Stat 375: Inference in Graphical Models
Lectures 5-6

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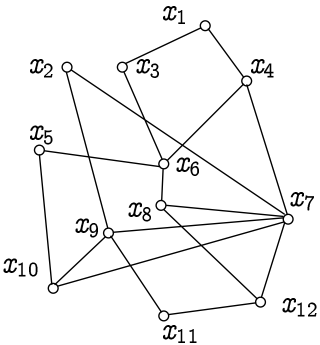
Undirected Pairwise Graphical Model

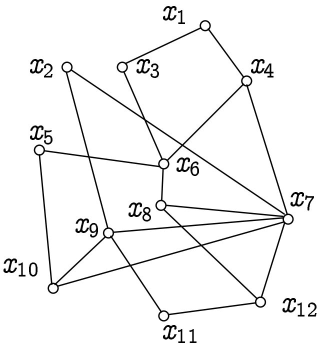


$G = (V, E)$, $V = [n]$, $x = (x_1, \dots, x_n)$, $x_i \in \mathcal{X}$, $|\mathcal{X}| < \infty$

$$\mu(x) = \frac{1}{Z} \prod_{(ij) \in E} \psi_{ij}(x_i, x_j) \, .$$

Computing marginals of μ

Undirected Pairwise Graphical Model



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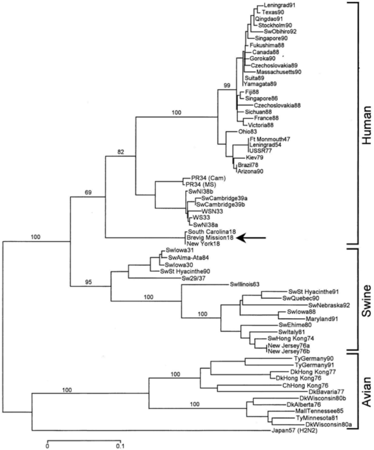
Computing marginals of μ

Outline

A motivating example

Influenza



[A.H. Reid, T.G. Fanning, J.V. Hultin, and J.K. Taubenberger, Proc. Natl. Acad. Sci. 96 (1999) 1651-1656]

Challenges in phylogeny

Phylogeny reconstruction: Given DNA sequences at vertices (only at leaves), infer the underlying tree $T = (V, E)$.

Phylogeny evaluation: Given a tree $T = (V, E)$ evaluate the probability of observed DNA sequences at vertices (only at leaves).

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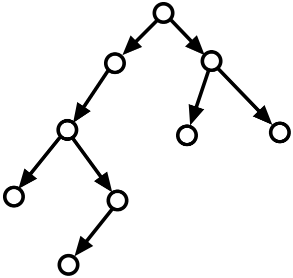
A Markov model

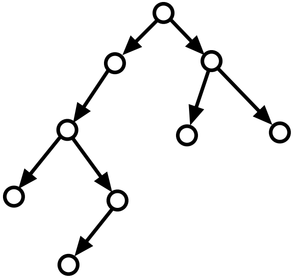


$T = (V, D)$ directed graph, observed $x = (x_i)_{i \in V} \in \mathcal{X}^V$

$$\mu_T(x) = q_o(x_o) \prod_{(i,j) \in D} q_{i,j}(x_i, x_j)\,,$$

$$q_{i,j}(x_i, x_j) = \text{Probability that the descendent is } x_j \text{ if ancestor is } x_i.$$

A Markov model



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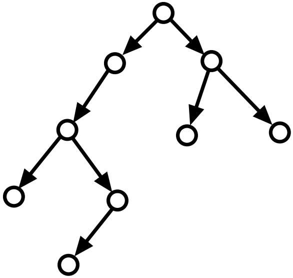

