BML. 6.2. Probabilistic graphical models aka Bayesian networks aka ...

DataLab CSIC

Objectives

Introduce key concepts about PGMs. Conditional independence. Representations: directed (and undirected). Hints on computations and inference. Influence diagrams. Gibbs sampling for BNs.

Contents

- Bayesian networks
- Conditional Independence
- Markov random fields
- Inference
- Influence diagrams

Bishop 8, Goodfellow et al 16

Lab

- A couple of labs around probabilistic graphical models
  - Handling PGMs
  - Structuring PGMs

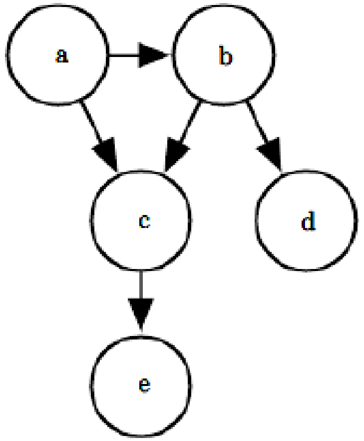
PGMs. Motivation

Motivation

- Simple way to visualize structure of probabilistic models
- Designing and motivating new models
- Understanding properties like conditional independence
- Complex computations viewed through simple graphical manipulations
- Explainable and interpretable
- Classification, generation.
- Deep belief nets in deep learning

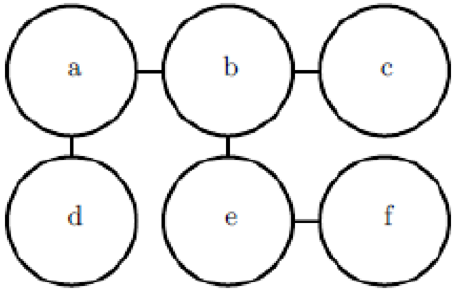
Concept

$$p(\mathbf{x}) = \prod_i p\left(\mathrm{x}_i \mid Pa_{\mathcal{G}}(\mathrm{x}_i)\right)$$



$$p(\mathrm{a}, \mathrm{b}, \mathrm{c}, \mathrm{d}, \mathrm{e}) = p(\mathrm{a})p(\mathrm{b} \mid \mathrm{a})p(\mathrm{c} \mid \mathrm{a}, \mathrm{b})p(\mathrm{d} \mid \mathrm{b})p(\mathrm{e} \mid \mathrm{c})$$

$$\tilde{p}(\mathbf{x}) = \Pi_{\mathcal{C} \in \mathcal{G}}\, \phi(\mathcal{C})$$



$$p(\mathrm{a}, \mathrm{b}, \mathrm{c}, \mathrm{d}, \mathrm{e}, \mathrm{f}) \quad \frac{1}{Z}\phi_{\mathrm{a},\mathrm{b}}(\mathrm{a}, \mathrm{b})\phi_{\mathrm{b},\mathrm{c}}(\mathrm{b}, \mathrm{c})\phi_{\mathrm{a},\mathrm{d}}(\mathrm{a}, \mathrm{d})\phi_{\mathrm{b},\mathrm{e}}(\mathrm{b}, \mathrm{e})\phi_{\mathrm{e},\mathrm{f}}(\mathrm{e}, \mathrm{f})$$

Bayesian networks. Directed, Acyclic

Markov fields. Undirected

Probabilistic graphical models. Directed Bayesian networks

Directed PGMs

As basic tools for qualitative modelling of uncertainty use probabilistic influence diagrams a.k.a. causal networks, Bayesian networks, Belief networks,…. See the excellent

http://en.wikipedia.org/wiki/Bayesian_network

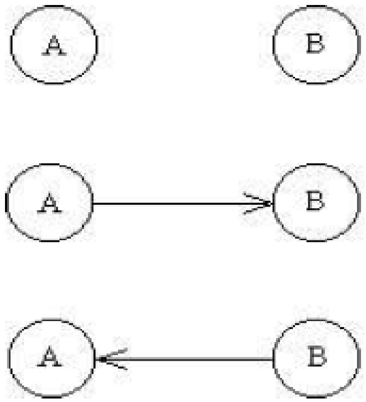
They are **influence diagrams** with chance nodes only. Qualitatively they describe a probabilistic model through

$$P(A1, A2,\ldots, An) = P(A1 \mid ant(A1))\ldots P(An \mid ant (An))$$

where ant (Ai) are the antecessors of node Ai.

In what follows we see several PIDs and we need to indicate the entailed probabilistic model

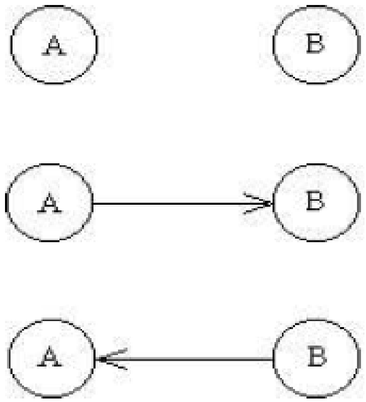
Probabilistic diagrams with two nodes



Before moving foreward, write the entailed probabilistic model

Probabilistic diagrams with two nodes

Model for P(A,B)



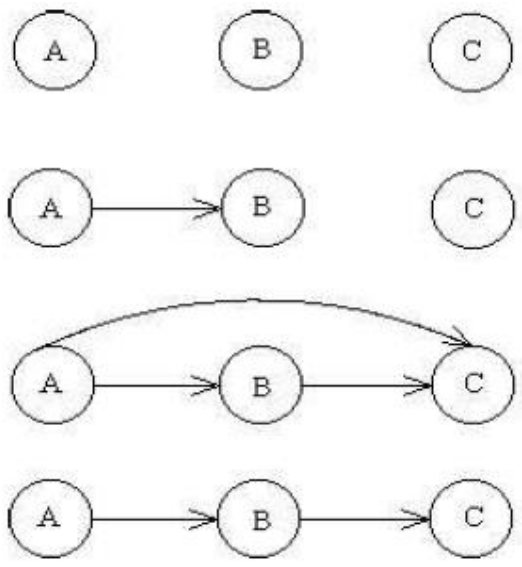
P(A)P(B)

P(A) P(B|A)

P(B) P(A|B)

First case, A and B are independent. We move from second to third, and viceversa, via Bayes formula

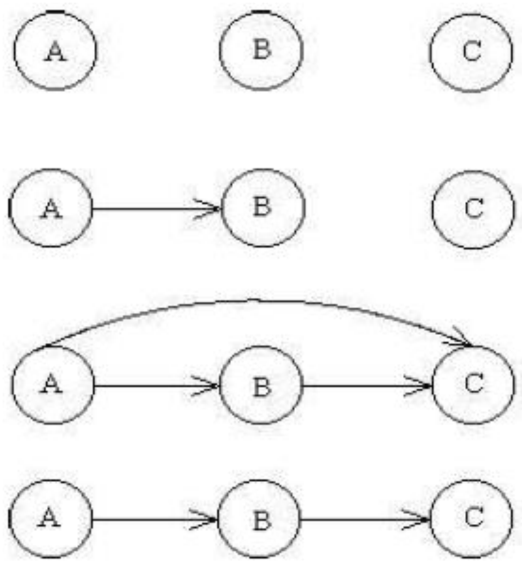
Probabilistic diagrams with three nodes



Before moving foreward, write the entailed probabilistic model

Probabilistic diagrams with three nodes

Model P(A ,B ,C)



