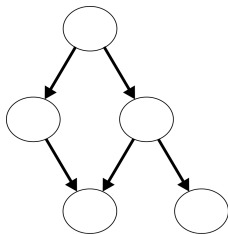


Probabilistic Graphical Models: Principles and Applications

Chapter 7: BAYESIAN NETWORKS: REPRESENTATION AND INFERENCE (Part II)

L. Enrique Sucar, INAOE



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- There are several classes of algorithms for probabilistic inference on multi connected BNs:
 - variable elimination,
 - conditioning,
 - junction tree.

Variable Elimination

- The variable elimination technique is based on the idea of calculating the probability by marginalizing the joint distribution
- It takes advantage of the independence conditions of the BN and the associative and distributive properties of addition and multiplication to do the calculations more efficiently:
 - 1 Represent the joint distribution as a product of local probabilities according to the network structure
 - 2 Summations can be carried out only on the subset of terms which are a function of the variables being normalized

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Variable Elimination

- Joint probability distribution of $\mathbf{X} = \{X_1, X_2, \dots, X_n\}$
- Posterior probability of a certain variable or subset of variables, X_H , given a subset of evidence variables, X_E ; the remaining variables are X_R , such that $\mathbf{X} = \{X_H \cup X_E \cup X_R\}$:

$$P(X_H | X_E) = P(X_H, X_E) / P(X_E) \quad (1)$$

- We can obtain both terms via marginalization of the joint distribution:

$$P(X_H, X_E) = \sum_{X_R} P(\mathbf{X}) \quad (2)$$

and

$$P(X_E) = \sum_{X_H} P(X_H, X_E) \quad (3)$$

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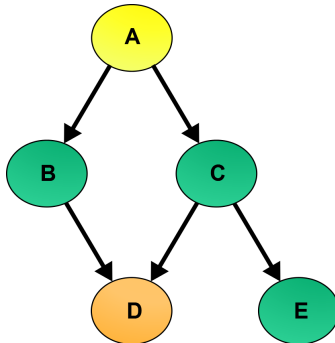
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VE - illustration



- Obtain $P(A | D)$ - we need to obtain $P(A, D)$ and $P(D)$.

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VE - calculations

- *Eliminate* B, C, E from the joint distribution, that is:

$$P(A, D) =$$

$$\sum_B \sum_C \sum_E P(A)P(B | A)P(C | A)P(D | B, C)P(E | C)$$

- By *distributing* the summations we can arrive to the following equivalent expression:

$$P(A, D) =$$

$$P(A) \sum_B P(B | A) \sum_C P(C | A)P(D | B, C) \sum_E P(E | C)$$

- If all variables are binary, this implies a reduction from 32 operations to 9 operations

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VE - example

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- Obtain $P(E | F = f_1) = P(E, F = f_1) / P(F = f_1)$
- Joint distribution:
$$P(C, E, F, D) = P(C)P(E | C)P(F | E)P(D | E)$$

VE - example

- First calculate $P(E, F)$; by reordering the operations:

$$P(E, F) = \sum_D P(F | E)P(D | E) \sum_C P(C)P(E | C)$$

- Calculation for each value of E , given $F = f_1$:

$$P(e_1, f_1) = \sum_D P(f_1 | e_1)P(D | e_1) \sum_C P(C)P(e_1 | C)$$

$$P(e_1, f_1) = \sum_D P(f_1 | e_1)P(D | e_1)[0.9 \times 0.8 + 0.7 \times 0.2]$$

$$P(e_1, f_1) = \sum_D P(f_1 | e_1)P(D | e_1)[0.86]$$

$$P(e_1, f_1) = [0.9 \times 0.7 + 0.9 \times 0.3][0.86]$$

$$P(e_1, f_1) = [0.9][0.86] = 0.774$$

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- In a similar way we obtain $P(e_2, f_1)$; and then from these values we can calculate $P(f_1) = \sum_E P(E, f_1)$

- Finally, we calculate the posterior probability of E given f_1 :

$$P(e_1 | f_1) = P(e_1, f_1) / P(f_1) \text{ and}$$

$$P(e_2 | f_1) = P(e_2, f_1) / P(f_1)$$

Analysis

- The critical aspect of the variable elimination algorithm is to select the appropriate order for eliminating each variable, as this has an important effect on the number of required operations
- The different terms that are generated during the calculations are known as *factors* which are functions over a subset of variables, in the previous example, one of the factors is $f(C, E) = P(C)P(E | C)$
- The computational complexity in terms of space and time of the variable elimination algorithm is determined by the size of the factors – is exponential on the number of variables in the factor.

