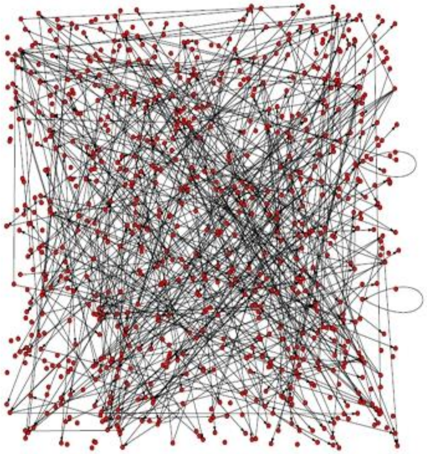
L10. Bayesian Network



Probability + Statistics + Graph Theory

L10. Bayesian Network

- (Static) Bayesian Network
- Dynamic Bayesian Network

(Static) Bayesian Network

Degree of Belief and Probability

How to compare the plausibility of different statements?

G : "we can be a billionaire if we go to graduate school"

vs

S : "we can be a billionaire if we go to Samsung"

- If you believe G more than S, you can write $G \succ S$
- If you believe S more than G, you can write $G \prec S$
- If you have the same belief, you can write $G \sim S$

Assumptions about relationships of $\succ$ and $\sim$

- *Universal comparability* : either $G \succ S$, $G \prec S$ or $G \sim S$
- *Transitivity* : if $G \succ S$ and $S \succ V$, then $G \succ V$

Due to the two assumptions, the degree of belief can be represented by a real-valued function:

- $P(G) > P(S)$ if and only if $G \succ V$
- $P(G) = P(S)$ if and only if $G \sim V$

Properties of probabilities for Bayesian Networks

We are going to use very simple probability theories to construct Probabilistic Graphical Model

- conditional probability :

$$P(A|B) = \frac{P(B|A)}{P(B)}$$

- Law of total probability :

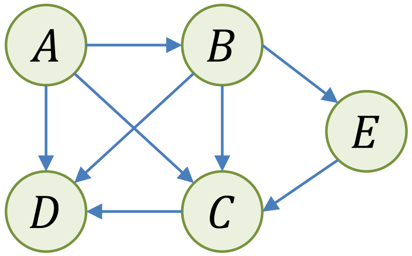
$$P(A) = \sum_{B \in \mathcal{B}} P(A|B)\, P(B) \quad \text{or} \quad P(A) = \int_B P(A|B) P(B) dB$$

- Bayes' rule:

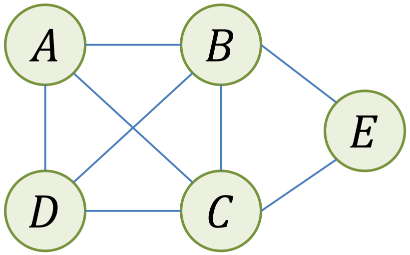
$$P(A|B) = \frac{P(B|A)P(A)}{P(B)}$$

Graph

- A graph G consists of nodes (also called vertices) and edges (also called links) between the nodes.



A directed graph G consists of directed edges between nodes

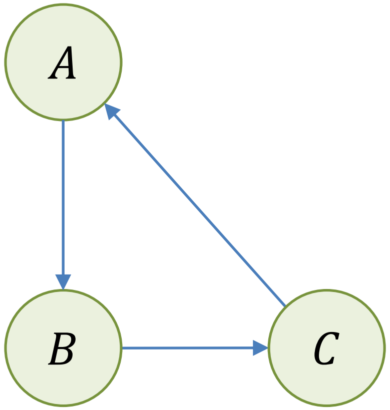


An undirected graph G consists of undirected edges between nodes

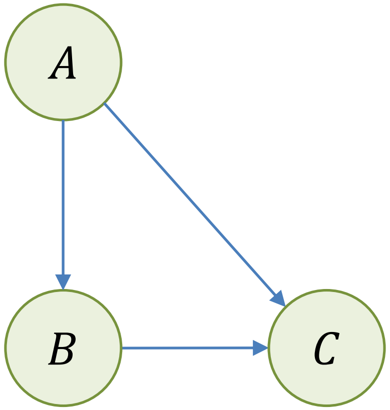
Directed Acyclic Graph (DAG)

- A DAG is a graph G with directed edges (arrows on each link) between the nodes such that by following a path of nodes from one node to another along the direction of each edge no path will revisit a node.

Cyclic Graph



Acyclic Graph



- DAG will play a central role in constructing probabilistic models with many variables
  → will be used for the belief networks
  → can encode the direction dependence between the parent nodes and child nodes.

Path

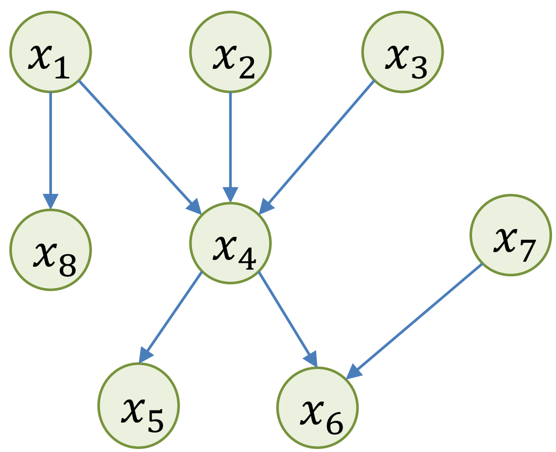
- A path $A \rightarrow B$ from node A to node B is a sequence of nodes that connects A to B

Ancestors

- In directed graph, the nodes A such that $A \rightarrow B$ and $B \nrightarrow A$ are the ancestors of B

Descendants

- In directed graph, the nodes B such that $A \rightarrow B$ and $B \nrightarrow A$ are the descendants of A



- ✓ A path $x_1 \rightarrow x_6$ is $x_1 \rightarrow x_4 \rightarrow x_6$
- ✓ The ancestors of x_6 are $\mathrm{ac}(x_6) = \{x_1, x_2, x_3, x_4, x_7\}$
- ✓ The descendants of x_2 are $\mathrm{dc}(x_2) = \{x_4, x_5, x_6\}$
- ✓ The parents of x_4 are $\mathrm{pa}(x_4) = \{x_1, x_2, x_3\}$
- ✓ The children of x_4 are $\mathrm{ch}(x_4) = \{x_5, x_6\}$

Representations

- Edge list

$$L = \{(x_1, x_4), (x_2, x_4), (x_3, x_4), (x_1, x_8), (x_4, x_5), (x_4, x_6), (x_7, x_6)\}$$

- Adjacency matrix

$$\begin{bmatrix} 0&0&0&1&0&0&0&1 \\ 0&0&0&1&0&0&0&0 \\ 0&0&0&1&0&0&0&0 \\ 0&0&0&0&1&1&0&0 \\ 0&0&0&0&0&0&0&0 \\ 0&0&0&0&0&0&0&0 \\ 0&0&0&0&0&1&0&0 \\ 0&0&0&0&0&0&0&0 \end{bmatrix}$$

Full Joint Distribution

Example distribution

A	B	C	$P(A,B,C)$
0	0	0	0.08
0	0	1	0.15
0	1	0	0.05
0	1	1	0.10
1	0	0	0.14
1	0	1	0.18
1	1	0	0.19
1	1	1	0.11

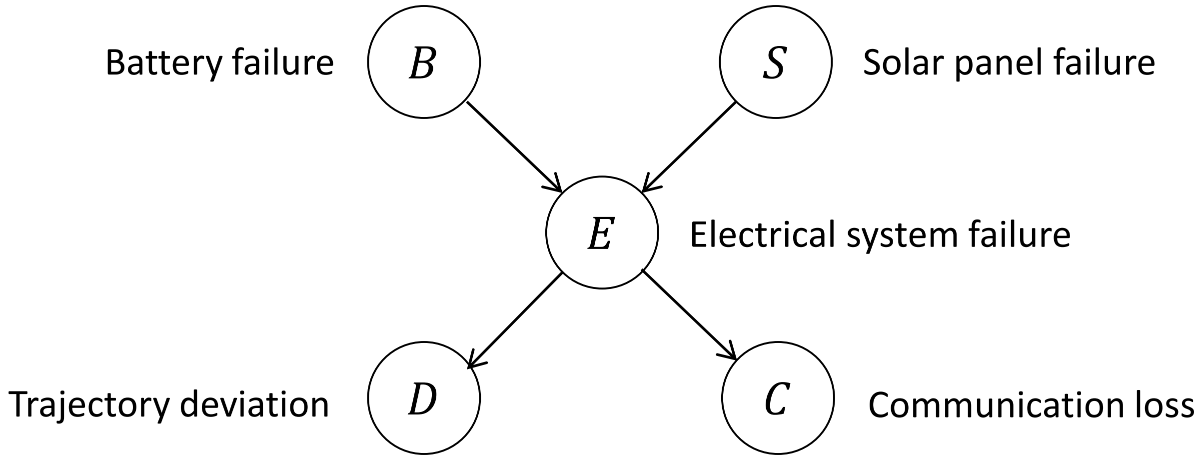
- Binary variables: A, B, C (e.g., $A = 1\ or\ 0$)
- 2^3 entities are required to construct the table
- $2^3 - 1$ independent parameters are required to fully specify the joint probability distribution
- $2^N - 1$ parameters are required for N binary variables

The number of parameters grows exponentially

→ **Difficult to represent Probability distribution and learn the parameters from data**

Motivation of Bayesian Network

Full Joint Probability Distribution



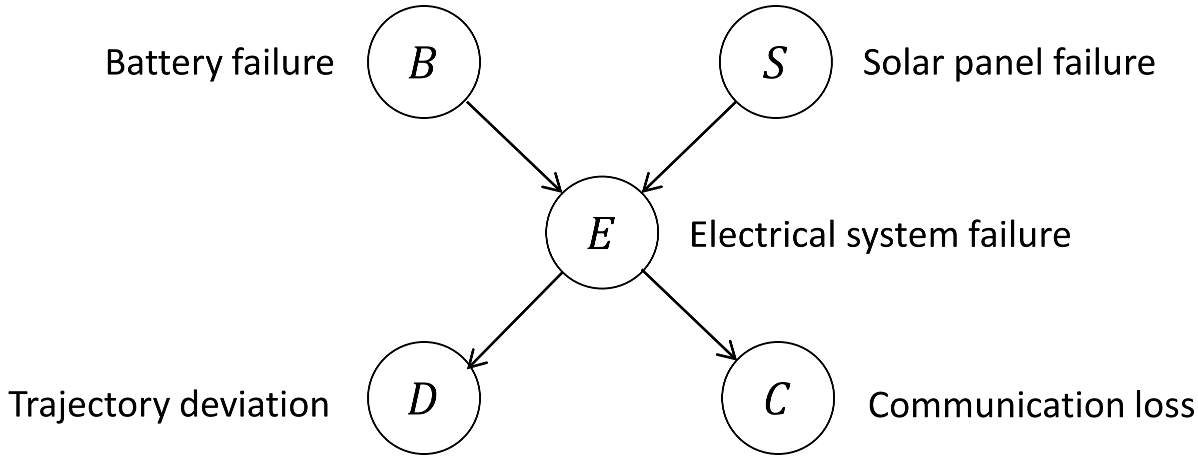
- Binary variables: B, S, E, D, C (e.g., $B = 1\ or\ 0$)
- 2^5 entities are required to construct the table
- $2^5 - 1$ independent parameters are required to fully specify the joint probability distribution
- $2^N - 1$ parameters are required for N binary variables
- If each variable has M different choices,
  $M^N - (M - 1)$ parameters are required

The number of parameters grows exponentially

→ **Difficult to represent Probability distribution and learn the parameters from data**

