

PGM 2 — Inference

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ML session 10

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 - VE for MAP inference

- 3 Message Passing
 - Sum-product
 - Max-product

Marginal and MAP Queries

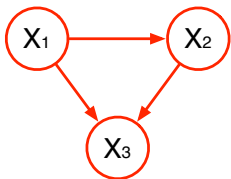
Given joint distribution $P(Y, E)$, where

- Y , query random variable(s), **unknown**
- E , evidence random variable(s), **observed** i.e. $E = e$.

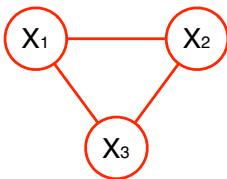
Two types of queries:

- **Marginal** queries (a.k.a. probability queries)
task is to compute $P(Y|E = e)$
- **MAP** queries (a.k.a. most probable explanation)
task is to find $y^* = \operatorname{argmax}_{y \in \text{Val}(Y)} P(Y|E = e)$

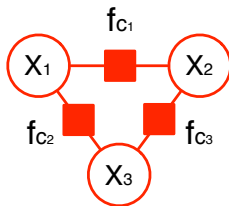
Marginal and MAP Inference



(a) Directed graph



(b) Undirected graph

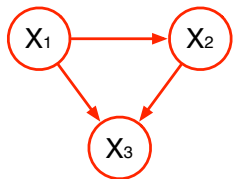


(c) Factor graph

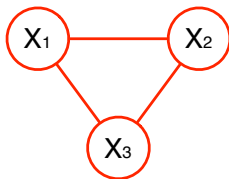
Marginal inference: $P(x_i) = \sum_{x_j: j \neq i} P(x_1, x_2, x_3)$

MAP inference: $(x_1^*, x_2^*, x_3^*) = \operatorname{argmax}_{x_1, x_2, x_3} P(x_1, x_2, x_3)$

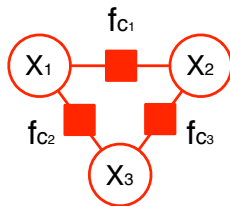
Marginal and MAP Inference



(d) Directed graph



(e) Undirected graph



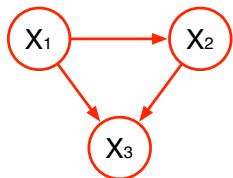
(f) Factor graph

Marginal inference: $P(x_i) = \sum_{x_j: j \neq i} P(x_1, x_2, x_3)$

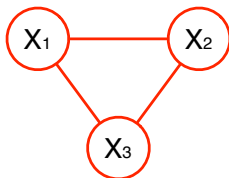
MAP inference: $(x_1^*, x_2^*, x_3^*) = \operatorname{argmax}_{x_1, x_2, x_3} P(x_1, x_2, x_3)$

Warning: $x_i^* \neq \operatorname{argmax} P(x_i)$ in general

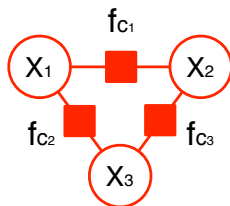
Marginal and MAP Inference



(g) Directed graph



(h) Undirected graph



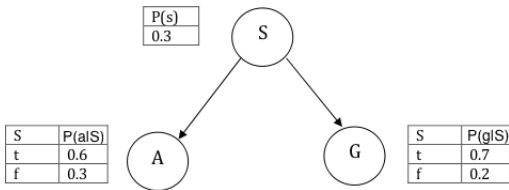
(i) Factor graph

Extends to seeing the evidence E ,

Marginal inference:
$$P(x_i|E) = \sum_{x_j:j \neq i} P(x_1, x_2, x_3|E)$$

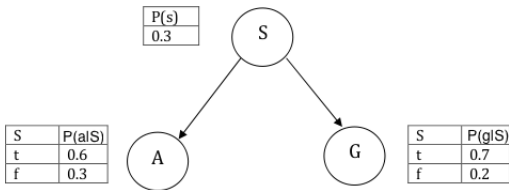
MAP inference:
$$(x_1^*, x_2^*, x_3^*) = \operatorname{argmax}_{x_1, x_2, x_3} P(x_1, x_2, x_3|E)$$

Example of 4WD



- $P(\neg g, a|s)$? (i.e. $P(G = \neg g, A = a|S = s)$)
- $P(S)$?

