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, oftened accompanied with cost-shifting schemes or re-parameterizations, that offers adjustable trade-off between accuracy and efficiency.

It was shown that deriving approximation scheme with a guaranteed relative error bounds, is NP-hard [Dagum and Luby, 1993, Roth, 1996]. 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 tighter bounds with more time and can therefore be responsive to the users allowing to be interrupted at any time producing the best solution found thus far.

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 [Dechter, 1999]. In the following sections we will introduce the weighted mini-bucket elimination scheme that approximates bucket-elimination, 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. These mini-bucket which belong to the class of variational decomposition bounds [Jaakola et al., 2005] are not fully anytime, because they may require significant memory on their

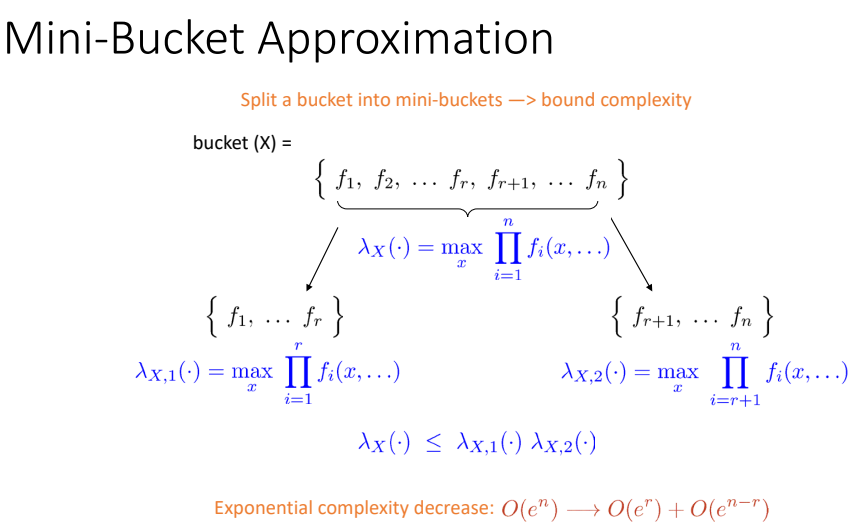


Figure 8.1: The idea of mini-bucket approximation.

way to exact solution and therefore may npot be able to produce an exact solution even with more time. However they can facilitate anytime schemes if they are used as heuristic functions within an anytime search algorithm [Marinescu and Dechter, 2009a,b].

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 applied separately to each function, thus requiring less computation.

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 exact messages with their upper bounds, it is easy to see that once all buckets are processed, the maximized product computed 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, since it is not necessarily optimal.

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,

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

□

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.

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:**

- Compute an mpe cost by maximizing over X_1, the product in $bucket_1$. Namely $U \leftarrow max_{X_1} \Pi_{h_j \in bucket_1} h_j$.
- (Generate an approximate mpe tuple): Given $\mathbf{x}_{(1...(i-1))} = (x_1, \ldots, x_{i-1})$ choose $x_i = argmax_{X_i} \Pi_{\{h_j \in \ bucket_i\}} h_j(\mathbf{x}_{(1...(i-1))})$. $L \leftarrow P(x_1, ..., x_n)$

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

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

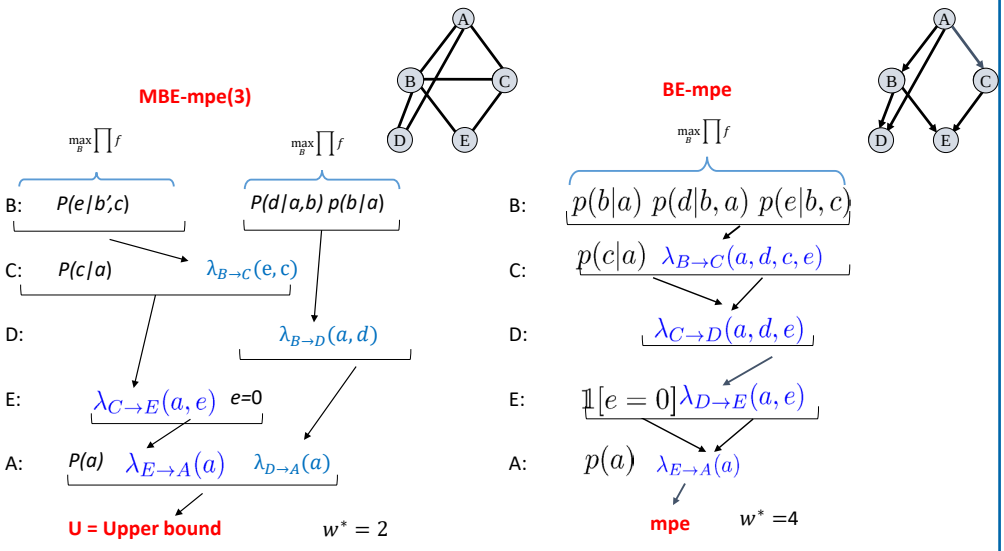


Figure 8.3: Comparison between (a) *BE-mpe* and (b) *MBE-mpe(3,2)*.