Motivation of Bayesian Network

A Bayesian network is a compact representation of a joint distribution

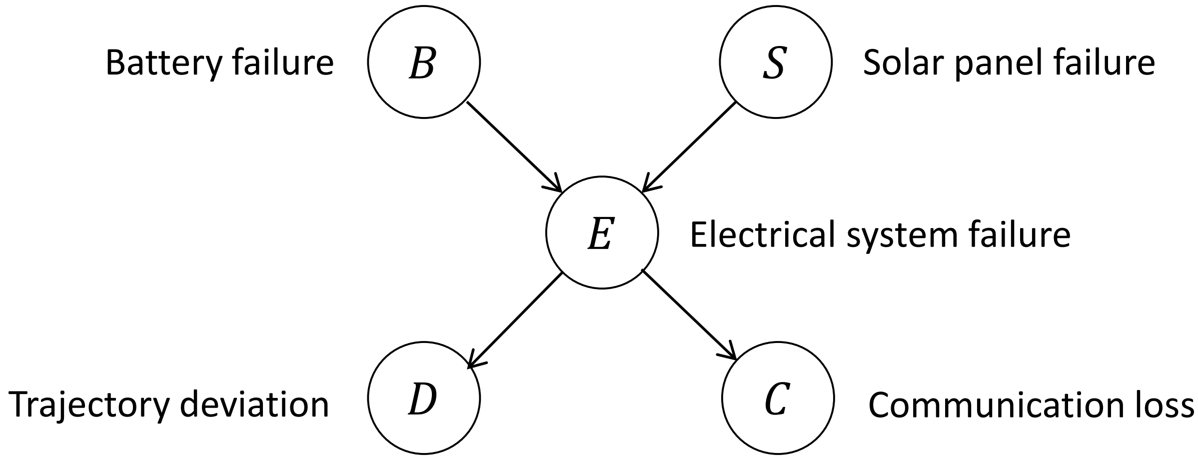


Probability + Statistics + Graph Theory

- A Bayesian Network introduces structure into a probabilistic model by using graphs to represent independence assumptions among the variables. For inferencing, it use statistics
- Provide a good representation to model the probabilistic structures between random variables.
  - Nodes represent random variables
  - Edges represent probabilistic dependency, namely conditional probability among variables
- Conditional independence described by the graph, greatly reduce the computational effort to learn the model and inferencing random variables.

Motivation of Bayesian Network

A Bayesian network is a compact representation of a joint distribution



- Each node corresponds to a random variable
- Directed edges connect pairs of nodes, indicating direct probabilistic relationships
- $P(x_i|\mathrm{pa}_{x_i})$ represents the probability distribution of x_i conditional on the parent nodes pa_{x_i} of X_i e.g., $P(E|B,S)$: B and S are the parent nodes of E

The chain rule for Bayesian networks specifies how to construct a joint distribution from the local conditional probability distribution

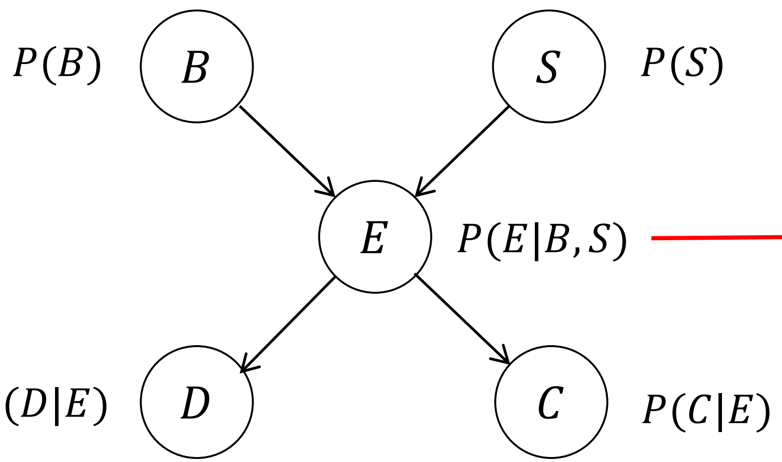
$$P(x_1, \dots, x_n) = \prod_{i=1}^{n} P(x_i|\mathrm{pa}_{x_i})$$

local conditional probability distribution

Motivation of Bayesian Network

A Bayesian network is a compact representation of a joint distribution

B	$P(B)$
0	
1	



E	B	S	$P(E|B,S)$
0	0	0	
1	0	0	
0	0	1	
1	0	1	
0	1	0	
1	1	0	
0	1	1	
1	1	1	

D	E	$P(D|E)$
0	0	
1	0	
0	1	
1	1	

- Chain rule: $P(B,S,E,D,C) = P(B)P(S)P(E|B,S)P(D|E)P(C|E)$
- Required independent parameters to fully specify the joint PDF

  $P(B)$: 1, $P(S)$: 1, $P(E|B,S)$: 4, $P(D|E)$: 2, $P(C|E)$: 2 (total 10 compared to 2^5-1 = 31)

Bayesian network can greatly reduce the number of parameters

Formal Definition Bayesian Network

- A Bayesian network (BN) is a distribution of the form

$$p(x_1, \dots, x_n) = \prod_{i=1}^{n} p(x_i | \mathrm{pa}_{x_i})$$

✓ pa_{x_i} represents the parental variables of variable x_i

✓ BN is represented as a directed acyclic graph (DAG) with an arrow pointing from a parent variable to child variable

- Every probability distribution can be written as a BN:

$$\begin{aligned} p(x_1, \dots, x_n) &= p(x_n | x_1, \dots, x_{n-1}) p(x_1, \dots, x_{n-1}) \\ &= p(x_n | x_1, \dots, x_{n-1}) p(x_{n-1} | x_1, \dots, x_{n-2}) p(x_1, \dots, x_{n-2}) \\ &= p(x_1) \prod_{i=2}^{n} p(x_i | \mathrm{pa}_{x_{i-1}}) \end{aligned}$$

- The particular role of BN is that the structure of the DAG corresponds to a set of conditional independence assumptions, namely which ancestral parental variables are sufficient to specify each conditional probability table

Conditional Independence

What causes the number of parameters to be reduced?

→ The conditional independence assumptions encoded by the structure of a Bayesian network

Definition : Independence

$$X \perp Y$$

$$p(X, Y) = p(X)p(Y) \text{ for all states of } X, Y$$

or equivalently $P(X|Y) = P(X)$

$$\because P(X|Y) = \frac{P(X, Y)}{P(Y)} = \frac{P(X)P(Y)}{P(Y)} = P(X)$$

Definition : Conditional Independence

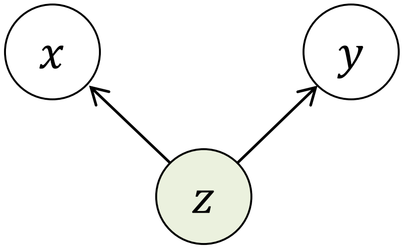
$$X \perp Y|Z$$

$$p(X, Y|Z) = p(X|Z)p(Y|Z) \text{ for all states of } X, Y, Z$$

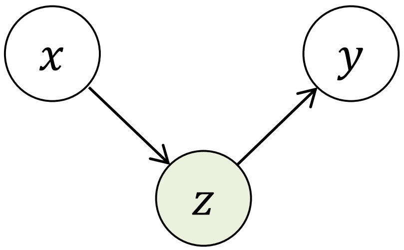
or equivalently $P(X|Y, Z) = P(X|Z)$

- ✓ The two sets of variables X and Y are independent of each other provided that we know the state of the set of variables Z
- ✓ The information of Y does not give further information on X

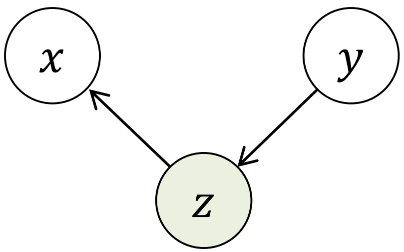
V-structure (or collider)



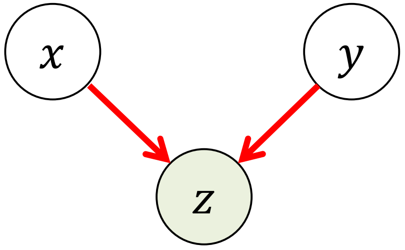
$$p(x,y|z)=\frac{p(x,y,z)}{p(z)}=\frac{p(z)p(x|z)p(y|z)}{p(z)}=p(x|z)p(y|z)$$



$$p(x,y|z)=\frac{p(x,y,z)}{p(z)}=\frac{p(x)p(z|x)p(y|z)}{p(z)}$$
$$=\frac{p(x,z)p(y|z)}{p(z)}=p(x|z)p(y|z)$$



$$p(x,y|z)=\frac{p(x,y,z)}{p(z)}=\frac{p(y)p(z|y)p(x|z)}{p(z)}$$
$$=\frac{p(y,z)p(x|z)}{p(z)}=p(y|z)p(x|z)$$



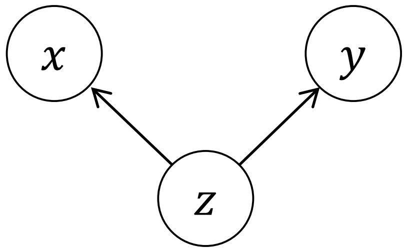
$$p(x,y|z)=\frac{p(x,y,z)}{p(z)}=\frac{p(x)p(y)p(z|x,y)}{p(z)}\neq p(y|z)p(x|z)$$

BN with $x \rightarrow z \leftarrow y$

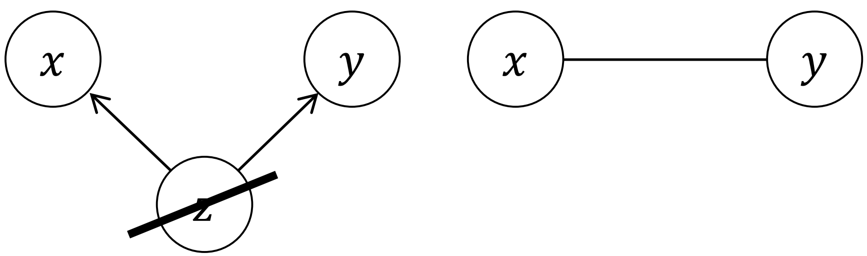
- ✓ x and y are unconditionally independent
- ✓ x and y are dependent conditional on z

V-structure (or collider)

