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SAMPLING WITHOUT REPLACEMENT IN JUNCTION TREES

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Sampling without replacement in junction trees

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Abstract

It is shown that a highly efficient algorithm recently presented by Nilsson (1997) for finding the M-most probable configurations in a probabilistic expert system can be adapted for generating samples without replacement from a junction-tree representation of the joint distribution.

Keywords: Probabilistic expert system, Bayesian network, junction tree, max-propagation, sampling without replacement.

1 Introduction

For a probabilistic expert system, (also called a Bayesian network), of discrete variables Dawid (1992) showed how one could find the most-probable configuration of the variables by a single max-propagation on an associated junction tree. Recently Nilsson (1997) exploited this calculational method and combined it with a clever partitioning scheme to formulate an efficient method for finding the M most likely configurations of the joint distribution for any integer M. In his paper Dawid also showed how one can sample directly and efficiently from the posterior distribution represented by the marginal-potential representation on the junction tree. It is the purpose of this short paper to show that, using the partitioning scheme of Nilsson, one can sample without replacement directly and efficiently from the posterior distribution. The next section presents a summary of the key points of Nilsson's method. Sampling without replacement is developed by analogy in the subsequent section. We shall assume the reader is familiar with the papers of (Dawid 1992) and (Nilsson 1997), and we will borrow notations, definitions and results from these papers.

2 Finding the M-most likely configurations

Suppose we are given a connected[1]junction tree $\mathcal{T}$ having a potential representation of a probability function f in the discrete variables $X_u, u \in U$ given by

$$f = \frac{\prod_{C \in \mathcal{C}} a_C}{\prod_{S \in \mathcal{S}} b_S}, \tag{1}$$

where the clique and separator potentials a_C and b_S are known non-negative functions. Then by a process called *max-propagation* on the junction tree, consisting of a set of local messages passed between the cliques, the joint distribution f can be

[1]This is not a problematic restriction, the disconnected case is readily treated.

expressed in the form

$$f = \frac{\prod_{C \in \mathcal{C}} \hat{f}_C}{\prod_{S \in \mathcal{S}} \hat{f}_S} \tag{2}$$

where $\hat{f}_C$ is the maximum of f over the subset of variables $x_C \subset U$. (See (Dawid 1992) for proof.) From this *max-marginal* representation one can readily find the configuration which has the highest probability, by the following search procedure (called *max-distribute*). First one designates a clique as the root, and orders the cliques starting with the root so that they obey the *running intersection property.* This is equivalent to making the junction tree directed, with all edges pointing away from the root, and then finding a topological ordering of the cliques beginning with the root. Such an ordering is always possible. For convenience label the ordered cliques sequentially thus $(C_0, C_1, \ldots, C_k)$, with separators $(S_1, \ldots, S_k)$ such that the separator S_j joins the clique C_j to the adjacent clique which is closer to the root. (see Figure 1 for an example). Denote the corresponding ordered *residual sets* by $(R_0, R_1, \ldots, R_k)$ where $R_j \equiv C_j \setminus S_j$ for every $j > 0$ and we define $R_0 \equiv C_0$.

To find the most likely configuration, one then proceeds outwards from the root as follows: First search the root clique C_0 for the configuration of its variables, $\hat{x}_{C_0}$ say, which maximizes the clique potential value (breaking ties arbitrarily). Distribute this as extra "evidence", fixing successively the remaining variables in the cliques further from the root in their running intersection order by finding a maximal configuration consistent with the neighbouring cliques which have also been fixed, and including the states of the newly fixed variables as extra evidence. Thus for clique C_j one finds the configuration of the residual variables R_j which maximizes $\hat{f}_{C_j}$ subject to the separator variables S_j taking the configuration fixed by the earlier steps. The union of the "evidence" yields the most likely configuration. If there is "real" evidence then this will have been incorporated by the original max-propagation which put the

junction tree into the max-marginal representation.

