Bounded inference non-iteratively; Mini-bucket elimination

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(Reading: Primary: Class Notes (10) Secondary: , Darwiche chapters 14)

Agenda

- Mini-bucket elimination
- Mini-clustering
- Iterative Belief propagation
- Iterative-join-graph propagation

Probabilistic Inference Tasks

Belief updating:

 $BEL(X_i) = P(X_i = x_i | evidence)$

Finding most probable explanation (MPE)
 x
 x
 x
 = argmax P(x, e)

• Finding maximum a-posteriory hypothesis $(a_1^*,...,a_k^*) = \arg\max_{\overline{a}} \sum_{XXA} P(\overline{x},e)$ $A \subseteq X:$ hypothesis variables

• Finding maximum-expected-utility (MEU) decision $(d_1^*,...,d_k^*) = \arg\max_{\overline{d}} \sum_{\overline{x}} P(\overline{x}, e) U(\overline{x})$ $D \subseteq X:$ decision variables $U(\overline{x}):$ utility function

Probability of evidence (or partition function)

Queries

$$P(e) = \sum_{X-\text{var}(e)} \prod_{i=1}^{n} P(x_i \mid pa_i)|_e \quad Z = \sum_X \prod_i \psi_i(C_i)$$

• Posterior marginal (beliefs):

$$P(x_i \mid e) = \frac{P(x_i, e)}{P(e)} = \frac{\sum_{X-\text{var}(e)-X_i} \prod_{j=1}^{n} P(x_j \mid pa_j)|_e}{\sum_{X-\text{var}(e)} \prod_{j=1}^{n} P(x_j \mid pa_j)|_e}$$

• Most Probable Explanation

$$\overline{\mathbf{x}^*} = \operatorname{argmax} \mathbf{P}(\overline{\mathbf{x}}, \mathbf{e})$$



Generating the MPE-tuple

- 5. b' = arg max P(b | a') × × P(d' | b, a') × P(e' | b, c')
- 4. c' = arg max P(c | a') ×
 × h^B(a', d^c, c, e')
- 3. $d' = \arg \max_{d} h^{c}(a', d, e')$
- 2. e' = 0

- B: P(b|a) P(d|b,a) P(e|b,c)
- C: P(c|a) $h^{B}(a, d, c, e)$
- D: $h^c(a, d, e)$
- E: e=0 *h^D* (a, e)
- **1.** $a' = \arg \max_{a} P(a) \cdot h^{E}(a)$ A: $P(a) = h^{E}(a)$

Return (a',b',c',d',e')



Approximate Inference

- Metrics of evaluation
- Absolute error: given e>0 and a query p= P(x|e), an estimate r has absolute error e iff | p-r|<e
- **Relative error**: the ratio r/p in [1-e,1+e].
- Dagum and Luby 1993: approximation up to a relative error is NP-hard.
- Absolute error is also NP-hard if error is less than .5

Mini-buckets: "local inference"

- Computation in a bucket is time and space exponential in the number of variables involved
- Therefore, partition functions in a bucket into "mini-buckets" on smaller number of variables

Mini-bucket approximation: MPE task

Split a bucket into mini-buckets =>bound complexity



Exponential complexity decrease : $O(e^n) \rightarrow O(e^r) + O(e^{n-r})$

Mini-Bucket Elimination



Semantics of Mini-Bucket: Splitting a Node

Variables in different buckets are renamed and duplicated (Kask *et. al.*, 2001), (Geffner *et. al.*, 2007), (Choi, Chavira, Darwiche , 2007)

Before Splitting: Network N After Splitting: Network N'





Relaxed network example



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)

MBE-mpe(i)

- Input: i max number of variables allowed in a mini-bucket
- Output: [lower bound (Probability of a sub-optimal solution), upper bound]



Example: <a>approx-mpe(3) versus <a>elim-mpe

(i,m) patitionings

Definition 7.1.1 ((i,m)-partitioning) Let H be a collection of functions $h_1, ..., h_t$ defined on scopes $S_1, ..., S_t$, respectively. We say that a function f is subsumed by a function h if any argument of f is also an argument of h. A partitioning of $h_1, ..., h_t$ is canonical if any function f subsumed by another function is placed into the bucket of 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.

