Slides Set 5: Exact Inference Algorithms Bucket-elimination

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(Dechter chapter 4, Darwiche chapter 6)

Inference for probabilistic networks

- Bucket elimination (Dechter chapter 4)
	- Belief-updating, P(e), partition function
	- Marginals, probability of evidence
	- The impact of evidence
	- \cdot for MPE (\rightarrow MAP)
	- for MAP $(\rightarrow$ Marginal Map)
	- Influence diagrams?
- Induced-Width (Dechter, Chapter 3.4)

Inference for probabilistic networks

- Bucket elimination
	- Belief-updating, P(e), partition function
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Bayesian networks: example (Pearl, 1988)

P(S, C, B, X, D) = P(S) P(C|S) P(B|S) P(X|C,S) P(D|C,B)

Belief Updating:

P (lung cancer=yes | smoking=no, dyspnoea=yes) = ?

A Bayesian Network

Types of queries

- **NP-hard**: exponentially many terms
- Difficulty (in part) due to restricted elimination orderings
- Focus is on **approximation** and Anytime algorithms
	- **Anytime**: very fast & very approximate ! Slower & more accurate

Belief updating is NP-hard

- Each SAT formula can be mapped into a belief updating query in a Bayesian network
- Example

A simple network

- How can we compute $P(D)?$, $P(D|A=0)?$ $P(A|D=0)?$
- **Brute force** $O(k^4)$
- Maybe $O(4k^2)$

A simple example

- Suppose we have two factors: $f(X) = f_{12}(X_1, X_2) f_{23}(X_2, X_3)$
- To compute the partition function (sum):

$$
Z = \sum_{x_1, x_2, x_3} f(x_1, x_2, x_3) = f(0, 0, 0) + f(0, 0, 1) + f(0, 0, 2) + f(0, 1, 0) + \dots
$$

+ $f(1, 0, 0) + f(1, 0, 1) + f(1, 0, 2) + f(1, 1, 0) + \dots$

Use the factorization of $f(x)$:
 $Z = f_{12}(0,0) f_{23}(0,0) + f_{12}(0,0) f_{23}(0,1) + f_{12}(0,0) f_{23}(0,2) + f_{12}(0,1) f_{23}(1,0) + ...$ $+f_{12}(1,0) f_{23}(0,0)+f_{12}(1,0) f_{23}(0,1)+f_{12}(1,0) f_{23}(0,2)+f_{12}(1,1) f_{23}(1,0)+\ldots$

 and apply the distributive rule:
 $f_{12}(0,1)$ $\left(f_{23}(1,0)+\ldots\right)$ + $f_{12}(1,0)\left(f_{23}(0,0)+f_{23}(0,1)+f_{23}(0,2)\right)+f_{12}(1,1)\left(f_{23}(1,0)+\ldots\right)$

We can pre-compute and re-use these terms in the sum!

$$
\lambda(x_2) = \left(\sum_{x_3} f_{23}(x_2, x_3)\right) \qquad \qquad Z = \sum_{276 \text{ sl\"{o}less } x_2} f_{12}(x_1, x_2) \lambda(x_2)
$$

Variable elimination

Product of factors:

 $p(X_1, X_2, X_3, X_4) = \frac{1}{Z} f_{12}(X_1, X_2) f_{13}(X_1, X_3) f_{24}(X_2, X_4) f_{34}(X_3, X_4).$ Compute:

$$
Z = \sum_{x_4} \sum_{x_3} \sum_{x_2} \sum_{x_1} f_{34}(x_3, x_4) f_{24}(x_2, x_4) f_{12}(x_1, x_2) f_{13}(x_1, x_3),
$$

Collect terms involving x_1 , then x_2 , and so on:

$$
Z = \sum_{x_4} \sum_{x_3} f_{34}(x_3, x_4) \sum_{x_2} f_{24}(x_2, x_4) \sum_{x_1} f_{12}(x_1, x_2) f_{13}(x_1, x_3),
$$

