# 10-601
# **Machine Learning**

## Graphical models and Bayesian networks

# Independence

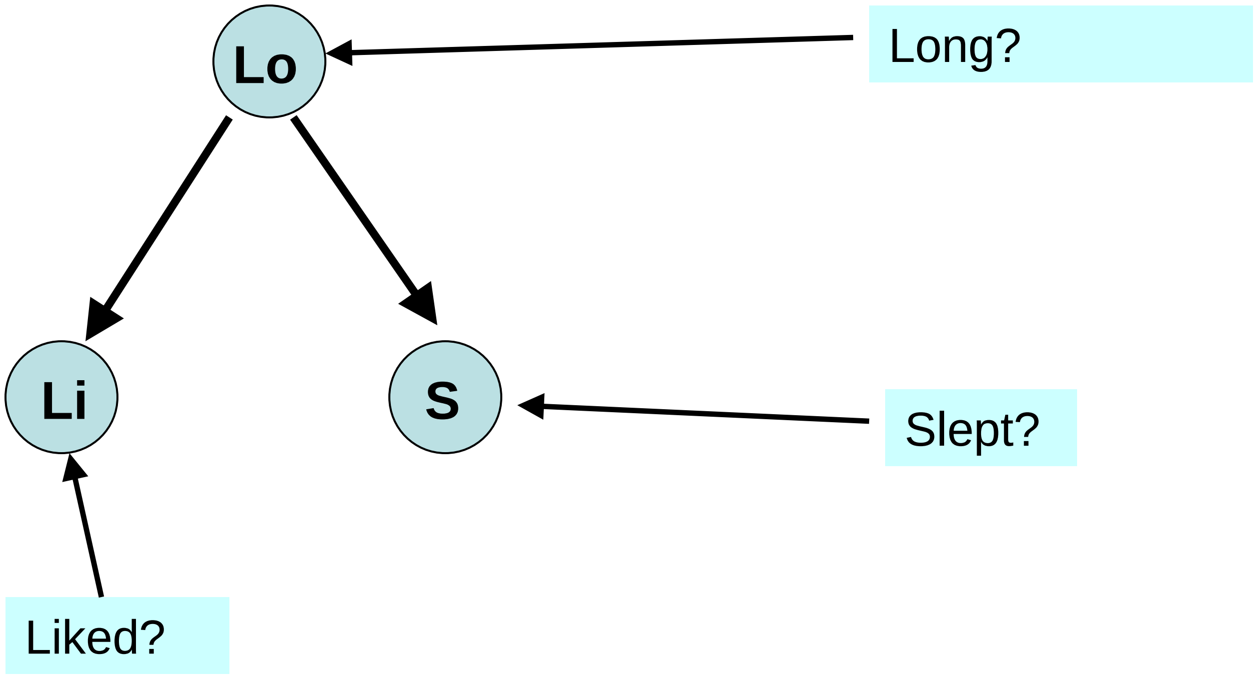
- In our density estimation class (and in the Naïve Bayes classifier class) we discussed at length the usefulness of the independence assumption
- However, we also mentioned its drawbacks

# Independence

- Independence allows for easier models, learning and inference
- For example, with 3 binary variables we only need 3 parameters rather than 7.
- The saving is even greater if we have many more variables …
- In many cases it would be useful to assume independence, even if its not the case
- Is there any middle ground?

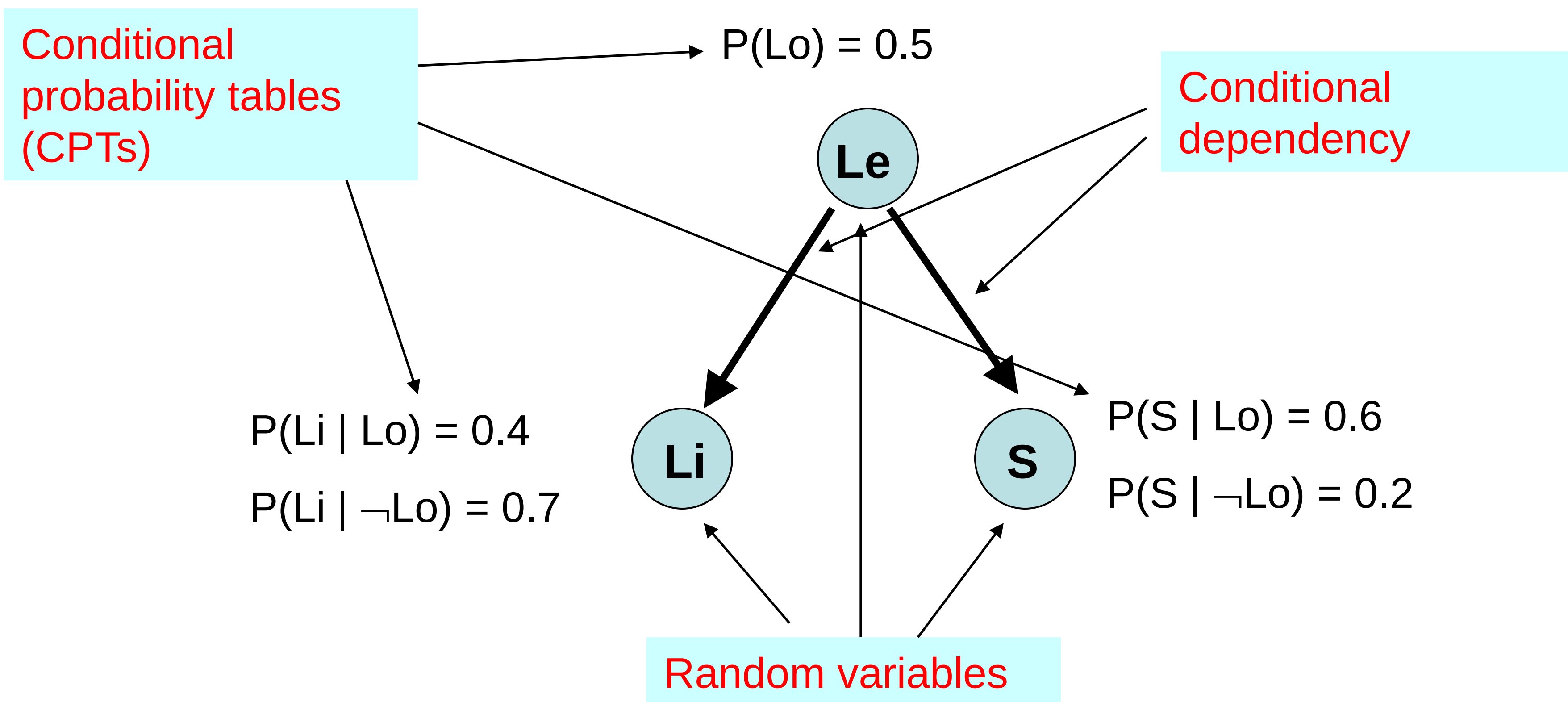
# Bayesian networks

- Bayesian networks are *directed graphs* with nodes representing *random variables* and edges representing *dependency assumptions*
- Lets use our movie example: We would like to determine the joint probability for length, liked and slept in a movie



# Bayesian networks: Notations

Bayesian networks are directed acyclic graphs.



