Lecture 14 - Inference, GraphEliminate; sum-product

Thursday, October 26, 2023 2:31 PM

today: inference & graphEliminate
sum-product alg.

<u>graph elimination alg</u> (for inference in generic UGM)

- consider $p \in \mathcal{F}(\mathcal{G})$ (undirected) $\quad p(x) = \frac{1}{Z}\prod_{C \in \mathcal{C}} \psi_C(x_C)$

say want to compute $p(x_F)$ for some $F \subseteq V$ "query nodes"

<u>main trick</u>: use distributivity of $\oplus$ over $\odot$ $\leadsto$ $c \odot (a \oplus b) = c\odot a + c \odot b$

$$\sum_{x_1, x_2} f(x_1) g(x_2) = \left(\sum_{x_1} f(x_1)\right)\left(\sum_{x_2} g(x_2)\right)$$

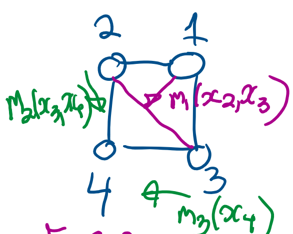
[convince yourself]

more generally

$$\sum_{x_{1:n}} \prod_i f_i(x_i) = \prod_{i=1}^{n}\left(\sum_{x_i} f_i(x_i)\right)$$

$$O(k^n n) \leadsto O(k \cdot n)$$

x_i takes k values



$F = \{4\}$

$$p(x_4) = \frac{1}{Z}\sum_{x_1, x_2, x_3} \psi(x_1, x_2)\psi(x_2, x_4)\psi(x_1, x_3)\psi(x_3, x_4)$$

$$= \frac{1}{Z}\left[\sum_{x_3}\psi(x_3,x_4)\left[\sum_{x_2}\psi(x_2,x_4)\underbrace{\left(\sum_{x_1}\psi(x_1,x_2)\psi(x_1,x_3)\right)}_{m_1(x_2,x_3)}\right]\right]$$

$m_1(x_2, x_3)$ "message"

$$\underbrace{\sum_{x_2}\psi(x_2,x_4)\, m_1(x_2,x_3)}_{\triangleq\, m_2(x_3,x_4)}$$

$$= \frac{1}{Z} m_3(x_4)$$

$\hookrightarrow$ last message is <u>proportional</u> to marginal $p(x_4)$

$$\sum_{x_4} m_3(x_4) = Z$$

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$$\boxed{p(x_4) = \frac{m_3(x_4)}{Z}} \quad = \sum_{x_4'} m_3(x_4')$$

<u>general alg: graph Eliminate</u>

init.: a) choose an elimination ordering s.t. F are the last nodes

b) put all $\psi_c(x_c)$ on "active list"

"update" c) repeat, in order of variables to eliminate

1) (say x_i is variable to eliminate)

remove all factors from active list with x_i in it & take their product

i.e. $\prod_{\substack{\alpha \in \text{s.t.} \\ i \in \alpha}} \psi_\alpha(x_\alpha)$

2) sum over x_i to get a new factor $m_i(x_{S_i})$ (think as $\psi_{S_i}(x_{S_i})$)

i.e. S_i are all variables in these factors except i

get $m_i(x_{S_i}) \triangleq \sum_{x_i} \underbrace{\prod_{\substack{\alpha \text{ s.t.} \\ i \in \alpha}} \psi_\alpha(x_\alpha)}_{\text{new clique to sum over } S_i \cup \{i\}}$

$S_i \triangleq \left(\bigcup_{\substack{\alpha \text{ s.t.} \\ i \in \alpha}} \alpha \right) \setminus \{i\}$