MBE(i,m), MBE(i)

- Input: Belief network (P1,...Pn)
- Output: upper and lower bounds
- Initialize: (put functions in buckets)
- Process each bucket from p=n to 1
 - Create (i,m)-mini-buckets partitions
 - Process each mini-bucket
- For mpe): assign values in ordering d
- Return: mpe-tuple, upper and lower bounds



Theorem 7.1.3 (mbe-mpe properties) Algorithm mbe-mpe(i, m) computes an upper bound on the MPE. Its time and space complexity is $O(n \cdot exp(i))$ where $i \leq n$.

Partitioning refinements

Clearly, as the mini-buckets get smaller, both complexity and accuracy decrease.

Definition 7.1.4 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 7.1.5 If Q'' is a refinement of Q' in bucket_p, then $h^p \leq g_{Q'}^p \leq g_{Q''}^p$.

Remember that *mbe-mpe* computes the bounds on $MPE = \max_{\bar{x}} P(\bar{x}, \bar{e})$, rather than on $M = \max_{\bar{x}} P(\bar{x}|\bar{e}) = MPE/P(\bar{e})$. Thus

$$\frac{L}{P(\bar{e})} \le M \le \frac{U}{P(\bar{e})}$$

Properties of MBE-mpe(i)

- Complexity: O(exp(i)) time and O(exp(i)) space.
- Accuracy: determined by upper/lower (U/L) bound.
- As *i* increases, both accuracy and complexity increase.
- Possible use of mini-bucket approximations:
 - As anytime algorithms
 - As heuristics in best-first search

Anytime Approximation

```
Algorithm anytime-mpe(\epsilon)
Input: Initial values of i and m, i_0 and m_0; increments i_{step} and m_{step},
and desired approximation error \epsilon.
Output: U and L
1. Initialize: i = i_0, m = m_0.
2. do
3.
      run mbe-mpe(i,m)
   U \leftarrow upper bound of mbe-mpe(i,m)
4.
5.
      L \leftarrow \text{lower bound of } mbe-mpe(i,m)
    Retain best bounds U, L, and best solution found so far
6.
       if 1 \leq U/L \leq 1 + \epsilon, return solution
7.
       else increase i and m: i \leftarrow i + i_{step} and m \leftarrow m + m_{step}
8.
9. while computational resources are available
10. Return the largest L
    and the smallest U found so far.
```

MBE for Belief Updating and for probability of evidence

Idea mini-bucket is the same:

$$\sum_{X} f(x) \bullet g(x) \le \sum_{X} f(x) \bullet \sum_{X} g(x)$$
$$\sum_{X} f(x) \bullet g(x) \le \sum_{X} f(x) \bullet \max_{X} g(X)$$

- So we can apply a sum in each mini-bucket, or better, one sum and the rest max, or min (for lower-bound)
- MBE-bel-max(i,m), MBE-bel-min(i,m) generating upper and lower-bound on beliefs approximates BE-bel
- MBE-map(i,m): max buckets will be maximized, sum buckets will be sum-max. Approximates BE-map.

Normalization

mbe-bel computes upper/lower bound on the joint marginal distributions.

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

$$\frac{L_i}{P(\bar{e})} \le P(x_i|\bar{e}) \le \frac{U_i}{P(\bar{e})}$$

We sometime use normalization of the approximation, but then no guarantee. The probable is that we have to approximate also the partition function.

Algorithm mbe-bel-max(i,m)

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 bucket₁, ..., 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)-mini-bucket-partitioning, $Q' = \{Q_1, ..., Q_r\}$ For each $Q_l \in Q'$, containing $h_{l_1}, \dots h_{l_t}$, do If l = 1 compute $h^l = \sum_{X_k} \prod_{j=1}^t h_{1_j}$ Else compute $h^l = max_{X_k} \prod_{i=1}^{t} h_{l_i}$ 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.

