INTRODUCTION TO INFERENCE FOR BAYESIAN NETWORKS

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1. Introduction

The field of Bayesian networks, and graphical models in general, has grown enormously over the last few years, with theoretical and computational developments in many areas. As a consequence there is now a fairly large set of theoretical concepts and results for newcomers to the field to learn. This tutorial aims to give an overview of some of these topics, which hopefully will provide such newcomers a conceptual framework for following the more detailed and advanced work. It begins with revision of some of the basic axioms of probability theory.

2. Basic axioms of probability

Probability theory, also known as inductive logic, is a system of reasoning under uncertainty, that is under the absence of certainty. Within the Bayesian framework, probability is interpreted as a numerical measure of the degree of consistent belief in a proposition, consistency being with the data at hand.

Early expert systems used deductive, or Boolean, logic, encapsulated by sets of production rules. Attempts were made to cope with uncertainty using probability theory, but the calculations became prohibitive, and the use of probability theory for inference in expert systems was abandoned. It is with the recent development of efficient computational algorithms that probability theory has had a revival within the AI community.

Let us begin with some basic axioms of probability theory. The probability of an event A, denoted by $P(A)$, is a number in the interval [0,1], which obeys the following axioms:

1 $P(A) = 1$ if and only if A is certain.

2 If A and B are mutually exclusive, then $P(A \text{ or } B) = P(A) + P(B)$.

We will be dealing exclusively with discrete random variables and their probability distributions. Capital letters will denote a variable, or perhaps a set of variables, lower case letter will denote values of variables. Thus suppose A is a random variable having a finite number of *mutually exclusive states* $(a_1, \ldots, a_n)$. Then $P(A)$ will be represented by a vector of non-negative real numbers $P(A) = (x_1, \ldots, x_n)$ where $P(A = a_i) = x_i$ is a scalar, and $\sum_i x_i = 1$.

A basic concept is that of conditional probability, a statement of which takes the form: *Given the event $B = b$ the probability of the event $A = a$ is x, written $P(A = a \mid B = b) = x$.* It is important to understand that this is not saying: "If $B = b$ is true then the probability of $A = a$ is x". Instead it says: "If $B = b$ is true, and any other information to hand is irrelevant to A, then $P(A = a) = x$". (To see this, consider what the probabilities would be if the state of A was part of the extra information).

Conditional probabilities are important for building Bayesian networks, as we shall see. But Bayesian networks are also built to facilitate the calculation of conditional probabilities, namely the conditional probabilities for variables of interest given the data (also called evidence) at hand.

The fundamental rule for probability calculus is the product rule[1]

$$P(A \text{ and } B) = P(A \mid B)P(B). \tag{1}$$

This equation tells us how to combine conditional probabilities for individual variables to define joint probabilities for sets of variables.

3. Bayes' theorem

The simplest form of Bayes' theorem relates the joint probability $P(A \text{ and } B)$ – written as $P(A, B)$ – of two events or hypotheses A and B in terms of marginal and conditional probabilities:

$$P(A, B) = P(A \mid B)P(B) = P(B \mid A)P(A). \tag{2}$$

By rearrangement we easily obtain

$$P(A \mid B) = \frac{P(B \mid A)P(A)}{P(B)}, \tag{3}$$

which is Bayes' theorem.

This can be interpreted as follows. We are interested in A, and we begin with a *prior* probability $P(A)$ for our belief about A, and then we observe

[1]Or more generally $P(A \text{ and } B \mid C) \equiv P(A \mid B, C)P(B \mid C)$.

B. Then Bayes' theorem, (3), tells us that our revised belief for A, the *posterior* probability $P(A \mid B)$ is obtained by multiplying the prior $P(A)$ by the ratio $P(B \mid A)/P(B)$. The quantity $P(B \mid A)$, as a function of varying A for fixed B, is called the *likelihood* of A. We can express this relationship in the form:

$$\begin{aligned} \textbf{posterior} &\propto \textbf{prior} \times \textbf{likelihood} \\ P(A \mid B) &\propto P(A)P(B \mid A). \end{aligned}$$

Figure 1 illustrates this prior-to-posterior inference process. Each diagram

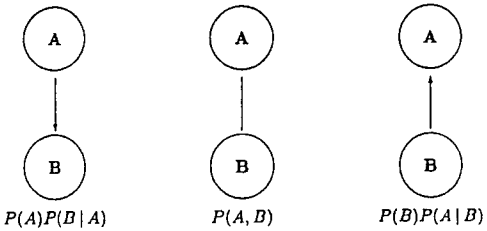


Figure 1. Bayesian inference as reversing the arrows

represents in different ways the joint distribution $P(A, B)$, the first represents the prior beliefs while the third represents the posterior beliefs. Often, we will think of A as a possible "cause" of the "effect" B, the downward arrow represents such a causal interpretation. The "inferential" upwards arrow then represents an "argument against the causal flow", from the observed effect to the inferred cause. (We will not go into a definition of "causality" here.)

Bayesian networks are generally more complicated than the ones in Figure 1, but the general principles are the same in the following sense. A Bayesian network provides a model representation for the joint distribution of a set of variables in terms of conditional and prior probabilities, in which the orientations of the arrows represent influence, usually though not always of a causal nature, such that these conditional probabilities for these particular orientations are relatively straightforward to specify (from data or eliciting from an expert). When data are observed, then typically an inference procedure is required. This involves calculating marginal probabilities conditional on the observed data using Bayes' theorem, which is diagrammatically equivalent to reversing one or more of the Bayesian network arrows. The algorithms which have been developed in recent years

allows these calculations to be performed in an efficient and straightforward manner.

4. Simple inference problems

Let us now consider some simple examples of inference. The first is simply Bayes' theorem with evidence included on a simple two node network; the remaining examples treat a simple three node problem.

4.1. PROBLEM I

Suppose we have the simple model $X \rightarrow Y$, and are given: $P(X)$, $P(Y \mid X)$ and $Y = y$. The problem is to calculate $P(X \mid Y = y)$.

Now from $P(X)$, $P(Y \mid X)$ we can calculate the marginal distribution $P(Y)$ and hence $P(Y = y)$. Applying Bayes' theorem we obtain

$$P(X \mid Y = y) = \frac{P(Y = y \mid X)P(X)}{P(Y = y)}. \tag{4}$$

4.2. PROBLEM II

Suppose now we have a more complicated model in which X is a parent of both Y and Z: $Z \leftarrow X \rightarrow Y$ with specified probabilities $P(X)$, $P(Y \mid X)$ and $P(Z \mid X)$, and we observe $Y = y$. The problem is to calculate $P(Z \mid Y = y)$. Note that the joint distribution is given by $P(X, Y, Z) = P(Y \mid X)P(Z \mid X)P(X)$. A 'brute force' method is to calculate:

1. The joint distribution $P(X, Y, Z)$.
2. The marginal distribution $P(Y)$ and thence $P(Y = y)$.
3. The marginal distribution $P(Z, Y)$ and thence $P(Z, Y = y)$.
4. $P(Z \mid Y = y) = P(Z, Y = y)/P(Y = y)$.

An alternative method is to exploit the given factorization:

1. Calculate $P(X \mid Y = y) = P(Y = y \mid X)P(X)/P(Y = y)$ using Bayes' theorem, where $P(Y = y) = \sum_X P(Y = y \mid X)P(X)$.
2. Find $P(Z \mid Y = y) = \sum_X P(Z \mid X)P(X \mid Y = y)$.