# Bayesian networks: Notations

The Bayesian network below represents the following joint probability distribution:

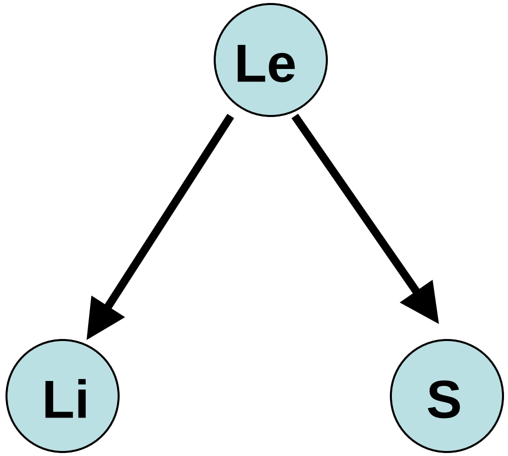
$$p(Le, Li, S) = P(Le)P(Li \mid Le)P(S \mid Le)$$

More generally Bayesian network represent the following joint probability distribution:

$$p(x_1 \cdots x_n) = \prod_i p(x_i \mid Pa(x_i))$$

The set of parents of $x_i$ in the graph

P(Lo) = 0.5




P(Li | Lo) = 0.4

P(Li | ¬Lo) = 0.7

P(S | Lo) = 0.6

P(S | ¬Lo) = 0.2

# Constructing a Bayesian network

- How do we go about constructing a network for a specific problem?
- Step 1: Identify the random variables
- Step 2: Determine the conditional dependencies
- Step 3: Populate the CPTs

Can be learned from observation data!

# A example problem

- An alarm system

  B – Did a burglary occur?

  E – Did an earthquake occur?

  A – Did the alarm sound off?

  M – Mary calls

  J – John calls

- How do we reconstruct the network for this problem?

# Factoring joint distributions

- Using the chain rule we can always factor a joint distribution as follows:

  P(A,B,E,J,M) =

  P(A | B,E,J,M) P(B,E,J,M) =

  P(A | B,E,J,M) P(B | E,J,M) P(E,J,M) =

  P(A | B,E,J,M) P(B | E, J,M) P(E | J,M) P(J,M)

  P(A | B,E,J,M) P(B | E, J,M) P(E | J,M)P(J | M)P(M)
- This type of conditional dependencies can also be represented graphically.

# A Bayesian network

P(A | B,E,J,M) P(B | E, J,M) P(E | J,M)P(J | M)P(M)

Number of parameters:

A: 2^4

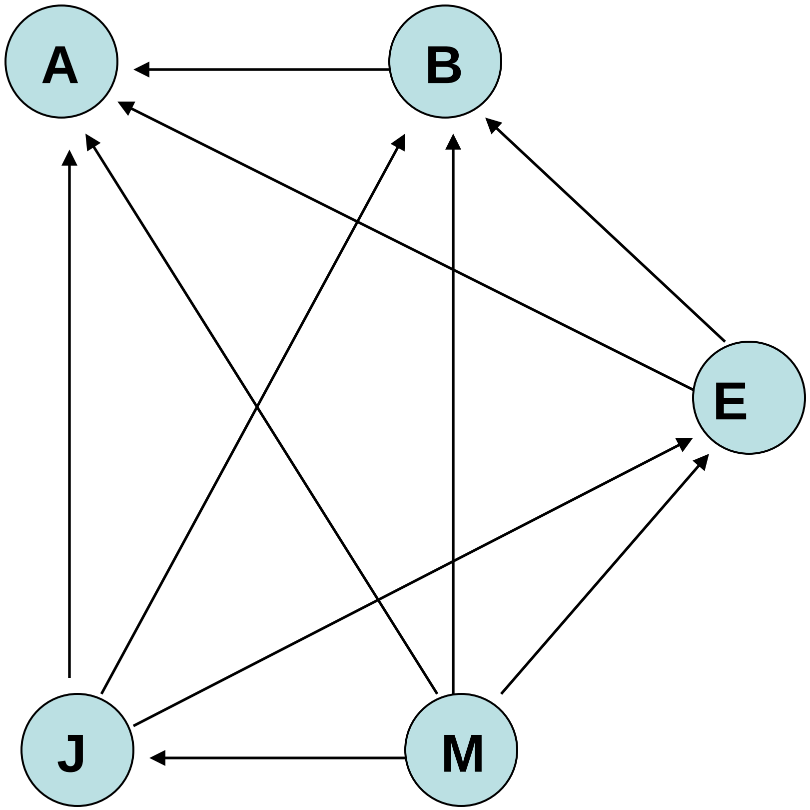
B: 2^3

E: 4

J: 2

M: 1

A total of 31 parameters



# A better approach

- An alarm system

  B – Did a burglary occur?

  E – Did an earthquake occur?

  A – Did the alarm sound off?

  M – Mary calls

  J – John calls

- Lets use our knowledge of the domain!

# Reconstructing a network

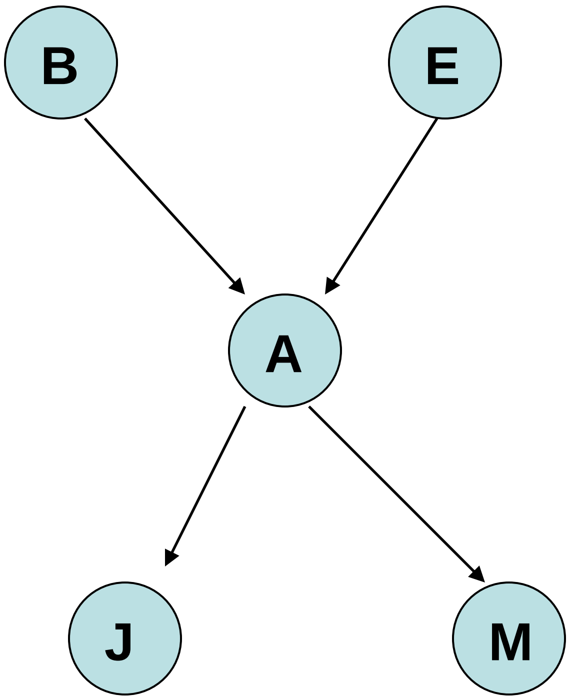
B – Did a burglary occur?

E – Did an earthquake occur?

A – Did the alarm sound off?

M – Mary calls

J – John calls



# Reconstructing a network

Number of parameters:

A: 4

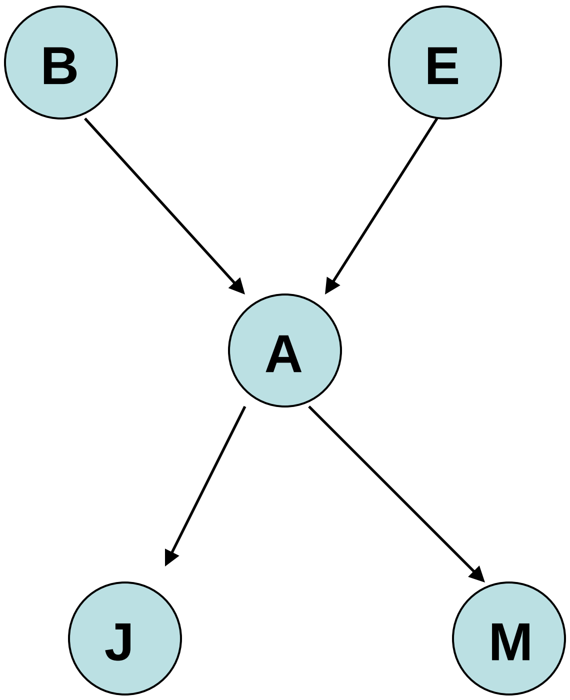
B: 1

E: 1

J: 2

M: 2

A total of 10 parameters




**By relying on domain knowledge we saved 21 parameters!**

# Constructing a Bayesian network: Revisited

- Step 1: Identify the random variables
- Step 2: Determine the conditional dependencies

  - Select on ordering of the variables

  - Add them one at a time

  - For each new variable X added select the minimal subset of nodes as parents such that X is independent from all other nodes in the current network given its parents.
- Step 3: Populate the CPTs

