Bayesian network

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Probabilistic graphical models

- Graphical models are a marriage between probability theory and graph theory (Michael Jordan, 1998)
- Graphical models use conditional independence assumptions for efficient representation, inference and learning of joint distributions
  - a compact representation of joint probability distributions;
  - a collection of conditional independence assumptions
- Graphs
  - nodes: random variables (probabilistic distribution over a fixed alphabet)
  - edges (arcs), or lack of edges: conditional independence assumptions

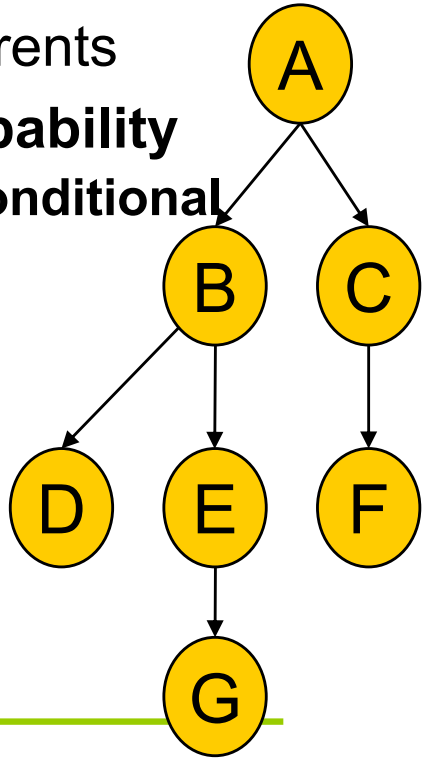
Classification of probabilistic graphical models

	Linear	Branching	Application
Directed	Markov Chain (HMM)	**Bayesian network** (BN)	Artificial Intelligence (AI) Statistics
Undirected	Linear chain conditional random field (CRF)	Markov network (MN)	Physics (Ising model) Image/Vision

Both directed and undirected arcs: chain graphs

Bayesian Network Structure

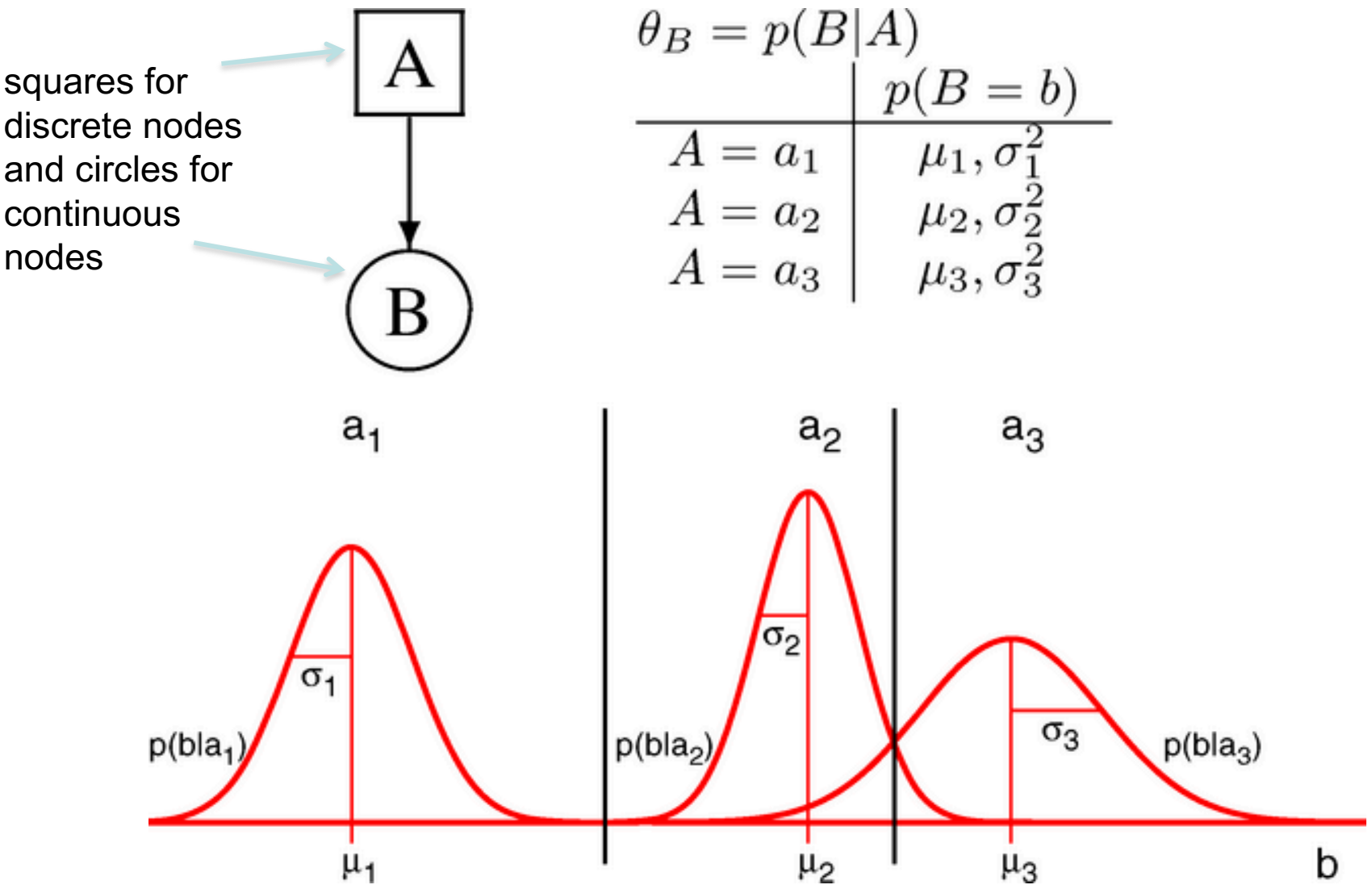
- Directed acyclic graph (DAG) G
  - Nodes $x_1,\ldots,x_n$ represent random variables; the parent nodes of x_i, (pa_i) represents the set of variables that x_i is dependent on.
  - The variables can be discrete or continuous
- G encodes ***local Markov assumptions***
  - ***Conditional independence*** $X_i \perp X_j | X_k$
  - x_i is independent of its non-descendants given its parents
  - The dependences are modeled by **Conditional Probability Distributions** (CPDs; for continuous variables) **or Conditional Probability Tables** (CPTs; for discrete variables)



P(A,B,C,D,E,F,G)=
P(A)P(B|A)P(C|A)P(D|B)P(E|B)P(G|E)P(F|C)
7 CPDs: each for one edge or one source node

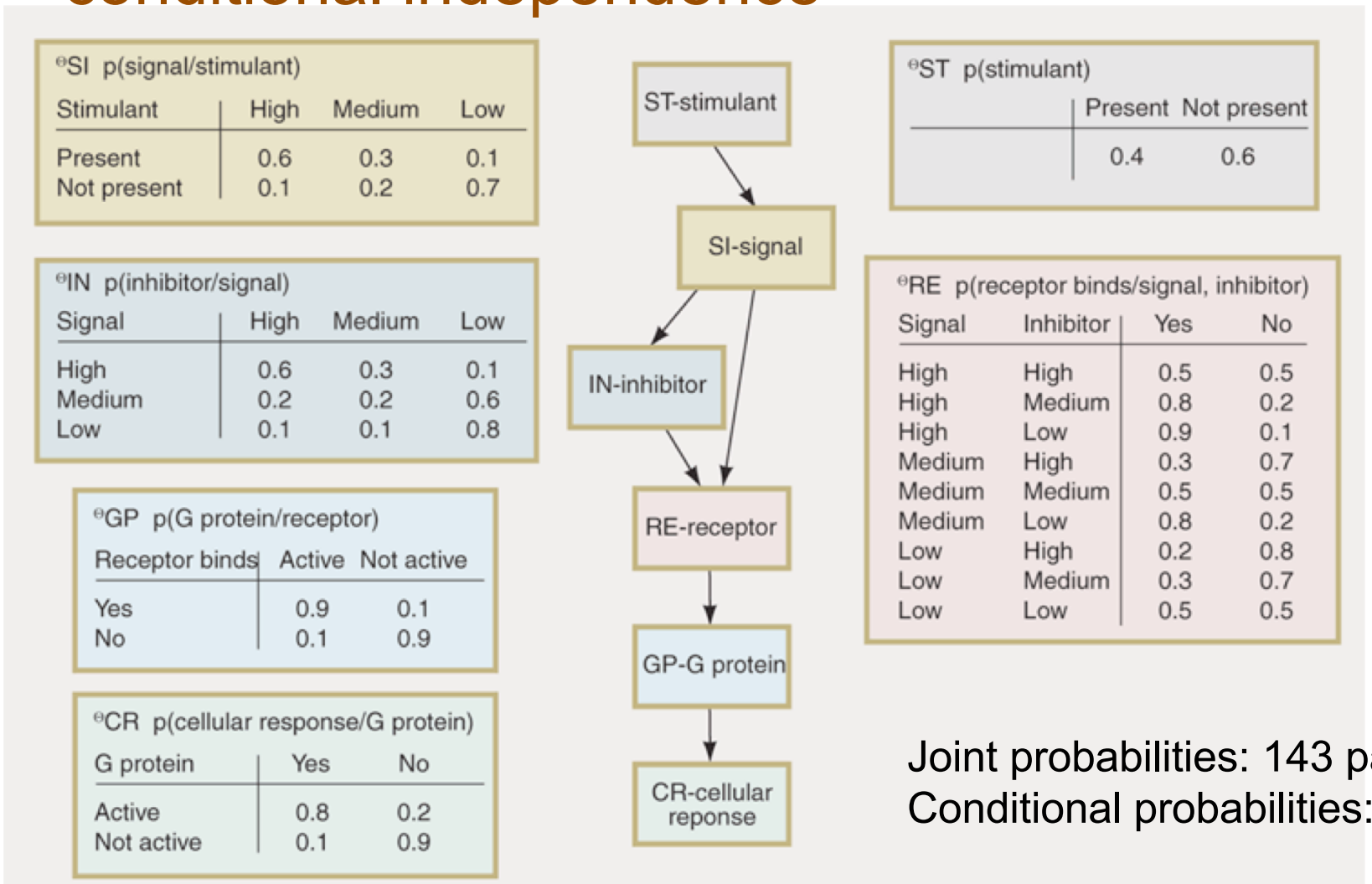
• BN computes the joint distribution of all random variables *compactly* in a *factorized* way.
• BN is a *compact* representation of *conditional independence* assumptions about a high dimension distribution.

