Discovering a junction tree behind a Markov network by a greedy algorithm

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Received: date / Accepted: date

Abstract In our paper [18] we introduced a special kind of k-width junction tree, called k-th order t-cherry junction tree in order to approximate a joint probability distribution. The approximation is the best if the Kullback-Leibler divergence between the true joint probability distribution and the approximating one is minimal. Finding the best approximating k-width junction tree is NP-complete if k > 2 (see in [12]). In [19] we also proved that the best approximating k-width junction tree can be embedded into a k-th order t-cherry junction tree. We introduce a greedy algorithm resulting very good approximations in reasonable computing time.

In this paper we prove that if the Markov network underlying fulfills some requirements then our greedy algorithm is able to find the true probability distribution or its best approximation in the family of the k-th order t-cherry tree probability distributions. Our algorithm uses just the k-th order marginal probability distributions as input.

We compare the results of the greedy algorithm proposed in this paper with the greedy algorithm proposed by Malvestuto [16].

Keywords Greedy algorithm · Conditional independence · Markov network · Triangulated graph · Graphical models · t-cherry junction tree · Contingency table

Mathematics Subject Classification (2000) 90C35 · 90C59 · 62B10 · 94A17 · 62H05 · 62H30

1 Introduction

The problem of approximating multivariate probability distributions is a central task of many fields. Unfortunately in most of the cases we know nothing about the theore-
cational probability distribution. It is useful to exploit the dependence structure between the random variables involved. The problem is: what should we do when correlation matrices cannot be used.

Starting from a discrete probability distribution, for example from a sample data, it is useful to discover some of the conditional independences between the variables. The Markov networks (Markov random fields) and Bayesian networks encode these conditional independences. In our paper we focus on the Markov networks. If the graph structure of the Markov network is known, many procedures were developed for its inference, see [17] and [8]. There are many cases where the graph structure of the Markov network is unknown. In [18] we proposed a method for discovering some of the conditional independences between the random variables by fitting a special type of multivariate probability distribution called $t$-cherry junction tree distribution to the sample data. The goodness of fit was quantified by the Kullback-Leibler divergence (see [14]). This relates the problem to information theory ([7]). On the other side, the graph underlying the Markov network links the problem to graph theory. For elements of graph theory see [2].

In the second section we introduce some concepts used in graph theory and probability theory that we need throughout the paper and present how these can be linked to each other. For a good overview see [15].

In the third part we introduce the Szántai-Kovács’s greedy algorithm which starting from the $k$-th order marginal probability distributions gives a $k$-th order $t$-cherry junction tree probability distribution as a result. For the same task Malvestuto gives another algorithm in [16]. First we compare these two algorithms from analytical point of view and then apply them on the example problem presented in Malvestuto’s paper [16].

In the fourth part we introduce the so called puzzle algorithm for $k$-th order $t$-cherry trees. This results in a puzzle numbering of the vertices. Using this we give some theoretical results related to our greedy algorithm.

The last part contains conclusions and some possible applications of our greedy algorithm.

2 Preliminaries

This part contains a summary of the concepts used throughout the paper. We first present the acyclic hypergraphs and junction trees. We then present a short reminder on Markov network. We finish this part with the multivariate joint probability distribution associated to a junction tree.

Let $V = \{1, \ldots, d\}$ be a set of vertices and $\Gamma$ a set of subsets of $V$ called set of hyperedges. A hypergraph consists of a set $V$ of vertices and a set $\Gamma$ of hyperedges. We denote a hyperedge by $C_i$, where $C_i$ is a subset of $V$. If two vertices are in the same hyperedge they are connected, which means, the hyperedge of a hypergraph is a complete graph on the set of vertices contained in it.

A vertex is called simplicial if it belongs to precisely one hyperedge.

An ordering of the vertices is a perfect elimination ordering if $\forall i, 1 \leq i \leq d$ the vertex $i$ is simplicial in the subhypergraph defined on the vertices $\{i, i+1, \ldots, d\}$.

The acyclic hypergraph is a special type of hypergraph which fulfills the following requirements:

- Neither of the edges of $\Gamma$ is a subset of another edge.
There exists a numbering of edges for which the running intersection property is fulfilled: \( \forall j \geq 2 \ \exists i < j : \ C_i \supseteq C_j \cap (C_1 \cup \ldots \cup C_{j-1}) \). (Other formulation is that for all hyperedges \( C_i \) and \( C_j \) with \( i < j - 1 \), \( C_i \cap C_j \subset C_s \) for all \( s, i < s < j \).

Let \( S_j = C_j \cap (C_1 \cup \ldots \cup C_{j-1}) \), for \( j > 1 \) and \( S_1 = \phi \). Let \( R_j = C_j \setminus S_j \). We say that \( S_j \) separates \( R_j \) from \( (C_1 \cup \ldots \cup C_{j-1}) \setminus S_j \), and call \( S_j \) separator set or shortly separator.

Now we link these concepts to the terminology of junction trees.

The junction tree is a special tree structure which is equivalent to the connected acyclic hypergraphs [15]. The nodes of the tree correspond to the hyperedges of the connected acyclic hypergraph and are called clusters, the edges of the tree correspond to the separator sets and called separators. The set of all clusters is denoted by \( C \), the set of all separators is denoted by \( S \). The junction tree with the largest cluster containing \( k \) variables is called \( k \)-width junction tree.

