

Graphical Models

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- ▶ Precursors originate mostly from Physics (Gibbs, 1902), Genetics (Wright, 1921, 1934), and Economics (Wold, 1954);

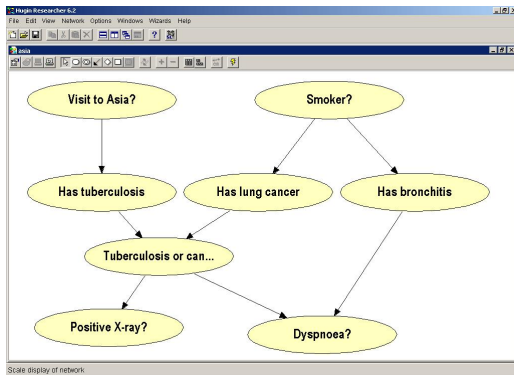
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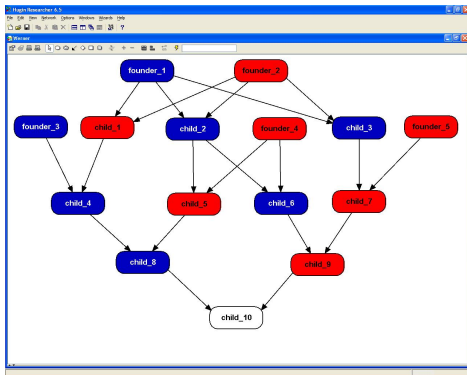
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- ▶ Developments now prolific and it is largely impossible to keep track. Google gives *7 420 000* hits.

A directed graphical model



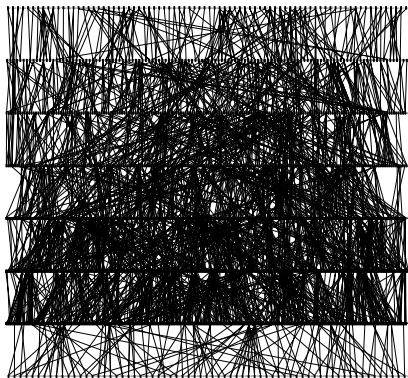
Directed graphical model (Bayesian network) showing relations between risk factors, diseases, and symptoms.

A pedigree



Graphical model for a pedigree from study of Werner's syndrome. Each node is itself a graphical model.

A large pedigree



Family relationship of 1641 members of Greenland Eskimo population.

Random variables X and Y are *conditionally independent* given the random variable Z if

$$\mathcal{L}(X | Y, Z) = \mathcal{L}(X | Z).$$

We then write $X \perp\!\!\!\perp Y | Z$ (or $X \perp\!\!\!\perp_P Y | Z$)

Intuitively:

Knowing Z renders Y *irrelevant* for predicting X .

Factorisation of densities:

$$\begin{aligned} X \perp\!\!\!\perp Y | Z &\iff f(x, y, z)f(z) = f(x, z)f(y, z) \\ &\iff \exists a, b : f(x, y, z) = a(x, z)b(y, z). \end{aligned}$$

Fundamental properties

For random variables X , Y , Z , and W it holds

- (C1) If $X \perp\!\!\!\perp Y \mid Z$ then $Y \perp\!\!\!\perp X \mid Z$;
- (C2) If $X \perp\!\!\!\perp Y \mid Z$ and $U = g(Y)$, then $X \perp\!\!\!\perp U \mid Z$;
- (C3) If $X \perp\!\!\!\perp Y \mid Z$ and $U = g(Y)$, then $X \perp\!\!\!\perp Y \mid (Z, U)$;
- (C4) If $X \perp\!\!\!\perp Y \mid Z$ and $X \perp\!\!\!\perp W \mid (Y, Z)$, then $X \perp\!\!\!\perp (Y, W) \mid Z$;

If density w.r.t. product measure $f(x, y, z, w) > 0$ also

- (C5) If $X \perp\!\!\!\perp Y \mid (Z, W)$ and $X \perp\!\!\!\perp Z \mid (Y, W)$ then $X \perp\!\!\!\perp (Y, Z) \mid W$.

