CENTRE FOR ARTIFICIAL INTELLIGENCE

Message Passing Algorithms in Machine Learning

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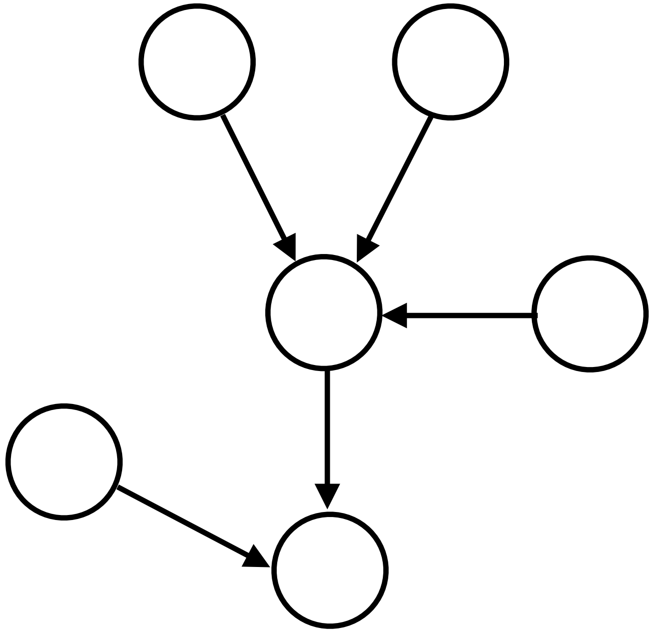
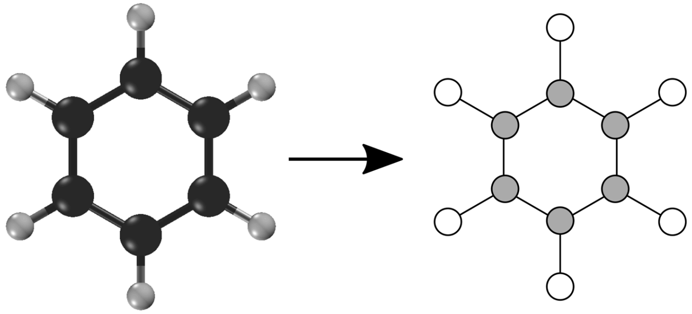
What we will cover in this lecture

We will study machine learning algorithms on **graphs**



Belief network

Images



Molecules

Social networks

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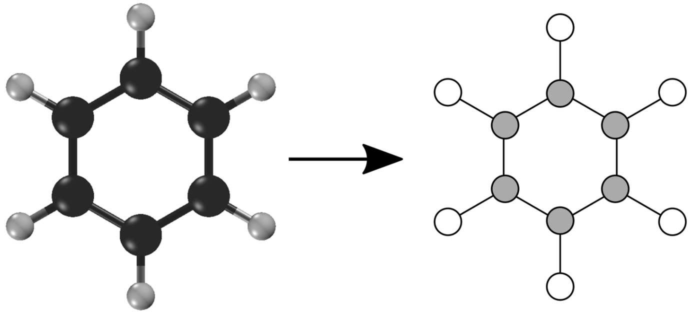
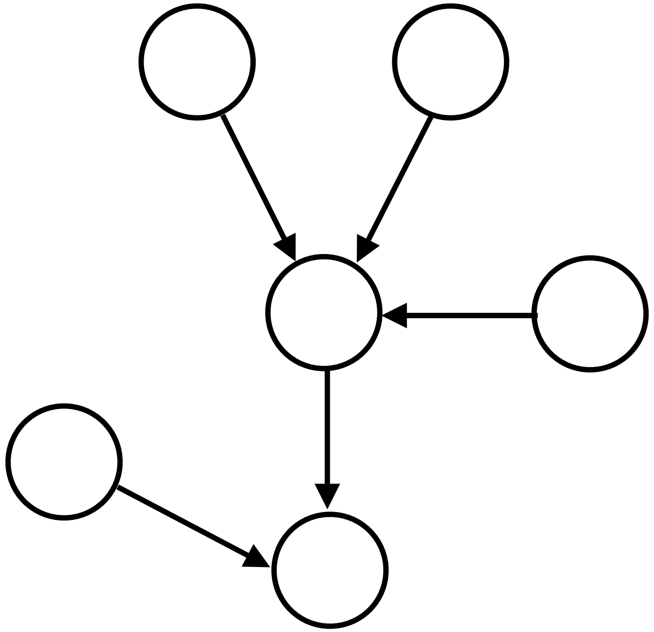


Molecules



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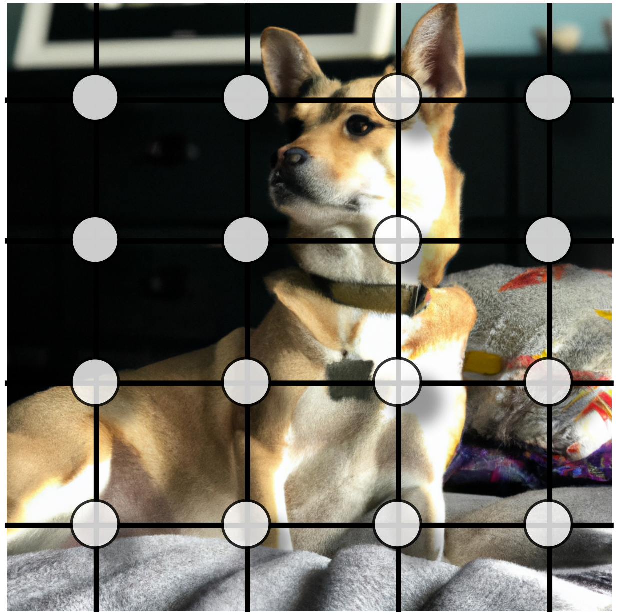


Images

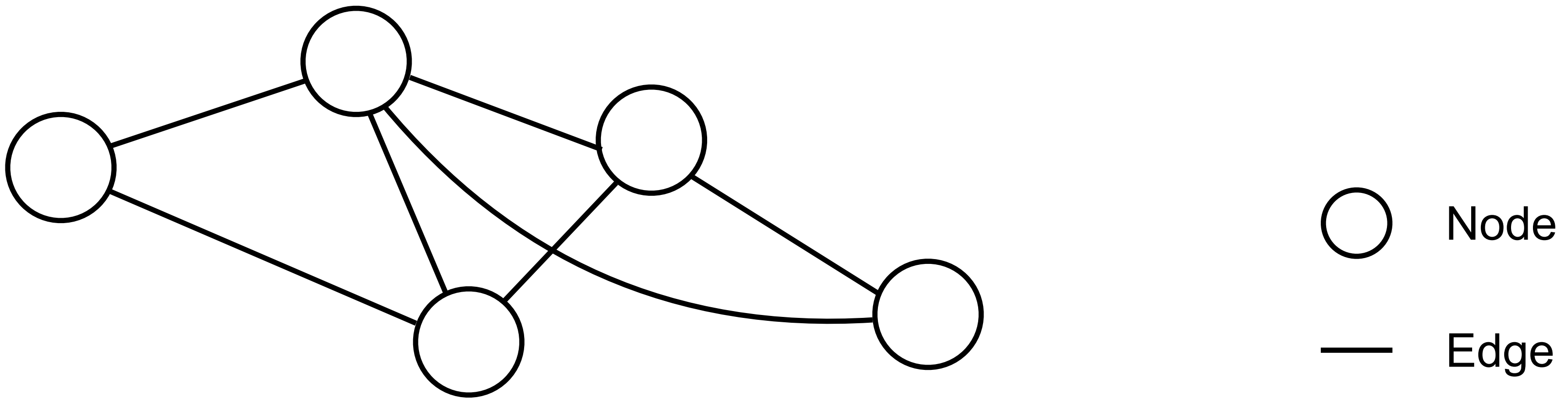
Social networks

What are graphs?

A **Graph** is a collection (V, E) of

- V: nodes
- E: edges

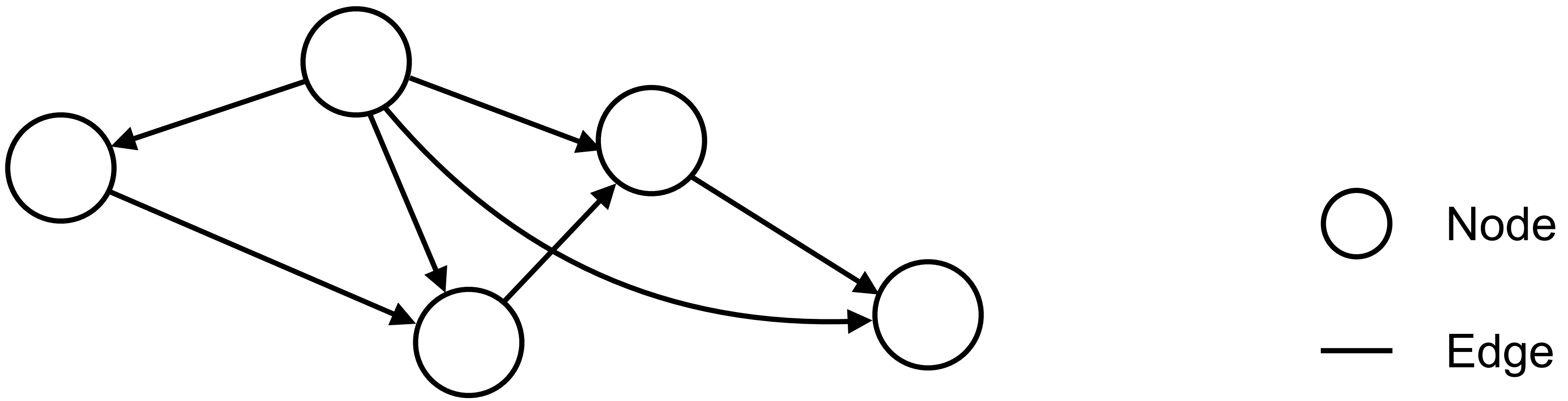
such that an edge $e \in E$ can be associated with a pair of nodes $u, v \in V$.



A graph

- A graph is *directed* if the ordering of nodes associated to an edge "matters"

i.e., $\exists\, \phi : E \rightarrow V \times V$ mapping an edge to an *ordered tuple* of nodes.



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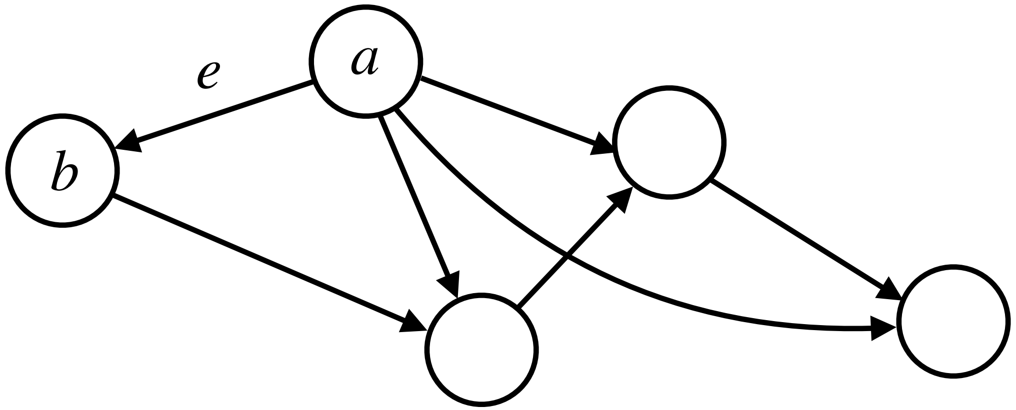

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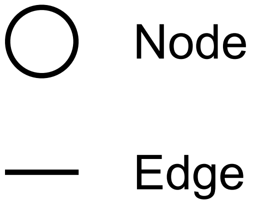

- Edges $\phi(e) = (a, b)$ in a directed graph represented graphically as arrows

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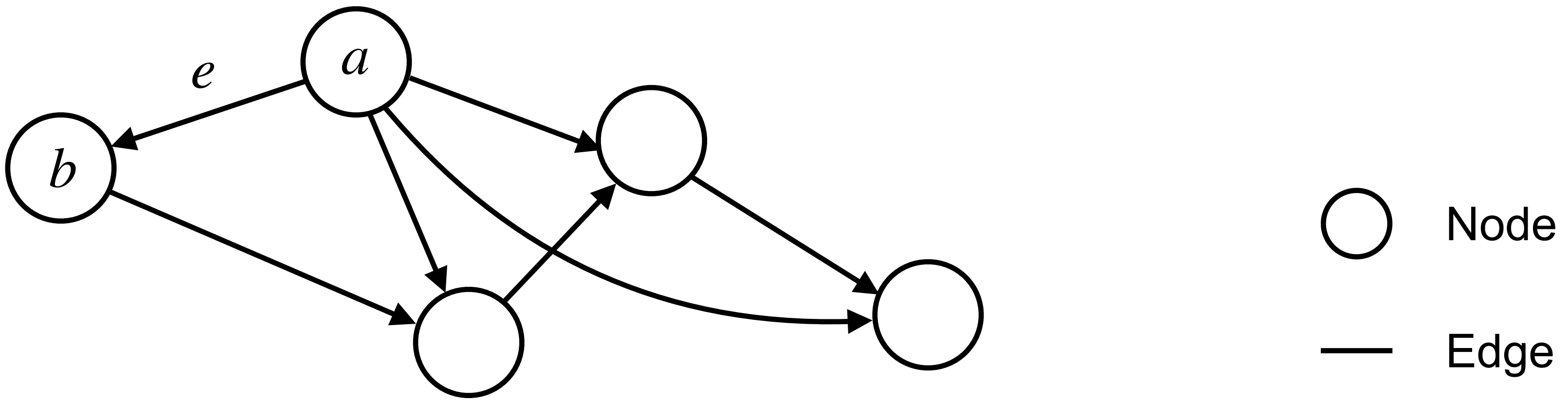


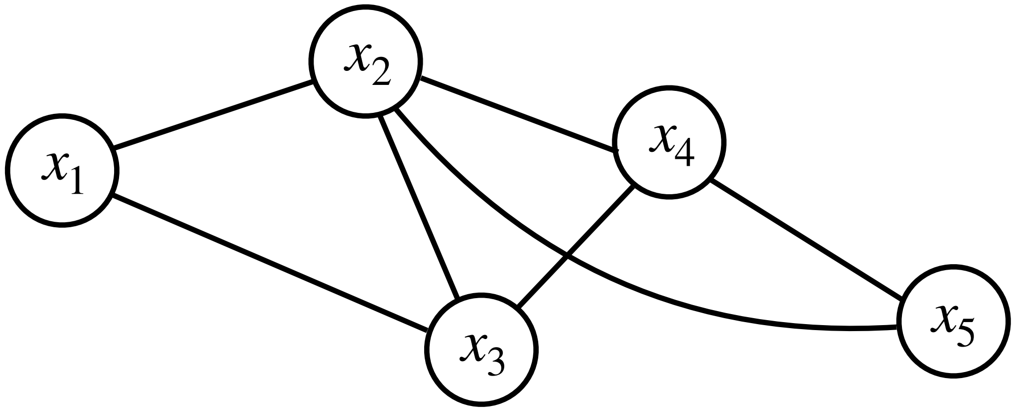
A directed graph

- Edges $\phi(e) = (a, b)$ in a directed graph represented graphically as arrows
- A graph is *undirected* if ordering of nodes in an edge doesn’t matter

- The edges E of a graph define an **adjacency relation** $\sim$ on V:

  For $x, y \in V$,

$$x \sim y \quad \Leftrightarrow \quad \{(x, y)\} \cup \{(y, x)\} \subset \phi(E).$$



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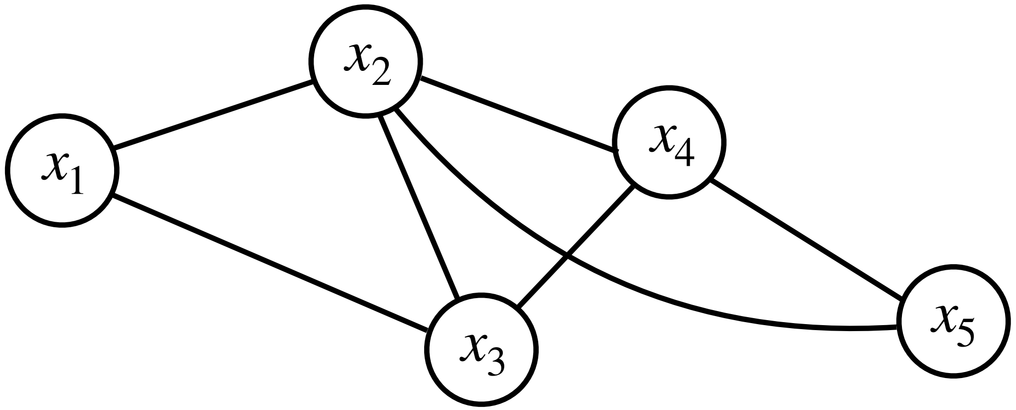

On the graph on the left, we have e.g.

- $x_1 \sim x_2$
- $x_4 \sim x_5$
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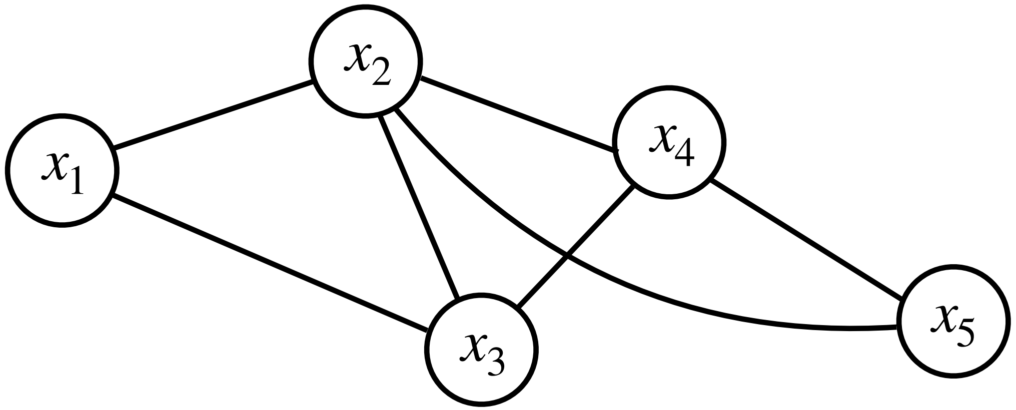

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- $x_1 \sim x_2$
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- If $x \sim y$, we say that y is a *neighbour* of x and vice versa

- Adjacency matrix $\mathbf{A}$ encodes the adjacency structure of G:

$$\mathbf{A}_{ij} = \begin{cases} 1, & \text{if } x_i \sim x_j, \\ 0, & \text{if } x_i \nsim x_j. \end{cases}$$

- Degree matrix $\mathbf{D}$ encodes the degree of connectivity of each node:

$$\mathbf{D}_{ij} = \begin{cases} |\text{Neighbours}(x_i)|, & \text{if } i = j, \\ 0, & \text{if } i \neq j. \end{cases}$$

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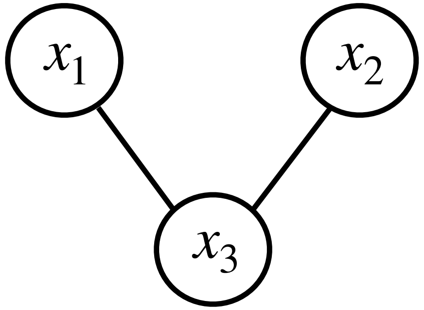

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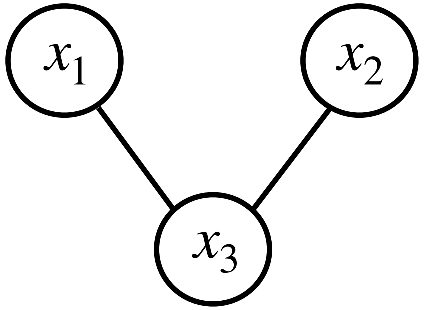

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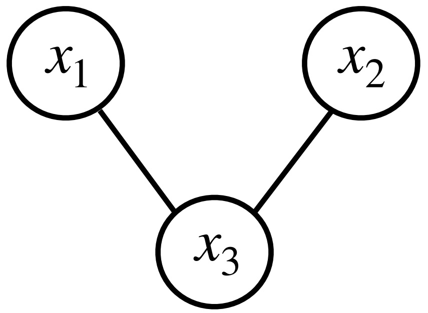

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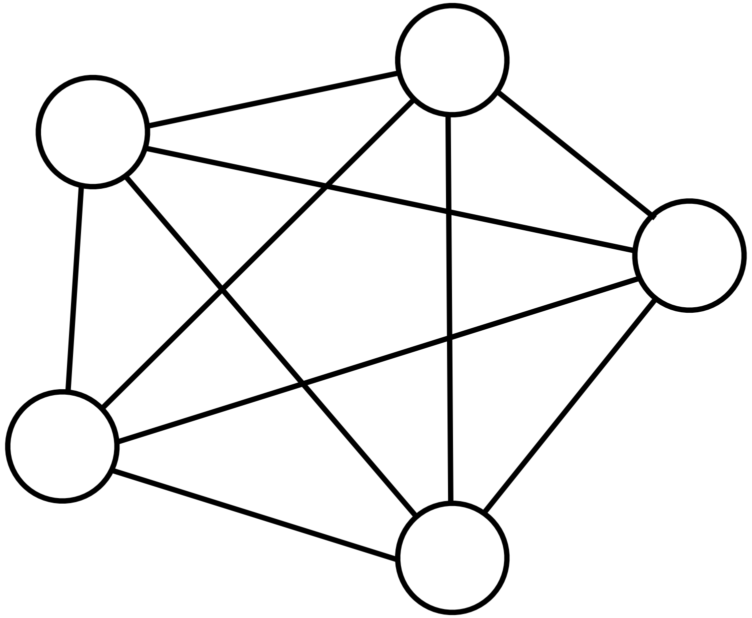
- Degree matrix $\mathbf{D}$ encodes the degree of connectivity of each node:

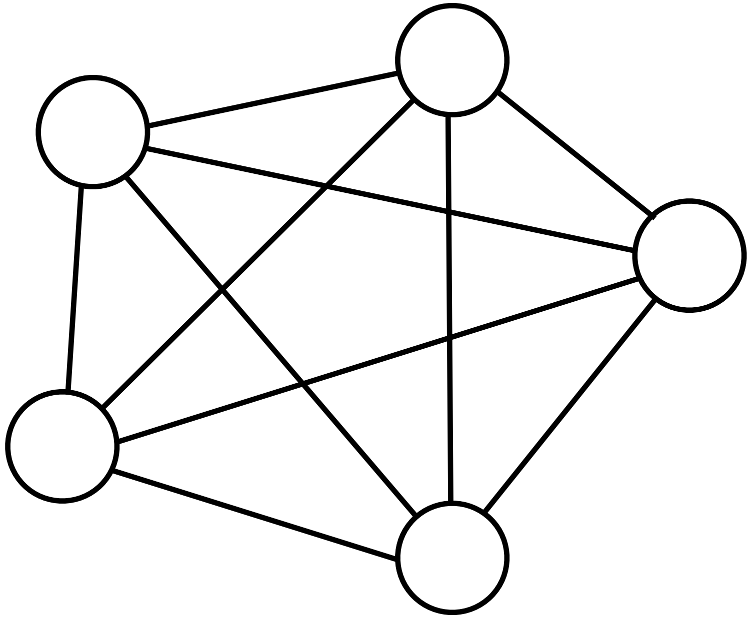
$$\mathbf{D} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 2 \end{pmatrix}$$

Types of Graphs



1. **Fully-connected graphs**

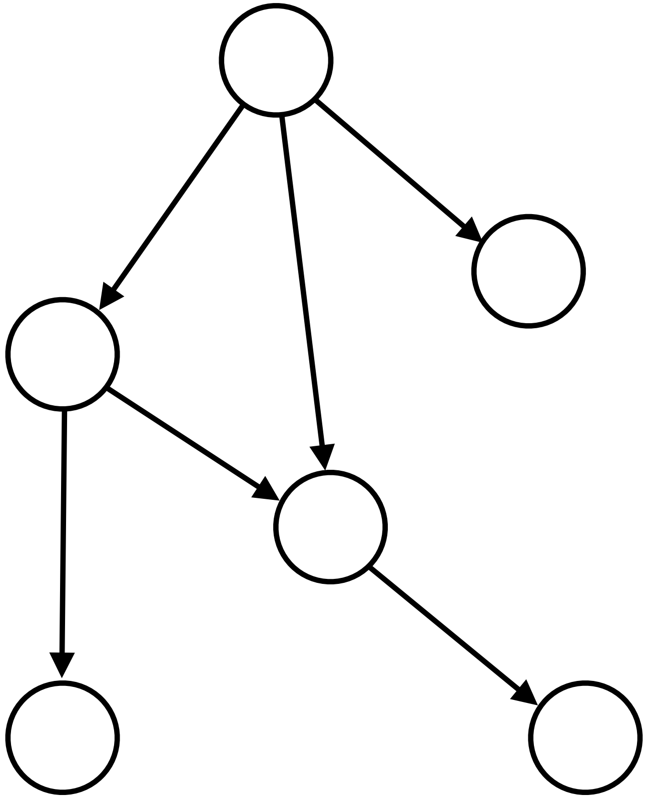
Types of Graphs



1. Fully-connected graphs

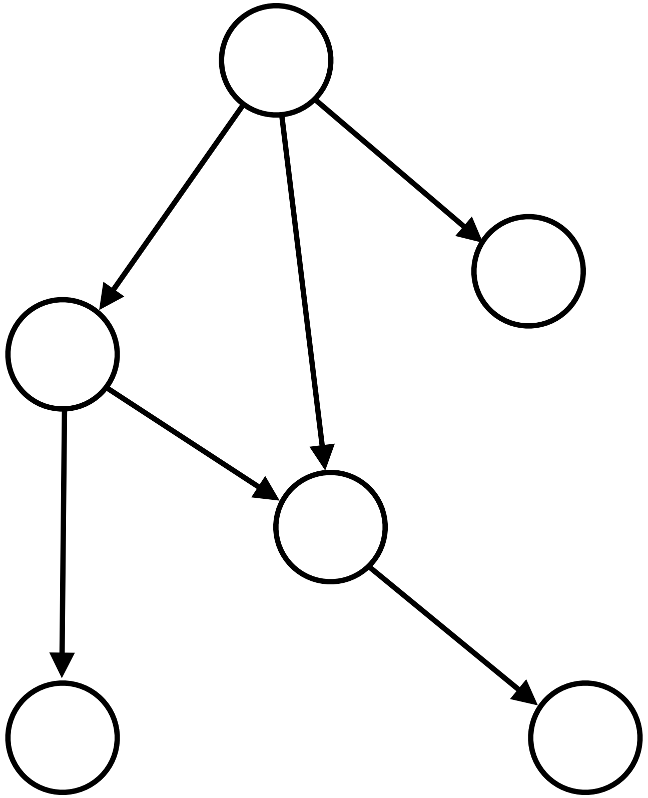
- Undirected
- Each node is connected to every other nodes

Types of Graphs



2. Directed Acyclic Graph (DAG)

Types of Graphs



2. Directed Acyclic Graph (DAG)

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- Does not contain any *directed* cycles

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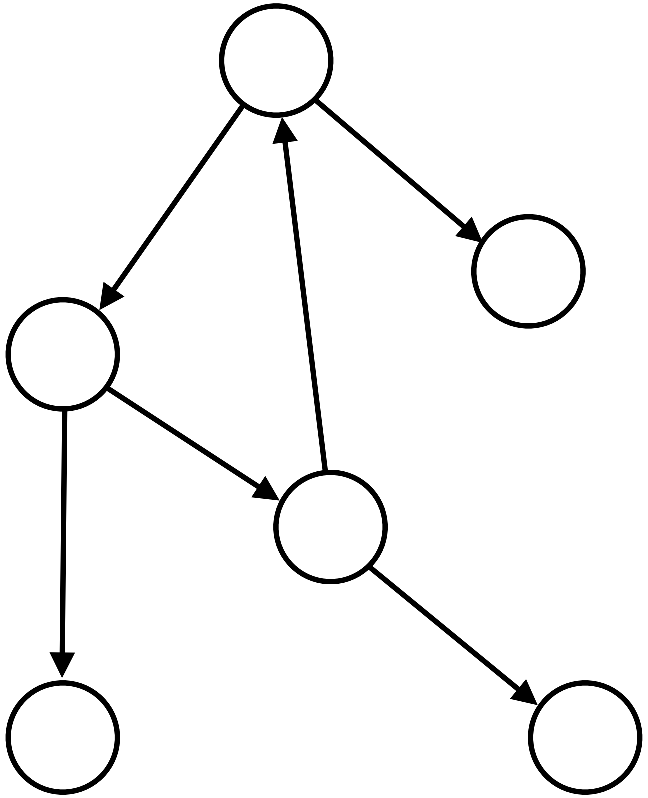

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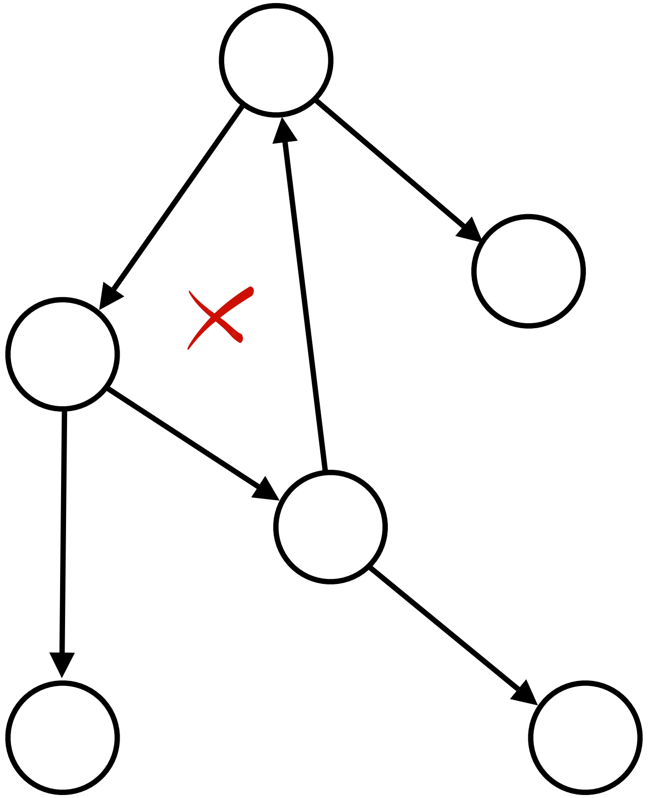

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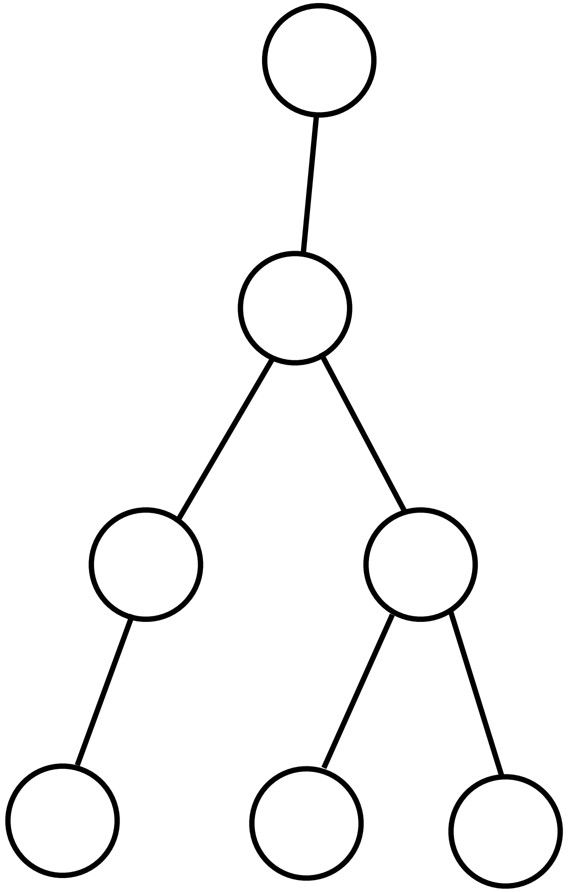
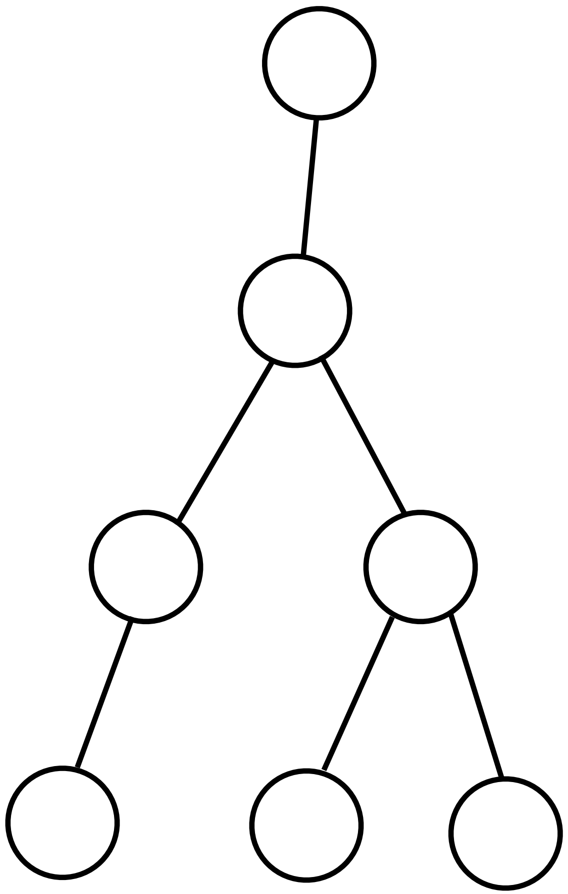


3. Trees and polytrees

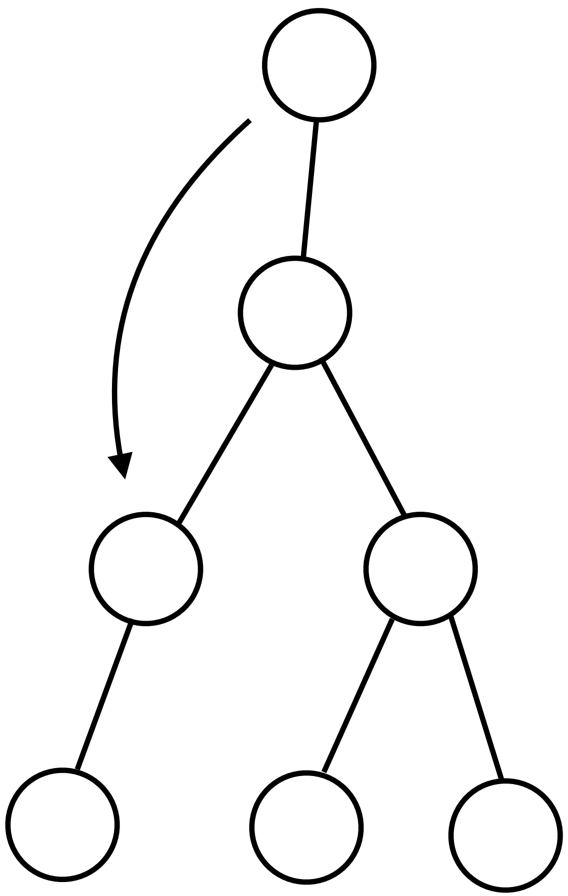
Types of Graphs



3. Trees and polytrees

- A tree is an *undirected* graph such that two nodes are connected by a unique path

Types of Graphs



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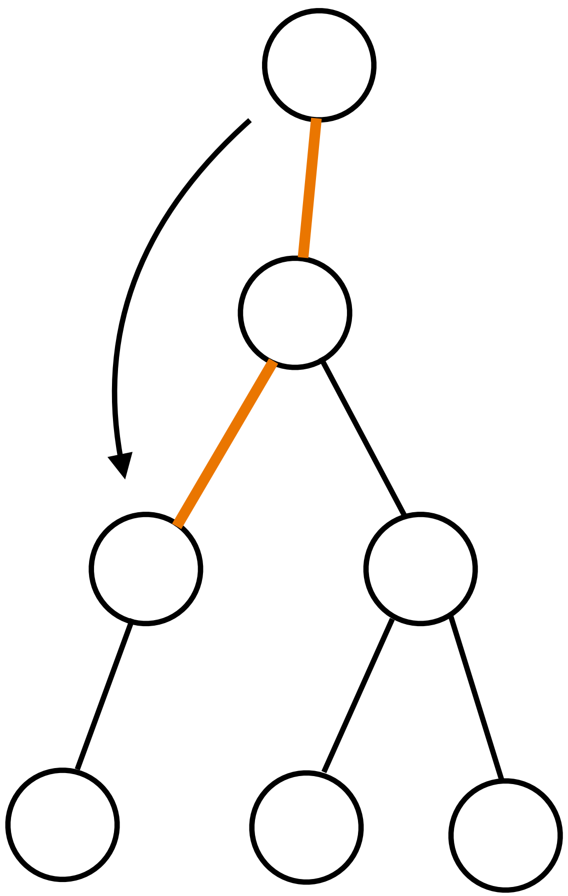

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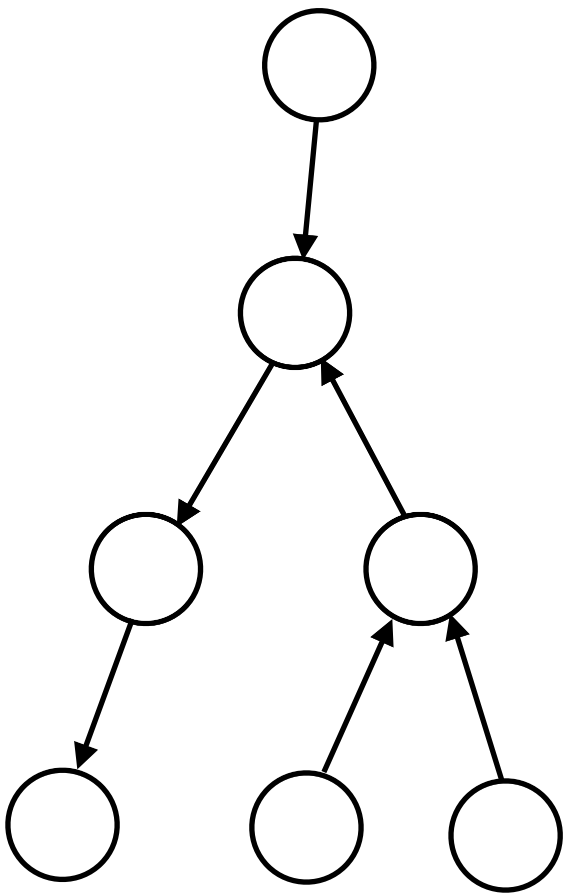

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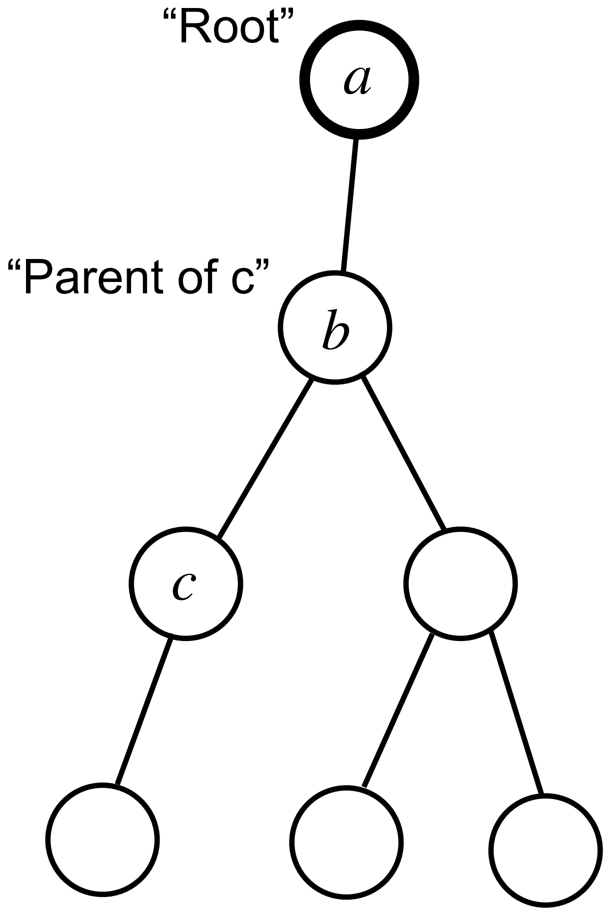

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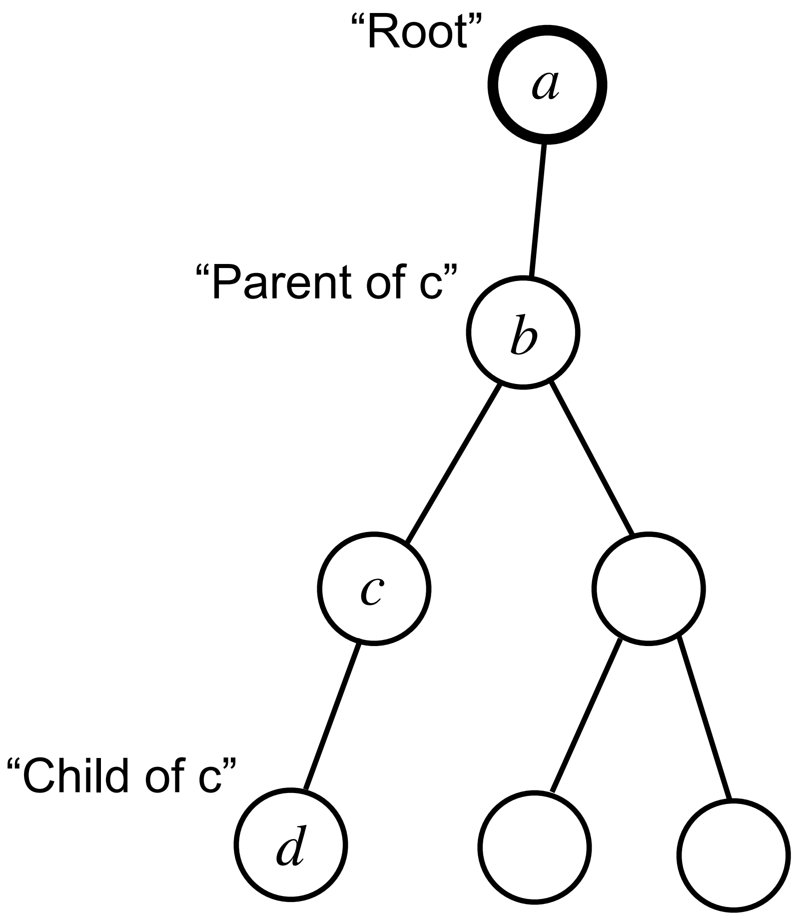

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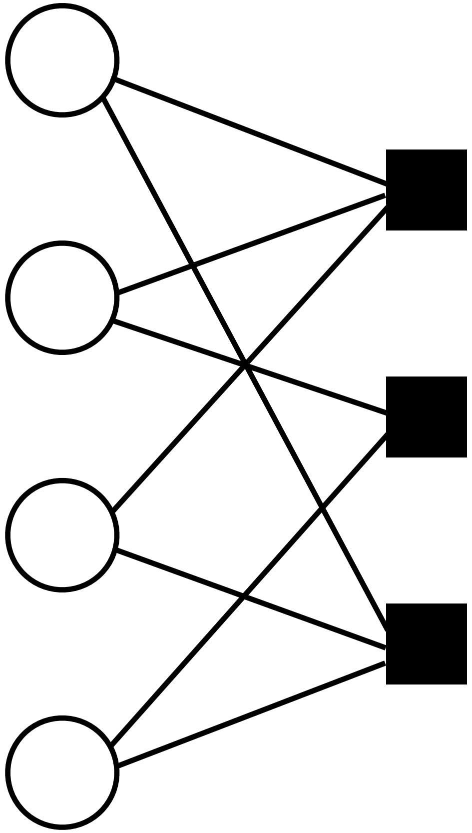
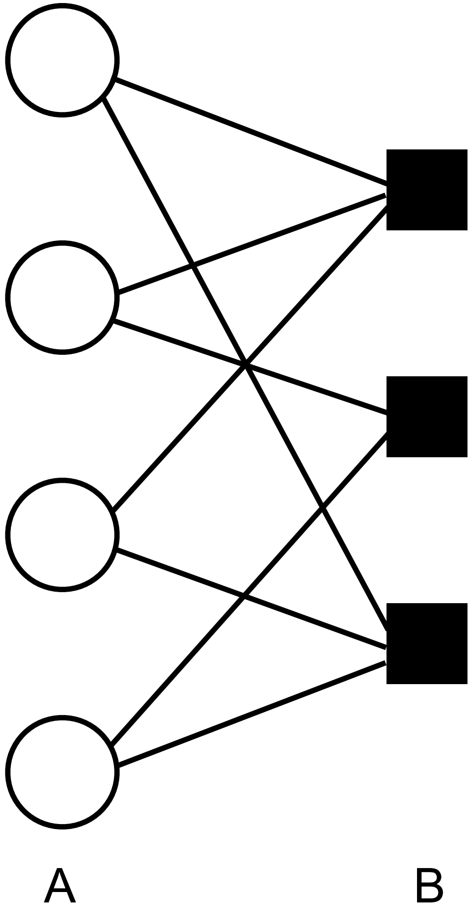
- Likewise d is a *child* of c if c is it’s parent

Types of Graphs



4. Bipartite graphs

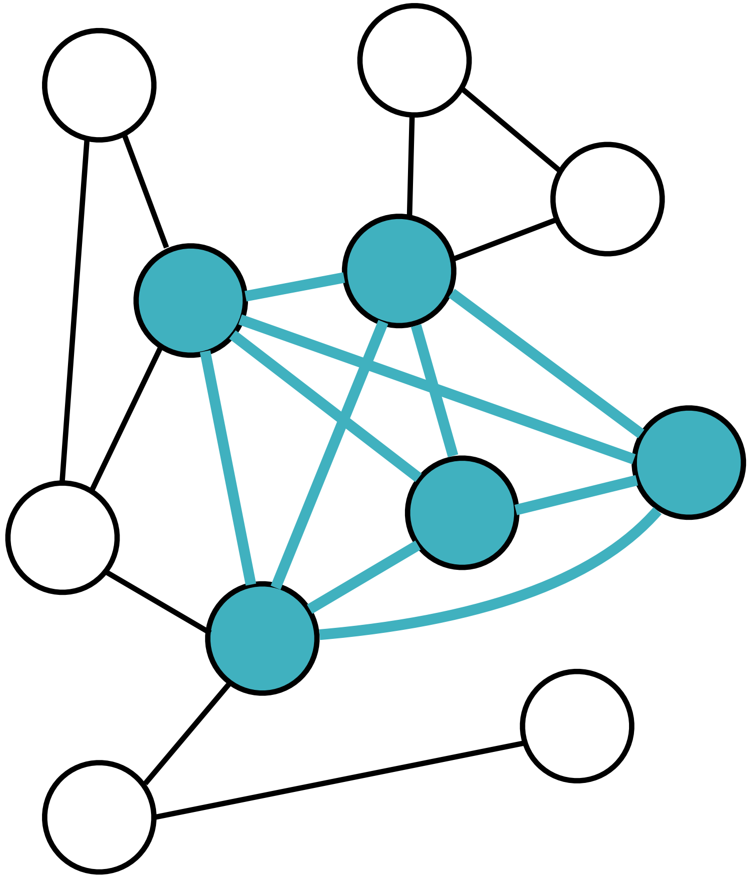
Types of Graphs



4. Bipartite graphs

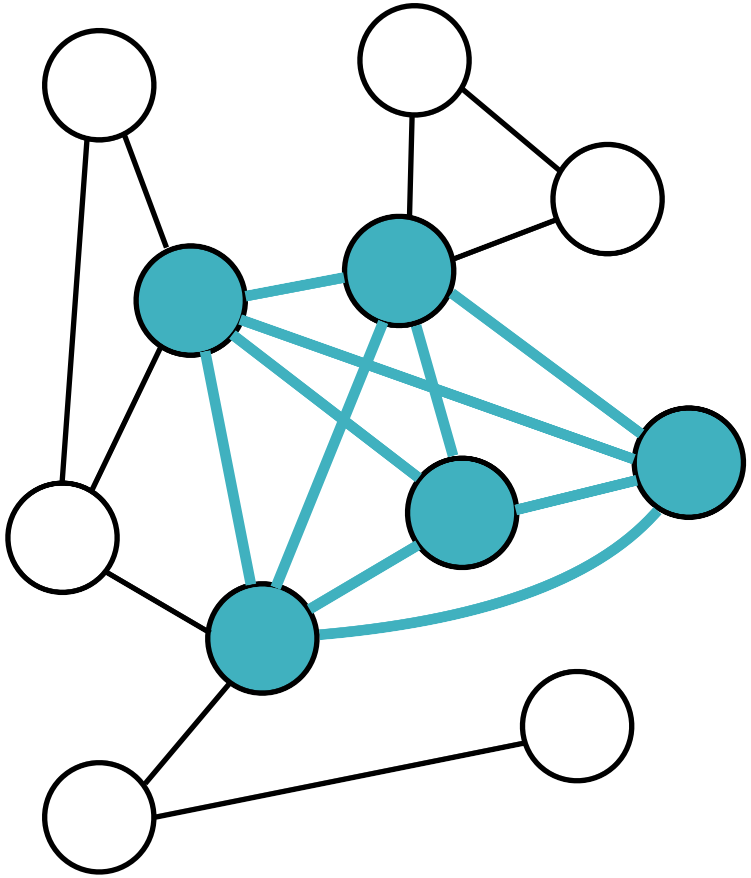
- Nodes can be divided into two “classes” (say A and B)
- Each edge connects a node in A with a node in B
- Can be either directed or undirected

Types of Graphs



5. Subgraphs

Types of Graphs



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Let $G = (V, E)$ be a graph.

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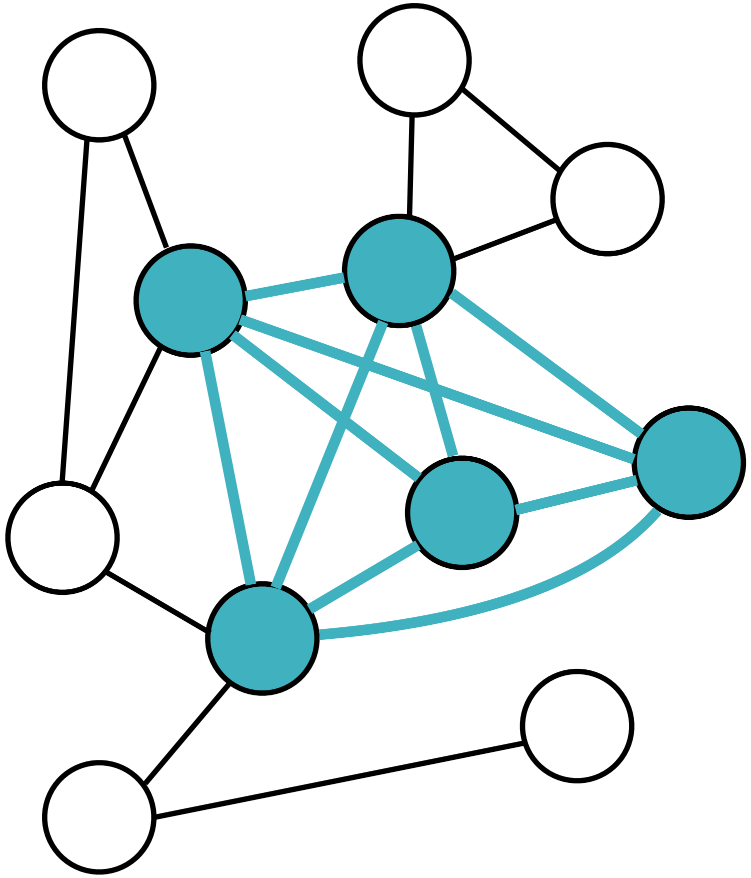

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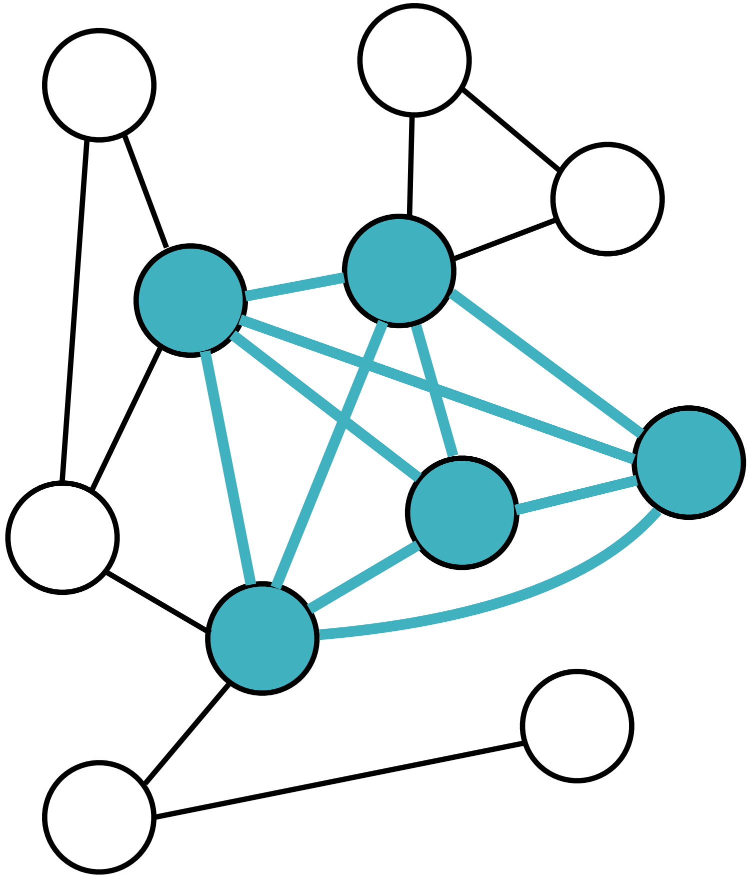

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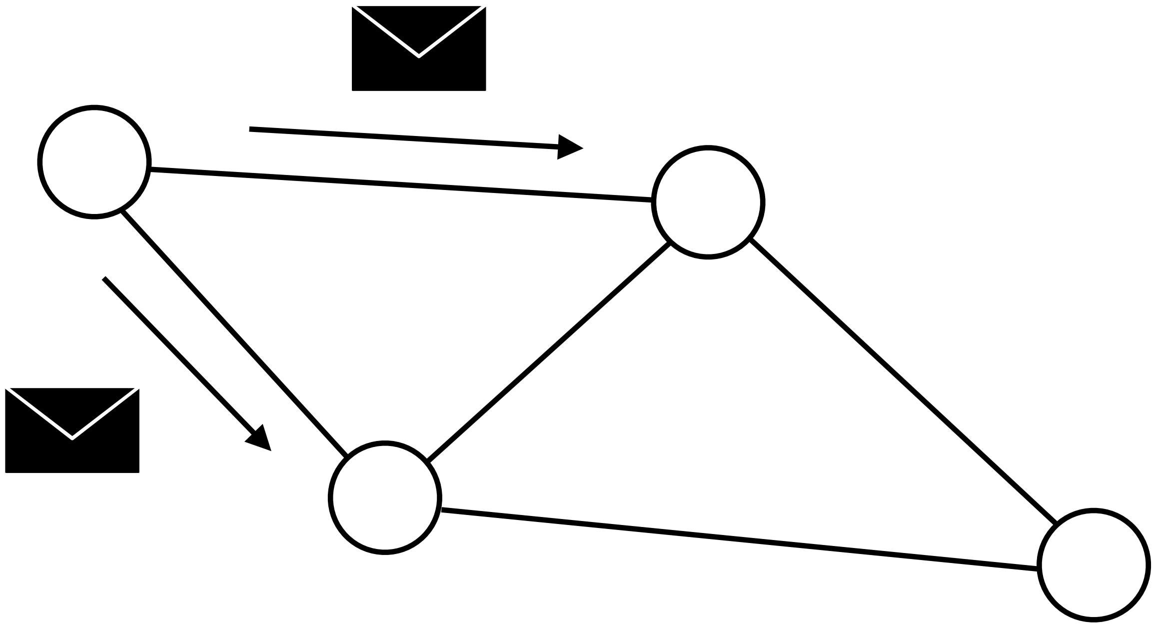
- A subgraph $G_1 = (V_1, E_1)$ of G is a graph such that $V_1 \subset V$ and $E_1 \subset E$
- If a subgraph is *fully-connected*, then we call it a **clique**

Message passing

Algorithms defined on graphs where information is passed between neighbours



Topics covered in this lecture

1. Probabilistic graphical models (PGMs)
2. Belief propagation on PGMs
3. Some extensions of belief propagation
4. Message passing neural networks

Supplementary materials

- Github link: https://github.com/sotakao/ml-seminar-ucl
- References provided at the end of each section
- See Bishop's book [1] for necessary background in graphs and probability theory

[1] Bishop, Christopher M. *Pattern Recognition and Machine Learning*. New York: springer, 2006.

1. Probabilistic Graphical Models (PGMs)

Example

$$p(x_1, x_2, x_3, x_4, x_5, x_6, x_7) = p(x_1)\, p(x_2)\, p(x_3)\, p(x_4 \mid x_1, x_2, x_3)$$
$$p(x_5 \mid x_1, x_3)\, p(x_6 \mid x_4)\, p(x_7 \mid x_4, x_5)$$

Example

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Questions:

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Questions:

- If x_4 is observed, are the variables x_2 and x_6 independent?

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- Which variable should we observe for x_6 and x_7 to be independent?

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- Which variable should we observe for x_6 and x_7 to be independent?

  i.e., $p(x_6, x_7 \,|\, ?) = p(x_6 \,|\, ?)\,p(x_7 \,|\, ?)$

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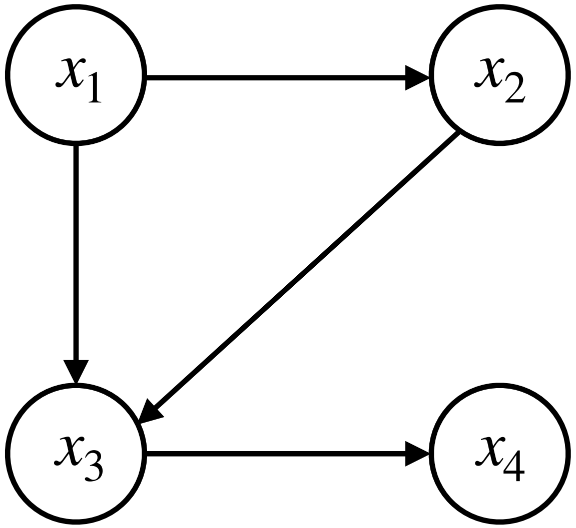
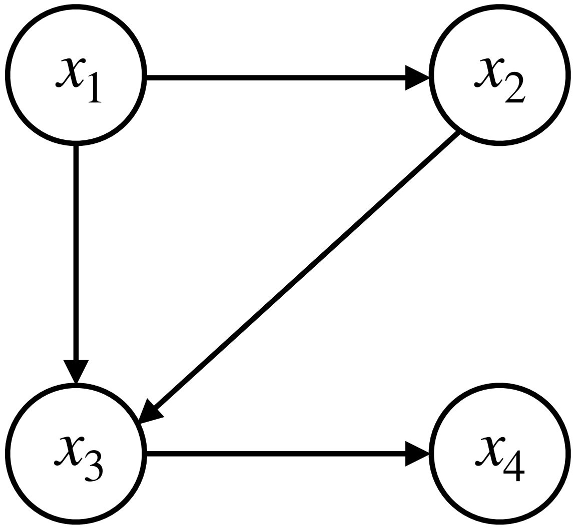
PGMs provide elegant answers to such questions!

