

Chapter 9

Bounding Inference by Iterative message-passing schemes

This section discusses Iterative bounded inference algorithms such as iterative belief propagation and iterative Join-Graph Propagation. One motivation for designing this algorithm is to combine the anytime feature of Mini-Clustering (MC) and the iterative virtues of Iterative Belief Propagation (IBP).

9.1 Iterative Join-Graph Propagation

Mini-clustering is, partially, an anytime algorithm. Partially, because, like the mini-bucket scheme, it may not be able to generate an exact solution when more time is available because it will run out of memory first. The scheme works on tree-decompositions and it converges in two passes, so iterating doesn't change the messages. IBP is an iterative algorithm that converges in many cases, and when it converges it does so very fast. However, allocating IBP more time doesn't improve its accuracy. The immediate question is if we can exploit the anytime property of MC obtained using its i -bound, with the iterative qualities of IBP. Algorithm Iterative Join-graph Propagation (IJGP) was designed to benefit from both these directions. It works on a general join-graph which may contain cycles. The cluster size of the graph is user adjustable by the i -bound and the cycles in the graph allow iterating.

The algorithm applies message computation over a join-graph decomposition, which has all the ingredients of a join-tree, except that the underlying graph may have cycles.

Definition 9.1.1 (join-graph decompositions) A join-graph decomposition for $\mathcal{B} = \langle \mathbf{X}, \mathbf{D}, \mathbf{P}_G, \mathbb{I} \rangle$, where $\mathcal{P} = \{P_1, \dots, P_n\}$, is a triple $D = \langle JG, \chi, \psi \rangle$, where $JG = (V, E)$ is a graph, and χ and ψ are labeling functions which associate with each vertex $v \in V$ two sets, $\chi(v) \subseteq X$ and $\psi(v) \subseteq P$ such that:

1. For each $P_i \in P$, there is exactly one vertex $v \in V$ such that $P_i \in \psi(v)$, and $\text{scope}(p_i) \subseteq \chi(v)$.
2. (connectedness) For each variable $X_i \in X$, the set $\{v \in V | X_i \in \chi(v)\}$ induces a connected subgraph of G , a property also called the running intersection property.

We will refer to a node and its CPT functions as a *cluster* (note that a node may be associated with an empty set of CPTs) and use the term *join-graph-decomposition* and *cluster graph* interchangeably. A *join-tree-decomposition* or a *cluster tree* is the special case when the join-graph JG is a tree.

It is clear that one of the problems of message propagation over cyclic join-graphs is *over-counting*. Various schemes were proposed to reduce this problem. We will describe here a scheme that avoids cycles relative to a single variable using the notion of arc-minimality also referred to as edge-minimality.

Definition 9.1.2 (arc-minimality) *A join-graph decomposition D is arc-minimal if none of its arcs can be removed while still satisfying the connectedness property of Definition 9.1.1.*

If a graph-decomposition is not arc-minimal it is easy to remove some of its arcs until it becomes arc-minimal. The property of arc-minimality is *not* sufficient to ensure such acyclicity though. What is required is that, for every variable X , the arc-subgraph that contains X be a tree.

Example 9.1.3 The example in Figure 9.1a shows an arc minimal join-graph which contains a cycle relative to variable 4, with arcs labeled with separators. Notice however that if we remove variable 4 from the label of one arc we will have no cycles (relative to single variables) while the connectedness property will still be maintained. \square

We next refine the definition of join-graph decompositions, when arcs can be labeled with a subset of their separator.