A distribution P is said to *factorize* w.r.t. and undirected graph if its joint density f can be written as

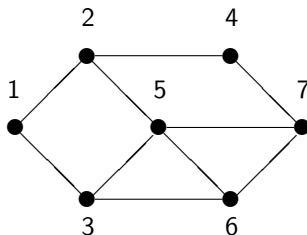
$$f(x) = Z^{-1} \prod_{A \in \mathcal{A}} \phi_A(x_A), \quad (1)$$

where \mathcal{A} are complete subsets of the graph.

Here $x = (x_v, v \in V)$, $x_A = (x_v, v \in A)$ so ϕ_A only depends the A -coordinates of x .

The factorization is matched by a *global Markov property*, ie that $A \perp\!\!\!\perp B \mid S$ if S separates A from B in \mathcal{G} , written as $A \perp_{\mathcal{G}} B \mid S$ (Hammersley and Clifford, 1971).

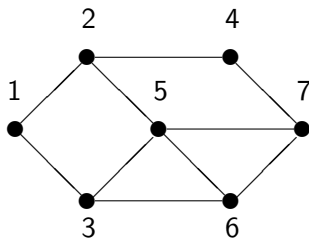
Factorization example



The graph above corresponds to a factorization as

$$\begin{aligned}
 f(x) &= \psi_{12}(x_1, x_2)\psi_{13}(x_1, x_3)\psi_{24}(x_2, x_4)\psi_{25}(x_2, x_5) \\
 &\times \psi_{356}(x_3, x_5, x_6)\psi_{47}(x_4, x_7)\psi_{567}(x_5, x_6, x_7).
 \end{aligned}$$

Global Markov property



To find conditional independence relations, one should look for separating sets, such as $\{2, 3\}$, $\{4, 5, 6\}$, or $\{2, 5, 6\}$.
 For example, it follows that $1 \perp\!\!\!\perp 7 \mid \{2, 5, 6\}$ and $2 \perp\!\!\!\perp 6 \mid \{3, 4, 5\}$.

Pairwise and local Markov properties

$\mathcal{G} = (V, E)$ simple undirected graph; A distribution P satisfies

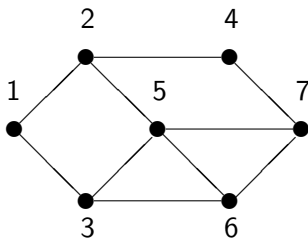
(P) *the pairwise Markov property* if

$$\alpha \not\sim \beta \Rightarrow \alpha \perp\!\!\!\perp_P \beta \mid V \setminus \{\alpha, \beta\};$$

(L) *the local Markov property* if

$$\forall \alpha \in V : \alpha \perp\!\!\!\perp_P V \setminus \text{cl}(\alpha) \mid \text{bd}(\alpha);$$

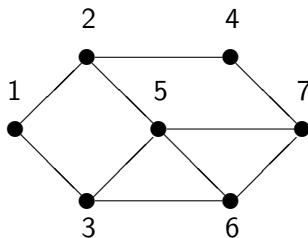
Pairwise Markov property



Any non-adjacent pair of random variables are conditionally independent given the remaining.

For example, $1 \perp\!\!\!\perp 5 \mid \{2, 3, 4, 6, 7\}$ and $4 \perp\!\!\!\perp 6 \mid \{1, 2, 3, 5, 7\}$.

Local Markov property



Every variable is conditionally independent of the remaining, given its neighbours.

For example, $5 \perp\!\!\!\perp \{1, 4\} \mid \{2, 3, 6, 7\}$ and $7 \perp\!\!\!\perp \{1, 2, 3\} \mid \{4, 5, 6\}$.

Let (F) denote the property that f factorizes w.r.t. \mathcal{G} and let (G), (L) and (P) denote the Markov properties as defined. *Then it holds that*

$$(F) \Rightarrow (G) \Rightarrow (L) \Rightarrow (P).$$

All *reverse implications are false in general.*

If $f(x) > 0$ for all x it further holds that

$$(P) \Rightarrow (F)$$

so then

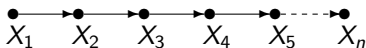
$$(F) \iff (G) \iff (L) \iff (P)$$

(Lauritzen, 1996, Chap. 3).