An important relation between graphs and hypergraphs is given in [15]: A hypergraph is acyclic if and only if it can be considered to be the set of cliques of a triangulated graph (a graph is triangulated if every cycle of length greater than 4 has a chord).

**Theorem 1** (Fulkerson and Gross, [12]): A graph is an acyclic hypergraph (triangulated graph or junction tree) if and only if it has an perfect elimination ordering.

**Algorithm 1** (Graham, [10]) A Graham reduction of a hypergraph \( H = (V, \Gamma) \) is defined by applying the following two operations to \( H \) until they can be applied no more.

- Node removal: If a node appears in only one hyperedge, delete it from \( V \) and from the edge.
- Hyperedge removal: In the transformed hyperedge set, delete a hyperedge if it is subset of another hyperedge.

In [1] is shown that a hypergraph reduces to nothing by this process if and only if the hypergraph is acyclic.

In the Figure 1 one can see a) a triangulated graph, b) the corresponding acyclic hypergraph and c) the corresponding junction tree.

We consider the random vector \( \mathbf{X} = (X_1, \ldots, X_d)^T \), with the set of indices \( V = \{1, \ldots, d\} \). Roughly speaking a Markov network encodes the conditional independences between the random variables. The graph structure associated to a Markov network consists in the set of nodes \( V \), and the set of edges \( E = \{(i, j) | i, j \in V\} \). We say the graph structure associated to the Markov network has

- the pairwise Markov (PM) property if \( \forall i, j \in V, i \) not connected to \( j \) implies that \( X_i \) and \( X_j \) are conditionally independent given all the other random variables;
- the local Markov (LM) property if \( \forall i \in V, \) and \( Ne(i) \) the neighbourhood of node \( i \) in the graph (the nodes connected with \( i \)) then \( X_i \) is conditionally independent from all \( X_j, j \notin Ne(i) \), given \( X_k, k \in Ne(i) \);
- the global Markov (GM) property states that if in the graph \( \forall A, B, C \subset V \) and \( C \) separates \( A \) and \( B \) in terms of graph then \( X_A \) and \( X_B \) are conditionally independent given \( X_C \), which means in terms of probabilities that

\[
P(X_{A \cup B | C}) = \frac{P(X_{A \cup C}) P(X_{A \cup B | C})}{P(X_C)};
\]
the factorization (F) property states that if \( C \) denotes the set of cliques of the graph (maximum complete graphs) then there exist positive functions \( \psi_C (X_C) \) that

\[
P (X_V) = \prod_{C \in C} \psi_C (X_C).
\]

The following implication is well known \[11\]: \( F \Rightarrow GM \Rightarrow LM \Rightarrow PM \). The Hammersley-Clifford theorem states that under assumption of positivity \( PM \Rightarrow F \). However positivity is a very strong condition. "The positivity condition is mathematically convenient; But it hardly seems necessary" \[11\]. In this paper we focus on Markov network characterized by the global Markov property.

The concept of junction tree probability distribution is related to the junction tree graph and to the global Markov property of the graph. A junction tree probability distribution is defined as a product and division of marginal probability distributions as follows:

\[
P(X) = \frac{\prod_{C \in C} P(X_C)}{\prod_{S \in S} [P(X_S)]^{\nu_S-1}},
\]

where \( C \) is the set of clusters of the junction tree, \( S \) is the set of separators, \( \nu_S \) is the number of those clusters which contain the separator \( S \). We emphasize here that the equalities written as \( P(X) = f(P(X_K), K \in C) \), where \( f : \Omega_X \rightarrow R \) hold for any possible realization of \( X \).

**Example 1** The probability distribution corresponding to Figure 1 is:

\[
P (X) = \frac{P(X_{\{1,3,5\}})P(X_{\{2,3,4\}})P(X_{\{3,4,5\}})}{P(X_{\{2,3\}})P(X_{\{1,4\}})} = \frac{P(X_1,X_2,X_5)P(X_2,X_3,X_4)P(X_3,X_4,X_5)}{P(X_2,X_5)P(X_3,X_4)}.
\]
In our paper [18] we introduced a special kind of $k$-width junction tree, called $k$-th order $t$-cherry junction tree in order to approximate a joint probability distribution. The $k$-th order $t$-cherry junction tree probability distribution is associates to the $k$-th order $t$-cherry tree, introduced in [4], [5].

Definition 1 The recursive construction of the $k$-th order $t$-cherry tree:

- (i) The complete graph of $(k - 1)$ nodes from $V$ represent the smallest $k$-th order $t$-cherry tree;
- (ii) By connecting a new vertex $i_k \in V$, with all $\{i_1, \ldots, i_{k-1}\}$ vertices of a $(k - 1)$-dimensional complete subgraph of the existing $k$-th order $t$-cherry tree, we obtain a new $k$-th order $t$-cherry tree. $\{\{i_k\} \{i_1, \ldots, i_{k-1}\}\}$ is called $k$-th order hypercherry.
- (iii) A $k$-th order $t$-cherry tree can be obtained from (i) by successive application of (ii).

The $k$-th order $t$-cherry tree is a special triangulated graph therefore a junction tree structure is associated to it.

Definition 2 ([18]) The $k$-th order $t$-cherry junction tree is defined in the following way:

- By using Definition 1 we construct a $k$-th order $t$-cherry tree over $V$.
- To each hypercherry $\{\{i_k\} \{i_1, \ldots, i_{k-1}\}\}$ is assigned a cluster $\{i_1, \ldots, i_{k-1}, i_k\}$ which a node of the junction tree and a separator $\{i_1, \ldots, i_{k-1}\}$ which is an edge of the junction tree.