Empirical Evaluation

(Dechter and Rish, 1997; Rish thesis, 1999)

- Randomly generated networks
 - Uniform random probabilities
 - Random noisy-OR
- CPCS networks
- Probabilistic decoding

Comparing MBE-mpe and anytime-mpe versus BE-mpe

Methodology for Empirical Evaluation (for mpe)

- U/L –accuracy
- Better (U/mpe) or mpe/L
- Benchmarks: Random networks
 - Given n,e,v generate a random DAG
 - For xi and parents generate table from uniform [0,1], or noisy-or
- Create k instances. For each, generate random evidence, likely evidence
- Measure averages

CPCS networks – medical diagnosis (noisy-OR model)



The effect of evidence

More likely evidence=>higher MPE => higher accuracy (why?)



Likely evidence versus random (unlikely) evidence

MBE-map

Process max buckets With max mini-buckets And sum buckets with sum Mini-bucket and max mini-buckets

Algorithm mbe-map(i,m) **Input:** A belief network BN = (G, P), a subset of variables $A = \{A_1, ..., A_k\}$, an ordering of the variables, o, in which the A's appear first, and evidence \bar{e} . Output: An upper bound U on the MAP and a suboptimal solution $A = \bar{a}_{\mu}^{a}$. 1. Initialize: Partition $P = \{P_1, ..., P_n\}$ into buckets bucket, ..., bucket_n where $bucket_P$ contains all CPTs, $h_1, ..., h_t$ whose highest index variable is X_p . 2. Backward: for p = n to 1 do • If X_p is observed $(X_p = a)$, assign $X_p = a$ in each h_i and put the result in its highest-variable bucket (put constants in bucket₁). Else for h₁, h₂, ..., h_j in bucket_p do Generate an (i, m)-partitioning, Q' of the matrices h_i into mini-buckets $Q_1, ..., Q_r$. If X_P ∉ A /* not a hypothesis variable */ for each $Q_l \in Q'$, containing $h_{l_1}, \dots h_{l_t}$, do If l = 1, compute $h^l = \sum_{X_n} \prod_{i=1}^t h_{1_i}$ Else compute $h^l = max_{X_p}\Pi_{i=1}^t h_{l_i}$ Add h^l to the bucket of the highest-index variable in $U_l \leftarrow \bigcup_{i=1}^t S_{l_i} - \{X_p\},\$ (put constants in bucket₁). Else (X_p ∈ A) /* a hypothesis variable */ for each $Q_l \in Q'$ containing $h_{l_1}, \dots h_{l_t}$ compute $h^l = max_{X_p} \prod_{i=1}^t h_{l_i}$ and place it in the bucket of the highest-index variable in $U_l \leftarrow \bigcup_{i=1}^t S_{l_i} - \{X_p\},\$ (put constants in bucket₁). 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. Return An upper bound U = max_{a1} ∏_{h_i∈bucket1} h_i on MAP, computed in the first bucket. and the assignment $\bar{a}_{k}^{a} = (a_{1}^{a}, ..., a_{k}^{a}).$

Probabilistic decoding

Error-correcting linear block code



State-of-the-art:

approximate algorithm – iterative belief propagation (IBP) (Pearl's poly-tree algorithm applied to loopy networks)



Figure 7.7: Belief network for a linear block code.

Example 7.3.1 We will next demonstrate the mini-bucket approximation for MAP on an example of *probabilistic decoding* (see Chapter 2) Consider a belief network which describes the decoding of a *linear block code*, shown in Figure 7.7. 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 access):

$$\begin{array}{l} \text{Initial} \\ \text{bucket}(X_0) &= P(y_0^x | X_0), P(X_0 | U_0, U_1, U_2), \\ \text{bucket}(X_1) &= P(y_1^x | X_1), P(X_1 | U_1, U_2, U_3), \\ \text{bucket}(X_2) &= P(y_2^x | X_2), P(X_2 | U_2, U_3, U_4), \\ \text{bucket}(X_3) &= P(y_3^x | X_3), P(X_3 | U_3, U_4, U_0), \\ \text{bucket}(X_4) &= P(y_4^x | X_4), P(X_4 | U_4, U_0, U_1), \\ \text{bucket}(U_0) &= P(U_0), P(y_0^u | U_0), \\ \text{bucket}(U_1) &= P(U_1), P(y_1^u | U_1), \\ \text{bucket}(U_2) &= P(U_2), P(y_2^u | U_2), \\ \text{bucket}(U_3) &= P(U_3), P(y_3^u | U_3), \\ \text{bucket}(U_4) &= P(U_4), P(y_4^u | U_4). \end{array} \right)$$