Definition 9.1.4 ((minimal) arc-labeled join-graph decompositions.) *An arc-labeled decomposition for $\mathcal{B} = \langle \mathbf{X}, \mathbf{D}, \mathbf{P}_G, \mathbf{\Pi} \rangle$ is a four-tuple $D = \langle JG, \chi, \psi, \theta \rangle$, where $JG = (V, E)$ is a graph, χ and ψ associate with each vertex $v \in V$ the sets $\chi(v) \subseteq X$ and $\psi(v) \subseteq P$ and θ associates with each edge $(v, u) \in E$ the set $\theta((v, u)) \subseteq X$ such that:*

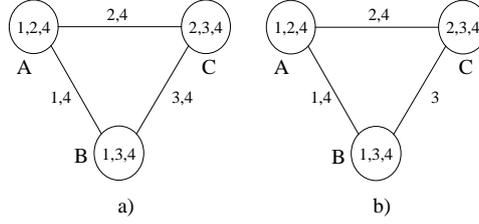


Figure 9.1: An arc-labeled decomposition

1. For each function $P_i \in \mathbf{P}_G$, there is exactly one vertex $v \in V$ such that $P_i \in \psi(v)$, and $\text{scope}(P_i) \subseteq \chi(v)$.
2. (arc-connectedness) For each arc (u, v) , $\theta(u, v) \subseteq \text{sep}(u, v)$, such that $\forall X_i \in X$, any two clusters containing X_i can be connected by a path whose every arc's label includes X_i .

Finally, an arc-labeled join-graph is minimal if no variable can be deleted from any label while still satisfying the arc-connectedness property.

Recall the following definitions of separators and eliminators.

Definition 9.1.5 (separator, eliminator) Given two adjacent vertices u and v of JG , the separator of u and v is defined as $\text{sep}(u, v) = \theta((u, v))$, and the eliminator of u with respect to v is $\text{elim}(u, v) = \chi(u) - \theta((u, v))$.

Arc-labeled join-graphs can be made label minimal by deleting variables from their labels while maintaining connectedness (if an edge label becomes empty, the edge can be deleted altogether). It is easy to see that,

Proposition 9.1.6 A minimal edge-labeled join-graph does not contain any cycle relative to any single variable. That is, any two clusters containing the same variable are connected by exactly one path labeled with that variable.

Notice that every minimal edge-labeled join-graph is edge-minimal (no edge can be deleted), but not vice-versa. The mini-clustering approximation presented in the previous section, works by relaxing the join-tree requirement of exact inference into a collection of join-trees having smaller cluster size. It introduces some independencies in the original problem via node duplication and applies exact inference on the relaxed model requiring

only 2 message passings. For the class of IJGP algorithms the idea is to relax the tree-structure requirement and use join-graphs, which do not introduce new independencies, and then utilize an iterative message-passing on the resulting cyclic structure.

Indeed, it can be shown that any join-graph of a belief network does not introduce any new independencies to the problem, namely it is an I-map (independency map [89]) of the underlying probability distribution relative to node-separation.

Since we plan to use minimally edge-labeled join-graphs to address over-counting problems, the question is what kind of independencies are captured by such graphs.

Definition 9.1.7 (edge-separation in (arc-labeled) join-graphs) Let $D = \langle JG, \chi, \psi, \theta \rangle$, $JG = (V, E)$ be an edge-labeled decomposition of a Bayesian network $\mathcal{B} = \langle \mathbf{X}, \mathbf{D}, \mathbf{P}_G, \Pi \rangle$. Let $N_W, N_Y \subseteq V$ be two sets of nodes, and $E_Z \subseteq E$ be a set of edges in JG . Let W, Y, Z be their corresponding sets of variables ($W = \cup_{v \in N_W} \chi(v)$, $Z = \cup_{e \in E_Z} \theta(e)$). We say that E_Z edge-separates N_W and N_Y in D if there is no path between N_W and N_Y in the JG graph whose edges in E_Z are removed. In this case we also say that W is separated from Y given Z in D , and write $\langle W|Z|Y \rangle_D$. Edge-separation in a regular join-graph is defined relative to its separators.

Theorem 9.1.8 Any arc-labeled join-graph decomposition $D = \langle JG, \chi, \psi, \theta \rangle$ of a belief network $\mathcal{B} = \langle \mathbf{X}, \mathbf{D}, \mathbf{P}_G, \Pi \rangle$ is an I-map of P relative to edge-separation. Namely, any edge separation in D corresponds to conditional independence in The probability distribution represented by \mathcal{B} .

