CHAPTER 8

Bounding Inference: Decomposition Bounds

Up to now we focused on exact algorithms for processing graphical models emphasizing the two reasoning styles of inference and search. We also showed that hybrids of AND/OR search and inference are effective and can be used to trade space for time.

Clearly, due to the hardness of the tasks, some networks cannot be processed exactly when their structure is not sparse thus having high treewidth and when their functions do not posses any internal structure. In such cases approximation algorithms are the only choice. Approximation algorithms can be designed to approximate either an inference, message-passing scheme, or a search scheme or their hybrid. Bounded inference algorithms, approximate inference schemes, while sampling schemes can be viewed as approximating search.

This chapter presents a class of approximation algorithms that bound the dimensionality of the dependencies created by inference. This yields a collection of parameterized schemes that often are called Decomposition Bounds, such as mini-bucket and weighted mini-bucket, mini-clustering and iterative join-graph propagation that offers adjustable trade-off between accuracy and efficiency. They can be accompanied by cost-shifting schemes.

It was shown that deriving approximation scheme with a guranateed relative error bounds, is NP-hard [Roth, **?**]. Nevertheless there are approximation strategies that work well in practice. One alternative for dealing with these bleak fact is to develop *anytime algorithms*. Such algorithms produce better and better solutions and better bounds with time and can therefore be interrupted at any time producing the best solution found thus far. This is our focus in this chapter.

As we showed (Chapter 4) the bucket-elimination scheme is a unifying algorithmic scheme for variable-elimination algorithms that is widely applicable. These include *directional-resolution* for propositional satisfiability *adaptive-consistency* for constraint satisfaction, *Fourier* and *Gaussian elimination* for linear inequalities, *dynamic-programming* for combinatorial optimization as well as many algorithms for probabilistic inference [**?**]. In the following sections we will introduce the mini-bucket elimination scheme that approximates bucket-elimination, and will subsequently generalize it into a scheme called weighted mini-bucket using the power-sum operator, allowing tightening the bounds for summation queries. Finally, we show how augmenting weighted mini-bucket by cost-shifting (e.g. re-parameterizations) yield a rich framework for bounding graphical models tasks that lend itself to anytime schemes.

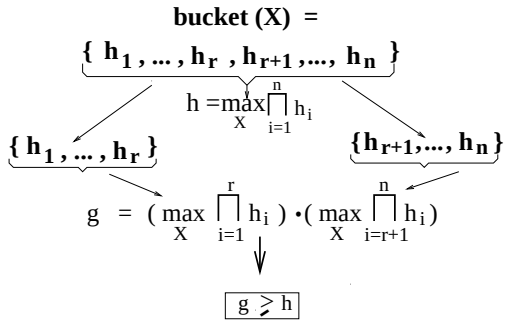


Figure 8.1: The idea of mini-bucket approximation.

8.1 MINI-BUCKET APPROXIMATION FOR MPE

Consider the bucket-elimination algorithm *BE-mpe* (Chapter 4). Since the complexity of processing a bucket depends on the number of arguments in the scope of the functions being recorded, we should consider approximating these functions by a collection of smaller-arity functions. Let $h_1, ..., h_t$ be the functions in the bucket of X_p, generated in earlier processed buckets and let $S_1, ..., S_t$ be their scopes. Recall that when *BE-mpe* processes bucket(X_p), the function $h_p = max_{X_p} \psi_p \Pi_{i=1}^t h_i$ is computed. A simple approximation idea is to compute an upper bound on h_p by exchanging summation and multiplication. Since, in general, for any two non-negative functions $Z(x)$ and $Y(x)$, $\max_x Z(x) \cdot Y(x) \leq \max_x Z(x) \cdot \max_x Y(x)$, this approximation will compute an upper bound on h_p. In particular, the function $g_p = \max_{X_p} \psi_P \cdot \prod_{i=1}^t \max_{X_p} h_i$, is an upper bound on $h_p = max_{X_p} \psi_p \prod_{i=1}^t h_i$. Procedurally it implies that the elimination operation of maximization is decomposed and is applied separately to each function, thus requiring less computation. This is because we wish to avoid the combinatorial explosion associated with generating a function oover the scope of all the bucket's variables, by applying multiplication first.

The idea is illustrated in Figure 8.1, where the bucket of variable X having n functions is split into two mini-buckets, one having r functions and the other having $n - r$ functions, where $r \leq n$. In general, the functions $h_1, ..., h_t$ can be partitioned into any set of subsets called *mini-buckets*. Let $Q = \{Q_1, ..., Q_r\}$ be a partitioning into mini-buckets of the functions $h_1, ..., h_t$ in X_p's bucket (these include both the original functions or messages sent from other buckets). Assume that the mini-bucket Q_l contains the functions $h_{l_1}, ..., h_{l_r}$. The exact *BE-mpe* algorithm computes $h_p = \max_{X_p} \prod_{i=1}^t h_i$, which can be rewritten as $h_p = \max_{X_p} \prod_{l=1}^r \prod_{h \in Q_l} h$. By migrating maximization into each mini-bucket we can compute, instead: $g_p = \prod_{l=1}^r \max_{X_p} \prod_{h \in Q_l} h$. Each new mini-bucket function (or message), $\max_{X_p} \prod_{h \in Q_l} h$, is computed independently and is placed separately into the bucket of the highest-variable in its scope. The algorithm then proceeds with the next variable. Functions without arguments (i.e., constants) are placed in the lowest bucket.

Since we replace functions with their upper bounds, it is easy to see that once all buckets are processed, the maximized product generated in the first bucket is an upper bound on the MPE

value. A lower bound can now be computed as the probability of any (suboptimal) assignment. In particular the suboptimal configuration that can be generated in a forward phase, similar to the way a solution is generated by the exact algorithm, can yield a good candidate solution whose cost will serve as a lower-bound.

It is convenient to control the algorithm's performance using two bounding parameters. Parameter i will bound the number of variables in each mini-bucket, while m will bound the number of its functions. The mini-bucket elimination (*MBE*) algorithm for finding an mpe, *MBE-mpe(i,m)*, is described in Figure 8.2.

Clearly, for efficiency, we would want the mini-buckets to be as small as possible yet we wish the scheme to be as accurate as possible. In general, as m and i increase, we get more accurate approximations. Note however, that a monotonic increase in accuracy as a function of the i-bound i, can be guaranteed only for restricted cases, as the refinement property that we discuss next, suggests.

Definition 8.1 refinement. Given two partitionings $Q^{'}$ and $Q^{''}$ over the same set of elements, $Q^{'}$ is a refinement of $Q^{''}$ if and only if for every set $A \in Q^{'}$ there exists a set $B \in Q^{''}$ such that $A \subseteq B$.

It is easy to see that:

Proposition 8.2 *If $Q^{''}$ is a refinement of $Q^{'}$ in $bucket_p$, then $h^p \leq g^p_{Q'} \leq g^p_{Q''}$.*

Proof. Clearly for any partitioning Q we have $h^p \leq g^p_Q$. By definition, given a refinement $Q'' = \{Q''_1, ..., Q''_k\}$ of a partitioning $Q' = \{Q'_1, ..., Q'_m\}$, each mini-bucket $i \in \{1, ..., k\}$ of Q'' belongs to some mini-bucket $j \in \{1, ..., m\}$ of Q'. In other words, each mini-bucket j of Q' is further partitioned into the corresponding mini-buckets of Q'', $Q'_j = \{Q''_{j_1}, ..., Q''_{j_l}\}$. Therefore,

$$g^p_{Q''} = \prod_{i=1}^{k} (\max_{X_p} \prod_{l \in Q''_i} h_l) = \prod_{j=1}^{m} \prod_{Q''_i \subseteq Q'_j} (\max_{X_p} \prod_{l \in Q''_i} h_l) \geq \prod_{j=1}^{m} (\max_{X_p} \prod_{l \in Q'_j} h_l) = g^p_{Q'}.$$

□

Definition 8.3 (i,m)-partitioning. A partitioning of $h_1, ..., h_t$ is *canonical* if any function f whose scope is subsumed by another's, is placed into a bucket containing one of those subsuming functions. A partitioning Q into mini-buckets is an (i, m)-partitioning if and only if (1) it is canonical, (2) at most m non-subsumed functions are included in each mini-bucket, (3) the total number of variables in a mini-bucket does not exceed i, and (4) the partitioning is *refinement-maximal*, namely, there is no other (i, m)-partitioning that it refines.

The i-bound, i (number of variables) and the m-bound, m (number of functions), are not independent, and some combinations of i and m do not yield a feasible (i,m)-partitioning. However,

Algorithm MBE-mpe(i,m)

Input: A belief network $\mathcal{B} =< X, D, G, \mathcal{P}_G, \prod >$, where $\mathcal{P} = \{P_1, ..., P_n\}$; an ordering of the variables, $d = X_1, ..., X_n$; observations $\mathbf{e}$.

Output: An upper bound U and a lower bound L on the most probable configuration given the evidence. A suboptimal solution $\bar{x}^a$ that provides the lower bound $L = P(\bar{x}^a)$.

1. **Initialize:** Generate an ordered partition of the conditional probability function, $bucket_1$, ..., $bucket_n$, where $bucket_i$ contains all functions whose highest variable is X_i. Put each observed variable in its bucket. Let ψ_i be the product of input function in a bucket and let h_i be the messages in the bucket.

2. **Backward:** For $p \leftarrow n$ downto 1, do
for all the functions $h_1, h_2, ..., h_j$ in $bucket_p$, do

- **If** (observed variable) $bucket_p$ contains $X_p = x_p$, assign $X_p = x_p$ to each function and put each in appropriate bucket.
- **else**, Generate an an (i, m)-partitioning, $Q' = \{Q_1, ..., Q_r\}$ of $h_1, h_2, ..., h_t$ in $bucket_p$.
- **for each** $Q_l \in Q'$ containing $h_{l_1}, ...h_{l_t}$, **do**

$$h_l \leftarrow max_{X_p} \prod_{j=1}^{t} h_{l_j} \tag{8.1}$$

Add h_l to the bucket of the largest-index in $scope(h_l)$.Put constants in $bucket_1$.

3. **Forward:**

- Generate an mpe upper bound cost by maximizing over X_1, the product in $bucket_1$. Namely $U \leftarrow max_{X_1} \psi_1 \prod_j h_{1_j}$.
- (Generate an approximate mpe tuple): Given $x_1^a, ..., x_{p-1}^a$, assign x_p^a to X_p that maximizes the product of all functions in $bucket_p$. $L \leftarrow P(x_1^a, ..., x_n^a)$

4. **Return** U and L and configuration: $\bar{x}^a = (x_1^a, ..., x_n^a)$

Figure 8.2: Algorithm *MBE-mpe(i,m)*.

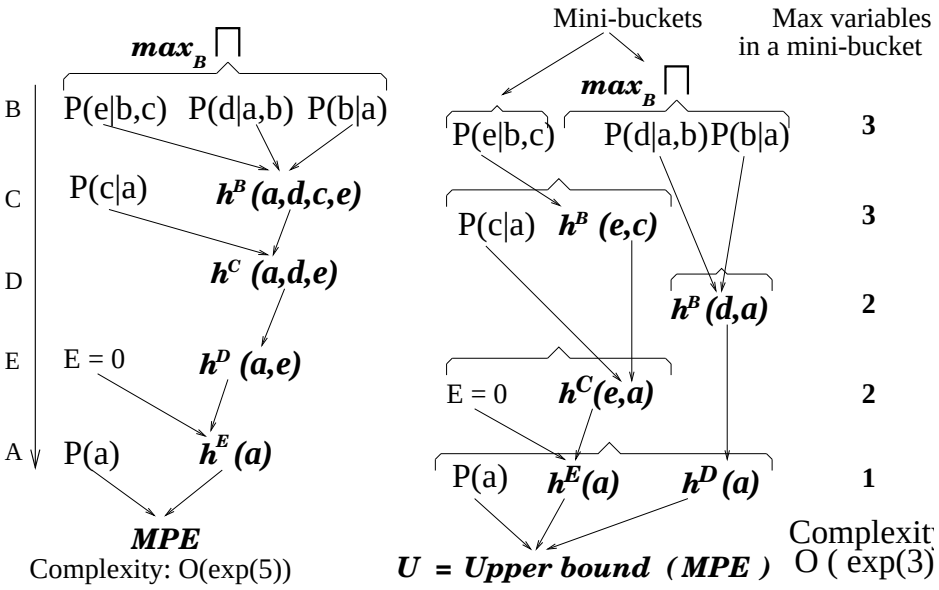


Figure 8.3: Comparison between (a) *BE-mpe* and (b) *MBE-mpe(3,2)*.

it is easy to see that if the i-bound is not smaller than the maximum scope size, then, for any value of $m > 0$, there exists an (i, m)-partitioning of each bucket. The use of the two parameters i and m, although not independent, allow considering a richer set of partitioning schemes, than using i or m alone. For flexibility reasons the i-bound would be the one mostly used in practice.

Clearly, since *MBE-mpe(i,m)* computes an upper bound in each bucket it yields an overall upper bound on the resulting mpe. Namely,

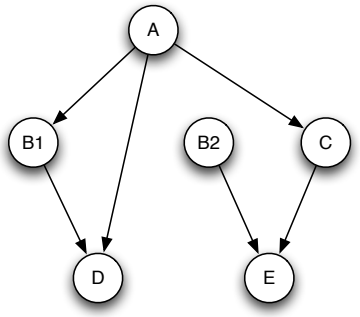
Theorem 8.4 MBE-mpe boundness. *Algorithm* MBE-mpe(i, m) *computes an upper and a lower bounds on the mpe.*

Example 8.5 Figure 8.3 compares algorithms *BE-mpe* and *MBE-mpe(i,m)* where $i = 3$ and $m = 2$ over the network in Figure 2.5a along the ordering $o = (A, E, D, C, B)$. The exact *BE-mpe* sequentially records the new functions (shown in boldface) $h_B(a, d, c, e)$, $h_C(a, d, e)$, $h_D(a, e)$, and $h_E(a)$. Then, in the bucket of A, it computes $M = \max_a P(a)h_E(a)$. Subsequently, an mpe configuration $(A = a', B = b', C = c', D = d', E = e')$ where $e' = 0$ is the evidence, can be computed along o by selecting a value that maximizes the product of functions in the corresponding buckets conditioned on the previously assigned values. Namely, $a' = \arg\max_a P(a)h_E(a)$, $e' = 0$, $d' = \arg\max_d h_C(a', d, e = 0)$, and so on.