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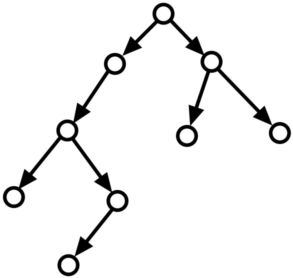
Simplified model: $\mathcal{X} = \{+1, -1\}$



$$\begin{aligned} q_o(x_o) &= \frac{1}{2}, \\ q(x_i, x_j) &= \begin{cases} 1-q & \text{if } x_j = x_i, \\ q & \text{if } x_i \neq x_j. \end{cases} \end{aligned}$$

$$q(x_i, x_j) \propto e^{\theta x_i x_j}.$$

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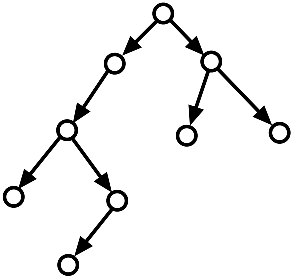

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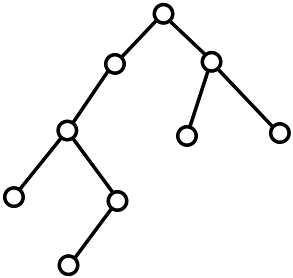

$T = (V, E)$ directed graph, observed $x = (x_i)_{i \in V} \in \mathcal{X}^V$

$$\mu_T(x) = \frac{1}{Z_\theta(T)} \prod_{(i,j) \in E} e^{\theta x_i x_j} \, .$$

Problem: For given T, compute $\mu_T(x)$. Difficult part: $Z_\theta(T)$.

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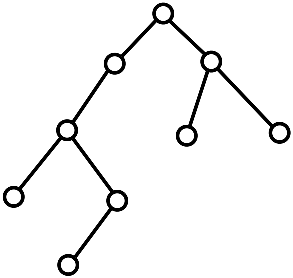

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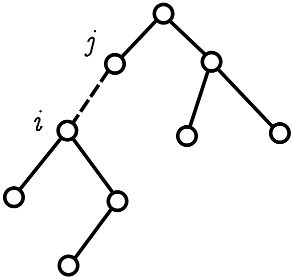
Recursion on trees

Subtree



$$
\begin{aligned}
T_{i\to j} = (V_{i\to j}, E_{i\to j}) \quad &= \quad \text{Subtree rooted at } i \text{ and excluding } j, \\
\mu_{i\to j}(x_{V_{i\to j}}) \quad &= \quad \frac{1}{Z(T_{i\to j})} \prod_{(u,v)\in E_{i\to j}} e^{\theta x_u x_v}, \\
\nu_{i\to j}(x_i) \quad &= \quad \sum_{x_{V_{i\to j}}\setminus i} \mu_{i\to j}(x_{V_{i\to j}})
\end{aligned}
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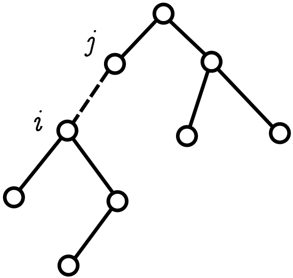
Subtree



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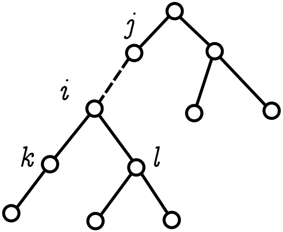
Merging trees



$$\mu_{i\to j}(x_{V_{i\to j}}) = \frac{1}{Z(T_{i\to j})}\, e^{\theta x_i x_k}\; e^{\theta x_i x_l} \Big\{ \prod_{(u,v)\in E_{k\to i}} e^{\theta x_i x_j} \Big\} \Big\{ \prod_{(u,v)\in E_{l\to i}} e^{\theta x_u x_v} \Big\}$$

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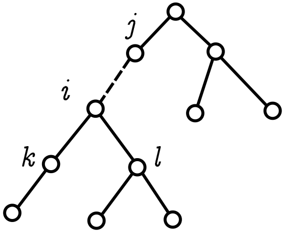