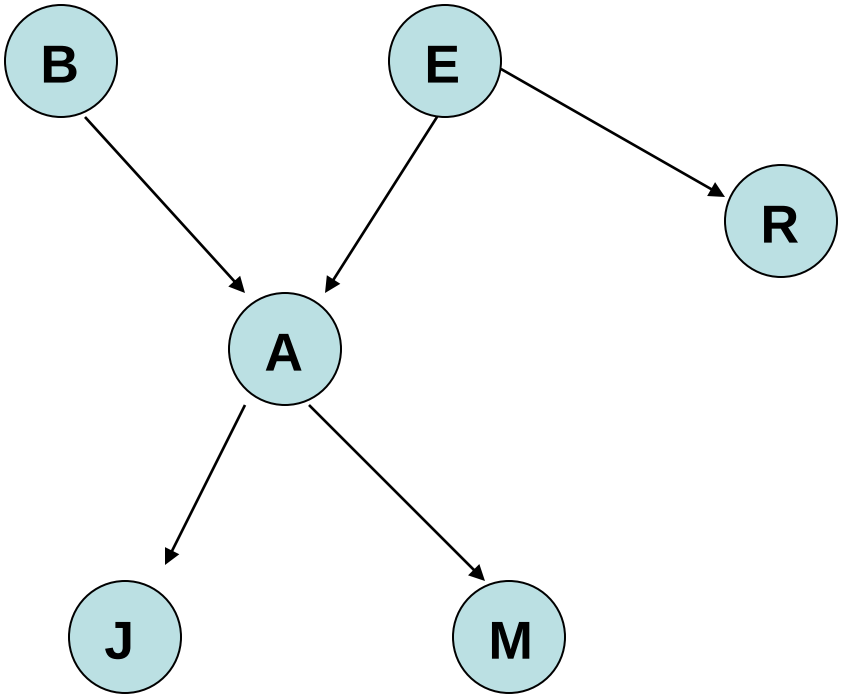
  - From examples using density estimation

# Reconstructing a network

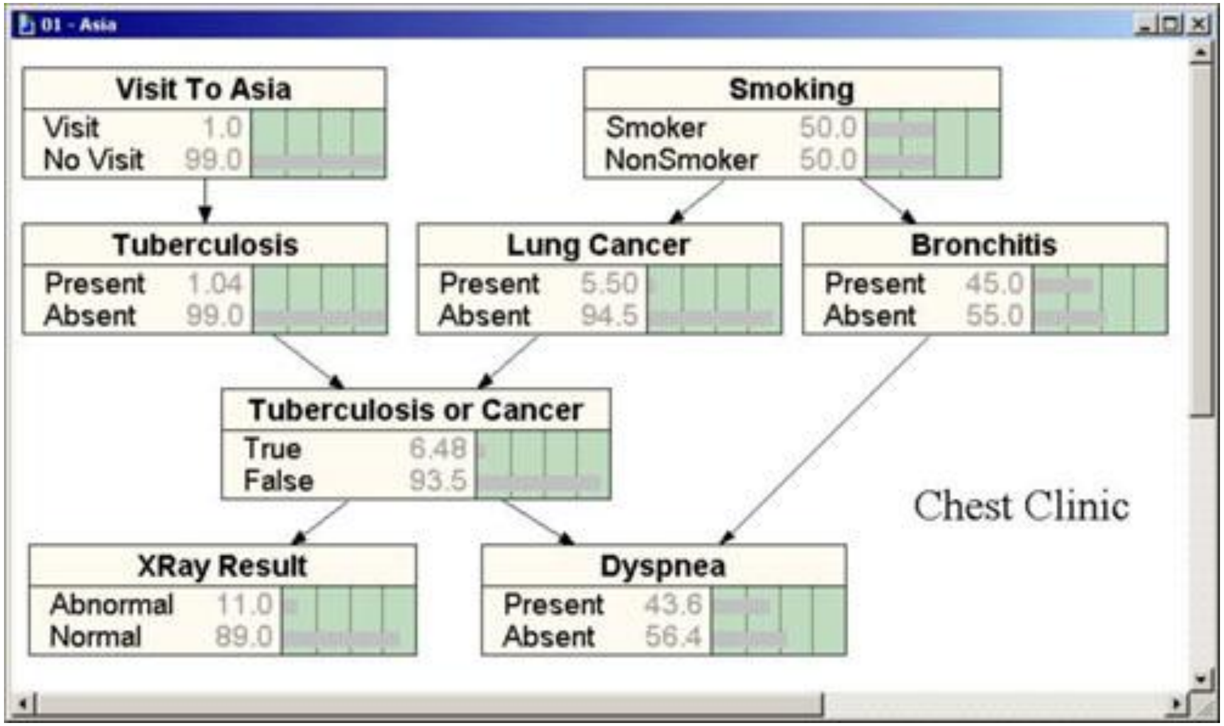
Suppose we wanted to add a new variable to the network:

R – Did the radio announce that there was an earthquake?

How should we insert it?



# Example: Bayesian networks for cancer detection



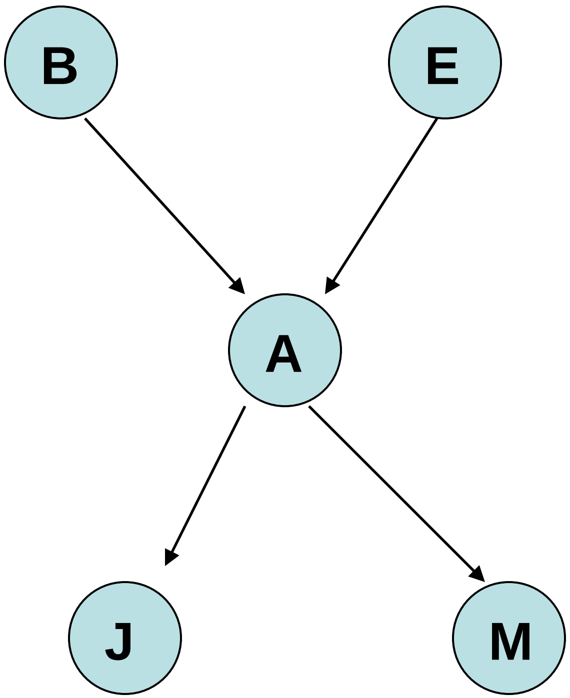
# Example: Gene expression network

QuickTime™ and a
TIFF (LZW) decompressor
are needed to see this picture.

# Conditional independence

- Two variables x,y are said to be conditionally independent given a third variable z if p(x,y|z) = p(x|z)p(y|z)
- In a Bayesian network a variable is conditionally independent of all other variables given it Markov blanket

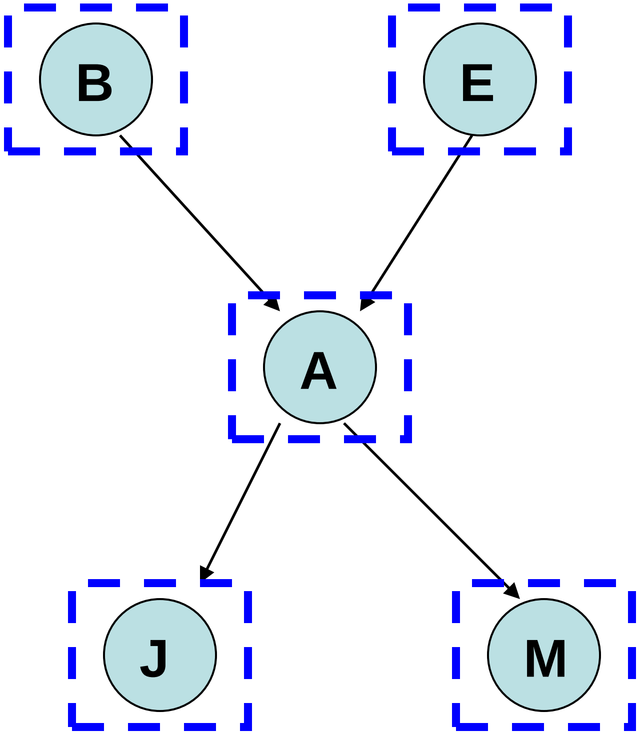
Markov blanket: All parent, children's and co-parents of children



# Markov blankets: Examples

Markov blanket for B:
E, A

Markov blanket for A:
B, E, J, M



# Bayesian network: Inference

- Once the network is constructed, we can use algorithms for inferring the values of unobserved variables.
- For example, in our previous network the only observed variables are the phone call and the radio announcement. However, what we are really interested in is whether there was a burglary or not.
- How can we determine that?