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Elimination Order

- Finding the *best* order is in general a NP-Hard problem
- There are several heuristics that help to determine a *good* ordering for variable elimination:

Min-degree: eliminate the variable that leads to the smallest possible factor; which is equivalent to eliminating the variable with the smallest number of neighbors in the current elimination graph.

Min-fill: eliminate the variable that leads to adding the minimum number of edges to the interaction graph.

- These heuristics can be explained based on the *interaction graph*—an undirected graph that is built during the process of variable elimination

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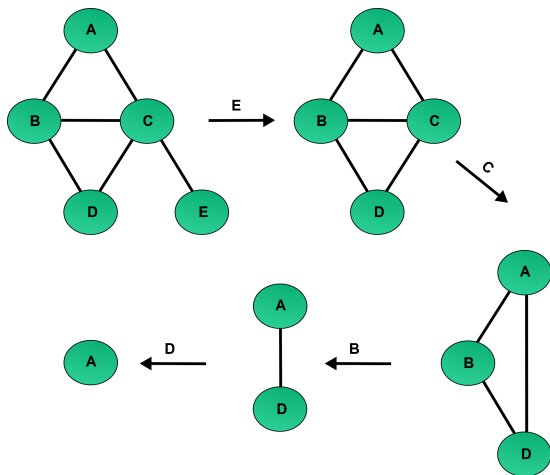
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Interaction graph



- When X_j is eliminated the interaction graph is modified:
 - (i) adding an arc between each pair of neighbors of X_j ,
 - (ii) deleting variable X_j from the graph

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- A disadvantage of variable elimination is that it only obtains the posterior probability of one variable
- To obtain the posterior probability of each non-instantiated variable in a BN, the calculations have to be repeated for each variable
- Next, we describe two algorithms that calculate the posterior probabilities for all variables at the same time

Conditioning

- The conditioning method is based on the fact that an instantiated variable *blocks* the propagation of the evidence in a Bayesian network
- It *cuts* the graph at the instantiated variables, and this can transform a multi connected graph into a polytree, for which we can apply the probability propagation algorithm
- If these variables are not actually known, we can set them to each of their possible values, and then do probability propagation for each value
- With each propagation we obtain a probability for each unknown variable – the final probability values are obtained as a weighted combination of these probabilities

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Formalization

- Formally, we want to obtain the probability of any variable, B , given the evidence E , conditioning on variable A . By the rule of total probability:

$$P(B | E) = \sum_i P(B | E, a_i)P(a_i | E) \quad (4)$$

- Where:

$P(B | E, a_i)$ is the posterior probability of B which is obtained by probability propagation for each possible value of A .

$P(a_i | E)$ is a *weight*.

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Formalization

- By applying the Bayes rule we obtain the following equation to estimate the weights:

$$P(a_i | E) = \alpha P(a_i) P(E | a_i) \quad (5)$$

- The first term, $P(a_i)$, can be obtained by propagating without evidence. The second term, $P(E | a_i)$, is calculated by propagation with $A = a_i$ to obtain the probability of the evidence variables. α is a normalizing constant

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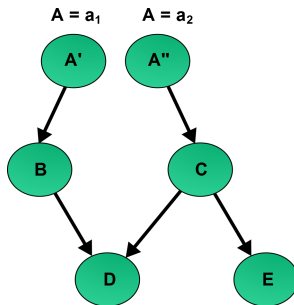
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Example



- If the evidence is D, E , then probabilities for the other variables, A, B, C can be obtained via conditioning

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Example

- 1 Obtain the prior probability of A (in this case it is already given as it is a root node).
- 2 Obtain the probability of the evidence nodes D, E for each value of A by propagation in the polytree.
- 3 Calculate the weights, $P(a_i | D, E)$, from (1) and (2) with the Bayes rule.
- 4 Estimate the probability of B and C for each value of A given the evidence by probability propagation in the polytree.
- 5 Obtain the posterior probabilities for B and C from (3) and (4) by applying equation 4.