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, 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 given in the figure (the directed and moral graphs) along the ordering $o = (A, E, D, C, B)$. Notice that we use the bucket-tree elimination notation where messages are indexed by their origin and destination bucket. The exact *BE-mpe* sequentially records the new functions (shown to the right) $\lambda_{B\to C}(a, d, c, e)$, $\lambda_{C\to D}(a, d, e)$, $\lambda_{D\to E}(a, e)$, and $\lambda_{E\to A}(a)$. Then, in the bucket of A, it computes $M = \max_a P(a)\lambda_{E\to A}(a)$. 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, $a' = \arg\max_a P(a)\lambda_{E\to A}(a)$, $e' = 0$, $d' = \arg\max_d \lambda_{C\to D}(a, d, e)$, 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 the left handside of Figure 8.3. There can be several (3,2)-partitionings, and any choice would be legitimate, and can be selected arbitrarily. The new functions $\lambda_{B\to C}(e, c)$ and $\lambda_{B\to D}(d, a)$ 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 variable A the product of functions in A's bucket: $U = max_a P(a)\lambda_{E\to A}(a)\lambda_{D\to A}(a)$.

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 $mpe = \max_{\mathbf{x}} P(\mathbf{x}, \mathbf{e})$, 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 happens to be 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 the duplicated variables, we know that the assignment is locally optimal, namely conditioned on the current partial configuration.

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.

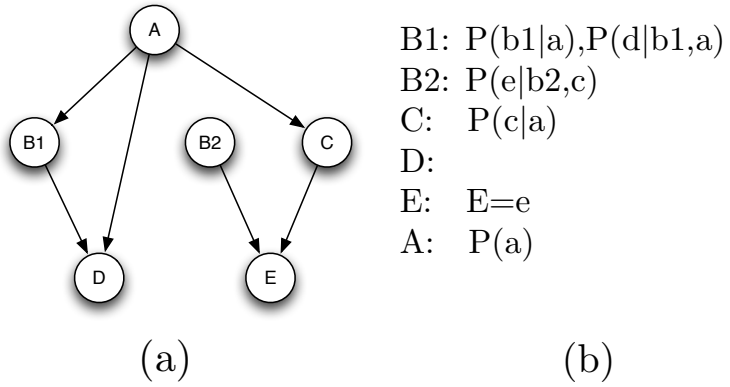


Figure 8.4: relaxed network corresponding to mini-bucket execution in Figure 8.3b

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 ($X_k = x_k$), 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 $h^l \leftarrow \sum_{X_k} \Pi_{j=1}^t h_{1_j}$
       Else compute $h^l \leftarrow max_{X_k} \Pi_{j=1}^t h_{l_j}$
       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** $P'(\bar{x_1}, e) \leftarrow$ 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)*.

Algorithm *BE-bel* computes $P(x_1, \mathbf{e})$, when X_1 is the first variable 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 apply summation in each mini-bucket, we will get the approximate bound of h_p by $f_p = \prod_{l=1}^{r} \sum_{X_p} \prod_{l_i} h_{l_i}$. 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 $\sum_{X_p} \prod_{l_i} h_{l_i}$, a constant function relative to X_p. Instead, let's distinguish one (arbitrary) mini-bucket (the first one here) and 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_p by its sum over X_p, we can bound $(i > 1)$, by its maximum operator over X_p, yielding

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

Therefore, an upper bound g_p of h_p is obtained by summing over one of X_p's mini-buckets and maximizing over the rest. This will lead to a tighter bound.

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. The *mean* operator is like the summation operator, divided by the number of elements in the sum. Notice however that the duplication semantics of MBE which implies summation for each of the mini-buckets does not extend here. This assymetry in mini-bucket processing for summation queries will be generalized and improved shortly using the notion of weighted mini-buckets. We can show that

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

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 which mini-bucket to select for summation.

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', whose sumed mini-bucket is a refinement of the sumed mini-bucket in 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 $P(X_1, \mathbf{e})$ 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.

