Bayesian Networks

5. Exact Inference / Clustering

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1. Trees
   2. Cluster Trees
   3. Recursive Computation of Link Potentials
   4. Clique (Cluster) Trees
   5. Triangulation
Components and cycles

**Definition 1.** Let $G$ be an undirected graph. $G$ is called **connected**, if there is a path from any vertex to any other vertex:

$$G^*(v, w) \neq \emptyset, \quad \forall v, w \in V$$

For a vertex $v \in V$ we call

$$\text{comp}_G(v) := \{w \mid G^*(v, w) \neq \emptyset\}$$

the *(connection) component of* $v$ in $G$.

A proper path $p = (v_1, \ldots, v_n)$ is called **cyclic**, if $v_1 = v_n$ and $v_i$ are pairwise different otherwise:

$$v_i = v_j \iff i = 1 \text{ and } j = n$$

A proper path $p = (v_1, \ldots, v_n)$ is called **simple**, if $v_i$ are pairwise different.

An undirected graph $G$ is called **acyclic**, if it does not contain a cyclic path.

Trees

**Definition 2.** An undirected graph $G$ is called **unrooted/undirected tree**, if

(i) it is connected and acyclic

or equivalently

(ii) there is exactly one simple path between any two vertices:

$$|G_{\text{simple}}^*(v, w)| = 1, \quad \forall v, w \in V$$

The unique simple path between $v$ and $w$ is denoted by $\text{path}_G(v, w)$.

A directed graph $G$ is called **rooted/directed tree**, if every vertex but one (called root) has exactly one parent and the root has no parents:

$$\exists r \in V : \text{pa}(r) = \emptyset \text{ and } \forall v \in V, v \neq r : |\text{pa}(v)| = 1$$

Rooted trees are special DAGs.
Definition 3. Let $G = (V, E)$ be an unrooted tree and $r \in V$ any vertex. Then the directed graph $\text{tree}(G, r) := (V, E')$ with 
\[ E' := \{(v, w) \mid \{v, w\} \in E, |\text{path}(r, v)| < |\text{path}(r, w)|\} \]
is called tree rooted at $r$ of $G$. Obviously the tree rooted at $r$ is a rooted tree with root $r$.

For an unrooted tree the vertices with only one neighbor are called leaves.

For a rooted tree vertices other than the root with only one neighbor are called leaves; the root is called a leaf if it is the only vertex of the tree.

Definition 4. Let $G$ be a DAG (e.g., a rooted tree). The length of the longest path is called the depth of $G$ and denoted by $\text{depth}(G)$.

Let $G := (V, E)$ be a DAG (e.g., a rooted tree). A map 
\[ \lambda : V \to \mathbb{N} \]
is called level map of $G$ if 
\[ \lambda(v) > \lambda(\text{pa}(v)), \quad \forall v \in V \]
For a rooted tree $G := (V, E)$ with root $r$, 
\[ \text{depth}(v) := |\text{path}(r, v)| \]
and 
\[ \text{height}(v) := \text{depth}(G) - \max\{|p| \mid w \in V \text{ leaf}, p \in G^*(v, w), r \notin p\} + 1 \]
are examples for level maps.
Definition 5. Let $G := (V, E)$ be an undirected graph. The set
$$L_G := \{(v, w) \mid \{v, w\} \in E\}$$
is called its set of links.

Definition 6. A directed graph $G$ is called polytree, if for each vertex $r$ without parents (called a root) its descendants $\text{desc } r \cup \{r\}$ form a tree.

or equivalently

if every vertex has at most one parent that is not a root (i.e., has parents itself).