Looking now at *MBE-mpe(3,2)*, since bucket(B) includes five variables, we *split* it into two mini-buckets $\{P(e|b, c)\}$ and $\{P(d|a, b), P(b|a)\}$, each containing no more than 3 variables, as shown in Figure 8.3b. There can be several (3,2)-partitionings, and any choice would be legitimate, and can be selected arbitrarily. The new functions $h_B(e, c)$ and $h_B(d, a)$ are generated in different mini-buckets and are placed independently into lower buckets. In each of the remaining lower buckets that still need to be processed, the number of variables is not larger than 3 and therefore no further partitioning occurs. An upper bound on the mpe value can be computed by maximizing over A the product of functions in A's bucket: $U = max_a P(a)h_E(a)h_D(a)$.

Once all the buckets are processed, a suboptimal mpe assignment (also called configuration) can be computed by instantiating a variable by one of its values that maximizes the product of functions in the corresponding bucket, in the same way this is done by exact *BE-mpe*. Clearly, any assignment to all the variables yields a lower bound, and one can use alternative methods to compute a configuration given the functions recorded by the mini-bucket algorithm. Note that by design *MBE-mpe(3,2)* does not produce functions on more than 2 variables, while the exact algorithm *BE-mpe* records a function on 4 variables.

In summary, *MBE-mpe(i,m)* computes an interval $[L, U]$ containing the mpe value where U is the upper bound computed by the backward phase and L is the probability or cost of the returned assignment. Note however that *MBE-mpe* computes the bounds on the joint probability



(a)

B1: P(b1|a),P(d|b1,a)
B2: P(e|b2,c)
C: P(c|a)
D:
E: E=e
A: P(a)

(b)

Figure 8.4: relaxed network corresponding to mini-bucket execution in Figure 8.3b

$mpe = \max_{\mathbf{x}} P(\mathbf{x}, \mathbf{e})$, rather than on the conditional probability $M = \max_{\mathbf{x}} P(\mathbf{x}|\mathbf{e}) = mpe/P(\mathbf{e})$. Thus

$$\frac{L}{P(\mathbf{e})} \leq M \leq \frac{U}{P(\mathbf{e})}$$

While the probability of evidence clearly influences the quality of the bound interval on M, the ratio between the upper and the lower bound is not affected.

As we will see in the next subsection, approximating posterior probabilities using bounds on joint probabilities may be more problematic.

8.1.1 THE MINI-BUCKET SEMANTICS

The Mini-Bucket computation can be given a useful interpretation. It can be viewed as an exact computation over a simplified graphical model where for every mini-bucket we use a new copy the bucket's variable. Namely, for each bucket and its partitioning into mini-buckets, a variable in the original problem is replaced by a set of new duplicate variables, each associated with a single mini-bucket. For example, the Mini-Bucket trace in Figure 8.3b, corresponds to solving exactly by full bucket-elimination the network of the problem in Figure 8.4. Variable B is replaced by two copies called variables B_1 and B_2, and the functions $P(e|b,c)$, $P(d|a,b)$, and $P(b|a)$ are replaced by $P(e|b_1,c)$, $P(d|a,b_2)$ and $P(b_2|a)$. Thus the two mini-buckets correspond to two full buckets in the new simplified or relaxed problem. The relaxed problem has a smaller width and can be solved efficiently, yielding a bound (upper or lower) as expected.

Certificate of optimality. Clearly when the lower bound equals to the upper bound we have an optimal solution. Alternatively, if we use the node duplication mechanism explicitly, whenever the optimal solution of the simplified problem allow assigning the same value to duplicated variables, we know that the assignment is locally optimal, namely conditioned on the current partial configuration.

Algorithm mbe-bel-max(i,m)
Input: A belief network $BN = (G, P)$, an ordering o, and evidence $\bar{e}$.
Output: an upper bound on $P(x_1, \bar{e})$ and an upper bound on $P(e)$.
1. **Initialize:** Partition $P = \{P_1, ..., P_n\}$ into buckets $bucket_1, \ldots, bucket_n$, where $bucket_k$ contains all CPTs $h_1, h_2, ..., h_t$ whose highest-index variable is X_k.
2. **Backward:** for $k = n$ to 2 do
   - **If** X_p is observed ($X_k = a$), assign $X_k \leftarrow a$ in each h_j and put the result in the highest-variable bucket of its scope (put constants in $bucket_1$).
   - **Else** for $h_1, h_2, ..., h_t$ in $bucket_k$ do
     Generate an (i, m)-partitioning, $Q' = \{Q_1, ..., Q_r\}$.
     For each $Q_l \in Q'$, containing $h_{l_1}, ...h_{l_t}$, do
       If $l = 1$ compute $h^l = \sum_{X_k} \Pi_{j=1}^t h_{1_j}$
       Else compute $h^l = max_{X_k} \Pi_{j=1}^t h_{l_j}$
       Add h^l to the bucket of the highest-index variable in $U_l \leftarrow \bigcup_{j=1}^t S_{l_j} - \{X_k\}$, (put constant functions in $bucket_1$).
3. **Return** $P'(\bar{x_1}, e) <-- $ the product of functions in the bucket of X_1, which is an upper bound on $P(x_1, \bar{e})$.
$P'(e) <-- \sum_{x_1} P'(\bar{x_1}, e)$, which is an upper bound on probability of evidence.

Figure 8.5: Algorithm *mbe-bel-max(i,m)*.

8.2 MINI-BUCKET APPROXIMATION FOR BELIEF UPDATING

As shown in Chapter 4, the bucket elimination algorithm *BE-bel* for belief assessment is similar to *BE-mpe* except that maximization is replaced by summation and no value assignment is generated. Algorithm *BE-bel* finds $P(x_1, \mathbf{e})$ and then computes $P(x_1|\mathbf{e}) = \alpha P(x_1, \mathbf{e})$ where α is the normalization constant (see Chapter 4).

The mini-bucket idea used for approximating MPE can be applied to belief updating. Let $Q\prime = \{Q_1, ..., Q_r\}$ be a partitioning of the functions $h_1, ...h_t$ in X_p's bucket. Algorithm *BE-bel* computes $h_p \leftarrow \sum_{X_p} \prod_{i=1}^t h_i$, over $scope(h_p) = \cup_i scope(h_i) - \{X_p\}$. (Again, we omit here the distinction between input functions and messages.) The function h_p can be rewritten as $h_p = \sum_{X_p} \prod_{l=1}^r \prod_{h_{l_i} \in Q_l} h_{l_i}$.

If we follow the mpe approximation precisely and migrate the summation operator into each mini-bucket, we will get $f_{Q\prime}^p = \prod_{l=1}^r \sum_{X_p} \prod_{l_i} h_{l_i}$. This, however, yields an unnecessarily weak upper bound of h_p where each $\prod_{l_i} h_{l_i}$ which is a function of X_p is bounded by $\sum_{X_p} \Pi_{l_i} h_{l_i}$, a constant function relative to X_p. Instead, we rewrite

$$h_p = \sum_{X_p} (\prod_{1_i} h_{1_i}) \cdot (\prod_{l=2}^{r} \prod_{l_i} h_{l_i})$$

and subsequently, instead of bounding a function of X by its sum over X, we can bound $(i > 1)$, by its maximum operator over X, yielding

$$g^p_{Q'} = (\sum_{X_p} \prod_{1_i} h_{1_i}) \cdot (\prod_{l=2}^{r} \max_{X_p} \prod_{l_i} h_{l_i}).$$

Therefore, an upper bound g_p of h_p can be obtained by processing one of X_p's mini-buckets by summation and the rest by maximization.

A lower bound on the belief, or its mean value, can be obtained in a similar way. Algorithm *MBE-bel-max(i,m)* that uses the max elimination operator is described in Figure 8.5. Algorithms *MBE-bel-min* and *MBE-bel-mean* can be obtained by replacing the operator max by min and by $mean$, respectively. Notice however that the node duplication semantics of MBE implies summation for each of the mini-buckets. This will be remedied shortly by an extension that generalize and improves the mini-bucket scheme, called *weighted mini-bucket*.

Theorem 8.6 *Given a Bayesian network with evidence e, algorithm MBE-bel-max(i,m) computes an upper bound on $P(X_1, \mathbf{e})$ and $P(\mathbf{e})$.*

We will have the same relationships between partitioning and their refinements as for the mpe case, but we have to be careful, since we have a new degree of freedom in selecting on which mini-bucket to maximize.

Proposition 8.7 *The following holds:*

1. *For every partitioning Q of a set of functions whose scopes include variable X_p, $h_p \leq g^p_Q \leq f^p_Q$, where f is obtained by processing each mini-bucket by summation while in g, one mini-bucket is processed by summation and the rest by maximization.*

2. *Also, if Q'' is a refinement partitioning of Q', then $h_p \leq g^p_{Q'} \leq g^p_{Q''}$.*

8.2.1 NORMALIZATION

Note that *MBE-bel-max* generates an upper bound on $P(x_1, \mathbf{e})$ but not on $P(x_1|\mathbf{e})$. If an exact value of $P(\mathbf{e})$ is not available, deriving a bound on $P(x_1|\mathbf{e})$ from a bound on $P(x_1, \mathbf{e})$ is not easy, because the normalization of upper-bounds is not an upper bound. Namely, $\frac{g(x_1)}{\sum_{x_1} g(x_1)}$, where $g(x)$ is the upper bound on $P(x_1, \mathbf{e})$, is not necessarily an upper bound on $P(x_1|\mathbf{e})$. As noted we can derive a lower bound, f, on $P(\mathbf{e})$ using *mbe-bel-min* and then compute $\frac{g(x_1)}{f}$ as an upper bound on $P(x_1|\mathbf{e})$. This however is likely to generate weak bounds due to compounded error.

Alternatively, let U_i and L_i be the upper bound and lower bounding functions on $P(X_1 = x_i, \mathbf{e})$ obtained by *mbe-bel-max* and *mbe-bel-min*, respectively. Then,

$$\frac{L_i}{P(\mathbf{e})} \leq P(x_i|\mathbf{e}) \leq \frac{U_i}{P(\mathbf{e})}$$

Therefore, although $P(\mathbf{e})$ is not known, the ratio of upper to lower bounds remains constant. Yet, the difference between the upper and the lower bounds can grow substantially, especially in cases of rare evidence. Note that if $P(\mathbf{e}) \leq U_i$, we get $\frac{L_i}{P(\bar{e})} \leq P(X_1|\bar{e}) \leq 1$, yielding a trivial upper bound. Finally, no guarantee is given for $g_{mean}(x_i)$, and therefore, the approximation of $\frac{g_{mean}(x_i)}{\sum_{x_1} g_{mean}(x_1)}$ can be below or above the exact value. Interestingly, the computation of $\frac{g_{mean}(X_1=x_i)}{\sum_{x_1} g_{mean}(x_1)}$ is automatically achieved when processing all the mini-buckets by summations, and subsequently normalizing. Namely, this is what is obtained when we transform the original network by node duplication and apply exact BE-bel to the simplified network.

8.3 WEIGHTED MINI-BUCKET ELIMINATION

The power sum is defined as follows:

$$\sum_x^w f(x) = (\sum_x f(x)^{\frac{1}{w}})^w \tag{8.2}$$

where w is a non-negative weight. The power sum reduce to a standard summation when $w = 1$ and approaches max when $w \to 0^+$.

Proposition 8.8 Holder inequality *Let $f_i(x)$, $i = 1..r$ be a set of functions and $w_1, ..., w_r$ be a set of non-zero weights, s.t., $w = \sum_{i=1}^r w_i$ then,*

$$\sum_x^w \prod_{i=1}^r f_i(x) \leq \prod_{i=1}^r \sum_x^{w_i} f_i(x)$$

This means that if we generalize to have a power-sum-product query over our graphical model relative to a given weight w, the bucket elimination immediately applies to yield an exact algorithm, when using $\otimes = \sum_x^w$. Most significantly, due to Holder inequality we get a *weighted*-mini-bucket algorithm which is correct for any set of weights satisfying EQ. (8.2). The case of w=1 specialize to summation and w=0 to maximization. When $w = 0$, the only consistent weight vector is $w_i = 0$, which means that each mini-bucket should be processed by maximization. But, when $w = 1$, namely for the summation query, an appropriate choice of the mini-bucket weights can tighten the obtained bound. We can try to select a good, or even optimal set of weights for each bucket to yield the tightest

Algorithm Weighted WMBE(i,m), $(w_1, ...w_n)$
Input: A belief network $\mathcal{B} = \langle \mathbf{X}, \mathbf{D}, \mathbf{P}_G, \prod \rangle$, an ordering $d = (X_1, \ldots, X_n)$; evidence $\mathbf{e}$
Output: an upper bound on $\sum_{\mathbf{X}}^{w} \prod_{i=1}^{n} P_i$
1. **Initialize:** Partition $P = \{P_1, ..., P_n\}$ into buckets $bucket_1$, ..., $bucket_n$, where $bucket_k$ contains all CPTs $h_1, h_2, ..., h_t$ whose highest-index variable is X_k.

2. **Backward:** for $k = n$ to 1 do

- **If** X_p is observed $(X_k = a)$, assign $X_k \leftarrow a$ in each h_j and put the result in the highest-variable bucket of its scope (put constants in $bucket_1$).
- **Else** for $h_1, h_2, ..., h_t$ in $bucket_k$, generate an (i, m)-partitioning, $Q' = \{Q_1, ..., Q_r\}$. Select a set of weights $w_1, ...w_r$ s.t $\sum_l w_l = w$., where w is the weight of the bucket
  For each $Q_l \in Q'$, containing $h_{l_1}, ...h_{l_t}$, do

$$h_l \leftarrow \sum_{X_k}^{w_l} \prod_{j=1}^{t} h_{l_j} = (\sum_{X_k} \prod_{j=1}^{t} (h_{l_j})^{w_l})^{\frac{1}{w_l}}$$

  Add h_l to the bucket of the highest-index variable in its scope.