Example of 4WD



- $P(\neg g, a|s)$? (i.e. $P(G = \neg g, A = a|S = s)$)
- $P(S)$?
- $\operatorname{argmax}_{G,A,S} P(G, A, S)$?

Marginals

- When do we need marginals? Marginals are used to compute
- query for probabilities like in W4D example.

Marginals

When do we need marginals? Marginals are used to compute

- **query for probabilities** like in W4D example.
- **normalisation constant**

$$Z = \sum_{x_i} q(x_i) = \sum_{x_j} q(x_j) \quad \forall i, j = 1, \dots$$

log loss in Conditional Random Fields (CRFs) is

$$-\log P(x_1, \dots, x_n) = \log(Z) + \dots$$

Here $q(x_i)$ is a **belief** (not necessarily a probability) in marginal inference.

Marginals

When do we need marginals? Marginals are used to compute

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- **normalisation constant**

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Here $q(x_i)$ is a **belief** (not necessarily a probability) in marginal inference.

- **expectations** like $\mathbb{E}_{P(x_i)}[\phi(x_i)]$ and $\mathbb{E}_{P(x_i, x_j)}[\phi(x_i, x_j)]$, where $\psi(x_i) = \langle \phi(x_i), w \rangle$ and $\psi(x_i, x_j) = \langle \phi(x_i, x_j), w \rangle$
Gradient of CRFs risk contains above expectations.

MAP

When do we need MAP?

- find the most likely configuration for $(x_i)_{i \in \mathcal{V}}$ in **testing**.

MAP

When do we need MAP?

- find the most likely configuration for $(x_i)_{i \in \mathcal{V}}$ in **testing**.
- find the most violated constraint generated by $(x_i^\dagger)_{i \in \mathcal{V}}$ in **training** (*i.e.* **learning**), *e.g.* by cutting plane method (used in SVM-Struct) or by Bundle method for Risk Minimisation (Teo JMLR2010).

How to infer?

How to infer?

How to infer by hand for Bayesian Networks? (previous lecture).

Problems: hand-tiring for many variables, and it's only for Bayesian Networks.

How to infer?

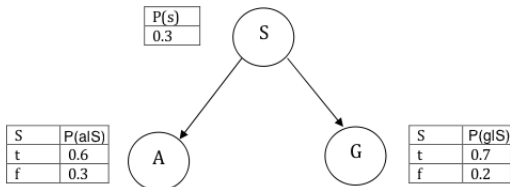
How to infer by hand for Bayesian Networks? (previous lecture).

Problems: hand-tiring for many variables, and it's only for Bayesian Networks.

How to infer for other graphical models and how to do it in a computer program?

Variable elimination

Variable elimination: infer by eliminating variables (works for both marginal and MAP inference)



$$\begin{aligned}
 P(A) &= \sum_{S,G} P(A, S, G) \\
 &= \sum_{S,G} P(S)P(A|S)P(G|S) \\
 &= \sum_S P(S)P(A|S) \left(\sum_G P(G|S) \right) = \sum_S P(S)P(A|S)
 \end{aligned}$$

VE for marginal inference

Step by step:

- 1 sum over missing variables (marginalisation) for the full distribution.

VE for marginal inference

Step by step:

- 1 sum over missing variables (marginalisation) for the full distribution.
- 2 factorise the full distribution.

VE for marginal inference

Step by step:

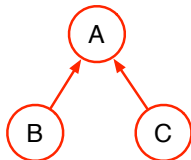
- 1 sum over missing variables (marginalisation) for the full distribution.
- 2 factorise the full distribution.
- 3 rearrange the sum operator to reduce the computation.

VE for marginal inference

Step by step:

- 1 sum over missing variables (marginalisation) for the full distribution.
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- 4 eliminate the variables.

