Probabilistic Graphical Models

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Today's lecture

1. Using VE for conditional queries
2. Running-time of variable elimination
    - Elimination as graph transformation
    - Fill edges, width, treewidth
3. Sum-product belief propagation (BP)
   Done on blackboard
4. Max-product belief propagation

How to introduce evidence?

- Recall that our original goal was to answer *conditional* probability queries,

$$p(\mathbf{Y}|\mathbf{E}=\mathbf{e}) = \frac{p(\mathbf{Y},\mathbf{e})}{p(\mathbf{e})}$$

- Apply variable elimination algorithm to the task of computing $P(\mathbf{Y}, \mathbf{e})$
- Replace each factor $\phi \in \Phi$ that has $\mathbf{E} \cap \mathrm{Scope}[\phi] \neq \emptyset$ with

$$\phi'(\mathbf{x}_{\mathrm{Scope}[\phi]-\mathbf{E}}) = \phi(\mathbf{x}_{\mathrm{Scope}[\phi]-\mathbf{E}}, \mathbf{e}_{\mathbf{E}\cap\mathrm{Scope}[\phi]})$$

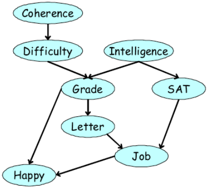
- Then, eliminate the variables in $\mathcal{X} - \mathbf{Y} - \mathbf{E}$. The returned factor $\phi^*(\mathbf{Y})$ is $p(\mathbf{Y}, \mathbf{e})$
- To obtain the conditional $p(\mathbf{Y} \mid \mathbf{e})$, normalize the resulting product of factors – the normalization constant is $p(\mathbf{e})$

Sum-product VE for conditional distributions

Algorithm 9.2 Using Sum-Product-Variable-Elimination **for computing conditional probabilities.**

Procedure Cond-Prob-VE (
  $\mathcal{K}$, // A network over $\mathcal{X}$
  $\boldsymbol{Y}$, // Set of query variables
  $\boldsymbol{E} = \boldsymbol{e}$ // Evidence
)
  $\Phi \leftarrow$ Factors parameterizing $\mathcal{K}$
  Replace each $\phi \in \Phi$ by $\phi[\boldsymbol{E} = \boldsymbol{e}]$
  Select an elimination ordering $\prec$
  $\boldsymbol{Z} \leftarrow \ = \mathcal{X} - \boldsymbol{Y} - \boldsymbol{E}$
  $\phi^* \leftarrow$ Sum-Product-Variable-Elimination($\Phi, \prec, \boldsymbol{Z}$)
  $\alpha \leftarrow \sum_{\boldsymbol{y} \in Val(\boldsymbol{Y})} \phi^*(\boldsymbol{y})$
  return α, ϕ^*

Running time of variable elimination

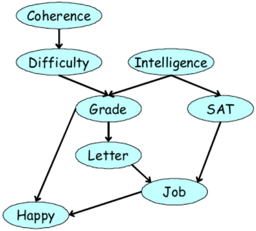


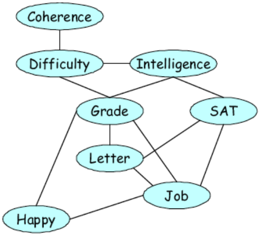
Step	Variable eliminated	Factors used	Variables involved	New factor
1	C	$\phi_C(C)$, $\phi_D(D,C)$	C, D	$\tau_1(D)$
2	D	$\phi_G(G,I,D)$, $\tau_1(D)$	G, I, D	$\tau_2(G,I)$
3	I	$\phi_I(I)$, $\phi_S(S,I)$, $\tau_2(G,I)$	G, S, I	$\tau_3(G,S)$
4	H	$\phi_H(H,G,J)$	H, G, J	$\tau_4(G,J)$
5	G	$\tau_4(G,J)$, $\tau_3(G,S)$, $\phi_L(L,G)$	G, J, L, S	$\tau_5(J,L,S)$
6	S	$\tau_5(J,L,S)$, $\phi_J(J,L,S)$	J, L, S	$\tau_6(J,L)$
7	L	$\tau_6(J,L)$	J, L	$\tau_7(J)$