Figure 2. Illustration of Model Parameters for Two-Node Bayesian Network



Needham CJ, Bradford JR, Bulpitt AJ, Westhead DR (2007) A Primer on Learning in Bayesian Networks for Computational Biology. PLoS Comput Biol 3(8): e129. doi:10.1371/journal.pcbi.0030129
http://www.ploscompbiol.org/article/info:doi/10.1371/journal.pcbi.0030129

BN provides compact representation of conditional independence



θSI p(signal/stimulant)

Stimulant	High	Medium	Low
Present	0.6	0.3	0.1
Not present	0.1	0.2	0.7

θST p(stimulant)

Present	Not present
0.4	0.6

θIN p(inhibitor/signal)

Signal	High	Medium	Low
High	0.6	0.3	0.1
Medium	0.2	0.2	0.6
Low	0.1	0.1	0.8

θRE p(receptor binds/signal, inhibitor)

Signal	Inhibitor	Yes	No
High	High	0.5	0.5
High	Medium	0.8	0.2
High	Low	0.9	0.1
Medium	High	0.3	0.7
Medium	Medium	0.5	0.5
Medium	Low	0.8	0.2
Low	High	0.2	0.8
Low	Medium	0.3	0.7
Low	Low	0.5	0.5

θGP p(G protein/receptor)

Receptor binds	Active	Not active
Yes	0.9	0.1
No	0.1	0.9

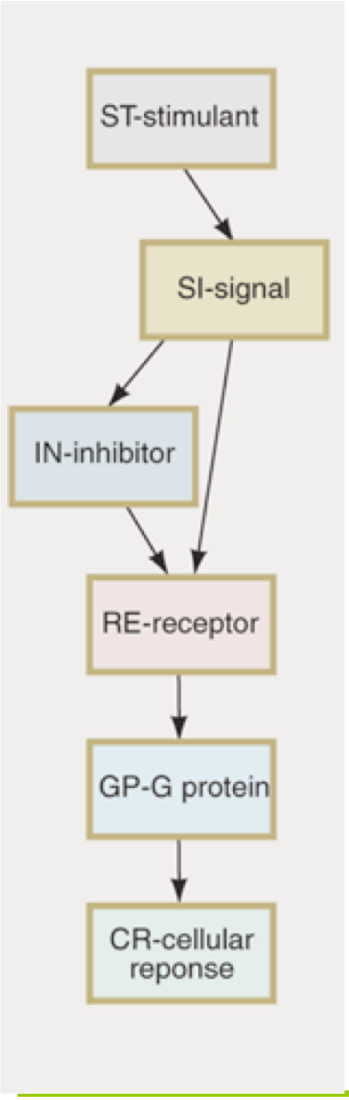
θCR p(cellular response/G protein)

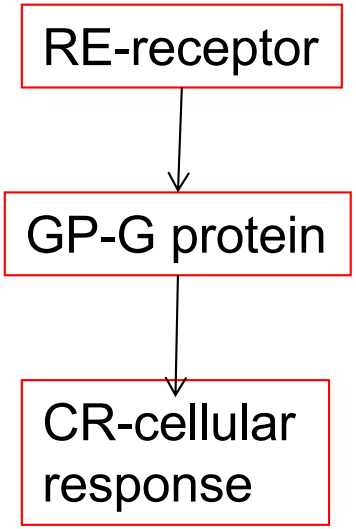
G protein	Yes	No
Active	0.8	0.2
Not active	0.1	0.9

Joint probabilities: 143 parameters
Conditional probabilities: 24

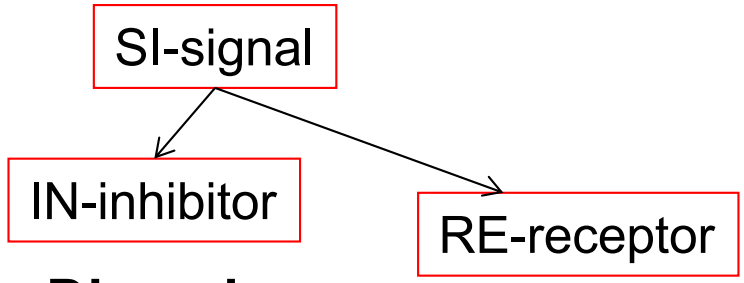
A network with 100 nodes, each with 3 possible values: > 10^{47} vs 1,800 parameters!

Conditional independence in BNs: Types of connections

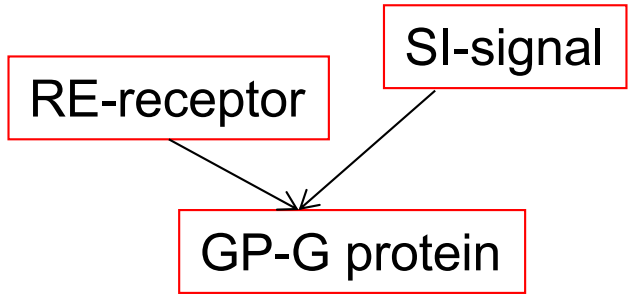




Serial
knowing GP makes RE and CR independent (intermediate cause)



Diverging
knowing SI makes IN and RE independent (common cause)



Converging
NOT knowing GP makes RE and SI independent (common effect)

Why Bayesian network?

- Combined with Bayesian method, Bayesian Network can offer solutions to a number of challenges
  - Facilitate the combination of domain knowledge and data
  - Handle incomplete data sets (marginalizing over unknown variables by considering all possible values the unknown variables may take, and averaging over them)
  - Offer an efficient and principled approach for avoiding the over fitting of data
  - Learn about causal relationships

Inference in a Bayesian network

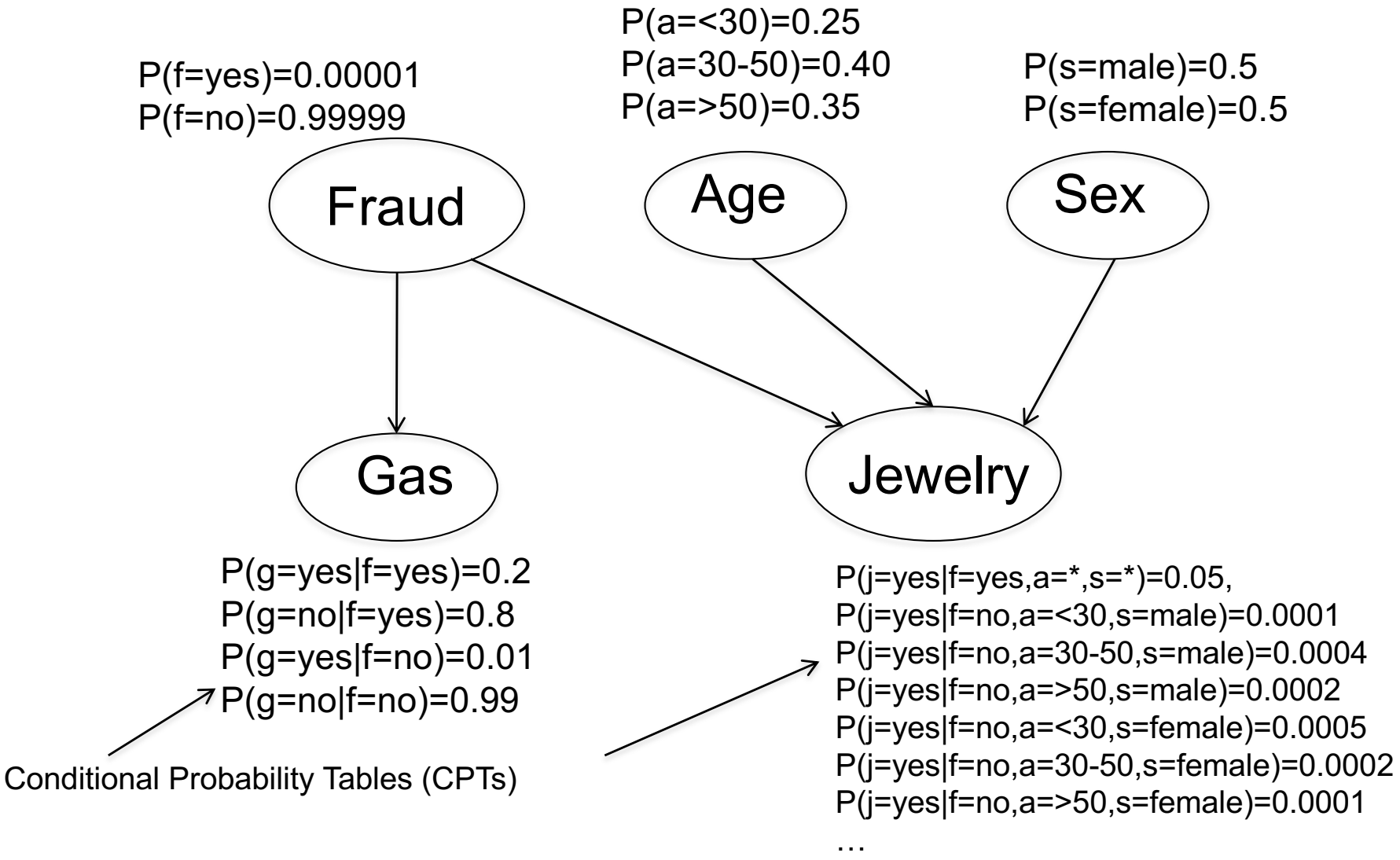
- Inference in probabilistic models in general asks the following questions: given $P(X_1, X_2, \ldots, X_m)$ and a set of observations e = $\{X_i=x_i, X_j=x_j, \ldots\}$ (or data) , compute
  - **Marginals: $P(X_k|e)$**
  - Probability of evidence: $P(e)$
  - Most probable explanation:

$$\arg\max_x P(x|e)$$

Approaches to inference

- Exact methods
  - **Enumeration**
  - **Variable elimination**
  - Belief propagation in polytrees
  - Clustering / join tree algorithms
- Approximate methods
  - **Stochastic simulation / sampling methods**
  - **Markov chain Monte Carlo**
  - Genetic algorithms
  - Neural networks
  - Simulated annealing
  - Mean field theory

A simple example: credit card fraud



Inference in the BN

- BN defines the joint probability for all involved random variables

$$p(f,a,s,g,j) = p(f)\cdot p(g \mid f)\cdot p(a)\cdot p(s)\cdot p(j \mid f,a,s)$$

- One can use BN to compute any probability of interest
  - Computing posterior marginal probability, e.g. The probability of fraud, given the ***evidences*** (a,s,g,j),

$$p(f \mid a,s,g,j) = \frac{p(f,a,s,g,j)}{\sum_{f'}(f',a,s,g,j)} = \frac{p(f)\cdot p(g \mid f)\cdot p(a)\cdot p(s)\cdot p(j \mid f,a,s)}{\sum_{f'} p(f')\cdot p(g \mid f')\cdot p(a)\cdot p(s)\cdot p(j \mid f',a,s)} = \frac{p(f)\cdot p(g \mid f)\cdot p(j \mid f,a,s)}{\sum_{f'} p(f')\cdot p(g \mid f')\cdot p(j \mid f',a,s)}$$

When variables are in a set of discrete values, this can be computed!

Inference by enumeration (examples)

- The probability of fraud (age=30-50,sex=female,gas=yes,jewelry=yes)

$$p(f \mid a,s,g,j) = \frac{p(f)\cdot\ p(g \mid f)\cdot\ p(j \mid f,a,s)}{\sum_{f'} p(f')\cdot\ p(g \mid f')\cdot\ p(j \mid f',a,s)}$$

$$p(f = yes \mid a = 30-50, s = female, g = yes, j = yes) =$$

$$\frac{0.00001 \times 0.2 \times 0.05}{10^{-7} + 0.99999 \times 0.01 \times 0.002} = 0.005$$ >> prior (0.00001)

- The probability that the card holder is female, if the card is not fraud

$$p(s \mid a,f,g,j) = \frac{p(s)\cdot\ p(j \mid f,a,s)}{\sum_{s'} p(s')\cdot\ p(j \mid f,a,s')}$$

$$p(s = female \mid a =< 30, f = no, g = yes, j = yes) =$$

$$\frac{0.5 \times 0.0005}{2.5 \times 10^{-4} + 0.5 \times 0.0001} = 5/6$$

Inference with missing data

- The probability of fraud, but the **gender of the card holder is unknown**

$$p(f \mid a,g,j) = \frac{\sum_{s'} (f) \cdot\ p(g \mid f) \cdot\ p(j \mid f,a,s')}{\sum_{f',s'} p(f') \cdot\ p(g \mid f') \cdot\ p(j \mid f',a,s')}$$

Don't see p(s'): $p(s = male) == p(s = female)\}$

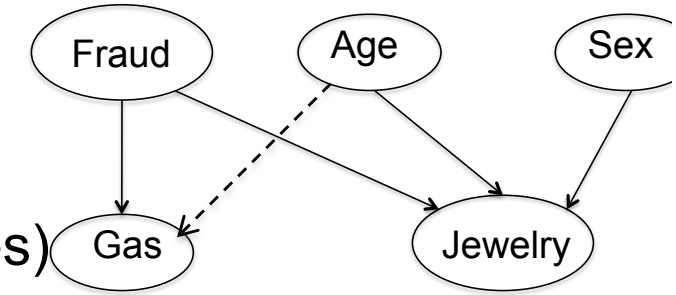
$$p(f = yes \mid a = 30-50, g = yes, j = yes) =$$

$$\frac{0.00001 \times 0.2 \times (0.05 + 0.05)}{2 \times 10^{-7} + 0.99999 \times 0.01 \times (0.002 + 0.0004)} = 0.004$$

(marginalizing over variable *s*)

Computational complexity of inference by enumeration

- Computing the joint probability
  - Multiplication of CPDs, $O(n^{|V|})$
    - n: # discrete values; v: # variables (nodes)



$$p(f) = \frac{\sum_{s',a',g',j'} p(f)\cdot p(a')\cdot p(s')\cdot p(g'\mid f)\cdot p(j'\mid f,a',s')}{\sum_{f',a',s',g',j'} p(f')\cdot p(a')\cdot p(s')\cdot p(g'\mid f')\cdot p(j\mid f',a',s')}$$

To compute the ***denominator,*** all combinations of (f, a, s, g, j) need to be enumerated, indicating the complexity of 2^5.
Exact inference in an arbitrary BN for discrete variables is NP-hard (Cooper, 1987). When BN contains many undirected cycles (e.g., adding an edge a→g forming a cycle f→g→a→j→f), inference is intractable.