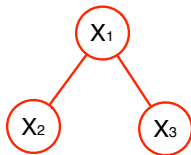
Variable elimination — BayesNets



Marginal inference $P(A)$?

$$\begin{aligned} P(A) &= \sum_{B,C} P(A, B, C) \\ &= \sum_{B,C} P(B)P(C)P(A|B, C) \\ &= \sum_B P(B) \sum_C P(C)P(A|B, C) \\ &= \sum_B P(B)m_1(A, B) \quad (C \text{ eliminated}) \\ &= m_2(A) \quad (B \text{ eliminated}) \end{aligned}$$

Variable elimination — MRFs

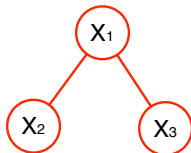


$$P(x_1, x_2, x_3) = \frac{1}{Z} \psi(x_1, x_2) \psi(x_1, x_3) \psi(x_1) \psi(x_2) \psi(x_3)$$

ψ are given. Show example using the document camera.

$$\begin{aligned}
 P(x_1) &= \sum_{x_2, x_3} \frac{1}{Z} \psi(x_1, x_2) \psi(x_1, x_3) \psi(x_1) \psi(x_2) \psi(x_3) \\
 &= \frac{1}{Z} \sum_{x_2, x_3} \psi(x_1, x_2) \psi(x_1, x_3) \psi(x_1) \psi(x_2) \psi(x_3) \\
 &= \frac{1}{Z} \psi(x_1) \sum_{x_2} \left(\psi(x_1, x_2) \psi(x_2) \right) \sum_{x_3} \left(\psi(x_1, x_3) \psi(x_3) \right) \\
 &= \frac{1}{Z} \psi(x_1) m_{2 \rightarrow 1}(x_1) m_{3 \rightarrow 1}(x_1)
 \end{aligned}$$

Variable elimination — MRFs



$$\begin{aligned}
 P(x_2) &= \sum_{x_1, x_3} \frac{1}{Z} \psi(x_1, x_2) \psi(x_1, x_3) \psi(x_1) \psi(x_2) \psi(x_3) \\
 &= \frac{1}{Z} \psi(x_2) \sum_{x_1} \left(\psi(x_1, x_2) \psi(x_1) \sum_{x_3} \left[\psi(x_1, x_3) \psi(x_3) \right] \right) \\
 &= \frac{1}{Z} \psi(x_2) \sum_{x_1} \psi(x_1, x_2) \psi(x_1) m_{3 \rightarrow 1}(x_1) \\
 &= \frac{1}{Z} \psi(x_2) m_{1 \rightarrow 2}(x_2)
 \end{aligned}$$

Variable elimination — factor graphical models

Works too.

Replace the ψ by factors f_1, f_2, \dots

VE for MAP inference

MAP inference:

$$(x_1^*, x_2^*, x_3^*, \dots, x_n^*) = \operatorname{argmax}_{x_1, x_2, x_3, \dots, x_n} P(x_1, x_2, x_3, \dots, x_n)$$

Step by step:

- 1 max over the full distribution.

VE for MAP inference

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Step by step:

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VE for MAP inference

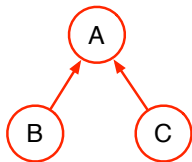
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Step by step:

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- 4 eliminate the variables.

Variable elimination — BayesNets

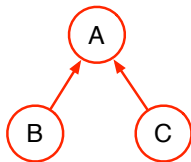


MAP inference $\operatorname{argmax}_{A,B,C} P(A, B, C)$?

$$\begin{aligned}
 \max_{A,B,C} P(A, B, C) &= \max_{A,B,C} P(B)P(C)P(A|B, C) \\
 &= \max_A \left\{ \max_B \left[P(B) \max_C \left(P(C)P(A|B, C) \right) \right] \right\} \\
 &= \max_A \left\{ \max_B \left[P(B)m_1(A, B) \right] \right\} \quad (C \text{ eliminated, record its best assignment}) \\
 &= \max_A m_2(A) \quad (B \text{ eliminated, record its best assignment, and A's best assignment})
 \end{aligned}$$

MAP solution?

