EE512A – Advanced Inference in Graphical Models

— Fall Quarter, Lecture 3 —

http://j.ee.washington.edu/~bilmes/classes/ee512a_fall_2014/

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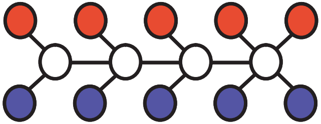


Announcements

- Reading assignments, posted to our canvas announcements page (`https://canvas.uw.edu/courses/914697/announcements`): `intro.pdf`, `ugms.pdf` on undirected graphical models, and `tree_inference.pdf` on trees.
- Slides from previous time this course was offered are at our previous web page (`http://j.ee.washington.edu/~bilmes/classes/ee512a_fall_2011/`) and even earlier at `http://melodi.ee.washington.edu/~bilmes/ee512fa09/`.

Class Road Map - EE512a

- L1 (9/29): Introduction, Families, Semantics
- L2 (10/1): MRFs, Inference on Trees
- L3 (10/6):
- L4 (10/8):
- L5 (10/13):
- L6 (10/15):
- L7 (10/20):
- L8 (10/22):
- L9 (10/27):
- L10 (10/29):
- L11 (11/3):
- L12 (11/5):
- L13 (11/10):
- L14 (11/12):
- L15 (11/17):
- L16 (11/19):
- L17 (11/24):
- L18 (11/26):
- L19 (12/1):
- L20 (12/3):
- Final Presentations: (12/10):

Finals Week: Dec 8th-12th, 2014.

Comparisons of families

- How do $\mathcal{F}(G, \mathcal{M}^{(\mathrm{cf})})$ and $\mathcal{F}(G, \mathcal{M}^{(\mathrm{mcf})})$ compare?

Lemma 3.2.1

$\mathcal{F}(G, \mathcal{M}^{(cf)}) \subseteq \mathcal{F}(G, \mathcal{M}^{(mcf)})$

Lemma 3.2.2

$\mathcal{F}(G, \mathcal{M}^{(cf)}) \supseteq \mathcal{F}(G, \mathcal{M}^{(mcf)})$

- Therefore

Corollary 3.2.3

$\mathcal{F}(G, \mathcal{M}^{(cf)}) = \mathcal{F}(G, \mathcal{M}^{(mcf)})$

- Since rules are identical, we use $\mathcal{M}^{(\mathrm{f})}$ for clique factorization, and family $\mathcal{F}(G, \mathcal{M}^{(\mathrm{f})})$.
- Often, it is not so obvious that different families are identical.
- Equally often, different families are indeed different.

Trees defined in many ways

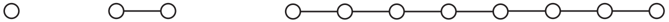
Theorem 3.2.2 (Trees, Berge)

Let $G = (V, E)$ be an undirected graph with $|V| = n > 2$. Then each of the following properties are equivalent and each can be used to define when G is a tree:

- *G is connected and has no cycles*
- *G has $n - 1$ edges and has no cycles,*
- *G is connected and contains exactly $n - 1$ edges,*
- *G has no cycles. Exactly one cycle created if edge added to G.*
- *G is connected, and if any edge is removed, the remaining graph is not connected,*
- *Every pair of vertices of G is connected by one unique path.*
- *G can be generated as follows: Start with v, repeatedly choose next vertex, and connect it with edge to exactly one previous vertex.*

Trees, inference, and distributive law

- Size of any maxclique in tree is two. Any set $S \subset V(T)$ with $|S| > 2$ induces a forest.
- Any $p \in \mathcal{F}(T, \mathcal{M}^{(\mathrm{f})})$ has factors of size at most two.
- This has important consequences for inference.
- A *chain* is a set of nodes connected in succession.



- A chain is a tree but not vice verse
- If p factors w.r.t. a chain then

$$p(x) = \prod_{i=1}^{N-1} \psi_{i,i+1}(x_i, x_{i+1}) \tag{3.8}$$

- Suppose we wish to compute $p(x_3, x_4)$. then

$$p(x_3, x_4) = \sum_{x_1} \sum_{x_2} \sum_{x_5} \sum_{x_6} \cdots \sum_{x_N} p(x_1, x_2, \ldots, x_N) \tag{3.9}$$

Summing, Marginalization, and variable elimination

- Problem: Sum over x_2 in Eq. **??** has cost $O(r^3)$. Total complexity is $O(r^3)$ which is unboundedly worse than $O(r^2)$.
- Some orders inextricably couple together factors, others don't.
- How do we ensure the best (fastest) elimination order? Graph tells us.
- Key Problem: there **exist no functions** $g(a)$ and $h(c)$ that constitute a factorization of a sum as in:

$$g(a)h(c) = \sum_b f_1(a,b) f_2(b,c) \tag{3.17}$$

- In general, for disjoint variables $A, B, C \subseteq V$, the function

$$f(x_A, x_C) = \sum_{x_B} f_1(x_A, x_B) f_2(x_B, x_C) \tag{3.18}$$

does not factor, exists no g, h such that $f(x_A, x_C) = g(x_A) h(x_C)$.

Elimination

- Existence of $f_1(x_A, x_B)$ suggests that $G[A \cup B]$ should be a clique, and existence of $f_2(x_B, x_C)$ suggests $G[B \cup C]$ should be a clique.
- After summation, existence of $f(x_A, x_C)$ suggests that $G[A \cup C]$ should also be a clique *(if it is not already)*.
- Graph-theoretic operation for eliminating a variable in a graph:

Definition 3.2.2

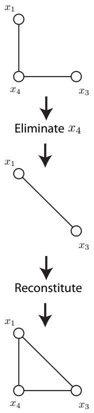
Elimination: To *eliminate* a node $v \in V$ in an undirected graph G, we first connect all neighbors of v and then remove v and all v's incident edges from the graph.

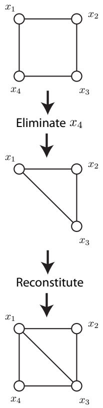
- Once eliminated, former neighbors of v form a clique.
- Additional edges added (if any) are called *fill-in* edges. We'll use $F \subseteq V \times V$ for these.

