CS 2750 Machine Learning
Lecture 14

Bayesian belief networks

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Density estimation

Data: $D = \{D_1, D_2, .., D_n\}$
$D_i = \mathbf{x}_i$ a vector of attribute values

Attributes:

- modeled by random variables $\mathbf{X} = \{X_1, X_2, \ldots, X_d\}$ with:
  - **Continuous values**
  - **Discrete values**

  E.g. ***temperature*** with numerical values
  or ***chest pain*** with discrete values
  [no-pain, mild, moderate, strong]

Underlying true probability distribution:

$p(\mathbf{X})$

Density estimation

Data: $D = \{D_1, D_2, .., D_n\}$

$D_i = \mathbf{x}_i$ a vector of attribute values

Objective: try to estimate the underlying true probability distribution over variables $\mathbf{X}$, $p(\mathbf{X})$, using examples in D

true distribution $p(\mathbf{X})$ → n samples $D = \{D_1, D_2, .., D_n\}$ → estimate $\hat{p}(\mathbf{X})$

Standard (iid) assumptions: Samples

- **are independent of each other**
- **come from the same (identical) distribution (fixed $p(\mathbf{X})$)**

Learning via parameter estimation

In this lecture we consider **parametric density estimation**

Basic settings:

- A set of random variables $\mathbf{X} = \{X_1, X_2, \ldots, X_d\}$
- **A model of the distribution** over variables in $\boldsymbol{X}$ with parameters Θ :

$$\hat{p}(\mathbf{X} \mid \Theta)$$

- **Data** $D = \{D_1, D_2, .., D_n\}$

Objective: find the parameters Θ that explain the observed data the best

Parameter estimation

- **Maximum likelihood (ML)**

  maximize $p(D \mid \Theta, \xi)$
  - yields: one set of parameters Θ_{ML}
  - the target distribution is approximated as:

$$\hat{p}(\mathbf{X}) = p(\mathbf{X} \mid \mathbf{\Theta}_{ML})$$

- **Bayesian parameter estimation**
  - uses the posterior distribution over possible parameters

$$p(\Theta \mid D, \xi) = \frac{p(D \mid \Theta, \xi)\, p(\Theta \mid \xi)}{p(D \mid \xi)}$$

  - Yields: all possible settings of Θ (and their "weights")
  - The target distribution is approximated as:

$$\hat{p}(\mathbf{X}) = p(\mathbf{X} \mid D) = \int_{\mathbf{\Theta}} p(X \mid \mathbf{\Theta})\, p(\mathbf{\Theta} \mid D, \xi)\, d\mathbf{\Theta}$$

Parameter estimation

Other possible criteria:

- **Maximum a posteriori probability (MAP)**

  maximize $p(\mathbf{\Theta} \mid D, \xi)$ (mode of the posterior)
  - Yields: one set of parameters $\mathbf{\Theta}_{MAP}$
  - Approximation:

$$\hat{p}(\mathbf{X}) = p(\mathbf{X} \mid \mathbf{\Theta}_{MAP})$$

- **Expected value of the parameter**

  $\hat{\mathbf{\Theta}} = E(\mathbf{\Theta})$ (mean of the posterior)
  - Expectation taken with regard to posterior $p(\mathbf{\Theta} \mid D, \xi)$
  - Yields: one set of parameters
  - Approximation:

$$\hat{p}(\mathbf{X}) = p(\mathbf{X} \mid \hat{\mathbf{\Theta}})$$

Density estimation

- **So far we have covered density estimation for "simple" distribution models:**
  - Bernoulli
  - Binomial
  - Multinomial
  - Gaussian
  - Poisson

But what if:

- The dimension of $\mathbf{X} = \{X_1, X_2, \ldots, X_d\}$ is large
  - Example: patient data
- Compact parametric distributions do not seem to fit the data
  - E.g.: multivariate Gaussian may not fit
- We have only a "small" number of examples to do accurate parameter estimates

How to learn complex distributions

How to learn complex multivariate distributions $\hat{p}(\mathbf{X})$ with large number of variables?