Bayesian Networks



Bayesian Networks



Bayesian networks (BN) visualise how a **joint probability distribution** factorises into **conditional probability distributions**

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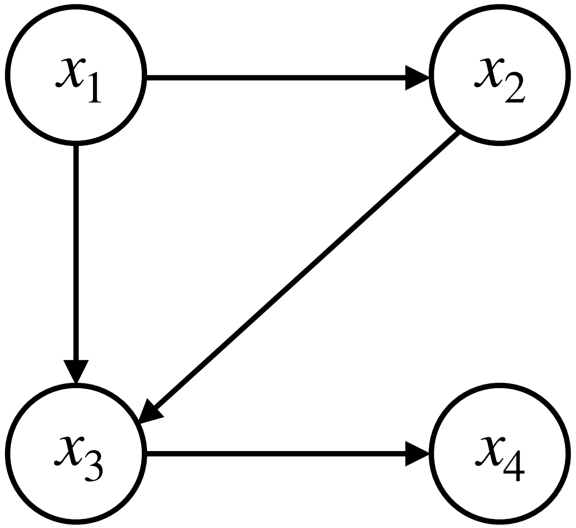
Bayesian Networks



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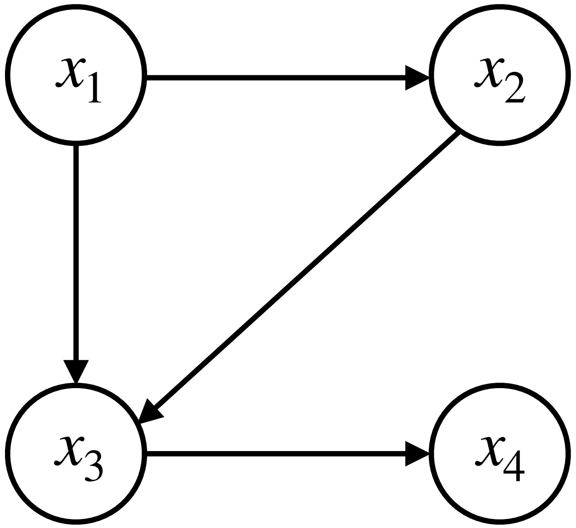
Bayesian Networks



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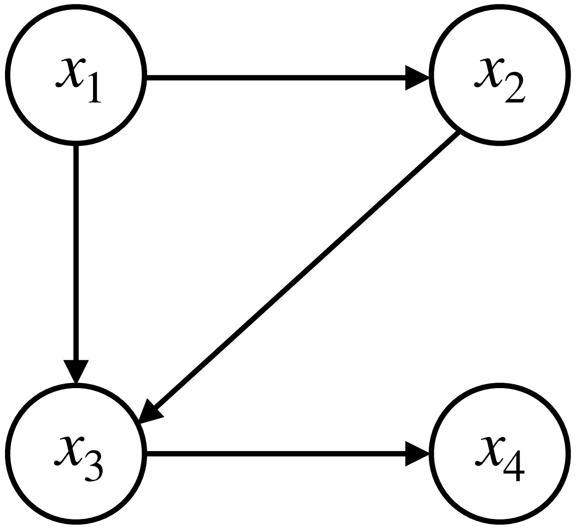

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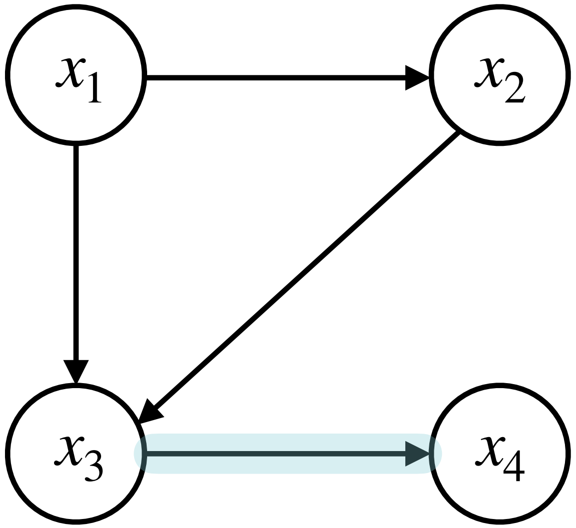

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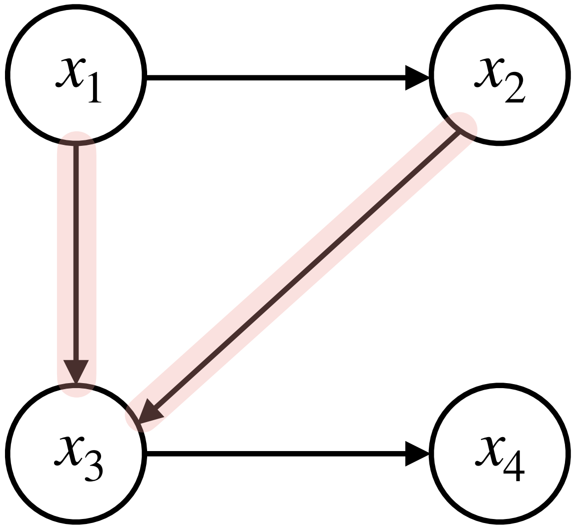

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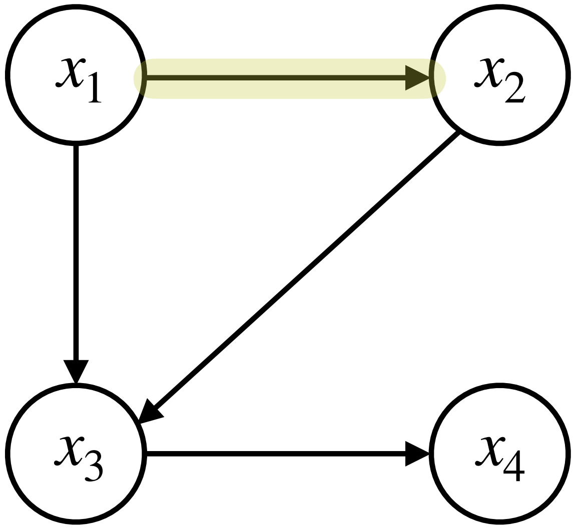

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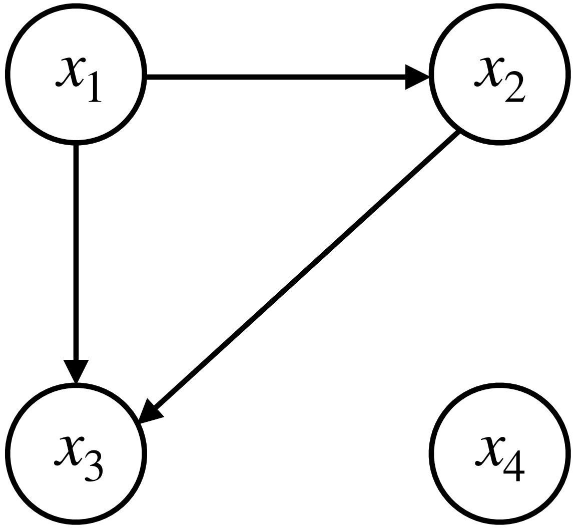

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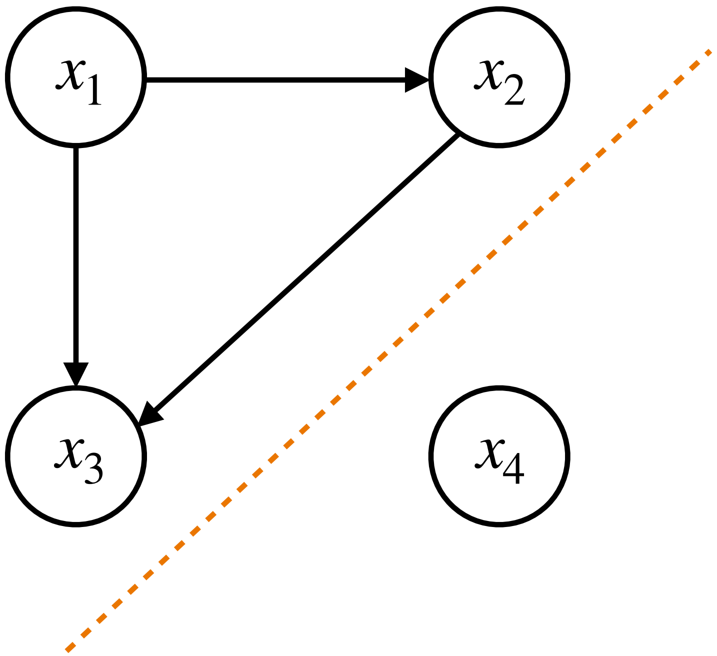

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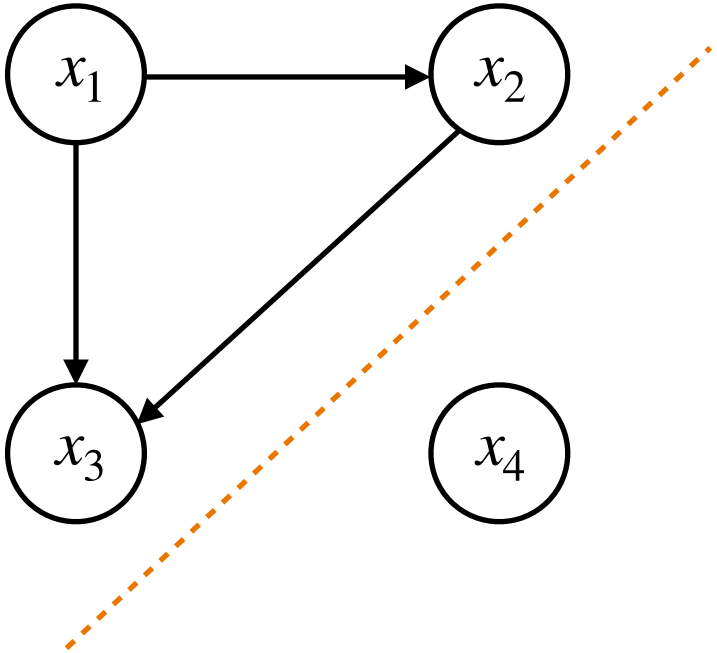

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x_4 is independent of all other nodes

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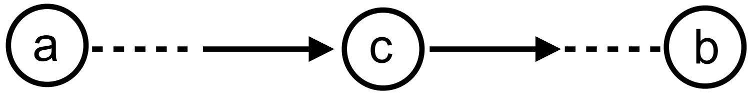
1. 

Path contains a **chain** and c belongs to Z.

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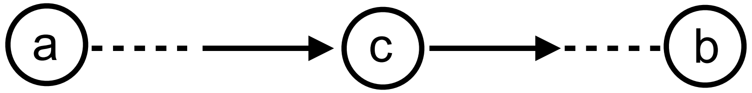
1. 

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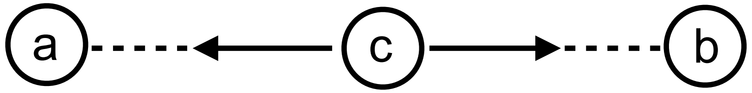
2. 

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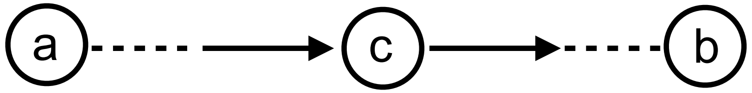
1. 

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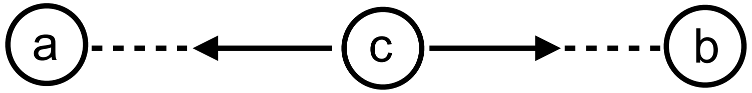
2. 

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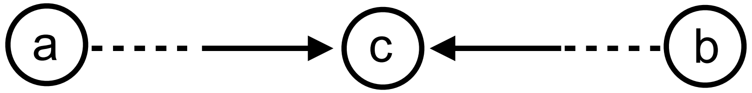
3. 

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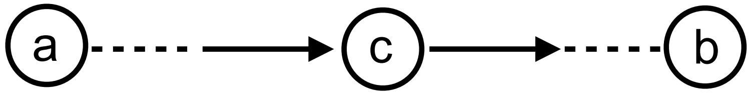
1. 

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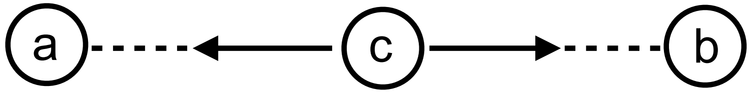
2. 

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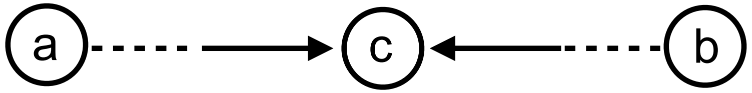
3. 

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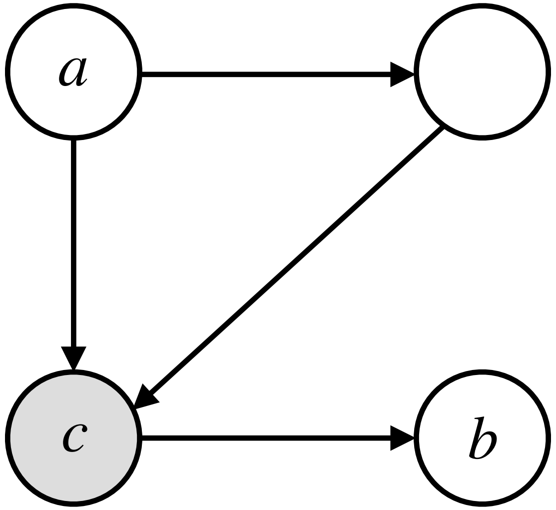
Property: variables a, b are independent given Z ⇔ they are d-separated by Z

Example of d-separation



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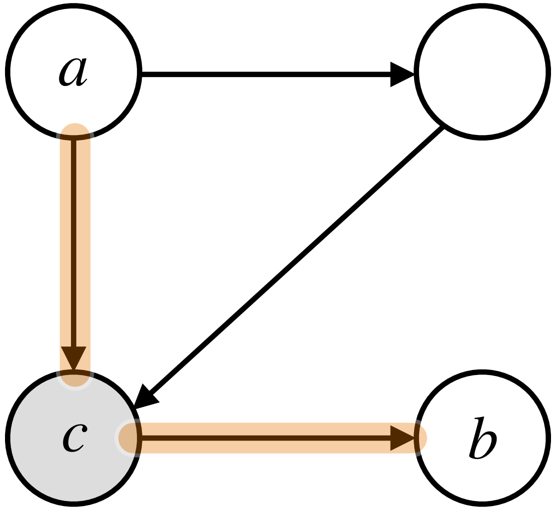

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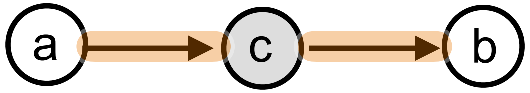
1. c is sandwiched by a **chain** in the path



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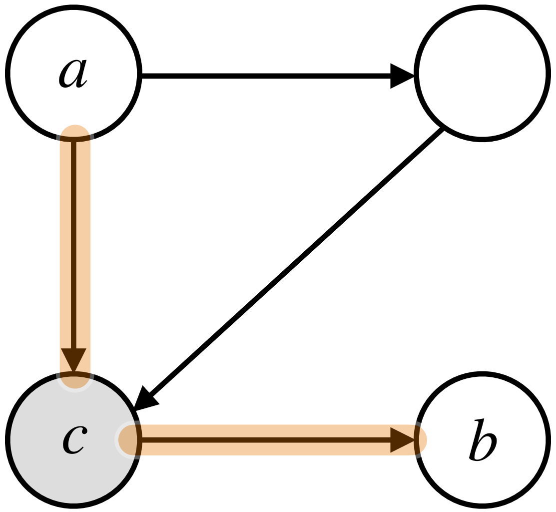

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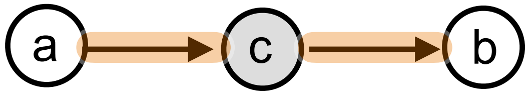

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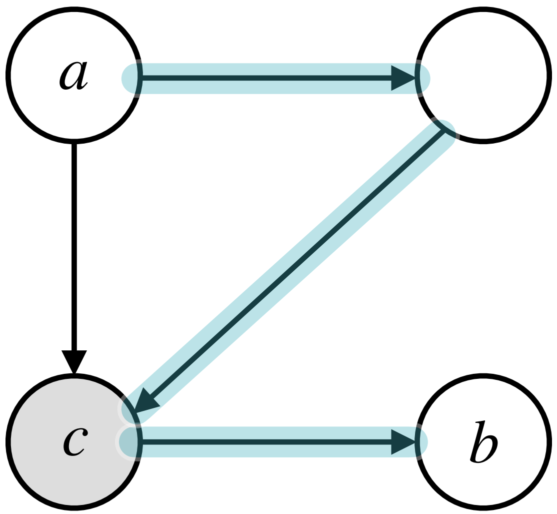

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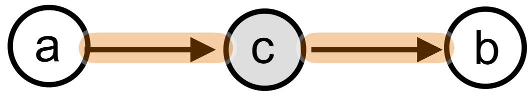

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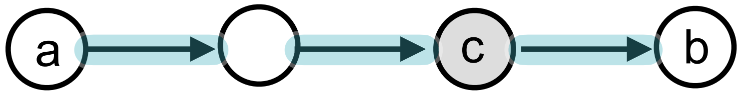

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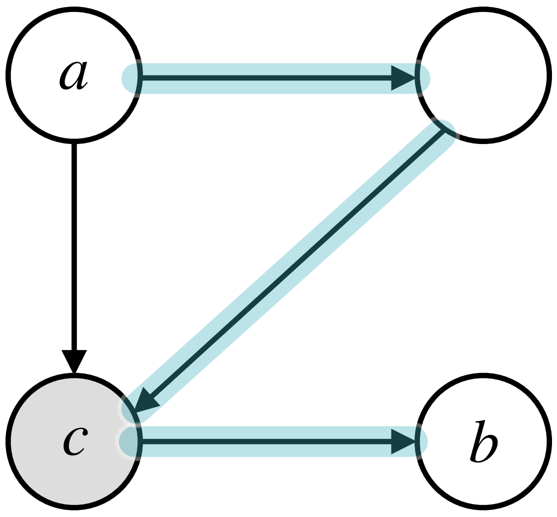

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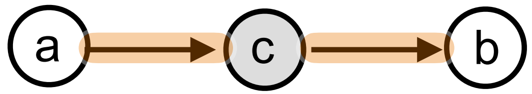

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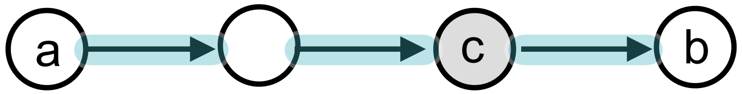

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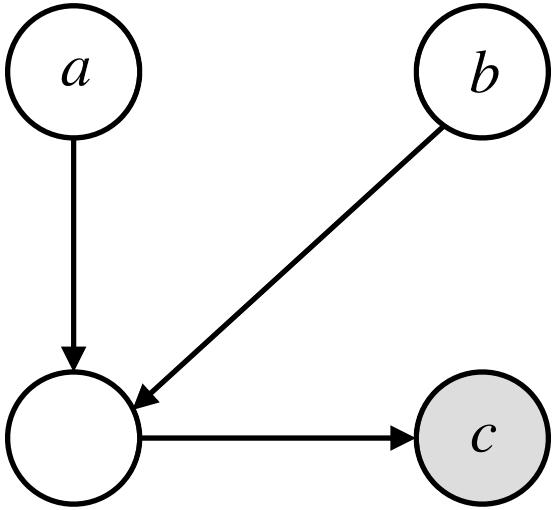

Nodes a and b are *not* d-separated by c

(i.e., a and b are d-connected)

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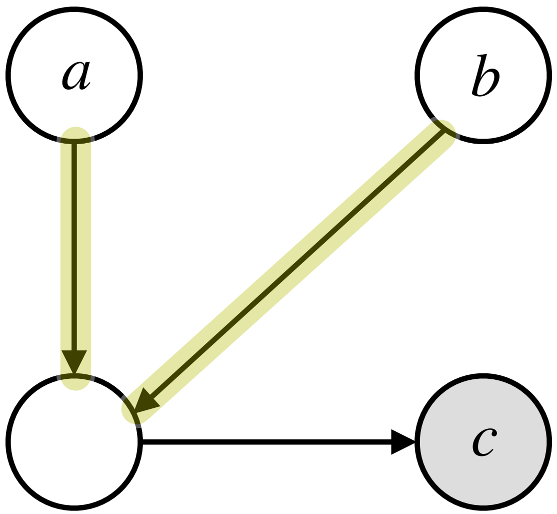

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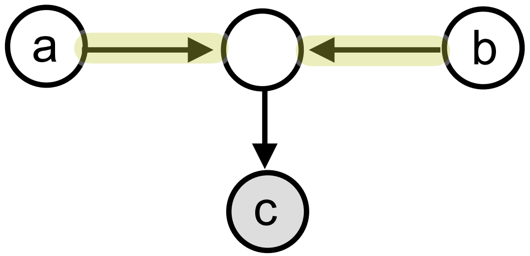

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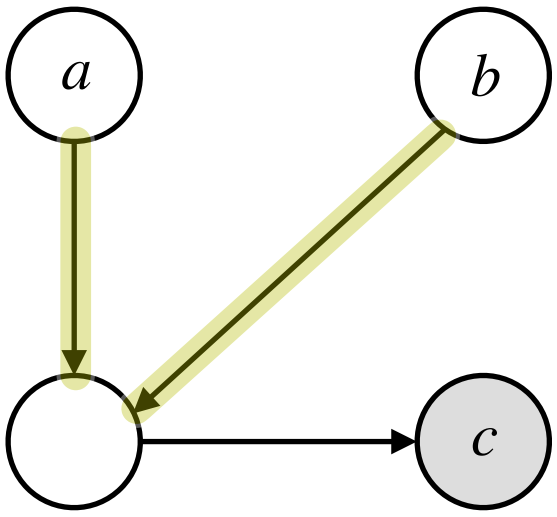

"Collider"

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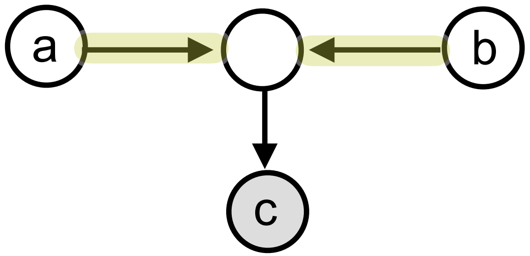

contains a **collider** and c is a descendant of the collider node

Markov Random Fields

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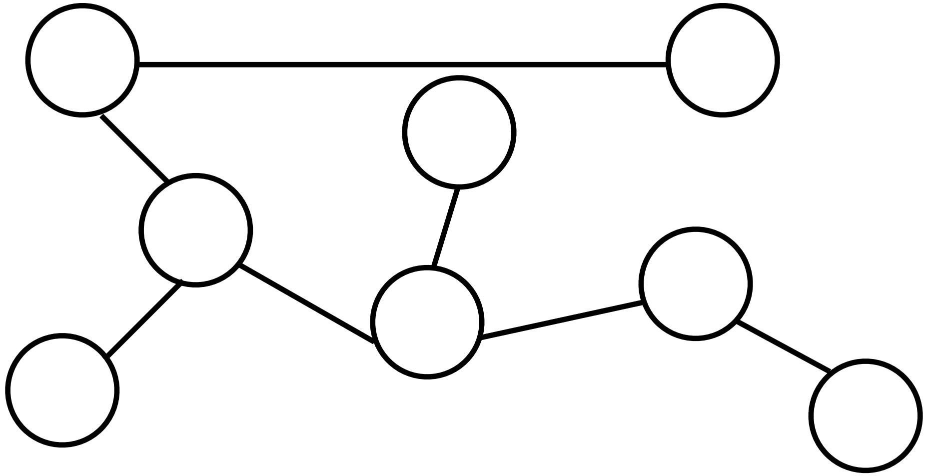
- **Markov random fields (MRF)** are represented by **undirected graphs**



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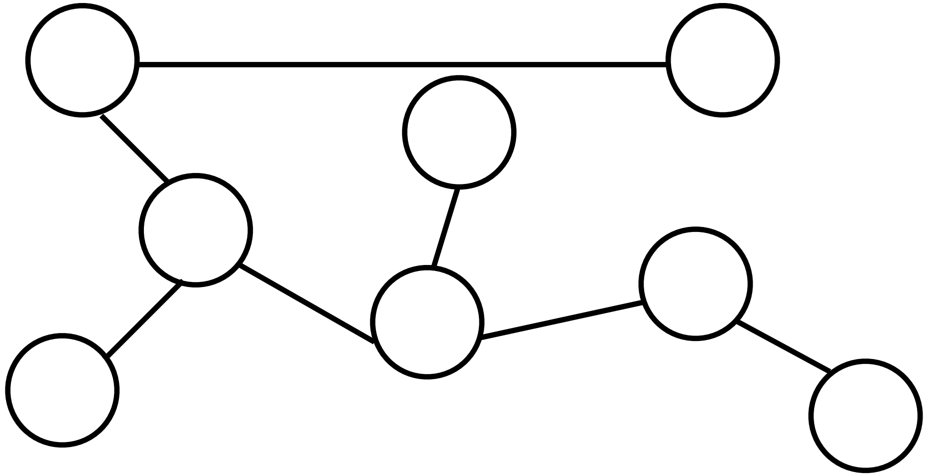

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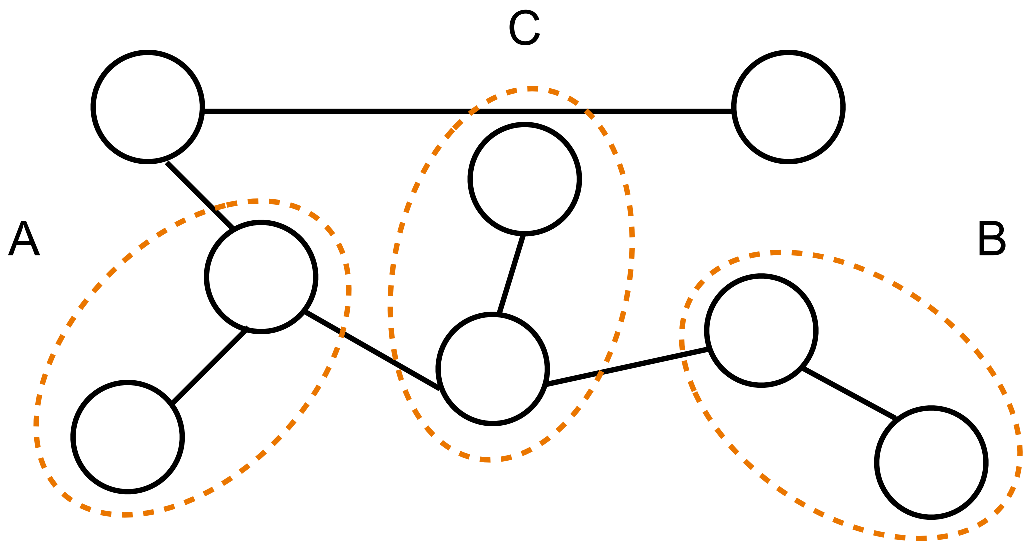

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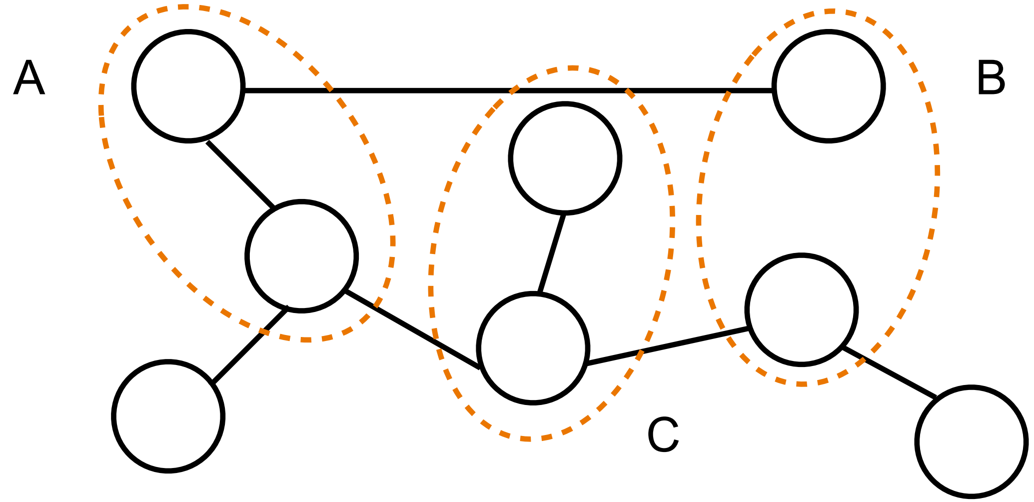

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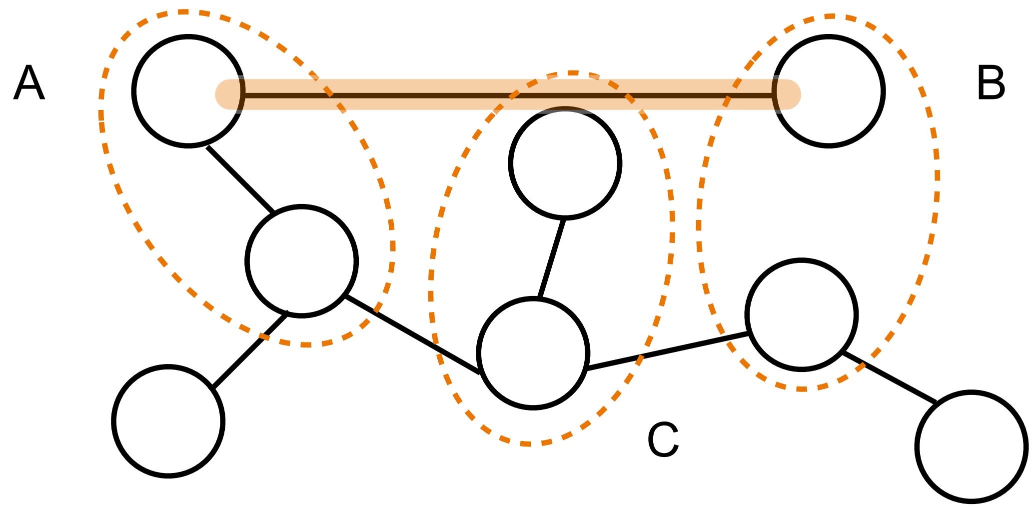

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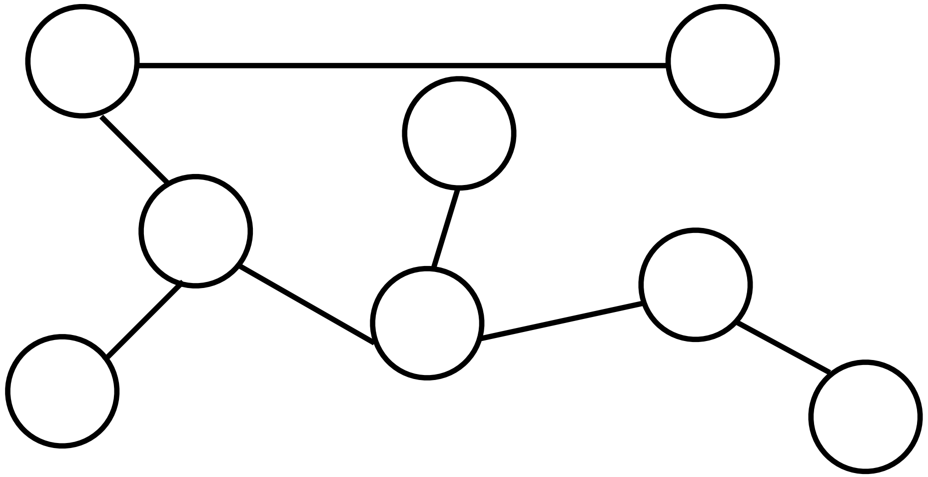

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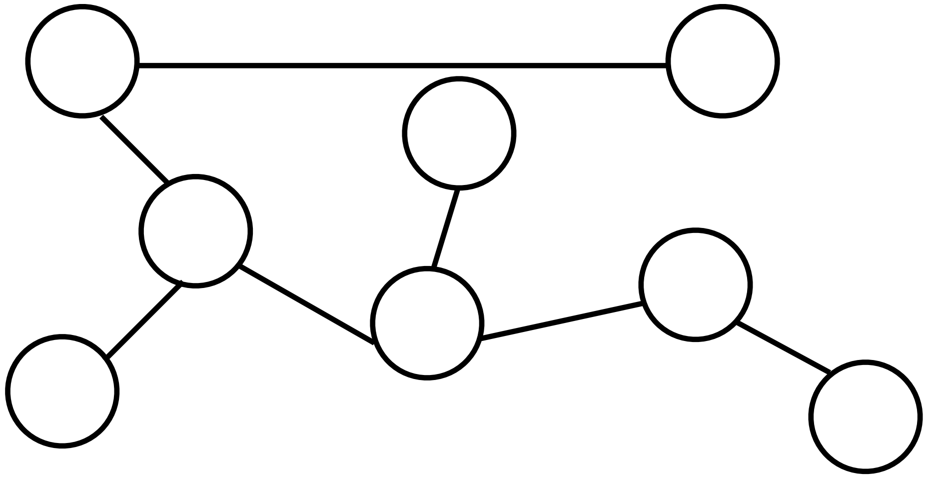

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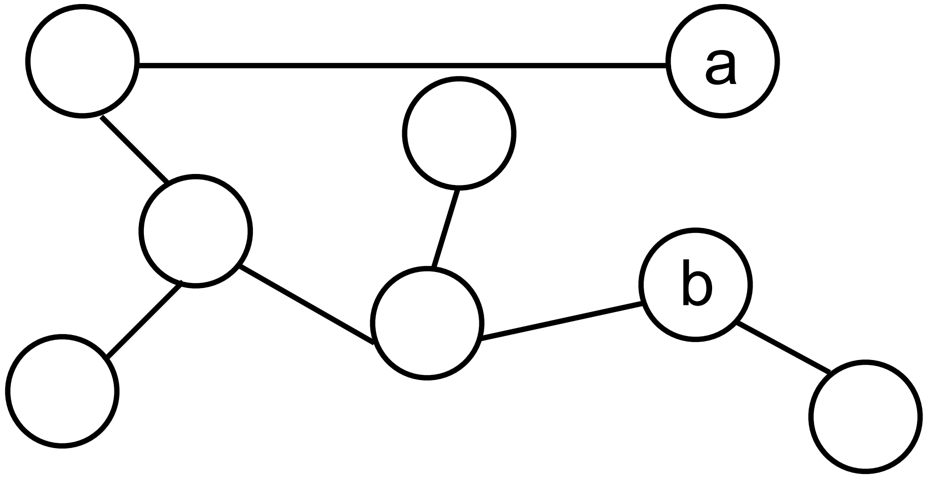

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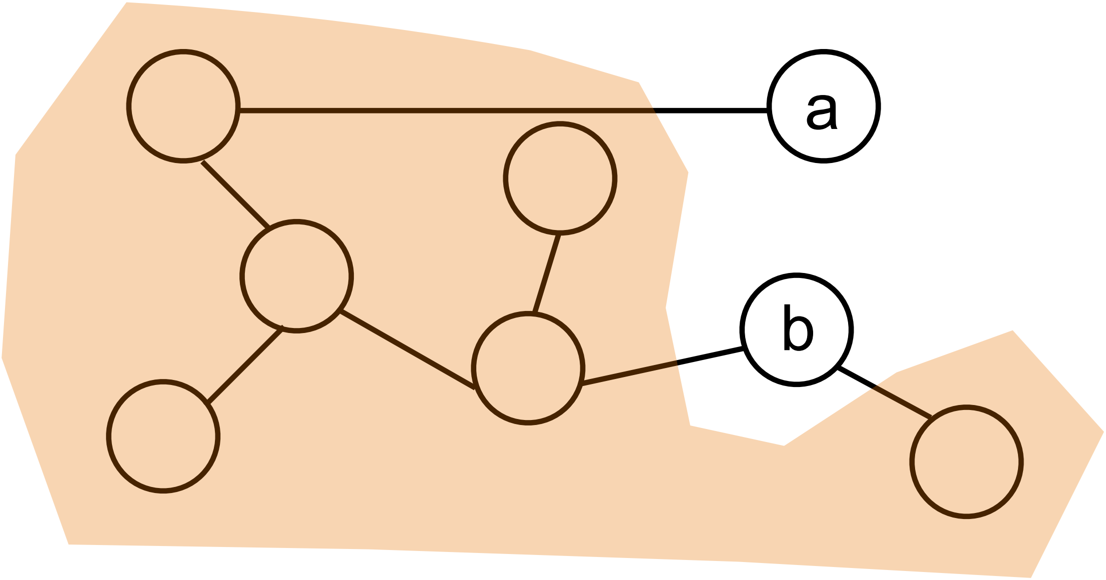

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In MRFs, we can consider factorisations into **potential functions** $\psi_C(\boldsymbol{x}_C) \geq 0$:

$$p(x_1, \ldots, x_n) \propto \prod_C \psi_C(\boldsymbol{x}_C),$$

where C is a clique of the graph*.

*Recall that a *clique* is a fully-connected subgraph of a graph

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Akin to factorising **joint distributions** into *conditional distributions* in BNs.

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- Factorisation is *not* unique

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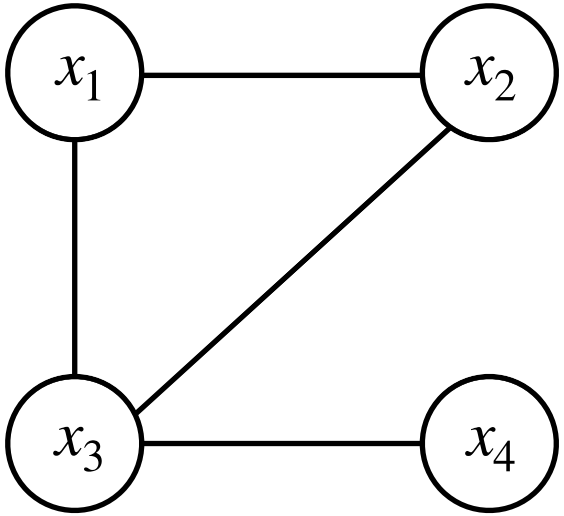
Example illustrating the Hammersley-Clifford theorem

1. Factorisation into maximal cliques



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Example illustrating the Hammersley-Clifford theorem

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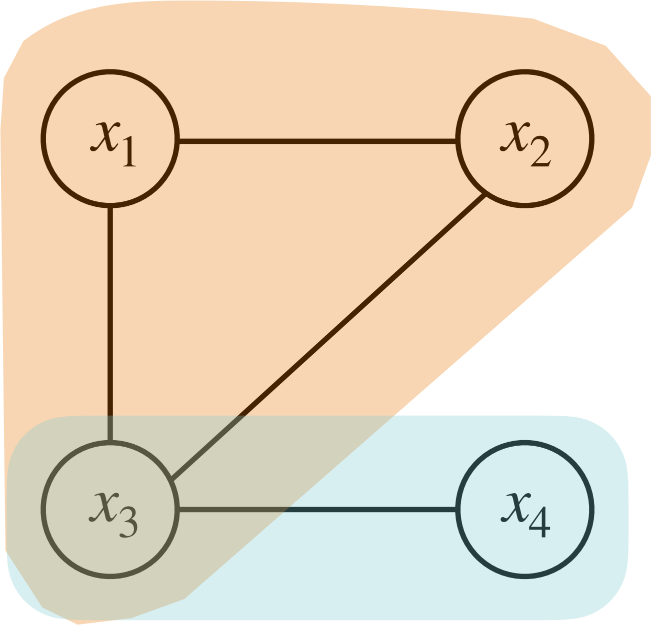
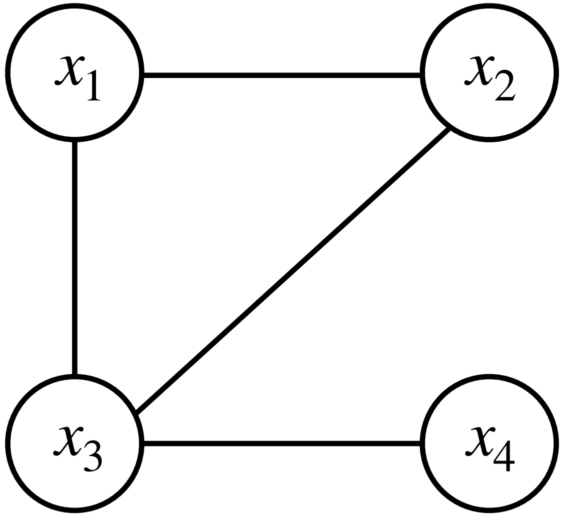


$$p(x_1, x_2, x_3, x_4)$$

$$= \psi_{123}(x_1, x_2, x_3)\,\psi_{34}(x_3, x_4)$$

Example illustrating the Hammersley-Clifford theorem

2. Factorisation into pairwise cliques



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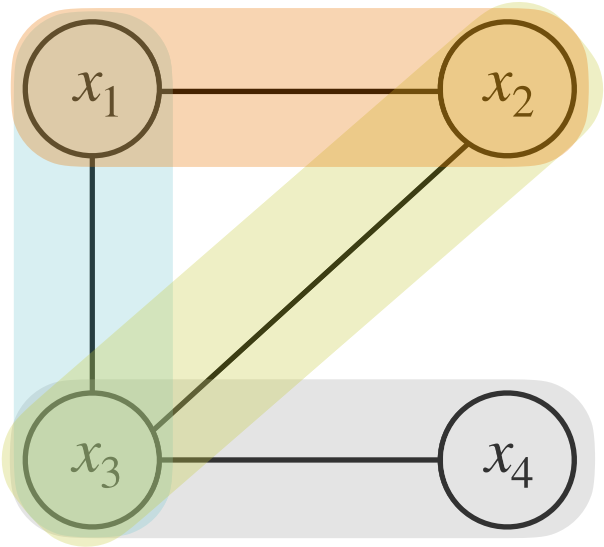
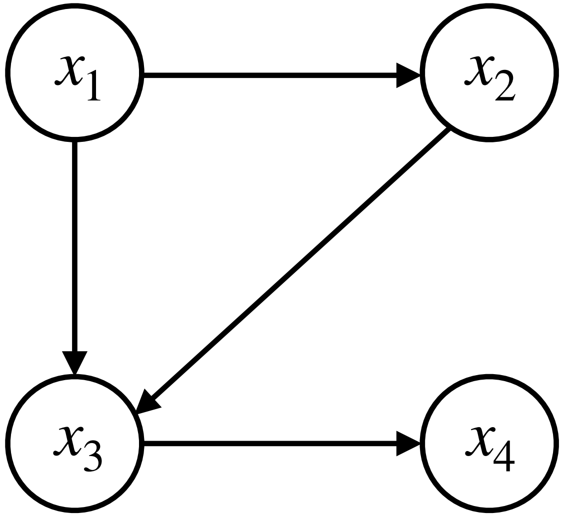


$$p(x_1, x_2, x_3, x_4)$$

$$= \psi_{12}(x_1, x_2)\,\psi_{13}(x_1, x_3)\,\psi_{23}(x_2, x_3)\,\psi_{34}(x_3, x_4)$$

Example illustrating the Hammersley-Clifford theorem

3. Factorisation of Bayesian networks



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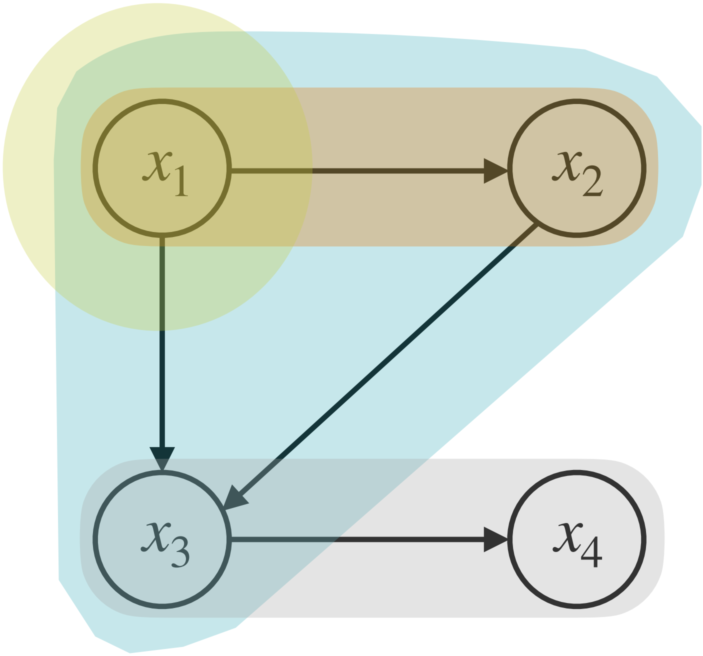

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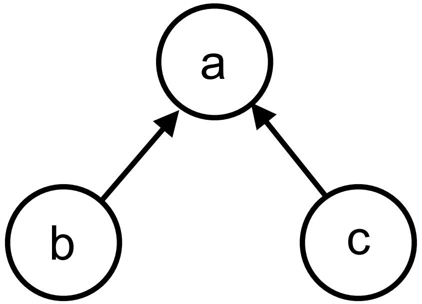

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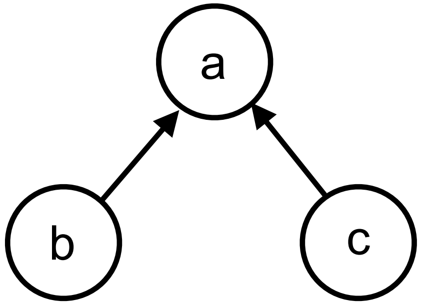

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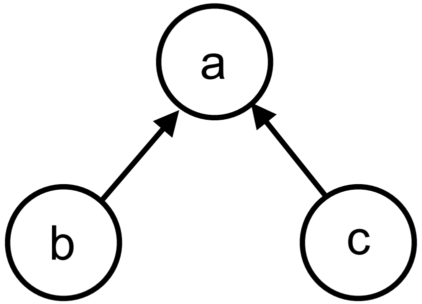

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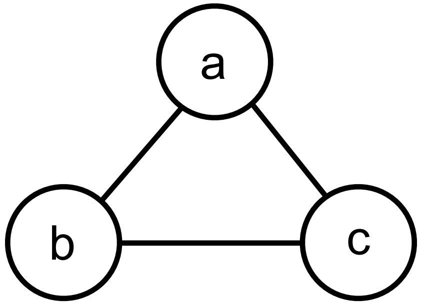

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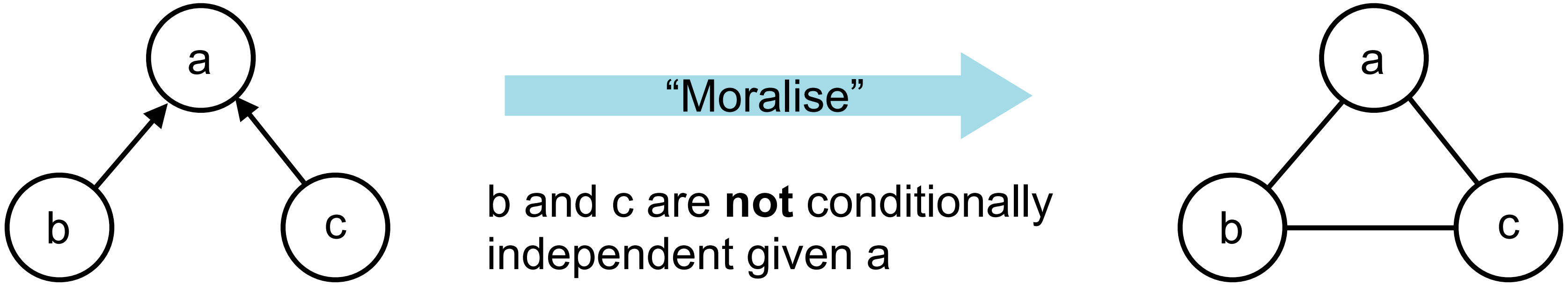

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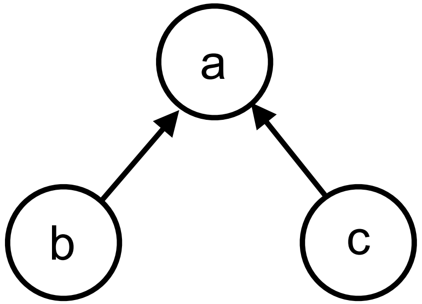

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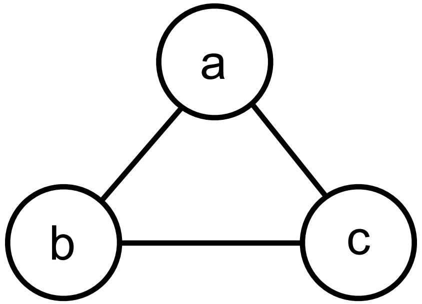

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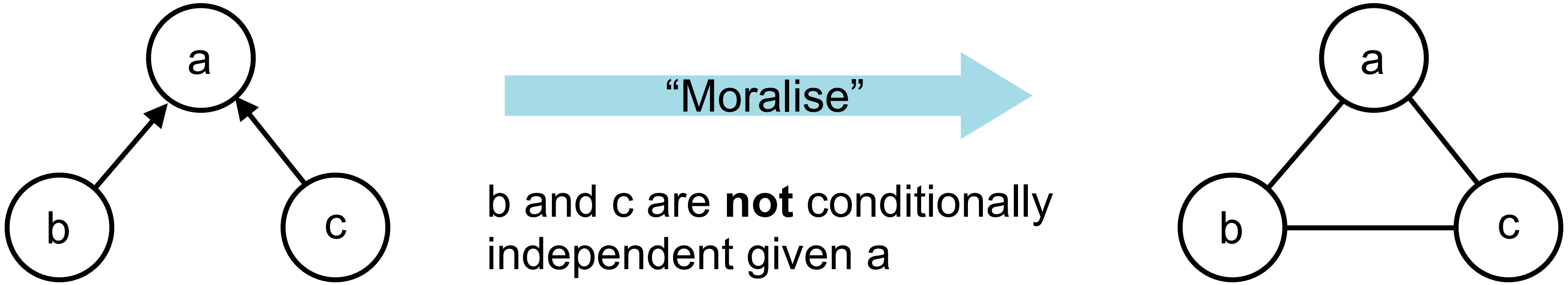

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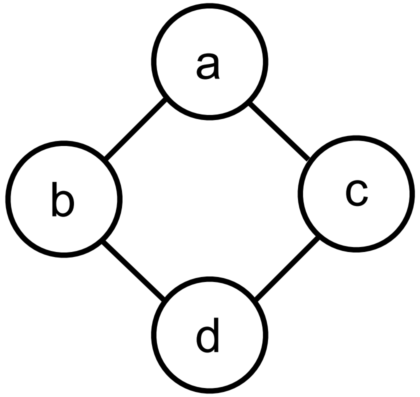

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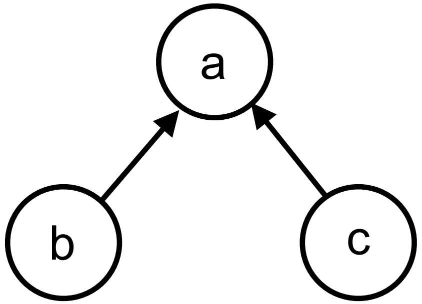

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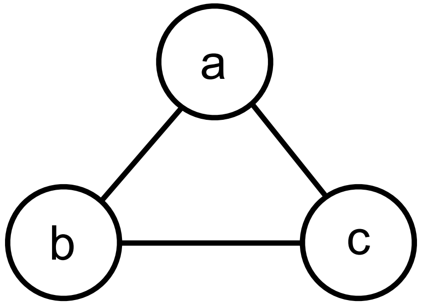

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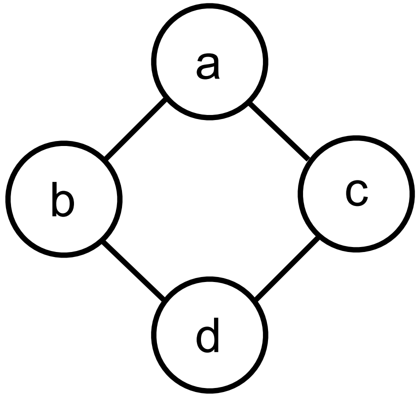

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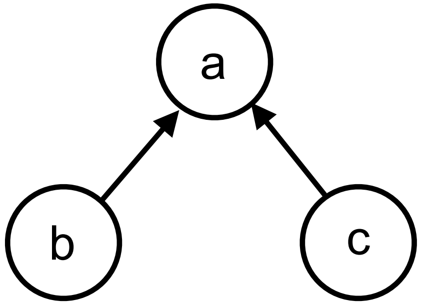

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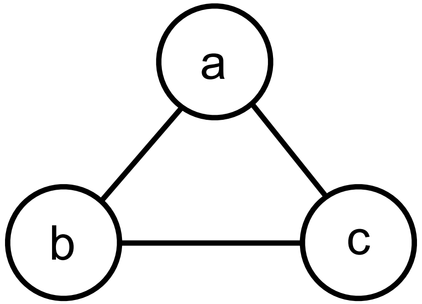

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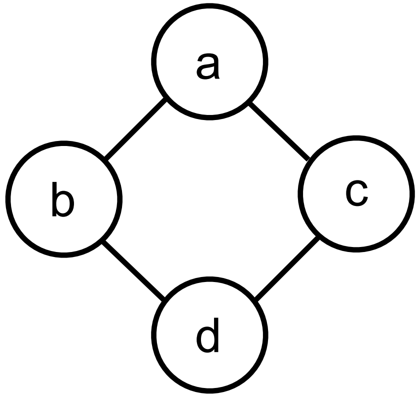

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Cannot happen in a DAG.

Factor Graphs

Factor Graphs

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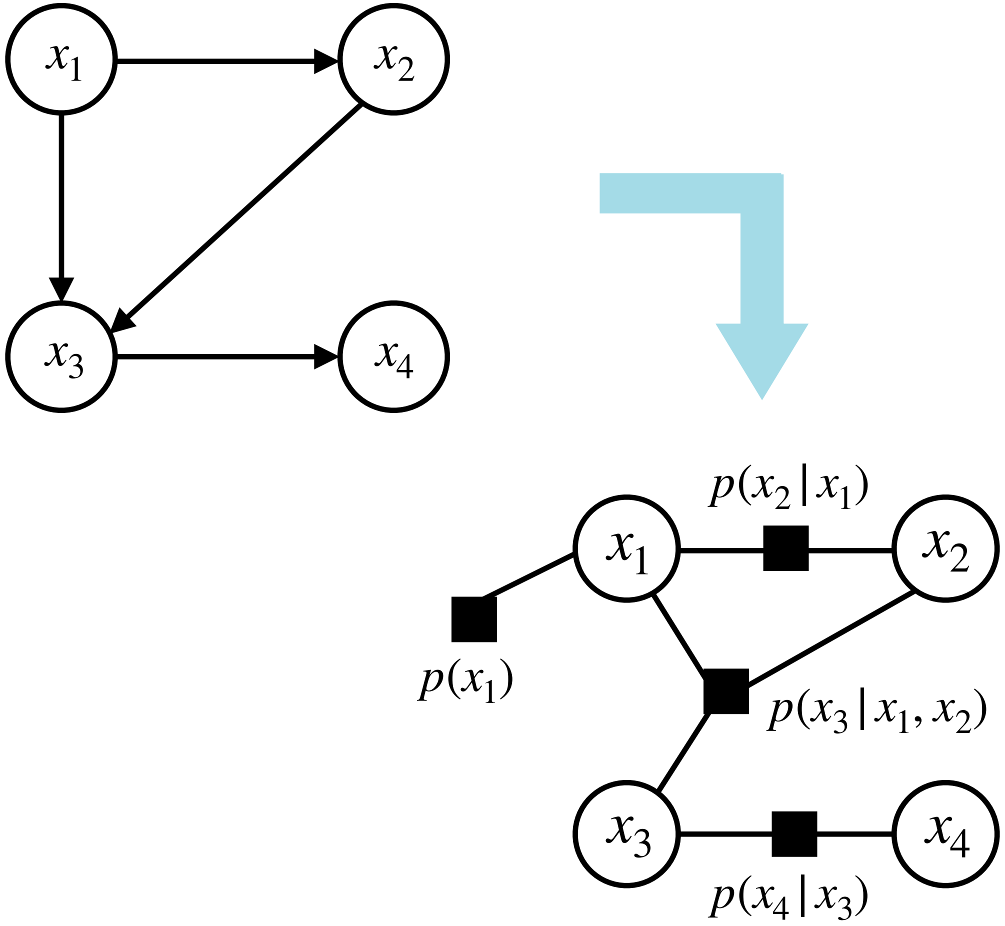

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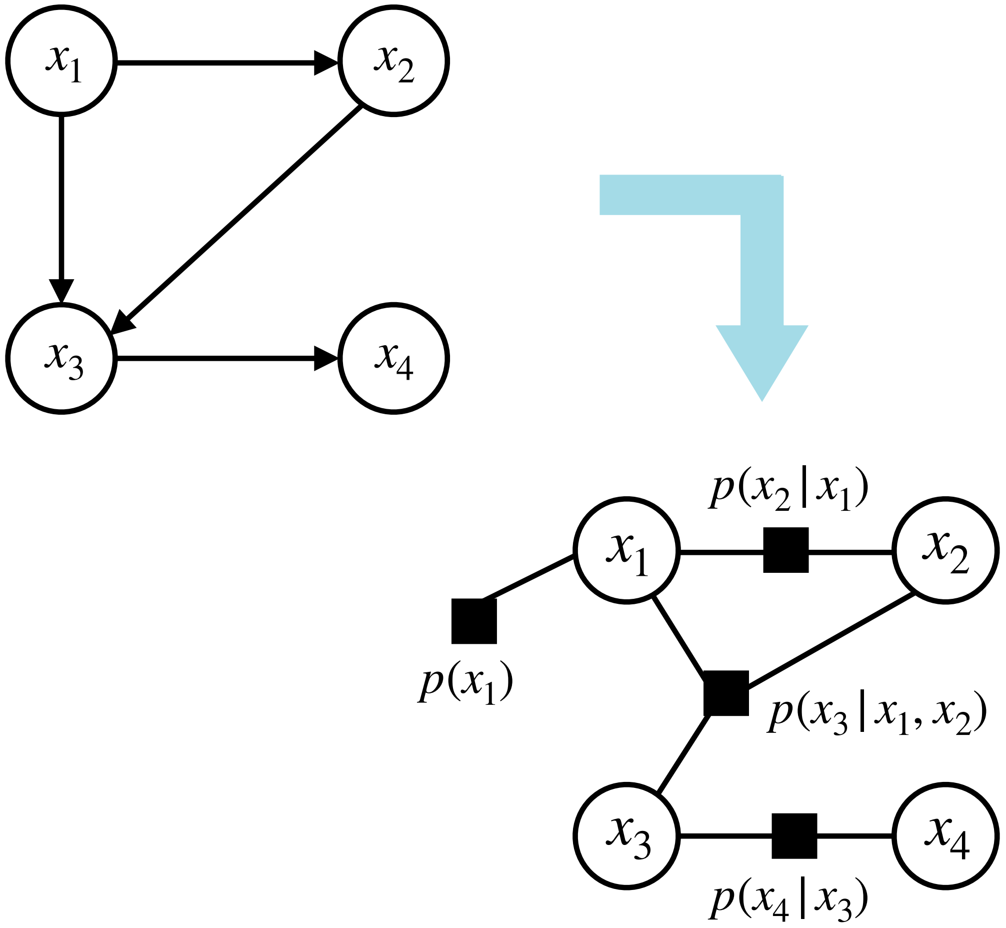

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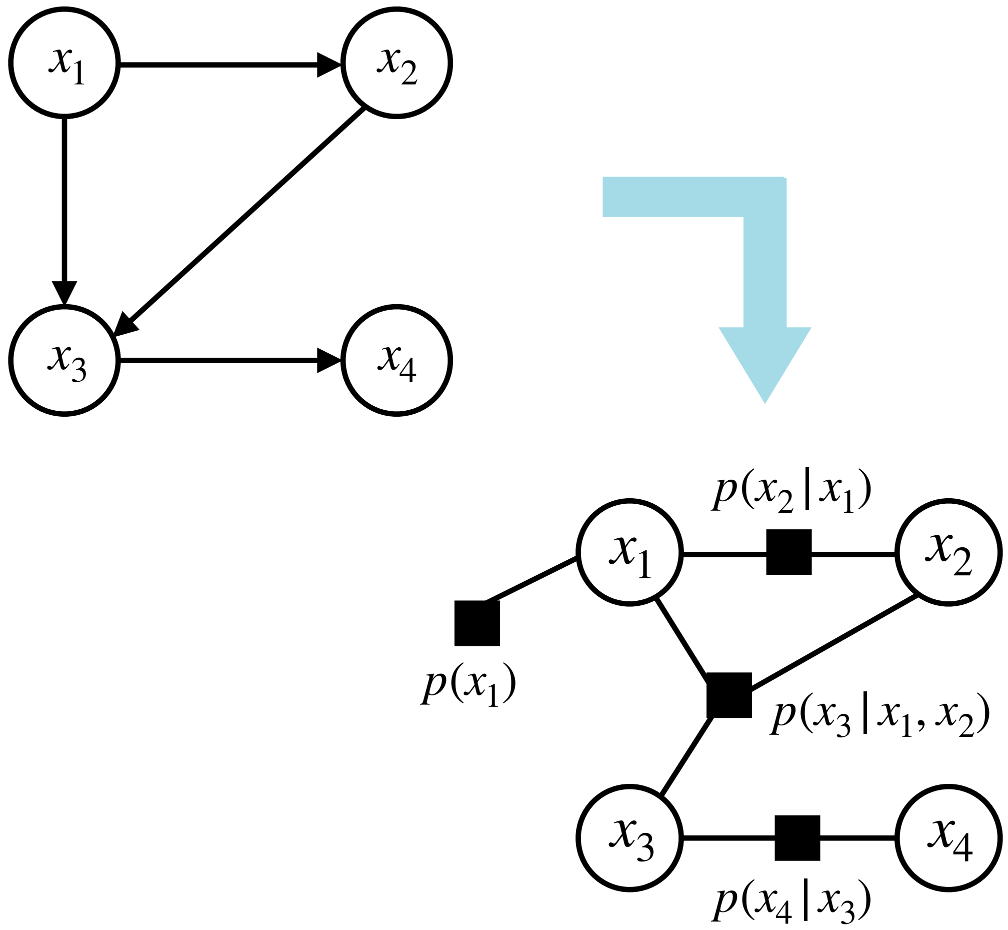

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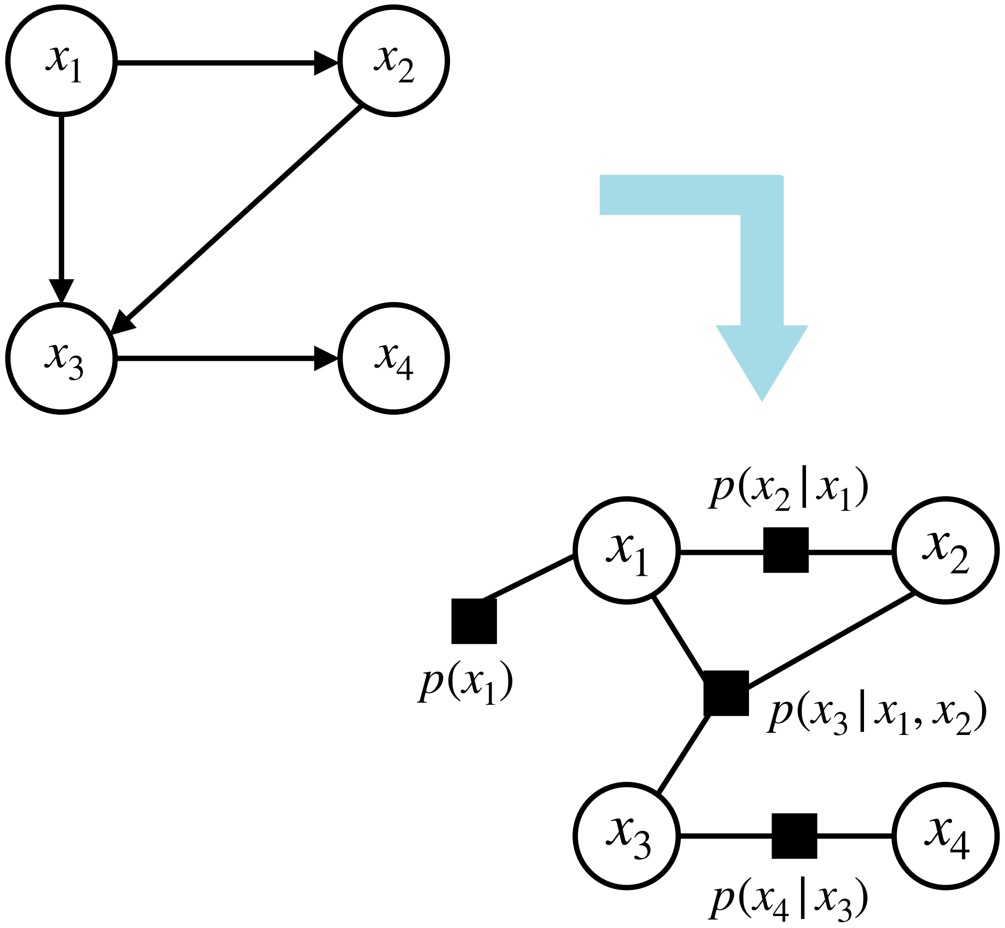

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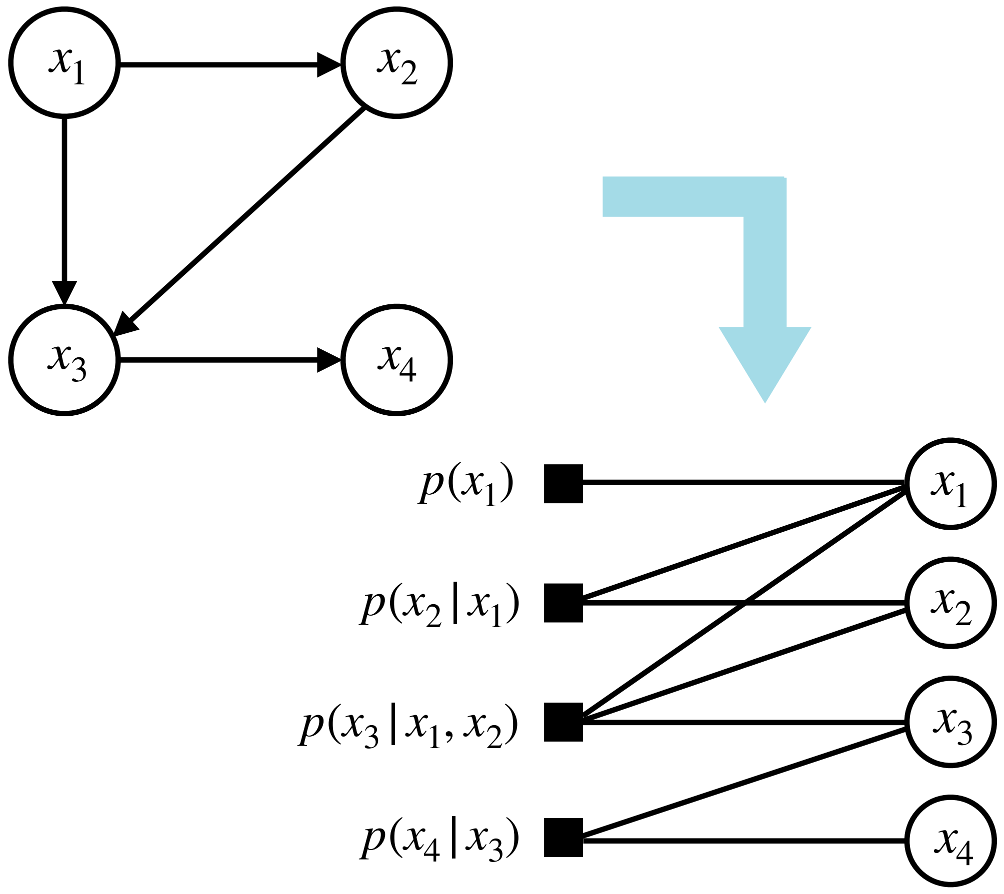