"Bucket elimination":

$$
\lambda_1(x_2, x_3) = \sum_{x_1} f_{12}(x_1, x_2) f_{13}(x_1, x_3),
$$

\n
$$
\lambda_2(x_3, x_4) = \sum_{x_2} f_{24}(x_2, x_4) \lambda_1(x_2, x_3),
$$

\n
$$
\lambda_3(x_4) = \sum_{x_3} f_{34}(x_3, x_4) \lambda_2(x_3, x_4),
$$

\n
$$
Z = \sum_{x_4} \lambda_3(x_4),
$$

Collect all factors with x_1 in a "bucket"

Collect all remaining factors with $x₂$

Place intermediate calculations in bucket of their earliest argument

slides₅ F₂₄

To compute the prior marginal on variable C , $Pr(C)$

we first eliminate variable A and then variable B

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- There are two factors that mention variable A, Θ_A and $\Theta_{B|A}$
- \bullet We multiply these factors first and then sum out variable A from the resulting factor.
- Multiplying Θ_A and $\Theta_{B|A}$:

 \bullet Summing out variable A :

- \bullet We now have two factors, $\sum_{A}\Theta_{A}\Theta_{B|A}$ and $\Theta_{C|B}$, and we want to eliminate variable B
- Since B appears in both factors, we must multiply them first and then sum out B from the result.
- Multiplying:

• Summing out:

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- \bullet We now have two factors, $\sum_{A}\Theta_{A}\Theta_{B|A}$ and $\Theta_{C|B}$, and we want to eliminate variable B
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- Multiplying:

• Summing out:

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Belief updating

P (lung cancer=yes | smoking=no, dyspnoea=yes $) = ?$

From essai

Belief updating

From essai

$$
P(a,g=1) = \sum_{c,b,e,d,g=1} P(a,b,c,d,e,g) = \sum_{c,b,f,d,g=1} P(g|f)P(f|b,c)P(d|a,b)P(c|a)P(b|a)P(a).
$$

$$
P(a, g = 1) = P(a) \sum_{c} P(c|a) \sum_{b} P(b|a) \sum_{f} P(f|b, c) \sum_{d} P(d|b, a) \sum_{g=1} P(g|f). \quad (4.1)
$$

\n
$$
P(a, g = 1) = P(a) \sum_{c} P(c|a) \sum_{b} P(b|a) \sum_{f} P(f|b, c) \lambda_G(f) \sum_{d} P(d|b, a). \quad (4.2)
$$

\n
$$
P(a, g = 1) = P(a) \sum_{c} P(c|a) \sum_{b} P(b|a) \lambda_D(a, b) \sum_{f} P(f|b, c) \lambda_G(f) \quad (4.3)
$$

\n
$$
P(a, g = 1) = P(a) \sum_{c} P(c|a) \sum_{b} P(b|a) \lambda_D(a, b) \lambda_F(b, c) \quad (4.4)
$$

\n
$$
P(a, g = 1) = P(a) \sum_{c} P(c|a) \lambda_B(a, c) \quad (4.5)
$$

A different ordering

Ordering: A,F,D,C,B,G

 $P(a, g = 1) = P(a) \sum_{f} \sum_{d} \sum_{c} P(c|a) \sum_{b} P(b|a) P(d|a, b) P(f|b, c) \sum_{g=1} P(g|f)$ $= P(a) \sum_f \lambda_G(f) \sum_d \sum_c P(c|a) \sum_b P(b|a) P(d|a, b) P(f|b, c)$ $= P(a) \sum_f \lambda_G(f) \sum_d \sum_c P(c|a) \lambda_B(a, d, c, f)$ ΣП $= P(a) \sum_f \lambda_g(f) \sum_d \lambda_C(a, d, f)$ Bucket G: $P(G|F)$ G=1 $= P(a) \sum_f \lambda_G(f) \lambda_D(a, f)$ Bucket B: $P(F|B,C)$ $P(D|B,A)$ $P(B|A)$ $= P(a)\lambda_F(a)$ Bucket C: $P(C|A)$ $\lambda^{B}(\overline{A},\overline{D},\overline{C},F)$