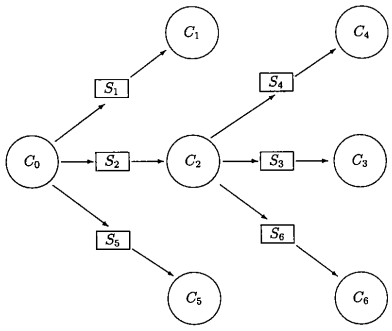

Figure 1: A junction tree as a directed acyclic graph.

The algorithm of (Nilsson 1997) for finding the M-most likely configurations is an iterative divide-and-conquer process built upon this algorithm for finding the most likely configuration. Following Nilsson, let H denote the complete set of configurations, and for $L = 1, 2,$ etc let x^L denote the Lth most probable configuration. The procedure for finding the $L+1$th configuration, which is essentially a search over the space $H \setminus \{x^1, \ldots, x^L\}$, consists of three steps:

1. **Partition phase:** Partition $H \setminus \{x^1, \ldots, x^L\}$ into disjoint representative subsets, which together are consistent with all remaining configurations.
2. **Candidate phase:** Search these partition-generated subsets for the set consistent with the $L+1$th most probably configuration.
3. **Identification phase:** Extract the configuration from the selected candidate.

First we discuss a simplified (and far less efficient) version to help explain Nilsson's algorithm. Denote the set of initial evidence (if any) by $\mathcal{E}$, and order the variables in some way, say $(X_1, X_2, \ldots, X_n)$ where the j-th node has T_j states $(x_j^1, \ldots x_j^{T_j})$.

From the preceding discussion, one can find the most likely configuration, $x^1 = (x_1^{t_1^1}, \ldots, x_n^{t_n^1})$. Now the second most likely configuration, x^2 must differ from x^1 in the state of at least one variable. So now perform a further n max-propagations, (each requires a re-initializing the junction tree), each with a distinct "pseudo-evidence" $\mathcal{E}^1_{j,\emptyset}$ defined by:

$$\begin{aligned}
\mathcal{E}^1_{1,\emptyset} &= \mathcal{E} \text{ and } X_1 \neq x_1^{t_1^1}, \\
\mathcal{E}^1_{2,\emptyset} &= \mathcal{E} \text{ and } X_1 = x_1^{t_1^1} \text{ and } X_2 \neq x_2^{t_2^1}, \\
\mathcal{E}^1_{3,\emptyset} &= \mathcal{E} \text{ and } X_1 = x_1^{t_1^1} \text{ and } X_2 = x_2^{t_2^1} \text{ and } X_3 \neq x_3^{t_3^1}, \\
&\vdots \\
\mathcal{E}^1_{n,\emptyset} &= X_1 = \mathcal{E} \text{ and } x_1^{t_1^1} \text{ and } \ldots X_{n-1} = x_{n-1}^{t_{n-1}^1} \text{ and } X_n \neq x_n^{t_n^1}.
\end{aligned} \tag{3}$$

By this procedure we partition the search space for the set of all configurations, excluding the most likely one x^1 we have already found. Hence one of these must be consistent with the second most likely configuration x^2, and only one if it is unique; which one can be found by calculating the max-normalizations of each and picking the one with the largest normalization.

If the second most likely configuration is found to arise from the jth set, then by a max-distribute operation it can found using initial evidence $\mathcal{E}^1_{j,\emptyset}$. Denote it by $x^2 = (x_1^{t_1^2}, \ldots, x_n^{t_n^2})$, (where by the partition constraint $t_i^1 = t_i^2$ for all $i < j$).