Inference by variable elimination (VE algorithm)

Consider a query that needs to compute the joint probability of $X=(x_1, x_2, \ldots, x_k)$, where x_i represents a random variable (i.e., node)

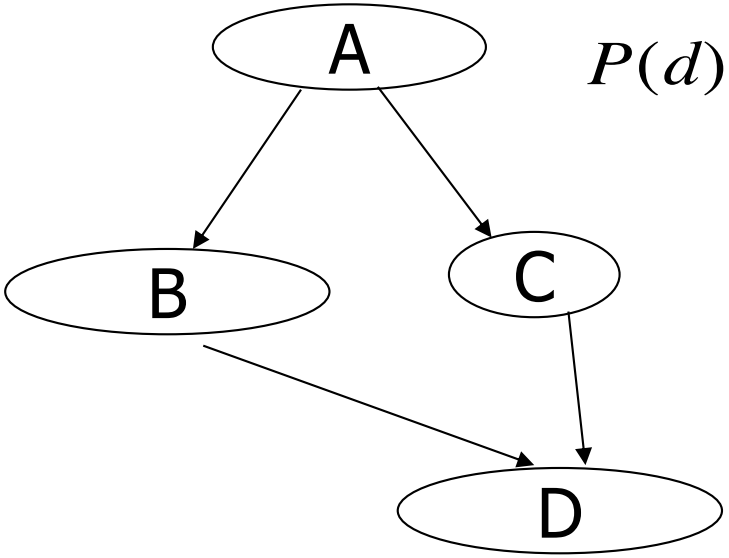
$$P(X \mid e) = \sum_{x_k} \cdots \sum_{x_2} \sum_{x_1} \prod_{i} P(x_i \mid pa_i)$$

where e represents a subset of variables outside X, pa_i represents the set of parent variables of x_i

The computation can be accelerated by a Dynamic Programming algorithm, which Iteratively

- move all irrelevant terms outside of innermost sum
- perform innermost sum, getting a new term
- insert the new term into the product

Variable elimination: Example



$$P(d) = \sum_{a,b,c} P(d \mid b,c)P(b \mid a)P(c \mid a)P(a)$$

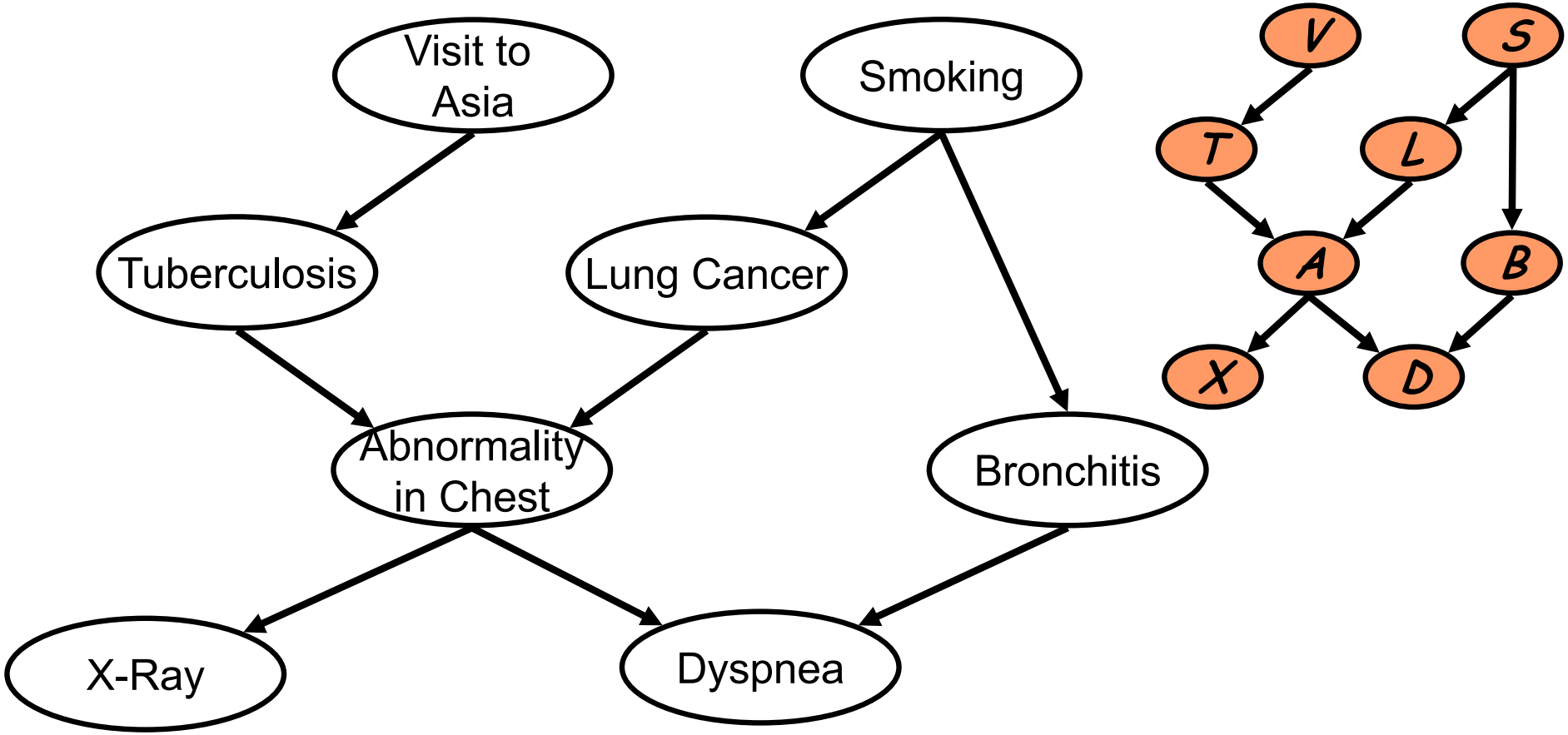
$$= \sum_{b,c} P(d \mid b,c) \sum_{a} P(b \mid a)P(c \mid a)P(a)$$

$$= \sum_{b,c} P(d \mid b,c) f_1(b,c)$$

$f_1(b,c)$

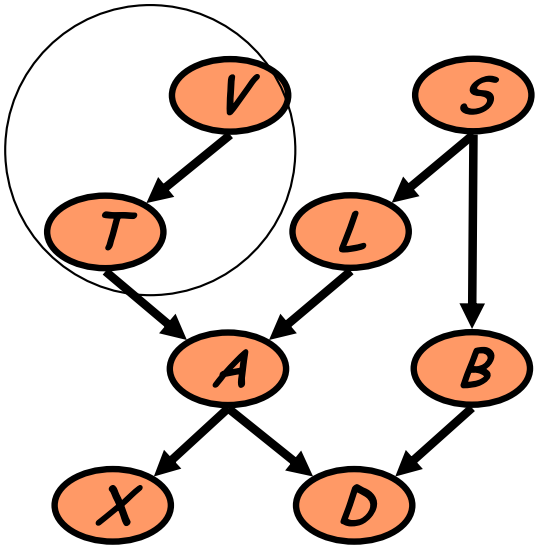
$f_1(b,c)$ can be computed for each combination of (b,c), and used for computing P(d).

A more complex example



$$\sum_{v,s,x,t,l,a,b} P(v)P(s)P(t \mid v)P(l \mid s)P(b \mid s)P(a \mid t,l)P(x \mid a)P(d \mid a,b)$$

Eliminate: v



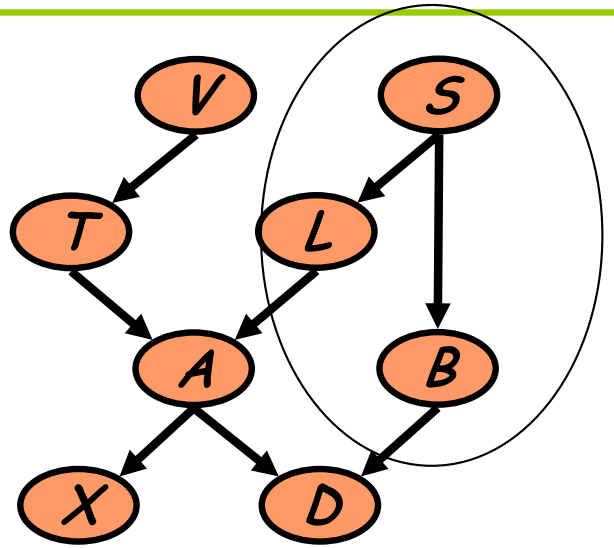
$$P(v)P(s)P(t \mid v)P(l \mid s)P(b \mid s)P(a \mid t,l)P(x \mid a)P(d \mid a,b)$$

Compute: $$f_v(t) = \sum_v P(v)P(t \mid v)$$

$$\Rightarrow f_v(t)P(s)P(l \mid s)P(b \mid s)P(a \mid t,l)P(x \mid a)P(d \mid a,b)$$

Note: let $f_v(t) = P(t)$
In general, however, result of elimination is not necessarily a probability term.

Eliminate: s



$$P(v)P(s)P(t \mid v)P(l \mid s)P(b \mid s)P(a \mid t,l)P(x \mid a)P(d \mid a,b)$$

$$\Rightarrow f_v(t)P(s)P(l \mid s)P(b \mid s)P(a \mid t,l)P(x \mid a)P(d \mid a,b)$$

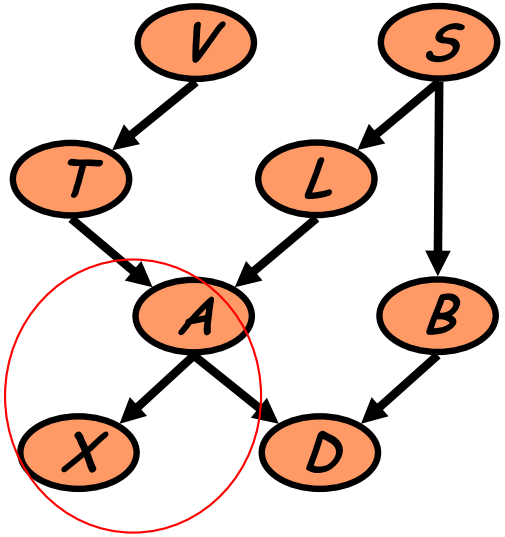
Compute: $$f_s(b,l) = \sum_s P(s)P(b \mid s)P(l \mid s)$$

$$\Rightarrow f_v(t)f_s(b,l)P(a \mid t,l)P(x \mid a)P(d \mid a,b)$$

Summing on s results in a dimensional matrix $f_s(b,l)$

In general, result of elimination may be a function of several variables.