A probability distribution P over $\mathcal{X} = \mathcal{X}_V$ *factorizes* over a DAG \mathcal{D} if its density or probability mass function f has the form

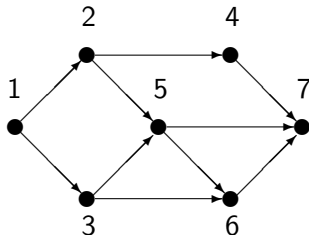
$$f(x) = \prod_{v \in V} f_v(x_v | x_{\text{pa}(v)}).$$

A well-known example is a Markov chain:



with $X_{i+1} \perp\!\!\!\perp (X_1, \dots, X_{i-1}) \mid X_i$ for $i = 3, \dots, n$.

Example of DAG factorization



The above graph corresponds to the factorization

$$\begin{aligned}
 f(x) &= f(x_1)f(x_2 | x_1)f(x_3 | x_1)f(x_4 | x_2) \\
 &\times f(x_5 | x_2, x_3)f(x_6 | x_3, x_5)f(x_7 | x_4, x_5, x_6).
 \end{aligned}$$

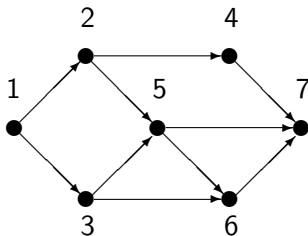
Local directed Markov property

A distribution P satisfies *the local Markov property* (L) w.r.t. a directed acyclic graph \mathcal{D} if

$$\forall \alpha \in V : \alpha \perp\!\!\!\perp_P \{nd(\alpha) \setminus pa(\alpha)\} \mid pa(\alpha).$$

Here $nd(\alpha)$ are the *non-descendants* of α .

Local directed Markov property



For example, the local Markov property says

$$4 \perp\!\!\!\perp \{1, 3, 5, 6\} \mid 2,$$

$$5 \perp\!\!\!\perp \{1, 4\} \mid \{2, 3\}$$

$$3 \perp\!\!\!\perp \{2, 4\} \mid 1.$$

A distribution satisfies the *global Markov property* w.r.t. \mathcal{D} if

$$A \perp_{\mathcal{D}} B \mid S \Rightarrow A \perp\!\!\!\perp B \mid S.$$

Here $\perp_{\mathcal{D}}$ is *d-separation*, which is somewhat subtle.

It is *always* true for a DAG that

$$(F) \iff (G) \iff (L)$$

(Pearl, 1986; Geiger and Pearl, 1990; Lauritzen et al., 1990).

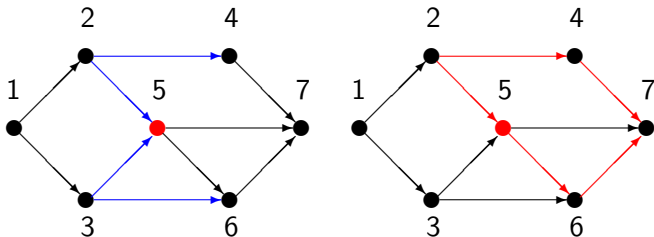
Separation in DAGs

A *trail* τ from vertex α to vertex β in a DAG \mathcal{D} is *blocked by* S if it contains a vertex $\gamma \in \tau$ such that

- ▶ either $\gamma \in S$ and edges of τ do not meet head-to-head at γ , or
- ▶ γ and all its descendants are not in S , and edges of τ meet head-to-head at γ .

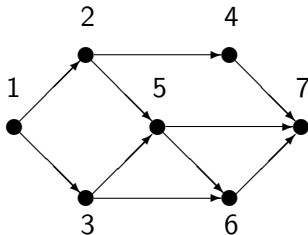
A trail that is not blocked is *active*. Two subsets A and B of vertices are *d-separated by* S if all trails from A to B are blocked by S . We write $A \perp_{\mathcal{D}} B \mid S$.

Separation by example



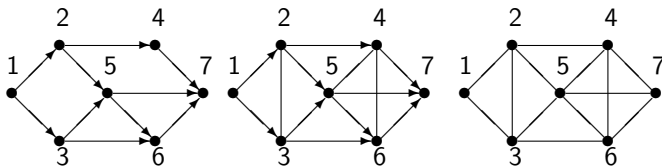
For $S = \{5\}$, the trail $(4, 2, 5, 3, 6)$ is *active*, whereas the trails $(4, 2, 5, 6)$ and $(4, 7, 6)$ are *blocked*.
 For $S = \{3, 5\}$, they are all blocked.

