4. Sum-product algorithm

- Elimination algorithm
- Sum-product algorithm on a line
- Sum-product algorithm on a tree

Inference tasks on graphical models

consider an undirected graphical model (a.k.a. Markov random field)

$$\mu(x) \;=\; \frac{1}{Z}\prod_{c\in\mathcal{C}}\psi_c(x_c)$$

where $\mathcal{C}$ is the set of all maximal cliques in G

we want to

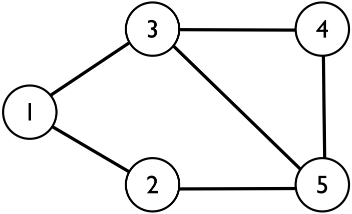
- calculate marginals: $\mu(x_A) = \sum_{x_{V\setminus A}} \mu(x)$
- calculating conditional distributions

$$\mu(x_A|x_B) \;=\; \frac{\mu(x_A, x_B)}{\mu(x_B)}$$

- calculation maximum a posteriori estimates: $\arg\max_{\hat{x}} \mu(\hat{x})$
- calculating the partition function Z
- sample from this distribution

Elimination algorithm for calculating marginals

Elimination algorithm is exact but can require $O(|\mathcal{X}|^{|V|})$ operations



$$\mu(x) \quad \propto \quad \psi_{12}(x_1, x_2)\psi_{13}(x_1, x_3)\psi_{25}(x_2, x_5)\psi_{345}(x_3, x_4, x_5)$$

- we want to compute $\mu(x_1)$
- brute force marginalization:

$$\mu(x_1) \propto \sum_{x_2, x_3, x_4, x_5 \in \mathcal{X}} \psi_{12}(x_1, x_2)\psi_{13}(x_1, x_3)\psi_{25}(x_2, x_5)\psi_{345}(x_3, x_4, x_5)$$

- requires $O(|\mathcal{C}| \cdot |\mathcal{X}|^5)$ operations, where big-O denotes that it is upper bounded by $c\,|\mathcal{C}|\,|\mathcal{X}|^5$ for some constant c and $|\mathcal{C}|$ is # of cliques

- consider an elimination ordering $(5, 4, 3, 2)$

$$
\begin{aligned}
\mu(x_1) \quad \propto \quad & \sum_{x_2,x_3,x_4,x_5 \in \mathcal{X}} \psi_{12}(x_1,x_2)\psi_{13}(x_1,x_3)\psi_{25}(x_2,x_5)\psi_{345}(x_3,x_4,x_5) \\
= \quad & \sum_{x_2,x_3,x_4 \in \mathcal{X}} \psi_{12}(x_1,x_2)\psi_{13}(x_1,x_3) \underbrace{\sum_{x_5 \in \mathcal{X}} \psi_{25}(x_2,x_5)\psi_{345}(x_3,x_4,x_5)}_{\equiv m_5(x_2,x_3,x_4)} \\
= \quad & \sum_{x_2,x_3,x_4 \in \mathcal{X}} \psi_{12}(x_1,x_2)\psi_{13}(x_1,x_3) m_5(x_2,x_3,x_4) \\
= \quad & \sum_{x_2,x_3 \in \mathcal{X}} \psi_{12}(x_1,x_2)\psi_{13}(x_1,x_3) \underbrace{\sum_{x_4 \in \mathcal{X}} m_5(x_2,x_3,x_4)}_{\equiv m_4(x_2,x_3)} \\
= \quad & \sum_{x_2,x_3 \in \mathcal{X}} \psi_{12}(x_1,x_2)\psi_{13}(x_1,x_3) m_4(x_2,x_3) \\
= \quad & \sum_{x_2 \in \mathcal{X}} \psi_{12}(x_1,x_2) \underbrace{\sum_{x_3 \in \mathcal{X}} \psi_{13}(x_1,x_3) m_4(x_2,x_3)}_{\equiv m_3(x_1,x_2)}
\end{aligned}
$$

$$
\begin{aligned}
\mu(x_1) &\propto \sum_{x_2 \in \mathcal{X}} \psi_{12}(x_1, x_2) \underbrace{\sum_{x_3 \in \mathcal{X}} \psi_{13}(x_1, x_3) m_4(x_2, x_3)}_{\equiv m_3(x_1, x_2)} \\
&= \sum_{x_2 \in \mathcal{X}} \psi_{12}(x_1, x_2) m_3(x_1, x_2) \\
&\equiv m_2(x_1)
\end{aligned}
$$

- normalize $m_2(\cdot)$ to get $\mu(x_1)$

$$
\mu(x_1) = \frac{m_2(x_1)}{\sum_{\hat{x}_1} m_2(\hat{x}_1)}
$$

- computational complexity depends on the elimination ordering
- how do we know which ordering is better?

Computational complexity of elimination algorithm

$$\mu(x_1) \propto \sum_{x_2,x_3,x_4,x_5\in\mathcal{X}} \psi_{12}(x_1,x_2)\psi_{13}(x_1,x_3)\psi_{25}(x_2,x_5)\psi_{345}(x_3,x_4,x_5)$$

$$= \sum_{x_2,x_3,x_4\in\mathcal{X}} \psi_{12}(x_1,x_2)\psi_{13}(x_1,x_3) \underbrace{\sum_{x_5\in\mathcal{X}} \psi_{25}(x_2,x_5)\psi_{345}(x_3,x_4,x_5)}_{\equiv m_5(S_5),\, S_5=\{x_2,x_3,x_4\},\, \Psi_5=\{\psi_{25},\psi_{345}\}}$$

$$= \sum_{x_2,x_3\in\mathcal{X}} \psi_{12}(x_1,x_2)\psi_{13}(x_1,x_3) \underbrace{\sum_{x_4\in\mathcal{X}} m_5(x_2,x_3,x_4)}_{\equiv m_4(S_4),\, S_4=\{x_2,x_3\},\Psi_4=\{m_5\}}$$