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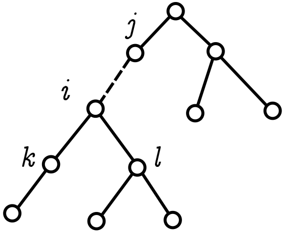

$$\mu_{i\to j}(x_{V_{i\to j}}) \cong e^{\theta x_i x_k}\, e^{\theta x_i x_l} \mu_{k\to i}(x_{V_{k\to i}}) \mu_{l\to i}(x_{V_{l\to i}})$$

$$\sum_{x_{v_{i\to j}\setminus i}} \mu_{i\to j}(x_{V_{i\to j}}) \cong \sum_{x_{V_{k\to i}}} e^{\theta x_i x_k} \mu_{k\to i}(x_{V_{k\to i}}) \sum_{x_{V_{l\to i}}} e^{\theta x_i x_l} \mu_{l\to i}(x_{V_{l\to i}}),$$

$$\nu_{i\to j}(x_i) \cong \Big\{ \sum_{x_k} e^{\theta x_i x_k} \nu_{k\to i}(x_k) \Big\} \Big\{ \sum_{x_l} e^{\theta x_i x_l} \nu_{l\to i}(x_l) \Big\}$$

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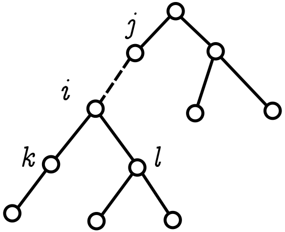

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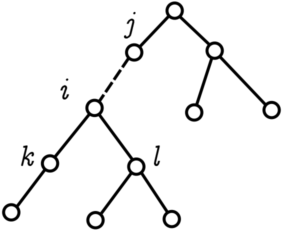

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\sum_{x_{v_{i\to j}\setminus i}} \mu_{i\to j}(x_{V_{i\to j}}) &\cong \sum_{x_{V_{k\to i}}} e^{\theta x_i x_k} \mu_{k\to i}(x_{V_{k\to i}}) \sum_{x_{V_{l\to i}}} e^{\theta x_i x_l} \mu_{l\to i}(x_{V_{l\to i}}), \\
\nu_{i\to j}(x_i) &\cong \Big\{ \sum_{x_k} e^{\theta x_i x_k} \nu_{k\to i}(x_k) \Big\} \Big\{ \sum_{x_l} e^{\theta x_i x_l} \nu_{l\to i}(x_l) \Big\}
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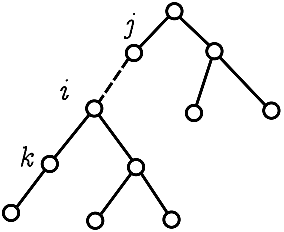

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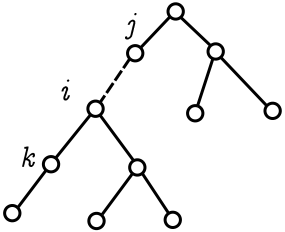

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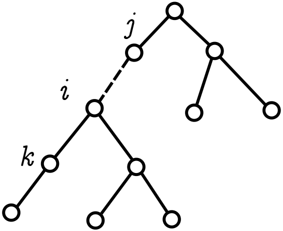
What about a general model ?



$$\nu_{i\to j}(x_i) \cong \prod_{k\in\partial i\setminus j}\Big\{\sum_{x_k\in\mathcal{X}}\psi_{ik}(x_i,x_k)\nu_{k\to i}(x_k)\Big\}$$

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Computes the marginals in $|\mathcal{X}|^2 n$ operations.

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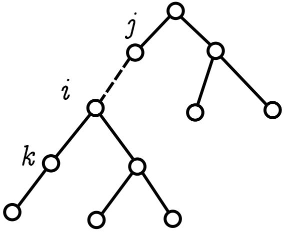

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Computes the marginals in $|\mathcal{X}|^2 n$ operations.

