

CMT311 Principles of Machine Learning

GM Inference (part 2)

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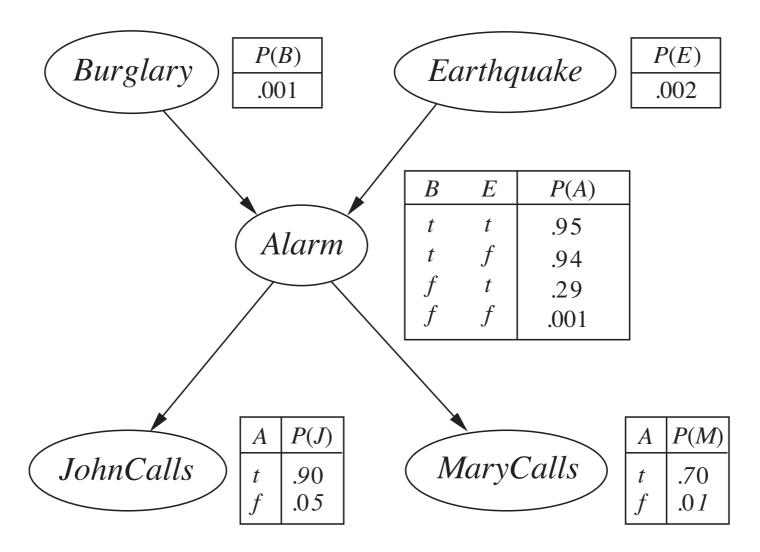
Coursework

- 30% of module marks
- now available on Learning Central under "Assessment"
- STRICT deadline: 28.02.2020, 9:30am
- You can update your submission as often as you want. Only your last submission counts: its timestamp determines whether you submitted on time, and only that submission will be marked.
- Questions: only via the "Coursework" forum on Learning Central (under "Discussions")

Last week

Judea Pearl's Alarm network

You have a new burglary alarm that is fairly reliable at detecting a burglary, but also responds to earthquakes. Your neighbours, Mary and John, promise to call you if they hear the alarm sounding.



Variable Elimination

$$P(B, J = t, M = t) = P(B) \sum_{E} P(E) \sum_{A} P(A \mid E, B) P(J = t \mid A) P(M = t \mid A)$$

$$f_{\overline{B}}(B) \qquad f_{\overline{E}}(E) \qquad f_{\overline{A}JM}(B, E)$$

$$f_{\overline{E}\overline{A}JM}(B)$$

$$P(B, J = t, M = t)$$

$$f_{\overline{A}JM}(B,E) = \sum_{a} f_A(A=a,B,E) \times f_J(A=a) \times f_M(A=a)$$

$$= f_A(A=t,B,E) \times f_J(A=t) \times f_M(A=t) + f_A(A=f,B,E) \times f_J(A=f) \times f_M(A=f)$$

$$f_{\overline{E}\overline{A}JM}(B) = f_E(E=t) \times f_{\overline{A}JM}(B,E=t) + f_E(E=f) \times f_{\overline{A}JM}(B,E=f)$$

 $P(B, J = t, M = t) = f_R(B) \times f_{\overline{FA}IM}(B)$

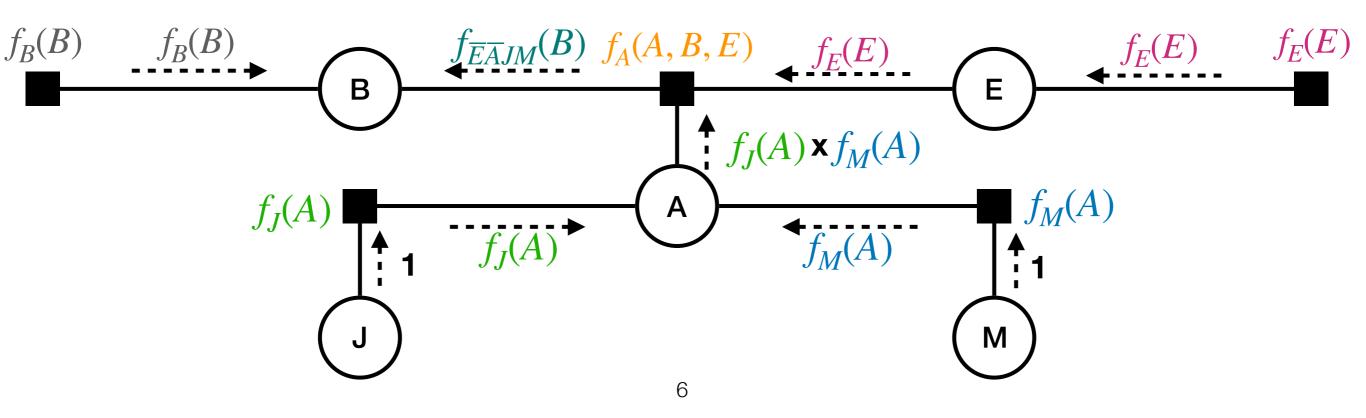
Variable Elimination as Message Passing

$$P(B, J = t, M = t) = P(B) \sum_{E} P(E) \sum_{A} P(A \mid E, B) P(J = t \mid A) P(M = t \mid A)$$

$$f_{B}(B) \qquad f_{E}(E) \qquad f_{A}(A, B, E) \qquad f_{J}(A) \qquad f_{M}(A)$$

$$f_{\overline{E}\overline{A}JM}(B)$$

$$P(B, J = t, M = t) = f_B(B) \times f_{\overline{EA}JM}(B)$$



Sum-product algorithm

- FGs can have **loops**, which cause a problem for message passing: eliminating a variable may introduce a factor that isn't in the graph yet
- what to do?
 - option 1: loopy belief propagation
 - use propagation rules anyways, hoping that messages will converge
 - no guarantees, but often works well enough in practice
 - option 2: bucket elimination
 - guaranteed to produce correct answers

Bucket Elimination

- computes the marginal of one variable only
- multi-variable messages need storage exponential in number of their variables
- for graphs without loops, computational complexity depends on ordering: there is an order with linear complexity, but others are much worse

Today

- Loopy structures revisited: junction trees
- Approximate inference using sampling