One solution:

- **Decompose the distribution using conditional independence relations**
- **Decompose the parameter estimation problem to a set of smaller parameter estimation tasks**

Decomposition of distributions under conditional independence assumption is the main idea behind **Bayesian belief networks**

Example

Problem description:

- **Disease:** pneumonia
- **Patient symptoms (findings, lab tests)**:
  - Fever, Cough, Paleness, WBC (white blood cells) count, Chest pain, etc.

Representation of a patient case:

- Symptoms and disease are represented as random variables

Our objectives:

- **Describe a multivariate distribution representing the relations between symptoms and disease**
- **Design of inference and learning procedures for the multivariate model**

Modeling uncertainty with probabilities

- **Full joint distribution:**
  - Assume $\mathbf{X} = \{X_1, X_2, \ldots, X_d\}$ are all random variables that define the domain
  - Full joint: $P(\mathbf{X})$ or $P(X_1, X_2, \ldots, X_d)$

Full joint it is sufficient to do any type of probabilistic inference:

- Computation of joint probabilities for sets of variables

  $P(X_1, X_2, X_3)$ $\quad$ $P(X_1, X_{10})$
- Computation of conditional probabilities

  $P(X_1 \mid X_2 = True, X_3 = False)$

Marginalization

Joint probability distribution (for a set variables)

- Defines probabilities for all possible assignments to values of variables in the set

$\mathbf{P}(pneumonia, WBCcount)$ 2×3 table

WBCcount

		high	*normal*	*low*	$\mathbf{P}(Pneumonia)$
Pneumonia	*True*	0.0008	0.0001	0.0001	0.001
	False	0.0042	0.9929	0.0019	0.999
$\mathbf{P}(WBCcount)$		0.005	0.993	0.002	

Marginalization (summing of rows, or columns)
- summing out variables

Variable independence

- **The joint distribution over a subset of variables can be always computed from the joint distribution through marginalization**
- **How about the opposite? Can we recover the joint from the joint over subsets?**

$\mathbf{P}(pneumonia, WBCcount)$

WBCcount

		high	*normal*	*low*	$\mathbf{P}(Pneumonia)$
Pneumonia	*True*	?	?	?	0.001
	False	?	?	?	0.999
$\mathbf{P}(WBCcount)$		0.005	0.993	0.002	

Variable independence

- **The joint distribution over a subset of variables can be always computed from the joint distribution through marginalization**
- **Can we recover the joint from the joint over subsets? NO !**
  - **Only exception:** **when variables are independent**

$$P(A, B) = P(A)P(B)$$

$\mathbf{P}(pneumonia, WBCcount)$

		WBCcount			$\mathbf{P}(Pneumonia)$
		high	*normal*	*low*	
Pneumonia	*True*	?	?	?	0.001
	False	?	?	?	0.999
$\mathbf{P}(WBCcount)$		0.005	0.993	0.002	

Conditional probability

Conditional probability :

- Probability of A given B

$$P(A \mid B) = \frac{P(A, B)}{P(B)}$$

- Conditional probability is defined in terms of joint probabilities
- Joint probabilities can be expressed in terms of conditional probabilities

$$P(A, B) = P(A \mid B)P(B) \quad \textbf{(product rule)}$$

$$P(X_1, X_2, \ldots X_n) = \prod_{i=1}^{n} P(X_i \mid X_{1,} \ldots X_{i-1}) \quad \textbf{(chain rule)}$$

- Conditional probability – is useful for **various probabilistic inferences**

$$P(Pneumonia = True \mid Fever = True, WBCcount = high, Cough = True)$$

Inference

Any query can be computed from the full joint distribution !!!