For a proof see [80].

9.1.1 Algorithm IJGP

Applying CTE iteratively to minimal edge-labeled join-graphs yields algorithm *Iterative Join-Graph Propagation (IJGP)* described in Figure 9.2. One iteration of the algorithm applies message-passing in a topological order over the join-graph, forward and back.

When node u sends a message (or messages) to a neighbor node v it operates on all the CPTs in its cluster and on all the messages sent from its neighbors excluding the ones received from v . First, all individual functions that share no variables with the eliminator are collected and sent to v . All the rest of the functions are *combined* in a product and summed over the eliminator between u and v .

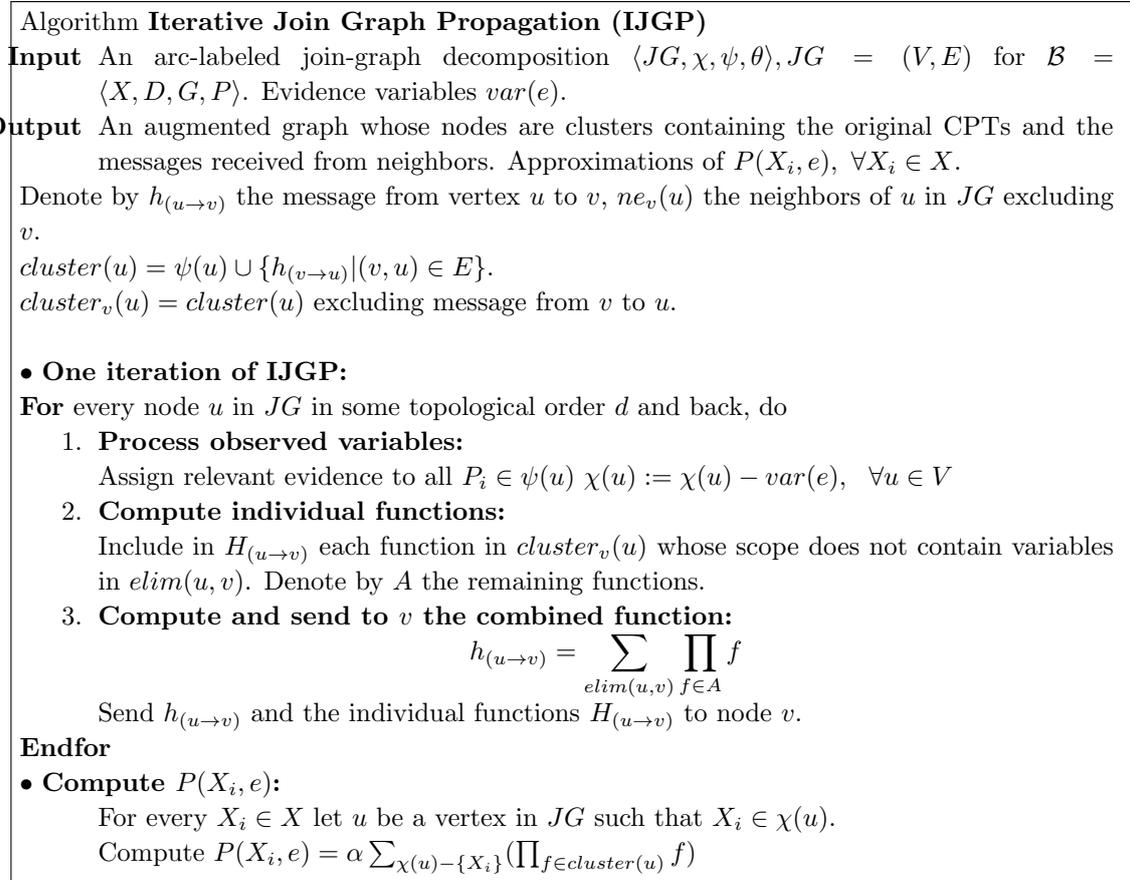


Figure 9.2: Algorithm Iterative Join-Graph Propagation (IJGP)

