CS 2750 Machine Learning
Lecture 12

Bayesian belief networks

Milos Hauskrecht
milos@cs.pitt.edu
5329 Sennott Square

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. ***blood pressure*** with numerical values
  or ***chest pain*** with discrete values
  [no-pain, mild, moderate, strong]

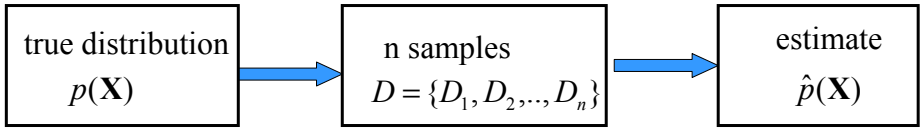
Underlying true probability distribution:

$p(\mathbf{X})$

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



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 description of parameters Θ so they fit the observed data

Parameter estimation

- **Maximum likelihood (ML)**

  maximize $p(D \mid \Theta, \xi)$

  – yields: one set of parameters Θ_{ML}

  – the target distribution is approximated as:

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

- **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:

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

Parameter estimation.

Other possible criteria:

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

  maximize $p(\boldsymbol{\Theta} \mid D, \xi)$ (mode of the posterior)

  – Yields: one set of parameters $\boldsymbol{\Theta}_{MAP}$

  – Approximation:

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

- **Expected value of the parameter**

  $\hat{\boldsymbol{\Theta}} = E(\boldsymbol{\Theta})$ (mean of the posterior)

  – Expectation taken with regard to posterior $p(\boldsymbol{\Theta} \mid D, \xi)$

  – Yields: one set of parameters

  – Approximation:

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

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 along 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

Joint probability distribution

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

$\mathbf{P}(Pneumonia)$

		WBCcount			
		high	*normal*	*low*	
Pneumonia	*True*	0.0008	0.0001	0.0001	0.001
	False	0.0042	0.9929	0.0019	0.999
		0.005	0.993	0.002	

$\mathbf{P}(WBCcount)$

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**
- **Not the other way around !!!**
  - **Only exception: when variables are independent**

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

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

		high	*normal*	*low*	
Pneumonia	*True*	0.0008	0.0001	0.0001	0.001
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		0.005	0.993	0.002	

$\mathbf{P}(WBCcount)$

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**

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

Modeling uncertainty with probabilities

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

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

- 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**

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

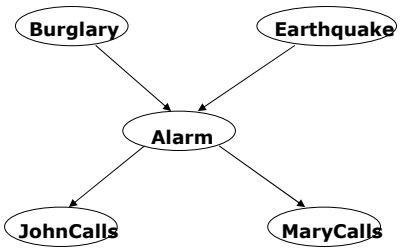
- **A and B are conditionally independent given C**

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

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

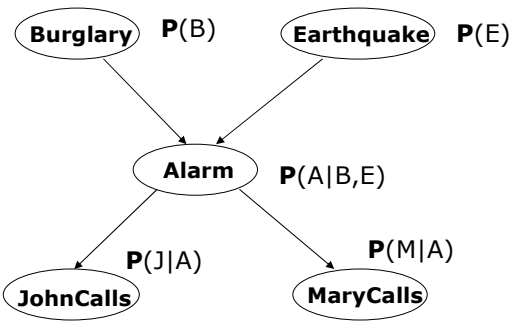
Causal relations



Bayesian belief network.

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

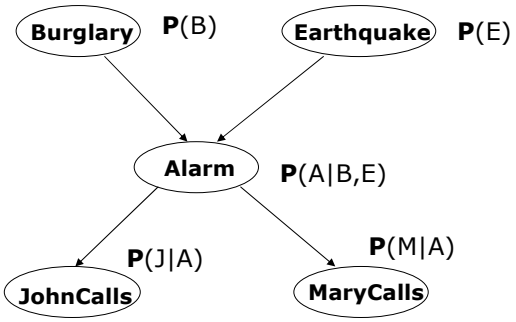
     The chance of Alarm being is influenced by Earthquake,
     The chance of John calling is affected by the Alarm