# Inference

- Lets start with a simpler question
  - How can we compute a joint distribution from the network?
  - For example, $P(B,\neg E,A,J,\neg M)$?
- Answer:
  - That's easy, lets use the network

# Computing: $P(B, \neg E, A, J, \neg M)$

$P(B, \neg E, A, J, \neg M) =$

$P(B)P(\neg E)P(A \mid B, \neg E)\, P(J \mid A)P(\neg M \mid A)$

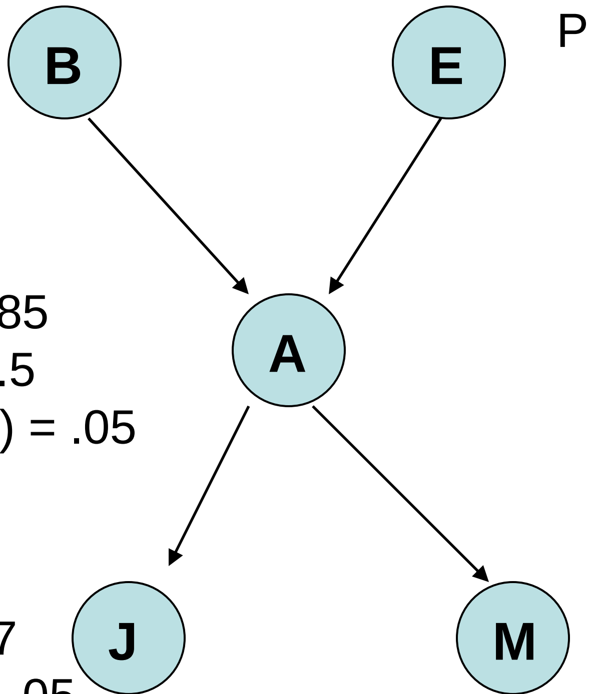
$= 0.05*0.9*.85*.7*.2$

$= 0.005355$

$P(B)=.05$

$P(E)=.1$

$P(A|B,E) =.95$
$P(A|B,\neg E) = .85$
$P(A|\neg B,E) =.5$
$P(A|\neg B, \neg E) = .05$




$P(J|A) =.7$
$P(J|\neg A) = .05$

$P(M|A) =.8$
$P(M|\neg A) = .15$

# Computing: P(B,¬E,A,J, ¬M)

P(B,¬E,A,J, ¬M) =

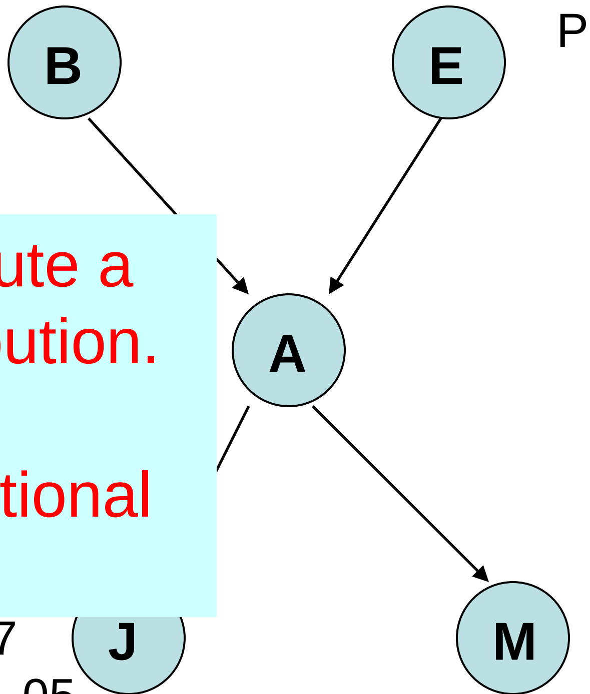
P(B)P(¬E)P(A | B, ¬E) P(J | A)P(¬M | A)

= 0.05*0.9*.85*.7*.2

= 0.005355

P(B)=.05

P(E)=.1




We can easily compute a complete joint distribution. What about partial distributions? Conditional distributions?

P(J|A) )=.7
P(J|¬A) = .05

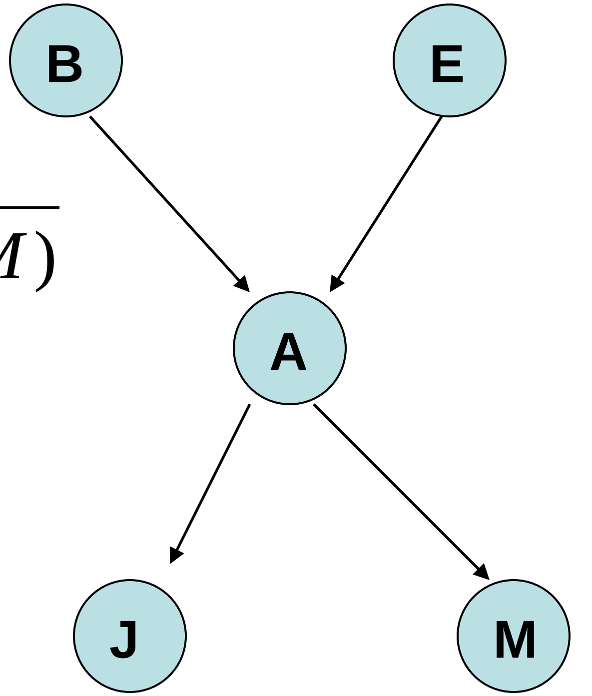
P(M|A) )=.8
P(M|¬A) = .15

# Inference

- We are interested in queries of the form:
  $P(B \mid J, \neg M)$
- This can also be written as a joint:

$$P(B \mid J, \neg M) = \frac{P(B, J, \neg M)}{P(B, J, \neg M) + P(\neg B, J, \neg M)}$$

- How do we compute the new joint?



# Inference in Bayesian networks

- We will discuss three methods:

1. Enumeration
2. Variable elimination
3. Stochastic inference

# Computing partial joints

$$P(B \mid J, \neg M) = \frac{P(B, J, \neg M)}{P(B, J, \neg M) + P(\neg B, J, \neg M)}$$

Sum all instances with these settings (the sum is over the possible assignments to the other two variables, E and A)

# Computing: $P(B,J,\neg M)$

$P(B,J,\neg M) =$

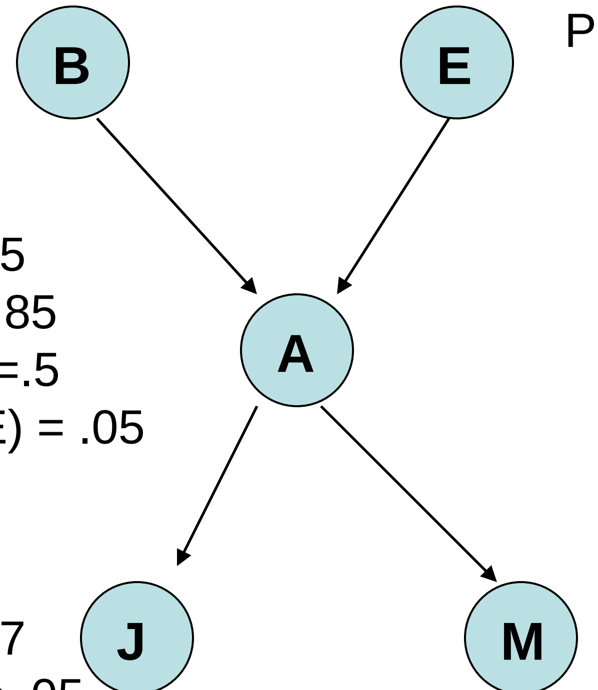
$P(B,J,\neg M,A,E)+$

$P(B,J,\neg M,\neg A,E) + P(B,J,\neg M,A,\neg E) + P(B,J,\neg M,\neg A,\neg E) =$

0.0007+0.00001+0.005+0.0003 = 0.00601

P(B)=.05

P(E)=.1




$P(A|B,E) )=.95$
$P(A|B,\neg E) = .85$
$P(A|\neg B,E) )=.5$
$P(A|\neg B,\neg E) = .05$