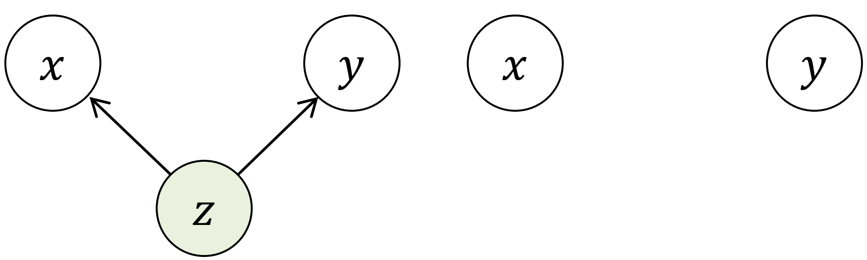
$$p(x, y, z) = p(x|z)p(y|z)$$



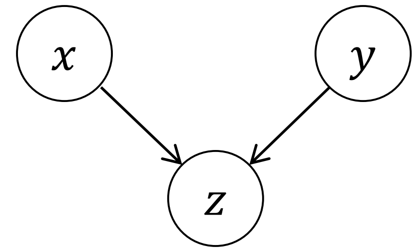
Marginalization over z



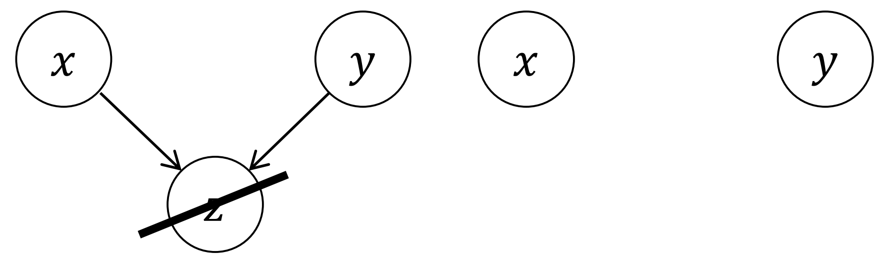
Conditionalization on z



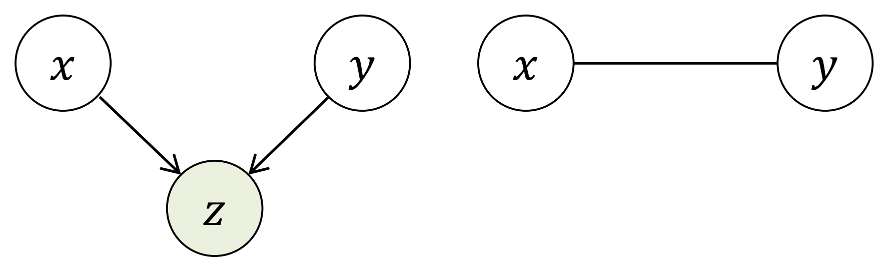
$$p(x, y, z) = p(z|x, y)p(x)p(y)$$



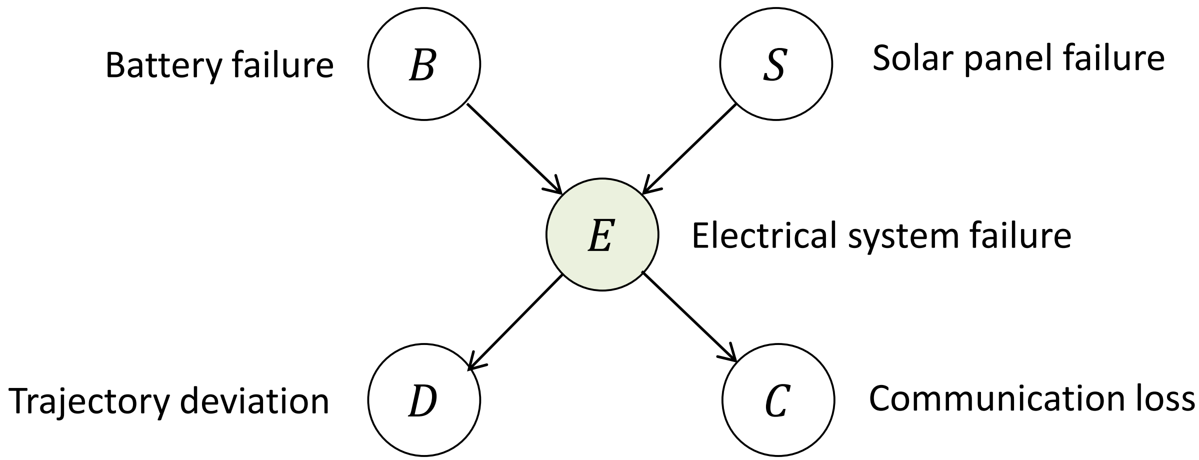
Marginalization over z



Conditionalization on z



Conditional Independence examples



- C is independent of B given E : $(C \perp B|E)$

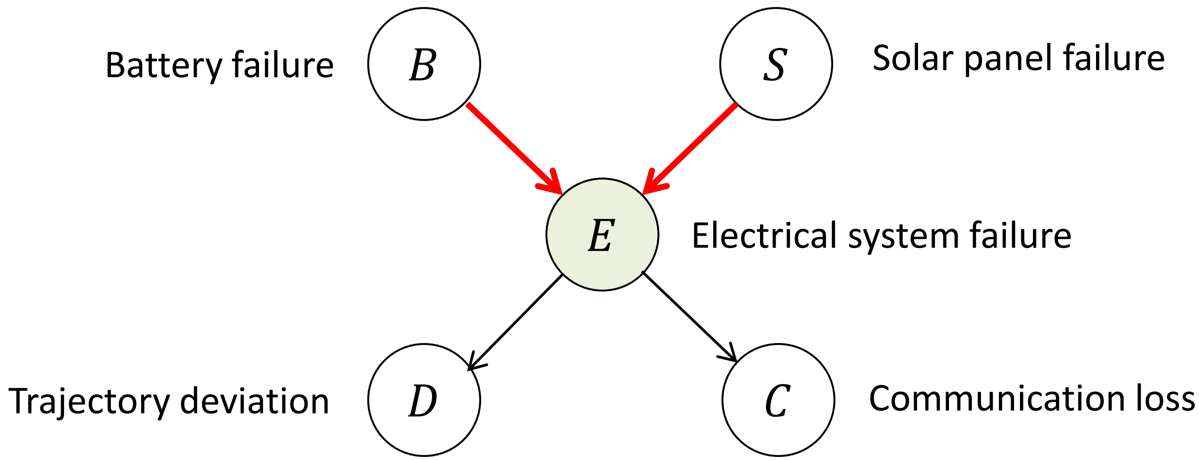
  → Information about Battery failure does not affect my belief on communication loss if I already know (observed) the status of electrical system failure

- D is independent of S given E : $(D \perp S|E)$

  → Information about Solar failure does not affect my belief on a trajectory deviation if I already know (observed) the status of electrical system failure

Conditional Independence examples

V-structure



- B is independent S (E is not observed)

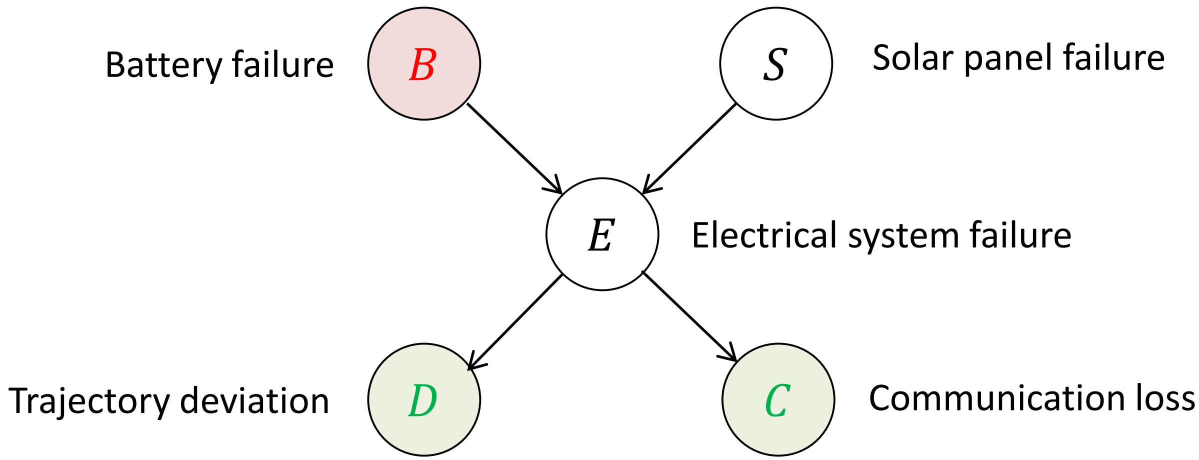
  → Knowing there is a battery failure does not affect my belief regarding solar panel failure

- B is dependent S given E

  → If there was an electrical system failure (observed) and there was no battery failure, there it is likely that a solar panel fails

- Influence flows only through $B \rightarrow E \leftarrow S$ when E is known

Inference



- Once a joint probability distribution is constructed, inference can be performed to determine the distribution over on or more unobserved variables given the values associated with a set of observed variables

$P(B|d^1, c^1)$ Probability distribution of Battery failure B

Query variable

given the trajectory deviation and the communication loss

Evidence variable D C

E S : Hidden variables

Inference

How to compute $P(B|d^1, c^1)$?

Exact inference

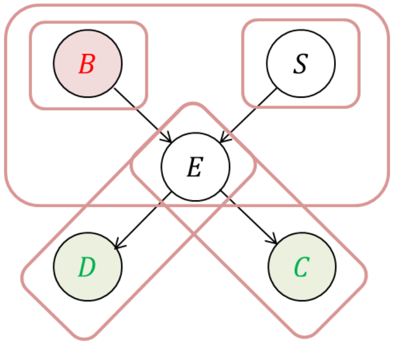
- $$P(b^1|d^1,c^1) \propto \sum_s \sum_e P(b^1, s, e, d^1, c^1)$$
$$= \sum_s \sum_e P(b^1)P(s)P(e|b^1,s)P(d^1|e)p(c^1|e)$$ By conditional independence
$$= P(b^1) \sum_e P(d^1|e)p(c^1|e) \sum_s P(s)P(e|b^1,s)$$

- $$P(b^0|d^1,c^1) = 1 - P(b^1|d^1,c^1)$$

The number of terms to be added together can grow exponentially with the number of hidden variables

How to compute $P(B|d^1, c^1)$?

Variable Elimination



Conditional distributions are represented by the following tables

$$T_1(B)T_2(S)T_3(E,B,S)T_4(d^1,E)T_5(c^1,E)$$

$$T_1(B)T_2(S)T_3(E,B,S)T_6(E)T_7(E)$$

Observe evidence (d^1 and c^1)

$$T_1(B)T_2(S)T_8(B,S)$$

$$T_8(B,S) = \sum_e T_3(e,B,S)T_6(e)T_7(e)$$

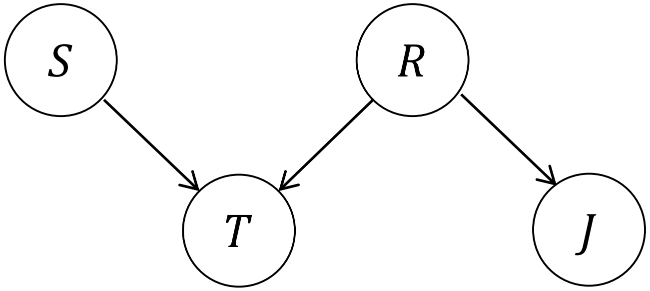
$$T_1(B)T_9(B)$$

$$T_9(B) = \sum_s T_2(s)T_8(B,s)$$

Normalizing the product of the two factors ($T_1(B)$ and $T_9(B)$) results in $P(B|d^1, c^1)$

Variable elimination algorithm relies on heuristic ordering of variables to eliminate in sequence
→ Often linear but sometimes exponential

Example : Wet Grass



$R \in \{0,1\}$: $R = 1$ means that it has been raining
$S \in \{0,1\}$: $S = 1$ Sprinkler is turned on
$J \in \{0,1\}$: $J = 1$ Jack's grass is wet
$T \in \{0,1\}$: $T = 1$ Tracey's grass is wet

Joint distribution based on chain rule

$$
\begin{aligned}
p(T,J,R,S) &= p(T|J,R,S)p(J,R,S) \\
&= p(T|J,R,S)p(J|R,S)p(R,S) \\
&= p(T|J,R,S)p(J|R,S)p(R|S)p(S)
\end{aligned}
$$

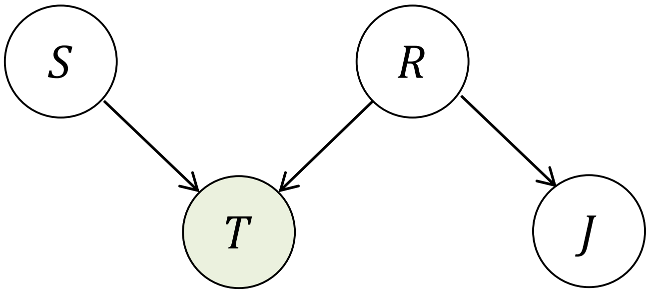
$8 + \quad 4 + \quad 2 + 1 \; = \; 2^4 - 1 = 15$ parameters are required

Joint distribution conditional independence

$$
\begin{aligned}
p(T,J,R,S) &= p(T|J,R,S)p(J|R,S)p(R|S)p(S) \\
&= p(T|R,S) \times p(J|R) \times p(R) \times p(S) \\
&= p(T|R,S)p(J|R)p(R)p(S)
\end{aligned}
$$