We denote by $C_{ch}$ and $S_{ch}$, the set of clusters and separators of the $t$-cherry junction tree.

Definition 3 ([18]) If the indices of the random vector $X = (X_1, \ldots, X_d)$ are assigned to a $t$-cherry junction tree structure then there exists a probability distribution called $t$-cherry junction tree probability distribution given by:

\[
P_{t-ch}(X) = \frac{\prod_{C \in C_{ch}} P(X_C)}{\prod_{S \in S_{ch}} (P(X_S))^{\nu_{S}} - 1}.
\]

Remark 1 The marginal probability distributions involved in the above formula are marginal probability distributions of $P(X)$.

Example 1 shows a 3-rd order $t$-cherry junction tree probability distribution.

In the following instead of probability distribution associated to a junction tree we will use shortly junction tree pd and similarly instead of $k$-th order $t$-cherry tree junction tree distribution we will use shortly $k$-th order $t$-cherry pd. Recently we found a paper [16] where Malvestuto introduced the same junction tree pd structure in a different way and named it elementary model of rank $k$.

The graph underlying the Markov network is usually unknown, the task of the following section is to give a greedy algorithm, for finding a junction tree starting from the $k$-th order marginal distributions, which are supposed to be known.
3 Szántai-Kovács’s greedy algorithm for finding an approximating junctoin tree probability distribution

The problem is finding a $k$-width junction tree pd which gives the best approximation for a discrete probability distribution $P(X)$. The goodness of the approximation is quantified by the Kullback-Leibler divergence, which have to be minimized:

$$KL(P(X), P_a(X)) = \sum_X P(X) \log_2 \frac{P(X)}{P_a(X)} \to \min.$$ 

This minimization problem for $k > 2$ can be solved in exact way only by exhaustive search [17]. For $k=2$ the problem can be solved using Kruskal’s algorithm, as was first proposed by Chow and Liu [6].

Malvestuto [16] and Szántai et.al. [19] proved independently and in different ways the following statement: If $P_k(X)$ is a $k$-width junction tree pd approximation then there exists $P_{t-ch}^k(X)$ a $k$-th order $t$-cherry tree pd which gives at least as good approximation as $P_k(X)$ does i.e.:

$$KL(P(X), P_k(X)) \geq KL(P(X), P_{t-ch}^k(X)).$$

Hence this result we consider as search space the $k$-th order $t$-cherry junction tree pd’s.

In this part we first give a greedy algorithm to minimize the Kullback-Leibler divergence between the true probability distribution and a $t$-cherry junction tree pd given the $k$-th order marginal probability distributions. We then compare our algorithm with Malvestuto’s algorithm from analytical point of view. Then we apply the two algorithms to the same sample data proposed in [16].

In [18] the authors give the following theorem.

**Theorem 2** The Kullback-Leibler divergence between the true $P(X)$ and the approximation given by the $k$-width junction tree probability distribution $P(X_j)$, determined by the set of clusters $C$ and the set of separators $S$ is:

$$KL(P(X), P_j(X)) = -H(X) - \left( \sum_{C \in C} I(X_C) - \sum_{S \in S} (\nu_S - 1) I(X_S) \right) + \sum_{i=1}^d H(X_i),$$

where $I(X_C) = \sum_{i \in C} H(X_i) - H(X_C)$ represents the information content of the random vector $X_C$ and similarly $I(X_S) = \sum_{i \in S} H(X_i) - H(X_S)$ represents the information content of the random vector $X_S$.

In Formula (1) $-H(X) + \sum_{i=1}^d H(X_i) = I(X)$ is independent from the structure of the junction tree. It is easy to see that minimizing the Kullback-Leibler divergence means maximizing $\sum_{C \in C} I(X_C) - \sum_{S \in S} (\nu_S - 1) I(X_S)$. We call this sum as weight of the junction tree pd. As larger this weight is, as better fits the approximation associated to the junction tree pd to the true probability distribution. It is well known that $KL = 0$ if $P(X) = P_j(X)$.
In the case when the approximating probability distribution is given by a \( k \)-th order \( t \)-cherry junction tree pd all of the clusters contain \( k \) and all of the separators contain \( k - 1 \) vertices in Formula (1).

Let \( X = \{X_1, \ldots, X_d\} \) a set of random variables.

**Definition 4** We define the following concepts:

– the search space:
\[
E = \{x_{i_1, \ldots, i_{k-1}} = \{X_{i_k} \}, \{X_{i_1}, \ldots, X_{i_{k-1}}\}\} | X_{i_1}, \ldots, X_{i_{k-1}}, X_{i_k} \in X,\]
– the independence set:
\[
\mathcal{F} = \phi \cup \{t - \text{cherry junction tree structure}\},
\]
– the weight function:
\[
w : E \to R \quad w \left( x_{i_1, \ldots, i_{k-1}} \right) = I \left( X_{i_1}, \ldots, X_{i_{k-1}}, X_{i_k} \right) - I \left( X_{i_1}, \ldots, X_{i_{k-1}} \right).
\]

**Algorithm 2** Szántai-Kovács’s greedy algorithm.

**Input:** Elements of \( E \) and their weights which can be calculated based on the \( k \)-th order marginal probability distributions.