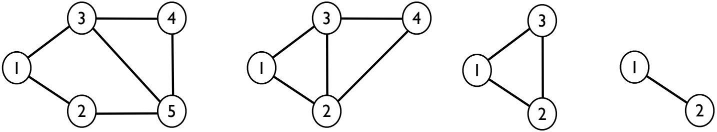
$$= \sum_{x_2\in\mathcal{X}} \psi_{12}(x_1,x_2) \underbrace{\sum_{x_3\in\mathcal{X}} \psi_{13}(x_1,x_3)m_4(x_2,x_3)}_{\equiv m_3(S_3),\, S_3=\{x_1,x_2\},\, \Psi_3=\{\psi_{13},m_4\}}$$

$$= \underbrace{\sum_{x_2\in\mathcal{X}} \psi_{12}(x_1,x_2)m_3(x_1,x_2)}_{\equiv m_2(S_2),\, S_2=\{x_1\},\, \Psi_2=\{\psi_{12},m_3\}} = m_2(x_1)$$

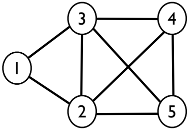
Total complexity: $\sum_i O(|\Psi_i|\cdot|\mathcal{X}|^{1+|S_i|}) = O(|V|\cdot\max_i|\Psi_i|\cdot|\mathcal{X}|^{1+max_i|S_i|})$

Induced graph

elimination algorithm as transformation of graphs



- **induced graph** $\mathcal{G}(G, I)$ for a graph G and an elimination ordering I
  - is the union of (the edges of) all the transformed graphs
  - or equivalently, start from G and for each $i \in I$ connect all pairs in S_i



- **theorem:** every maximal clique in $\mathcal{G}(G, I)$ corresponds to a domain of a message $S_i \cup \{i\}$ for some i
- size of the largest clique in $\mathcal{G}(G, I)$ is $1 + \max_i |S_i|$
- different orderings I's give different cliques, resulting in varying complexity

- **theorem:** finding optimal elimination ordering is NP-hard
- any suggestions?
- greedy heuristic gives $I = (4, 5, 3, 2, 1)$

- for Bayesian networks
  - the same algorithm works with conditional probabilities instead of compatibility functions
  - complexity analysis can be done on moralized undirected graph
  - intermediate messages do not correspond to a conditional distribution

Elimination algorithm

- **input**: $\{\psi_c\}_{c \in \mathcal{C}}$, alphabet $\mathcal{X}$, subset $A \subseteq V$, elimination ordering I
- **output**: marginal $\mu(x_A)$

1. initialize active set Ψ to be the set of input compatibility functions
2. **for** node i in I that is not in A **do**

   let S_i be the set of nodes, not including i, that share a compatibility function with i

   let Ψ_i be the set of compatibility functions in Ψ involving x_i

   compute $m_i(x_{S_i}) = \sum_{x_i} \prod_{\psi \in \Psi_i} \psi(x_i, x_{S_i})$

   remove elements of Ψ_i from Ψ

   add m_i to Ψ

   end
3. normalize $\mu(x_A) = \prod_{\psi \in \Psi} \psi(x_A) \,/\, \sum_{x_A} \prod_{\psi \in \Psi} \psi(x_A)$

Role of the messages $m_i(x_{S_i})$

- messages capture local information about what one side of the edge needs to know about the other side of the edge
- this intuition is exactly correct when the graph is a tree
- we provide a heuristic (called sum-product algorithm or belief propagation) that is accurate when the graph is a tree
- but also provides surprisingly good approximate solutions, even when the underlying graph has loops

$$m_i(x_i) = \sum_{x_a \in \mathcal{X}} \left\{ \psi_{i,a}(x_i, x_a) \sum_{x_A} \psi_A(x_a, x_A) \right\}$$

Role of the messages

$$
\begin{aligned}
m_i(x_i) &= \sum_{x_a, x_b \in \mathcal{X}, x_A, x_B} \psi_{i,a}(x_i, x_a)\psi_A(x_a, x_A)\psi_{i,b}(x_i, x_b)\psi_B(x_b, x_B) \\
&= \Big\{ \sum_{x_a \in \mathcal{X}} \{\psi_{i,a}(x_i, x_a) \sum_{x_A} \psi_A(x_a, x_A)\}\Big\} \Big\{ \sum_{x_b \in \mathcal{X}} \{\psi_{i,b}(x_i, x_b) \sum_{x_B} \psi_B(x_b, x_B)\}\Big\}
\end{aligned}
$$

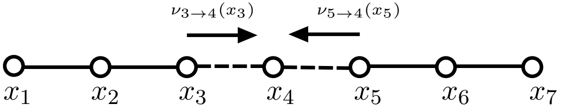
Belief Propagation for approximate inference

- given a pairwise MRF: $\mu(x) = \frac{1}{Z} \prod_{(i,j)\in E} \psi_{i,j}(x_i, x_j)$
- compute marginal: $\mu(x_i)$ for all $i \in V$
- message update: set of $2|E|$ messages on each (directed) edge $\{\nu_{i\to j}(x_i)\}_{(i,j)\in E}$, where $\nu_{i\to j} : \mathcal{X} \to \mathbb{R}^+$ encoding our belief (or approximate $\mathbb{P}(x_i)$)
  - $\nu_{i\to j}^{(t+1)}(x_i) = \prod_{k\in\partial i\setminus j} \Big\{ \sum_{x_k} \nu_{k\to i}^{(t)}(x_k)\psi_{i,k}(x_i, x_k) \Big\}$
  - $O(d_i|\mathcal{X}|^2)$ computations
- decision:

$$\nu_i^{(t)}(x_i) \quad = \quad \prod_{k\in\partial i} \Big\{ \sum_{x_k} \nu_{k\to i}^{(t)}(x_k)\psi_{i,k}(x_i, x_k) \Big\}$$