8.3 WEIGHTED MINI-BUCKET ELIMINATION

The asymetry in processing mini-buckets for summation queries is annoying, especially when we lack and criterion for chhosing the summation mini-bucket. We will next see a generalization of the mini-bucket scheme in *weighted mini-bucket (wmb)* which facilitate tighter bounds by associating mini-buckets with weights. This is facilitated using Holder inequality [Hardy et al., 1952], which uses the notion of a power-sum 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 reduces to a standard summation when $w = 1$ and approaches max when $w \to 0^+$ as shown in Figure 8.6. For 2 functions, when $w = w_1 + w_2$, Holder inequality looks as follows.

$$\sum_x f_1(x) \cdot f_2(x) \leq (\sum_x f_1(x)^{\frac{1}{w_1}})^{w_1} \cdot (\sum_x f_2(x)^{\frac{1}{w_2}})^{w_2}$$

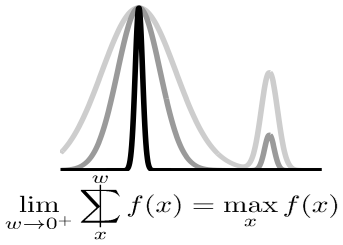


Figure 8.6: The impact of w on the power sum.

The general Holder inequality is:

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 summation to power-sum 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, any choice of the mini-bucket weights will tighten the obtained bound. It is easy to see that uniform weights will yield superior bounds to simple summation (that correspond to node duplication) (prove as an exercise). We can try to select a good, or even optimal set of weights for each bucket to yield the tightest 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 mini-bucket (WMB)E is given in Figure 8.7. It is parameterized 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 the weights based on variables, so that buckets of sum variables will be assigned $w = 1$ and others $w = 0$ for maximization. This makes WMB algorithm not only poetntially better, by optimizing the weight parameters, but also provide a uniform way for expressing the mini-bucket scheme.

Weighted mini-buckets for lower bounds. WMB can also be used to compute a lower bound when the factors are strictly positive; this is obtained by requesting that exactly one weight, say, w_{l_k} is positive, and the rest are negative: $w_{l_k} > 0, w_{l_j} < 0$ [Hardy et al., 1952].

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

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

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

  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 8.7: Algorithm *WMBE(i,m)*.

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 $w = 1$, where the selected mini-bucket weights is left as a hypr-parameter. The rest of the buckets are processed by the mini-bucket rule with $w = 0$, yielding maximization. In other words, 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 8.8.

Decoding the map assignment and the issue with lower-bounds. Once the backwards phase of *MBE-map* ends, we have an upper bound and, in principle, we can compute a map assignment in the forward phase. While the probability of any 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 served 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 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 8.9. 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 $Y = (Y^u, Y^x)$. 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):
$bucket(X_0) = P(y_0^x|X_0), P(X_0|U_0, U_1, U_2),$
$bucket(X_1) = P(y_1^x|X_1), P(X_1|U_1, U_2, U_3),$

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 $bucket_1, \ldots, bucket_n$, 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

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

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

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

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 messages. Three are placed in bucket U_0 ($h_{X_0}, h_{X_3}, h_{X_4}$), one in bucket U_1 (h_{U_0}) and one in bucket U_2 (h_{X_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 $Upper$ on the map value, namely $Upper \geq P(U, \bar{y}^u, \bar{y}^x)$ 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?

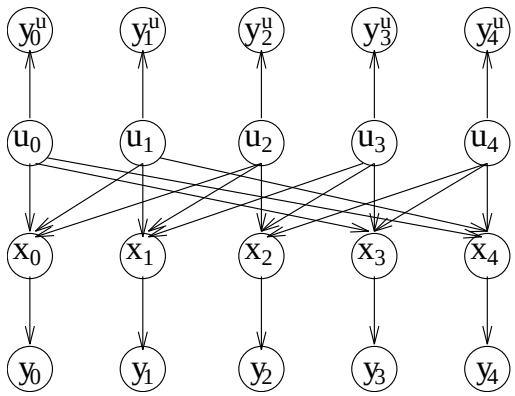


Figure 8.9: Belief network for a linear block code.

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 [Bertele and Brioschi, 1972]. 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 8.10. 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 provides another one way to generalize this scheme, leading to Weighted mini-bucket elimination [Liu and Ihler, 2011].

8.6 COMPLEXITY AND TRACTABILITY

8.6.1 THE CASE OF LOW INDUCED WIDTH

We denote by *weighted mini-bucket-elimination(i,m)*, or simply *WMB(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 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* WMB(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,* $|S| \leq i \leq n$.

