(X_i \mid X_{i+1}, \ldots, X_n)P(X_n) \end{aligned}$$

Definition Bayesian network (BN)

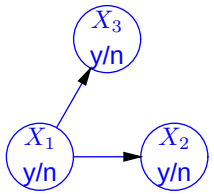
A Bayesian network $\mathcal{B}$ is a pair $\mathcal{B} = (G, P)$, where:

- $G = (V(G), A(G))$ is an acyclic directed graph, with
  - $V(G) = \{v_1, v_2, \ldots, v_n\}$, a set of vertices (nodes)
  - $A(G) \subseteq V(G) \times V(G)$ a set of arcs
- $P : \wp(V(G)) \rightarrow [0, 1]$ is a joint probability distribution, such that

$$P(V(G)) = \prod_{i=1}^{n} P(v_i \mid \pi_G(v_i))$$

  where $\pi_G(v_i)$ denotes the set of immediate ancestors (parents) of vertex v_i in G
- Notational convenience: $v_i \longrightarrow X_i$

Example of a Bayesian network



Bayesian network $\mathcal{B} = (G, P)$, where $G = (V(G), A(G))$, with

- Set of vertices: $V(G) = \{X_1, X_2, X_3\}$
- Set of arcs: $A(G) = \{(X_1, X_2), (X_1, X_3)\}$
- Joint probability distribution:

$$P(X_1, X_2, X_3) = P(X_1) \cdot P(X_2 \mid X_1) \cdot P(X_3 \mid X_1)$$

Example (cont.)

$$P(X_1, X_2, X_3) = P(X_1) \cdot P(X_2 \mid X_1) \cdot P(X_3 \mid X_1)$$

with for example:

$$\begin{aligned} P(x_1) &= 0.7 \\ P(\neg x_1) &= 0.3 = 1 - P(x_1) \end{aligned}$$

$$\begin{aligned} P(x_2 \mid x_1) &= 0.6 & \qquad P(x_3 \mid x_1) &= 0.1 \\ P(\neg x_2 \mid x_1) &= 0.4 & \qquad P(\neg x_3 \mid x_1) &= 0.9 \end{aligned}$$

$$\begin{aligned} P(x_2 \mid \neg x_1) &= 0.1 & \qquad P(x_3 \mid \neg x_1) &= 0.8 \\ P(\neg x_2 \mid \neg x_1) &= 0.9 & \qquad P(\neg x_3 \mid \neg x_1) &= 0.2 \end{aligned}$$

Conditional independence relation

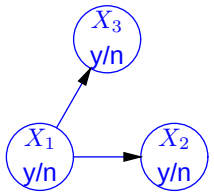
Let X, Y, Z be *sets* of variables, such that $X, Y, Z \subseteq V(G)$, then X is called conditionally independent of Y given Z, denoted as

$$X \perp\!\!\!\perp_P Y \mid Z$$

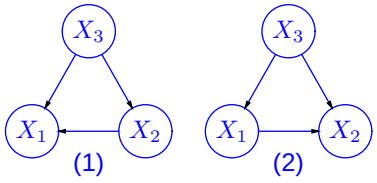
if and only if

$$P(X \mid Y, Z) = P(X \mid Z)$$

Example: Representation of $X_2 \perp\!\!\!\perp_P X_3 \mid X_1$ in a directed graph



Chain rule - digraph



Factorisation (1):

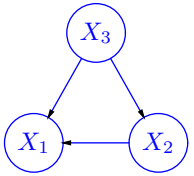
$$P(X_1, X_2, X_3) = P(X_1 \mid X_2, X_3) P(X_2 \mid X_3) P(X_3)$$

Other factorisation (2):

$$P(X_1, X_2, X_3) = P(X_2 \mid X_1, X_3) P(X_1 \mid X_3) P(X_3)$$

$\Rightarrow$ different *factorisations* possible

Does the chain rule help?



$$P(X_1, X_2, X_3) = P(X_1 \mid X_2, X_3)P(X_2 \mid X_3)P(X_3)$$

i.e. we need:

$$\begin{array}{ll} P(x_1 \mid x_2, x_3) & P(x_1 \mid x_2, \neg x_3) \\ P(\neg x_1 \mid x_2, x_3) & P(\neg x_1 \mid x_2, \neg x_3) \\ P(x_1 \mid \neg x_2, x_3) & P(x_1 \mid \neg x_2, \neg x_3) \\ P(\neg x_1 \mid \neg x_2, x_3) & P(\neg x_1 \mid \neg x_2, \neg x_3) \\ \vdots & \vdots \end{array}$$

Does the chain rule help?

