Exact Inference

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Recap

$$p(\mathbf{x}|\mathbf{y}_o) = \frac{\sum_{\mathbf{z}} p(\mathbf{x},\mathbf{y}_o,\mathbf{z})}{\sum_{\mathbf{x},\mathbf{z}} p(\mathbf{x},\mathbf{y}_o,\mathbf{z})}$$

Assume that $\mathbf{x}, \mathbf{y}, \mathbf{z}$ each are $d = 500$ dimensional, and that each element of the vectors can take $K = 10$ values.

- Issue 1: To specify $p(\mathbf{x}, \mathbf{y}, \mathbf{z})$, we need to specify $K^{3d} - 1 = 10^{1500} - 1$ non-negative numbers, which is impossible.

  Topic 1: Representation What reasonably weak assumptions can we make to efficiently represent $p(\mathbf{x}, \mathbf{y}, \mathbf{z})$?
- Directed and undirected graphical models
- Factorisation and independencies

Recap

$p(\mathbf{x}|\mathbf{y}_o) = \frac{\sum_{\mathbf{z}} p(\mathbf{x},\mathbf{y}_o,\mathbf{z})}{\sum_{\mathbf{x},\mathbf{z}} p(\mathbf{x},\mathbf{y}_o,\mathbf{z})}$

- Issue 2: The sum in the numerator goes over the order of $K^d = 10^{500}$ non-negative numbers and the sum in the denominator over the order of $K^{2d} = 10^{1000}$, which is impossible to compute.

  Topic 2: Exact inference Can we further exploit the assumptions on $p(\mathbf{x}, \mathbf{y}, \mathbf{z})$ to efficiently compute the posterior probability or derived quantities?
- Note: we do not want to introduce new assumptions but exploit those that we made to deal with issue 1.
- Quantities of interest:
  - $p(\mathbf{x}|\mathbf{y}_o)$ (marginal inference)
  - $\mathrm{argmax}_{\mathbf{x}}\, p(\mathbf{x}|\mathbf{y}_o)$ (inference of most probable states)
  - $\mathbb{E}\left[g(\mathbf{x}) \mid \mathbf{y}_o\right]$ for some function g (posterior expectations)

Assumptions

Unless otherwise mentioned, we here assume discrete valued random variables whose joint pmf is a Gibbs distribution factorising as

$$p(x_1, \dots, x_d) \propto \prod_{i=1}^{m} \phi_i(\mathcal{X}_i),$$

with $\mathcal{X}_i \subseteq \{x_1, \dots, x_d\}$ and $x_i \in \{1, \dots, K\}$.

Note:

- Includes case where (some of) the ϕ_i are conditionals
- The x_i could be categorical taking on maximally K different values.

Program

1. Factor graphs
2. Marginal inference by variable elimination
3. Marginal inference for factor trees (sum-product algorithm)
4. Inference of most probable states for factor trees

Program

1. Factor graphs
   - Definition
   - Visualising Gibbs distributions as factor graphs
   - Factor graphs represent factorisations better than undirected graphs
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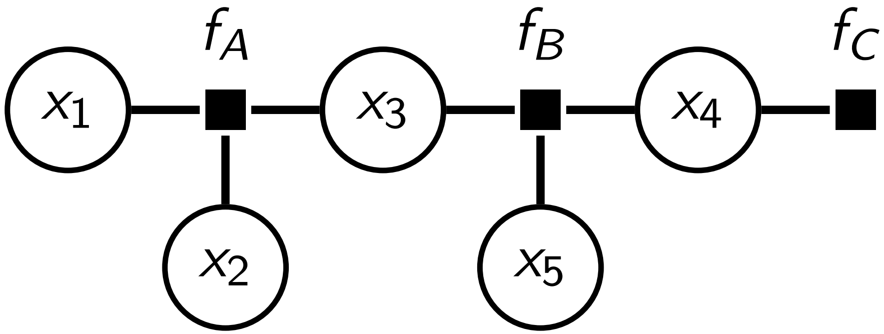
Definition of factor graphs

- A factor graph represents the factorisation of an arbitrary function (not necessarily related to pdfs/pmfs)
- Example: $h(x_1, \ldots, x_5) = f_A(x_1, x_2, x_3) f_B(x_3, x_4, x_5) f_C(x_4)$

  Factor graph (FG):



- Two types of nodes: factor and variable nodes
- Convention: squares for factors, circles for variables (other conventions are used too)

Definition of factor graphs

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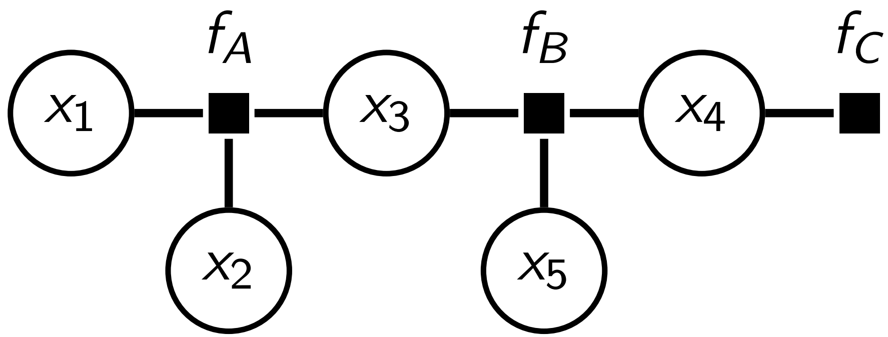
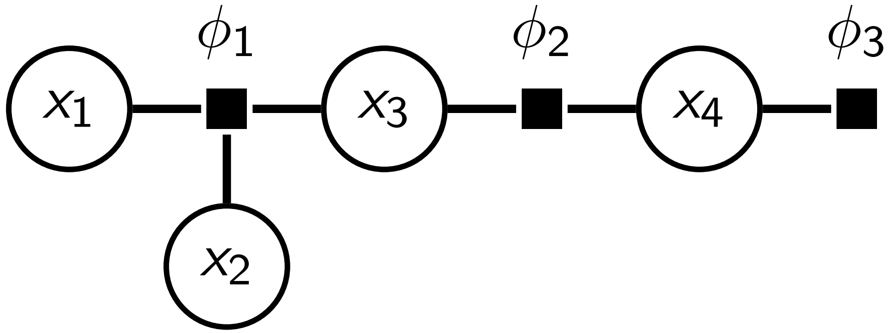
  Factor graph (FG):



- Edge between variable x and factor f $\Leftrightarrow$ x is an argument of f
- Variable nodes are always connected to factor nodes; no direct links between factor or variable nodes (FGs are bipartite graphs)
- FGs can have directed edges to indicate conditionals (not needed here).

Visualising Gibbs distributions as factor graphs

- Example: $p(x_1, x_2, x_3, x_4) = \frac{1}{Z}\phi_1(x_1, x_2, x_3)\phi_2(x_3, x_4)\phi_3(x_4)$



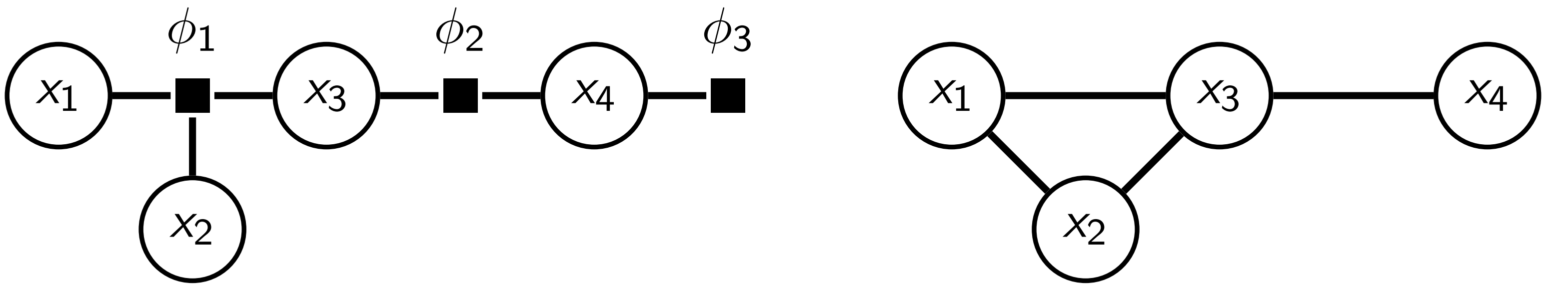
- General case: $p(x_1, \ldots, x_d) \propto \prod_c \phi_c(\mathcal{X}_c)$
  - Factor node for all ϕ_c
  - For all factors ϕ_c:
    draw an undirected edge between ϕ_c and all $x_i \in \mathcal{X}_c$.
- Can visualise any undirected graphical model as a factor graph.

Differences to undirected graphs

Some differences to visualising Gibbs distributions with undirected graph:

- Factors ϕ_c are shown, which makes the graphs more informative (see next slide).
- Variables x_i are neighbours if they are connected to the same factor.

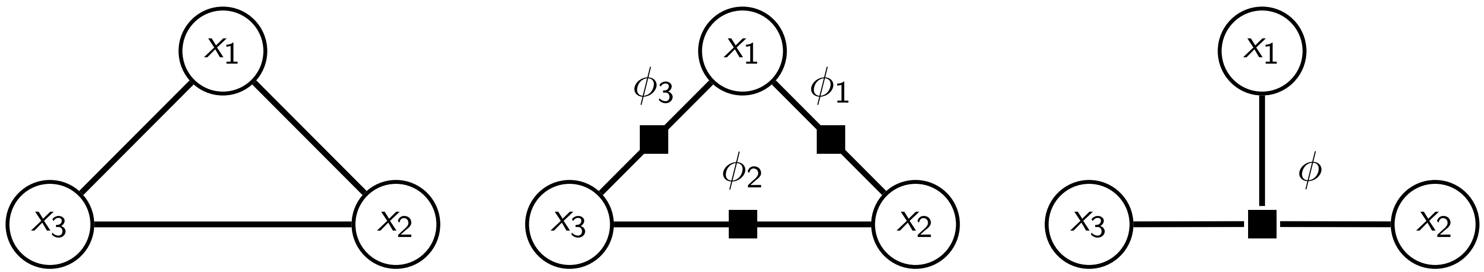
$p(x_1, x_2, x_3, x_4) = \frac{1}{Z}\phi_1(x_1, x_2, x_3)\phi_2(x_3, x_4)\phi_3(x_4)$



More informative than undirected graphs

- Mapping from Gibbs distribution to undirected graph is many to one but one-to-one for factor graphs.
- Example

$$p_A(x_1, x_2, x_3) \propto \phi_1(x_1, x_2)\phi_2(x_2, x_3)\phi_3(x_3, x_1)$$
$$p_B(x_1, x_2, x_3) \propto \phi(x_1, x_2, x_3)$$

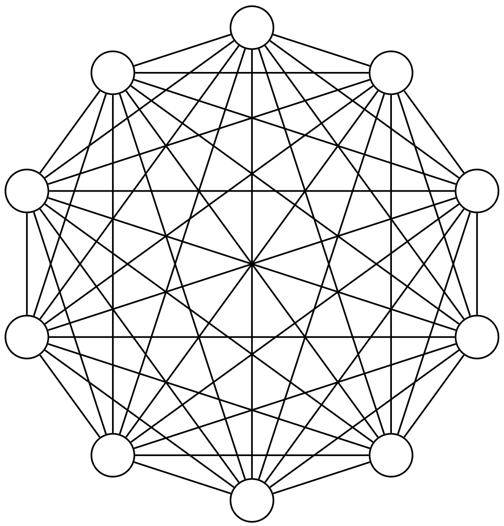


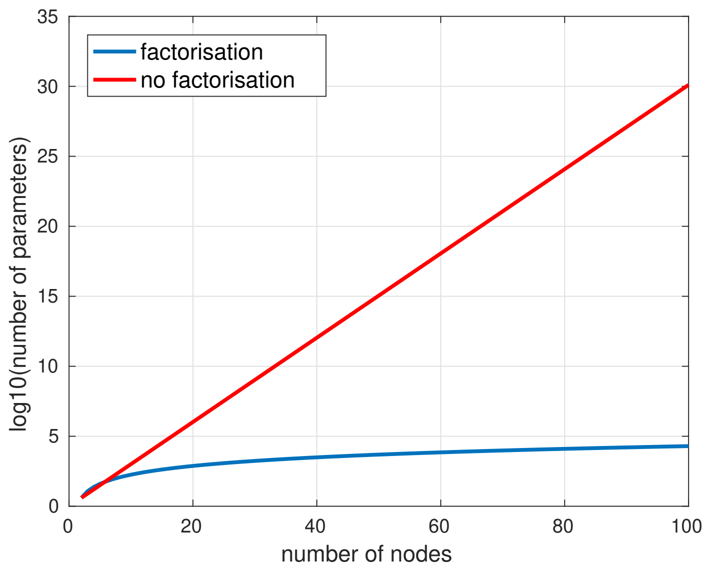
UG for p_A and p_B — FG for p_A — FG for p_B

More informative than undirected graphs

Assume binary random variables x_i.

- Same undirected graph but
  $p(x_1, \ldots, x_d) \propto \phi(x_1, \ldots, x_d)$ has 2^d free parameters,
  $p(x_1, \ldots, x_d) \propto \prod_{i<j} \phi_{ij}(x_i, x_j)$ has $\binom{d}{2} 2^2$ free parameters
  parameters $\equiv$ entries to specify in a table representation
- The difference matters for learning and inference when the number of variables is large.





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1. Factor graphs
   - Definition
   - Visualising Gibbs distributions as factor graphs
   - Factor graphs represent factorisations better than undirected graphs

2. Marginal inference by variable elimination

3. Marginal inference for factor trees (sum-product algorithm)

4. Inference of most probable states for factor trees

Program

1. Factor graphs

2. Marginal inference by variable elimination
   - Exploiting the factorisation by using the distributive law $ab + ac = a(b + c)$ and by caching computations
   - Variable elimination for general factor graphs
   - The principles of variable elimination also apply to continuous random variables

3. Marginal inference for factor trees (sum-product algorithm)

4. Inference of most probable states for factor trees

Basic ideas of variable elimination

1. Use the distributive law $ab + ac = a(b + c)$ to exploit the factorisation ($\sum\prod \to \prod\sum$):
   reduces the overall dimensionality of the domain of the factors in the sum and thereby the computational cost.
2. Recycle/cache results

Example: full factorisation

- Consider discrete-valued random variables $x_1, x_2, x_3 \in \{1, \ldots, K\}$
- Assume pmf factorises $p(x_1, x_2, x_3) \propto \phi_1(x_1)\phi_2(x_2)\phi_3(x_3)$
- Task: compute $p(x_1 = k)$ for $k \in \{1, \ldots, K\}$
- We can use the sum-rule

  $$p(x_1 = k) = \sum_{x_2, x_3} p(x_1 = k, x_2, x_3)$$

  Sum over K^2 terms for each k (value of x_1).
- Pre-computing $p(x_1, x_2, x_3)$ for all K^3 configurations and then computing the sum is neither necessary nor a good idea
- Exploit factorisation when computing $p(x_1 = k)$.

Example: full factorisation

$$
\begin{aligned}
&\text{(sum rule)} & p(x_1 = k) &= \sum_{x_2, x_3} p(x_1 = k, x_2, x_3) & (1)\\
&\text{(factorisation)} & &\propto \sum_{x_2} \sum_{x_3} \phi_1(k)\phi_2(x_2)\phi_3(x_3) & (2)\\
&\text{(distr. law)} & &\propto \phi_1(k) \sum_{x_2} \sum_{x_3} \phi_2(x_2)\phi_3(x_3) & (3)\\
&\text{(distr. law)} & &\propto \phi_1(k) \left[\sum_{x_2} \phi_2(x_2)\right] \left[\sum_{x_3} \phi_3(x_3)\right] & (4)
\end{aligned}
$$

Distributive law changes $\sum \prod$ in (2) to $\prod \sum$ in (4).

Example: full factorisation

$$p(x_1 = k) \propto \phi_1(k) \left[\sum_{x_2} \phi_2(x_2)\right] \left[\sum_{x_3} \phi_3(x_3)\right] \tag{5}$$

What's the point?