$P(J|A) )=.7$
$P(J|\neg A) = .05$

$P(M|A) )=.8$
$P(M|\neg A) = .15$

# Computing partial joints

$$P(B \mid J, \neg M) = \frac{P(B, J, \neg M)}{P(B, J, \neg M) + P(\neg B, J, \neg M)}$$

Sum all instances with these settings (the sum is over the possible assignments to the other two variables, E and A)

- This method can be improved by re-using calculations (similar to dynamic programming)
- Still, the number of possible assignments is exponential in the unobserved variables?
- That is, unfortunately, the best we can do. General querying of Bayesian networks is NP-complete

# Inference in Bayesian networks if NP complete (sketch)

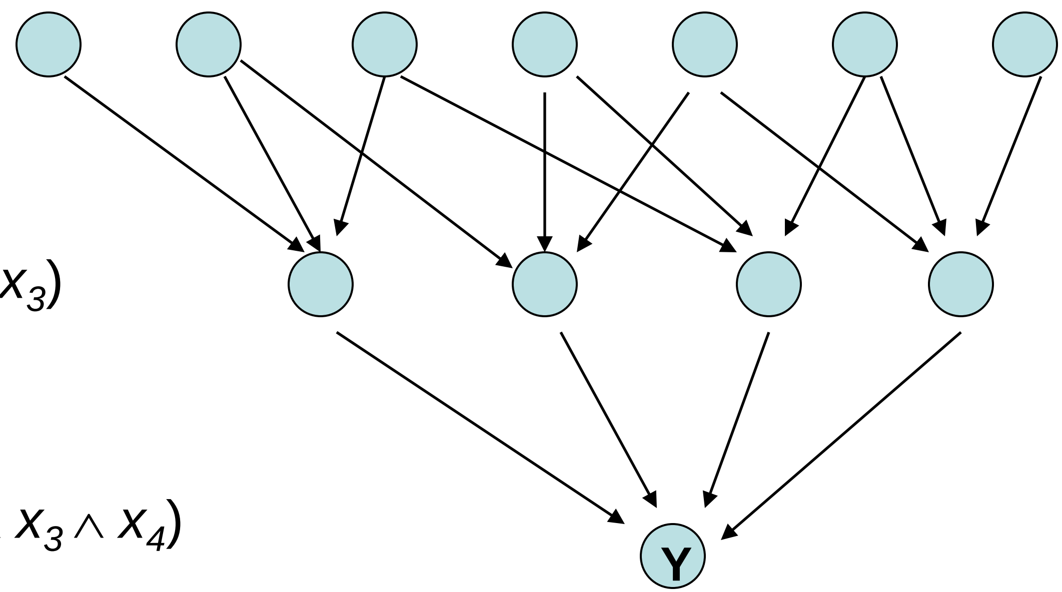
- Reduction from 3SAT
- Recall: 3SAT, find satisfying assignments to the following problem: $(a \vee b \vee c) \wedge (d \vee \neg b \vee \neg c) \ldots$

**What is P(Y=1)?**

$P(x_i=1) = 0.5$

$P(x_i=1) = (x_1 \vee x_2 \vee x_3)$

$P(Y=1) = (x_1 \wedge x_2 \wedge x_3 \wedge x_4)$



# Inference in Bayesian networks

- We will discuss three methods:

1. Enumeration
2. Variable elimination
3. Stochastic inference

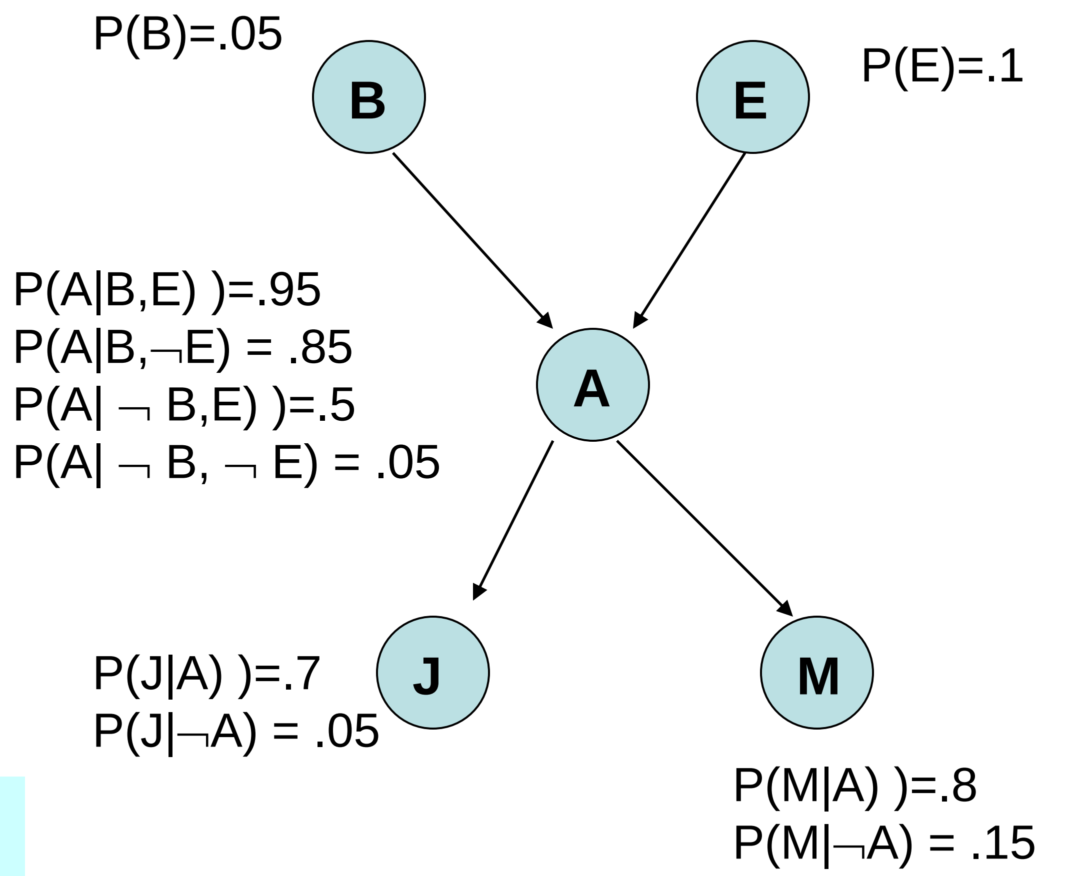
# Variable elimination

P(B,J, ¬M) =

P(B,J, ¬M,A,E)+

P(B,J, ¬M, ¬ A,E) + P(B,J,¬M,A, ¬ E) + P(B,J, ¬M, ¬ A, ¬ E) =

0.0007+0.00001+0.005+0.0003 = 0.00601




Reuse computations rather than recompute probabilities

# Computing: P(B,J, ¬M)

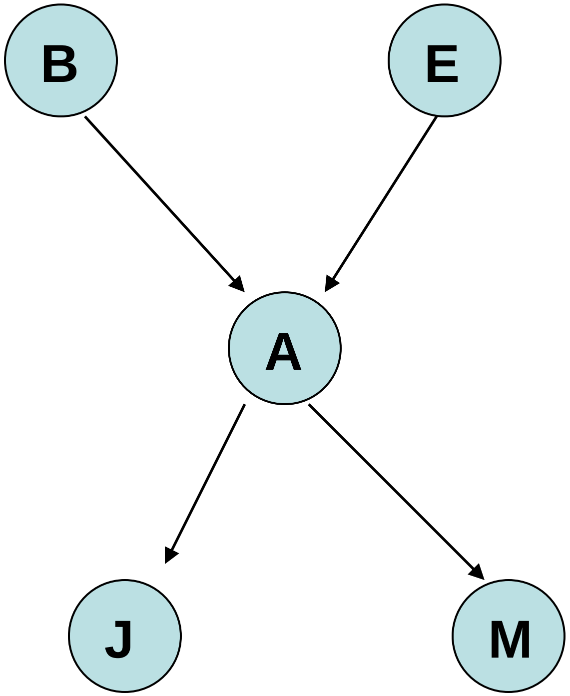
P(B,J, ¬M) =

P(B,J, ¬M,A,E)+

P(B,J, ¬M, ¬ A,E) + P(B,J, ¬M,A, ¬ E) + P(B,J, ¬M, ¬ A, ¬ E) =

$$\sum_a \sum_e P(B)P(e)P(a \mid B,e)P(M \mid a)P(J \mid a)$$

Store as a function of a and use whenever necessary (no need to recompute each time)