Eliminate: x



$$P(v)P(s)P(t \mid v)P(l \mid s)P(b \mid s)P(a \mid t,l)P(x \mid a)P(d \mid a,b)$$

$$\Rightarrow f_v(t)P(s)P(l \mid s)P(b \mid s)P(a \mid t,l)P(x \mid a)P(d \mid a,b)$$

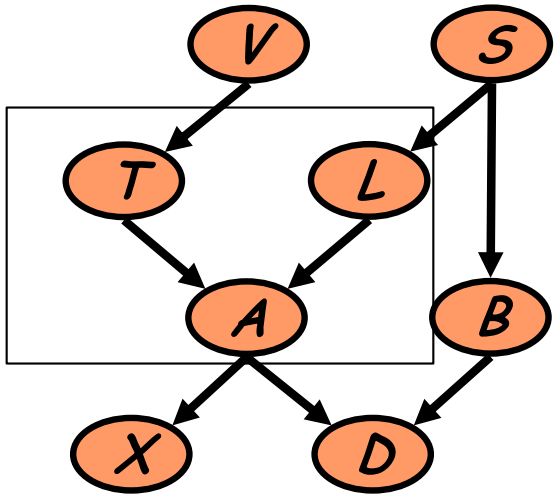
$$\Rightarrow f_v(t)f_s(b,l)P(a \mid t,l)P(x \mid a)P(d \mid a,b)$$

Compute: $$f_x(a) = \sum_x P(x \mid a)$$

$$\Rightarrow f_v(t)f_s(b,l)f_x(a)P(a \mid t,l)P(d \mid a,b)$$

Note: $f_x(a) = 1$ for all values of a !!

Eliminate: t



$$P(v)P(s)P(t \mid v)P(l \mid s)P(b \mid s)P(a \mid t,l)P(x \mid a)P(d \mid a,b)$$

$$\Rightarrow f_v(t)P(s)P(l \mid s)P(b \mid s)P(a \mid t,l)P(x \mid a)P(d \mid a,b)$$

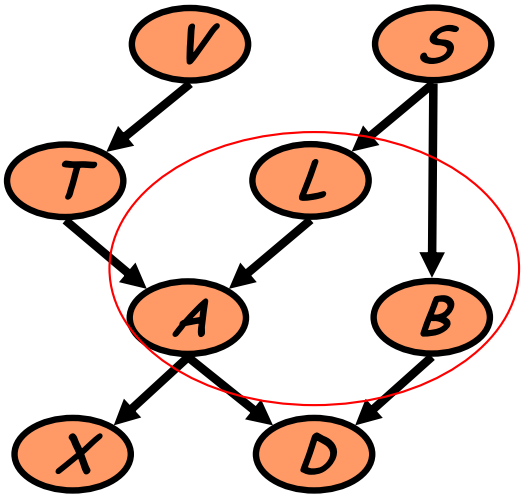
$$\Rightarrow f_v(t)f_s(b,l)P(a \mid t,l)P(x \mid a)P(d \mid a,b)$$

$$\Rightarrow f_v(t)f_s(b,l)f_x(a)P(a \mid t,l)P(d \mid a,b)$$

Compute: $$f_t(a,l) = \sum_t f_v(t)P(a \mid t,l)$$

$$\Rightarrow f_s(b,l)f_x(a)f_t(a,l)P(d \mid a,b)$$

Eliminate: l



$$P(v)P(s)P(t \mid v)P(l \mid s)P(b \mid s)P(a \mid t,l)P(x \mid a)P(d \mid a,b)$$

$$\Rightarrow f_v(t)P(s)P(l \mid s)P(b \mid s)P(a \mid t,l)P(x \mid a)P(d \mid a,b)$$

$$\Rightarrow f_v(t)f_s(b,l)P(a \mid t,l)P(x \mid a)P(d \mid a,b)$$

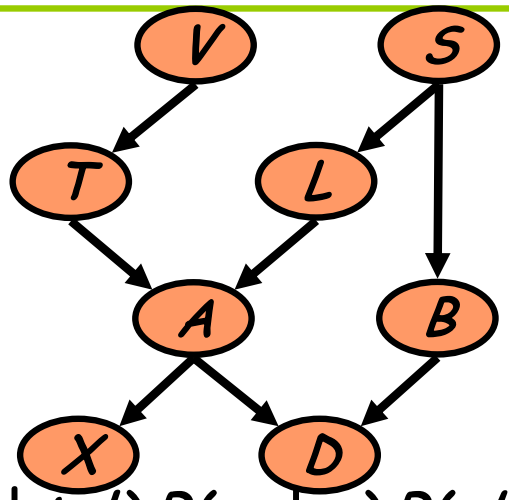
$$\Rightarrow f_v(t)f_s(b,l)f_x(a)P(a \mid t,l)P(d \mid a,b)$$

$$\Rightarrow f_s(b,l)f_x(a)f_t(a,l)P(d \mid a,b)$$

Compute: $f_l(a,b) = \sum_l f_s(b,l)f_t(a,l)$

$$\Rightarrow f_l(a,b)f_x(a)P(d \mid a,b)$$

Eliminate: a,b



$$P(v)P(s)P(t \mid v)P(l \mid s)P(b \mid s)P(a \mid t,l)P(x \mid a)P(d \mid a,b)$$

$$\Rightarrow f_v(t)P(s)P(l \mid s)P(b \mid s)P(a \mid t,l)P(x \mid a)P(d \mid a,b)$$

$$\Rightarrow f_v(t)f_s(b,l)P(a \mid t,l)P(x \mid a)P(d \mid a,b)$$

$$\Rightarrow f_v(t)f_s(b,l)f_x(a)P(a \mid t,l)P(d \mid a,b)$$

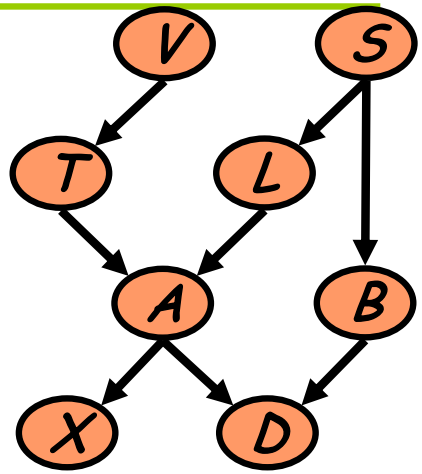
$$\Rightarrow f_s(b,l)f_x(a)f_t(a,l)P(d \mid a,b)$$

$$\Rightarrow \underline{f_l(a,b)}\,\underline{f_x(a)}\,\underline{P(d \mid a,b)} \Rightarrow \underline{f_a(b,d)} \Rightarrow \underline{f_b(d)}$$

Compute:

$$f_a(b,d) = \sum_a f_l(a,b)f_x(a)p(d \mid a,b) \qquad f_b(d) = \sum_b f_a(b,d)$$

Complexity of VE algorithm



$$P(v)P(s)P(t \mid v)P(l \mid s)P(b \mid s)P(a \mid t,l)P(x \mid a)P(d \mid a,b)$$

$$\Rightarrow f_v(t)P(s)P(l \mid s)P(b \mid s)P(a \mid t,l)P(x \mid a)P(d \mid a,b)$$

$$\Rightarrow f_v(t)f_s(b,l)P(a \mid t,l)P(x \mid a)P(d \mid a,b)$$

$$\Rightarrow f_v(t)f_s(b,l)f_x(a)P(a \mid t,l)P(d \mid a,b)$$

$$\Rightarrow f_s(b,l)f_x(a)f_t(a,l)P(d \mid a,b)$$

$$\Rightarrow \underline{f_l(a,b)}\,\underline{f_x(a)}\,\underline{P(d \mid a,b)} \Rightarrow \underline{f_a(b,d)} \Rightarrow \underline{f_b(d)}$$

Complexity: $O(|V| \bullet n^{k+1})$ instead of $O(n^{|V|})$, where *k* is the ***maximum in-degree*** of a node in the graph (here k=2).

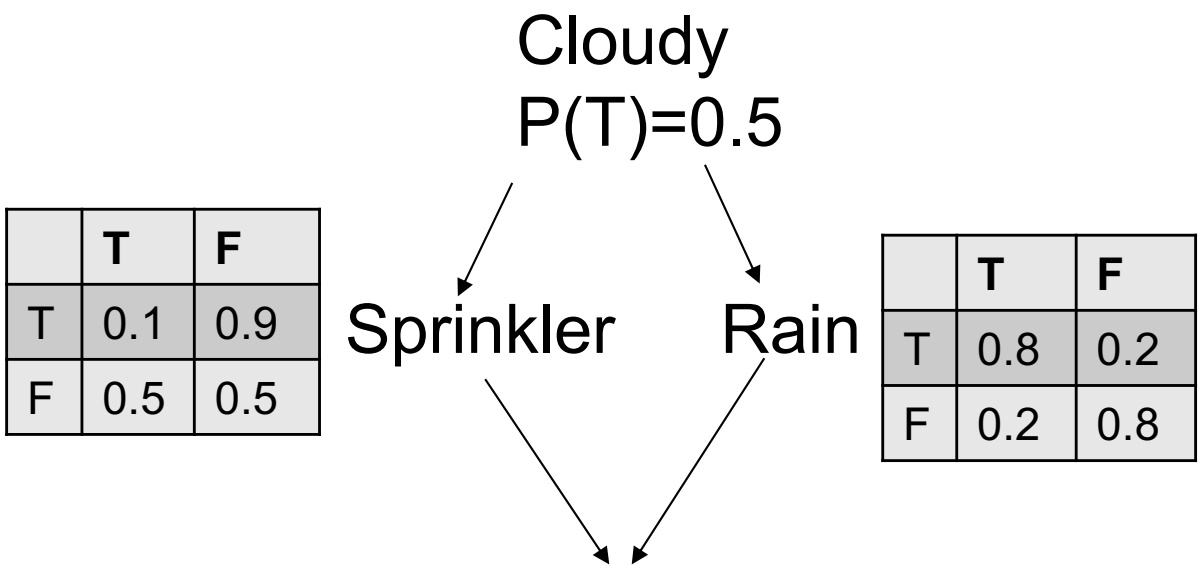
Variable elimination

- Can be exponential for arbitrary graph;
- **Hard to determine the order of variables to be eliminated**
  - **Find the optimal order is NP-hard**
- In practice, it may be quite efficient on sparse graph
- However, hard for inference problems in bioinformatics.

Approximate inference: sampling

- Suppose you are given values for some subset of the variables (evidences), E, and want to infer values for unknown variables, Z
- Randomly sample a very large number of instances from BN
  - Generate instances for **all** variables – start at root variables and move "forward" in a **"topological order"** of the nodes
    - **topological ordering** of a directed graph is a linear ordering of its vertices such that for every directed edge *uv* from vertex *u* to vertex *v*, *u* comes before *v* in the ordering
    - There always exists a topological order in a DAG.
  - This is much easier to compute than the joint probability
- **Reject the instances inconsistent with E**
- Use the frequency of values for Z in the **retained instances** to get estimated probabilities
- Accuracy of the results depends on the size of the sample (asymptotically approaches the exact results)

An example



	T	F
T	0.1	0.9
F	0.5	0.5

	T	F
T	0.8	0.2
F	0.2	0.8

S	R	T	F
T	T	0.99	0.01
T	F	0.90	..
F	T		
F	F		

P(Rain=T|Sprinkler=T)?