- Because of the factorisation (independencies) we do not need to evaluate and store the values of $p(x_1, x_2, x_3)$ for all K^3 configurations of the random variables.
- 2 sums over K numbers vs. 1 sum over K^2 numbers
- Recycling/caching of already computed quantities: we only need to compute

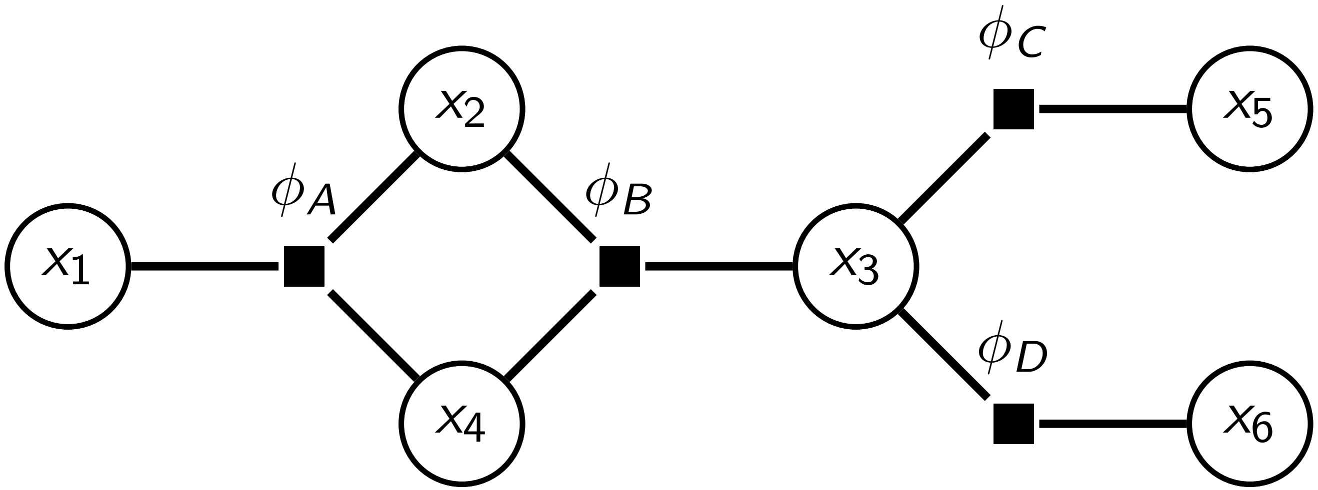
$$\left[\sum_{x_2} \phi_2(x_2)\right] \left[\sum_{x_3} \phi_3(x_3)\right]$$

  once; the value can be re-used when computing $p(x_1 = k)$ for different k.

Example: general factor graph

- Example:

$$p(x_1, \ldots, x_6) \propto \phi_A(x_1, x_2, x_4)\phi_B(x_2, x_3, x_4)\phi_C(x_3, x_5)\phi_D(x_3, x_6)$$



- Task: Compute $p(x_1, x_3)$
- Note the structural changes in the graph during variable elimination

Example: general factor graph (cont)

Task: Compute $p(x_1, x_3)$

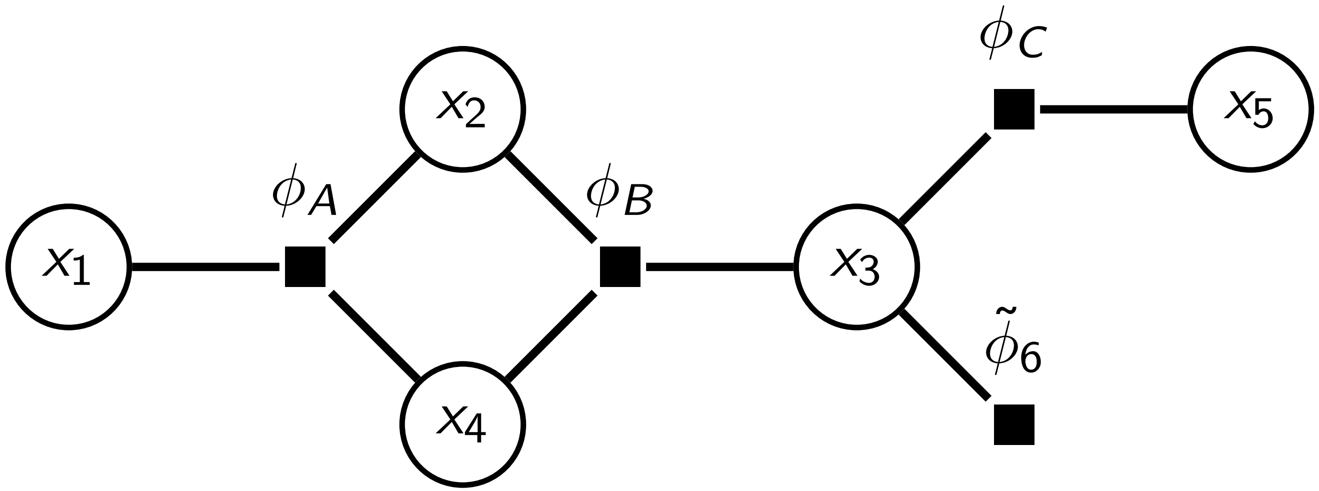
First eliminate x_6

$$p(x_1, \ldots, x_5) = \sum_{x_6} p(x_1, \ldots, x_6)$$

$$\text{(factorisation)} \propto \sum_{x_6} \phi_A(x_1, x_2, x_4)\phi_B(x_2, x_3, x_4)\phi_C(x_3, x_5)\phi_D(x_3, x_6)$$

$$\text{(distr. law)} \propto \phi_A(x_1, x_2, x_4)\phi_B(x_2, x_3, x_4)\phi_C(x_3, x_5) \sum_{x_6} \phi_D(x_3, x_6)$$

$$\propto \phi_A(x_1, x_2, x_4)\phi_B(x_2, x_3, x_4)\phi_C(x_3, x_5)\tilde{\phi}_6(x_3)$$

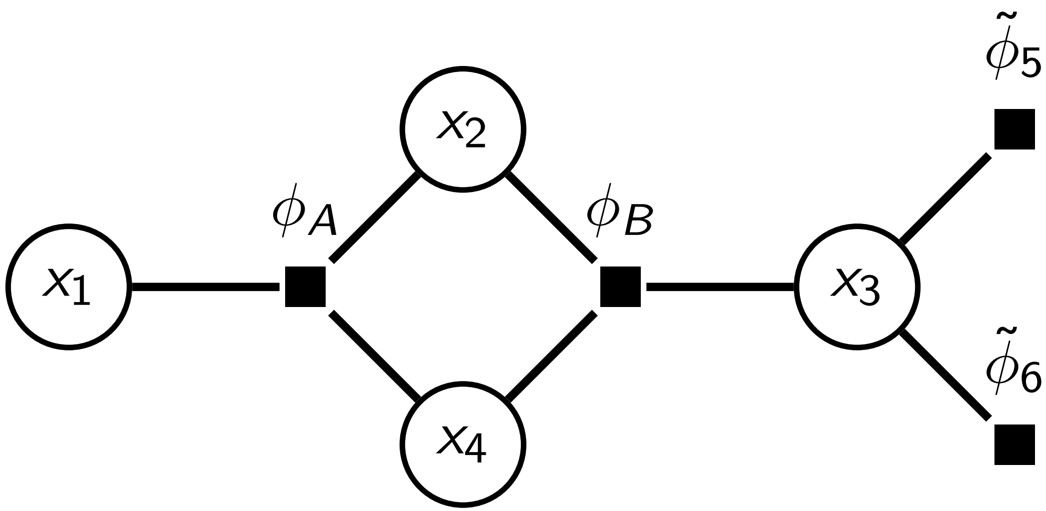


Example: general factor graph (cont)

Task: Compute $p(x_1, x_3)$

Eliminate x_5

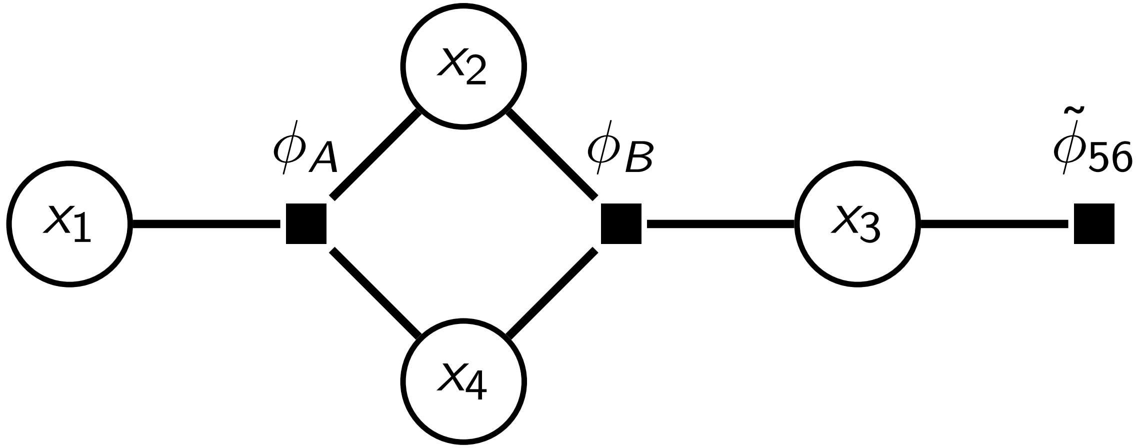
$$
\begin{aligned}
p(x_1, \ldots, x_4) &\propto \sum_{x_5} \phi_A(x_1, x_2, x_4)\phi_B(x_2, x_3, x_4)\phi_C(x_3, x_5)\tilde{\phi}_6(x_3) \\
&\propto \phi_A(x_1, x_2, x_4)\phi_B(x_2, x_3, x_4)\tilde{\phi}_6(x_3) \sum_{x_5} \phi_C(x_3, x_5) \\
&\propto \phi_A(x_1, x_2, x_4)\phi_B(x_2, x_3, x_4)\tilde{\phi}_6(x_3)\tilde{\phi}_5(x_3)
\end{aligned}
$$



Example: general factor graph (cont)

Define $\tilde{\phi}_{56}(x_3) = \tilde{\phi}_6(x_3)\tilde{\phi}_5(x_3)$

$$
\begin{aligned}
p(x_1, \ldots, x_4) &\propto \phi_A(x_1, x_2, x_4)\phi_B(x_2, x_3, x_4)\tilde{\phi}_6(x_3)\tilde{\phi}_5(x_3) \\
&\propto \phi_A(x_1, x_2, x_4)\phi_B(x_2, x_3, x_4)\tilde{\phi}_{56}(x_3)
\end{aligned}
$$



Example: general factor graph (cont)

Task: Compute $p(x_1, x_3)$

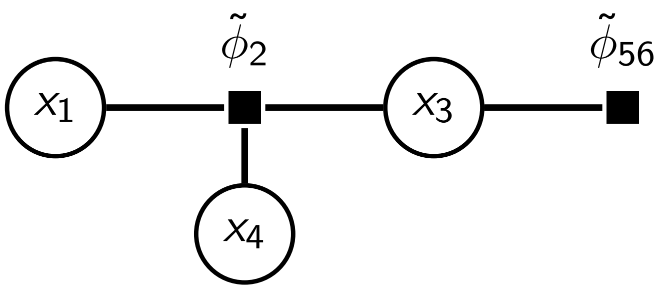
Eliminate x_2

$$p(x_1, x_3, x_4) \propto \sum_{x_2} \phi_A(x_1, x_2, x_4)\phi_B(x_2, x_3, x_4)\tilde{\phi}_{56}(x_3)$$

$$\propto \tilde{\phi}_{56}(x_3) \underbrace{\sum_{x_2} \phi_A(x_1, x_2, x_4)\phi_B(x_2, x_3, x_4)}_{K^3 \text{ times } K \text{ add/mult} \Rightarrow O(K^4) \text{ cost}}$$

$$\propto \tilde{\phi}_{56}(x_3)\tilde{\phi}_2(x_1, x_3, x_4)$$

Other justification for the cost: $\phi_A(x_1, x_2, x_4)\phi_B(x_2, x_3, x_4)$ equals a compound factor $\phi_*(x_1, x_2, x_3, x_4)$ that requires K^4 space when represented as a table. Summing out x_2 for all combinations of (x_1, x_3, x_4) touches each table-entry once $\Rightarrow O(K^4)$ cost.

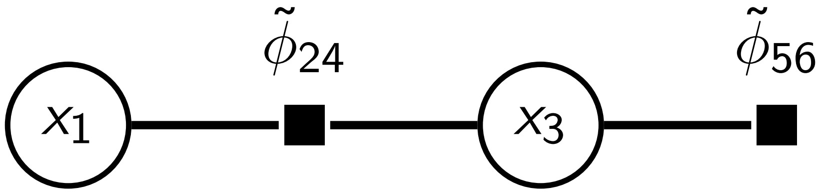


Example: general factor graph (cont)

Task: Compute $p(x_1, x_3)$

Eliminate x_4

$$
\begin{aligned}
p(x_1, x_3) &\propto \sum_{x_4} \tilde{\phi}_{56}(x_3)\tilde{\phi}_2(x_1, x_3, x_4) \\
&\propto \tilde{\phi}_{56}(x_3) \sum_{x_4} \tilde{\phi}_2(x_1, x_3, x_4) \\
&\propto \tilde{\phi}_{56}(x_3)\tilde{\phi}_{24}(x_1, x_3)
\end{aligned}
$$



Normalisation to obtain $p(x_1 = k, x_3 = k')$ for any k, k':

$$
p(x_1 = k, x_3 = k') = \frac{\tilde{\phi}_{56}(x_3 = k')\tilde{\phi}_{24}(x_1 = k, x_3 = k')}{\sum_{x_1, x_3} \tilde{\phi}_{56}(x_3)\tilde{\phi}_{24}(x_1, x_3)}
$$

Remarks

- Compared to precomputing K^6 numbers and then marginalising out variables, using the factorisation reduces the cost to $O(K^4)$.
- Caching: Intermediate quantities can be re-used when computing $p(x_1 = k, x_3 = k')$ for different k, k'
- Structural changes in the graph during variable elimination:
  - Eliminated leaf-variable and factor node $\to$ factor node
  - Factor nodes that depend on the same variables $\to$ single factor node
  - Factor nodes between neighbours of the eliminated variable $\to$ single factor node connecting all neighbours

Variable (bucket) elimination

Without loss of generality: Given $p(x_1, \ldots, x_d) \propto \prod_i^m \phi_i(\mathcal{X}_i)$ compute the marginal $p(\mathcal{X}_{\text{target}})$ for some $\mathcal{X}_{\text{target}} \subseteq \{x_1, \ldots, x_d\}$.

- Assume that at iteration k, you have the pmf over $d^k = d - k$ variables $X^k = (x_{i_1}, \ldots, x_{i_{d^k}})$ that factorises as

$$p(X^k) \propto \prod_{i=1}^{m^k} \phi_i^k(\mathcal{X}_i^k)$$

- Decide which variable to eliminate. Call it x^*. ($x^* \in X^k$, $x^* \notin \mathcal{X}_{\text{target}}$)
- Let X^{k+1} be equal to X^k with x^* removed. We have

$$\text{(sum rule)} \qquad p(X^{k+1}) = \sum_{x^*} p(X^k) \tag{6}$$

$$\text{(factorisation)} \qquad \propto \sum_{x^*} \prod_{i=1}^{m^k} \phi_i^k(\mathcal{X}_i^k) \tag{7}$$

Variable (bucket) elimination (cont.)

$$p(X^{k+1}) \propto \sum_{x^*} \prod_{i:x^* \notin \mathcal{X}_i^k} \phi_i^k(\mathcal{X}_i^k) \prod_{i:x^* \in \mathcal{X}_i^k} \phi_i^k(\mathcal{X}_i^k) \tag{8}$$

$$\text{(distr. law)} \propto \prod_{i:x^* \notin \mathcal{X}_i^k} \phi_i^k(\mathcal{X}_i^k) \sum_{x^*} \underbrace{\prod_{i:x^* \in \mathcal{X}_i^k} \phi_i^k(\mathcal{X}_i^k)}_{\text{compound factor } \phi_*^k(\mathcal{X}_*^k)} \tag{9}$$

$$\propto \left[\prod_{i:x^* \notin \mathcal{X}_i^k} \phi_i^k(\mathcal{X}_i^k) \right] \underbrace{\sum_{x^*} \phi_*^k(\mathcal{X}_*^k)}_{\text{new factor } \tilde{\phi}_*^k(\tilde{\mathcal{X}}_*^k)} \tag{10}$$

$\mathcal{X}_*^k$ is the union of all $\mathcal{X}_i^k$ that contain x^*, and $\tilde{\mathcal{X}}_*^k$ is $\mathcal{X}_*^k$ with x^* removed,

$$\mathcal{X}_*^k = \bigcup_{i:x^* \in \mathcal{X}_i^k} \mathcal{X}_i^k \qquad \tilde{\mathcal{X}}_*^k = \mathcal{X}_*^k \setminus x^* \tag{11}$$

Variable (bucket) elimination (cont.)