Example : Wet Grass

Modeling



$R \in \{0,1\}$: $R = 1$ means that it has been raining
$S \in \{0,1\}$: $S = 1$ Sprinkler is turned on
$J \in \{0,1\}$: $J = 1$ Jack's grass is wet
$T \in \{0,1\}$: $T = 1$ Tracey's grass is wet

$$p(T, J, R, S) = p(T|R, S)p(J|R)p(R)p(S)$$

$p(T|S, E)$

Tracey's Grass wet=1	Rain	Sprinkler
1	1	1
1	1	0
0.9	0	1
0	0	0

$p(J|R)$

Jack's Grass wet=1	Rain
1	1
0.2	0

$p(S = 1) = 0.1$

$p(R = 1) = 0.2$

The tables and graphical structure fully specify the distribution

Inference

$$p(S=1|T=1) = \frac{p(S=1,T=1)}{p(T=1)} = \frac{\sum_{J,R} p(T=1,J,R,S=1)}{\sum_{J,R,S} p(T=1,J,R,S)}$$

$$= \frac{\sum_{J,R} p(J|R) p(T=1|R,S=1)p(R)p(S=1)}{\sum_{J,R,S} p(J|R) p(T=1|R,S)p(R)p(S)}$$

$$= \frac{\sum_{R} p(T=1|R,S=1)p(R)p(S=1)}{\sum_{R,S} p(T=1|R,S)p(R)p(S)} \qquad \because \sum_J p(J|R) = 1$$

$$= \frac{0.9 \times 0.8 \times 0.1 + 1 \times 0.2 \times 0.1}{0.9 \times 0.8 \times 0.1 + 1 \times 0.2 \times 0.1 + 0 \times 0.8 \times 0.9 + 1 \times 0.2 \times 0.9} = 0.3382$$

$$p(S=1|T=1,J=1) = \frac{p(S=1,T=1,J=1)}{p(T=1,J=1)}$$

$$= \frac{\sum_{R} p(T=1,J=1,R,S=1)}{\sum_{R,S} p(T=1,J=1,R,S)}$$

$$= \frac{\sum_{R} p(J=1|R)p(T=1|R,S=1)p(R)p(S=1)}{\sum_{R,S} p(J=1|R)p(T=1|R,S)p(R)p(S)}$$

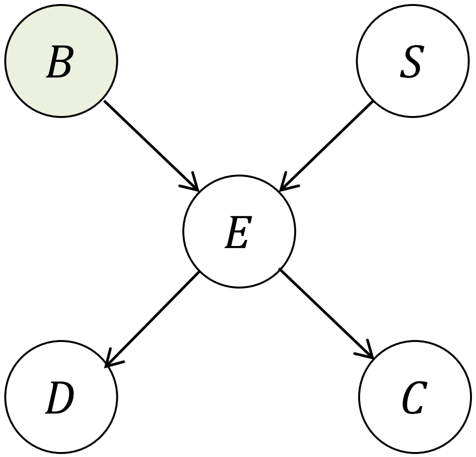
$$= \frac{0.0344}{0.2144} = 0.1604$$

The fact that Jack's grass is also wet increases the chance that the rain has played a role in making Tracey's grass wet

Inference

How to compute $P(B|d^1, c^1)$?

Approximate inference (Sampling based methods)



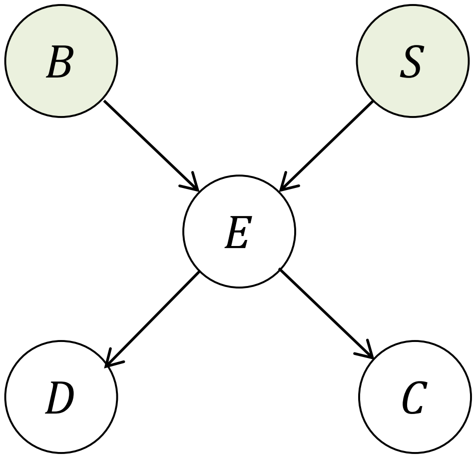
B	S	E	D	C
1				

Sample from $P(B)$

Inference

How to compute $P(B|d^1, c^1)$?

Approximate inference (Sampling based methods)

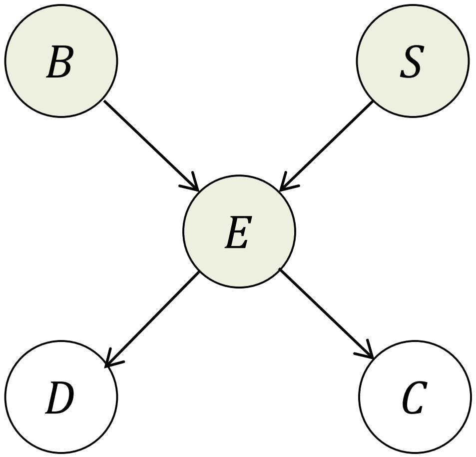


B	S	E	D	C
1	1			

Sample from $P(S)$

How to compute $P(B|d^1, c^1)$?

Approximate inference (Sampling based methods)

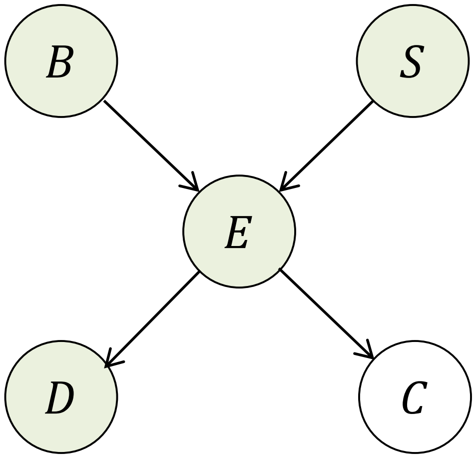


B	S	E	D	C
1	1	1		

Sample from $P(E|B = 1, S = 1)$

How to compute $P(B|d^1, c^1)$?

Approximate inference (Sampling based methods)



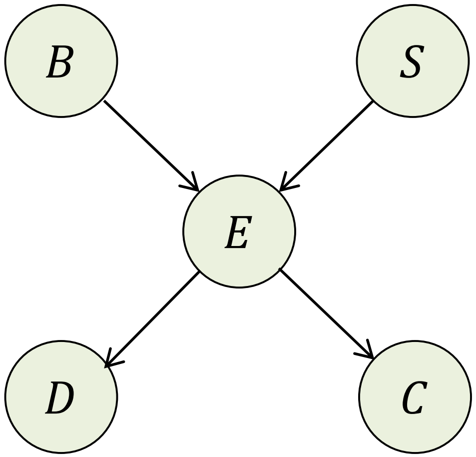
B	S	E	D	C
1	1	1	0	

Sample from $P(D|E = 1)$

Inference

How to compute $P(B|d^1, c^1)$?

Approximate inference (Sampling based methods)



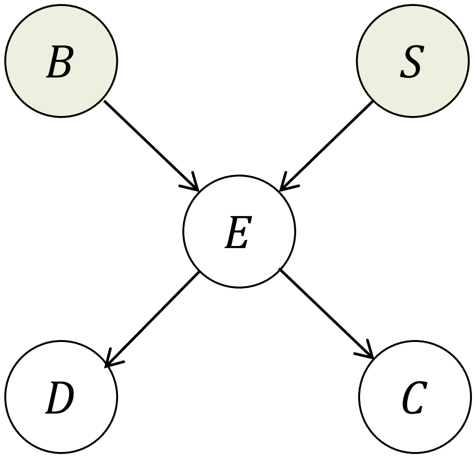
B	S	E	D	C
1	1	1	0	0

Sample from $P(C|E = 1)$

Inference

How to compute $P(B|d^1, c^1)$?

Approximate inference (Sampling based methods)



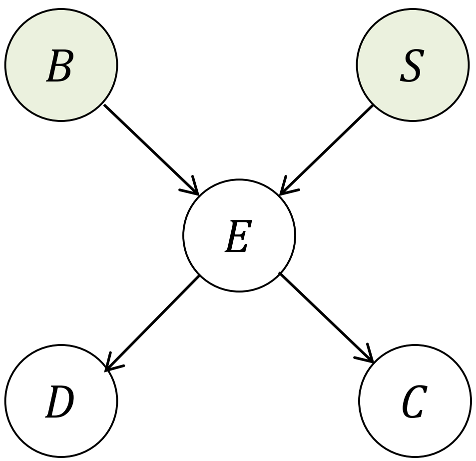
$$P(b^1|d^1, c^1) = 1/3$$
$$P(b^0|d^1, c^1) = 2/3$$

B	S	E	D	C
1	1	1	0	0
0	1	0	1	0
1	0	1	1	1
0	1	0	0	1
0	1	1	1	1
0	1	0	0	1
0	0	0	1	0
0	1	1	1	0
0	1	0	1	1

Three cases coincide observations d^1, c^1

How to compute $P(B|d^1, c^1)$?

Approximate inference (Sampling based methods)



$P(b^1|d^1, c^1) = 1/3$
$P(b^0|d^1, c^1) = 2/3$

B	S	E	D	C
1	1	1	0	0
0	1	0	1	0
1	0	1	1	1
0	1	0	0	1
0	1	1	1	1
0	1	0	0	1
0	0	0	1	0
0	1	1	1	0
0	1	0	1	1

Three cases coincide observations d^1, c^1

If likelihood of evidence is small, then many samples are required!!

Inference

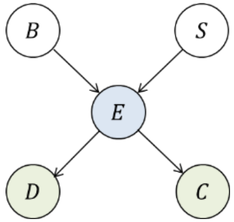
How to compute $P(B|d^1, c^1)$?

Likelihood sampling

Algorithm 2.5 Likelihood-weighted sampling from a Bayesian network

```
function LikelihoodWeightedSample(B, o_{1:n})
    X_{1:n} ← a topological sort of nodes in B
    w ← 1
    for i ← 1 to n
        if o_i = NIL
            x_i ← a random sample from P(X_i | pa_{x_i})
        else
            x_i ← o_i
            w ← w × P(x_i | pa_{x_i})
    return (x_{1:n}, w)
```

B	S	E	D	C
1	1	1	0	0
0	1	0	1	0
1	0	1	1	1
0	1	0	0	1
0	1	1	1	1
0	1	0	0	1
0	0	0	1	0
0	1	1	1	0
0	1	0	1	1

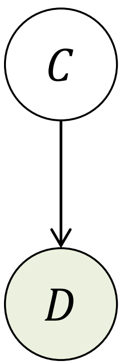


B	S	E	D	C	weight
1	0	1	1	1	$P(d^1|e^1)\ P(c^1|e^1)$
0	1	1	1	1	$P(d^1|e^1)\ P(c^1|e^1)$
0	1	0	1	1	$P(d^1|e^0)\ P(c^1|e^0)$

$$P(b^1|d^1, c^1) = \frac{P(d^1|e^1)\ P(c^1|e^1)}{P(d^1|e^1)\ P(c^1|e^1) + P(d^1|e^1)\ P(c^1|e^1) + P(d^1|e^0)\ P(c^1|e^0)}$$

How to compute $P(B|d^1, c^1)$?

Likelihood sampling has a still problem!



$P(c^1) = 0.001$

$P(d^1|c^0) = 0.001$
$P(d^1|c^1) = 0.999$

Bayesian approach :

$$P(c^1|d^1) = \frac{P(d^1|c^1)P(c^1)}{P(d^1|c^1)P(c^1) + P(d^1|c^0)P(c^0)}$$

$$= \frac{0.999 \times 0.001}{0.999 \times 0.001 + 0.001 \times 0.999}$$

$$= 0.5$$

To use likelihood weighting sampling approach:

$$c^0, c^0, c^0, c^0, c^0, c^0, c^0, c^0, c^0, c^0, c^0, c^0, c^0, c^0, c^0, \dots, c^1$$

$P(d^1|c^1) = 0$ because c^1 is not sampled due to the low prior

How to compute $P(B|d^1, c^1)$?