It is straightforward to show that:

Theorem 9.1.9 *We can show the following:*

- [74] If IJGP is applied to a join-tree decomposition it reduces to join-tree clustering and it therefore is guaranteed to compute the exact beliefs in one iteration.*
- [70] The time complexity of one iteration of IJGP is $O(deg \cdot (n + N) \cdot k^{w^*+1})$ and its space complexity is $O(N \cdot k^\theta)$, where deg is the maximum degree of a node in the join-graph, n is the number of variables, N is the number of nodes in the graph decomposition, k is the maximum domain size, w is the maximum cluster size and θ is the maximum label size.*

Proof: The number of cliques in the chordal graph G' corresponding to G is at most n , so the number of nodes in the join-tree is at most n . The complexity of processing a

node u in the join-tree is $deg_u \cdot (|\psi(u)| + deg_u - 1) \cdot k^{|\chi(u)|}$, where deg_u is the degree of u . By bounding deg_u by deg , $|\psi(u)|$ by n and $\chi(u)$ by $w + 1$ and knowing that $deg < N$, by summing over all nodes, we can bound the entire time complexity by $O(deg \cdot (n + N) \cdot k^{w+1})$.

For each edge JTC records functions. Since the number of edges is bounded by n and the size of each message is bounded by k^{sep} we get space complexity of $O(n \cdot k^{sep})$. ■

One question which we did not address at all in this section is why propagating the messages iteratively should help. Why is IJGP upon convergence, superior to IJGP with one iteration and is superior to MC? One clue can be provided when considering deterministic constraint networks which can be viewed as “extreme probabilistic networks”. It is known that constraint propagation algorithms, which are analogous to the messages sent by belief propagation, are guaranteed to converge and are guaranteed to improve with convergence. The propagation scheme presented here works like constraint propagation relative to the flat network abstraction of P (where all non-zero entries are normalized to a positive constant), and propagation is guaranteed to be more accurate for that abstraction at least. Another explanation will be provided by showing a connection between the probability distribution generated by IJGP (upon convergence) and the distribution that minimize a distance function to the exact distribution, as we (may) discuss later.

Next we will demonstrate that the well-known algorithm IBP (also called belief propagation) is a special case of IJGP.

9.1.2 The Case of Iterative Belief Propagation

Iterative belief propagation (IBP) is an iterative application of Pearl’s algorithm for poly-trees [89], to any Bayesian network. We will describe IBP as an instance of join-graph propagation over a *dual graph*.

Definition 9.1.10 (dual graphs) *Given a set of functions $F = \{f_1, \dots, f_l\}$ over scopes S_1, \dots, S_l , the dual graph of F is a graph $DG = (V, E, L)$ that associates a node with each function, namely $V = F$ and an edge connects any two nodes whose function’s scope share a variable, $E = \{(f_i, f_j) | S_i \cap S_j \neq \Phi\}$. L is a set of labels for the arcs, each being labeled by the shared variables of its nodes, $L = \{l_{ij} = S_i \cap S_j | (i, j) \in E\}$. A dual join-graph is an edge-labeled edge subgraph of DG . A minimal dual join-graph is a dual join-graph for which none of the edge labels can be reduced while maintaining the connectedness property.*

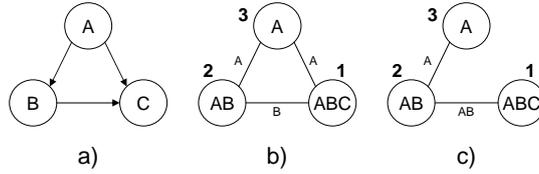


Figure 9.3: a) A belief network; b) A dual join-graph with singleton labels; c) A dual join-graph which is a join-tree

Interestingly, there may be many minimal dual join-graphs of the same dual graph. We will define Iterative Belief Propagation on a dual join-graph. Each node sends a message over an edge whose scope is identical to the label on that edge. Since Pearl’s algorithm sends messages whose scopes are singleton variables only, we highlight minimal singleton-label dual join-graphs.