- **Joint over a subset of variables** is obtained through marginalization

$$P(A=a, C=c) = \sum_i \sum_j P(A=a, B=b_i, C=c, D=d_j)$$

- **Conditional probability over a set of variables**, given other variables' values is obtained through marginalization and definition of conditionals

$$P(D=d \mid A=a, C=c) = \frac{P(A=a, C=c, D=d)}{P(A=a, C=c)}$$

$$= \frac{\sum_i P(A=a, B=b_i, C=c, D=d)}{\sum_i \sum_j P(A=a, B=b_i, C=c, D=d_j)}$$

Inference

- Any joint probability can be expressed as a product of conditionals via the **chain rule**.

$$P(X_1, X_2, \ldots X_n) = P(X_n \mid X_{1,} \ldots X_{n-1}) P(X_{1,} \ldots X_{n-1})$$

$$= P(X_n \mid X_{1,} \ldots X_{n-1}) P(X_{n-1} \mid X_{1,} \ldots X_{n-2}) P(X_{1,} \ldots X_{n-2})$$

$$= \prod_{i=1}^{n} P(X_i \mid X_{1,} \ldots X_{i-1})$$

- It is often easier to define the distribution in terms of conditional probabilities:
  - E.g. $\mathbf{P}(Fever \mid Pneumonia = T)$
    $\mathbf{P}(Fever \mid Pneumonia = F)$

Modeling uncertainty with probabilities

- **Full joint distribution:** joint distribution over all random variables defining the domain
  - it is sufficient to represent the complete domain and to do any type of probabilistic inferences

Problems:

- **Space complexity.** To store full joint distribution requires to remember $O(d^n)$ numbers.

  n – number of random variables, d – number of values
- **Inference complexity.** To compute some queries requires $O(d^n)$ steps.
- **Acquisition problem.** Who is going to define all of the probability entries?

Pneumonia example. Complexities.

- **Space complexity**.
  - Pneumonia (2 values: T,F), Fever (2: T,F), Cough (2: T,F), WBCcount (3: high, normal, low), paleness (2: T,F)
  - Number of assignments: 2*2*2*3*2=48
  - We need to define at least 47 probabilities.
- **Time complexity**.
  - Assume we need to compute the probability of Pneumonia=T from the full joint

$$P(Pneumonia = T) =$$

$$= \sum_{i \in T,F} \sum_{j \in T,F} \sum_{k=h,n,l} \sum_{u \in T,F} P(Fever = i, Cough = j, WBCcount = k, Pale = u)$$

  - Sum over 2*2*3*2=24 combinations

Bayesian belief networks (BBNs)

Bayesian belief networks.

- Represent the full joint distribution over the variables more compactly with a **smaller number of parameters**.
- Take advantage of **conditional and marginal independences** among random variables

- **A and B are independent**

$$P(A,B) = P(A)P(B)$$

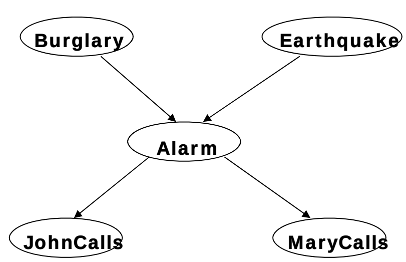
- **A and B are conditionally independent given C**

$$P(A,B \mid C) = P(A \mid C)P(B \mid C)$$
$$P(A \mid C,B) = P(A \mid C)$$

Alarm system example

- Assume your house has an **alarm system** against **burglary**. You live in the seismically active area and the alarm system can get occasionally set off by an **earthquake**. You have two neighbors, **Mary** and **John**, who do not know each other. If they hear the alarm they call you, but this is not guaranteed.
- We want to represent the probability distribution of events:
  - Burglary, Earthquake, Alarm, Mary calls and John calls