**Output:** set \( A \) which contains the clusters of the \( k \)-th order \( t \)-cherry junction tree pd and the weight of the \( k \)-th order \( t \)-cherry junction tree pd.

**The algorithm:**

\[
A := \phi
\]

Sort \( E \) into monotonically decreasing order by weight \( w \);

Choose \( x = \arg \max_{x \in E} \left( w \left( x \right) \right) \);

let \( A := A \cup \{x\} \); \( E := E \setminus \{x\} \); \( w := I \left( x \right) \);

Do for each \( x \in E \) taken in monotonically decreasing order

if \( A \cup \{x\} \in \mathcal{F} \) then let \( A := A \cup \{x\} \); \( E := E \setminus \{x\} \); \( w := w + w \left( x \right) \);

if the union of subsets of \( A \) is \( X \), then Stop;

else take the next element of \( E \).

In our \( t \)-cherry junction tree terminology the KL divergence formula used by Malvestuto in his paper \[16\] is:

\[
KL \left( P \left( X \right), P_{t-ch} \left( X \right) \right) = -H \left( X \right) + \sum_{C \in \mathcal{C}} H \left( X_C \right) - \sum_{S \in \mathcal{S}} \left( \nu_S - 1 \right) H \left( X_S \right). \quad (2)
\]

In order to minimize the KL divergence Malvestuto had to minimize

\[
\sum_{C \in \mathcal{C}} H \left( X_C \right) - \sum_{S \in \mathcal{S}} \left( \nu_S - 1 \right) H \left( X_S \right)
\]

in a greedy way.

Malvestuto’s algorithm uses the same search space \( E \) and independence set \( F \). The weight function however is different:

\[
\omega : E \to R \quad \omega \left( x_{i_1, \ldots, i_{k-1}} \right) = H \left( X_{i_1}, \ldots, X_{i_{k-1}}, X_{i_k} \right) - H \left( X_{i_1}, \ldots, X_{i_{k-1}} \right).
\]
Algorithm 3 Malvestuto’s greedy algorithm.

**Input:** Elements of E and their weights which can be calculated based on the k-th order marginal probability distributions.

**Output:** set A which contains the clusters of the k-th order t-cherry junction tree probability distribution and the weight of the k-th order t-cherry junction tree.

A := φ

Sort E into monotonically increasing order by weight \( w \);

Chose \( x = \arg \min_{x \in E} (H(x)) \);

let \( A := A \cup \{x\} \); \( E := E \setminus \{x\} \); \( \omega := H(x) \);

Do for each \( x \in E \) taken in monotonically increasing order

if \( A \cup \{x\} \in F \) then let \( A := A \cup \{x\} \); \( E := E \setminus \{x\} \); \( \omega := \omega + H(x) \);

if the union of subsets of \( A \) is \( X \), then Stop;

else take the next element of \( E \).

We present experimental results on the application of the two algorithms to the probability distribution obtained from the sample data published in the paper [16]. These data contain informations on the structural habitat of grahami and opalinus lizards. They were published originally by Bishop et al [3] and we give them in Table 1.

| Cell \((X_1, X_2, X_3, X_4, X_5)\) | Observed | Cell \((X_1, X_2, X_3, X_4, X_5)\) | Observed |
|----------------------------------|----------|----------------------------------|----------|
| 1 1 1 1 1 | 20       | 1 2 2 3 1 | 8        |
| 2 1 1 1 1 | 13       | 2 2 2 3 1 | 4        |
| 1 2 1 1 1 | 8        | 1 1 1 2 2 | 2        |
| 2 2 1 1 1 | 6        | 1 2 1 1 2 | 3        |
| 1 1 2 1 1 | 34       | 1 1 2 1 2 | 11       |
| 2 1 2 1 1 | 31       | 2 1 2 1 2 | 5        |
| 1 2 2 1 1 | 17       | 1 2 2 1 2 | 15       |
| 2 2 2 1 1 | 12       | 2 2 2 1 2 | 1        |
| 1 1 1 2 1 | 8        | 1 1 1 2 2 | 1        |
| 2 1 1 2 1 | 8        | 1 2 1 2 2 | 1        |
| 1 2 1 2 1 | 4        | 1 1 2 2 2 | 20       |
| 1 1 2 2 1 | 69       | 2 1 2 2 2 | 4        |
| 2 1 2 2 1 | 55       | 1 2 2 2 2 | 32       |
| 1 2 2 2 1 | 60       | 2 2 2 2 2 | 5        |
| 2 2 2 2 1 | 21       | 1 1 1 3 2 | 4        |
| 1 1 1 3 1 | 4        | 1 2 1 3 2 | 3        |
| 2 1 1 3 1 | 12       | 2 2 1 3 2 | 1        |
| 1 2 1 3 1 | 5        | 1 1 2 3 2 | 10       |
| 2 2 1 3 1 | 1        | 2 1 2 3 2 | 3        |
| 1 1 2 3 1 | 18       | 1 2 2 3 2 | 8        |
| 2 1 2 3 1 | 13       | 2 2 2 3 2 | 4        |

The data consists of observed counts for perch height \(< 2' \) or \( \geq 2' \)-- \( X_1 \), perch diameter \(< 5'' \) or \( \geq 5'' \)-- \( X_2 \), insolation (sun, shade)-- \( X_3 \), time of day categories (early, midday, late)-- \( X_4 \), lizard type (grahami, opalinus)-- \( X_5 \). The size of the contingency table is \( 2 \times 2 \times 2 \times 3 \times 2 \).