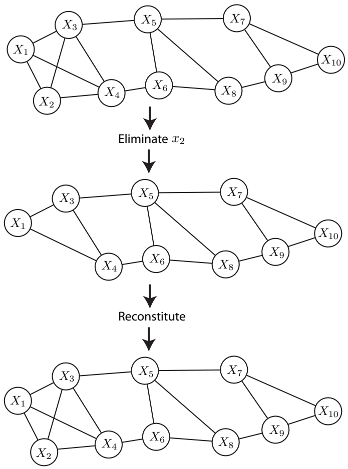
Review: graph theoretic node elimination

- Let $\delta_G(v)$ denote the neighbors of node $v \in V$ in graph G.
- Elimination of a node $v \in V(G)$ from G forms graph G_1
- $G_1 = (V_1, E_1)$ where $V_1 = V \setminus \{v\}$, and where $E_1 = (E \cap V_1 \times V_1) \cup \delta_G(v) \times \delta_G(v)$.
- In G_1, $\delta_G(v)$ forms a clique.
- Any edges in G_1 not in G are part of the fill-in edges F.
- We can say that $G_1 = G_{\sigma_1}$ is the result of eliminating σ_1 from G
- Also, that $G_2 = (G_{\sigma_1})_{\sigma_2}$ is the result of eliminating σ_2 starting from G_{σ_1}, that $G_3 = ((G_{\sigma_1})_{\sigma_2})_{\sigma_3}$ is the result of eliminating σ_3 starting from G_2 and so on.
- Therefore, the ordering σ defines a sequence of graphs $(G_0, G_1, G_2, \dots, G_{N-1})$ where $G_0 = G$ and where G_{N-1} consists of only one node σ_N.
- Reconstituted graph is $G' = (V, E \cup F)$.

Example elimination on graphs





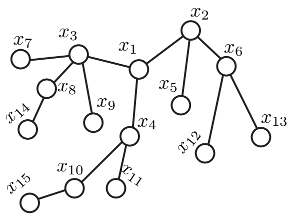


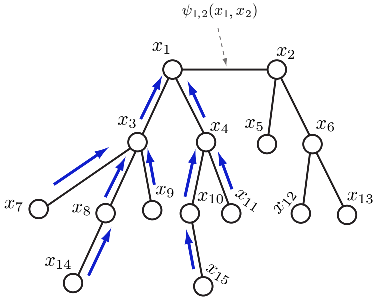
Review: Other facts about node elimination

- A tree always has ≥ 2 leaf nodes.
- Eliminating leaf node always yields sub-tree
- Can continue eliminating nodes in a tree graph.
- Eliminating leaf-nodes never produce fill-in edges.
- data-structure for leaf nodes is easy
- Computation corresponding to tree-elimination is fast $O(Nr^2)$.

Morphing from elimination to belief propagation

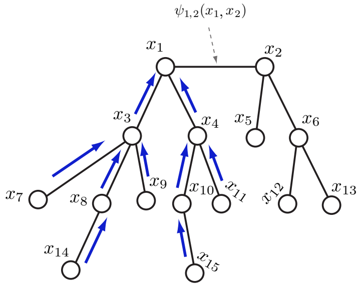
- elimination can be seen as a message passing scheme on a graph
- Tree on left, goal is to produce computation for $p(x_1, x_2)$. We rooted at edge $(1, 2)$ on the right





- blue arrows show elimination steps starting at leaf nodes and continuing until we have reached the root.

Computations for marginal "rooted" at edge (x_1, x_2)



$$\phi_{\cancel{14},8}(x_8) = \sum_{x_{14}} \psi_{8,14}(x_8, x_{14}) \tag{3.19a}$$

$$\phi_{\cancel{7},3}(x_3) = \sum_{x_7} \psi_{7,3}(x_7, x_3) \tag{3.19b}$$

$$\phi_{\cancel{8},\cancel{14},3}(x_3) = \sum_{x_8} \psi_{8,3}(x_8, x_3)\phi_{\cancel{14},8}(x_8) \tag{3.19c}$$

$$\phi_{\cancel{9},3}(x_3) = \sum_{x_9} \phi_{9,3}(x_9, x_3) \tag{3.19d}$$

$$\phi_{\cancel{7},\cancel{14},\cancel{8},\cancel{9},\cancel{3},1}(x_1) = \sum_{x_3} \psi_{1,3}(x_1, x_3)\phi_{\cancel{7},3}(x_3)\phi_{\cancel{8},\cancel{14},3}(x_3)\phi_{\cancel{9},3}(x_3) \tag{3.19e}$$

$$\phi_{\cancel{15},10}(x_{10}) = \sum_{x_{15}} \psi_{10,15}(x_{10}, x_{15}) \tag{3.19f}$$

$$\phi_{\cancel{15},\cancel{10},4}(x_4) = \sum_{x_{10}} \psi_{4,10}(x_4, x_{10})\phi_{\cancel{15},10}(x_{10}) \tag{3.19g}$$

$$\phi_{\cancel{11},4}(x_4) = \sum_{x_{11}} \psi_{4,11}(x_4, x_{11}) \tag{3.19h}$$

$$\phi_{\cancel{10},\cancel{11},\cancel{15},\cancel{4},1}(x_1) = \sum_{x_4} \psi_{1,4}(x_1, x_4)\phi_{\cancel{15},\cancel{10},4}(x_4)\phi_{\cancel{11},4}(x_4) \tag{3.19i}$$

Elimination $\rightarrow$ message passing

- Each node receives a "message" from children in rooted tree, once received enough "messages" can send a "message" to parent.
- General, node i may send message to parent j when i has received message from all of i's children
- at that point, i has become a leaf node in the tree (all children eliminated)
- The parent is chosen arbitrarily (it depends on root).
- There is a general pattern that is true regardless of root designation.

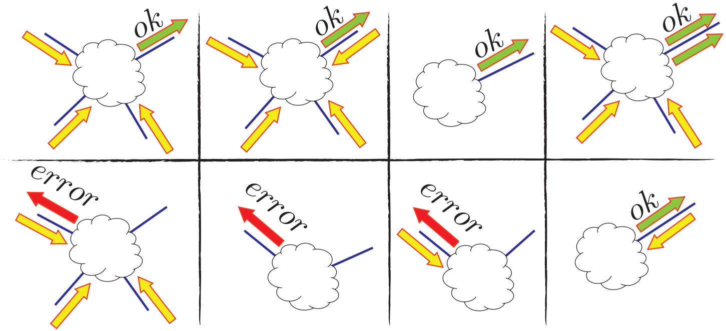
Message passing protocol

Definition 3.2.4

Message passing protocol (MPP): A message may be sent from node i to a neighbor node j only when node i has received a message from all its other neighbors besides j.

- Notationally, if $i \to j$ indicates a message from i to j, then the protocol may be written as $i \to j$ only when $\forall k \in \delta(i) \setminus \{j\}, k \to i$, where $\delta(i)$ are the neighbors of node i in G.
- If MPP is followed but otherwise the ordering of the messages is arbitrary, then we are guaranteed that the end result will be the correct marginal. That is, the protocol specifies only a *partial* (rather than a total) order on messages.

Message passing protocol examples



- Examples of valid and invalid messages. Yellow arrows correspond to incoming messages. Green outgoing arrows correspond to messages that obey MPP, and red outgoing arrows are messages that disobey MPP.
- Note that the 2nd from left example on top row corresponds to what happens at the root of a tree.