Proposition 9.1.11 *Any Bayesian network has a minimal dual join-graph where each edge is labeled by a single variable.*

Proof: Consider a topological ordering of the nodes in the acyclic directed graph of the Bayesian network $d = X_1, \dots, X_n$. We define the following dual join-graph. Every node in the dual graph \mathcal{D} , associated with P_i is connected to node P_j , $j < i$ if $X_j \in pa(X_i)$. We label the edge between P_j and P_i by variable X_j , namely $l_{ij} = \{X_j\}$. It is easy to see that the resulting edge-labeled subgraph of the dual graph satisfies connectedness. The resulting labeled graph is a dual graph with singleton labels. ■

Example 9.1.12 Consider the belief network on 3 variables A, B, C with CPTs. 1. $P(C|A, B)$, 2. $P(B|A)$ and 3. $P(A)$, given in Figure 9.3a. Figure 9.3b shows a dual graph with singleton labels on the edges. Figure 9.3c shows a dual graph which is a join-tree, on which belief propagation can solve the problem exactly in one iteration (two passes up and down the tree). □

For completeness, we present algorithm IBP in Figure 9.5, which is a special case of IJGP. It is easy to see that one iteration of IBP is time and space linear in the size of the belief network. It is also easy to show that when IBP is applied to a minimal singleton-labeled dual graph it coincides with Pearl’s belief propagation applied directly to the