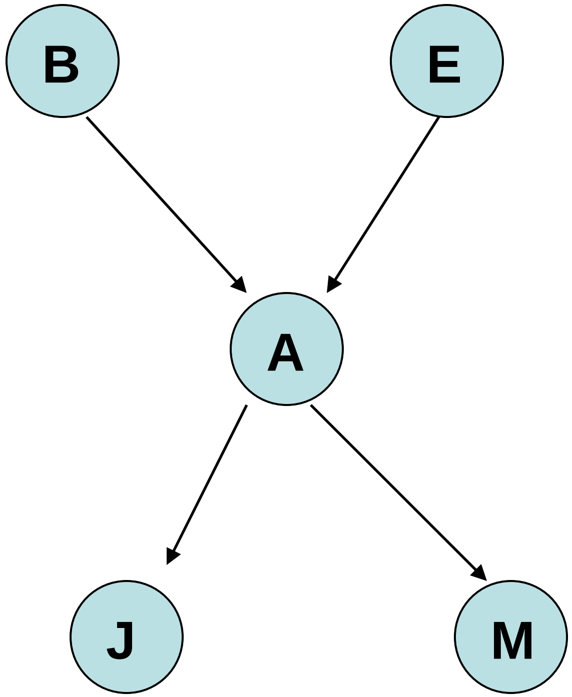
# Variable elimination

$$P(B,J,M) = \sum_a \sum_e P(B)P(e)P(a \mid B,e)P(M \mid a)P(J \mid a)$$

$$= P(B)\sum_e P(e)\sum_a P(a \mid B,e)P(M \mid a)P(J \mid a)$$

Set: $f_M(A) = \begin{pmatrix} P(M \mid A) \\ P(M \mid \neg A) \end{pmatrix}$

$$f_J(A) = \begin{pmatrix} P(J \mid A) \\ P(J \mid \neg A) \end{pmatrix}$$



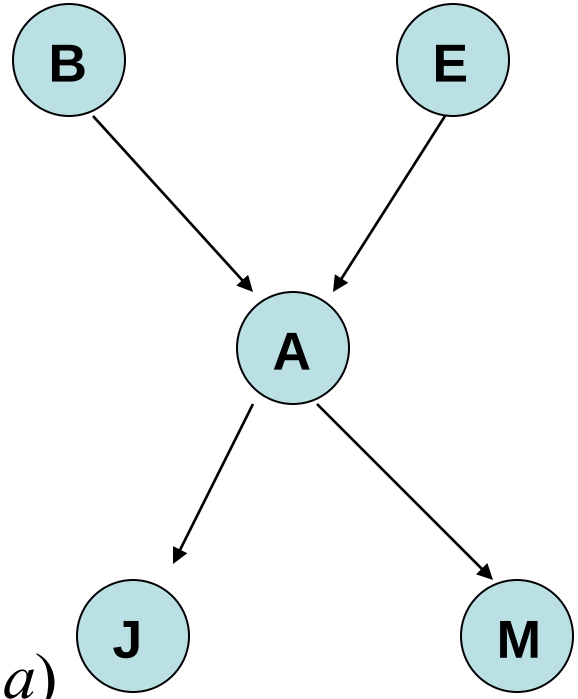
# Variable elimination

$$P(B,J,M) = \sum_a \sum_e P(B)P(e)P(a \mid B,e)P(M \mid a)P(J \mid a)$$

$$= P(B)\sum_e P(e)\sum_a P(a \mid B,e)P(M \mid a)P(J \mid a)$$

Set: $f_M(A) = \begin{pmatrix} P(M \mid A) \\ P(M \mid \neg A) \end{pmatrix}$

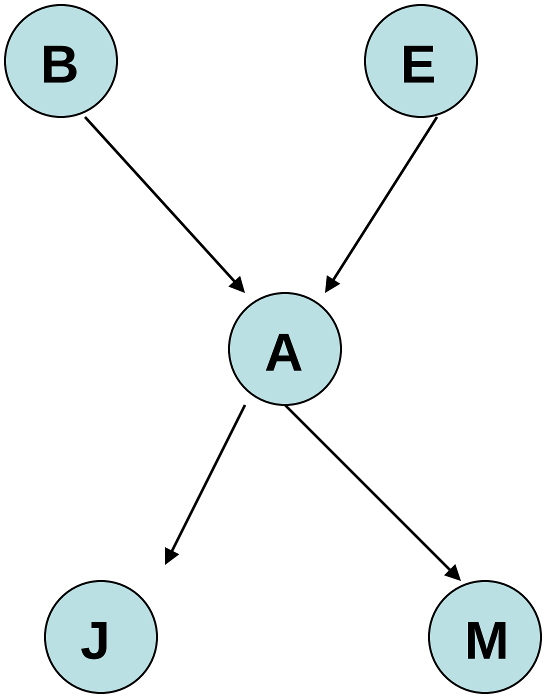
$$f_J(A) = \begin{pmatrix} P(J \mid A) \\ P(J \mid \neg A) \end{pmatrix}$$




$$P(B,J,M) = P(B)\sum_e P(e)\sum_a P(a \mid B,e) f_M(a) f_J(a)$$

# Variable elimination

$$= P(B)\sum_{e} P(e)\sum_{a} P(a \mid B,e) f_M(a) f_J(a)$$




Lets continue with these functions:

$$f_A(a,B,e) = P(a \mid B,e)$$

We can now define the following function:

$$f_{A,J,M}(B,e) = \sum_{a} f_A(a,B,e) f_J(a) f_M(a)$$

And so we can write:

$$P(B,J,M) = P(B)\sum_{e} P(e) f_{A,J,M}(B,e)$$

# Variable elimination

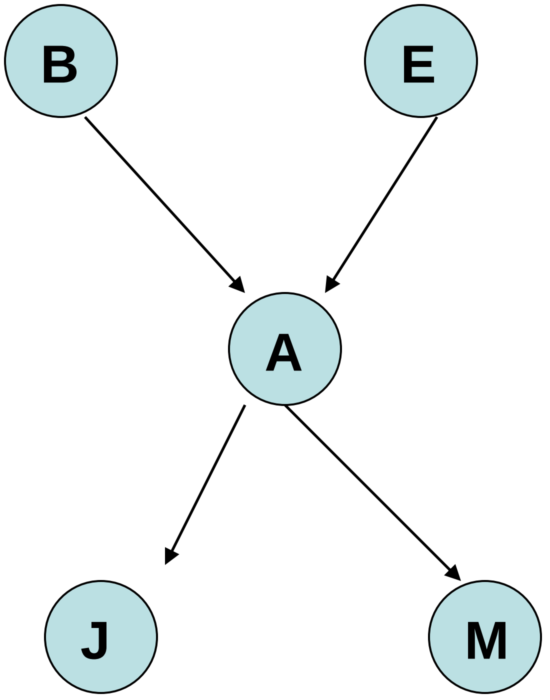
$$P(B,J,M) = P(B)\sum_{e} P(e) f_{A,J,M}(B,e)$$