- By re-labelling the factors and variables, we obtain

$$p(X^{k+1}) \propto \left[\prod_{i: x^* \notin \mathcal{X}_i^k} \phi_i^k(\mathcal{X}_i^k) \right] \tilde{\phi}_*^k(\tilde{\mathcal{X}}_*^k) \tag{12}$$

$$\propto \prod_{i=1}^{m^{k+1}} \phi_i^{k+1}(\mathcal{X}_i^{k+1}), \tag{13}$$

  which has the same form as $p(X^k)$.
- Set $k = k + 1$ and decide which variable x^* to eliminate next.
- To compute $p(\mathcal{X}_{\text{target}})$ stop when $X^k = \mathcal{X}_{\text{target}}$, followed by normalisation.

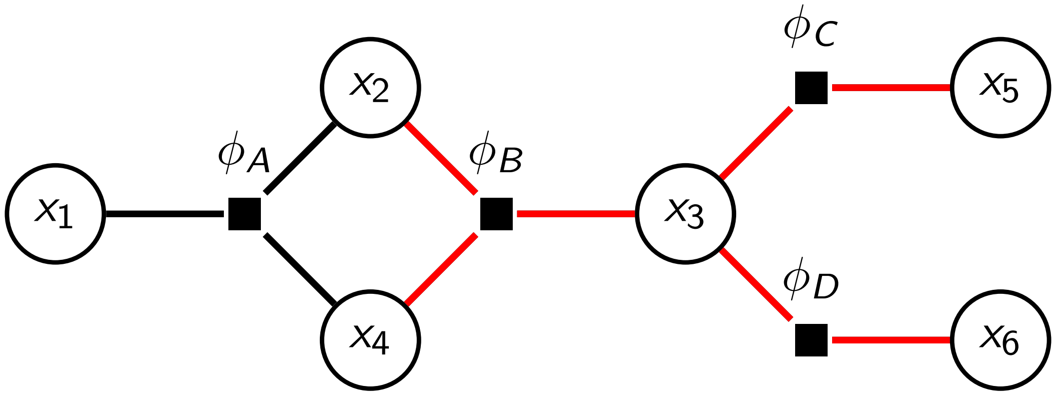
How to choose the elimination variable x^*?

- When we marginalise over x^* in iteration k, we generate the temporary compound factor ϕ_*^k that depends on

$$\mathcal{X}_*^k = \bigcup_{i:x^*\in\mathcal{X}_i^k} \mathcal{X}_i^k \tag{14}$$

Contains x^* and the variables with which x^* shares a factor node in the factor graph ("neighbours").

- Ex.: $p(x_1, \ldots, x_6) \propto \phi_A(x_1, x_2, x_4)\phi_B(x_2, x_3, x_4)\phi_C(x_3, x_5)\phi_D(x_3, x_6)$
If we eliminated $x^* = x_3$: $\mathcal{X}_* = \{x_2, x_3, x_4, x_5, x_6\}$



How to choose the elimination variable x^*?

- When we marginalise over x^* in iteration k, we generate the temporary compound factor ϕ_*^k that depends on

$$\mathcal{X}_*^k = \bigcup_{i:x^* \in \mathcal{X}_i^k} \mathcal{X}_i^k \tag{15}$$

  Contains x^* and the variables with which x^* shares a factor node in the factor graph ("neighbours").
- Eliminating x^* costs K^{M_k} where M_k is the number of variables in $\mathcal{X}_*^k$.
- Optimal choice of elimination order is difficult since the size of the factors can change when we eliminate variables (for details, see e.g. Koller, Section 9.4, not examinable)
- Heuristic: in each iteration, choose x^* in a greedy way so that $\mathcal{X}_*^k$ is small, i.e. the variable with the least number of neighbours in the factor graph (e.g. x_5 or x_6 in the example)

Computing conditionals

- The same approach can be used to compute conditionals.
- Example: Given

  $$p(x_1, \ldots, x_6) \propto \phi_A(x_1, x_2, x_4)\phi_B(x_2, x_3, x_4)\phi_C(x_3, x_5)\phi_D(x_3, x_6)$$

  assume you want to compute $p(x_1|x_3 = \alpha)$
- We can write

  $$\begin{aligned} p(x_1, x_2, x_4, x_5, x_6|x_3 = \alpha) &\propto p(x_1, x_2, x_3 = \alpha, x_4, x_5, x_6) \\ &\propto \phi_A(x_1, x_2, x_4)\phi_B^\alpha(x_2, x_4)\phi_C^\alpha(x_5)\phi_D^\alpha(x_6) \end{aligned}$$

  and consider $p(x_1, x_2, x_4, x_5, x_6|x_3 = \alpha)$ to be a pdf/pmf $\tilde{p}(x_1, x_2, x_4, x_5, x_6)$ defined up to the proportionality factor.
- We can compute $p(x_1|x_3 = \alpha) = \tilde{p}(x_1)$ by applying variable elimination to $\tilde{p}(x_1, x_2, x_4, x_5, x_6)$.

What if we have continuous random variables?

- Conceptually, all stays the same but we replace sums with integrals
  - Simplifications due to distributive law remain valid
  - Caching of results remains valid
- In special cases, integral can be computed in closed form (e.g. Gaussian family)
- If not: need for approximations (see later)
- Approximations are also needed for discrete random variables when K is large.

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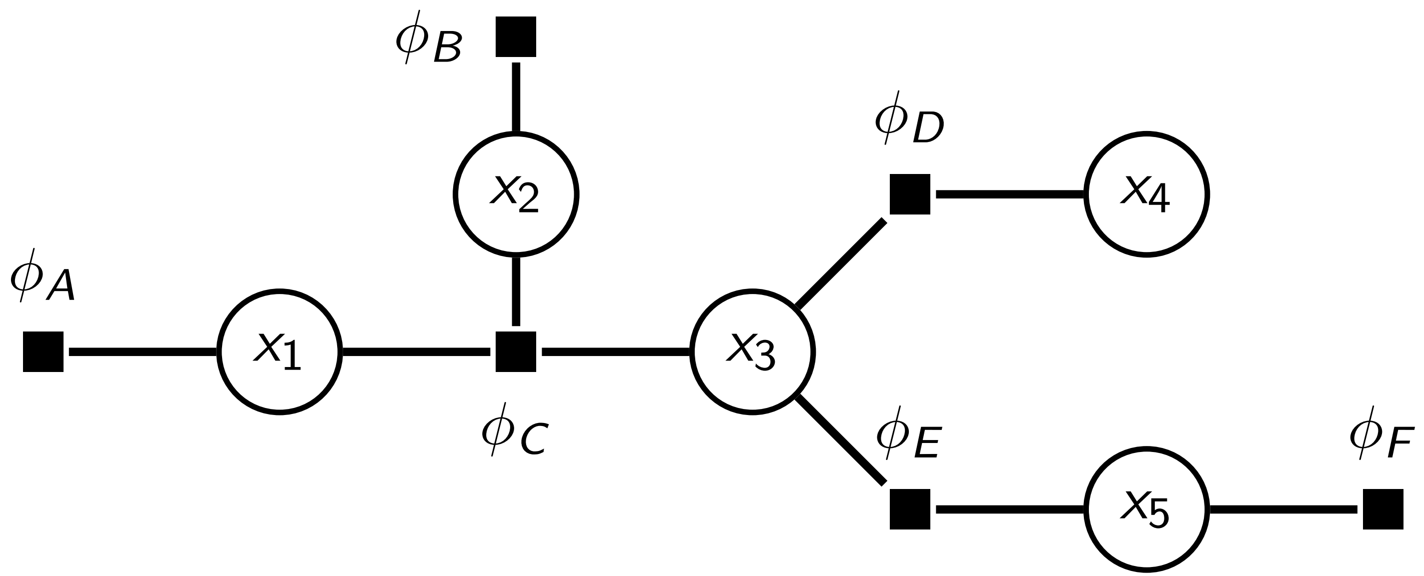
2. Marginal inference by variable elimination
   - Exploiting the factorisation by using the distributive law $ab + ac = a(b + c)$ and by caching computations
   - Variable elimination for general factor graphs
   - The principles of variable elimination also apply to continuous random variables
3. Marginal inference for factor trees (sum-product algorithm)
4. Inference of most probable states for factor trees

Program

1. Factor graphs
2. Marginal inference by variable elimination
3. Marginal inference for factor trees (sum-product algorithm)
    - Factor trees
    - Sum-product algorithm = variable elimination for factor trees
    - Messages = effective factors
    - The rules for sum-product message passing
4. Inference of most probable states for factor trees

Factor trees

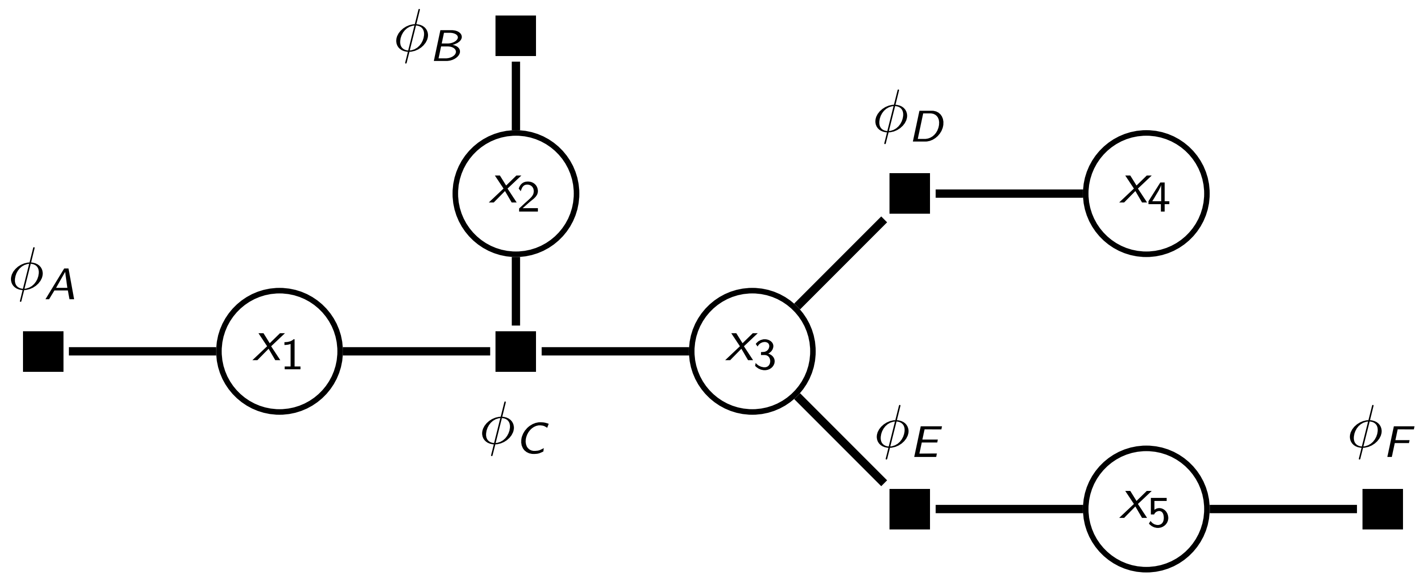
- We next consider the class of models (pmfs/pdfs) for which the factor graph is a tree.
- Tree: graph where there is only one path connecting any two nodes (no loops!)
- Chain is an example of a factor tree. (see later: inference for HMMs)
- Useful property: the factor tree obtained after summing out a leaf variable is still a factor tree.



Variable elimination for factor trees

Task: Compute $p(x_1)$ for

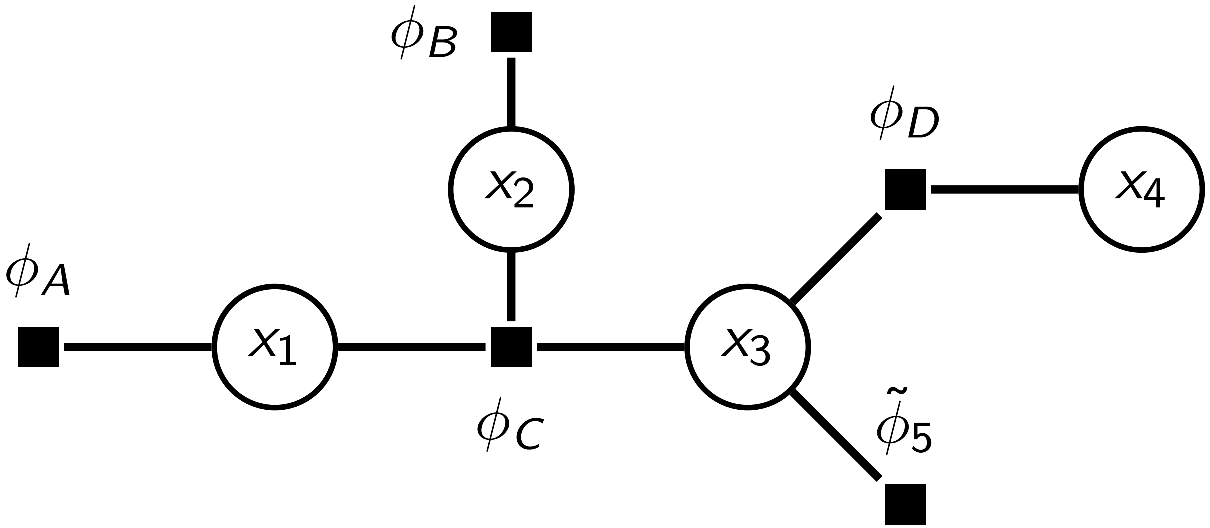
$$p(x_1, \dots, x_5) \propto \phi_A(x_1)\phi_B(x_2)\phi_C(x_1, x_2, x_3)\phi_D(x_3, x_4)\phi_E(x_3, x_5)\phi_F(x_5)$$



Sum out leaf-variable x_5

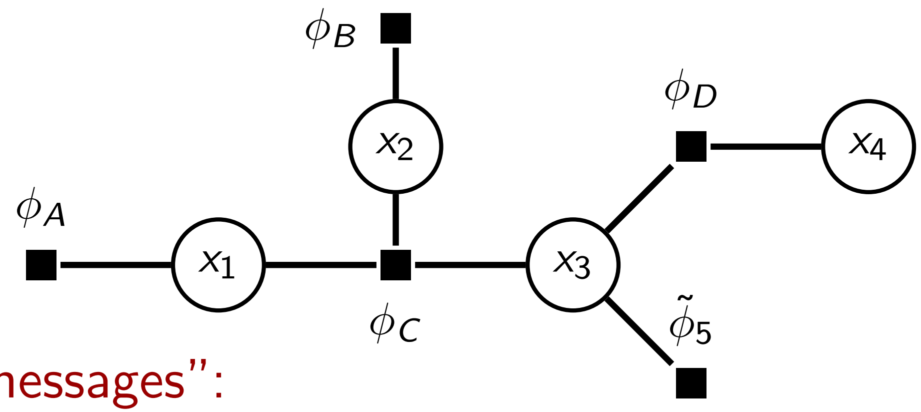
Task: Compute $p(x_1)$

$$
\begin{aligned}
p(x_1, \ldots, x_4) &= \sum_{x_5} p(x_1, \ldots, x_5) \\
&\propto \sum_{x_5} \phi_A(x_1)\phi_B(x_2)\phi_C(x_1, x_2, x_3)\phi_D(x_3, x_4)\phi_E(x_3, x_5)\phi_F(x_5) \\
&\propto \phi_A(x_1)\phi_B(x_2)\phi_C(x_1, x_2, x_3)\phi_D(x_3, x_4) \sum_{x_5} \phi_E(x_3, x_5)\phi_F(x_5) \\
&\propto \phi_A(x_1)\phi_B(x_2)\phi_C(x_1, x_2, x_3)\phi_D(x_3, x_4)\tilde{\phi}_5(x_3)
\end{aligned}
$$