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

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

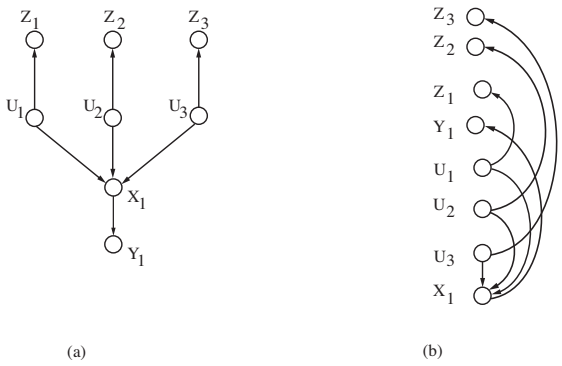
Figure 8.10: Algorithm *MBE-opt(i,m)*.

Proof. 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 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. This is illustrated in Example 8.11. We conclude,

Example 8.11 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 8.11a, where the last four variables $Y_1,\ Z_1,\ Z_2,\ Z_3$ in the ordering are observed. Once those four buckets are processed as observation buckets, we get (where 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.



(a) (b)

Figure 8.11: (a) A polytree and (b) a legal ordering, assuming that nodes Z_1, Z_2, Z_3 and Y_1 are observed.

Theorem 8.12 *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.*

8.6.2 HEURISTIC FOR MINI-BUCKET PARTITIONINGS

Clearly, given the parameters i and m, there are many (i, m) partitioning. These partitionings can be guided by the graph, or by the content of the actual functions, aiming to minimize the error incurred by the partitioning. 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 because controlling the mini-bucket size by the number of variables is less restricting. 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)*.

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. 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 `Partition`(B, i) , where B is the partitioned bucket, using the SCP heuristic is $O(|B| \log(|B|) + |B|^2)$ 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 that can be considered include *log relative error*, *maximum log relative error*, *KL divergence* and *absolute error*. For example:

- Log relative error, (RE):

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

- 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

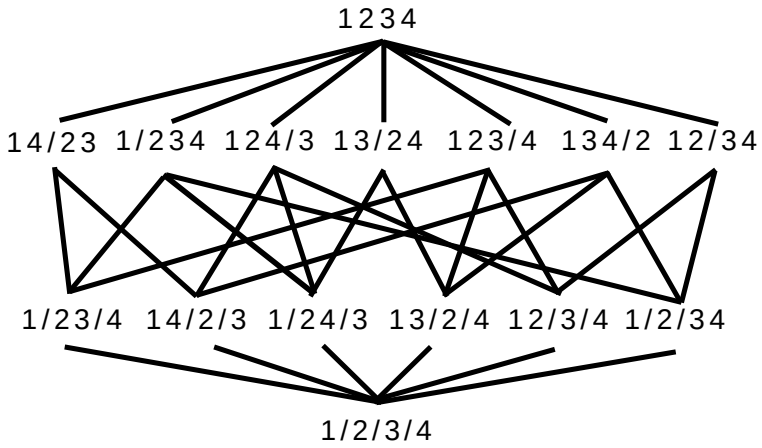


Figure 8.12: Partitioning lattice of bucket $\{f_1, f_2, f_3, f_4\}$. We specify each function by its subindex.

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, as dictated by Proposition 8.2 .

Example 8.13 Consider a bucket $\mathcal{B}_x = \{f_1, f_2, f_3, f_4\}$. Its Hasse diagram in depicted in Figure 8.12. 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 were 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 [Rollon et. al., 2010]). At each step, the algorithm ranks 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 8.13.

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.

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 8.13: Greedy partitioning

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 8.14: Algorithm *ANYTIME-mpe(ϵ)*.

8.6.3 DISCUSSION

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 variable C and then go back and process another mini-bucket of variable 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.

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-mpe(ϵ)* is presented in Figure 8.14, where ϵ is 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 summation 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.)

Mini-bucket as heuristic generation for search. An orthogonal anytime extension of the mini-bucket, is to embed it 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 (e.g., by branch and bound schemes), while using the mini-bucket functions to guide and prune the search. This approach was explored extensively in recent years yielding state-of the art algorithms both for finding an mpe assignment as well as for constraint optimization problems [Kask and Dechter, 2001, 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 $h_{u\to v} = \sum_{elim(u,v)} \prod_{f\in cluster(u)} f = \sum_{elim(u,v)} \prod_{k=1}^{p} \prod_{f\in mc(k)} f$. 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 8.15 (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 and each associated with a weight w_j s.t. $\sum_j w_j = 1$. Each mini-cluster is processed by the power-sum over the eliminator and the resulting set of 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 the joint beliefs. We can also use power sums exactly as we did for WMB, where all the weights are positive for deriving upper bounds and all above 1 or, for lower-bounds, all but one are negative.