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- In general, to transform a multi connected BN to a polytree we need to instantiate m variables
- Thus, propagation must be performed for all the combinations of values (cross product) of the instantiated variables
- If each variable has k values, then the number of propagations is k^m

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- The junction tree method is based on a transformation of the BN to a junction tree, where each node in this tree is a group or cluster of variables
- Probabilistic inference is performed over this new representation, via propagation over the junction tree
- The probability of a variable is obtained by marginalization over the corresponding “junction” (clique)

Transformation

- 1 Eliminate the directionality of the arcs.
- 2 Order the nodes in the graph (based on *maximum cardinality*).
- 3 Moralize the graph (add an arc between pairs of nodes with common children).
- 4 If necessary add additional arcs to make the graph *triangulated*.
- 5 Obtain the *cliques* of the graph (subsets of nodes that are fully connected and are not subsets of other fully connected sets).
- 6 Build a junction tree in which each node is a clique and its parent is any node that contains all common previous variables according to the ordering.

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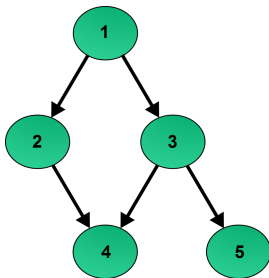
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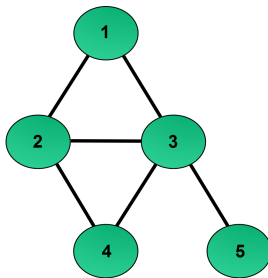
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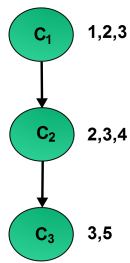
Transformation - example



(a)



(b)



(c)

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Inference

- Once the junction tree is built, inference is based on probability propagation over the junction tree
- Initially the joint probability (potential) of each macro node is obtained, and given some evidence, this is propagated to obtain the posterior probability of each junction
- The individual probability of each variable is obtained from the joint probability of the appropriate junction via marginalization

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Preprocessing

In the preprocessing phase the potentials of each clique are obtained following the next steps:

- 1 Determine the set of variables for each clique, C_i .
- 2 Determine the set of variables that are common with the previous (parent) clique, S_i .
- 3 Determine the variables that are in C_i but not in S_i :
 $R_i = C_i - S_i$.
- 4 Calculate the potential of each clique, clq_i , as the product of the corresponding CPTs:
 $\psi(clq_i) = \prod_j P(X_j | Pa(X_j))$; where X_j are the variables in clq_i .

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Preprocessing - example

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Cliques: $clq_1 = \{1, 2, 3\}$, $clq_2 = \{2, 3, 4\}$, $clq_3 = \{3, 5\}$.

Then the preprocessing phase is:

$$C: C_1 = \{1, 2, 3\}, C_2 = \{2, 3, 4\}, C_3 = \{3, 5\}.$$

$$S: S_1 = \emptyset, S_2 = \{2, 3\}, S_3 = \{3\}.$$

$$R: R_1 = \{1, 2, 3\}, R_2 = \{4\}, R_3 = \{5\}.$$

Potentials: $\psi(clq_1) = P(1)P(2 | 1)P(3 | 2),$

$$\psi(clq_2) = P(4 | 3, 2), \psi(clq_3) = P(5 | 3).$$

Propagation

- The propagation phase proceeds in a similar way to belief propagation for trees, by propagating λ messages bottom-up and π messages top-down
- **Bottom-Up Propagation**
 - 1 Calculate the λ message to send to the parent clique:
$$\lambda(C_i) = \sum_R \psi(C_j).$$
 - 2 Update the potential of each clique with the λ messages of its sons: $\psi(C_j)' = \lambda(C_i)\psi(C_j).$
 - 3 Repeat the previous two steps until reaching the root clique.
 - 4 When reaching the root node obtain $P'(C_r) = \psi(C_r)'$.