Figure 4.3: The bucket's output when processing along $d_2 = A, F, D, C, B, G$

The operation in a bucket

- Multiplying functions
- Marginalizing (summing-out) functions

Combination of Cost Functions

= 0.1 x 0.8

Elimination in a factor

Factors: Sum-Out Operation

The result of summing out variable X from factor $f(\mathbf{X})$

is another factor over variables $Y = X \setminus \{X\}$:

$$
\left(\sum_{X} f\right) (\mathbf{y}) \stackrel{\text{def}}{=} \sum_{X} f(x, \mathbf{y})
$$

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Thanks to Darwiche

ALGORITHM BE-BEL

Input: A belief network $B = \langle X, D, P_G, \Pi \rangle$, an ordering $d = (X_1, \dots, X_n)$; evidence e output: The belief $P(X_1 | e)$ and probability of evidence $P(e)$

- Partition the input functions (CPTs) into $bucket_1, ..., bucket_n$ as follows: 1. for $i \leftarrow n$ downto 1, put in *bucket_i* all unplaced functions mentioning X_i . Put each observed variable in its bucket. Denote by ψ_i the product of input functions in $bucket_i$.
- backward: for $p \leftarrow n$ downto 1 do 2.

\n- \n 3. for all the functions
$$
\psi_{S_0}, \lambda_{S_1}, \ldots, \lambda_{S_j}
$$
 in *bucket* do\n $\text{If (observed variable)} \ X_p = x_p \text{ appears in } bucket_p,$ \n assign $X_p = x_p$ to each function in *bucket* and then put each resulting function in the bucket of the *closest* variable in its scope.\n
	\n- else,
	\n- 1. $\lambda_p \leftarrow \sum_{X_p} \psi_p \cdot \prod_{i=1}^j \lambda_{S_i}$
	\n- 5. place λ_p in bucket of the latest variable in scope(λ_p),
	\n- 6. return (as a result of processing *bucket*1):\n $P(\epsilon) = \alpha = \sum_{X_1} \psi_1 \cdot \prod_{\lambda \in bucket_1} \lambda$
	\n- $P(X_1 | \epsilon) = \frac{1}{\alpha} \psi_1 \cdot \prod_{\lambda \in bucket_1} \lambda$
	\n\n
\n

Figure 4.5: BE-bel: a sum-product bucket-elimination algorithm.

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Student network example

Induced width

- Width is the max number of parents in the ordered graph
- Induced-width is the width of the induced ordered graph: recursively connecting parents going from last node to first.
- Induced-width $w^*(d)$ is the max induced-width over all nodes in ordering d
- Induced-width of a graph, w^* is the min $w^*(d)$ over all orderings d

Complexity of bucket elimination

Bucket-Elimination is **time** and **space** $O(r \exp(w_d^*))$

The effect of the ordering: $r =$ number of functions w_d^* : the induced width of the primal graph along ordering d

Inference for probabilistic networks

■ Bucket elimination

- Belief-updating, P(e), partition function
- Marginals, probability of evidence
- The impact of evidence
- \blacksquare for MPE (\rightarrow MAP)
- \bullet for MAP $(\rightarrow$ Marginal Map)
- Induced-Width

The impact of evidence? Algorithm BE-bel

The impact of evidence? Algorithm BE-bel

The impact of observations

Figure 4.9: Adjusted induced graph relative to observing B.