Algorithm *MC-bel* for upper bounds can be obtained from CTE (see Chapter 5) 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 8.15. The partitioning of clusters to mini-clusters can be done in an identical manner to partitioning buckets into mini-buckets.

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 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 $cluster_v(u)$, $\{mc(1), \ldots, mc(p)\}$;
- $h^j_{u \to v} = (\sum_{elim(u,v)} \prod_{f \in mc(j)} f^{\frac{1}{w_j}})^{w_j}$
- 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** $U(X_i, e)$ **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 $\overline{P}(X_i, e) = \prod_{k=1}^{p} (\sum_{\chi(u) - X_i} (\prod_{f \in mc(k)} f)^{\frac{1}{w_k}})^{w_k}$.

Figure 8.15: Procedure Mini-Clustering for Belief Updating (MC-bel)

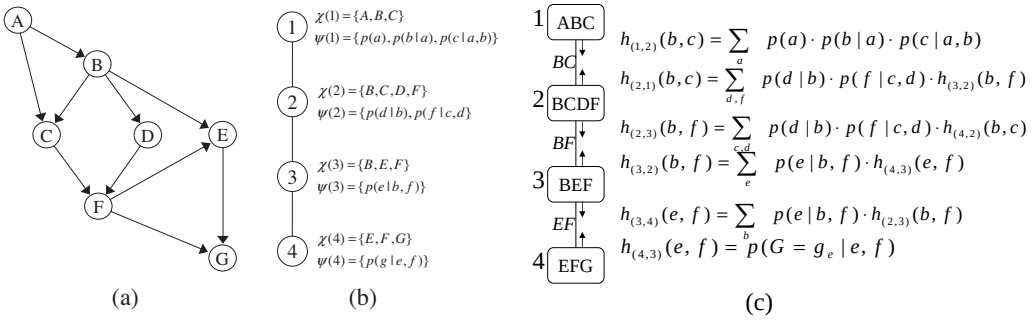


Figure 8.16: (a) A belief network; (b) A join-tree decomposition; (c) Execution of CTE-BU.

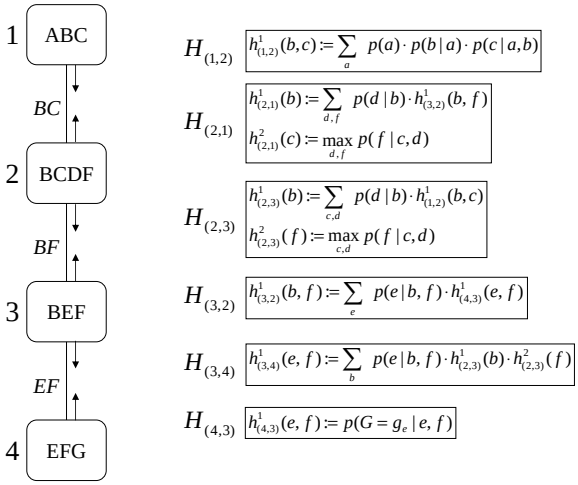


Figure 8.17: Execution of MC-bel for $i = 3$

Example 8.15 Figure 8.17 shows the trace of running MC-bel(3) on the problem in Figure 8.16. 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, $\chi(1) = \{A, B, C\}$, therefore it is not partitioned. The combined function $h^1_{1\to2}(b, c) = \sum_a p(a) \cdot p(b|a) \cdot p(c|a, b)$ is computed and the message $H_{1\to2} = \{h^1_{1\to2}(b, c)\}$ 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 $mc(1) = \{p(d|b), h_{1\to2}(b, c)\}$ and $mc(2) = \{p(f|c, d)\}$. The combined functions using power sum is $h^1_{2\to3}(b) = (\sum_{c,d}(p(d|b) \cdot h_{1\to2}(b, c))^{\frac{1}{w_1}})w_1$ and $h^2_{2\to3}(f) = (\sum_{c,d}(p(f|c, d))^{\frac{1}{w_2}})^{w_2}$ where $w_1 + w_2 = 1$ are computed and the message $H_{4\to3} = \{h^1_{2\to3}(b), h^2_{2\to3}(f)\}$ 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 $\sum_{b,c} p(a) \cdot p(b|a) \cdot p(c|a,b) \cdot h^1_{2\to1}(b) \cdot h^2_{2\to1}(c)$. 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).

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