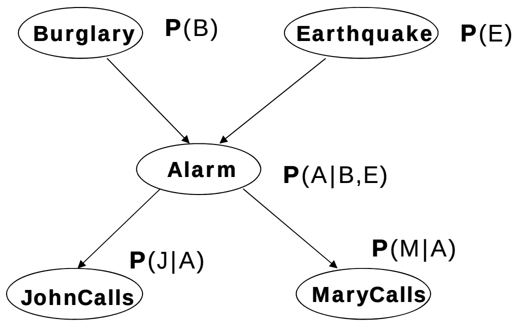
Causal relations



Bayesian belief network

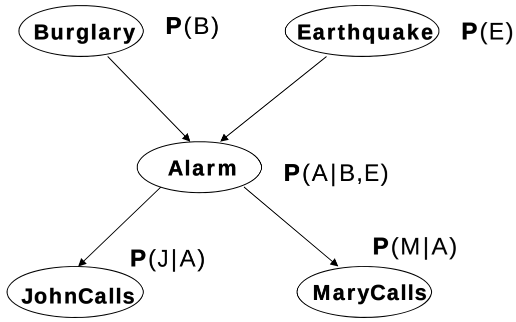
1. **Directed acyclic graph**
   - **Nodes** = random variables
     Burglary, Earthquake, Alarm, Mary calls and John calls
   - **Links** = direct (causal) dependencies between variables.

     The chance of Alarm being is influenced by Earthquake,
     The chance of John calling is affected by the Alarm

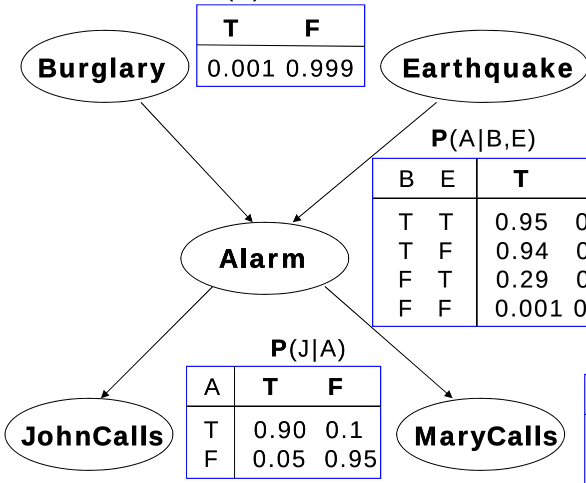


Bayesian belief network

2. **Local conditional distributions**
   - relating variables and their parents



Bayesian belief network



P(B)

T	F
0.001	0.999

P(E)

T	F
0.002	0.998

P(A|B,E)

B	E	T	F
T	T	0.95	0.05
T	F	0.94	0.06
F	T	0.29	0.71
F	F	0.001	0.999

P(J|A)

A	T	F
T	0.90	0.1
F	0.05	0.95

P(M|A)

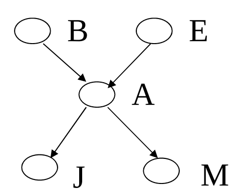
A	T	F
T	0.7	0.3
F	0.01	0.99

Full joint distribution in BBNs

Full joint distribution is defined in terms of local conditional distributions (obtained via the chain rule):

$$\mathbf{P}(X_1, X_2, .., X_n) = \prod_{i=1,..n} \mathbf{P}(X_i \mid pa(X_i))$$

Example:



Assume the following assignment of values to random variables

$B = T, E = T, A = T, J = T, M = F$

Then its probability is:

$P(B = T, E = T, A = T, J = T, M = F) =$

$P(B = T)P(E = T)P(A = T \mid B = T, E = T)P(J = T \mid A = T)P(M = F \mid A = T)$

Bayesian belief networks (BBNs)

Bayesian belief networks

- Represent the full joint distribution over the variables more compactly using the product of local conditionals.
- **But how did we get to local parameterizations?**

Answer:

- **Graphical structure** encodes **conditional and marginal independences** among random variables
- **A and B are independent** $P(A,B) = P(A)P(B)$
- **A and B are conditionally independent given C**