P(A)P(B)P(C)

P(A) P(B|A) P(C)

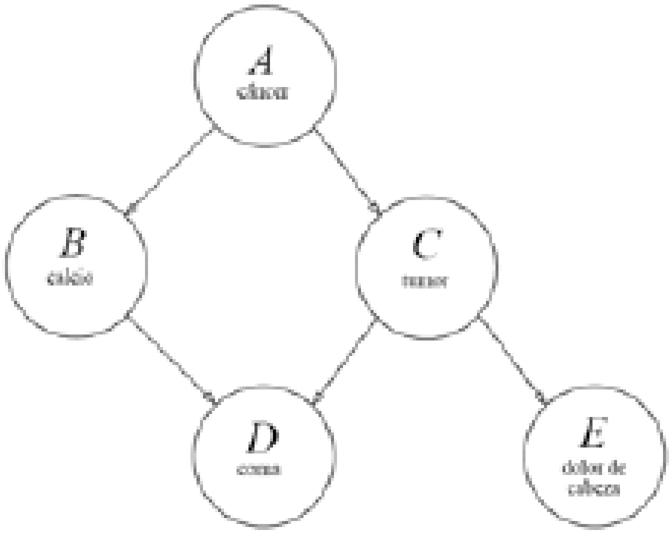
P(A)P(B|A)P(C|A,B)

P(A)P(B|A)P(C|B)

First case, independence. Third case, A and C are conditionally independent given B.

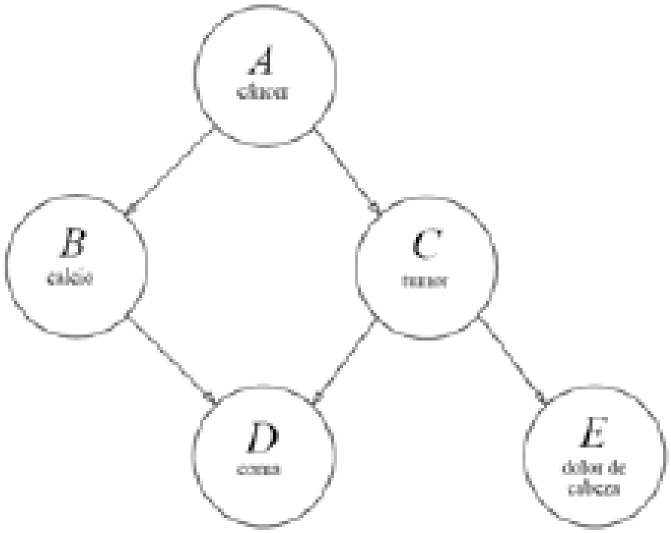
Read http://en.wikipedia.org/wiki/Conditional_independence

The hidden info



$$P(A, B, C, D, E) = P(A)P(B|A)P(C|A)P(D|B, C)P(E|C)$$

The hidden info



a	0.2

	a	$\overline{a}$
b	0.8	0.2

	a	$\overline{a}$
c	0.2	0.05

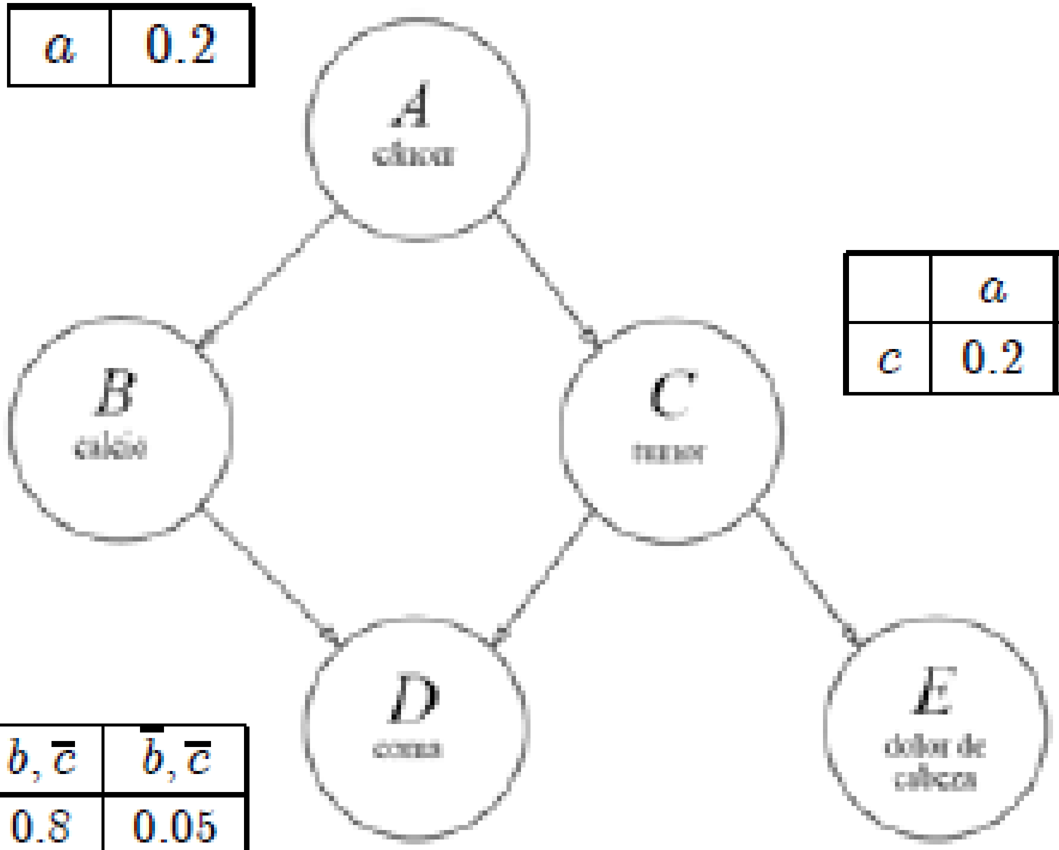
	b, c	$\overline{b}, c$	$b, \overline{c}$	$\overline{b}, \overline{c}$
d	0.8	0.8	0.8	0.05

	c	$\overline{c}$
e	0.8	0.6

$$P(A, B, C, D, E) = P(A)P(B|A)P(C|A)P(D|B, C)P(E|C)$$

The hidden info

a	0.2



	a	$\overline{a}$
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	b, c	$\overline{b}, c$	$b, \overline{c}$	$\overline{b}, \overline{c}$
d	0.8	0.8	0.8	0.05

	c	$\overline{c}$
e	0.8	0.6

No need to be discrete!!!!

Conditional Independence I

A and B conditional independent given C if

$$p(A|B,C)=p(A|C)$$

or

$$p(A,B|C) = p(A|C)\, p(B|C)$$

$$a \perp\!\!\!\perp b \mid c$$

d-separation etc..
De Finetti's representation theorem

Probabilistic diagrams. Asia

An example referring to lung diseases

A breathing condition (dyspnea) may be due to tuberculosis, lung cancer or bronchitis, none of them or several of them. A recent visit to Asia, increases the chances of tuberculosis, whereas smoking is a risk factor for lung cancer and bronchitis. The results of an X-ray may not discriminate between cancer and tuberculosis, as neither the presence or absence of dyspnea does.