Better notation

- Notation is unwieldy. Rather than keep track of entire history, as in $\phi_{\cancel{1}5,\cancel{1}0,4}(x_4)$, use notation that only indicates neighbors in a message

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- Before

$$\phi_{\cancel{1}4,8}(x_8) = \sum_{x_{14}} \psi_{8,14}(x_8, x_{14}) \tag{3.1}$$

After

$$\mu_{14\to 8}(x_8) = \sum_{x_{14}} \psi_{8,14}(x_8, x_{14}) \tag{3.2}$$

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- Before

$$\phi_{\cancel{7},\cancel{1}4,\cancel{8},\cancel{9},\cancel{3},1}(x_1) = \sum_{x_3} \psi_{1,3}(x_1, x_3)\phi_{\cancel{7},3}(x_3)\phi_{\cancel{8},\cancel{1}4,3}(x_3)\phi_{\cancel{9},3}(x_3) \tag{3.3}$$

  After

$$\mu_{3\to 1}(x_1) = \sum_{x_3} \psi_{1,3}(x_1, x_3)\mu_{7\to 3}(x_3)\mu_{8\to 3}(x_3)\mu_{9\to 3}(x_3) \tag{3.4}$$

Generic form of message

$$\mu_{i \to j}(x_j) = \sum_{x_i} \left(\psi_{i,j}(x_i, x_j) \prod_{k \in \delta(i) \setminus \{j\}} \mu_{k \to i}(x_i) \right) \tag{3.5}$$

Message is of form:

1. First, collect messages from all neighbors of i other than j,
2. next, incorporate these incoming messages by multiplying them in along with the factor $\psi_{i,j}(x_i, x_j)$,
3. the factor $\psi_{i,j}(x_i, x_j)$ relates x_i and x_j, and can be seen as a representation of a "communications channel" relating how the information x_i transforms into the information in x_j, thus motivating the terminology of a "message", and
4. then finally marginalizing away x_i thus yielding the desired message to be delivered at the destination node x_j.

Multiple Tree Queries

- Rather than one S we may have $\{S_1, S_2, \ldots, S_k\} = \mathcal{S}$ and wish to compute $p(x_{S_i})$ for all $i \in \{1, 2, \ldots, k\}$. Ex: all cliques/edges.

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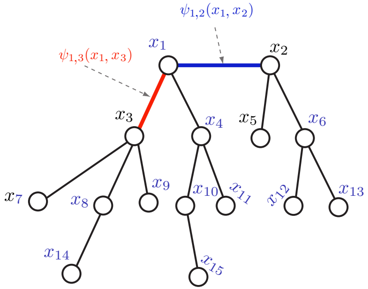
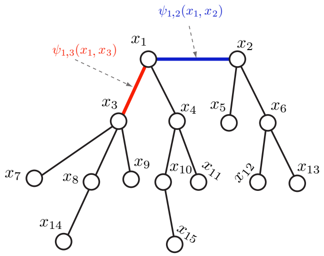
- Example: compute both $p(x_1, x_2)$ and $p(x_1, x_3)$ as before.



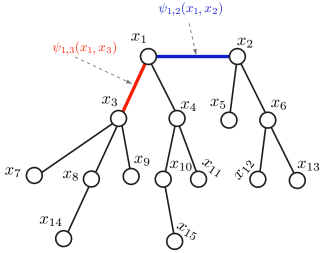
Multiple Tree Queries: Variable elimination

- For $p(x_1, x_2)$, the variable elimination ordering $(14, 7, 8, 9, 15, 10, 11, 4, 12, 13, 5, 6, 3)$ would suffice



Multiple Tree Queries: Variable elimination

- For $p(x_1, x_2)$, the variable elimination ordering $(14, 7, 8, 9, 15, 10, 11, 4, 12, 13, 5, 6, 3)$ would suffice
- 13 messages: $\mu_{14\to8}(x_8)$, $\mu_{7\to3}(x_3)$, $\mu_{8\to3}(x_3)$, $\mu_{9\to3}(x_3)$, $\mu_{15\to10}(x_{10})$, $\mu_{10\to4}(x_4)$, $\mu_{11\to4}(x_4)$, $\mu_{4\to1}(x_1)$, $\mu_{12\to6}(x_6)$, $\mu_{13\to6}(x_6)$, $\mu_{5\to2}(x_2)$, $\mu_{6\to2}(x_2)$, and $\mu_{3\to1}(x_1)$.



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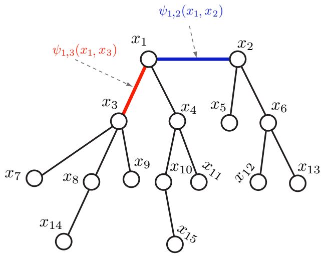
- For $p(x_1, x_3)$, the variable ordering $(14, 7, 8, 9, 15, 10, 11, 4, 12, 13, 5, 6, 2)$ would suffice



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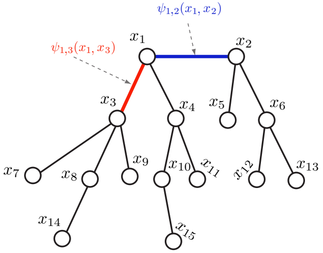

- For $p(x_1, x_3)$, the variable ordering $(14, 7, 8, 9, 15, 10, 11, 4, 12, 13, 5, 6, 2)$ would suffice
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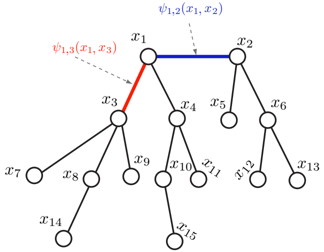
Multiple Tree Queries: Variable elimination



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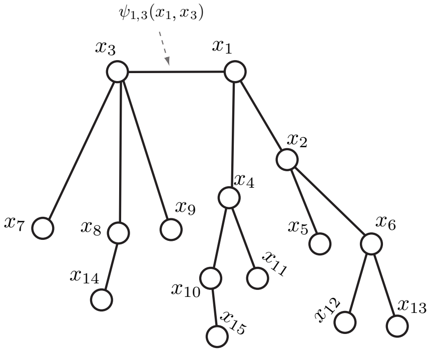
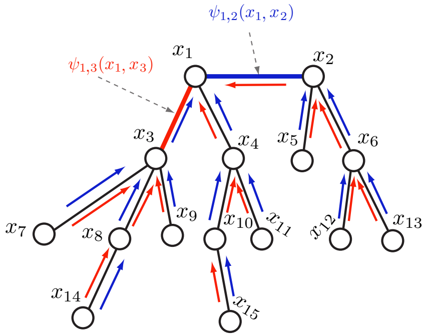
- First 12 of variables in each order are identical! Results in marginal $p(x_1, x_2, x_3)$ from which both results are easy.