Gibbs sampling, a kind of Markov chain Monte Carlo technique

- The sequence of samples forms a Markov chain
- In the limit, samples are drawn exactly from the joint distribution over the unobserved variables given the observations
- Simulate samples by sweeping through all the posterior conditionals, one random variables at a time

---

Algorithm : Gibbs sampler

Initialize $X^{(0)} \sim q(x)$

for iteration $i = 1, \dots do$

$$x_1^{(i)} \sim P\left(X_1 = x_1 \middle| X_2 = x_2^{(i-1)}, X_3 = x_3^{(i-1)}, \dots, X_D = x_D^{(i-1)}\right)$$
$$x_2^{(i)} \sim P\left(X_2 = x_2 \middle| X_1 = x_1^{(i)}, X_3 = x_3^{(i-1)}, \dots, x_D = x_D^{(i-1)}\right)$$
$$x_3^{(i)} \sim P\left(X_3 = x_2 \middle| X_1 = x_1^{(i)}, X_2 = x_2^{(i)}, \dots, x_D = x_D^{(i-1)}\right)$$
$$\vdots$$
$$x_D^{(i)} \sim P\left(X_D = x_D \middle| X_1 = x_1^{(i)}, X_2 = x_2^{(i)}, \dots, X_{D-1} = x_{D-1}^{(i)}\right)$$

end for

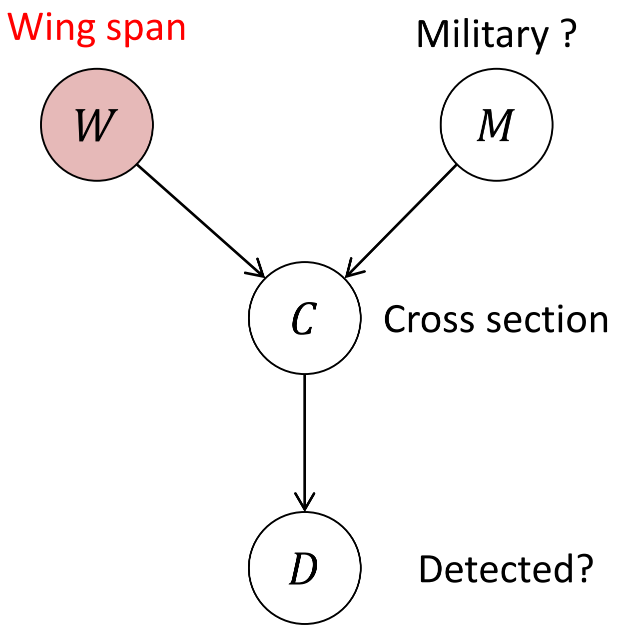
Because samples from the early iterations are not from the target posterior, it is common to discard these samples "burn-in" period"

Sampling method comparisons

Jupyter Demo Simulation
Wet grass (PyMC)

Hybrid Bayesian Networks

Bayesian networks can contain a mixture of both discrete and continuous variables

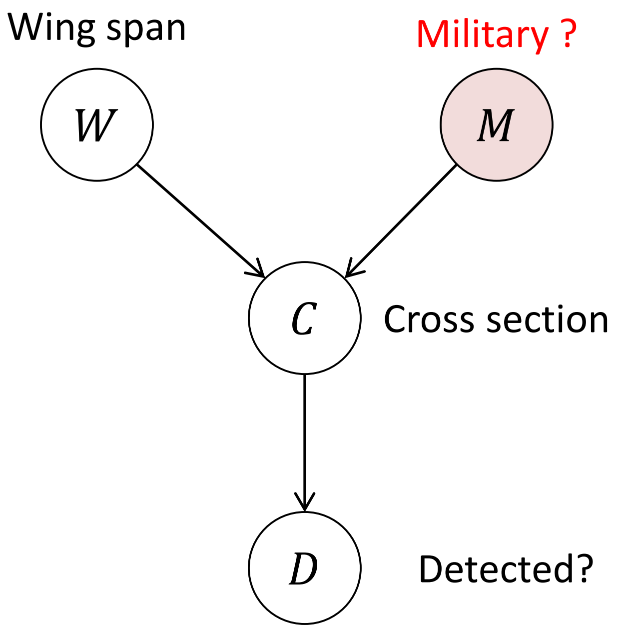


Wing span is a continuous variable and modeled as a Gaussian distribution

$$P(w) = N(w|\mu, \sigma^2) = \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{1}{2}\left(\frac{w-\mu}{\sigma}\right)^2}$$

Hybrid Bayesian Networks

Bayesian networks can contain a mixture of both discrete and continuous variables



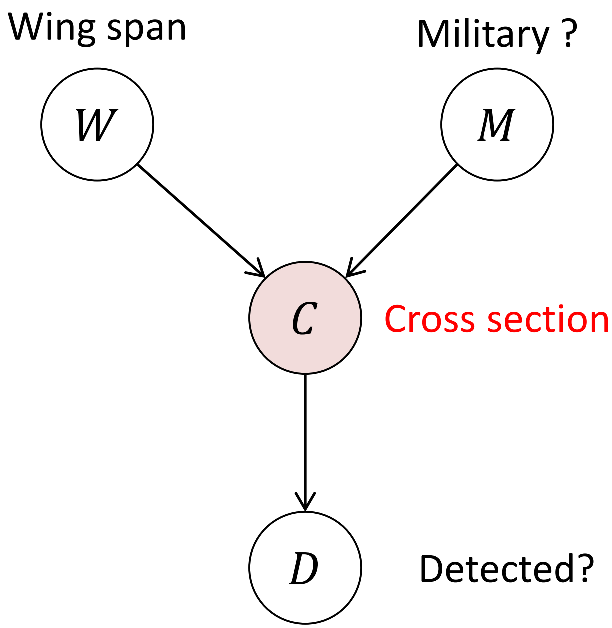
Whether a target is a military vehicle can be modeled with a single parameter θ

$$P(m^1) = \theta$$

$$P(m^0) = 1 - \theta$$

Hybrid Bayesian Networks

Bayesian networks can contain a mixture of both discrete and continuous variables



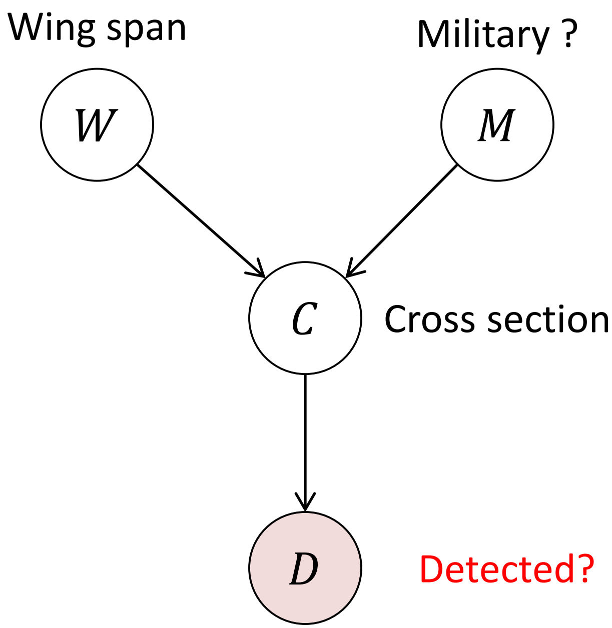
Radar cross section can be modeled as a conditional Gaussian

$$P(c|w,m) = \begin{cases} N(c|a_0 w + b_0, \sigma_0^2) & \text{if } m = m^0 \\ N(c|a_1 w + b_1, \sigma_1^2) & \text{if } m = m^1 \end{cases}$$

(Conditional linear Gaussian)

Hybrid Bayesian Networks

Bayesian networks can contain a mixture of both discrete and continuous variables

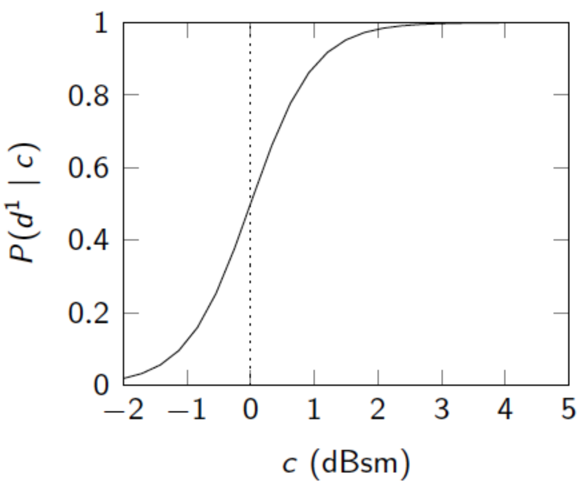


- Logit model:

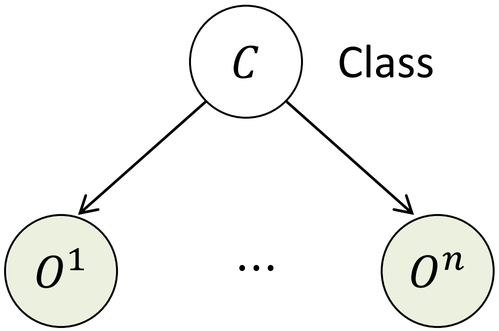
$$P(d^1|c) = \frac{1}{1 + \exp\left(-2\frac{c-\alpha}{\beta}\right)}$$

- Probit model:

$$P(d^1|c) = \Phi\left(\frac{c-\alpha}{\beta}\right)$$



Naïve Bayes Model



- Prior: $\mathrm{P}(C)$
- Likelihood: $P(O^i|C)$ *for single obs. and* $P(O^{1:n}|C) = \prod_{i=1}^{n} P(O^i|C)$ *for set of i.i.d. obs.*
- Posterior on the class given the observation:

$$P(C|O^{1:n}) = \frac{P(C, O^{1:n})}{P(O^{1:n})} = \frac{P(C) \prod_{i=1}^{n} P(O^i|C)}{P(O^{1:n})}$$

$$P(O^{1:n}) = \sum_{c} P(C, O^{1:n})$$

$$P(C|O^{1:n}) \propto P(C) \prod_{i=1}^{n} P(O^i|C)$$

Parameter Learning

We already know how to estimate the parameters for probability distributions

MLE or Bayesian approach

Structure learning

- Bayesian Score $P(G|D)$ for a certain graph G given data D is defined as

$$P(G|D) = \frac{P(G)P(D|G)}{P(D)}$$
$$= \frac{P(G)\int_{\theta} P(D|\theta, G)P(\theta|G)d\theta}{P(D)}$$

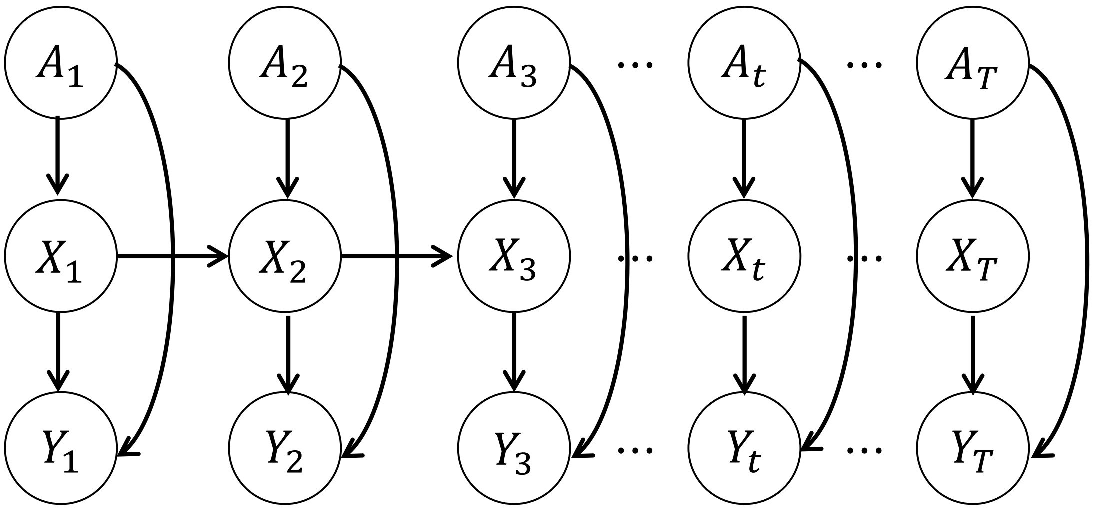
- A Bayesian approach to structure learning involves finding the graph G that maximizes the Bayesian Score $P(G|D)$ as

$$G^* = \underset{G}{\operatorname{argmax}}\, P(G|D)$$

- Not feasible to enumerate every possible structure, so use local search for graph with largest Bayesian score

Dynamic Bayesian Network

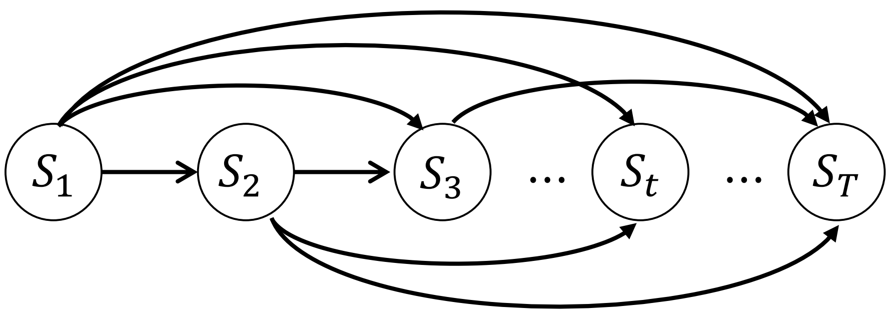
Dynamic Bayesian Network relates variables to each other over adjacent time steps.