Figure 8: A polytree with roots $A$ and $B$. 
Definition 7. Let \( V \) be a set (of variables).
An unrooted tree \( G := (V, E) \) on \( V \subseteq \mathcal{P}(V) \) is called a **cluster tree on** \( V \), if

(i) the induced subgraph on all vertices containing a given variable \( v \), i.e.,

\[
\{ W \in V \mid v \in W \}
\]

is connected for all variables \( v \in V \).

or equivalently

(ii) for any \( U, W \in V \):

\[
U \cap W = U \cap \bigcup \text{comp}_{G \setminus \{v\}}(W)
\]

For two vertices \( U, W \) of a cluster tree \( U \cap W \) is called their **separator**.

Cluster trees are also called **join trees** and **junction trees**.

\[\{A, C\}\quad \{B, D, E\}\quad \{C, E, F\}\quad \{D\}\quad \{C, D, E\}\]

Figure 9: A cluster tree on \( V := \{A, B, C, D, E, F\} \).

\[\{A, C\}\quad \{B, D, E\}\quad \{C, E, F\}\quad \{A, D\}\quad \{C, D, E\}\]

Figure 10: Not a cluster tree.

Definition 8. Let \( V \) be a set of variables and \( Q \) be a set of potentials on \( V \).
A cluster tree \( G := (V, E) \) on \( V \) with a map

\[Q_G : V \to \mathcal{P}(Q)\]

s.t.

(i) \( \text{dom}(q) \subseteq C \) for all \( q \in Q_G(C), C \in V \),

(ii) \( \text{Im}(Q_G) \) covers \( Q \), i.e.,

\[
\bigcup_{W \in V} Q_G(W) = Q
\]

and

(iii) \( Q_G(W) \) and \( Q_G(U) \) are pairwise disjoint, i.e.,

\[
Q_G(W) \cap Q_G(U) \neq \emptyset \Rightarrow W = U, \quad \forall W, U \in V
\]

is called a **cluster tree for** \( Q \).

\[Q := \{p(D), p(B), p(C|D), p(E|D, B), p(A|C), p(F|C, E)\}\]

are the conditional probabilities of the bayesian network

A cluster tree for \( Q \) is, e.g.,

\[\{B, D, E\} \quad p(B), p(E|B, I)\]

\[p(A|C) \quad \{A, C\} \quad \{C, D, E\} \quad p(C|D)\]

\[p(D) \quad \{D\} \quad \{C, E, F\} \quad p(F|C, E)\]
A simple cluster tree for polytree Bayesian networks

Let $G$ be a directed graph. For $v \in V$

$$\text{fam}(v) := \{v\} \cup \text{pa}(v)$$

is called the family of $v$.

Let $(G = (V,E), (p_v)_{v \in V})$ be a polytree Bayesian network. Let

$$V := \{\text{fam}(v) \mid v \in V\}$$

and

$$F := \{(\text{fam}(\text{pa}(v)), \text{fam}(v)) \mid v \in V, \text{pa}(v) \neq \emptyset\}$$

Then $H := (V,F)$ is a cluster tree for $Q := \{p_v \mid v \in V\}$ called family tree.

Clique cluster tree for Markov networks

Markov networks $(G,(q_C)_{C \in \mathcal{C}(G)})$ use potentials on cliques to specify the JPD. If $G$ is triangulated, it allows a chain of cliques, i.e., an ordering $C_1, \ldots, C_n$ of the cliques that satisfies the running intersection property:

$$C_i \cap \bigcup_{j<i} C_j \subseteq C_{k(i)}, \quad \forall i \exists k(i) < i$$

We can construct the clique (cluster) tree $H := (V,F)$ from

$$V := \mathcal{C}(G) = \{C_1, \ldots, C_n\}$$

and

$$F := \{(C_{k(i)}, C_i) \mid i = 2, \ldots, n\}$$

We will later address the problem of cluster trees for non-triangulated Markov networks.
Cluster trees for Bayesian networks can be constructed by a two phase approach:

(i) construct an equivalent Markov network representation of the Bayesian network,

(ii) construct the clique cluster tree for the Markov network.