Note that the first step essentially reverses the arrow between X and Y. Although the two methods give the same answer, the second is generally more efficient. For example, suppose that all three variables have 10 states. Then the first method in explicitly calculating $P(X, Y, Z)$ requires a table of 1000 states. In contrast the largest table required for the second method has size 100. This gain in computational efficiency by exploiting the given factorizations is the basis of the arc-reversal method for solving influence

diagrams, and of the junction-tree propagation algorithms. The following example shows the same calculation using propagation on a junction tree.

4.3. PROBLEM III

Suppose now that we are given the *undirected* structure $ZX - X - XY$, and probabilities $P(Z, X)$, $P(X)$ and $P(Y, X)$. Again the problem is to calculate $P(Z \mid Y = y)$. Note that:

$$\begin{aligned} P(Z, X) &= P(Z \mid X)P(X) \\ P(Y, X) &= P(Y \mid X)P(X) \\ P(X, Y, Z) &= P(Z, X)P(Y, X)/P(X). \end{aligned}$$

The calculational steps now proceeds using a 'message' in step 1 which is 'sent' in step 2:

1. Calculate $\bar{P}(X) \equiv \sum_Y P(X, Y = y)$.
2. Find $\bar{P}(Z, X) \equiv P(Z, X)\bar{P}(X)/P(X)$.
3. Find $P(Z, Y = y) = \sum_X \bar{P}(Z, X)$.
4. Find $P(Z \mid Y = y) = P(Z, Y = y)/\sum_Z P(Z, Y = y)$

5. Conditional independence

In the last example we had that

$$P(X, Y, Z) = P(Y \mid X)P(Z \mid X)P(X),$$

from which we get

$$\begin{aligned} P(Y \mid Z, X) &= \frac{P(X, Y, Z)}{P(Z, X)} \\ &= \frac{P(Y \mid X)P(Z \mid X)P(X)}{P(Z, X)} \\ &= P(Y \mid X) \end{aligned}$$

and likewise for $P(Z \mid Y, X) = P(Z \mid X)$. Hence given $X = x$ say, we obtain $P(Y \mid Z, X = x) = P(Y \mid X = x)$ and $P(Z \mid Y, X = x) = P(Z \mid X = x)$. This is an example of conditional independence (Dawid(1979)). We associated the graph $Z \leftarrow X \rightarrow Y$ with this distribution, though this is not unique. In fact the joint probability can be factorized according to three distinct directed graphs:

$Z \leftarrow X \rightarrow Y : P(X, Y, Z) = P(X)P(Y \mid X)P(Z \mid X)$.
$Z \rightarrow X \rightarrow Y : P(X, Y, Z) = P(Y \mid X)P(X \mid Z)P(Z)$.
$Z \leftarrow X \leftarrow Y : P(X, Y, Z) = P(X \mid Y)P(Z \mid X)P(Y)$.

Each of these factorizations follows from the conditional independence properties which each graph expresses, viz $Z \perp\!\!\!\perp Y \mid X$, (which is to be read as "Z is conditionally independent of Y given X") and by using the general factorization property:

$$\begin{aligned} P(X_1, \ldots X_n) &= P(X_1 \mid X_2, \ldots, X_n) P(X_2, \ldots, X_n) \\ &= P(X_1 \mid X_2, \ldots, X_n) P(X_2 \mid X_3, \ldots, X_n) P(X_3, \ldots, X_n) \\ &= \vdots \\ &= P(X_1 \mid X_2, \ldots, X_n) \ldots P(X_{n-1} \mid X_n) P(X_n). \end{aligned}$$

Thus for the third example

$$P(X,Y,Z) = P(Z \mid X,Y) P(X \mid Y) P(Y) = P(Z \mid X) P(X \mid Y) P(Y).$$

Note that the graph $Z \rightarrow X \leftarrow Y$ does not obey the conditional independence property $Z \perp\!\!\!\perp Y \mid X$ and is thus excluded from the list; it factorizes as $P(X,Y,Z) = P(X \mid Y,Z) P(Z) P(Y)$.

This example shows several features of general Bayesian networks. Firstly, the use of the conditional independence properties can be used to simplify the general factorization formula for the joint probability. Secondly, that the result is a factorization that can be expressed by the use of directed acyclic graphs (DAGs).

6. General specification in DAGs

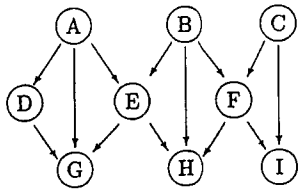
It is these features which work together nicely for the general specification of Bayesian networks. Thus a Bayesian network is a directed acyclic graph, whose structure defines a set of conditional independence properties. These properties can be found using graphical manipulations, eg *d-separation* (see eg Pearl(1988)). To each node is associated a conditional probability distribution, conditioning being on the parents of the node: $P(X \mid \mathrm{pa}(X))$. The joint density over the set of all variables U is then given by the product of such terms over all nodes:

$$P(U) = \prod_X P(X \mid \mathrm{pa}(X)).$$

This is called a *recursive factorization* according to the DAG; we also talk of the distribution being graphical over the DAG. This factorization is equivalent to the general factorization but takes into account the conditional independence properties of the DAG in simplifying individual terms in the product of the general factorization. Only if the DAG is complete will this formula and the general factorization coincide, (but even then only for one ordering of the random variables in the factorization).

6.1. EXAMPLE

Consider the graph of Figure 2.



$$\begin{aligned} &P(A,B,C,D,E,F,G,H,I) \\ &= P(A)P(B)P(C) \\ &\quad P(D \mid A)P(E \mid A,B)P(F \mid B,C) \\ &\quad P(G \mid A,D,E)P(H \mid B,E,F)P(I \mid C,F). \end{aligned}$$

Figure 2. Nine node example.

It is useful to note that marginalising over a childless node is equivalent to simply removing it and any edges to it from its parents. Thus for example, marginalising over the variable H in the above gives:

$$\begin{aligned} P(A,B,C,D,E,F,G,I) &= \sum_H P(A,B,C,D,E,F,G,H,I) \\ &= \sum_H P(A)P(B)P(C)P(D \mid A)P(E \mid A,B)P(F \mid B,C) \\ &\qquad P(G \mid A,D,E)P(H \mid B,E,F)P(I \mid C,F) \\ &= P(A)P(B)P(C)P(D \mid A)P(E \mid A,B)P(F \mid B,C) \\ &\qquad P(G \mid A,D,E)P(I \mid C,F) \sum_H P(H \mid B,E,F) \\ &= P(A)P(B)P(C)P(D \mid A)P(E \mid A,B)P(F \mid B,C) \\ &\qquad P(G \mid A,D,E)P(I \mid C,F), \end{aligned}$$

which can be represented by Figure 2 with H and its incident edges removed.

Directed acyclic graphs can always have their nodes linearly ordered so that for each node X all of its parents $\mathrm{pa}(X)$ precedes it in the ordering. Such and ordering is called a *topological ordering* of the nodes. Thus for example (A,B,C,D,E,F,G,H,I) and (B,A,E,D,G,C,F,I,H) are two of the many topological orderings of the nodes of Figure 2.

A simple algorithm to find a topological ordering is as follows: Start with the graph and an empty list. Then successively delete from the graph any node which does not have any parents, and add it to the end of the list. Note that if the graph is not acyclic, then at some stage a graph will be obtained in which no node has no parent nodes, hence this algorithm can be used as an efficient way of checking that the graph is acyclic.