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:





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 U satisfying $U \ge MAP = P(U, \bar{y}^u, \bar{y}^x)$ 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 $P(\bar{e})$ which is not available. Yet, again, in most cases we are interested in the ratio $P(U = \bar{u}_1|\bar{e})/P(U = \bar{u}_2|\bar{e})$ for competing hypotheses $U = \bar{u}_1$ and $U = \bar{u}_2$ rather than in the absolute values. Since $P(U|\bar{e}) = P(U,\bar{e})/P(\bar{e})$ and the probability of the evidence is just a constant factor independent of U, the ratio is equal to $P(U_1,\bar{e})/P(U_2,\bar{e})$.

Complexity and tractability of MBE(i,m)

Theorem 7.6.1 Algorithm mbe(i,m) takes $O(r \cdot exp(i))$ time and space, where r is the number of input functions², and where |F| is the maximum scope of any input function, $|F| \le i \le n$. For m = 1, the algorithm is time and space $O(r \cdot exp(|F|))$.

Belief propagation is easy on polytree: Pearl's Belief Propagation

A polytree: a tree with Larger families

A polytree decomposition





- Running CTE = running Pearl's BP over the dual graph
- Dual-graph: nodes are cpts, arcs connect non-empty
- intersections. BP is Time and space linear

Iterative Belief Proapagation

- Belief propagation is exact for poly-trees
- IBP applying BP iteratively to cyclic networks



- No guarantees for convergence
- Works well for many coding networks

MBE-mpe vs. IBP

mbe - mpe is better on low - w * codes

IBP is better on randomly generated (high - w*) codes

Bit error rate (BER) as a function of noise (sigma):



Mini-buckets: summary

- Mini-buckets local inference approximation
- Idea: bound size of recorded functions
- MBE-mpe(i) mini-bucket algorithm for MPE
 - Better results for noisy-OR than for random problems
 - Accuracy increases with decreasing noise in coding
 - Accuracy increases for likely evidence
 - Sparser graphs -> higher accuracy
 - Coding networks: MBE-mpe outperforms IBP on lowinduced width codes
Agenda

- Mini-bucket elimination
- Mini-clustering
- Iterative Belief propagation
- Iterative-join-graph propagation

Cluster Tree Elimination - properties

- Correctness and completeness: Algorithm CTE is correct, i.e. it computes the exact joint probability of a single variable and the evidence.
- Time complexity: $O(deg \times (n+N) \times d^{w^{*+1}})$
- Space complexity:

 $O(N \times d^{sep})$

where

- *deg* = the maximum degree of a node
- n = number of variables (= number of CPTs)
- N = number of nodes in the tree decomposition
- d = the maximum domain size of a variable
- w^* = the induced width
- sep = the separator size





Exponential complexity decrease $O(e^n) \rightarrow O(e^{\operatorname{var}(r)}) + O(e^{\operatorname{var}(n-r)})$



Semantic of variable duplication for mini-clustering

We can have a different duplication of nodes going up and down. Example: going down (left) and up (right)





(a)

(b)

Figure 1.14: Node duplication semantics of MC: (a) trace of MC-BU(3); (b) trace of CTE-BU.

Mini-Clustering

- Correctness and completeness: Algorithm MC-bel(*i*) computes a bound (or an approximation) on the joint probability *P*(*X_i*,*e*) of each variable and each of its values.
- Time & space complexity: O(n × hw* × kⁱ)

where $hw^* = max_u | \{f | f \cap \chi(u) \neq \phi\} |$



We can replace *max* operator by

- min => lower bound on the joint
- mean => approximation of the joint

Grid 15x15 - 10 evidence



CPCS422 - Absolute error



evidence=0

evidence=10

Coding networks - Bit Error Rate

Coding networks, N=100, P=4, sigma=.22, w*=12, 50 instances



Coding networks, N=100, P=4, sigma=.51, w*=12, 50 instances



sigma=0.22

sigma=.51

Heuristic for partitioning

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 minibucket 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 minibucket is absorbed into the left-most minibucket 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 $O(|B| \log (|B|) + |B| ^2)$ and O(exp(i)), respectively.