3) put back $m_i(x_{S_i})$ in active list $(\psi_{S_i}(x_{S_i}))$

"normalize": d) last product of factors has only x_F $\Rightarrow$ proportional $p(x_F)$

suppose $x_i \in \{0,1\}$ memory needed? $\approx 2^{\overbrace{\max_i |S_i|}^{\leq |C|}}$ (max size of active list)

computational $= \underbrace{\left(2^{\max_i |S_i| + 1}\right)}_{\text{later, related to "treewidth" of a graph}} \cdot n$

☆ "augmented graph" $\rightarrow$ graph obtained by running graph Eliminate (for specific ordering) + keeping track of all edges added

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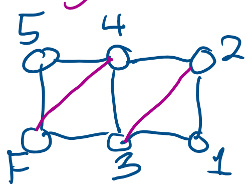
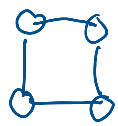
(*) "augmented graph" → graph obtained by running graphEliminate + keeping track of all edges added (for specific ordering)



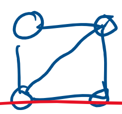
(*) note: augmented graph obtained after graphEliminate is always a triangulated graph

def: graph with no cycle of size 4 or more that cannot be broken by a "chord"

"chord": an edge between two non-neighboring nodes in a cycle



e.g. not triangulated



e.g. Δ-graph

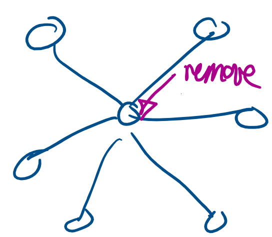
treewidth of a graph $\triangleq$ min over all possible elimination orderings { size of biggest clique in augmented graph − 1 }

→ convention: tree width (tree) = 1

both memory & running time of graphEliminate is dominated by $2^{\text{size of biggest clique}}$

best ordering $\approx$ $2^{\text{tree width}+1}$

not all orderings are good



→

bad news:

a) NP hard to compute treewidth of a general graph (or find best ordering)

b) NP hard to do (exact) inference in general UGM

⟹ approximate methods

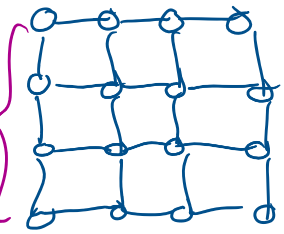
examples:

$\Rightarrow$ approximate methods

example: treewidth of a grid

$\approx \sqrt{|V|}$

side length $\approx$ treewidth



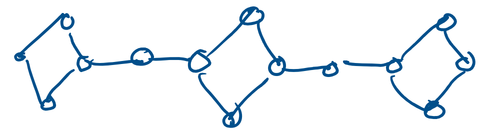
good news:

* inference is linear time for tree (treewidth $=1$) ("sum-product alg.")

  $\hookrightarrow |V| + |E|$ (~~H~~HMM, Markov chain)

* efficient for "small treewidth graph"

  $\rightsquigarrow$ use junction tree alg.



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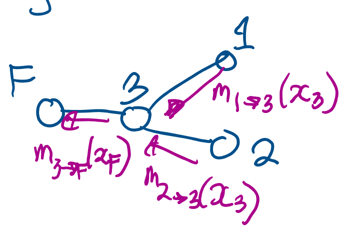
inference on trees

graphEliminate on a tree

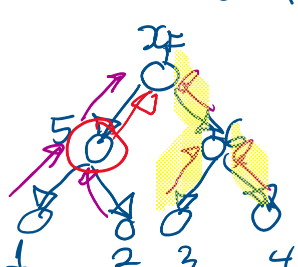
$\rightarrow$ good order is to eliminate leaves first



$$p(x) = \frac{1}{Z} \prod_i \psi_i(x_i) \prod_{\{i,j\}\in E} \psi_{ij}(x_i, x_j)$$

(assuming F is singleton)