  - $\widehat{\mu}(x_i) = \frac{\nu_i(x_i)}{\sum_{x'} \nu_i(x')}$

Sum-product algorithm on a line



Remove node i and recursively compute marginals on sub-graphs

$$\mu(x) = \frac{1}{Z}\prod_{i=1}^{n-1}\psi_{i,i+1}(x_i, x_{i+1})$$

$$\mu(x_i) = \sum_{x_{[n]\setminus\{i\}}} \mu(x)$$

$$\propto \sum_{x_{[n]\setminus\{i\}}} \underbrace{\psi(x_1,x_2)\cdots\psi(x_{i-2},x_{i-1})}_{\mu_{(i-1)\to i}\text{:joint dist. on a sub-graph}} \psi(x_{i-1},x_i)\psi(x_i,x_{i+1}) \underbrace{\psi(x_{i+1},x_{i+2})\cdots\psi(x_{n-1},x_n)}_{\mu_{(i+1)\to i}}$$

$$\propto \sum_{x_{i-1},x_{i+1}} \underbrace{\nu_{(i-1)\to i}(x_{i-1})}_{\text{marginal dist. on a subrgaph}} \psi(x_{i-1},x_i)\psi(x_i,x_{i+1})\nu_{(i+1)\to i}(x_{i+1})$$

$$\nu_{(i-1)\to i}(x_{i-1}) \equiv \sum_{x_1,\ldots,x_{i-2}} \mu_{(i-1)\to i}(x_1,\ldots,x_{i-1})$$

$$\nu_{(i+1)\to i}(x_{i+1}) \equiv \sum_{x_{i+2},\ldots,x_n} \mu_{(i+1)\to i}(x_{i+1},\ldots,x_n)$$

$$\nu_i(x_i) \equiv \sum_{x_{i-1},x_{i+1}} \nu_{(i-1)\to i}(x_{i-1})\psi(x_{i-1},x_i)\psi(x_i,x_{i+1})\nu_{(i+1)\to i}(x_{i+1})$$

$$\mu(x_i) = \frac{\nu_i(x_i)}{\sum_{x_i}\nu_i(x_i)}$$

definitions: of joint distribution and marginal on sub-graphs

$$\begin{aligned}
\mu_{(i-1)\to i}(x_1,\ldots,x_{i-1}) &\equiv \frac{1}{Z_{(i-1)\to i}} \prod_{k\in[i-2]} \psi(x_k,x_{k+1}) \\
\nu_{(i-1)\to i}(x_{i-1}) &\equiv \sum_{x_1,\ldots,x_{i-2}} \mu_{(i-1)\to i}(x_1,\ldots,x_{i-1}) \\
\mu_{(i+1)\to i}(x_{i+1},\ldots,x_n) &\equiv \frac{1}{Z_{(i+1)\to i}} \prod_{k\in\{i+2,\ldots,n\}} \psi(x_{k-1},x_k) \\
\nu_{(i+1)\to i}(x_{i+1}) &\equiv \sum_{x_{i+2},\ldots,x_n} \mu_{(i+1)\to i}(x_{i+1},\ldots,x_n)
\end{aligned}$$

how can we compute the messages ν, recursively?

$$\begin{aligned}
\mu_{i\to i+1}(x_1,\ldots,x_i) &\propto \mu_{i-1\to i}(x_1,\ldots,x_{i-1})\psi(x_{i-1},x_1) \\
\nu_{i\to i+1}(x_i) &= \sum_{x_1,\ldots,x_{i-1}} \mu_{i\to i+1}(x_1,\ldots,x_i) \\
&\propto \sum_{x_1,\ldots,x_{i-1}} \mu_{i-1\to i}(x_1,\ldots,x_{i-1})\psi(x_{i-1},x_i) \\
&= \sum_{x_{i-1}} \nu_{i-1\to i}(x_{i-1})\psi(x_{i-1},x_i) \\
\nu_{1\to 2}(x_1) &= 1/|\mathcal{X}| \\
\nu_{2\to 3}(x_2) &\propto \sum_{x_1} \frac{1}{|\mathcal{X}|}\psi(x_1,x_2)
\end{aligned}$$

how many operations are required?

- $O(n\,|\mathcal{X}|^2)$ operations to compute one marginal $\mu(x_i)$

what if we want all the marginals?

- compute all the messages forward and backward $O(n\,|\mathcal{X}|^2)$
- then compute all the marginals in $O(n\,|\mathcal{X}|^2)$ operations

Computing partition function is as easy as computing marginals

recall

$$\mu_{(i-1)\to i}(x_1,\dots,x_{i-1}) \equiv \frac{1}{Z_{(i-1)\to i}} \prod_{k\in[i-2]} \psi(x_k,x_{k+1})$$

$$\nu_{(i-1)\to i}(x_{i-1}) \equiv \sum_{x_1,\dots,x_{i-2}} \mu_{(i-1)\to i}(x_1,\dots,x_{i-1})$$

computing the partition function from the messages

$$\begin{aligned} Z_{i\to(i+1)} &= \sum_{x_1,\dots,x_i} \prod_{k\in[i-1]} \psi(x_k,x_{k+1}) \\ &= \sum_{x_i,x_{i-1}} Z_{(i-1)\to i}\,\nu_{(i-1)\to i}(x_{i-1})\,\psi(x_{i-1},x_i) \\ Z_1 &= 1 \\ Z_n &= Z \end{aligned}$$

how many operations do we need?

- $O(n\,|\mathcal{X}|^2)$ operations

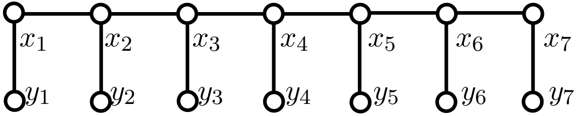
Sum-product algorithm for hidden Markov models

- hidden Markov model

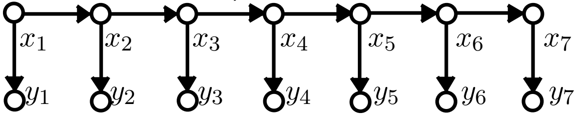
Sequence of r.v.'s $\{(X_1, Y_1); (X_2, Y_2); \dots; (X_n, Y_n)\}$

hidden state $\{X_i\}$ Markov Chain $\mathbb{P}\{x\} = \mathbb{P}\{x_1\} \prod_{i=1}^{n-1} \mathbb{P}\{x_{i+1}|x_i\}$

$\{Y_i\}$ noisy observations $\mathbb{P}\{y|x\} = \prod_{i=i}^{n} \mathbb{P}\{y_i|x_i\}$