Now the third most likely configuration x^3 is either consistent with one of the set alternative evidences of (3) excluding the jth, or it has a configuration which disagrees with both the x^1 and x^2 configurations in at least one place for some variable having index $\geq j$ while agreeing for all indices less that j. To find out which perform a further partition of the search space to obtain an extra set of $n - j + 1$

disjoint evidences of the form:

$$\begin{aligned}
\mathcal{E}^2_{j,j} =& \mathcal{E}^1_{j,\emptyset} \text{ and } X_j \neq x_j^{t_j^2}, \\
\mathcal{E}^2_{j+1,j} =& \mathcal{E}^1_{j,\emptyset} \text{ and } \; X_j = x_j^{t_j^2} \text{and } X_{j+1} \neq x_{j+1}^{t_{j+1}^2}, \\
& \vdots \\
\mathcal{E}^2_{n,j} =& \mathcal{E}^1_{j,\emptyset} \text{ and } \; \ldots X_{n-1} = x_{n-1}^{t_{n-1}^2} \text{and } X_n \neq x_n^{t_n^2}.
\end{aligned} \tag{4}$$

Finding the max-normalizations of these, and comparing with those of (3) (excluding the jth) we pick out that which attains the highest max-normalization and the use max-distribute to find the actual configuration. The representative evidence is then further partitioned, etc, until the desired number M of configurations have been found.

The partitioning the search space is one of the key steps in Nilsson's method, and will work with any ordering of the variables. However it does require a large number of junction tree initializations and propagations. The other key step is to select a specific ordering of the variables so that only one max-propagation is required, thus making the process much more efficient. Specifically, one orders the variables according to the ordered residual sets R, and in the partitioning phase excludes joint states of the residual variables (rather than states of individual variables). Thus, in terms of the residual sets, suppose the most likely configuration has the form $x^1 = (r_0^{t_0^1}, \ldots, r_k^{t_k^1})$, (where now the ts range over the configurations of the residuals). Then as dummy evidence for finding the second most likely configuration, one could perform $k+1$ propagations of the form:

$$
\begin{aligned}
\mathcal{E}^1_{0,\emptyset} =& \mathcal{E} \text{ and } R_0 \neq r_0^{t_0^1}, \\
\mathcal{E}^1_{1,\emptyset} =& \mathcal{E} \text{ and } R_0 = r_0^{t_0^1} \text{ and } R_1 \neq r_1^{t_1^1}, \\
\mathcal{E}^1_{2,\emptyset} =& \mathcal{E} \text{ and } R_0 = r_0^{t_0^1} \text{ and } R_1 = r_1^{t_1^1} \text{ and } R_2 \neq r_2^{t_2^1}, \\
& \vdots \\
\mathcal{E}^1_{k,\emptyset} =& \mathcal{E} \text{ and } R_0 = r_1^{t_1^1} \text{ and } \ldots R_{k-1} = r_{k-1}^{t_{k-1}^1} \text{ and } R_k \neq r_k^{t_k^1}.
\end{aligned} \tag{5}
$$

The point about using this ordering is that, for example, if one were to do a max-collect using $\mathcal{E}^1_{j,\emptyset}$ then, because no new dummy-evidence has been entered beyond the jth residual set or clique, all messages received by the subtree induced by $(C_0, \ldots, C_j)$ are identical to those which were sent in the original max-propagation using the evidence $\mathcal{E}$. This means that sending such messages is unnecessary, and one need only consider the max-collect operation on the subtree $(C_0, \ldots, C_j)$ to find the max-normalization. But such an operation is trivial in that, because of the evidence $\mathcal{E}^1_{j,\emptyset}$ entered, only one non-zero value from each clique and separator (denoted by $x^*_{C_i}$ and $x^*_{S_i}$) survive for all indices $i < j$, thus the normalization can be found very efficiently by the simple formula:

$$
\frac{\prod_{i=0}^{j-1} \hat{f}_{C_i}(x^*_{C_i})}{\prod_{i=0}^{j-1} \hat{f}_{S_i}(x^*_{S_i})} \max \hat{f}_{C_j}(x_{C_j}, \mathcal{E}^1_{j,\emptyset}) \tag{6}
$$

which requires a simple search in the jth clique for the last term. This is Theorem 3 of (Nilsson 1997). $\mathcal{E}^1_{j,\emptyset}$ is then partitioned similarly to (4) into:

$$
\begin{aligned}
\mathcal{E}^2_{j,j} =& \mathcal{E}^1_{j,\emptyset} \text{ and } R_j \neq rj^{t_j^2}, \\
\mathcal{E}^2_{j+1,j} =& \mathcal{E}^1_{j,\emptyset} \text{ and } R_j = r_j^{t_j^2} \text{and } R_{j+1} \neq r_{j+1}^{t_{j+1}^2}, \\
& \vdots \\
\mathcal{E}^2_{n,j} =& \mathcal{E}^1_{j,\emptyset} \text{ and } \ldots R_{n-1} = r_{k-1}^{t_{k-1}^2} \text{and } R_k \neq r_k^{t_k^2}.
\end{aligned} \tag{7}
$$