The scope-based

heuristic is is quite fast, its shortcoming is that it does not consider the actual information in the functions.

Content-based heuristics

(Rollon and Dechter 2010)



- Log relative error:

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

- Max log relative error:

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

Partitioning lattice of bucket $\{f_1, f_2, f_3, f_4\}$.

Use greedy heuristic derived from a distance function to decide which functions go into a single mini-bucket

Agenda

- Mini-bucket elimination
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- Iterative-join-graph propagation

Iterative Join Graph Propagation

- Loopy Belief Propagation
 - Cyclic graphs
 - Iterative
 - Converges fast in practice (no guarantees though)
 - Very good approximations (e.g., turbo decoding, LDPC codes, SAT – survey propagation)
- Mini-Clustering(i)
 - Tree decompositions
 - Only two sets of messages (inward, outward)
 - Anytime behavior can improve with more time by increasing the i-bound
- We want to combine:
 - Iterative virtues of Loopy BP
 - Anytime behavior of Mini-Clustering(i)

IJGP - The basic idea

- Apply Cluster Tree Elimination to any *join-graph*
- We commit to graphs that are *I-maps*
- Avoid cycles as long as I-mapness is not violated
- Result: use *minimal arc-labeled* join-graphs

Minimal arc-labeled join-graph



Figure 1.17: a) A belief network; b) A dual join-graph with singleton labels; c) A dual join-graph which is a join-tree



Figure 1.15: An arc-labeled decomposition









Message propagation

Minimal arc-labeled: $sep(1,2) = \{D,E\}$ $elim(1,2) = \{A,B,C\}$ $h_{(1,2)}(de) = \sum_{a,b,c} p(a) p(c) p(b \mid ac) p(d \mid abe) p(e \mid bc) h_{(3,1)}(bc)$

Non-minimal arc-labeled: $sep(1,2) = \{C,D,E\}$ $elim(1,2) = \{A,B\}$

$$h_{(1,2)}(cde) = \sum_{a,b} p(a)p(c)p(b \mid ac)p(d \mid abe)p(e \mid bc)h_{(3,1)}(bc)$$
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Bounded decompositions

- We want arc-labeled decompositions such that:
 - the cluster size (internal width) is bounded by *i* (the accuracy parameter)
 - the width of the decomposition as a graph (external width) is as small as possible
- Possible approaches to build decompositions:
 - partition-based algorithms inspired by the mini-bucket decomposition
 - grouping-based algorithms

a) schematic mini-bucket(i), i=3

b) arc-labeled join-graph decomposition

IJGP properties

- IJGP(*i*) applies BP to min arc-labeled join-graph, whose cluster size is bounded by *i*
- On join-trees IJGP finds exact beliefs
- IJGP is a Generalized Belief Propagation algorithm (Yedidia, Freeman, Weiss 2001)
- Complexity of one iteration:
 - time: *O(deg•(n+N) •dⁱ⁺¹)*
 - space: $O(N \bullet d^{\theta})$

Empirical evaluation

Measures:

- Algorithms:
 - Exact
 - IBP
 - MC
 - IJGP

- Absolute error
- Relative error
- Kulbach-Leibler (KL) distance
- Bit Error Rate
- Time
- Networks (all variables are binary):
 - Random networks
 - Grid networks (MxM)
 - CPCS 54, 360, 422
 - Coding networks

Coding networks - BER

Coding, N=400, 500 instances, 30 it, w*=43, sigma=.32

CPCS 422 – KL Distance

evidence=0

evidence=30

CPCS 422 – KL vs. Iterations

evidence=0

evidence=30

More On the Power of Belief Propagation

- BP as local minima of KL distance
- BP's power from constraint propagation perspective.

More On the Power of Belief Propagation

BP as local minima of KL distance

 BP's power from constraint propagation perspective.

The Kullback-Leibler Divergence

The Kullback-Leibler divergence (KL-divergence)

$$\mathrm{KL}(\mathrm{Pr}'(\mathbf{X}|\mathbf{e}), \mathrm{Pr}(\mathbf{X}|\mathbf{e})) = \sum_{\mathbf{x}} \mathrm{Pr}'(\mathbf{x}|\mathbf{e}) \log \frac{\mathrm{Pr}'(\mathbf{x}|\mathbf{e})}{\mathrm{Pr}(\mathbf{x}|\mathbf{e})}$$

- KL(Pr'(X|e), Pr(X|e)) is non-negative
- equal to zero if and only if Pr'(X|e) and Pr(X|e) are equivalent.