(equivalent directed form)

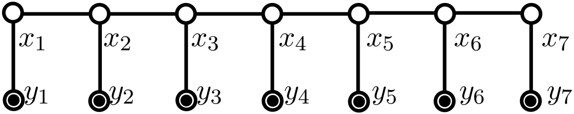


- time homogeneous hidden Markov models

$$\begin{aligned} &\text{Sequence of r.v.'s} && \{(X_1,Y_1);(X_2,Y_2);\dots;(X_n,Y_n)\} \\ &\{X_i\}\ \text{Markov Chain} && \mathbb{P}\{x\} = q_0(x_1)\prod_{i=1}^{n-1} q(x_i,x_{i+1}) \\ &\{Y_i\}\ \text{noisy observations} && \mathbb{P}\{y|x\} = \prod_{i=i}^{n} r(x_i,y_i) \end{aligned}$$

$$\begin{aligned} \mu(x,y) &= \frac{1}{Z}\prod_{i=1}^{n-1}\psi_i(x_i,x_{i+1})\prod_{i=1}^{n}\tilde{\psi}_i(x_i,y_i)\,, \\ & \psi_i(x_i,x_{i+1}) = q(x_i,x_{i+1})\,, \qquad \tilde{\psi}_i(x_i,y_i) = r(x_i,y_i)\,. \end{aligned}$$

- we want to compute marginals of the following graphical model on a line (q_0 uniform)



$$\mu_y(x) = \mathbb{P}\{x|y\} \stackrel{\text{Bayes thm}}{=} \frac{1}{Z(y)} \prod_{i=1}^{n-1} q(x_i, x_{i+1}) \prod_{i=1}^{n} r(x_i, y_i)\,.$$

$$\begin{aligned}
\mu_y(x) &= \frac{1}{Z(y)} \prod_{i=1}^{n-1} q(x_i, x_{i+1}) \prod_{i=1}^{n} r(x_i, y_i) \\
&= \frac{1}{Z(y)} \prod_{i=1}^{n-1} \psi_i(x_i, x_{i+1}) \\
&\quad \psi_i(x_i, x_{i+1}) = q(x_i, x_{i+1})\, r(x_i, y_i) \qquad \text{(for } i < n-1\text{)} \\
&\quad \psi_{n-1}(x_{n-1}, x_n) = q(x_{n-1}, x_n)\, r(x_{n-1}, y_{n-1})\, r(x_n, y_n)\,.
\end{aligned}$$

- apply sum-product algorithm to compute marginals in $O(n|\mathcal{X}|^2)$ time

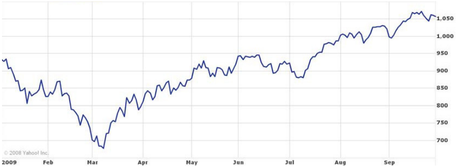
$$\nu_{i\to(i+1)}(x_i) \propto \sum_{x_{i-1}\in\mathcal{X}} q(x_{i-1},x_i)\, r(x_{i-1},y_{i-1})\, \nu_{(i-1)\to i}(x_{i-1})\,,$$

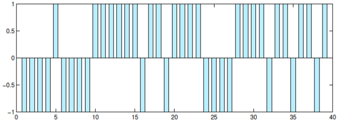
$$\nu_{(i+1)\to i}(x_i) \propto \sum_{x_{i+1}\in\mathcal{X}} q(x_i,x_{i+1})\, r(x_i,y_i)\, \nu_{(i+2)\to(i+1)}(x_{i+1})\,.$$

- known as forward-backward algorithm
  - a special case of the sum-product algorithm
  - BCJR algorithm for convolutional codes ([Bahl, Cocke, Jelinek and Raviv 1974])
  - cannot find the maximum likelihood estimate (cf. Viterbi algorithm)
  - this requires max-product algorithm

- implement sum-product algorithm for HMM [Exercise 4.3]
- consider an extension of inference on HMM [Exercise 4.4]

Exercise 4.3





- S&P 500 index over a period of time
- For each week, measure the price movement relative to the previous week: $+1$ indicates up and -1 indicates down
- a hidden Markov model in which x_t denotes the economic state (good or bad) of week t and y_t denotes the price movement (up or down)
- $x_{t+1} = x_t$ with probability 0.8
- $\mathbb{P}_{Y_t|X_t}(y_t = +1 | x_t = \text{'good'}) = \mathbb{P}_{Y_t|X_t}(y_t = -1 | x_t = \text{'bad'}) = q$

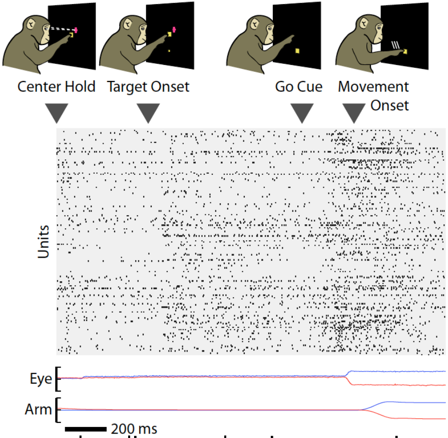
Example: Neuron firing patterns

Hypothesis

Assemblies of neurones activate in a coordinate way in correspondence to specific cognitive functions. Performing of the function corresponds sequence of these activity states.

