Lecture 8: PGM — Inference

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Intro. to Stats. Machine Learning
COMP SCI 4401/7401

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Marginal and MAP Queries

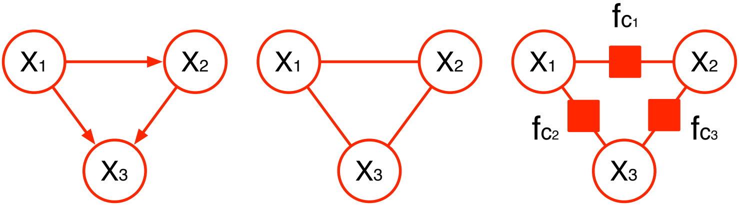
Given joint distribution $P(Y, E)$, where

- 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 $y^* = \mathrm{argmax}_{y \in Val(Y)} P(Y|E = e)$

Marginal and MAP Inference

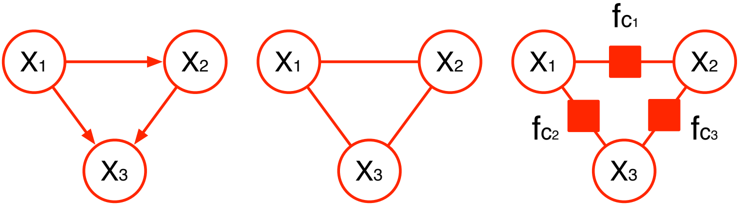


(a) Directed graph (b) Undirected graph (c) Factor graph

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

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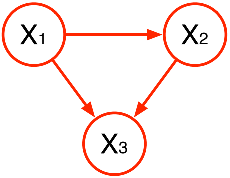
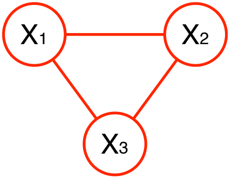
Warning: $x_i^* \neq \operatorname*{argmax}_{x_i} P(x_i)$ in general

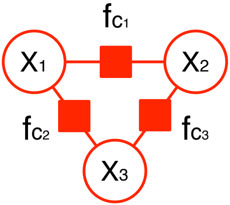
Marginal and MAP Inference



(g) Directed graph



(h) Undirected graph



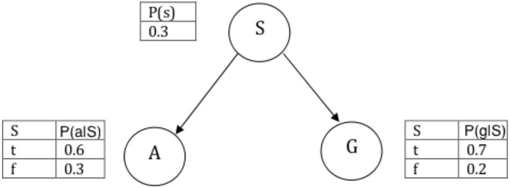
(i) Factor graph

Extends to seeing the evidence E,

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

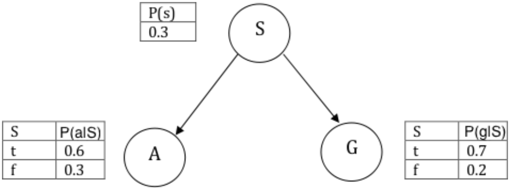
MAP inference: $(x_1^*, x_2^*, x_3^*) = \operatorname{argmax}_{x_1, x_2, x_3} P(x_1, x_2, x_3|E)$

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

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- query for probabilities like in W4D example.
- normalisation constant
  $Z = \sum_{x_i} q(x_i) = \sum_{x_j} q(x_j) \quad \forall i, j = 1, \ldots.$
  log loss in Conditional Random Fields (CRFs) is
  $-\log P(x_1, \ldots, x_n) = \log(Z) + \ldots.$
  Here $q(x_i)$ is a belief (not necessarily a probability) in marginal inference.

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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?

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

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

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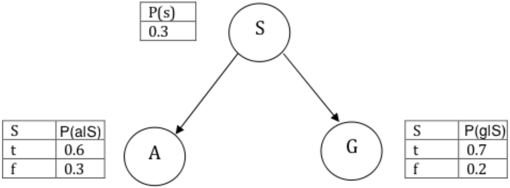
How to infer by hand for Bayesian Networks? (previous lecture).

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)



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

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.

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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.
2. factorise the full distribution.
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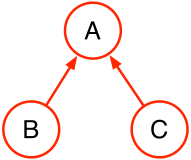
4. eliminate the variables.

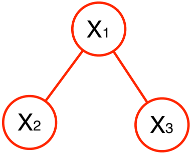
Variable elimination — BayesNets



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

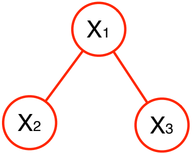


$$P(x_1, x_2, x_3) = \frac{1}{Z}\psi(x_1, x_2)\psi(x_1, x_3)\psi(x_1)\psi(x_2)\psi(x_3)$$

ψ are given. Show example using the document camera.