Belief propagation

Notation

$$\vec{E} \equiv \text{Directed edges},$$

$$\nu \equiv \{\nu_{i\to j}(\,\cdot\,)\}_{(i,j)\in\vec{E}}\} \in \mathsf{M}(\mathcal{X})^{\vec{E}}, \text{ messages}$$

$$\mathsf{F} \quad \mathsf{M}(\mathcal{X})^{\vec{E}} \to \mathsf{M}(\mathcal{X})^{\vec{E}}$$

$$\nu \mapsto \mathsf{F}(\nu), \quad \mathsf{F}(\nu)_{i\to j}(x_i) \cong \prod_{k\in\partial i\setminus j} \Big\{ \sum_{x_k\in\mathcal{X}} \psi_{ik}(x_i, x_k)\nu_{k\to i}(x_k) \Big\}$$

$$\mathsf{F}^{\mathsf{v}} \quad \mathsf{M}(\mathcal{X})^{\vec{E}} \to \mathsf{M}(\mathcal{X})^{V}$$

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Belief propagation (sequential version)

Belief propagation(Tree $T = (V, E)$, $\psi = \{\psi_{ij}\}$)

1: Initialize $\nu_{i\to k}(x_i) = 1/|\mathcal{X}|$ for all i leaves;
2: Recursively over $(i,j) \in \vec{E}$ compute (from leaves):
3: $\quad \nu_{i\to j} = \mathsf{F}(\nu)_{i\to j}$;
4: For each $i \in V$ output the estimated marginal;
5: $\quad \nu_i = \mathsf{F}^{\mathsf{v}}(\nu)_i$;

Belief propagation (parallel version)

Messages: $\nu_{i\to j}^{(t)}(\,\cdot\,)$, $t \in \{0, 1, 2, \dots\}$

BELIEF PROPAGATION(Tree $T = (V, E)$, $\psi = \{\psi_{ij}\}$)

1: Initialize $\nu_{i\to k}^{(0)}(x_i) = 1/|\mathcal{X}|$ for all i leaves;
2: For $t \in \{0, 1, 2, \dots, t_{\max} \equiv \text{diam}(T)\}$
3: $\quad \nu^{(t+1)} = \mathsf{F}(\nu^{(t)})$;
4: For each $i \in V$ output the estimated marginal;
5: $\quad \nu_i = \mathsf{F}^{\mathsf{v}}(\nu)_i$;

Computes all the marginals in $|\mathcal{X}|^2 n \cdot \text{diam}(T)$ operations.

Belief propagation (parallel version)

Messages: $\nu_{i\to j}^{(t)}(\,\cdot\,)$, $t \in \{0, 1, 2, \dots\}$

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Computes all the marginals in $\lvert\mathcal{X}\rvert^2 n \cdot \mathrm{diam}(T)$ operations.

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Computes all the marginals in $|\mathcal{X}|^2 n \cdot \text{diam}(T)$ operations.

Belief propagation (loopy version)

Messages: $\nu^{(t)}_{i\to j}(\,\cdot\,)$, $t \in \{0,1,2,\dots\}$

BELIEF PROPAGATION(Graph $T=(V,E)$, $\psi = \{\psi_{ij}\}$)

1: Initialize $\nu^{(0)}_{i\to k}(x_i) = 1/|\mathcal{X}|$ for all i leaves;
2: For $t \in \{0,1,2,\dots,t_{\max}\}$
3: $\quad \nu^{(t+1)} = \mathsf{F}(\nu^{(t)})$;
4: For each $i \in V$ output the estimated marginal;
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Folklore about Loopy BP

Generally it does not converge, and if it does, the output is incorrect.
This does not stop people from using it!

- Works better when $\psi_{i,j}(x_i, x_j) = \psi_{ij,1}(x_i)\psi_{ij,2}(x_j) + \text{small}(x_i, x_j)$.
- Works better when G has few short loops.
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A couple of exercises

Exercise #1: Partition function on trees

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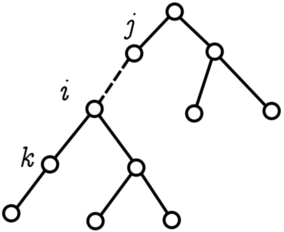

$$Z(T_{i\to j}) = \prod_{k\in\partial i\setminus j} Z(T_{k\to i}) \sum_{x_i\in\mathcal{X}} \prod_{k\in\partial i\setminus j} \Big\{ \sum_{x_k\in\mathcal{X}} \psi_{ik}(x_i,x_k)\nu_{k\to i}(x_k) \Big\}$$