Approach

Firing process	$\leftrightarrow$	Observed variables
Activity states	$\leftrightarrow$	Hidden variables



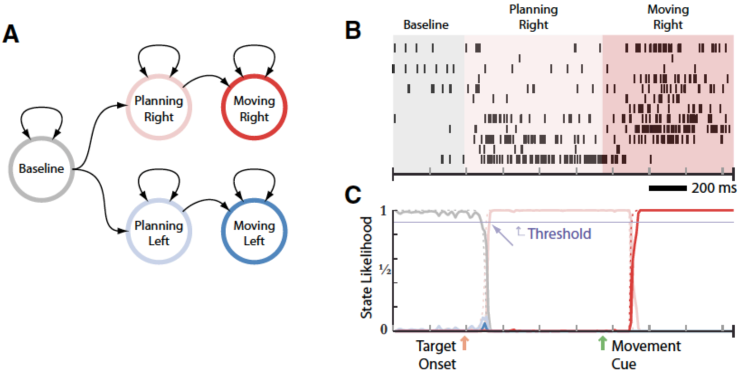
single subject ensemble neural spikes

horizontal eye position
vertical eye position

baseline → planning → moving

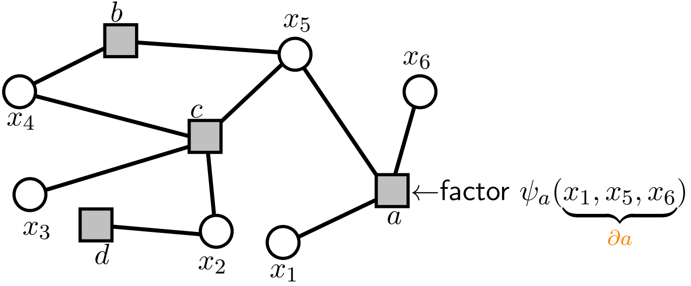
- automatically detect (as opposed to manually specify) baseline, plan, and perimovement epochs of neural activity
- detect target movement in advance
- goal: neural prosthesis to help patients with spinal cord injury or neurodegenerative disease and significantly impaired motor control

[C. Kemere, G. Santhanam, B. M. Yu, A. Afshar, S.I. Ryu, T. H. Meng and K. V. Shenoy, J. Neurophysiol. 100:2441-2452 (2008)]



- discrete time 10ms
- $\mathbb{P}(x_{t+1}|x_t) = A_{ij}$,
  $\mathbb{P}(\#$ spikes for measurement $k = d | x_t = i) \propto e^{-\lambda_{k,i}} \lambda_{k,i}^d$
- likelihood: $\frac{\mathbb{P}(x_t = s)}{\sum_{s'} \mathbb{P}(x_t = s')}$

Belief propagation for factor graphs



$$\mu(x) = \frac{1}{Z} \prod_{a \in F} \psi_a(x_{\partial a})$$

- variable nodes i, j, etc.; factor nodes a, b, etc.
- set of messages $\{\nu_{i\to a}\}_{(i,a)\in E}$ and $\{\tilde{\nu}_{a\to i}\}_{(a,i)\in E}$
- messages from variables to factors

$$\nu_{i\to a}(x_i) = \prod_{b\in\partial i\setminus\{a\}} \tilde{\nu}_{b\to i}(x_i)$$

- messages from factors to variables

$$\tilde{\nu}_{a\to i}(x_i) = \sum_{x_{\partial a\setminus\{i\}}} \psi_a(x_{\partial a}) \prod_{j\in\partial a\setminus\{i\}} \nu_{j\to a}(x_j)$$

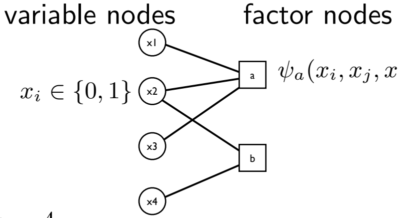
- marginal distribution at variables

$$\nu_i(x_i) = \prod_{b\in\partial i} \tilde{\nu}_{b\to i}(x_i)$$

- this includes belief propagation (=sum-product algorithm) on (general) Markov random fields
- exact on factor trees

Example: decoding LDPC codes

- LDPC code is defined by a factor graph model



$x_i \in \{0,1\}$ $\quad$ $\psi_a(x_i, x_j, x_k) = \mathbb{I}(x_i \oplus x_j \oplus x_k = 0)$

  - block length $n = 4$
  - number of factors $m = 2$
  - allowed messages $= \{0000, 0111, 1010, 1101\}$
- decoding using belief propagation (for BSC with $\epsilon = 0.3$)

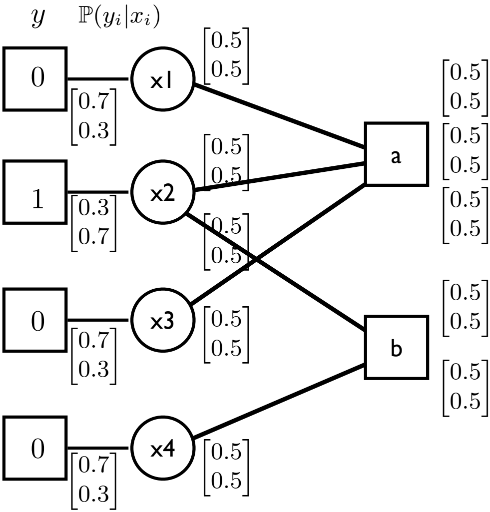
$$\mu_y(x) = \frac{1}{Z} \prod_{i \in V} \mathbb{P}_{Y|X}(y_i|x_i) \prod_{a \in F} \mathbb{I}(\oplus x_{\partial a} = 0)$$

- use (parallel) sum-product algorithm to find $\mu(x_i)$ and let

$$\hat{x}_i = \arg\max \mu(x_i)$$

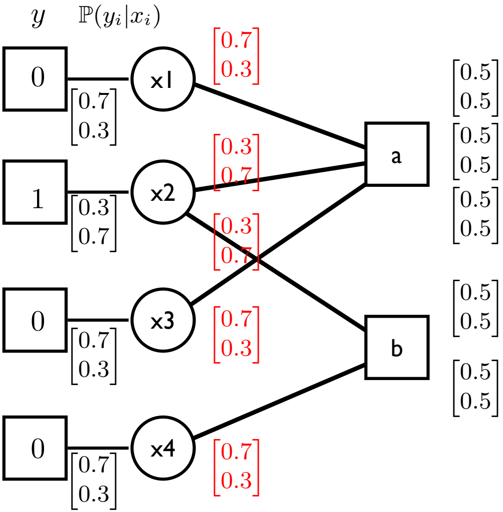
  - minimizes bit error rate

Decoding by sum-product algorithm



$$\nu_{i \to a}^{(t+1)}(x_i) = \mathbb{P}(y_i|x_i) \prod_{b \in \partial i \setminus \{a\}} \tilde{\nu}_{b \to i}^{(t)}(x_i)$$
$$\tilde{\nu}_{a \to i}^{(t+1)}(x_i) = \sum_{x_{\partial a \setminus \{i\}}} \prod_{j \in \partial a \setminus \{i\}} \nu_{j \to a}(x_j) \mathbb{I}(\oplus x_{\partial a} = 0)$$