100 samples

27 samples have Sprinkler=T

Out of 27 samples, 8 have Rain=T

P(Rain=T|Sprinkler=T)=8/27

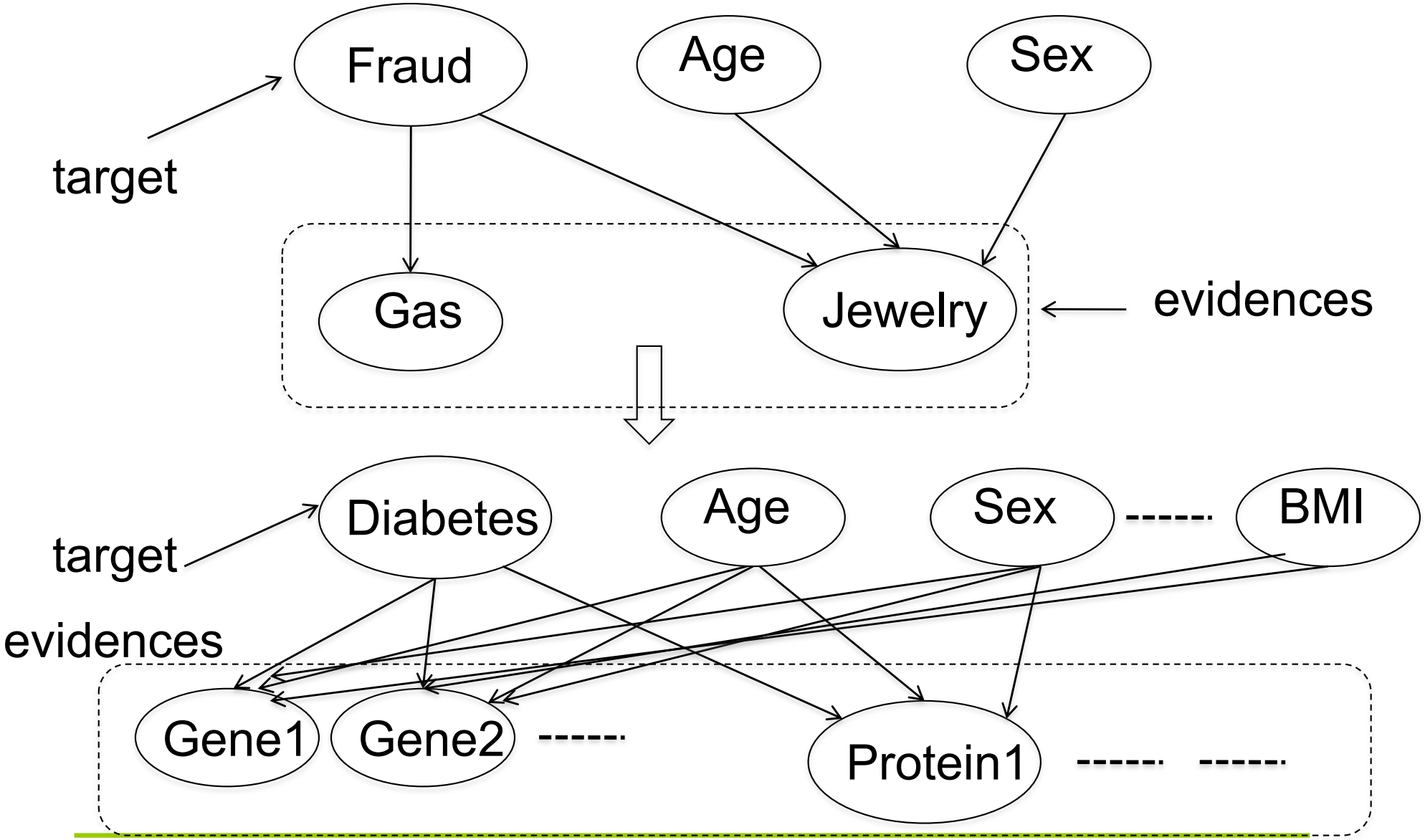
Likelihood weighting

- Idea: do not sample instances that need to be rejected
  - Sample only from the unknown variables Z
  - weight each sample according to the likelihood that it would occur, given the evidence E
  - Markov Chain Monte Carlo (MCMC) algorithm

MCMC algorithm

- A random walk through variable space, counting instances during sampling
  - Initialize with a random instance, consistent with evidence variables E
  - At each step, for a ***non-evidence*** variable, randomly sample its value, based on the other current assigned variables
  - When samples approach infinite, MCMC reaches an accurate estimate of the actual joint distribution
- MCMC approaches
  - The Metropolis-Hastings (MH) algorithm is the most popular MCMC method; Most practical MCMC algorithms can be interpreted as special cases or extensions of this algorithm
  - Gibbs sampling is a MCMC algorithm that generates samples by sampling from **conditional** distributions (instead of the marginal distribution (motif finding)

Predicting diseases from BN



BMI: body mass index

Learning Bayesian networks: four cases

- Known graph—learn parameters
  - Complete data (ML, MAP)
  - Incomplete data (EM)

- Unknown graph—learn graph and parameters
  - Complete data; optimization problem (search in space of graphs)
  - Incomplete data; structural EM

Learning parameters: complete data

The **maximum likelihood estimate (MLE)** of $\boldsymbol{\theta}_{ij}$ can be computed by a frequency model,

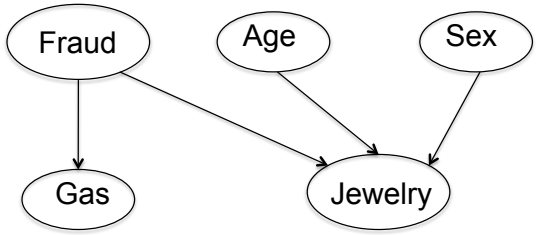
$$\theta_{ijk} = \frac{N_{ijk}}{\sum_{k} N_{ijk}}$$

where θ_{ijk} is the number of cases in D in which $X_i = x_i^k$ and $Pa_i = pa_i^j$. If we assume the prior distribution of $\boldsymbol{\theta}_{ij}$ follow a Dirichlet distribution with parameters $\boldsymbol{\alpha}_{ij}=(\alpha_{ij1},\ldots, \alpha_{ijri})$, i.e., the pseudo-counts, we have the MAP estimates,

$$\theta_{ijk} = \frac{\alpha_{ijk} + N_{ijk}}{\sum_{k}\left(\alpha_{ijk} + N_{ijk}\right)}$$

Assumption: the *parameters are independent (i.e.,* $\boldsymbol{\theta}_{ij}$ are mutually independent)

An example



Fraud	Age	Sex	Gas	Jewelry
no	35	M	no	no
no	22	F	no	yes
no	55	M	no	no
no	42	M	no	no
no	51	F	no	no
no	32	F	no	yes
no	28	F	no	no
yes	25	M	yes	no
yes	53	M	yes	yes
yes	24	F	yes	yes

Adding pseudo-count
1 for each case

P(j=yes|f=yes,a=*,s=*)=0.6,
P(j=yes|f=no,a=<30,s=male)=0.5
P(j=yes|f=no,a=30-50,s=male)=0.25
P(j=yes|f=no,a=>50,s=male)=0.33
P(j=yes|f=no,a=<30,s=female)=0.50
P(j=yes|f=no,a=30-50,s=female)=0.67
P(j=yes|f=no,a=>50,s=female)=0.33

P(f=yes)=0.33
P(s=male)=0.5

P(a=<30)=0.40
P(a=30-50)=0.30

P(g=yes|f=yes)=0.8
P(g=yes|f=no)=0.1

Sample size is too small!

Learning parameters with missing data

- Important property of the missing data
  - the absence of the data is dependent on the actual state of the variable
    - e.g., a missing datum in a drug study may indicate that a patient became too sick, perhaps due to the side effects of the drug, to continue in the study.
  - the absence of the data and the state of the variable are independent
- BN can handle both situations; the 2nd one is simpler and will be discussed here.

Learning parameters: missing data

- Gibbs sampling (MCMC) algorithm
  - Randomly choose an initial state for each of the variables without observations, forming the initial configuration
  - Pick a random variable x_i, compute its probability distribution **given the states of the other n-1 variables**
  - Sample a state of variable x_i, forming a new configuration
  - Iterate the two previous steps, and record all visited configurations
  - Compute the MLE parameters involving the variables with missing data

Learning parameters: missing data

- EM algorithm: finding a local ML
  - Randomly assign parameters to the distribution involving the variables without observations
  - E-step: using BN inference algorithm to obtain the probability distribution of these variables, given the entire network
  - M-step: update model parameters by using MLE based on the frequencies derived from E-step
  - Iterate between E and M steps until the model converges

Learning graph structure

- Constraint-based structure learning algorithms (**dependence analysis and search**)
  - Independence test: P(X,Y)=P(X)*P(Y)
- Structure scoring methods (optimization of a scoring function) (**scoring and search**)

$$\text{Find } \hat{G} = \arg\max_{G} \text{Score}(G)$$

- Hybrid methods
  - Constraint-based methods can be more efficient for large samples; the detection of conditional independencies may be sensitive; and may not assign a direction to every edge
  - Score-based approach is generally preferred, esp when dealing with small sample size and noisy data.

Constraint-based methods

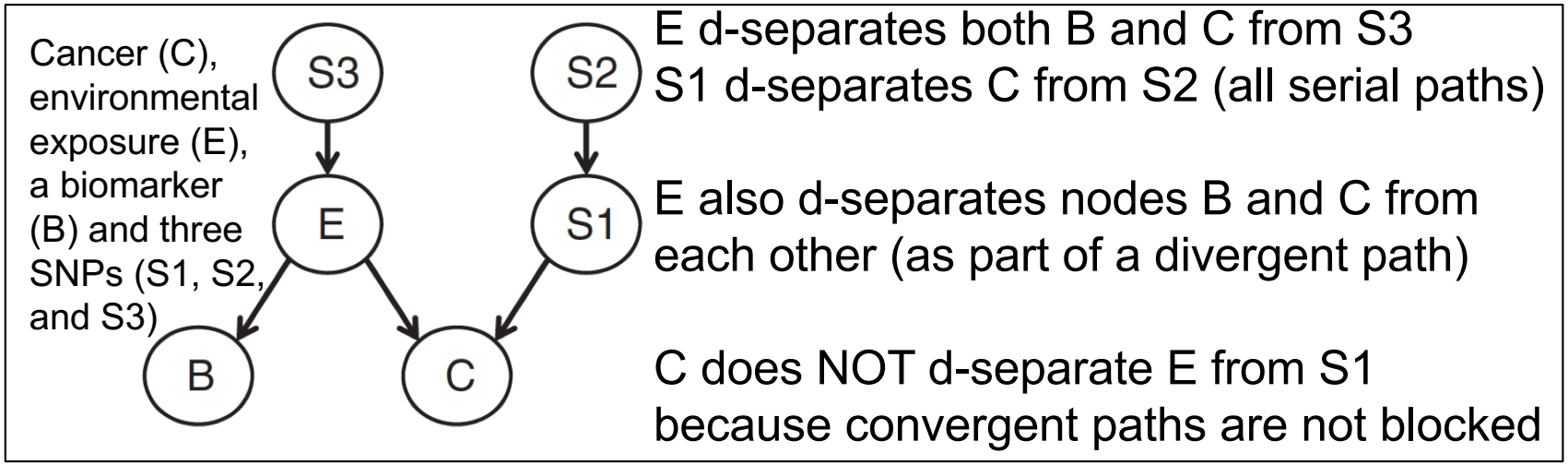
- Constraint-based methods focus on identifying conditional independence relationships (i.e., Markov conditions) between variable using observed data; conditional independencies are used to constrain the underlying network structure.
- Typically, hypothesis testing procedures, such as the chi-square test and mutual information test, are first used to remove edges from a fully connected undirected graph based on findings of unconditional independence.
- Then directions are added to edges between nodes according to the d-separation (directed separation) criteria.