KL-divergence is not a true distance measure in that it is not symmetric. In general:

 $\mathrm{KL}(\mathrm{Pr}'(\mathbf{X}|\mathbf{e}), \mathrm{Pr}(\mathbf{X}|\mathbf{e})) \neq \mathrm{KL}(\mathrm{Pr}(\mathbf{X}|\mathbf{e}), \mathrm{Pr}'(\mathbf{X}|\mathbf{e})).$

- KL(Pr'(X|e), Pr(X|e)) weighting the KL-divergence by the approximate distribution Pr'
- We shall indeed focus on the KL-divergence weighted by the approximate distribution as it has some useful computational properties.

The Kullback-Leibler Divergence

Let Pr(X) be a distribution induced by a Bayesian network \mathcal{N} having families $X\mathbf{U}$

The KL-divergence between \Pr and another distribution \Pr' can be written as a sum of three components:

$$\begin{aligned} &\operatorname{KL}(\operatorname{Pr}'(\mathbf{X}|\mathbf{e}), \operatorname{Pr}(\mathbf{X}|\mathbf{e})) \\ &= -\operatorname{ENT}'(\mathbf{X}|\mathbf{e}) - \sum_{X\mathbf{U}} \operatorname{AVG}'(\log \lambda_{\mathbf{e}}(X)\Theta_{X|\mathbf{U}}) + \log \operatorname{Pr}(\mathbf{e}), \end{aligned}$$

where

- $\text{ENT}'(\mathbf{X}|\mathbf{e}) = -\sum_{\mathbf{x}} \Pr'(\mathbf{x}|\mathbf{e}) \log \Pr'(\mathbf{x}|\mathbf{e})$ is the entropy of the conditioned approximate distribution $\Pr'(\mathbf{X}|\mathbf{e})$.
- $\operatorname{AVG}'(\log \lambda_{\mathbf{e}}(X)\Theta_{X|\mathbf{U}}) = \sum_{x\mathbf{u}} \operatorname{Pr}'(x\mathbf{u}|\mathbf{e}) \log \lambda_{\mathbf{e}}(x)\theta_{x|\mathbf{u}}$ is a set of expectations over the original network parameters weighted by the conditioned approximate distribution.

The Kullback-Leibler Divergence

A distribution Pr'(X|e) minimizes the KL-divergence KL(Pr'(X|e), Pr(X|e)) if it maximizes

$$\mathrm{ENT}'(\mathbf{X}|\mathbf{e}) + \sum_{X\mathbf{U}} \mathrm{AVG}'(\log \lambda_{\mathbf{e}}(X)\Theta_{X|\mathbf{U}})$$

Competing properties of $Pr'(\mathbf{X}|\mathbf{e})$ that minimize the KL-divergence:

- Pr'(X|e) should match the original distribution by giving more weight to more likely parameters λ_e(x)θ_{x|u} (i.e, maximize the expectations).
- Pr'(X|e) should not favor unnecessarily one network instantiation over another by being evenly distributed (i.e., maximize the entropy).
Optimizing the KL-Divergence

The approximations computed by IBP are based on assuming an approximate distribution $Pr'(\mathbf{X})$ that factors as follows:

$$\Pr'(\mathbf{X}|\mathbf{e}) = \prod_{X\mathbf{U}} \frac{\Pr'(X\mathbf{U}|\mathbf{e})}{\prod_{U \in \mathbf{U}} \Pr'(U|\mathbf{e})}$$

- This choice of Pr'(X|e) is expressive enough to describe distributions Pr(X|e) induced by polytree networks N
- In the case where N is not a polytree, then we are simply trying to fit Pr(X|e) into an approximation Pr'(X|e) as if it were generated by a polytree network.
- The entropy of distribution $Pr'(\mathbf{X}|\mathbf{e})$ can be expressed as:

$$\mathrm{ENT}'(\mathbf{X}|\mathbf{e}) = -\sum_{x\mathbf{u}} \sum_{x\mathbf{u}} \mathrm{Pr}'(x\mathbf{u}|\mathbf{e}) \log \frac{\mathrm{Pr}'(x\mathbf{u}|\mathbf{e})}{\prod_{u \sim \mathbf{u}} \mathrm{Pr}'(u|\mathbf{e})}$$