Decoding by sum-product algorithm



$$\nu_{i\to a}^{(t+1)}(x_i) = \mathbb{P}(y_i|x_i)\prod_{b\in\partial i\setminus\{a\}}\tilde{\nu}_{b\to i}^{(t)}(x_i)$$

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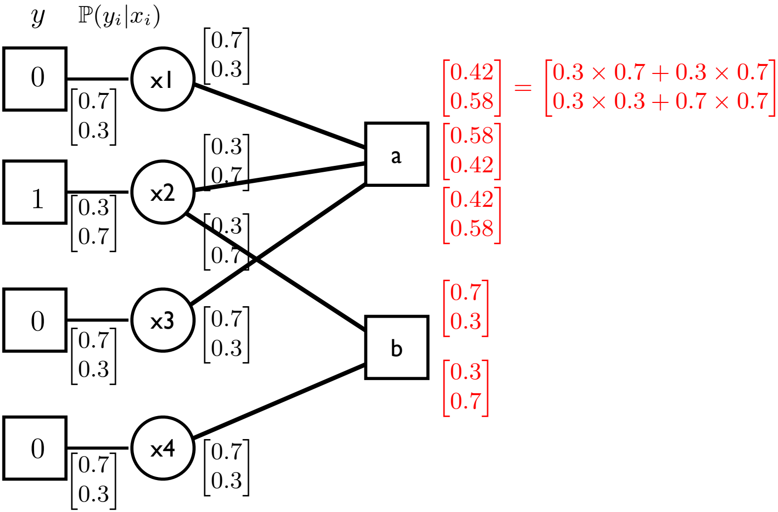
Decoding by sum-product algorithm



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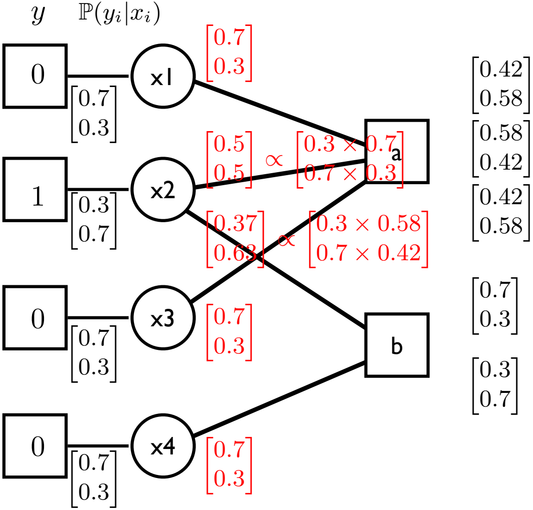
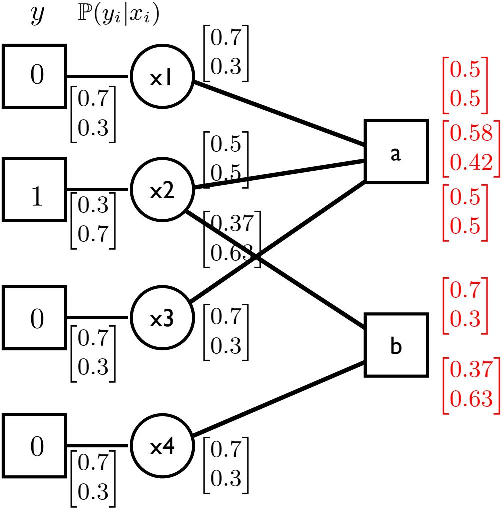
Decoding by sum-product algorithm



$$\nu_{i\to a}^{(t+1)}(x_i) = \mathbb{P}(y_i|x_i) \prod_{b\in\partial i\setminus\{a\}} \tilde{\nu}_{b\to i}^{(t)}(x_i)$$

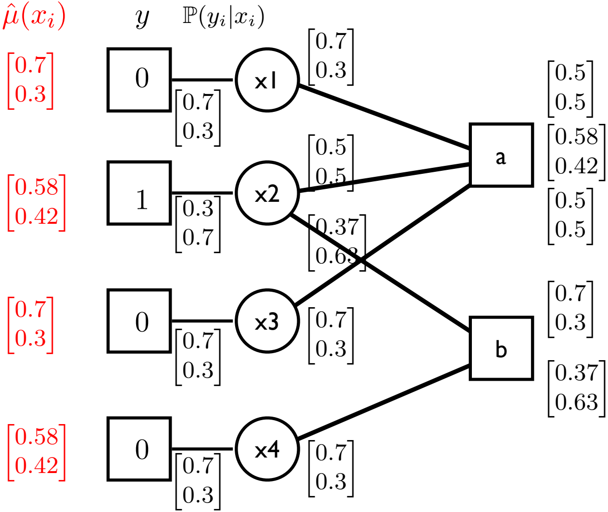
$$\tilde{\nu}_{a\to i}^{(t+1)}(x_i) = \sum_{x_{\partial a\setminus\{i\}}} \prod_{j\in\partial a\setminus\{i\}} \nu_{j\to a}(x_j)\mathbb{I}(\oplus x_{\partial a} = 0)$$

Decoding by sum-product algorithm



$$\nu_{i\to a}^{(t+1)}(x_i) = \mathbb{P}(y_i|x_i) \prod_{b\in\partial i\setminus\{a\}} \tilde{\nu}_{b\to i}^{(t)}(x_i)$$
$$\tilde{\nu}_{a\to i}^{(t+1)}(x_i) = \sum_{x_{\partial a\setminus\{i\}}} \prod_{j\in\partial a\setminus\{i\}} \nu_{j\to a}(x_j)\mathbb{I}(\oplus x_{\partial a} = 0)$$