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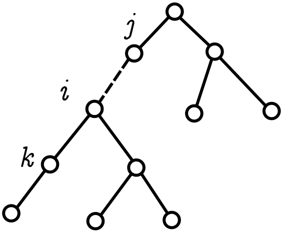

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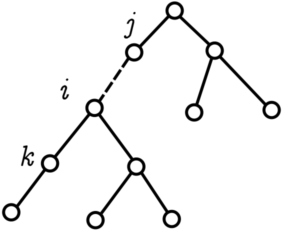

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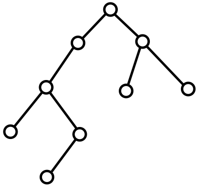

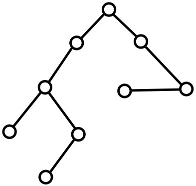

$$\mu(x) = \frac{1}{Z(T)} \prod_{(i,j)\in E} e^{\theta x_i x_j} \prod_{i \in V} e^{\gamma x_i}$$

Which one has highest likelihood?

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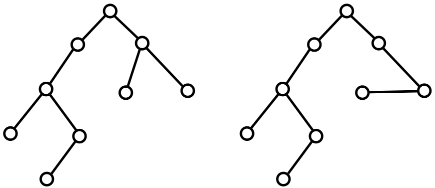

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Exercise #2: Sampling from on the tree

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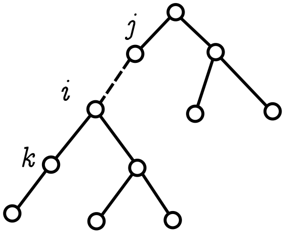

SAMPLING(Tree $T = (V, E)$, $\psi = \{\psi_{ij}\}_{(ij)\in E}$)

1: Choose a root $o \in V$;
2: Sample $X_o \sim \mu_o(\,\cdot\,)$;
2: Recursively over $i \in V$ (from root to leaves):
3: Compute $\mu_{i|\pi(i)}(x_i|x_{\pi(i)})$;
4: Sample $X_i \sim \mu_{i|\pi(i)}(\,\cdot\,|x_{\pi(i)})$;

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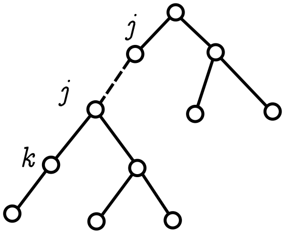

$$\mu_T(x_{V_{i\to j}}|x_j) \;\cong\; \psi_{ij}(x_i x_j)\,\mu_{T_{i\to j}}(x_{V_{i\to j}})\,,$$

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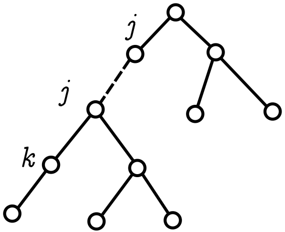

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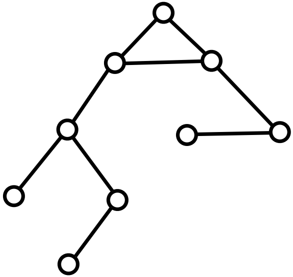
Tree decomposition

Idea



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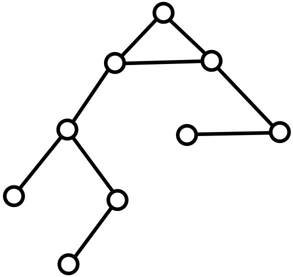

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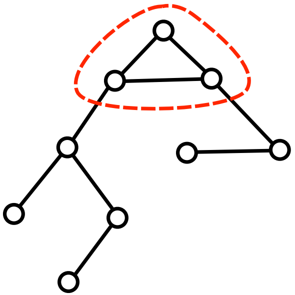

Create an equivalent tree graph.

Price: enlarging the alphabet to $\mathcal{X}^3$.

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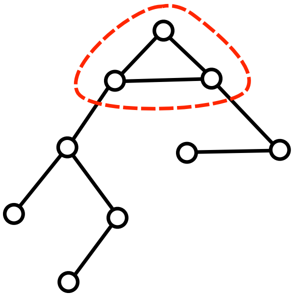

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How you do this in general?