Another equivalent way is to start with the graph and an empty list, and successively delete nodes which have no children and add them to the beginning of the list (cf. marginalisation of childless nodes.)

6.2. DIRECTED MARKOV PROPERTY

An important property is the *directed Markov property*. This is a conditional independence property which states that a variable is conditionally independent of its non-descendents given it parents:

$$X \perp\!\!\!\perp \mathrm{nd}(X) \,|\, \mathrm{pa}(X).$$

Now recall that the conditional probability $P(X \,|\, \mathrm{pa}(X))$ did not necessarily mean that if $\mathrm{pa}(X) = \pi^*$ say, then $P(X = x) = P(x \,|\, \pi^*)$, but included the caveat that any other information is irrelevant to X for this to hold. For the DAGs this 'other information' means, from the directed Markov property, knowledge about the node itself or any of its descendents. For if all of the parents of X are observed, but additionally observed are one or more descendents D_X of X, then because X influences D_X, knowing D_X and $\mathrm{pa}(X)$ is more informative than simply knowing about $\mathrm{pa}(X)$ alone. However having information about a non-descendent does not tell us anything more about X, because either it cannot influence or be influenced by X either directly or indirectly, or if it can influence X indirectly, then only through influencing the parents which are all known anyway.

For example, consider again Figure 2. Using the previous second topological ordering we may write the general factorization as:

$$\begin{aligned} P(A,B,C,D,E,F,G,I,H) = & P(B) \\ & * P(A \,|\, B) \\ & * P(E \,|\, B, A) \\ & * P(D \,|\, B, A, E) \\ & * P(G \,|\, B, A, E, D) \\ & * P(C \,|\, B, A, E, D, G) \\ & * P(F \,|\, B, A, E, D, G, C) \\ & * P(I \,|\, B, A, E, D, G, C, F) \\ & * P(H \,|\, B, A, E, D, G, C, F, I) \end{aligned} \tag{5}$$

but now we can use $A \perp\!\!\!\perp B$ from the directed Markov property to simplify $P(A \,|\, B) \rightarrow P(A)$, and similarly for the other factors in (5) etc, to obtain the factorization in Figure 2. We can write the general pseudo-algorithm of what we have just done for this example as

Topological ordering +
General factorization +
Directed Markov property
$\Longrightarrow$ Recursive factorization.

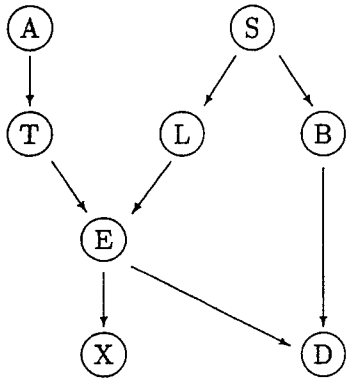
7. Making the inference engine

We shall now move on to building the so called "inference engine" to introduce new concepts and to show how they relate to the conditional independence/recursive factorization ideas that have already been touched upon. Detailed justification of the results will be omitted, the aim here is to give an overview, using the use the fictional ASIA example of Lauritzen and Spiegelhalter.

7.1. ASIA: SPECIFICATION

Lauritzen and Spiegelhalter describe their fictional problem domain as follows:

> Shortness-of-breath (Dyspnoea) may be due to Tuberculosis, Lung cancer or Bronchitis, or none of them, or more than one of them. A recent visit to Asia increases the chances of Tuberculosis, while Smoking is known to be a risk factor for both Lung cancer and Bronchitis. The results of a single X-ray do not discriminate between Lung cancer and Tuberculosis, as neither does the presence or absence of Dyspnoea.



$$\begin{aligned} P(U) = & P(A)P(S) \\ & P(T \,|\, A)P(L \,|\, S) \\ & P(B \,|\, S)P(E \,|\, L, T) \\ & P(D \,|\, B, E)P(X \,|\, E) \end{aligned}$$

Figure 3. ASIA

The network for this fictional example is shown in Figure 3. Each variable is a binary with the states ("yes", "no"). The **E** node is a logical node taking value "yes" if either of its parents take a "yes" value, and "no" otherwise; its introduction facilitates modelling the relationship of X-ray to Lung cancer and Tuberculosis.

Having specified the relevant variables, and defined their dependence with the graph, we must now assign (conditional) probabilities to the nodes. In real life examples such probabilities may be elicited either from some large database (if one is available) as frequency ratios, or subjectively from the expert from whom the structure has been elicited (eg using a fictitious gambling scenario or probability wheel), or a combination of both. However as this is a fictional example we can follow the third route and use made-up values. (Specific values will be omitted here.)

7.2. CONSTRUCTING THE INFERENCE ENGINE

With our specified graphical model we have a representation of the joint density in terms of a factorization:

$$P(U) = \prod_V P(V \mid \mathrm{pa}(V)) \tag{6}$$

$$= P(A) \ldots P(X \mid E). \tag{7}$$

Recall that our motivation is to use the model specified by the joint distribution to calculate marginal distributions conditional on some observation of one or more variables. In general the full distribution will be computationally difficult to use directly to calculate these marginals directly. We will now proceed to outline the various stages that are performed to find a representation of $P(U)$ which makes the calculations more tractable. (The process of constructing the inference engine from the model specification is sometimes called *compiling* the model.)

The manipulations required are almost all graphical. There are five stages in the graphical manipulations. Let us first list them, and then go back and define new terms which are introduced.

1. Add undirected edges to all co-parents which are not currently joined (a process called *marrying parents*).
2. Drop all directions in the graph obtained from Stage 1. The result is the so-called *moral graph.*
3. *Triangulate the moral graph*, that is, add sufficient additional undirected links between nodes such that there are no cycles (ie. closed paths) of length 4 or more distinct nodes without a short-cut.
4. Identify the *cliques* of this triangulated graph.
5. Join the cliques together to form the *junction tree.*

Now let us go through these steps, supplying some justification and defining the new terms just introduced as we go along. Consider first the joint density again. By a change of notation this can be written in the form

$$P(U) = \prod_V a(V, \mathrm{pa}(V)) \tag{8}$$

$$= a(A) \ldots a(X, E). \tag{9}$$

where $a(X, \mathrm{pa}(X)) \equiv P(V \mid \mathrm{pa}(V))$. That is, the conditional probability factors for V can be considered as a function of V and its parents. We call such functions *potentials.* Now after steps 1 and 2 we have an undirected graph, in which for each node both it and its set of parents in the original graph form a complete subgraph in the moral graph. (A complete graph is one in which every pair of nodes is joined together by an edge.) Hence, the original factorization of $P(U)$ on the DAG G goes over to an equivalent factorization on these complete subsets in the moral graph G^m. Technically we say that the distribution is graphical on the undirected graph G^m. Figure 4 illustrates the moralisation process for the Asia network. Now let us de-

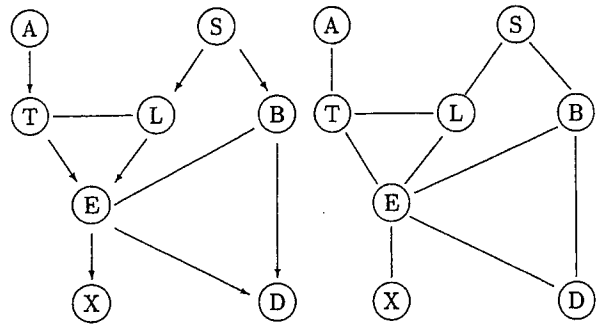


Figure 4. Moralising Asia: Two extra links are required, $A - S$ and $L - B$. Directionality is dropped after all moral edges have been added.

note the set of cliques of the moral graph by C^m. (A clique is a complete subgraph which is not itself a proper subgraph of a complete subgraph, so it is a maximal complete subgraph.) Then each of the complete subgraphs formed from $\{V\} \cup \mathrm{pa}(V)$ is contained within at least one clique. Hence we can form functions a_C such that

$$P(U) = \prod_{c \in C^m} a_C(V_C)$$

where $a_C(V_C)$ is a function of the variables in the clique C. Such a factorization can be constructed as follows: Initially define each factor as unity, i.e.,

$a_C(V_C) = 1$ for all cliques in C^m. Then for each factor $P(V \mid \mathrm{pa}(V))$ find one and only one clique which contains the complete subgraph of $\{V\} \cup \mathrm{pa}(V)$ and multiply this conditional distribution into the function of that clique to obtain a new function. When this is done the result is a potential representation of the joint distributions in terms of functions on the cliques of the moral G^m.