3. **Return** $U \leftarrow$ the sum over X_1 of the product of functions in the bucket of X_1, which is an upper bound on $\sum_{\mathbf{X}}^{w} \prod_{i=1}^{n} P_i(\cdot|\mathbf{e})$.

Figure 8.6: Algorithm *WMBE(i,m)*.

bounds, at least in principle. The max-sum case that we proposed in MBE-max-bel, correspond to assigning one mini-bucket with $w = 1$ and the rest with $w = 0$.

Algorithm weighted WMBE is given in Figure 8.6. It is paramaterized by a set of n weights, one for each variable, so it can accomodate a variety of tasks. When we solve a pure summation task such as the probability of evidence or the posterior probability the weight for each variable is $w = 1$. For pure optimization the weights are all $w = 0$. But, as we will see next, for mixed max-sum product queries such as marginal maps (mmap), we can specialize weights based on variables, so that buckets of sum variables will be assigned $w = 1$ and others $w = 0$ for maximization. This yields an elegant framework expressing the mini-bucket algorithms and permits the additional control via splitting the weights for each mini-bucket of a summation variable.

8.4 MINI-BUCKET ELIMINATION FOR MARGINAL MAP

Algorithm *BE-map* is a combination of *BE-mpe* and *BE-bel* as we have shown in Chapter 4; some of the variables are eliminated by summation, while the others by maximization.

Given a belief network, a subset of hypothesis variables $A = \{A_1, ..., A_k\}$, which we call MAP variables, and evidence $\mathbf{e}$, the problem is to find an assignment to the hypothesized variables that maximizes their probability conditioned on $\mathbf{e}$. Formally, we wish to find

$$\bar{a}_k^{map} = \arg\max_{\bar{a}_k} P(\bar{a}_k|\mathbf{e}) = \arg\max_{\bar{a}_k} \frac{\sum_{\mathbf{x}_{(k+1)..n}} \prod_{i=1}^{n} P(x_i, \mathbf{e}|\mathbf{x}_{pa_i})}{P(\mathbf{e})} \tag{8.3}$$

where $\mathbf{x} = (a_1, ..., a_k, x_{k+1}, ..., x_n)$ denotes an assignment to all variables, while $\bar{a}_k = (a_1, ..., a_k)$ and $\mathbf{x}_{(k+1)..n} = (x_{k+1}, ..., x_n)$ denote assignments to the MAP and SUM variables, respectively. Since $P(\mathbf{e})$ is a normalization constant, the same maximum is obtained for $P(\bar{a}_k, \mathbf{e})$.

As we know, the bucket-elimination algorithm for finding the exact mmap, *BE-map*, assumes constrained orderings in which the MAP variables appear first and thus are processed last by the algorithm. This restriction makes this MMAP task more difficult because it implies higher induced widths. The algorithm has the usual backward phase and its forward phase however is relative to the MAP variables only.

The mini-bucket scheme for MAP is a straightforward extension of the mini-bucket algorithms for summation and maximization and easy to express using the weighted mini-bucket scheme. As usual, we partition each bucket into mini-buckets as before. If the bucket's variable can be eliminated by summation, we apply the power-sum with $w = 1$. The rest of the buckets are processed by the mini-bucket rule with $w = 0$, yielding maximization. Namely, when the algorithm reaches the MAP buckets, their processing is identical to that of *MBE-mpe*. Algorithm *WMBE-map(i,m)* is described in Figure 8.7.

Decoding the map assignment and the issue with lower-bounds. Once the backwards phase of *MBE-map* terminates, we have an upper bound and, in principle, we can compute a map assignment in the forward phase. While the probability of this assignment is a lower bound on the MMAP value, computing the actual probability is no longer a simple forward step over the generated buckets but requires an exact inference. We cannot use the functions generated by *WMBE* in the buckets of summation variables since those serve as upper bounds. One possibility is, once an assignment is obtained, to rerun the mini-bucket algorithm over the SUM variables using the min operator with $w = -1$ and then compute a lower bound on the assigned tuple in another forward step over the first k buckets. We will leave the details of this idea as an exercise.

Example 8.9 Consider a belief network which describes the decoding of a *linear block code*, shown in Figure 8.8. In this network, U_i are *information bits* and X_j are *code bits*, which are functionally dependent on U_i. The vector (U, X), called the channel input, is transmitted through a noisy channel which adds Gaussian noise and results in the channel output vector $Y = (Y^u, Y^x)$

Algorithm WMBE-map(i,m)

Input: A Bayesian network $\mathcal{B} = \langle \mathbf{X}, \mathbf{D}, \mathbf{P}_G, \prod \rangle$, $P = \{P_1, ..., P_n\}$; a subset of hypothesis variables $A = \{A_1, ..., A_k\}$; an ordering of the variables, d, in which the A's are first in the ordering; observations $\mathbf{e}$.

Output: An upper bound on the map and a and a suboptimal solution $A = \bar{a}_k^a$.

1. **Initialize:** Partition $P = \{P_1, ..., P_n\}$ into $bucket_1$, ..., $bucket_n$, where $bucket_i$ contains all functions whose highest variable is X_i.

2. **Backwards** For $p \leftarrow n$ downto 1, do

for all the functions $h_1, h_2, ..., h_j$ in $bucket_p$ do

- **If** (observed variable) $bucket_p$ contains the observation $X_p = x_p$, assign $X_p = x_p$ to each h_i and and put each in appropriate bucket.
- **Else** for $h_1, h_2, ..., h_j$ in $bucket_p$ generate an (i, m)-partitioning, $Q^{'} = \{Q_1, ..., Q_r\}$.
- **If** $X_P \notin A$ assign $w_p = 1$, otherwise $w_p = 0$. Select weights for the mini-buckets in X_p bucket: $w_{p_1}, ..., w_{p_r}$. s.t $\sum_i w_{p_i} = w_p$.
  foreach $Q_l \in Q^{'}$, containing $h_{l_1}, ...h_{l_t}$, do

$$h_l \leftarrow \sum_{X_k}^{w_{p_l}} \prod_{j=1}^{t} h_{l_j} = (\sum_{X_k} (\prod_{j=1}^{t} h_{l_j})^{w_{p_l}})^{\frac{1}{w_{p_l}}}$$

  Add h_l to the bucket of the highest-index variable in its scope.

3. **Forward: for** $p = 1$ to k, given $A_1 = a_1^a, ..., A_{p-1} = a_{p-1}^a$, assign a value a_p^a to A_p that maximizes the product of all functions in $bucket_p$. conditioned on earlier assignments.

4. **Return** An upper bound $U = max_{a_1} \prod_{h_i \in bucket_1} h_i$ on the map value, computed in the first bucket, and the assignment $\bar{a}_k^a = (a_1^a, ..., a_k^a)$.

Figure 8.7: Algorithm *WMBE-map(i,m)*.

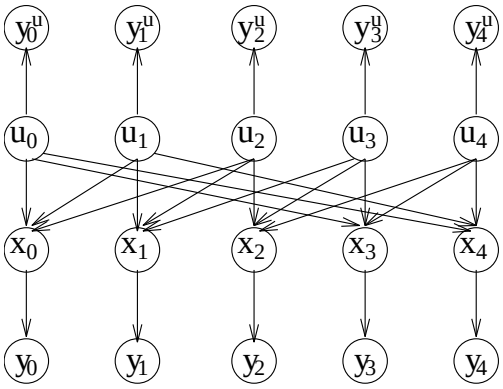


Figure 8.8: Belief network for a linear block code.

. The decoding task is to assess the most likely values for the U's given the observed values $Y = (\bar{y}^u, \bar{y}^x)$, which is the map task where U is the set of hypothesis variables, and $Y = (\bar{y}^u, \bar{y}^x)$ is the evidence. After processing the observed buckets we get the following bucket configuration (lower case y's are observed values):

$bucket(X_0) = P(y_0^x|X_0), P(X_0|U_0, U_1, U_2),$
$bucket(X_1) = P(y_1^x|X_1), P(X_1|U_1, U_2, U_3),$
$bucket(X_2) = P(y_2^x|X_2), P(X_2|U_2, U_3, U_4),$
$bucket(X_3) = P(y_3^x|X_3), P(X_3|U_3, U_4, U_0),$
$bucket(X_4) = P(y_4^x|X_4), P(X_4|U_4, U_0, U_1),$
$bucket(U_0) = P(U_0), P(y_0^u|U_0),$
$bucket(U_1) = P(U_1), P(y_1^u|U_1),$
$bucket(U_2) = P(U_2), P(y_2^u|U_2),$
$bucket(U_3) = P(U_3), P(y_3^u|U_3),$
$bucket(U_4) = P(U_4), P(y_4^u|U_4).$

Processing by *MBE-map(4,1)* of the first top five buckets by summation and the rest by maximization, results in the following mini-bucket partitionings and function generation:

$bucket(X_0) = \{P(y_0^x|X_0), P(X_0|U_0, U_1, U_2)\},$
$bucket(X_1) = \{P(y_1^x|X_1), P(X_1|U_1, U_2, U_3)\},$
$bucket(X_2) = \{P(y_2^x|X_2), P(X_2|U_2, U_3, U_4)\},$
$bucket(X_3) = \{P(y_3^x|X_3), P(X_3|U_3, U_4, U_0)\},$
$bucket(X_4) = \{P(y_4^x|X_4), P(X_4|U_4, U_0, U_1)\},$
$bucket(U_0) = \{P(U_0), P(y_0^u|U_0), h^{X_0}(U_0, U_1, U_2)\}, \{h^{X_3}(U_3, U_4, U_0)\}, \{h^{x_4}(U_4, U_0, U_1)\},$
$bucket(U_1) = \{P(U_1), P(y_1^u|U_1), h^{x_1}(U_1, U_2, U_3), h^{U_0}(U_1, U_2)\}, \{h^{u_0}(U_4, U_1)\},$
$bucket(U_2) = \{P(U_2), P(y_2^u|U_2), h^{x_2}(U_2, U_3, U_4), h^{U_1}(U_2, U_3)\},$
$bucket(U_3) = \{P(U_3), P(y_3^u|U_3), h^{u_0}(U_3, U_4), h^{U_1}(U_3, U_4), h^{u_2}(U_3, U_4)\},$
$bucket(U_4) = \{P(U_4), P(y_4^u|U_4), h^{u_1}(U_4), h^{u_3}(U_4)\}.$

The first five buckets are not partitioned at all and are processed as full buckets, since in this case a full bucket is a (4,1)-partitioning. This processing generates five new functions, three are placed in bucket U_0, one in bucket U_1 and one in bucket U_2. Then bucket U_0 is partitioned into three mini-buckets processed by maximization, creating two functions placed in bucket U_1 and one function placed in bucket U_3. Bucket U_1 is partitioned into two mini-buckets, generating functions placed in bucket U_2 and bucket U_3. Subsequent buckets are processed as full buckets. Note that the scope of recorded functions is bounded by 3.

In the bucket of U_4 we get an upper bound $Upper$ satisfying $Upper \geq map = P(U, \bar{y}^u, \bar{y}^x)$ where $\bar{y}^u$ and , $\bar{y}^x$ are the observed outputs for the U's and the X's bits transmitted. In order to bound $P(U|\bar{e})$, where $\bar{e} = (\bar{y}^u, \bar{y}^x)$, we need $P(\mathbf{e})$ which is not available. Yet, again, in most cases we are interested in the ratio $P(U = \bar{u_1}|\mathbf{e})/P(U = \bar{u_2}|\mathbf{e})$ for competing hypotheses $U = \bar{u_1}$ and

$U = \bar{u_2}$ rather than in the absolute values. Since $P(U|\mathbf{e}) = P(U, \mathbf{e})/P(\mathbf{e})$ and the probability of the evidence is just a constant factor independent of U, the ratio is equal to $P(U_1, \mathbf{e})/P(U_2, \mathbf{e})$.

Exercise: What is the relaxed network that corresponds to the above computation? How would you generate a candidate map assignment? how would you compute its probability? What is the relationship between the map and the mpe assignments?

8.5 MINI-BUCKETS FOR GENERAL DISCRETE OPTIMIZATION; THE MIN-SUM QUERY

The mini-bucket principle can also be applied to deterministic discrete optimization problems which can be defined over *cost networks*, yielding approximation to dynamic programming for discrete optimization [**?**]. In fact, as we showed (Chapter 2) the mpe task is a special case of combinatorial optimization and its approximation via mini-buckets can be straightforwardly extended to the general case. For completeness we present the algorithm explicitly for cost networks, namely, for the min-sum problem.

As defined earlier a *cost network* is a triplet (X, D, C), where X is a set of discrete variables, $X = \{X_1, ..., X_n\}$, over domains $D = \{D_1, ..., D_n\}$, and C is a set of real-valued cost functions $C_1, ..., C_l$. The *cost function* is defined by $C(X) = \sum_{i=1}^{l} C_i$. The optimization (minimization) problem is to find an assignment $x^{opt} = ({x_1}^{opt}, ..., {x_n}^{opt})$ such that $C(x^{opt}) = \min_{x=(x_1,...,x_n)} C(x)$.

Algorithm *mbe-opt* is described in Figure 8.9. Step 2 (backward step) computes a lower bound on the cost function while Step 3 (forward step) generates a suboptimal solution which provides an upper bound on the cost function.

Unified presentation of MBE. Clearly the mini-bucket scheme is applicable to any bucket-elimination scheme and can be described within the general framework using the combination and marginalization operators. The power-sum provide one way to generalize this scheme, leading to Weighted mini-bucket elimination [**?**].

8.6 COMPLEXITY AND TRACTABILITY

8.6.1 THE CASE OF LOW INDUCED WIDTH

We denote by *mini-bucket-elimination(i,m)*, or simply *MBE(i,m)*, a generic mini-bucket scheme with parameters i and m, without specifying the particular task it solves.