$$\begin{array}{ll} \vdots & \vdots \\ P(x_2 \mid x_3) & P(x_3) \\ P(\neg x_2 \mid x_3) & P(\neg x_3) \\ P(x_2 \mid \neg x_3) & \\ P(\neg x_2 \mid \neg x_3) & \end{array}$$

So, 14 probabilities; however
$P(x_1 \mid X_2, X_3) = 1 - P(\neg x_1 \mid X_2, X_3)$,
$P(x_2 \mid X_3) = 1 - P(\neg x_2 \mid X_3)$, and $P(x_3) = 1 - P(\neg x_3)$

$\Rightarrow$ 7 probabilities required

How many did we have originally for $P(X_1, X_2, X_3)$?

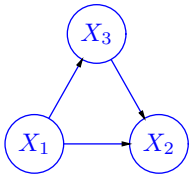
Does the chain rule help?

$$\begin{array}{ll} P(x_1, x_2, x_3) & P(x_1, x_2, \neg x_3) \\ P(\neg x_1, x_2, x_3) & P(\neg x_1, x_2, \neg x_3) \\ P(x_1, \neg x_2, x_3) & P(x_1, \neg x_2, \neg x_3) \\ P(\neg x_1, \neg x_2, x_3) & P(\neg x_1, \neg x_2, \neg x_3) \end{array}$$

8 required? No, because $\sum_{X_1, X_2, X_3} P(X_1, X_2, X_3) = 1$
Hence, e.g.

$$\begin{aligned} P(x_1, x_2, x_3) &= 1 - \sum_{X_2, X_3} P(\neg x_1, X_2, X_3) \\ &\quad - \sum_{X_3} P(x_1, \neg x_2, X_3) - P(x_1, x_2, \neg x_3) \end{aligned}$$

Let's use stochastic independence



$$P(X_1, X_2, X_3) = P(X_2 \mid X_1, X_3)P(X_3 \mid X_1)P(X_1)$$

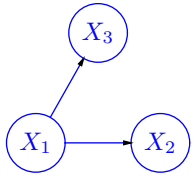
Now assume that X_2 and X_3 are conditionally independent given X_1:

$$P(X_2 \mid X_1, X_3) = P(X_2 \mid X_1)$$

and

$$P(X_3 \mid X_1, X_2) = P(X_3 \mid X_1)$$

Stochastic independence: does it help?



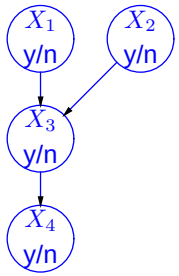
$$P(X_2 \mid X_1, X_3) = P(X_2 \mid X_1)$$

$$\begin{aligned} P(X_1, X_2, X_3) &= P(X_2 \mid X_1, X_3)P(X_3 \mid X_1)P(X_1) \\ &= P(X_2 \mid X_1)P(X_3 \mid X_1)P(X_1) \end{aligned}$$

Only $5 = 2 + 2 + 1$ probabilities required instead of 7

Probabilistic inference

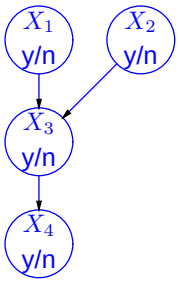
Given:



$P(x_4 \mid x_3) = 0.4$
$P(x_4 \mid \neg x_3) = 0.1$
$P(x_3 \mid x_1, x_2) = 0.3$
$P(x_3 \mid \neg x_1, x_2) = 0.5$
$P(x_3 \mid x_1, \neg x_2) = 0.7$
$P(x_3 \mid \neg x_1, \neg x_2) = 0.9$
$P(x_1) = 0.6$
$P(x_2) = 0.2$

Then:
$$\begin{aligned} P(x_4) &= P(x_4, x_3) + P(x_4, \neg x_3) \\ &\quad \text{(marginalisation)} \\ &= P(x_4 \mid x_3)P(x_3) + P(x_4 \mid \neg x_3)P(\neg x_3) \\ &\quad \text{(conditioning)} \\ &= \sum_{X_3} P(x_4 \mid X_3)P(X_3) \end{aligned}$$