Probabilistic diagrams

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A breathing condition (dyspnea) may be due to tuberculosis, lung cancer or bronchitis, none of them or several of them. A recent visit to Asia, increases the chances of tuberculosis, whereas smoking is a risk factor for lung cancer and bronchitis. The results of an X-ray may not discriminate between cancer and tuberculosis, as neither the presence or absence of dyspnea does.

Probabilistic diagrams

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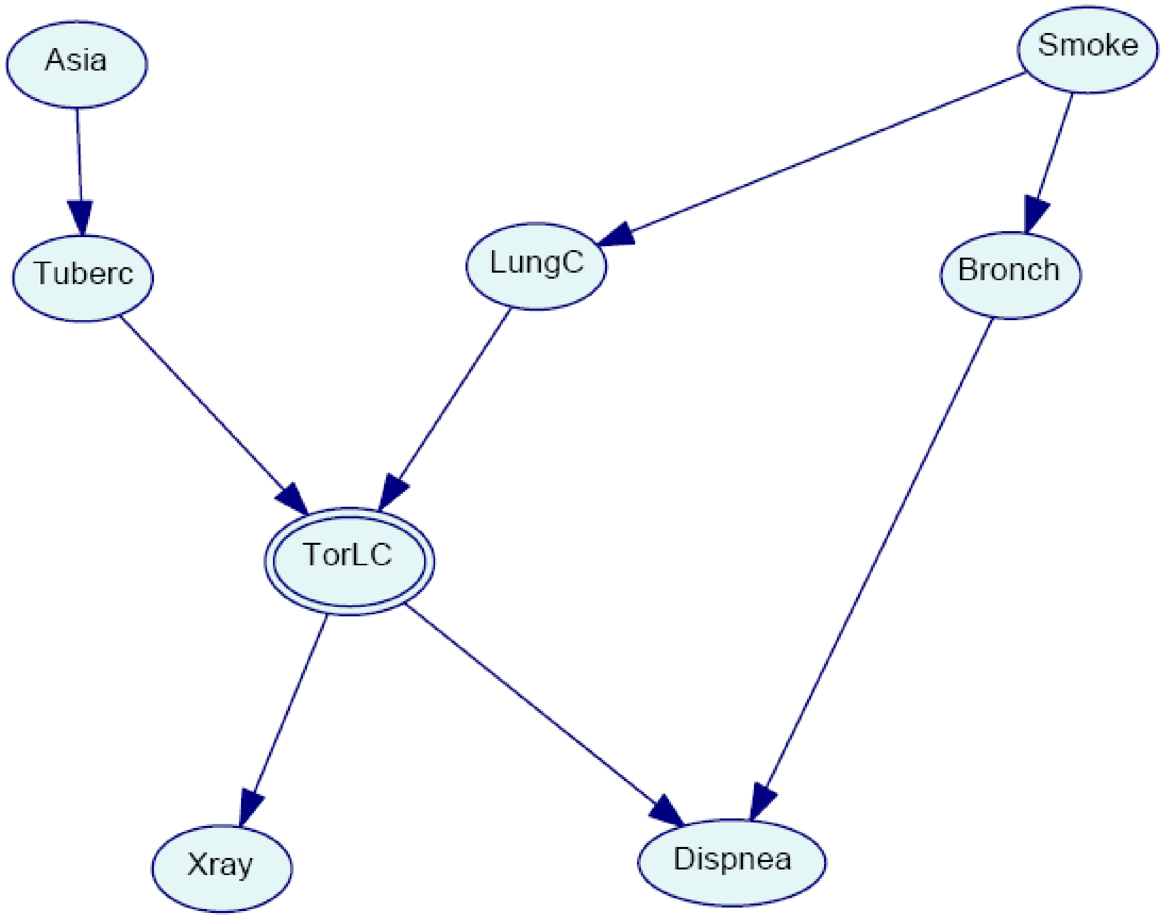
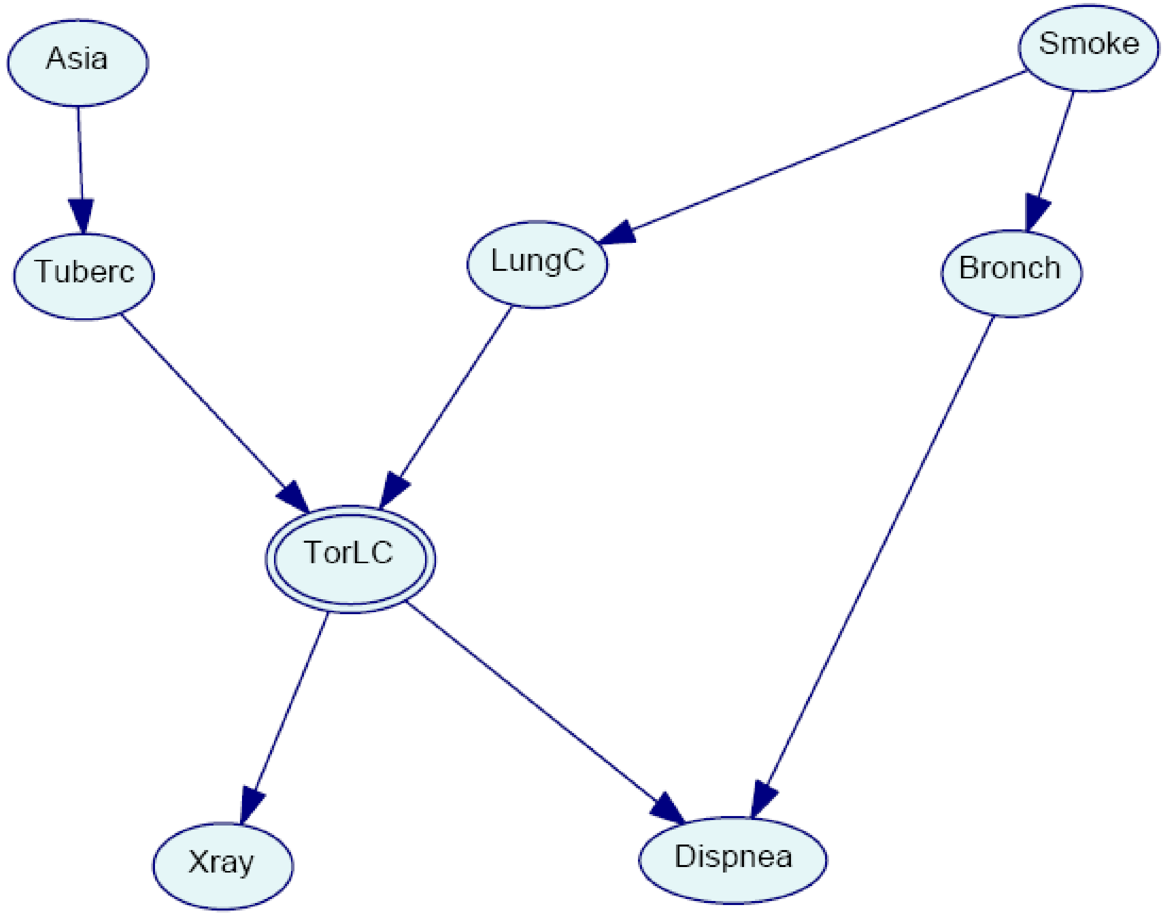
Probabilistic diagrams