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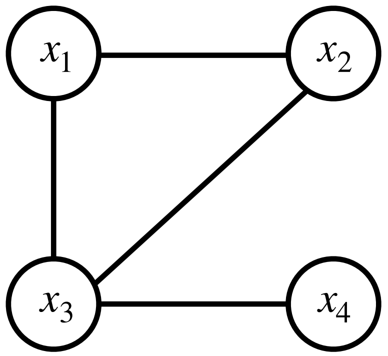
Factor graphs make the factorisation explicit

$\Rightarrow$ Useful for MRFs where factorisation is non-unique



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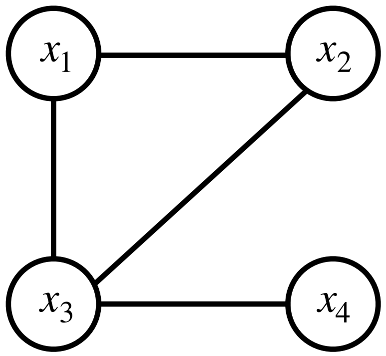
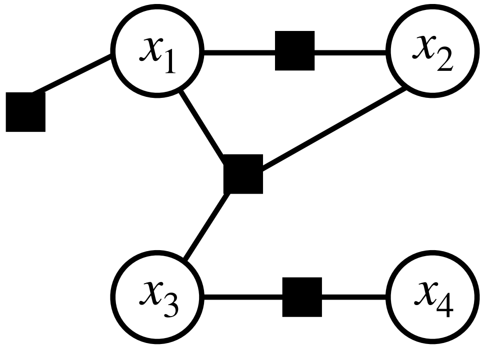
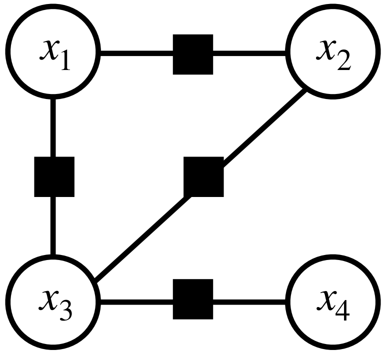
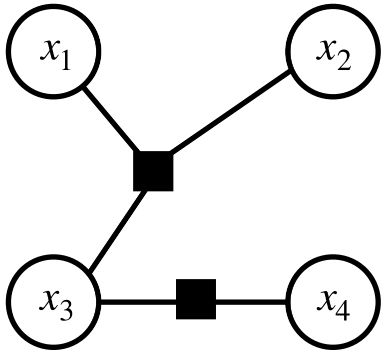


There are many ways of factorising into potentials:







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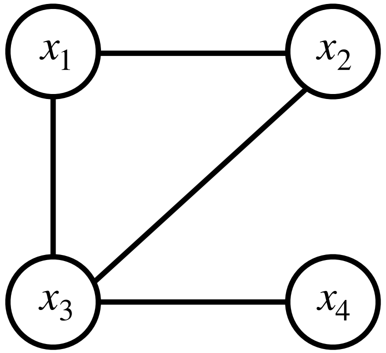

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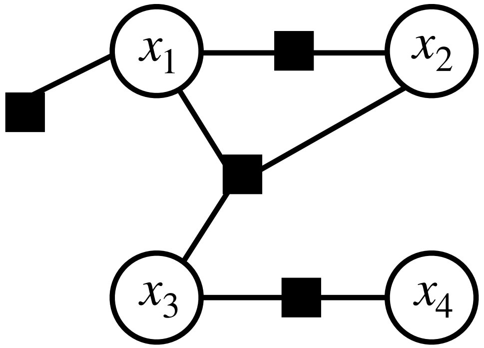

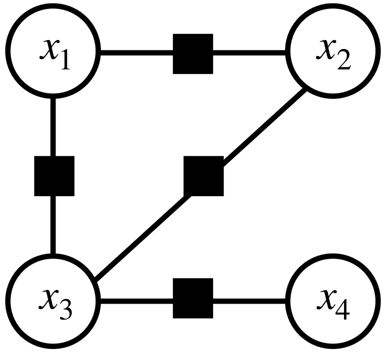

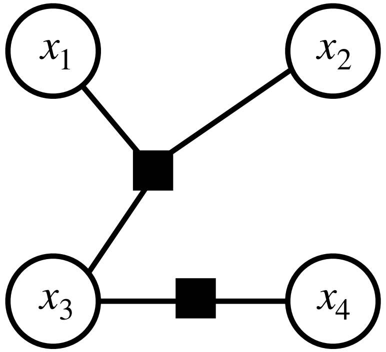

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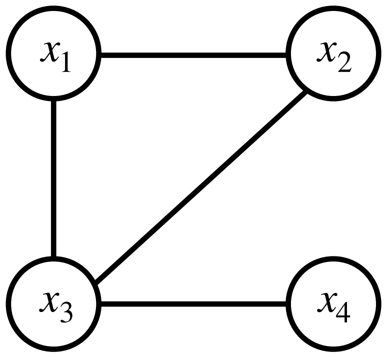

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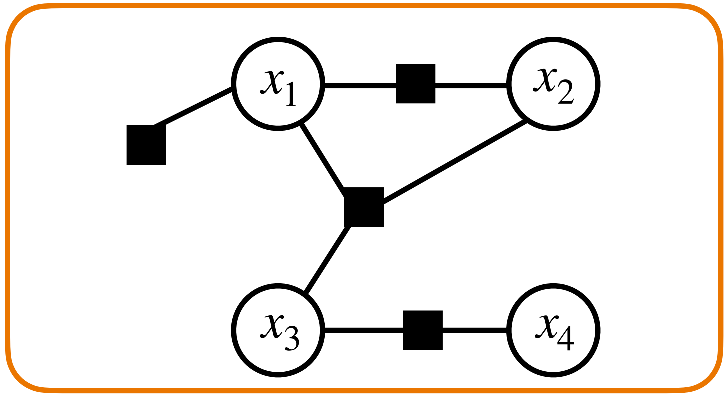

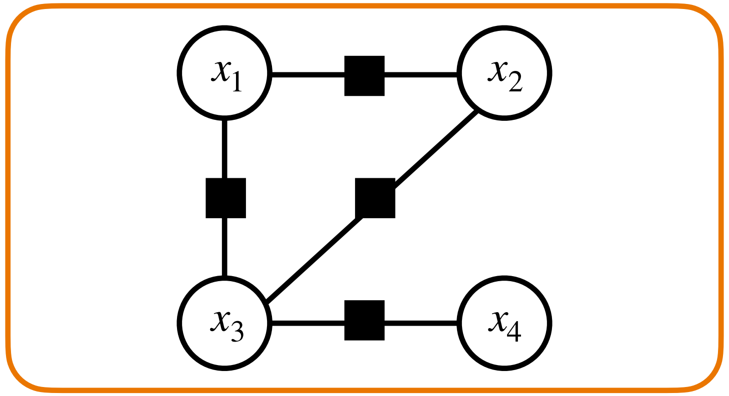

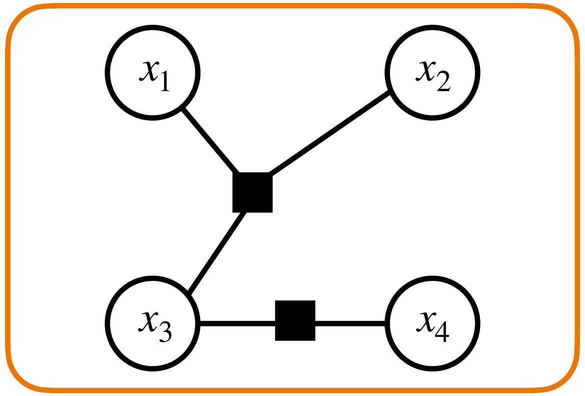

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Useful notations

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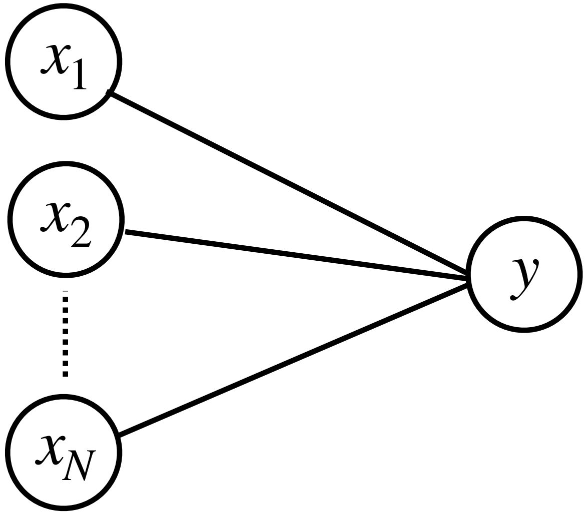

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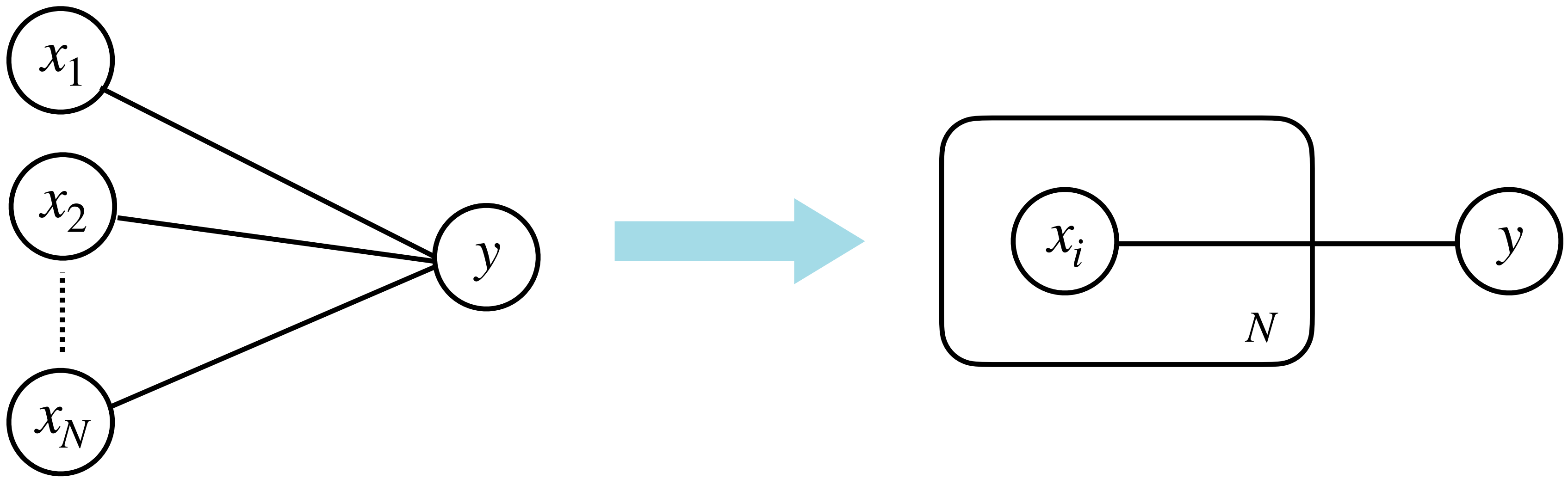

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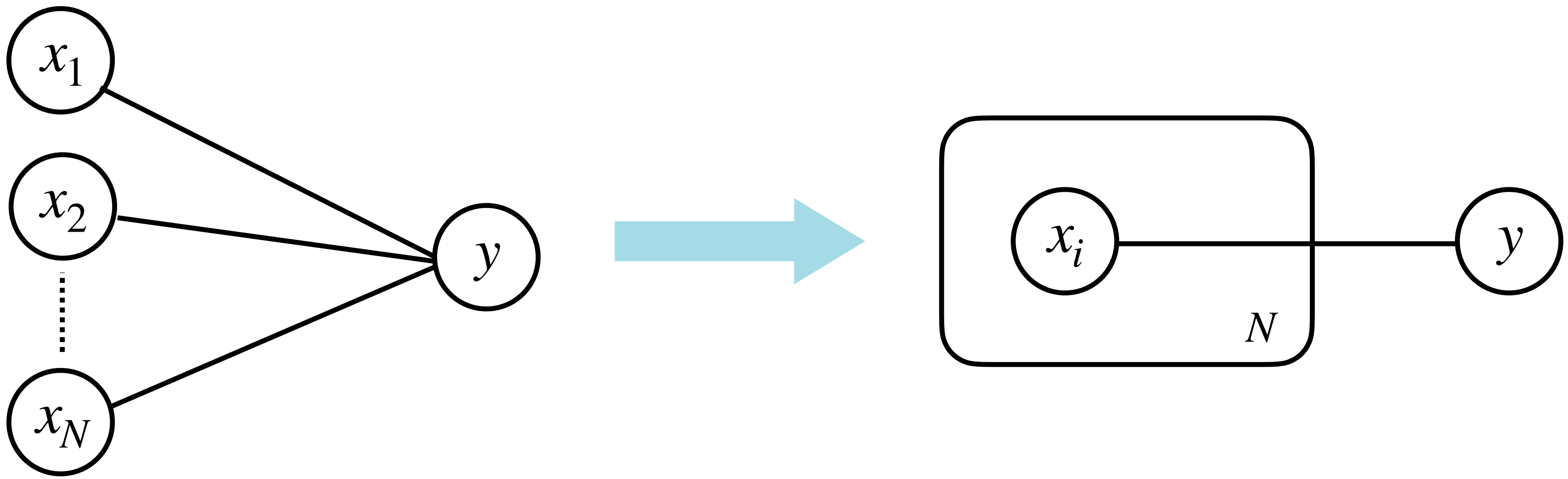
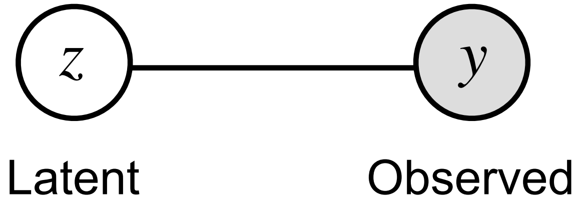


- Shaded vs. unshaded nodes



Examples of Bayesian networks

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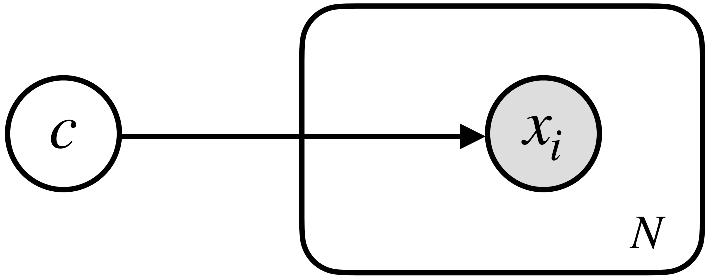
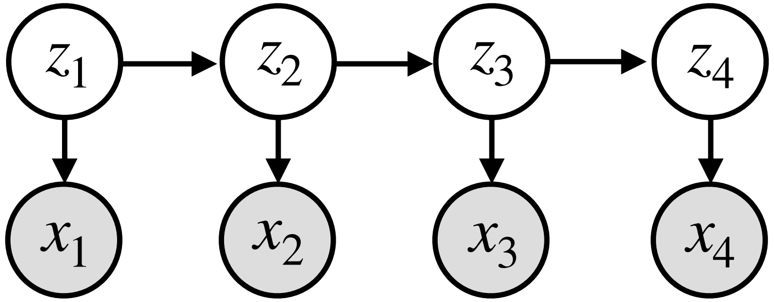
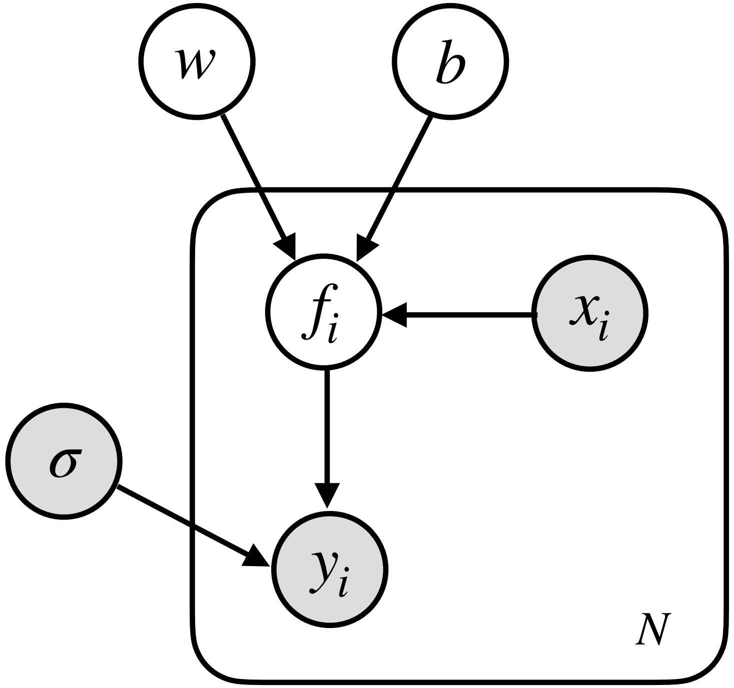


- Hidden Markov model



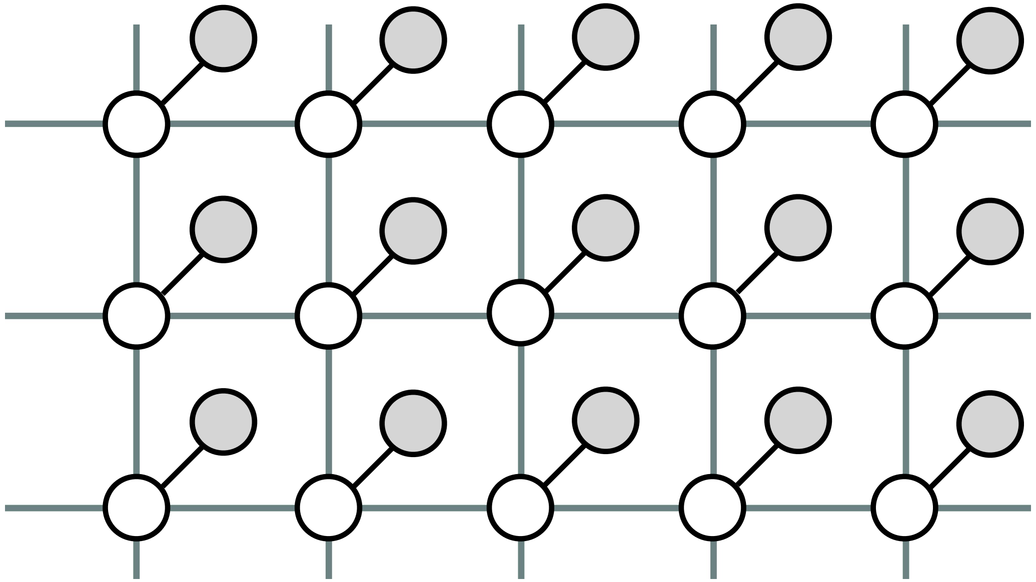
- Bayesian linear regression



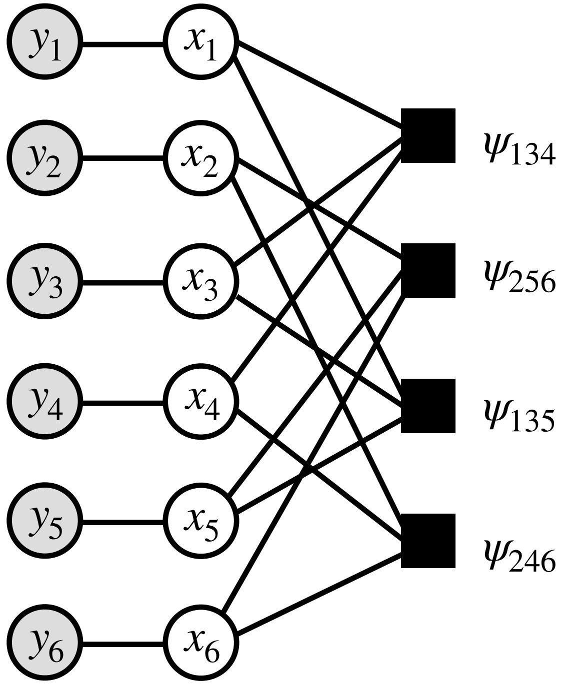
$$y_i = f_i + \epsilon_i, \quad \epsilon_i \sim \mathcal{N}(0, \sigma),$$
$$f_i = w x_i + b\,.$$

Examples of Markov random fields

- Spatial analysis / image processing [3,4]



- Error-correcting codes [5]



References

[1] Bishop, Christopher M. *Pattern Recognition and Machine Learning*. New York: springer, 2006.

[2] Koller, Daphne, and Nir Friedman. *Probabilistic Graphical Models: Principles and Techniques*. MIT press, 2009.

[3] Besag, Julian. *Spatial interaction and the statistical analysis of lattice systems*. Journal of the Royal Statistical Society: Series B (Methodological). 1974.

[4] Besag, Julian. *On the statistical analysis of dirty pictures.* Journal of the Royal Statistical Society: Series B (Methodological). 1986.

[5] Gallager, Robert. *Low-density parity-check codes.* IRE Transactions on information theory. 1962.

2. Belief Propagation on PGMs

Statistical inference with PGMs

In Bayesian statistics, we often need to compute:

1. The marginal likelihood $p(y)$ of observed data
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3. The conditional distribution $p(x_i \mid x_j)$ for any $i, j \in V$
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This has computational cost $\mathcal{O}(K^N)$

Example

Let $X_1, \ldots, X_N$ be random variables, each with K discrete states and p is the joint probability mass function.

Question: What is the *marginal distribution* $p(X_i = x_i)$ for all $i = 1, \ldots, N$?

A naive solution:

$$p(X_i = x_i) = \sum_{j \neq i}^{N} \left(\sum_{x_j \in \{1, \ldots, K\}} p(x_1, \ldots, x_N) \right).$$

This has computational cost $\mathcal{O}(K^N)$ 👎

Assuming independence

Let $N = 3$ and assume we can write $p(x_1, x_2, x_3) = p(x_1, x_2)p(x_3)$.

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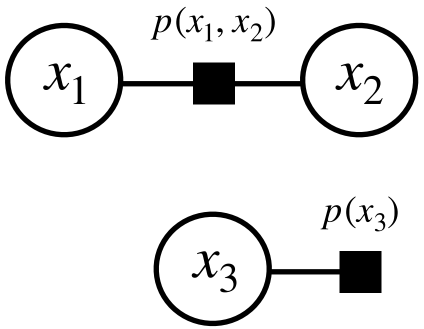

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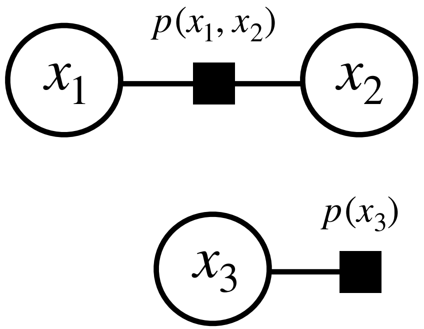

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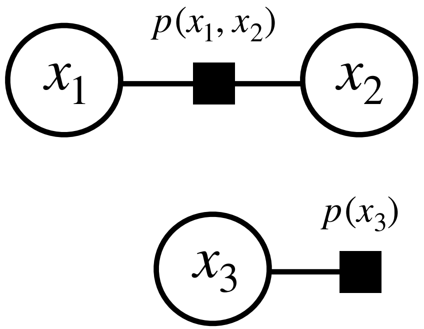

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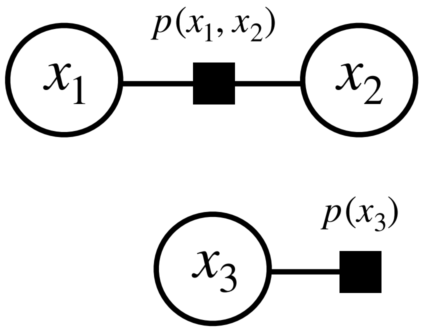

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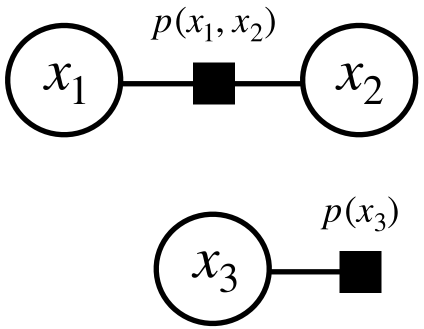

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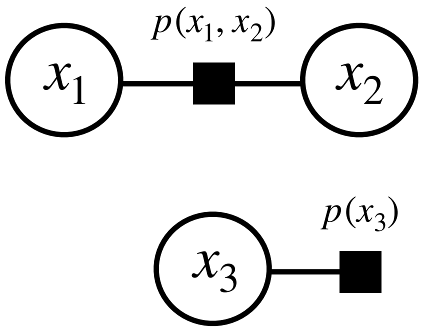

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A single sum is cheaper to compute than a double sum!

Assuming conditional independence

Now assume we have $p(x_1, x_2, x_3) = p(x_1 \mid x_3)p(x_2 \mid x_3)p(x_3)$.

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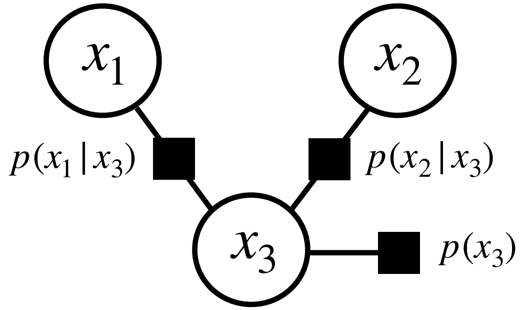

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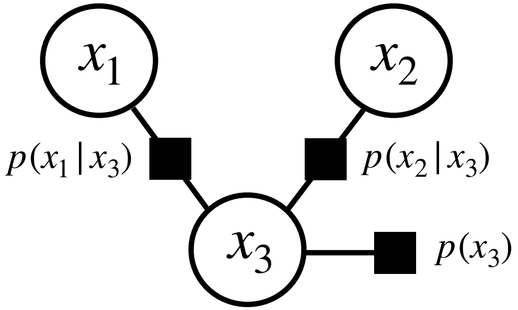

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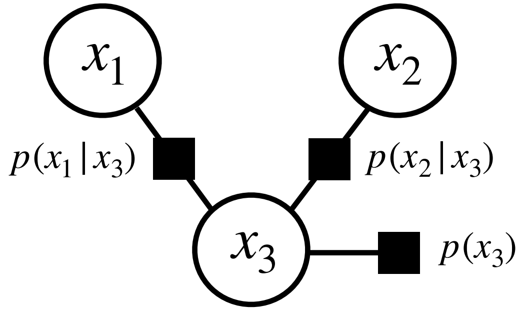

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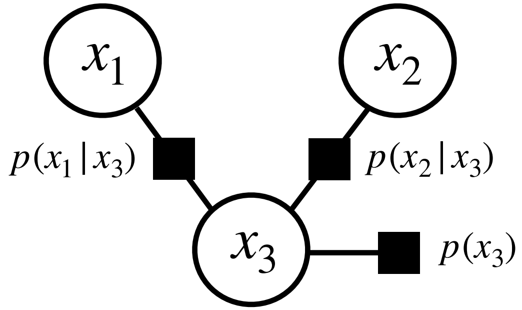

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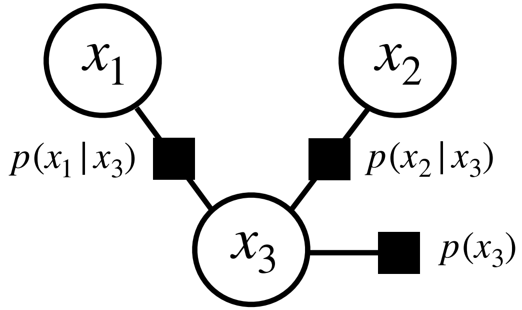

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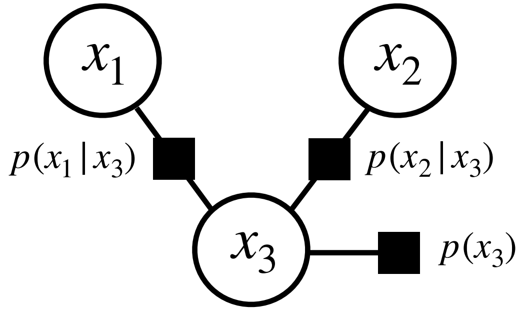

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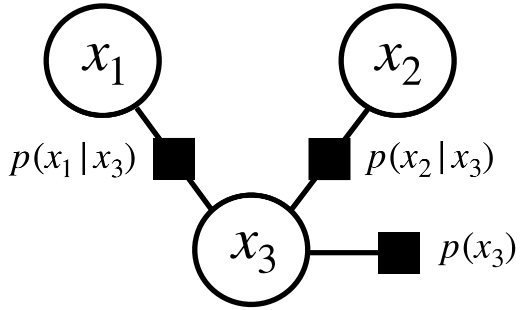

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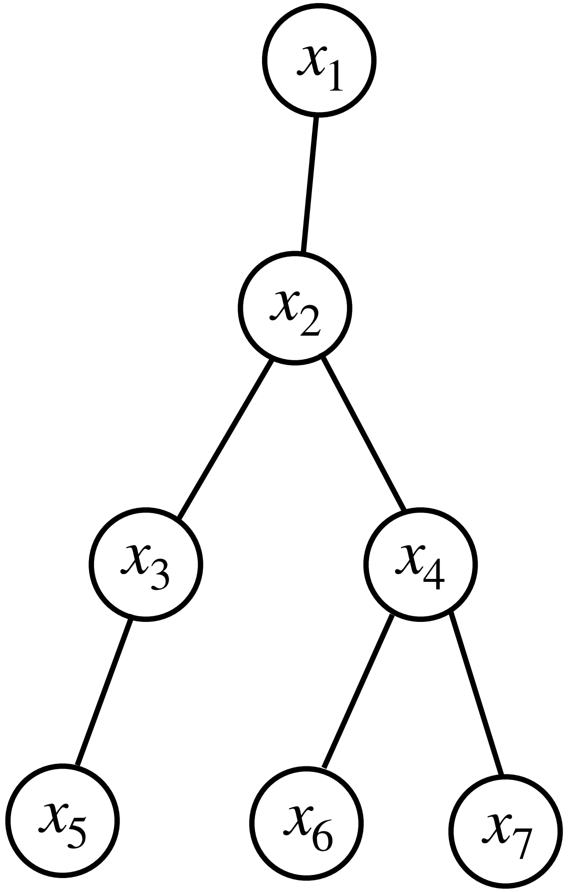
$\equiv$ *sparsity of graph*

Belief propagation algorithm



- **Belief propagation** efficiently computes *marginal probabilities* $p(x_i)$ on trees
- Assume that the graph is **tree-structured**
- Operate on factor graphs

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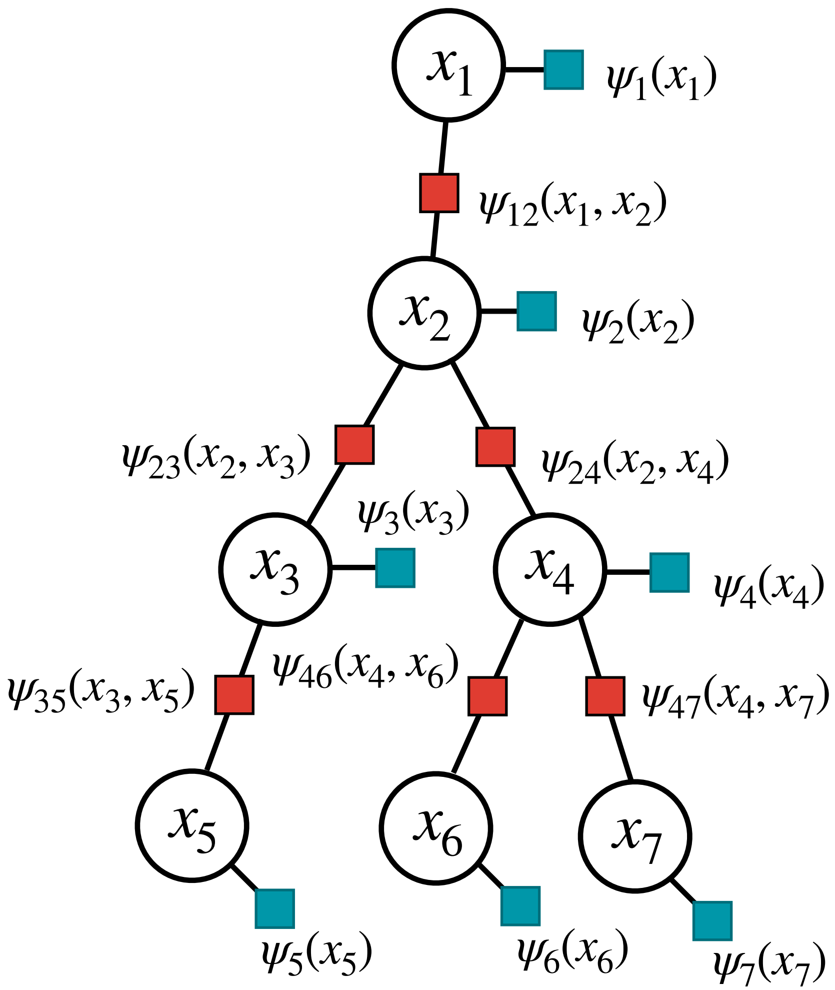

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$$p(\mathbf{x}) = \prod_{i \in V} \psi_i(x_i) \prod_{(i,j) \in E} \psi_{ij}(x_i, x_j).$$

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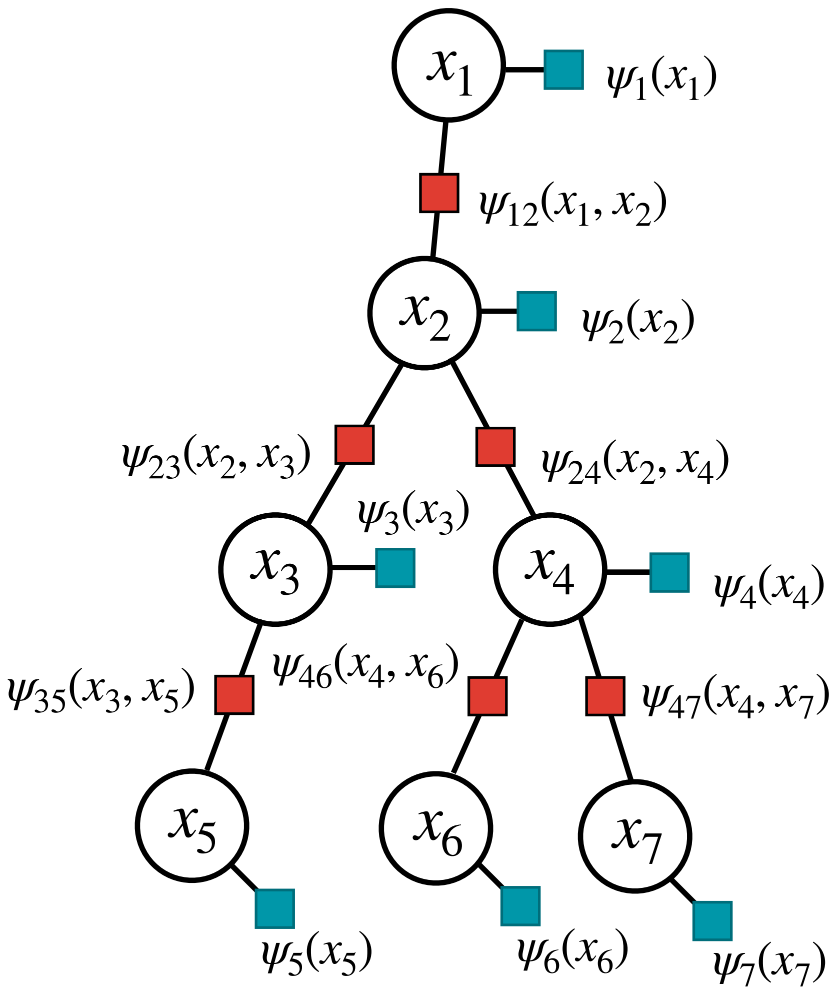
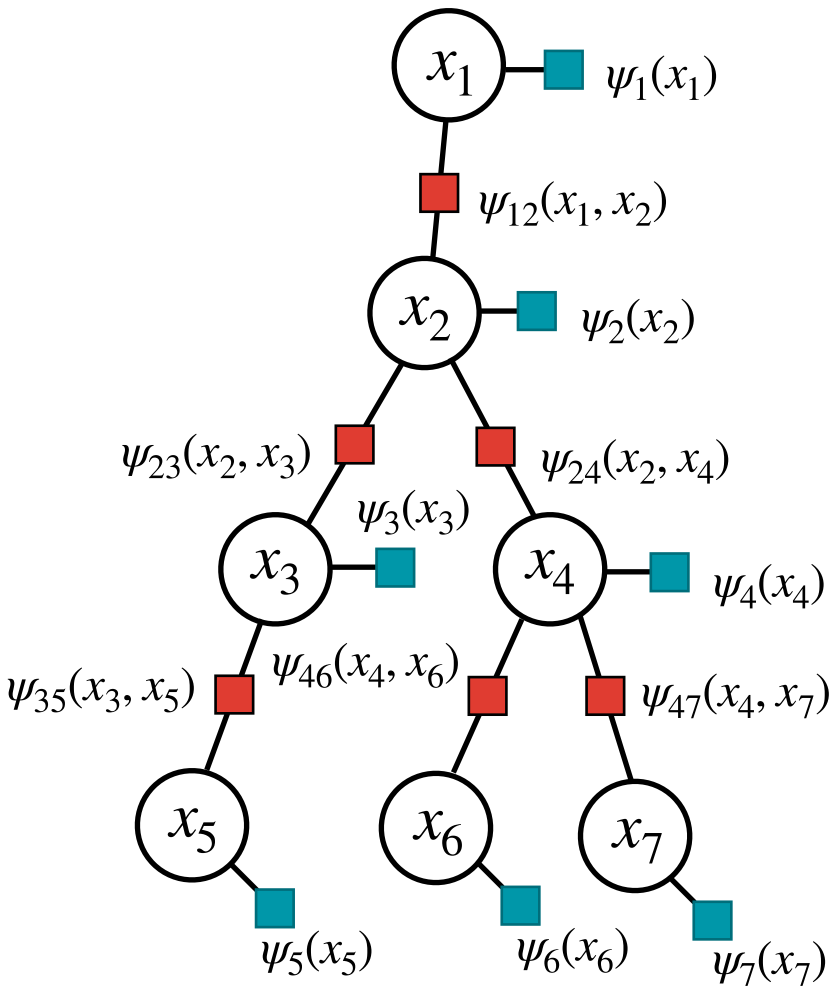


BP proceeds by iteratively updating:

Belief propagation algorithm



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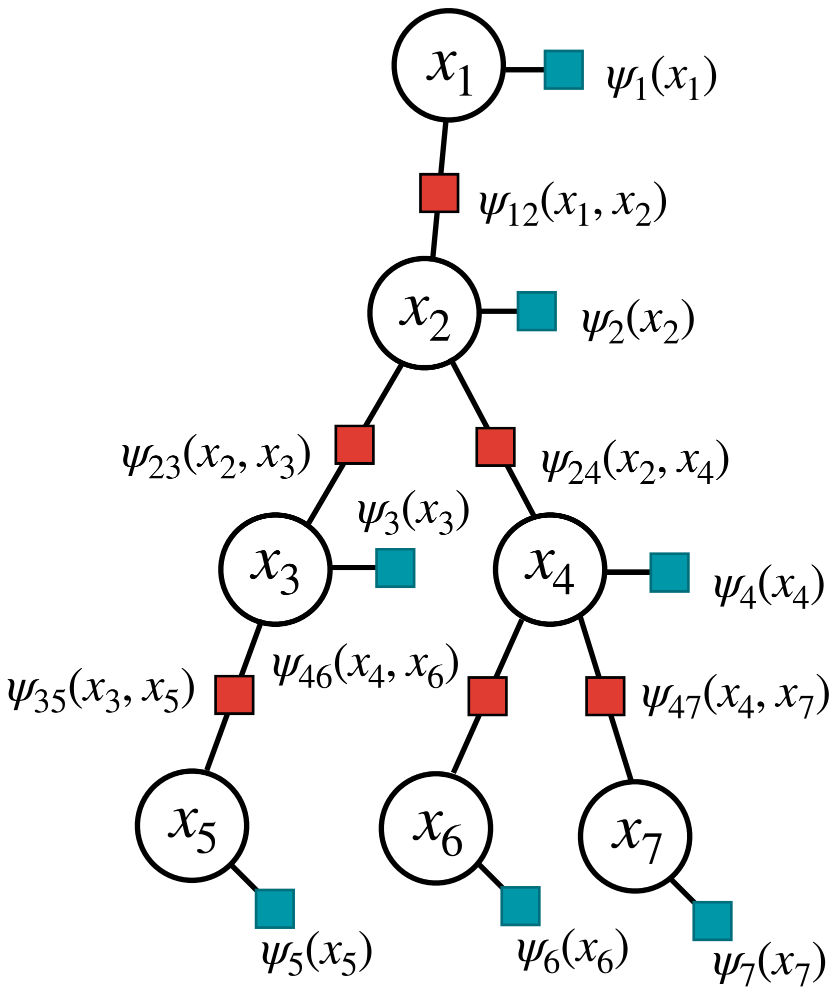
1. The “**messages**” between two nodes

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

Belief propagation algorithm



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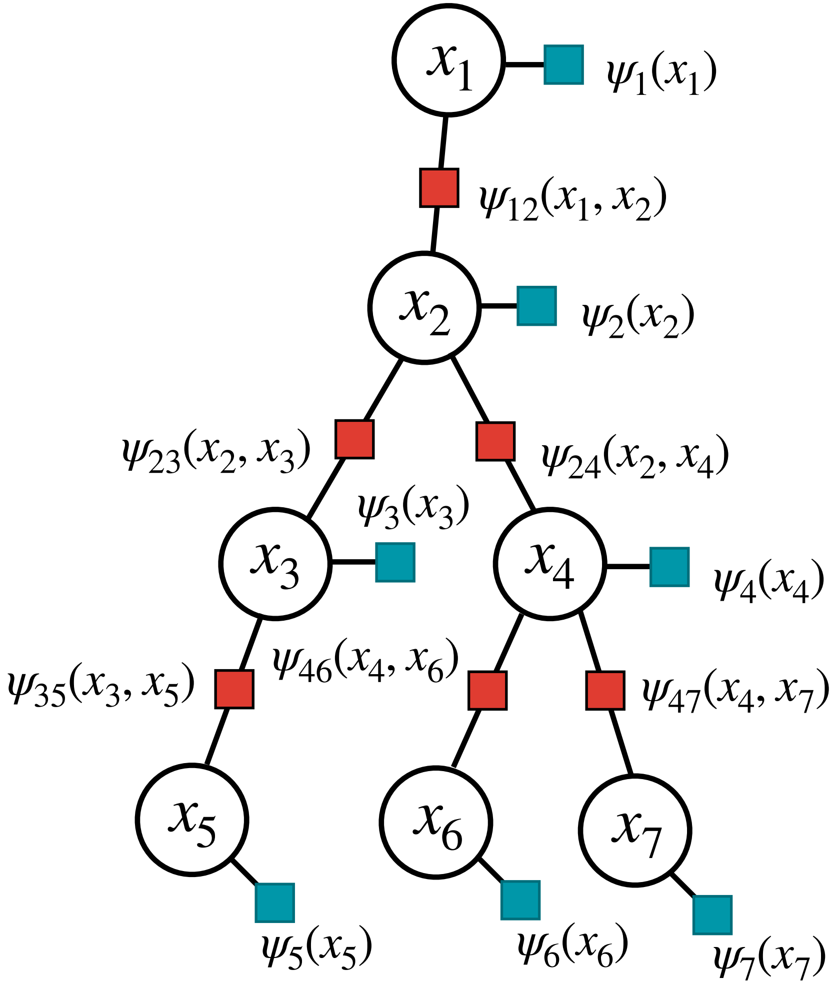

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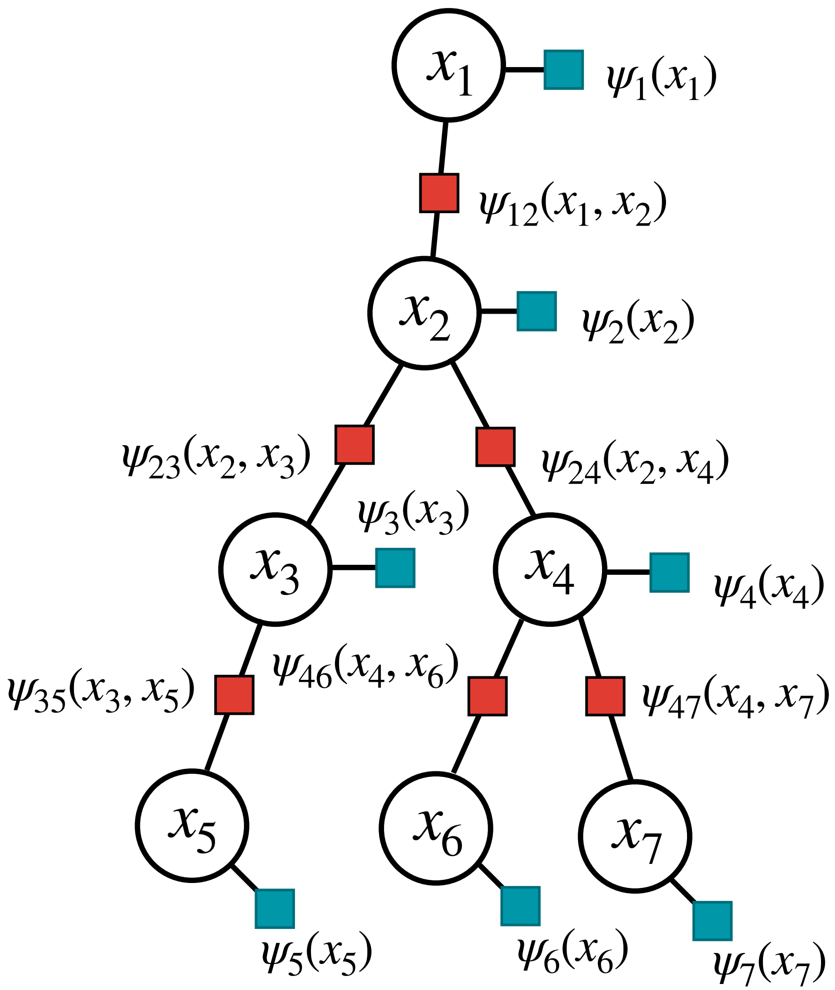

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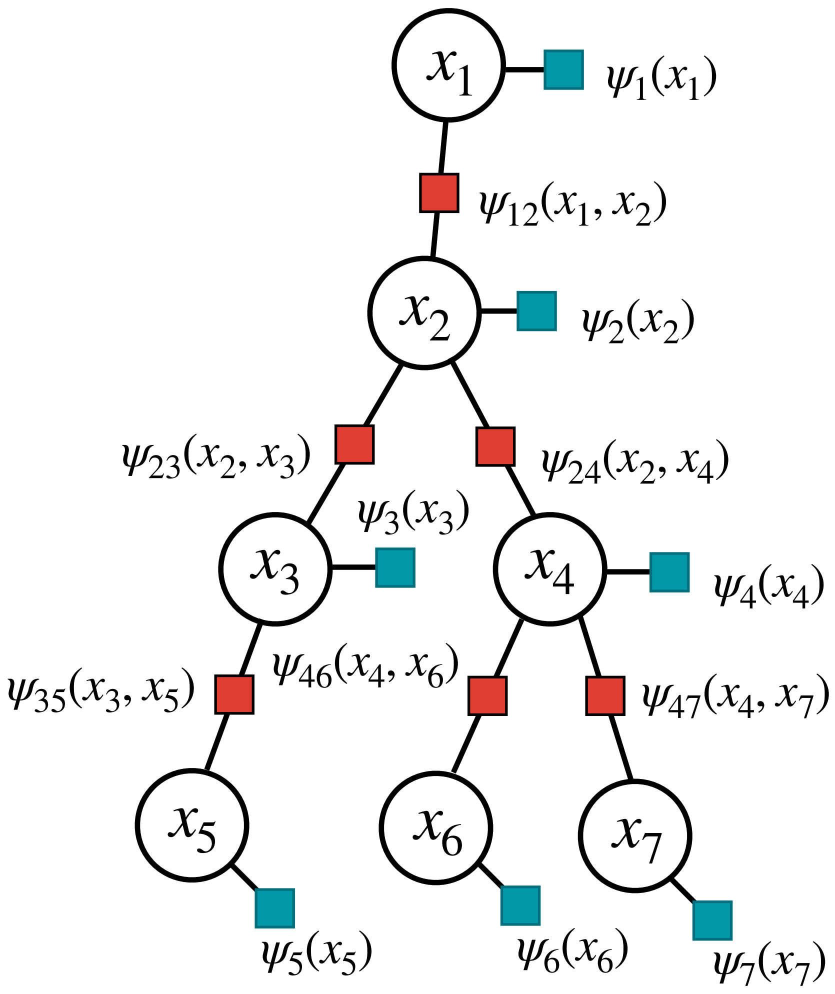

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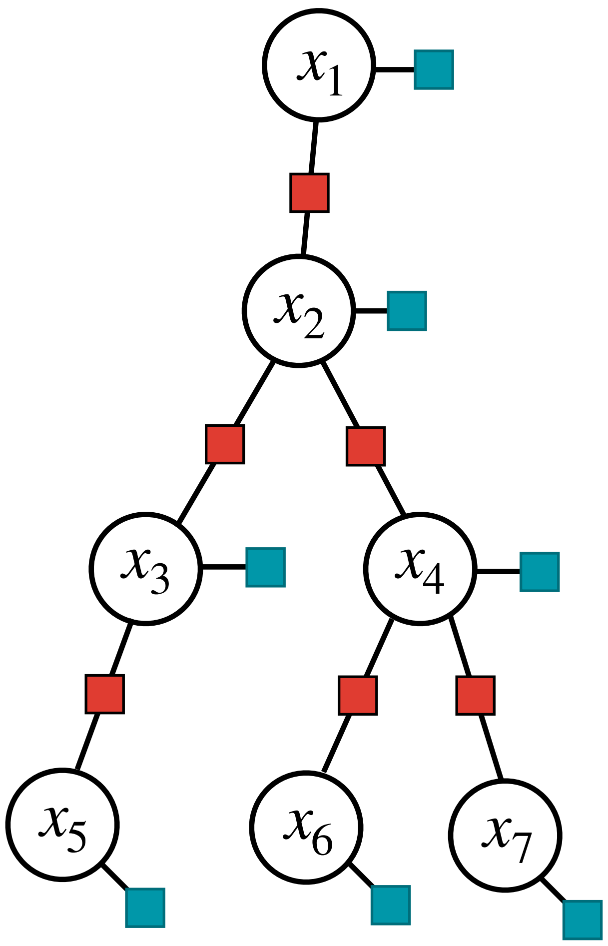

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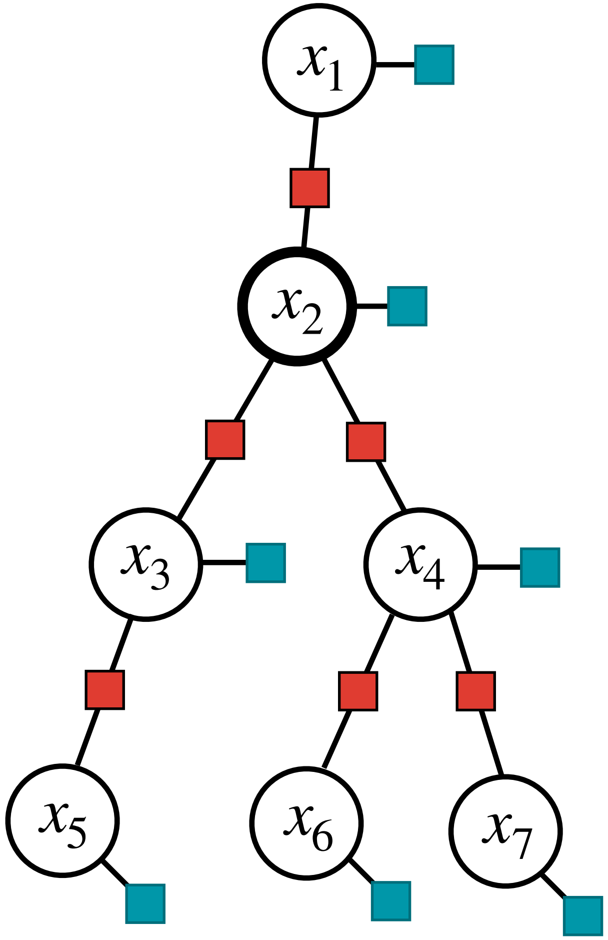

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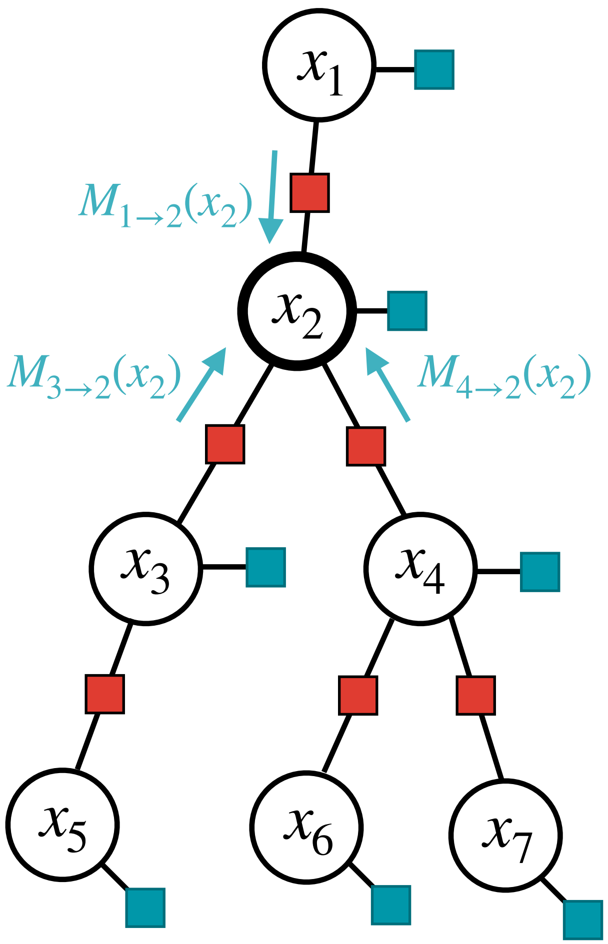

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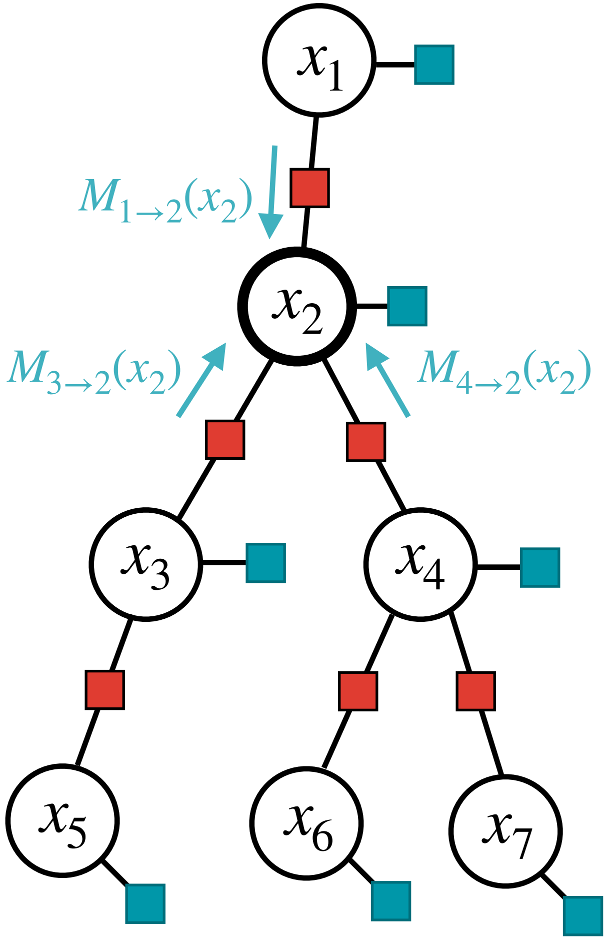

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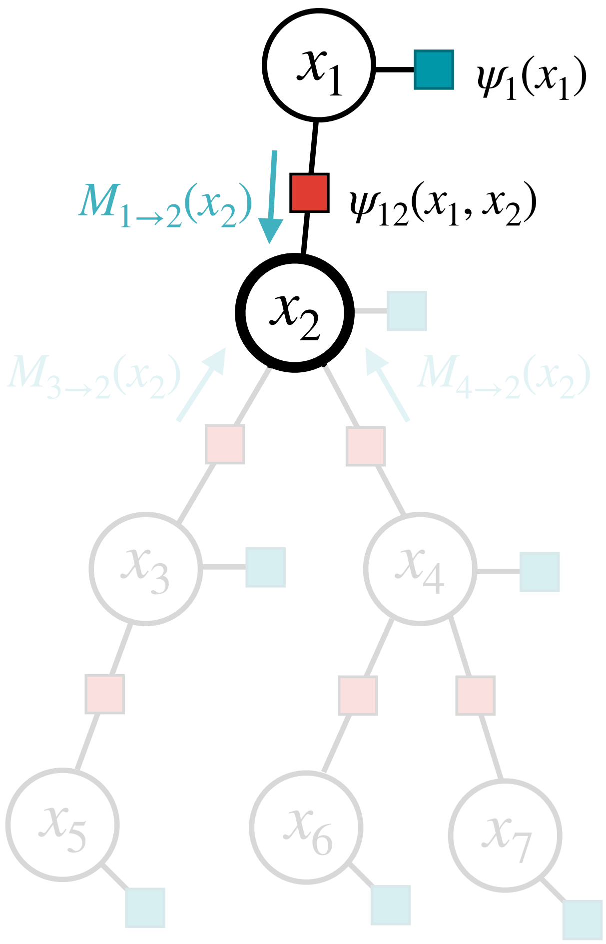

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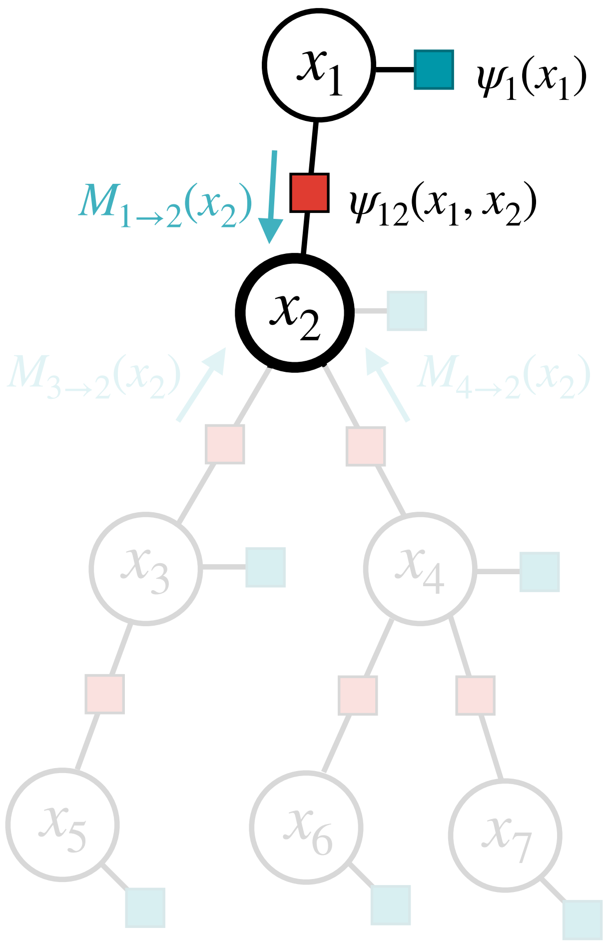

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$$M_{1\to 2}(x_2) = \sum_{x_1 \in \{1,\ldots,K\}} \psi_{12}(x_1, x_2)\, \psi_1(x_1) \prod_{k \sim 1, k \neq 2} M_{k\to 1}(x_1)$$

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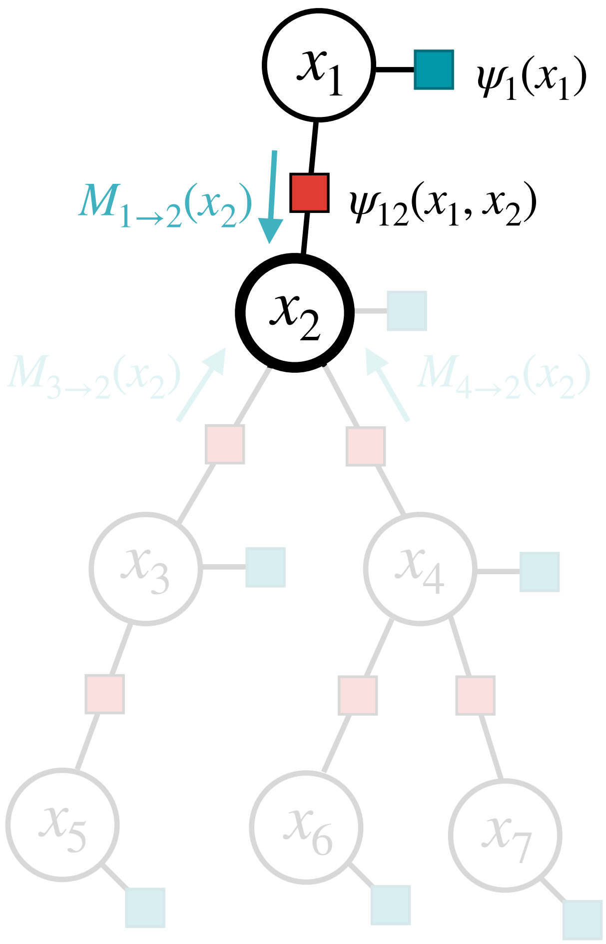

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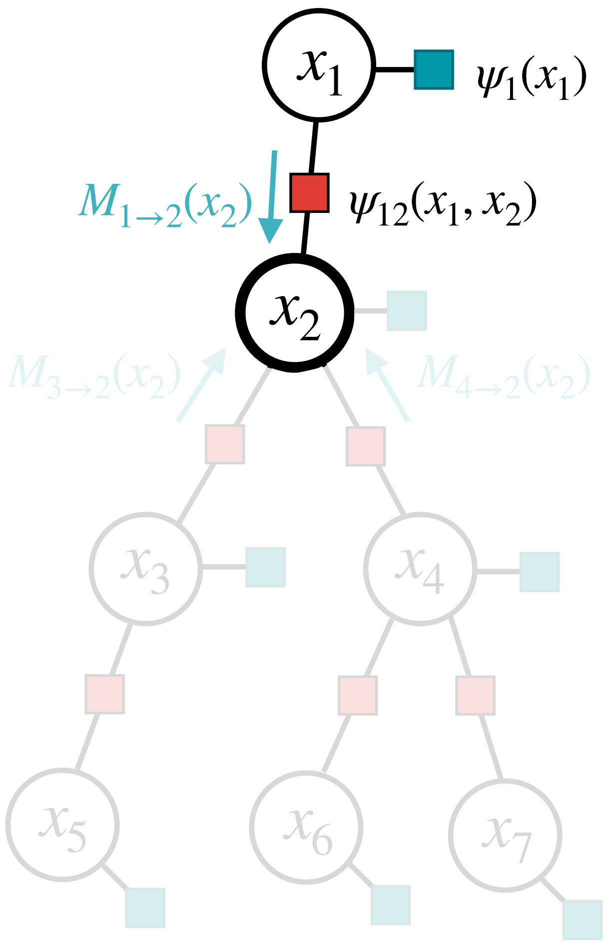