Variable elimination — BayesNets



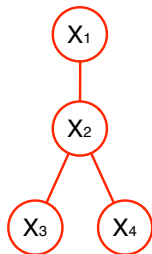
MAP inference $\operatorname{argmax}_{A,B,C} P(A, B, C)$?

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 &= \max_A m_2(A) \quad (B \text{ eliminated, record its best assignment, and } A\text{'s best assignment})
 \end{aligned}$$

MAP solution? $\operatorname{argmax} = A, B, C$'s best assignments.

Variable elimination — MRFs

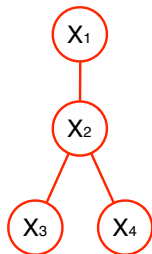
$$\begin{aligned}
 & \max_{x_1, x_2, x_3, x_4} P(x_1, x_2, x_3, x_4) \\
 &= \max_{x_1, x_2, x_3, x_4} \psi(x_1, x_2) \psi(x_2, x_3) \psi(x_2, x_4) \psi(x_1) \psi(x_2) \psi(x_3) \psi(x_4) \\
 &= \max_{x_1, x_2} \left[\dots \max_{x_3} \left(\psi(x_2, x_3) \psi(x_3) \right) \max_{x_4} \left(\psi(x_2, x_4) \psi(x_4) \right) \right] \\
 &= \max_{x_1} \left[\psi(x_1) \max_{x_2} \left(\psi(x_2) \psi(x_1, x_2) m_{3 \rightarrow 2}(x_2) m_{4 \rightarrow 2}(x_2) \right) \right] \\
 &= \max_{x_1} \left(\psi(x_1) m_{2 \rightarrow 1}(x_1) \right)
 \end{aligned}$$



Variable elimination — MRFs

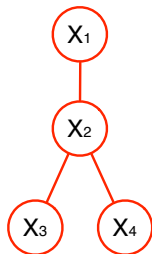
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 &= \max_{x_1, x_2} \left[\dots \max_{x_3} \left(\psi(x_2, x_3) \psi(x_3) \right) \max_{x_4} \left(\psi(x_2, x_4) \psi(x_4) \right) \right] \\
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 \end{aligned}$$

argmax = recorded best assignments.



Variable elimination — MRFs

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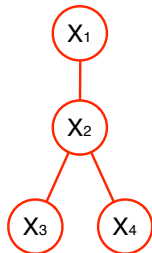
argmax = recorded best assignments.

What if you didn't (or don't want to) record the assignments?

How to get them back?

Variable elimination — MRFs

$$\begin{aligned}
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Hint: $x_1^* = \operatorname{argmax}_{x_1} \left(\psi(x_1) m_{2 \rightarrow 1}(x_1) \right)$

Variable elimination — MRFs

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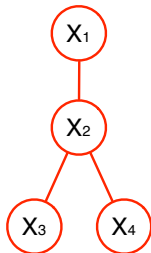
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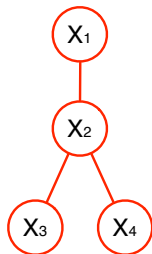
Hint: $x_1^* = \operatorname{argmax}_{x_1} \left(\psi(x_1) m_{2 \rightarrow 1}(x_1) \right)$

x_2^* ?



Variable elimination — MRFs

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argmax = recorded best assignments.

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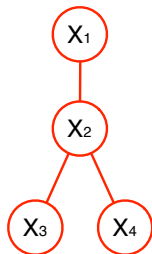
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$x_2^* = \operatorname{argmax}_{x_2} \left(\psi(x_2) \psi(x_1^*, x_2) m_{3 \rightarrow 2}(x_2) m_{4 \rightarrow 2}(x_2) \right)$