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Propagation

- **Top-Down Propagation**

- 1 Calculate the π message to send to each child node i :

$$\pi(C_i) = \sum_{C_j - S_i} P'(C_j).$$
- 2 Update the potential of each clique when receiving the π message of its parent: $P'(C_i) = \pi(C_i)\psi(C_i)'$.
- 3 Repeat the previous two steps until reaching the leaf nodes in the junction tree.

- When there is evidence, the potentials for each clique are updated based on the evidence, and the same propagation procedure is followed
- Finally, the marginal posterior probabilities of each variable are obtained from the clique potentials via marginalization: $P(X) = \sum_{C_i - X} P'(C_i)$

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Complexity analysis

- In the worst case, probabilistic inference for Bayesian networks is NP-Hard
- The time and space complexity is determined by what is known as the *tree-width* - a tree-structured BN (maximum one parent per variable) has a tree-width of one. A polytree with at most k parents per node has a tree-width of k
- In general, the tree-width is determined by how *dense* the topology of the network is, and this affects:
 - (i) the size of the largest factor in the variable elimination algorithm;
 - (ii) the number of variables that need to be instantiated in the conditioning algorithm,
 - (iii) the size of the largest clique in the junction tree algorithm

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Loopy Propagation

- This is simply the application of the probability propagation algorithm for multi connected networks
- Although in this case the conditions for this algorithm are not satisfied, and it only provides an approximate solution
- Given that the BN is not singly connected, as the messages are propagated, these can *loop* through the network

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Procedure

- 1 Initialize the λ and π values for all nodes to random values.
- 2 Repeat until convergence or a maximum number of iterations:
 - 1 Do probability propagation according to the algorithm for singly connected networks.
 - 2 Calculate the posterior probability for each variable.

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Convergence

- The algorithm converges when the difference between the posterior probabilities for all variables of the current and previous iterations is below a certain threshold
- It has been found empirically that for certain structures this algorithm converges to the true posterior probabilities; however, for other structures it does not converge
- An important application of loopy belief propagation is in “Turbo Codes”; which is a popular error detection and correction scheme used in data communications

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Stochastic simulation

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- Stochastic simulation algorithms consist in *simulating* the BN several times, where each simulation gives a sample value for all non-instantiated variables
- These values are chosen randomly according to the conditional probability of each variable
- This process is repeated N times, and the posterior probability of each variable is approximated in terms of the frequency of each value in the sample space

Logic Sampling

- Logic sampling is a basic stochastic simulation algorithm that generates samples according to the following procedure:
 - ① Generate sample values for the root nodes of the BN according to their prior probabilities. That is, a random value is generated for each root variable X , following a distribution according to $P(X)$.
 - ② Generate samples for the next *layer*, that is the sons of the already sampled nodes, according to their conditional probabilities, $P(Y | Pa(Y))$, where $Pa(Y)$ are the parents of Y .
 - ③ Repeat (2) until all the leaf nodes are reached.
- The previous procedure is repeated N times to generate N samples. The probability of each variable is estimated as the fraction of times (frequency) that a value occurs in the N samples, that is, $P(X = x_i) \sim No(x_i)/N$

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Example

10 samples generated by logic sampling (assuming all variables are binary):

variables	A	B	C	D	E
<i>sample₁</i>	T	F	F	F	T
<i>sample₂</i>	F	T	T	F	F
<i>sample₃</i>	T	F	F	T	F
<i>sample₄</i>	F	F	T	F	T
<i>sample₅</i>	T	F	T	T	F
<i>sample₆</i>	F	F	F	F	T
<i>sample₇</i>	F	T	T	T	F
<i>sample₈</i>	F	F	F	F	F
<i>sample₉</i>	F	F	F	T	F
<i>sample₁₀</i>	T	T	T	T	F

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Probabilities - no evidence

If there is no evidence, then given these samples, the marginal probabilities are estimated as follows:

- $P(A = T) = 4/10 = 0.4$
- $P(B = T) = 3/10 = 0.3$
- $P(C = T) = 5/10 = 0.5$
- $P(D = T) = 5/10 = 0.5$
- $P(E = T) = 3/10 = 0.3$