Ordered graph Induced graph Ordered conditioned graph

Types of queries

- **NP-hard**: exponentially many terms
- Difficulty (in part) due to restricted elimination orderings
- We will focus on **approximation** algorithms
	- **Anytime**: very fast & very approximate ! Slower & more accurate

Inference for Probabilistic Networks

■ Bucket elimination

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- Marginals, probability of evidence
- The impact of evidence
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- Induced-Width

²⁷⁶ slides5 F24

Generating the optimal assignment

• Given BE messages, select optimum config in reverse **order**
 b^{*} = arg max $p(b|a^*) p(d^*|b, a^*) p(e^*|b, c^*)$ **B:** $p(b|a) p(d|b, a) p(e|b, c)$ **C:** $p(c|a)$ $\lambda_{B\to C}(a, c, d, e)$ $\mathbf{c}^* = \arg \max_{a} p(c|a^*) \lambda_{B \to C}(a^*, c, d^*, e^*)$ $\lambda_{C\to D}(a,d,e)$ $\mathbf{d}^* = \arg \max_{d} \lambda_{C \to D}(a^*, d, e^*)$ **D:** $\mathbf{e}^* = \arg \max \mathbb{1}[e = 0] \lambda_{D \to E}(a^*, e)$ **E:** $\mathbb{1}[e=0] \quad \lambda_{D\to E}(a,e)$ $p(a) \lambda_{E\to A}(a)$ **A:** $\mathbf{a}^* = \arg \max_a p(a) \cdot \lambda_{E \to A}(a)$

Return optimal configuration (a*,b*,c*,d*,e*)

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OPT = optimal value

Complexity of bucket elimination

Bucket-Elimination is **time** and **space** $O(r \exp(w_d^*))$

The effect of the ordering: $r =$ number of functions w_d^* : the induced width of the primal graph along ordering d

A Bayesian Network

Example with mpe?

Try to compute MPE when $E=0$

■ **Theorem:**

BE is $O(n \exp(w^*+1))$ time and $O(n \exp(w^*))$ space, when w^* is the induced-width of the moral graph along d when evidence nodes are processed (edges from evidence nodes to earlier variables are removed.)

More accurately: $O(r \exp(w^*(d))$ where r is the number of CPTs. For Bayesian networks r=n. For Markov networks?

Inference for probabilistic networks

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- Induced-Width (Dechter 3.4,3.5)

Variable ordering heuristics

- What makes a good order?
	- Low induced width
	- Elimination creates a function over neighbors
- Finding the best order is hard (NP-complete!)
	- But we can do well with simple heuristics
		- Min-induced-width, Min-Fill, …
	- Anytime algorithms

Min-width ordering

MIN-WIDTH (MW) **input:** a graph $G = (V, E), V = \{v_1, ..., v_n\}$ **output:** A min-width ordering of the nodes $d = (v_1, ..., v_n)$. 1. for $j = n$ to 1 by -1 do $r \leftarrow$ a node in G with smallest degree. 2. put r in position j and $G \leftarrow G - r$. $3.$ (Delete from V node r and from E all its adjacent edges) 4. endfor

276 slides5 F24 **Proposition:** algorithm min-width finds a min-width ordering of a graph **What is the Complexity of MW?** O(e)

Variable ordering heuristics

- Min (induced) width heuristic
- 1. for $i=1$ to n (# of variables)
- 2. Select a node X_i with smallest degree as next eliminated
- 3. Connect Xi's neighbors:
- 4. $E = E + \{ (X_i, X_k) : (X_i, X_j) \text{ and } (X_i, X_k) \text{ in } E \}$
- 5. Remove X_i from the graph: $V = V \{X_i\}$

6. end

("Weighted" version: weight edges by domain size)

Variable ordering heuristics

- Min fill heuristic
- 1. for $i=1$ to n (# of variables)
- 2. Select a node X_i with smallest "fill edges" as next eliminated
- 3. Connect Xi's neighbors:
- 4. $E = E + \{ (X_i, X_k) : (X_i, X_j) \text{ and } (X_i, X_k) \text{ in } E \}$
- 5. Remove X_i from the graph: $V = V \{X_i\}$

6. end

("Weighted" version: weight edges by domain size)

Tree-structured graphs

- If the graph is a tree, the best ordering is easy:
	- B, E have only one neighbor; no "fill"
	- Select one to eliminate; remove it
	- Now D or E have only one neighbor; no "fill"...
- **Order**
	- leaves to root
	- never increases the size of the factors

Greedy orderings heuristics

- Min-induced-width
	- From last to first, pick a node with smallest width, then connect parent and remove
- Min-Fill
	- From last to first, pick a node with smallest fill-edges

Complexity? $O(n^3)$

Different induced-graphs

 (a)

Let's find a miw ordering and a min-fill ordering

Different induced-graphs

Which greedy algorithm is best?