Optimizing the KL-Divergence

Let $Pr(\mathbf{X})$ be a distribution induced by a Bayesian network \mathcal{N} having families $X\mathbf{U}$. Then IBP messages are a fixed point if and only if IBP marginals $\mu_u = BEL(u)$ and $\mu_{xu} = BEL(xu)$ are a stationary point of:

$$\operatorname{ENT}'(\mathbf{X}|\mathbf{e}) + \sum_{X\mathbf{U}} \operatorname{AVG}'(\log \lambda_{\mathbf{e}}(X)\Theta_{X|\mathbf{U}})$$
$$= -\sum_{X\mathbf{U}} \sum_{x\mathbf{u}} \mu_{x\mathbf{u}} \log \frac{\mu_{x\mathbf{u}}}{\prod_{u \sim \mathbf{u}} \mu_{u}} + \sum_{X\mathbf{U}} \sum_{x\mathbf{u}} \mu_{x\mathbf{u}} \log \lambda_{\mathbf{e}}(x)\theta_{x|\mathbf{u}},$$

under normalization constraints:

$$\sum_{u} \mu_{u} = \sum_{\mathbf{x}\mathbf{u}} \mu_{\mathbf{x}\mathbf{u}} = 1$$

for each family $X\mathbf{U}$ and parent U, and under consistency constraints:

$$\sum_{\mathbf{x}\mathbf{u}\sim y}\mu_{\mathbf{x}\mathbf{u}}=\mu_{y}$$

for each family instantiation $x\mathbf{u}$ and value y of family member $Y \in X\mathbf{U}$.

Optimizing the KL-Divergence

- IBP fixed points are stationary points of the KL-divergence: they may only be local minima, or they may not be minima.
- When IBP performs well, it will often have fixed points that are indeed minima of the KL-divergence.
- For problems where IBP does not behave as well, we will next seek approximations Pr' whose factorizations are more expressive than that of the polytree-based factorization.

Generalized Belief Propagation

If a distribution Pr' has the form:

$$\Pr'(\mathbf{X}|\mathbf{e}) = \frac{\prod_{\mathbf{C}} \Pr'(\mathbf{C}|\mathbf{e})}{\prod_{\mathbf{S}} \Pr'(\mathbf{S}|\mathbf{e})},$$

then its entropy has the form:

$$\mathrm{ENT}'(\mathbf{X}|\mathbf{e}) = \sum_{\mathbf{C}} \mathrm{ENT}'(\mathbf{C}|\mathbf{e}) - \sum_{\mathbf{S}} \mathrm{ENT}'(\mathbf{S}|\mathbf{e}).$$

When the marginals Pr'(C|e) and Pr'(S|e) are readily available, the ENT component of the KL-divergence can be computed efficiently.

While a jointree induces an exact factorization of a distribution, a joingraph G induces an approximate factorization:

$$\Pr'(\mathbf{X}|\mathbf{e}) = \frac{\prod_{i} \Pr'(\mathbf{C}_{i}|\mathbf{e})}{\prod_{ij} \Pr'(\mathbf{S}_{ij}|\mathbf{e})}$$

which is a product of cluster marginals over a product of separator marginals. When the joingraph corresponds to a jointree, the above factorization will be exact.



A dual joingraph leads to the factorization used by IBP.