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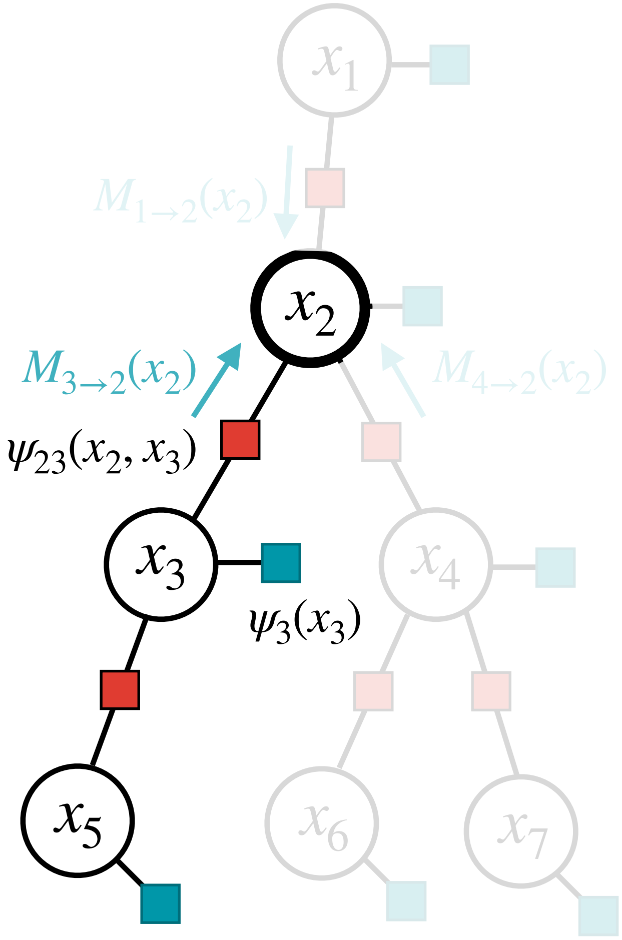
Rule: Ignore "incoming messages" to node i if there are none

Step 1. Message update



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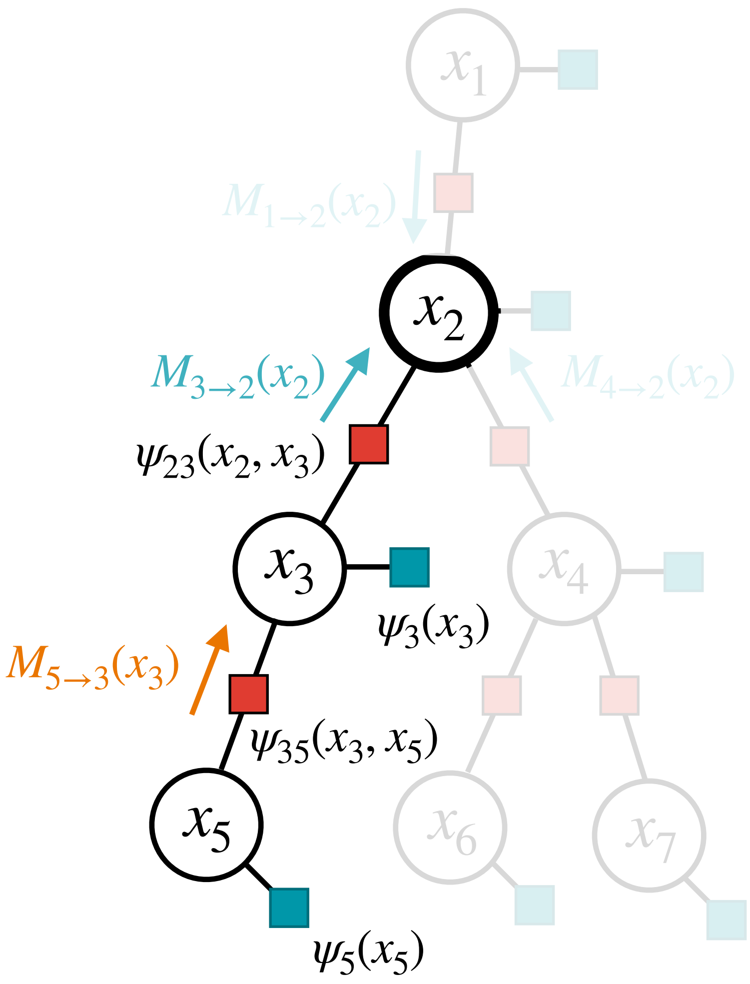

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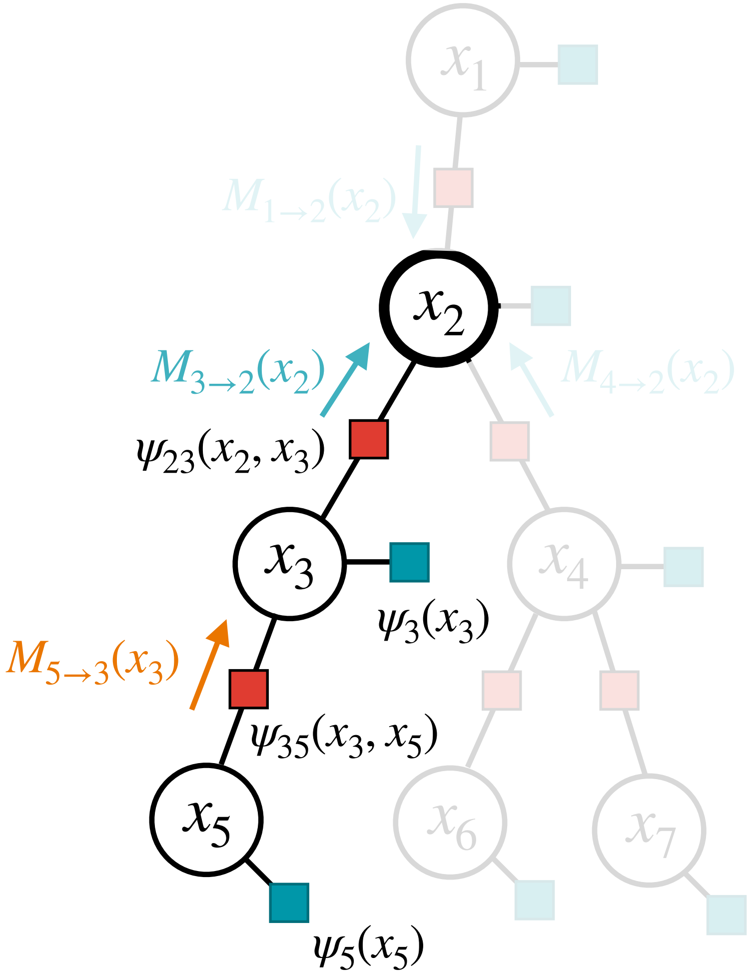

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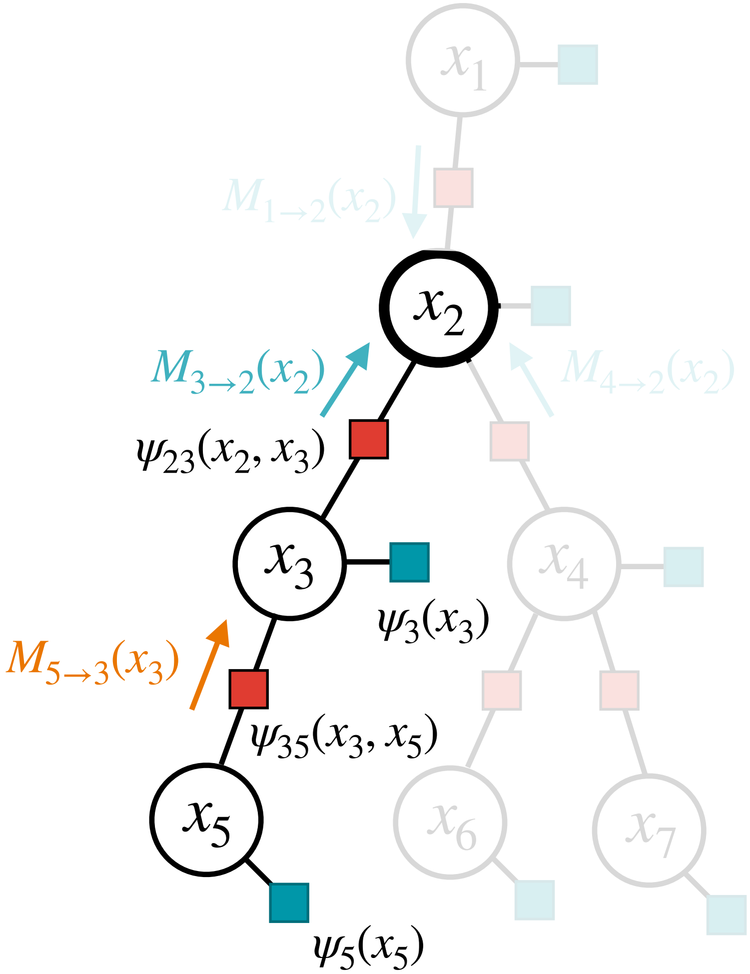
$$M_{5\to 3}(x_3) = \sum_{x_5 \in \{1,\ldots,K\}} \psi_{35}(x_3, x_5)\psi_5(x_5) \prod_{k\sim 5, k\neq 3} M_{k\to 5}(x_5)$$

Step 1. Message update



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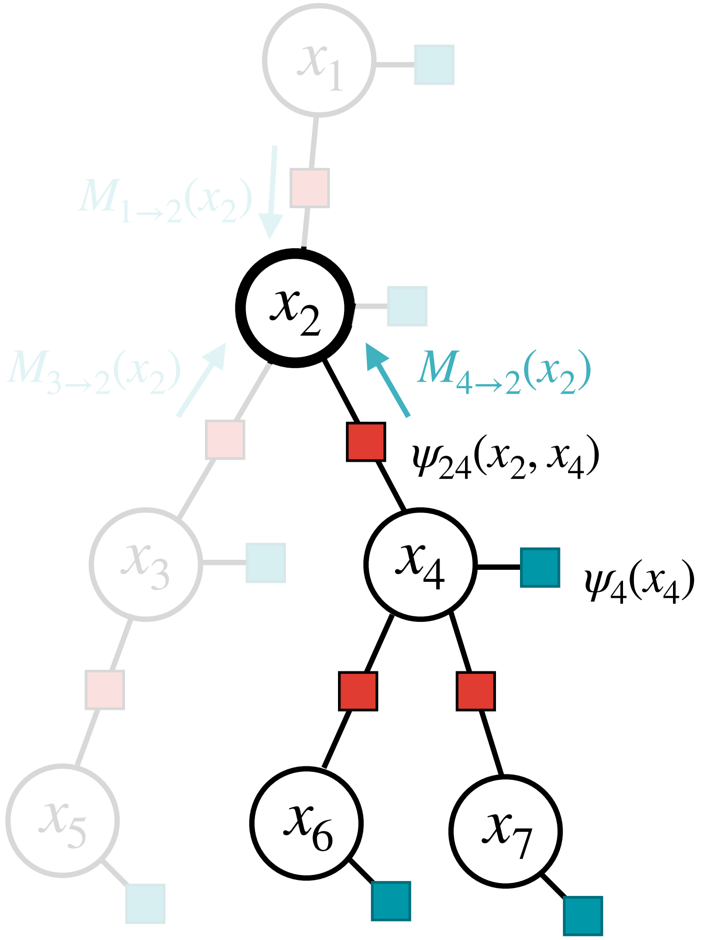
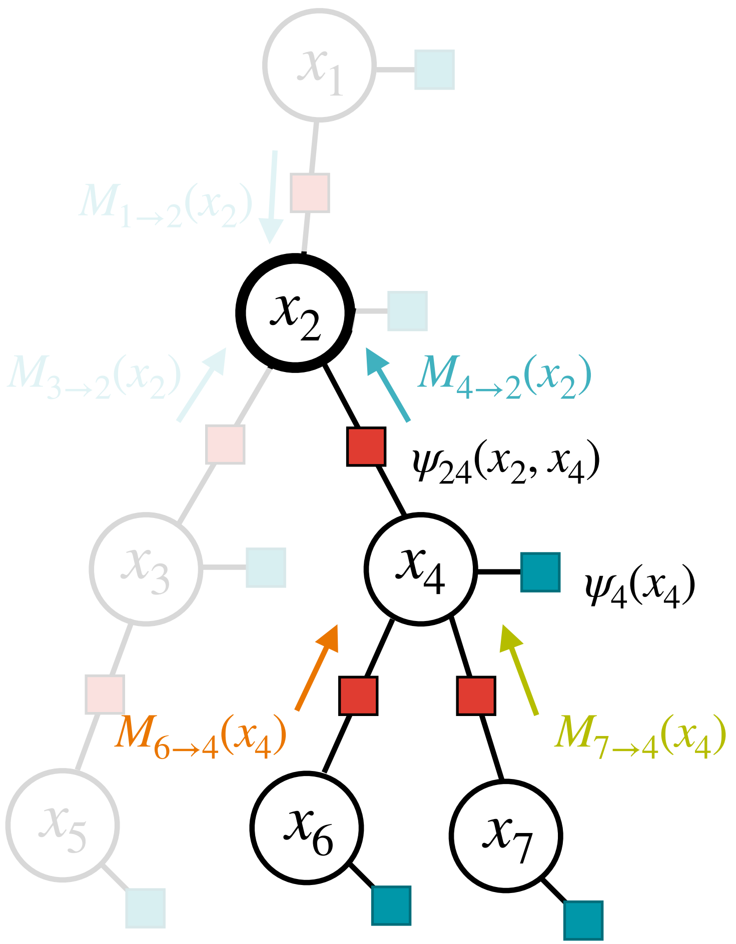
Step 1. Message update



Finally, compute the message $x_4 \to x_2$:

$$\boxed{M_{4\to2}(x_2)} = \sum_{x_4\in\{1,\ldots,K\}} \psi_{24}(x_2, x_4)\, \psi_4(x_4) \underbrace{\prod_{k\sim4,k\neq2} M_{k\to4}(x_4)}_{??}$$

Step 1. Message update



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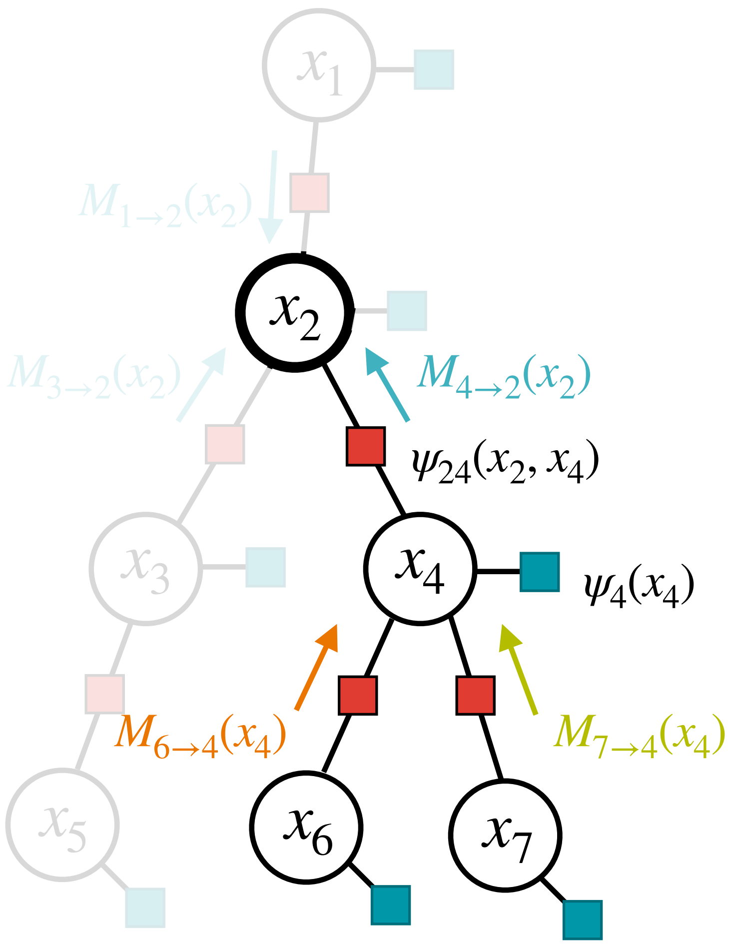
$$M_{4\to2}(x_2) = \sum_{x_4\in\{1,\ldots,K\}} \psi_{24}(x_2, x_4)\, \psi_4(x_4)\, M_{6\to4}(x_4)\, M_{7\to4}(x_4)$$

Step 1. Message update



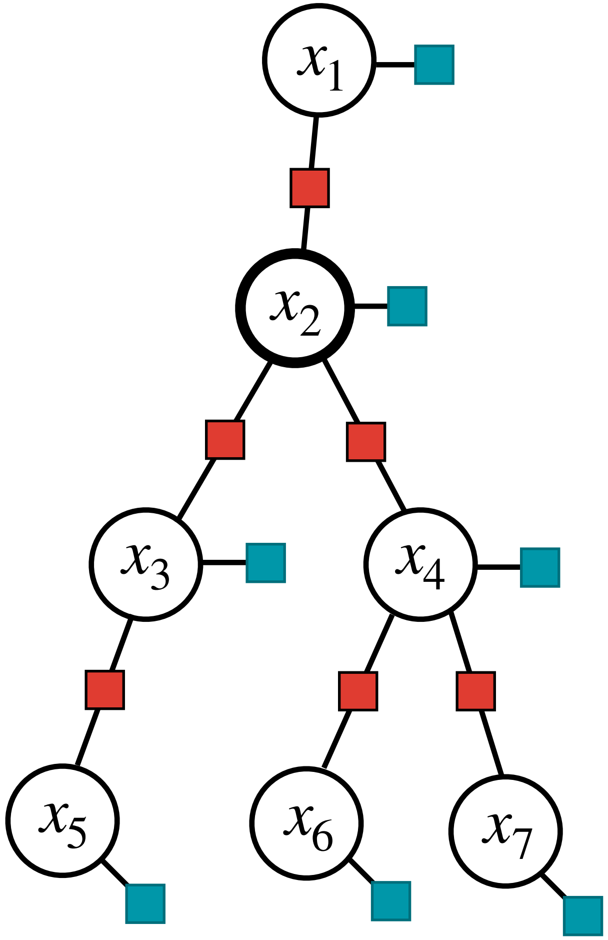
Finally, compute the message $x_4 \to x_2$:

$$M_{4\to 2}(x_2) = \sum_{x_4 \in \{1,\ldots,K\}} \psi_{24}(x_2, x_4)\, \psi_4(x_4)\, M_{6\to 4}(x_4)\, M_{7\to 4}(x_4)$$

$$M_{6\to 4}(x_4) = \sum_{x_6 \in \{1,\ldots,K\}} \psi_{46}(x_4, x_6)\psi_6(x_6)$$

$$M_{7\to 4}(x_4) = \sum_{x_7 \in \{1,\ldots,K\}} \psi_{47}(x_4, x_7)\psi_7(x_7)$$

Belief propagation algorithm



BP proceeds by iteratively updating:

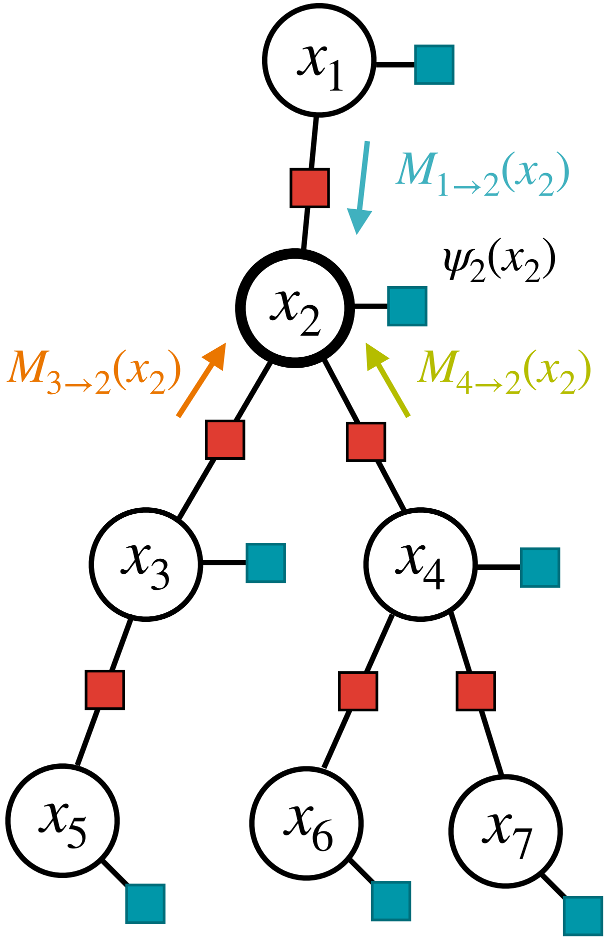
1. The "**messages**" between two nodes

$$M_{j\to i}(x_i) \to \sum_{x_j\in\{1,\ldots,K\}} \psi_{ij}(x_i, x_j)\,\psi_j(x_j) \prod_{k\sim j, k\neq i} M_{k\to j}(x_j)$$

- 2. The "**state**" of each node

$$p(x_i) \to \psi_i(x_i) \prod_{j\sim i} M_{j\to i}(x_i)$$

Step 2. State update



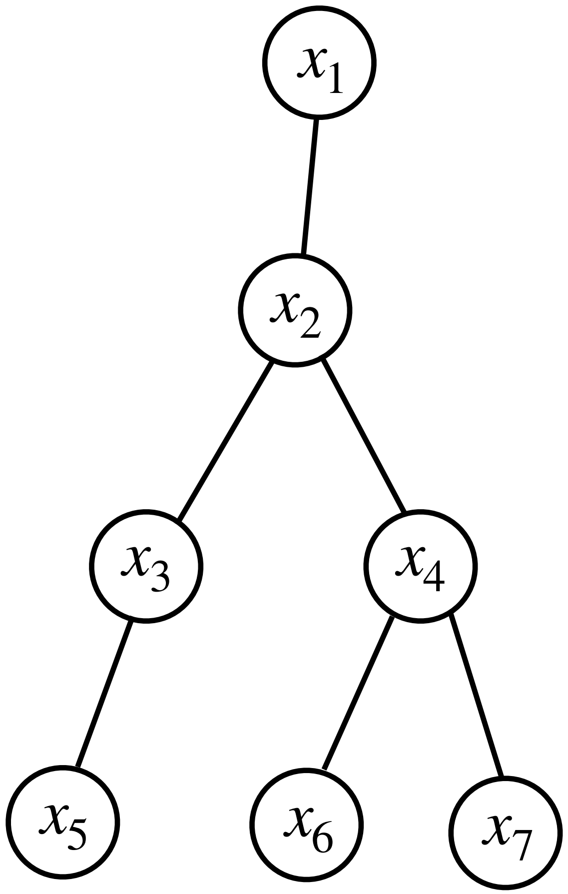
Now we can compute $p(x_2)$:

$$p(x_2) = \frac{1}{Z}\,\psi_2(x_2) \times M_{1\to2}(x_2) \times M_{3\to2}(x_2) \times M_{4\to2}(x_2)$$

where

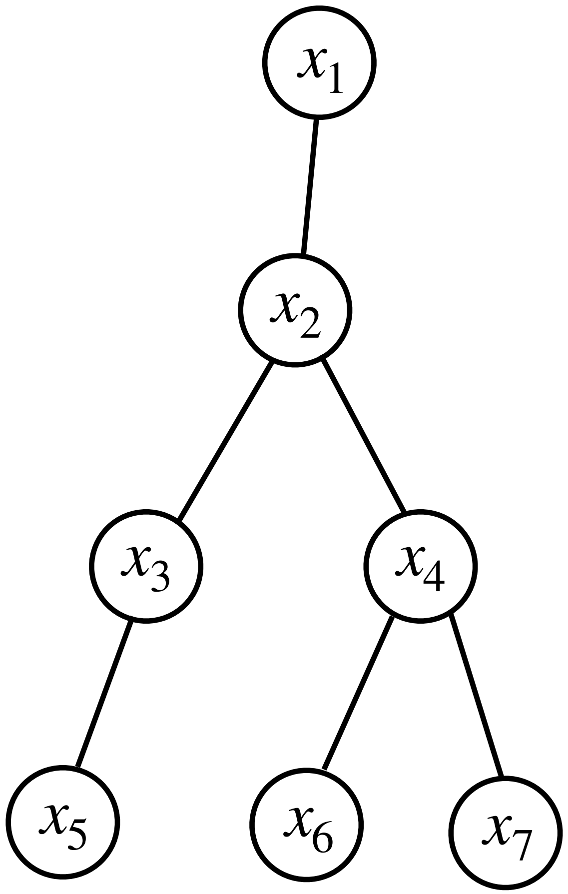
$$Z = \sum_{x_2 \in \{1,\ldots,K\}} \psi_2(x_2) \times M_{1\to2}(x_2) \times M_{3\to2}(x_2) \times M_{4\to2}(x_2)$$

Efficient implementation



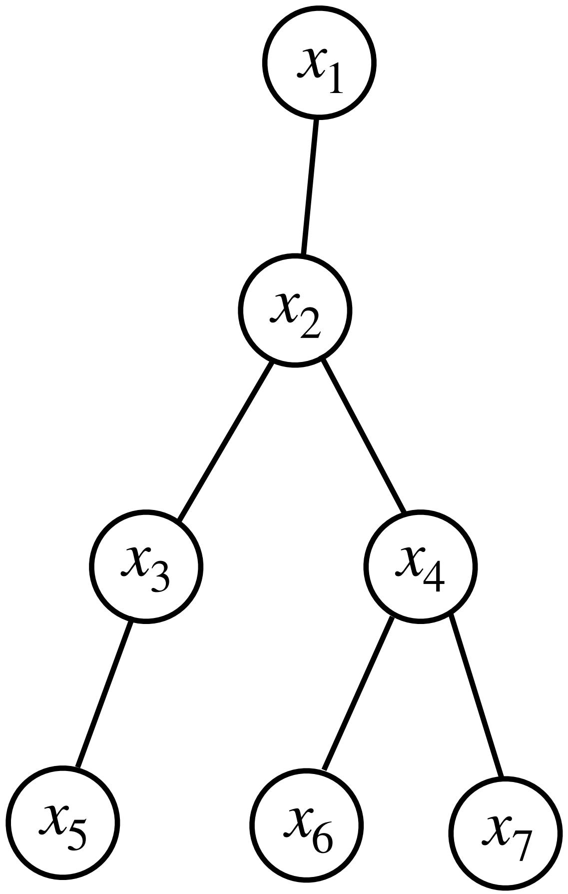
Efficient implementation

Exploiting the tree-structure, we can compute *all* the marginals efficiently



Efficient implementation

Step 0. Initialise



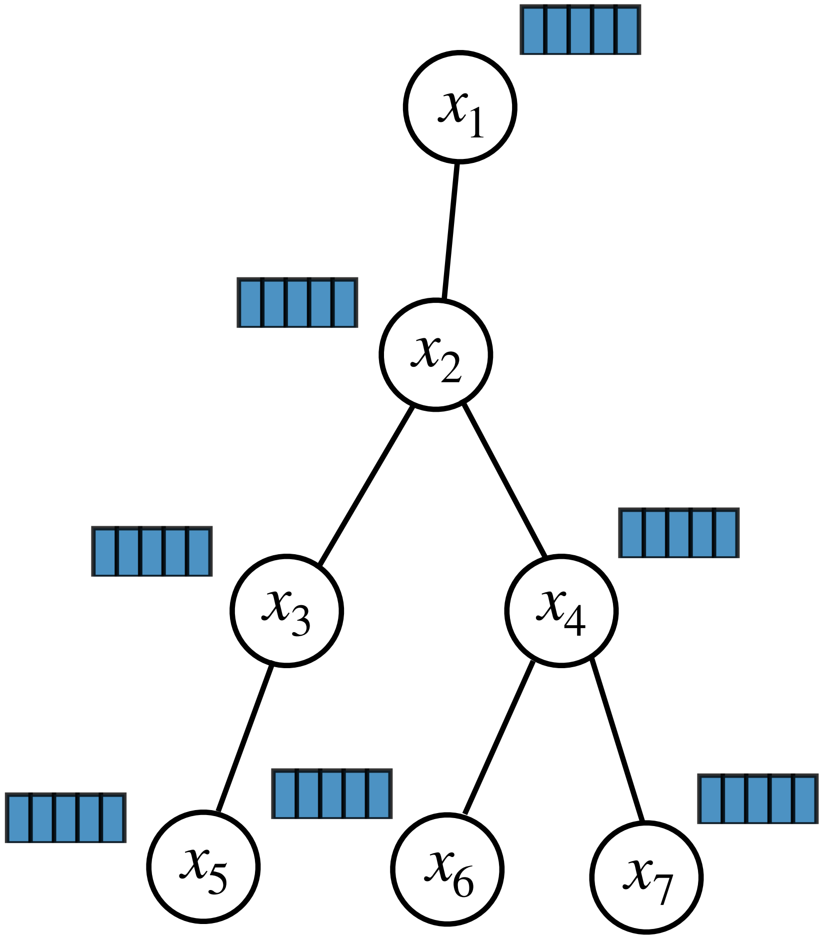
Efficient implementation

Step 0. Initialise

- the **states** as

$$p(x_i) = \frac{1}{K}\mathbf{1},$$

for all $i \in V$, and



Efficient implementation

Step 0. Initialise

- the **states** as

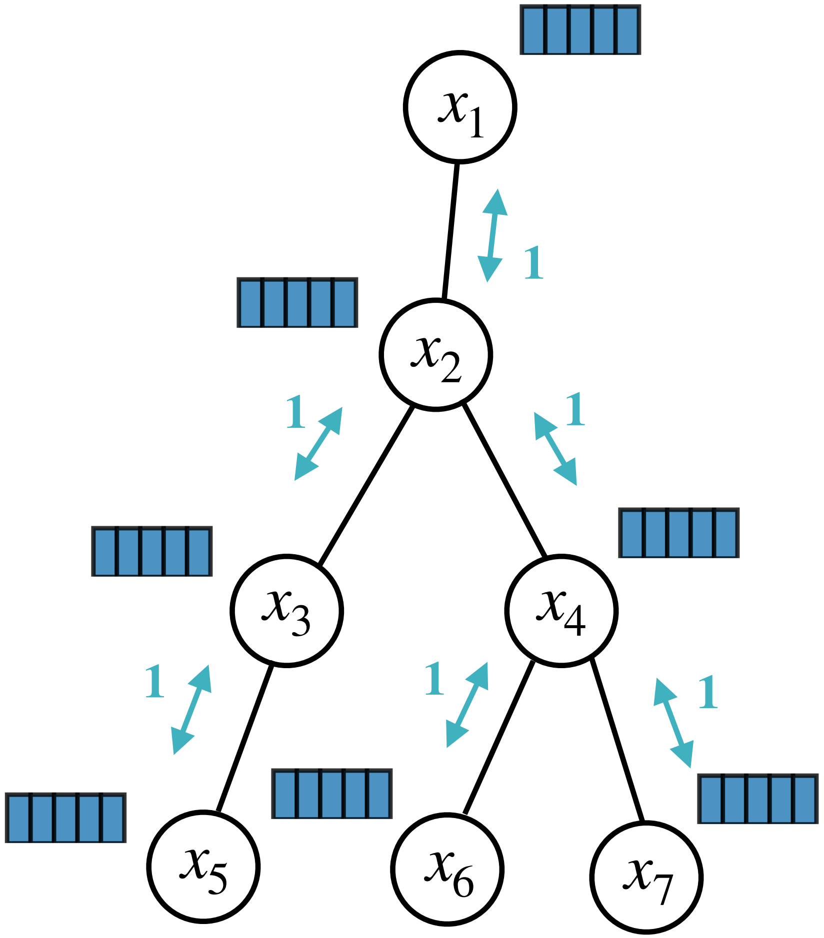
$$p(x_i) = \frac{1}{K}\mathbf{1},$$

  for all $i \in V$, and

- the **messages** as

$$M_{j\to i}(x_i) = \mathbf{1}$$

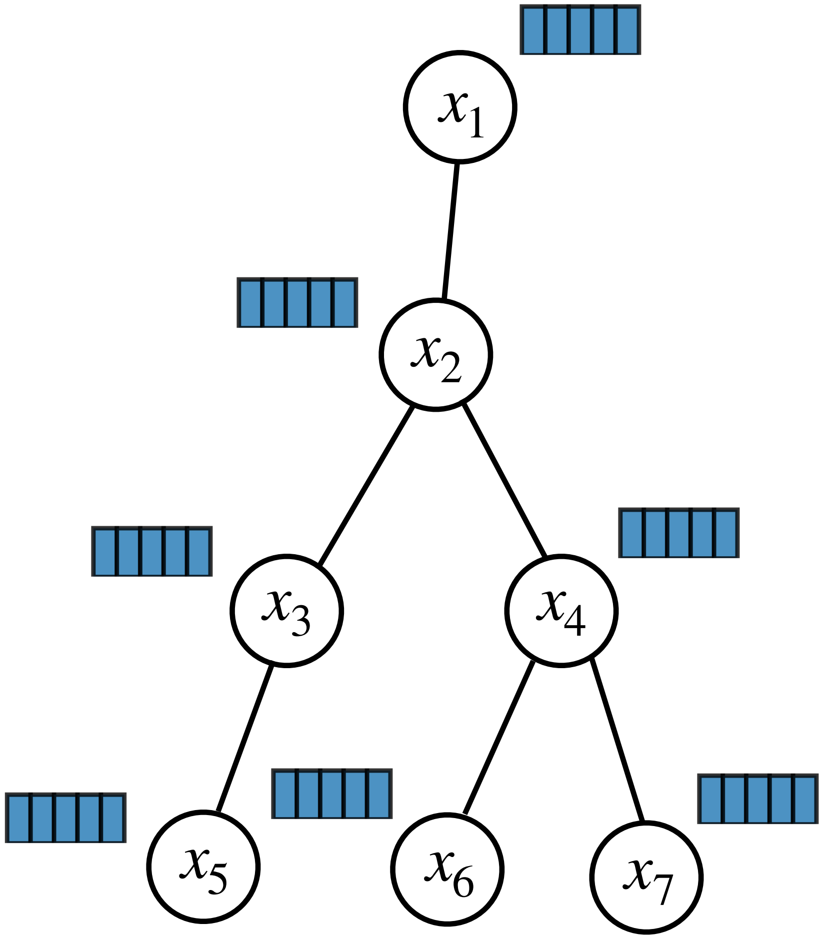
  for all $(i, j) \in E$.



Efficient implementation

Step 1. Choose a "**root**" node and identify the corresponding "**leaf**" nodes

Note: The leaves are the furthest descendants of the root



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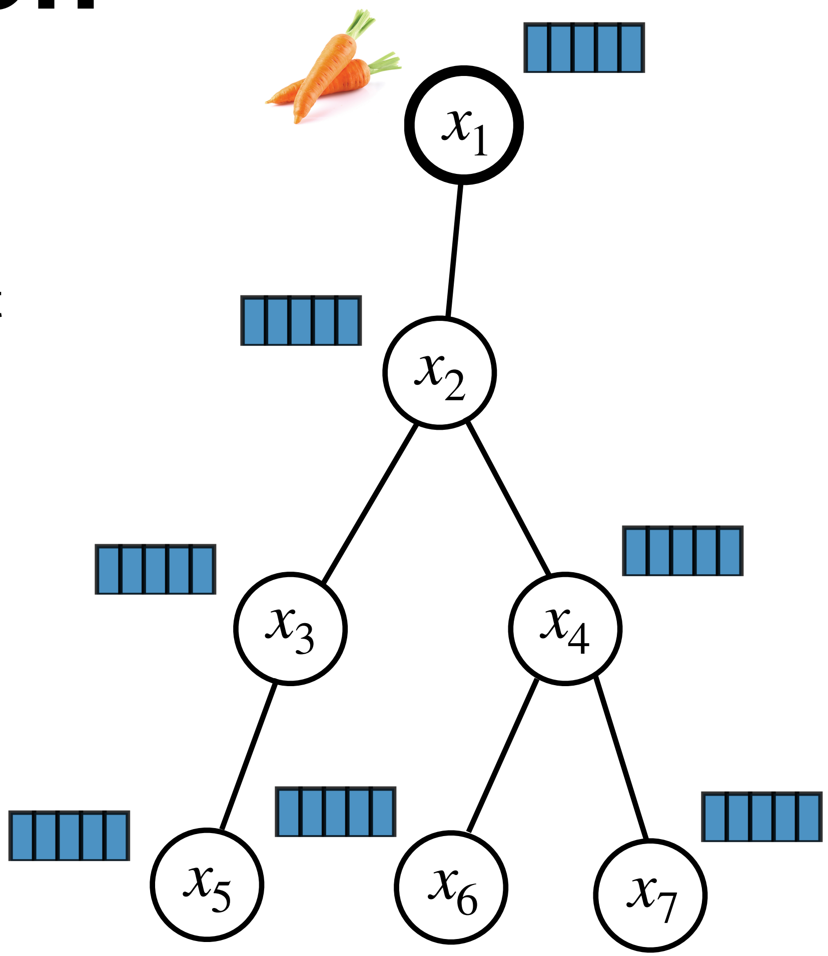

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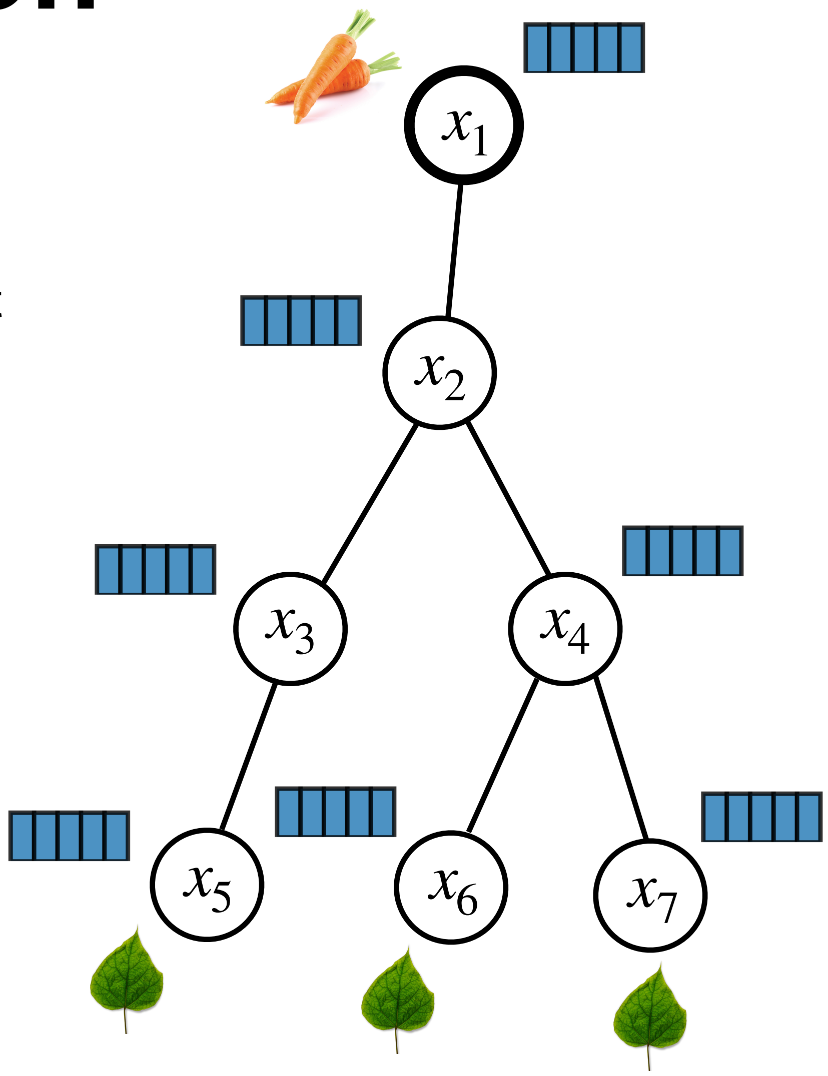
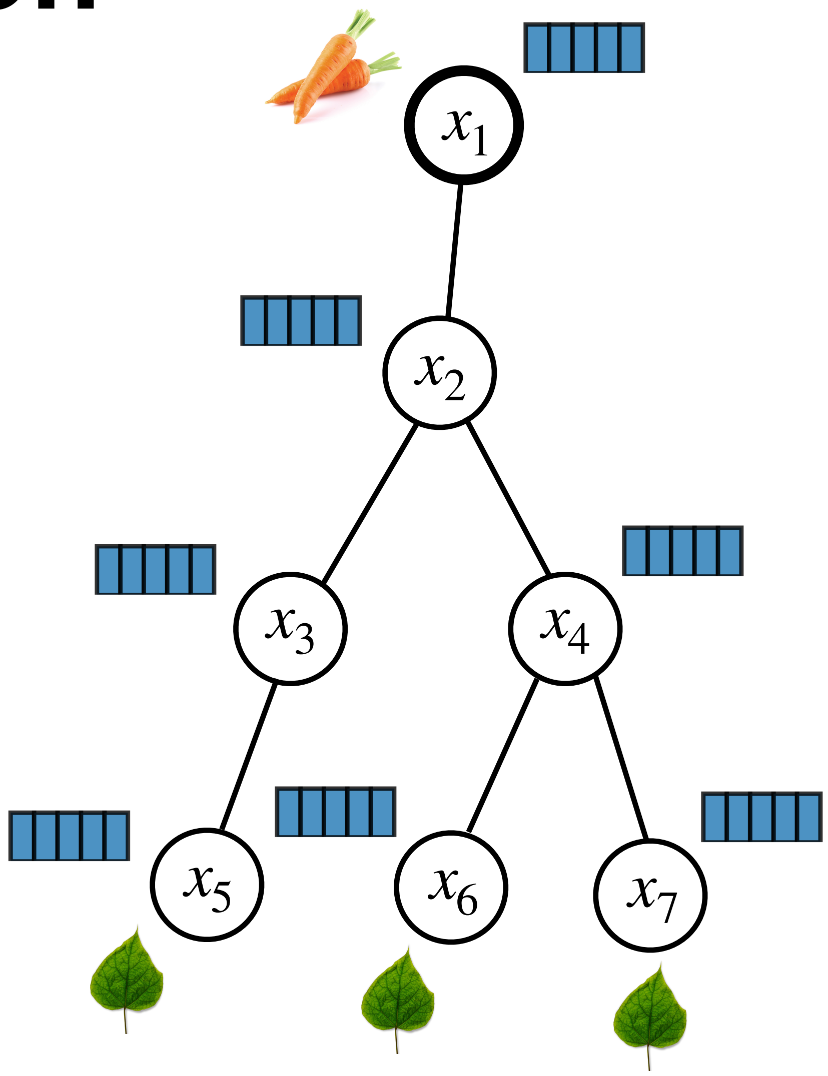


Efficient implementation

Step 2. Update

- all **messages** propagating from the leaf nodes, and
- all the **states** of their parent nodes



Efficient implementation

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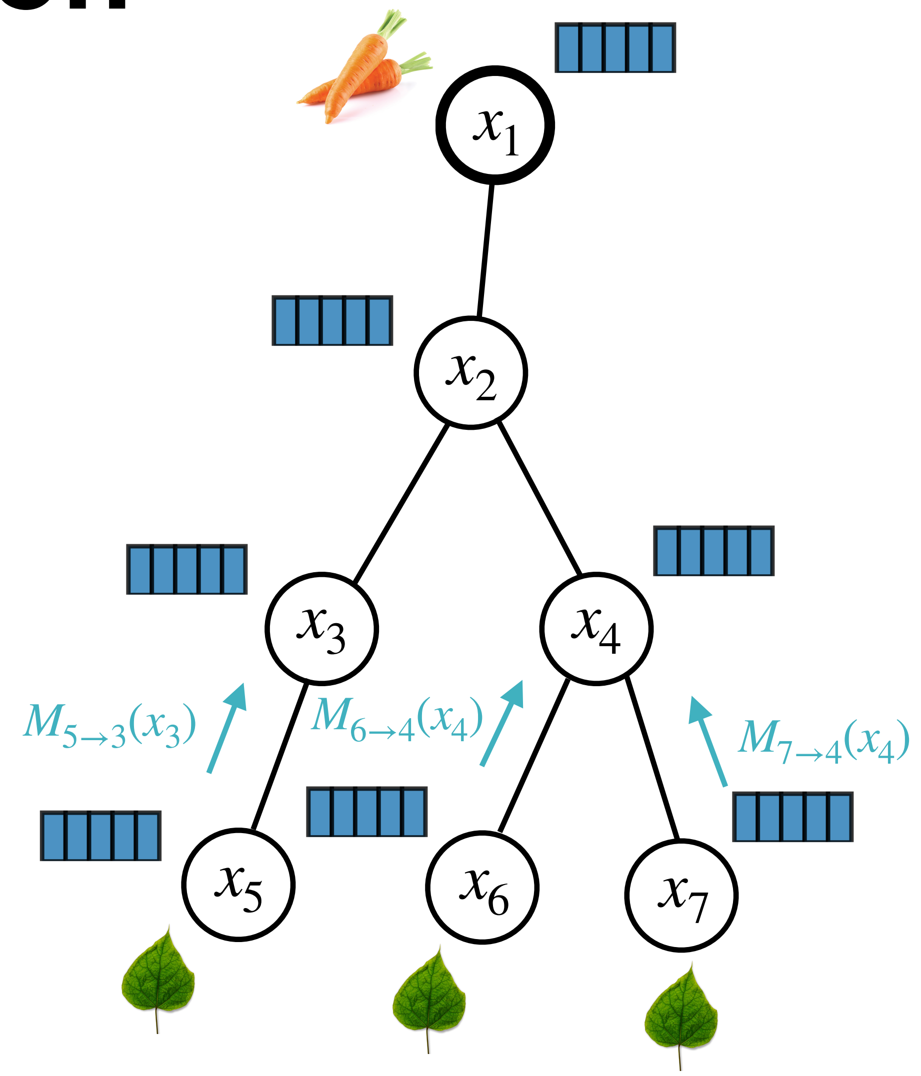

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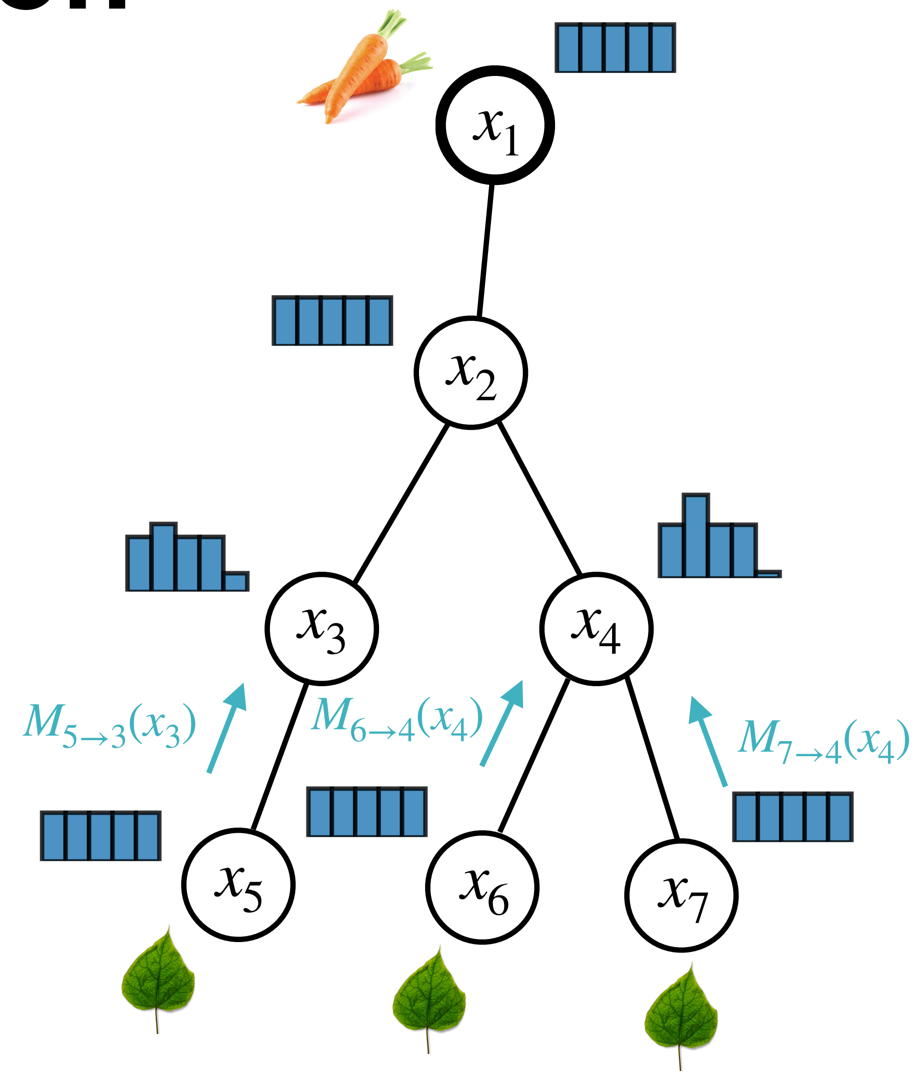
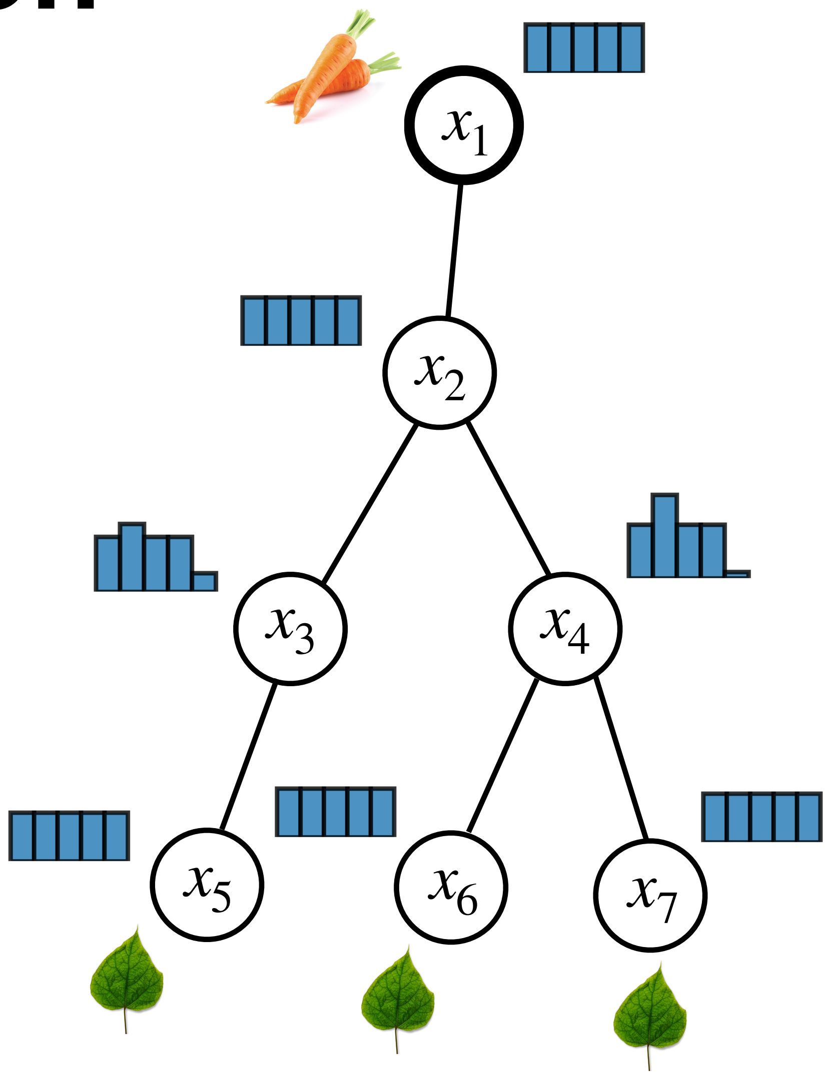


Efficient implementation

Step 3. Update the **messages** and **states** all the way up to the root



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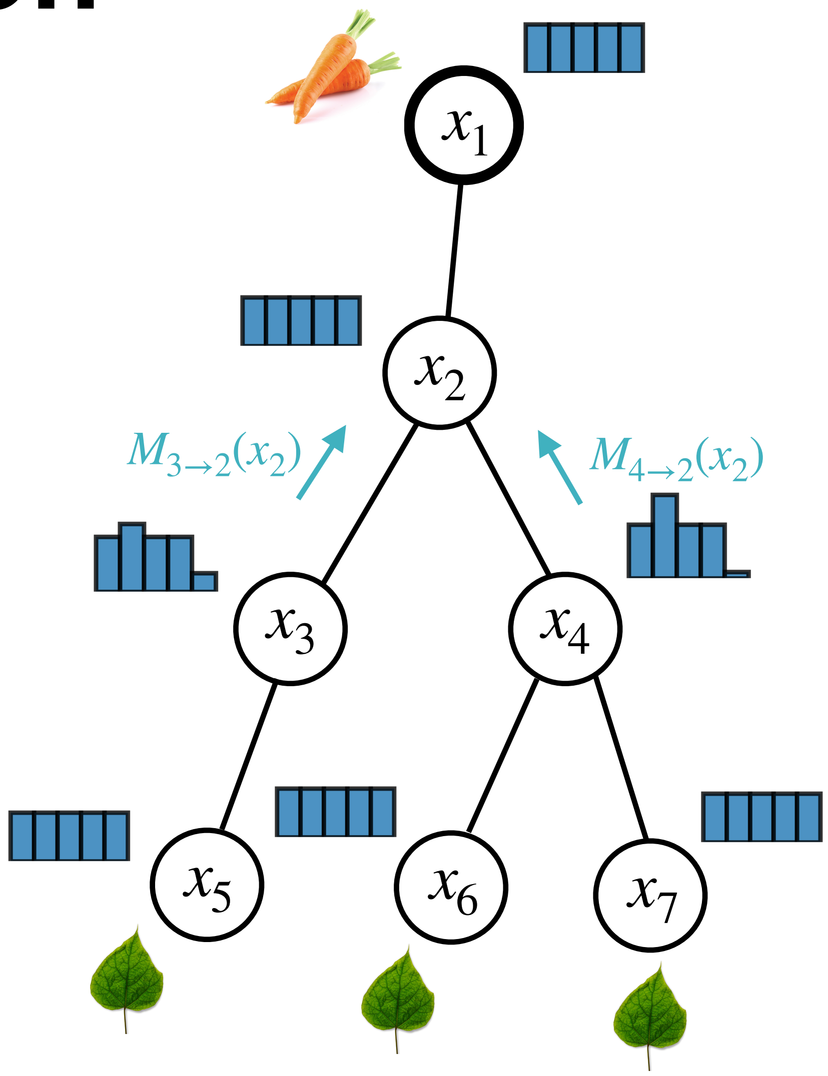

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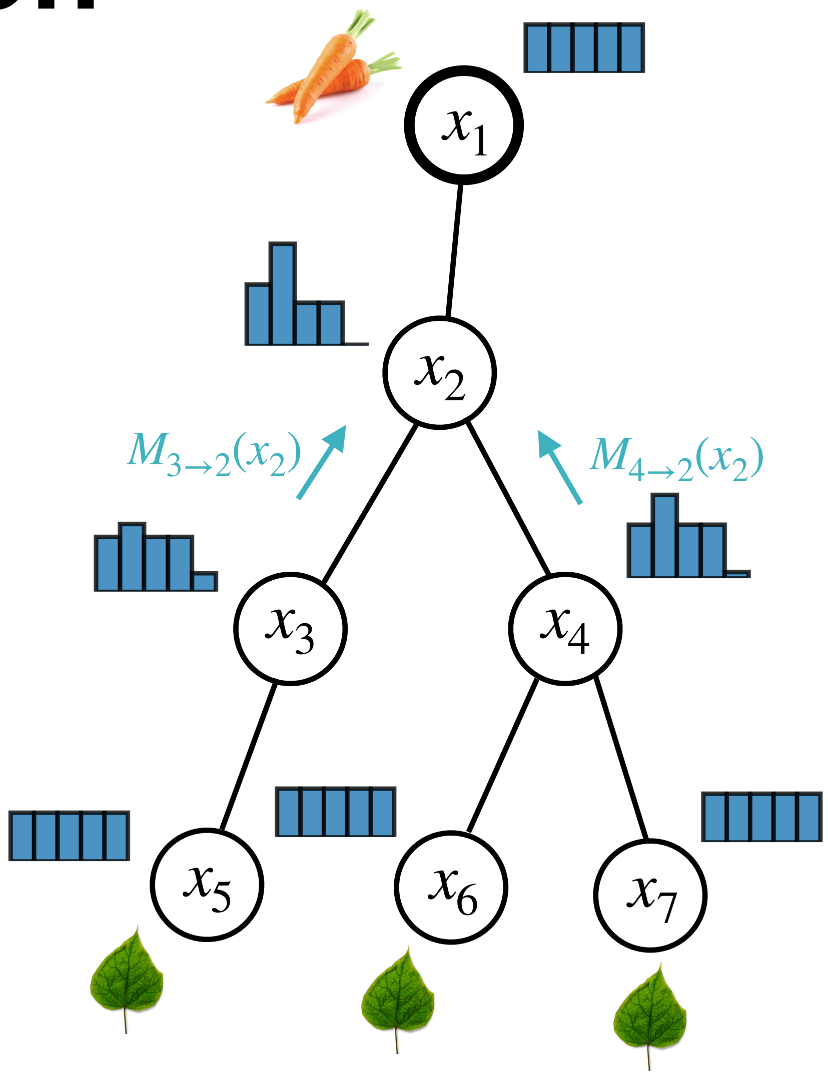

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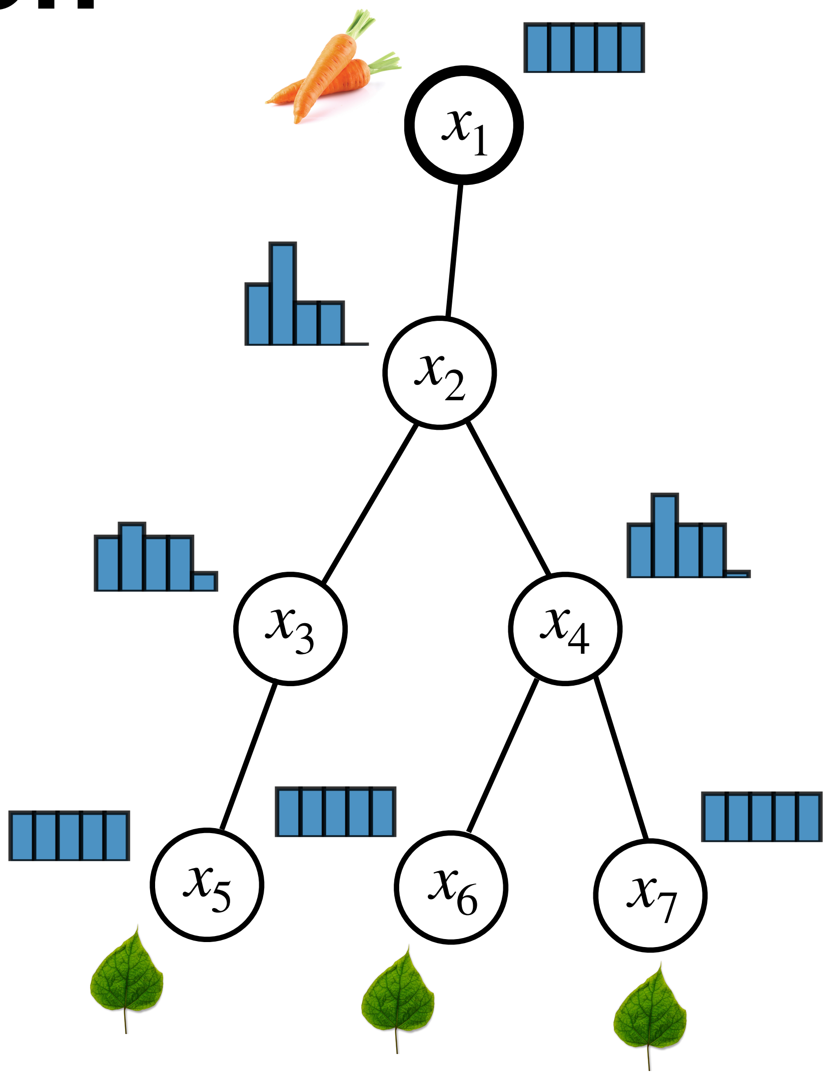

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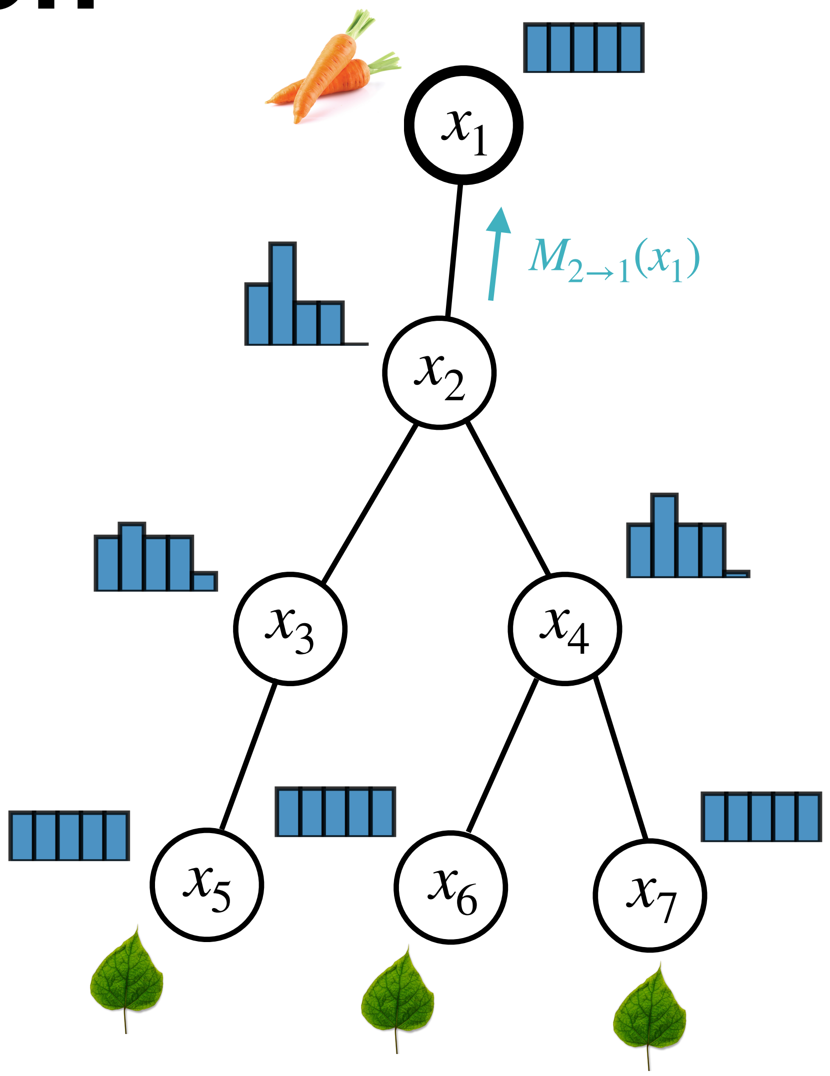