Multiple Tree Queries





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- Another look: Left tree rooted at $(1,3)$, right rooted at $(1,2)$.
- Red arrows are messages are for $(1,3)$, blue arrows are messages for $(1,2)$.
- most messages are the same.

Multiple Tree Queries

- Amount of available re-use depends on the desired queries

Multiple Tree Queries

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- Ex: compute $p(x_8, x_{14})$ and $p(x_6, x_{13})$.

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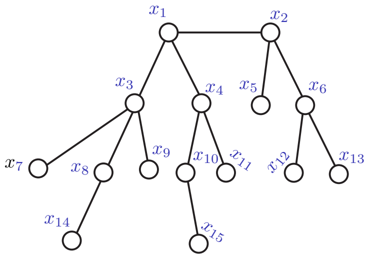

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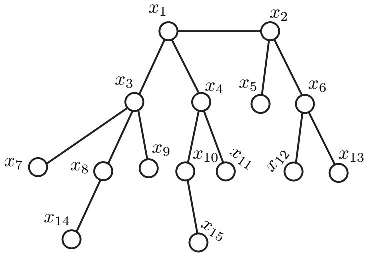

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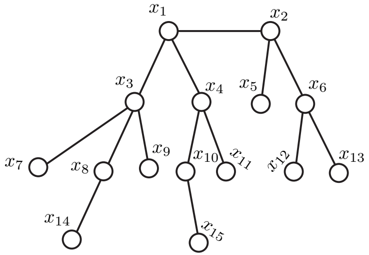

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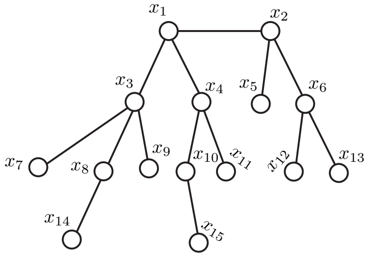
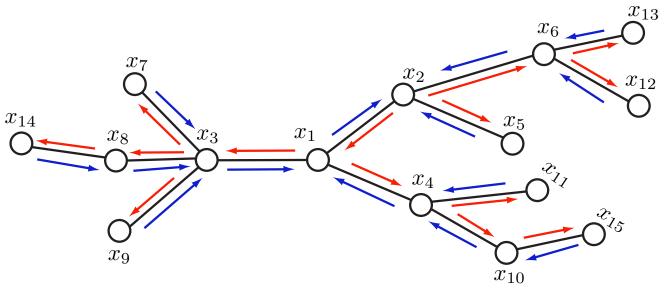


- remaining messages, from x_{14} to x_{13} and from x_{13} back to x_{14}.
- Chain has least re-use for these queries (since they are on ends)
- Still, have saved quite a bit by "trimming" off branches tree relative to naive strategy.

All edge Queries

- As number of queries increases, so does efficiency (queries/message)
- Consider computing $p(x_i, x_j)$ for all $(i, j) \in E(G)$.
- Naive case, $N - 1$ edges $O(N^2 r^2)$.
- Smart case, only $O(N r^2)$ still.
- consider: root tree at all $(i, j) \in E(G)$ in turn
- mark edge with arrow only once (so don't redundantly send message)
- result is each edge has two arrows in each direction

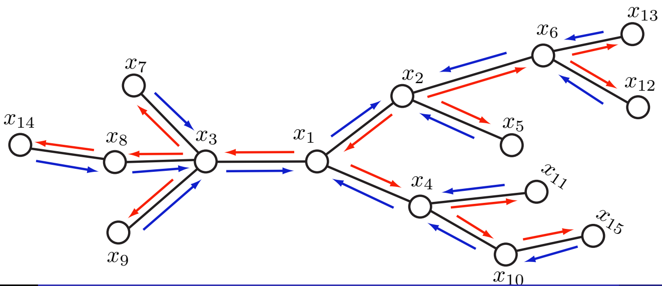


All edge Queries

- When done, each edge $(i,j) \in E(G)$ is now in possession of $\psi_{i,j}(x_i, x_j)$ as well as $\mu_{k\to i}(x_i)$ for all $k \in \delta(i) \setminus \{j\}$ as well as $\mu_{k\to j}(x_j)$ for all $k \in \delta(j) \setminus \{i\}$.
- Thus, can compute the marginals

$$p(x_i, x_j) = \psi_{i,j}(x_i, x_j) \prod_{k\in\delta(i)\setminus\{j\}} \mu_{k\to i}(x_i) \prod_{k\in\delta(j)\setminus\{i\}} \mu_{k\to j}(x_j) \quad (3.6)$$

- Overall computation $O(Nr^2)$.



All edge Queries

Theorem 3.3.1

Given a tree $G = (V, E)$ and some $p \in \mathcal{F}(G, \mathcal{M}^{(f)})$, if messages are sent obeying the message passing protocol so that all edges have two messages across them in each direction, then the computation given above will correctly produce all marginals for all edges in $E(G)$.

Proof.

Consider any edge $(i, j) \in E(G)$ and consider rooting the graph at that edge, as described above. Since all messages obey the MPP, the messages correspond to eliminating the variables in an order from leaf to root, which precisely gives $p(x_i, x_j)$. □

All edge queries - algorithm

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- Once root has received all messages from children, start sending messages back out to children.
- when done all nodes have all messages, MPP obeyed, and any marginal can be computed.
- This procedure is formalized by algorithms *collect evidence* and *distribute evidence* as follows

Collect Evidence

Algorithm 1: CollectEvidence($c \to p$)

Input: A rooted tree $G = (V, E)$ with a child node $c \in V$ and its parent $p \in V$.

Result: A message propagated from c to p that obeys the message passing protocol.

```
1 foreach $u \in \text{child}(c)$ do
2     call CollectEvidence($u \to c$)
3 Compute
```

$$\mu_{c\to p}(x_p) = \sum_{x_c} \psi_{c,p}(x_c, x_p) \prod_{u\in\text{child}(c)} \mu_{u\to c}(x_c)$$

Distribute Evidence

Algorithm 2: DistributeEvidence($p \to c$)

Input: A rooted tree $G = (V, E)$ with a parent node $p \in V$ and a child $c \in \text{child}(p)$.