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

Variable elimination — MRFs



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

Variable elimination — factor graphical models

Works too.
Replace the ψ by factors $f_1, f_2, \ldots$

Break

Take a break ...

VE for MAP inference

MAP inference:

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

Step by step:

1. max over the full distribution.

VE for MAP inference

MAP inference:

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

Step by step:

1. max over the full distribution.
2. factorise the full distribution.

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MAP inference:

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Step by step:

1. max over the full distribution.
2. factorise the full distribution.
3. rearrange the max operator to reduce the computation.

VE for MAP inference

MAP inference:

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

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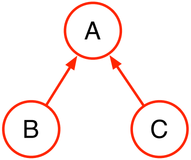
Variable elimination — BayesNets

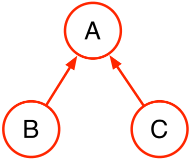


MAP inference $\mathrm{argmax}_{A,B,C}\, P(A, B, C)$?

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

MAP solution?

Variable elimination — BayesNets



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

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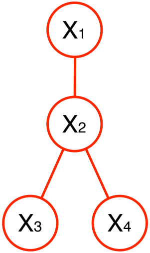
\max_{A,B,C} P(A,B,C) &= \max_{A,B,C} P(B)P(C)P(A|B,C) \\
&= \max_{A} \left\{ \max_{B} \left[P(B) \max_{C} \Big(P(C)P(A|B,C) \Big) \right] \right\} \\
&= \max_{A} \left\{ \max_{B} \left[P(B) m_1(A,B) \right] \right\} \quad (C \text{ eliminated, record its best assignment}) \\
&= \max_{A} m_2(A) \quad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

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

Variable elimination — MRFs

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



Variable elimination — MRFs

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\begin{aligned}
&\max_{x_1,x_2,x_3,x_4} P(x_1,x_2,x_3,x_4)\\
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&= \max_{x_1,x_2} \left[\ldots \max_{x_3}\Big(\psi(x_2,x_3)\psi(x_3)\Big) \max_{x_4}\Big(\psi(x_2,x_4)\psi(x_4)\Big)\right]\\
&= \max_{x_1}\left[\psi(x_1)\max_{x_2}\Big(\psi(x_2)\psi(x_1,x_2)m_{3\to 2}(x_2)m_{4\to 2}(x_2)\Big)\right]\\
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\end{aligned}
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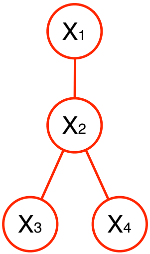
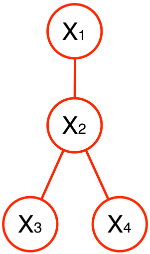


argmax = recorded best assignments.

Variable elimination — MRFs

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



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}
&\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)\\
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\end{aligned}
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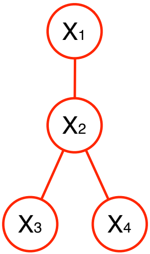

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How to get them back?
Hint: $x_1^* = \mathrm{argmax}_{x_1}\Big(\psi(x_1)m_{2\to 1}(x_1)\Big)$

Variable elimination — MRFs

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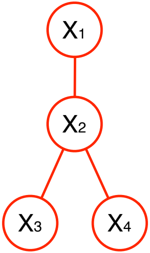

argmax = recorded best assignments.
What if you didn't (or don't want to) record the assignments?
How to get them back?

Hint: $x_1^* = \mathrm{argmax}_{x_1}\Big(\psi(x_1)m_{2\to 1}(x_1)\Big)$

x_2^*?

Variable elimination — MRFs

$$\max_{x_1,x_2,x_3,x_4} P(x_1,x_2,x_3,x_4)$$
$$= \max_{x_1,x_2,x_3,x_4} \psi(x_1,x_2)\psi(x_2,x_3)\psi(x_2,x_4)\psi(x_1)\psi(x_2)\psi(x_3)\psi(x_4)$$
$$= \max_{x_1,x_2}\left[\ldots \max_{x_3}\Big(\psi(x_2,x_3)\psi(x_3)\Big)\max_{x_4}\Big(\psi(x_2,x_4)\psi(x_4)\Big)\right]$$
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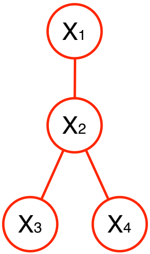
$$= \max_{x_1}\Big(\psi(x_1)m_{2\to 1}(x_1)\Big)$$



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Hint: $x_1^* = \mathrm{argmax}_{x_1}\Big(\psi(x_1)m_{2\to 1}(x_1)\Big)$
x_2^*? $\quad x_2^* = \mathrm{argmax}_{x_2}\Big(\psi(x_2)\psi(x_1^*,x_2)m_{3\to 2}(x_2)m_{4\to 2}(x_2)\Big)$
x_3^*, x_4^*?