An equivalent Markov network for a Bayesian network \( G = (V, E), (p_v)_{v \in V} \) can be constructed by

\[
\text{moral}(G)
\]

and assigning the conditional probabilities to cliques that contain their domain.
Let $Q$ be a set of potentials and $G$ be a cluster tree for $Q$.
Inference for all variables separately can be accomplished by
(i) adding the evidence potentials to $Q$ (and to $Q_G$),
(ii) computing the vertex marginals
$$q_V := (\prod_{q \in Q} q)_{\downarrow V}$$
(iii) computing the single variable marginals
$$q_v := (q_V)_{\downarrow v}, \text{ for } V \in \mathcal{V} \text{ with } v \in V$$
This can be done by a recursive computation of the link potentials:
$$q_{U,W} := (\prod_{q \in Q_G(\text{comp}_{G\setminus\{O\}}(U))} q)_{\downarrow U \cap W}$$
traditionally called messages.

**Lemma 1.** Vertex marginals and link potentials can be expressed by link potentials:

(i)
$$q_U = \prod_{q \in Q_G(U)} q \prod_{T \in \text{fan}(U)} q_{T,U}$$

(ii)
$$q_{U,W} = (\prod_{q \in Q_G(U)} q \prod_{T \in \text{fan}(U), T \neq W} q_{T,U})_{\downarrow U \cap W}$$

Figure 18: The link potential $q_{C,O}$ describes the potentials in the component $\text{comp}_{G\setminus\{O\}}(C)$ (orange).

Figure 19: Expressing the vertex potential $q_O$ by the link potentials $q_{.,O}$. 
Lemma 1. **Vertex marginals and link potentials can be expressed by link potentials:**

(i) \[ q_U = \prod_{q \in Q_G(U)} q \prod_{T \in \text{fan}(U)} q_{T,U} \]

(ii) \[ q_{U,W} = (\prod_{q \in Q_G(U)} q \prod_{T \in \text{fan}(U), T \neq W} q_{T,U})^{|U \cap W|} \]

Figure 20: Expressing the link potential \( q_{O,N} \) by the linkpotentials \( q_{.,O} \).

Lemma 2. The formula of the previous lemma allows the recursive computation of link potentials in a cluster tree \( G \).

**Proof.** Choose an arbitrary vertex as root and replace \( G \) by its rooted tree. Let \( \lambda \) be a level map of \( G \) and \( \lambda_{\min}, \lambda_{\max} \) its minimal and maximal values.

1. **up links (collect evidence):** induction on \( n := \lambda(U) \) for link potentials \( q_{U,\text{pa}(U)} \).

   - \( n = \lambda_{\max} \): \( U \) is a leaf and has no other neighbors other than its parent.
   - \( n \rightarrow n - 1 \): the link potentials from childs into \( U \) have already been computed by induction hypothesis. \( q_{U,\text{pa}(U)} \) can be computed (\( G \) is a tree, thus \( U \) has at most one parent).

Figure 21: Collect evidence.

Figure 22: Collect evidence.
Recursive computation of link potentials

**Lemma 2.** The formula of the previous lemma allows the recursive computation of link potentials in a cluster tree $G$.

**Proof (cont.).**

II. down links (distribute evidence): induction on $n := \lambda(\text{pa}(U))$ for link potentials $q_{\text{pa}(U),U}$.

$n = \lambda_{\text{min}}: \text{pa}(U)$ is the root. All of its neighboring link potentials have been computed by step I. $\Rightarrow q_{\text{pa}(U),U}$ can be computed.

$n \rightarrow n + 1$: the link potentials from childs into $\text{pa}(U)$ have already been computed by step I, the link potential $q_{\text{pa}(\text{pa}(U)),\text{pa}(U)}$ has already been computed by induction hypothesis. $\Rightarrow q_{\text{pa}(U),U}$ can be computed.