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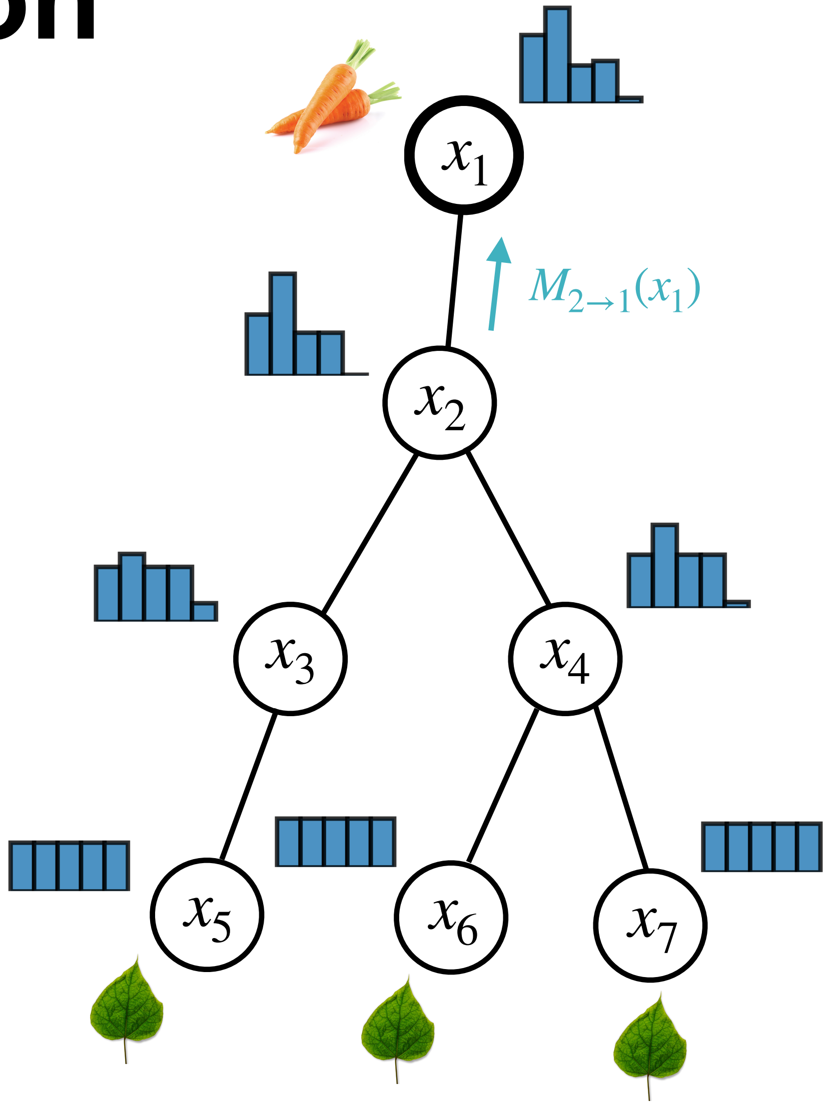
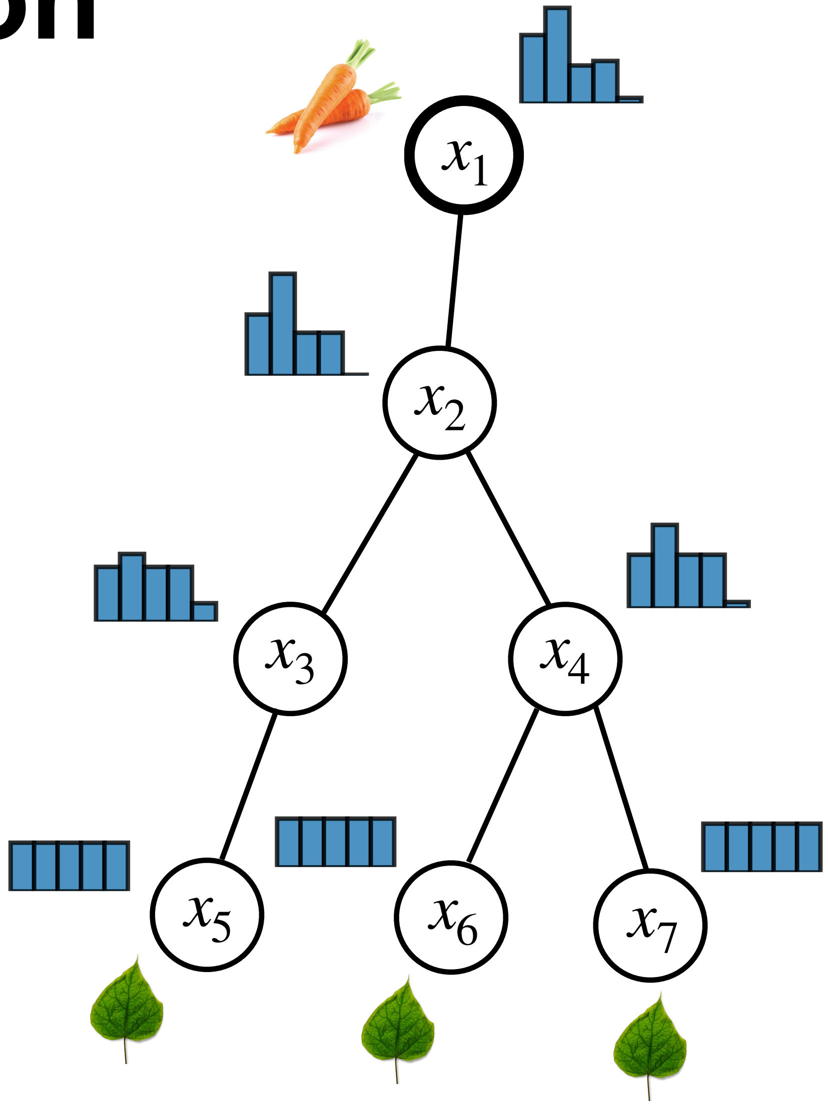


Efficient implementation

Step 4. Do the same, starting from the root and going down to the leaves



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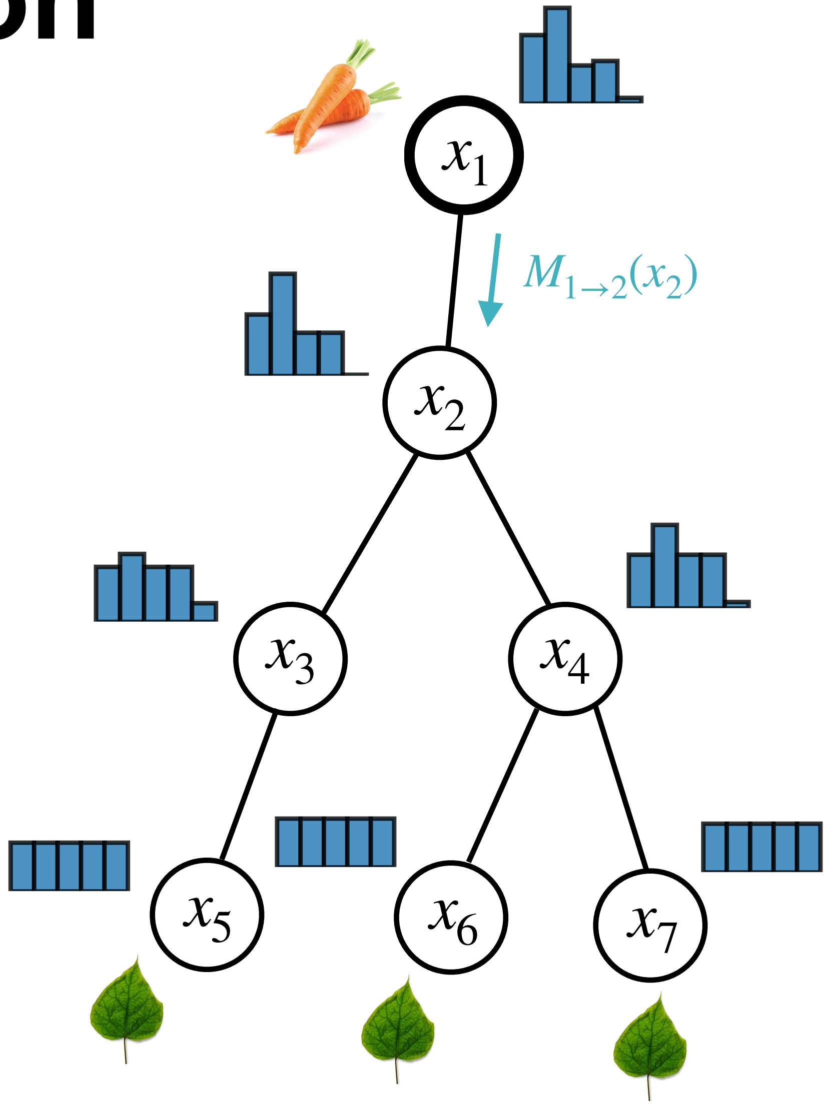

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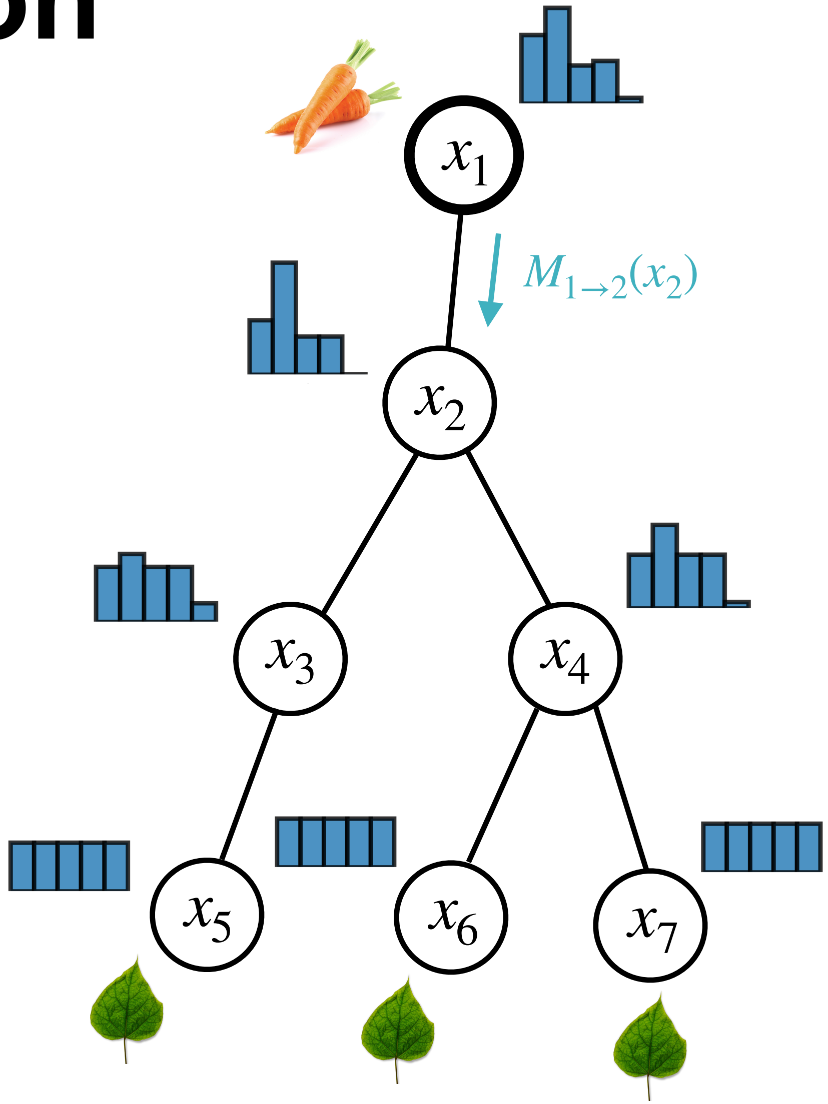

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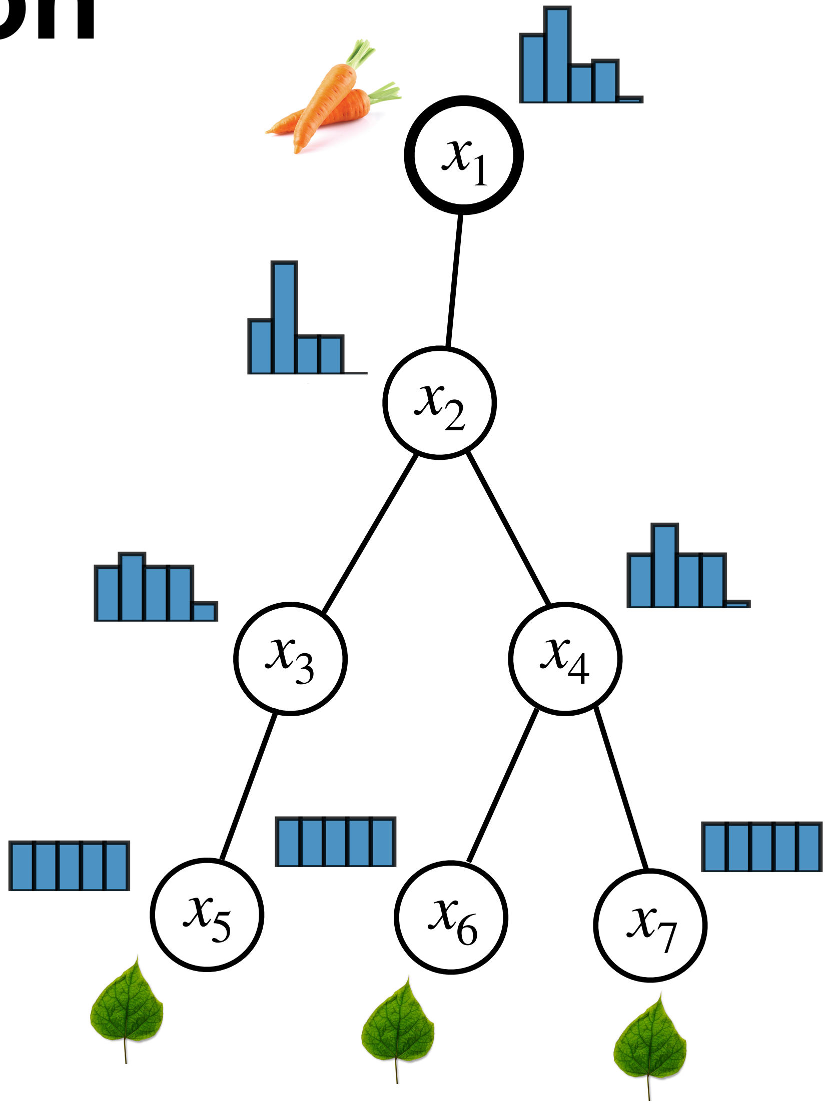

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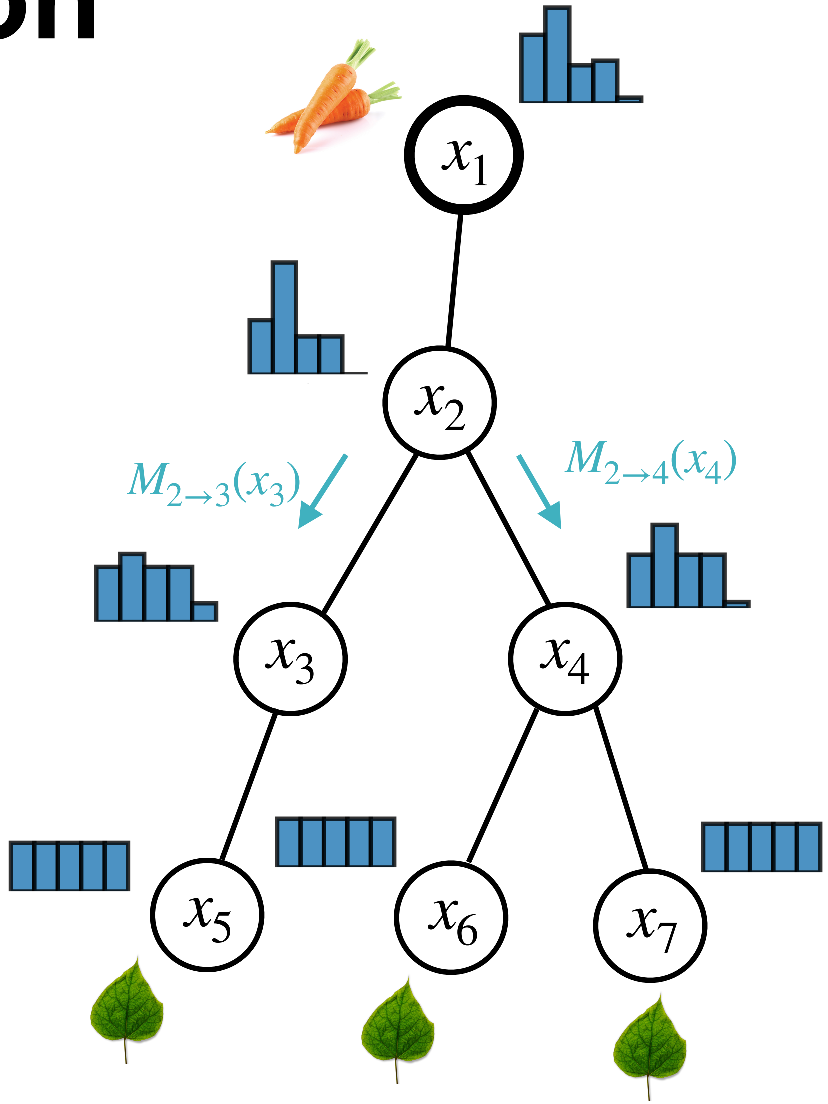

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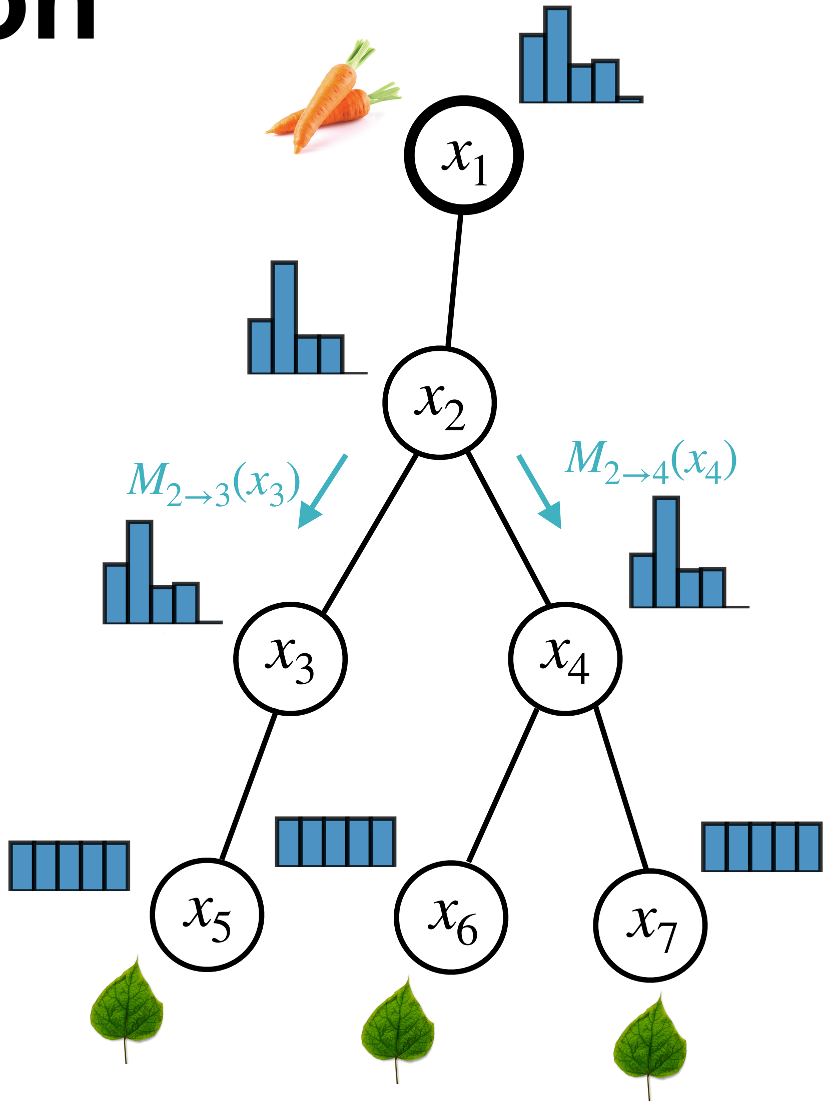

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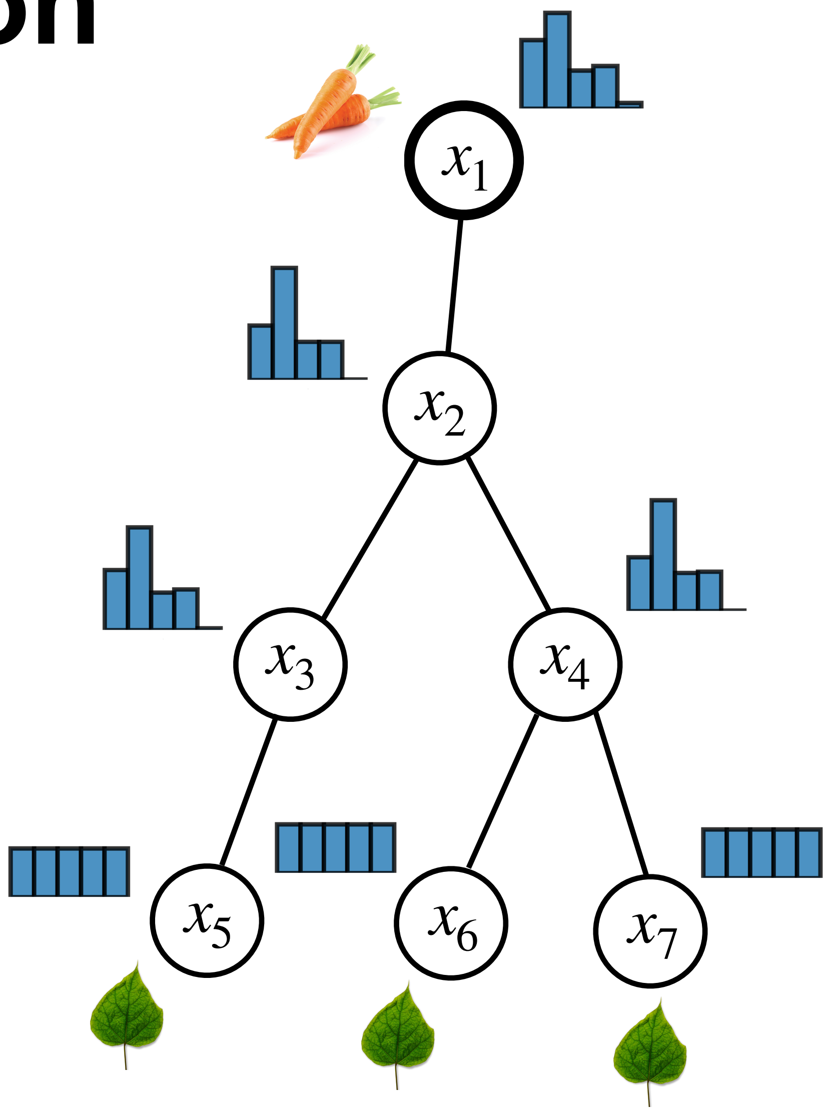

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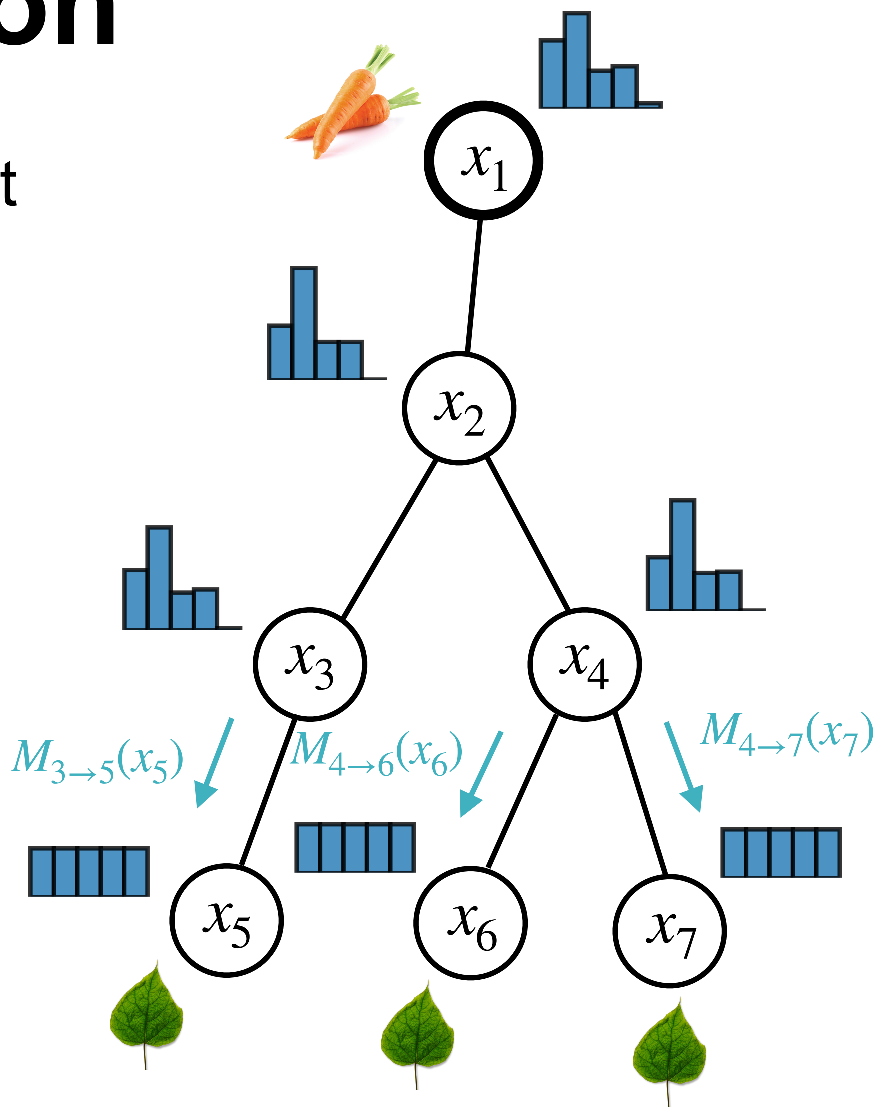

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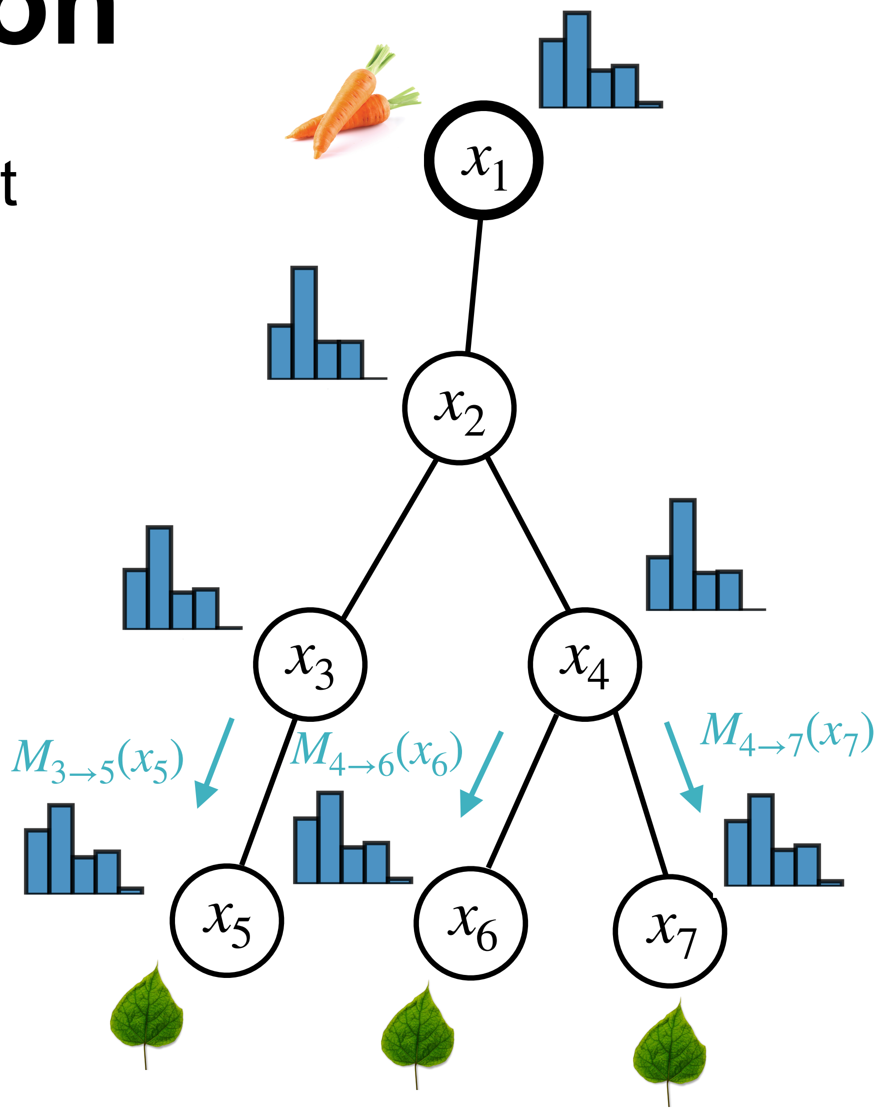

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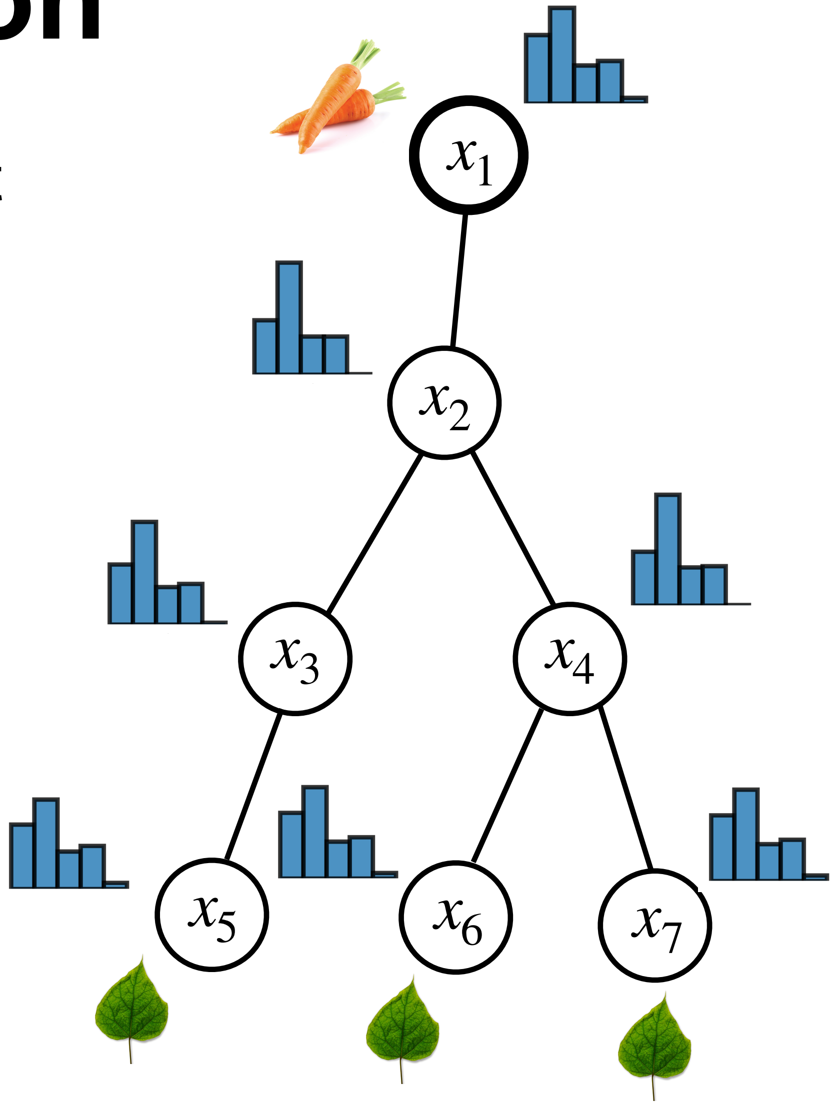
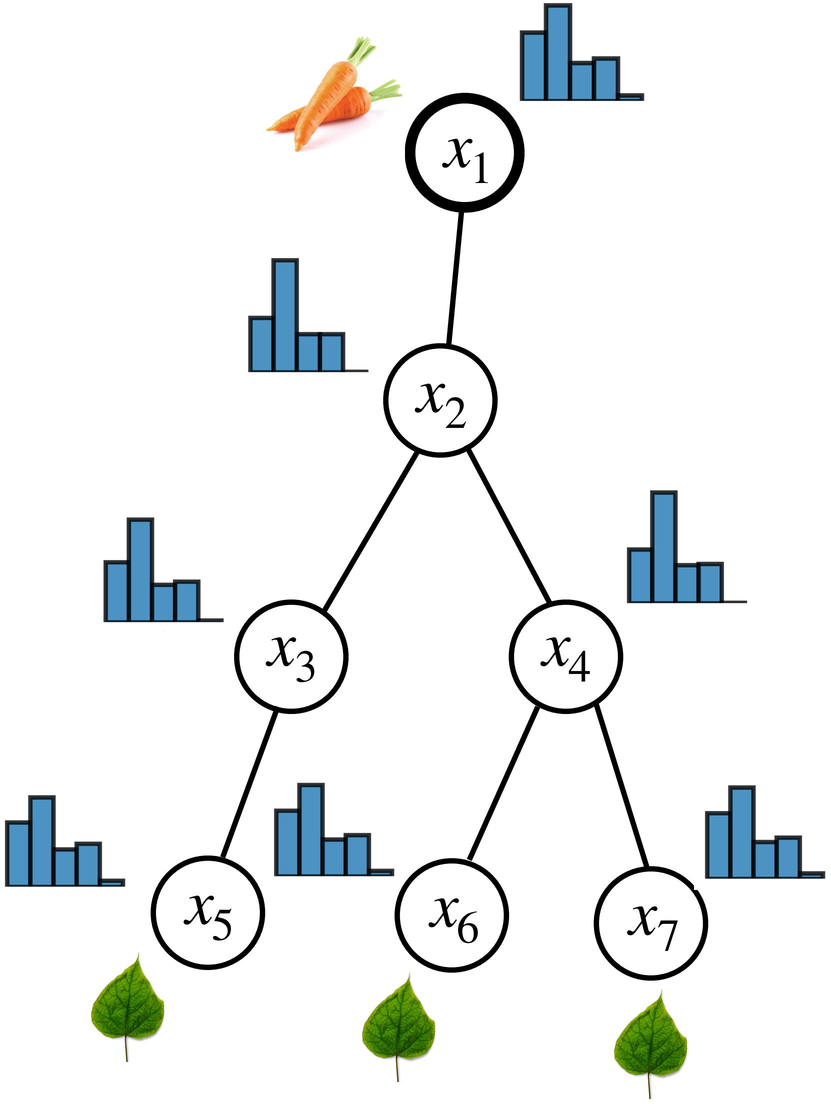
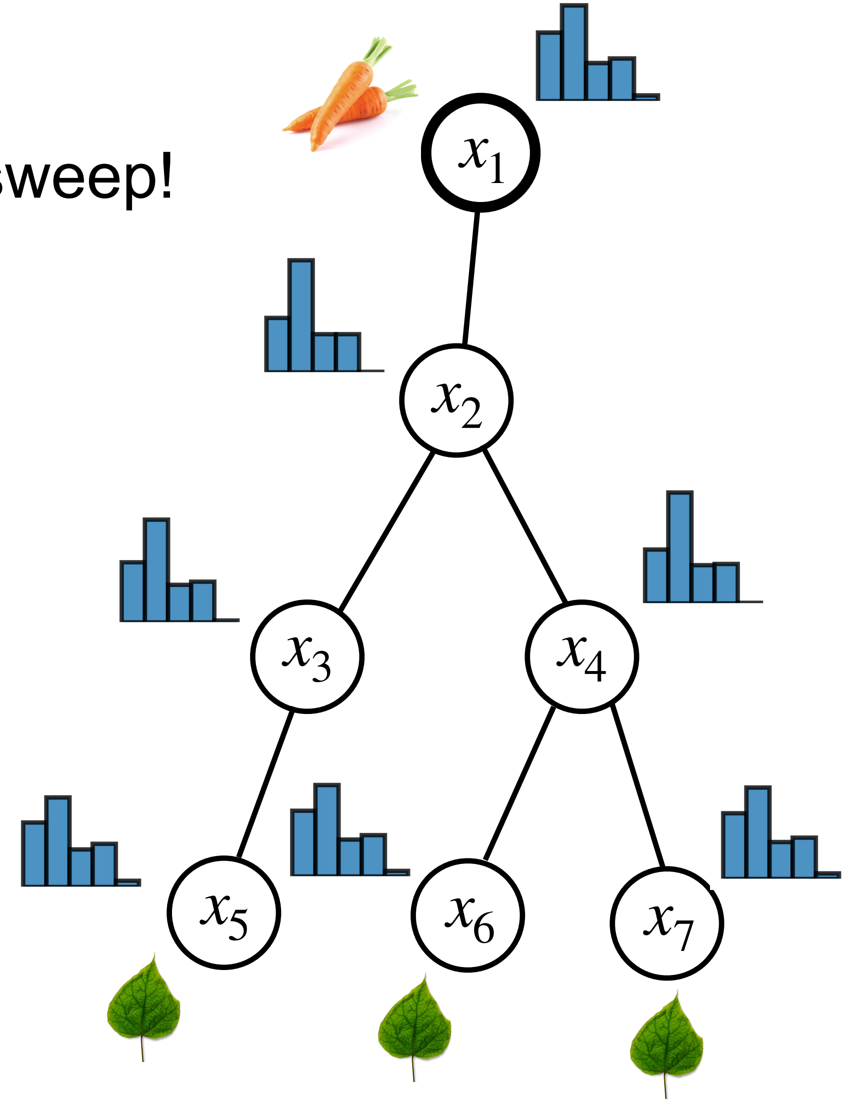


Remarks



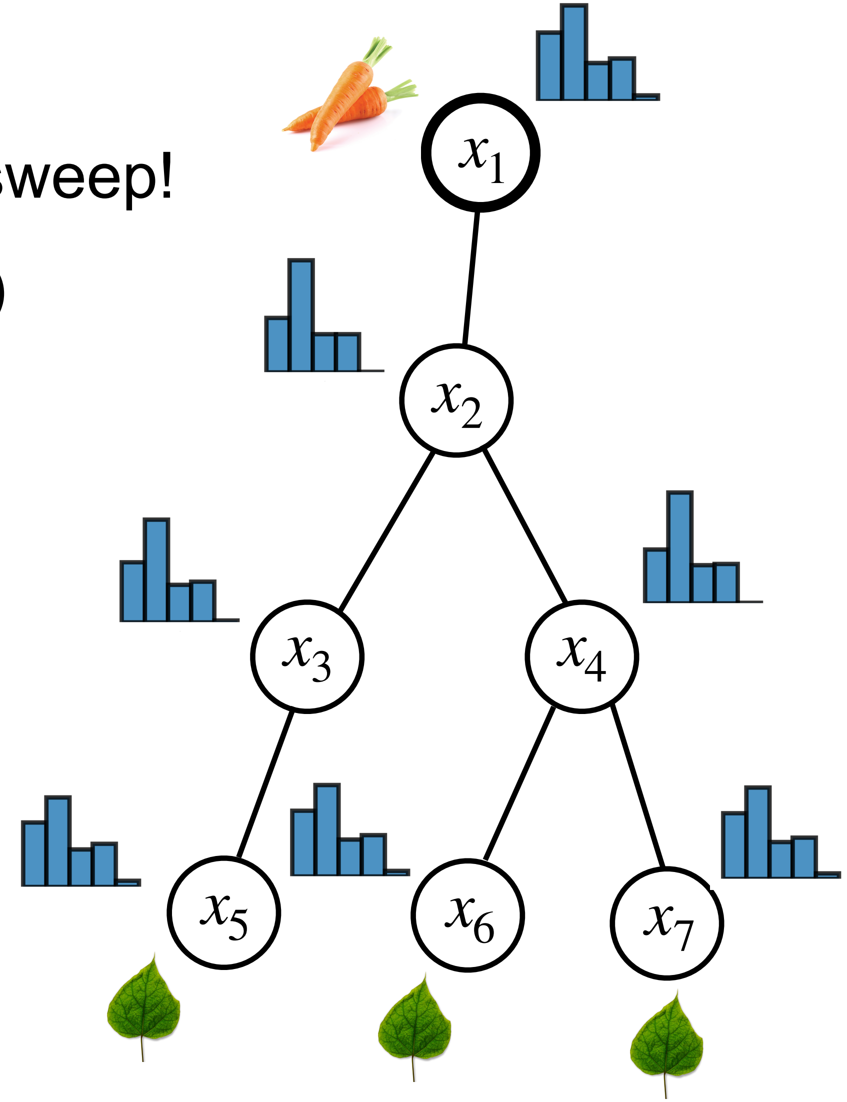
Remarks

- Guaranteed convergence after a single sweep!



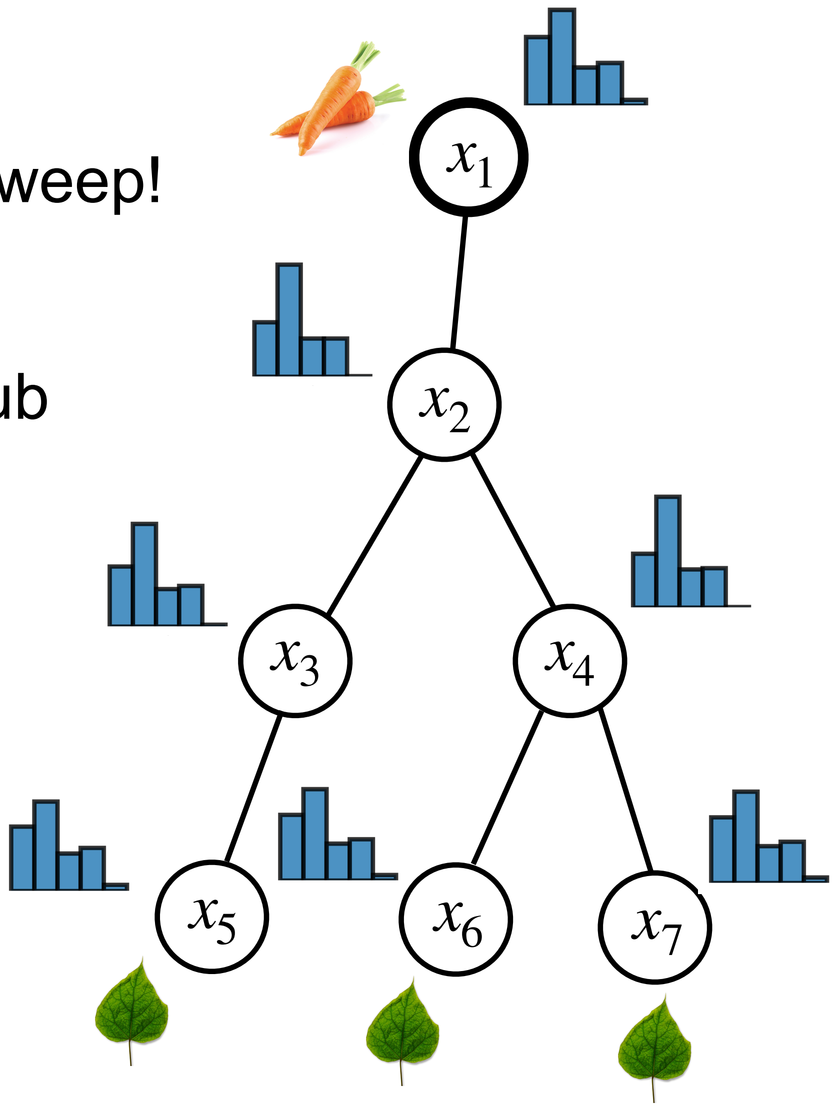
Remarks

- Guaranteed convergence after a single sweep!
- *Linear* complexity in N (**not** exponential!)



Remarks

- Guaranteed convergence after a single sweep!
- *Linear* complexity in N (**not** exponential!)
- See example implementation in my GitHub



Checklist

If $G = (V, E)$ is a tree, can we compute:

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1. The marginal likelihood $p(y)$ of observed data

2. The marginal distribution $p(z)$ of latent variables

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If $G = (V, E)$ is a tree, can we compute:

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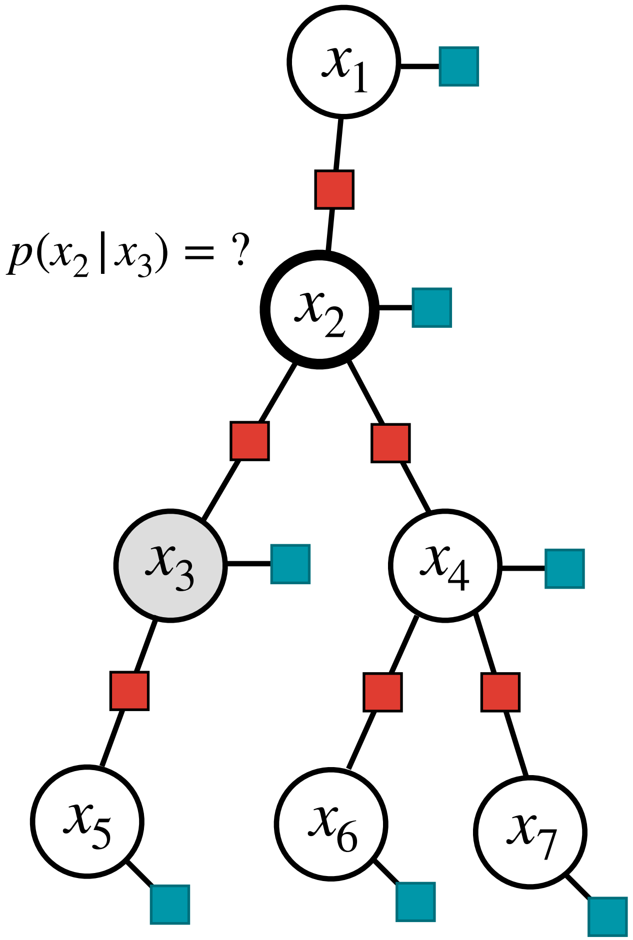
3. The conditional distribution $p(x_i \mid x_j)$ for any $i, j \in V$



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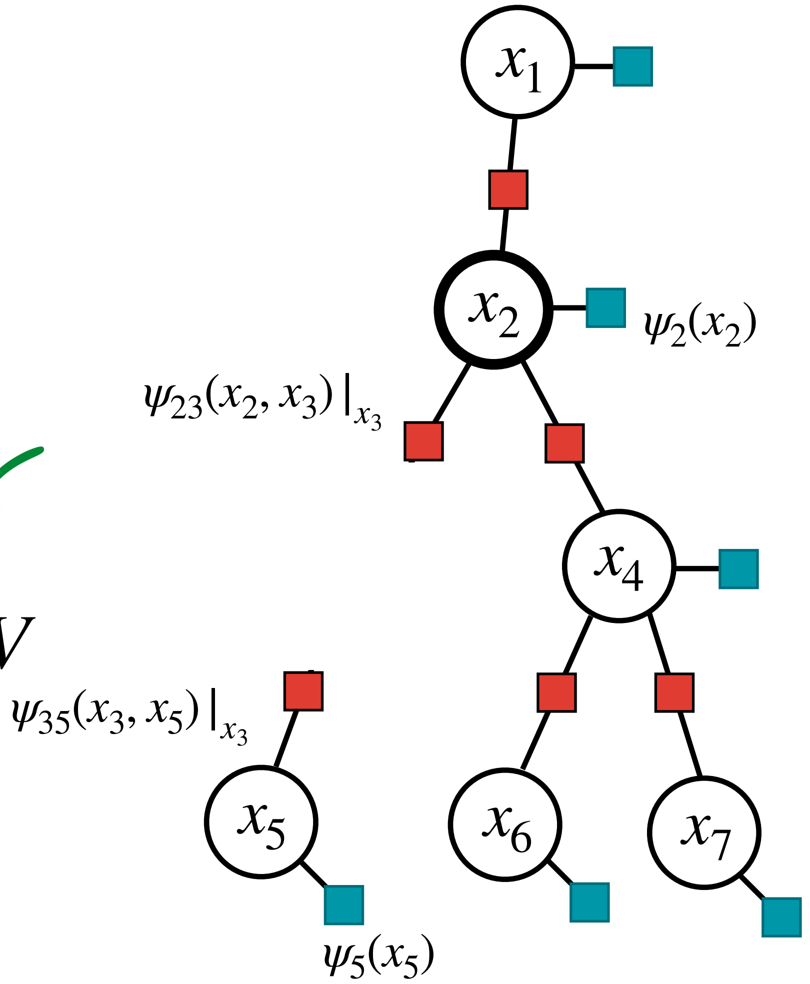

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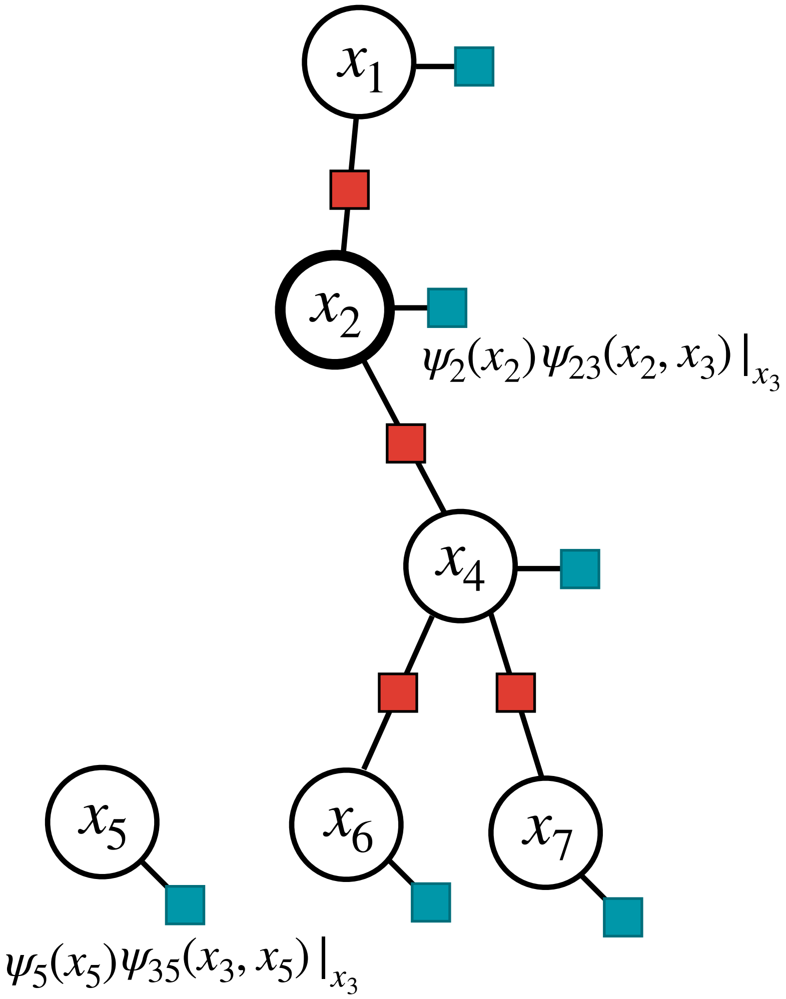

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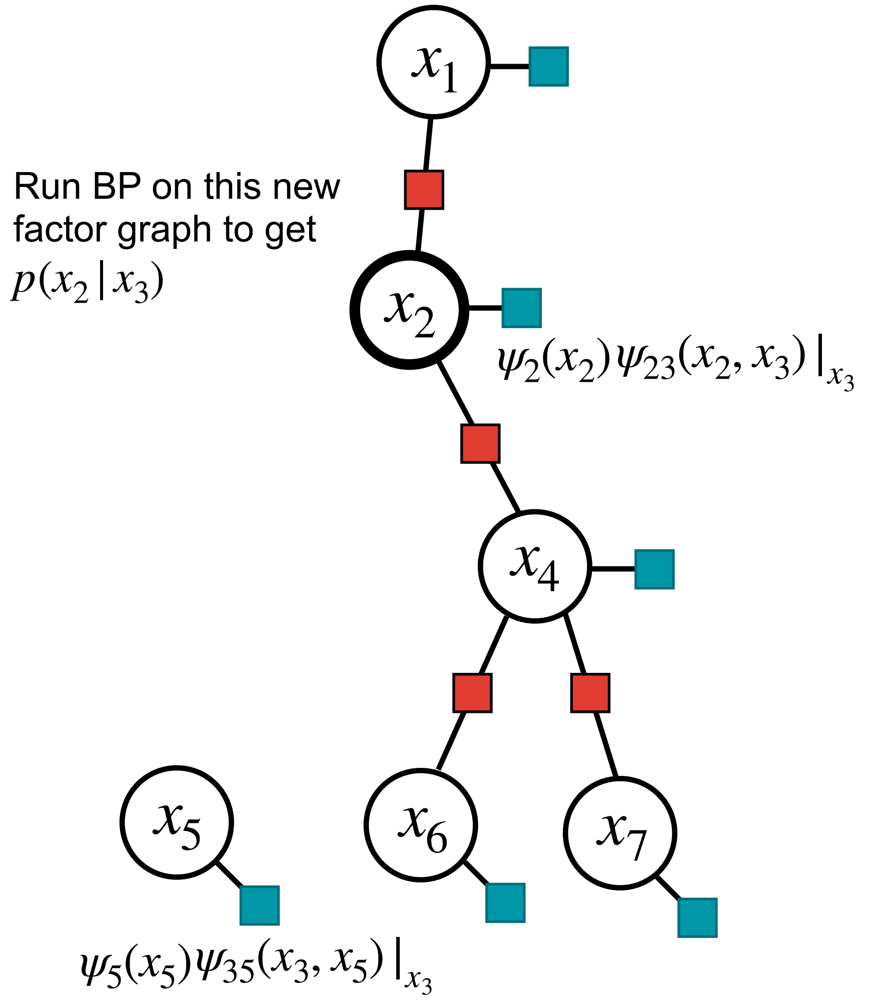

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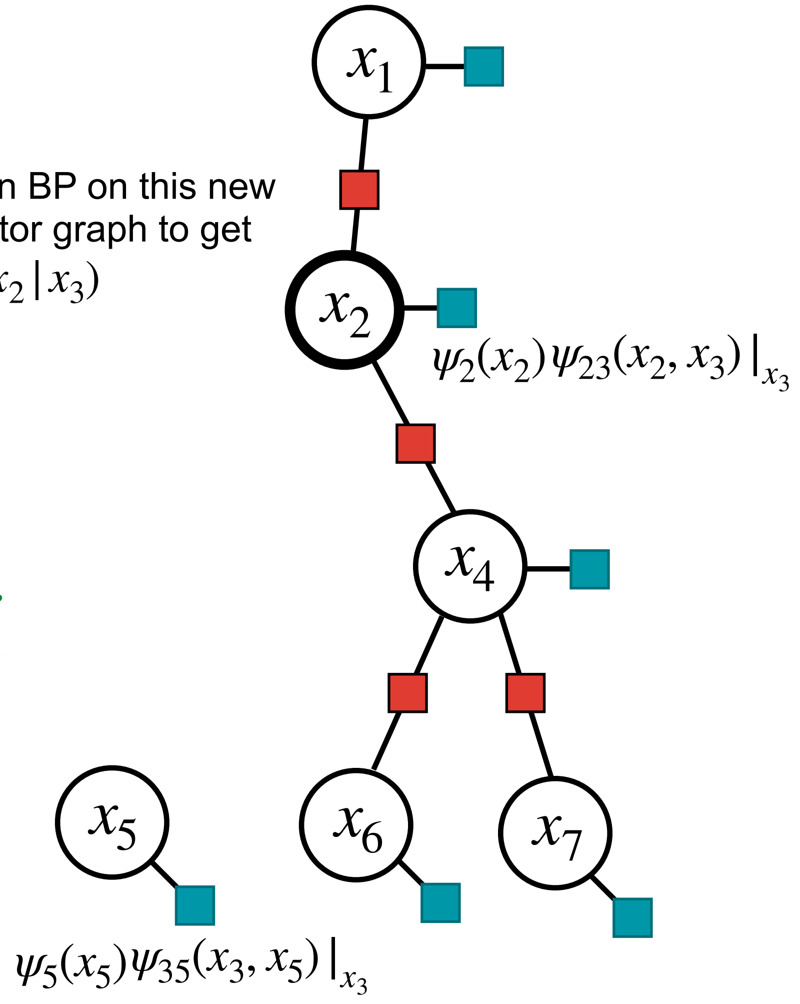
3. The conditional distribution $p(x_i \mid x_j)$ for any $i, j \in V$ ✓

Run BP on this new factor graph to get $p(x_2 \mid x_3)$



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4. The mode $\boldsymbol{x}^* = \text{argmax}_{\boldsymbol{x}} p(\boldsymbol{x})$

Checklist

If $G = (V, E)$ is a tree, can we compute:

1. The marginal likelihood $p(y)$ of observed data ✓

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3. The conditional distribution $p(x_i \mid x_j)$ for any $i, j \in V$ ✓

4. The mode $\boldsymbol{x}^* = \mathrm{argmax}_{\boldsymbol{x}} p(\boldsymbol{x})$ ✗

References

[1] Bishop, Christopher M. *Pattern Recognition and Machine Learning*. New York: springer, 2006.

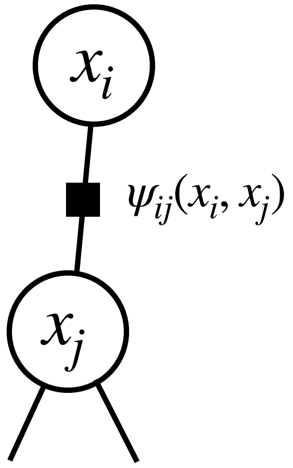
[2] Wainwright, Martin J., and Michael I. Jordan. *Graphical Models, Exponential Families, and Variational Inference*. Foundations and Trends in Machine Learning, 2008.

3. Some Extensions of Belief Propagation

Recall the message passing protocol in BP:

Message update:

$$M_{j\to i}(x_i) = \sum_{x_j \in \{1,\dots,K\}} \psi_{ij}(x_i, x_j)\, \psi_j(x_j) \prod_{k\sim j, k\neq i} M_{k\to j}(x_j),$$



State update:

$$p(x_i) \propto \psi_i(x_i) \prod_{j\sim i} M_{j\to i}(x_i).$$

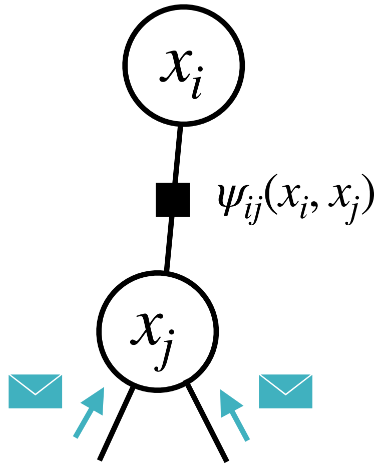
Recall the message passing protocol in BP:

Message update:

$$M_{j\to i}(x_i) = \sum_{x_j \in \{1,\ldots,K\}} \psi_{ij}(x_i, x_j)\, \psi_j(x_j) \prod_{k\sim j, k\neq i} M_{k\to j}(x_j),$$

State update:

$$p(x_i) \propto \psi_i(x_i) \prod_{j\sim i} M_{j\to i}(x_i).$$



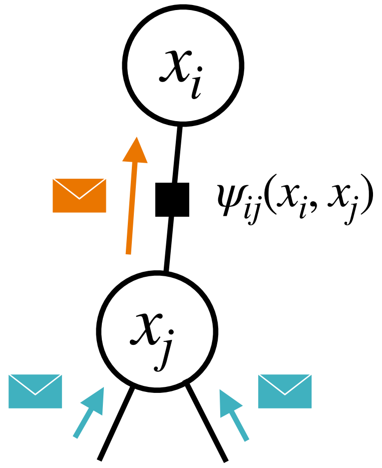
Recall the message passing protocol in BP:

Message update:

$$\boxed{M_{j\to i}(x_i)} = \sum_{x_j\in\{1,\ldots,K\}} \psi_{ij}(x_i, x_j)\,\boxed{\psi_j(x_j)} \prod_{k\sim j, k\neq i} \boxed{M_{k\to j}(x_j)},$$

State update:

$$p(x_i) \propto \psi_i(x_i) \prod_{j\sim i} M_{j\to i}(x_i).$$



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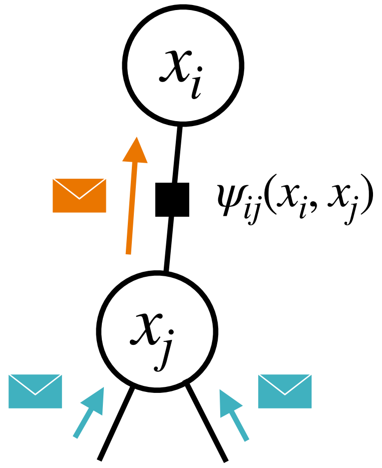
State update:

$$p(x_i) \propto \psi_i(x_i) \prod_{j\sim i} M_{j\to i}(x_i).$$



We assume that the graph is **tree-structured**.

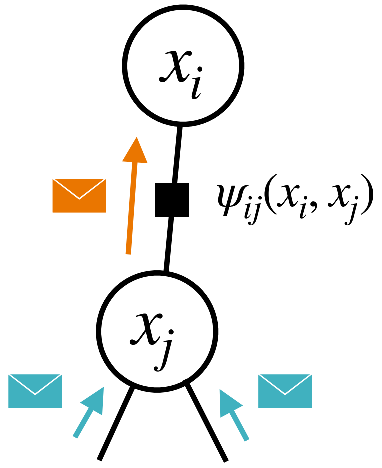
Recall the message passing protocol in BP:

Message update:

$$M_{j\to i}(x_i) = \sum_{x_j \in \{1,\ldots,K\}} \psi_{ij}(x_i, x_j)\, \psi_j(x_j) \prod_{k\sim j, k\neq i} M_{k\to j}(x_j),$$

State update:

$$p(x_i) \propto \psi_i(x_i) \prod_{j\sim i} M_{j\to i}(x_i).$$



We assume that the graph is **tree-structured**.

What extensions can we consider?

Extension 1. Continuous states

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When states are *continuous* $x_i \in \mathbb{R}^d$, we replace the sum by an integral:

Message update:

$$M_{j\to i}(x_i) = \int_{\mathbb{R}^d} \psi_{ij}(x_i, x_j)\, \psi_j(x_j) \prod_{k\sim j, k\neq i} M_{k\to j}(x_j)\, \mathrm{d}x_j,$$

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For e.g. **Gaussian belief propagation**.