- Min-Fill, prefers a node who adds the least number of fill-in arcs.
- Empirically, fill-in is the best among the greedy algorithms (MW,MIW,MF,MC)
- Complexity of greedy orderings?
- MW is O(e), MIW: $O(n^3)$ MF $O(n^3)$ MC is $O(e+n)$

Inference for probabilistic networks

- Bucket elimination (Dechter chapter 4)
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	- Influence diagrams?
- Induced-Width (Dechter, Chapter 3.4)

Marginal Map

■ **NP-hard**: exponentially many terms

Example for MMAP Applications

- Haplotype in Family pedigrees
- Coding networks

 (s_o)

 $A_{\mathcal{O}}$

 S_2

 $o₂$

• Probabilistic planning

■ Diagnosis

Marginal MAP is not easy on trees

- Pure MAP or summation tasks
	- Dynamic programming
	- Ex: efficient on trees

- Marginal MAP
	- Operations do not commute:
	- Sum must be done first!

Bucket elimination for MMAP

Bucket Elimination

Why is MMAP harder?

Inference for probabilistic networks

- Bucket elimination (Dechter chapter 4)
	- Belief-updating, P(e), partition function
	- Marginals, probability of evidence
	- The impact of evidence
	- \blacksquare for MPE (\rightarrow MAP)
	- \bullet for MAP (\rightarrow) Marginal Map)
- Induced-Width (Dechter, Chapter 3.4)
- Mixed networks
- Influence diagrams?

Ex: "oil wildcatter"

e.g., [Raiffa 1968; Shachter 1986]

Influence diagram:

- Three actions: test, drill, sales policy
- Chance variables: ۰

P(oil) P(seismic|oil) P(result | seismic, test) P(produced | oil, drill) P(market)

Utilities capture costs of actions, rewards of sale \bullet Oil sales - Test cost - Drill cost - Sales cost

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Influence Diagrams

Influence diagram ID = (X,D,P,R).

Chance variables over domains. Decision variables CPT's for chance variables Reward components Utility function

Common examples

- Markov decision process
	- Markov chain state sequence
	- Actions "di" influence state transition
	- Rewards based on action, new state
	- Temporally homogeneous
- Partially observable MDP \bullet
	- Hidden Markov chain state sequence -
	- Generate observations
	- Actions based on observations

A decision rule for is a mapping:

where is the cross product of domains in S.

A policy is a list of decision rules

Task: Find an optimal policy that maximizes the expected utility.

The Car Example (Howard 1976)

A car buyer needs to buy one of two used cars. The buyer can carry out tests with various costs, and then, decide which car to buy.

T: Test variable (t_0, t_1, t_2) $(t_1$ test car 1, t_2 test car 2)

D: the decision of which car to buy, $D \in \{buy1, buy2\}$

C_i: the quality of car *i*, $C_i \in \{q_1, q_2\}$

 t_i : the outcome of the test on car *i*, $t_i \in \{pass, fail, null\}$.

r(T): The cost of testing,

 $r(C₁,D)$, $r(C₂,D)$: the reward in buying cars 1 and 2.

The utility is: $r(T) + r(C_1, D) + r(C_2, D)$.