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Probabilities - with evidence

In the case where there is evidence with $D = T$, we eliminate all the samples where $D = F$, and estimate the posterior probabilities from the remaining 5 samples:

- $P(A = T \mid D = T) = 3/5 = 0.6$
- $P(B = T \mid D = T) = 2/5 = 0.4$
- $P(C = T \mid D = T) = 3/5 = 0.6$
- $P(E = T \mid D = T) = 1/5 = 0.2$

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Likelihood Weighting

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- A disadvantage of logic sampling when evidence exists is that many samples have to be discarded
- Likelihood weighting generates samples in the same way as logic sampling, however when there is evidence the non-consistent samples are not discarded
- Each sample is given a weight according to the weight of the evidence for this sample

Weighting

- Given a sample s and the evidence variables $\mathbf{E} = \{E_1, \dots, E_m\}$, the weight of sample s is estimated as:

$$W(\mathbf{E} | s) = P(E_1)P(E_2)\dots P(E_m) \quad (6)$$

where $P(E_i)$ is the probability of the evidence variable E_i for that sample

- The posterior probability for each variable X taking value x_i is estimated by dividing the sum of the weights $W_i(X = x_i)$ for each sample where $X = x_i$ by the total weight for all the samples:

$$P(X = x_i) \sim \sum_i W_i(X = x_i) / \sum_i W_i \quad (7)$$

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MPE

- The *most probable explanation* (MPE) or *abduction* problem consists in determining the most probable values for a subset of variables (explanation subset) in a BN given some evidence
- Two variants: *total abduction* and *partial abduction*
- In the total abduction problem, the explanation subset is the set of all non-instantiated variables
- In partial abduction, the explanation subset is a proper subset of the non-instantiated variables

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- Consider the set of variables $\mathbf{X} = \{X_E, X_R, X_H\}$, where X_E is the subset of instantiated variables; then we can formalize the MPE problems as follows:

Total abduction: $ArgMax_{X_H, X_R} P(X_H, X_R | X_E)$.

Partial abduction: $ArgMax_{X_H} P(X_H | X_E)$.

Solution

- One way to solve the MPE problem is based on a modified version of the variable elimination algorithm
- Total abduction, we substitute the summations by maximizations:

$$\max_{X_H, X_R} P(X_H, X_R \mid X_E)$$

- Partial abduction, we sum over the variables that are not in the explanation subset and maximize over the explanation subset:

$$\max_{X_H} \sum_{X_R} P(X_H, X_R \mid X_E)$$

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- When dealing with continuous variables, one option is to discretize them; however, this could result in a loss of information or in an unnecessary increase in computational requirements
- Another alternative is to operate directly on the continuous distributions
- Probabilistic inference techniques have been developed for some distribution families, in particular for Gaussian variables

Gaussian variables

The basic algorithm makes the following assumptions:

- 1 The structure of the network is a polytree.
- 2 All the sources of uncertainty are Gaussians and uncorrelated.
- 3 There is a linear relationship between each variable and its parents:

$$X = b_1 U_1 + b_2 U_2 + \dots + b_n U_n + W_X$$

Where U_j are parents of variable X , b_i are constant coefficients and W_X represents Gaussian noise with a zero mean.

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Inference

- The inference procedure is analogous to belief propagation in discrete BNs, but instead of propagating probabilities, it propagates means and standard deviations
- The posterior probability of a variable can be written as:

$$P(X | E) = N(\mu_X, \sigma_X)$$

Where μ_X and σ_X are the mean and standard deviation of X given the evidence E , respectively.

- We calculate the mean and standard deviation for each variable via a propagation algorithm

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Propagation

- Each variable sends to its parent variable i :

$$\mu_i^- = (1/b_i)[\mu_\lambda - \sum_{k \neq i} b_k \mu_k^+] \quad (8)$$

$$\sigma_i^- = (1/b_i^2)[\sigma_\lambda - \sum_{k \neq i} b_k^2 \sigma_k^+] \quad (9)$$