Note that by adding the extra edges in the moralisation process it is not possible to read of all of the conditional independences of the original DAG, though they are still there "buried" in the numerical specification. Those which remain "visible" in the moral graph are used to exploit the efficient local computations which will be described later.

8. Aside: Markov properties on ancestral sets

In fact the moral graph is a powerful construction for elicudating conditional independence. First we require some more definitions. A node A is an ancestor of a node B if either (i) A is a parent of B or (ii) A is an ancestor of (at least) one of the parents of B. The ancestral set of a node is the node itself and the set of its ancestors. The ancestral set of a set of nodes Y is the union of the ancestral sets of the nodes in Y. A set S *separates* the sets A and B if every path between a node $a \in A$ and $b \in B$ passes through some node of S. With these definitions we have:

Lemma 1

Let P factorize recursively according to $\mathcal{G}$. Then

$$A \perp\!\!\!\perp B \mid S$$

whenever A and B are separated by S in $(\mathcal{G}_{\mathrm{An}(A \cup B \cup S)})^m$, the moral graph of the smallest ancestral set containing $A \cup B \cup S$.

Lemma 2

Let A, B and S be disjoint subsets of a directed, acyclic graph $\mathcal{G}$. Then S d-separates A from B if and only if S separates A from B in $(\mathcal{G}_{\mathrm{An}(A \cup B \cup S)})^m$.

What these lemmas tell us is that if we want to check conditional independences we can either look at d-separation properties or the smallest ancestral sets of the moral graphs – they are alternative ways of calculation.

To understand why ancestral set come into the picture, let us consider the following simple algorithm for finding them. Suppose that we have the graph G and that we wish to find the ancestral set of a set of nodes $Y \subseteq U$. Then successively delete nodes from G which have no children, provided they are not in the set Y. When it is not possible any longer delete any nodes, the subgraph left is the minimal ancestral set.

Now recall that deleting a childless node is equivalent to marginalising over that node. Hence the marginal distribution of the minimal ancestral set containing $A \perp\!\!\!\perp B \mid S$ factorizes according to the sub-factors of the original joint distribution. So these lemmas are saying that rather than go through the numerical exercise of actually calculating such marginals we can read it off from the graphical structure instead, and use that to test conditional independences. (Note also that the directed Markov property is also lurking behind the scenes here.) The "moral" is that when ancestral sets appear in theorems like this it is likely that such marginals are being considered.

9. Making the junction tree

The remaining three steps of the inference-engine construction algorithm seem more mysterious, but are required to ensure we can formulate a consistent and efficient message passing scheme. Consider first step 3 – adding edges to the moral graph G^m to form a triangulated graph G^t. Note that adding edges to the graph does not stop a clique of the moral graph formed from being a complete subgraph in G^t. Thus for each clique in C^m of the moral graph there is at least one clique in the triangulated graph which contains it. Hence we can form a potential representation of the joint probability in terms of products of functions of the cliques in the triangulated graph:

$$P(U) = \prod_{c \in C^t} a_C(X_C)$$

by analogy with the previous method outline for the moral graph. The point is that after moralisation and triangulation there exists for each a node-parent set at least one clique which contains it, and thus a potential representation can be formed on the cliques of the triangulated graph.

While the moralisation of a graph is unique, there are in general many alternative triangulations of a moral graph. In the extreme, we can always add edges to make the moral graph complete. There is then one large clique. The key to the success of the computational algorithms is to form triangulated graphs which have small cliques, in terms of their state space size.

Thus after finding the cliques of the triangulated graph – stage 4 – we are left with joining them up to form a junction tree. The important property of the junction tree is the *running intersection property* which means that if variable V is contained in two cliques, then it is contained in every clique along the path connecting those two cliques. The edge joining two cliques is called a separator. This joining up property can always be done, not necessarily uniquely for each triangulated graph. However the choice of

tree is immaterial except for computational efficiency considerations. The junction tree captures many, but not necessarily all, of the conditional independence properties of the distribution on the original DAG. It loses some of the conditional independences by the process of adding extra edges to the moral graph. However it does retain conditional independence between (not necessarily neighbouring) cliques given separators between them. It is because of this fact that local computation with message passing becomes possible. The running intersection property ensures *consistence* in the message passing between cliques, and the cliques become the basic unit of the local computation, ie., they define the granularity of the computational algorithms. If the cliques are of manageable size then local computation is possible. Figure 5 shows a triangulated version of Asia and a possible junction tree.

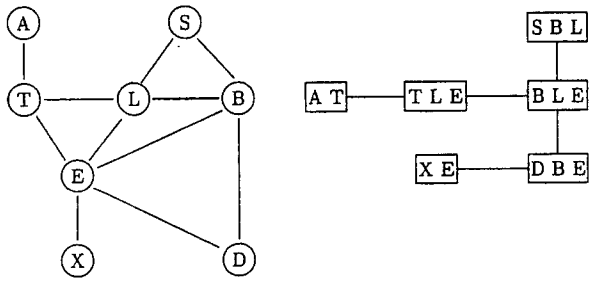


Figure 5. Junction tree for Asia

10. Inference on the junction tree

We will summarise some of the basic results of message passing on the junction tree. We have seen that we can form a potential representation of the joint probability using functions defined on the cliques:

$$P(U) = \prod_{C \in \mathcal{C}'} a_C(X_C).$$

This can be generalized to include functions on the separators (the intersections of neighbouring cliques) to form the following so called *generalized potential representation*:

$$P(U) = \frac{\prod_{C \in \mathcal{C}'} a_C(X_C)}{\prod_{S \in \mathcal{S}'} b_S(X_S)}.$$

(for instance by making the separator functions the identity). Now, by sending messages between neighbouring cliques consisting of functions of the separator variables only, which modify the intervening separator and the clique receiving the message, but in such a way that the overall ratio of products remains invariant, we can arrive at the following *marginal representation*:

$$p(U) = \frac{\prod_{C \in \mathcal{C}} p(C)}{\prod_{S \in \mathcal{S}} p(S)}. \tag{10}$$

Marginals for individual variables can be obtained from these clique (or separator) marginals by further marginalisation.