Task: determine decision rules T and D such that:

Bucket Elimination for meu (Algorithm Elim-meu-id)

Input: An Influence diagram $ID = \{P_1, ..., P_n, r_1, ..., r_j\}$ *Output: Meu and optimizing policies.*

- *1. Order the variables and partition into buckets.*
- *2. Process buckets from last to first:*

$$
o = T, t2, t2, D, C2, C1\nbucket(C1): P(C1), P(t1|C1, T), r(C1, D)\nbucket(C2): P(C2), P(t2|C2, T), r(C2, D)\nbucket(D): $\frac{\theta}{C_1} \frac{(t_1, T, D), \frac{\theta}{C_2} (t_2, T, D)}{(t_1, T, D), \frac{\theta}{C_1} (t_1, T, D)}$
\nbucket(t₁): $\frac{\theta}{C_2} \frac{(t_1, T)}{(t_1, T)} \frac{\theta}{C_1} \frac{(t_1, t_2, T)}{(t_2, T)}$
\nbucket(t₂): $\frac{\theta}{C_2} \frac{(t_2, T)}{(t_2, T)} \frac{\theta}{C_1} \frac{(t_2, T)}{(t_2, T)}$
\nbucket(T): r(T) $\frac{\theta}{C_1} \frac{\theta}{C_2} \frac{(T)}{(T)}$
\n θ
\n θ
\n θ
\n θ
$$

3. Forward: Assign values in ordering d

The Bucket Description

*Final buckets: (*λ*s or Ps) utility components (*θ*'s or r's).*

bucket(C_1): $P(C_1)$, $P(t_1|C_1, T)$, $r(C_1, D)$

bucket(C_2): $P(C_2)$, $P(t_2|C_2, T)$, $r(C_2, D)$

bucket(D): $bucket(t_l):$

 $bucket(t₂):$ *bucket(T): r(T)*

Optimizing policies: is argmax of computed in bucket(T), and *in bucket(t₁).*

 t_2

T

 C_1

 C_2

D

 t_1

General Graphical Models

Definition 2.2 Graphical model. A graphical model M is a 4-tuple, $M = \langle X, D, F, \otimes \rangle$, where:

- 1. $X = \{X_1, \ldots, X_n\}$ is a finite set of variables;
- 2. $\mathbf{D} = \{D_1, \ldots, D_n\}$ is the set of their respective finite domains of values;
- 3. $F = \{f_1, \ldots, f_r\}$ is a set of positive real-valued discrete functions, defined over scopes of variables $S = \{S_1, ..., S_r\}$, where $S_i \subseteq X$. They are called *local* functions.
- 4. \otimes is a *combination* operator (e.g., $\otimes \in \{\Pi, \Sigma, \bowtie\}$ (product, sum, join)). The combination operator can also be defined axiomatically as in [Shenoy, 1992], but for the sake of our discussion we can define it explicitly, by enumeration.

The graphical model represents a *global function* whose scope is X which is the combination of all its functions: $\bigotimes_{i=1}^r f_i$.

General bucket elimination

Algorithm General bucket elimination (GBE)

Input: $\mathcal{M} = \langle X, D, F, \otimes \rangle$. $F = \{f_1, ..., f_n\}$ an ordering of the variables, $d = X_1, ..., X_n$; $Y \subset X$.

Output: A new compiled set of functions from which the query $\psi_Y \otimes_{i=1}^n f_i$ can be derived in linear time.

1. Initialize: Generate an ordered partition of the functions into buck $et_1, ..., \text{bucket}_n$, where bucket_i contains all the functions whose highest variable in their scope is X_i . An input function in each bucket ψ_i , $\psi_i = \otimes_{i=1}^n f_i$. 2. Backward: For $p \leftarrow n$ downto 1, do for all the functions ψ_p , λ_1 , λ_2 , ..., λ_j in *bucket_p*, do

- If (observed variable) $X_p = x_p$ appears in bucket_p, assign $X_p = x_p$ in ψ_p and to each λ_i and put each resulting function in appropriate bucket.
- else, (combine and marginalize) $\lambda_p \leftarrow \mathcal{L}_{S_p}$ $\psi_p \otimes (\otimes_{i=1}^j \lambda_i)$ and add λ_p to the largest-index variable in $scope(\lambda_p)$.

3. Return: all the functions in each bucket.

Theorem 4.23 Correctness and complexity. Algorithm GBE is sound and complete for its task. Its time and space complexities is exponential in the $w^*(d) + 1$ and $w^*(d)$, respectively, along the order of processing d.