Decoding by sum-product algorithm

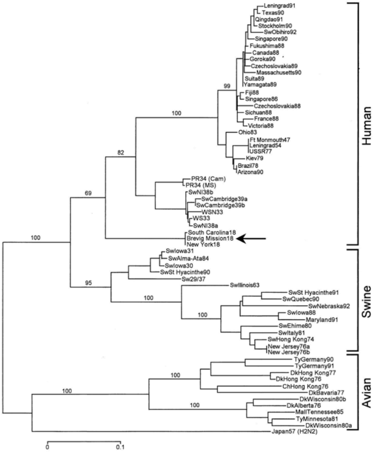


$$\nu_{i\to a}^{(t+1)}(x_i) = \mathbb{P}(y_i|x_i) \prod_{b\in\partial i\setminus\{a\}} \tilde{\nu}_{b\to i}^{(t)}(x_i)$$
$$\tilde{\nu}_{a\to i}^{(t+1)}(x_i) = \sum_{x_{\partial a\setminus\{i\}}} \prod_{j\in\partial a\setminus\{i\}} \nu_{j\to a}(x_j)\mathbb{I}(\oplus x_{\partial a} = 0)$$

Sum-product algorithm on trees

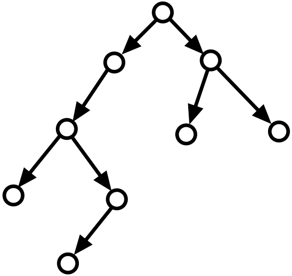
a motivating example: influenza virus

complete sequence of the gene of the 1918 influenza virus



[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).
- Bayesian network model for phylogeny evaluation



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

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

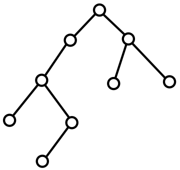
$q_{i,j}(x_i, x_j)$ = Probability that the descendent is x_j if ancestor is x_i.

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

$$q_o(x_o) = \frac{1}{2}$$

$$q(x_i, x_j) = \begin{cases} 1-q & \text{if } x_j = x_i \\ q & \text{if } x_i \neq x_j \end{cases}$$

MRF representation: $q(x_i, x_j) \propto e^{\theta x_i x_j}$ with $\theta = \frac{1}{2}\log\frac{q}{1-q}$

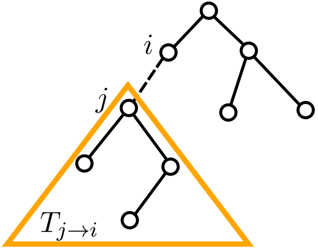


probability of certain tree of mutations x:

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

- **problem:** for given T, compute marginal $\mu_T(x_i)$
- we prove the correctness of sum-product algorithm for this model, but the same proof holds for any general pairwise MRF (and also for general MRF and FG)

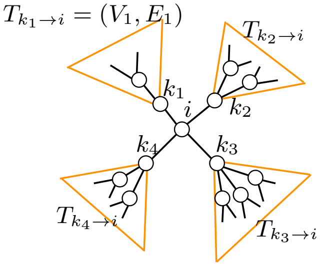
- define graphical model on sub-trees



$$T_{j\to i} = (V_{j\to i}, E_{j\to i}) \equiv \text{Subtree rooted at } j \text{ and excluding } i$$

$$\mu_{j\to i}(x_{V_{j\to i}}) \equiv \frac{1}{Z(T_{j\to i})} \prod_{(u,v)\in E_{j\to i}} e^{\theta x_u x_v}$$

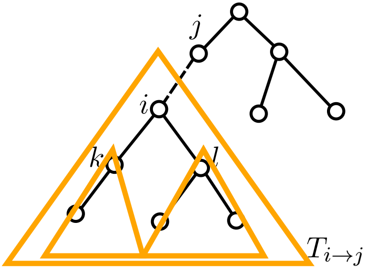
$$\nu_{j\to i}(x_j) \equiv \sum_{x_{V_{j\to i}\setminus\{j\}}} \mu_{j\to i}(x_{V_{j\to i}})$$



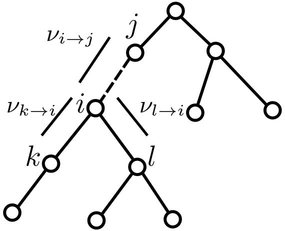
the messages from neighbors k_1, k_2, k_3, k_4 are sufficient to compute the marginal $\mu(x_i)$

$$
\begin{aligned}
\mu_T(x_i) &\propto \sum_{x_{V\setminus\{i\}}} \prod_{(u,v)\in E} e^{\theta x_u x_v} \\
&= \sum_{x_{V_1}, x_{V_2}, x_{V_3}, x_{V_4}} \prod_{\ell=1}^{4} \Big\{ e^{\theta x_i x_{k_\ell}} \prod_{(u,v)\in E_\ell} e^{\theta x_u x_v} \Big\} \\
&= \prod_{\ell=1}^{4} \sum_{x_{k_\ell}, x_{V_\ell\setminus\{k_\ell\}}} \Big\{ e^{\theta x_i x_{k_\ell}} \prod_{(u,v)\in E_\ell} e^{\theta x_u x_v} \Big\} \\
&\propto \prod_{\ell=1}^{4} \Big\{ \sum_{x_{k_\ell}} e^{\theta x_i x_{k_\ell}} \underbrace{\sum_{x_{V_\ell\setminus\{k_\ell\}}} \mu_{k_\ell\to i}(x_{V_\ell})}_{\nu_{k_\ell\to i}(x_{k_\ell})} \Big\}
\end{aligned}
$$