Returning to example



Hence $4 \perp_{\mathcal{D}} 6 \mid 3, 5$, but it is *not* true that $4 \perp_{\mathcal{D}} 6 \mid 5$ nor that $4 \perp_{\mathcal{D}} 6$.

The *moral graph* \mathcal{D}^m of a DAG \mathcal{D} is obtained by adding undirected edges between unmarried parents and subsequently dropping directions, as in the example below:



Undirected factorizations

If P factorizes w.r.t. \mathcal{D} , it factorizes w.r.t. the moralised graph \mathcal{D}^m .

This is seen directly from the factorization:

$$f(x) = \prod_{v \in V} f(x_v | x_{\text{pa}(v)}) = \prod_{v \in V} \psi_{\{v\} \cup \text{pa}(v)}(x),$$

since $\{v\} \cup \text{pa}(v)$ are all complete in \mathcal{D}^m .

Hence if P satisfies any of the directed Markov properties w.r.t. \mathcal{D} , it satisfies all Markov properties for \mathcal{D}^m .

Alternative equivalent separation

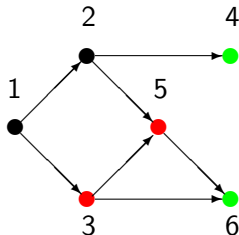
To resolve query involving three sets A , B , S :

1. Reduce to subgraph induced by ancestral set $\mathcal{D}_{\text{An}(A \cup B \cup S)}$ of $A \cup B \cup S$;
2. Moralize to form $(\mathcal{D}_{\text{An}(A \cup B \cup S)})^m$;

It then holds that $A \perp_{\mathcal{D}} B \mid S$ if and only if S separates A from B in this undirected graph.

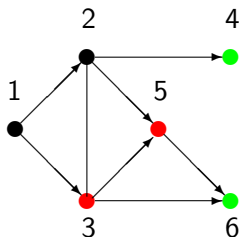
Proof in Lauritzen (1996) needs to allow self-intersecting paths to be correct.

Forming ancestral set



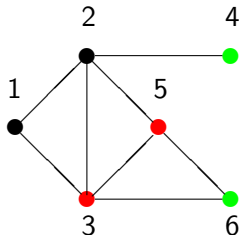
The subgraph induced by all ancestors of nodes involved in the query $4 \perp_{\mathcal{D}} 6 \mid 3, 5$?

Adding links between unmarried parents



Adding an undirected edge between 2 and 3 with common child 5 in the subgraph induced by all ancestors of nodes involved in the query $4 \perp_{\mathcal{D}} 6 \mid 3, 5$?

Dropping directions



Since $\{3, 5\}$ separates 4 from 6 in this graph, we can conclude that $4 \perp_{\mathcal{D}} 6 \mid 3, 5$

A particular successful development is associated with BUGS, (Gilks et al., 1994) (WinBUGS, OpenBUGS).

- ▶ enables a Bayesian analyst to focus on substantive modelling whereas the technical model specification and computational side is taken care of automatically,

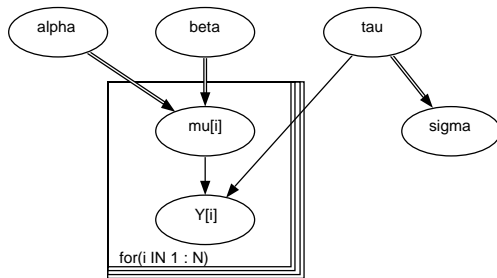
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- ▶ enables a Bayesian analyst to focus on substantive modelling whereas the technical model specification and computational side is taken care of automatically,
- ▶ exploiting modularity, factorization, and MCMC methodology, including the Gibbs and Metropolis–Hastings sampler.
- ▶ Conforming with Bayesian paradigm, parameters and observations are explicitly represented in model as nodes in graph, all being observables;

Linear regression



Linear regression as a full Bayesian graphical model.