It is easy to derive *MBE(i,m)* complexity can be derived from the bucket-elimination complexity applied to the relaxed problem generated by variable duplication. Since variable duplication can generate at most r additional variables, where r is the number of functions, but will leave the

Algorithm MBE-opt(i,m)
Input: A cost network (X, D, C), $C = \{C_1, ..., C_l\}$; ordering o, a set of assignments e.
Output: A lower and an upper bound on the optimal cost.
1.**Initialize:** Partition C into $bucket_1$, ..., $bucket_n$, where $bucket_p$ contains all components $h_1, h_2, ..., h_t$ whose highest-index variable is X_p.
2. **Backward:** for $p = n$ to 2 do

- **If** X_p is observed ($X_p = a$), replace X_p by a in each h_i and put the result in its highest-variable bucket (put constants in $bucket_1$).
- **Else** for $h_1, h_2, ..., h_t$ in $bucket_p$ generate an (i, m)-partitioning, $Q' = \{Q_1, ..., Q_r\}$.
- **For each** $Q_l \in Q'$ containing $h_{l_1}, ...h_{l_t}$,

$$h_l \leftarrow min_{X_p} \sum_{i=1}^{t} h_{l_i}$$

  and add it to the bucket of the highest-index variable in its scope. (put constants in $bucket_1$).

3. **Forward: for** $p = 1$ to n, given $X_1 = x_1^{opt}, ..., X_{p-1} = x_{p-1}^{opt}$,
assign a value x_p^{opt} to X_p that minimizes the sum of all functions in $bucket_p$.
4. **Return** the assignment $x^{opt} = (x_1^{opt}, ..., x_n^{opt})$, an upper bound $U = C(x^{opt})$, and a lower bound $L = min_{x_1} \sum_{h_i \in bucket_1} h_i$ on the optimal cost.

Figure 8.9: Algorithm *MBE-opt(i,m)*.

number of functions fixed at r, and since the resulting problem has induced-width bounded by i, *MBE's* complexity obeys the following:

Theorem 8.10 *Algorithm* MBE(i,m) *takes* $O(r \cdot k^i)$ *time and space, where,* k *bounds the domain size and* r *is the number of input functions*[1]. *For* $m = 1$ *the algorithm is time and space linear and is bounded by* $O(r \cdot exp(|S|))$, *where* $|S|$ *is the maximum scope of any input function,* $|S| \leq i \leq n$.

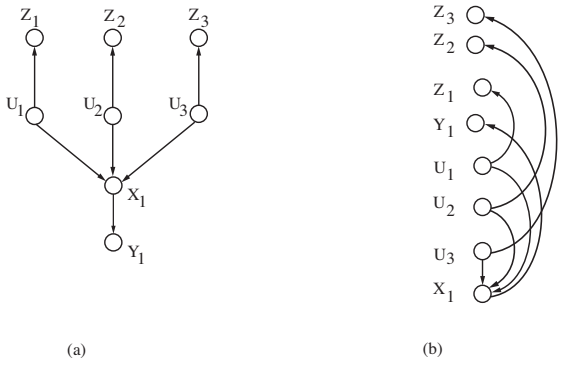
We can associate a bucket-elimination or a mini-bucket elimination algorithm with a *computation tree* where leaf nodes correspond to the original input functions (CPTs or cost functions), and each internal node v corresponds to the result of applying an elimination operator (e.g., product followed by summation) to the set of node's children, denoted $ch(v)$ where children correspond to all the functions in the corresponding bucket or mini-bucket). We can compress the computation tree so that each node having a single child will be merged into one node with its parent, so that the branching degree in the resulting tree is not less than 2. Computing an internal node that is a compressed sequence of single-child nodes takes $O(exp(|S|)$ time and space since it only requires a sequence of elimination operations over a single function which can be accomplished in one pass through the tuples (accumulating appropriate running summations over the relevant variables). The cost of computing any other internal node v is $O(|ch(v)| \cdot exp(i))$ where $|ch(v)| \leq m$, and where i bounds the resulting scope size of the generated functions. Since the number of leaf nodes is bounded by r, the number of internal nodes in the computation tree is bounded by r as well (since the branching factor of each internal node is at least 2). Thus the total amount of computation over all internal nodes in the computation tree is time and space $O(r \cdot exp(i))$ in general, which becomes to $O(n \cdot exp(i))$ for Bayesian networks.

Clearly, when the induced-width along the processing order is smaller than i, MBE(i, n) coincides with bucket-elimination and is therefore exact. This is because each full bucket satisfies the condition of being an (i, n)-partitioning.

Interestingly, algorithm *MBE(i,m=1)* is exact for acyclic networks, and in particular for polytrees, if applied along a proper orderings. Such orderings are determined by consulting a rooted join-tree of the acyclic network (we know that such a join-tree exists from the definition of an acyclic network as discussed in Chapter 5). We then order the variables from last to first by selecting and removing a leaf function from the rooted join-tree and placing as next all its variables that were not ordered yet. This way, each bucket would contain at most one non-subsumed function. Thus,

Theorem 8.11 *Given an acyclic network, there exists an ordering such that algorithm* MBE(n,1) *is exact and is time and space* $O(n \cdot exp(|S|))$, *where* $|S|$ *is the largest scope size of any input function.*

[1] Note that $r = n$ for Bayesian networks, but can be higher or lower for general constraint optimization tasks



(a) (b)

Figure 8.10: (a) A polytree and (b) a legal ordering, assuming that nodes Z_1, Z_2, Z_3 and Y_1 are observed.

Example 8.12 Consider an ordering $o = (X_1, U_3, U_2, U_1, Y_1, Z_1, Z_2, Z_3)$ of the polytree in Figure 8.10a, where the last four variables $Y_1,\ Z_1,\ Z_2,\ Z_3$ in the ordering are observed. Once the last four buckets are processed as observation buckets, we get (observed values shown in low-case):
$bucket(U_1) = P(U_1), P(X_1|U_1, U_2, U_3), P(z_1|U_1),$
$bucket(U_2) = P(U_2), P(z_2|U_2),$
$bucket(U_3) = P(U_3), P(z_3|U_3)$
$bucket(X_1) = P(y_1|X_1).$
We can see that when $m = 1$ the algorithm will have no partitioning in any bucket, because each bucket has at most one non-subsumed function.

8.6.2 HEURISTIC FOR MINI-BUCKET PARTITIONINGS

Clearly, there are many ways to partition a bucket into a collection of mini-buckets having parameters i and m. These partitionings can be guided by the graph, or by the content of the actual functions, aiming to minimize the error incurred by a particular partition. In practice the mini-bucket scheme is used primarily with the i-bound and ignores the m-bound. Namely, the mini-bucket is bounded by the number of variables it contains regardless of the number of function it has. This is because controlling the mini-bucket size by the number of variables allows more flexibility. One popular partitioning heuristic, is scope-based, relying solely on the scopes of the functions. We refer to the procedure that takes a bucket B and partition it into mini-buckets having at most i variables as *partitioning(B,i)*, and it outputs an i-partition. It outputs an i-partition.

Scope-based Partitioning Heuristic. The *scope-based* partition heuristic (SCP) aims at minimizing the number of mini-buckets in the partition by including in each mini-bucket as many functions as possible as long as the i bound is satisfied. This is equivalent to minimizing the number of copies of each variable. According to this scheme, first, single function mini-buckets are decreasingly ordered according to their arity. Then, each mini-bucket, from first to last, is absorbed into the earliest mini-bucket with whom it can be merged. The time and space complexity of $\texttt{Partition}(B, i)$, where B is the partitioned bucket, using the SCP heuristic is $O(|B| \log(|B|) + |B|^2)$ and $O(exp(i))$, respectively, where $|B|$ is the number of variables in the bucket. (Exercise: prove this complexity).

Content-based Partitioning Heuristic. The scope-based heuristic can be computed quickly, but its shortcoming is that it does not consider the actual information contained in each function. Bucket partitioning strategies that take into account the functions themselves were also explored. Given a bucket B, the goal of the partition process is to find an i-partition Q of B such that the function computed by the collection of mini-buckets g_Q is the *closest* to the exact bucket function g, according to some distance measure $dist$. Thus, the partition task is to find an i-partition Q^* of B such that $Q^* = \arg\min_Q dist(g_Q, g)$. Distance measures considered include *log relative error*, *maximum log relative error*, *KL divergence* and *absolute error*. For example:

- *Log relative error, (RE)*:

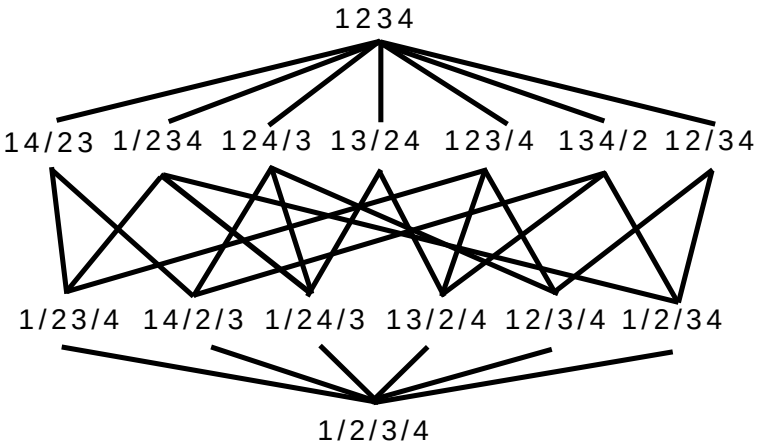


Figure 8.11: Partitioning lattice of bucket $\{f_1, f_2, f_3, f_4\}$. We specify each function by its subindex.

$$RE(f,h) = \sum_t (\log(f(t)) - \log(h(t)))$$

- *Max log relative error (MRE)* :

$$MRE(f,h) = \max_t \{\log(f(t)) - \log(h(t))\}$$

We can organize the space of partitions in a lattice using the *refinement* relation since it yields a partial order. Each partition Q of bucket B is a vertex in the lattice. There is an upward edge from Q to Q' if Q' results from merging two mini-buckets of Q in which case Q' is a *child* of Q. The set of all children of Q is denoted by $ch(Q)$. The *bottom* partition in the lattice is $Q^{\perp}$ while the *top* partition is $Q^{\top}$. For any two partitions Q and Q', if Q' is a descendent of Q then $g^{Q'}$ is clearly tighter than g^{Q} .

Example 8.13 Consider a bucket $\mathcal{B}_x = \{f_1, f_2, f_3, f_4\}$. Its Hasse diagram in depicted in Figure 8.11. As observed, the finest partition is $Q^{\perp} = \{\{f_1\}, \{f_2\}, \{f_3\}, \{f_4\}\}$ (depicted in the bottom of the diagram). The coarsest partition is $Q^{\top} = \{\{f_1, f_2, f_3, f_4\}\}$ (depicted in the top of the diagram).

Since an optimal partition-seeking algorithm may need to traverse the partitioning lattice bottom-up along all paths, yielding a computationally hard task, only depth-first greedy traversals schemes may be considered. A guiding heuristic function along the lattice can be constructed based on the error that occur when combining two functions into a single mini-bucket versus keeping them separate,

The traversal can be guided by a heuristic function h defined for a partition Q and its child partition Q', denoted $Q \rightarrow Q'$. The local distance heuristics derived from the above distance measures yield *content-based* local partitioning heuristics(see [**?**]). At each step, the algorithm ranks

function `GreedyPartition`($\mathcal{B}$,i, h)
1. **Initialize** Q as the bottom partition of B;
2. **While** $\exists Q' \in ch(Q)$ which is a i-partition
$Q \leftarrow \arg\min_{Q'}\{h(Q \rightarrow Q')\}$ among child i-partitions of Q;
3.Return Q;

Figure 8.12: Greedy partitioning

each child Q' of the current partition Q according to such an h. Clearly, each iteration is guaranteed to tighten the resulting bound. Algorithm GreedyPartition is given in Figure 8.12.

Proposition 8.14 *The time complexity of* `GreedyPartition` *is* $O(|B| \times T)$ *where* $O(T)$ *is the time complexity of selecting the* min *child partition according to* h.

8.6.3 GENERALIZED MBE

The schedule by which mini-buckets are identified and processed can be relaxed. It does not have to be regimented to be processed in blocks for each variable. In other words, we can process just a single mini-bucket of B first, yielding a new, relaxed problem to which we can apply the mini-bucket recursively. In particular we can identify, and process a mini-bucket of C and then go back and process another mini-bucket of B and so on. This alternative schedule is apparent once we reason about partitioning heuristics as variable duplications. Finally, a relaxed network due to variable-duplication can be processed by any means, not necessarily by bucket-elimination. This observation open ups a richer collection of bounding schemes that can be considered.

8.7 USING THE MINI-BUCKET AS AN ANYTIME SCHEME

The mini-bucket scheme can be used as a stand alone approximation. Yet it can be extended into an anytime scheme or can be augmented within a search scheme as described next.

An important property is that the scheme provides an adjustable trade-off between accuracy of a solution and the complexity of deriving it. Both the accuracy and the complexity increase monotonically with the parameters i and m. While in general it may not be easy to predict the algorithm's performance for a particular parameter setting, it is possible to use this scheme within an *anytime* framework. *Anytime algorithms* can be interrupted at any time producing the best solution found thus far. As more time is available, better solutions will be generated.

We can have an anytime algorithm by running a sequence of mini-bucket algorithms with increasing values of i and m until either a desired level of accuracy is obtained, or until the computational resources are exhausted. To illustrate, such an anytime scheme for finding the mpe, *ANYTIME-*

Algorithm ANYTIME-mpe(ϵ)
Input: A belief network $\mathcal{B} =< X, D, G, \mathcal{P} >$, where $\mathcal{P} = \{P_1, ..., P_n\}$;
an ordering of the variables, $d = X_1, ..., X_n$; observations $\mathbf{e}$.
Initial values, i_0 and m_0; increments i_{step} and m_{step}, approximation error ϵ.
Output: An upper bound U and a lower bound L on the $MPE = \max_{\bar{x}} P(\bar{x}, \bar{e})$, and a suboptimal solution $\bar{x}^a$ that provides a lower bound $L = P(\bar{x}^a)$.
1. **Initialization:** $i = i_0, m = m_0$.
2. **while resources are available, do**

- run *MBE-mpe(i,m)*
- $U \leftarrow$ upper bound of *MBE-mpe(i,m)*
- $L \leftarrow$ lower bound of *MBE-mpe(i,m)*
- Retain best bounds U, L, and best solution found so far
- **if** $1 \leq U/L \leq 1 + \epsilon$, return solution
- **else** increase i and m: $i \leftarrow i + i_{step}$ and $m \leftarrow m + m_{step}$

3. **Return** the largest L and the smallest U found so far.
Return the corresponding mpe assignment.