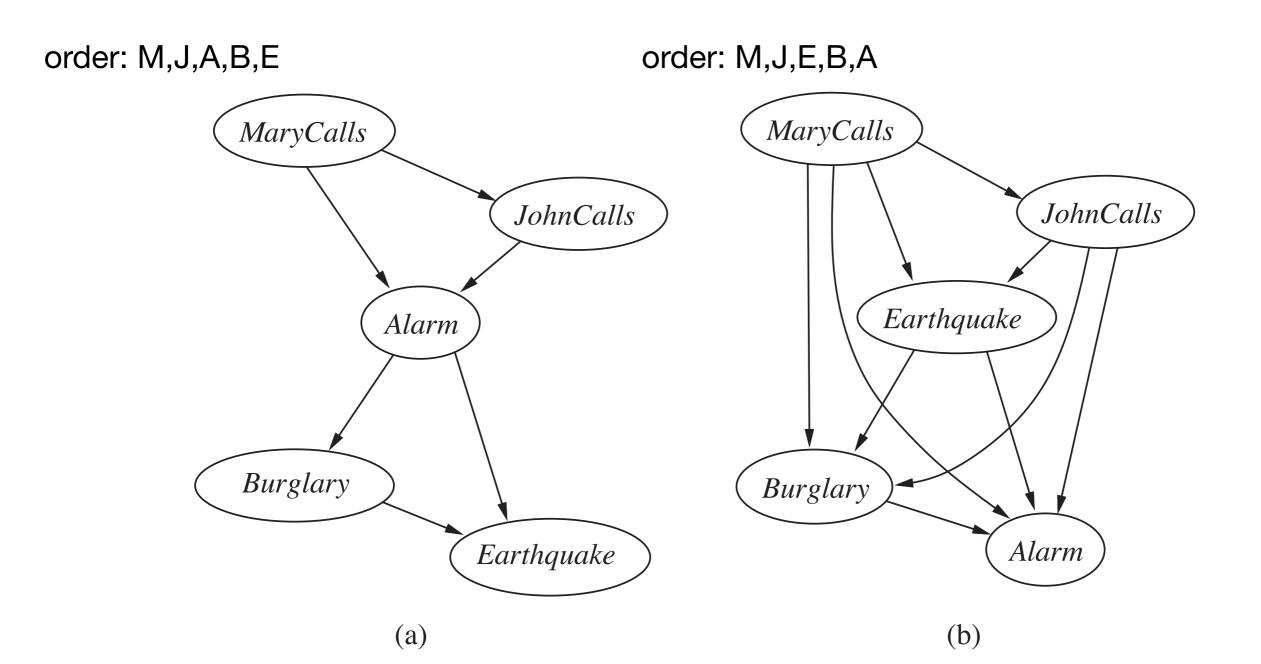
The cost of BN inference

- Time and space requirements of variable elimination are dominated by the size of the largest factor constructed.
- If the DAG of a BN is **singly connected** (no loops), then the time and space complexity of exact inference is **linear** in the size of the network (=number of parameters).
 - If the number of parents per node is bounded, also linear in the number of variables.
- If the DAG has loops, VE can take exponential time and space, even for bounded number of parents.

The cost of BN inference

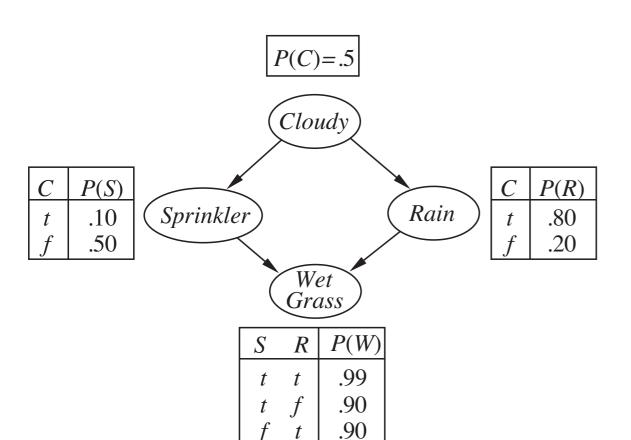
- As inference in propositional logic is a special case of BN inference, BN inference is (at least) NP-hard.
- More precisely, inference in BNs is as hard as computing the number of satisfying assignments for a propositional formula, which is #P-hard (strictly harder than NPcomplete problems)
- Yet another reason for careful modelling...

Judea Pearl's Alarm network



The junction tree algorithm

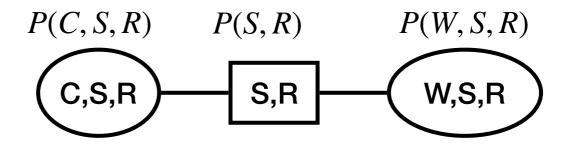
- Loops cannot always be avoided.
- Bucket elimination handles loops, but needs a separate run for each variable's marginal.
- The junction tree algorithm computes marginals for all variables:
 - construct a new graph without loops, but with more complicated nodes (called junction tree)
 - perform a form of message passing on the junction tree (linear in the size of the junction tree)
 doesn't make the problem less hard!
- the result explicitly represents marginals