- Each variable sends to its child node j :

$$\mu_j^+ = \frac{\sum_{k \neq j} \mu_k^- / \sigma_k + \mu_\pi / \sigma_\pi}{\sum_{k \neq j} 1 / \sigma_k + \mu_\pi / \sigma_\pi} \quad (10)$$

$$\sigma_j^+ = \left[\sum_{k \neq j} 1 / \sigma_k^- + 1 / \sigma_\pi \right]^{-1} \quad (11)$$

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Propagation

- Each variable integrates the messages it receives from its sons and parents via the following equations:

$$\mu_{\pi} = \sum_i b_i \mu_i^+ \quad (12)$$

$$\sigma_{\pi} = \sum_i b_i^2 \sigma_i^+ \quad (13)$$

$$\mu_{\lambda} = \sigma_{\lambda} \sum_j \mu_j^- / \sigma_j^- \quad (14)$$

$$\sigma_{\lambda} = \left[\sum_j 1 / \sigma_j^- \right]^{-1} \quad (15)$$

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- Finally, each variable obtains its mean and standard deviation by combining the information from its parent and children nodes:

$$\mu_X = \frac{\sigma_\pi \mu_\lambda + \sigma_\lambda \mu_\pi}{\sigma_\pi + \sigma_\lambda} \quad (16)$$

$$\sigma_X = \frac{\sigma_\pi \sigma_\lambda}{\sigma_\pi + \sigma_\lambda} \quad (17)$$

- Propagation for other distributions is more difficult, as they do not have the same properties of the Gaussian; in particular, the product of Gaussians is also a Gaussian

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- Many systems use information to make decisions; if this information is erroneous it could lead to non-optimal decisions
- In many applications there are different sources of information, i.e. sensors, which are not independent; the information from one source gives us clues about the other sources
- If we can represent these dependencies between the different sources, then we can use it to detect possible errors and avoid erroneous decisions

Algorithm

- The algorithm starts by building a model of the dependencies between sources of information (variables) represented as a Bayesian network
- The validation is done in two phases. In the first phase, potential faults are detected by comparing the actual value with the one predicted from the related variables
- In the second phase, the real faults are isolated by constructing an additional Bayesian network based on the Markov blanket property

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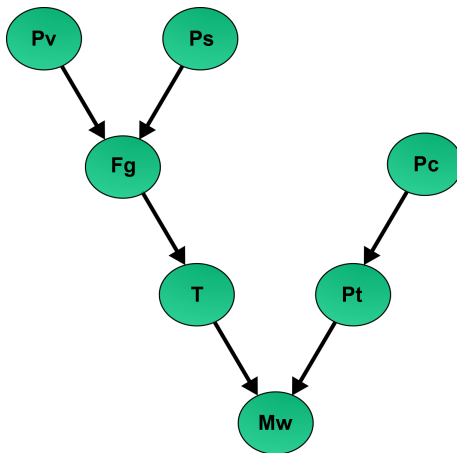
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Fault detection

- Build a probabilistic model relating all the variables in the application domain
- Example - gas turbine:



Fault detection

- Suppose it is required to validate the temperature measurements in the turbine
- By reading the values of the rest of the sensors, and applying probability propagation, it is possible to calculate a posterior probability distribution of the temperature given all the evidence, i.e.,
$$P(T \mid Mw, P, Fg, Pc, Pv, Ps)$$
- If the real observed value coincides with a *valid* value – that has a *high* probability, then the sensor is considered correct; otherwise it is considered faulty

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Fault detection

- If a validation of a single sensor is made using a faulty sensor, then a faulty validation can be expected
- In the example above, what happens if T is validated using a faulty Mw sensor?
- By applying this validation procedure, we may only detect a faulty condition, but we are not able to identify which is the real faulty sensor – *apparent fault*
- An isolation stage is needed
- S is the set of variables with apparent faults detected in the first phase

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Fault isolation

- The isolation phase is based on the *Markov Blanket* (MB) property
- The *Extended Markov Blanket* of a node X ($EMB(X)$) as the set of sensors formed by the sensor itself plus its MB
- For example, $EMB(Fg) = \{Fg, Pv, Ps, T\}$
- Utilizing this property, if a fault exists in one of the sensors, it will be revealed in all of the sensors in its EMB. On the contrary, if a fault exists outside a sensors' EMB, it will not affect the estimation of that sensor
- The EMB is used to create a *fault isolation* module that distinguishes the *real faults* from the apparent faults