First we compare the goodness of fit of the 4-th order t-cherry junction tree found by Szántai-Kovács’s algorithm, then by Malvestuto’s algorithm.
In Table 2 one can see the information contents of the marginal probability distribution of 4 random variables, 3 random variables and the weights used in Szántai-Kovács’s algorithm, ordered in decreasing way.

Table 2 Illustration of Szántai–Kovács’s algorithm

| Indices of the cluster variables | Indices of the separator variables | \( I(X_C) \) | \( I(X_S) \) | \( I(X_C) - I(X_S) \) |
|----------------------------------|-----------------------------------|-------------|-------------|------------------|
| 1 3 4 5                          | 1 3 5                             | 0.129381    | 0.045701    | 0.083680         |
| 1 3 4 5                          | 1 4 5                             | 0.129381    | 0.047533    | 0.081848         |
| 2 3 4 5                          | 2 3 5                             | 0.116608    | 0.035137    | 0.081470         |
| 1 2 3 4                          | 1 2 3                             | 0.105531    | 0.026624    | 0.078907         |
| 1 2 3 4                          | 1 2 4                             | 0.100251    | 0.029315    | 0.070936         |
| 1 3 4 5                          | 1 3 4                             | 0.129381    | 0.066088    | 0.063294         |
| 1 2 3 5                          | 1 2 3                             | 0.089070    | 0.026624    | 0.062446         |
| 1 2 4 5                          | 2 4 5                             | 0.100251    | 0.038063    | 0.062160         |
| 1 2 3 5                          | 2 3 5                             | 0.089070    | 0.035137    | 0.053933         |
| 1 2 4 5                          | 1 4 5                             | 0.100251    | 0.047533    | 0.052718         |

The junction tree obtained by Szántai-Kovács’s algorithm has two clusters \( \{1, 3, 4, 5\} \), \( \{1, 2, 4, 5\} \) and one separator \( \{1, 4, 5\} \). The KL divergence in this case is:

\[
KL = I(X) - (I(X_{\{1,3,4,5\}}) - I(X_{\{1,4,5\}}) + I(X_{\{1,2,4,5\}}))
\]

\[
= 0.19519 - (0.129381 - 0.045701 + 0.100251) = 0.013091
\]

In Table 3 one can see the entropy of the marginal probability distribution of 4 random variables, 3 random variables and the weights used in Malvestuto’s algorithm, ordered in increasing way.

The junction tree obtained by Malvestuto’s algorithm has two clusters \( \{1, 2, 3, 5\} \), \( \{1, 3, 4, 5\} \) and one separator \( \{1, 4, 5\} \). The KL divergence in this case is:

\[
KL = -H(X) + H(X_{\{1,2,3,5\}}) - H(X_{\{1,3,5\}}) + H(X_{\{1,3,4,5\}})
\]

\[
= -4.64164 + 3.288813 - 2.36849 + 3.743757 = 0.02244
\]

Table 3 Illustration of Malvestuto’s algorithm

| Indices of the cluster variables | Indices of the separator variables | \( H(X_C) \) | \( H(X_S) \) | \( H(X_C) - H(X_S) \) |
|----------------------------------|-----------------------------------|-------------|-------------|------------------|
| 1 2 3 5                          |                                  | 3.288813    |              |                  |
| 1 3 4 5                          | 1 3 5                             | 3.743757    | 2.368490    | 1.375267         |
| 2 3 4 5                          | 2 3 5                             | 3.783647    | 2.406170    | 1.377478         |
| 1 2 3 4                          | 1 2 3                             | 3.943287    | 2.563246    | 1.380041         |
| 1 2 4 5                          | 1 2 5                             | 4.046977    | 2.615873    | 1.431104         |

The two results of KL divergence reflect that the junction tree obtained by our algorithm fits better to the probability distribution of the sample data.
If the task is fitting a third order $t$-cherry junction tree, then our algorithm finds a $t$-cherry junction tree probability distribution, with $KL = 0.0355415$. The third order $t$-cherry junction tree given by Malvestuto’s algorithm has the $KL = 0.0375077$. The clusters found by our algorithm were $\{3, 4, 5\}, \{1, 4, 5\}, \{1, 2, 5\}$ and those found by Malvestuto’s algorithm were $\{1, 3, 5\}, \{1, 2, 5\}, \{3, 4, 5\}$.

4 Theorems related to the Szántai-Kovács’s algorithm

This part contains some theoretical discussions on the algorithm introduced, regarding assumptions related to the Markov network underlying the variables.

As we remind in the preliminary part a triangulated graph can be represented as a junction tree structure. If the graph is complete then the junction tree has only one cluster.

If a graph is not triangulated, then by adding edges it can be transformed into a triangulated graph. The problem of „fill in as few edges as possible“ is known to be NP complete ([21]). A greedy algorithm was given by Tarjan and Yanakakis [20].

If the vertices of a graph represent the indices of the random variables of a Markov network with global Markov property then by adding new edges to the graph results a Markov network having the global Markov property, too.

If the graph associated to a Markov network is not complete then it can be transformed into a triangulated graph by adding edges which is equivalent with a junction tree structure, let say of order $k$. Since the global Markov property holds for this graph the probability distribution can be written as a product-division type, where the largest marginal probability distribution contains $k$ variables. A logical question which arises here is if the greedy algorithm does find the $k$-th order junction tree which gives the true probability distribution. For this question the answer is that under some assumption our greedy algorithm guarantees the optimal solution, which in this context is the true probability distribution.