Gaussian belief propagation

Properties of Gaussians:

Gaussian belief propagation

Properties of Gaussians:

1. Product of two Gaussians is Gaussian:

$$\mathcal{N}(x \,|\, a, A)\, \mathcal{N}(x \,|\, b, B) = \mathcal{N}(x \,|\, c, C),$$

Gaussian belief propagation

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Gaussian belief propagation

Properties of Gaussians:

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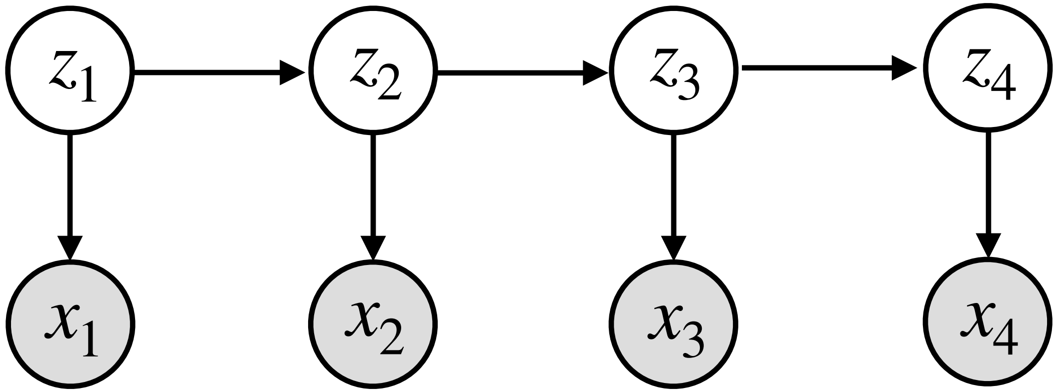
Example: Timeseries modelling



Bayesian network representation of a state-space model

Example: Timeseries modelling

Consider a linear state-space model:

$$z_{n+1} = Mz_n + \epsilon_n, \quad \epsilon_n \sim \mathcal{N}(0, Q),$$
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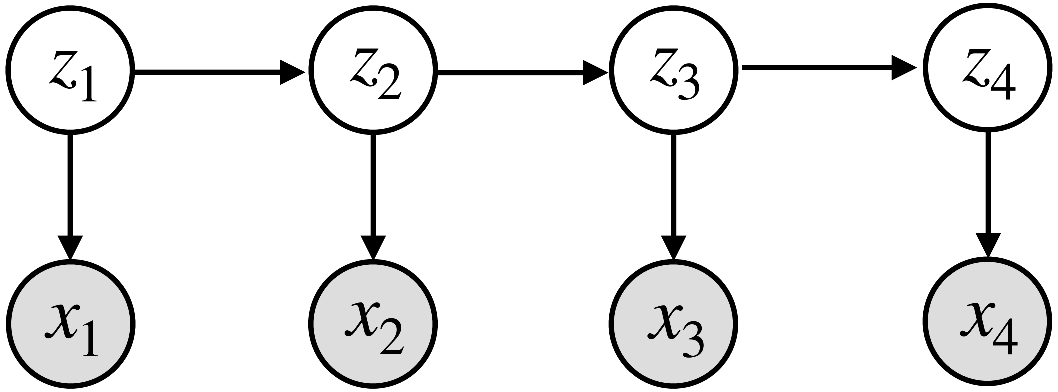

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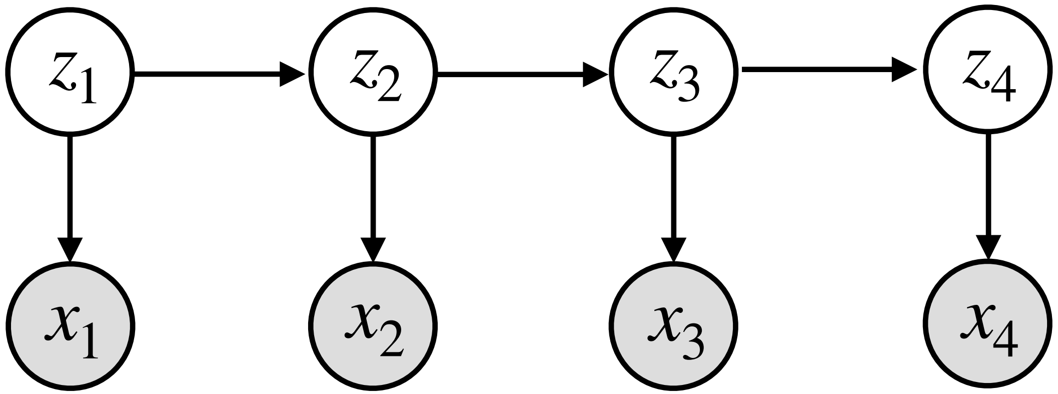

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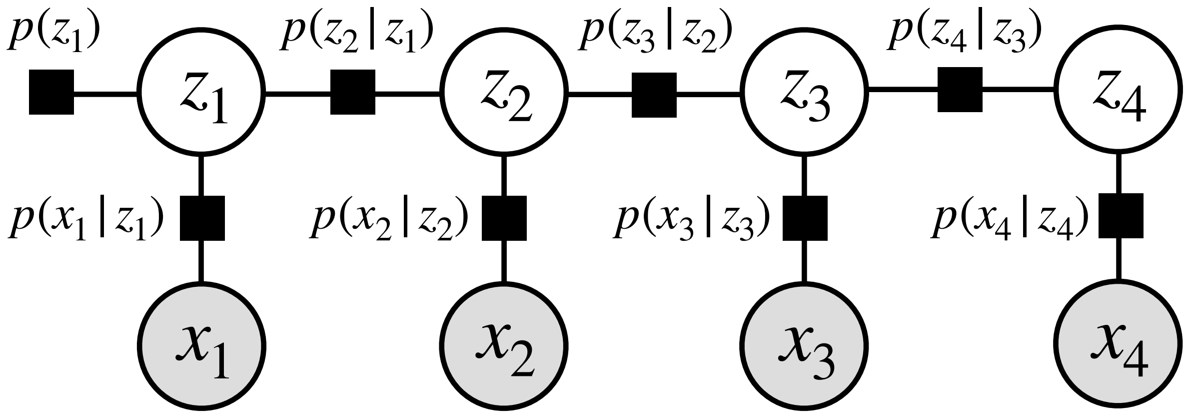

Factor graph representation of a state-space model

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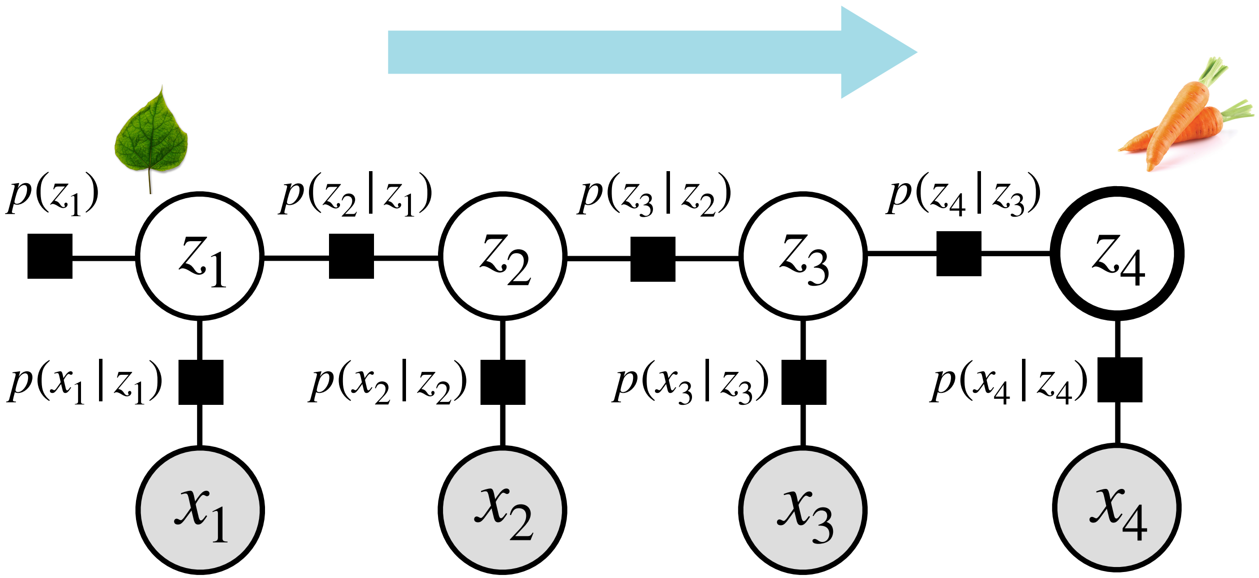

Forward sweep ≡ Kalman filter

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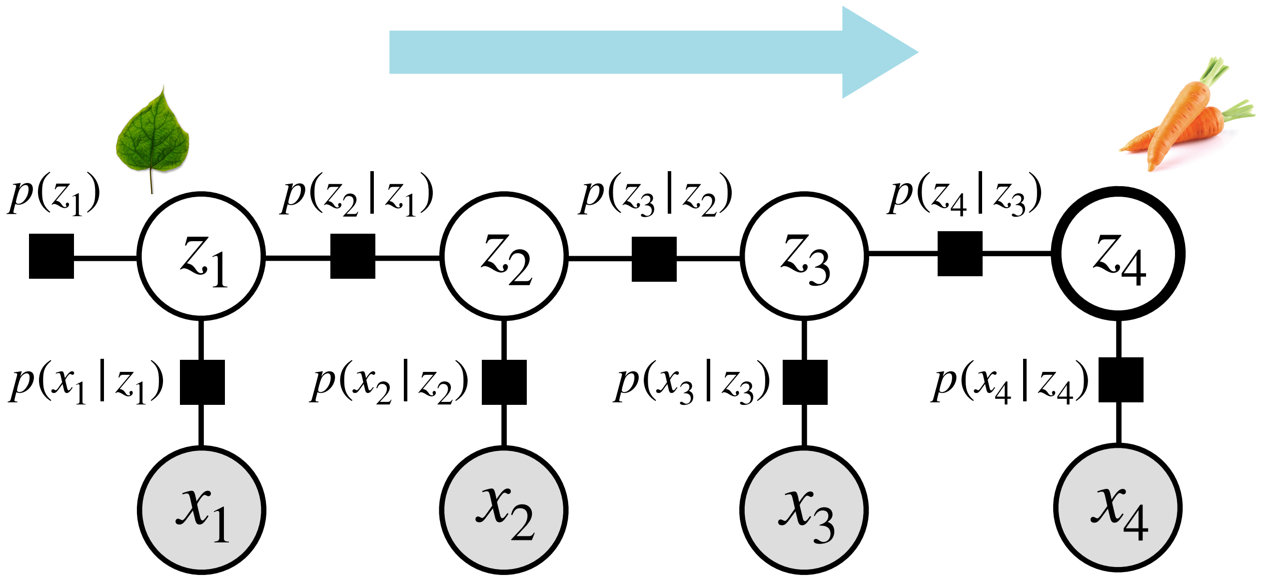

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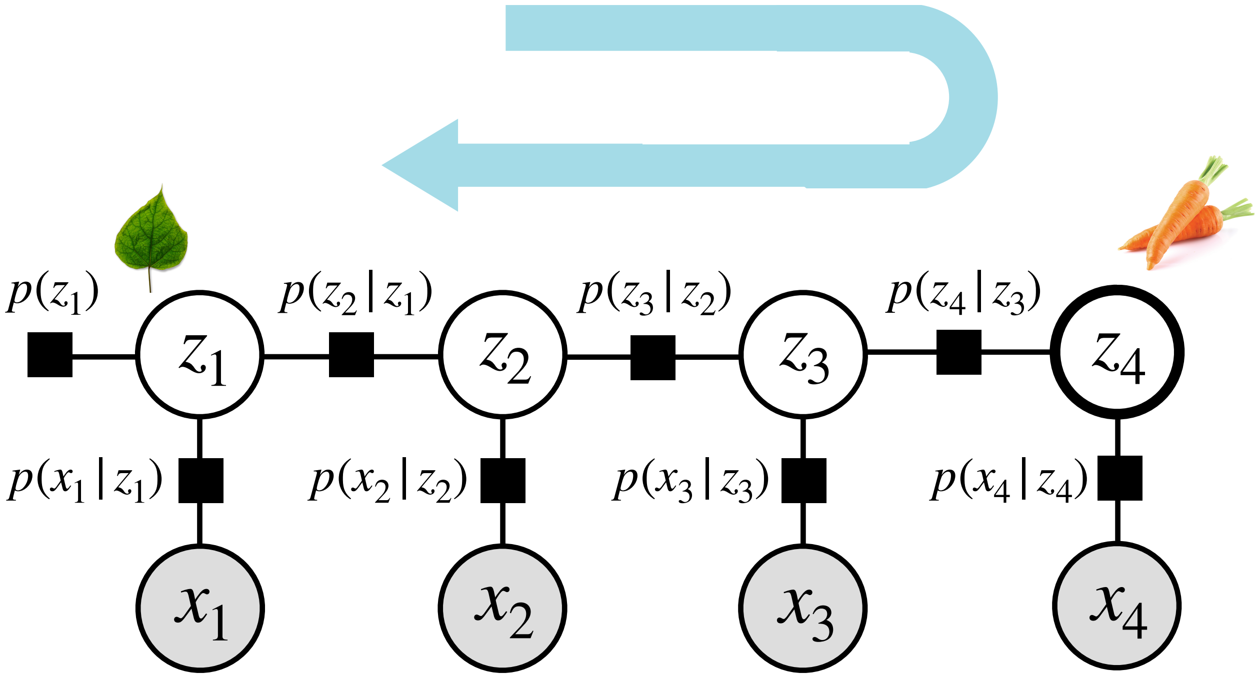
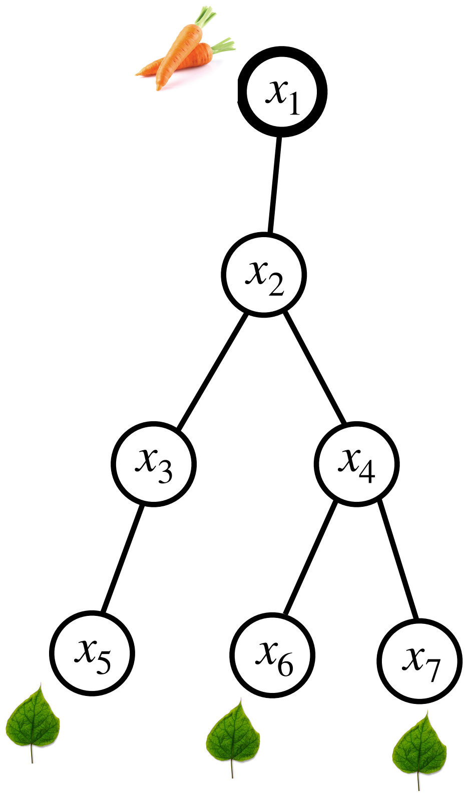


Forward-backward sweep ≡ RTS smoother

- Running only the forward sweep of BP is equivalent to the *Kalman filter*
- Running a full BP is equivalent to the *Rauch-Tung Striebel smoother*

Extension 2. Max-product algorithm



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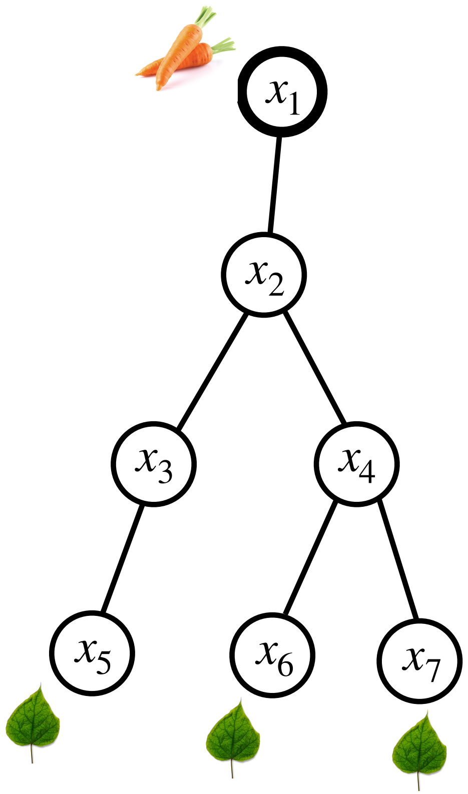
$$M_{j\to i}(x_i) = \max_{x_j\in\{1,\dots,K\}} \psi_{ij}(x_i, x_j)\, \psi_j(x_j) \prod_{k\sim j, k\neq i} M_{k\to j}(x_j),$$



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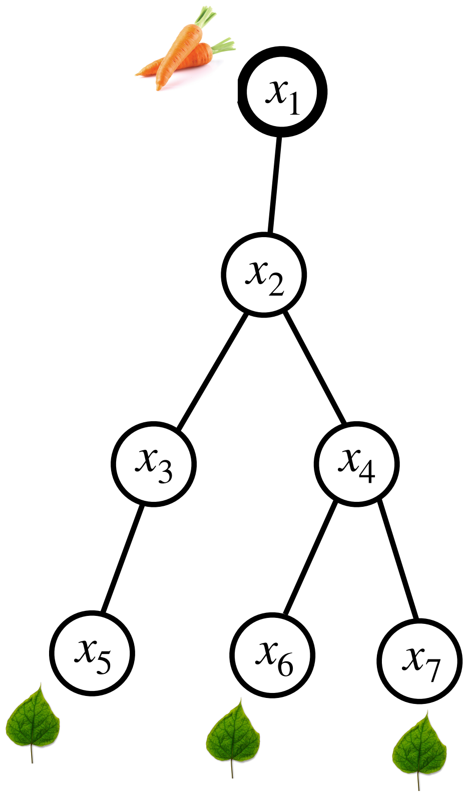

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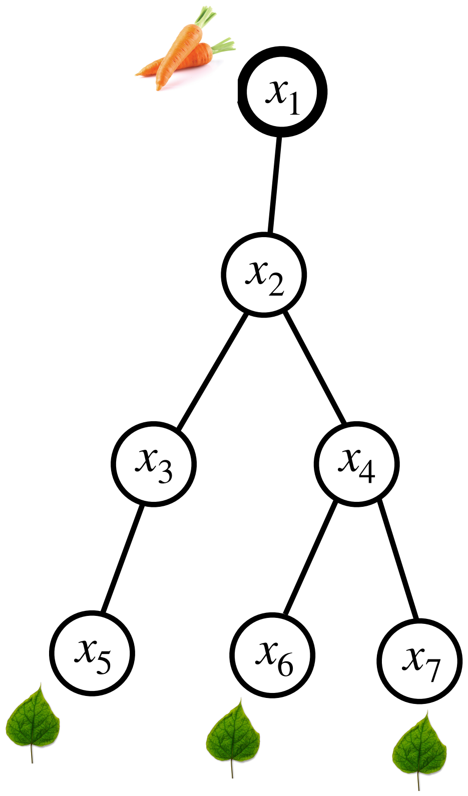

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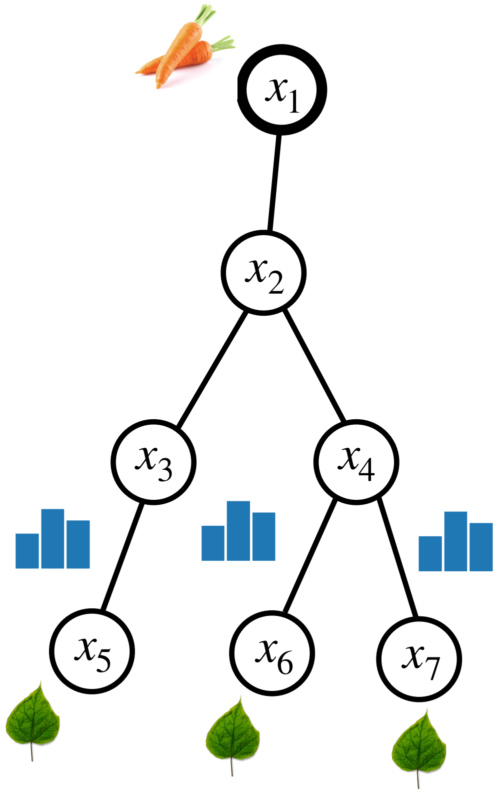

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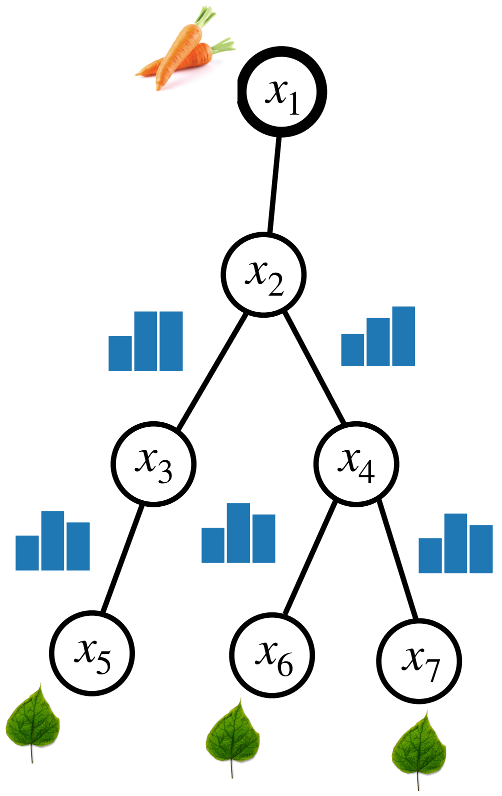

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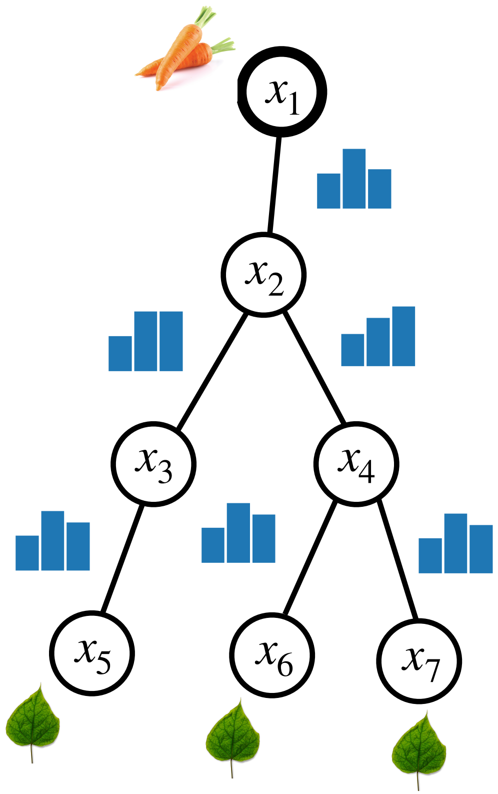

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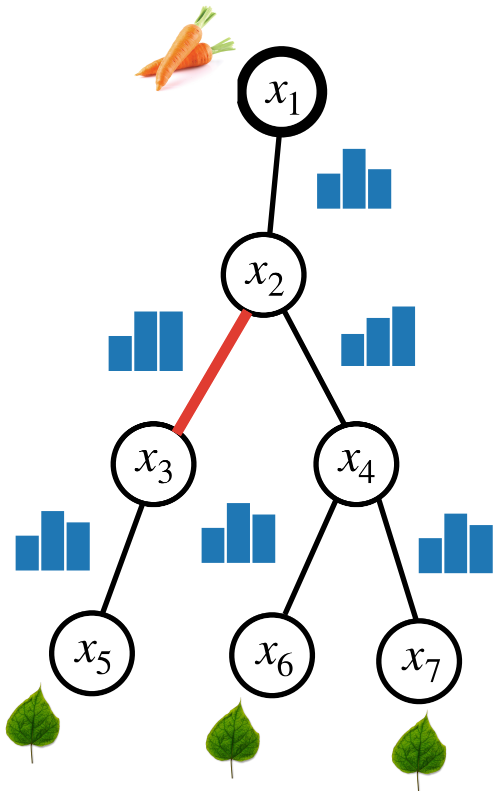

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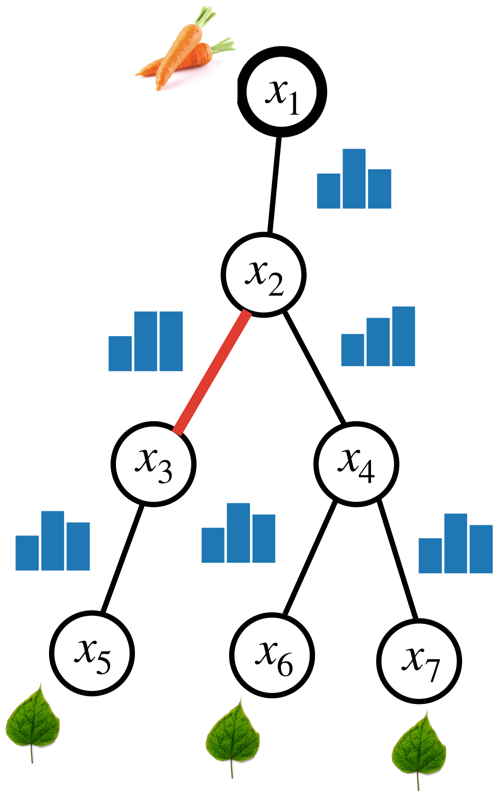

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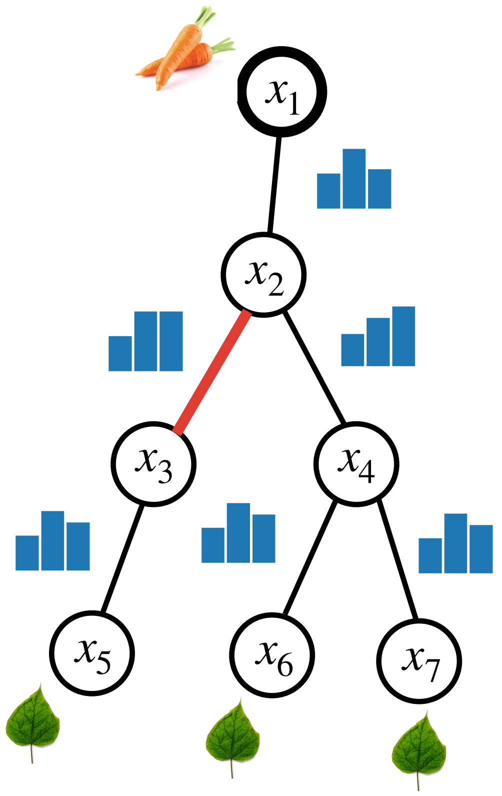

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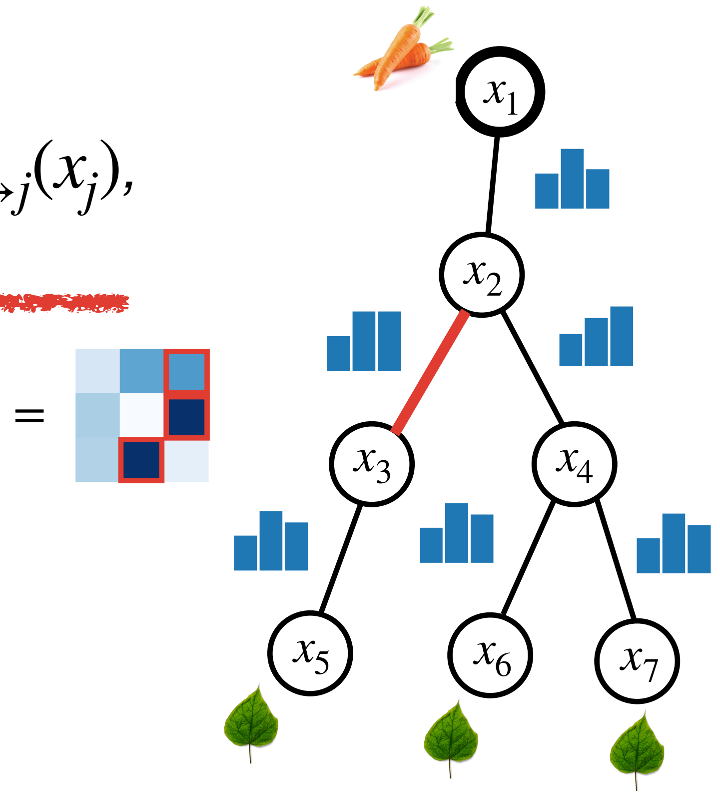

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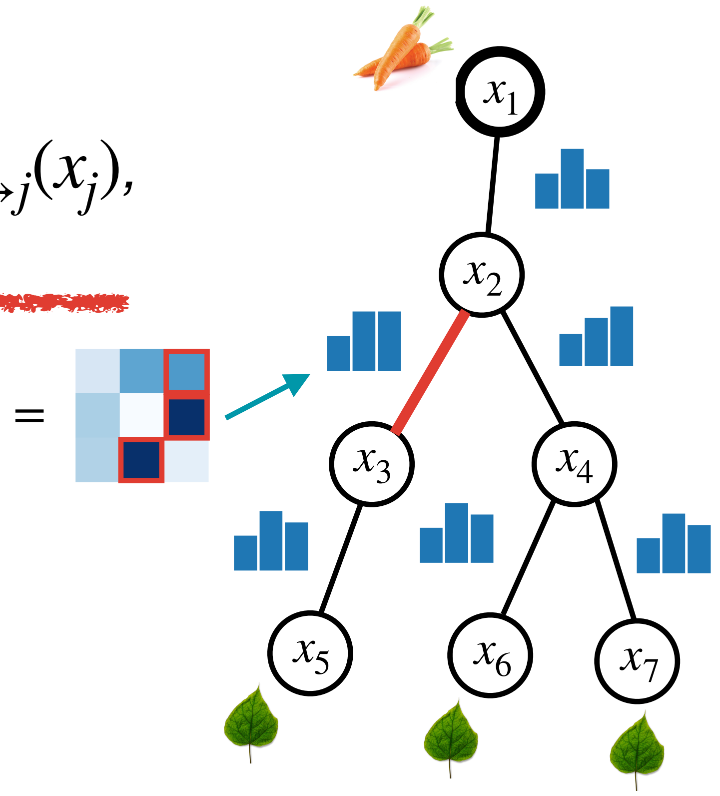

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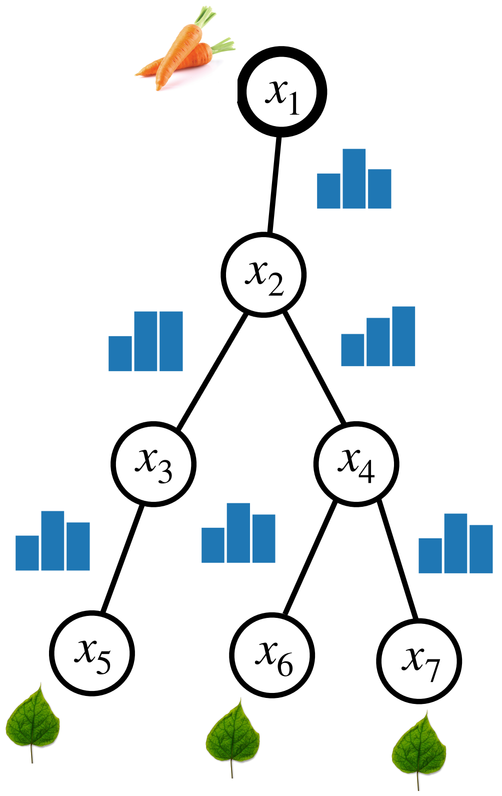

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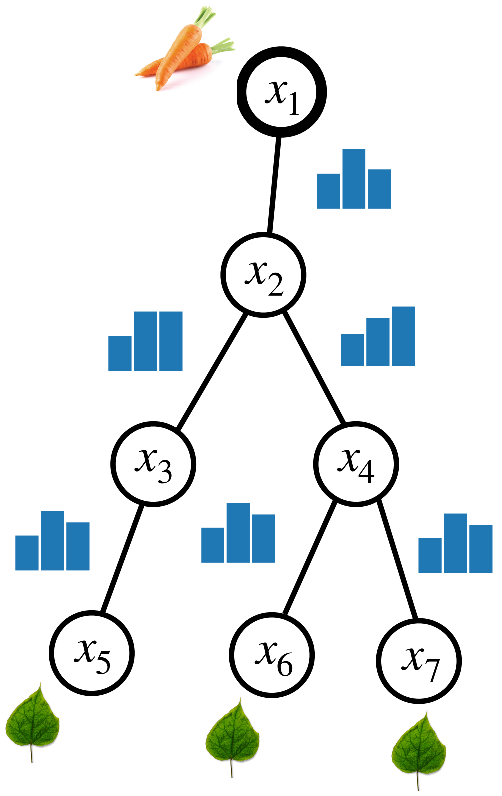
$$\max_{\boldsymbol{x}} p(\boldsymbol{x}) = \max_{x_{\text{root}}\in\{1,\ldots,K\}} \frac{1}{Z} \prod_{j\sim\text{root}} M_{j\to\text{root}}(x_{\text{root}}).$$



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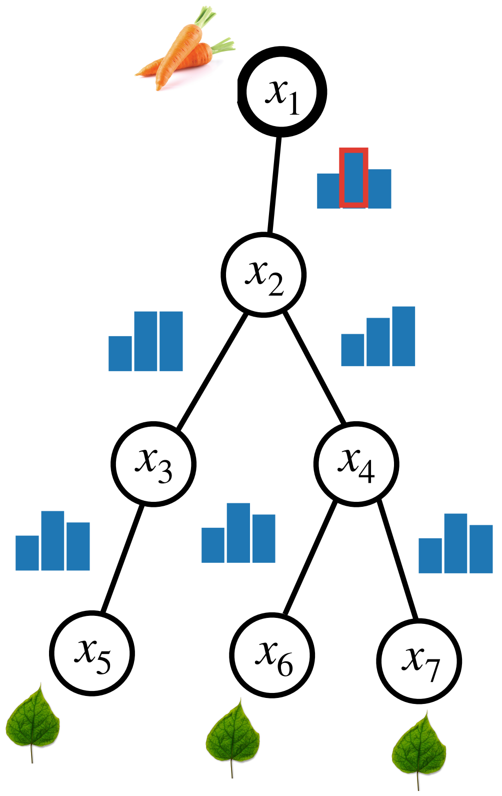

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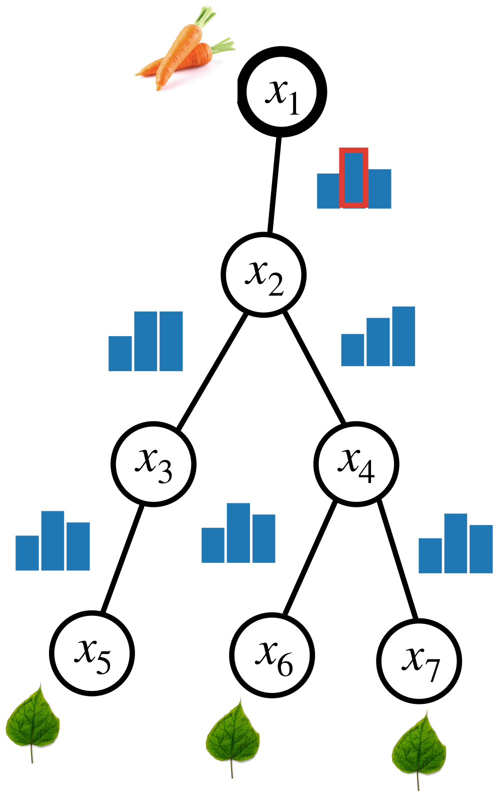
$$\boldsymbol{x}^* = \text{argmax}_{\boldsymbol{x}} p(\boldsymbol{x}),$$

using a procedure called *back-tracking:*



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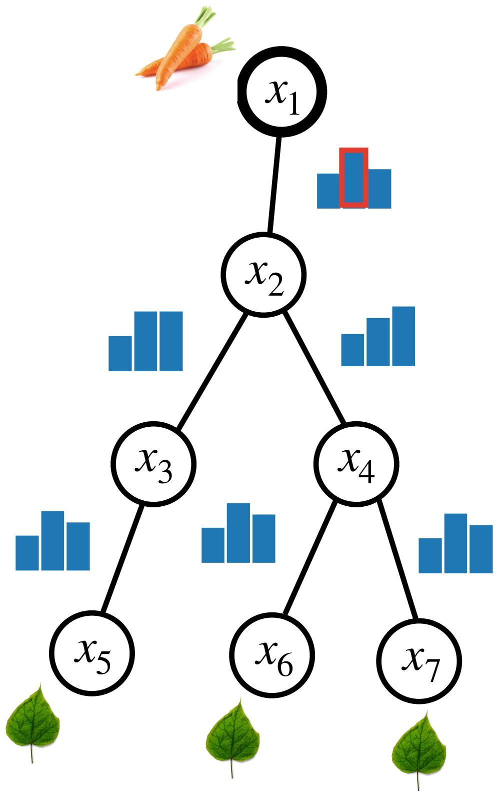

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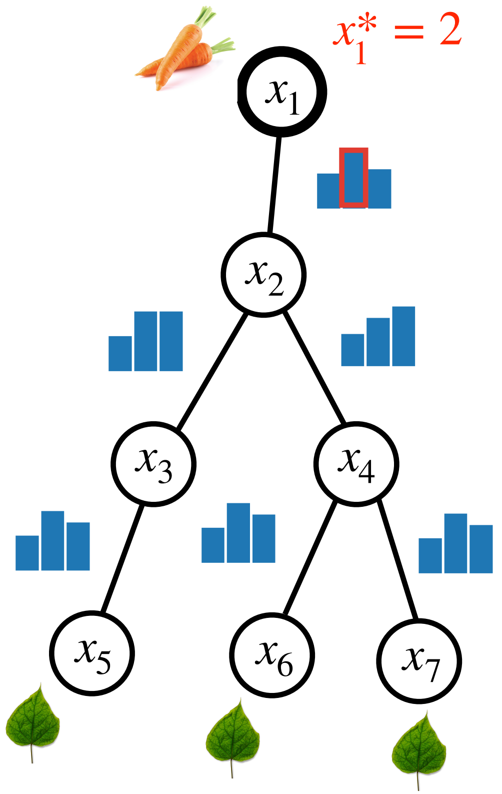

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1. At the root node, compute

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2. From the root node back to the leaf nodes, compute

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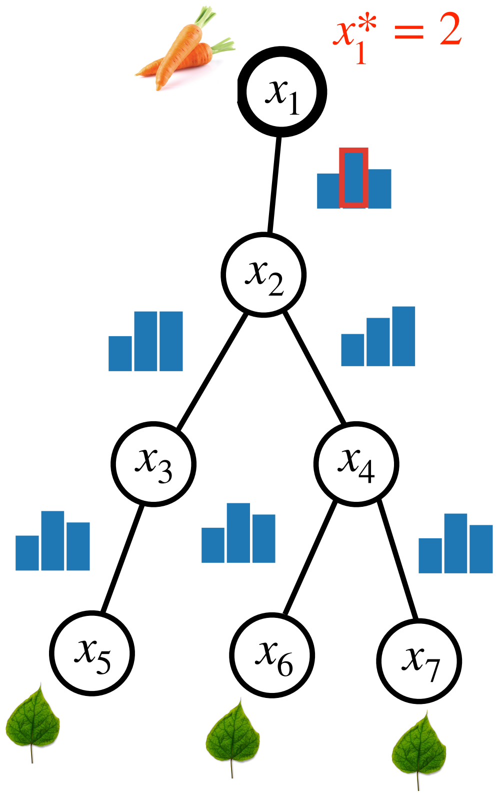

Extension 2. Max-product algorithm

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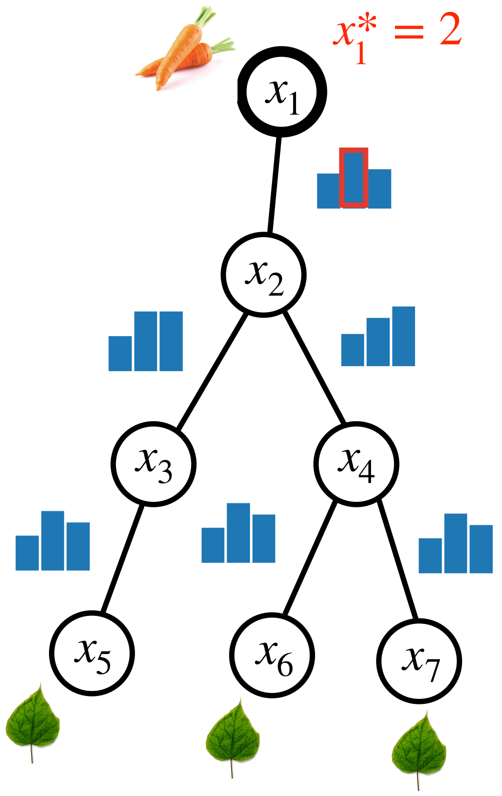

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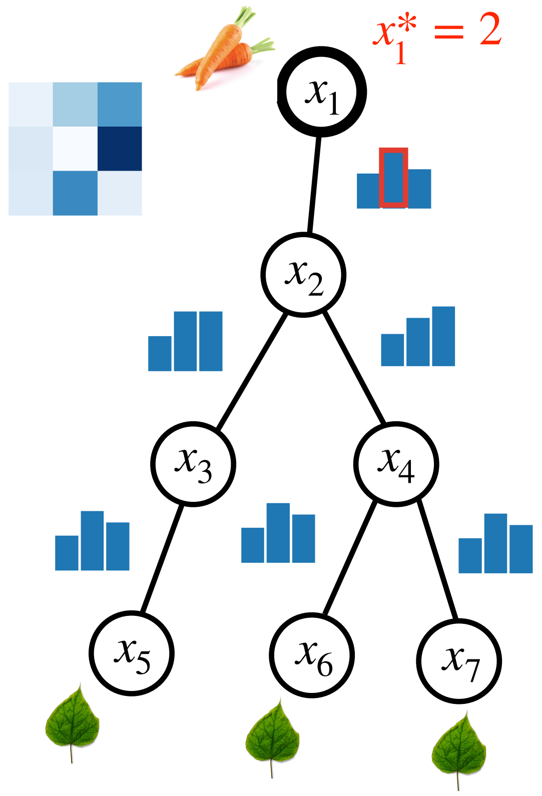

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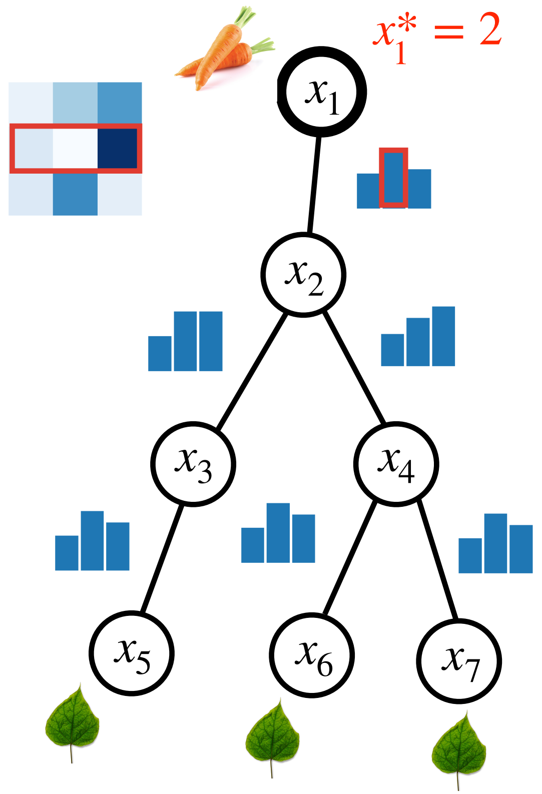

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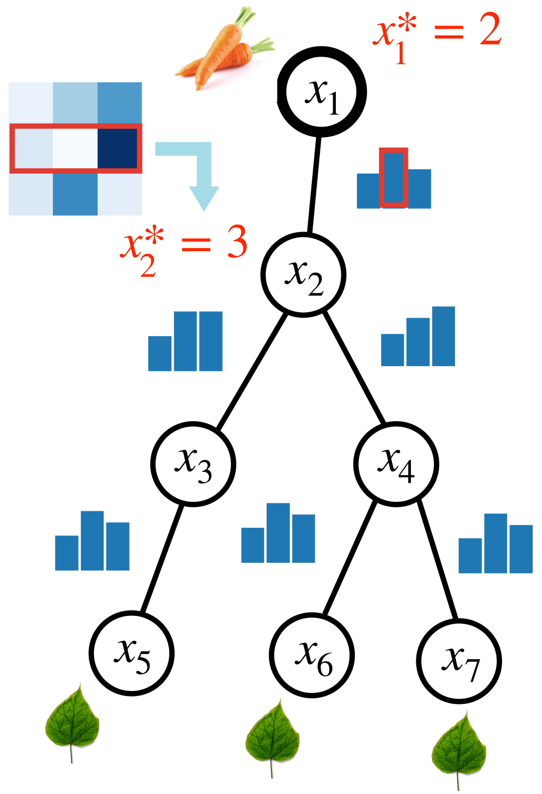

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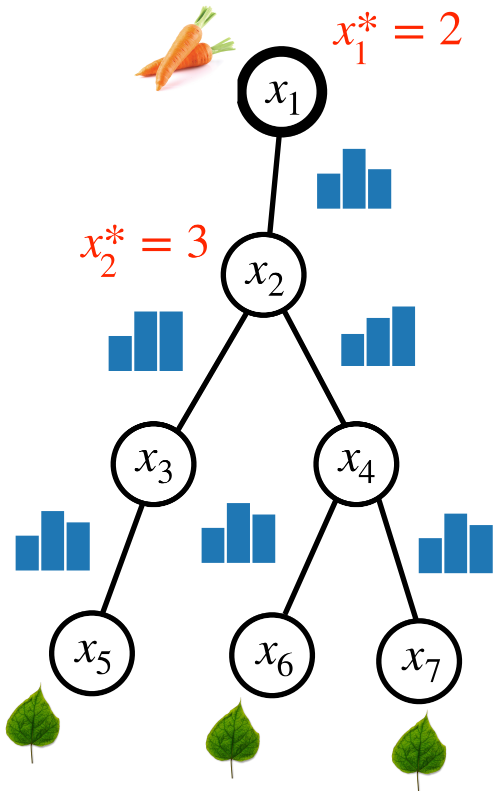

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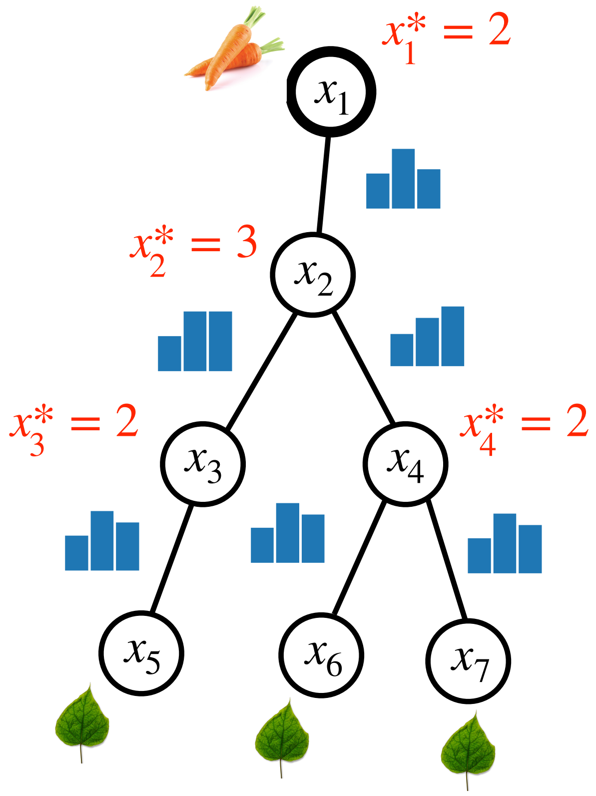

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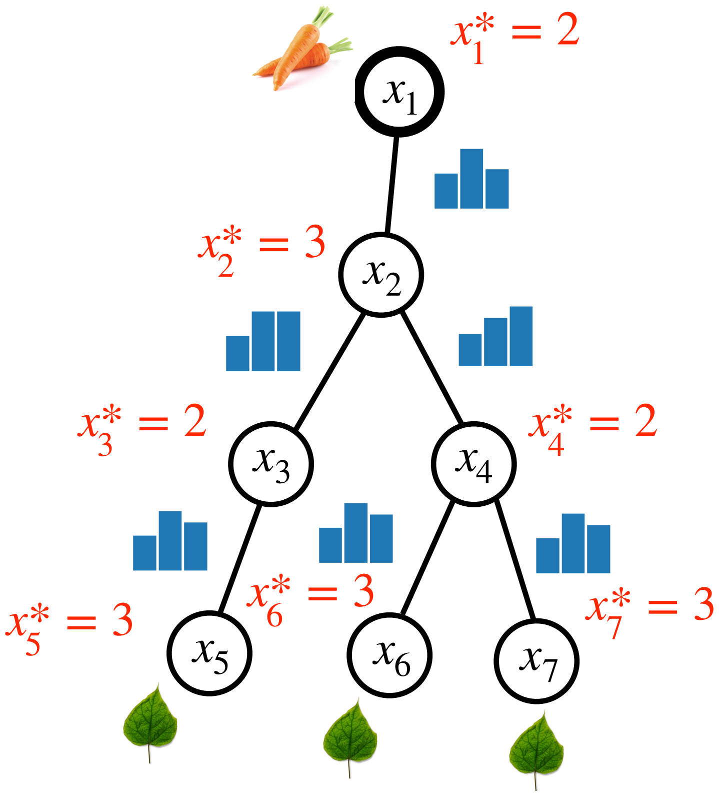

Extension 3. Polytrees and other graphs

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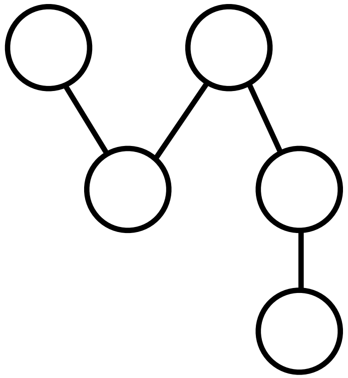
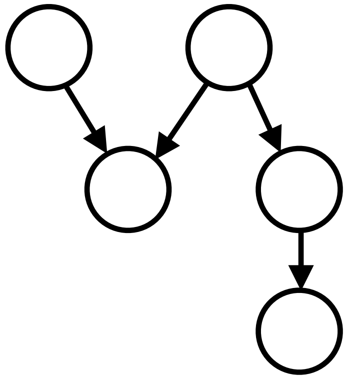
A **polytree** is a directed tree



A tree



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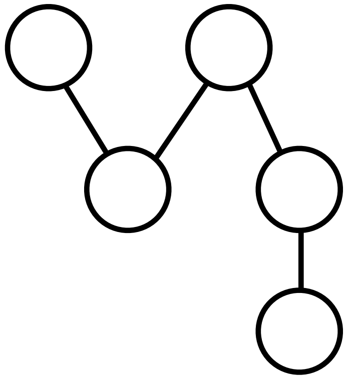

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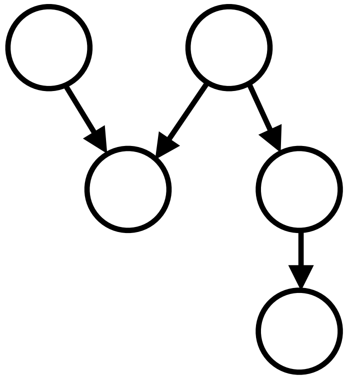

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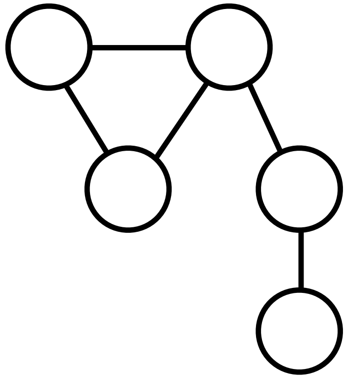

A polytree as a MRF

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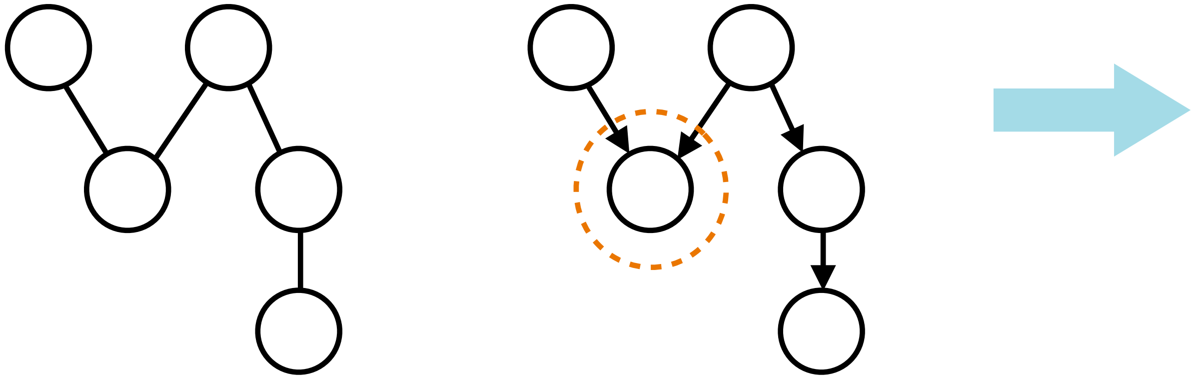

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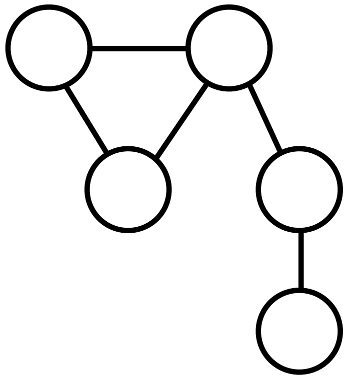

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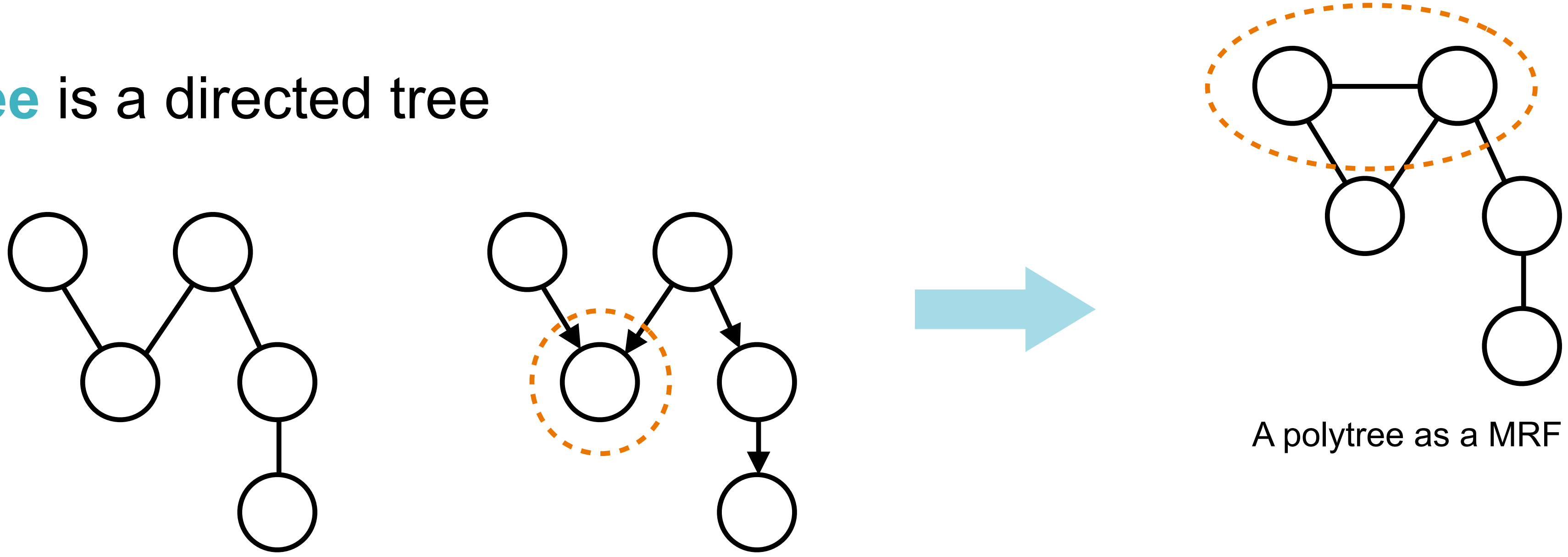

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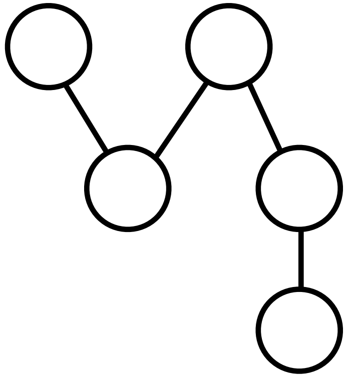

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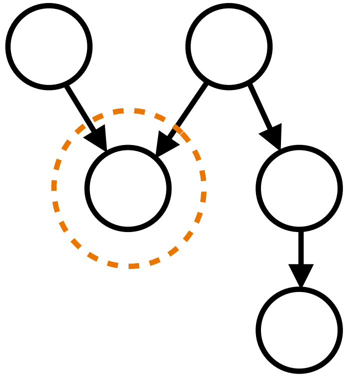

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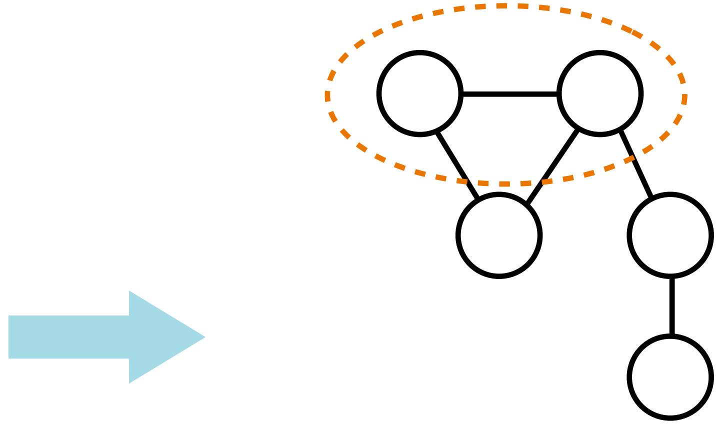

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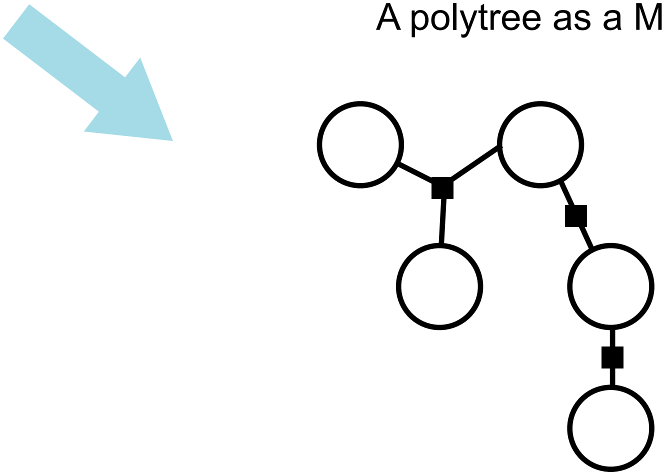

A polytree as a factor graph

Extension 3. Polytrees and other graphs

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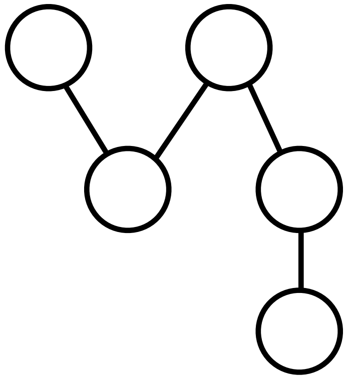

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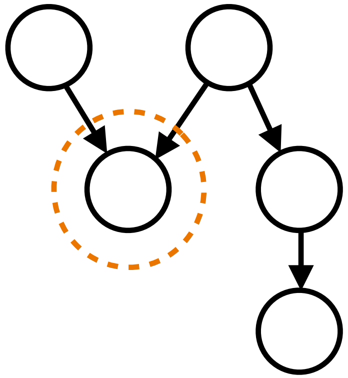

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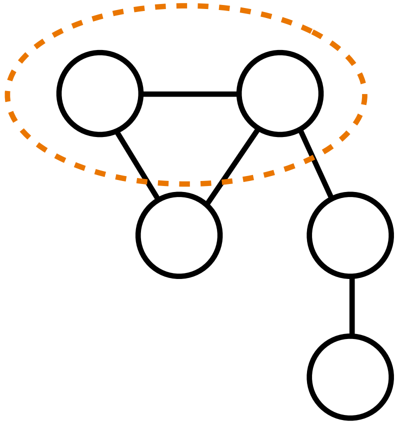

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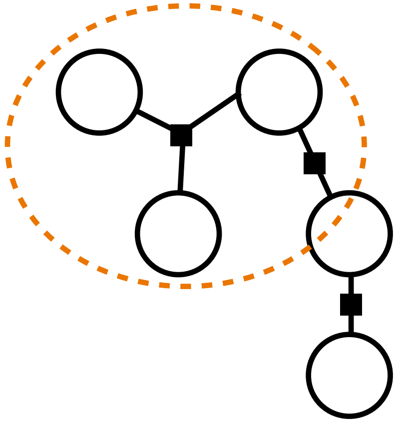


A polytree as a factor graph

Note: factors are not necessarily pairwise!