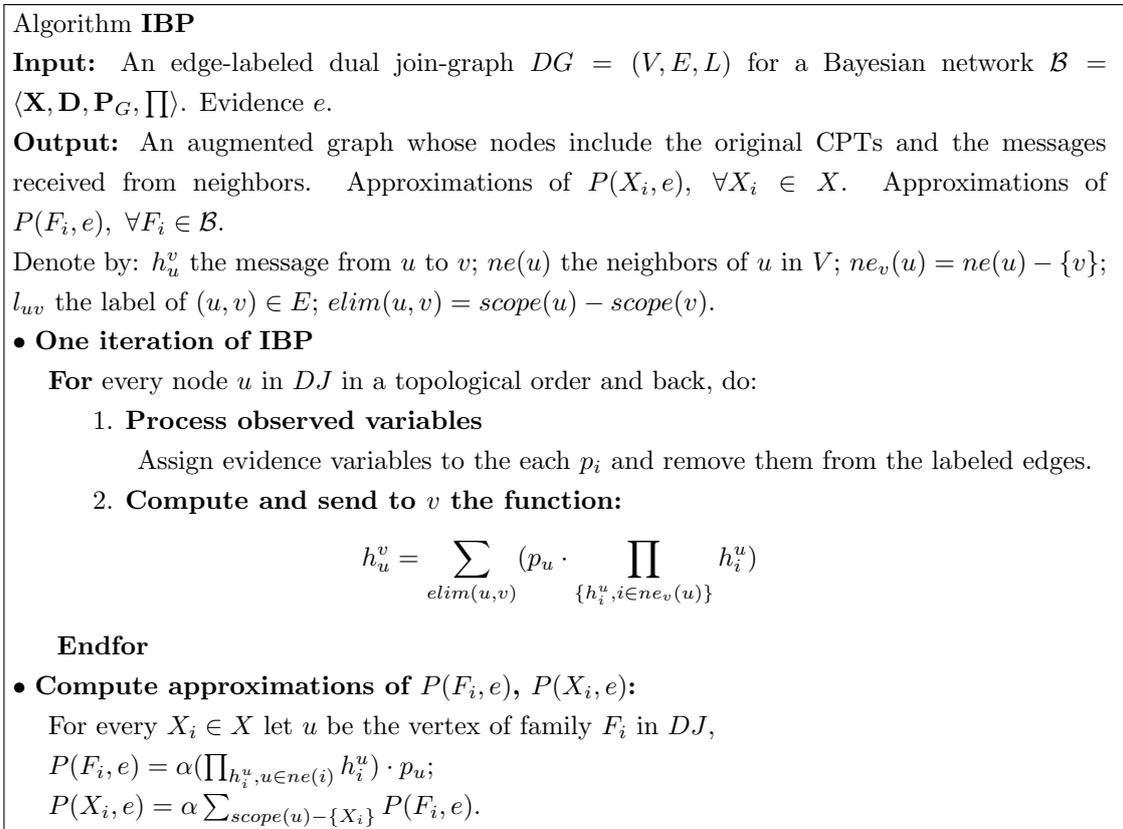


Figure 9.4: Algorithm Iterative Belief Propagation

acyclic graph representation. Also, when the dual join-graph is a tree IBP converges after one iteration (two passes, up and down the tree) to the exact beliefs.

: Algorithm Iterative Belief Propagation

9.1.3 Bounded Join-Graph Decompositions

Since we want to control the complexity of join-graph algorithms, we will define it on decompositions having bounded cluster size. If the number of variables in a cluster is bounded by i , the time and space complexity of processing one cluster is exponential in i .

Given a join-graph decomposition $D = \langle JG, \chi, \psi, \theta \rangle$, the accuracy and complexity on the (iterative) join-graph propagation algorithm depends on the joinwidth of D defined

as $\max_{v \in V} |\chi(v)|$. Intuition also suggests that the accuracy depends on how far the join-graph is from a join-tree, which may be captured by the treewidth of JG which we would call *external width*.

We can now state our target decomposition as follows. Given a graph G , and a bounding parameter i we wish to find a join-graph decomposition D of G whose internal width is bounded by i and whose external width is minimized.

We can consider two classes of algorithms. One class is *partition-based*. It starts from a given tree-decomposition and then partitions the clusters until the decomposition has clusters bounded by i . An alternative approach is *grouping-based*. It starts from a minimal dual-graph-based join-graph decomposition (where each cluster contains a single CPT) and groups clusters into larger clusters as long as the resulting clusters do not exceed the given i -bound. In both methods one should attempt to reduce the external width of the generated graph-decomposition.

We will next present a partition-based approach which is based on the decomposition suggested by the mini-bucket scheme. Given a bound i , algorithm *Join-Graph Structuring*(i) applies the procedure *Schematic Mini-Bucket*(i), described in Figure 9.7. The procedure only traces the scopes of the functions that would be generated by the full mini-bucket procedure, avoiding actual function computation. The procedure ends with a collection of mini-bucket trees, each rooted in the mini-bucket of the first variable. Each of these trees is minimally edge-labeled. Then, *in-edges* labeled with only one variable are introduced, and they are added only to obtain the running intersection property between branches of these trees.

Proposition 9.1.13 *Algorithm Join-Graph Structuring*(i) *generates a minimal edge-labeled join-graph decomposition having bound* i .

Proof: The construction of the join-graph specifies the vertices and edges of the join-graph, as well as the variable and function labels of each vertex. We need to demonstrate that 1) the connectedness property holds, and 2) that edge-labels are minimal.

Connectedness property specifies that for any 2 vertices u and v , if vertices u and v contain variable X , then there must be a path u, w_1, \dots, w_m, v between u and v such that every vertex on this path contains variable X . There are two cases here. 1) u and

v correspond to 2 mini-buckets in the same bucket, or 2) u and v correspond to mini-buckets in different buckets. In case 1 we have 2 further cases, 1a) variable X is being eliminated in this bucket, or 1b) variable X is not eliminated in this bucket. In case 1a, each mini-bucket must contain X and all mini-buckets of the bucket are connected as a chain, so the connectedness property holds. In case 1b, vertexes u and v connect to their (respectively) parents, who in turn connect to their parents, etc. until a bucket in the scheme is reached where variable X is eliminated. All nodes along this chain include variable X , so the connectedness property holds. Case 2 resolves like case 1b.