$x_3^*, x_4^*?$

Variable elimination — MRFs

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 & \max_{x_1, x_2, x_3, x_4} P(x_1, x_2, x_3, x_4) \\
 &= \max_{x_1, x_2, x_3, x_4} \psi(x_1, x_2) \psi(x_2, x_3) \psi(x_2, x_4) \psi(x_1) \psi(x_2) \psi(x_3) \psi(x_4) \\
 &= \max_{x_1, x_2} \left[\dots \max_{x_3} \left(\psi(x_2, x_3) \psi(x_3) \right) \max_{x_4} \left(\psi(x_2, x_4) \psi(x_4) \right) \right] \\
 &= \max_{x_1} \left[\psi(x_1) \max_{x_2} \left(\psi(x_2) \psi(x_1, x_2) m_{3 \rightarrow 2}(x_2) m_{4 \rightarrow 2}(x_2) \right) \right] \\
 &= \max_{x_1} \left(\psi(x_1) m_{2 \rightarrow 1}(x_1) \right)
 \end{aligned}$$



argmax = recorded best assignments.

What if you didn't (or don't want to) record the assignments?

How to get them back?

Hint: $x_1^* = \operatorname{argmax}_{x_1} \left(\psi(x_1) m_{2 \rightarrow 1}(x_1) \right)$

x_2^* $x_2^* = \operatorname{argmax}_{x_2} \left(\psi(x_2) \psi(x_1^*, x_2) m_{3 \rightarrow 2}(x_2) m_{4 \rightarrow 2}(x_2) \right)$

x_3^*, x_4^* ? $x_3^* = \operatorname{argmax}_{x_3} \left(\psi(x_2^*, x_3) \psi(x_3) \right)$

$x_4^* = \operatorname{argmax}_{x_4} \left(\psi(x_2^*, x_4) \psi(x_4) \right)$

Answer: backtrack the best assignments (in the reversed the elimination order)

Variable elimination — factor graphical models

Works too.

Replace the ψ by factors f_1, f_2, \dots

Message Passing

Reuse the intermediate results (called messages) of VE

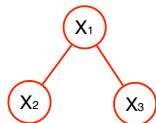
⇒ **Message Passing**:

- VE for marginal inference ⇒ **sum-product** message passing
- VE for MAP inference ⇒ **max-product** message passing

Revisit VE for marginal

$$\text{Assume } P(x_1, x_2, x_3) = \frac{1}{Z} \psi(x_1, x_2) \psi(x_1, x_3) \psi(x_1) \psi(x_2) \psi(x_3)$$

$$\begin{aligned} P(x_1) &= \frac{1}{Z} \psi(x_1) \sum_{x_2} (\psi(x_1, x_2) \psi(x_2)) \sum_{x_3} (\psi(x_1, x_3) \psi(x_3)) \\ &= \frac{1}{Z} \psi(x_1) m_{2 \rightarrow 1}(x_1) m_{3 \rightarrow 1}(x_1) \end{aligned}$$



$$\begin{aligned} P(x_2) &= \frac{1}{Z} \psi(x_2) \sum_{x_1} (\psi(x_1, x_2) \psi(x_1) \sum_{x_3} [\psi(x_1, x_3) \psi(x_3)]) \\ &= \frac{1}{Z} \psi(x_2) \sum_{x_1} \psi(x_1, x_2) \psi(x_1) m_{3 \rightarrow 1}(x_1) \\ &= \frac{1}{Z} \psi(x_2) m_{1 \rightarrow 2}(x_2) \end{aligned}$$

$m_{3 \rightarrow 1}(x_1)$ can be reused instead of computing twice.

Sum-product

Can we compute all messages first, and then use them to compute all marginal distributions?

Sum-product

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Yes, it's called **sum-product**.

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Yes, it's called **sum-product**.

In general,

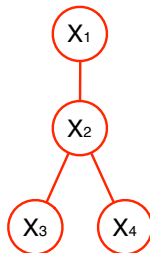
$$P(x_i) = \frac{1}{Z} \left(\psi(x_i) \prod_{j \in Ne(i)} m_{j \rightarrow i}(x_i) \right)$$
$$m_{j \rightarrow i}(x_i) = \sum_{x_j} \left(\psi(x_j) \psi(x_i, x_j) \prod_{k \in Ne(j) \setminus \{i\}} m_{k \rightarrow j}(x_j) \right)$$

$Ne(i)$: neighbouring nodes of i (*i.e.* nodes that connect with i).