Dynamic Bayesian Networks (temporal model)

- We are interested in reasoning about the state of the world as it evolves over time
- System state S_t is a snapshot of the relevant attributes of the system at time t
- Trajectory of states $S_1, \ldots, S_t$ represents the evolution of the target system
- $P(S_1, \ldots, S_t)$ is very complex probability space

→ we need a series of simplifying assumptions

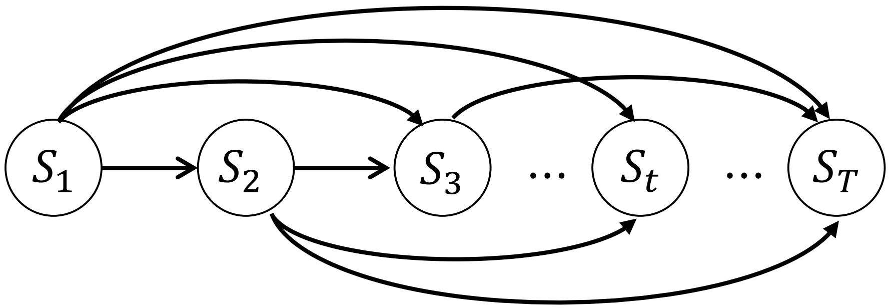


Discrete-State Markov models

Consider a distribution over trajectories sampled over a prefix of time $t = 1, \dots, T$

$$P(S_1, S_2, \dots, S_T) = P(S_1) \prod_{t=2}^{T} P(S_t | S_{1:t-1})$$

Cascade decomposition



Discrete-State Markov models

Consider a distribution over trajectories sampled over a prefix of time $t = 1, \dots, T$

$$P(S_1, S_2, \dots, S_T\ ) = P(S_1) \prod_{t=2}^{T} P(S_t | S_{1:t-1})$$

Cascade decomposition

1. Markov Chain:

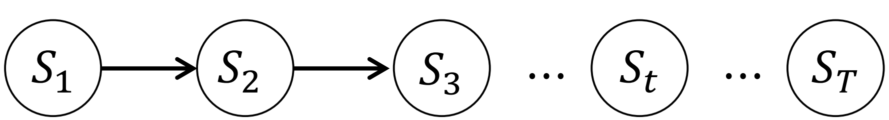
A Markov chain is defined on either discrete or continuous variables $S_{1:t}$ and the following conditional independence assumption holds:

$$P(S_t | S_1, \dots, S_{t-1}) = P(S_t | S_{t-L}, \dots, S_{t-1})$$

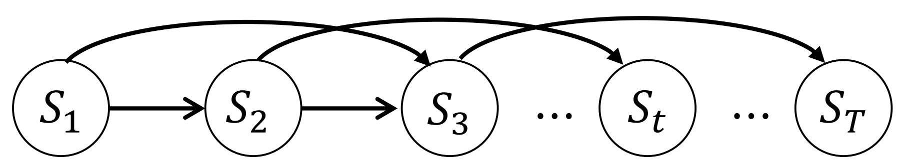
where $L \geq$ is the order of the Markov chain. First order Markov chain can be represented

$$P(S_1, S_2, \dots, S_T) = P(S_1) \prod_{t=2}^{T} P(S_t | S_{t-1})$$

the future is conditionally independent of the past given the present: $\left(S^{t+1} \perp S^{(1:t-1)} | S^t\right)$



First Order Markov Chain



Second Order Markov Chain

Discrete-State Markov models

Consider a distribution over trajectories sampled over a prefix of time $t = 1, \ldots, T$

$$P(S_1, S_2, \ldots, S_T\ ) = P(S_1) \prod_{t=2}^{T} P(S_t | S_{1:t-1})$$

Cascade decomposition

1. Markov Chain:

A Markov chain is defined on either discrete or continuous variables $S_{1:t}$ and the following conditional independence assumption holds:

$$P(S_t | S_1, \ldots, S_{t-1}) = P(S_t | S_{t-L}, \ldots, S_{t-1})$$

where $L \geq$ is the order of the Markov chain. First order Markov chain can be represented

$$P(S_1, S_2, \ldots, S_T) = P(S_0) \prod_{t=1}^{T} P(S_t | S_{t-1})$$

2. Stationary assumption

The state transition probability $P(S^{t+1} | S^t)$ is the same for all t

$$P(S^{t+1} = s' | S^t = s) = P(S' = s' | S = s) \text{ for any } t$$

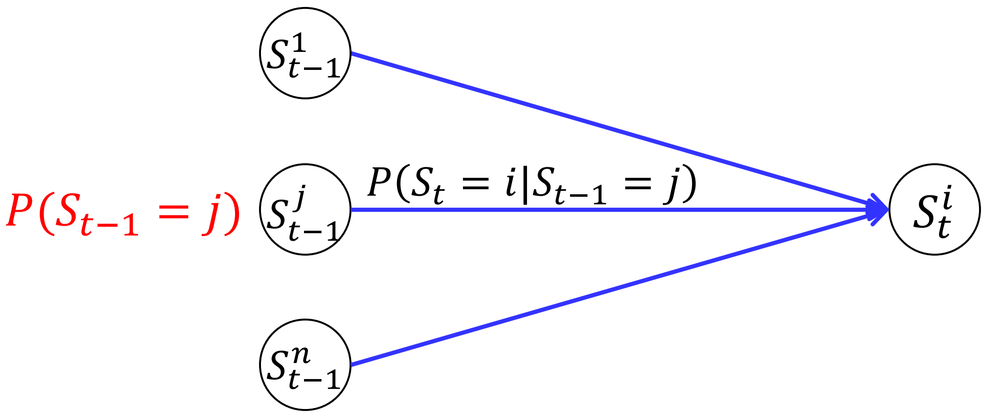
→The number of parameters are reduced substantially

Equilibrium and stationary distribution of a Markov chain

- The marginal $P(S_t)$ evolves through time. For discrete time,

$$P(S_t = i) = \sum_j P(S_t = i|S_{t-1} = j)P(S_{t-1} = j)$$

✓ $P(S_t = i)$: the frequency that we visit state i at time t, given we started with a sample from $P(S_1)$ and subsequently repeatedly drew samples from the transition $P(S_\tau|S_{\tau-1})$



- Denoting $(\mathbf{p}_t)_i = P(S_t = i)$,

$$\mathbf{p}_t = \mathbf{M}\mathbf{p}_{t-1} = \mathbf{M}^{t-1}\mathbf{p}_1$$

- If, for $t \to \infty$, $\mathbf{p}_t$ is independent of the initial distribution $\mathbf{p}_1$, then $\mathbf{p}_\infty$ is called the equilibrium distribution (stationary distribution) of the chain, that is

$$\mathbf{p}_\infty = \mathbf{M}\mathbf{p}_\infty$$

Fitting Markov Models

$$S_1 \rightarrow S_2 \rightarrow S_3 \quad \cdots \quad S_t \quad \cdots \quad S_T$$

Given a sequence $(S_1 = s_1, S_2 = s_2, \ldots, S_T = s_T)$, how to construct the transition matrix?

$$\theta_{i|j} = P(S_\tau = i | S_{\tau-1} = j) \propto \sum_{t=2}^{T} \mathbb{I}[S_\tau = i, S_{\tau-1} = j]$$

$$\boldsymbol{\theta} = \begin{bmatrix} \theta_{1|1} \theta_{1|2} \theta_{1|3} \theta_{1|4} \theta_{1|5} \\ \theta_{2|1} \theta_{2|2} \theta_{2|3} \theta_{2|4} \theta_{2|5} \\ \theta_{3|1} \theta_{3|2} \theta_{3|3} \theta_{3|4} \theta_{3|5} \\ \theta_{4|1} \theta_{4|2} \theta_{4|3} \theta_{4|4} \theta_{4|5} \\ \theta_{5|1} \theta_{5|2} \theta_{5|3} \theta_{5|4} \theta_{5|5} \end{bmatrix}$$

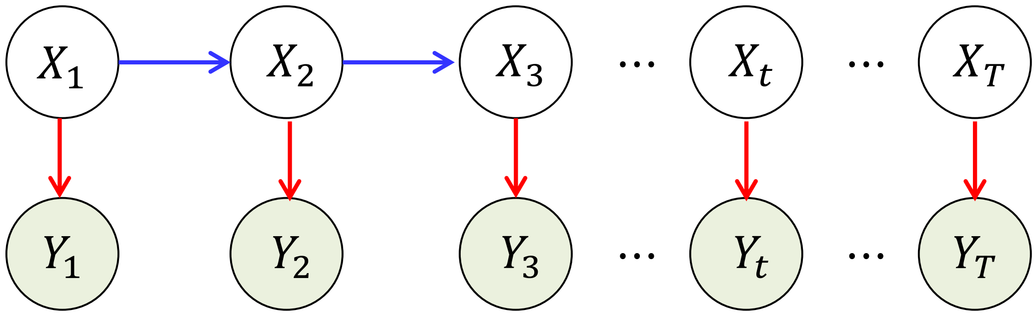
State transition matrix

$$\sum_i \theta_{i|j} = 1$$

If we have $s_{1:t} = 1, 3, 2, 4, 1, 4, 3, 5, 1, 3, 4, 2, 1, 4, 4, 2, 4, 5, 1, 3, 3, 4, \ldots$ $\quad \theta_{3|1} = \frac{3}{5}$

Definition of Hidden Markov Models

- The Hidden Markov Model (HMM) defines a Markov chain on hidden variables $X_{1:t}$
- The observed variables are dependent on the hidden variables through an emission $P(Y_t|X_t)$



- The joint distribution on the hidden variables and observations are

$$P(X_{1:t}, Y_{1:t}) = P(X_1)P(Y_1|X_1)\prod_{t=2}^{T} P(X_t|X_{t-1})P(Y_t|X_t)$$