Lets continue with another function:

$$f_{E,A,J,M}(B) = \sum_{e} P(e) f_{A,J,M}(B,e)$$

And finally we can write:

$$P(B,J,M) = P(B) f_{E,A,J,M}(B)$$



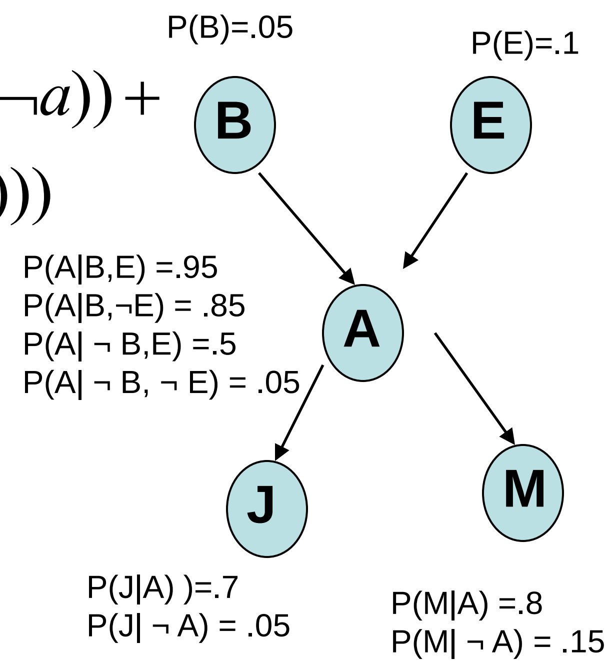
# Example

$$P(B,J,M) = P(B) f_{E,A,J,M}(B)$$

$$= 0.05 \sum_e P(e) f_{A,J,M}(B,e) = 0.05(0.1 f_{A,J,M}(B,e) + 0.9 f_{A,J,M}(B,\neg e))$$

$$0.05(0.1(0.95 f_J(a) f_M(a) + 0.05 f_J(\neg a) f_M(\neg a)) +$$

$$0.9(.85 f_J(a) f_M(a) + .15 f_J(\neg a) f_M(\neg a)))$$




Calling the same function multiple times

# Final computation (normalization)

$$P(B \mid J, \neg M) = \frac{P(B, J, \neg M)}{P(B, J, \neg M) + P(\neg B, J, \neg M)}$$

# Algorithm

- *e* - evidence (the variables that are known)
- *vars* - the conditional probabilities derived from the network in reverse order (bottom up)
- For each *var* in *vars*

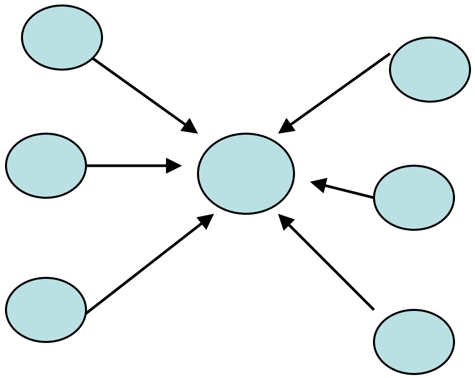
  - *factors* <- make_factor (*var*,*e*)

  - if *var* is a hidden variable then create a new factor by summing out *var*
- Compute the product of all factors
- Normalize

# Computational complexity

- We are reusing computations so we are reducing the running time.
- However, there are still cases in which this algorithm we lead to exponential running time.
- Consider the case of $f_x(y_1 \ldots y_n)$. When factoring x out we would need to account for all possible values of the y's.

Variable elimination can lead to significant costs saving but its efficiency depends on the network structure



# Inference in Bayesian networks

- We will discuss three methods:

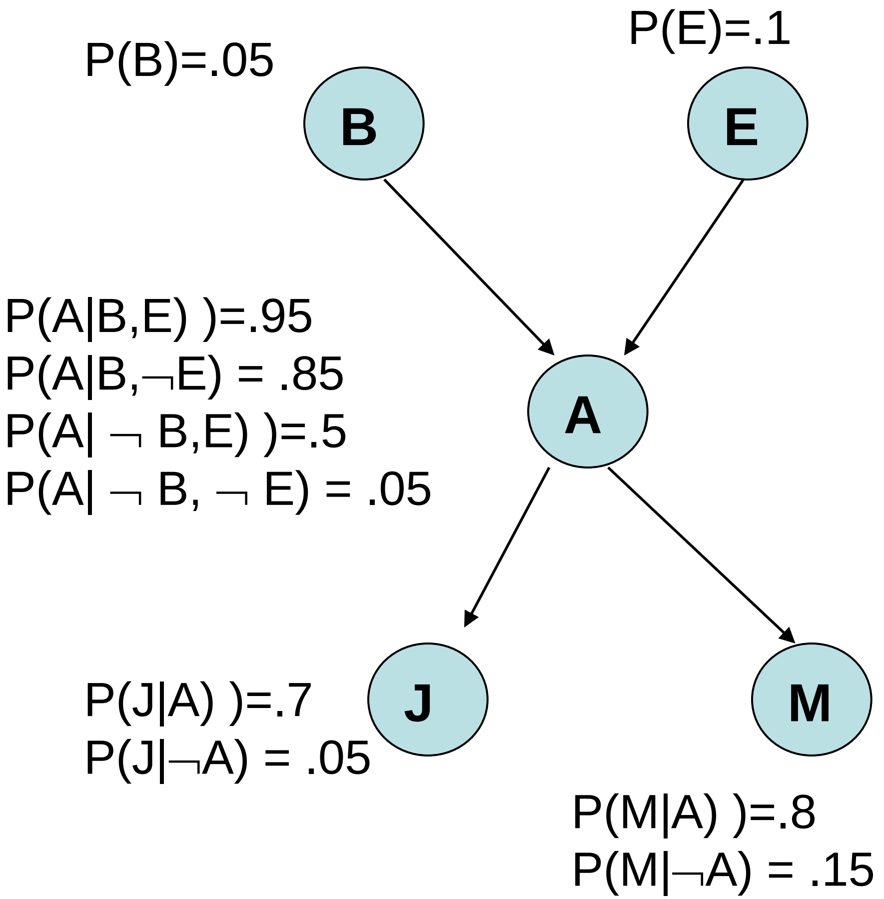
1. Enumeration
2. Variable elimination
3. Stochastic inference

# Stochastic inference

- We can easily sample the joint distribution to obtain possible instances

1. Sample the free variable
2. For every other variable:
   - If all parents have been sampled, sample based on conditional distribution

We end up with a new set of assignments for B,E,A,J and M which are a random sample from the joint

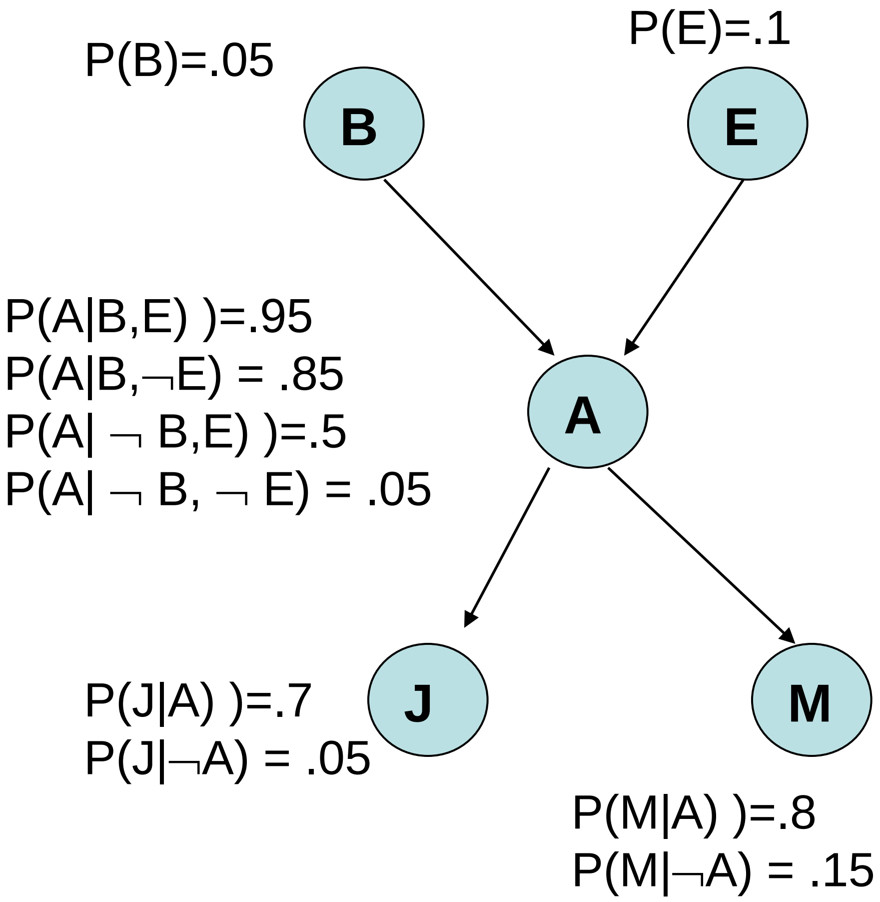


# Stochastic inference

- We can easily sample the joint distribution to obtain possible instances

1. Sample the free variable
2. For every other variable:
   - If all parents have been sampled, sample based on conditional distribution

Its always possible to carry out this sampling procedure, why?