Suppose that we observe "evidence" $\mathcal{E} : X_A = x_A^*$. Define a new function P^* by

$$P^*(x) = \begin{cases} P(x) & \text{if } X_A = x_A^* \\ 0 & \text{otherwise.} \end{cases} \tag{11}$$

Then $P^*(U) = P(U, \mathcal{E}) = P(\mathcal{E})P(U \mid \mathcal{E})$. We can rewrite (11) as

$$P^*(U) = P(U) \prod_{v \in A} l(v), \tag{12}$$

where $l(v)$ is 1 if $x_v = x_v^*$, 0 otherwise. Thus $l(v)$ is the *likelihood function* based on the partial evidence $X_v = x_v^*$. Clearly this also factorizes on the junction tree, and by message passing we may obtain the following *clique-marginal representation*

$$p(V \mid \mathcal{E}) = \frac{\prod_{C \in \mathcal{C}} p(C \mid \mathcal{E})}{\prod_{S \in \mathcal{S}} p(S \mid \mathcal{E})}. \tag{13}$$

or by omitting the normalization stage,

$$p(V, \mathcal{E}) = \frac{\prod_{C \in \mathcal{C}} p(C, \mathcal{E})}{\prod_{S \in \mathcal{S}} p(S, \mathcal{E})}. \tag{14}$$

Again marginal distributions for individual variables, conditional upon the evidence, can be obtained by further marginalisation of individual clique tables, as can the probability (according to the model) of the evidence, $P(\mathcal{E})$.

11. Why the junction tree?

Given that the moral graph has nice properties, why is it necessary to go on to form the junction tree? This is best illustrated by an example, Figure 6:

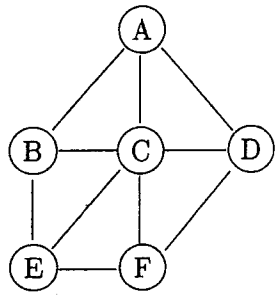


Figure 6. A non-triangulated graph

The cliques are (A, B, C), (A, C, D), (C, D, F), (C, E, F) and (B, C, E) with successive intersections (A, C), (C, D), (C, F), (C, E) and (B, C). Suppose we have clique marginals $P(A, B, C)$ *etc.*. We cannot express $P(A, B, C, D)$ in terms of $P(A, B, C)$ and $P(A, C, D)$ – the graphical structure does *not* imply $B \perp\!\!\!\perp D|(A, C)$. In general there is no closed for expression for the joint distribution of all six variables in terms of its cliques marginals.

12. Those extra edges again

Having explained why the cliques of the moral graph are generally not up to being used for local message passing, we will now close by indicating where the extra edges to form a triangulated graph come from.

Our basic message passing algorithm will be one in which marginals of the potentials in the cliques will form the messages on the junction tree. So let us begin with our moral graph with a potential representation in terms of functions on the cliques, and suppose we marginalise a variable Y say,which belongs to more than one clique of the graph, say two cliques, C_1 and C_2, with variables $Y \cup Z_1$ and $Y \cup Z_2$ respectively. They are cliques, but the combined set of variables do not form a single clique, hence there must be at least one pair of variables, one in each clique, which are not joined to each other, u_1 and u_2 say.

Now consider the effect of marginalisation of the variable Y. We will have

$$\sum_Y a_{C_1}(Y \cup Z_1) a_{C_2}(Y \cup Z_2) \equiv f(Z_1 \cup Z_2),$$

a function of the combined variables of the two cliques minus Y. Now this function cannot be accommodated by a clique in the moral graph because the variables u_1 and u_2 are not joined (and there may be others).

Hence we cannot form a potential representation of the joint distribution of $P(U - Y)$ on the moral graph with node Y removed. However, if we fill in the missing edges between the pairs of variables of the two cliques, then this marginal can be accommodated, and we can find a potential representation for $P(U - Y)$ on the reduced moral graph having these extra edges. This is why one adds edges to the moral graph, to be able to accommodate such intermediate marginal expressions. It turns out that one must fill-in sufficiently to form a triangulated graph, and doing so results in being able to set up a consistent message passing scheme.

13. Suggested further reading

Pearl is one of the pioneers who helped Bayesian methods for uncertain reasoning become popular in the artificial intelligence community. His textbook (Pearl, 1988) contains a wealth of material, from introducing probability theory and arguments for its use; axiomatics for graphical models; Markov properties; etc, to propagation in singly connected DAGs (ie prior to the development of making junction trees and propagating with them.) A good collection of papers on uncertain reasoning is Shafer and Pearl(1990), which covers not only probabilistic reasoning but also other formalisms for handling uncertainty. This also contains good overviews by the editors explaining the historical significance of the selected papers. An introductory review for probabilistic expert systems is (Spiegelhalter *et al.*, 1993). Each of these three references contain a large number of references for further reading.

Dawid(1979) introduced the axiomatic basis for treating conditional independence. More recent accounts of conditional independence with emphasis on graphical models and their Markov properties are given by Whittaker(1990) and Lauritzen(1996). (The latter also contains proofs of the lemmas stated in section 8.)

The Asia example was given by Lauritzen and Spiegelhalter(1988), who showed how to do consistent probability calculations in multiply connected DAG's using propagation, (it is also reprinted in (Shafer and Pearl, 1990)). Junction trees arise in other areas and are known by different names (eg join trees in relational databases); see (Lauritzen and Spiegelhalter, 1988) for more on this and also the discussion section of that paper. A recent and general formulation of propagation in junction trees is given by Dawid(1992). A recent introductory textbook on Bayesian networks is (Jensen, 1996).

References

Dawid, A. P. (1979). Conditional independence in statistical theory (with discussion). *Journal of the Royal Statistical Society, Series B*, **41**, pp. 1–31.

6. Modelling with continuous variables

All examples and discussion has have been restricted to the special case of discrete random variables. In principle, however, there is no reason why we should not build models having continuous random variables as well as, or instead of, discrete random variables, with more general conditional probability densities to represent the joint density, and use local message passing to simplify the calculations. In practice the barrier to such general applicability is the inability of performing the required integrations in closed form representable by a computer. (Such general models can be analyzed by simulation, for example Gibbs sampling.)

However there is a case for which such message passing is tractable, and that is when the random variables are such that the overall distribution is multivariate-Gaussian. This further extends to the situation where both discrete and continuous random variables coexist within a model having a so called *conditional-gaussian* joint distribution.

We will first discuss Gaussian models, and then discuss the necessary adjustments to the theory enabling analysis of mixed models with local computation.

7. Gaussian models

Structurally, the directed Gaussian model looks very much like the discrete models we have already seen. The novel aspect is in their numerical specification. Essentially, the conditional distribution of a node given its parents is given by a Gaussian distribution with expectation linear in the values of the parent nodes, and variance independent of the parent nodes. Let us take a familiar example:

$$\boxed{Y} \rightarrow \boxed{X} \rightarrow \boxed{Z}.$$

Node Y, which has no parents, has a normal distribution given by

$$N_Y(\mu_Y; \sigma_Y^2) \propto \exp\left(\frac{-(y-\mu_Y)^2}{2\sigma_Y^2}\right),$$

where μ_Y and σ_Y are constants. Node X has node Y as a parent, and has the conditional density:

$$N_X(\mu_X + \beta_{X,Y} y; \sigma_X^2) \propto \exp\left(\frac{-(x-\mu_X-\beta_{X,Y}y)^2}{2\sigma_X^2}\right),$$

where μ_X, $\beta_{X,Y}$ and σ_X are constants. Finally, node Z has only X as a parent; its conditional density is given by

$$N_Z(\mu_Z + \beta_{Z,X} x; \sigma_Z^2) \propto \exp\left(\frac{-(z-\mu_Z-\beta_{Z,X}x)^2}{2\sigma_Z^2}\right).$$