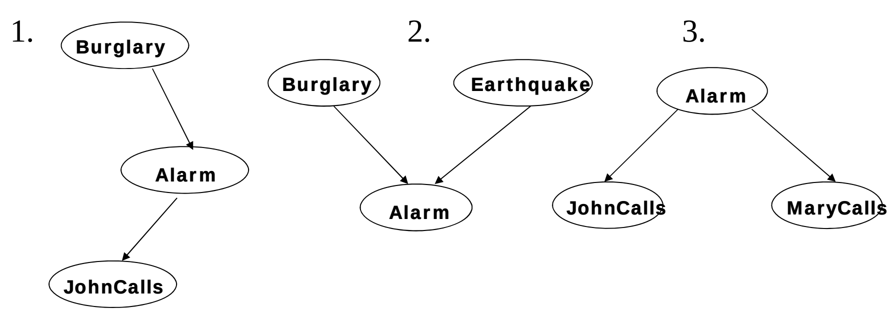
$$P(A \mid C, B) = P(A \mid C)$$

$$P(A, B \mid C) = P(A \mid C)P(B \mid C)$$

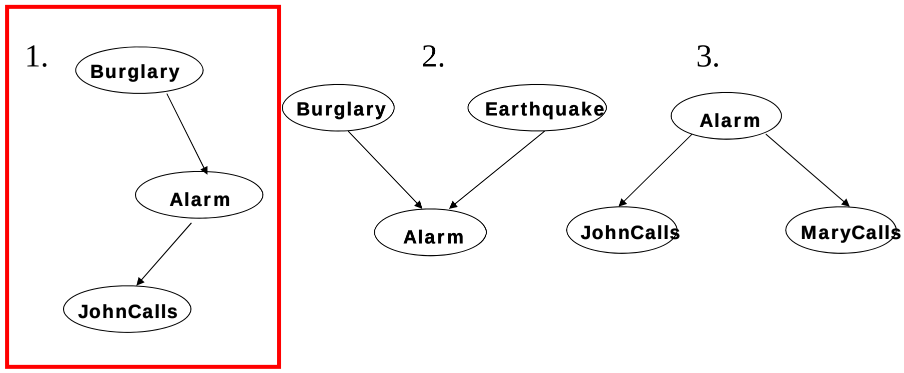
- **The graph structure implies the decomposition !!!**

Independences in BBNs

3 basic independence structures:



Independences in BBNs

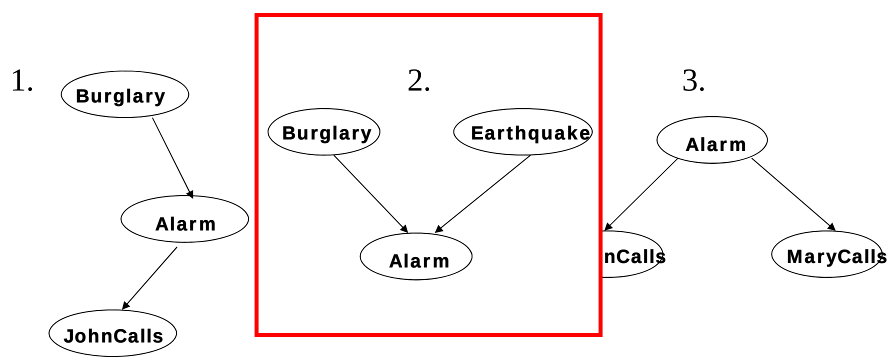


1. JohnCalls **is independent** of Burglary given Alarm

$$P(J \mid A, B) = P(J \mid A)$$

$$P(J, B \mid A) = P(J \mid A) P(B \mid A)$$

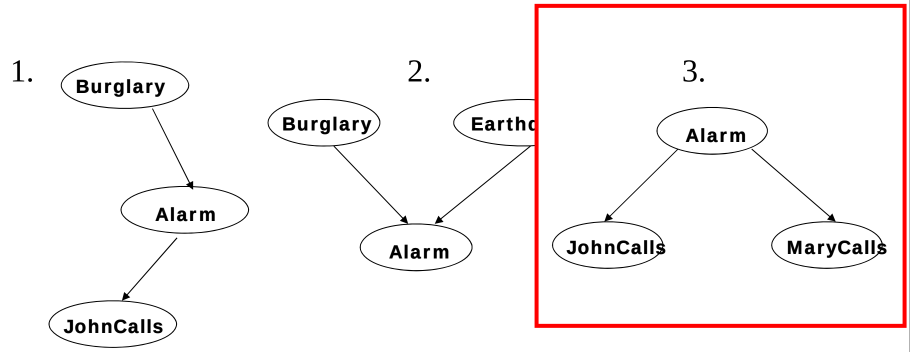
Independences in BBNs



2. Burglary **is independent** of Earthquake (not knowing Alarm)
   Burglary and Earthquake **become dependent** given Alarm !!