- Tree decomposition.

- Equivalent graphical model.

- Alphabet enlargement $\mathcal{X} \to \mathcal{X}^k$.

- Treewidth$(G) \equiv$ Minimum such k.

Problem: In general Treewidth$(G) = \Theta(n)$.

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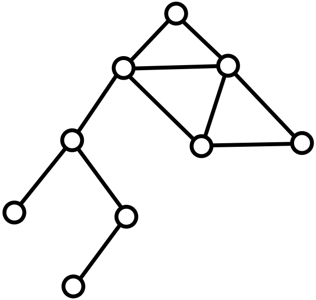
Tree decomposition of $G = (V, E)$

A tree $T = (V_T, E_T)$ and a mapping $V : V_T \to$SUBSETS(V) s.t.:

- For each $i \in V$ there exists at least one $u \in V_T$ with $i \in V(u)$.
- For each $(i, j) \in E$ there exists at least one $u \in V_T$ with $i, j \in V(u)$.
- If $i \in V(u_1)$ and $i \in V(u_2)$, then $i \in V(w)$ for any w on the path between u_1 and u_2 in T.

For instance



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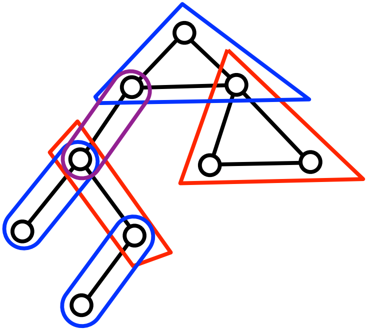

You see the tree, right?

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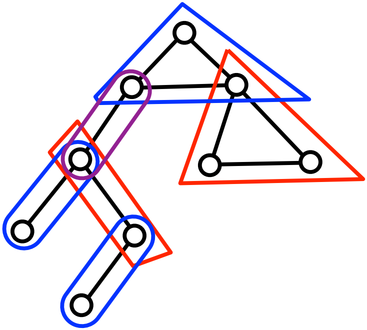

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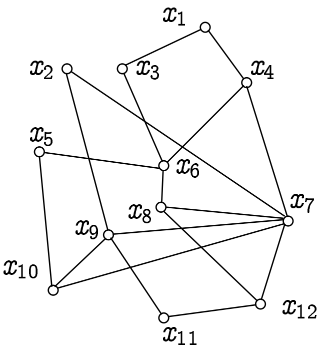
General methods to prove convergence

- Monotonicity.

- Contraction.

The max-product algorithm

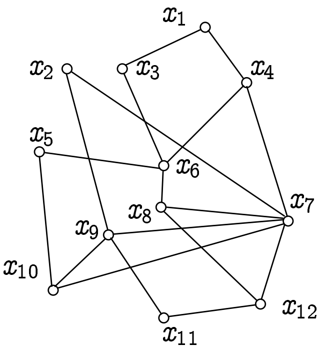
Optimization – Mode computation



$G = (V, E)$, $V = [n]$, $x = (x_1, \dots, x_n)$, $x_i \in \mathcal{X}$, $|\mathcal{X}| < \infty$
Compute

$$\arg\max_{x \in \mathcal{X}^V} \mu(x) = \arg\max_{x \in \mathcal{X}^V} \prod_{(ij) \in E} \psi_{ij}(x_i, x_j) \, .$$

Equivalently



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Everything goes through: Max-Marginals

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Normalization $\max_{x_v} \mu_v(x_v) = 1$

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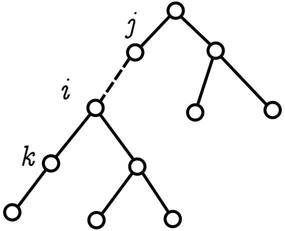

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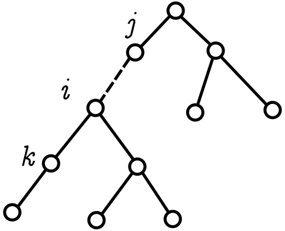

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