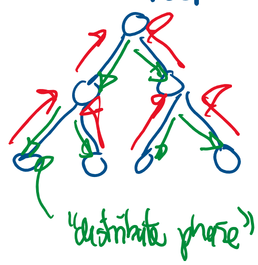
order: make a directed tree by using x_F as a root



$$\boxed{m_{\underset{\text{child}}{i}\to\underset{\text{parent}}{j}}(x_j) = \sum_{x_i} \psi_i(x_i)\psi_{ij}(x_i,x_j) \underbrace{\prod_{k\in \text{children}(i)} m_{k\to i}(x_i)}_{\text{new factors containing } i \text{ in the active list}}}$$

sum-product alg. (for trees)

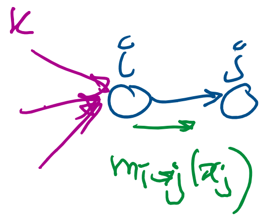
alg. to get all node/edge marginals cheaply by storing (caching) & re-using messages alg. to get all node/edge marginals cheaply by storing (caching) & re-using messages (dynamic programming)



goal: $\{i,j\} \in E$, compute $m_{i\to j}(x_j)$

$m_{j\to i}(x_i)$

rule: i can only send message to neighbor j when it has received all messages from other neighbors



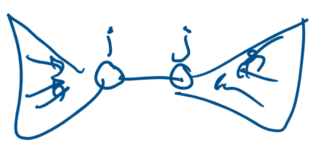
$$\boxed{m_{i\to j}(x_j) = \sum_{x_i} \psi_i(x_i)\,\psi_{ij}(x_i,x_j) \prod_{k\in N(i)\setminus\{j\}} m_{k\to i}(x_i)}$$

at end:

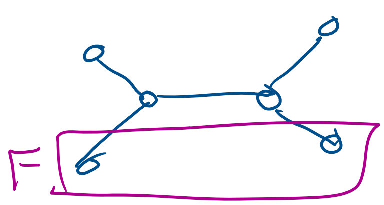
(node marginal) $$p(x_i) \propto \underbrace{\psi_i(x_i) \prod_{j\in N(i)} m_{j\to i}(x_i)}$$

normalize $Z = \sum_{x_i} (\;{''}\;)$

(edge marginal)



$$\boxed{p(x_i,x_j) = \frac{1}{Z}\,\psi_i(x_i)\,\psi_j(x_j)\,\psi_{ij}(x_i,x_j) \cdot \prod_{k\in N(i)\setminus\{j\}} m_{k\to i}(x_i) \cdot \prod_{k'\in N(j)\setminus\{i\}} m_{k'\to j}(x_j)}$$



for this marginal, need to use graph eliminate

sum-product schedules:

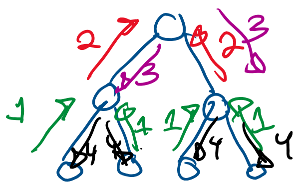
a) above, collect / distribute schedule

b) (flooding) parallel schedule

1) initialize all $m^{0}_{i\to j}(x_j)$ messages to uniform dist $\forall\, (i,j)$ s.t. $\{i,j\} \in E$
(j,i)

2) at every step (in parallel) compute $m^{(new)}_{i\to j}(x_j)$
as if the neighbors were correctly computed

$\rightarrow$ one can prove that after "diameter of tree" # of steps,
all messages are correctly computed (for a tree)
(and are fixed to a fixed point)



loopy belief propagation (loopy BP): approximate inference for graphs with cycles

$$m^{new}_{i\to j}(x_j) = \left(m^{old}_{i\to j}(x_j)\right)^{1-\alpha} \left(\sum_{x_i} \psi_i(x_i)\, \psi_{ij}(x_i, x_j) \prod_{k \in N(i)\setminus\{j\}} m^{old}_{k\to i}(x_i) \right)^{\alpha}$$

$\alpha \in [0,1]$ "damping"
step-size

$\oplus$ this gives exact answer on trees
(fixed pt. $\rightarrow$ yields correct marginals)

$*$ on (not too loopy) graphs $\rightarrow$ "nice" approximate solution