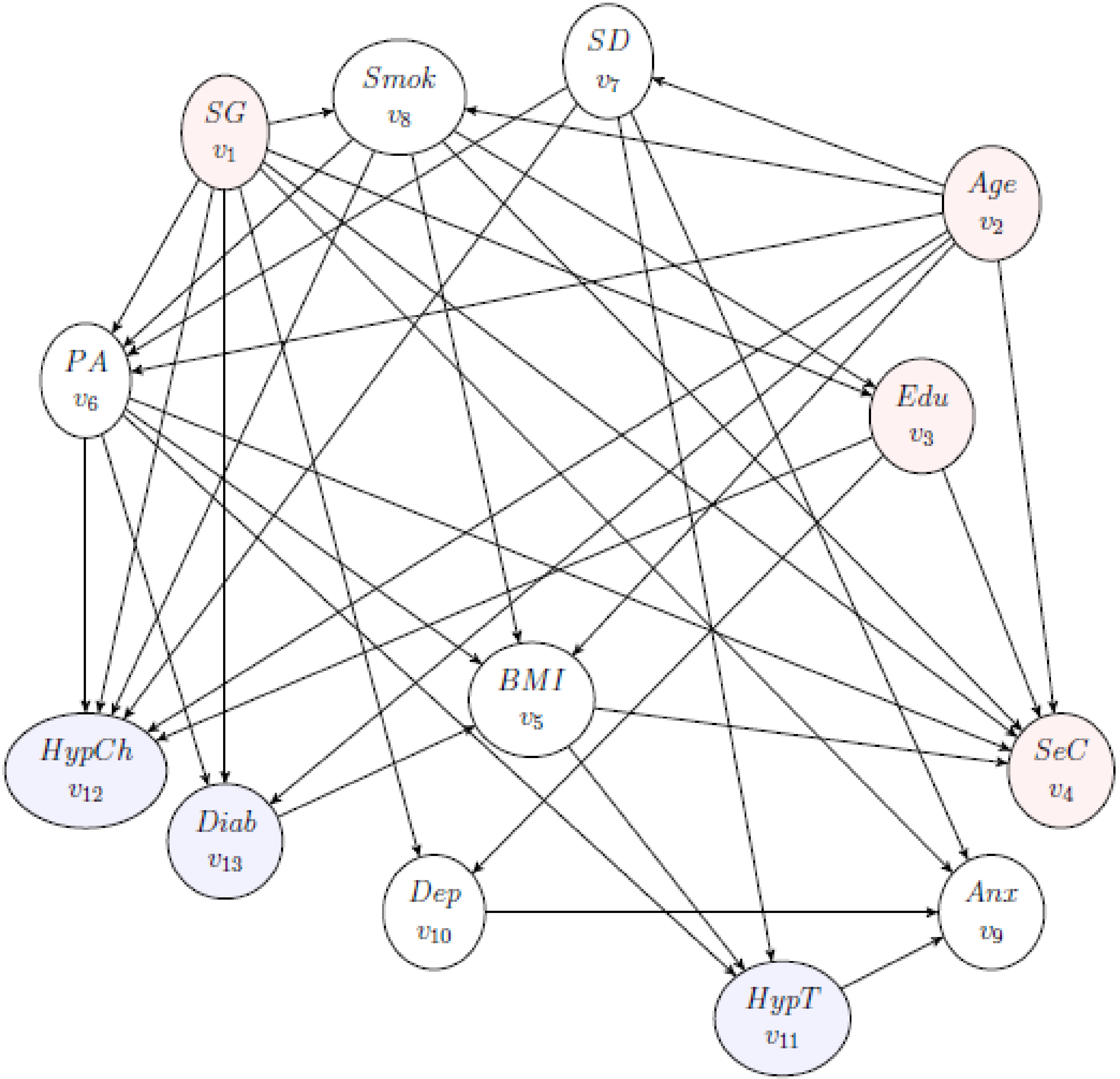
Provide the model

Probabilistic diagrams



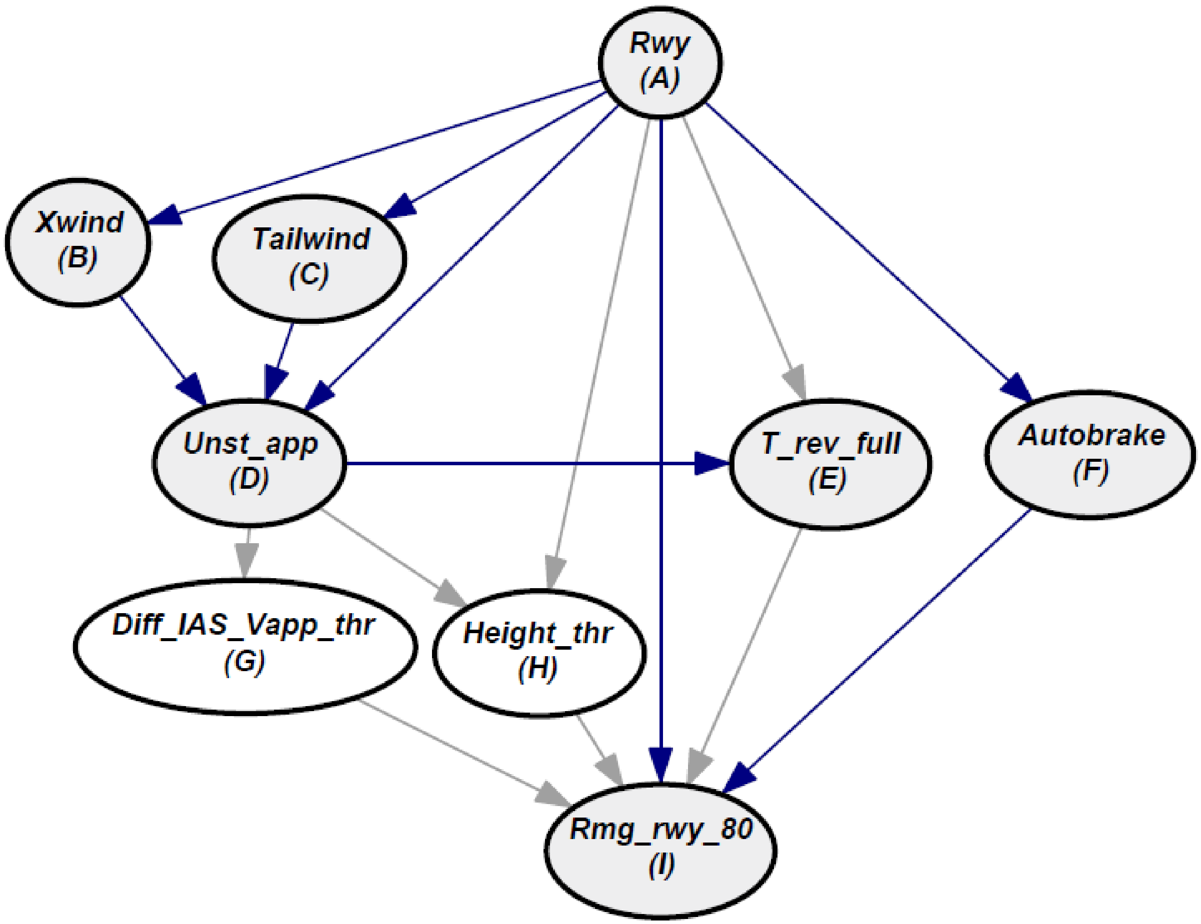
P(A,T,S,L,B,O,X,D) = P(A)P(T|A)P(S)P(L|S)P(B|S)P(0|T,L)P(X|O)P(D|O,B)