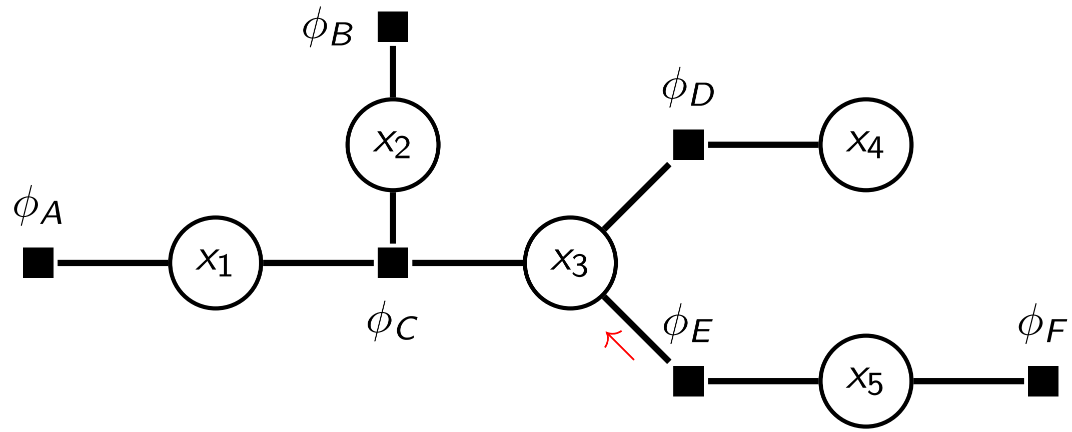


Visualising the computation

Graph with transformed factors:



Graph with "messages":



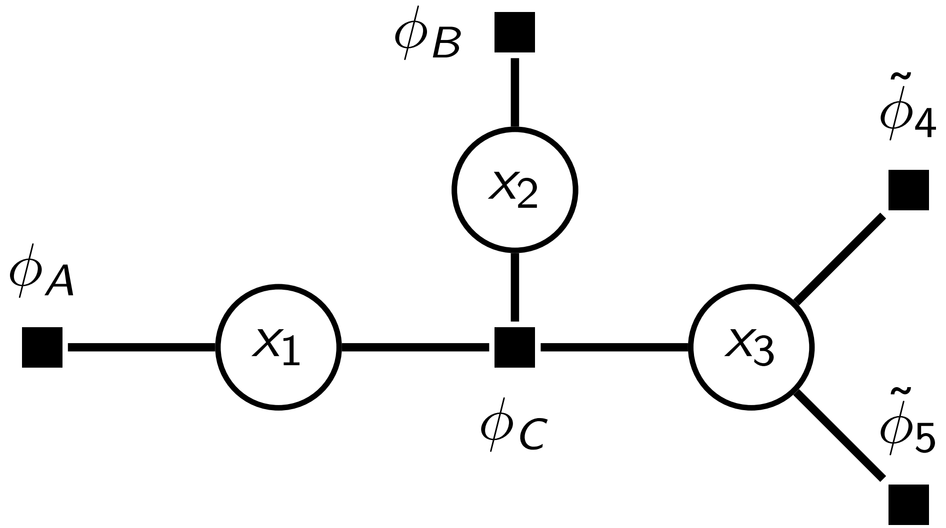
Message: $\mu_{\phi_E \to x_3}(x_3) = \tilde{\phi}_5(x_3) = \sum_{x_5} \phi_E(x_3, x_5)\phi_F(x_5)$

Effective factor for x_3 if all variables in the subtree attached to ϕ_E are eliminated (subtree does *not* include x_3)

Sum out leaf-variable x_4

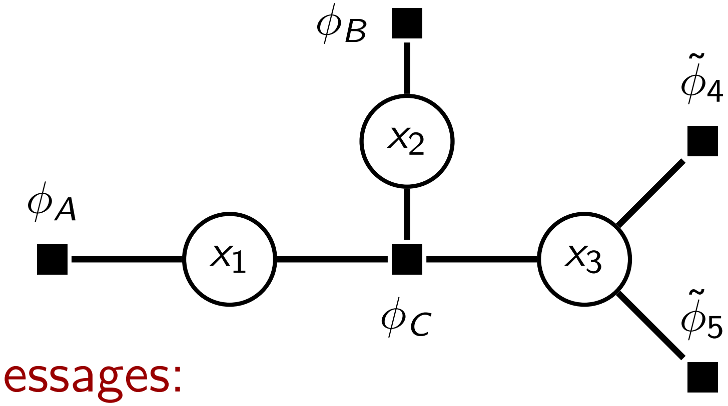
Task: Compute $p(x_1)$

$$
\begin{aligned}
p(x_1, \dots, x_3) &= \sum_{x_4} p(x_1, \dots, x_4) \\
&\propto \sum_{x_4} \phi_A(x_1)\phi_B(x_2)\phi_C(x_1, x_2, x_3)\phi_D(x_3, x_4)\tilde{\phi}_5(x_3) \\
&\propto \phi_A(x_1)\phi_B(x_2)\phi_C(x_1, x_2, x_3)\tilde{\phi}_5(x_3) \sum_{x_4} \phi_D(x_3, x_4) \\
&\propto \phi_A(x_1)\phi_B(x_2)\phi_C(x_1, x_2, x_3)\tilde{\phi}_5(x_3)\tilde{\phi}_4(x_3)
\end{aligned}
$$

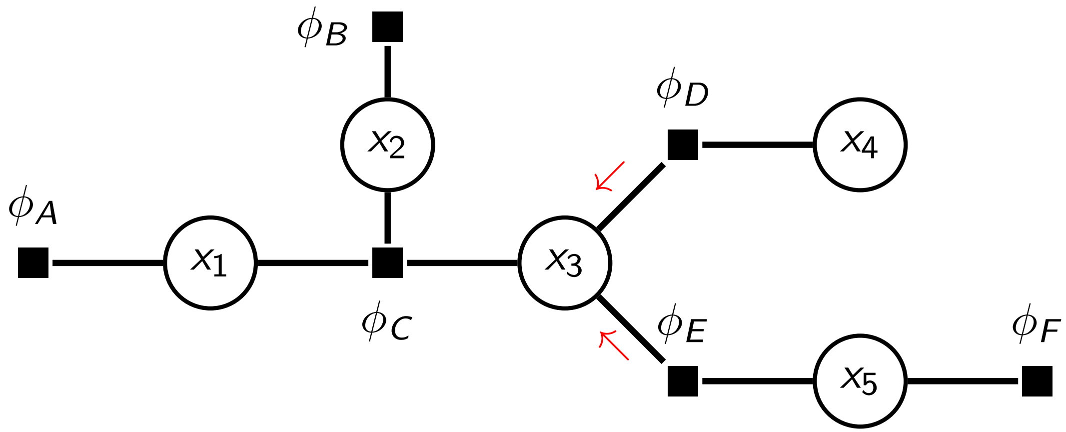


Visualising the computation

Graph with transformed factors:



Graph with messages:



Message: $\mu_{\phi_D \to x_3}(x_3) = \tilde{\phi}_4(x_3) = \sum_{x_4} \phi_D(x_3, x_4)$

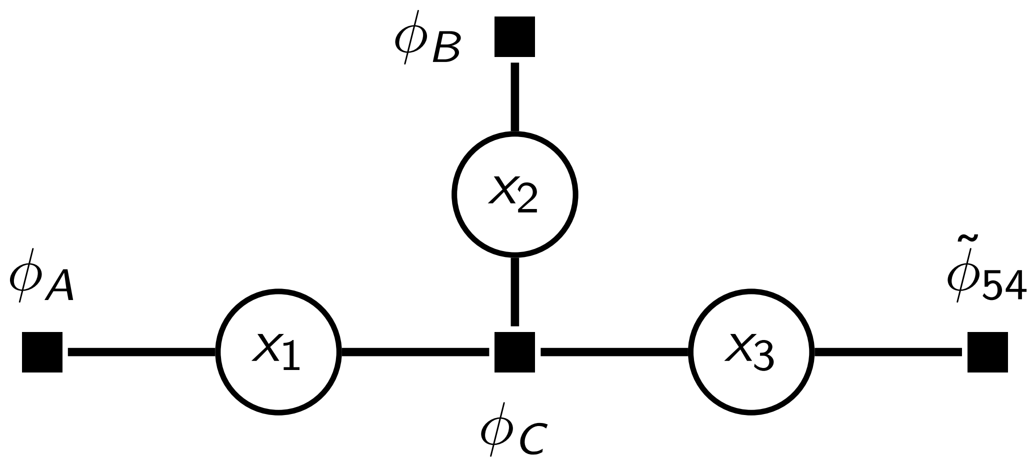
Effective factor for x_3 if all variables in the subtree attached to ϕ_D are eliminated (subtree does *not* include x_3)

Simplify by multiplying factors with common domain

Task: Compute $p(x_1)$

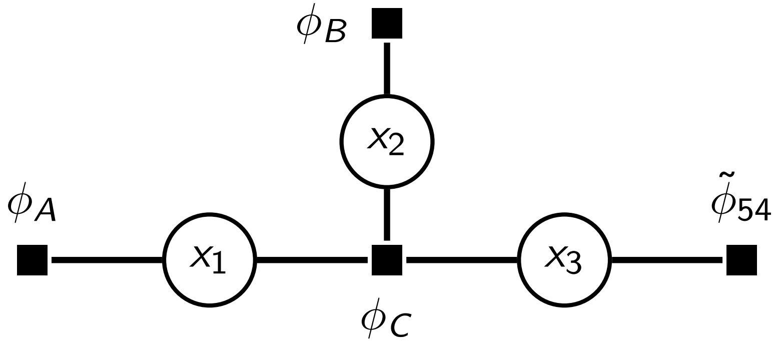
$$p(x_1, \ldots, x_3) \propto \phi_A(x_1)\phi_B(x_2)\phi_C(x_1, x_2, x_3) \underbrace{\tilde{\phi}_5(x_3)\tilde{\phi}_4(x_3)}_{\tilde{\phi}_{54}(x_3)}$$

$$\propto \phi_A(x_1)\phi_B(x_2)\phi_C(x_1, x_2, x_3)\tilde{\phi}_{54}(x_3)$$

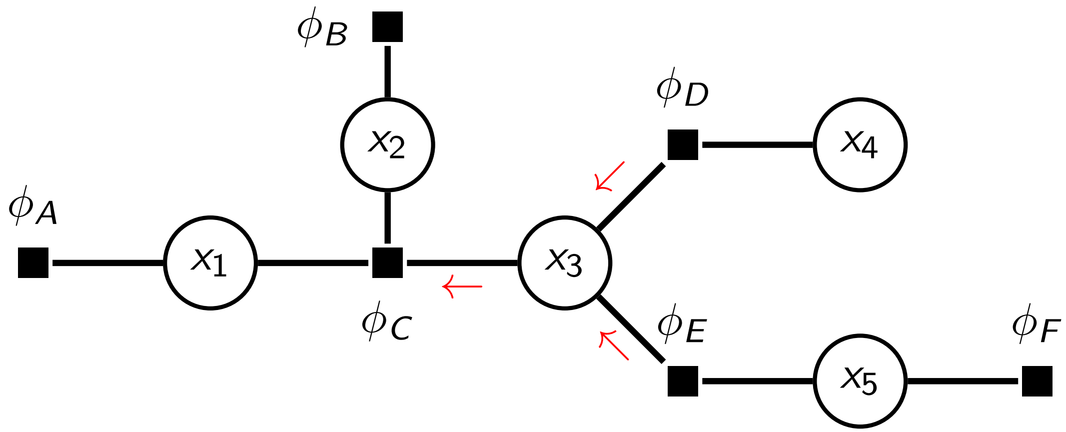


Visualising the computation

Graph with transformed factors:



Graph with messages:



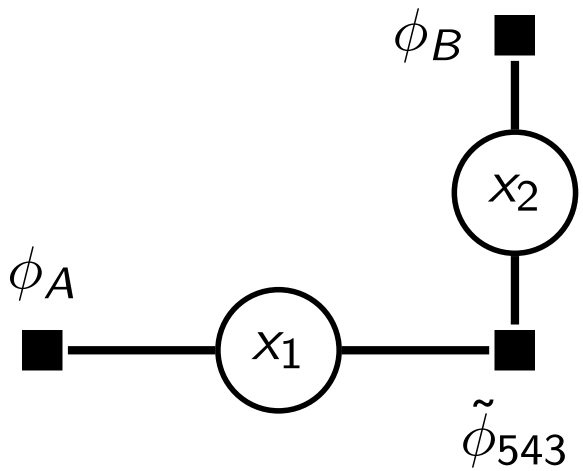
Message: $\mu_{x_3 \to \phi_C}(x_3) = \tilde{\phi}_{54}(x_3) = \tilde{\phi}_4(x_3)\tilde{\phi}_5(x_3) = \mu_{\phi_D \to x_3}(x_3)\mu_{\phi_E \to x_3}(x_3)$

Effective factor for x_3 if all variables in the subtrees attached to x_3 are eliminated (subtrees do *not* include ϕ_c)

Sum out leaf-variable x_3

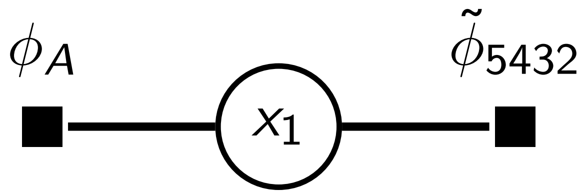
Task: Compute $p(x_1)$

$$
\begin{aligned}
p(x_1, x_2) &= \sum_{x_3} p(x_1, x_2, x_3) \\
&\propto \sum_{x_3} \phi_A(x_1)\phi_B(x_2)\phi_C(x_1, x_2, x_3)\tilde{\phi}_{54}(x_3) \\
&\propto \phi_A(x_1)\phi_B(x_2) \sum_{x_3} \phi_C(x_1, x_2, x_3)\tilde{\phi}_{54}(x_3) \\
&\propto \phi_A(x_1)\phi_B(x_2)\tilde{\phi}_{543}(x_1, x_2)
\end{aligned}
$$



Sum out leaf-variable x_2 and normalise

$$p(x_1) = \sum_{x_2} p(x_1, x_2) \propto \sum_{x_2} \phi_A(x_1)\phi_B(x_2)\tilde{\phi}_{543}(x_1, x_2)$$
$$\propto \phi_A(x_1) \sum_{x_2} \phi_B(x_2)\tilde{\phi}_{543}(x_1, x_2)$$
$$\propto \phi_A(x_1)\tilde{\phi}_{5432}(x_1)$$



$$p(x_1) = \frac{\phi_A(x_1)\tilde{\phi}_{5432}(x_1)}{\sum_{x_1} \phi_A(x_1)\tilde{\phi}_{5432}(x_1)}$$

Alternative: sum out both x_2 and x_3

Since

$$\begin{aligned}\tilde{\phi}_{5432}(x_1) &= \sum_{x_2} \phi_B(x_2)\tilde{\phi}_{543}(x_1, x_2) \\ &= \sum_{x_2} \phi_B(x_2) \sum_{x_3} \phi_C(x_1, x_2, x_3)\tilde{\phi}_{54}(x_3) \\ &= \sum_{x_2, x_3} \phi_C(x_1, x_2, x_3)\phi_B(x_2)\tilde{\phi}_{54}(x_3)\end{aligned}$$

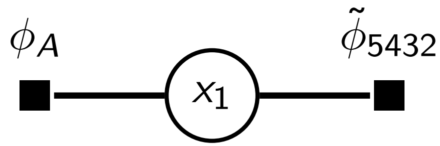
we obtain the same result by first summing out x_2 and then x_3, or both at the same time.