Figure 8.13: Algorithm *ANYTIME-mpe(ϵ)*.

mpe(ϵ) is presented in Figure 8.13, where using a parameter ϵ to express the desired accuracy level. The algorithm uses initial parameter settings, i_0 and m_0, and increments i_{step} and m_{step}. *MBE-mpe(i,m)* computes a suboptimal *mpe* solution and the corresponding lower and upper bounds L, and U for increasing values of i and m. The algorithm terminates when either $1 \leq U/L \leq 1 + \epsilon$, or when the computational resources (i.e., memory) are exhausted, returning the largest lower bound and the smallest upper bound found so far, as well as the current highest suboptimal solution. This scheme is not fully anytime due to the memory restriction of MBE. In other words, it is not *any space*.

For other queries, such as belief computations deriving the upper and lower bound can be done using two runs of WMBE to generate both an upper bound and a lower bound using all-positive, or a single negative weight, respectively.

The above scheme can be refined and improved to save redundant computation in the repeated mini-bucket runs and also in controlling the partitioning from one run to the next in a manner that will

guarantee improvements by combining some mini-buckets, from one iteration to the next. (Exercise: design an anytime scheme that allows computation sharing between subsequent mbe processing.)

Embedding mini-bucket as heuristic generation for search. An orthogonal anytime extension of the mini-bucket, is to embed it within a complete anytime heuristic search algorithm such as *branch-and-bound* for optimization tasks. Since, the mini-bucket scheme computes bounds (upper or lower) on the exact quantities, these bounds can be used as heuristic functions to guide search algorithms and for pruning the search space. In other words, rather than stopping with the first solution found (which is a lower bound for maximization), as it is done in the forward step of *MBE-mpe*, we can continue searching for better solutions, while using the mini-bucket functions to guide and prune the search. This approach was explored extensively in recent year yielding state-of the art algorithms both for finding an mpe assignment as well as for constraint optimization problems [Marinescu and Dechter, 2009b, **?**].

In the context of sum-product queries such as belief updating and probability of evidence, the mini-bucket's output can be viewed as approximating the probability distribution of the Bayesian network. This can be used as a basis for sampling (e.g., importance sampling) and for guiding search to bound quantities of interest. More on this in future chapters. For details on this direction see [Gogate, 2009, **?**, **?**, **?**].

8.8 FROM MINI-BUCKET TO MINI-CLUSTERING

The mini-bucket idea can be extended to any tree-decomposition scheme. In this section we will describe one such extension called *Mini-Clustering (MC)*. The benefit of this algorithm is that all single-variable beliefs are computed (approximately) at once, using a two-phase message-passing process along the cluster tree like in the mini-bucket bounded inference.

We focus on likelihood computations (belief-updating and probability of evidence) for which such extensions (from mini-bucket to mini-clustering) are most relevant. We will consider a general belief network $BN =< X, D, G, P >$ and its *tree-decomposition* defined as usual by $< T, \chi, \psi >$, where $T = (V, E)$ is a tree, and χ and ψ are the labeling functions which associate with each vertex $v \in V$ two sets, $\chi(v) \subseteq X$ and $\psi(v) \subseteq P$.

Rather than computing the mini-bucket approximation n times, one for each variable as would be required by the mini-bucket approach, *mini-clustering* performs an equivalent computation with just two message passings along each arc of the tree-decomposition. Remember that a tree-decomposition assigns to each node u in the tree T a set of variables $\chi(u)$ and a set of functions $\psi(u)$ (see Chapter 5). During CTE's processing of a cluster u, the cluster contains the original functions as well as messages from neighboring clusters which we denote as $cluster(u)$ (see Algorithm 5.10). We can partition $cluster(u)$ into p mini-clusters $mc(1), \ldots, mc(p)$, each having at most i variables, where i is the i-bound controlling the accuracy. Instead of computing the message $h_{u\to v} = \sum_{elim(u,v)} \prod_{f\in cluster(u)} f$ by CTE-bel from node u to node v; we can divide the functions of $cluster(u)$ into p mini-clusters and rewrite $h_{u\to v} = \sum_{elim(u,v)} \prod_{f\in cluster(u)} f =$

Weighted Mini-Clustering Elimination for Belief Updating (MC-bel-max(i))
Input: A tree decomposition $\langle T, \chi, \psi \rangle T = (V, E)$ for
$\mathcal{B} = \langle X, D, G, P \rangle$. Evidence variables $var(e)$. An i-bound parameter i.
Output: An augmented tree whose nodes are clusters containing the original CPTs as well as messages received from neighbors. An upper bound for $P(X_i, e)$. Denote by $H_{u \to v}$ the message sent by vertex u to vertex v, $ne_v(u)$ the neighbors of u in T excluding v.
$cluster(u) = \psi(u) \cup \{H_{v \to u} | (v, u) \in E\}$.
1. **Compute the combined mini-functions: For** every node u in the cluster tree, T, once u has received messages from all $ne_v(u)$, compute message to node v:

- **Process observed variables:**
  For each $u \in T$ assign relevant evidence to all $p_i \in \psi(u)$.
- **Compute the combined mini-functions:** Make an (i)-partitioning of $cluster_v(u)$, $\{mc(1), \ldots, mc(p)\}$;
- $h^j_{u \to v} = (\sum_{elim(u,v)} \prod_{f \in mc(j)} f^{w_j})^{\frac{1}{w_j}}$
- add $\{h^j_{u \to v} | j = 1, \ldots, p\}$ to $H_{u \to v}$. Send the ste of messages $H_{u \to v}$ to v.

2. **Compute upper bounds $\overline{P}(X_i, e)$ on $P(X_i, e)$:**
For every $X_i \in X$ let $u \in V$ be a cluster such that $X_i \in \chi(u)$. Apply (i)-partition mini-clusters for $cluster(u)$, $\{mc(1), \ldots, mc(p)\}$; Compute $\overline{P}(X_i, e) = \prod_{k=1}^{p} (\sum_{\chi(u) - X_i} (\prod_{f \in mc(k)} f)^{w_k})^{\frac{1}{w_k}}$.

Figure 8.14: Procedure Mini-Clustering for Belief Updating (MC-bel)

$\sum_{elim(u,v)} \prod_{k=1}^{p} \prod_{f \in mc(k)} f$. By migrating the summation operator into each mini-cluster, yielding $\prod_{k=1}^{p} \sum_{elim(u,v)} \prod_{f \in mc(k)} f$, we get an upper bound on $h_{u \to v}$. The resulting algorithm, called MC-bel(i) is presented in Figure 8.14 (notice that we dropped the m parameter for simplicity).

The combined functions are approximated via mini-clusters, as follows. Suppose $u \in V$ has received messages from all its neighbors other than v (the message from v is ignored even if received). The functions in $cluster_v(u)$ that are to be combined are partitioned into mini-clusters $\{mc(1), \ldots, mc(p)\}$, each one containing at most i variables. Each mini-cluster is processed by summation over the eliminator, or by maximization, and the resulting combined functions as well as all the individual functions (not dependant on the separator) are sent to v.

As in the mini-bucket case we can also derive a lower-bound on beliefs by replacing the max operator with min operator. This allows computing both an upper bound and a lower bound on

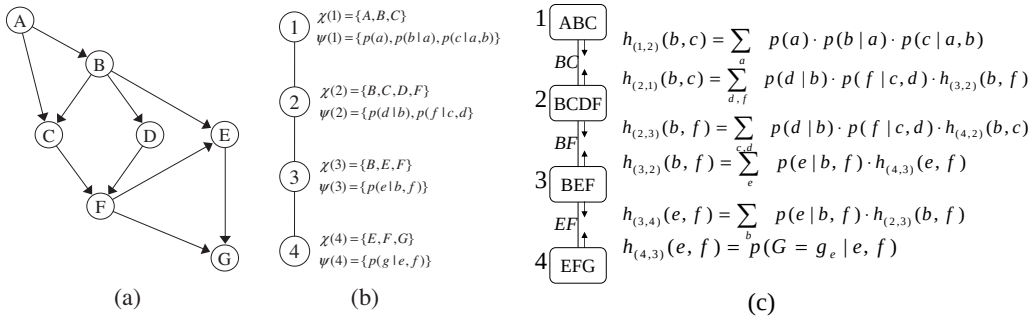


Figure 8.15: (a) A belief network; (b) A join-tree decomposition; (c) Execution of CTE-BU.

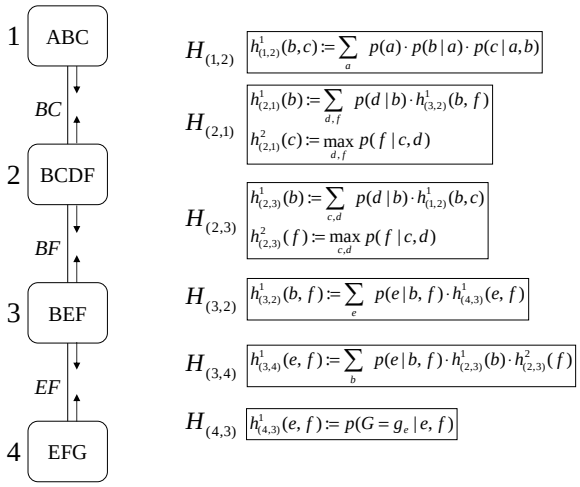


Figure 8.16: Execution of MC-bel for $i = 3$

the joint beliefs. Alternatively, if we forgo the desire to derive a bound, we can replace max by a $mean$ operator (taking the sum and dividing by the number of elements in the sum), deriving an approximation of the joint belief.

Algorithm *MC-bel* for upper bounds can be obtained from CTE by replacing step 2 of the main loop and the final part of computing the upper bounds on the joint belief by the procedure given in Figure 5.10 yielding the Algorithm in Figure 8.14. The partitioning of clusters to mini-clusters can be done in an identical manner to partitioning buckets into mini-buckets as discussed earlier.

Example 8.15 Figure 8.16 shows the trace of running MC-bel(3) on the problem in Figure 8.15. First, evidence $G = g_e$ is assigned in all CPTs. There are no individual functions to be sent from cluster 1 to cluster 2. Cluster 1 contains only 3 variables, $\chi(1) = \{A, B, C\}$, there-

fore it is not partitioned. The combined function $h^1_{1\to 2}(b,c) = \sum_a p(a) \cdot p(b|a) \cdot p(c|a,b)$ is computed and the message $H_{1\to 2} = \{h^1_{1\to 2}(b,c)\}$ is sent to node 2. Now, node 2 can send its message to node 3. Again, there are no individual functions. Cluster 2 contains 4 variables, $\chi(2) = \{B, C, D, F\}$, and a partitioning is necessary: MC-bel(3) can choose $mc(1) = \{p(d|b), h_{1\to 2}(b,c)\}$ and $mc(2) = \{p(f|c,d)\}$. The combined functions using power sum is $h^1_{2\to 3}(b) = (\sum_{c,d}(p(d|b) \cdot h_{1\to 2}(b,c))^{w_1})^{\frac{1}{w_1}}$ and $h^2_{2\to 3}(f) = (\sum_{c,d}(p(f|c,d))^{w_2})^{\frac{1}{w_2}}$ where $w_1 + w_2 = 1$ are computed and the message $H_{4\to 3} = \{h^1_{2\to 3}(b), h^2_{2\to 3}(f)\}$ is sent to node 3. The algorithm continues until every node has received messages from all its neighbors. An upper bound on $P(a, G = g_e)$ can now be computed by choosing cluster 1, which contains variable A. It doesn't need partitioning, so the algorithm just computes $\sum_{b,c} p(a) \cdot p(b|a) \cdot p(c|a,b) \cdot h^1_{2\to 1}(b) \cdot h^2_{2\to 1}(c)$. Notice that unlike CTE-bel which processes 4 variables in cluster 2, MC-bel(3) never processes more than 3 variables at a time. It is easy to see that,

Theorem 8.16 *Given a Bayesian network $\mathcal{B} = \langle X, D, G, P\rangle$, MC-bel(i) computes an upper bound on the joint probability $P(X, e)$ of each variable and each of its values.*

You can also convince yourself about the complexity: (or consult the proof in [**?**])

Theorem 8.17 Complexity of MC-bel(i). *Given a Bayesian network $\mathcal{B} = \langle X, D, G, P\rangle$ and a tree-decomposition $\langle T, \chi, \psi\rangle$ of $\mathcal{B}$, the time and space complexity of MC-bel(i) is $O(n \cdot hw^* \cdot k^i)$, where n is the number of variables, k is the maximum domain size of a variable and $hw^* = max_{u\in T}|\{f \in P|scope(f) \cap \chi(u) \neq \Phi\}|$, which bounds the number of mini-clusters.*

The mini-clustering scheme for posterior marginals suffers from the same normalization issues as the mini-bucket scheme. As noted, MC-bel(i) is an improvement over the Mini-Bucket algorithm MBE-bel(i), in that it allows the computation of $\overline{P}(X_i, e)$ for all variables with a single run, whereas MBE(i) computes $\overline{P}(X_i, e)$ for just one variable, with a single run [**?**]. When computing $\overline{P}(X_i, e)$ for each variable, MBE-bel(i) has to be run n times, once for each variable (an algorithm we call nMBE(i)). In [**?**] it was demonstrated that MC-bel(i) has up to linear speed-up over nMBE(i). For a given i, the accuracy of MC-bel(i) can be shown to be not worse than that of nMBE(i).