Hypertension



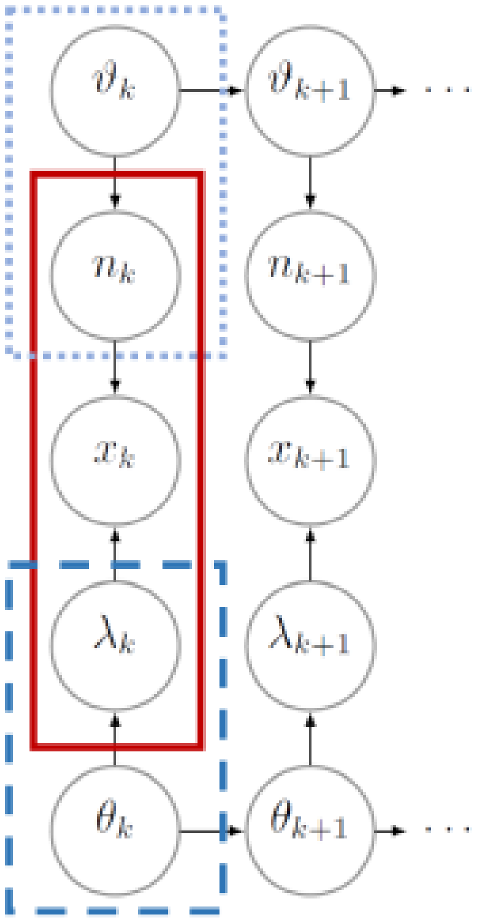
Build the probabilistic model

Runway excursions at airports



Build the probabilistic model

National aviation safety plan



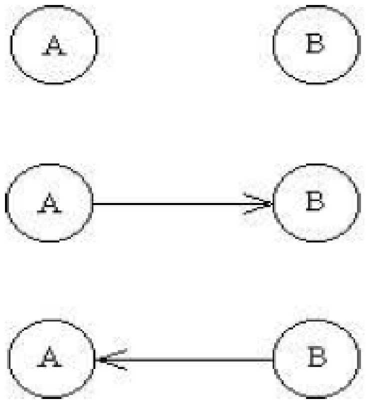
$$
\begin{cases}
\begin{cases}
\begin{cases}
n_k = \boldsymbol{H}_k \vartheta_k + z_k, \;\; z_k \sim N(0, \Sigma_k) \\
\vartheta_k = \boldsymbol{J}_k \vartheta_{i-1} + \xi_k, \;\; \xi_k \sim N(\boldsymbol{0}, \boldsymbol{S}_k)
\end{cases} \\
\vartheta_0 \sim N(\boldsymbol{\eta}_0, \boldsymbol{S}_0)
\end{cases} \\
x_k | \lambda_k, n_k \sim Po(\lambda_k n_k), \quad \lambda_k = \exp(u_k) \\
\begin{cases}
\begin{cases}
u_k = \boldsymbol{F}_k \boldsymbol{\theta}_k + v_k, \;\; v_k \sim N(0, V_k) \\
\boldsymbol{\theta}_k = \boldsymbol{G}_k \boldsymbol{\theta}_{k-1} + \boldsymbol{w}_k, \;\; \boldsymbol{w}_k \sim N(\boldsymbol{0}, \boldsymbol{W}_k)
\end{cases} \\
\boldsymbol{\theta}_0 \sim N(\boldsymbol{m}_0, \boldsymbol{C}_0),
\end{cases}
\end{cases}
$$

Assessments. Discrete case

1 node

$$p(x|\mu) = \prod_{k=1}^{K} \mu_k^{x_k} \longrightarrow K-1$$

2 nodes



$$p(x_1,x_2|\mu) = \prod_{k=1}^{K}\prod_{l=1}^{K} \mu_{kl}^{x_{1k}x_{2l}} \longrightarrow K^2-1$$

$$p(x_1,x_2) = p(x_2|x_1)\,p(x_1) \quad \begin{matrix}(K-1)\\ + \\ K(K-1)\end{matrix} \longrightarrow K^2-1$$

$$p(x_1,x_2) = p(x_1)\,p(x_2) \longrightarrow 2(K-1)$$

M nodes

FULLY CONNECTED $\longrightarrow K^M-1$

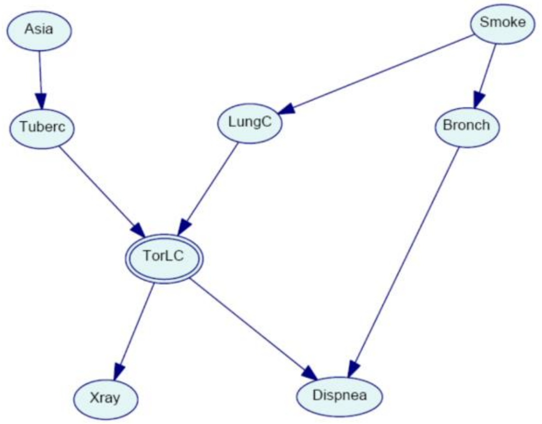
INDEPENDENT $\longrightarrow M(K-1)$

M.CHAIN $(K-1)+(M-1)K(K-1)$ $\longrightarrow O(K^2)$, $O(M)$

Inference in graphical models

General problem

Assuming DAG (arcs and distributions at nodes):

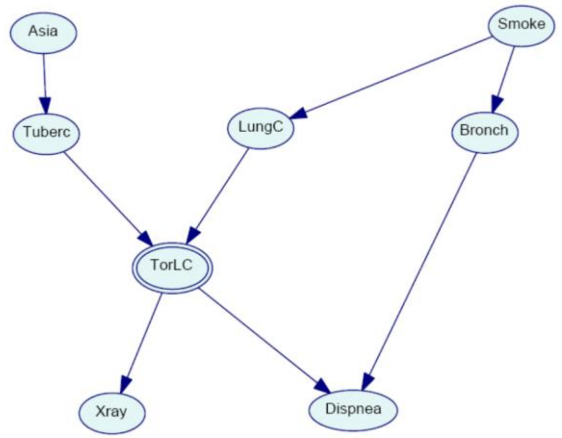


1. Initialisation
2. Absorption of evidence
3. Global propagation of evidence
4. Hypothesising and propagating single pieces of evidence
5. Planning
6. Influential findings

Core ideas

Model $p(\alpha, \tau, \xi, \varepsilon, \delta, \lambda, \beta, \sigma)$

expressed as $p(\alpha)p(\tau \mid \alpha)p(\xi \mid \varepsilon)p(\varepsilon \mid \tau, \lambda)p(\delta \mid \varepsilon, \beta)p(\lambda \mid \sigma)p(\beta \mid \sigma)p(\sigma)$



Typical (probabilistic) query $p(x \mid a, d)$

Trivially $p(x, a, d)/p(a, d)$ and can be computed by brute force.....