We need the following assertion:

Lemma 1 $H(X_1|X_2, \ldots, X_k) = H(X_1) - [I(X_1, \ldots, X_k) - I(X_2, \ldots, X_k)]$.

Proof

\[
H(X_1|X_2, \ldots, X_k) = H(X_1, X_2, \ldots, X_k) - H(X_2, \ldots, X_k) \\
= H(X_1, X_2, \ldots, X_k) - \sum_{i=1}^{k} H(X_i) \\
- \left( H(X_2, \ldots, X_k) - \sum_{i=2}^{k} H(X_i) \right) + H(X_1) \\
= H(X_1) - (I(X_1, X_2, \ldots, X_k) - I(X_2, \ldots, X_k)).
\]

Remark 2. It is easy to see that maximizing $I(X_1, \ldots, X_k) - I(X_2, \ldots, X_k)$ is the same as maximizing $H(X_1) - H(X_1|X_2, \ldots, X_k)$.

We introduce the following notations.

Let $K = \{ K = \{i_1, \ldots, i_k\} | i_1, \ldots, i_k \in V \}$ be the set of all possible $k$-element subsets of $V$.

Let $M_K : K \to R$ be defined as $M_K = \max_{i \in K} \{ I(X_K) - I(X_{K-\{i\}}) \}$ and let
\[ K^* = \arg \max_{K \in \mathcal{K}} M_K. \] (3)

We prove the following two theorems.

**Theorem 3** If \( X \) has a \( k \)-th order \( t \)-cherry tree representation then \( K^* \) is a cluster of the junction tree.

**Proof** We make the proof by contradiction. We suppose \( K^* = \{i_1, \ldots, i_k\} \notin \mathcal{C} \). Let us consider the smallest subjunction tree which contains all the vertices \( i_1, \ldots, i_k \) at least once. In this subjunction tree one of the vertices \( i_1, \ldots, i_k \) is a simplicial vertex (a vertex which is contained in one cluster only). For simplicity let this vertex be \( i_1 \) and the cluster which contains it \( \{i_1, s_1, \ldots, s_{k-1}\} \), with \( \{s_1, \ldots, s_{k-1}\} \neq \{i_2, \ldots, i_k\} \).

We emphasize here that it is not necessary that \( \{s_1, \ldots, s_{k-1}\} \cap \{i_2, \ldots, i_k\} = \emptyset \).

Since \( i_1 \) is a simplicial vertex \( X_{i_1} \) depends on all the other random variables of the subjunction tree only through its neighbours \( X_{s_1}, \ldots, X_{s_{k-1}} \), therefore

\[ H(X_{i_1}|X_{s_1}, \ldots, X_{s_{k-1}}) < H(X_{i_1}|X_{i_2}, \ldots, X_{i_k}). \]

Using Lemma this inequality is equivalent to:

\[
H(X_{i_1}) - \left[I(X_{i_1}, X_{s_1}, \ldots, X_{s_{k-1}}) - I(X_{s_1}, \ldots, X_{s_{k-1}})\right]
< H(X_{i_1}) - \left[I(X_{i_1}, X_{i_2}, \ldots, X_{i_k}) - I(X_{i_2}, \ldots, X_{i_k})\right]
\]

that is

\[
I(X_{i_1}, X_{s_1}, \ldots, X_{s_{k-1}}) - I(X_{s_1}, \ldots, X_{s_{k-1}}) > I(X_{i_1}, X_{i_2}, \ldots, X_{i_k}) - I(X_{i_2}, \ldots, X_{i_k})
\]

which is in contradiction with the hypothesis that \( \{i_1, \ldots, i_k\} = K^* \).

In the following we introduce the so called puzzle-algorithm, which results a special numbering of the vertices of \( t \)-cherry junction tree.

**Algorithm 4** Puzzle algorithm.

**Input:** a \( k \)-th order \( t \)-cherry junction tree \( H(V, \Gamma) \), (acyclic hypergraph with edges of size \( k \), and separators of size \( k-1 \))

**Output:** a numbering \( \{i_1, \ldots, i_d\} \) of the vertices of \( V = \{1, \ldots, d\} \).

**Step 1. Initialization.**

Let \( e_i \in \Gamma \), call it parent edge. The vertices belonging to the parent edge are numbered in an arbitrary order by \( i_1, \ldots, i_k \).

\[ s := k, \ S_s := \{S_{i_1}, \ldots, S_{i_k}\}, \text{ where for } j = 1, \ldots, k, S_{i_j} \text{ are all the } k-1 \text{ element subset of } e_i. \]

**Step 2. Iteration.**

Do \( \Gamma = \Gamma \setminus e_i \).

Do if \( \Gamma \neq \emptyset \) then take \( e_i \in \Gamma \), which contains one of the elements \( S \) of \( S_s \).

Set \( s := s + 1 \),

assign \( i_s \) to \( i = e_i \setminus S \).

\[ S_s = S_{s-1} \cup \{S_{i_1}, \ldots, S_{i_k}\}, \text{ where for } j = 1, \ldots, k, S_{i_j} \text{ are all the } k-1 \text{ element subset of } e_i. \] Go to Step 2.

else Stop.
Definition 5 The numbering \( \{i_1, \ldots, i_d\} \) of the vertices of \( V = \{1, \ldots, d\} \), obtained using Algorithm 4, is called puzzle numbering.