In any case:

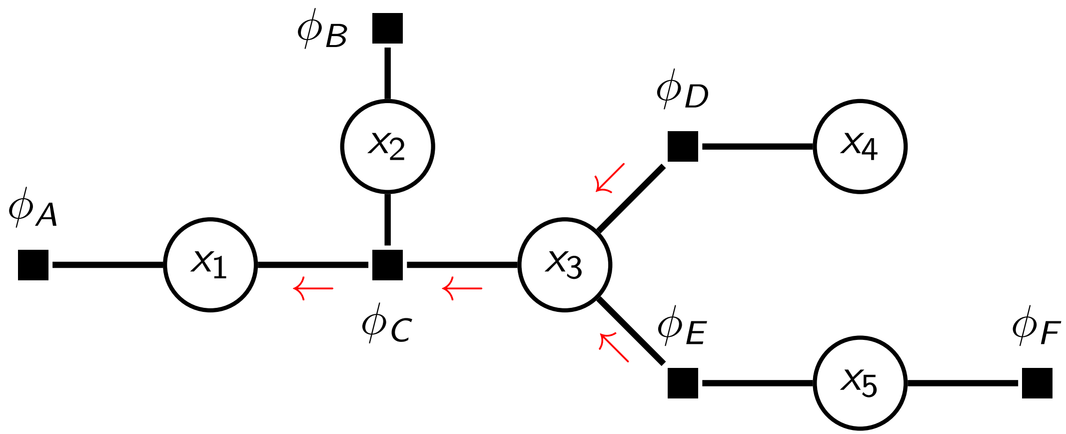
$$p(x_1) \propto \phi_A(x_1) \sum_{x_2, x_3} \phi_C(x_1, x_2, x_3)\phi_B(x_2)\tilde{\phi}_{54}(x_3)$$

Visualising the computation

Graph with transformed factors:



Graph with messages:



Message:

$\mu_{\phi_C \to x_1}(x_1) = \tilde{\phi}_{5432}(x_1) = \sum_{x_2, x_3} \phi_C(x_1, x_2, x_3)\phi_B(x_2)\mu_{x_3 \to \phi_C}(x_3)$

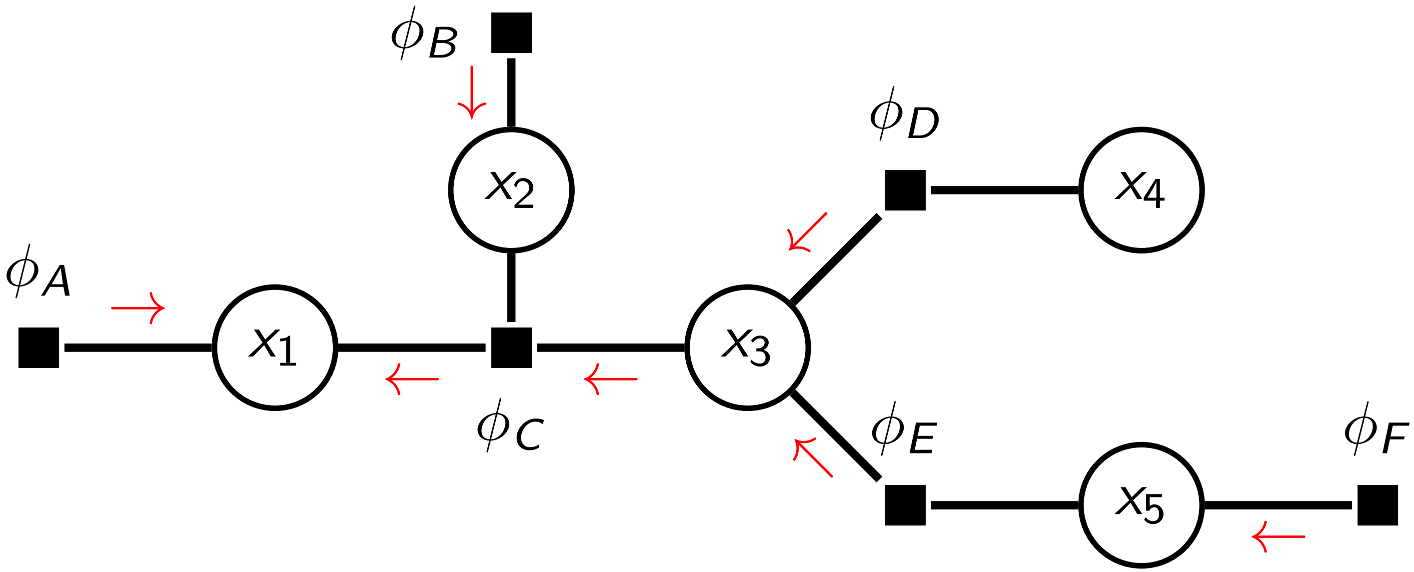
Effective factor for x_1 if all variables in the subtrees attached to ϕ_C are eliminated (subtrees do *not* include x_1)

Representing leaf-factors with messages

Since there are no variables "behind" the leaf-factors, we can consider all leaf-factors to be effective factors themselves:

$$\mu_{\phi_A \to x_1}(x_1) = \phi_A(x_1)$$
$$\mu_{\phi_B \to x_2}(x_2) = \phi_B(x_2)$$
$$\mu_{\phi_F \to x_5}(x_5) = \phi_F(x_5)$$

We then obtain



Variables with single incoming messages copy the message

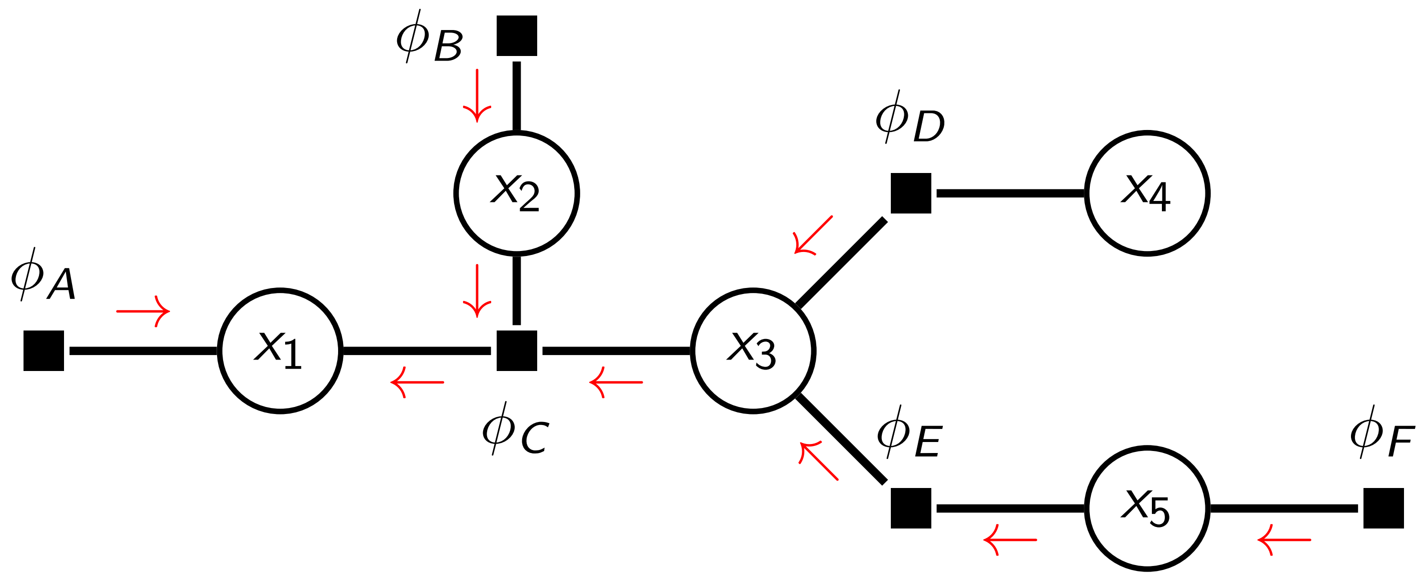
We had

$$\mu_{x_3 \to \phi_C}(x_3) = \mu_{\phi_D \to x_3}(x_3)\mu_{\phi_E \to x_3}(x_3)$$

which corresponded to simplifying the factorisation by multiplying effective factors defined on the same domain. Special cases:

$$\mu_{x_5 \to \phi_E}(x_5) = \mu_{\phi_F \to x_5}(x_5)$$
$$\mu_{x_2 \to \phi_C}(x_2) = \mu_{\phi_B \to x_2}(x_2)$$

We then obtain



Messages from leaf variable nodes

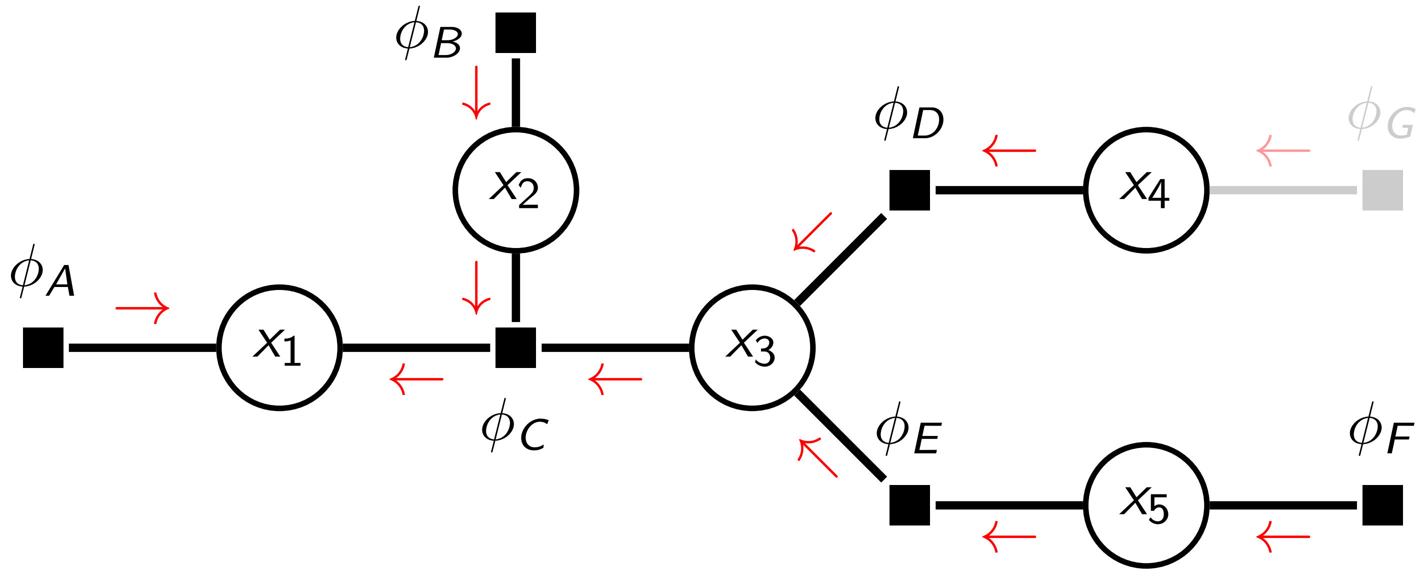
What about x_4? We can consider

$$p(x_1, \ldots, x_5) \propto \phi_A(x_1)\phi_B(x_2)\phi_C(x_1, x_2, x_3)\phi_D(x_3, x_4)\phi_E(x_3, x_5)\phi_F(x_5)$$

to include an additional factor $\phi_G(x_4) = 1$. We can thus set

$$\mu_{\phi_G \to x_4}(x_4) = 1$$
$$\mu_{x_4 \to \phi_D}(x_4) = \mu_{\phi_G \to x_4}(x_4) = 1$$

Graph:

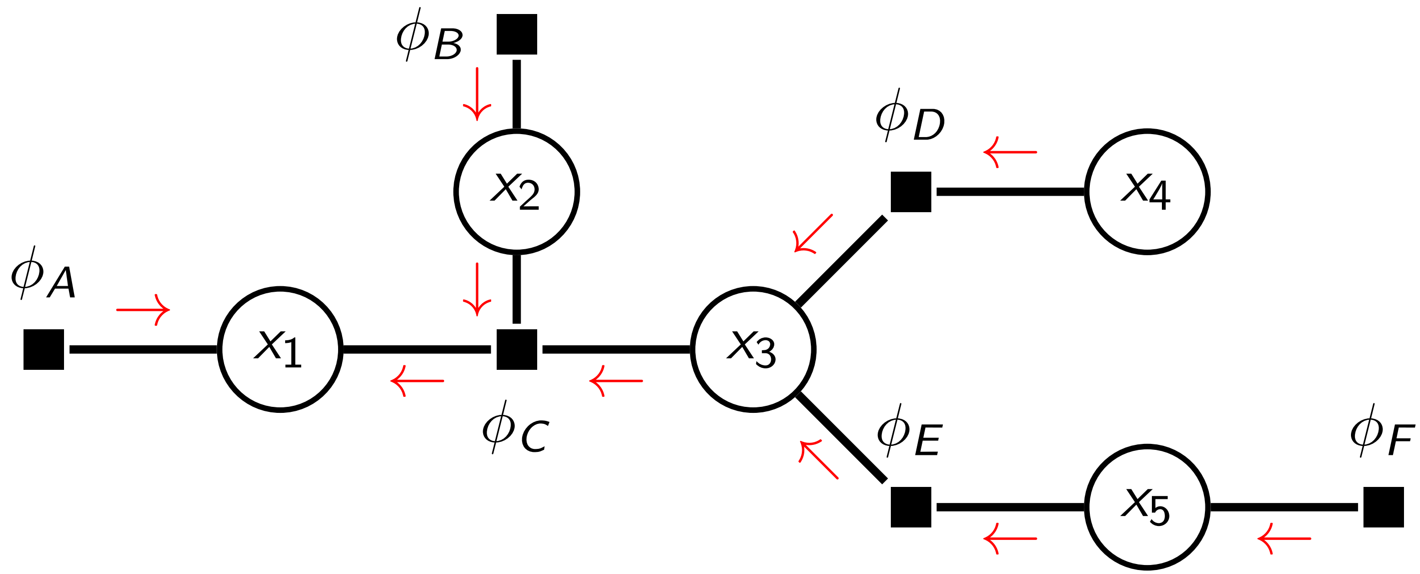


Single marginal from messages

We have seen that

$$\begin{aligned} p(x_1) &\propto \phi_A(x_1)\tilde{\phi}_{5432}(x_1) \\ &\propto \mu_{\phi_A \to x_1}(x_1)\mu_{\phi_C \to x_1}(x_1) \end{aligned}$$

Marginal is proportional to the product of the incoming messages.



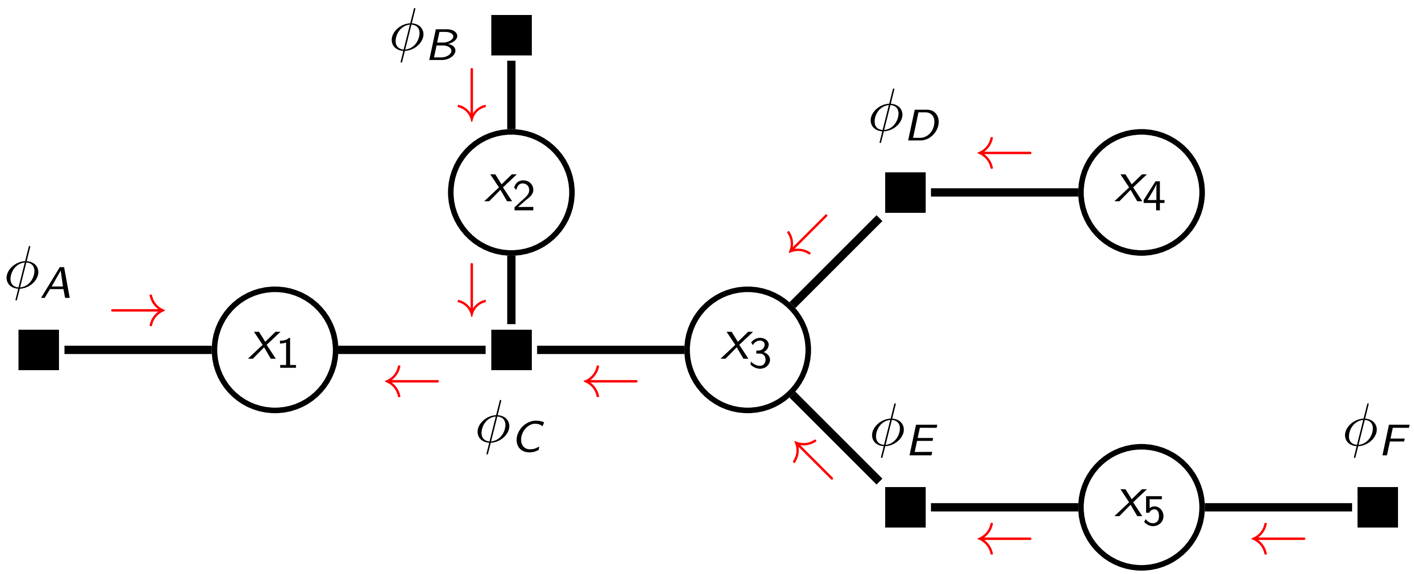
Single marginal from messages

Cost (due to properties of variable elimination):

- Linear in number of variables d, exponential in maximal number of variables attached to a factor node.