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 because it is not anyspace. Namely it is limited by the available memory. It 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. Allowing it 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 join-graph decompositions. A *join-graph decomposition* for $BN =< X, D, G, P >$ is a triple $D =< JG, \chi, \psi >$, 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 $scope(p_i) \subseteq \chi(v)$.
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.

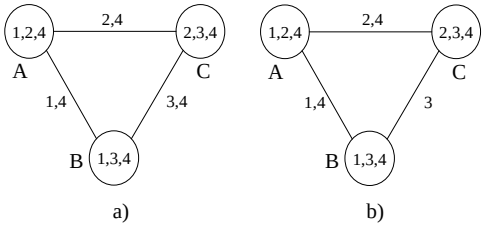


Figure 9.1: An arc-labeled decomposition

It is clear that one of the problems of message propagation over cyclic join-graphs is *over-counting*. Various schemes were proposed to overcome this problem. We will describe here a scheme that avoids cycles relative to a single variable.

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 9.2 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.

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

Definition 9.3 ((minimal) arc-labeled join-graph decompositions.) An *arc-labeled decomposition* for $BN =< X, D, P_G, \prod$ 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 $(v, u) \subset E$ the set $\theta((v, u)) \subseteq X$ such that:

1. For each function $p_i \in P$, there is *exactly* one vertex $v \in V$ such that $p_i \in \psi(v)$, and $scope(p_i) \subseteq \chi(v)$.
2. (arc-connectedness) For each arc (u, v), $\theta(u, v) \subseteq sep(u, v)$, 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 9.4 separator, eliminator. Given two adjacent vertices u and v of JG, the *separator* of u and v is defined as $sep(u, v) = \theta((u, v))$, and the *eliminator* of u with respect to v is $elim(u, v) = \chi(u) - \theta((u, v))$.

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

Proposition 9.5 *A* minimal arc-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 arc-labeled join-graph is arc-minimal (no arc 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,and then which do not introduce new independencies, 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 [Pearl, 1988]) of the underlying probability distribution relative to node-separation. Since we plan to use minimally arc-labeled join-graphs to address over-counting problems, the question is what kind of independencies are captured by such graphs.

Definition 9.6 **(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 $\mathcal{B} = \langle X, D, P_G, \prod \rangle$. 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 9.7 *Any arc-labeled join-graph decomposition $D = \langle JG, \chi, \psi, \theta \rangle$ of a belief network $\mathcal{B} = \langle X, D, G, P \rangle$ is an I-map of P relative to edge-separation. Namely, any edge separation in D corresponds to conditional independence in P.*

For a proof see [Mateescu *et al.*, 2010].

Algorithm **Iterative Join Graph Propagation (IJGP)**

Input An arc-labeled join-graph decomposition $\langle JG, \chi, \psi, \theta \rangle$, $JG = (V, E)$ for $\mathcal{B} = \langle X, D, P_G, \prod \rangle$. Evidence variables $var(e)$.

Output An augmented graph whose nodes are clusters containing the original CPTs and the messages received from neighbors. Approximations of $P(X_i, e)$, $\forall X_i \in X$.

Denote by $h_{(u \to v)}$ the message from vertex u to v, $ne_v(u)$ the neighbors of u in JG excluding v.
$cluster(u) = \psi(u) \cup \{h_{(v \to u)} | (v, u) \in E\}$.
$cluster_v(u) = cluster(u)$ excluding message from v to u.

• **One iteration of IJGP:**
For every node u in JG in some topological order d and back, do

1. **Process observed variables:**
   Assign relevant evidence to all $p_i \in \psi(u)$ $\chi(u) := \chi(u) - var(e), \ \forall u \in V$
2. **Compute individual functions:**
   Include in $H_{(u \to v)}$ each function in $cluster_v(u)$ whose scope does not contain variables in $elim(u, v)$. Denote by A the remaining functions.
3. **Compute and send to v the combined function:** $h_{(u \to v)} = \sum_{elim(u,v)} \prod_{f \in A} f$.
   Send $h_{(u \to v)}$ and the individual functions $H_{(u \to v)}$ to node v.

Endfor
• **Compute** $P(X_i, e)$**:**

For every $X_i \in X$ let u be a vertex in JG such that $X_i \in \chi(u)$.
Compute $P(X_i, e) = \alpha \sum_{\chi(u) - \{X_i\}} (\prod_{f \in cluster(u)} f)$

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

9.1.1 ALGORITHM IJGP

Applying CTE iteratively to minimal arc-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.

It is straightforward to show that:

Theorem 9.8

1. *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.*
2. *[Mateescu et al., 2010] 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 decompo-*

sition, k is the maximum domain size, w is the maximum cluster size and θ is the maximum label size.

For proof see properties of CTE in [**?**].

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.

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

9.1.2 ITERATIVE BELIEF PROPAGATION

Iterative belief propagation (IBP) is an iterative application of Pearl's algorithm for poly-trees [Pearl, 1988] to any Bayesian network. We will describe IBP as an instance of join-graph propagation over a *dual graph*.

Definition 9.9 dual graphs. Given a set of functions $F = \{f_1, ..., f_l\}$ over scopes $S_1, ..., S_l$, 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 arc-labeled edge subgraph of DG. A *minimal* dual join-graph is a dual join-graph for which none of the edge labels can be further reduced while maintaining the connectedness property.

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 9.10 *Any Bayesian network has a minimal dual join-graph where each arc is labeled by a single variable.*

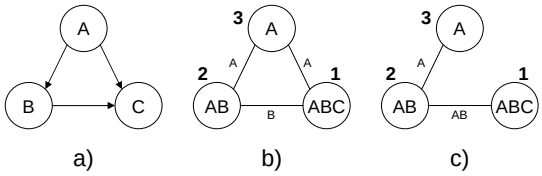


Figure 9.3: a) A belief network; b) A dual join-graph with singleton labels; c) A dual join-graph which is a join-tree

Proof. Consider a topological ordering of the nodes in the acyclic directed graph of the Bayesian network $d = X_1, ..., X_n$. 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 arc between p_j and p_i by variable X_j, namely $l_{ij} = \{X_j\}$. It is easy to see that the resulting arc-labeled subgraph of the dual graph satisfies connectedness. The resulting labeled graph is a dual graph with singleton labels. □

Example 9.11 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 9.4. It 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 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.

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.

Algorithm **IBP**
Input: An edge-labeled dual join-graph $DG = (V, E, L)$ for a Bayesian network $\mathcal{B} = \langle X, D, P_G, \prod \rangle$. Evidence e.
Output: An augmented graph whose nodes include the original CPTs and the messages received from neighbors. Approximations of $P(X_i, e)$, $\forall X_i \in X$. Approximations of $P(F_i, e)$, $\forall F_i \in \mathcal{B}$.
Denote by: $h_{u\to v}$ the message from u to v; $ne(u)$ the neighbors of u in V; $ne_v(u) = ne(u) - \{v\}$; l_{uv} the label of $(u, v) \in E$; $elim(u, v) = scope(u) - scope(v)$.
• **One iteration of IBP**
For every node u in DJ in a topological order and back, do:
1. **Process observed variables**
Assign evidence variables to the each p_i and remove them from the labeled edges.
2. **Compute and send to v the function:**

$$h_{u\to v} = \sum_{elim(u,v)} (p_u \cdot \prod_{\{h_{i\to u}, i\in ne_v(u)\}} h_{i\to v})$$

Endfor
• **Compute approximations of $P(F_i, e)$, $P(X_i, e)$:**
For every $X_i \in X$ let u be the vertex of family F_i in DJ,
$P(F_i, e) = \alpha(\prod_{h_{i\to u}, u\in ne(i)} h_{i\to u}) \cdot p_u$;
$P(X_i, e) = \alpha \sum_{scope(u)-\{X_i\}} P(F_i, e)$.

Figure 9.4: Algorithm Iterative Belief Propagation

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 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 9.6. 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 9.12 *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.

Algorithm **Join-Graph Structuring(*i*)**

1. Apply procedure schematic mini-bucket(i).
2. Associate each resulting mini-bucket with a node in the join-graph, the variables of the nodes are those appearing in the mini-bucket, the original functions are those in the mini-bucket.
3. Keep the edges created by the procedure (called out-edges) and label them by the regular separator.
4. Connect the mini-bucket clusters belonging to the same bucket in a chain by in-edges labeled by the single variable of the bucket.

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

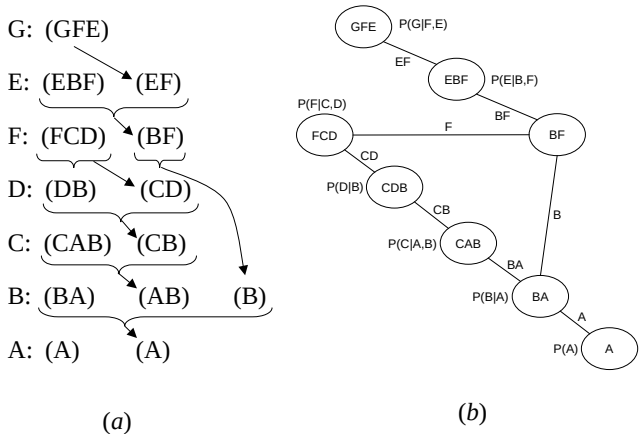
Procedure **Schematic Mini-Bucket(*i*)**

1. Order the variables from X_1 to X_n minimizing (heuristically) induced-width, and associate a bucket for each variable.
2. Place each CPT in the bucket of the highest index variable in its scope.
3. For $j = n$ to 1 do:
   Partition the functions in $bucket(X_j)$ into mini-buckets having at most i variables.
   For each mini-bucket mb create a new scope-function (message) f where $scope(f) = \{X | X \in mb\} - \{X_i\}$ and place scope(f) in the bucket of its highest variable. Maintain an edge between mb and the mini-bucket (created later) of f.

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

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 $u, w_1, ..., w_m, v$ 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. □



(*a*) (*b*)

Figure 9.7: Join-graph decompositions.

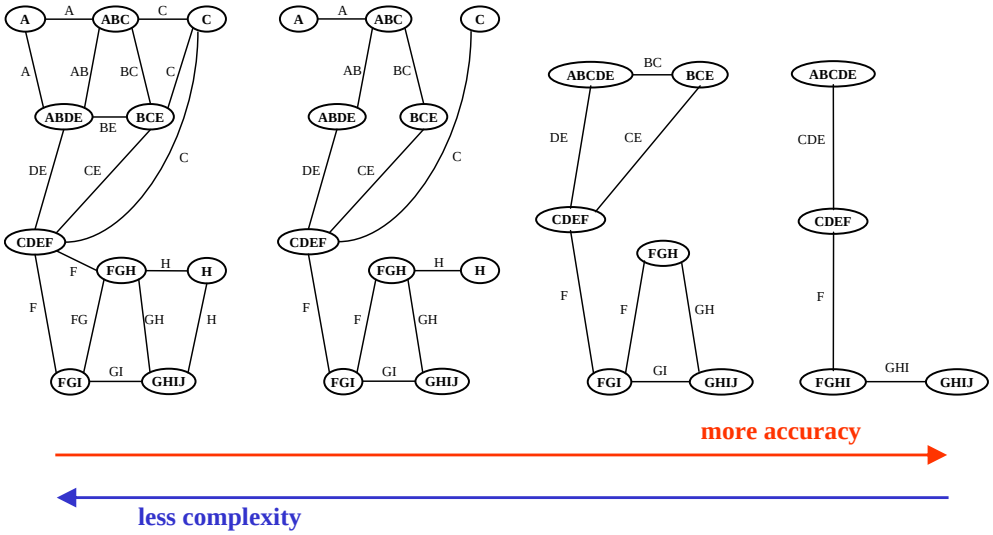


Figure 9.8: Join-graphs.

Example 9.13 Figure 9.7a shows the trace of procedure schematic mini-bucket(3) applied to the problem described in Figure 8.15a. The decomposition in Figure 9.7b 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 9.14 Figure 9.8 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.

9.2 COST-SHIFTING FOR BETTER APPROXIMATION

The relaxation view of MBE is closely related to a family of iterative approximation techniques based on linear programming (LP). These include "re-weighted" max-product [**?**], Max-Product Linear Programming (MPLP) [**?**], dual decomposition [**?**], and soft arc consistency [**??**]. Like the mini-bucket scheme these algorithms simplify the graphical model into independent components and tighten the resulting bound via iterative cost-shifting updates. They can be thought of as "re-parametrizing" the original functions without changing the global model. Most of the schemes operate on the original factors of the model, although some works tighten the approximations by introducing larger clusters [**?**].

We can combine the ideas of MBE and re-parametrization to define two new hybrid schemes. We will introduce mini-bucket elimination with max-marginal matching (MBE-MM), which is a non-iterative algorithm that applies a single pass of cost-shifting during the mini-bucket construction bucket by bucket. The second approach, Join Graph Linear Programming (JGLP), iteratively applies cost-shifting updates to the full mini-bucket join-graph. Empirical evaluation demonstrated the increased power of these hybrid approximation schemes over their individual components.

9.2.1 LINEAR PROGRAMMING METHODS

We discussed the mini-bucket elimination algorithm in Section **??**. Here we provide background on the alternative approximation approach for solving optimization tasks, using existing LP-relaxation methods. Note that throughout we describe algorithms in terms of a maximization task, unless specified otherwise.