- Let n be the number of variables, and m the number of initial factors
- At each step, we pick a variable X_i and multiply all factors involving X_i, resulting in a single factor ψ_i
- Let N_i be the number of variables in the factor ψ_i, and let $N_{max} = \max_i N_i$
- The running time of VE is then $O(mk^{N_{max}})$, where $k = |\mathrm{Val}(X)|$. Why?
- The primary concern is that N_{max} can potentially be as large as n

Running time in graph-theoretic concepts

- Let's try to analyze the complexity in terms of the graph structure
- G_Φ is the undirected graph with one node per variable, where there is an edge (X_i, X_j) if these appear together in the scope of some factor ϕ
- Ignoring evidence, this is either the original MRF (for sum-product VE on MRFs) or the moralized Bayesian network:





Elimination as graph transformation

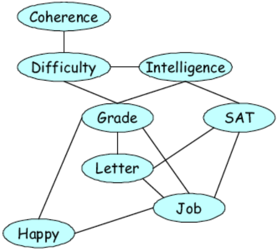
When a variable X is eliminated,

- We create a single factor ψ that contains X and all of the variables $\mathbf{Y}$ with which it appears in factors
- We eliminate X from ψ, replacing it with a new factor τ that contains all of the variables $\mathbf{Y}$, but not X. Let's call the new set of factors Φ_X

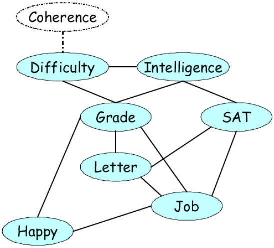
How does this modify the graph, going from G_Φ to G_{Φ_X}?

- Constructing ψ generates edges between all of the variables $Y \in \mathbf{Y}$
- Some of these edges were already in G_Φ, some are new
- The new edges are called **fill edges**
- The step of removing X from Φ to construct Φ_X removes X and all its incident edges from the graph

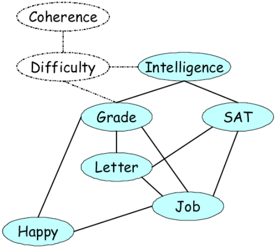
Example



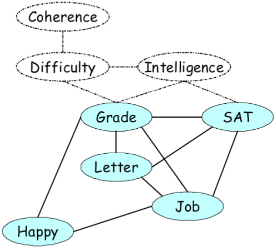
(Graph)



(Elim. C)



(Elim. D)

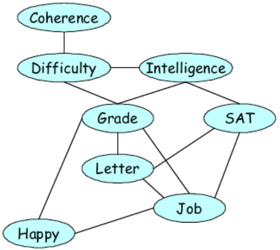


(Elim. I)

Induced graph

- We can summarize the computation cost using a single graph that is the union of all the graphs resulting from each step of the elimination
- We call this the **induced graph** $\mathcal{I}_{\Phi,\prec}$, where $\prec$ is the elimination ordering

Example



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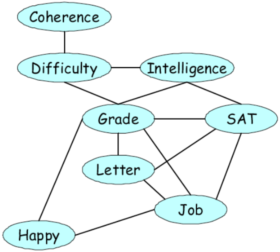
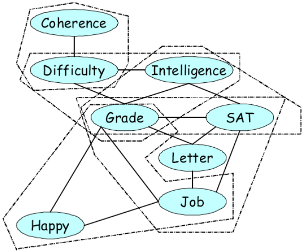


(Induced graph)



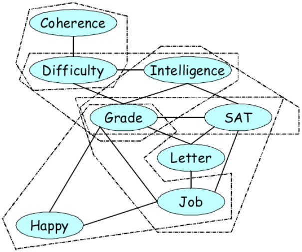
(Maximal Cliques)

Properties of the induced graph

- **Theorem**: Let $\mathcal{I}_{\Phi,\prec}$ be the induced graph for a set of factors Φ and ordering $\prec$, then
  1. Every factor generated during VE has a scope that is a clique in $\mathcal{I}_{\Phi,\prec}$
  2. Every maximal clique in $\mathcal{I}_{\Phi,\prec}$ is the scope of some intermediate factor in the computation