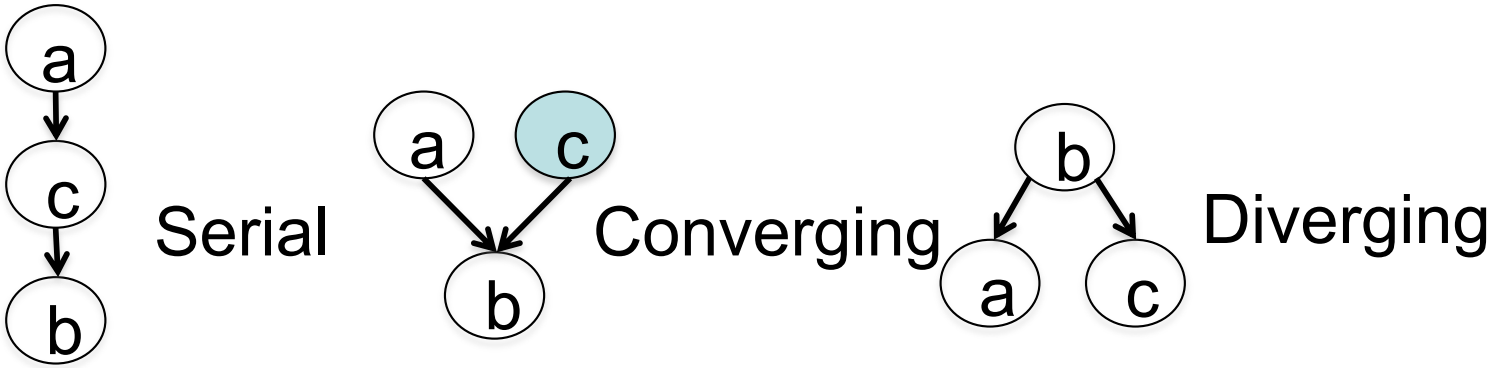
Grow-shrink method

- Based on the concept of Markov blanket
  - The **Markov blanket** of a node in a BN consists of its parents, children, and its children's other parents.
- The GS algorithm
  - Starts with a variable X and an empty set S. The growing phase adds variables to S if they are dependent on X, conditional on the variables currently in S. In the shrinking phase, variables that are rendered independent of X, based on the current members of S, are then removed from S.
  - Represent S (together with X) as a fully connected, undirected network.
  - Examining triples of variables using **the d-separation criteria** (e.g., remove spousal links between two nodes Y and Z by looking for a d-separating set around Y and Z, and give directions to edges if conditioning on a middle node creates a dependency.

D-separation criteria

- If X, Y and Z are three disjoint sets of nodes in a BN, then Y is said to d-separate X from Z if and only if Y blocks every path from a node in X to a node in Z.



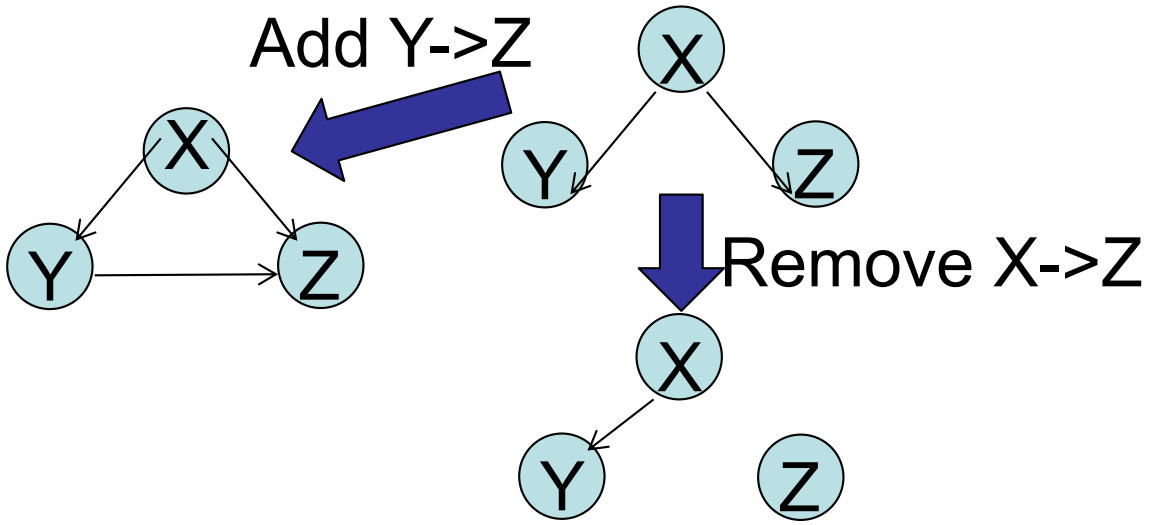


Score-based methods

Find $\hat{G} = \arg\max_{G}$ **Score(G)**

Score(G) – measures how well a model fits the data
Finding the best model is NP-hard optimization; Use heuristic search algorithms instead

- Scoring function
- Search space
- Search strategy



Scoring functions

- Likelihood scores

$$\max_{(G,\theta_G)} L\left(\langle G,\theta_G\rangle \mid D\right) = \max_S\left(\max_{\theta_S}\left(L\left(\langle S,\theta_S\rangle \mid D\right)\right)\right) = \max_S\left(L\left(\langle S,\hat{\theta}_S\rangle \mid D\right)\right)$$

- Penalized log-likelihood scores
  - BIC Bayesian information criteria
  - MDL Minimum description length
- Bayesian scores

$$\max_G P(G \mid D) \propto \max_S P(D \mid S)P(S) = \int_{\theta_S} P\left(D \mid \theta_S, S\right)P\left(\theta_S \mid S\right)d\theta_S$$

  - Prior probability used for $P(S)$ and $P(\theta_S|S)$

Search methods

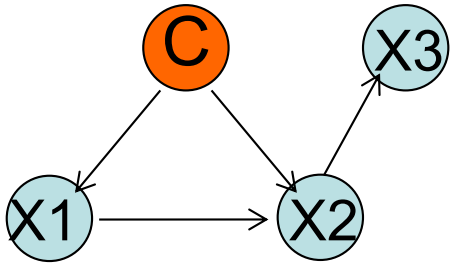
- Most search methods make successive changes of edge linkages to the network, and employ the local criterion to assess the merit of each change.
- One simple heuristic search algorithm is greedy search
  - may be stuck at local minima; can start from multiple initial points
  - global optimization approaches can apply: simulated annealing, best-first search, etc

Bayesian networks as classifiers

- Two types of nodes: a class node (C) and attribute nodes
- A BN can be used as a classifier that gives the posterior probability distribution of the class node, given attributes X.

$$P(C|x,G) = \frac{P(C,x|G)}{P(x|G)} \propto P(C,x|G)$$

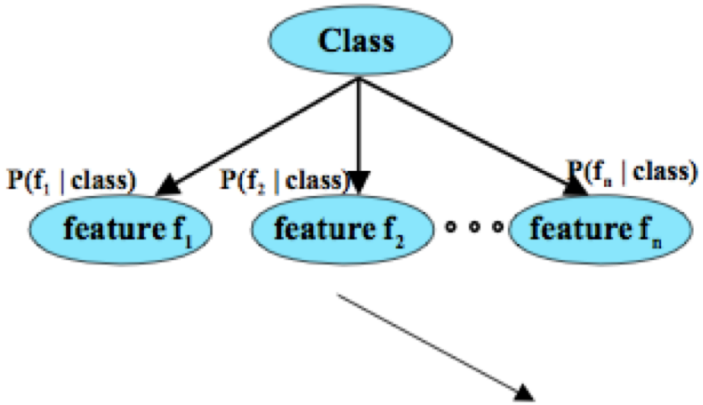
$$c^* = \arg\max_j P(c_j,x|G)$$



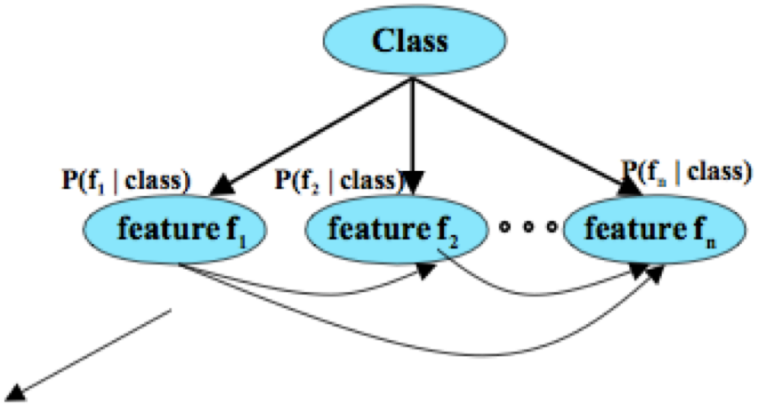
- A NB (Naïve Bayes) classifier can be viewed as a BN classifier with a simple structure

Model selection trade-offs

Naïve Bayes – too simple
(less parameters, but bad model)



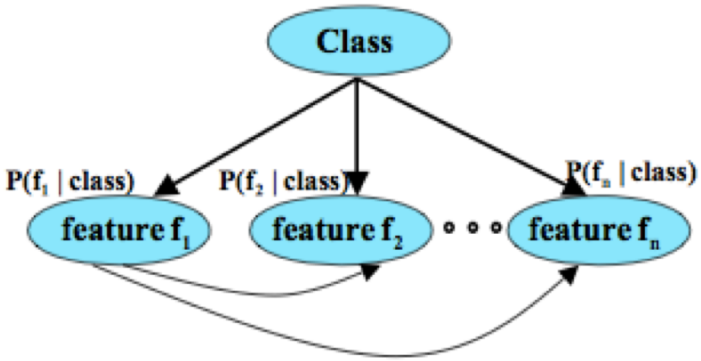
Unrestricted BN – too complex
(possible overfitting + complexity)



Various approximations between the two extremes

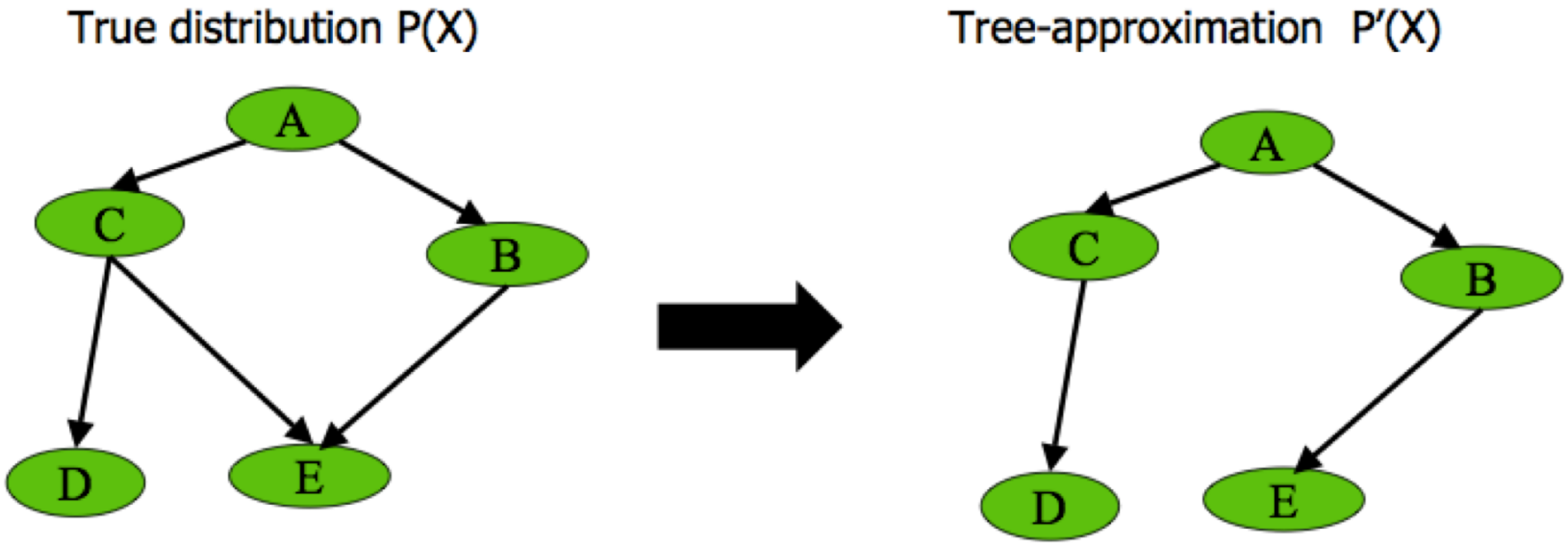
TAN:
tree-augmented Naïve Bayes
[Friedman et al. 1997]