To introduce the idea assume for simplicity that the network consists only of pairwise functions $f_{ij}(X_i, X_j)$ and that the problem is max-sum, i.e., to compute $C^* = \max_{\mathbf{X}} \sum_{f_{ij} \in F} f_{ij}(X_i, X_j)$. A simple bound on the max-sum objective is then given by maxima of the individual functions, exchanging the sum and max operators:

$$C^* = \max_{\mathbf{X}} \sum_{f_{ij} \in F} f_{ij}(X_i, X_j) \leq \sum_{f_{ij} \in F} \max_{\mathbf{X}} f_{ij}(X_i, X_j) = \sum_{f_{ij} \in F} \max_{X_i, X_j} f_{ij}(X_i, X_j) \qquad (9.1)$$

As noted for the mini-bucket case we can interpret this operation as making an individual copy of each variable for each function, and optimizing over them separately. See, for example, the problem in Figure 9.9(a) with 3 variables and 3 functions. Figure 9.9(e). We can also derive a bound on the optimal cost by introducing a collection of functions $\{\lambda_{ij}(X_i), \lambda_{ji}(X_j)\}$ for each edge (ij) and requiring

$$\lambda \in \Lambda \quad \Leftrightarrow \quad \forall i, \quad \sum_j \lambda_{ij}(X_i) = 0 \tag{9.2}$$

Then, we have

$$\begin{aligned} C^* &= \max_{\mathbf{X}} \sum_{f_{ij} \in F} f_{ij}(X_i, X_j) \\ &= \max_{\mathbf{X}} \sum_{f_{ij} \in F} f_{ij}(X_i, X_j) + \sum_i \sum_j \lambda_{ij}(X_i) \\ &\leq \min_{\lambda \in \Lambda} \sum_{f_{ij} \in F} \max_{X_i, X_j} \left(f_{ij}(X_i, X_j) + \lambda_{ij}(X_i) + \lambda_{ji}(X_j) \right) \end{aligned} \tag{9.3}$$

The last expression is obtained by distributing each λ_{ij} to its associated factor and applying the inequality (9.1).

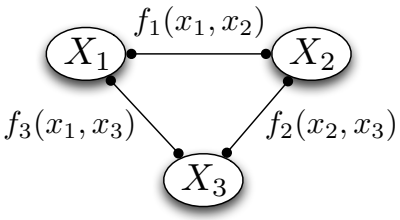
The new functions $\tilde{f}_{ij} = f_{ij}(X_i, X_j) + \lambda_{ij}(X_i) + \lambda_{ji}(X_j)$ define a *re-parametrization* of the original distribution, i.e., they change the individual functions without modifying the global function $F(\mathbf{X}) = \sum_{\mathbf{X}} f_{ij} = \sum_{\mathbf{X}} \tilde{f}_{ij}$. Depending on the literature, the λ_{ij} are interpreted as "cost-shifting" operations that transfer cost from one function to another while preserving the overall cost [**??**], or as Lagrange multipliers enforcing consistency among the copies of X_i [**??**]. In the former interpretation, the updates are called "soft arc-consistency" due to their similarity to arc-consistency for constraint satisfaction [**?**]. Under the latter view, the bound corresponds to a *dual decomposition* solver for a linear programming (LP) relaxation of the original problem [**??**].

The main distinguishing feature among such dual decomposition approaches is the way in which the bound is tightened by updating the functions λ. This is done either by sub-gradient or gradient approaches [**??**] or by coordinate descent updates that can be interpreted as "message passing" [**??**]. Without going into the details of these approaches, we refer to these iterative bound improvement updates as "LP-tightening" updates, although technically we are tightening the decomposition bound (9.3) which is the dual of the LP.

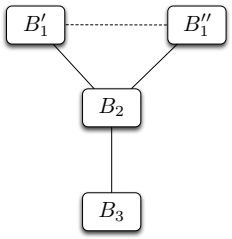
LP-tightening algorithm. Next we will show a derivation of a particular simple, yet effective scheme that minimizes over λs the expression

$$\sum_{f_{ij} \in F} \max_{X_i, X_j} \left(f_{ij}(X_i, X_j) + \lambda_{ij}(X_i) + \lambda_{ji}(X_j) \right) \tag{9.4}$$

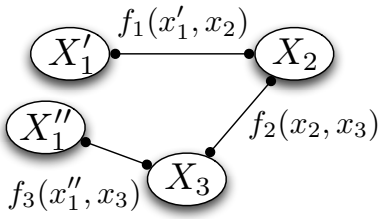
tightening the upper bound on C^* (Eq. 9.3). This scheme, though formulated by us, is closely related to the "tree-block" coordinate descent updates derived by Sontag and Jaakkola [**?**]. The intuition behind the iterative updates used in this scheme is very similar to the ones employed by our algorithms JGLP (Section 9.2.2) and MBE-MM (Section 9.2.3).



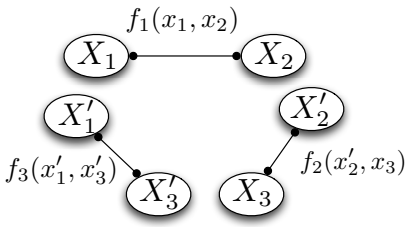
(a) (a) Original model



(b) (c) Join graph



(c) (d) Model with duplicated variables in a mini-bucket



(d) (e) Model with all variables duplicated

Figure 9.9: The mini-bucket procedure for a simple graph. (a) Primal graph; (b) the buckets and messages computed in MBE; (c) join-graph, dotted line corresponds to an edge absent from a mini-bucket tree; (d) interpreting MBE as variable duplication, X_1 is duplicated in each of two mini-buckets $q_1^1 = \{f_1(X_1, X_2)\}$ and $q_1^2 = \{f_3(X_1, X_3)\}$; (e) The graph on which FGLP runs with all variables duplicated and each factor processed separately.

The LP-tightening scheme is initialized with all $\lambda_{ij}(X_i) = 0$. In the spirit of well-known coordinate descent approaches we iteratively minimize expression 9.4 with respect to each $\lambda_{ij}(X_i)$ separately, while fixing the values of all other λs. For simplicity of derivation, without loss of generality, we assume that each variable X_i appears in scope of at most two functions, $f_{ij}(X_i, X_j)$ and $f_{ik}(X_i, X_k)$. Identifying only the terms relevant to variable X_i, we obtain:

$$\min_{\lambda_{ij}(X_i),\lambda_{ik}(X_i)} \Big[\big[\max_{X_i,X_j} f_{ij}(X_i, X_j) + \lambda_{ij}(X_i) \big] + \big[\max_{X_i,X_k} f_{ik}(X_i, X_k) + \lambda_{ik}(X_i) \big] \Big]$$
$$= \min_{\lambda_{ij}(X_i),\lambda_{ik}(X_i)} \Big[\max_{X_i} \big[\max_{X_j} f_{ij}(X_i, X_j) + \lambda_{ij}(X_i) \big] + \max_{X_i} \big[\max_{X_k} f_{ik}(X_i, X_k) + \lambda_{ik}(X_i) \big] \Big]$$

Algorithm 6: LP-tightening (based on [**?**])

Input: A graphical model $\mathcal{M} = \langle \mathbf{X}, \mathbf{D}, \mathbf{F}, \sum \rangle$, where $f_{\mathbf{S}_i}$ is a potential defined on variables $\mathbf{S}_i$
Output: Upper bound on the optimum value of $\max_{\mathbf{X}} \sum \mathbf{F}$
while *NOT converged* **do**
  for *any pair of function scopes* $\boldsymbol{S}_i, \boldsymbol{S}_j$ *such that* $\boldsymbol{S}_{ij} = \boldsymbol{S}_i \cap \boldsymbol{S}_j \neq \emptyset$ **do**
    Compute max-marginals:
    $\gamma_{\mathbf{S}_i}(\mathbf{S}_{ij}) = \max_{\mathbf{S}_i \setminus \mathbf{S}_{ij}} f_{\mathbf{S}_i}$;
    $\gamma_{\mathbf{S}_j}(\mathbf{S}_{ij}) = \max_{\mathbf{S}_j \setminus \mathbf{S}_{ij}} f_{\mathbf{S}_j}$;
    Update parametrization:
    $f_{\mathbf{S}_i} \leftarrow f_{\mathbf{S}_i} + \frac{1}{2}\big(\gamma_{\mathbf{S}_j}(\mathbf{S}_{ij}) - \gamma_{\mathbf{S}_i}(\mathbf{S}_{ij})\big)$;
    $f_{\mathbf{S}_j} \leftarrow f_{\mathbf{S}_j} + \frac{1}{2}\big(\gamma_{\mathbf{S}_i}(\mathbf{S}_{ij}) - \gamma_{\mathbf{S}_j}(\mathbf{S}_{ij})\big)$;

Let us define the so-called "max-marginals" $\gamma_{ij}(X_i) = \max_{X_j} f_{ij}(X_i, X_j)$ and re-arrange the terms in the above expression, yielding the following bound:

$$
\begin{aligned}
&\min_{\lambda_{ij}(X_i), \lambda_{ik}(X_i)} \Big[\max_{X_i} \big[\max_{X_j} f_{ij}(X_i, X_j) + \lambda_{ij}(X_i) \big] + \max_{X_i} \big[\max_{X_k} f_{ik}(X_i, X_k) + \lambda_{ik}(X_i) \big] \Big] \\
&= \min_{\lambda_{ij}(X_i), \lambda_{ik}(X_i)} \Big[\max_{X_i} \big[\gamma_{ij}(X_i) + \lambda_{ij}(X_i) \big] + \max_{X_i} \big[\gamma_{ik}(X_i) + \lambda_{ik}(X_i) \big] \Big] \\
&\geq \min_{\lambda_{ij}(X_i), \lambda_{ik}(X_i)} \Big[\max_{X_i} \big[\gamma_{ij}(X_i) + \gamma_{ik}(X_i) + \lambda_{ij}(X_i) + \lambda_{ik}(X_i) \big] \Big]
\end{aligned}
\tag{9.5}
$$

We require that $\lambda_{ij}(X_i) + \lambda_{ik}(X_i) = 0$ to make sure that the total cost of the problem is not changed (Equation 9.2).

Many choices of λ_{ij} are known to achieve the minimum of the right-hand side of expression 9.5. We chose to use the following one:

$$
\lambda_{ij}(X_i) = \frac{1}{2}\big(\gamma_{ik}(X_i) - \gamma_{ij}(X_i)\big) = \frac{1}{2}\big(\max_{X_k} f_{ik}(X_i, X_k) - \max_{X_j} f_{ij}(X_i, X_j)\big) \tag{9.6}
$$

Iterating over all functions, while updating each function $\forall i, j, f_{ij}(X_i, X_j) \leftarrow f_{ij}(X_i, X_j) + \lambda_{ij}(X_i)$ and recalculating λ_{ij} at each step until convergence, yields a minimization procedure that can be interpreted as a *max-marginal* or *moment-matching* procedure on the functions $f_{ij}(X_i, X_j)$. Intuitively, we would like the updates to diminish in magnitude and converge to zero as fast as possible. To achieve that, taking into account Equation 9.6, we would like to make the max-marginals $\gamma_{ij}(X_i)$ and $\gamma_{ik}(X_i)$ of each variable X_i to be equal. Algorithm 6 generalizes this update to higher-order functions $f_{\mathbf{S}_i}$ over scopes of variables $\mathbf{S}_i \subseteq \mathbf{X}$.

A well-known algorithm quite similar to our LP-tightening in Algorithm 6 is a message-passing scheme called Max-Product Linear Programming (MPLP) [**?**]. Algorithm 7 presents a version of MPLP that we call Factor Graph Linear Programming (FGLP). At each step FGLP simultaneously updates all functions $f_{ij}(X_i, X_j)$ involving a single variable X_i. The messages sent by the algorithms on a factor graph are schematically illustrated in Figure **??**. In this example vari-

Algorithm 7: Factor Graph Linear Programming (FGLP, based on [**?**])

Input: A graphical model $\mathcal{M} = \langle \mathbf{X}, , \mathbf{F}, \sum \rangle$, variable ordering o
Output: Upper bound on the optimum value of MPE cost
while *NOT converged* **do**
  for *each variable* X_i **do**
    Get factors $F_i = f_{\mathbf{S}_k} : X_i \in \mathbf{S}_k$ with X_i in their scope;
    //for each function compute max-marginals γ marginalizing out all variables except for X_i:
    $\forall f_{\mathbf{S}_k}\ \gamma_{\mathbf{S}_k}(X_i) = \max_{\mathbf{S}_k \setminus X_i} f_{\mathbf{S}_k}$;
    // compute messages $\beta_{\mathbf{S}_k}(X_i)$ from X_i back to a function $f_{\mathbf{S}_k}$ correcting for the function's own max-marginal $\gamma_{\mathbf{S}_k}$:
    $\forall f_{\mathbf{S}_k}\ \beta_{\mathbf{S}_k} = \frac{1}{|F_i|} \sum_{\{\mathbf{S}_j | f_{\mathbf{S}_j} \in F_i\}} \gamma_{\mathbf{S}_j}(X_i) - \gamma_{\mathbf{S}_k}(X_i)$
    // update (re-parametrize) each function:
    $\forall f_{\mathbf{S}_k}, f_{\mathbf{S}_k} \leftarrow f_{\mathbf{S}_k} + \beta_{\mathbf{S}_k}$;

able X_i is in the scope of three functions: $f_{\mathbf{S}_t}(X_i, X_k, X_m)$, $f_{\mathbf{S}_p}(X_i, X_j)$ and $f_{\mathbf{S}_q}(X_i, X_n)$, where $\mathbf{S}_t = \{X_i, X_k, X_m\}$, $\mathbf{S}_p = \{X_i, X_j\}$ and $\mathbf{S}_q = \{X_i, X_n\}$. Note that in the figure we only show the messages involving X_i. The max-marginals are: $\gamma_{\mathbf{S}_q}(X_i) = \max_{X_n} f_{\mathbf{S}_q}(X_i, X_n)$, $\gamma_{\mathbf{S}_p}(X_i) = \max_{X_j} f_{\mathbf{S}_p}(X_i, X_j)$ and $\gamma_{\mathbf{S}_t}(X_i) = \max_{X_k, X_m} f_{\mathbf{S}_t}(X_i, X_k, X_m)$. The update messages from variable X_i back to the functions are:

$$\beta_{\mathbf{S}_q}(X_i) = \frac{1}{3}(\gamma_{\mathbf{S}_q}(X_i) + \gamma_{\mathbf{S}_p}(X_i) + \gamma_{\mathbf{S}_t}(X_i)) - \gamma_{\mathbf{S}_q}(X_i)$$
$$\beta_{\mathbf{S}_p}(X_i) = \frac{1}{3}(\gamma_{\mathbf{S}_q}(X_i) + \gamma_{\mathbf{S}_p}(X_i) + \gamma_{\mathbf{S}_t}(X_i)) - \gamma_{\mathbf{S}_p}(X_i)$$
$$\beta_{\mathbf{S}_t}(X_i) = \frac{1}{3}(\gamma_{\mathbf{S}_q}(X_i) + \gamma_{\mathbf{S}_p}(X_i) + \gamma_{\mathbf{S}_t}(X_i)) - \gamma_{\mathbf{S}_t}(X_i)$$

The benefit of messages passing is that it can be performed asynchronously. The issue of efficient message scheduling has been extensively studied [e.g., **???**].