- Transition distribution: For a stationary HMM the transition distribution $P(X_t|X_{t-1})$ is defined as the $H \times H$ matrix

$$M_{i,j} = P(X_t = i|X_{t-1} = j)$$

- Emission distribution: For a stationary HMM and emission distribution with discrete states $Y_t \in \{1, \ldots, V\}$, we define $V \times H$ matrix

$$O_{i,j} = P(Y_t = i|X_t = j)$$

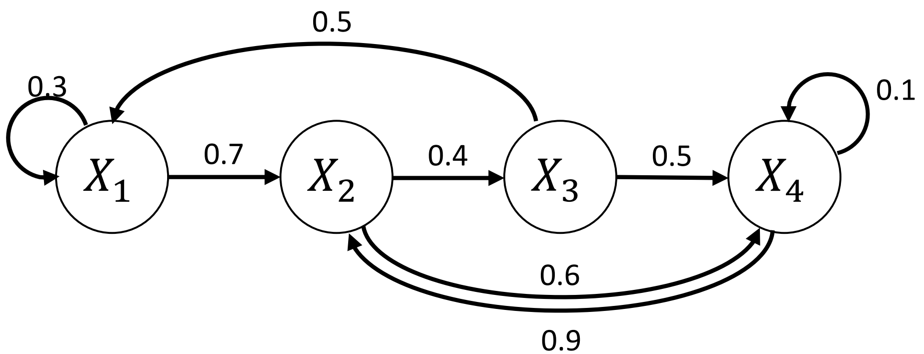
Hidden Markov Model

The state variable X_t is discrete

- The state transition model $P(X'|X)$ is usually sparse,

  $\rightarrow$can be represented as a directed graph

$X = (X_1, X_2, X_3, X_4\ )$: 4 discretized states

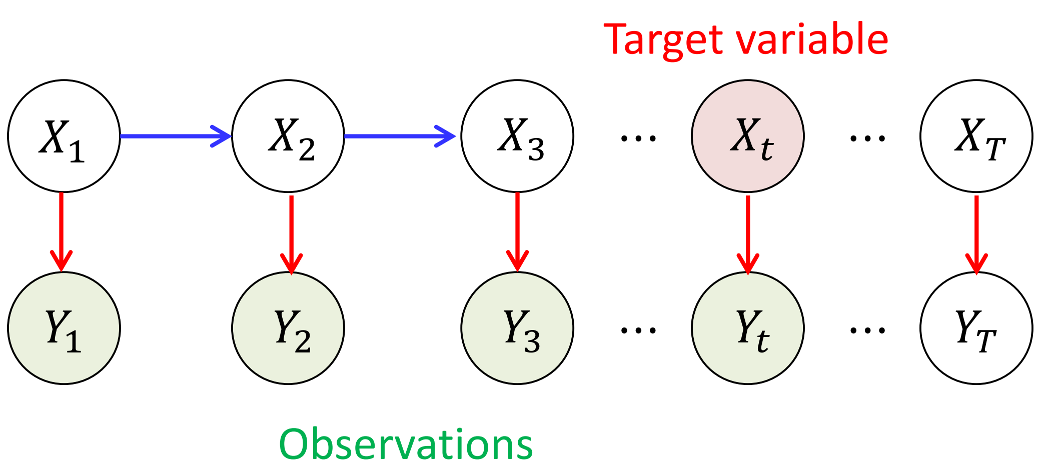


$\sum_i P(X_i'|X) = 1$

- The observation model : $P(Y\ |X)$ can be deterministic or random

Inferencing of Hidden Markov Models

- Filtering (inferencing the present) $P(x_t|y_{1:t})$
- Prediction (inferencing the future) $P(x_t|y_{1:s}) \quad t > s$
- Smoothing (inferencing the past) $P(x_t|y_{1:u}) \quad t < u$
- Likelihood (inferencing the past) $P(x_{1:t})$
- Most likely hidden path (Viterbi alignment) $\underset{x_{1:t}}{\operatorname{argmax}} P(x_{1:t}|y_{1:t})$



Inferencing of Hidden Markov Models

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- Smoothing (inferencing the past) $P(x_t|y_{1:u})$ $t < u$
- Likelihood (inferencing the past) $P(x_{1:t})$
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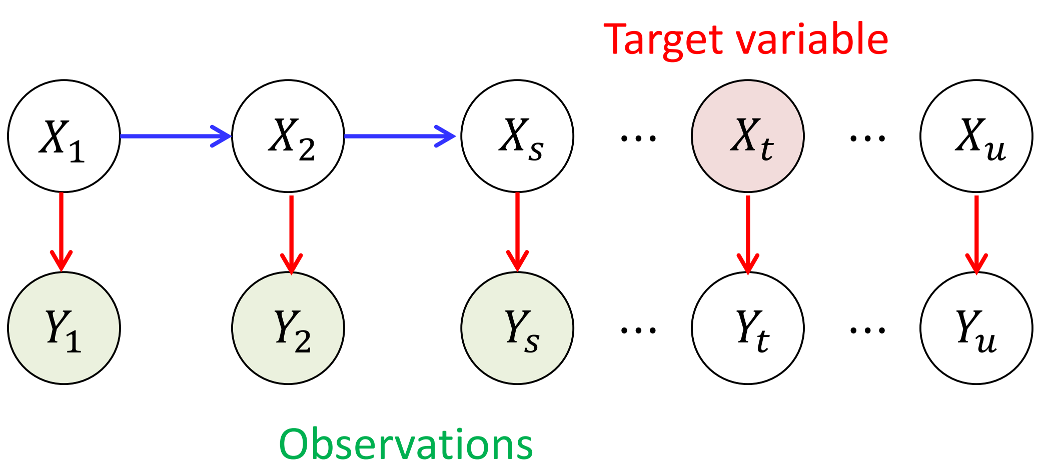

Inferencing of Hidden Markov Models

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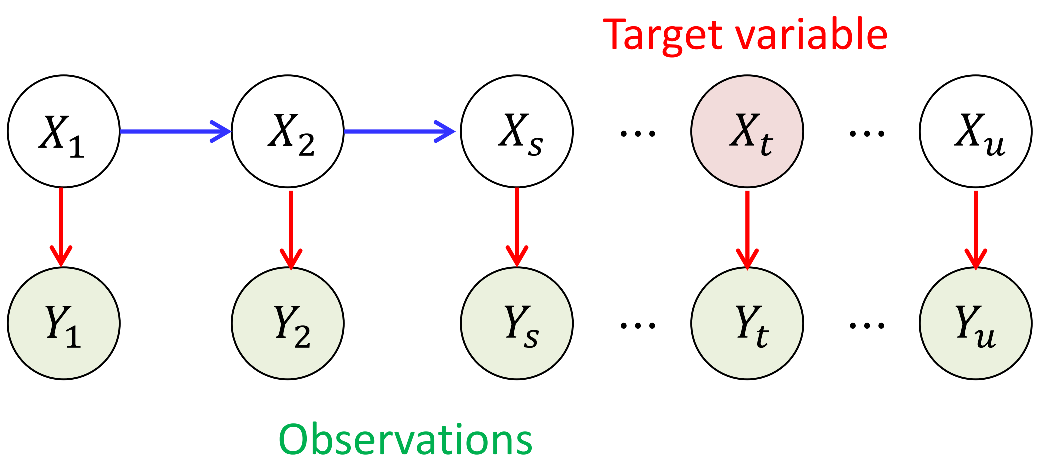

Inferencing of Hidden Markov Models

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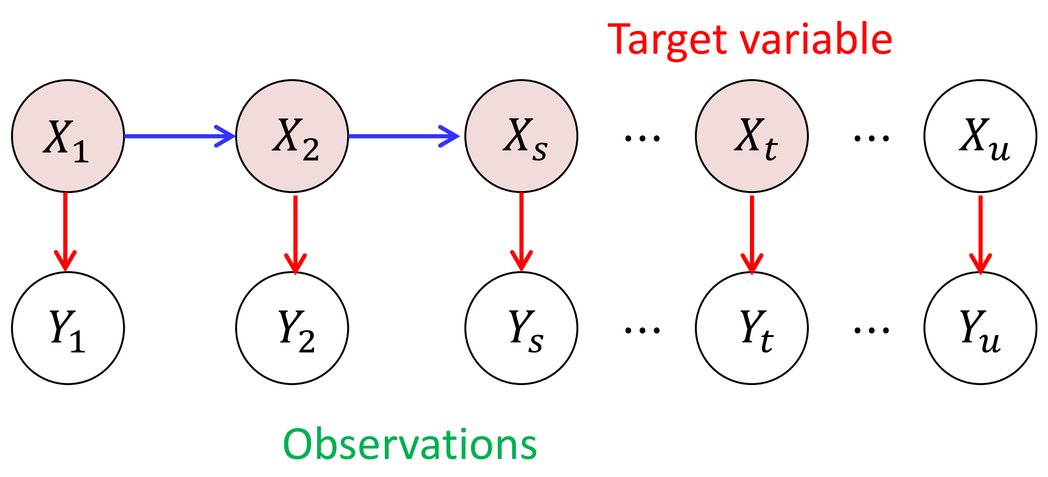

Inferencing of Hidden Markov Models

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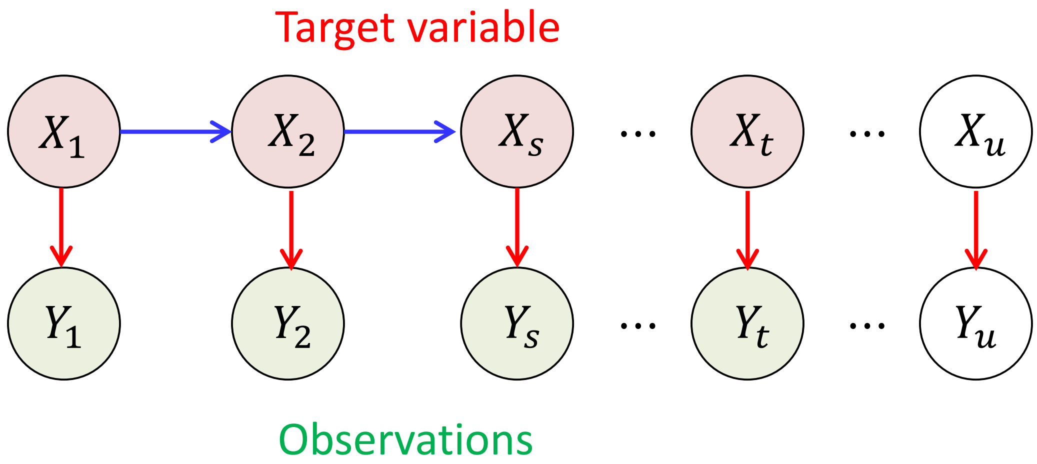


Inferencing of Hidden Markov Models

- Filtering (inferencing the present) $P(x_t|y_{1:t})$

$$P(x_t|y_{1:t}) = \frac{P(x_t, y_{1:t})}{P(y_{1:t})} \propto P(x_t, y_{1:t})$$

$$P(x_t, y_{1:t}) = \sum_{x_{t-1}} P\left(x_t, x_{t-1}, y_{1:t-1}, y_t\right)$$

$$\sum_{x_{t-1}} P(y_t|\cancel{y_{1:t-1}}, x_t, \cancel{x_{t-1}})P(x_t|\, \cancel{y_{1:t-1}}, x_{t-1})P(x_{t-1}, y_{1:t-1})$$

$$\sum_{x_{t-1}} P(y_t|x_t)P(x_t|\, x_{t-1})P(x_{t-1}, y_{1:t-1})$$

∵Conditional independence

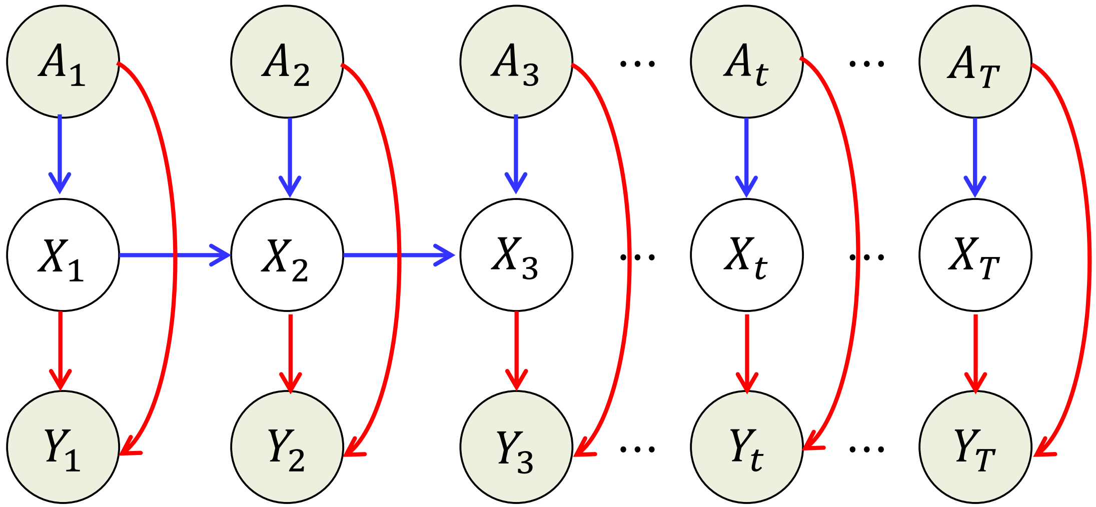
$$\underbrace{P(y_t|x_t)}_{\text{corrector}} \underbrace{\sum_{x_{t-1}} P(x_t|\, x_{t-1})P(x_{t-1}, y_{1:t-1})}_{\text{predictor}}$$