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**Shafer-Shenoy propagation**

The following computation scheme is called **Shafer-Shenoy propagation** []:

1. **Collect evidence**:
   
   $$q_{U,W} = \left( \prod_{q \in Q_G(U)} q \right) \prod_{T \in \text{fan}(U), T \neq W} q_{T,U} \downarrow_{U \cap W} = \left( \prod_{q \in Q_G(U)} q \right) \cdot q_{T_1,U} \cdots q_{T_n,U} \downarrow_{U \cap W}$$

2. **Distribute evidence**:

   $$q_{U,T_i} = \left( \prod_{q \in Q_G(U)} q \right) \prod_{T \in \text{fan}(U), T \neq T_i} q_{T,U} \downarrow_{U \cap T_i} = \left( \prod_{q \in Q_G(U)} q \right) \cdot q_{W,U} \cdot q_{T_1,U} \cdots q_{T_i,U} \cdots q_{T_n,U} \downarrow_{U \cap T_i}$$

3. **Marginalize**:

   $$q_U = \prod_{q \in Q_G(U)} q \prod_{T \in \text{fan}(U)} q_{T,U} = \left( \prod_{q \in Q_G(U)} q \right) \cdot q_{W,U} \cdot q_{T_1,U} \cdots q_{T_n,U}$$
The following computation scheme is called Hugin propagation []:

(i) collect evidence:

\[ q'_U = \prod_{q \in Q_G(U)} q \prod_{T \in \text{fan}(U), T \neq W} q_{T,U} = ( \prod_{q \in Q_G(U)} q ) \cdot q_{T_1,U} \cdots q_{T_n,U} \]

\[ q_{U,W} = q'_U \cap W \]

(ii) marginalize and distribute evidence:

\[ q_U = q'_U \cdot q_{W,U} \]

\[ q_{U,T_i} = \left( \frac{q_U}{q_{T_i,U}} \right) \downarrow U \cap T_i \]

but store separator marginal \((q_U) \downarrow U \cap T_i\)

Shafer-Shenoy vs. Hugin propagation

Hugin propagation compared to Shafer-Shenoy propagation:

(i) Hugin propagation allows the reuse of the storage space of the link potentials \(q_{U,W}\) for \(q_{W,U}\) (one "postbox" instead of two),

(ii) Hugin propagation affords extra storage space for the vertex potentials \(q_U\) and thus its overall space requirements are higher,

(iii) Hugin propagation requires a smaller number of total operations (additions, multiplications, divisions) than Shafer-Shenoy propagation at vertices with degree \(> 3\) (that can be avoided by the use of binary cluster trees),

(iv) Hugin propagation allows the marginalization of the smaller separator marginals,

(v) Some of the operations required by Hugin propagation are more costly (divisions) than those required by Shafer-Shenoy.
Lazy propagation

The idea of lazy propagation [MJ98] is to keep the link potentials in factored form, i.e., to replace the link potential $q_{U,W}$ with a set of potentials $Q_{U,W}$ with

$$q_{U,W} = \prod_{q \in Q_{U,W}} q$$

The formulas of lemma 1 then read as:

(i)

$$q_U = \prod_{q \in Q_G(U)} q \prod_{T \in \text{fan}(U)} \prod_{q \in Q(T,U)} q$$

(ii)

$$q_{U,W} = \text{elim}(Q_G(U) \cup \bigcup_{T \in \text{fan}(U), \ T \neq W} Q_{T,U}, c(U \cap W))$$
Clique trees for triangulated graphs (1/3)

Clique cluster trees can easily be computed of triangulated graphs.

(i) Triangulated graphs admit a perfect ordering of $G$, i.e., an ordering $\sigma$ with

$$\text{fam}_{\sigma\{1, \ldots, i\}}(\sigma(i))$$

is complete.

(ii) A perfect ordering can be computed by the maximum cardinality search algorithm (MCS).