Based on Chow-Liu Tree Method
(CL) for learning trees
[Chow-Liu, 1968]

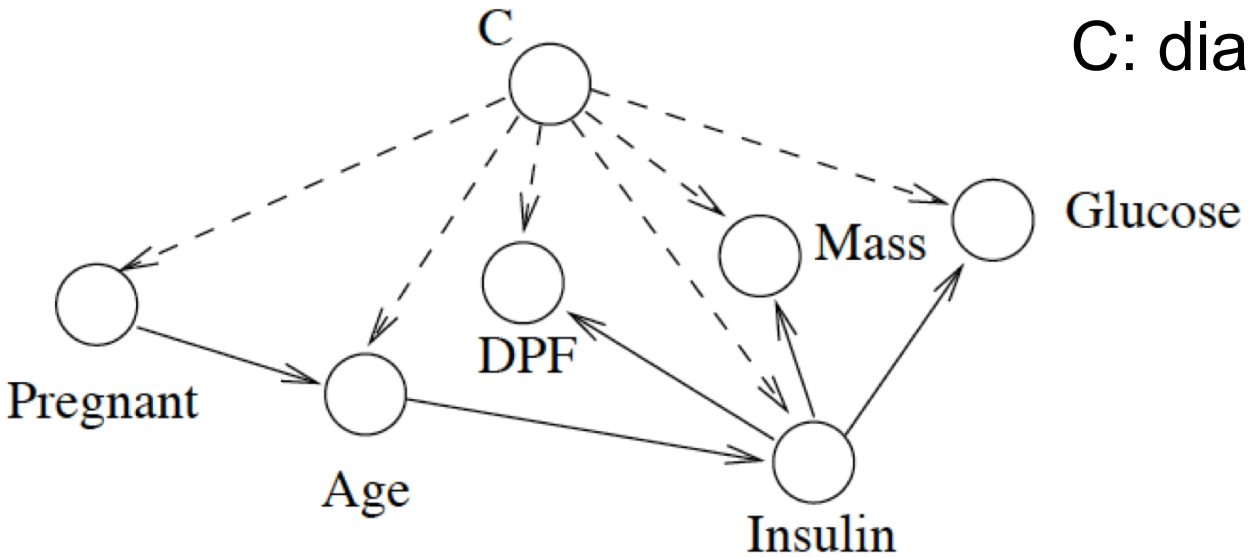


Ref: http://www.ee.columbia.edu/~vittorio/Lecture12.pdf

Tree-approximation



Extensions to NB classifier



C: diabetes (yes/no)

TAN model: A network with an edge between the class node and each of the attributes (to ensure that all attributes are part of the class variable Markov blanket)

- Dashed lines, edges required by NB classifier
- Solid lines, correlation edges between attributes (relax the independence assumption between the attributes)

Ref: Friedman et al, 1997

CL algorithm for constructing a tree BN from data

1. Compute $I_{\hat{P}_D}(X_i; X_j)$ between each pair of variables, $i \neq j$, where

$$I_P(\mathbf{X}; \mathbf{Y}) = \sum_{\mathbf{x},\mathbf{y}} P(\mathbf{x}, \mathbf{y}) \log \frac{P(\mathbf{x}, \mathbf{y})}{P(\mathbf{x})P(\mathbf{y})}$$

   is the *mutual information* function. Roughly speaking, this function measures how much information $\mathbf{Y}$ provides about $\mathbf{X}$. See Appendix A for a more detailed description of this function.

2. Build a complete undirected graph in which the vertices are the variables in $\mathbf{X}$. Annotate the weight of an edge connecting X_i to X_j by $I_{\hat{P}_D}(X_i; X_j)$.

3. Build a maximum weighted spanning tree.

4. Transform the resulting undirected tree to a directed one by choosing a root variable and setting the direction of all edges to be outward from it.

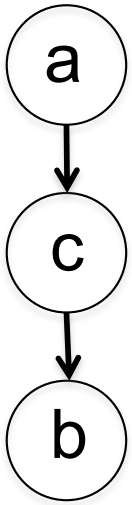
CL prove that this procedure finds the tree that maximizes the likelihood given the data D.

Ref: Chou and Liu, 1968

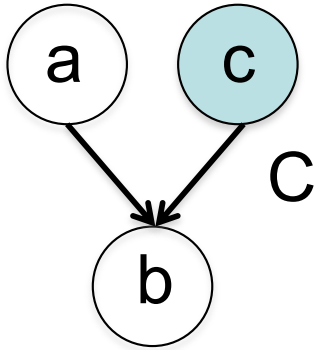
Learning of causal relationships

- *Causal Markov condition*:
  - Variable *a* is a *direct* cause of variable *b* if and only if there is a direct edge from *a* to *b*; then the BN is called a *causal graph*.
  - Variable *a* is a cause of variable *b* (or b is dependent on a) if there exists a *d-connecting* path from *a* to *b* given *evidence* E (a set of variables)
    - A path from *a* to *b* is *d-connecting* if each interior node n in the path is either
      - Linear or diverging and not a member of E; or
      - Converging, and either n or one of its descendants is in E.

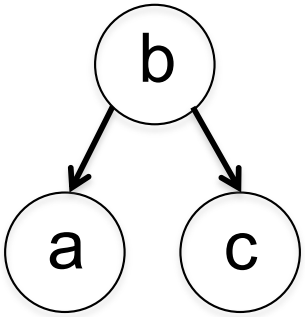
d-separation path



Serial



Converging



Diverging

a is the cause of b; but
a is not the cause of b, given c as evidence

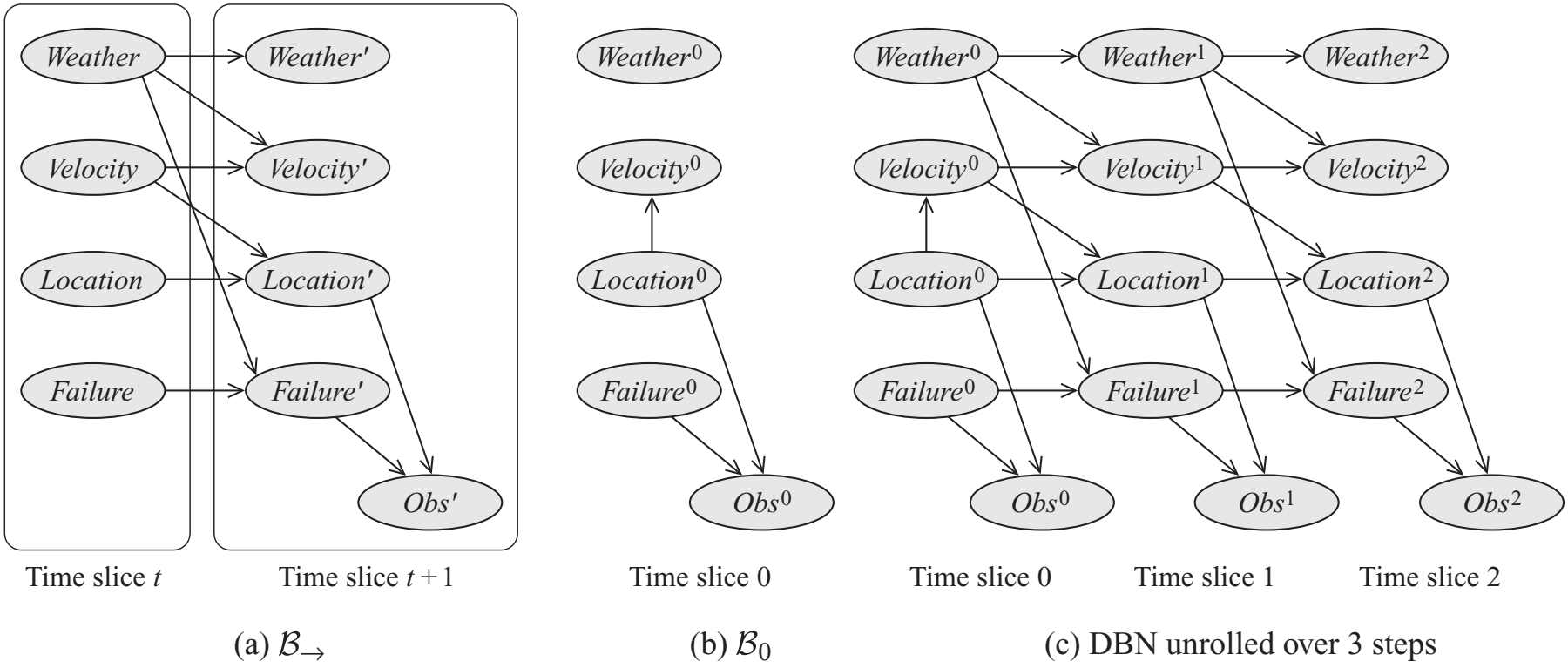
a is not the cause of b; but
a is the cause of b, given c as evidence

b is the cause of a; b may not be the cause of a, if c is given as evidence

Dynamic Bayesian network (DBN)

(Vehicle localization task) A moving car tried to track its current location using the data obtained from a, possibly faulty sensor. The system state can be encoded (very simply) using the: Location – the car's current location, Velocity – the car's current velocity; Weather – the current weather; Failure – the failure status of the sensor; and Obs – the current observation. We have one such set of variables for every time point t. *A joint probability distribution* over all of these sets defines a probability distribution over trajectories of the car. Using this distribution, we want to ask a variety of queries, such as 1) given a sequence of observations about the car, where is it now? 2) where is it likely to be in 10 minutes? 3) did it stop at the red light?

DBN for monitoring a car
a 2-time-slice DBN (2-DBN)

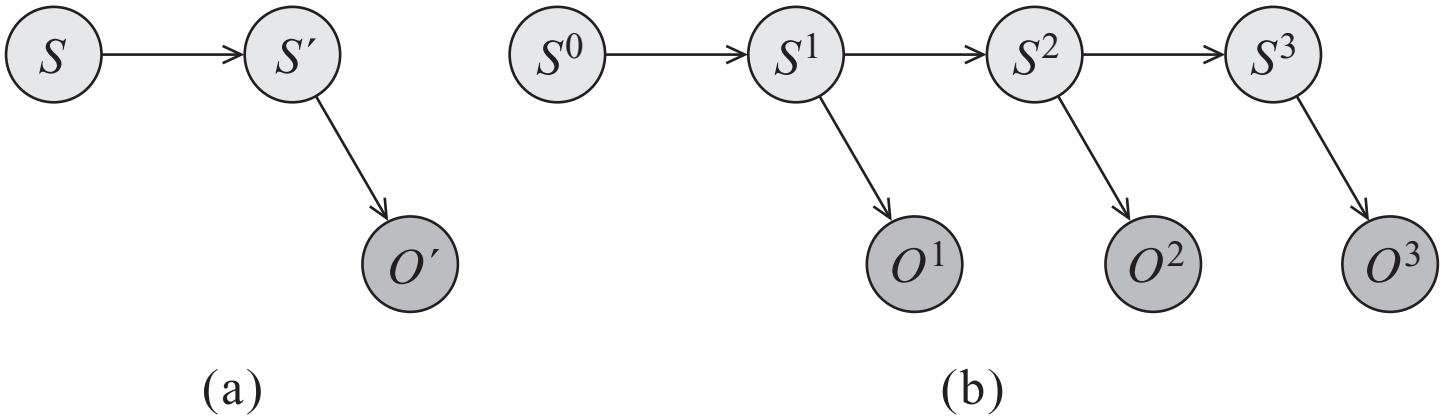


Assumptions: 1) the sensor observation is generated at each time point independently given other variables; 2) all variables are interface variables except for obs.