The jointree induces the following factorization, which is exact:

$$\Pr'(\mathbf{X}|\mathbf{e}) = \frac{\Pr'(ABC|\mathbf{e})\Pr'(ABD|\mathbf{e})\Pr'(ABCD|\mathbf{e})\Pr'(CDE|\mathbf{e})}{\Pr'(ABC|\mathbf{e})\Pr'(ABD|\mathbf{e})\Pr'(CD|\mathbf{e})}$$



The joingraph induces the following factorization:

$$\Pr'(\mathbf{X}|\mathbf{e}) = \frac{\Pr'(ABC|\mathbf{e})\Pr'(ABD|\mathbf{e})\Pr'(ACD|\mathbf{e})\Pr'(CDE|\mathbf{e})}{\Pr'(B|\mathbf{e})\Pr'(AC|\mathbf{e})\Pr'(AD|\mathbf{e})\Pr'(CD|\mathbf{e})}$$

terative Joingraph Propagation

Computing cluster marginals $\mu_{\mathbf{c}_i} = \Pr'(\mathbf{c}_i | \mathbf{e})$ and separator marginals $\mu_{\mathbf{s}_{ij}} = \Pr'(\mathbf{s}_{ij} | \mathbf{e})$ that minimize the KL-divergence between $\Pr'(\mathbf{X} | \mathbf{e})$ and $\Pr(\mathbf{X} | \mathbf{e})$

This optimization problem can be solved using a generalization of IBP, called iterative joingraph propagation (IJGP), which is a message passing algorithm that operates on a joingraph.

Iterative Joingraph Propagation

 $IJGP(G, \Phi)$

input:

- G: a joingraph
- Φ : factors assigned to clusters of G

output: approximate marginal $BEL(C_i)$ for each node *i* in the joingraph *G*.

main:

1: $t \leftarrow 0$ 2: initialize all messages M_{ij}^t (uniformly) 3: while messages have not converged do 4: $t \leftarrow t + 1$ 5: for each joingraph edge i-j do 6: $M_{ij}^t \leftarrow \eta \sum_{\mathbf{C}_i \setminus \mathbf{S}_{ij}} \Phi_i \prod_{k \neq j} M_{ki}^{t-1}$ 7: $M_{ji}^t \leftarrow \eta \sum_{\mathbf{C}_j \setminus \mathbf{S}_{ij}} \Phi_j \prod_{k \neq i} M_{kj}^{t-1}$ 8: end for 9: end while 10: return $BEL(\mathbf{C}_i) \leftarrow \eta \Phi_i \prod_k M_{ki}^t$ for each node i

terative Joingraph Propagation

Let Pr(X) be a distribution induced by a Bayesian network \mathcal{N} having families XU, and let C_i and S_{ij} be the clusters and separators of a joingraph for \mathcal{N} .

Then messages M_{ij} are a fixed point of IJGP if and only if IJGP marginals $\mu_{c_i} = BEL(c_i)$ and $\mu_{s_{ij}} = BEL(s_{ij})$ are a stationary point of:

$$\begin{aligned} & \text{ENT}'(\mathbf{X}|\mathbf{e}) + \sum_{\mathbf{C}_i} \text{AVG}'(\log \Phi_i) \\ & = -\sum_{\mathbf{C}_i} \sum_{\mathbf{c}_i} \mu_{\mathbf{c}_i} \log \mu_{\mathbf{c}_i} + \sum_{\mathbf{S}_{ij}} \sum_{\mathbf{s}_{ij}} \mu_{\mathbf{s}_{ij}} \log \mu_{\mathbf{s}_{ij}} + \sum_{\mathbf{C}_i} \sum_{\mathbf{c}_i} \mu_{\mathbf{c}_i} \log \Phi_i(\mathbf{c}_i), \end{aligned}$$

under normalization constraints:

$$\sum_{\mathbf{c}_{i}} \mu_{\mathbf{c}_{i}} = \sum_{\mathbf{s}_{ij}} \mu_{\mathbf{s}_{ij}} = 1$$

for each cluster C_i and separator S_{ij} , and under consistency constraints:

$$\sum_{\mathbf{c}_i \sim \mathbf{s}_{ij}} \mu_{\mathbf{c}_i} = \mu_{\mathbf{s}_{ij}} = \sum_{\mathbf{c}_j \sim \mathbf{s}_{ij}} \mu_{\mathbf{c}_j}$$

for each separator S_{ij} and neighboring clusters C_j and C_j .

Summary of IJGP so far

A spectrum of approximations.

IBP: results from applying IJGP to the dual joingraph.

Jointree algorithm: results from applying IJGP to a jointree (as a joingraph).

In between these two ends, we have a spectrum of joingraphs and corresponding factorizations, where IJGP seeks stationary points of the KL-divergence between these factorizations and the original distribution.