Theorem 9.15 Complexity of FGLP. *The total time complexity of a single iteration of FGLP is* $O(n \cdot Q \cdot k^{Sc})$*, where* n *is the number of variables in the problem,* k *is the largest domain size,* $|\boldsymbol{F}|$ *is the number of functions,* Sc *bounds the largest scope of the original functions,* Q *is the largest number of functions having the same variable* X_j *in their scopes. The space complexity is* $O(|\boldsymbol{F}| \cdot k^{Sc})$.

9.2.2 JOIN GRAPH LINEAR PROGRAMMING

Join-Graph MBE Structuring. The mini-bucket procedure defines a mini-bucket tree. Each mini-bucket defines a cluster. Two mini-buckets are connected if there exists a message between them. Once the mini-buckets of the same variables are connected, the mini-bucket tree yields a join-graph, where each cluster has at most $i + 1$ variables, where i is the i-bound.

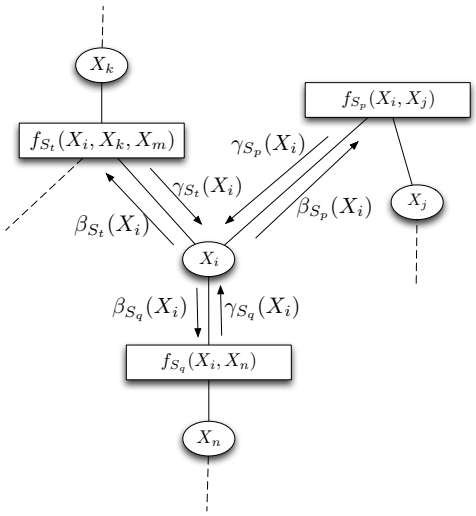


Figure 9.10: FGLP example: local messages involving variable X_i.

Algorithm 8: Algorithm JGLP

Input: A graphical model $\mathcal{M} = \langle \mathbf{X}, , \mathbf{F}, \sum \rangle$, variable order $o = \{X_1, \ldots, X_n\}$, parameter i.
Output: Upper bound on the optimum value of MPE cost
//Initialize: Partition the functions in $\mathbf{F}$ into $\mathbf{B}_{X_1}, \ldots, \mathbf{B}_{X_n}$, where $\mathbf{B}_{X_p}$ contains all functions f_{S_j} whose highest variable is X_p;
Build mini-bucket join graph; // (Algorithm **??**)
Find the function of each mini-bucket q_k^p:
$F_k^p = \sum_{f_{\mathbf{S}_j} \in q_k^p} f_{\mathbf{S}_j}$
while *NOT converged OR NOT time limit reached* **do**
  for *all pairs of mini-buckets* q_k^p, q_k^l *connected by an edge* **do**
    Find the separators $S = Scope(q_k^p) \cap Scope(q_k^l)$;
    Find the max-marginals of each mini-bucket
    q_k^p: $\gamma_k^p = \max_{Scope(q_k^p)-S}(F_k^p)$;
    q_k^j: $\gamma_k^l = \max_{Scope(q_k^l)-S}(F_k^l)$;
    Update functions in both mini-buckets
    q_k^p: $F_k^p \leftarrow F_k^p - \frac{1}{2}(\gamma_k^p - \gamma_k^l)$
    q_k^l: $F_k^l \leftarrow F_k^l + \frac{1}{2}(\gamma_k^p - \gamma_k^l)$;

Join-Graph MBE Structuring (Algorithm **??**) constructs a join-graph using the mini-bucket elimination. Note that the separators between the clusters corresponding to the mini-buckets of the same variable may be over more than a single variable, so the resulting graph may not be a join-graph in a strict sense, not satisfying the induced tree property. However, this minor point does not impact the use of the graph by our algorithms. The structure is the same as the mini-bucket-tree assuming variable duplication with additional arcs connecting mini-buckets of the same bucket in a line.

Figure 9.9 presents an example of a problem with 3 variables, whose primal graph is shown in Figure 9.9(a). In Figure 9.9(b) we see the trace of MBE on the problem, namely the buckets and the messages computed. Figure 9.9(c) shows the join-graph created by Join-Graph MBE Structuring. The dotted line corresponds to an edge absent from a mini-bucket tree and added during step at line 8.

Join-Graph Linear Programming. From the perspective of linear programming relaxation (Section 9.2.1) mini-bucket elimination can be interpreted as running a single pass of LP-tightening, sending messages top down only along edges of the spanning tree of the mini-bucket join graph. A straightforward extension of MBE can be an iterative procedure that repeatedly performs LP-tightening along all of the join graph edges. Algorithm 8 shows the resulting Join-Graph Linear Programming (JGLP) scheme. It constructs the join graph (line 1), calculated mini-bucket functions F_k^p (line 2) and performs re-parametrization updates to F_k^p (as in Algorithm 6) until convergence (lines 2-7). Note that once JGLP converges, performing mini-bucket elimination on the resulting graph will not change the bound value.

Theorem 9.16 Complexity of JGLP. *Given a problem with n variables with largest domains of size k, where at most Q functions have the same variable in their scope, and i-bound i, the time com-*

Algorithm 9: Algorithm MBE-MM

Input: A graphical model $\mathcal{M} = \langle \mathbf{X}, , \mathbf{F}, \sum \rangle$, variable order $o = \{X_1, \ldots, X_n\}$, i-bound parameter i
Output: Upper bound on the optimum value of MPE cost
//Initialize:
Partition the functions in $\mathbf{F}$ into $\mathbf{B}_{X_1}, \ldots, \mathbf{B}_{X_n}$, where $\mathbf{B}_{X_k}$ contains all functions f_j whose highest variable is X_k;
//processing bucket $\mathbf{B}_{X_k}$
for $k \leftarrow n$ *down to 1* **do**
  Partition functions g (both original and messages generated in previous buckets) in $\mathbf{B}_{X_k}$ into the mini-buckets defined $Q_{X_k} = \{q_k^1, \ldots, q_k^t\}$, where each q_k^p has no more than $i+1$ variables;
  Find the set of variables common to all the mini-buckets of variable X_k: $\mathbf{S}_k = Scope(q_k^1) \cap \cdots \cap Scope(q_k^t)$;
  Find the function of each mini-bucket
  q_k^p: $F_k^p \leftarrow \prod_{g \in q_k^p} g$;
  Find the max-marginals of each mini-bucket
  q_k^p: $\gamma_{X_k}^p = \max_{Scope(q_k^p) \setminus \mathbf{S}_k} (F_k^p)$;
  Update functions of each mini-bucket
  $F_k^p \leftarrow F_k^p - \gamma_{X_k}^p + \frac{1}{t} \sum_{j=1}^t \gamma_{X_k}^j$;
  Generate messages $h_{X_k \rightarrow X_m}^p = \max_{X_k} F_k^p$ and place each in the bucket of highest in the ordering o variable X_m in $Scope(q_k^p)$;
return *All the buckets and the cost bound from* $\boldsymbol{B}_1$*;*

plexity of a single iteration of JGLP is $O(n \cdot Q \cdot k^i)$*. The time complexity of join-graph construction step is* $O(n \cdot k^{i+1})$*. The overall space complexity is* $O(n \cdot k^{i+1} + n \cdot k^i)$*.*

Proof. The complexity of constructing a join-tree is the same as the complexity of running full mini-bucket elimination algorithm, namely $O(n \cdot k^{i+1})$. The time complexity of a single iteration of JGLP consists of performing for each edge the following steps: 1. compute max-marginals of a pair of clique functions, requires time equal to $O(2 \cdot k^{i+1-|S|})$, where $|S|$ is the size of a separator between the mini-buckets of the same variable. 2. compute the mean, which takes $O(2 \cdot k^{|S|})$ time. 3. update the clique functions, requiring $O(2 \cdot k^{i+1})$ time.

The space complexity of the algorithm is dominated by the necessity of storing in memory the join-graph, whose size is bounded by $O(n \cdot k^{i+1})$ and the messages between the clusters of size $O(n \cdot k^i)$, yielding the overall space complexity of $O(n \cdot k^{i+1})$. □

9.2.3 MBE-MM

While the iterative nature of JGLP yields more accurate bounds, in practice it can have a significant additional time and space overhead compared to MBE. The latter scheme does not need to store the entire functions computed in mini-buckets, requiring space of $O(nk^{(i+1)} + nk^i)$, only the messages between them, reducing the space complexity to $O(nk^i)$ [**?**]. The difference may seem insignificant worst-case wise, but makes a practical impact, as we will see in the empirical section.

We we next present a non-iterative scheme that performs re-parametrization between the mini-buckets of the same variable only. The algorithm mini-bucket elimination with max-marginal

matching (MBE-MM, Algorithm 9) proceeds by following the standard mini-bucket downward pass. When each mini-bucket $q_k^p \in Q_k$ is processed, before eliminating variable X_k, we first perform an LP-tightening update (that is, a re-parametrization) to the mini-bucket functions $f_{q_k^p}$. For storage and computational efficiency reasons, we perform a single update on all mini-buckets of the same variable simultaneously, matching their max-marginals on their joint intersection. Alternatively, the updates can be done between all possible pairs of mini-buckets. Although any max-marginal matching step strictly improves the bound within each bucket (Equation 9.3), it is not guaranteed to increase the overall accuracy. However, it is reasonable to expect that the update will help, and in practice we find that the bounds are almost always significantly improved (see the experiments, Section **??**).

Theorem 9.17 Complexity of MBE-MM. *Given a problem with n variables having domain of size k and an i-bound i, the worst-case time complexity of MBE-MM is $O(n \cdot Q \cdot k^{i+1})$ and its space complexity is $O(n \cdot k^i)$, where Q bounds the number of functions having the same variable X_i in their scopes.*

Interestingly, our algorithms are related to known methods in constraint satisfaction. MBE(i) and JGLP(i), parametrized by an i-bound, are analogous to directional i-consistency and full i-consistency, respectively. Our algorithm MBE-MM represents an intermediate step between these two, and is analogous to an improvement of directional i-consistency with full iterative relational consistency schemes within each bucket [**?**].

CHAPTER 10

Conclusion

We covered the principles of *exact* algorithms in graphical models, organized along the two styles of reasoning: *inference* and *search*. We focused on methods that are applicable to general graphical models, whose functions can come from a variety of frameworks and applications (constraints, Boolean, probabilities, costs etc.). These include, constraint networks and SAT models, Bayesian networks, Markov random fields, Cost networks, and Influence diagrams. Therefore, the primary features that capture structure in a unified way across all these models are graph features. The main graph property is the *induced-width* also known as *treewidth*, but we also showed the relevance of related features such as *height* of pseudo trees, *cycle-cutsets, q-cutsets* and *separator width*. We showed that both inference and search scheme are bounded exponentially by any of these parameters, and some combination of those hint at how we can trade memory for time.

With the exception of constraints, we did not discuss internal function structure as a potential feature. These function-structure features are sometimes addressed as *language* (e.g., Horn clauses, linear functions, convex functions) and can lead to various tractable classes. Other terms used are *context-sensitive* or *context specific independence*. In the constraint literature, tractability based on the language of constraints was investigated thoroughly (see Chapter 10 in[Dechter, 2003].) Likewise, focus on language is a central research activity in probabilistic reasoning. An example of a structure exploited in probabilistic graphical models are the sub-modular functions [Dughmi, 2009].

The next thing on our agenda is to extend the book with a second part focusing on approximation schemes. This obviously is necessary since exact algorithms cannot scale-up to many realistic applications that are complex and quite large and appropriately, current research centered on developing approximation schemes. But, we believe that **in order to have effective approximation algorithms we have to be equipped with the best exact algorithms, first.**

Approximation algorithms can be organized along the dimensions of inference and search as well. Given a general algorithmic architecture (such as Adaptive AND/OR search with caching (AOC(q)), or, alternatively, AO-VEC(q), we can approximate either the inference part or the search part or both, systematically yielding an ensemble of candidates approximation algorithms that can be studied. We can view messages-passing and variational algorithms such as generalized belief propagation, the mini-bucket and weighted mini-bucket schemes [Dechter and Rish, 2002, Liu and Ihler, 2011] as approximations that bound inference. We can view Monte Carlo sampling methods, as approximations to search. The hybrid schemes can be used to focus on approximating only those portions of the problem instance that appear non-tractable for exact processing. Namely, for a given problem instances, it can suggest a balance between approximate and exact and the type of approximation that should be utilized.

One should note that approximate reasoning in graphical modeling with any guarantees was shown to be hard as well [Dagum and Luby, 1993, Roth]. Yet, algorithms that generate bounds or anytime schemes that can improve their bounds if allowed more time, and even get to an exact solution when time permits, are highly desirable. Pointers to some literature on approximations can be found in recent PhD theses [Kask, 2001] [Bidyuk, 2006] and [Gogate, 2009] [Mateescu, 2007] [Marinescu, 2007] and in a variety of articles in the field such as (on message-passing variational approaches) [Mateescu *et al.*, 2010] [J. S. Yedidia and Weiss, 2005, M. J. Wainwright and Willskey, 2005, Wainwright and Jordan, 2008, Wainwright *et al.*, 2003], [Ihler *et al.*, 2012, Liu and Ihler, 2013], and [Sontag *et al.*, 2008]. On Sampling and hybrid of sampling and bounded inference see [Bidyuk and Dechter, 2007, Bidyuk *et al.*, 2010], [Gogate and Dechter, 2010, 2011, 2012]. On anytime schemes for optimization see [Marinescu and Dechter, 2009b, Otten and Dechter, 2012].

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