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Fault isolation theory

- 1 If $S = \phi$ there are no faults.
- 2 If S is equal to the EMB of a sensor X , and there is no other EMB which is a subset of S , then there is a *single real fault* in X .
- 3 If S is equal to the EMB of a sensor X , and there are one or more EMBs which are subsets of S , then there is a real fault in X , and possibly, real faults in the sensors whose EMBs are subsets of S . In this case, there are possibly *multiple indistinguishable* real faults.
- 4 If S is equal to the union of several EMBs and the combination is unique, then there are *multiple distinguishable* real faults in all the sensors whose EMB are in S .
- 5 If none of the above cases is satisfied, then there are multiple faults but they can not be distinguished

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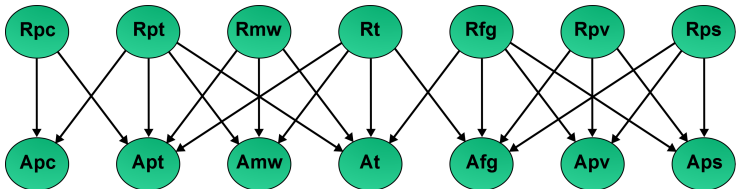
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Isolation network

- The isolation network is formed by two levels:
 - The root nodes represent the real faults, where there is one per sensor or variable
 - The lower level is formed by one node representing the apparent fault for each variable. Notice that the arcs are defined by the EMB of each variable



Reliability analysis

- In the reliability analysis of a complex system, a common approach is to divide the system into smaller elements, units, subsystems, or components
- This subdivision generates a “block diagram” that is similar to the description of the system in operation
- For each element, the *failure rate* is specified, and based on these, the reliability of the complete system is obtained
- Traditional techniques assume that faults are independent

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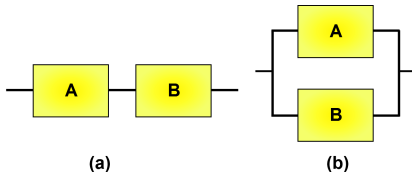
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Reliability modeling with BN

- In a block diagram representation there are two basic structures: serial and parallel components
- A serial structure implies that the two components should operate correctly for the system to function
- In parallel structures, it is sufficient for one of the components to operate for the system to function



(a)

(b)

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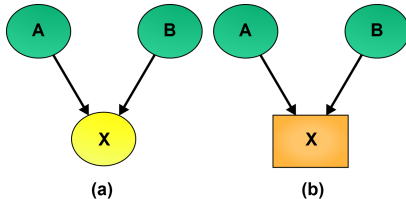
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Basic structures

- The basic series and parallel block diagrams can be represented with a Bayesian network
- The structure is the same in both cases, the difference is the conditional probability matrix



CPTs

- Series (AND):

X	A, B	$A, \neg B$	$\neg A, B$	$\neg A, \neg B$
Success	1	0	0	0
Failure	0	1	1	1

- Parallel (OR):

X	A, B	$A, \neg B$	$\neg A, B$	$\neg A, \neg B$
Success	1	1	1	0
Failure	0	0	0	1

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Extending the basic models

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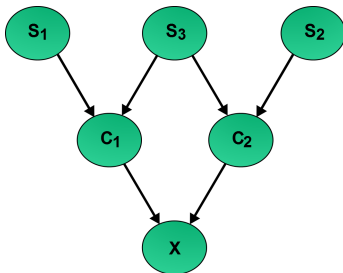
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- The BN representation of the basic serial/parallel cases can be directly generalized to represent any block diagram that can be reduced to a set of serial and parallel combinations of components
- There are some structures that can not be decomposed to a serial/parallel combination, such as a *bridge*. However, it is also possible to model these cases using BNs

Example

- Suppose that a system has two components that are affected by three possible failure sources. Source S_1 affects component C_1 , source S_2 affects component C_2 , and source S_3 affects both components (common cause)
- In the BN, the CPT for all three non root nodes (C_1 , C_2 , X) is equivalent to that of a serial component combination



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Additional Reading - Books on BNs

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