Result: A message propagated from p to c that obeys the message passing protocol.

```
1 Compute
      $$\mu_{p\to c}(x_c) = \sum_{x_p} \psi_{p,c}(x_p, x_c) \prod_{u \in \delta(p) \setminus \{c\}} \mu_{u \to p}(x_p)$$
2 foreach $u \in \text{child}(c)$ do
3     call DistributeEvidence($c \to u$)
```

Collect/Distribute Evidence

Algorithm 3: CollectDistributeEvidence

Input: A tree graph $G = (V, E)$
Result: All messages propagated between all pairs of nodes so that we may compute the marginals on all edges $(i, j) \in E(G)$ as shown in Equation 3.6.

```
1 Designate an arbitrary node $r \in V$ as the root.
2 foreach $c \in \text{child}(r)$ do
3     call CollectEvidence($c \to r$)
4 foreach $c \in \text{child}(r)$ do
5     call DistributeEvidence($r \to c$)
```

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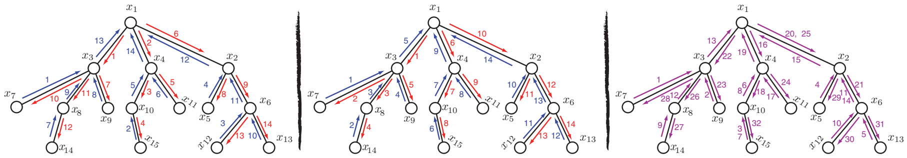
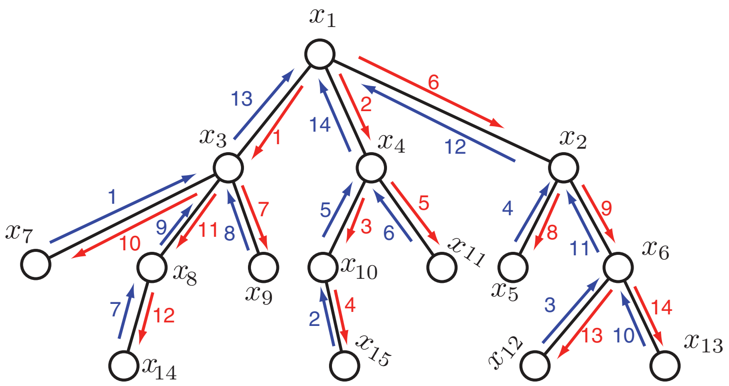
- All messages obey the message passing protocol.
- At the collect evidence stage, a message is not sent to a node's (single) parent until it has received messages from all its children, so there is only one node it has not yet received a message from, namely the parent.
- At the distribute evidence stage, once a node has received a message from its parent, it has received a message from all of its neighbors (since it received a message from all its children earlier, during the collect evidence phase) so it is free to send a message to any child that it likes.

Collect/Distribute Evidence



- Pictures show messages to compute all edge queries.
- Blue arrows indicate messages towards the root (node 1)
- Red arrow indicate messages away from the root.
- The numbers next to each arrow indicate the order of the message.
- Messages abide by MPP? Correspond to collect/distribute evidence?
- We'll next zoom into each one ...

Collect/Distribute Evidence



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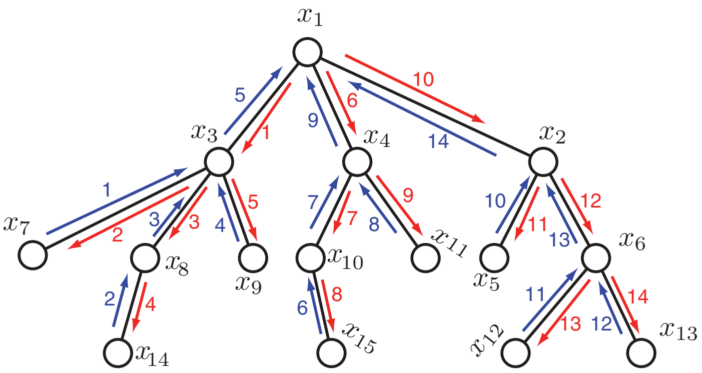

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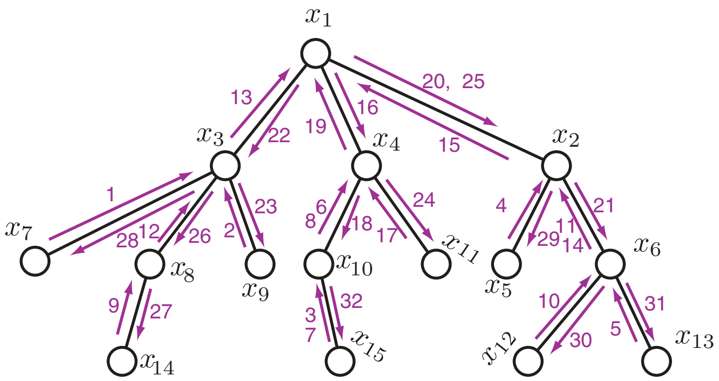

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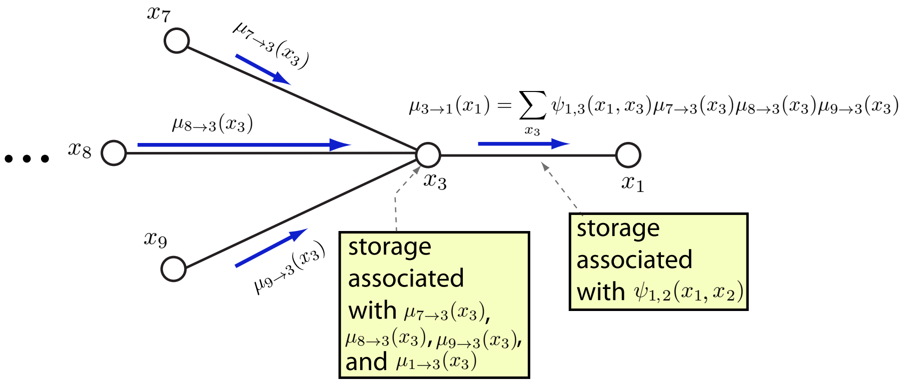
- Collect/Distribute Evidence allows many orders, different roots, different orders too/from the roots, and also parallel implementations.

Associated storage with message propagation


x_7
$\mu_{7\to 3}(x_3)$
$\mu_{8\to 3}(x_3)$
$\cdots$ x_8
x_9
$\mu_{9\to 3}(x_3)$
x_3
x_1
$\mu_{3\to 1}(x_1) = \sum_{x_3} \psi_{1,3}(x_1,x_3)\mu_{7\to 3}(x_3)\mu_{8\to 3}(x_3)\mu_{9\to 3}(x_3)$
storage associated with $\mu_{7\to 3}(x_3)$, $\mu_{8\to 3}(x_3)$, $\mu_{9\to 3}(x_3)$, and $\mu_{1\to 3}(x_3)$
storage associated with $\psi_{1,2}(x_1,x_2)$

- for each edge (i,j), is storage associated with edge itself, $\psi_{i,j}(x_i,x_j)$, and all incoming messages, $\mu_{k\to i}(x_i)$ for all $k \in \delta(i) \setminus \{j\}$.
- $O(|E|(2r + r^2))$ total storage.