  (see book for proof)
- Thus, N_{max} is equal to the size of the largest clique in $\mathcal{I}_{\Phi,\prec}$
- The running time, $O(mk^{N_{max}})$, is exponential in the size of the largest clique of the induced graph

Example



(Maximal Cliques)

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(VE)

- The maximal cliques in $\mathcal{I}_{G,\prec}$ are

$$
\begin{aligned}
\mathbf{C}_1 &= \{C, D\} \\
\mathbf{C}_2 &= \{D, I, G\} \\
\mathbf{C}_3 &= \{G, L, S, J\} \\
\mathbf{C}_4 &= \{G, J, H\}
\end{aligned}
$$

Induced width

- The **width** of an induced graph is #nodes in largest clique - 1
- We define the **induced width** $w_{\mathcal{G},\prec}$ to be the width of the graph $\mathcal{I}_{\mathcal{G},\prec}$ induced by applying VE to $\mathcal{G}$ using ordering $\prec$
- The **treewidth**, or "minimal induced width" of graph $\mathcal{G}$ is

$$w^*_{\mathcal{G}} = \min_{\prec} w_{\mathcal{G},\prec}$$

- The treewidth provides a bound on the best running time achievable by VE on a distribution that factorizes over $\mathcal{G}$: $O(mk^{w^*_{\mathcal{G}}})$,
- Unfortunately, finding the **best** elimination ordering (equivalently, computing the treewidth) for a graph is NP-hard
- In practice, heuristics (e.g., min-fill) are used to find a good elimination ordering

Chordal Graphs

Graph is **chordal**, or triangulated, if every cycle of length ≥ 3 has a shortcut (called a "chord")

Theorem: Every induced graph is chordal
Proof: (by contradiction)

- Assume we have a chordless cycle $X_1 - X_2 - X_3 - X_4 - X_1$ in the induced graph
- Suppose X_1 was the first variable that we eliminated (of these 4)
- After a node is eliminated, no fill edges can be added to it. Thus, $X_1 - X_2$ and $X_1 - X_4$ must have pre-existed
- Eliminating X_1 introduces the edge $X_2 - X_4$, contradicting our assumption

Chordal graphs

- **Thm:** Every induced graph is chordal
- **Thm:** Any chordal graph has an elimination ordering that does not introduce any fill edges

Algorithm 9.3 Maximum Cardinality Algorithm for constructing an elimination ordering

Procedure Max-Cardinality (
  $\mathcal{H}$ // An undirected graph over $\mathcal{X}$
)
  Initialize all nodes in $\mathcal{X}$ as unmarked
  for $k = |\mathcal{X}| \ldots 1$
    $X \leftarrow$ unmarked variable in $\mathcal{X}$ with largest number of marked neighbors
    $\pi(X) \leftarrow k$
    Mark X
  return π

(The elimination ordering is REVERSE)

- **Conclusion:** Finding a good elimination ordering is equivalent to making graph chordal with minimal width

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MAP inference

- Recall the MAP inference task,

$$\arg\max_{\mathbf{x}} p(\mathbf{x}), \qquad p(\mathbf{x}) = \frac{1}{Z} \prod_{c \in C} \phi_c(\mathbf{x}_c)$$

  (we assume any evidence has been subsumed into the potentials, as discussed in the last lecture)

- Since the normalization term is simply a constant, this is equivalent to

$$\arg\max_{\mathbf{x}} \prod_{c \in C} \phi_c(\mathbf{x}_c)$$

  (called the *max-product* inference task)

- Furthermore, since log is monotonic, letting $\theta_c(\mathbf{x_c}) = \lg \phi_c(\mathbf{x_c})$, we have that this is equivalent to

$$\arg\max_{\mathbf{x}} \sum_{c \in C} \theta_c(\mathbf{x}_c)$$

  (called *max-sum*)

Semi-rings

- Compare the sum-product problem with the max-product (equivalently, max-sum in log space):

$$\text{sum-product} \qquad \sum_{\mathbf{x}} \prod_{c \in C} \phi_c(\mathbf{x}_c)$$

$$\text{max-sum} \qquad \max_{\mathbf{x}} \sum_{c \in C} \theta_c(\mathbf{x}_c)$$