Extension 3. Polytrees and other graphs

On trees, the message passing updates read:

Message update:

$$M_{j\to i}(x_i) = \sum_{x_j \in \{1,\ldots,K\}} \psi_{ij}(x_i, x_j)\, \psi_j(x_j) \prod_{k\sim j, k\neq i} M_{k\to j}(x_j),$$

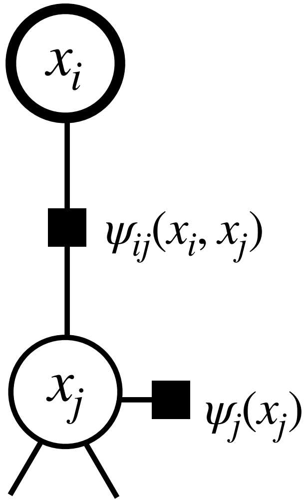
State update:

$$p(x_i) \propto \psi_i(x_i) \prod_{j\sim i} M_{j\to i}(x_i).$$

Extension 3. Polytrees and other graphs

First, break down the message update step into two sub-steps:

$$M_{j\to i}(x_i) = \sum_{x_j\in\{1,\ldots,K\}} \psi_{ij}(x_i, x_j)\, \psi_j(x_j) \prod_{k\sim j, k\neq i} M_{k\to j}(x_j),$$



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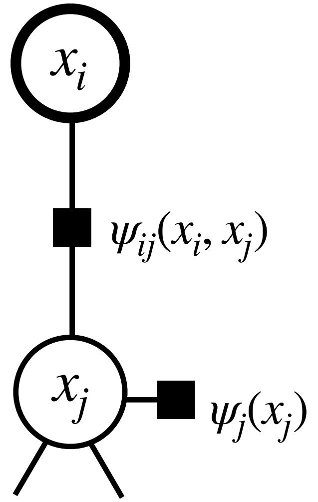

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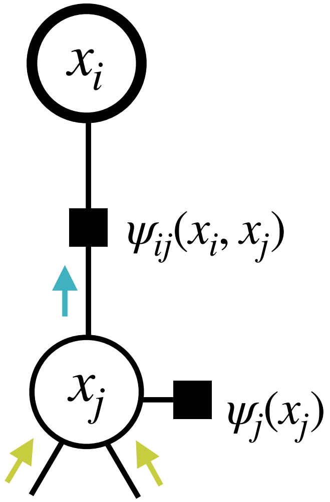

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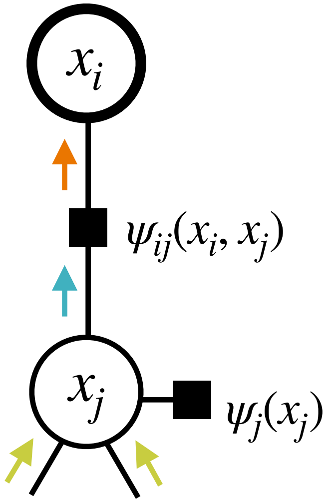

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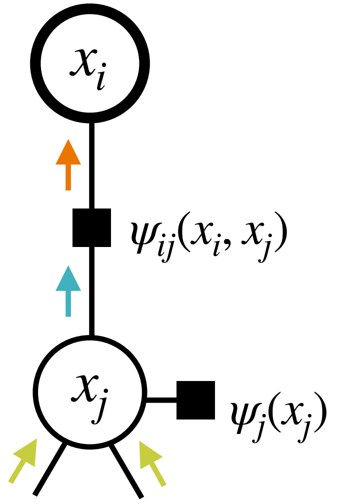
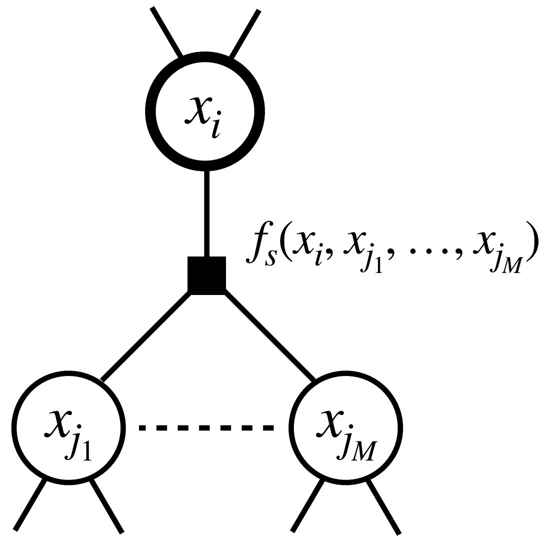


Extension 3. Polytrees and other graphs

Extending to polytrees:



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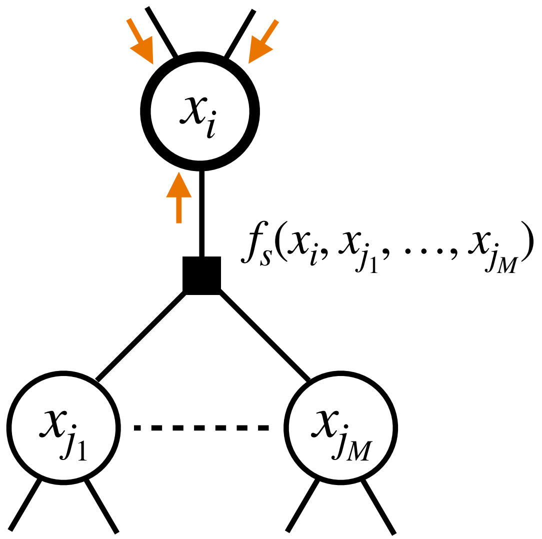

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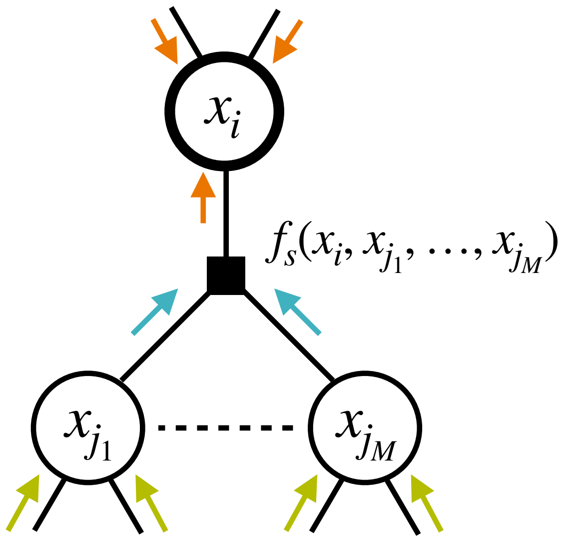
1. $\mu_{x_j \to f_s}(x_j) = \prod_{l \in \mathrm{ne}(x_j) \setminus s} \mu_{f_l \to x_j}(x_j)$



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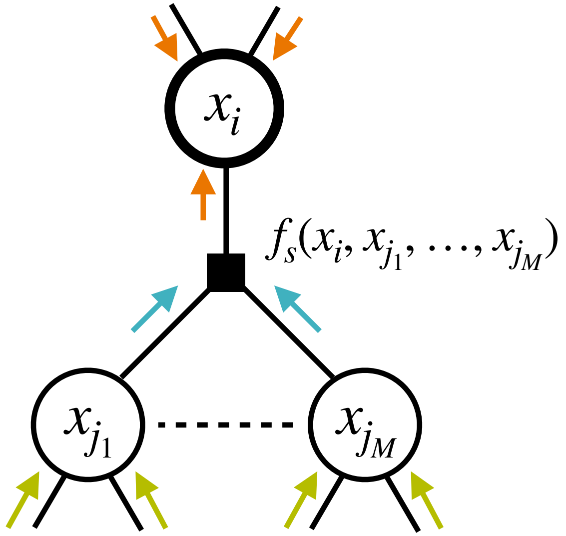

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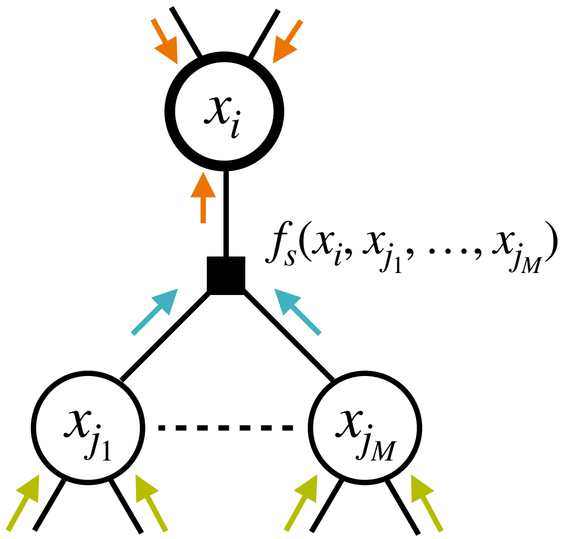

The state updates read:

$$p(x_i) = \prod_{s \in \mathrm{ne}(x_i)} \mu_{f_s \to x_i}(x_i).$$

Extension 3. Polytrees and other graphs

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This is called **Loopy Belief Propagation (LBP)**.

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State update (same as before):

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- LBP is iterative and can be started off by setting

$$\mu_{x \to f}(x) = 1,$$

for all variables x and factors f.

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$$p(x_i) = \prod_{s \in \mathrm{ne}(x_i)} \mu_{f_s \to x_i}(x_i).$$

- LBP is iterative and can be started off by setting

$$\mu_{x \to f}(x) = 1,$$

for all variables x and factors f.

Extension 3. Polytrees and other graphs

We can apply the same update rules to more general graphs with loops.

This is called **Loopy Belief Propagation (LBP)**.

Message update (same as before):

1. $\mu_{x_j \to f_s}(x_j) = \prod_{l \in \mathrm{ne}(x_j) \setminus s} \mu_{f_l \to x_j}(x_j)$

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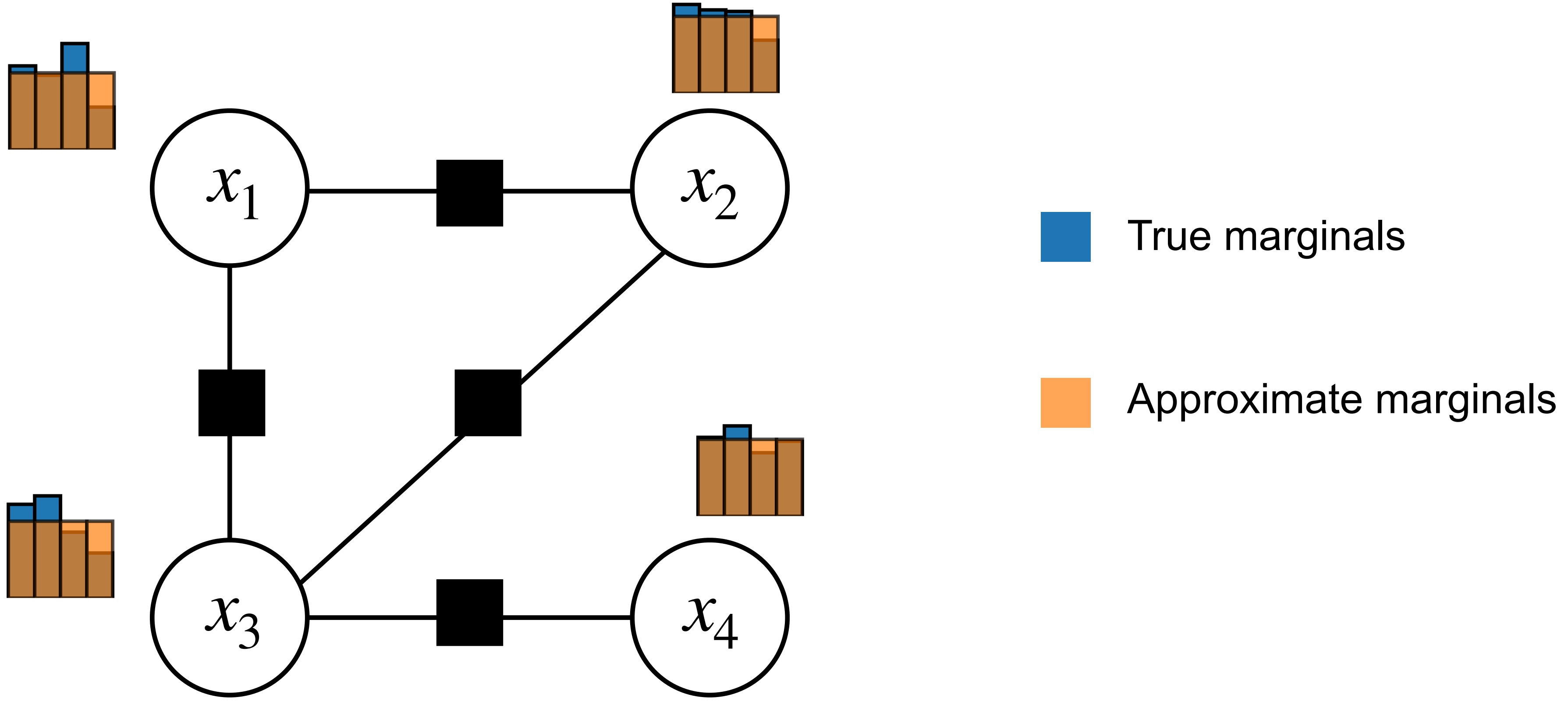
  for all variables x and factors f.

- Updates can be done in parallel (flooding schedule).

Implementation (flooding schedule)

Iteration 1



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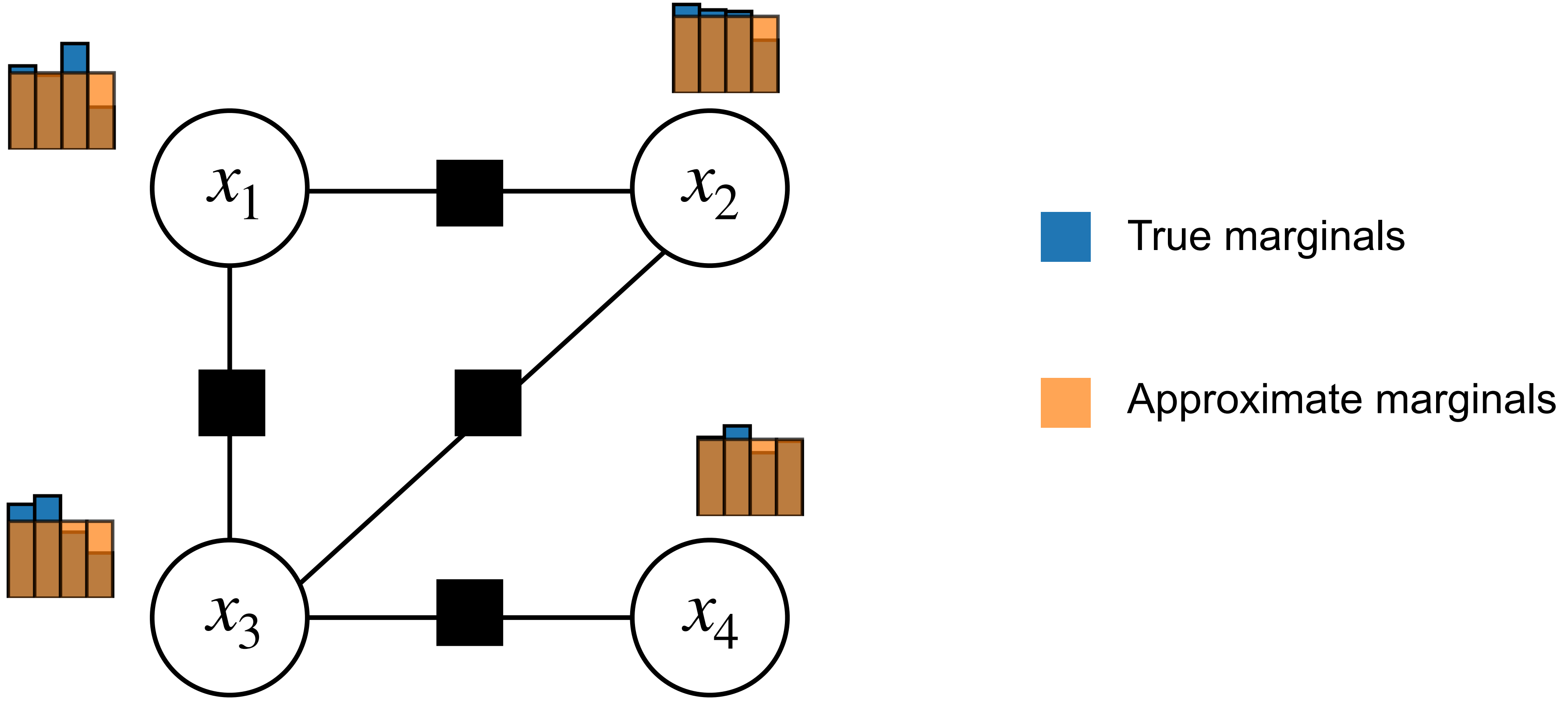

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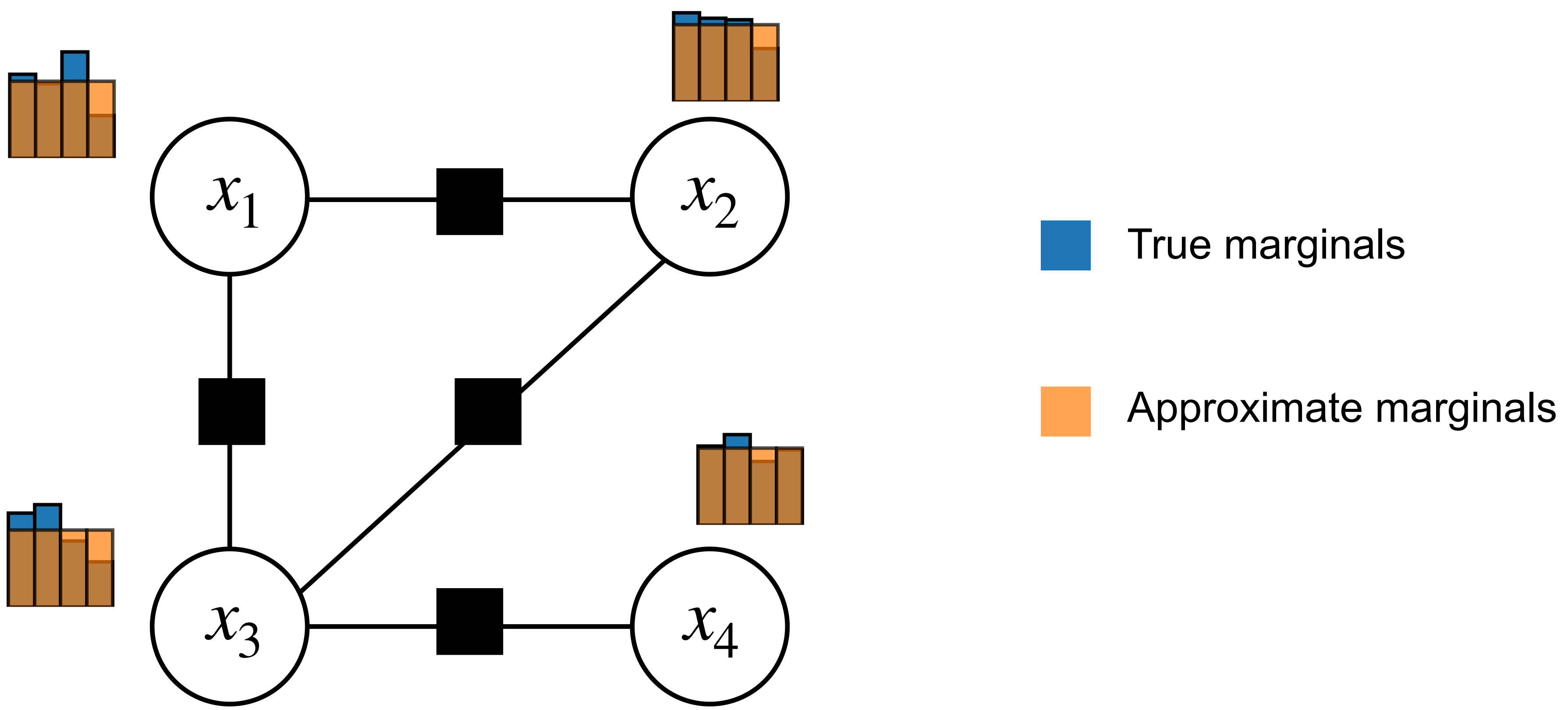

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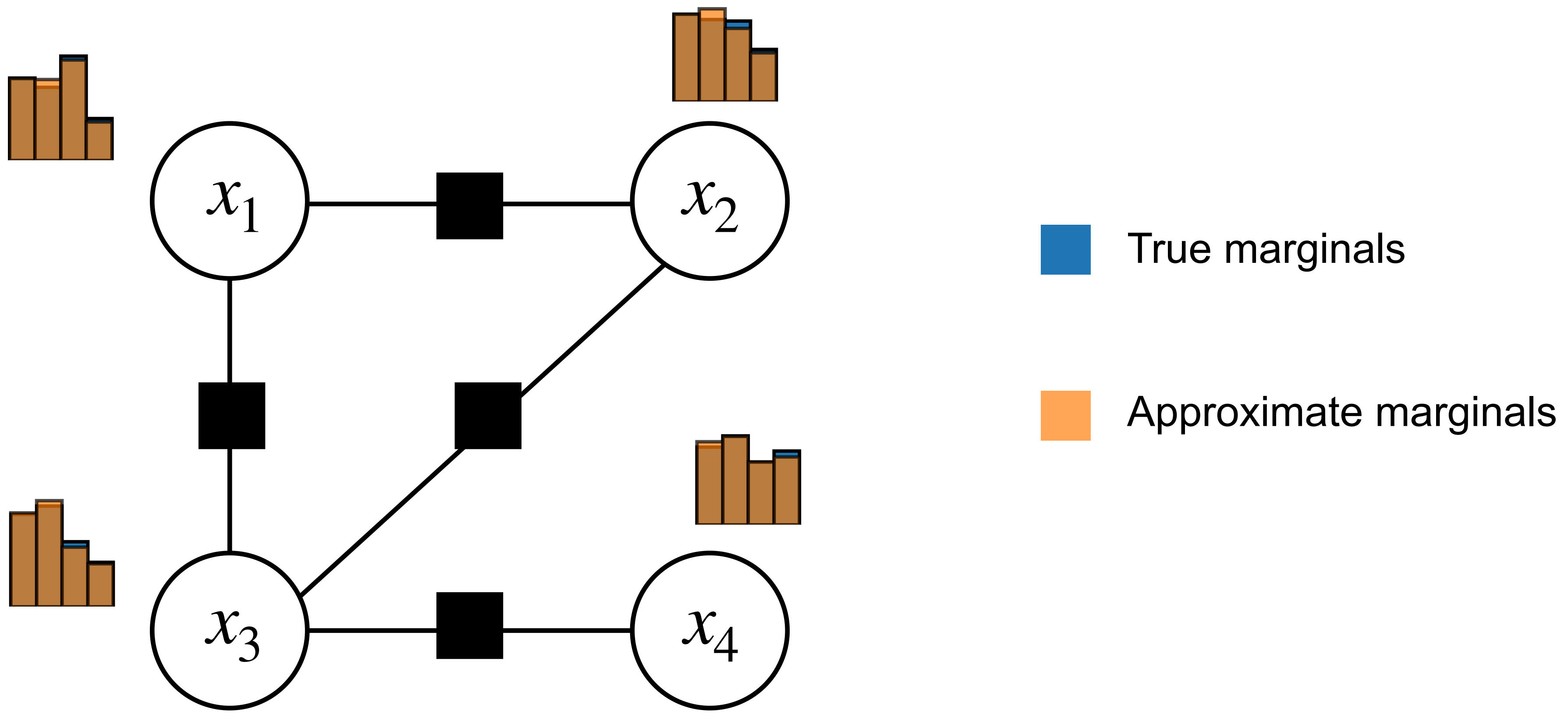

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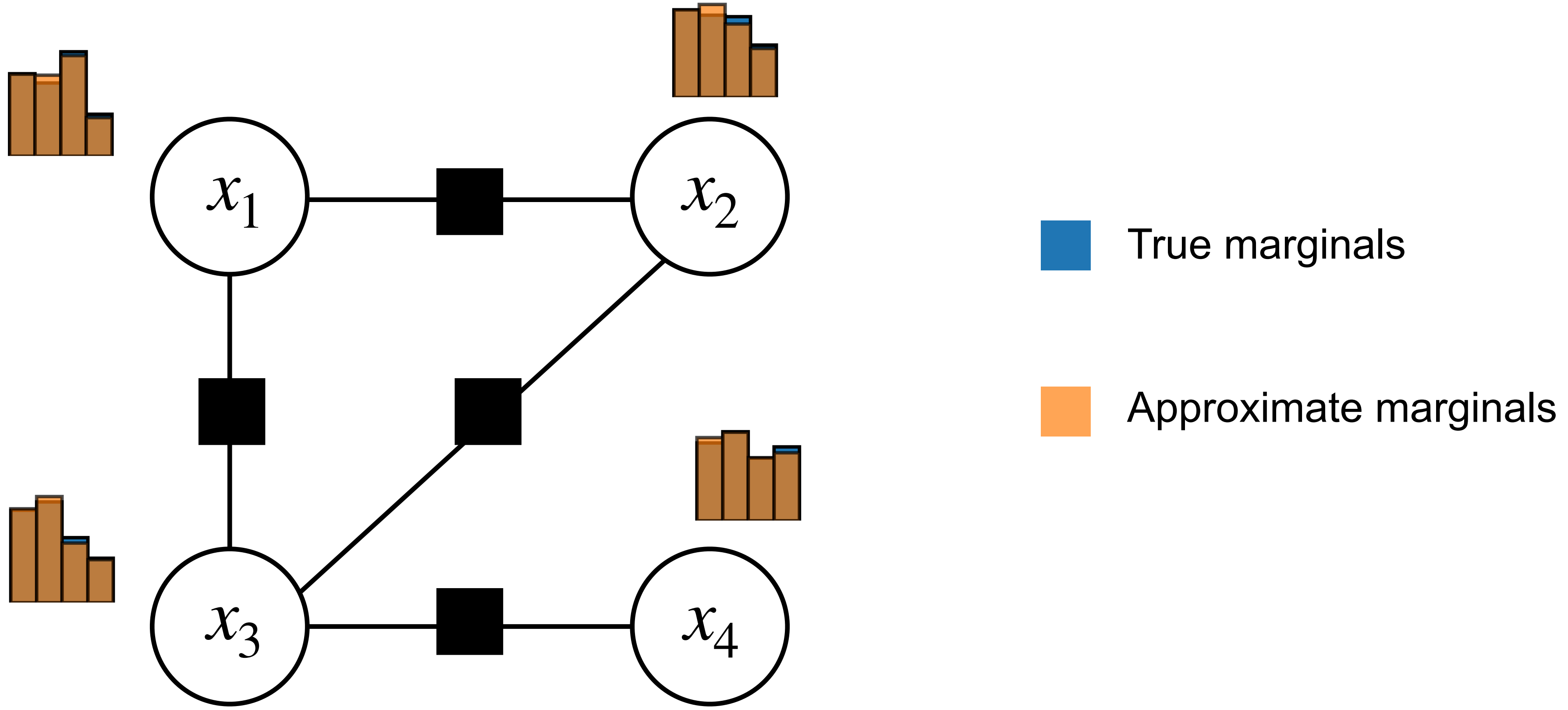

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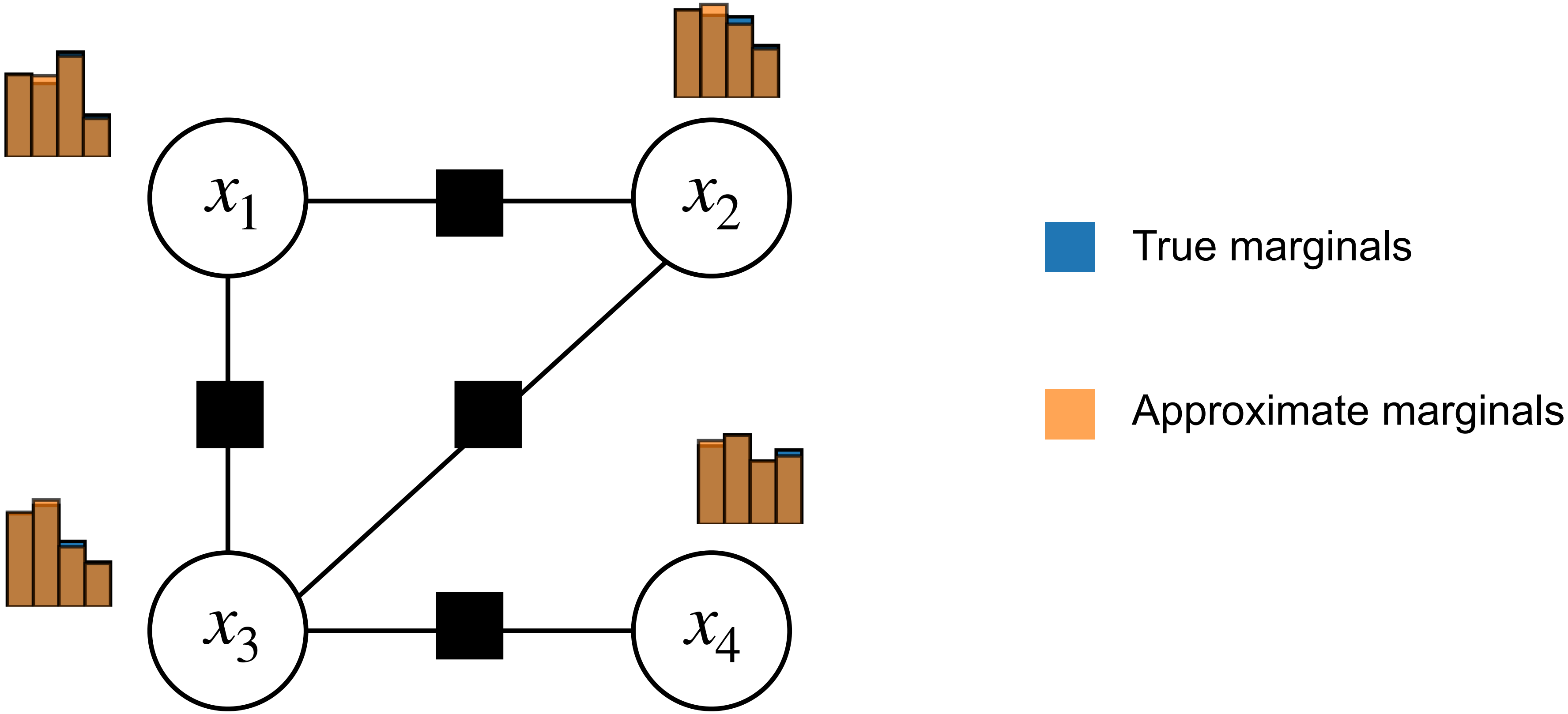
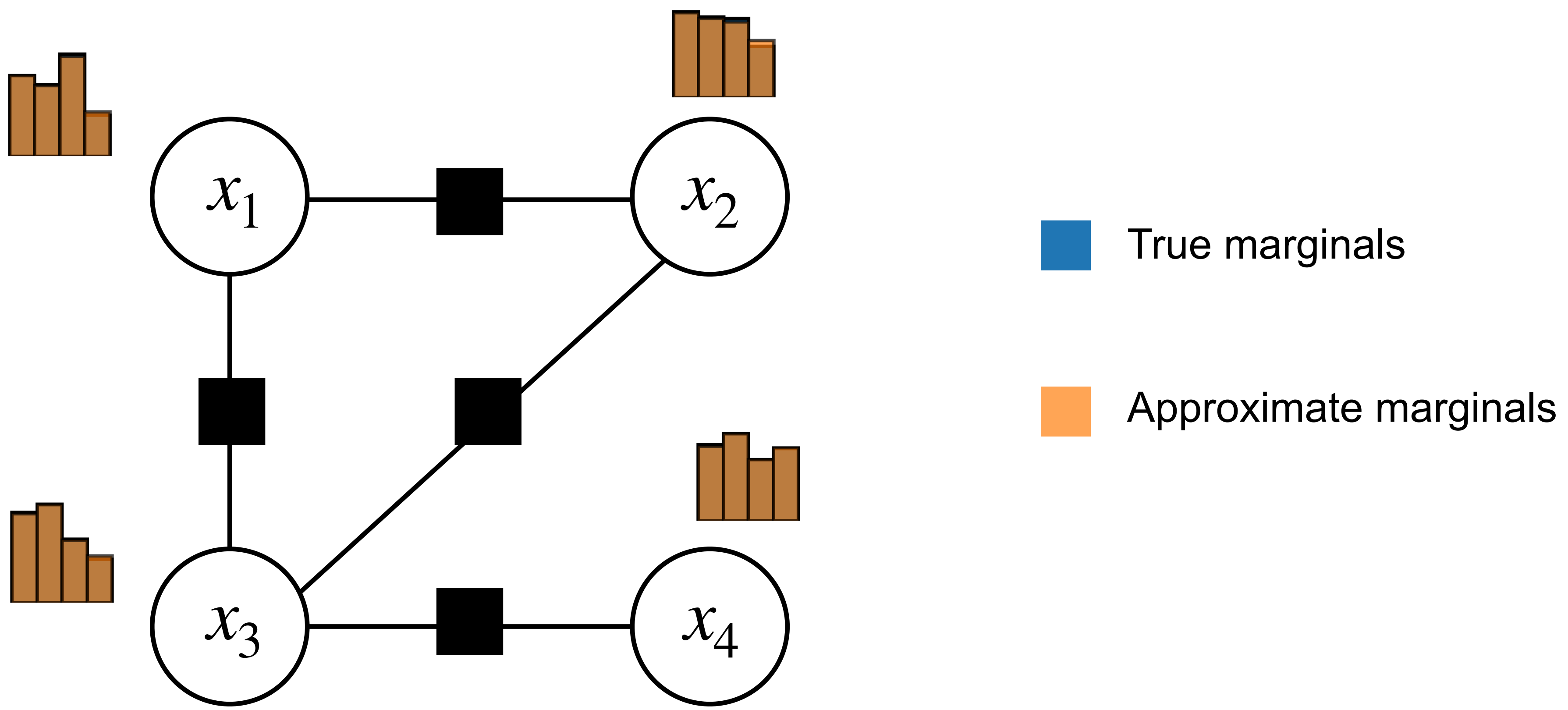


Implementation (flooding schedule)

Iteration 2



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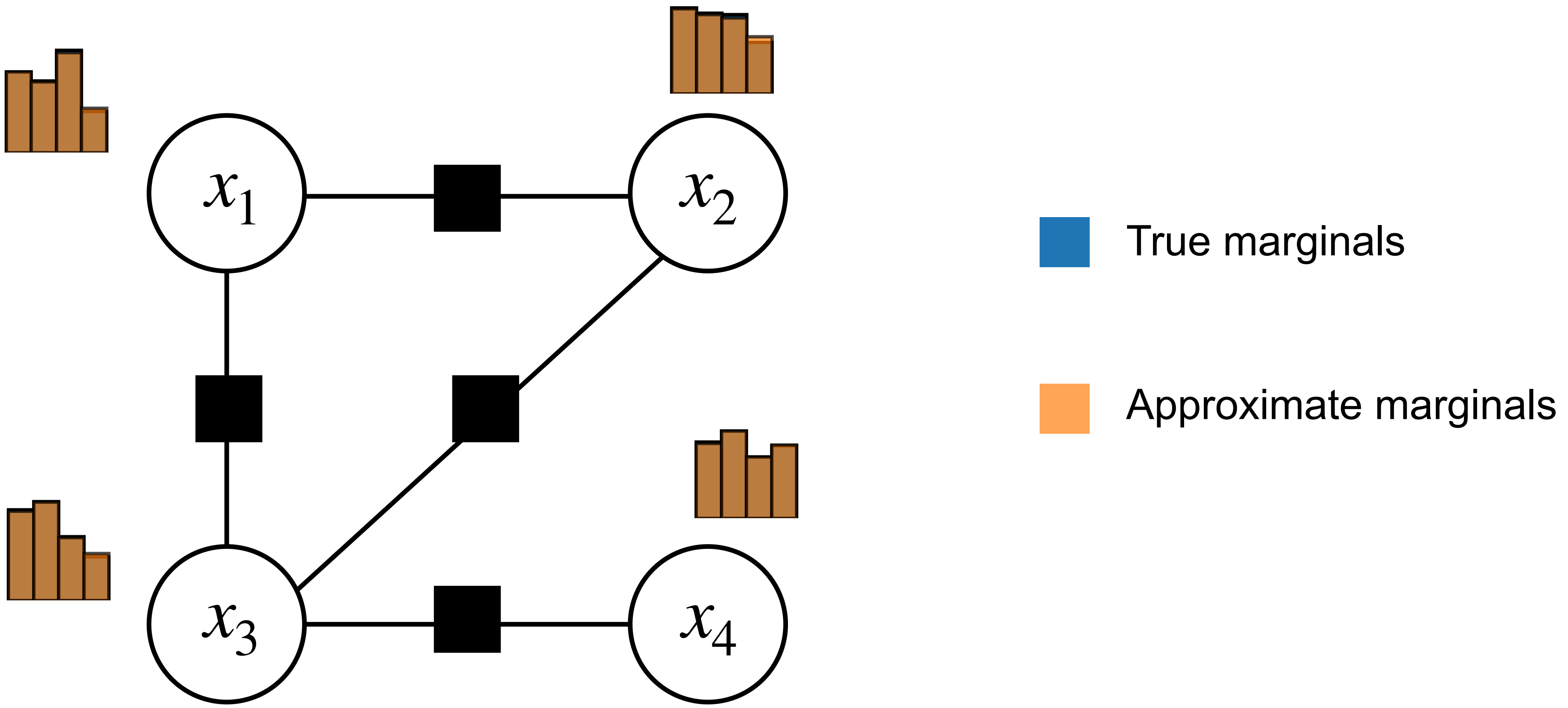

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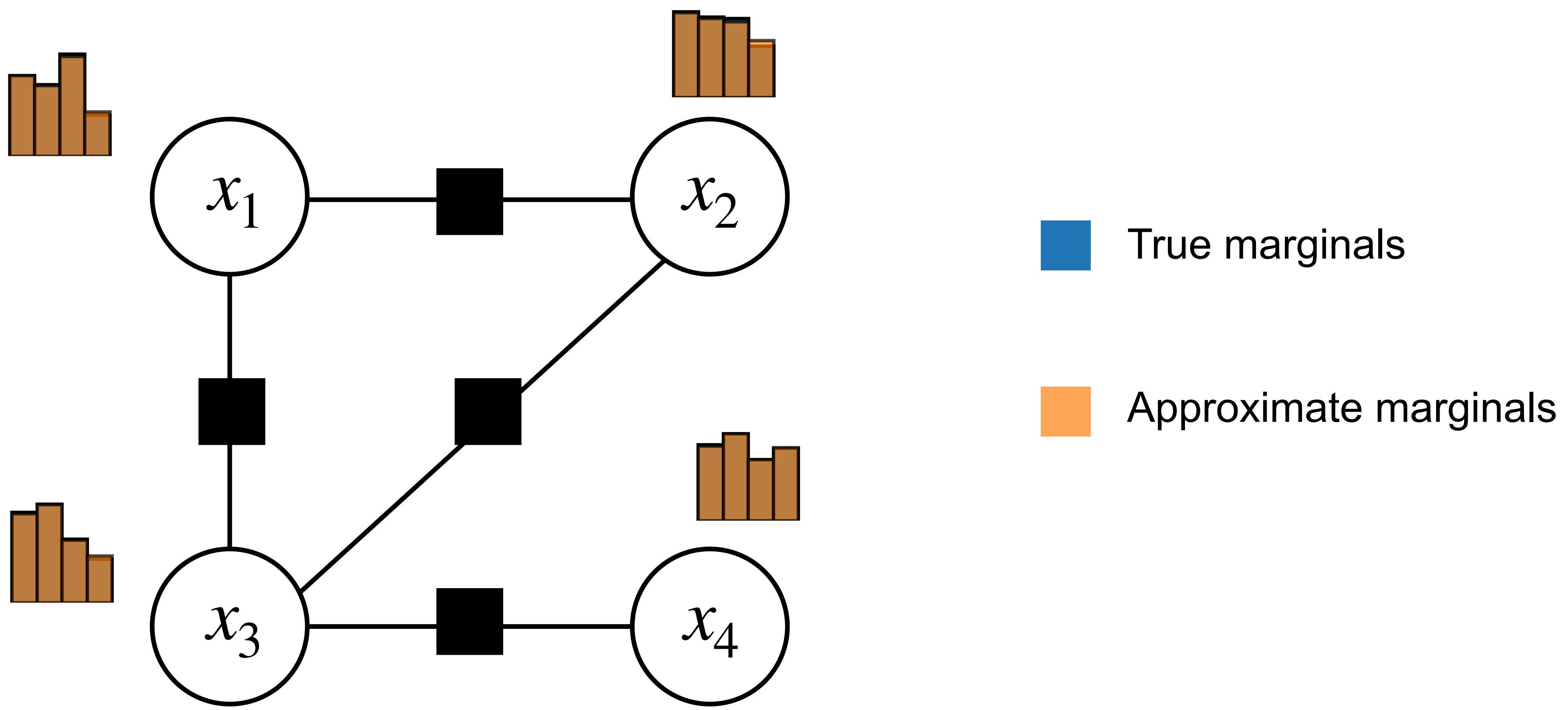

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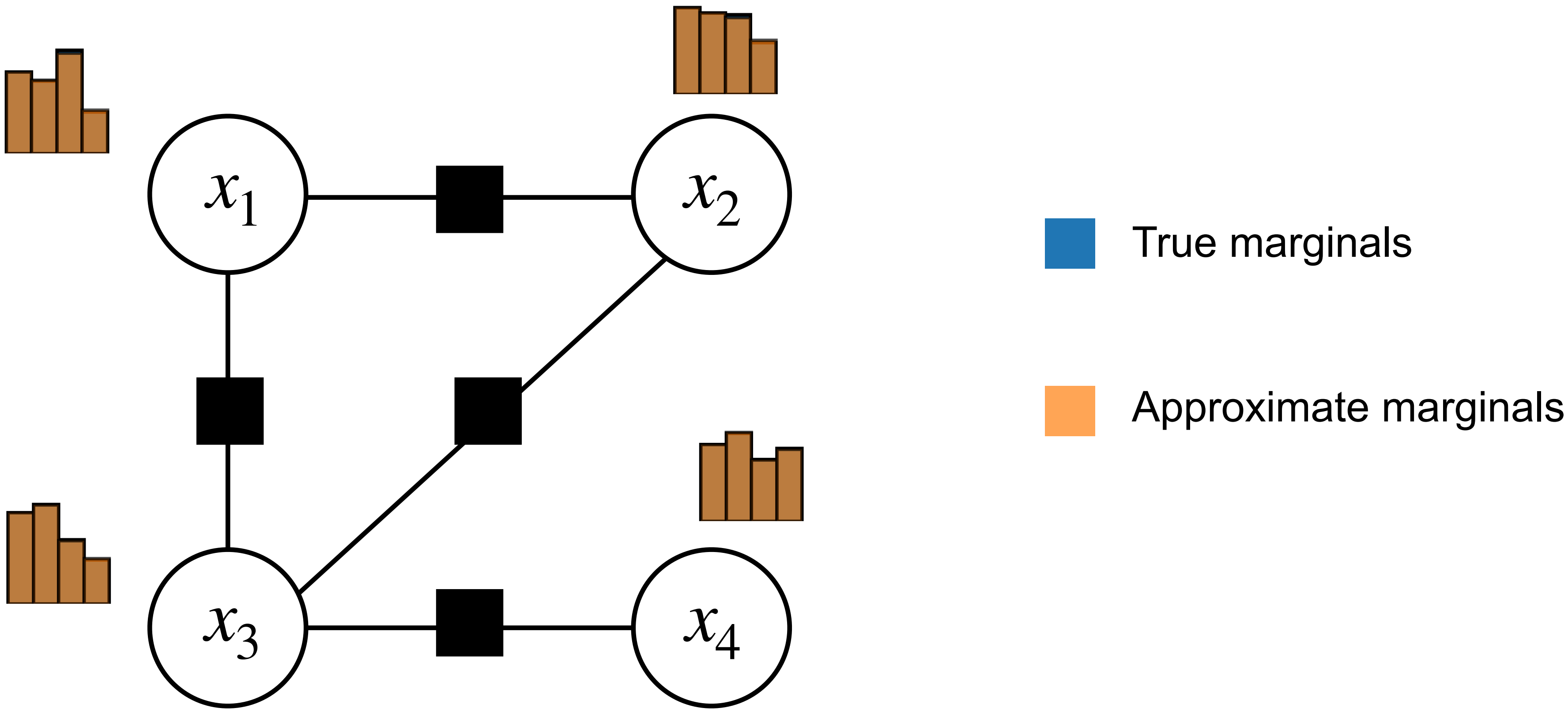
Iteration 3



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  - When applied to graphs, it generalises LBP [4]
- LBP is closely related to Bethe free energy optimisation [5]

References

[1] Bishop, Christopher M. *Pattern Recognition and Machine Learning*. New York: springer, 2006.

[2] Wainwright, Martin J., and Michael I. Jordan. *Graphical Models, Exponential Families, and Variational Inference*. Foundations and Trends in Machine Learning, 2008.

[3] Ortiz, Joseph, Talfan Evans, and Andrew J. Davison. *A Visual Introduction to Gaussian Belief Propagation.* 2021. (https://gaussianbp.github.io/)

[4] Minka, Thomas P. *Expectation propagation for approximate Bayesian inference*. Proceedings of the Seventeenth conference on Uncertainty in artificial intelligence, 2001.

[5] Yedidia, Jonathan S., William T. Freeman, and Yair Weiss. *Understanding belief propagation and its generalizations.* Exploring artificial intelligence in the new millennium, 2003.

4. Message Passing Neural Networks

Neural networks

Neural networks have dominated ML in the past decade.

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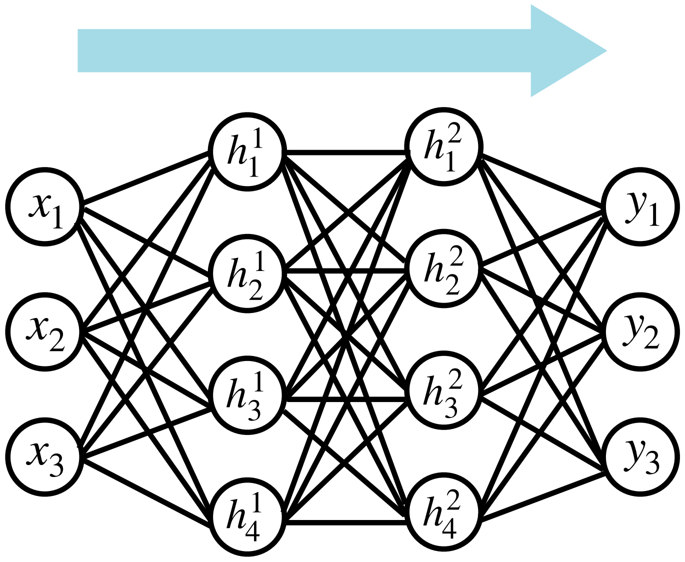
$$h^0 = x$$
$$h^{l+1} = \mathrm{ReLU}(Wh^l + b), \quad t = 0, \ldots, L-1$$
$$y = \mathrm{Softmax}(Wh^L + b)$$



Multilayer perceptron

A zoo of graphs in the real world

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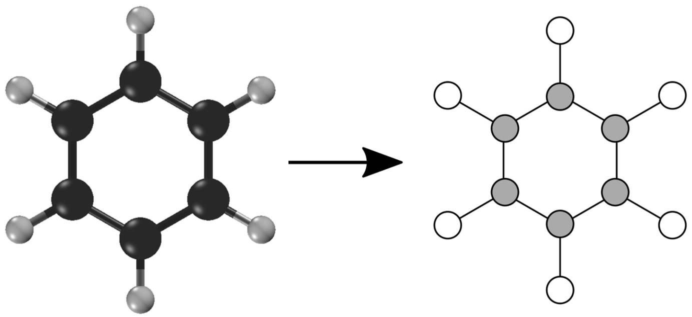

Molecules as graphs
Image from: https://www.oreilly.com/library/view/deep-learning-for/9781492039822/ch04.html

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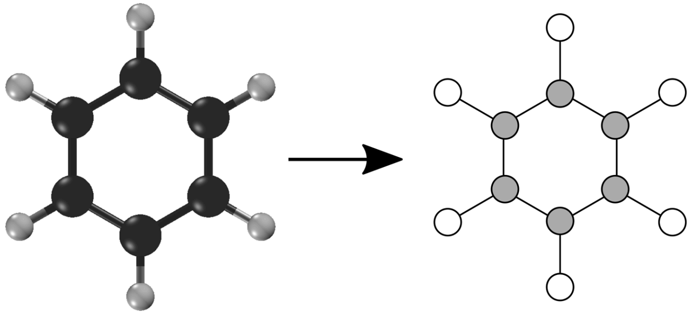

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Social networks
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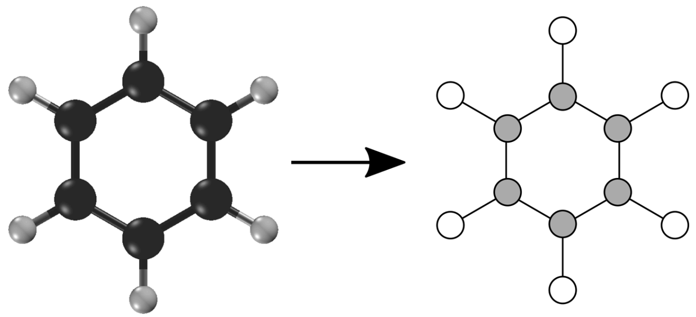

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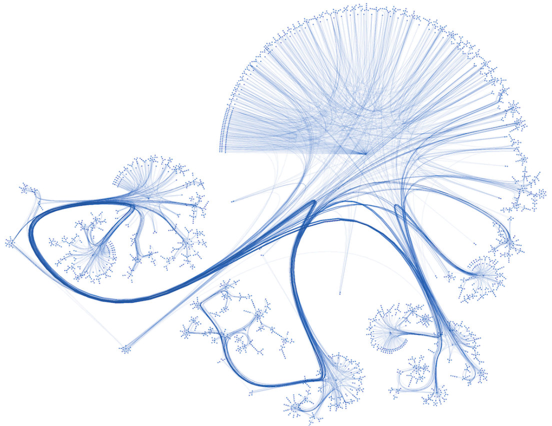

Citation networks
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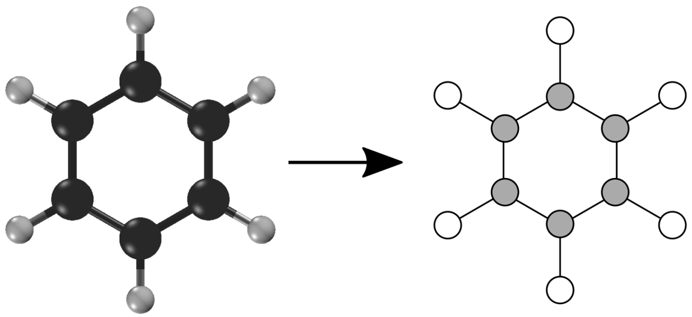

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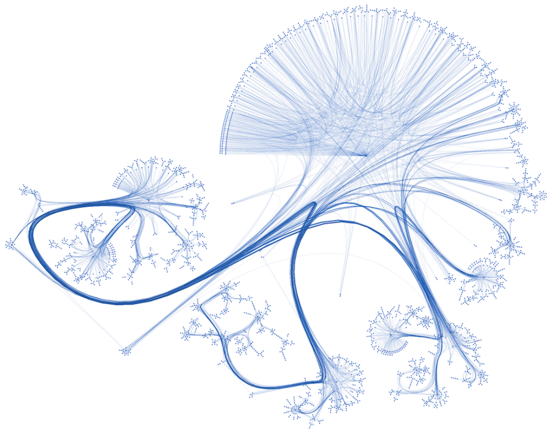

Citation networks
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Social networks
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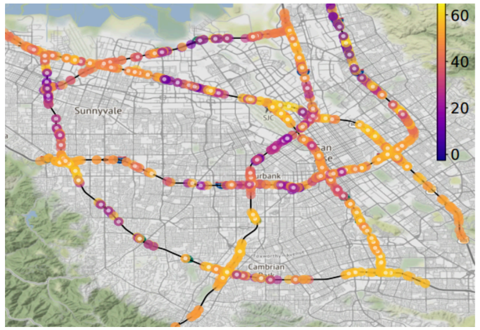
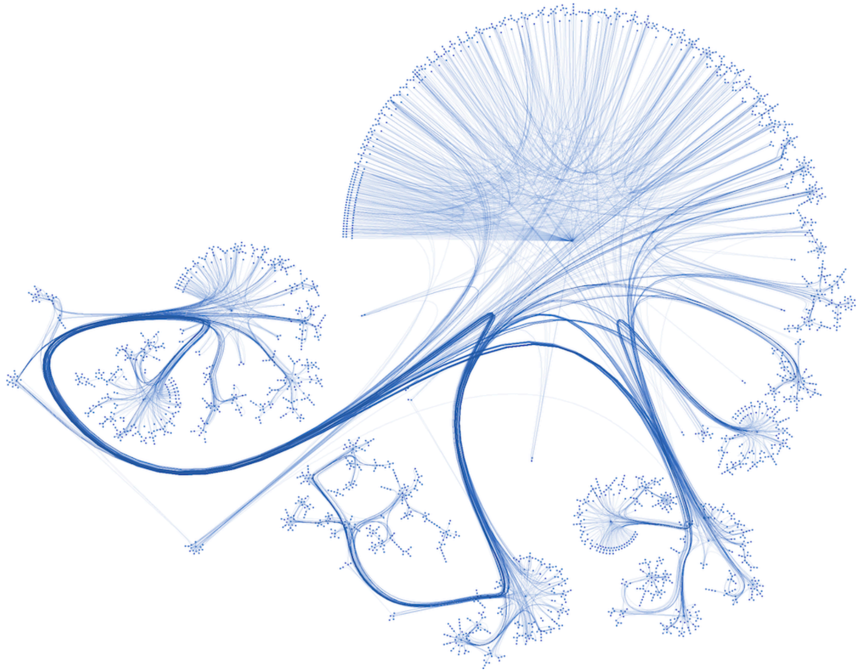


Traffic networks
Image from: http://proceedings.mlr.press/v130/borovitskiy21a/borovitskiy21a.pdf

Example: Cora dataset

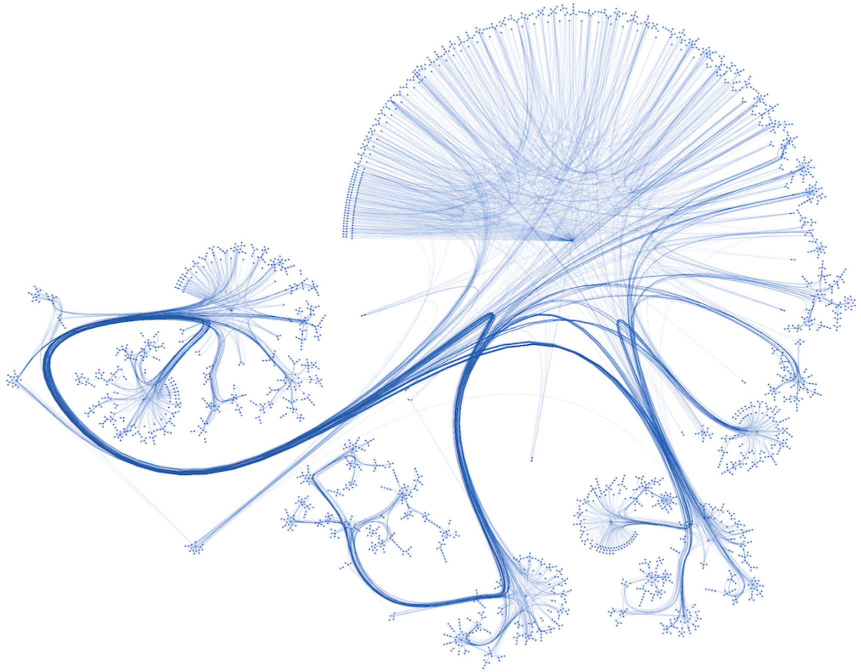


Overview of dataset:

- 2708 ML publications
- 5429 citation links
- Node feature size: 1433
- Seven classes

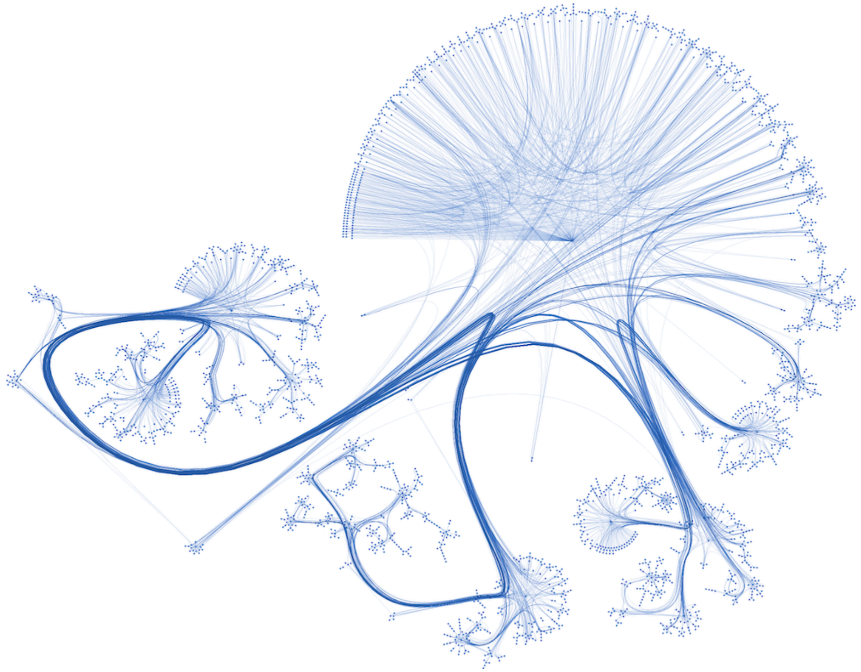
Task: classify nodes according to topic

Example: Cora dataset



Using MLP:

Example: Cora dataset



Using MLP:

Do MLP classification with

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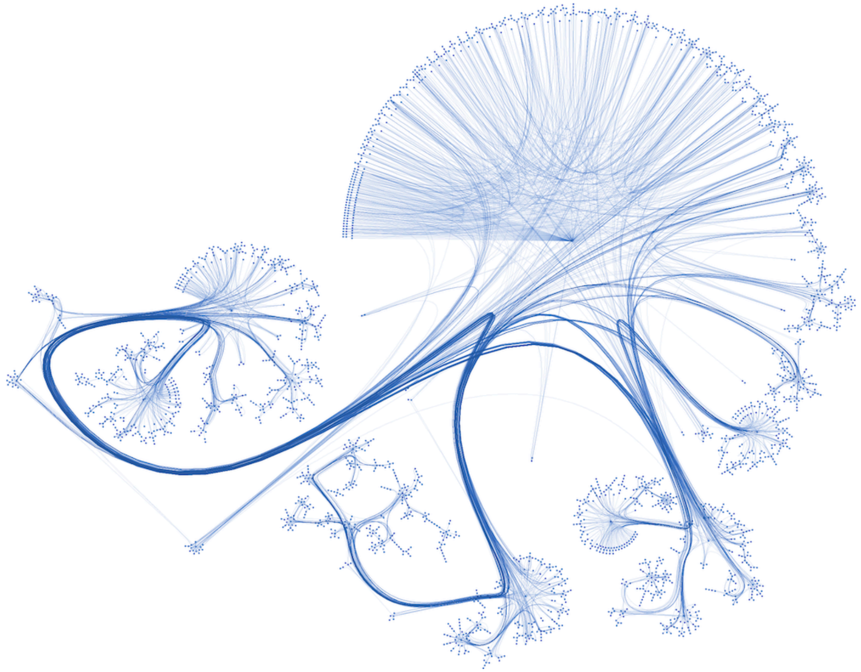

Using MLP:

Do MLP classification with

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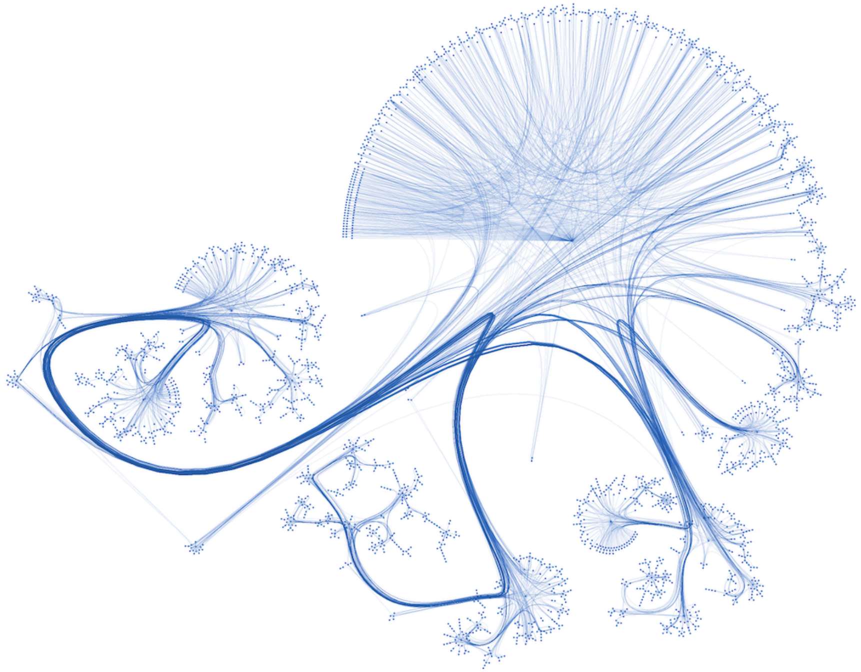

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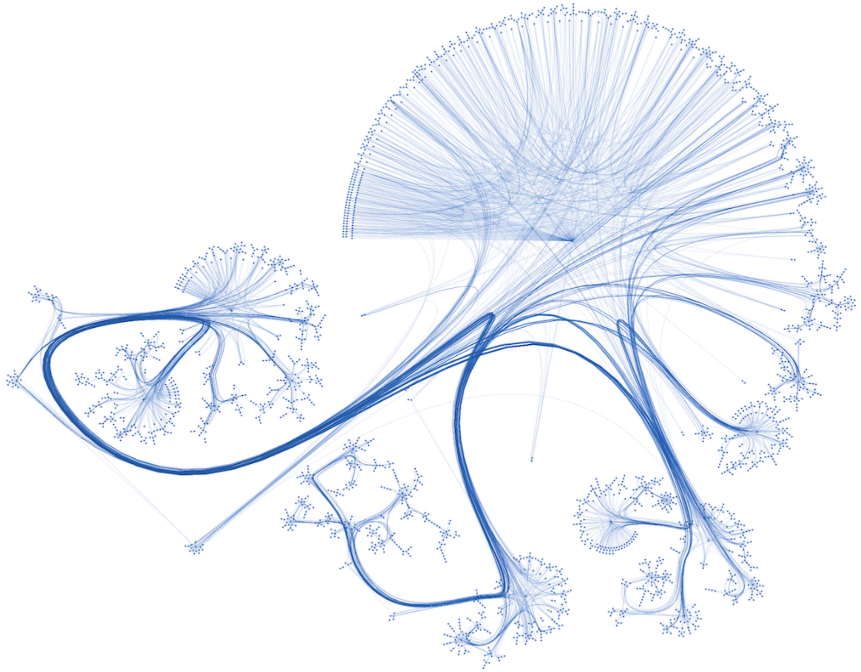

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Do MLP classification with

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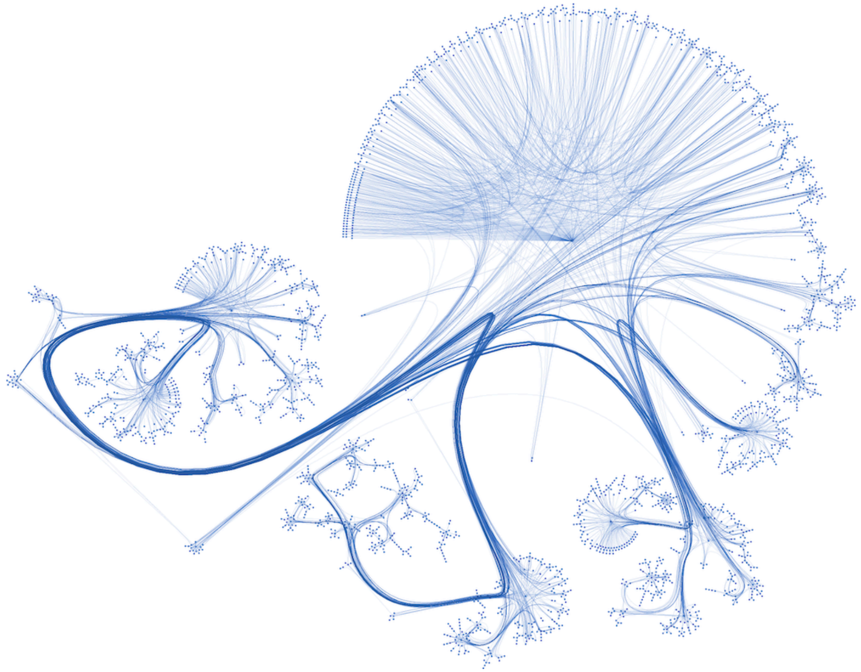