Alternative propagation styles

- Alternatively, incorporate in and then forget message as soon as it arrives
- Result of message would be new edge table:

$$\psi'_{i,j}(x_i, x_j) \leftarrow \psi_{i,j}(x_i, x_j)\mu_{k\to i}(x_i) \tag{3.7}$$

- Final factor, *after* incorporating all messages, has value $\psi'_{i,j}(x_i, x_j)$ where:

$$\psi'_{i,j}(x_i, x_j) = \psi_{i,j}(x_i, x_j) \prod_{k\in\delta(i)\setminus\{j\}} \mu_{k\to i}(x_i) \tag{3.8}$$

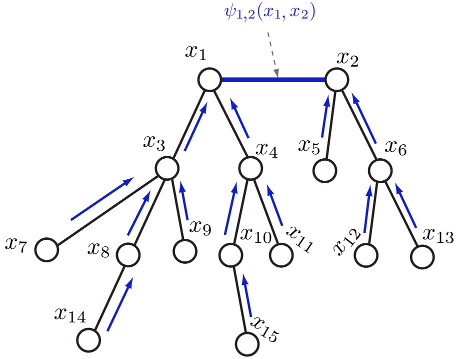
- Outgoing message to j depends only on the edge function, and becomes

$$\mu_{i\to j}(x_j) = \sum_{x_i} \psi'_{i,j}(x_i, x_j). \tag{3.9}$$

- Never require storage at only node i

Alternative propagation styles

- Never require storage at only nodes, only at edges.
- This can be good for certain queries. For example, for computing **just** $p(x_i)$, or $p(x_i, x_j)$ for $(i, j) \in E(G)$, this works out fine.



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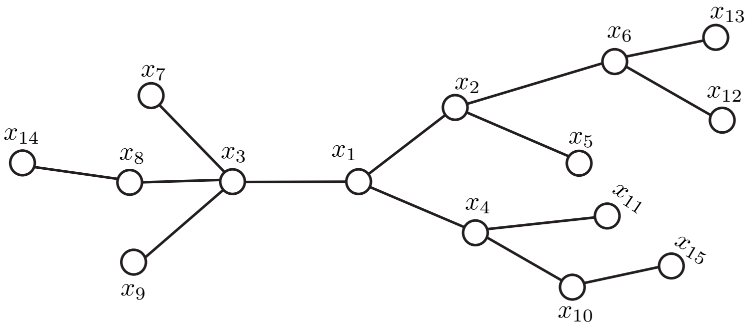

Alternative propagation styles

- Intuitively, we want to avoid double-counting the information sent from i to j, when a message is sent from j back to i — i (and the subtree rooted at i when the (i, j) edge is severed) already has that information, it doesn't need it again.

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- Mathematically, from the elimination perspective, this would be equivalent to squaring the marginal functions after they have been constructed (i.e., ϕ^2 rather than ϕ).
- $\therefore$ need somehow to divide out first set of messages before sending back, but can't do that if lost that info.

Alternative propagation styles

- Solution 1: divide out the outgoing message from an edge as soon as it is ready, when it comes back it is multiplied back in and counted one time.
- During the first phase of message passing (e.g., collect evidence) we re-define our message definition as follows:

Algorithm 4: First phase message update $\mu_{i\to j}(x_j)$

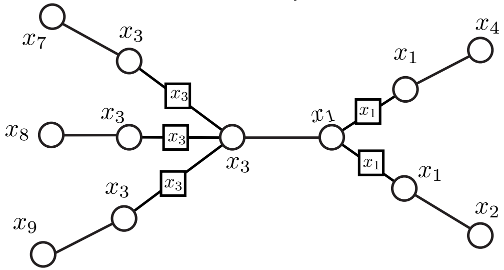
```
1 $\mu_{i\to j}(x_j) = \sum_{x_i} \psi_{i,j}(x_i, x_j) \prod_{k\in\delta(i)\setminus\{j\}} \mu_{k\to i}(x_i)$ ; /* message as normal */
2 $\psi'_{i,j}(x_i, x_j) \leftarrow \psi_{i,j}(x_i, x_j)/\mu_{i\to j}(x_j)$ ; /* table update - divide outgoing message out */
3 if $j$ is not the root then
4     Let $k \in \delta(j)$ be the neighbor of $j$ towards the root ;
5     $\psi'_{j,k}(x_j, x_k) \leftarrow \psi_{j,k}(x_j, x_k)\mu_{i\to j}(x_j)$ ; /* table update - multiply in incoming message */
```

Alternative propagation styles

- By dividing out $\mu_{i \to j}(x_j)$ from $\psi_{i,j}(x_i, x_j)$, we are sure that the $\mu_{i \to j}(x_j)$ will not be double counted once it is multiplied back in from the message coming back from k in $\mu_{k \to j}(x_j)$.
- when root has received all messages, start propagating messages towards leaves using standard message definition.
- No longer valid to send multiple messages along an edge in same direction
- new scheme is asymmetric, different message definitions during the collect vs. the distribute evidence phase of message passing.

Alternative propagation styles

- Solution 2: maintain distinct node separator functions



- every pair of edges that shares a common node has an extra node potential (shown as a square node) corresponding to that common node.
- common node separates tree into two separate sub-trees.
- edge $(7,3)$ and $(3,1)$ share the common node 3 and so there is a distinct square x_3 node corresponding to the edge pair $((7,3),(3,1))$ and separator potential function $\phi_{7,3,1}(x_3)$.

Alternative propagation styles

- Use only two extra tables per separator (square) node $i \in V$, which store incoming messages at i
- The two tables $\phi^n_{ijk}(x_j)$ (new) and $\phi^p_{ijk}(x_j)$ (previous) at each separator node, which keeps track of incoming messages.
- At start, initialize both tables to unity $\phi^n_{ijk}(x_j) = 1$, $\phi^p_{ijk}(x_j) = 1$ $\forall x_j \in \mathsf{D}_{X_j}$.
- Always update "new" table and divide out previous. Once "new" is used, it becomes "previous".
- we follow the collect/distribute evidence schedule for sending messages

Alternative propagation styles

Algorithm 5: collect evidence message update $\mu_{i\to j}(x_j)$

```
1 $\phi^n_{i,j,k}(x_j) = \sum_{x_i} \psi_{i,j}(x_i, x_j)$ ; /* message as normal stored in node */
2 $\psi_{j,k}(x_j, x_k) \leftarrow \psi_{j,k}(x_j, x_k)\frac{\phi^n_{i,j,k}(x_j)}{\phi^p_{i,j,k}(x_j)}$ ; /* update $(j,k)$ edge potential. */
```

- At this point, step 2 same as $\psi_{j,k}(x_j, x_k) \leftarrow \psi_{j,k}(x_j, x_k)\phi^n_{i,j,k}(x_j)$
- we must ensure that there is no double counting of $\phi_{i,j,k}(x_j)$ when we do the distribute evidence phase, which is given in the next messages for the distribute evidence phase of the algorithm.