Bayesian view

$$P(x_t|y_{1:t}) \propto \sum_{x_{t-1}} \underbrace{P(y_t|x_t)P(x_t|\, x_{t-1})}_{\text{Regarded as likelihood}}\underbrace{P(x_{t-1}|y_{1:t-1})}$$

Modified prior distribution has an effect of removing all nodes in the graph before time $t-1$

Input and output hidden Markov Model (IOHMM)



The state transition model : $P(X_t | X_{t-1}, A_t)$

The observation model : $P(Y_t | X_t, A_t)$

Continuous-state Markov models

- In many practical time series applications, the data is naturally continuous (i.e., variables are not discretized), particularly for models of the physical environment

- Restrict the form of the continuous transition $p(X_t|X_{t-1})$

- A simple yet powerful class of such transitions are the linear dynamical systems

- A *deterministic linear dynamical system* defines the temporal evolution of a vector x_t according to the discrete-time update equation

$$x_t = A_t x_{t-1}$$

where A_t is the transition matrix at time t

- If A_t is invariant with t, the process is called stationary or time-invariant

Observed linear dynamic system

- A *stochastic linear dynamical system* defines the temporal evolution of a vector x_t according to the discrete-time update equation

$$x_t = A_t x_{t-1} + \eta_t$$

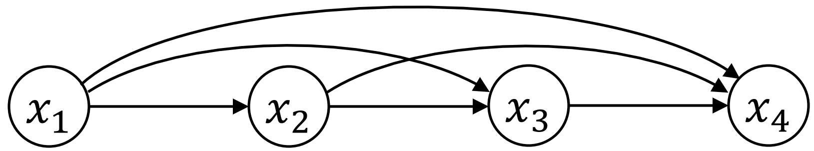
where η_t is a noise vector sampled from a Gaussian distribution

$$\eta_t \sim N(0, \Sigma_t)$$

- This is equivalent to a first-order Markov model with transition

$$p(x_t | x_{t-1}) = N(x_t | A_t x_{t-1}, \Sigma_t)$$

Auto-regressive models



- A scalar time-invariant Auto-Regressive (AR) model is defined by

$$x_t = \sum_{l=1}^{L} a_l x_{t-l} + \eta_t\,, \qquad \eta_t \sim N(0, \sigma^2)$$

where $a = (a_1, a_2, \dots, a_L)^T$ are AR coefficients and σ^2 is innovation noise.

- As a belief network, the AR model can be written as an Lth-order Markov model:

$$p(x_{1:T}) = \prod_{t=1}^{T} p(x_t | x_{t-1}, \dots, x_{t-L}), \qquad \text{with } x_i = 0 \text{ for } i \leq 0$$

$\hat{x}_{t-1} = (x_{t-1}, \dots, x_{t-L})$

with $p(x_t | x_{t-1}, \dots, x_{t-L)} = N\left(x_t \middle| \sum_{l=1}^{L} a_l x_{t-l}\,, \sigma^2\right) = N(x_t | a^T \hat{x}_{t-1}, \sigma^2)$

Similar to Bayesian Regression

- Heavily used in financial time series prediction, being able to capture simple trends in the data
- ***The AR coefficients form a compressed representation of the signal***

Training Auto-regressive model

- Maximum likelihood training of the AR coefficients is straightforward based on

$$
\begin{aligned}
\log p(x_{1:T}) &= \log \prod_{t=1}^{T} p(x_t | x_{t-1}, \dots, x_{t-L}) \\
&= \sum_{t=1}^{T} \log(x_t | \hat{x}_{t-1}) \\
&= -\frac{1}{2\sigma^2} \sum_{t=1}^{T} (x_t - a^T \hat{x}_{t-1})^2 - \frac{T}{2} \log(2\pi\sigma^2)
\end{aligned}
$$

- Differentiating w.r.t. a and equating to zero we arrive at

$$\sum_{t=1}^{T} (x_t - a^T \hat{x}_{t-1}) \hat{x}_{t-1} = 0$$

$$\rightarrow a = \left[\sum_t \hat{x}_{t-1} \hat{x}_{t-1}^T\right]^{-1} \sum_t x_t \hat{x}_{t-1}$$

x_t : target output (scalar)

- Similarly,

$$\sigma^2 = \frac{1}{T} \sum_{t=1}^{T} (x_t - a^T \hat{x}_{t-1})^2$$

Time-varying Auto-regressive model

- Learning the AR coefficients as a problem in inference in a latent linear dynamical system (LDS):

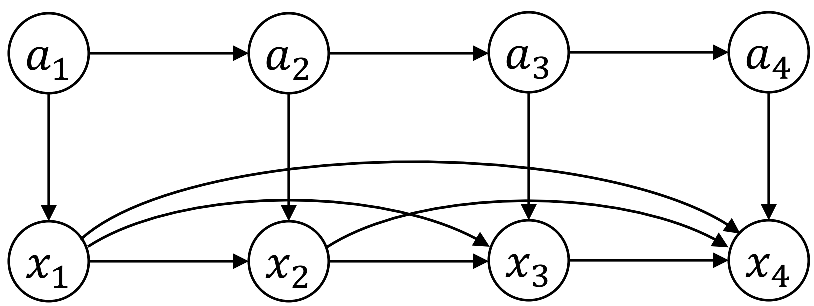
$$x_t = \hat{x}_{t-1}^T a_t + \eta_t, \qquad \eta_t \sim N(0, \sigma^2)$$

which can be viewed as the emission distribution of a latent LDS in which the hidden variable is a_t and the time dependent emission matrix is given by $\hat{x}_{t-1}^T$

- By placing a simple latent transition

$$a_t = a_{t-1} + \eta_t^a, \qquad \eta_t^a \sim N(0, \sigma_a^2 \mathbf{I})$$

which encourages the AR coefficients to change slowly with time



Time-varying Auto-regressive model

- Learning the AR coefficients as a problem in inference in a latent linear dynamical system (LDS):

$$x_t = \hat{x}_{t-1}^T a_t + \eta_t, \qquad \eta_t \sim N(0, \sigma^2)$$

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- By placing a simple latent transition

$$a_t = a_{t-1} + \eta_t^a, \qquad \eta_t^a \sim N(0, \sigma_a^2 \mathbf{I})$$

which encourages the AR coefficients to change slowly with time

- The joint distribution between the observation $x_{1:T}$ and the coefficients $\boldsymbol{a}_{1:t}$

$$p(a_{1:T} | x_{1:T}) \propto p(x_{1:T}, a_{1:T}) = \prod_{t=2}^{T} p(x_t | a_t, \hat{x}_{t-1}) p(a_t | a_{t-1})$$

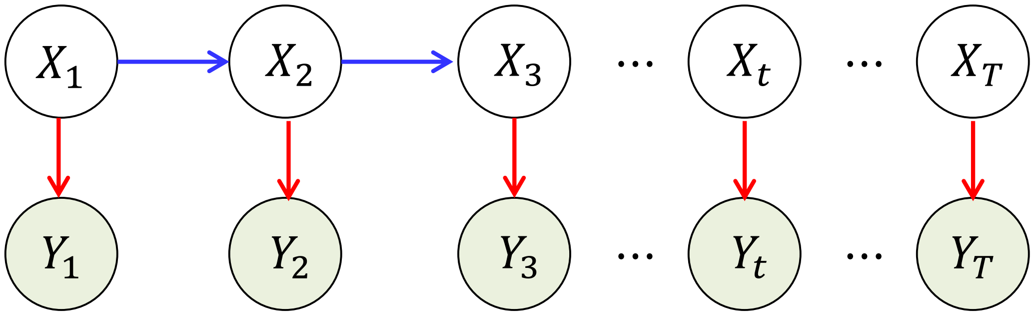
then we can compute

$$a_{1:T}^* = \underset{a_{1:T}}{\operatorname{argmax}}\, p(a_{1:T} | x_{1:T})$$

from which the MAP estimates for the AR coefficients can be determined

Linear Gaussian State Space Model

- The latent LDS defines a stochastic linear dynamical system in a latent space on a sequence of states $x_{1:T}$
- Observations $y_{1:T}$ are used to infer the hidden states that tracks or explains the system evolution



Transition model : $x_t = A_t x_{t-1} + \eta_t^x, \quad \eta_t^x \sim N(\bar{x}_t, \Sigma_t^x)$
Emission model : $y_t = B_t x_t + \eta_t^y, \quad \eta_t^y \sim N(\bar{y}_t, \Sigma_t^y)$

A_t: transition matrix
B_t: emission matrix

η_t^x transition noise vector with a hidden bias $\bar{x}_t$
η_t^y emission noise vector with a hidden bias $\bar{y}_t$

Linear Gaussian State Space Model

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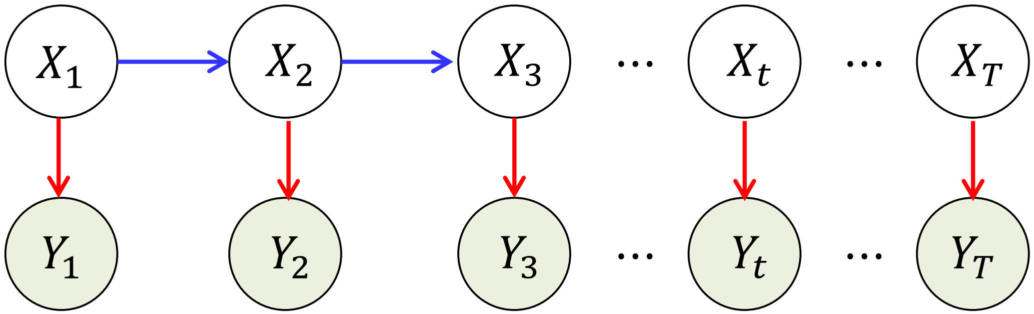

Transition model : $p(x_t|x_{t-1}) = N(x_t|A_t x_{t-1} + \bar{x}_t, \Sigma_t^x)$, $\quad p(x_1) = N(x_1|\mu_\pi, \Sigma_\pi)$
Emission model : $p(y_t|x_t) = N\left(y_t\middle|B_t x_t + \bar{y}_t, \Sigma_t^y\right)$

- The first order Markov model is then defined as

$$p(x_{1:T}, y_{1:T}) = p(x_1)p(y_1|x_1)\prod_{t=2}^{T} p(x_t|x_{t-1})p(y_t|x_t)$$

Kalman Filter

- Recall the filtering recursion for HMM:

$$P(x_t|y_{1:t}) \propto \sum_{x_{t-1}} P(y_t|x_t)P(x_t|\, x_{t-1})P(x_{t-1}|y_{1:t-1})$$

- For linear Gaussian State-space model, the recursion becomes

$$P(x_t|y_{1:t}) \;\propto \int_{x_{t-1}} P(y_t|x_t)P(x_t|x_{t-1})P(x_{t-1}|y_{1:t-1}) \quad \text{for} \quad t > 1$$

- Since the product of two Gaussians is another Gaussian, and the integral of a Gaussian is another Gaussian, $P(x_t|y_{1:t})$ is Gaussian:

$$P(x_t|y_{1:t})=N(x_t|f_t, F_t)$$

- Thus the recursion is for computing the mean μ_t and the variance V_t for $P(x_t|y_{1:t})$ using μ_{t-1} and the variance V_{t-1} for $P(x_{t-1}|y_{1:t-1})$

$P(x_{t-1}|y_{1:t-1}) = N(x_{t-1}|\mu_{t-1}, V_{t-1})$ $\qquad$ $P(x_t|y_{1:t}) = N(x_t|\mu_t, V_t)$