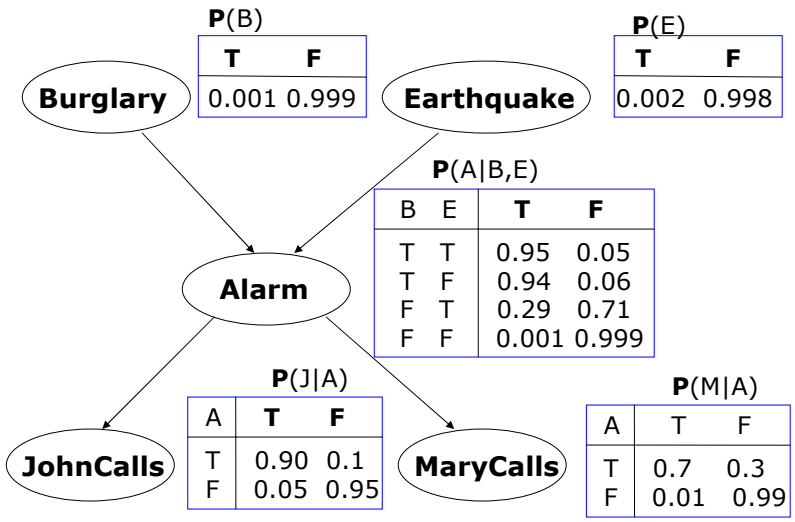
Bayesian belief network.

2. Local conditional distributions

- relate variables and their parents

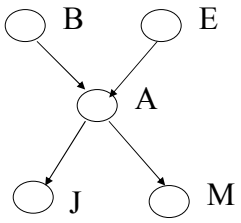


Bayesian belief network.



Bayesian belief networks (general)

Two components: $B = (S, \Theta_S)$



- **Directed acyclic graph**
  - Nodes correspond to random variables
  - (Missing) links encode independences
- **Parameters**
  - Local conditional probability distributions for every variable-parent configuration

$$\mathbf{P}(X_i \mid pa(X_i))$$

Where:

$pa(X_i)$ - stand for parents of X_i

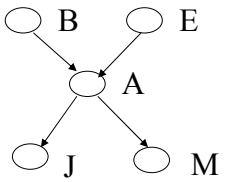
P(A|B,E)

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

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**

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

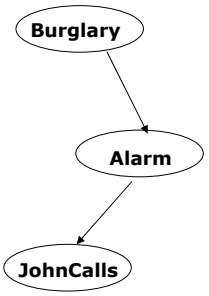
$$P(A, B \mid C) = P(A \mid C)P(B \mid C)$$

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

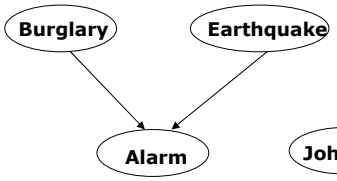
Independences in BBNs

3 basic independence structures:

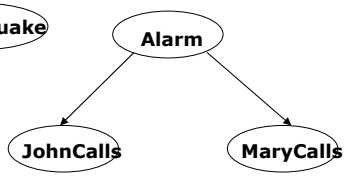
1.



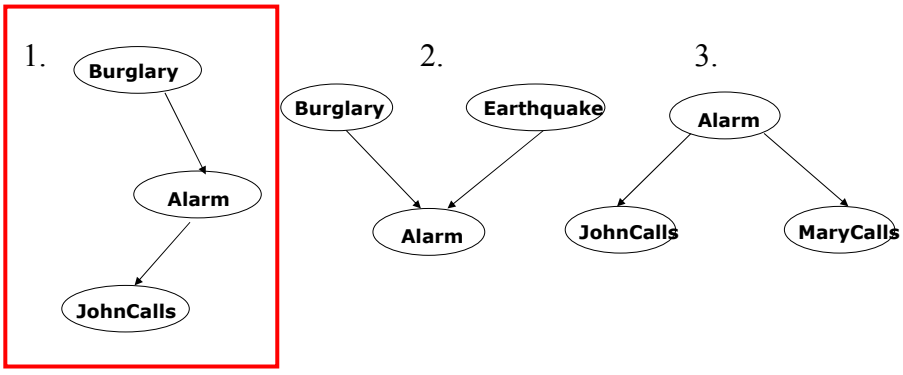
2.



3.