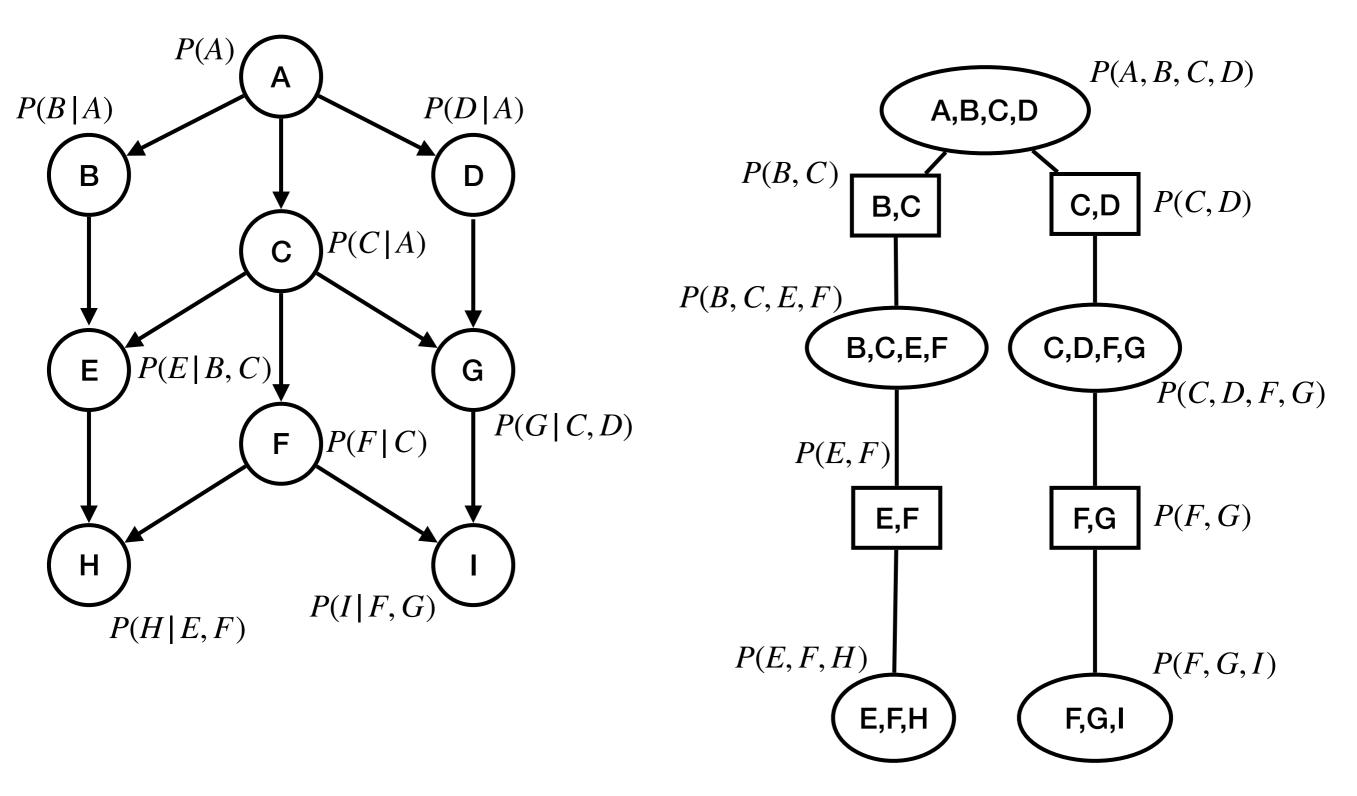
Idea

$$P(C, S, R, W) = P(C)P(S|C)P(R|C)P(W|S, R)$$
$$= P(C, S, R) \frac{P(W, S, R)}{P(S, R)}$$

if we can transform the BN into a representation of this factorisation, then we can compute marginals as local summation operators



P(A)P(B|A)P(C|A)P(D|A)P(E|B,C)P(F|C)P(G|C,D)P(H|E,F)P(I|F,G)



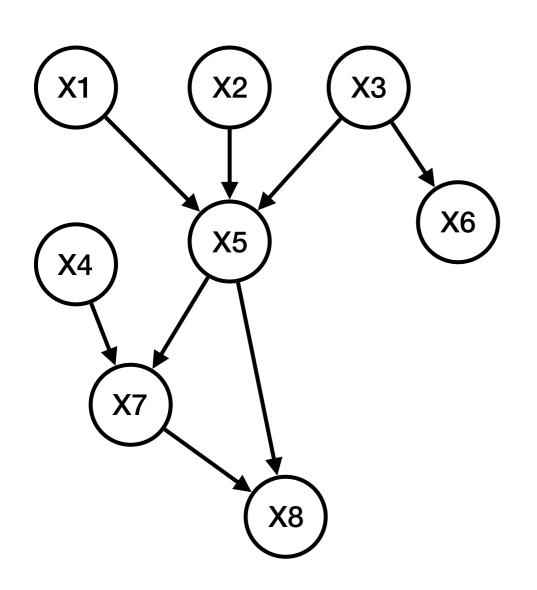
 $\frac{P(A,B,C,D)P(B,C,E,F)P(C,D,F,G)P(E,F,H)P(F,G,I)}{P(B,C)P(C,D)P(E,F)P(F,G)}$

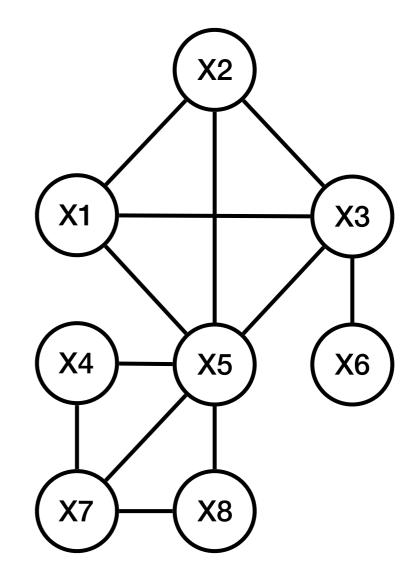
Junction Tree Algorithm

[see Barber ch 6 for correctness]

- 1. **Moralise**: if input is BN, turn it into an MN (marry all unmarried parents + drop edge directions)
- 2. **Triangulate**: ensure that every loop involving four or more edges has a chord (a shortcut edge)
- Construct junction tree: turn the triangulated graph into a socalled clique graph and find a maximal weighted spanning tree of that graph
- 4. Assign potentials to nodes
- 5. Pass messages

Moralisation

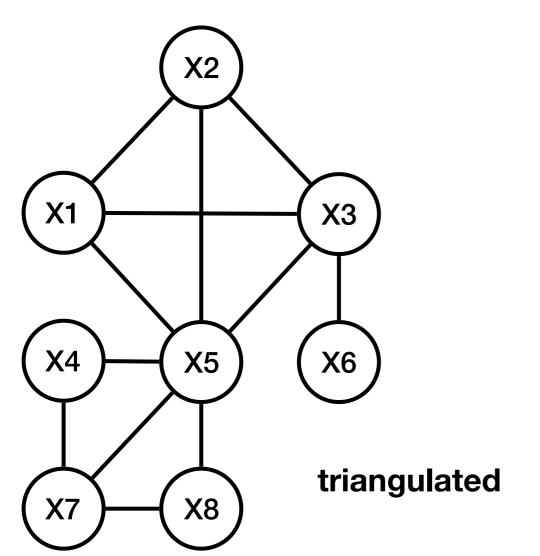




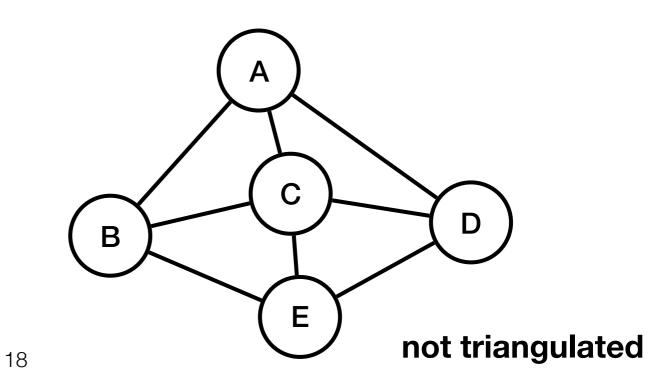
Triangulation

An undirected graph is triangulated if every loop of length four or more has a chord.

- choose an arbitrary node and label it 1
- for i = 2 to n
 - choose a node with the highest number of labeled neighbours and label it i
 - if i has two labeled neighbours without an edge between them, FAIL