- Can exchange operators $(+, *)$ for $(\max, +)$ and, because both are semirings satisfying associativity and commutativity, everything works!
- We get "max-product variable elimination" and "max-product belief propagation"

Simple example

- Suppose we have a simple chain, $A - B - C - D$, and we want to find the MAP assignment,

$$\max_{a,b,c,d} \phi_{AB}(a, b)\phi_{BC}(b, c)\phi_{CD}(c, d)$$

- Just as we did before, we can push the maximizations inside to obtain:

$$\max_{a,b} \phi_{AB}(a, b) \max_{c} \phi_{BC}(b, c) \max_{d} \phi_{CD}(c, d)$$

  or, equivalently,

$$\max_{a,b} \theta_{AB}(a, b) + \max_{c} \theta_{BC}(b, c) + \max_{d} \theta_{CD}(c, d)$$

- To find the actual maximizing assignment, we do a traceback (or keep back pointers)

Max-product variable elimination

Procedure Max-Product-VE (
Φ, // Set of factors over $\boldsymbol{X}$
$\prec$ // Ordering on $\boldsymbol{X}$
)
Let $X_1, \ldots, X_k$ be an ordering of $\boldsymbol{X}$ such that
$X_i \prec X_j$ iff $i < j$
for $i = 1, \ldots, k$
$(\Phi, \phi_{X_i}) \leftarrow$ Max-Product-Eliminate-Var(Φ, X_i)
$\boldsymbol{x}^* \leftarrow$ Traceback-MAP$(\{\phi_{X_i} \ : \ i = 1, \ldots, k\})$
return $\boldsymbol{x}^*, \Phi$ // Φ contains the probability of the MAP

Procedure Max-Product-Eliminate-Var (
Φ, // Set of factors
Z // Variable to be eliminated
)
$\Phi' \leftarrow \{\phi \in \Phi \ : \ Z \in \mathit{Scope}[\phi]\}$
$\Phi'' \leftarrow \Phi - \Phi'$
$\psi \leftarrow \prod_{\phi \in \Phi'} \phi$
$\tau \leftarrow \max_Z \psi$
return $(\Phi'' \cup \{\tau\}, \psi)$

Procedure Traceback-MAP (
$\{\phi_{X_i} \ : \ i = 1, \ldots, k\}$
)
for $i = k, \ldots, 1$
$\boldsymbol{u}_i \leftarrow (x^*_{i+1}, \ldots, x^*_k)\langle \mathit{Scope}[\phi_{X_i}] - \{X_i\}\rangle$
// The maximizing assignment to the variables eliminated after X_i
$x^*_i \leftarrow \arg\max_{x_i} \phi_{X_i}(x_i, \boldsymbol{u}_i)$
// x^*_i is chosen so as to maximize the corresponding entry in the factor, relative to the previous choices $\boldsymbol{u}_i$
return $\boldsymbol{x}^*$

Max-product belief propagation (for tree-structured MRFs)

- Same as sum-product BP except that the messages are now:

$$m_{j\to i}(x_i) = \max_{x_j} \phi_j(x_j)\phi_{ij}(x_i, x_j) \prod_{k\in N(j)\setminus i} m_{k\to j}(x_j)$$

- After passing all messages, can compute single node *max-marginals*,

$$m_i(x_i) = \phi_i(x_i) \prod_{j\in N(i)} m_{j\to i}(x_i) \qquad \propto \qquad \max_{\mathbf{x}_{V\setminus i}} p(\mathbf{x}_{V\setminus i}, x_i)$$

- If the MAP assignment $\mathbf{x}^*$ is **unique**, can find it by locally decoding each of the single node max-marginals, i.e.

$$x_i^* = \arg\max_{x_i} m_i(x_i)$$

Exactly solving MAP, beyond trees

- MAP as a discrete optimization problem is

$$\arg\max_{\mathbf{x}} \sum_{i \in V} \theta_i(x_i) + \sum_{ij \in E} \theta_{ij}(x_i, x_j)$$

- Very general discrete optimization problem – many hard combinatorial optimization problems can be written as this (e.g., 3-SAT)
- Studied in operations research communities, theoretical computer science, AI (constraint satisfaction, weighted SAT), etc.
- Very fast moving field, both for theory and heuristics