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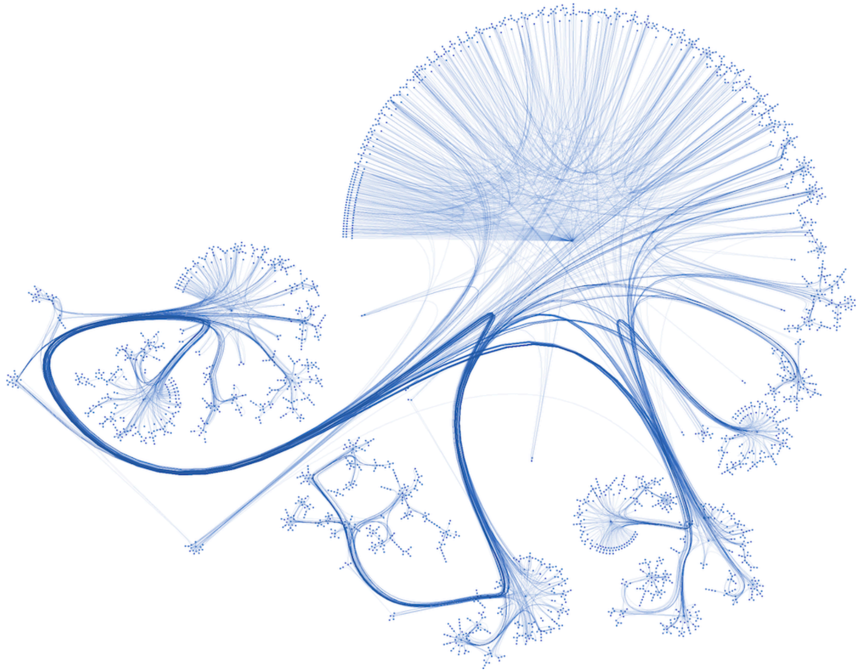

Using MLP:

Do MLP classification with

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However,

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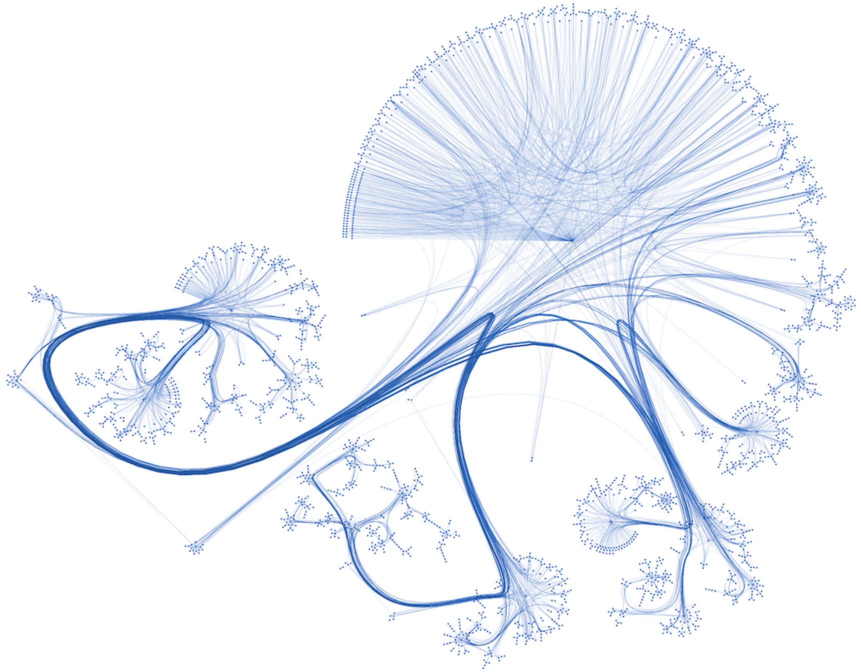
- Data size is small

Example: Cora dataset



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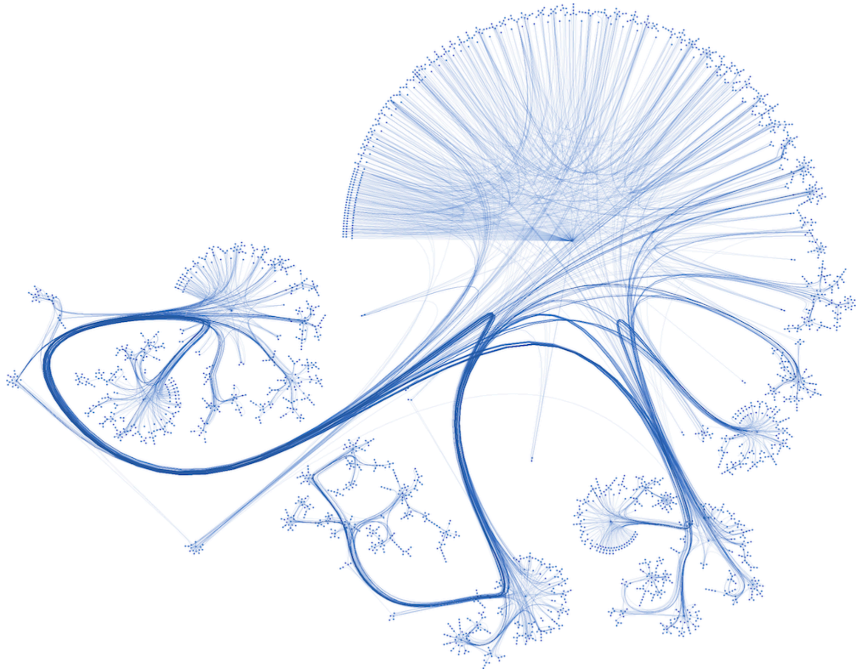

Using belief propagation:

- Create a MRF with pairwise potential [12]

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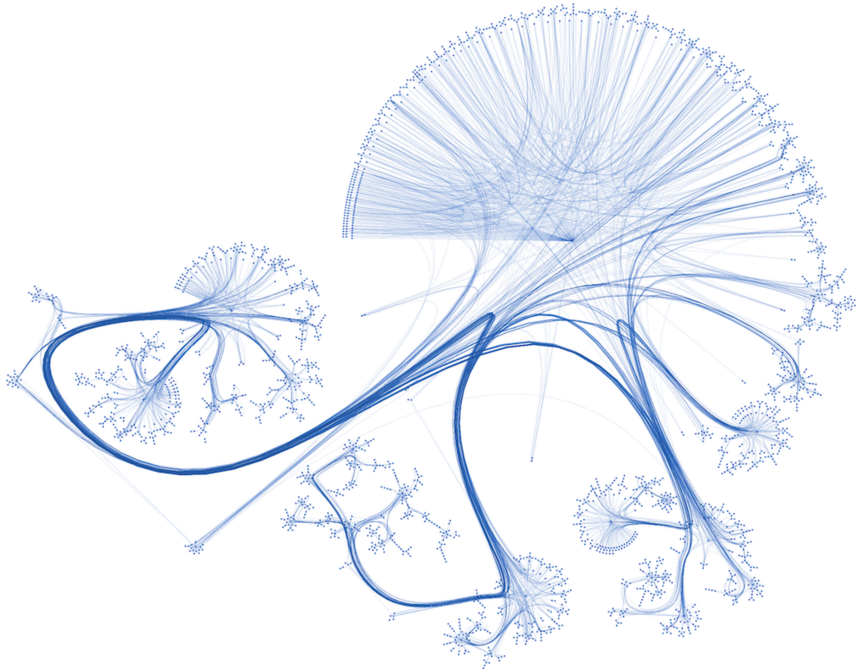

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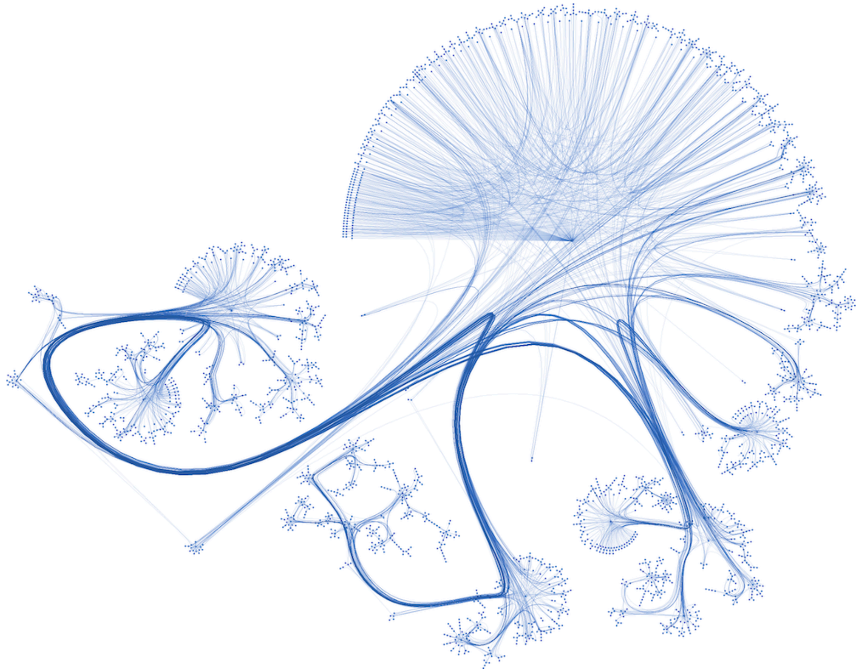

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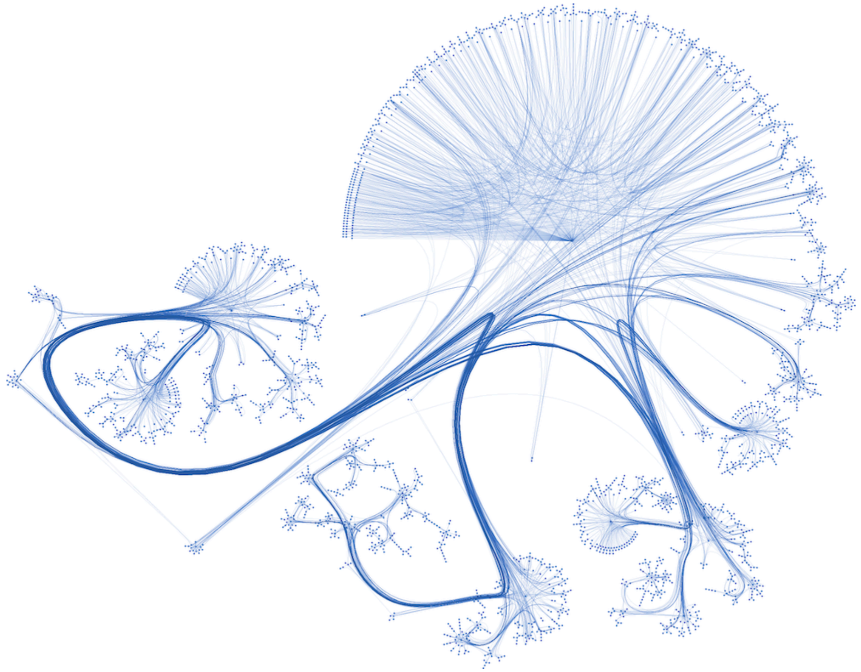

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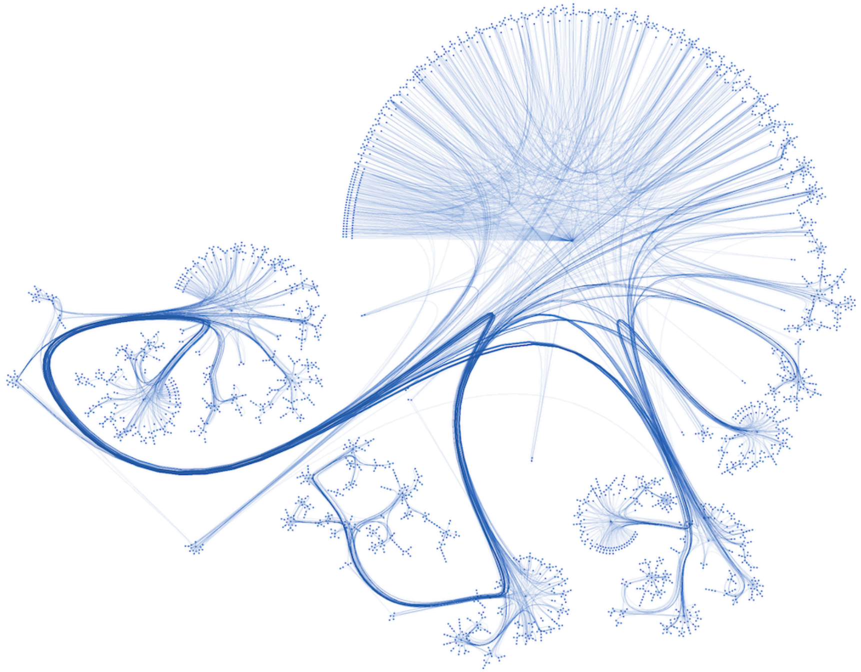

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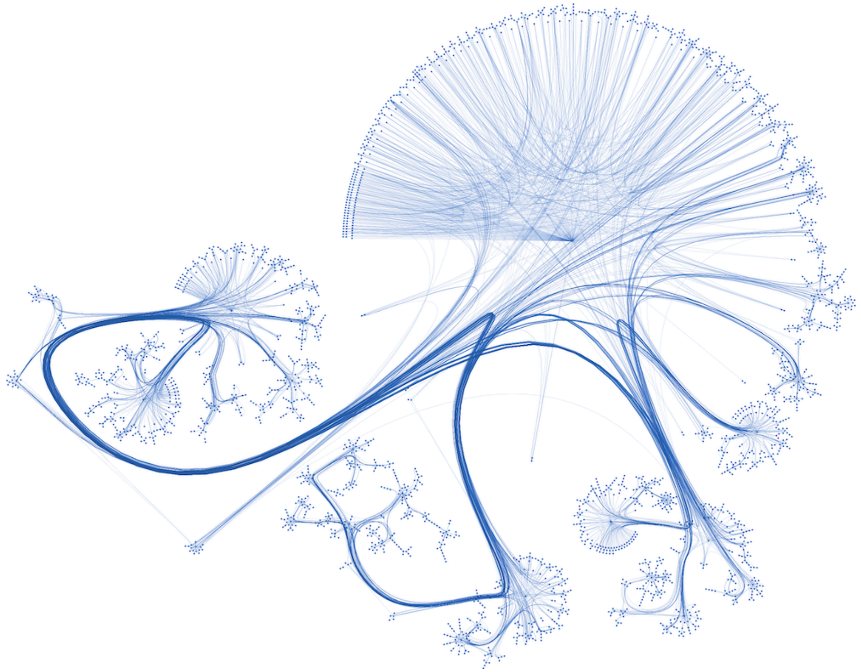

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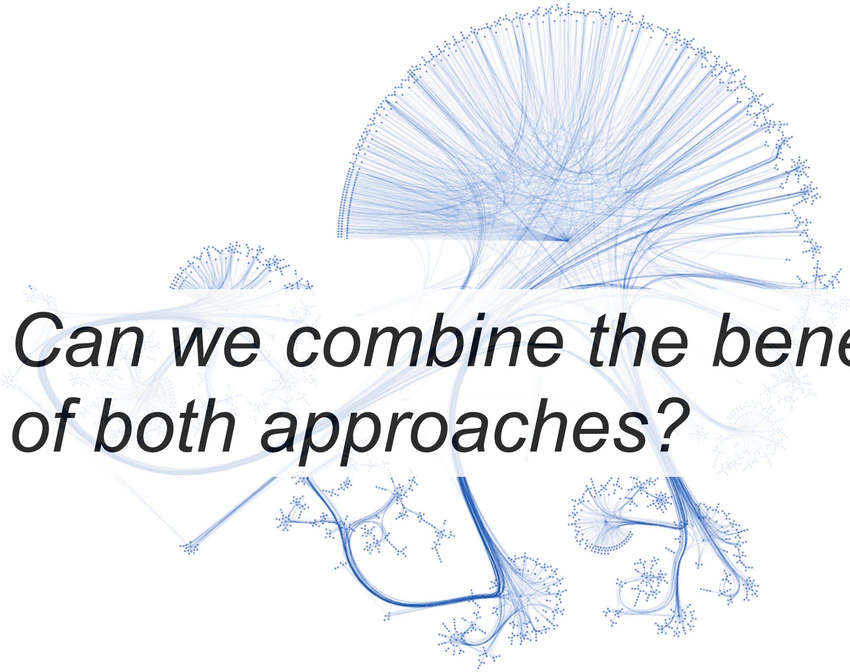

Can we combine the benefits of both approaches?

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Convolutional neural networks

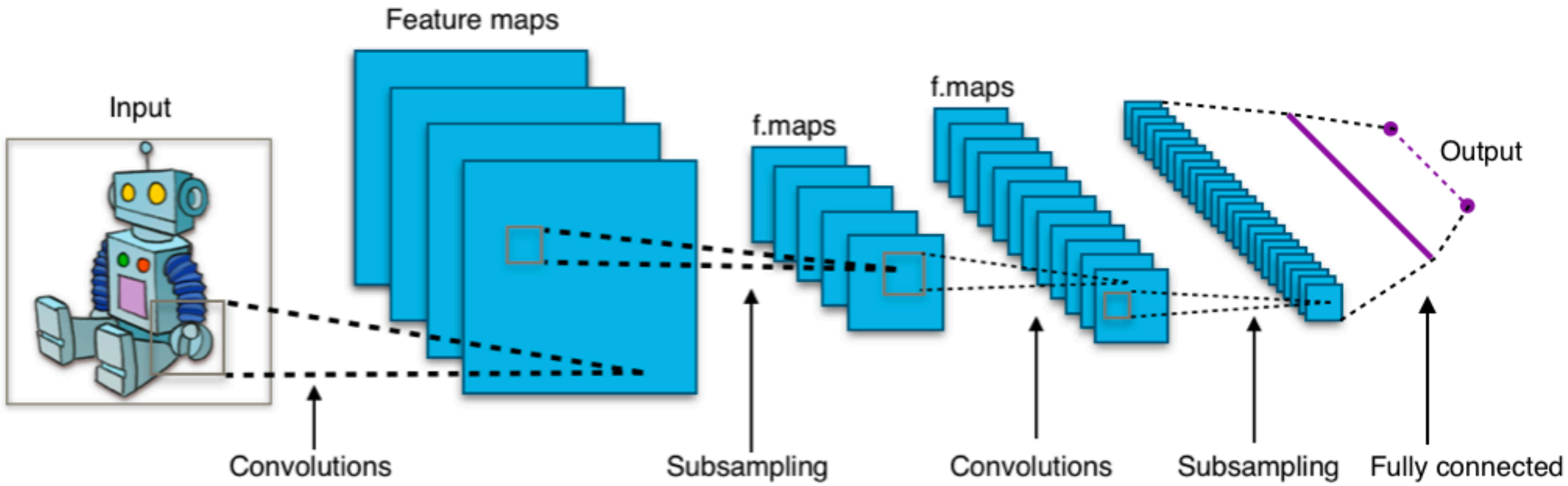
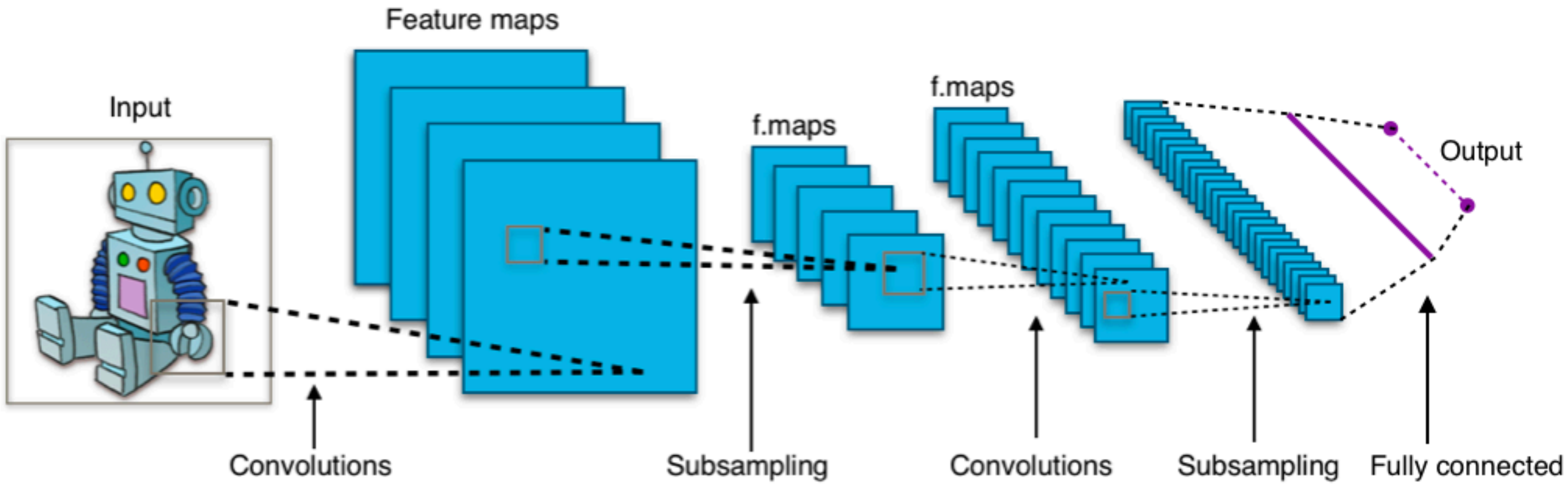


Image from: https://en.wikipedia.org/wiki/Convolutional_neural_network

Convolutional neural networks

- Incorporates inductive bias of grid-inputs



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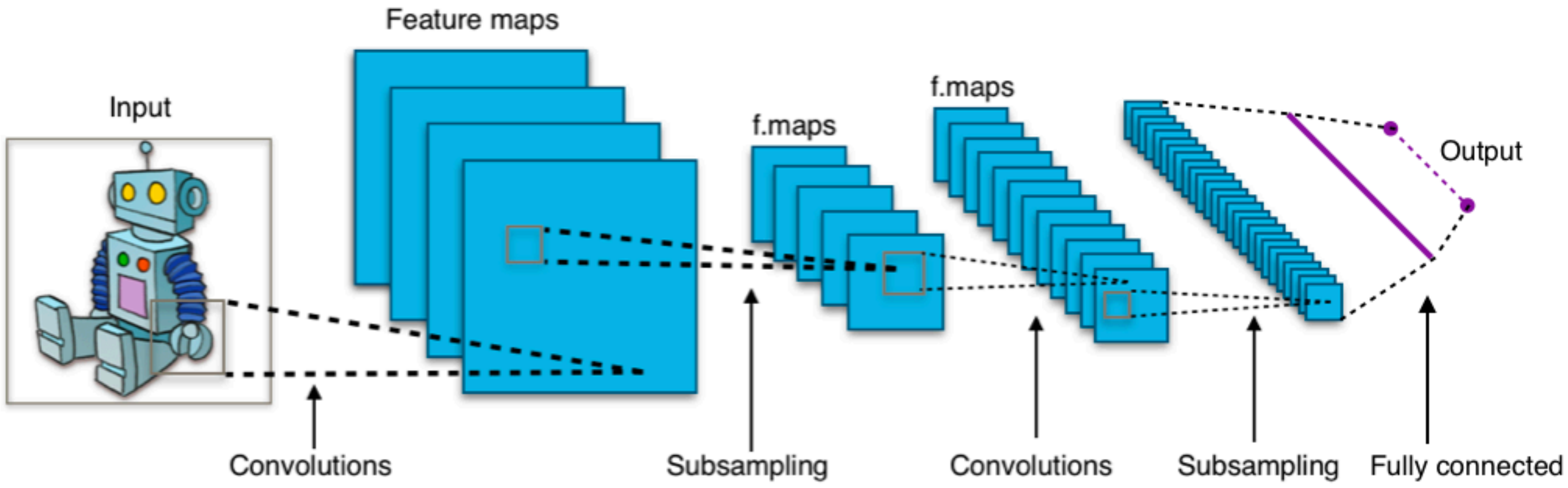
Convolutional neural networks

- Incorporates inductive bias of grid-inputs
- Sparse connectivity owing to local receptive field



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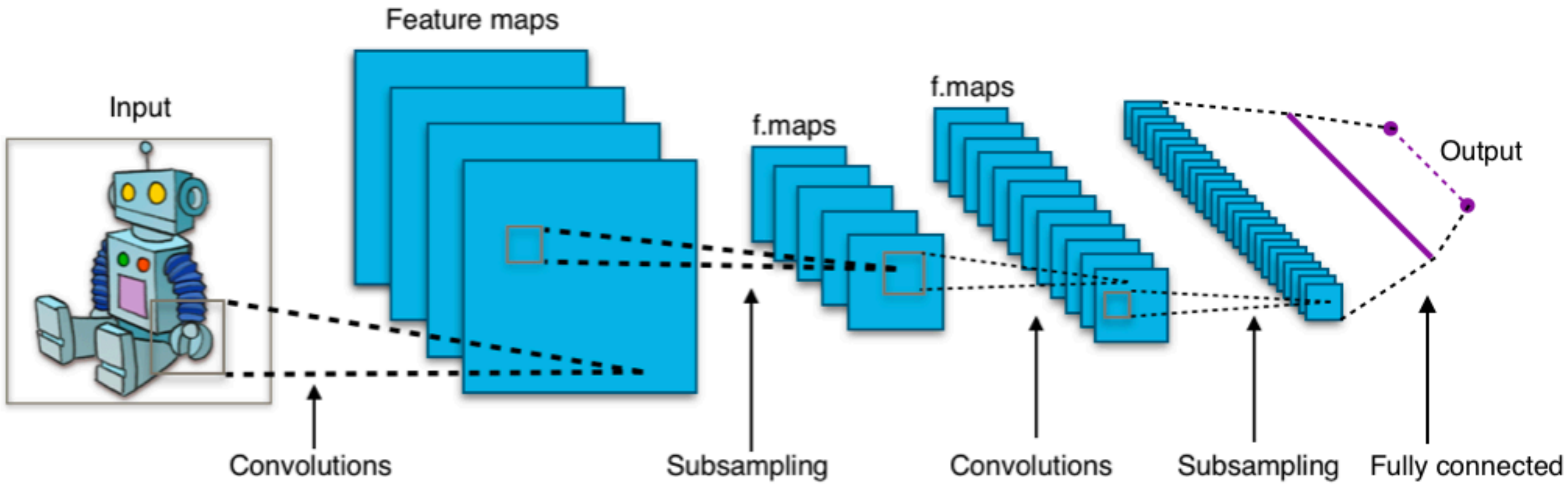
Convolutional neural networks

- Incorporates inductive bias of grid-inputs
- Sparse connectivity owing to local receptive field
- Shared parameters



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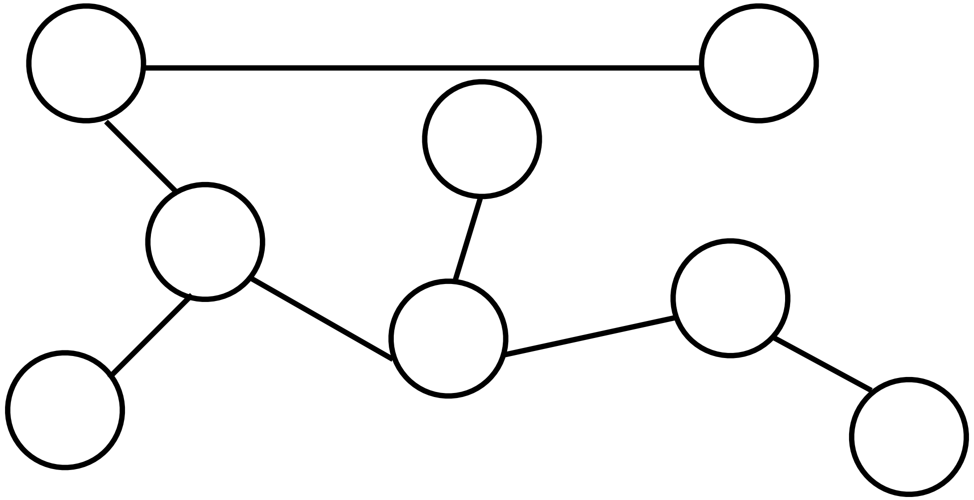
3. Use local information to construct hidden features

4. Can use edge features in addition to node features

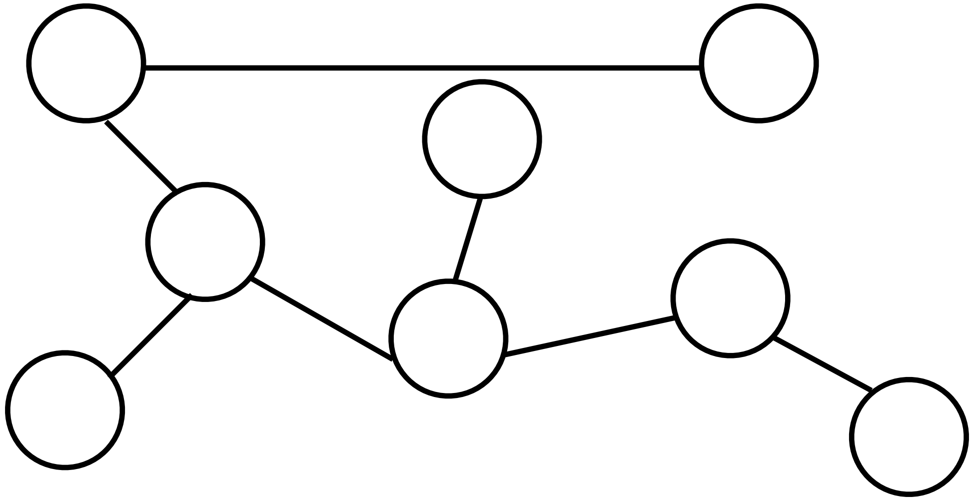
Extending convolutions to graphs?



Can we define convolutions on graphs?

Extending convolutions to graphs?

CNNs are based on discretisation of the *convolution operator*



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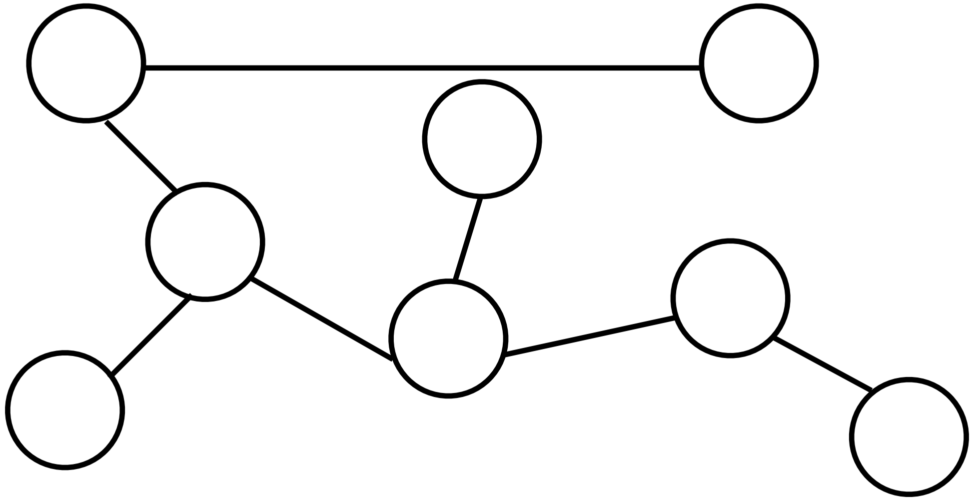

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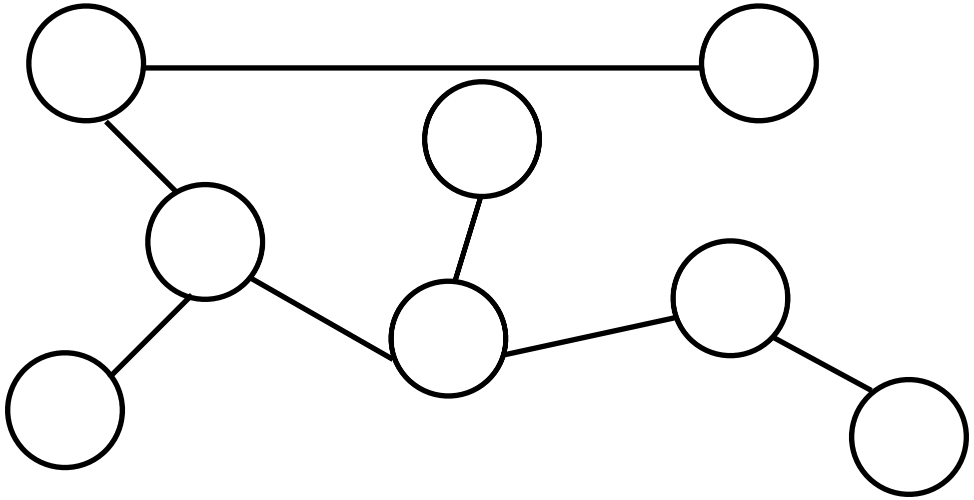

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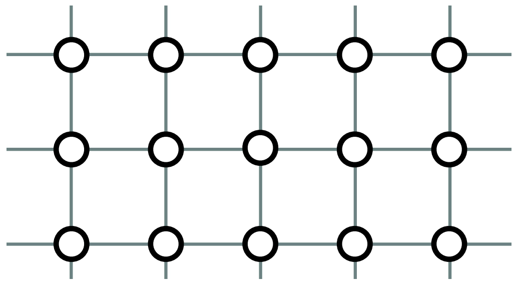
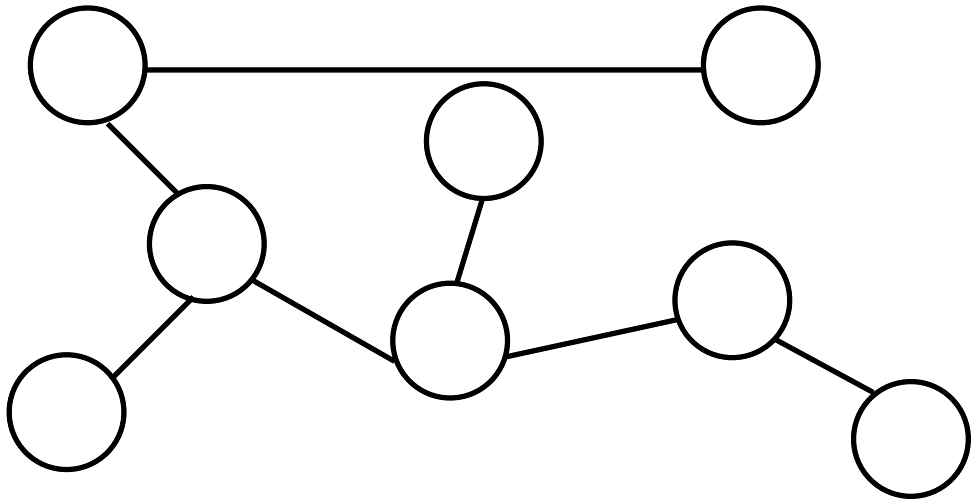


Convolution applies to grids



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Spectral graph convolution

Bruna et al. [1] introduced SpectralNet based on the following property of $\star$

$$f \star \psi_\theta(x) = \mathscr{F}^{-1}\left(\mathscr{F}f \odot \mathscr{F}\psi_\theta\right)(x),$$

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Alternatively, consider a “spatial” approach (Duvenaud et al. [3]):

$$h_{v_i}^{l+1} = \sigma\Big(\sum_{j \in \mathcal{N}_i} h_{v_j}^{l} W_{|\mathcal{N}_i|}^{l} \Big), \quad v_i \in V.$$

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- Can be derived from *ChebNet* [2], a variant of spectral graph convolution

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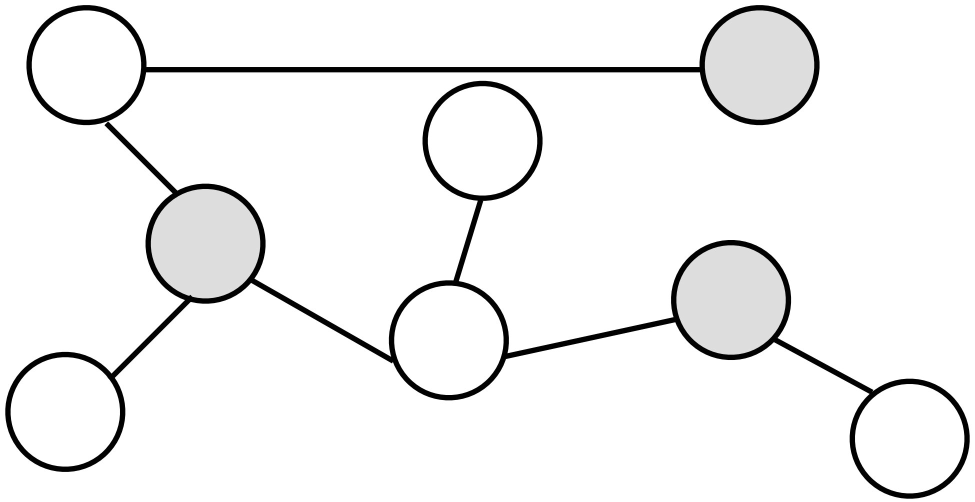
Semi-supervised learning

- Applies when the number of labelled datapoints are *small*
- But relations between labelled and unlabelled data exist



Semi-supervised learning

Experiment with Cora dataset:

- Use only 140 nodes for training data
- 1000 nodes for testing

Train with cross-entropy loss over labelled data $\mathscr{D}_L$ (i.e. training data):

$$L = -\sum_{(y,X)\in\mathscr{D}_L} y \log \mathrm{GCN}(X).$$

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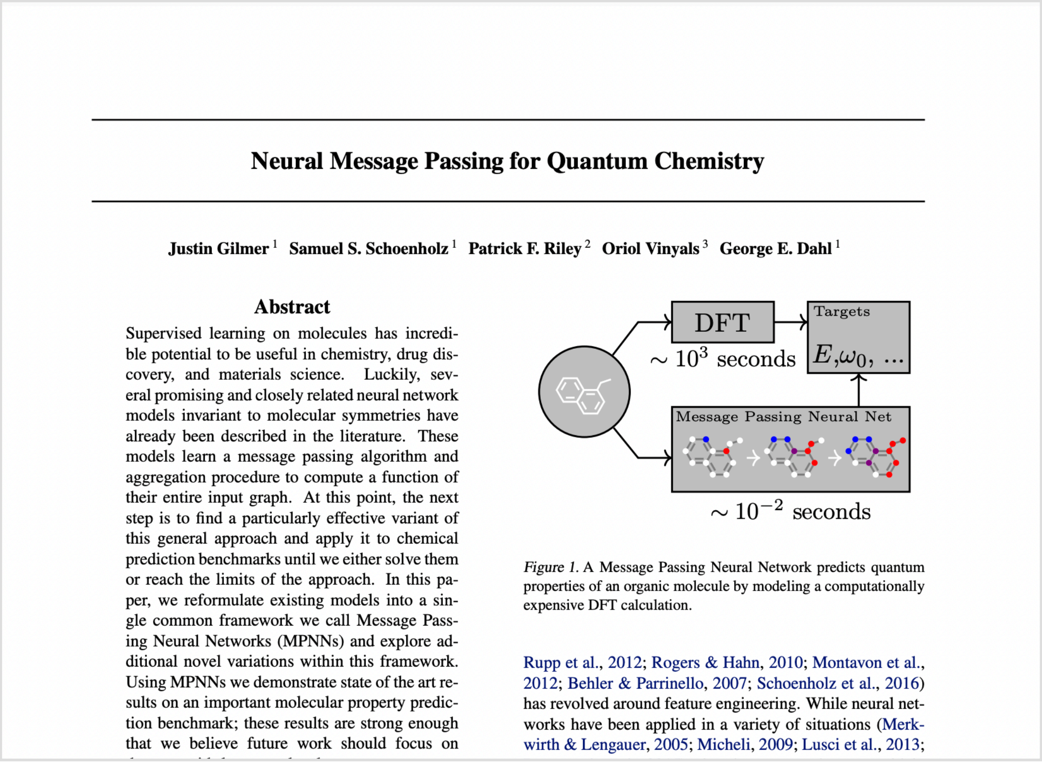
Kipf and Welling [4] reports accuracy of:

- $81.5\,\%$ using GCN
- $55.1\,\%$ using MLP

Message Passing Neural Networks



Neural Message Passing for Quantum Chemistry

Justin Gilmer [1] Samuel S. Schoenholz [1] Patrick F. Riley [2] Oriol Vinyals [3] George E. Dahl [1]

Abstract

Supervised learning on molecules has incredible potential to be useful in chemistry, drug discovery, and materials science. Luckily, several promising and closely related neural network models invariant to molecular symmetries have already been described in the literature. These models learn a message passing algorithm and aggregation procedure to compute a function of their entire input graph. At this point, the next step is to find a particularly effective variant of this general approach and apply it to chemical prediction benchmarks until we either solve them or reach the limits of the approach. In this paper, we reformulate existing models into a single common framework we call Message Passing Neural Networks (MPNNs) and explore additional novel variations within this framework. Using MPNNs we demonstrate state of the art results on an important molecular property prediction benchmark; these results are strong enough that we believe future work should focus on

Figure 1. A Message Passing Neural Network predicts quantum properties of an organic molecule by modeling a computationally expensive DFT calculation.

Rupp et al., 2012; Rogers & Hahn, 2010; Montavon et al., 2012; Behler & Parrinello, 2007; Schoenholz et al., 2016) has revolved around feature engineering. While neural networks have been applied in a variety of situations (Merkwirth & Lengauer, 2005; Micheli, 2009; Lusci et al., 2013;

Gilmer et. al. [5] (ICML, 2017)

- Developed to predict properties of molecules
- Introduces a general framework for learning features on graphs based on message passing
- Can handle graph data containing both node and edge features

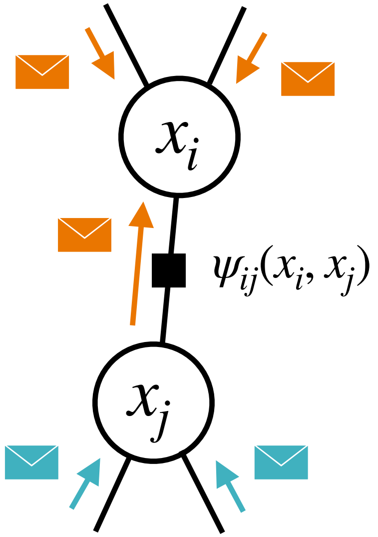
Recall the message passing protocol in BP:

Message update:

$$M_{j\to i}(x_i) = \sum_{x_j \in \{1,\ldots,K\}} \psi_{ij}(x_i, x_j)\, \psi_j(x_j) \prod_{k\sim j, k\neq i} M_{k\to j}(x_j),$$

State update:

$$p(x_i) = \psi_i(x_i) \prod_{j\sim i} M_{j\to i}(x_i).$$



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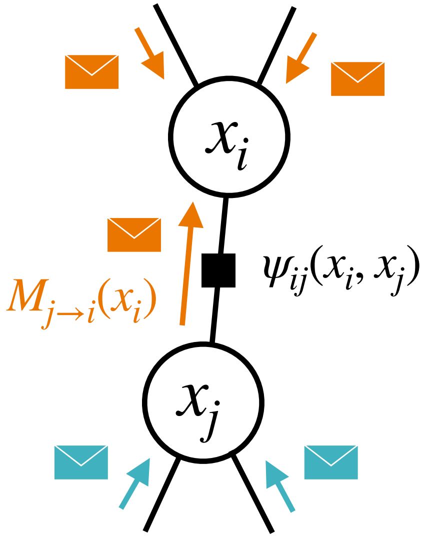

Message passing in MPNN [6]:

Message update:

$$M_{j\to i}^{l} = M_{\theta}^{l}(h_{v_i}^{l}, h_{v_j}^{l}, e_{ij}),$$

State update:

$$h_{v_i}^{l+1} = U_{\theta}^{l}(h_{v_i}^{l}, \square_{j\sim i}\, M_{j\to i}^{l}).$$

Readout:

$$y = R_{\theta}(\{h_{v_i}^{L} \,|\, v_i \in V\}).$$

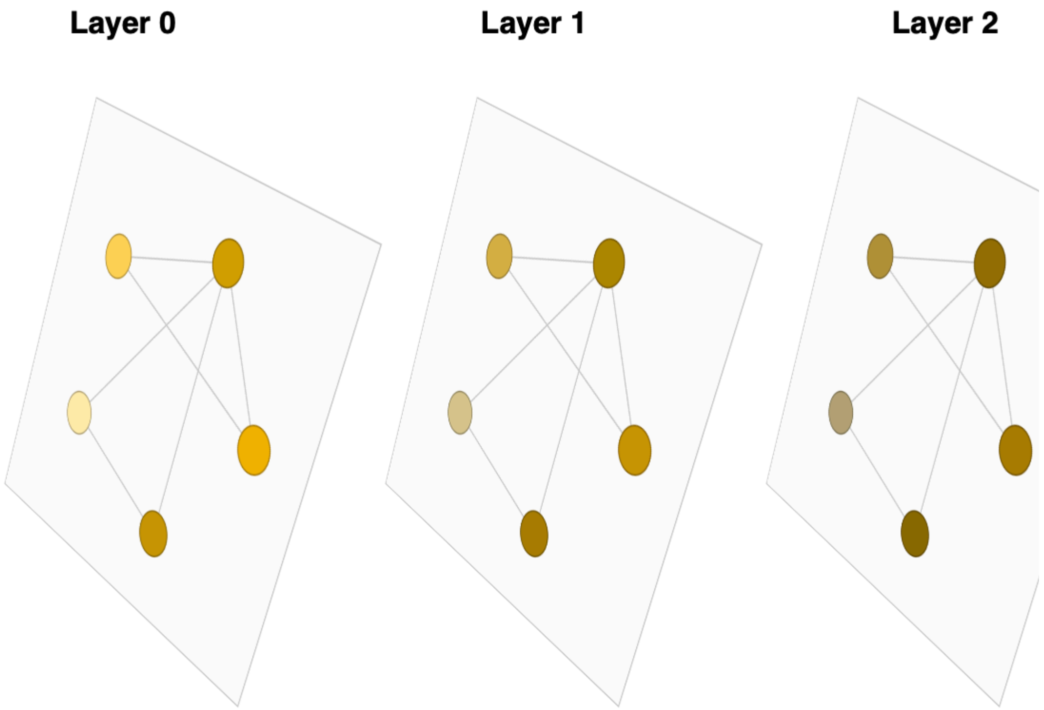

Image from: https://distill.pub/2021/gnn-intro/

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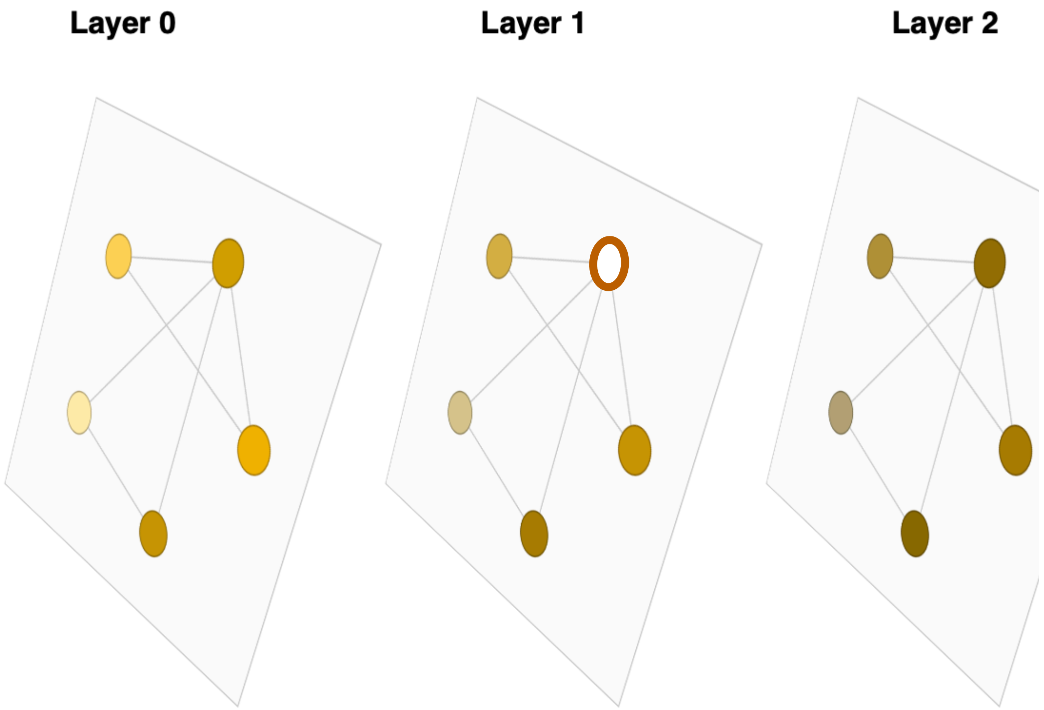

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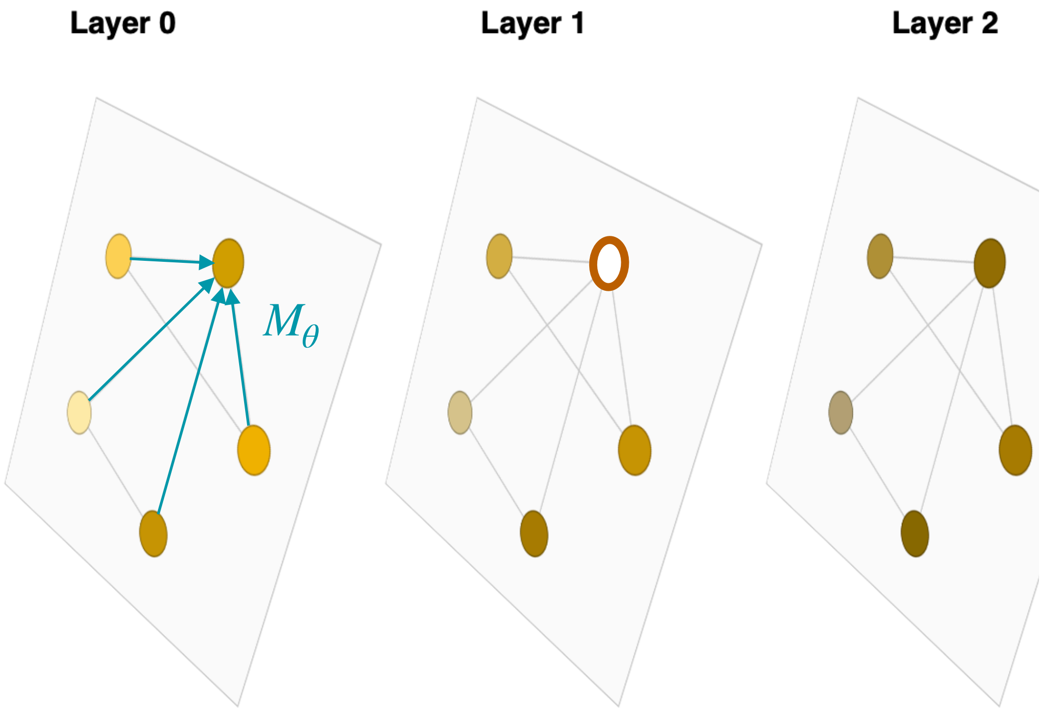

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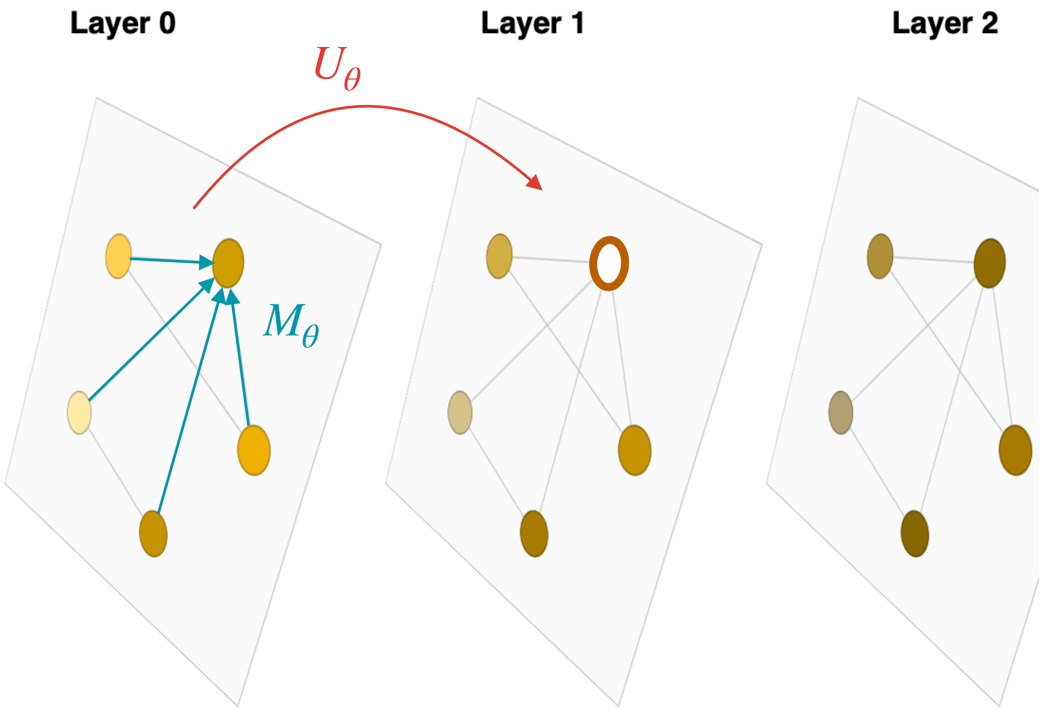

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$$h^{l+1}_{v_i} = U^l_\theta(h^l_{v_i}, \square_{j\sim i} M^l_{j\to i}).$$

Readout:

$$y = R_\theta(\{h^L_{v_i} \,|\, v_i \in V\}).$$

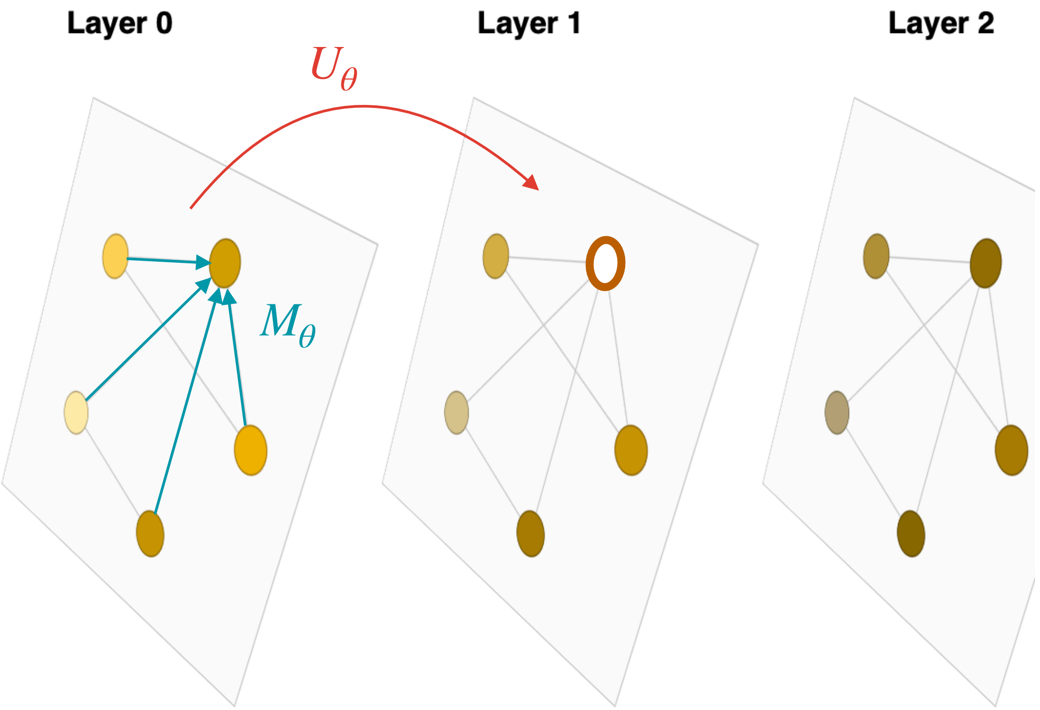

Image from: https://distill.pub/2021/gnn-intro/

Most GNN architectures can be expressed as an MPNN!

Example 1: GCNs as MPNN

Recall the GCN architecture:

$$h_{v_i}^{l+1} = \mathrm{ReLU}\left(\sum_{j \in \mathcal{N}_i} h_{v_j}^{l} \frac{W^l}{\sqrt{|\mathcal{N}_i||\mathcal{N}_j|}} \right), \quad v_i \in V.$$

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This can be expressed as an MPNN with:

- $M_\theta^l(h_{v_i}^l, h_{v_j}^l, e_{ij}) = \dfrac{1}{\sqrt{|\mathcal{N}_i||\mathcal{N}_j|}} h_{v_j}^l$
- $U_\theta^l(h_{v_i}^l, \square_{j\sim i} M_{j\to i}^l) = \mathrm{ReLU}\left(\left(\dfrac{1}{|\mathcal{N}_i|} h_{v_i}^l + \sum_{j\sim i} M_\theta^l(h_{v_i}^l, h_{v_j}^l, e_{ij}) \right) W^l \right)$

Example 2: MPNN in Gilmer et al. [5]

The original work of Gilmer et al. [5] used the following MPNN model

- $M_\theta^l(h_{v_i}^l, h_{v_j}^l, e_{ij}) = \mathrm{MLP}(e_{ij})\, h_{v_j}^l$
- $U_\theta^l(h_{v_i}^l, \square_{j\sim i} M_{j\to i}^l) = \mathrm{GRU}\left(h_{v_i}^l, \sum_{j\sim i} M_{j\to i}^l\right)$

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Model performs extremely well with 11 out of 13 properties reaching "chemical accuracy".

Example 3: Transformers

MPNNs also encompass the transformer [9] model:

- $M^l_\theta(h^l_{v_i}, h^l_{v_j}, e_{ij}) = \mathrm{MultiheadAttention}(h^l_{v_i}, h^l_{v_j})$

$$= \left\{ w^k_{ij}(h^l_{v_i}, h^l_{v_j}), V^k_j(h^l_{v_j}) \right\}_{k=1}^{K}$$

- $U^l_\theta(h^l_{v_i}, \square_{j\sim i} M^l_{j\to i}) = \mathrm{LN}\Big(\mathrm{MLP}\Big(\mathrm{LN}\Big(\sum_{j\sim i} w^k_{ij} V^k_j\Big)\Big)\Big)$

where the graph is assumed to be *fully-connected.*

(See blogpost [8] for more details)

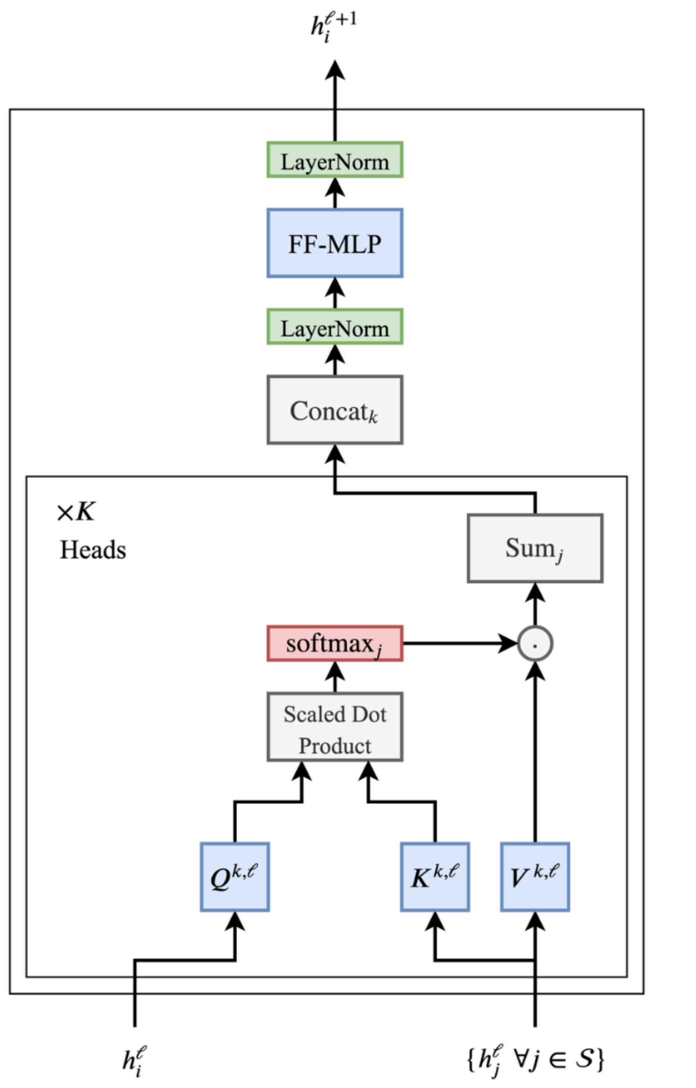

Image from [8]

Comparison of MPNN with LBP

LBP	MPNN
Bayesian. Coupling between neighbours arise from prior knowledge of model. Message passing rule follows from laws of probability.	**Frequentist.** Message and state update rules are learned from data to obtain useful feature representations.
Iterative. States are updated iteratively to obtain better estimates of marginals.	**Deep.** Uses the power of deep learning to extract increasingly complex features with depth.
Interpretable. Prior assumptions are usually quite simple, making predictions interpretable.	**Flexible.** Processes high-dimensional node and edge features easily to model complex relations between inputs and outputs.

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Many recent works aim to combine benefits of both approaches ([10] - [14])!

References

[1] Bruna, Joan, Wojciech Zaremba, Arthur Szlam, and Yann LeCun. "Spectral networks and deep locally connected networks on graphs." *ICLR*, 2014.

[2] Defferrard, Michaël, Xavier Bresson, and Pierre Vandergheynst. "Convolutional neural networks on graphs with fast localized spectral filtering." *NeurIPS, 2016*.

[3] Duvenaud, David K., Dougal Maclaurin, Jorge Iparraguirre, Rafael Bombarell, Timothy Hirzel, Alán Aspuru-Guzik, and Ryan P. Adams. "Convolutional networks on graphs for learning molecular fingerprints." *NeurIPS,* 2015.

[4] Welling, Max, and Thomas N. Kipf. "Semi-supervised classification with graph convolutional networks." *ICLR,* 2017.

[5] Gilmer, Justin, Samuel S. Schoenholz, Patrick F. Riley, Oriol Vinyals, and George E. Dahl. "Neural message passing for quantum chemistry." *ICML*, 2017.

References

[6] PyTorch Geometric. “Creating Message Passing Networks”: https://pytorch-geometric.readthedocs.io/en/latest/notes/create_gnn.html

[7] Sanchez-Lengeling, Benjamin, Emily Reif, Adam Pearce and Alexander B. Wiltschko, "A Gentle Introduction to Graph Neural Networks”. *Distill*, 2021.

[8] Joshi, Chaitanya K. "Transformers are Graph Neural Networks", *The Gradient*, 2020.

[9] Vaswani, Ashish, Noam Shazeer, Niki Parmar, Jakob Uszkoreit, Llion Jones, Aidan N. Gomez, Łukasz Kaiser, and Illia Polosukhin. "Attention is all you need." *NeurIPS,* 2017.

[10] Ying, Zhitao, Dylan Bourgeois, Jiaxuan You, Marinka Zitnik, and Jure Leskovec. "GNNexplainer: Generating explanations for graph neural networks." *NeurIPS,* 2019.

References

[11] Yoon, KiJung, Renjie Liao, Yuwen Xiong, Lisa Zhang, Ethan Fetaya, Raquel Urtasun, Richard Zemel, and Xaq Pitkow. "Inference in probabilistic graphical models by graph neural networks." *53rd Asilomar Conference on Signals, Systems, and Computers,* 2019.

[12] Kuck, Jonathan, Shuvam Chakraborty, Hao Tang, Rachel Luo, Jiaming Song, Ashish Sabharwal, and Stefano Ermon. "Belief propagation neural networks." *NeurIPS,* 2020.

[13] Wang, Binghui, Jinyuan Jia, and Neil Zhenqiang Gong. "Semi-Supervised Node Classification on Graphs: Markov Random Fields vs. Graph Neural Networks." *AAAI*, 2021.

[14] Satorras, Victor Garcia, and Max Welling. "Neural enhanced belief propagation on factor graphs." *AISTATS*, 2021.

[15] Hua, Chenqing, Sitao Luan, Qian Zhang and Jie Fu. "Graph Neural Networks Intersect Probabilistic Graphical Models: A Survey." *arXiv preprint arXiv:2206.06089,* 2022.