Idea 1. Take advantage of structure

$$p(a) \sum_{\tau} p(\tau \mid a)\left[\sum_{\varepsilon} p(x \mid \varepsilon)\left[\sum_{\lambda} p(\varepsilon \mid \tau, \lambda)\left[\sum_{\beta} p(d \mid \varepsilon, \beta)\left[\sum_{\sigma} p(\lambda \mid \sigma)p(\beta \mid \sigma)p(\sigma)\right]\right]\right]\right]$$

Core ideas

Idea 2. Full calculation not needed until the end

$$p(\alpha)p(\tau \mid \alpha)p(\xi \mid \varepsilon)p(\varepsilon \mid \tau, \lambda)p(\delta \mid \varepsilon, \beta)p(\lambda \mid \sigma)p(\beta \mid \sigma)p(\sigma)$$

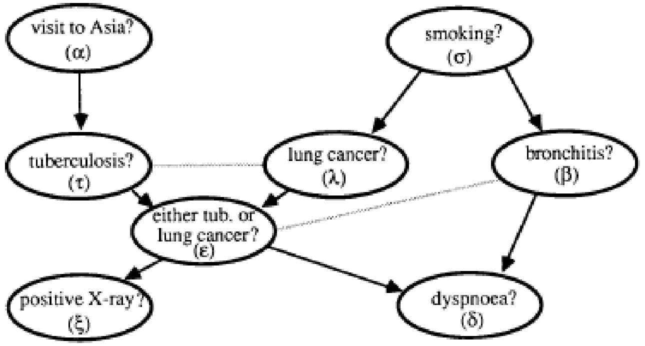
Rewritten (initially) as

$$\psi(\alpha)\psi(\tau, \alpha)\psi(\xi, \varepsilon)\psi(\varepsilon, \tau, \lambda)\psi(\delta, \varepsilon, \beta)\psi(\lambda, \sigma)\psi(\beta, \sigma)\psi(\sigma)$$

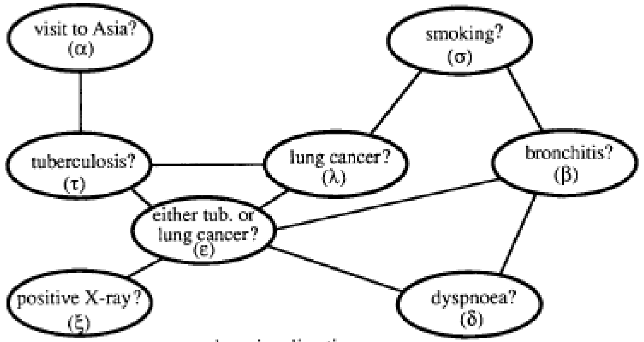
Idea 3. Track computations through moral graph

Idea 4. Actually track it through triangulated mg

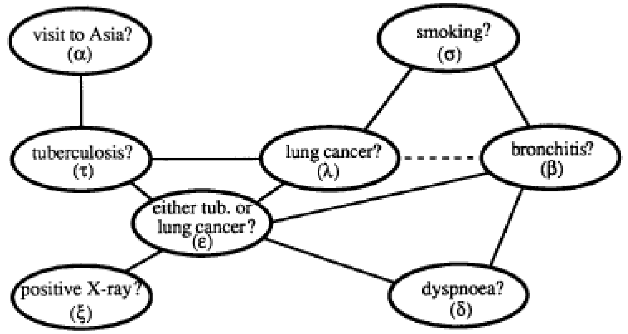
$$p \propto \psi(\alpha, \tau)\psi(\tau, \lambda, \varepsilon)\psi(\lambda, \varepsilon, \beta)\psi(\lambda, \beta, \sigma)\psi(\varepsilon, \beta, \delta)\psi(\varepsilon, \xi)$$



marrying parents



dropping directions

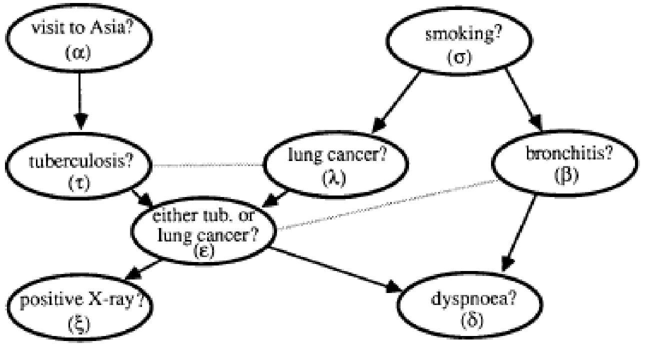


Core ideas

Idea 6. Represent joint in terms of marginals on cliques

$$\frac{p(\alpha,\ \tau)p(\tau,\ \lambda,\ \varepsilon)p(\lambda,\ \varepsilon,\ \beta)p(\lambda,\ \beta,\ \sigma)p(\varepsilon,\ \beta,\ \delta)p(\varepsilon,\ \xi)}{p(\tau)p(\lambda,\ \varepsilon)p(\lambda,\ \beta)p(\varepsilon,\ \beta)p(\varepsilon)}$$

Idea 7. Store clique marginals



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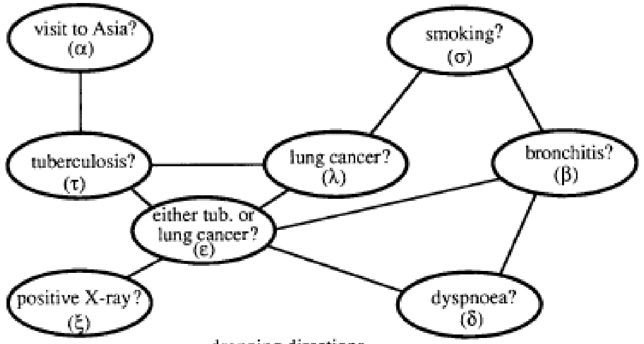
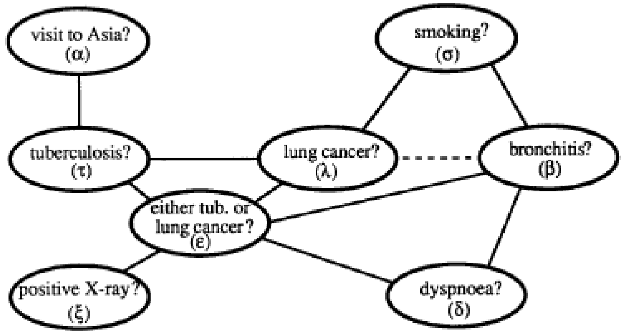


dropping directions



Algos

Sum-product

Max-product

Junction tree

……

Simulation based

Sampling from a belief network. Generative model

$$p(\mathbf{x}) = \prod_i p\left(\mathrm{x}_i \mid Pa_{\mathcal{G}}(\mathrm{x}_i)\right)$$

For $i = 1$ to n

Sample $x_i \sim p(x_i \mid Pa_{\mathcal{G}}(x_i))$

Generic Gibbs sampler

$$X = (X_1, \dots, X_p) \sim \pi$$

Sample from $X_s \mid X_{-s} = (X_1, \dots, X_{s-1}, X_{s+1}, \dots, X_p)$

Initialize $X_1^0, \dots, X_p^0$, $i = 1$

Iterate

Sample $X_1^i \sim X_1 \mid X_2^{i-1}, \dots, X_p^{i-1}$

Sample $X_2^i \sim X_2 \mid X_1^i, X_3^{i-1}, \dots, X_p^{i-1}$

...