$$P(B, E) = P(B) P(E)$$

Independences in BBNs



3. MaryCalls **is independent** of JohnCalls given Alarm

$$P(J \mid A, M) = P(J \mid A)$$

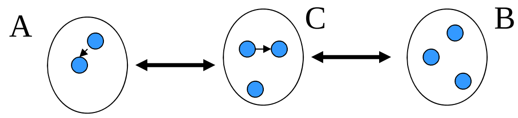
$$P(J, M \mid A) = P(J \mid A) P(M \mid A)$$

Independence in BBN

- BBN distribution models many conditional independence relations relating distant variables and sets
- These are defined in terms of the graphical criterion called d-separation
- **D-separation in the graph**
  - Let X,Y and Z be three sets of nodes
  - If X and Y are d-separated by Z then X and Y are conditionally independent given Z
- **D-separation :**
  - **A is d-separated from B given C** if every undirected path between them is **blocked with C**
- **Path blocking**
  - 3 cases that expand on three basic independence structures

Undirected path blocking

A is d-separated from B given C if every undirected path between them is **blocked**



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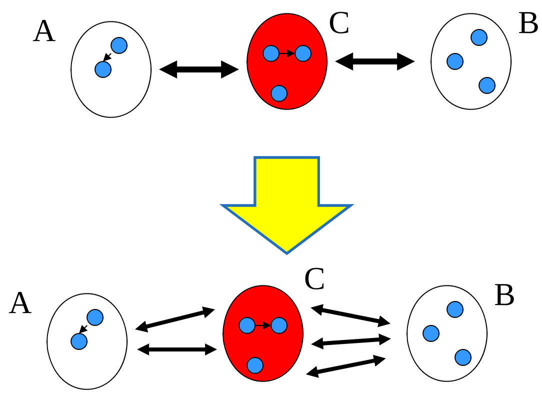

Undirected path blocking

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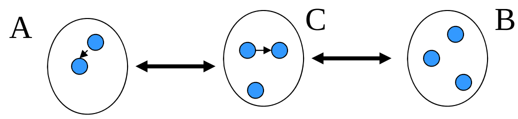
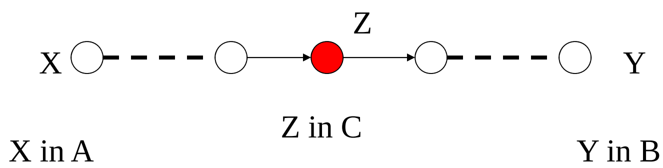


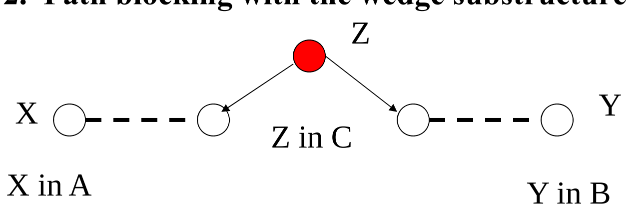
- **1. Path blocking with a linear substructure**



Undirected path blocking

A is d-separated from B given C if every undirected path between them is **blocked**

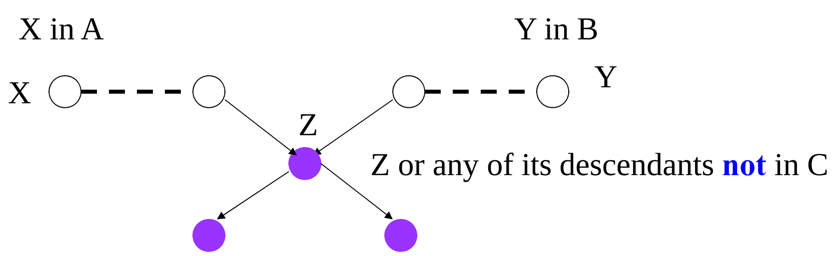
- **2. Path blocking with the wedge substructure**