Reasoning if the model is given

- Given a sequence of observations about the car, where is it now?
  - $P(obs^t|obs^0,\ldots, obs^{t-2}, obs^{t-1})$
- Where is it likely to be in 10 minutes?
  - $P(obs^{t+10}|obs^0,\ldots, obs^{t-2}, obs^{t-1})$
- Did it stop at the red light?
  - $P(V^t|obs^0,\ldots, obs^{t-2}, obs^{t-1})$

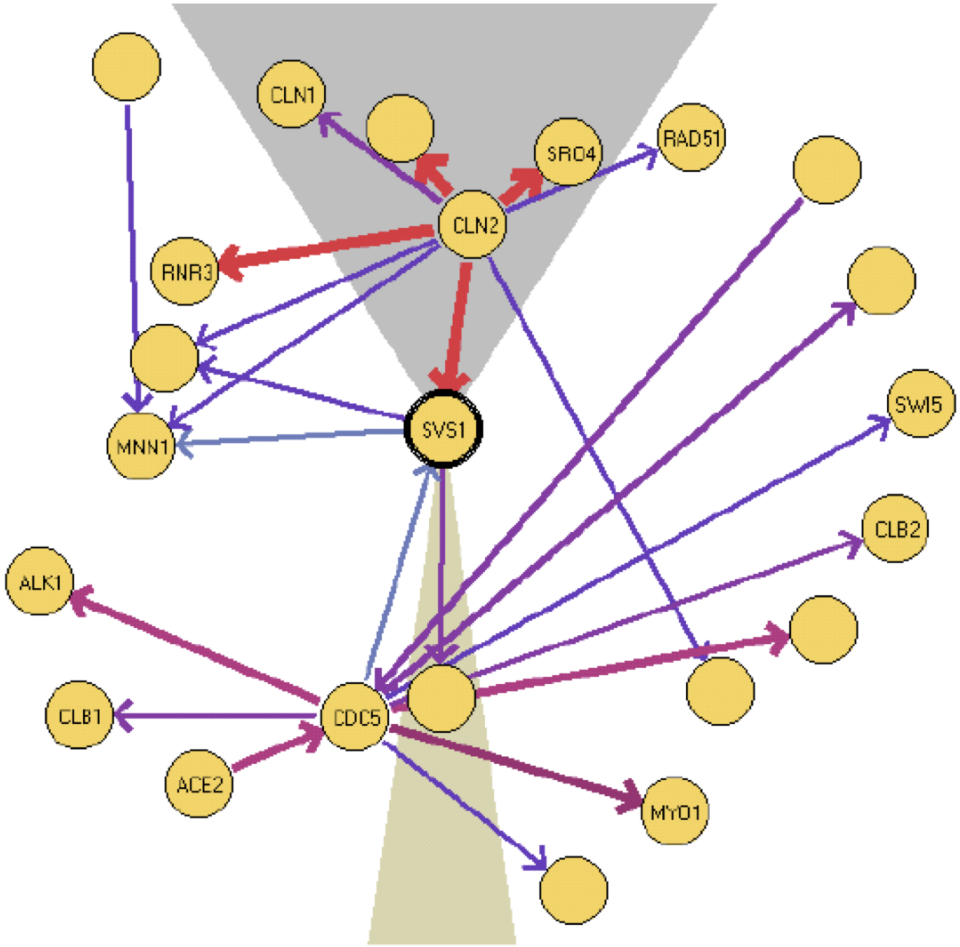
HMM as a 2-DBN



DBN is more general than HMM: 1) the CPD of hidden states can be modeled by a BN, rather than a simple Markov chain; 2) more than one observation variable can be modeled simultaneously (like multivariate HMM).

Applications of BN and DBN

- Friedman et al. Using Bayesian network to analyze expression data. 2000, JCB, 7:601-620.
- Troyanskaya et al. A Bayesian framework for combining heterogeneous data sources for gene function prediction (in *Saccharomyces Cerevisiae*). PNAS, 2003, 100: 8348–8353.
- Jansen et al. A Bayesian networks approach for predicting protein-protein interactions from genomic data. Science 2003, 302:449-453
- Friedman et al. Inferring cellular networks using probabilistic graphical models. Science, 2004, 303:799-805
- Sachs et al. Causal protein-signaling networks derived from multi-parameter single-cell data. Science, 2005, 308:523-529
- …
- Predicting gene regulatory networks by combining spatial and temporal gene expression data in Arabidopsis root stem cells. PNAS, 2017, 114 (36) E7632-E7640



Sparse candidate algorithm:
Only consider a small number of parent candidates for each gene to constrain the search space of the network

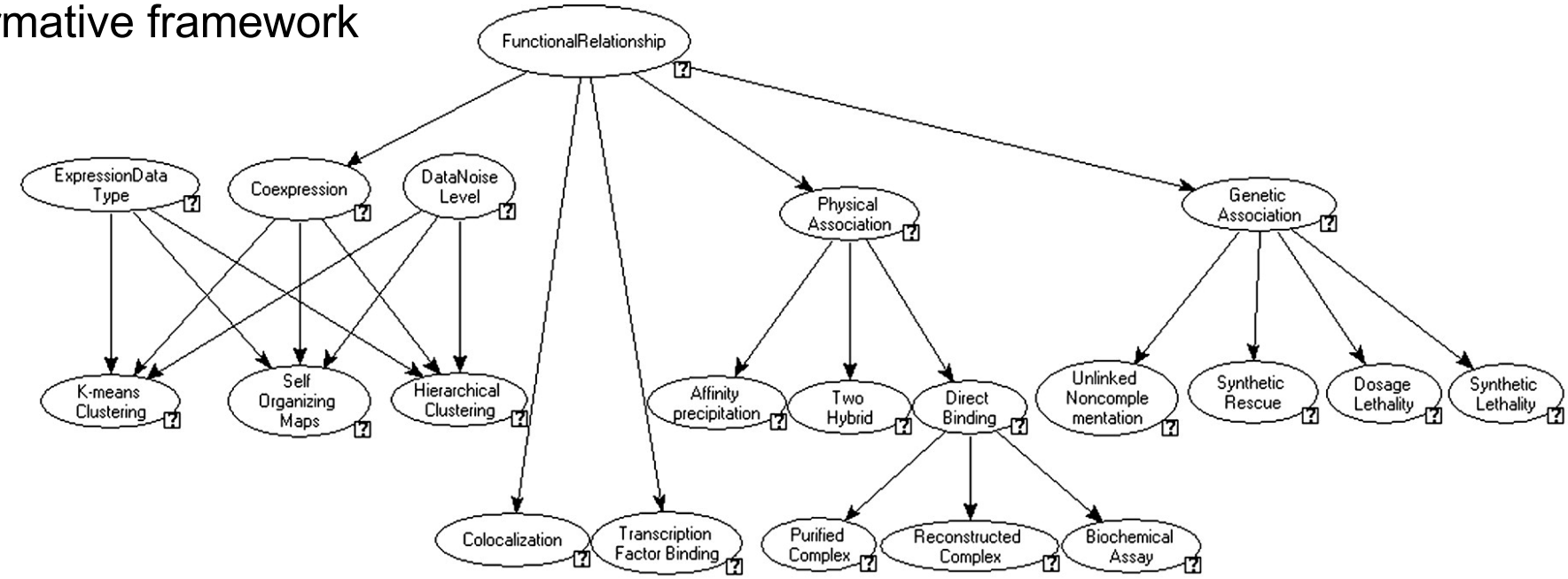
Local probability models:
Multinomial model
Linear Gaussian model

Figure 2: An example of the graphical display of Markov features. This graph shows a "local map" for the gene SVS1. The width (and color) of edges corresponds to the computed confidence level. An edge is directed if there is a sufficiently high confidence in the order between the genes connected by the edge. This local map shows that CLN2 separates SVS1 from several other genes. Although there is a strong connection between CLN2 to all these genes, there are no other edges connecting them. This indicates that, with high confidence, these genes are conditionally independent given the expression level of CLN2.

Friedman et al. Using Bayesian network to analyze expression data. 2000, JCB, 7:601-620.

General architecture of the magic Bayesian Network.

The system (MAGIC) formally incorporates expert knowledge about relative accuracies of data sources to combine them within a normative framework



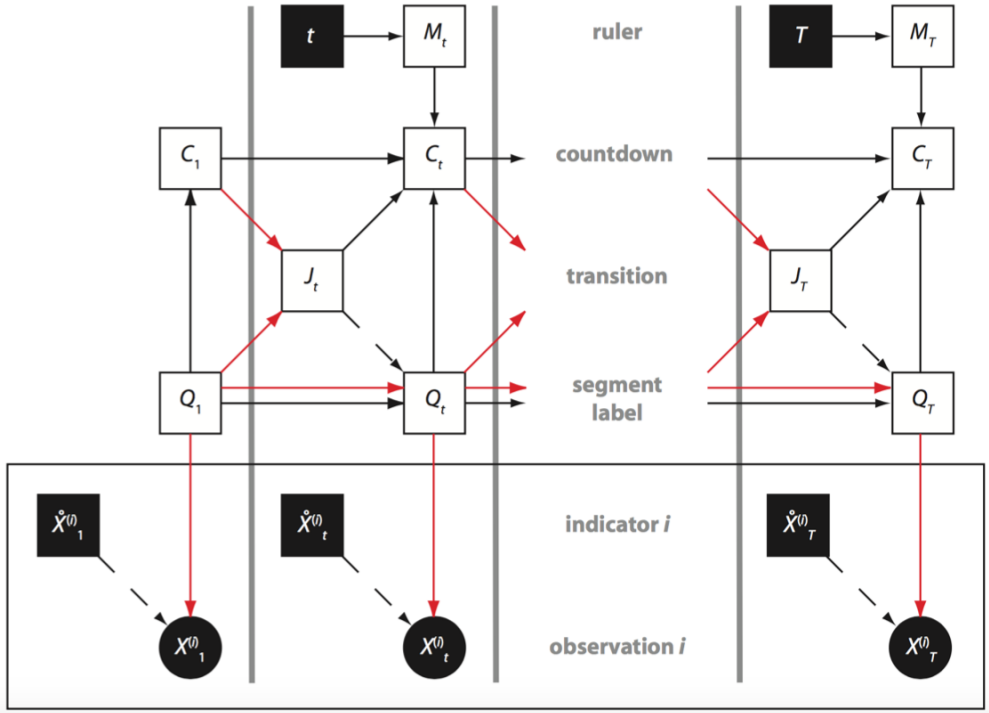
Conditional probability tables for each connection were assessed formally from yeast genetics expert

Troyanskaya O G et al. PNAS 2003;100:8348-8353

Segway (based on DBN)

- Ref: Unsupervised pattern discovery in human chromatin structure through genomic segmentation
- Uses a dynamic Bayesian network (DBN) model, which enables it to analyze the entire genome at 1-bp resolution even in the face of heterogeneous patterns of missing data.
- Uses the Graphical Models Toolkit (GMTK) for efficient DBN inference.

Supplementary Fig. 11: Graphical model representation of the default Segway DBN.



Nature Methods 9, 473–476 (2012)

GENIST

- GENIST: gene regulatory network inference from spatiotemporal data algorithm, a DBN-based algorithm capable of integrating transcriptional datasets of different characteristics to reconstruct GRNs.
- “we transcriptionally profiled several stem cell populations and developed a gene regulatory network inference algorithm that combines clustering with dynamic Bayesian network inference. ”
- Ref: PNAS, 2017, 114 (36) E7632-E7640

Packages

- Scikit-learn: naïve bayes (http://scikit-learn.org/stable/modules/naive_bayes.html)
- bnlearn - an R package for Bayesian network learning and inference (http://www.bnlearn.com/)
- GMTK (DGM & DBN) http://melodi.ee.washington.edu/gmtk/
- mlbench
  - machine learning benchmark problems
  - E.g., pima data: PimaIndiansDiabetes2