Variable elimination — MRFs

$$
\begin{aligned}
&\max_{x_1,x_2,x_3,x_4} P(x_1,x_2,x_3,x_4)\\
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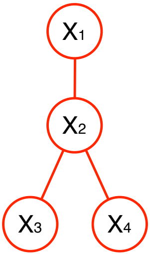

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What if you didn't (or don't want to) record the assignments?
How to get them back?

Hint: $x_1^* = \mathrm{argmax}_{x_1}\Big(\psi(x_1)m_{2\to 1}(x_1)\Big)$

x_2^*? $\quad x_2^* = \mathrm{argmax}_{x_2}\Big(\psi(x_2)\psi(x_1^*,x_2)m_{3\to 2}(x_2)m_{4\to 2}(x_2)\Big)$

x_3^*, x_4^*? $\quad x_3^* = \mathrm{argmax}_{x_3}\Big(\psi(x_2^*,x_3)\psi(x_3)\Big)$

$x_4^* = \mathrm{argmax}_{x_4}\Big(\psi(x_2^*,x_4)\psi(x_4)\Big)$

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

Variable elimination — factor graphical models

Works too.

Replace the ψ by factors $f_1, f_2, \ldots$

Message Passing

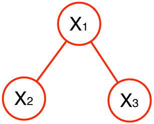
Reuse the intermediate results (called messages) of VE
$\Rightarrow$ Message Passing:

- VE for marginal inference $\Rightarrow$ sum-product message passing
- VE for MAP inference $\Rightarrow$ max-product message passing

Revisit VE for marginal

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

$$\begin{aligned} P(x_1) &= \frac{1}{Z}\psi(x_1)\sum_{x_2}\Big(\psi(x_1, x_2)\psi(x_2)\Big)\sum_{x_3}\Big(\psi(x_1, x_3)\psi(x_3)\Big) \\ &= \frac{1}{Z}\psi(x_1)m_{2\to1}(x_1){\color{blue}m_{3\to1}(x_1)} \end{aligned}$$



$$\begin{aligned} P(x_2) &= \frac{1}{Z}\psi(x_2)\sum_{x_1}\Big(\psi(x_1, x_2)\psi(x_1)\sum_{x_3}\Big[\psi(x_1, x_3)\psi(x_3)\Big]\Big) \\ &= \frac{1}{Z}\psi(x_2)\sum_{x_1}\psi(x_1, x_2)\psi(x_1){\color{blue}m_{3\to1}(x_1)} \\ &= \frac{1}{Z}\psi(x_2)m_{1\to2}(x_2) \end{aligned}$$

$m_{3\to1}(x_1)$ can be reused instead of computing twice.

Sum-product

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

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In general,

$$P(x_i) = \frac{1}{Z}\Big(\psi(x_i) \prod_{j \in Ne(i)} m_{j\to i}(x_i)\Big)$$

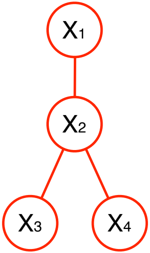
$$m_{j\to i}(x_i) = \sum_{x_j} \Big(\psi(x_j)\psi(x_i, x_j) \prod_{k \in Ne(j)\backslash\{i\}} m_{k\to j}(x_j)\Big)$$

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

Revisit VE for MAP

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

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



Max-product

Variable elimination for MAP $\Rightarrow$ Max-product:

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

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

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

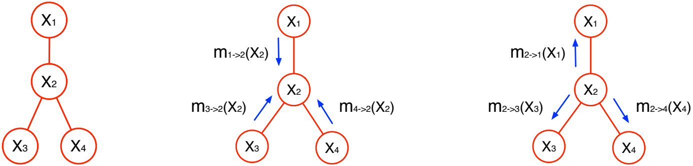
$Ne(j) \setminus \{i\} = \emptyset$ if j has only one edge connecting it. *e.g.* x_1, x_3, x_4. For such node j,

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

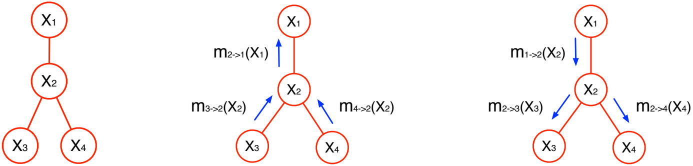
Easier computation!

Max-product

Order matters: message $m_{2\to3}(x_3)$ requires $m_{1\to2}(x_2)$ and $m_{4\to2}(x_2)$.



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!