Linear regression

```
model
{
  for( i in 1 : N ) {
    Y[i] ~ dnorm(mu[i],tau)
    mu[i] <- alpha + beta * (x[i] - xbar)
  }
  tau ~ dgamma(0.001,0.001) sigma <- 1 / sqrt(tau)
  alpha ~ dnorm(0.0,1.0E-6)
  beta ~ dnorm(0.0,1.0E-6)
}
```

Data and BUGS model for pumps

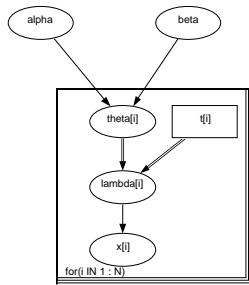
The number of failures X_i is assumed to follow a Poisson distribution with parameter $\theta_i t_i$, $i = 1, \dots, 10$ where θ_i is the failure rate for pump i and t_i is the length of operation time of the pump (in 1000s of hours). The data are shown below.

Pump	1	2	3	4	5	6	7	8	9	10
t_i	94.5	15.7	62.9	126	5.24	31.4	1.05	1.05	2.01	10.5
x_i	5	1	5	14	3	19	1	1	4	22

A gamma prior distribution is adopted for the failure rates:

$$\theta_i \sim \Gamma(\alpha, \beta), i = 1, \dots, 10$$

Gamma model for pumpdata



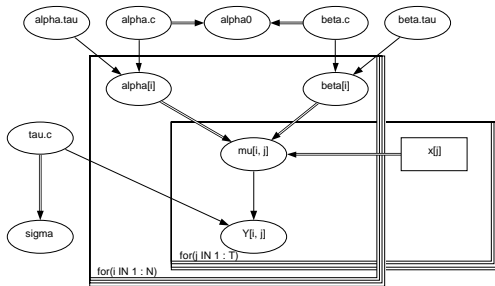
Failure of 10 power plant pumps.

BUGS program for pumps

With suitable priors the program becomes

```
model
{
  for (i in 1 : N) {
    theta[i] ~ dgamma(alpha, beta)
    lambda[i] <- theta[i] * t[i]
    x[i] ~ dpois(lambda[i])
  }
  alpha ~ dexp(1)
  beta ~ dgamma(0.1, 1.0)
}
```


Growth of rats



Growth of 30 young rats.

Finding full conditionals for Gibbs sampler

Inference in Bayesian complex graphical models as above uses the Gibbs sampler.

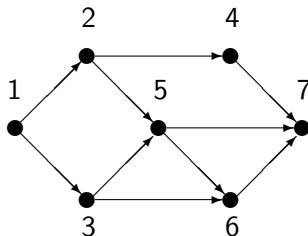
For a *DAG* the densities of full conditional distributions are:

$$\begin{aligned}
 f(x_i | x_{V \setminus i}) &\propto \prod_{v \in V} f(x_v | x_{\text{pa}(v)}) \\
 &\propto f(x_i | x_{\text{pa}(i)}) \prod_{v \in \text{ch}(i)} f(x_v | x_{\text{pa}(v)}) \\
 &= f(x_i | x_{\text{bl}(i)}),
 \end{aligned}$$

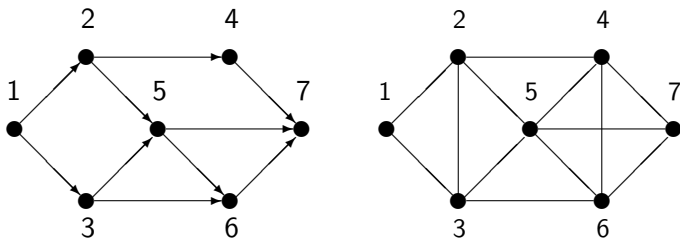
x where $\text{bl}(i)$ is the *Markov blanket* of node i :

$$\text{bl}(i) = \text{pa}(i) \cup \text{ch}(i) \cup \left\{ \bigcup_{v \in \text{ch}(i)} \text{pa}(v) \setminus \{i\} \right\}.$$

Markov blanket



Markov blanket of 6 is $bl(6) = \{3, 5, 7, 4\}$.



The Markov blanket is just the neighbours of in the moral graph:

$bl(v) = ne^m(v)$ so $bl(6) = \{3, 5, 7, 4\}$ and $bl(3) = \{1, 5, 6, 2\}$.

The *DAG is used for modular specification* of the model, and *the moral graph for local computation*.

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- ▶ distinction prior/likelihood and parameter/random variable less well defined;

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- ▶ distinction prior/likelihood and parameter/random variable less well defined;
- ▶ If founder nodes in network are considered fixed and unknown, *no reason not to consider models in Fisherian paradigm.*

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