# Using sampling for inference

- Lets revisit our problem: Compute $P(B \mid J, \neg M)$
- Looking at the samples we can count:

  - $N$: total number of samples

  - $N_c$ : total number of samples in which the condition holds $(J, \neg M)$

  - $N_B$: total number of samples where the joint is true $(B, J, \neg M)$
- For a large enough N
  - $N_c$ / N $\approx P(J, \neg M)$
  - $N_B$ / N $\approx P(B, J, \neg M)$
- And so, we can set

$$P(B \mid J, \neg M) = P(B, J, \neg M) / P(J, \neg M) \approx N_B / N_c$$

# Using sampling for inference

- Lets revisit our problem: Compute P(B | J,¬M)
- Looking at the samples we can count:

  - *N*: total number o

  - $N_c$ : total number

  - $N_B$: total number

- For a large enoug

  - $N_c$ / N ≈ P(J,¬M)

  - $N_B$ / N ≈ P(B,J,¬M)

- And so, we can set

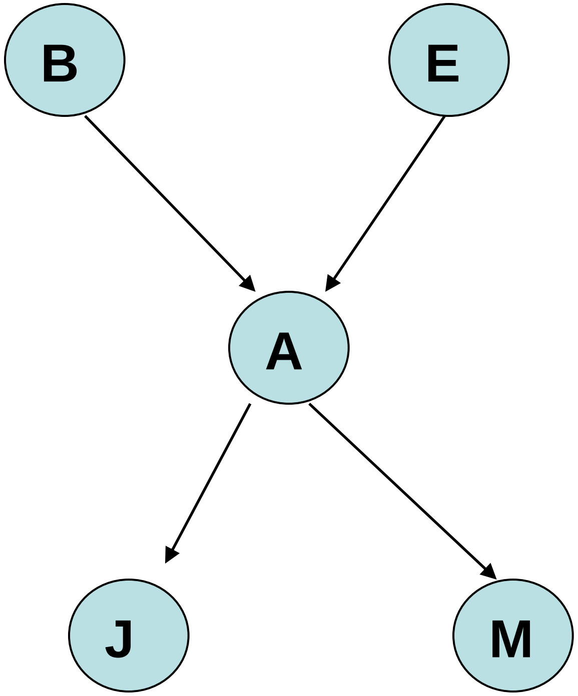
P(B | J,¬M) = P(B,J,¬M) / P(J,¬M) ≈ $N_B$ / $N_c$

Problem: What if the condition rarely happens?

We would need lots and lots of samples, and most would be wasted

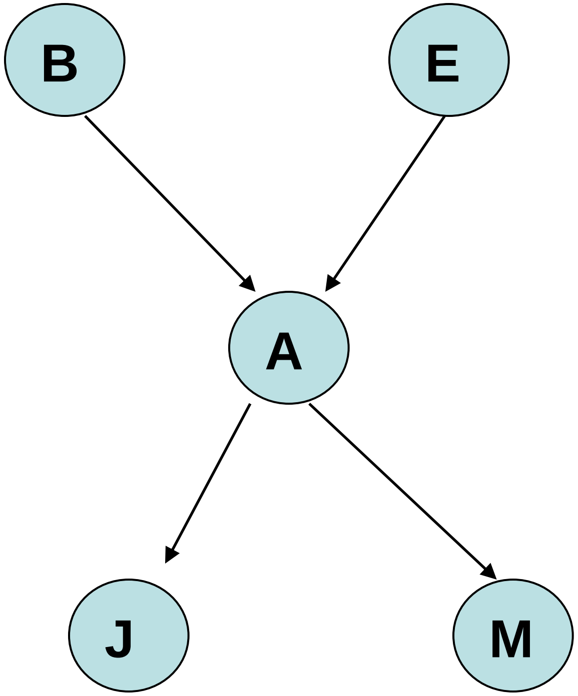
# Weighted sampling

- Compute P(B | J,¬M)
- We can manually set the value of J to 1 and M to 0
- This way, all samples will contain the correct values for the conditional variables
- Problems?



# Weighted sampling

- Compute P(B | J,¬M)
- Given an assignment to parents, we assign a value of 1 to J and 0 to M.
- We record the *probability* of this assignment ($w = p_1 * p_2$) and we weight the new joint sample by *w*



# Weighted sampling algorithm for computing P(B | J,¬M)

- Set $N_B, N_c = 0$
- Sample the joint setting the values for *J* and *M*, compute the weight, *w,* of this sample
- $N_c = N_c + w$
- If $B = 1$, $N_B = N_B + w$

- After many iterations, set

P(B | J,¬M) = $N_B / N_c$

# Important points

- Bayes rule
- Joint distribution, independence, conditional independence
- Attributes of Bayesian networks
- Constructing a Bayesian network
- Inference in Bayesian networks

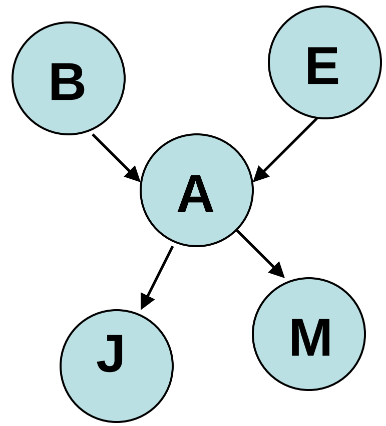
# Other inference methods

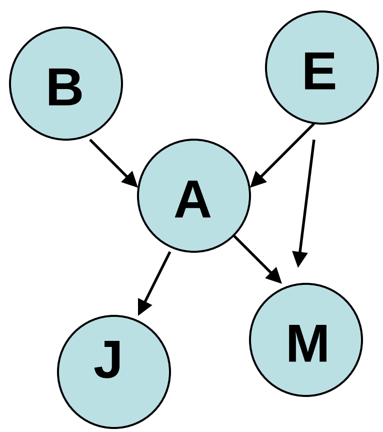
- Convert network to a polytree

  - In a polytree no two nodes have more than one path between them

  - We can convert arbitrary networks to a polytree by clustering (grouping) nodes. For such a graph there is a algorithm which is linear in the number of nodes

  - However, converting into a polytree can result in an exponential increase in the size of the CPTs



# d-separation

- In some cases it would be useful for us to know under which conditions two variables are independent of each other
  - Helps when trying to do inference
  - Can help determine causality from structure
- Two variables x and y are d-separated given a set of variables Z (which could be empty) if x and y are conditionally independent given Z
- We denote such conditional independence as I(x,y|Z)

# d-separation

- We will give rules to identify d-connected variables. Variables that are not d-connected are d-separated.
- The following three rules can be used to determine if x and y are d-connected given Z:

1. If Z is empty then x and y are d-connected if there exists a path between them does not contain a collider.
2. x and y are d-connected given Z if there exists a path between them that does not  contain a collider and does not contain any member of Z
3. If Z contains a collider or one of its descendents then if a path between x and y contains this node they are d-connected