3 Sampling without replacement algorithm

Besides showing how one can find the most likely configuration, in his paper Dawid (1992) also showed how one can sample with replacement directly from the posterior distribution using the junction tree. The first stage is to put the junction tree potentials into their marginal-potential form by a sum-propagation of evidence, thus:

$$f(U,\mathcal{E}) = \frac{\prod_C f(C,\mathcal{E})}{\prod_S f(S,\mathcal{E})}. \tag{8}$$

Then to get a sample, one uses again the ordering of the cliques as for the previous maximization story. One begins by sampling a configuration in the root clique, drawing from $f(R_0,\mathcal{E})$ to obtain $r_0^{t_0^1}$ say. Next one samples from $f(R_1 \mid R_0 = r_0^{t_0^1},\mathcal{E})$ found from clique C_1, etc, processing the cliques in their running intersection ordering, so that when sampling for R_i from clique C_i the variables X_{S_i} will already have been fixed by earlier sampling. When all cliques have been so processed a configuration will have been generated with its correct probability. This process can be repeated to draw as many independent samples as may be required. We shall call such a search process a *sample-distribute* operation.

However, instead of sampling independent samples we can employ Nilsson's partitioning scheme to draw samples without replacement correctly from the posterior distribution. The differences are (1) sum-propagation rather than max-propagation is used to initialize the tree, and (2) sampling rather than maximization is performed in the candidate partition search stages.

Specifically, suppose that we have put the junction tree into sum-marginal representation by sum-propagation of evidence. Then one samples one configuration by the method described above - denote this first sample by x^1 writing it in terms of the residual sets as: $x^1 = (r_0^{t_0^1},\ldots,r_k^{t_k^1})$. Then to sample a second configuration, in analogy to finding the second most likely configuration one generates $k+1$ candi-

dates using evidences given by (5), with the evidence defined by $\mathcal{E}^1_{j,\emptyset}$ being assigned a weight given by

$$\frac{\prod_{i=0}^{j-1} f_{C_i}(x^*_{C_i})}{\prod_i^j f_{S_i}(x^*_{S_i})} \sum f_{C_j}(x_{C_j}, \mathcal{E}^1_{j,\emptyset}) \tag{9}$$

(cf (6)). This weight could alternatively be found much more inefficiently using a sum-collect operation with evidence $\mathcal{E}^1_{j,\emptyset}$, but again in direct analogy to the max-collect operation, by sum-consistence the cliques and separators having indices greater than j have their contributions cancel.

Next from this set of weighted candidates one samples a candidate according to its weight, (max-distribute-search picks the highest weight configuration), and then proceed to complete the configuration by a sample-distribute operation, which ensures that the final configuration obtained is drawn from the distribution correctly.

Thus assume that in this process the jth term was sampled. Then in analogy to drawing a single sample, the configuration is completed by a sample-distribute-search using $\mathcal{E}^1_{j,\emptyset}$, (which can begin from the j clique as all previous cliques have completely specified residuals). Its probability can then be found easily. After completion, if a third configuration is required then this must also be partitioned to form new extra candidates. These candidates will have respective evidences as in (7), with weights given in analogy to (9).

4 Conclusions

We have shown informally how samples may be drawn without replacement using a variation of the top M-configuration search algorithm of Nilsson (1997), in which max-propagation is replaced with sum-propagation, and max-distribute-searching with sample-distribute-searching etc. With these simple replacements, plus sampling

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