  (cost known upfront since no new factors are created unlike in the general case considered before)

- Recycling: most messages do not depend on x_1 and can be re-used for computing $p(x_1)$ for any value of x_1 (as well as for computing the marginal distribution of other variables, see next slides)

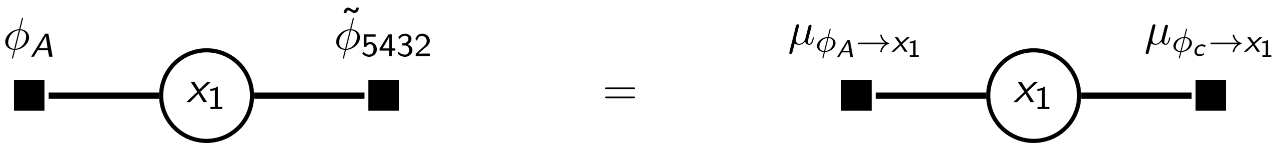


Further marginals from messages

- We have seen that

$$
\begin{aligned}
p(x_1) &\propto \phi_A(x_1)\tilde{\phi}_{5432}(x_1) \\
&\propto \mu_{\phi_A \to x_1}(x_1)\mu_{\phi_C \to x_1}(x_1)
\end{aligned}
$$

- Remember: Messages are effective factors

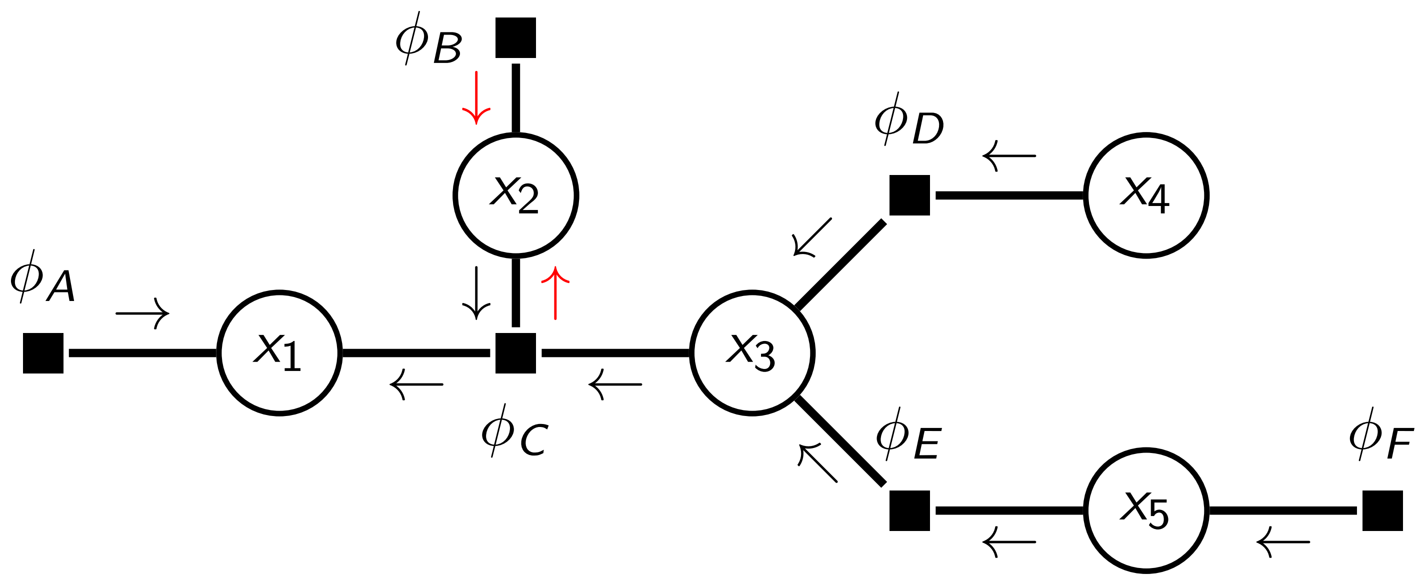


- This correspondence allows us to write down the marginal for other variables too. The incoming messages are all we need.

Further marginals from messages

- Example: For $p(x_2)$ we need $\mu_{\phi_B \to x_2}$ and $\mu_{\phi_C \to x_2}$
- $\mu_{\phi_B \to x_2}$ is known but $\mu_{\phi_C \to x_2}$ needs to be computed
- $\mu_{\phi_C \to x_2}$ is the effective factor for x_2 if all variables of the subtrees attached to ϕ_c are eliminated.
- Can be computed from previously computed factors:

$$\mu_{\phi_A \to x_1} \quad \text{and} \quad \mu_{x_3 \to \phi_C}$$



Further marginals from messages

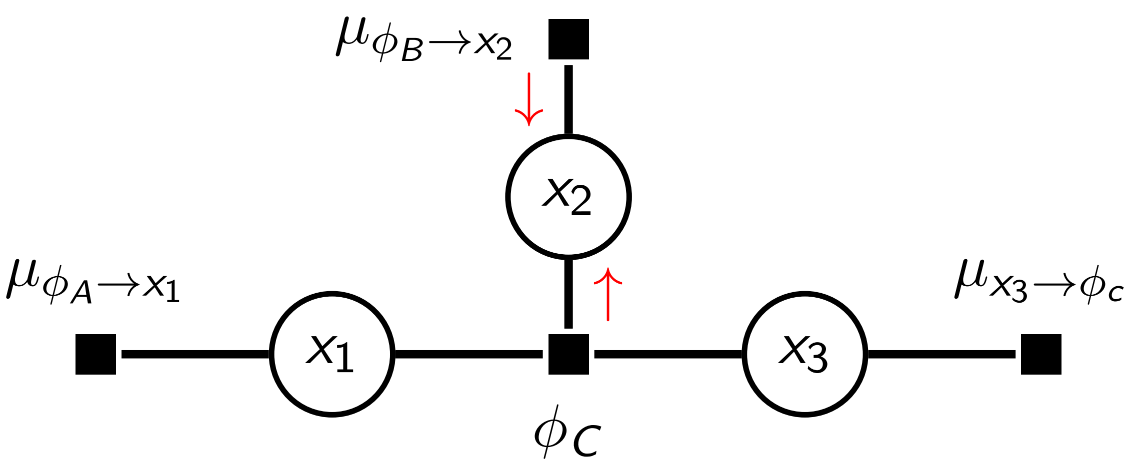
- By definition of the messages, and their correspondence to effective factors, we have

$$p(x_1, x_2, x_3) \propto \phi_C(x_1, x_2, x_3)\mu_{\phi_A \to x_1}(x_1)\mu_{\phi_B \to x_2}(x_2)\mu_{x_3 \to \phi_C}(x_3)$$

- Eliminating x_1 and x_3 gives

$$p(x_2) \propto \mu_{\phi_B \to x_2}(x_2) \underbrace{\sum_{x_1, x_3} \phi_c(x_1, x_2, x_3)\mu_{x_3 \to \phi_C}(x_3)\mu_{\phi_A \to x_1}(x_1)}_{\mu_{\phi_C \to x_2}(x_2)}$$

$$\propto \mu_{\phi_B \to x_2}(x_2)\mu_{\phi_C \to x_2}(x_2)$$



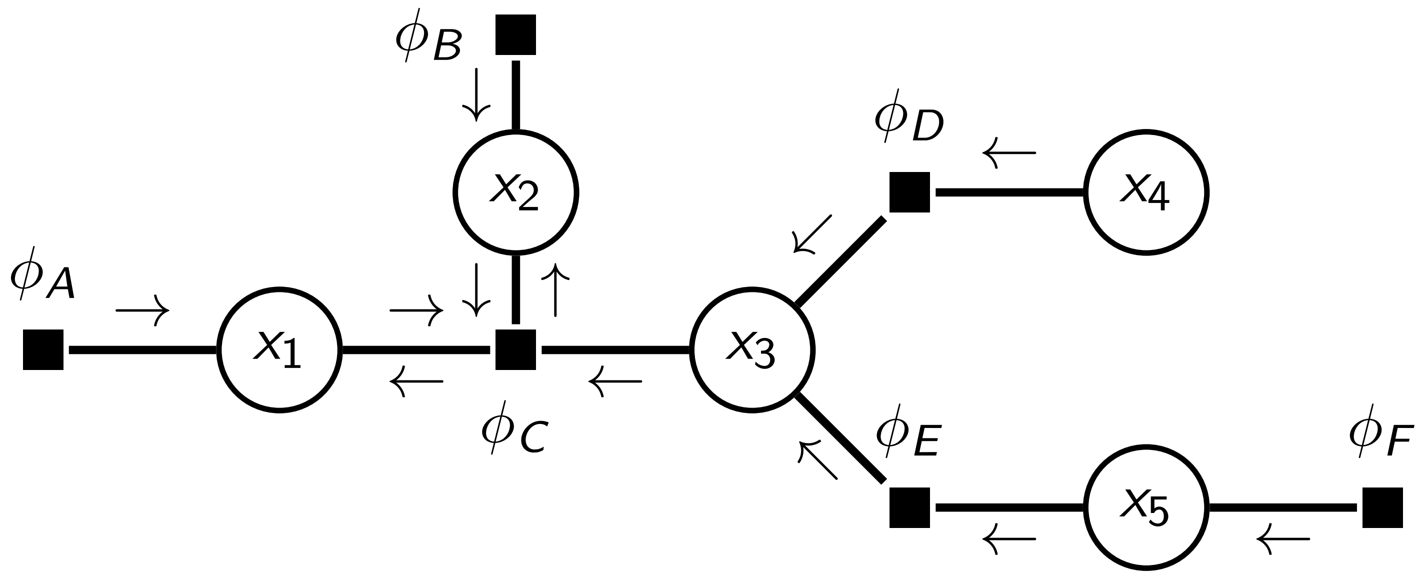
Further marginals from messages

We had

$$\mu_{\phi_C \to x_2}(x_2) = \sum_{x_1, x_3} \phi_c(x_1, x_2, x_3) \mu_{x_3 \to \phi_C}(x_3) \mu_{\phi_A \to x_1}(x_1)$$

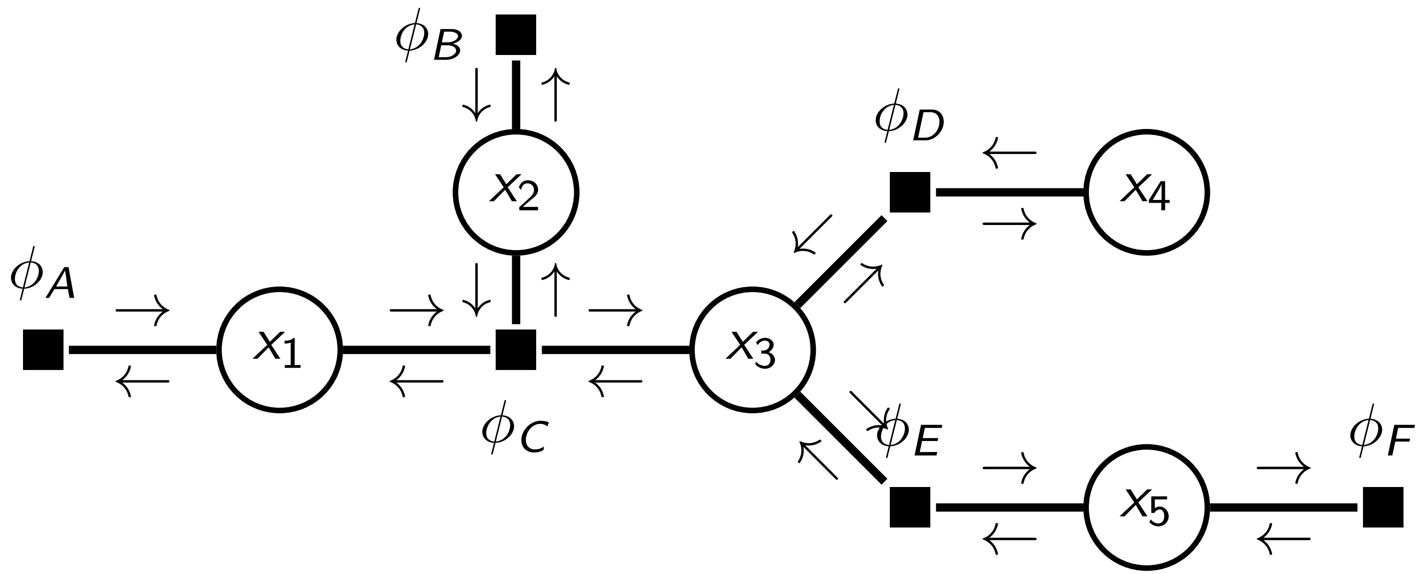
Introducing variable to factor message $\mu_{x_1 \to \phi_c} = \mu_{\phi_A \to x_1} = \phi_A$

$$\mu_{\phi_C \to x_2}(x_2) = \sum_{x_1, x_3} \phi_c(x_1, x_2, x_3) \mu_{x_3 \to \phi_C}(x_3) \mu_{x_1 \to \phi_c}(x_1)$$



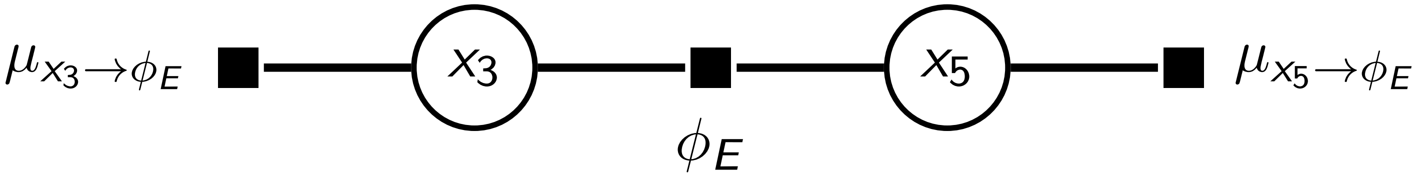
All (univariate) marginals from messages

- We can use the messages to compute the marginals of all variables in the graph.
- For the marginal of a variable x we need to know the incoming messages $\mu_{\phi_i \to x}$ from all factor nodes ϕ_i connected to x.
- This means that if each edge has a message in both directions, we can compute the marginals of all variables in the graph.



Joint distributions from messages

- The correspondence between messages and effective factors allows us to find the joint distribution for variables connected to the same factor node (neighbours).
- For example, we can compute $p(x_3, x_5)$ from messages
- The messages $\mu_{x_3 \to \phi_E}$ and $\mu_{x_5 \to \phi_E}$ correspond to effective factors attached to x_3 and x_5, respectively.



- Factor graph corresponds to

$$p(x_3, x_5) \propto \phi_E(x_3, x_5)\mu_{x_3 \to \phi_E}(x_3)\mu_{x_5 \to \phi_E}(x_5)$$

Rules of message passing: initialisation

Note: The rules come from the fact that messages correspond to effective factors obtained after marginalisation.

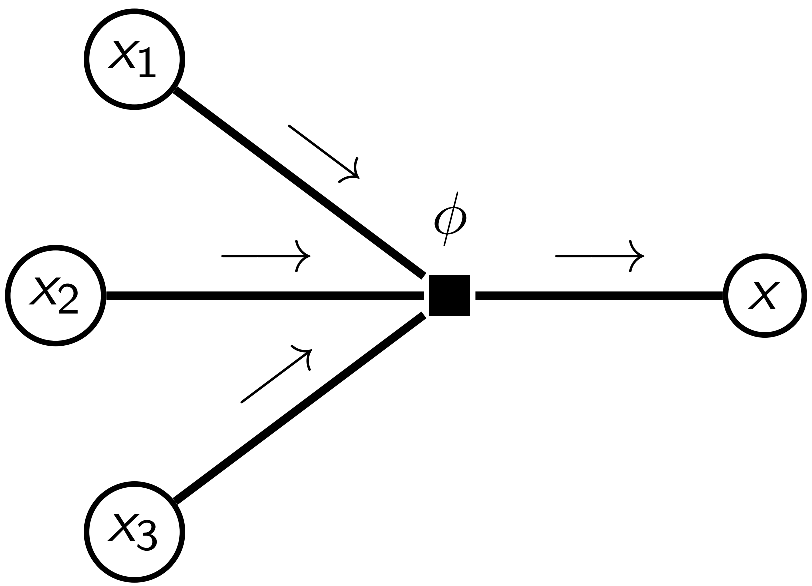
- From a leaf variable node x to a factor node ϕ, the message $\mu_{x \to \phi}(x) = 1$.
- From a leaf factor node ϕ to a variable node x, the message $\mu_{\phi \to x}(x) = \phi(x)$.

Rules of message passing: factor to variable messages

Note: The rules come from the fact that messages correspond to effective factors obtained after marginalisation.