To show that edge labels are minimal, we need to prove that there are no cycles with respect to edge labels. If there is a cycle with respect to variable X , then it must involve at least one in-edge (edge connecting two mini-buckets in the same bucket). This means variable X must be the variable being eliminated in the bucket of this in-edge. Therefore, variable X is not contained in any of the parents of the mini-buckets of this bucket. Therefore, in order for the cycle to exist, another in-edge down the bucket-tree from this bucket must contain X . However, this is impossible as this would imply that variable X is eliminated twice. ■

Example 9.1.14 Figure 9.8a shows the trace of procedure schematic mini-bucket(3) applied to the problem described in Figure 8.15a. The decomposition in Figure 9.8b is created by the algorithm graph structuring. The only cluster partitioned is that of F into two scopes (FCD) and (BF), connected by an in-edge labeled with F . □

Example 9.1.15 Figure 9.9 shows a range of edge-labeled join-graphs. On the left extreme we have a graph with smaller clusters, but more cycles. This is the type of graph IBP works on. On the right extreme we have a tree decomposition, which has no cycles but has bigger clusters. In between, there could be a number of join-graphs where maximum cluster size can be traded for number of cycles. Intuitively, the graphs on the left present less complexity for join-graph algorithms because the cluster size is small, but they are also likely to be less accurate. The graphs on the right side are computationally more complex, because of larger cluster size, but are likely to be more accurate. □

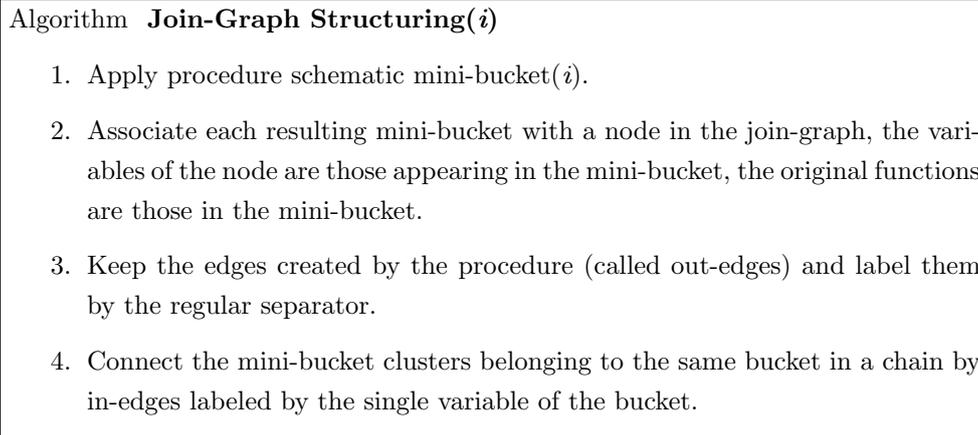


Figure 9.5: Algorithm Join-Graph Structuring(i).