Alternative propagation styles

Algorithm 6: distribute evidence message update $\mu_{i \to j}(x_j)$

```
1 $\phi^n_{i,j,k}(x_j) = \sum_{x_i} \psi_{i,j}(x_i, x_j)$ ;   /* message as normal stored in node */
2 $\psi_{j,k}(x_j, x_k) \leftarrow \psi_{j,k}(x_j, x_k) \frac{\phi^n_{i,j,k}(x_j)}{\phi^p_{i,j,k}(x_j)}$ ;   /* update $(j,k)$ edge potential. */
```

- Line 2 is where the double counting is avoided, divide out the previous separator potential table when we update the (j, k) edge function.
- General principle: at destination, multiply in new, and divide out old.
- uniform message style, and can once again send multiple messages along an edge if we want. ☺
- If divide same cost as multiply, less compute than previous style. ☺
- On the other hand, once again more storage, even more than originally!! ☹

Alternative propagation styles

Algorithm 7: collect evidence message update $\mu_{i\to j}(x_j)$

```
1 $\phi_{i,j,k}(x_j) = \sum_{x_i} \psi_{i,j}(x_i, x_j)$ ; /* message as normal stored in node */
2 $\psi_{j,k}(x_j, x_k) \leftarrow \psi_{j,k}(x_j, x_k)\phi_{i,j,k}(x_j)$ ; /* update $(j,k)$ edge potential. */
```

Algorithm 8: asymmetric distribute evidence message update $\mu_{i\to j}(x_j)$

```
1 foreach $x_j \in \mathsf{D}_{X_j}$ do
2     $\phi_{i,j,k}(x_j) \leftarrow \frac{1}{\phi_{i,j,k}(x_j)} \sum_{x_i} \psi_{i,j}(x_i, x_j)$ ; /* message as normal stored in node */
3     $\psi_{j,k}(x_j, x_k) \leftarrow \psi_{j,k}(x_j, x_k)\phi_{i,j,k}(x_j)$ ; /* update $(j,k)$ edge potential. */
```

- One table per separator.
- Recovered some storage ☺ but lost uniformity ☹ and multiple message sends ☹.

Three propagation styles

- The three different message styles we have described are called, respectively, the Shenoy-Shafer, the Lauritzen-Speigelhalter, and the Hugin message passing strategies.
- Normally given w.r.t. a junction tree (which we have not yet defined)
- Style of message can have practical consequences in an implementation.

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- Ex: 4-node Markov chain: $G = x_1 — x_2 — x_3 — x_4$ with $p(x_1, x_2, x_3, x_4) \in \mathcal{F}(G, \mathcal{M}^{(\mathsf{f})})$, goal is $p(x_1, x_2, x_3)$
- We eliminate x_4 in

$$\sum_{x_4} \psi_{1,2}(x_1, x_2)\psi_{2,3}(x_2, x_3)\psi_{3,4}(x_3, x_4) \tag{3.10}$$

Tree queries with arbitrary S

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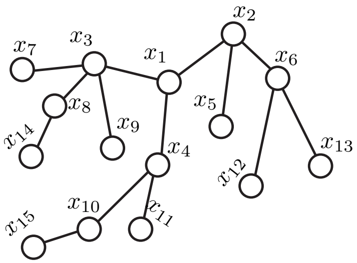
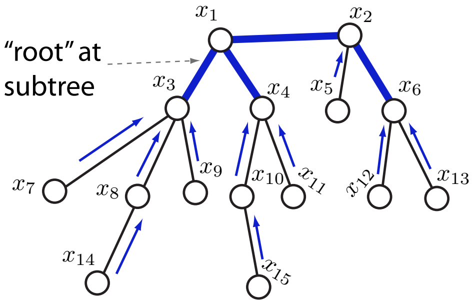
- $O(r^2)$ computation.
- General property: if S is a sub-tree in $G = (V, E)$ then can do the trick above, resulting $p(x_S)$ can be obtained by "rooting" the tree at the subtree S, and still have $O(r^2)$ computation.

Tree queries with arbitrary S





- Above, $S = \{1, 2, 3, 4, 6\}$ which induces a sub-tree in G, so all messages sent towards nearest node inside of S.
- Once we have $p(x_S)$ we have efficient representation for it, using only r^2 tables.

Tree queries with arbitrary S

- what if S is not a sub-tree?
- Ex: 3-node Markov chain: $G = x_1 — x_2 — x_3$ with $p(x_1, x_2, x_3) \in \mathcal{F}(G, \mathcal{M}^{(\mathrm{f})})$, goal is $p(x_1, x_3)$
- Only choice is to eliminate x_2 in

$$\sum_{x_2} \psi_{1,2}(x_1, x_2)\psi_{2,3}(x_2, x_3) \tag{3.11}$$

- $O(r^3)$ computation.
- fill-in edge has occurred (might as well have started with larger family with additional edge $x_1 — x_3$.

Tree queries with arbitrary S

- We eliminate $x_{V \setminus S}$, which might introduce edges.
- Let $\sigma = (\sigma_1, \sigma_2, \ldots, \sigma_N)$ be an ordering of the nodes. Also $\sigma^{-1}(v)$ for $v \in V(G)$ gives number that node v is eliminated by order σ. We have following theorem

Theorem 3.4.1

Let $G = (V, E)$ be an undirected graph with a given elimination ordering σ that maps G to $G' = (V, E')$ where $E' = E \cup F_\sigma$, and where F_σ are the fill-in edges added during elimination with order σ. Then $(v, w) \in E'$ is an edge in G' **iff** *there is a path in G with endpoints v and w, and where any nodes on the path other than v and w are eliminated before v and w in order σ. I.e., if there is a path $(v = v_1, v_2, \ldots, v_{k+1} = w)$ in G such that*

$$\sigma^{-1}(v_i) < \min(\sigma^{-1}(v), \sigma^{-1}(w)), \text{ for } 2 \leq i \leq k \tag{3.12}$$

Tree queries with arbitrary S

Proof.

First part: Induction on $\ell = \min(\sigma^{-1}(v), \sigma^{-1}(w))$ that given any $(v, w) \in G'$ the equation holds. If $\ell = 1$ then $(v, w) \in E$ and $(v, w) \in E'$. Suppose holds for $\ell \leq \ell_0$ and consider $\ell = \ell_0 + 1$. If $(v, w) \in E$ then the equation holds. Otherwise, $(v, w) \in F_\sigma$, and by definition, we have an $x \in V$ with $\sigma^{-1}(x) \leq \min(\sigma^{-1}(v), \sigma^{-1}(w))$ and x—v, x—w in G'. Induction hypothesis implies existence of x, v and x, w paths in G satisfying the equation, combining these chains gives the required v, w path.