Probabilistic inference

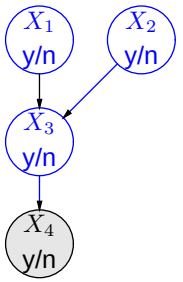


$P(x_4 \mid x_3) = 0.4$
$P(x_4 \mid \neg x_3) = 0.1$
$P(x_3 \mid x_1, x_2) = 0.3$
$P(x_3 \mid \neg x_1, x_2) = 0.5$
$P(x_3 \mid x_1, \neg x_2) = 0.7$
$P(x_3 \mid \neg x_1, \neg x_2) = 0.9$
$P(x_1) = 0.6$
$P(x_2) = 0.2$

$$\begin{aligned} P(x_3) &= \textstyle\sum_{X_1,X_2} P(x_3, X_1, X_2) \\ &= \textstyle\sum_{X_1,X_2} P(x_3 \mid X_1, X_2)P(X_1, X_2) \\ &= \textstyle\sum_{X_1,X_2} P(x_3 \mid X_1, X_2)P(X_1)P(X_2) \end{aligned}$$

$\Rightarrow P(x_4) = \sum_{X_3} P(x_4 \mid X_3) \sum_{X_1,X_2} P(X_3 \mid X_1, X_2)P(X_1, X_2)$
= 0.31

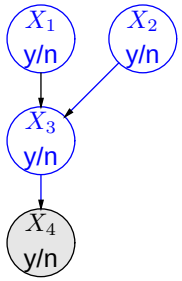
Probabilistic inference: evidence



$P(x_4 \mid x_3) = 0.4$
$P(x_4 \mid \neg x_3) = 0.1$
$P(x_3 \mid x_1, x_2) = 0.3$
$P(x_3 \mid \neg x_1, x_2) = 0.5$
$P(x_3 \mid x_1, \neg x_2) = 0.7$
$P(x_3 \mid \neg x_1, \neg x_2) = 0.9$
$P(x_1) = 0.6$
$P(x_2) = 0.2$

$$\begin{aligned} P^*(x_4) = P(x_4 \mid x_2) &= \textstyle\sum_{X_3} P(x_4 \mid x_2, X_3)P(X_3 \mid x_2) \\ &= \textstyle\sum_{X_3} P(x_4 \mid X_3)P(X_3 \mid x_2) \\ &= \textstyle\sum_{X_3} P(x_4|X_3) \sum_{X_1} P(X_3|X_1, x_2)P(X_1|x_2) \\ &= \textstyle\sum_{X_3} P(x_4|X_3) \sum_{X_1} P(X_3|X_1, x_2)P(X_1) \\ &= 0.214 \end{aligned}$$

Probabilistic inference: evidence

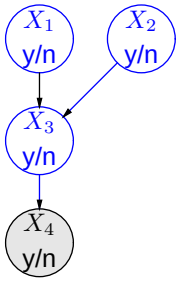


$P(x_4 \mid x_3) = 0.4$
$P(x_4 \mid \neg x_3) = 0.1$
$P(x_3 \mid x_1, x_2) = 0.3$
$P(x_3 \mid \neg x_1, x_2) = 0.5$
$P(x_3 \mid x_1, \neg x_2) = 0.7$
$P(x_3 \mid \neg x_1, \neg x_2) = 0.9$
$P(x_1) = 0.6$
$P(x_2) = 0.2$

$$P^*(x_2) = P(x_2 \mid x_4) = \frac{P(x_4 \mid x_2)P(x_2)}{P(x_4)} \text{ (Bayes' rule)}$$

$$\begin{aligned} P(x_4 \mid x_2) &= 0.214, \quad P(x_4) = 0.31 \\ \Rightarrow P^*(x_2) &= 0.214 \cdot 0.2/0.31 \\ &\approx 0.1381 \end{aligned}$$

Probabilistic inference: evidence



$P(x_4 \mid x_3) = 0.4$
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$P(x_1) = 0.6$
$P(x_2) = 0.2$

$$\begin{aligned} P^*(x_2) &= P(x_2 \mid x_4) = P(x_4 \mid x_2)P(x_2)/P(x_4) \\ &= \frac{\sum_{X_3} P(x_4|X_3) \sum_{X_1} P(X_3|X_1, x_2) P(X_1) P(x_2)}{\sum_{X_3} P(x_4 \mid X_3) \sum_{X_1, X_2} P(X_3 \mid X_1, X_2) P(X_1) P(X_2)} \end{aligned}$$

Bayesian software and links

- Some software companies in this area:
  - Hugin (Denmark): `www.hugin.dk`
  - Norsys (USA): `www.norsys.com`
  - Knowledge Industries (USA): `www.kic.com`
  - BayesWare (USA): `www.bayesware.com`
  - Bayesia (France): `www.bayesia.com`
- Some public domain software:
  - JavaBayes: `www-2.cs.cmu.edu/~javabayes`
  - BayesBuilder: `www.snn.ru.nl/nijmegen/`
  - Ideal: Lisp based
  - Elvira: `leo.ugr.es/~elvira`
  - BNT (Murphy's toolbox, Matlab based): `http://bnt.sourceforge.net/`