Let $C_i := \text{fam}_{\sigma\{1, \ldots, i\}}(\sigma(i))$ and

$$C_i = \{\sigma(j_1), \ldots, \sigma(j_n), \sigma(i)\}$$

with $j_1 < j_2 < \ldots < j_n$. Due to the completeness of $C_i$ then $\sigma(j_n)$ is a neighbor of all $\sigma(j_l)$, $l = 1, \ldots, n - 1$, and thus

$$C_i \cap \bigcup_{k<i} C_k \subseteq C_{j_n}$$

i.e., the sequence $(C_i)_{i=1, \ldots, |V|}$ has the running intersection property (that can be telescoped if a $C_i$ gets pruned).

Proving the correctness of MCS affords some work (e.g., [Sha94, p. 43–46]).

Figure 25: Perfect ordering of a triangulated graph obtained by MCS.

Clique trees for triangulated graphs (2/3)

All cliques can be enumerated by a variant of the MCS algorithm:

1. if $G$ is triangulated, MCS computes a perfect ordering of $G$, i.e., $\text{fam}_{\sigma\{1, \ldots, i\}}(\sigma(i))$ is complete.

2. we get all cliques this way, as for each clique $C$ let $i := \max \sigma^{-1}(C)$, then $C = \text{fam}_{\sigma\{1, \ldots, i\}}(\sigma(i))$.

Let $C := \text{fam}_{\sigma\{1, \ldots, i\}}(\sigma(i))$ and

$$C_i = \{\sigma(j_1), \ldots, \sigma(j_n), \sigma(i)\}$$

with $j_1 < j_2 < \ldots < j_n$. Due to the completeness of $C_i$ then $\sigma(j_n)$ is a neighbor of all $\sigma(j_l)$, $l = 1, \ldots, n - 1$, and thus

$$C_i \cap \bigcup_{k<i} C_k \subseteq C_{j_n}$$

i.e., the sequence $(C_i)_{i=1, \ldots, |V|}$ has the running intersection property (that can be telescoped if a $C_i$ gets pruned).

Figure 27: MCS algorithm to compute cliques of a triangulated graph [TY84].
BAYESIAN NETWORKS / 4. CLIQUE (CLUSTER) TREES

Clique trees for triangulated graphs (3/3)

Figure 28: Perfect ordering of a triangulated graph obtained by MCS.

Figure 29: Clique cluster tree for triangulated graph at the left (blue nodes are temporary and pruned).

1. Trees
2. Cluster Trees
3. Recursive Computation of Link Potentials
4. Clique (Cluster) Trees
5. Triangulation
Triangulation of graphs (1/3)

As clique cluster trees can easily be computed of triangulated graphs, we triangulate non-triangulated graphs by filling-in additional edges.

However, additional edges mean, that the graph represents a smaller portion of the independency statements, and thus, inference becomes harder.

The fewer edges have to be filled-in, the better.

```
1 triangulate-MCS(G = (V, E)) :
2 σ := perfect-ordering-MCS(G)
3 fillin := ∅
4 for i = |V|, . . . , 1 do
5    fillin := fillin ∪ {(u, w) | u, w ∈ fan(V,E∪fillin)(σ(i)) ∩ σ({1, . . . , i − 1}), {u, w} ∉ E}
6 od
7 return G′ := (V, E ∪ fillin)
```

Figure 31: Maximum cardinality search algorithm for triangulating a graph [TY84].

MCS does not guarantee to give best results (i.e., minimal fill-ins). It is just a heuristics that gives useable results (in most cases).

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Figure 32: Optimal triangulation.

Figure 33: Non-optimal triangulation obtained by MCS (with smallest index rule).
Triangulation of graphs (3/3)

Beneath the heuristic triangulation algorithms one distinguishes between:

**minimum triangulations:** no other triangulation has a smaller number of filled-in edges (global minimum).

This task is known to be NP-complete [Yan81].

**minimal triangulations:** no subset of the filled-in edges results in a triangulation (local minimum).

There are several algorithms for the minimal triangulation task, e.g., Lex-M [RTL76], MCS-M [BBH02], and LB-triang [BBH0+03].

Figure 34: A minimum triangulation (here: unique).

Figure 35: A minimal triangulation.

References