Converse: Induction on k, length of path. If $k = 1$ clearly $(v, w) \in E'$. Suppose holds for $k \leq k_0$ and consider $k = k_0 + 1$. From path $(v = v_1, v_2, \ldots, v_{k+1} = w)$, choose $x = v_i$ where $\sigma^{-1}(v_i) = \max\left\{\sigma^{-1}(v_j) | 2 \leq j \leq k\right\}$. Induction hypothesis implies v—x and x—w in G'. Therefore v—w in G'. □

Tree queries with arbitrary S

- So if there are $v, w \in S$ that are connected by a path strictly within $V \setminus S$, then v, w will be connected once elimination has run.

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- typical case: somewhere in between, depends on the query.
- Bad news for scientists who want to do exact inference! ☹

Perfect elimination orders

Definition 3.5.1 (perfect elimination order)

Order σ is called perfect for G if when we eliminate nodes in G according to σ, there are zero fill edges in the resulting reconstituted graph.

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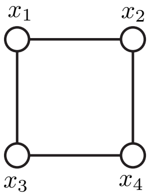
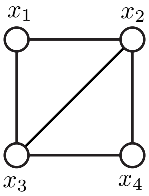
- For a tree, there is always a perfect elimination order. Why? Because there are always leaf nodes available.
- For arbitrary graphs, must there be a perfect elimination order?

Non-tree graphs

- If not tree, might not be a fill-in-free elimination order. Example:



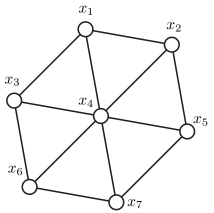


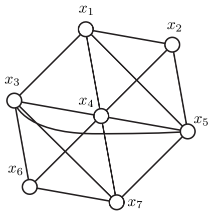
- Any node will produce a fill in. $O(r^3)$ query seems unavoidable.
- There are no leaf nodes, and no node v such that $\delta(v)$ induces a clique in G.
- Might as well have started with graph on the right, no penalty for eliminating x_1 first (but there is for x_2).
- Consider message passing on this graph, could oscillate.

Non-tree graphs

- 4-cycle states both $X_1 \perp\!\!\!\perp X_4 | \{X_2, X_3\}$ and $X_2 \perp\!\!\!\perp X_3 | \{X_1, X_4\}$, while right graph only requires first property.
- extra independence properties of the 4-cycle does not help us computationally.

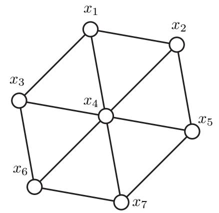
Non-tree graphs

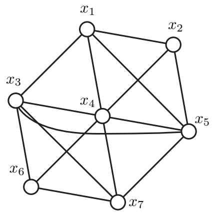




- Left: Eliminating x_4 is bad, but other nodes are better.

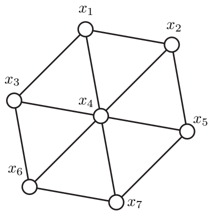
Non-tree graphs

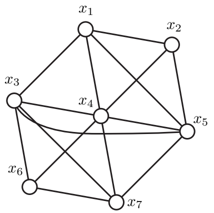




- Left: Eliminating x_4 is bad, but other nodes are better.
- Left: No node results in zero fill in! ☹

Non-tree graphs





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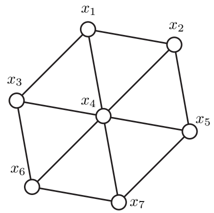
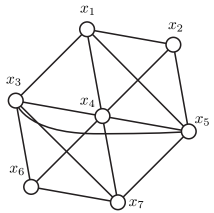
- Right: Is there a perfect elimination order?

Non-tree graphs





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- Right: Is there a perfect elimination order?
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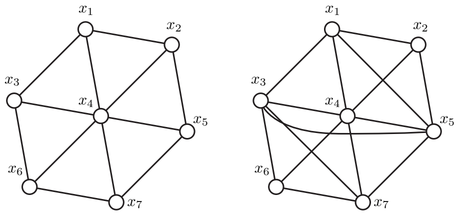
Non-tree graphs



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- Appears to be computational equivalence classes of families of models.

Non-tree graphs

Lemma 3.5.2

The reconstituted graph on which elimination has been run is the family on which we are running inference. If fill-in is caused by elimination, inference is solved on a family larger than that specified by the original graph, and we might as well have started with that family to begin with. If an elimination order produces no fill-in, we are solving the inference query optimally.

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- Also, ordering σ matters. Using σ a second time results in a perfect elimination order.

Non-tree graphs

Lemma 3.5.3

When elimination is run for a second time on the reconstituted graph with the same order, the set of neighbors v at the time v is eliminated is the same in both the original and in the reconstituted graph.

Proof.

Any neighbor of v in the reconstituted graph must be either an original-graph edge, or it must be due to a fill-in edge between v and some other node that is not an original graph neighbor. All of the fill-in neighbors must be due to elimination of nodes before v since after v is eliminated no new neighbors can be added to v. But the point at which v is eliminated at the original graph and the point at which it v is eliminated in the reconstituted graph, the same previous set of nodes have been eliminated, so any neighbors of v in the reconstituted graph will have been already added to the original graph when v is eliminated in the original graph.

Non-tree graphs

Lemma 3.5.4

Given an elimination order, the computational complexity of the elimination process is $O(r^{k+1})$ where k is the largest set of neighbors encountered during elimination. This is the size of the largest clique in the reconstituted graph.

Proof.

First, when we eliminate σ_i in G_{i-1}, eliminating variable v when it is in the context of its current neighbors will cost $O(r^\ell)$ where $\ell = |\delta(v) + 1|$ — thus, the overall cost will be $O(r^{k+1})$.
Next, we show that largest clique in the reconstituted graph is equal to the complexity. Consider the reconstituted graph, and assume its largest clique is of size $k+1$. When we re-run elimination on this graph, there will be no fill in. . . .

Proof cont.

. . . continued.

However, the cost of the elimination step upon reaching the first vertex v of the clique of size $k+1$ will be $O(r^{k+1})$ since k of the variables of the clique will be neighbors of v, but no other nodes will be neighbors since it is a perfect elimination order in the reconstituted graph. This will be the same cost as what was incurred during the initial elimination procedure since v has the same set of neighbors. Therefore, the largest clique in the reconstituted graph is the complexity of doing elimination. □

- This means that any perfect elimination ordering on a perfect-elimination graph will have complexity exponential in the size of the largest clique in that graph.

Non-tree graphs

Summarizing what we've got so far:

- $G' = (V, E \cup F_\sigma)$ always has at least one perfect elimination order

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- $G' = (V, E \cup F_\sigma)$ always has at least one perfect elimination order
- When we run elimination algorithm, we will always end up with such a graph - inevitable
- Perhaps we should deal only with such graphs?
- Is finding the order that minimizes fill-in optimal? (HW problem)
- We can characterize the complexity of a given elimination order.

Sources for Today's Lecture

- Most of this material comes from the reading handout `tree_inference.pdf`