Let $x_1, \ldots, x_j$ be the neighbours of factor node ϕ, without variable x.

$$\mu_{\phi \to x}(x) = \sum_{x_1, \ldots, x_j} \phi(x_1, \ldots, x_j, x) \prod_{i=1}^{j} \mu_{x_i \to \phi}(x_i)$$



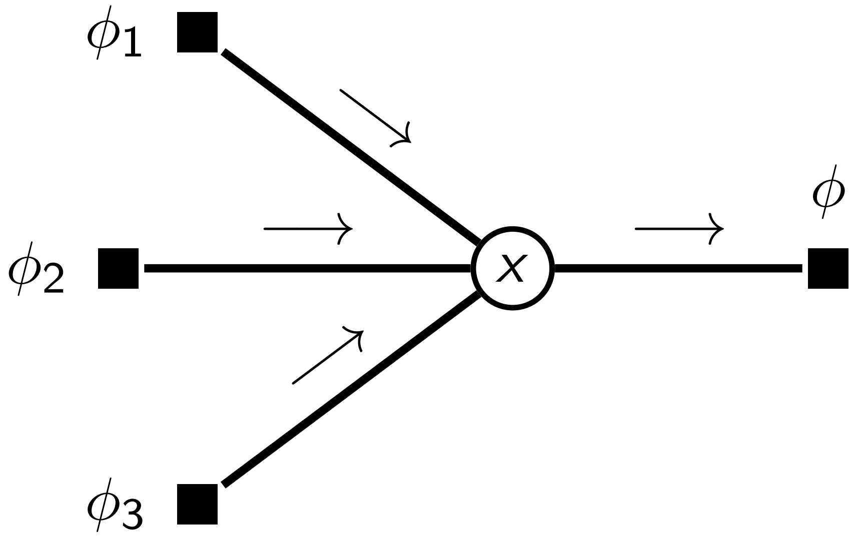
Rule corresponds to eliminating variables $x_1, \ldots, x_j$

Rules of message passing: variable to factor messages

Note: The rules come from the fact that messages correspond to effective factors obtained after marginalisation.

Let $\phi_1, \ldots, \phi_j$ be the neighbours of variable node x, without factor ϕ.

$$\mu_{x \to \phi}(x) = \prod_{i=1}^{j} \mu_{\phi_i \to x}(x)$$



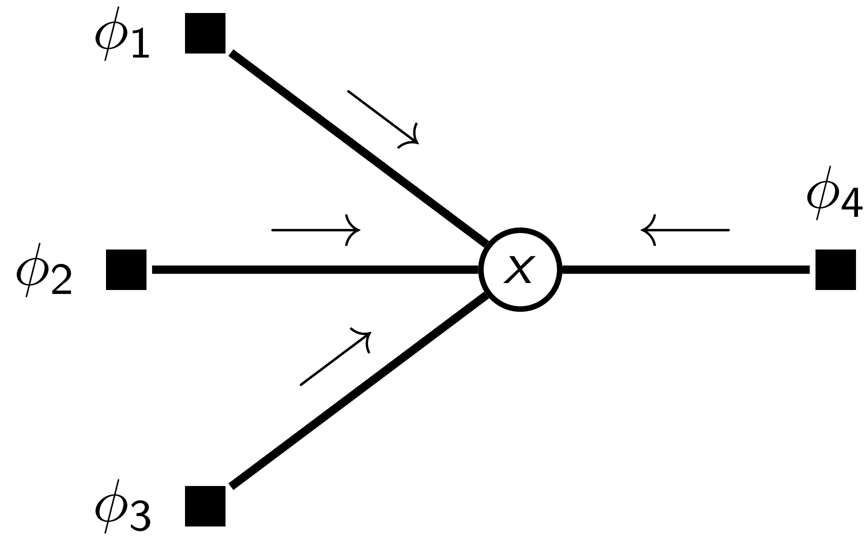
Rule corresponds to simplifying the factorisation by multiplying effective factors defined on the same domain.

Rules of message passing: univariate marginals

Note: The rules come from the fact that messages correspond to effective factors obtained after marginalisation.

Let $\phi_1, \ldots, \phi_j$ be all neighbours of variable node x.

$$p(x) = \frac{1}{Z} \prod_{i=1}^{j} \mu_{\phi_i \to x}(x) \qquad Z = \sum_x \prod_i \mu_{\phi_i \to x}(x)$$



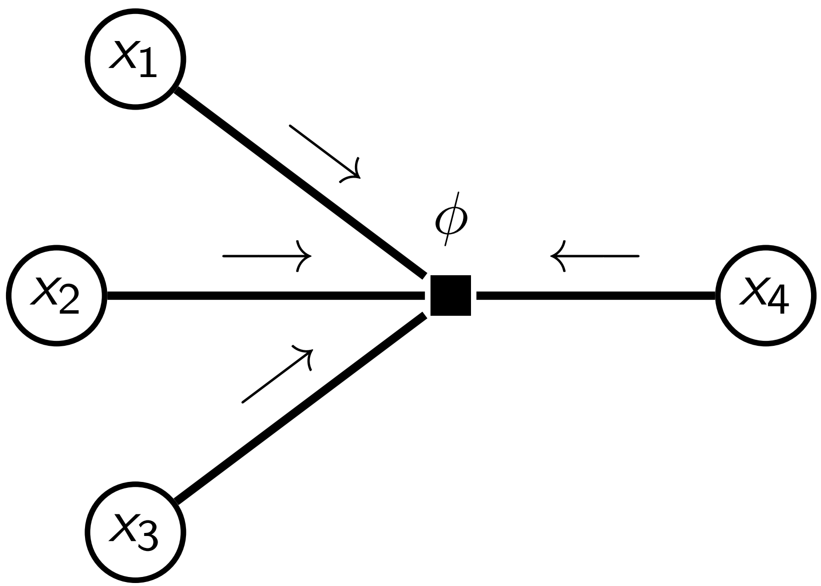
Note: The normalising constant Z can be computed for any of the marginals. Same as the normaliser for $p(x_1, \ldots, x_d) \propto \prod_i \phi_i(\mathcal{X}_i)$.

Rules of message passing: joint marginals

Note: The rules come from the fact that messages correspond to effective factors obtained after marginalisation.

Let $x_1, \ldots, x_j$ be all neighbours of factor node ϕ.

$$p(x_1, \ldots, x_j) = \frac{1}{Z}\phi(x_1, \ldots, x_j) \prod_{i=1}^{j} \mu_{x_i \to \phi}(x_i)$$



Other names for the sum-product algorithm

- Other names for the sum-product algorithm include
  - sum-product message passing
  - message passing
  - belief propagation
- Whatever the name: it is variable elimination applied to factor trees
- For numerical stability, often implemented in the log-domain.

Key advantages of the sum-product algorithm

Assume $p(x_1, \ldots, x_d) \propto \prod_{i=1}^m \phi_i(\mathcal{X}_i)$, with $\mathcal{X}_i \subseteq \{x_1, \ldots, x_d\}$, can be represented as a factor tree.

- The sum-product algorithm allows us to compute
  - *all* univariate marginals $p(x_i)$.
  - *all* joint distributions $p(\mathcal{X}_i)$ for the variables $\mathcal{X}_i$ that are part of the same factor ϕ_i.
- Cost: If variables can take maximally K values and there are maximally M elements in the $\mathcal{X}_i$: $O(2dK^M) = O(dK^M)$
- Note the linear increase in the number of variables d.

Applicability of the sum-product algorithm

- Factor graph must be a tree
- Can be used to compute conditionals (same argument as for variable elimination)
- May be used for continuous random variables (same caveats as for variable elimination)

If the factor graph is not a tree

- Use variable elimination
- Group variables together so that the factor graph becomes a tree (for details, see Chapter 6 in Barber, or Section V in Kschischang et al, *Factor Graphs and the Sum-Product Algorithm*, 2001; not examinable)
- Pretend the factor graph is a tree and use message passing (loopy belief propagation; not examinable)
- Can you condition on some variables so that the conditional is a tree? Message passing can then be used to solve part of the inference problem.

  Example: $p(x_1, x_2, x_3, x_4)$ is not a tree but $p(x_1, x_2, x_3 | x_4)$ is.
  Use law of total probability

$$p(x_1) = \sum_{x_4} \underbrace{\sum_{x_2, x_3} p(x_1, x_2, x_3 | x_4)}_{\text{by message passing}} p(x_4)$$

(see Barber Section 5.3.2, "Loop-cut conditioning"; not examinable)

Program

1. Factor graphs
2. Marginal inference by variable elimination
3. Marginal inference for factor trees (sum-product algorithm)
   - Factor trees
   - Sum-product algorithm = variable elimination for factor trees
   - Messages = effective factors
   - The rules for sum-product message passing
4. Inference of most probable states for factor trees

Program

1. Factor graphs
2. Marginal inference by variable elimination
3. Marginal inference for factor trees (sum-product algorithm)
4. Inference of most probable states for factor trees
    - Maximisers of the marginals $\neq$ maximiser of joint
    - We can exploit the factorisation (in the log-domain) using the distributive law $\max(u + v, u + w) = u + \max(v, w)$
    - Max-sum message passing

Inference task

- So far: given a joint distribution $p(\mathbf{x})$, find marginals or conditionals over variables
- Inference task of interest here:
  - Find a setting of the variables that maximises $p(\mathbf{x})$, i.e.

$$\hat{\mathbf{x}} = \underset{\mathbf{x}}{\operatorname{argmax}}\, p(\mathbf{x}) = \underset{\mathbf{x}}{\operatorname{argmax}} \log p(\mathbf{x})$$

  - Find the corresponding value maximal value of $p(\mathbf{x})$, i.e.

$$p_{\max} = p(\hat{\mathbf{x}}) = \max_{\mathbf{x}} p(\mathbf{x}) \quad \text{or}$$

$$\log p_{\max} = \log p(\hat{\mathbf{x}}) \stackrel{(*)}{=} \max_{\mathbf{x}} \log p(\mathbf{x})$$

    $(*)$ holds since log is monotonically increasing

- Note: the task includes $\operatorname{argmax}_{\mathbf{x}} \tilde{p}(\mathbf{x}|\mathbf{y}_o)$, which is known as maximum a-posteriori (MAP) estimation or inference.

Maximisers of the marginals $\neq$ maximiser of joint

- The sum-product algorithm gives us the univariate marginals $p(x_i)$ for all variables $x_1, \ldots, x_d$.
- But the vector with the $\operatorname{argmax}_{x_i} p(x_i)$, $x_1, \ldots, x_d$, is not the same as $\operatorname{argmax}_{\mathbf{x}} p(\mathbf{x})$
- Example (Bishop Table 8.1):

x_1	x_2	$p(x_1, x_2)$
0	0	0.3
1	**0**	0.4
0	1	0.3
1	1	0.0

x_1	$p(x_1)$
0	0.6
1	0.4

x_2	$p(x_2)$
0	0.7
1	0.3

Distributive law to exploit the factorisation

- We use that

$$\max_{\mathbf{x}} \log p(\mathbf{x}) = \max_{x_d} \max_{x_1,\ldots,x_{d-1}} \log p(\mathbf{x}) \tag{16}$$

  where x_d is an arbitrarily chosen variable that serves as "sink" (conceptually easiest: choose a leaf variable).
- Denote $\max_{x_1,\ldots,x_{d-1}} \log p(\mathbf{x})$ by $\gamma^*(x_d)$
- Inserting the assumed factorisation gives

$$\gamma^*(x_d) = \max_{x_1,\ldots,x_{d-1}} \log \frac{1}{Z} \prod_{i=1}^{m} \phi_i(\mathcal{X}_i) \tag{17}$$

$$= -\log Z + \max_{x_1,\ldots,x_{d-1}} \sum_{i=1}^{m} \log \phi_i(\mathcal{X}_i) \tag{18}$$

- Compare to formula for marginal $p(x_d)$

$$p(x_d) = \sum_{x_1,\ldots,x_{d-1}} p(\mathbf{x}) \propto \sum_{x_1,\ldots,x_{d-1}} \prod_{i=1}^{m} \phi_i(\mathcal{X}_i) \tag{19}$$

Distributive law to exploit the factorisation

- Correspondences

$$\sum_{x_1,\ldots,x_{d-1}} \longleftrightarrow \max_{x_1,\ldots,x_{d-1}}, \quad \prod_{i=1}^{m} \longleftrightarrow \sum_{i=1}^{m}, \quad \phi_i(\mathcal{X}_i) \longleftrightarrow \log \phi_i(\mathcal{X}_i)$$

- To compute $p(x_d)$, we relied on the distributive law

$$\text{sum}(ab, ac) = a\,\text{sum}(b, c)$$

- To compute $\gamma^*(x_d)$, we can use the distributive law

$$\max(\log a + \log b, \log a + \log c) = \log a + \max(\log b, \log c)$$

- Message passing algorithm by replacing sum with max, products with sums, and factors with log-factors.

Use correspondence to derive the algorithm

- In the sum-product algorithm to compute the marginal, consider the computation of the message $\mu_{\phi \to x}(x)$

$$\mu_{\phi \to x}(x) = \sum_{x_1,\ldots,x_j} \phi(x_1, \ldots, x_j, x) \cdot \prod_{i=1}^{j} \mu_{x_i \to \phi}(x_i) \tag{20}$$

- Replace sum with max, products with sums, and factors with log-factors to obtain the computation for the corresponding message $\gamma_{\phi \to x}(x)$

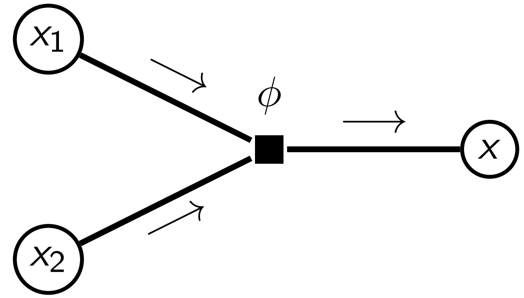
$$\gamma_{\phi \to x}(x) = \max_{x_1,\ldots,x_j} \log \phi(x_1, \ldots, x_j, x) + \sum_{i=1}^{j} \gamma_{x_i \to \phi}(x_i) \tag{21}$$

- Resulting algorithm is called max-sum message passing (max-product if we do not work in the log-domain)

Sum-product algorithm with x_d as sink (recap)

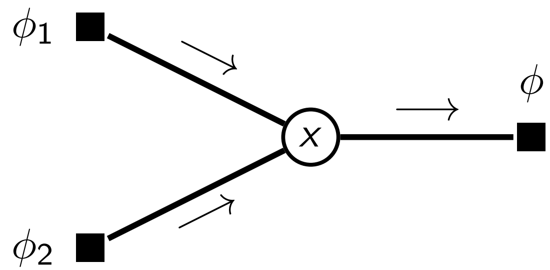
Factor to variable

$\mu_{\phi \to x}(x) = \sum_{x_1,\ldots,x_j} \phi(x_1,\ldots,x_j,x) \prod_{i=1}^{j} \mu_{x_i \to \phi}(x_i)$
where $\{x_1,\ldots,x_j\} = \mathrm{ne}(\phi) \setminus \{x\}$



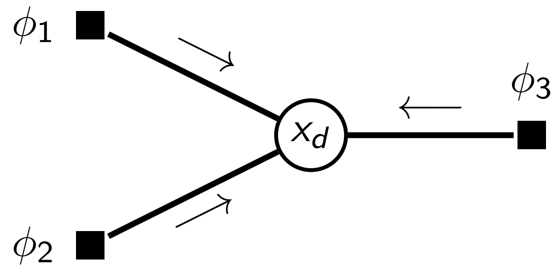
Variable to factor

$\mu_{x \to \phi}(x) = \prod_{i=1}^{j} \mu_{\phi_i \to x}(x)$
where $\{\phi_1,\ldots,\phi_j\} = \mathrm{ne}(x) \setminus \{\phi\}$



Univariate marginal

$p(x_d) = \frac{1}{Z} \prod_{i=1}^{j} \mu_{\phi_i \to x_d}(x_d)$
$Z = \sum_{x_d} \prod_{i=1}^{j} \mu_{\phi_i \to x_d}(x_d)$
where $\{\phi_1,\ldots,\phi_j\} = \mathrm{ne}(x_d)$

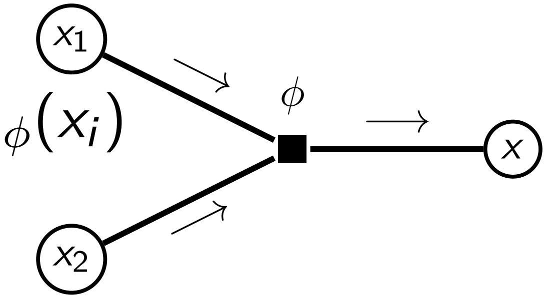


Initialisation

At leaf variable nodes: $\mu_{x \to \phi}(x) = 1$
At leaf factor nodes: $\mu_{\phi \to x}(x) = \phi(x)$