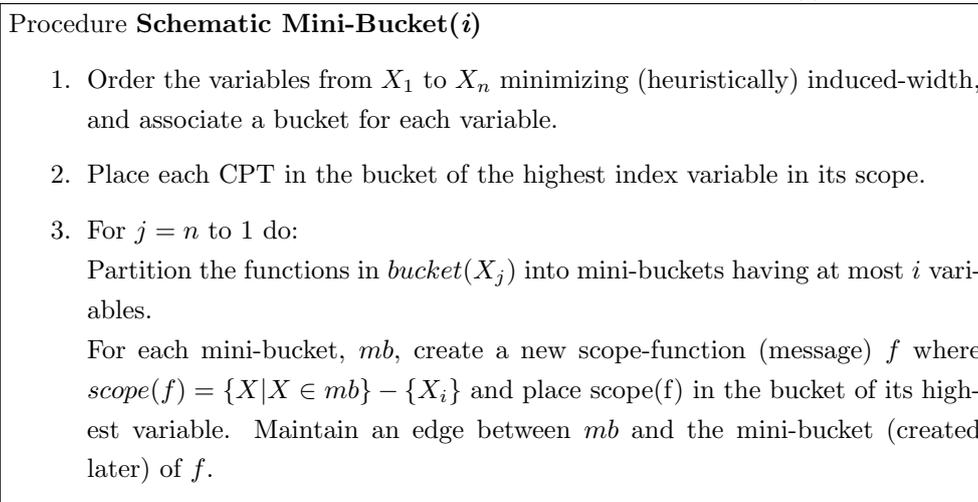


Figure 9.6: Procedure Schematic Mini-Bucket(i).

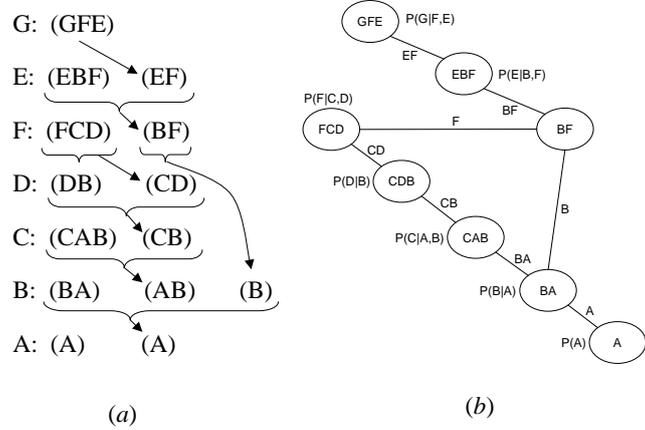


Figure 9.7: Join-graph decompositions.

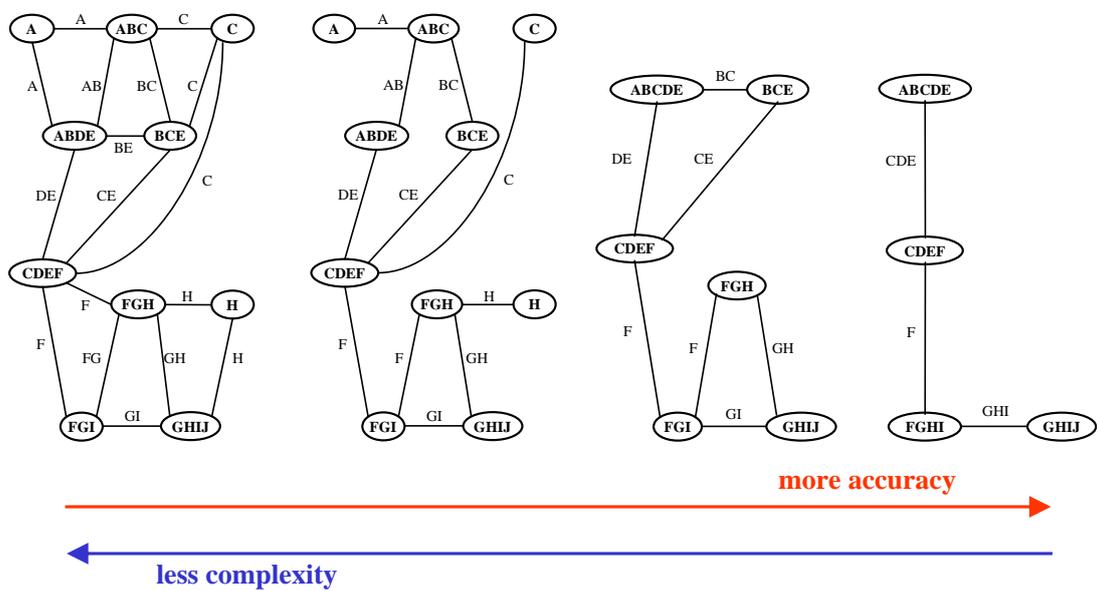


Figure 9.8: Join-graphs.

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