In general, if a node X had parents $\{Y_1, \ldots, Y_n\}$ it would have a conditional density:

$$N_X(\mu_X + \sum_i \beta_{X,Y_i} y_i; \sigma_X^2) \propto \exp\left(\frac{-(x-\mu_X-\sum_i \beta_{X,Y_i} y_i)^2}{2\sigma_X^2}\right).$$

Now the joint density is obtained by multiplying together the separate component Gaussian distributions:

$$\begin{aligned} P(X,Y,Z) &= N_Y(\mu_Y; \sigma_Y^2) N_X(\mu_X + \beta_{X,Y} y; \sigma_X^2) N_Z(\mu_Z + \beta_{Z,X} x; \sigma_Z^2) \\ &\propto \exp\left(-\frac{1}{2}(x-\mu_X, y-\mu_Y, z-\mu_Z) K (x-\mu_X, y-\mu_Y, z-\mu_Z)^T\right), \end{aligned}$$

where K is a symmetric (positive definite) 3×3 matrix, and T denotes transpose. In a more general model with n nodes, one obtains a similar expression with an $n \times n$ symmetric (positive definite) matrix.

Expanding the exponential, the joint density can be written as:

$$\exp\left((x \;\; y \;\; z)\begin{pmatrix} h_X \\ h_Y \\ h_Z \end{pmatrix} - \frac{1}{2}(x \;\; y \;\; z)\begin{pmatrix} K_{XX} & K_{XY} & K_{XZ} \\ K_{YX} & K_{YY} & K_{YZ} \\ K_{ZX} & K_{ZY} & K_{ZZ} \end{pmatrix}\begin{pmatrix} x \\ y \\ z \end{pmatrix}\right)$$

where $h_X = \mu_X/\sigma_X^2 + \mu_Z \beta_{Z,X}/\sigma_Z^2$ etc. This form of the joint density is the most useful for constructing local messages, and indeed local messages will consist of functions of this type. Let us now define them and list the properties we shall be using.

7.1. GAUSSIAN POTENTIALS

Suppose we have n continuous random variables $X_1, \ldots, X_n$. A Gaussian potential in a subset $\{Y_1, \ldots, Y_k\}$ of variables is a function of the form:

$$\exp\left(g + (y_1 \;\; \ldots \;\; y_k)\begin{pmatrix} h_1 \\ \vdots \\ h_k \end{pmatrix} - \frac{1}{2}(y_1 \;\; \ldots \;\; y_k)\begin{pmatrix} K_{1,1} & \ldots & K_{1,k} \\ \vdots & \ddots & \vdots \\ K_{k,1} & \ldots & K_{k,k} \end{pmatrix}\begin{pmatrix} y_1 \\ \vdots \\ y_k \end{pmatrix}\right)$$

where K is a constant positive definite $k \times k$ matrix, h is a k dimensional constant vector and g is a number. For shorthand we write this as a

triple, $\phi = (g, h, K)$. Gaussian potentials can be multiplied by adding their respective triples together:

$$\phi_1 * \phi_2 = (g_1 + g_2, h_1 + h_2, K_1 + K_2).$$

Similarly division is easily handled:

$$\phi_1 / \phi_2 = (g_1 - g_2, h_1 - h_2, K_1 - K_2).$$

These operations will be used in passing the "update factor" from separator to clique.

To initialize cliques we shall require the extension operation combined with multiplication. Thus a Gaussian potential defined on a set of variables Y is extended to a larger set of variables by enlarging the vector h and matrix K to the appropriate size and setting the new slots to zero. Thus for example: $\phi(x) = \exp(g + x^T h - \frac{1}{2} x^T K x)$ extends to

$$\phi(x, y) = \phi(x) = \exp\left(g + \begin{pmatrix} x & y \end{pmatrix} \begin{pmatrix} h \\ 0 \end{pmatrix} - \frac{1}{2} \begin{pmatrix} x & y \end{pmatrix} \begin{pmatrix} K & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix}\right).$$

Finally, to form the messages we must define marginalisation, which is now an integration. Let us take Y_1 and Y_2 to be two sets of distinct variables, and

$$\phi(y_1, y_2) = \exp\left(g + \begin{pmatrix} y_1 & y_2 \end{pmatrix} \begin{pmatrix} h_1 \\ h_2 \end{pmatrix} - \frac{1}{2} \begin{pmatrix} y_1 & y_2 \end{pmatrix} \begin{pmatrix} K_{1,1} & K_{1,2} \\ K_{2,1} & K_{2,2} \end{pmatrix} \begin{pmatrix} y_1 \\ y_2 \end{pmatrix}\right)$$

so that the h and K are in blocks. Then integrating over Y_1 yields a new vector h and matrix K as follows:

$$h = h_2 - K_{2,1} K_{1,1}^{-1} h_1$$

$$K = K_{2,2} - K_{2,1} K_{1,1}^{-1} K_{1,2}.$$

(Discussion of the normalization will be omitted, because it is not required except for calculating probability densities of evidence.) Thus integration has a simple algebraic structure.

7.2. JUNCTION TREES FOR GAUSSIAN NETWORKS

Having defined the directed Gaussian model, the construction of the junction tree proceeds exactly as for the discrete case, as far as the structure is concerned. The difference is with the initialization.

A Gaussian potential of correct size is allocated to each clique and separator. They are initialized with all elements equal to zero.

Next for each conditional density for the DAG model, a Gaussian potential is constructed to represent it and multiplied into any one clique which contains the node and its parents, using extension if required.

The result is a junction tree representation of the joint density. Assuming no evidence, then sending the clique marginals as messages results in the clique marginal representation, as for the discrete case:

$$P(U) = \prod_C P(X_C) / \prod_S P(X_S).$$

Care must be taken to propagate evidence. By evidence $\mathcal{E}$ on a set of nodes Y we mean that each node in Y is observed to take a definite value. (This is unlike the discrete case in which some states of a variable could be excluded but more than one could still be entertained.) Evidence about a variable must be entered into every clique and separator in which it occurs. This is because when evidence is entered on a variable it reduces the dimensions of every h vector and K matrix in the cliques and separators in which it occurs.

Thus for example, let us again take Y_1 and Y_2 to be two sets of distinct variables, and

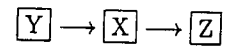
$$\phi(y_1, y_2) \propto \exp\left(\begin{pmatrix} y_1 & y_k \end{pmatrix} \begin{pmatrix} h_1 \\ h_k \end{pmatrix} - \frac{1}{2} \begin{pmatrix} y_1 & y_k \end{pmatrix} \begin{pmatrix} K_{1,1} & K_{1,2} \\ K_{2,1} & K_{2,2} \end{pmatrix} \begin{pmatrix} y_1 \\ y_2 \end{pmatrix}\right)$$

so that the h and K are again in blocks. Suppose we now observe the variables of Y_2 to take values y_2^*. Then the potentials become modified to $h = h_1 - y_2^* K_{2,1}$ and $K = K_{1,1}$.

After such evidence has been entered in every clique and separator, then the standard propagation will yield the clique-marginal density representation with evidence included. Further within clique marginals then gives the (Gaussian) distributions on individual nodes.