Theorem 4 If the following two assumptions are fulfilled then the Szántai-Kovács algorithm finds the true probability distribution.

(i) The Markov network can be transformed into a \( k \)-th order \( t \)-cherry tree by adding some edges if it is necessary.

(ii) Starting from the parent cluster defined by (3) there exists a puzzle numbering with the following property: for all \( i_r < i_s \) and for any \( S \in S_r \)

\[
H(X_{i_r}) - H(X_{i_r}|S) < H(X_{i_r}) - H(X_{i_r}|S_{i_r}),
\]

where \( S_{i_r} \) is the separator which separates \( i_r \) from the tree containing the vertices \( \{i_1, \ldots, i_{r-1}\} \).

Proof We proved in Theorem 3 that the cluster \( K^* \) which satisfies (3) is a cluster of the junction tree associated to the Markov network. We choose this cluster as parent edge.

Let us suppose that the Szántai-Kovács Algorithm, has in the constructed junction tree already \( m-1 \) verticies. We denote this set of verticies by \( V_{m-1} \). The set of possible separators at this end is \( S_{m-1} \).

The Szántai-Kovács algorithm adds a new cluster by maximizing

\[
I(X_{i_m}, X_{S_i}) - I(X_{S_i}), \text{ where } i_m \in V \setminus V_{m-1} \text{ and } S_i \in S_{m-1}
\]

According to Remark 4 this is equivalent with maximizing

\[
H(X_{i_m}) - H(X_{i_m}|S_{i}), \text{ where } i_m \in V \setminus V_{m-1} \text{ and } S_i \in S_{m-1}.
\]

(4)

We suppose now by contradiction that \( i_m \) is not connected to the existing junction tree through \( S_i \). Since the junction tree is a connected hypergraph, there exist two possibilities:

1. \( i_m \) is separated from the existing tree \( T_{m-1} \) by another separator \( S_j \in S_{m-1} \);
2. There exists \( i_n \in V \setminus V_{m-1} \) which is connected with the existing junction tree by \( S_i \in S_{m-1} \), and the cluster \( (S_i, i_n) \) is on the path between the existing tree \( T_{m-1} \) and the cluster which contains \( i_m \).

Now we pove that none of the two possibilities can occur.

1. If \( i_m \) is separated from the existing tree \( T_{m-1} \) by another separator \( S_j \in S_{m-1} \) then according to the global Markov property we have:

\[
P(X_{T_{m-1}}, X_{i_m}) = \frac{P(X_{T_{m-1}}) P(X_{S_j}, X_{i_m})}{P(X_{S_j})}.
\]

This implies that the Kullback Leibler between

\[
P(X_{T_{m-1}}, X_{i_m}) \text{ and } \frac{P(X_{T_{m-1}}) P(X_{S_j}, X_{i_m})}{P(X_{S_j})}
\]

is 0:

\[
KL = I(X_{T_{m-1}}, X_{i_m}) - \left( I(X_{T_{m-1}}) + I(X_{S_j}, X_{i_m}) - I(X_{S_j}) \right) = 0.
\]
Thus
\[ I(X_S, X_{i_m}) - I(X_T, X_{i_m}) = I(X_{T_{m-1}}, X_{i_m}) - I(X_{T_{m-1}}). \] (5)
On the other hand if \( S_i \) does not separate \( i_m \) from the existing tree then the KL between
\[ P(X_{T_{m-1}}, X_{i_m}) \quad \text{and} \quad \frac{P(X_{S_i}, X_{i_m})}{P(X_{S_i})} \]
is positive:
\[ KL = I(X_{T_{m-1}}, X_{i_m}) - (I(X_{T_{m-1}}) + I(X_{S_i}, X_{i_m}) - I(X_{S_i})) > 0. \]
Thus
\[ I(X_{S_i}, X_{i_m}) - I(X_{S_i}) < I(X_{T_{m-1}}, X_{i_m}) - I(X_{T_{m-1}}). \] (6)
From (5) and (6) we have \( I(X_{S_i}, X_{i_m}) = I(X_{S_i}) < I(X_{S_j}, X_{i_m}) - I(X_{S_j}). \)
According to Remark 1 this implies
\[ H(X_{i_m}) - H(X_{i_m}|X_{S_i}) < H(X_{i_m}) - H(X_{i_m}|X_{S_j}) \]
which is in contradiction with maximization of (4).

2. If on the path between the existing \( T_{m-1} \) tree and the cluster which contains \( i_m \) there exists a cluster \( (S_i, i_n) \), where \( i_n \in V \setminus V_{m-1} \) and \( S_i \in \mathcal{S}_{m-1} \), then according to the puzzle numbering \( i_n < i_m \). Using and (ii) we have:
\[ H(X_{i_m}) - H(X_{i_m}|S) \quad \text{and} \quad H(X_{i_m}) - H(X_{i_m}|S_i) \]
for any \( S \in \mathcal{S}_{m-1} \), and \( S_i \in \mathcal{S}_{m-1} \) separator between \( i_m \) and the existing tree \( T_{m-1} \). This is in contradiction with maximization of (4).