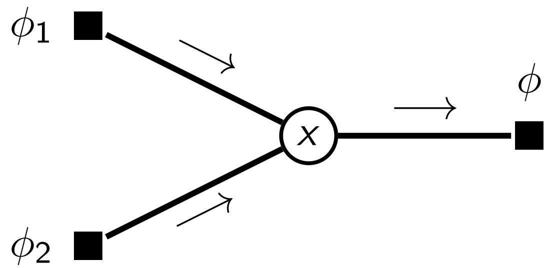
Max-sum algorithm with x_d as sink

Factor to variable



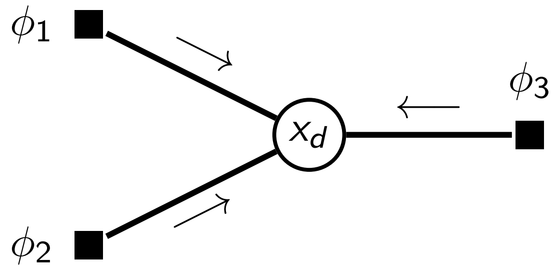
$\gamma_{\phi \to x}(x) = \max_{x_1,\ldots,x_j} \log \phi(x_1, \ldots, x_j, x) + \sum_{i=1}^{j} \gamma_{x_i \to \phi}(x_i)$
where $\{x_1, \ldots, x_j\} = \mathrm{ne}(\phi) \setminus \{x\}$

Variable to factor



$\gamma_{x \to \phi}(x) = \sum_{i=1}^{j} \gamma_{\phi_i \to x}(x)$
where $\{\phi_1, \ldots, \phi_j\} = \mathrm{ne}(x) \setminus \{\phi\}$

Maximum probability



$\gamma^*(x_d) = -\log Z + \sum_{i=1}^{j} \gamma_{\phi_i \to x_d}(x_d)$
$\log p_{\max} = \max_{x_d} \gamma^*(x_d)$
where $\{\phi_1, \ldots, \phi_j\} = \mathrm{ne}(x_d)$

Initialisation

At leaf variable nodes: $\gamma_{x \to \phi}(x) = 0$
At leaf factor nodes: $\gamma_{\phi \to x}(x) = \log \phi(x)$

Backward pass to compute $\mathrm{argmax}_{\mathbf{x}}\, p(\mathbf{x})$

- The max-sum algorithm computes $\gamma^*(x_d)$ and $\log p_{\max} = \max_{x_d} \gamma^*(x_d)$ in a forward pass through the graph.
- We can compute $\hat{\mathbf{x}} = \mathrm{argmax}_{\mathbf{x}}\, p(\mathbf{x})$ in a backward pass.
- When solving the optimisation problem in the forward pass

$$\gamma_{\phi \to x}(x) = \max_{x_1, \ldots, x_j} \log \phi(x_1, \ldots, x_j, x) + \sum_{i=1}^{j} \gamma_{x_i \to \phi}(x_i)$$

  we also build the function (look-up table)

$$\gamma^*_{\phi \to x}(x) = \mathop{\mathrm{argmax}}_{x_1, \ldots, x_j} \log \phi(x_1, \ldots, x_j, x) + \sum_{i=1}^{j} \gamma_{x_i \to \phi}(x_i)$$

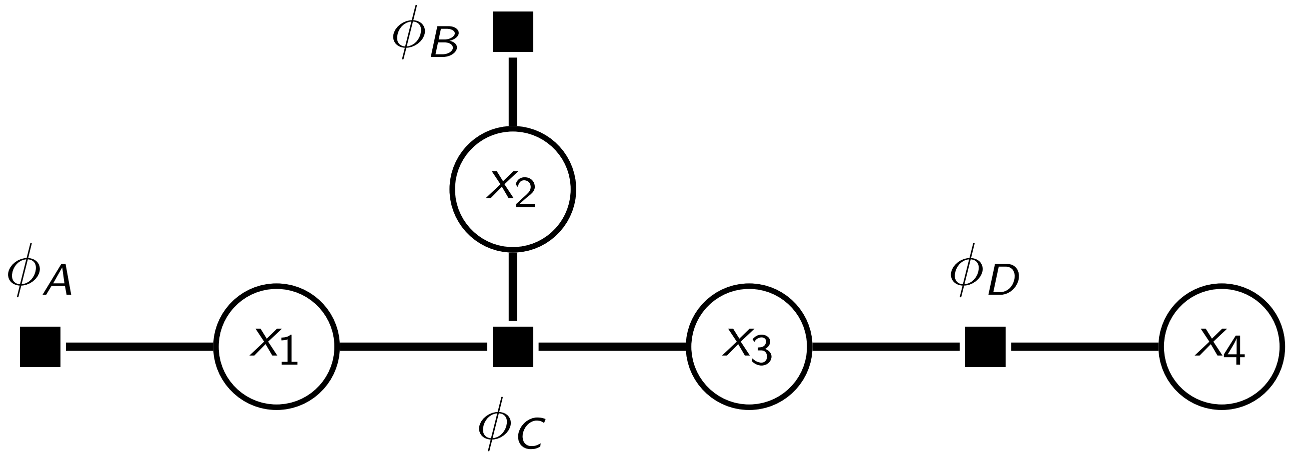
  which returns the maximiser $(\hat{x}_1, \ldots, \hat{x}_j)$ for each value of x.
- We then compute $\hat{\mathbf{x}}$ recursively, starting with $\hat{x}_d = \mathrm{argmax}_{x_d}\, \gamma^*(x_d)$ and backtrack to the earlier variables, obtaining further dimensions of $\hat{\mathbf{x}}$ with the look-up tables.

Example

Model (pmf):

$$p(x_1, x_2, x_3, x_4) \propto \phi_A(x_1)\phi_B(x_2)\phi_C(x_1, x_2, x_3)\phi_D(x_3, x_4)$$

Factor graph (tree):

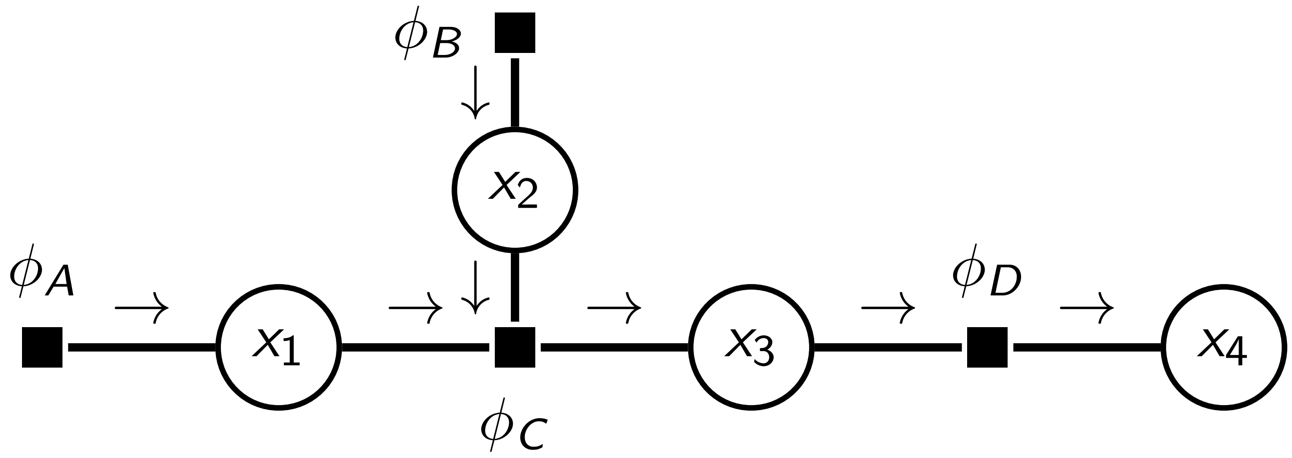


Goal:

$$\begin{aligned}(\hat{x}_1, \hat{x}_2, \hat{x}_3, \hat{x}_4) &= \underset{x_1,\ldots,x_4}{\operatorname{argmax}}\, p(x_1, x_2, x_3, x_4) \\ &= \underset{x_1,\ldots,x_4}{\operatorname{argmax}}\, \log p(x_1, x_2, x_3, x_4)\end{aligned}$$

Example: forward pass

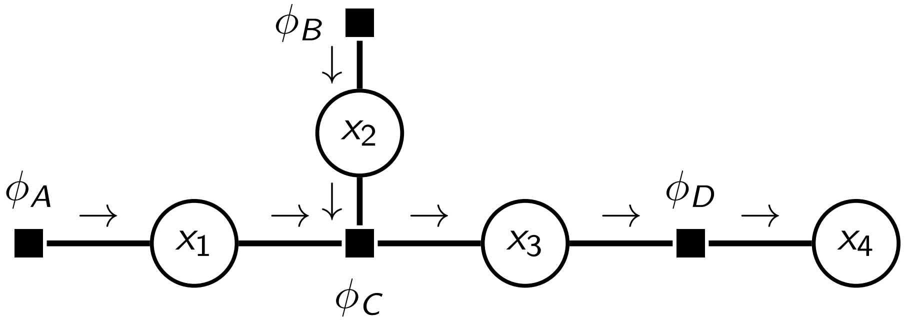
- Select sink towards which we send messages. Here: x_4 (arbitary choice).
- Messages that we need to send:



- Initialise:

$$\gamma_{\phi_A \to x_1}(x_1) = \log \phi_A(x_1)$$
$$\gamma_{\phi_B \to x_2}(x_2) = \log \phi_B(x_2)$$

Example: forward pass



- x_1 and x_2 copy the messages:

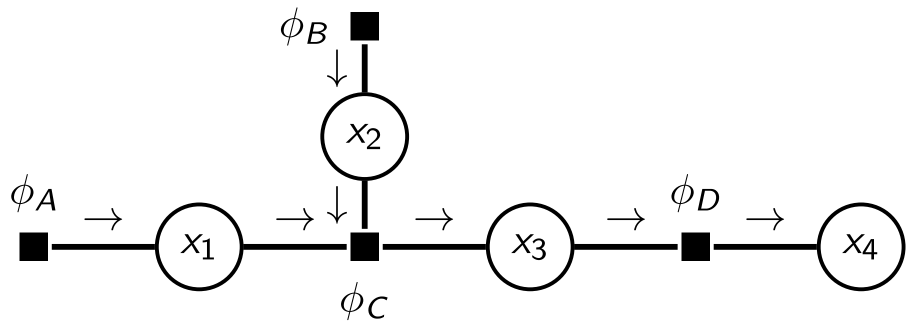
$$\gamma_{x_1 \to \phi_C}(x_1) = \gamma_{\phi_A \to x_1}(x_1)$$
$$\gamma_{x_2 \to \phi_C}(x_2) = \gamma_{\phi_B \to x_2}(x_2)$$

- For $\gamma_{\phi_C \to x_3}(x_3)$ solve optimisation problem

$$\gamma_{\phi_C \to x_3}(x_3) = \max_{x_1, x_2} [\log \phi_C(x_1, x_2, x_3) + \gamma_{x_1 \to \phi_C}(x_1) + \gamma_{x_2 \to \phi_C}(x_2)]$$
$$\gamma^*_{\phi_C \to x_3}(x_3) = \operatorname*{argmax}_{x_1, x_2} [\log \phi_C(x_1, x_2, x_3) + \gamma_{x_1 \to \phi_C}(x_1) + \gamma_{x_2 \to \phi_C}(x_2)]$$

for all values of x_3.

Example: forward pass

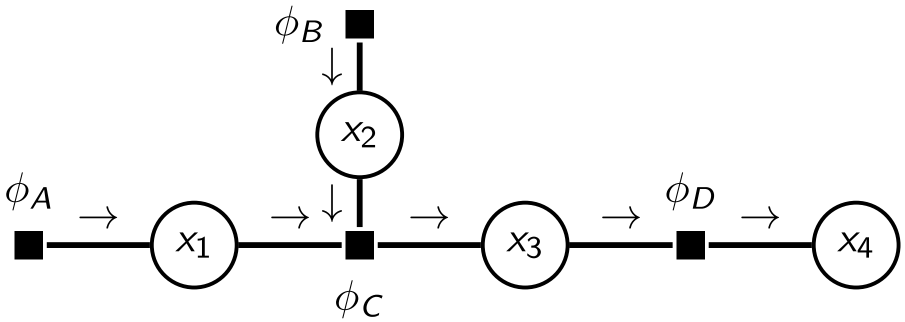


- x_3 copies the message: $\gamma_{x_3 \to \phi_D}(x_3) = \gamma_{\phi_C \to x_3}(x_3)$
- For $\gamma_{\phi_D \to x_4}(x_4)$ solve optimisation problem

$$\gamma_{\phi_D \to x_4}(x_4) = \max_{x_3} \left[\log \phi_D(x_3, x_4) + \gamma_{x_3 \to \phi_D}(x_3)\right]$$
$$\gamma^*_{\phi_D \to x_4}(x_4) = \operatorname*{argmax}_{x_3} \left[\log \phi_D(x_3, x_4) + \gamma_{x_3 \to \phi_D}(x_3)\right]$$

for all values of x_4.

Example: forward pass



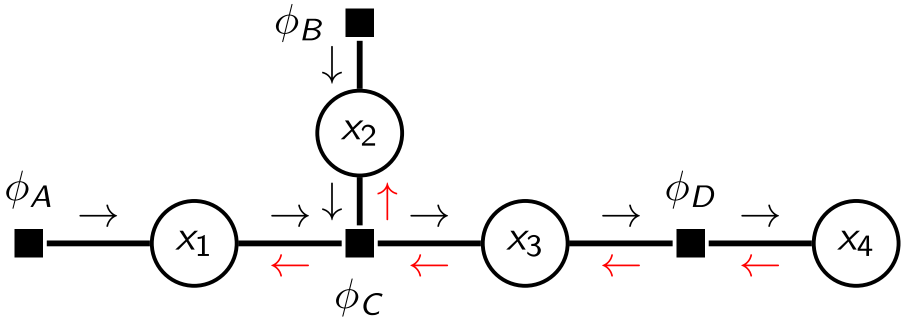
- After computation of $\gamma_{\phi_D \to x_4}(x_4)$, we obtain $\log p_{\max}$ as

$$\log p_{\max} = \max_{x_d} \gamma^*(x_d)$$

$$\gamma^*(x_4) = -\log Z + \gamma_{\phi_D \to x_4}(x_4)$$

- This requires knowledge of Z. We can compute Z via the sum-product algorithm.
- Z not needed if we are only interested in $\operatorname{argmax} p(x_1, \ldots, x_4)$

Example: backward pass



Backtracking:

- Compute $\hat{x}_4 = \mathrm{argmax}_{x_4} \gamma^*(x_4) = \mathrm{argmax}_{x_4} \gamma_{\phi_D \to x_4}(x_4)$
- Plug $\hat{x}_4$ into look-up table $\gamma^*_{\phi_D \to x_4}(x_4)$ to look up best value of x_3:
$$\hat{x}_3 = \gamma^*_{\phi_D \to x_4}(\hat{x}_4)$$
- Plug $\hat{x}_3$ into look-up table $\gamma^*_{\phi_C \to x_3}(x_3)$ to look up best values of (x_1, x_2):
$$(\hat{x}_1, \hat{x}_2) = \gamma^*_{\phi_C \to x_3}(\hat{x}_3)$$
- This gives $(\hat{x}_1, \hat{x}_2, \hat{x}_3, \hat{x}_4) = \mathrm{argmax}_{x_1,\ldots,x_4} p(x_1, x_2, x_3, x_4)$

Program recap

1. Factor graphs
   - Definition
   - Visualising Gibbs distributions as factor graphs
   - Factor graphs represent factorisations better than undirected graphs
2. Marginal inference by variable elimination
   - Exploiting the factorisation by using the distributive law $ab + ac = a(b + c)$ and by caching computations
   - Variable elimination for general factor graphs
   - The principles of variable elimination also apply to continuous random variables
3. Marginal inference for factor trees (sum-product algorithm)
   - Factor trees
   - Sum-product algorithm = variable elimination for factor trees
   - Messages = effective factors
   - The rules for sum-product message passing
4. Inference of most probable states for factor trees
   - Maximisers of the marginals $\neq$ maximiser of joint
   - We can exploit the factorisation (in the log-domain) using the distributive law $\max(u + v, u + w) = u + \max(v, w)$
   - Max-sum message passing