7.3. EXAMPLE

Let us take out three node example again, with initial conditional distributions as follows:



$$\begin{aligned} N(Y) &= N(0, 1) \\ N(X \mid Y) &= N(y, 1) \\ N(Z \mid X) &= N(x, 1) \end{aligned}$$

The cliques for this tree are $\boxed{\text{X Y}}$ and $\boxed{\text{X Z}}$. After initializing and propagating, the clique potentials are

$$\phi(x,y) \propto \exp\left(-\frac{1}{2}\begin{pmatrix}x & y\end{pmatrix}\begin{pmatrix}1 & -1\\ -1 & 2\end{pmatrix}\begin{pmatrix}x\\ y\end{pmatrix}\right)$$
$$\phi(x,z) \propto \exp\left(-\frac{1}{2}\begin{pmatrix}x & z\end{pmatrix}\begin{pmatrix}1.5 & -1\\ -1 & 1\end{pmatrix}\begin{pmatrix}x\\ z\end{pmatrix}\right)$$

with separator $\phi(x) \propto \exp(-x^2/4)$; Now if we enter evidence $X = 1.5$, say, then the potentials reduce to:

$$\phi(X = 1.5, y) \propto \exp(1.5y - y^2)$$

and

$$\phi(X = 1.5, z) \propto \exp(1.5z - \frac{1}{2}z^2),$$

because in this example X makes up the separator between the two cliques. The marginal densities are then:

$$P(Y) = N(0.75, 0.5) \text{ and } P(Z) = N(1.5, 1).$$

Alternatively, suppose we take $\boxed{\text{X Y}}$ as the root clique, and enter evidence that $Z = 1.5$. Then the message from $\boxed{\text{X Z}}$ to $\boxed{\text{X Y}}$ is given by $\phi(X) \propto \exp(1.5x - 0.75x^2)$ so that after propagation the clique potential on $\boxed{\text{X Y}}$ is of the form:

$$\phi(x,y) \propto \exp\left(\begin{pmatrix}x & y\end{pmatrix}\begin{pmatrix}1.5\\ 0\end{pmatrix} - \frac{1}{2}\begin{pmatrix}x & y\end{pmatrix}\begin{pmatrix}2 & -1\\ -1 & 2\end{pmatrix}\begin{pmatrix}x\\ y\end{pmatrix}\right)$$

with marginal densities

$$P(X) = N(1, 2/3) \text{ and } P(Y) = N(1/2, 2/3).$$

8. Conditional Gaussian models

As we have seen, the treatment of Gaussian networks is much the same as for discrete models. The minor differences are in (1) the nature of the potentials employed, and (2) evidence has to be entered into every clique and separator.

The passage to mixed models proceeds with some more important differences. The first is a restriction in the modeling stage: *continuous variables are not allowed to have discrete children*, ie. discrete nodes can only have discrete parents. The conditional probabilities specified for discrete nodes differ in character to those of continuous nodes. The former are again simple tables, as for discrete models, the latter are Gaussian potentials, but with the constants g, vectors h and matrices K indexed by the parent configurations of the discrete parents. Also, because certain sub configurations of discrete variables might not be allowed, we need to include indicator functions on the Gaussian potentials and we have to more careful with the normalization constants g.

The following is a brief guide to the theory, for more details see the original paper by Lauritzen, whose notation we follow closely here.

8.1. CG-POTENTIALS

The set of variables V is partitioned into the *discrete* variables (Δ) and continuous variables (Γ), thus $V = \Delta \cup \Gamma$. Let $x = (i, y)$ denote a typical element of the joint state space with i denoting the values of the discrete variables and y the values of the continuous variables. The joint density is assumed to be a *CG distribution*, which means that it has the form f with

$$f(x) = f(i,y) = \chi(i) \exp\left\{g(i) + y^T h(i) - y^T K(i) y/2\right\},$$

where $\chi(i) \in \{0, 1\}$ indicates whether f is positive at i. The triple (g, h, K) is called the *canonical characteristics* of the distribution; it is only defined for $\chi(i) > 0$ but when that is the case one can define the *moment characteristics*, denoted by the triple $\{p, \xi, \Sigma\}$ and given by

$$\xi(i) = K(i)^{-1} h(i), \quad \Sigma(i) = K(i)^{-1}.$$

Inverting, we have the canonical characteristics are $K(i) = \Sigma(i)^{-1}$, $h(i) = K(i)\xi(i)$, and

$$g(i) = \log p(i) + \left\{\log\det K(i) - |\Gamma|\log(2\pi) - \xi(i)^T K(i)\xi(i)\right\}/2.$$

As for the Gaussian networks, we generalize CG distributions to *CG potentials* which are any functions ϕ of the form

$$\phi(x) = \phi(i,y) = \chi(i)\exp\{g(i) + y^T h(i) - y^T K(i) y/2\}.$$

$K(i)$ is restricted to be symmetric, though not necessarily invertible. However we still call the triple (g, h, K) the canonical characteristics, and if for all i, $\chi(i) > 0$ and $K(i)$ is positive definite then the moment characteristics are given as before.

Multiplication, division and extension proceed as for the Gaussian potentials have already been discussed. Marginalisation is however different,

because adding two CG potentials in general will result in a mixture of CG potentials – a function of a different algebraic structure. Thus we need to distinguish two types of marginalisation – *strong* and *weak*.

8.2. MARGINALISATION

Marginalising continuous variables corresponds to integration. Let

$$y = \begin{pmatrix} y_1 \\ y_2 \end{pmatrix}, \quad h = \begin{pmatrix} h_1 \\ h_2 \end{pmatrix}, \quad K = \begin{pmatrix} K_{11} & K_{12} \\ K_{21} & K_{22} \end{pmatrix}$$

with y_1 having dimension p and y_2 dimension q with K_{11} is positive definite. Then the integral $\int \phi(i, y_1, y_2)\, dy_1$ is finite and equal to a CG potential $\tilde{\phi}$ with canonical characteristics given as

$$\begin{aligned} \tilde{g}(i) &= g(i) + \{p \log(2\pi) - \log\det K_{11}(i) + h_1(i)^T K_{11}(i)^{-1} h_1(i)\}/2 \\ \tilde{h}(i) &= h_2(i) - K_{21}(i) K_{11}(i)^{-1} h_1(i) \\ \tilde{K}(i) &= K_{22}(i) - K_{21}(i) K_{11}(i)^{-1} K_{12}(i). \end{aligned}$$

Marginalising discrete variables corresponds to summation. Since in general addition of CG potentials results is a mixture of CG potentials, an alternative definition based upon the moment characteristics $\{p, \xi, \Sigma\}$ is used which does result in a CG potential; however it is only well defined for $K(i,j)$ positive definite. Specifically, the marginal over the discrete states of ϕ is *defined* as the CG potential with moment characteristics $\{\tilde{p}, \tilde{\xi}, \tilde{\Sigma}\}$ where

$$\tilde{p}(i) = \sum_j p(i,j), \quad \tilde{\xi}(i) = \sum_j \xi(i,j) p(i,j)/\tilde{p}(i), \text{ and}$$

$$\tilde{\Sigma}(i) = \sum_j \Sigma(i,j) p(i,j)/\tilde{p}(i) + \sum_j \left(\xi(i,j) - \tilde{\xi}(i)\right)^T \left(\xi(i,j) - \tilde{\xi}(i)\right) p(i,j)/\tilde{p}(i).$$

Note that the latter can be written as

$$\tilde{p}(i) \left(\tilde{\Sigma}(i) + \tilde{\xi}(i)^T \tilde{\xi}(i)\right) = \sum_j p(i,j) \left(\Sigma(i,j) + \xi(i,j)^T \xi(i,j)\right).$$

so that if $\Sigma(i,j)$ and $\xi(i,j)$ are independent of j then they can be taken through the summations as constants. This observation is used to define a marginalisation over both continuous and discrete variables: First marginalise over the the continuous variables and then over the discrete variables. If, after marginalising over the continuous variables the resulting pair (h, K) is independent of the discrete variables to be marginalised over, (summation over these discrete variables then leaves the pair (h, K)

unmodified), we say that we have a *strong marginalisation*. Otherwise one sums over the discrete variables using the moment characteristics, and the overall marginalisation is called a *weak marginalisation*.