Revisit VE for MAP

$$\begin{aligned}
 & \max_{x_1, x_2, x_3, x_4} P(x_1, x_2, x_3, x_4) \\
 &= \max_{x_1, x_2, x_3, x_4} \psi(x_1, x_2)\psi(x_2, x_3)\psi(x_2, x_4)\psi(x_1)\psi(x_2)\psi(x_3)\psi(x_4) \\
 &= \max_{x_1, x_2} \left[\dots \max_{x_3} \left(\psi(x_2, x_3)\psi(x_3) \right) \max_{x_4} \left(\psi(x_2, x_4)\psi(x_4) \right) \right] \\
 &= \max_{x_1} \left[\psi(x_1) \max_{x_2} \left(\psi(x_2)\psi(x_1, x_2)m_{3 \rightarrow 2}(x_2)m_{4 \rightarrow 2}(x_2) \right) \right] \\
 &= \max_{x_1} \left(\psi(x_1)m_{2 \rightarrow 1}(x_1) \right)
 \end{aligned}$$

$$\begin{aligned}
 x_1^* &= \operatorname{argmax}_{x_1} \left(\psi(x_1)m_{2 \rightarrow 1}(x_1) \right) \\
 x_2^* &= \operatorname{argmax}_{x_2} \left(\psi(x_2)\psi(x_1^*, x_2)m_{3 \rightarrow 2}(x_2)m_{4 \rightarrow 2}(x_2) \right) \\
 x_3^* &= \operatorname{argmax}_{x_3} \left(\psi(x_2^*, x_3)\psi(x_3) \right) \\
 x_4^* &= \operatorname{argmax}_{x_4} \left(\psi(x_2^*, x_4)\psi(x_4) \right)
 \end{aligned}$$



Max-product

Variable elimination for MAP \Rightarrow Max-product:

$$x_i^* = \operatorname{argmax}_{x_i} \left(\psi(x_i) \prod_{j \in \text{Ne}(i)} m_{j \rightarrow i}(x_i) \right)$$

$$m_{j \rightarrow i}(x_i) = \max_{x_j} \left(\psi(x_j) \psi(x_i, x_j) \prod_{k \in \text{Ne}(j) \setminus \{i\}} m_{k \rightarrow j}(x_j) \right)$$

$\text{Ne}(i)$: neighbouring nodes of i (i.e. nodes that connect with i).

$\text{Ne}(j) \setminus \{i\} = \emptyset$ if j has only one edge connecting it. e.g. x_1, x_3, x_4 .

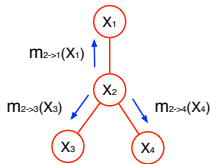
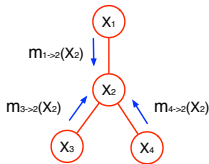
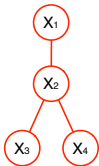
For such node j ,

$$m_{j \rightarrow i}(x_i) = \max_{x_j} \left(\psi(x_j) \psi(x_i, x_j) \right)$$

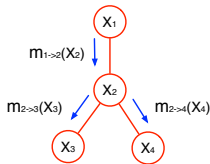
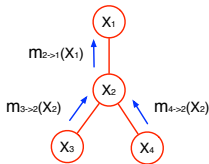
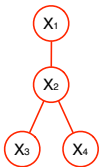
Easier computation!

Max-product

Order matters: message $m_{2 \rightarrow 3}(x_3)$ requires $m_{1 \rightarrow 2}(x_2)$ and $m_{4 \rightarrow 2}(x_2)$.



Alternatively, leaves to root, and root to leaves.



Extension

To avoid over/under flow, often operate in the **log space**.

Max/sum-product is also known as **Message Passing** and **Belief Propagation** (BP).

In graphs with loops, running BP for several iterations is known as **Loopy BP** (neither convergence nor optimal guarantee in general).

Extend to Junction Tree Algorithm (exact, but expensive) and Clusters-based BP.

That's all

Thanks!