**Theorem 5** If the the best approximating \( k \)-th order \( t \)-cherry probability distribution has a puzzle numbering which starting from the parent cluster defined by (3) satisfies (i) and (ii) then the Szántai-Kovács Algorithm finds the best approximating \( k \)-th order \( t \)-cherry probability distribution.

i) for all \( i_r < i_s \), for any \( S \in \mathcal{S}_r \), \( H(X_{i_r}) - H(X_{i_r}|S) < H(X_{i_r}) - H(X_{i_r}|S_i) \), where \( S_i \in \mathcal{S}_r \) is the separator which separates \( i_r \) from the tree containing the vertices \( \{i_1, \ldots, i_{r-1}\} \)

ii) for all \( i_r > k \)
\[ X_{i_r} = \arg \min_{i \in V \setminus \{i_1, \ldots, i_{r-1}\}} KL(P_{app}(X_{i_1}, \ldots, X_{i_{r-1}}, X_i), P(X_{i_1}, \ldots, X_{i_{r-1}}, X_i)) \]

**Proof** Let the cluster \( K^* \) which satisfies (3) the first cluster of the junction tree. We choose this cluster as parent edge.

Let us suppose that the Szántai-Kovács Algorithm, has in the constructed junction tree already \( m - 1 \) vertices. The set of possible separators at this end is \( \mathcal{S}_{m-1} \).

The Szántai-Kovács algorithm adds a new cluster by maximizing
\[ I(X_{i_m}, X_{S_i}) = I(X_{T_{m-1}}, X_{i_m}) \]
According to Remark 1 this is equivalent with maximizing
\[ H(X_{i_m}) - H(X_{i_m}|S_i) \]
We suppose now by contradiction that in the best approximating junction tree \( i_m \) is not connected to the existing junction tree through \( S_i \). Since the best approximating junction tree is a connected hypergraph there exist two possibilities:
1. $i_m$ is separated from the existing tree $T_{m-1}$ by another separator $S_j \in S_{m-1}$;
2. In the best approximating junction tree there exists $i_n \in V \setminus V_{m-1}$ which is connected with the existing junction tree by $S_i \in S_{m-1}$, and the cluster $(S_i,i_n)$ is on the path between the existing tree and the cluster which contains $i_m$.

Now we prove that none of the two possibilities can occur.

1. If $i_m$ is separated from the existing tree $T_{m-1}$ by another separator $S_j$ then according to the Markov property we have:

$$P^j_{\text{app}}(X_{T_{m-1}},X_{i_m}) = \frac{P(X_{T_{m-1}})P(X_{S_j}X_{i_m})}{P(X_{S_j})}.$$  

This implies that the Kullback Leibler between

$$P \left( X_{T_{m-1}}, X_{i_m} \right) \text{ and } P^j_{\text{app}} \left( X_{T_{m-1}}, X_{i_m} \right)$$

is given by:

$$KL \left( P^j_{\text{app}} \left( X_{T_{m-1}}, X_{i_m} \right), P \left( X_{T_{m-1}}, X_{i_m} \right) \right) \leq I \left( X_{T_{m-1}}, X_{i_m} \right) - \left( I \left( X_{T_{m-1}} \right) + I \left( X_{S_j}, X_{i_m} \right) - I \left( X_{S_j} \right) \right)$$

According to (7)

$$I \left( X_{S_i}, X_{i_m} \right) - I \left( X_{S_j} \right) < I \left( X_{S_i}, X_{i_m} \right) - I \left( X_{S_j} \right)$$

and this implies that

$$KL \left( P^j_{\text{app}} \left( X_{T_{m-1}}, X_{i_m} \right), P \left( X_{T_{m-1}}, X_{i_m} \right) \right) \leq I \left( X_{T_{m-1}}, X_{i_m} \right) - \left( I \left( X_{T_{m-1}} \right) + I \left( X_{S_j}, X_{i_m} \right) - I \left( X_{S_j} \right) \right) < KL \left( P^j_{\text{app}}, P \right) .$$

This is in contradiction with (ii).

2. If on the path between the existing $T_{m-1}$ tree and the cluster which contains $i_m$ there exists a cluster $(S_i,i_n)$, where $i_n \in V \setminus V_{m-1}$ and $S_i \in S_{m-1}$, then according to the puzzle numbering $i_n < i_m$ and (i) we have:

$$H \left( X_{i_m} \right) - H \left( X_{i_m} \mid S \right) < H \left( X_{i_n} \right) - H \left( X_{i_n} \mid S_{i_n} \right)$$

for any $S \in S_{m-1}$, and $S_{i_n} \in S_{m-1}$ separator between $i_n$ and the existing tree $T_{m-1}$. This is in contradiction with maximizing (8).
5 Conclusions

We give in this paper a greedy algorithm for fitting $k$-width junction tree approximation by minimizing the Kullback-Leibler divergence. The problem of finding the best approximation of this kind is generally an NP-hard problem. We reduce the search space to the so called $k$-th order $t$-cherry junction tree probability distributions. We then compare our algorithm to Malvestuto’s algorithm. We proved that our algorithm in the first step finds a cluster which belongs to the junction tree. Malvestuto’s algorithm has not guarantee for this. Beside this our formula for Kullback-Leibler divergence detached a greater part which does not depend on the structure of the tree than Malvestuto’s formula.

We proved that under some assumptions our algorithm finds the optimal solution.

By discovering the $t$-cherry junction tree probability distribution assigned to a Markov network we can obtain many information on the dependence structure underlying the random variables. This information can be used for storing the data in lower dimensional contingency tables. The method can be applied in classification problems where it is possible to select the ”informative” variables which influence directly the classification variable, see [19].

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