Weak and strong marginalisation satisfy composition:

$$\sum_A \left(\sum_B \phi_{A \cup B \cup C} \right) = \sum_{A \cup B} \phi_{A \cup B \cup C},$$

but in general only the strong marginalisation satisfies

$$\sum_A (\phi_{A \cup B} \psi_B) = \psi_B \left(\sum_A \phi_{A \cup B} \right).$$

Under both type of marginalisation, a 'marginalised' density will then have the correct moments to order 2, i.e.

$$P(I = i) = \tilde{p}(i), \quad \mathbf{E}(Y \mid I = i) = \tilde{\xi}(i), \quad \mathbf{V}(Y \mid I = i) = \tilde{\Sigma}(i),$$

where the correct CG distribution is used to take expectations.

8.3. MAKING THE JUNCTION TREE

The non-closure of cg-potentials under marginalisation of discrete variables means that we have to adjust to how we construct the junction tree and pass messages in it. The first step is to construct the junction tree. First we moralize the DAG in the usual way. Then we triangulate by a restricted elimination ordering.[2] Specifically, we first eliminate all of the continuous variables, and then we eliminate the discrete variables. Then from the resulting cliques we can construct a junction tree. Now we must select a root. Unlike the previous pure cases, we cannot freely choose any clique of the junction tree. Instead we choose a so called *strong root* defined as follows:

> *Any clique R which for any pair A, B of cliques themselves neighbours on the tree with A closer to R than B satisfies*
>
> $$(B \setminus A) \subseteq \Gamma \text{ or } (B \cap A) \subseteq \Delta.$$

Thus, when a separator between two neighbouring cliques is not purely discrete, the clique furthest away from the root has only continuous vertices extra beyond the separator.

[2] One way to triangulate a graph is to take an ordering of the nodes and give all of the nodes the status 'unmarked'. One then works through each node in turn, marking it and joining all pairs of its unmarked neighbours. The ordering is called an *elimination ordering*. Finding good triangulations is then equivalent to finding good elimination orderings.

8.4. PROPAGATION ON THE JUNCTION TREE

The point of this restriction is that on the collect operation, only strong marginalisations are required to be performed. This is because our restricted elimination ordering - getting rid of the continuous variables first, is equivalent to doing the integrations over the continuous variables before marginalising any of the discrete variables.

Thus our message passing algorithm takes the form:

1. Initialization: Set all clique and separator potentials to zero with unit indicators, and multiply in the model specifying potentials using the extension operation where appropriate.
2. Enter evidence into all clique and separator potentials, reducing vector and matrix sizes as necessary.
3. Perform a collect operation to the strong root, where the messages are formed by strong marginalisation by first integrating out the redundant continuous variables, and then summing over discrete variables.
4. Perform a distribute operation, using weak marginalisation where appropriate when mixtures might be formed on marginalising over the discrete variables.

The result is a representation of the joint CG-distribution including evidence, because of the invariant nature of the message passing algorithm. Furthermore, because of the use of weak marginalisation for the distribute operation, the marginals on the cliques will themselves be CG-distributions whose first two moments match that of the full distribution. The following is an outline sketch of why this could be.

First by the construction of the junction tree, all collect operations are strong marginals, so that after a collect-to-root operation the root clique contains a strong marginal. Now suppose, for simplicity, that before the distribute operation we move to a set-chain representation (cf. section 2.2). Then apart from the strong root, each clique will have the correct joint density $P(X_{C_i \setminus S_i} \mid X_{S_i})$ where S_i is the separator adjacent to the clique C_i on the path between it and the strong root. Now on the distribute operation the clique C_i will be multiplied by a CG-potential which will either be a strong marginal or a weak marginal. If the former then the clique potential will be the correct marginal joint density. If the latter then we may write the clique potential as the product $P(X_{C_i \setminus S_i}) * Q(X_{S_i})$ where Q is the correct weak marginal for the variables X_{S_i}. Now consider taking an expectation of any linear or quadratic function of the X_{C_i} with respect to this "density". We are free to integrate by parts. However, choosing to integrate wrt. $X_{C_i \setminus S_i}$ first means that we form the expectation wrt the correct CG-density $P(X_{C_i \setminus S_i} \mid X_{S_i})$, and will thus end up with a correct expectation (which will be a linear or quadratic function in the X_{S_i}) multiplied

by the correct weak marginal $Q(X_{S_i})$. Hence performing these integrations we will obtain the correct expectation of the original function wrt the true joint density.

For brevity some details have been skipped over here, such as showing that the separator messages sent are correct weak marginals. Detailed justifications and proofs use induction combined with a careful analysis of the messages sent from the strong root on the distribute operation. See the original paper for more details.

9. Summary

This tutorial has shown the variety of useful applications to which the junction-tree propagation algorithm can be used. It has not given the most general or efficient versions of the algorithms, but has attempted to present the main points of each so that the more detailed descriptions in the original articles will be easier to follow. There are other problems, to which the junction-tree propagation algorithm can be applied or adapted to, not discussed here, such as:

- Influence diagrams: Discrete models, with random variables, decisions and utilities. Potentials are now doublets representing probabilities and utilities. Junction tree is generated with a restricted elimination generalising that for cg-problems to emulate solving the decision tree.
- Learning probabilities. Nodes presenting parametrisations of probabilities can be attached to networks, and Bayesian updating performed using the same framework.
- Time series. A network can represent some state at a given time, and they can be chained together to form a time-window for dynamic modelling. The junction tree can be expanded and contracted to allow forward-prediction or backward smoothing.

Doubtless new examples will appear in the future.

10. Suggested further reading

Probabilistic logic sampling for Bayesian networks is described by Henrion(1988). A variation of the method – *likelihood-weighting sampling* – in which rejection steps are replaced by a weighting scheme is given by Shachter and Peot(1989). Drawing samples directly from the junction tree is described by Dawid(1992), which also shows how the most likely configuration can be found from the junction tree. The algorithm for finding the N- most likely configurations is due to Nilsson(1994), who has also developed a more efficient algorithm requiring only one max-propagation on the junction tree. L^P-propagation is not described anywhere but here.

Fast retraction is introduced in (Dawid, 1992) and developed in more detail in (Cowell and Dawid, 1992).

Gaussian networks are described by Shachter and Kenley(1989), who use arc-reversal and barren-node reduction algorithms for their evaluation. (The equivalence of various evaluation schemes is given in (Shachter *et al.*, 1994).) The treatment of Gaussian and conditional-gaussian networks is based on the original paper by Lauritzen(1992). For pedagogical reasons this chapter specialized the conditional-gaussian presentation of (Lauritzen, 1992) to the pure gaussian case, to show that the latter is not so different from the pure discrete case. Evaluating influence diagrams by junction-trees is treated in (Jensen *et al.*, 1994). For an extensive review on updating probabilities (Buntine, 1994). Dynamic junction trees for handling time series is described by Kjærulff(1993). See also (Smith *et al.*, 1995) for an application using dynamic junction trees not derived from a DAG model.

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