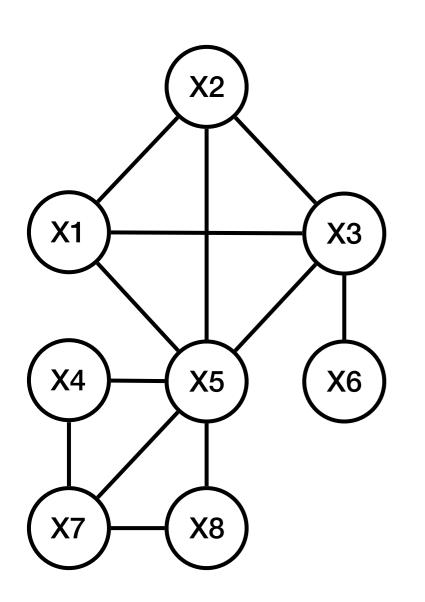


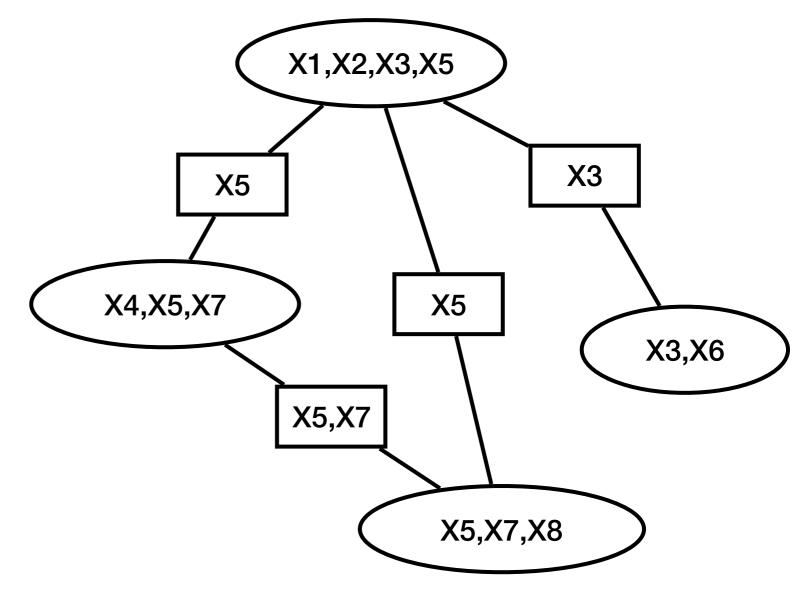
can be used to triangulate: in case of FAIL, add the edge(s) causing the failure & restart



Clique Graph

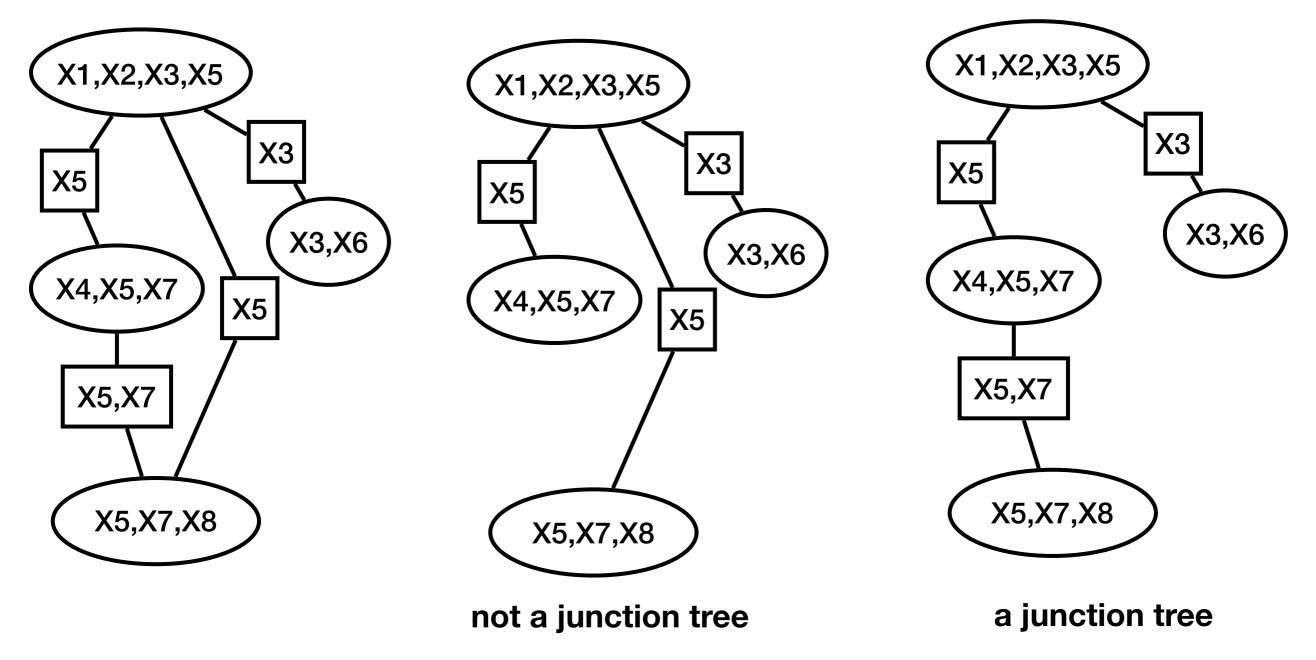
A **clique graph** contains a **clique node** for the set of variables of each potential, a **separator node** for each pair of neighbouring cliques' shared variables, and edges between the separators and their cliques.