Independences in BBNs

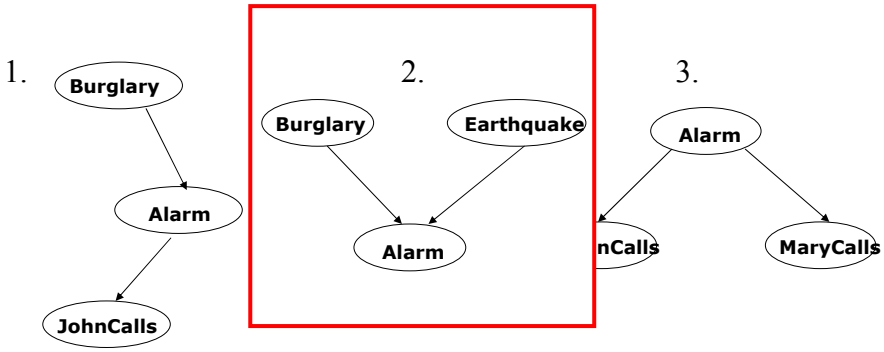


1. JohnCalls **is independent** of Burglary given Alarm

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

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

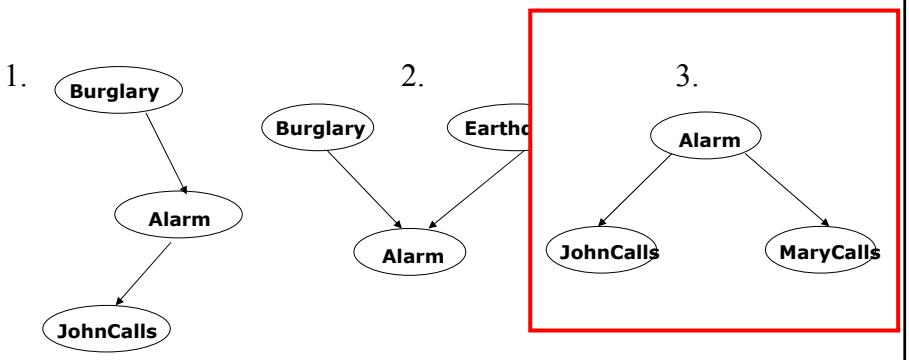
Independences in BBNs



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

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

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

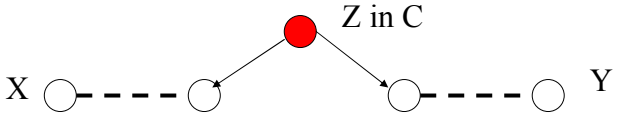
Independences in BBN

- 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**
- **Path blocking**
  - 3 cases that expand on three basic independence structures

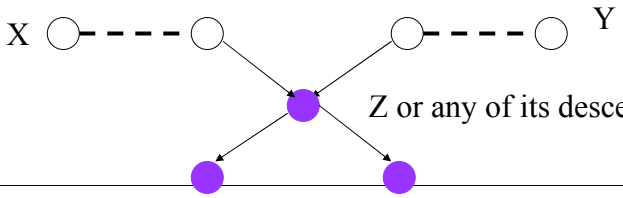
Undirected path blocking

- **1. With linear substructure**

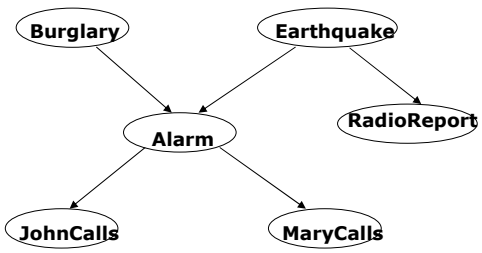
- **2. With wedge substructure**



- **3. With vee substructure**



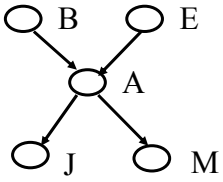
Independences in BBNs



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



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

Full joint distribution in BBNs

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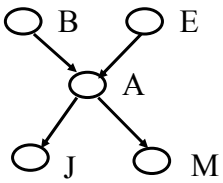

$$P(B=T,E=T,A=T,J=T,M=F)=$$

$$=P(J=T\,|\,B=T,E=T,A=T,M=F)P(B=T,E=T,A=T,M=F)$$
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Full joint distribution in BBNs

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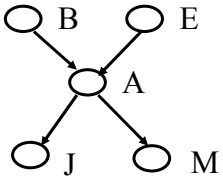

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$$P(M=F\mid B=T,E=T,A=T)P(B=T,E=T,A=T)$$
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Full joint distribution in BBNs

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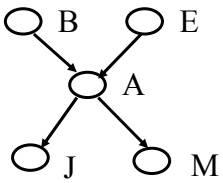

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Full joint distribution in BBNs

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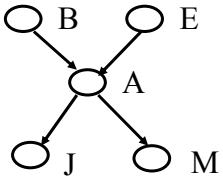

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$$P(B=T)P(E=T)$$

Full joint distribution in BBNs

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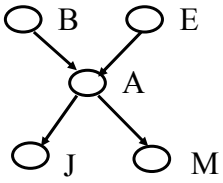

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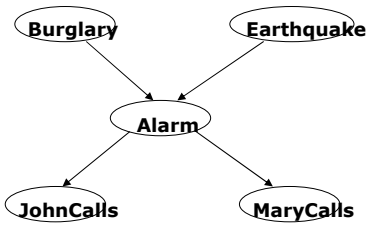
$$P(M=F\mid A=T)P(B=T,E=T,A=T)$$
$$P(A=T\mid B=T,E=T)P(B=T,E=T)$$
$$P(B=T)P(E=T)$$
$$=P(J=T\mid A=T)P(M=F\mid A=T)P(A=T\mid B=T,E=T)P(B=T)P(E=T)$$

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: $2^5 = 32$

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

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

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