Sample $X_p^i \sim X_p \mid X_1^i, X_2^i, \dots, X_{p-1}^{i}$

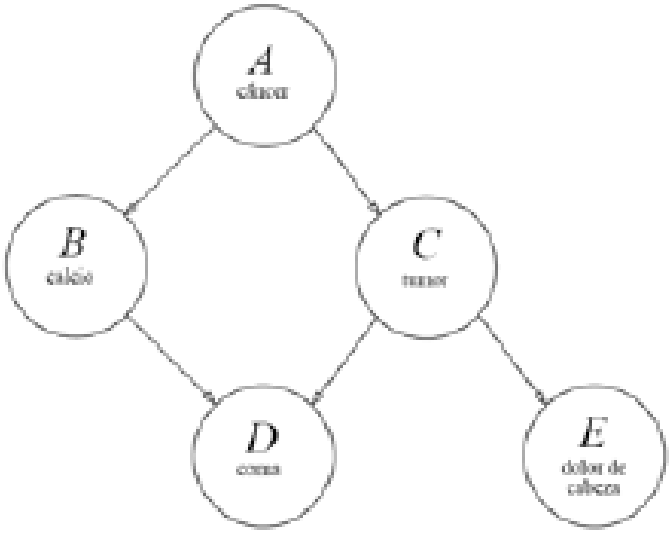
$i = i + 1$

Gibbs sampler for belief nets

Conditionals

$$P(X_j = x_j | X_{-j} = x_{-j}) = \alpha P(X_j = x_j | \Pi_{X_j}(x_{-j})) \prod_{Y_j \in S_j} P(Y_j = y_j | \Pi_{Y_j}(x_j))$$

Back to example



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	b, c	$\overline{b}, c$	$b, \overline{c}$	$\overline{b}, \overline{c}$
d	0.8	0.8	0.8	0.05

	c	$\overline{c}$
e	0.8	0.6

$$P(c|\overline{d}, e) = \frac{P(c, \overline{d}, e)}{P(\overline{d}, e)}$$

$$\begin{aligned} P(c, \overline{d}, e) &= \sum_{\alpha,\beta} P(\alpha, \beta, c, \overline{d}, e) = \sum_{\alpha,\beta} P(\alpha)P(\beta|\alpha)P(c|\alpha)P(\overline{d}|\beta, c)P(e|c) \\ &= P(a)P(b|a)P(c|a)P(\overline{d}|b, c)P(e|c) + P(a)P(\overline{b}|a)P(c|a)P(\overline{d}|\overline{b}, c)P(e|c) + \\ &\quad P(\overline{a})P(b|\overline{a})P(c|\overline{a})P(\overline{d}|b, c)P(e|c) + P(\overline{a})P(\overline{b}|\overline{a})P(c|\overline{a})P(\overline{d}|\overline{b}, c)P(e|c) \\ &= 0.0118 \end{aligned}$$

$$P(\overline{d}, e) = \sum_{\alpha,\beta,\gamma} P(\alpha, \beta, \gamma, \overline{d}, e) = 0.410$$

$$P(A, B, C, D, E) = P(A)P(B|A)P(C|A)P(D|B, C)P(E|C)$$

$$P(c|\overline{d}, e) = 0.0287$$

Back to example

$$
\begin{aligned}
P(A|B,C,\overline{d},e) &= P(A|x_{-A}) = \alpha_1 P(A)P(B|A)P(C|A) \\
P(B|A,C,\overline{d},e) &= P(B|x_{-B}) = \alpha_2 P(B|A)P(\overline{d}|B,C) \\
P(C|A,B,\overline{d},e) &= P(C|x_{-C}) = \alpha_3 P(C|A)P(\overline{d}|B,C)P(e|C)
\end{aligned}
$$

Seleccionar $B = b_0$, $C = c_0$ arbitrariamente
Hacer $j = 1$
Mientras no se juzgue convergencia,
    Generar $A_j = a_j \sim P(A|x_{-A}) = \alpha_{1j} P(A)P(b_{j-1}|A)P(c_{j-1}|A)$
    Generar $B_j = b_j \sim P(B|x_{-B}) = \alpha_{2j} P(B|a_j)P(\overline{d}|B,c_{j-1})$
    Generar $C_j = c_j \sim P(C|x_{-C}) = \alpha_{3j} P(C|a_j)P(\overline{d}|b_j,C)P(e|C)$
    Hacer $j = j + 1$