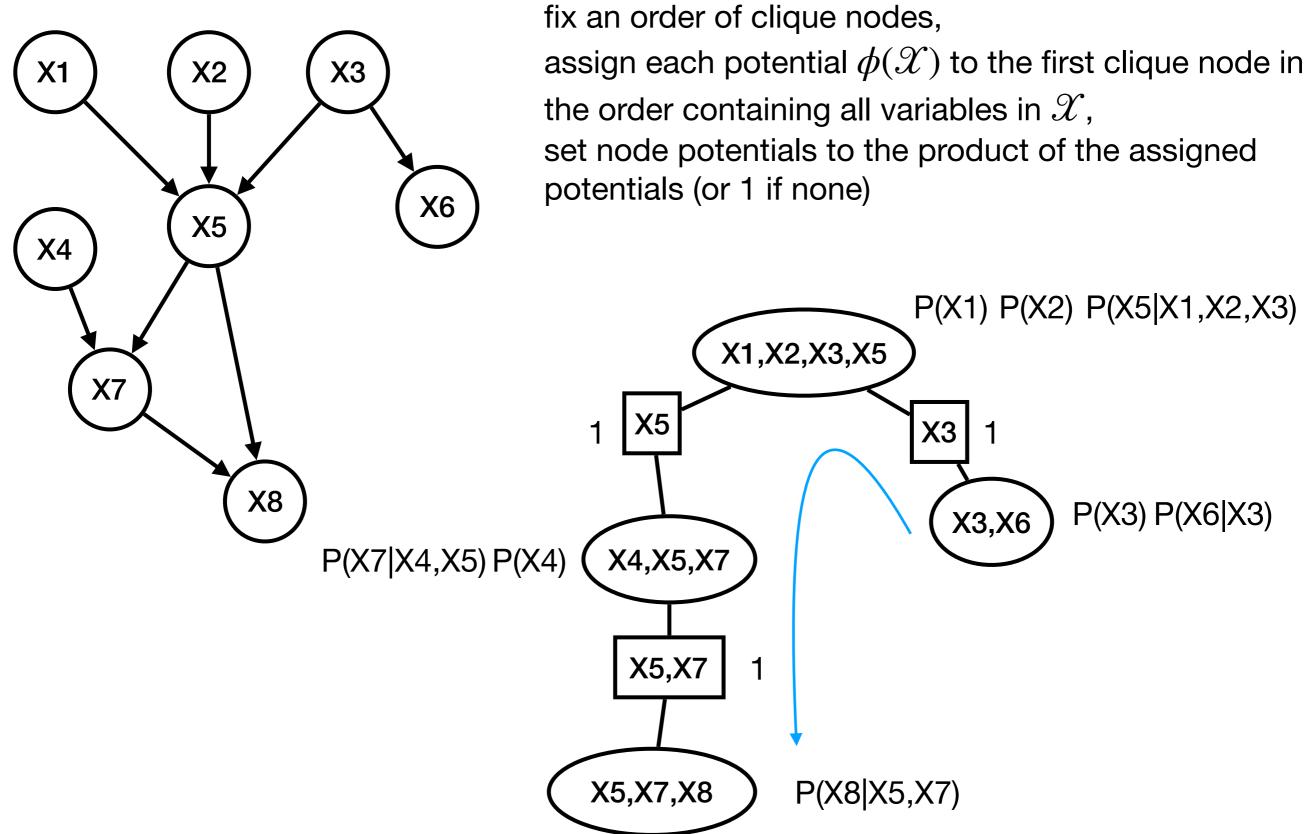


Junction Tree

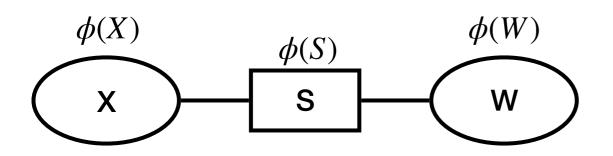
A junction tree is a clique graph without loops that satisfies the running intersection property, i.e., for all pairs of nodes \mathcal{X} and \mathcal{Y} , all nodes on the path between \mathcal{X} and \mathcal{Y} contain $\mathcal{X} \cap \mathcal{Y}$

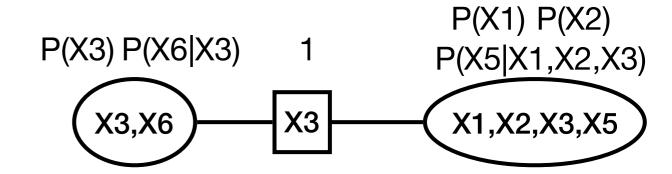


Junction Tree Potentials

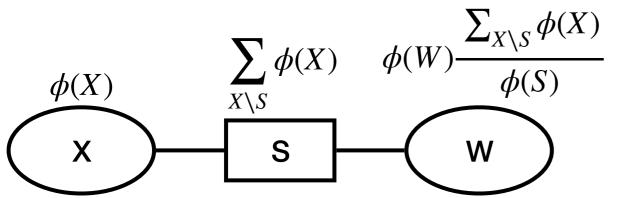


JT Message Passing



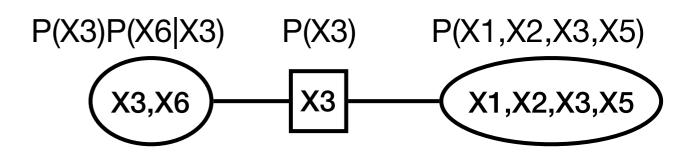


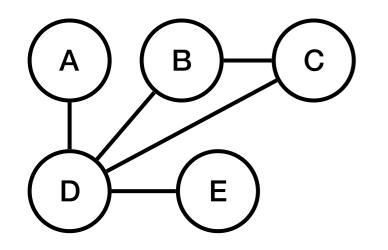
after sending a message from X to W, we get:



$$\sum_{X6} P(X3)P(X6 | X3) = P(X3)$$

$$P(X1)P(X2)P(X5 \mid X1, X2, X3) \frac{P(X3)}{1} = P(X1, X2, X3, X5)$$



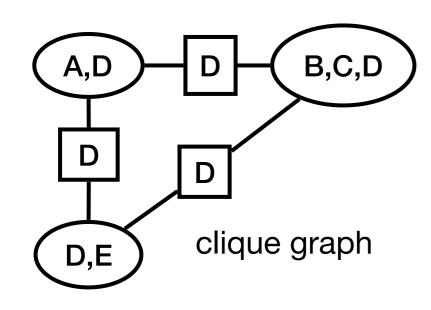


Α	D	f ₁ (A,D)
0	0	5
0	1	2
1	0	1
1	1	1

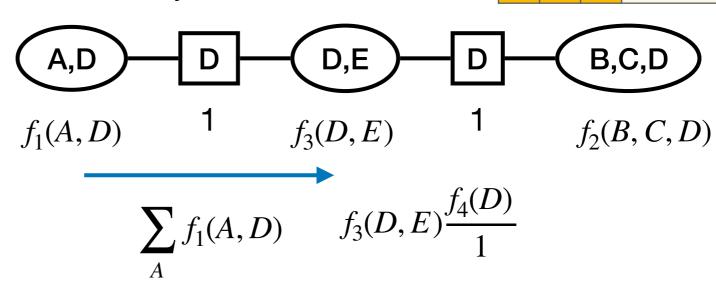
D	Ε	f ₃ (D,E)
0	0	1
0	1	0
1	0	0
1	1	1

В	С	D	f ₂ (B,C,D)
0	0	0	10
0	0	1	1
0	1	0	1
0	1	1	5
1	0	0	1
1	0	1	5
1	1	0	5
1	1	1	10

is triangulated



junction tree



D	f ₄ (D)
0	6
1	3

D	Ε	f ₅ (D,E)
0	0	6
0	1	0
1	0	0
1	1	3



Α	D	f ₁ (A,D)
0	0	5
0	1	2
1	0	1
1	1	1

D	f ₄ (D)
0	6
1	3

D	Е	f ₅ (D,E)
0	0	6
0	1	0
1	0	0
1	1	3

$$\sum_{E} f_5(D, E)$$

D	f ₆ (D)
0	6
1	3

В	С	D	f ₂ (B,C,D)
0	0	0	10
0	0	1	1
0	1	0	1
0	1	1	5
1	0	0	1
1	0	1	5
1	1	0	5
1	1	1	10

В	С	D	f ₇ (B,C,D)
0	0	0	60
0	0	1	3
0	1	0	6
0	1	1	15
1	0	0	6
1	0	1	15
1	1	0	30
1	1	1	30

$$f_2(B, C, D) \frac{f_6(D)}{1}$$



Α	D	$f_1(A,D)$
0	0	5
0	1	2
1	0	1
1	1	1

D	f ₄ (D)
0	6
1	3

$$f_5(D, E) \frac{f_8(D)}{f_6(D)}$$

D	Е	f ₉ (D,E)
0	0	102
0	1	0
1	0	0
1	1	63

D	f ₆ (D)
0	6
1	3

$$\sum_{B,C} f_7(B,C,D)$$

D	f ₈ (D)
0	102
1	63

В	С	D	f ₇ (B,C,D)
0	0	0	60
0	0	1	3
0	1	0	6
0	1	1	15
1	0	0	6
1	0	1	15
1	1	0	30
1	1	1	30

D	f ₈ (D)/f ₆ (D)			
0	102/6=17			
1	63/3=21			



Α	D	$f_1(A,D)$
0	0	5
0	1	2
1	0	1
1	1	1

D	f ₄ (D)
0	6
1	3

$$\sum_{E} f_9(D, E)$$

D	f ₁₀ (D)
0	102
1	63

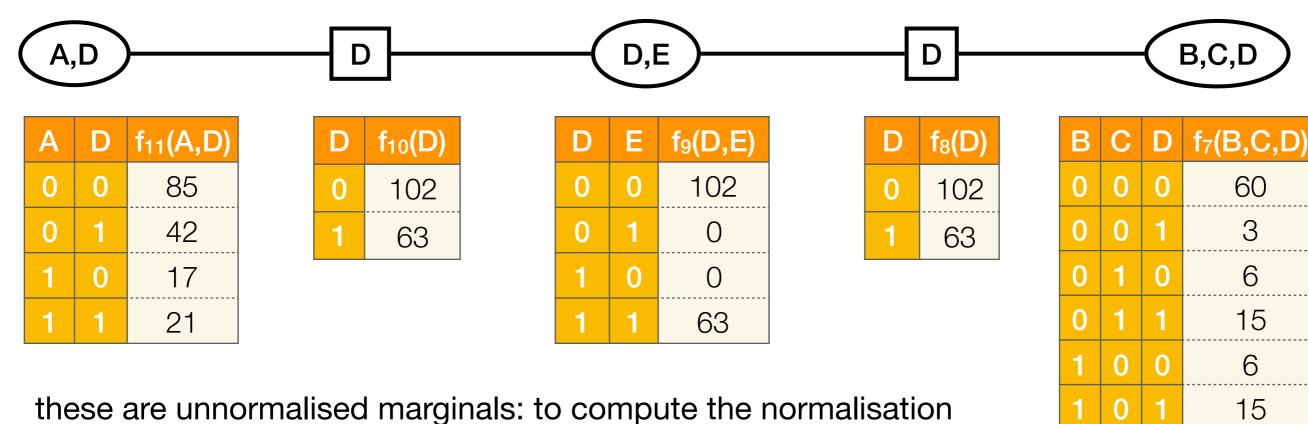
D	Е	f ₉ (D,E)
0	0	102
0	1	0
1	0	0
1	1	63

D	f ₈ (D)
0	102
1	63

В	С	D	f ₇ (B,C,D)
0	0	0	60
0	0	1	3
0	1	0	6
0	1	1	15
1	0	0	6
1	0	1	15
1	1	0	30
1	1	1	30

$$f_1(A, D) \frac{f_{10}(D)}{f_4(D)}$$

Α	D	f ₁₁ (A,D)
0	0	85
0	1	42
1	0	17
1	1	21



constant Z, pick one of the tables and sum out all variables

$$Z = \sum_{D} f_{10}(D) = 102 + 63 = 165$$

to compute the marginal P(A,D), normalise $f_{11}(A,D)$:

A	D	P(A,D)
0	0	85/165=0.515
0	1	42/165=0.255
1	0	17/165=0.103
1	1	21/165=0.127

to compute the marginal P(A), sum out D:

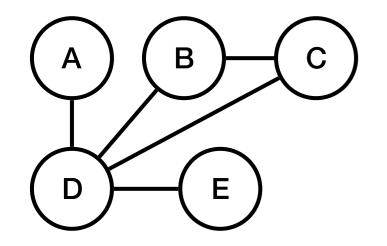
A	P(A)
0	85/165+42/165=0.7697
1	17/165+21/165=0.2303

similar for marginals of other variables

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Homework



Α	D	f ₁ (A,D)
0	0	5
0	1	2
1	0	1
1	1	1

D	Е	f ₃ (D,E)
0	0	1
0	1	0
1	0	0
1	1	1

В	С	D	f ₂ (B,C,D)
0	0	0	10
0	0	1	1
0	1	0	1
0	1	1	5
1	0	0	1
1	0	1	5
1	1	0	5
1	1	1	10

- From the information on the previous slide, compute the marginals of the other variables, P(B), P(C), P(D) and P(E), as well.
- Compute the marginal of each variable using the original Markov network (repeated above) and the definition of the marginals, i.e.,

$$P(A) = \frac{1}{Z} \sum_{B,C,D,E} f_1(A,D) f_2(B,C,D) f_3(D,E) \text{ etc, where}$$

$$Z = \sum_{A,B,C,D,E} f_1(A,D) f_2(B,C,D) f_3(D,E)$$

• Construct the factor graph for the Markov network and use the sum-product algorithm (seen last week) to compute the marginal of each variable.

Where are we?

- Variable elimination: use the definition of marginal probability, but exploit distributivity and caching of intermediate results to save steps
- Sum-product algorithm: message passing on singly connected factor graph to compute all single variable marginals
- Bucket elimination: compute the marginal of one variable on any graph, using buckets to organise computation
- Junction tree algorithm: compute all single variable marginals on any graph
- All of these perform exact inference & can get expensive
- Alternative: approximate inference by sampling

Sampling

- sampling = randomly selecting elements from Ω according to a distribution P over Ω
- remember data generation in the statistical learning framework
- a large number of i.i.d. (independently and identically distributed) samples from P can be used to estimate the probability of any event $E\subseteq\Omega$

C	P(C)
England	0.9
Scotland	0.1
Wales	0.0

E,E,E,E,E,S,E,E,E,E

С	P(C)
England	0.85
Scotland	0.05
Wales	0.10

С	P(C)
England	0.83
Scotland	0.07
Wales	0.10

С	P(C)
England	0.85
Scotland	0.075
Wales	0.075

Example

E,E,E,E,E,E,E,E,E,W,W,E,E,E,E,E,E,E,E

С	P(C)
England	0.86
Scotland	0.08
Wales	0.06

• • •

С	P(C)
England	0.88
Scotland	0.08
Wales	0.04

Sampling in practice

- Assumption: we have a random number generator that generates i.i.d. samples from the uniform distribution over the interval [0,1], e.g., {0.432,0.100,0.773,0.310,0.130,0.004,0.055,0.931,0.445,0.723}
- hardware random number generators harvest "entropy" to generate random numbers (measuring atmospheric noise, thermal noise or other external phenomena, see also https://en.wikipedia.org/wiki//dev/random)
- pseudo random number generators generate "random" numbers deterministically from an initial "seed" number

Sampling for a single RV

to sample from P(C), create the cumulant:

$$t_0 = 0$$

 $t_1 = t_0 + P(C = England) = 0.88$
 $t_2 = t_1 + P(C = Scotland) = 0.96$
 $t_3 = t_2 + P(C = Wales) = 1.00$