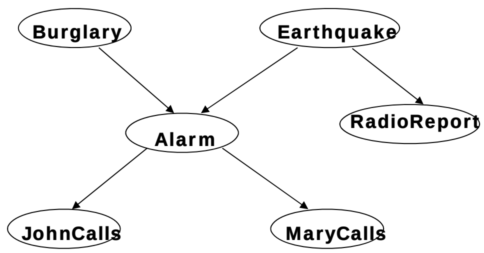
Undirected path blocking

A is d-separated from B given C if every undirected path between them is **blocked**

- **3. Path blocking with the vee substructure**

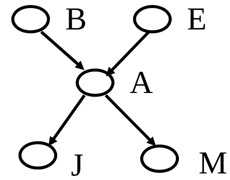


Independences in BBNs



- Earthquake and Burglary are independent given MaryCalls **F**
- Burglary and MaryCalls are independent (not knowing Alarm) **F**
- Burglary and RadioReport are independent given Earthquake **T**
- Burglary and RadioReport are independent given MaryCalls **F**

Full joint distribution in BBNs



Rewrite the full joint probability using the product rule:

$$P(B=T,E=T,A=T,J=T,M=F)=$$

$$=P(J=T \mid B=T,E=T,A=T,M=F)P(B=T,E=T,A=T,M=F)$$

$$=\underline{P(J=T \mid A=T)}P(B=T,E=T,A=T,M=F)$$

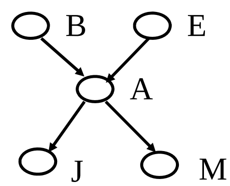
$$P(M=F \mid B=T,E=T,A=T)P(B=T,E=T,A=T)$$

$$\underline{P(M=F \mid A=T)}P(B=T,E=T,A=T)$$

$$\underline{P(A=T \mid B=T,E=T)}P(B=T,E=T)$$

$$P(B=T)P(E=T)$$

Full joint distribution in BBNs



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$$=\underline{P(J=T \mid A=T)}P(B=T,E=T,A=T,M=F)$$

$$P(M=F \mid B=T,E=T,A=T)P(B=T,E=T,A=T)$$

$$\underline{P(M=F \mid A=T)}P(B=T,E=T,A=T)$$

$$\underline{P(A=T \mid B=T,E=T)}P(B=T,E=T)$$

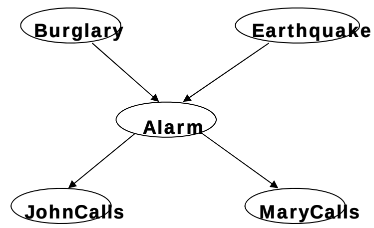
$$P(B=T)P(E=T)$$

$$=P(J=T \mid A=T)P(M=F \mid A=T)P(A=T \mid B=T,E=T)P(B=T)P(E=T)$$

Parameter complexity problem

- In the BBN the full joint distribution is expressed as a product of conditionals (of smaller) complexity

$$\mathbf{P}(X_1, X_2,.., X_n) = \prod_{i=1,..n} \mathbf{P}(X_i \mid pa(X_i))$$



Parameters:
full joint: ?

BBN: ?

Parameter complexity problem

- In the BBN the full joint distribution is expressed as a product of conditionals (of smaller) complexity

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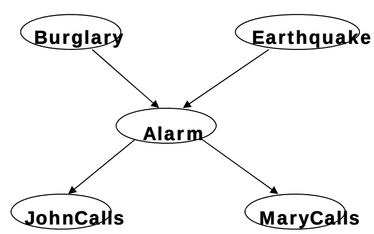

Parameters:
full joint: $2^5 = 32$

BBN: $2^3 + 2(2^2) + 2(2) = 20$

Parameters to be defined:
full joint: $2^5 - 1 = 31$

BBN: $2^2 + 2(2) + 2(1) = 10$