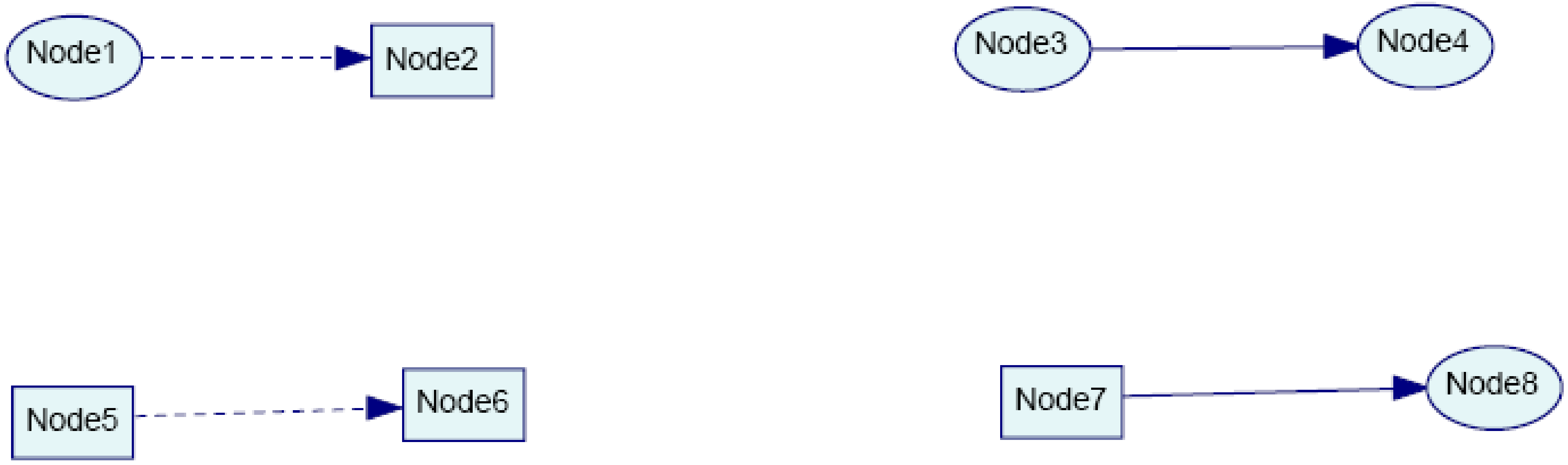
$$\frac{\#\{C_j = c\}}{M}$$

Final comments: Influence diagrams

Influence Diagrams

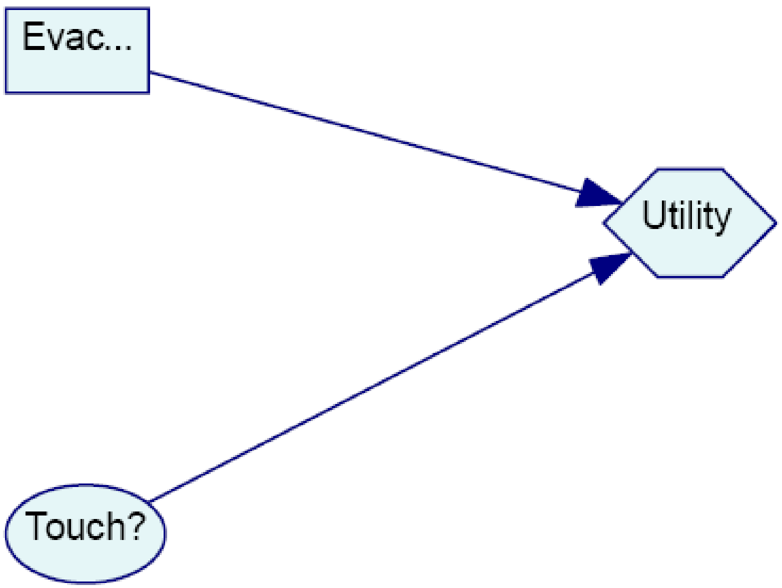
- Tool to structure (and solve) decision making problems
- Graph with nodes and arcs. No cycles
- Three main types of nodes.
  - Chance. Circle
  - Decision. Square
  - Value. Hexagon, Diamond
    - Fourth type of node. Deterministic. Double circle
- Two types of arcs
  - Arcs into decision nodes
  - Arcs into chance and value nodes

Influence Diagrams. Interpretation?



Suppose you’re Nags Head mayor. There is a hurricane threat. Would you issue an evacuation order?

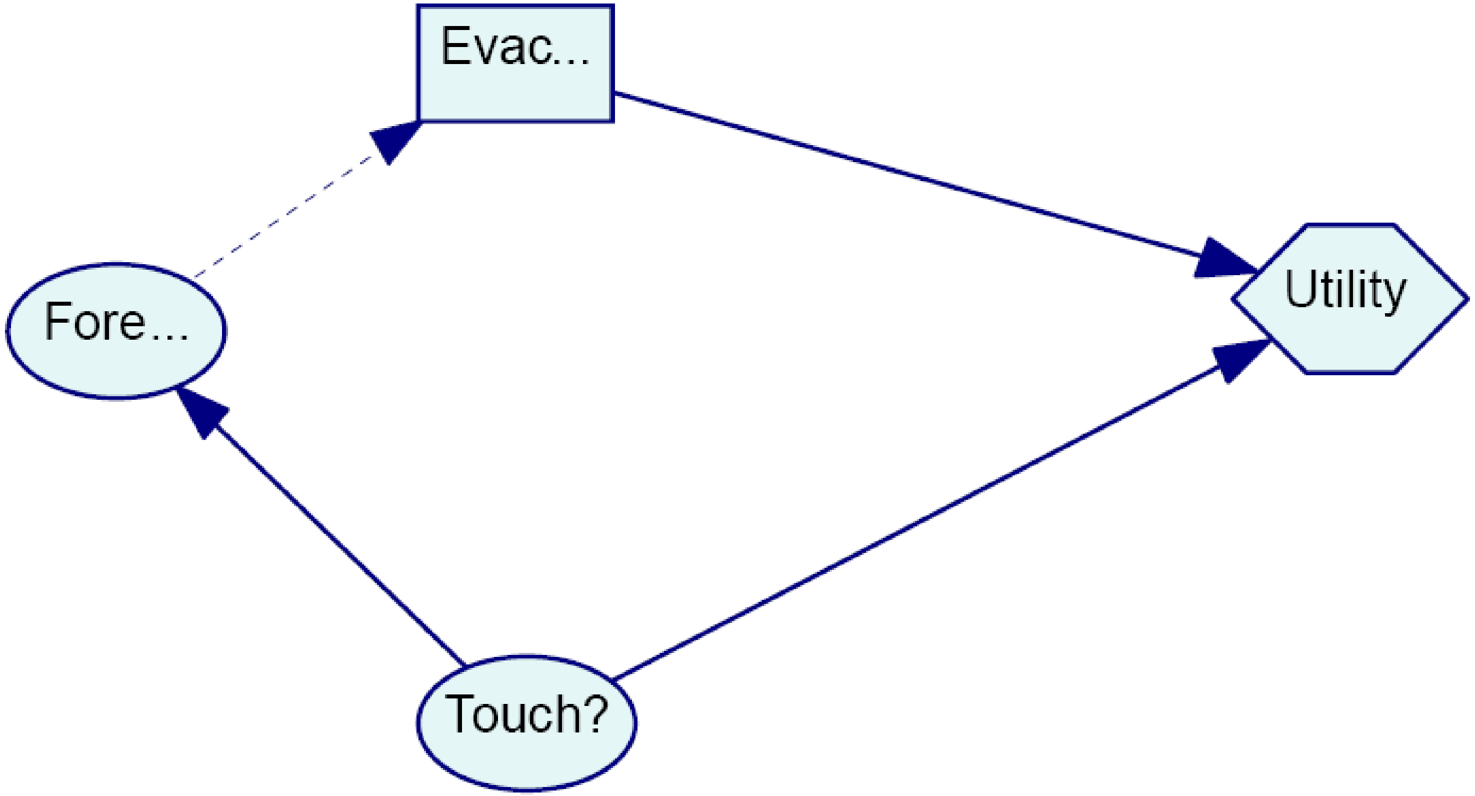
Decision under risk



Suppose you’re Nags Head mayor. There is a hurricane threat. Would you issue an evacuation order?

You have as info a forecast from the NHC. But the forecast is not perfect…

Decision under risk with imperfect information



Additional comments

Learning structure from data: **Structure learning**. Greedy search based on a scoring function based on an information measure.

Tens of methods

Learning node distributions….

Causal inference and causal discovery

https://www.youtube.com/watch?v=wPuJ8tR_05s&list=PLH_XnVAPg2hwSIGIvgK7aCd0U0TYnblFq&index=7

GeNIe

https://www.bayesfusion.com/influence-diagrams/

https://download.bayesfusion.com/files.html?category=Academia

Deep belief nets include belief nets (to be seen)