С	P(C)
England	0.88
Scotland	0.08
Wales	0.04

0.88 0.96

Е

S

random numbers {0.432, 0.100, 0.773, 0.310, 0.130, 0.004, 0.055, 0.931, 0.445, 0.723}

sample

E

E E

E

S

E

E

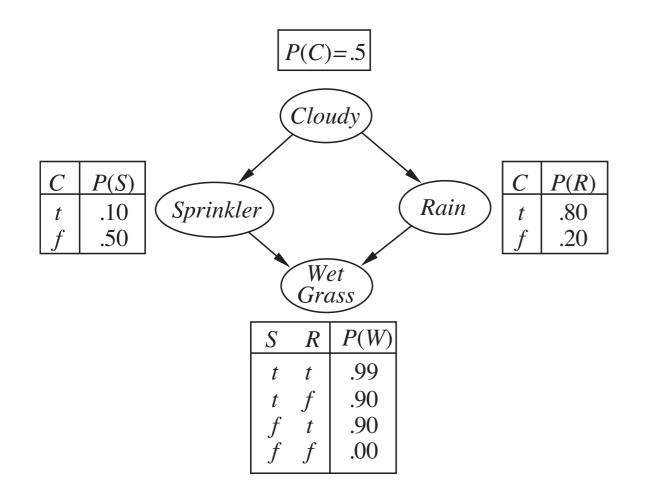
Sampling from a joint distribution

 the same idea can in principle be used for joint distributions: we simply get a more fine grained cumulant

	P(C,L)	C=E	C=S	C=W	
	L=Eng	0.836	0.056	0.024	
	L=Scot	0.0352	0.024	0	
	L=Wel	0.0088	0	0.016	0.936 0.871 0.
					0.836 0.88 0.9
7					
Eng,E)			(;	Scot,E) —— (Wel,E) — (Eng,S)	(Scot,S) (Wel,W)
			34	· · · · /	(Eng,W) (vvei,vv)

Sampling from a BN

- If the joint distribution is given as BN, we can use the structure:
 - fix an order of the variables such that every child comes after its parents
 - sample each node in order from its conditional distribution



C,S,R,W

sample C from P(C) -> t sample S from P(S|C=t) -> f sample R from P(R|C=t) -> t sample W from P(W|S=f,R=t) -> t

full sample (C=t,S=f,R=t,W=t)

Estimating probabilities from samples

 Given a set of samples from the joint distribution, we can estimate answers to general probability questions

marginal of S?
$$P(S=0)=7/10$$

$$P(S=1)=3/10$$
 conditional distribution of C given W=1?
$$P(C=0 \mid W=1)=5/6$$

$$P(C=1 \mid W=1)=1/6$$

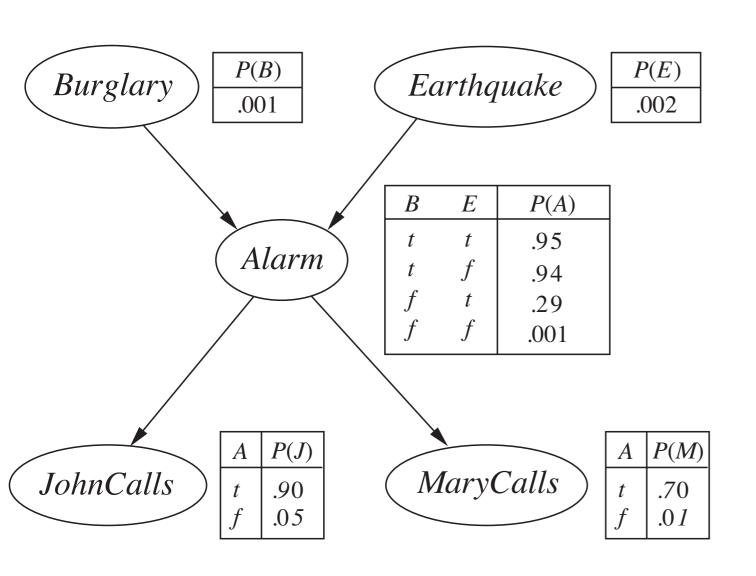
Sampling from a BN

- How to sample from a conditional distribution, say P(C|W=t)?
- Rejection sampling: sample from the joint distribution as before, but throw away all samples where W≠t
- Problem: the more observations we condition on, the more samples are thrown away
 - observing N Boolean variables rules out all but one of their 2^N possible states

Sampling from a BN

- Likelihood weighting avoids this problem by only generating samples that are consistent with the evidence
- Sample unobserved variables as in the case of the joint distribution, but set observed ones to their given value
- no longer i.i.d.: we cannot just compute frequencies
- instead: each sample is weighted by its likelihood, i.e., the product of the conditional probabilities of the observations given their parents in the sample

Example



$$P(B \mid J = t, E = t)$$

$$B = f$$
 1

$$E = t$$
 1*0.002

$$A = f$$
 0.002

$$J = t$$
 0.002*0.05

$$M = t$$
 0.0001

Likelihood weighting

- can be much more efficient than rejection sampling
- performance can suffer as number of observations increases, especially if evidence variables are late in the order the variables are sampled in

Gibbs sampling

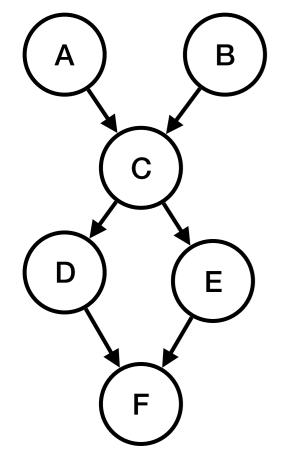
- Gibbs sampling generates a chain of samples by sampling each variable in turn, conditioned on the current values of all other variables
- given current state $(X_1=v_1,\ldots,X_n=v_n)$, sample new value for X_i from

$$P(X_i | X_1 = v_1, \dots, X_{i-1} = v_{i-1}, X_{i+1} = v_{i+1}, \dots, X_n = v_n)$$

often easier to sample from a distribution over just one variable

Gibbs sampling

- In a Bayesian network, each variable is conditionally independent of all others given its Markov blanket
- thus, need to sample from $P(X_i | MB(X_i))$ knowing the values of the variables in the Markov blanket, where $P(X_i | MB(X_i)) \propto P(X_i | parents(X_i)) \prod_{j \in ch(X_i)} P(X_j | parents(X_j))$
- easy to obtain (and normalise)
- observed variables can simply be fixed and excluded from sampling



P(A=1) P(B=1)

0.3

0.5

С	P(D=1 C)	P(D=0 C)
0	0.1	0.9
1	0.2	8.0

Α	В	P(C=1 A,B)	P(C=0 A,B)
0	0	0.9	0.1
0	1	0.3	0.7
1	0	0.2	8.0
1	1	0.2	0.8

С	P(E=1 C)	P(E=0 C)
0	0.3	0.7
1	0.6	0.4

D	Е	P(F=1 D,E)	P(F=0 D,E)
0	0	0.5	0.5
0	1	0.9	0.1
1	0	0.5	0.5
1	1	0.6	0.4

start with arbitrary sample:

(A=1,B=0,C=0,D=1,E=1,F=0)

sample from $P(A | B = 0, C = 0) \propto P(A)P(C = 0 | A, B = 0)$

$$P(A = 1)P(C = 0 | A = 1, B = 0) = 0.3 \cdot 0.7 = 0.21$$

$$P(A = 0)P(C = 0 | A = 0, B = 0) = 0.7 \cdot 0.1 = 0.07$$

$$P(A = 1 | B = 0, C = 0) = 0.75$$

$$P(A = 0 | B = 0, C = 0) = 0.25$$

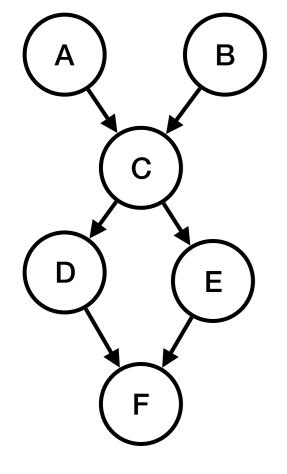
say, A=1, i.e., next sample: (A=1,B=0,C=0,D=1,E=1,F=0)

sample from
$$P(B|A=1,C=0) \propto P(B)P(C=0|A=1,B)$$

$$P(B = 1 | A = 1, C = 0) = 0.5$$

$$P(B = 0 | A = 1, C = 0) = 0.5$$

say, B=1, i.e., next sample: (A=1,B=1,C=0,D=1,E=1,F=0)



P(A=1)		P(B=1)
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0.3

0.5

С	P(D=1 C)	P(D=0 C)
0	0.1	0.9
1	0.2	0.8

A	В	P(C=1 A,B)	P(C=0 A,B)
0	0	0.9	0.1
0	1	0.3	0.7
1	0	0.2	8.0
1	1	0.2	0.8

C	P(E=1 C)	P(E=0 C)
0	0.3	0.7
1	0.6	0.4

D	Е	P(F=1 D,E)	P(F=0 D,E)
0	0	0.5	0.5
0	1	0.9	0.1
1	0	0.5	0.5
1	1	0.6	0.4

current sample: (A=1,B=1,C=0,D=1,E=1,F=0)

sample from
$$P(C|A = 1,B = 1,D = 1,E = 1) \propto P(C|A = 1,B = 1)P(D = 1|C)P(E = 1|C)$$

$$P(C = 1 | A = 1, B = 1)P(D = 1 | C = 1)P(E = 1 | C = 1) = 0.2 \cdot 0.2 \cdot 0.6$$

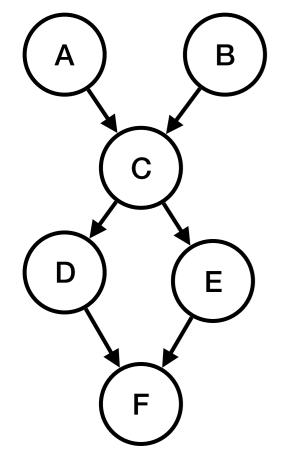
$$P(C = 0 | A = 1, B = 1)P(D = 1 | C = 0)P(E = 1 | C = 0) = 0.8 \cdot 0.1 \cdot 0.3$$

say, C=1, i.e., next sample: (A=1,B=1,C=1,D=1,E=1,F=0)

sample from
$$P(D \mid C = 1, E = 1, F = 0) \propto P(D \mid C = 1)P(F = 0 \mid D, E = 1)$$

$$P(D = 1 | C = 1)P(F = 0 | D = 1, E = 1) = 0.2 \cdot 0.4$$

$$P(D = 0 | C = 1)P(F = 0 | D = 0, E = 1) = 0.8 \cdot 0.1$$



P(A=1)	P(B=1)

0.3

0.5

С	P(D=1 C)	P(D=0 C)
0	0.1	0.9
1	0.2	8.0

A	В	P(C=1 A,B)	P(C=0 A,B)
0	0	0.9	0.1
0	1	0.3	0.7
1	0	0.2	8.0
1	1	0.2	8.0

С	P(E=1 C)	P(E=0 C)
0	0.3	0.7
1	0.6	0.4

D	Е	P(F=1 D,E)	P(F=0 D,E)
0	0	0.5	0.5
0	1	0.9	0.1
1	0	0.5	0.5
1	1	0.6	0.4

current sample: (A=1,B=1,C=1,D=0,E=1,F=0)

sample from
$$P(E \mid C = 1, D = 0, F = 0) \propto P(E \mid C = 1)P(F = 0 \mid D = 0, E)$$

$$P(E = 1 | C = 1)P(F = 0 | D = 1, E = 1) = 0.6 \cdot 0.4$$

$$P(E = 0 | C = 1)P(F = 0 | D = 1, E = 0) = 0.4 \cdot 0.5$$

sample from
$$P(F|D = 0,E = 0)$$

$$(A=1,B=0,C=0,D=1,E=1,F=0)$$

$$(A=1,B=0,C=0,D=1,E=1,F=0)$$

$$(A=1,B=1,C=0,D=1,E=1,F=0)$$

$$(A=1,B=1,C=1,D=1,E=1,F=0)$$

$$(A=1,B=1,C=1,D=0,E=1,F=0)$$

$$(A=1,B=1,C=1,D=0,E=0,F=0)$$

$$(A=1,B=1,C=1,D=0,E=0,F=1)$$

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Gibbs sampling

- straightforward to implement, but samples are strongly dependent
- therefore, it is common to
 - discard a fixed number of samples at the start (burn-in)
 - only use every k-th sample to estimate answers
- Gibbs sampling belongs to the wider class of Markov Chain Monte Carlo (MCMC) algorithms

MCMC algorithms

- MCMC algorithms generate the next sample by random modification of the current one
- if the random modification satisfies certain properties, in the long run, this generates each possible state with the correct frequency
- however, can be difficult to detect when this has happened, i.e., when estimates converge

Probabilistic Inference

- Inference uses a distribution to answer questions, e.g., to compute the conditional distribution of a variable given observations
- Exact algorithms manipulate formulas to obtain these answers; this can be done efficiently for singly-connected BNs or MNs, but is hard in general
- Sampling resorts to generating large numbers of examples from the distribution and uses these to estimate answers

Looking forward

- How to learn Bayesian networks from data?
 - given the graph, learn the parameters
 - learn both the graph structure & the parameters
 - learning as inference
- Probabilistic models involving time
- Probabilistic models involving objects and relations

Reading Material

- Today:
 - Russell & Norvig: 14.5
 - Barber: 6 & 27 (yes, that's 27)

- Parts of slides based on
 - David Barber's slides for the BRML book
 - Tinne De Laet & Luc De Raedt's slides for the UAI course at KU Leuven