- recursion on sub-trees to compute the messages ν



$$\begin{aligned}
\mu_{i\to j}(x_{V_{i\to j}}) &= \frac{1}{Z(T_{i\to j})} \prod_{(u,v)\in E_{i\to j}} e^{\theta x_u x_v} \\
&= \frac{1}{Z(T_{i\to j})} e^{\theta x_i x_k}\, e^{\theta x_i x_l} \left\{ \prod_{(u,v)\in E_{k\to i}} e^{\theta x_u x_v} \right\} \left\{ \prod_{(u,v)\in E_{l\to i}} e^{\theta x_u x_v} \right\} \\
&\propto e^{\theta x_u x_v}\, e^{\theta x_i x_l} \left\{ \prod_{(u,v)\in E_{k\to i}} e^{\theta x_u x_v} \right\} \left\{ \prod_{(u,v)\in E_{l\to i}} e^{\theta x_u x_v} \right\} \\
&\propto e^{\theta x_i x_k}\, e^{\theta x_i x_l} \mu_{k\to i}(x_{V_{k\to i}}) \mu_{l\to i}(x_{V_{l\to i}})
\end{aligned}$$



$$
\begin{aligned}
\nu_{i\to j}(x_i) &= \sum_{x_{V_{i\to j}\setminus i}} \mu_{i\to j}(x_{V_{i\to j}}) \\
&\propto \sum_{x_{V_{i\to j}\setminus i}} e^{\theta x_i x_k}\, e^{\theta x_i x_l}\, \mu_{k\to i}(x_{V_{k\to i}}) \mu_{l\to i}(x_{V_{l\to i}}) \\
&\propto \Big\{ \sum_{x_{V_{k\to i}}} e^{\theta x_i x_k} \mu_{k\to i}(x_{V_{k\to i}}) \Big\} \Big\{ \sum_{x_{V_{l\to i}}} e^{\theta x_i x_l} \mu_{l\to i}(x_{V_{l\to i}}) \Big\} \\
&= \Big\{ \sum_{x_k} e^{\theta x_i x_k} \sum_{x_{V_{k\to i}\setminus\{k\}}} \mu_{k\to i}(x_{V_{k\to i}}) \Big\} \Big\{ \sum_{x_l} e^{\theta x_i x_l} \sum_{x_{V_{l\to i}\setminus\{l\}}} \mu_{l\to i}(x_{V_{l\to i}}) \Big\} \\
&\propto \Big\{ \sum_{x_k} e^{\theta x_i x_k} \nu_{k\to i}(x_k) \Big\} \Big\{ \sum_{x_l} e^{\theta x_i x_l} \nu_{l\to i}(x_l) \Big\}
\end{aligned}
$$

with uniform initialization $\nu_{i\to j}(x_i) = \frac{1}{|\mathcal{X}|}$ for all leaves i

- sum-product algorithm (for our example)

$$\nu_{i\to j}(x_i) \propto \prod_{k\in\partial i\setminus j}\Big\{\sum_{x_k} e^{\theta x_i x_k}\nu_{k\to i}(x_k)\Big\}$$

$$\nu_i(x_i) \equiv \prod_{k\in\partial i}\Big\{\sum_{x_k} e^{\theta x_i x_k}\nu_{k\to i}(x_k)\Big\}$$

$$\mu_T(x_i) = \frac{\nu_i(x_i)}{\sum_{x_i}\nu_i(x_i)}$$

- what if we want all the marginals?
  - choose an arbitrary root ϕ
  - compute all the messages towards the root ($|E|$ messages)
  - then compute all the messages outwards from the root ($|E|$ messages)
  - then compute all the marginals (n marginals)
- how many operations are required?
  - naive implementation requires $O(|\mathcal{X}|^2\sum_i d_i^2)$ per iteration
    - ★ if i has degree d_i, then computing $\nu_{i\to j}$ requires $d_i|\mathcal{X}|^2$ operations
    - ★ d_i messages start at each node i, each require $d_i|\mathcal{X}|^2$ operations
    - ★ total computation for $2|E|$ messages is $\sum_i\Big\{d_i\cdot(d_i|\mathcal{X}|^2)\Big\}$
  - however, we can compute all marginals in $O(n\,|\mathcal{X}|^2)$ operations

- let $D = \{(i,j),(j,i)|(i,j) \in E\}$ be the directed version of E (cf. $|D| = 2|E|$)
- **(sequential) sum-product algorithm**
  1. initialize $\nu_{i\to j}(x_i) = 1/|\mathcal{X}|$ for all leaves i
  2. recursively over $(i,j) \in D$ compute (from leaves)

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

  3. for each $i \in V$ compute marginal

$$\nu_i(x_i) = \prod_{k\in\partial i} \Big\{ \sum_{x_k} \psi_{ik}(x_i,x_k)\nu_{k\to i}(x_k) \Big\}$$

$$\mu_T(x_i) = \frac{\nu_i(x_i)}{\sum_{x_i} \nu_i(x_i)}$$

- **(parallel) sum-product algorithm**
  1. initialize $\nu^{(0)}_{i\to j}(x_i) = 1/|\mathcal{X}|$ for all $(i,j) \in D$
  2. for $t \in \{0, 1, \dots, t_{\max}\}$
     for all $(i,j) \in D$ compute

$$\nu^{(t+1)}_{i\to j}(x_i) \;=\; \prod_{k\in\partial i\setminus j} \Big\{ \sum_{x_k} \psi_{ik}(x_i, x_k)\nu^{(t)}_{k\to i}(x_k) \Big\}$$

  3. for each $i \in V$ compute marginal

$$\nu_i(x_i) \;=\; \prod_{k\in\partial i} \Big\{ \sum_{x_k} \psi_{ik}(x_i, x_k)\nu^{(t_{\max}+1)}_{k\to i}(x_k) \Big\}$$

$$\mu_T(x_i) \;=\; \frac{\nu_i(x_i)}{\sum_{x_i} \nu_i(x_i)}$$

- also called **belief propagation**
- when $t_{\max}$ is larger than the diameter of the tree (the length of the longest path), this converges to the correct marginal [Exercise 4.1]
- more operations than the sequential version ($O(n|\mathcal{X}|^2 \cdot \mathrm{diam}(T))$)
  - a naive implementation requires $O(|\mathcal{X}|^2 \cdot \mathrm{diam}(T) \cdot \sum d_i^2)$
- naturally extends to general graphs but no proof of exactness

Sum-product algorithm on general graphs

- **(loopy) belief propagation**
  1. initialize $\nu_{i\to j}(x_i) = 1/|\mathcal{X}|$ for all $(i,j) \in D$
  2. for $t \in \{0, 1, \ldots, t_{\max}\}$

     for all $(i,j) \in D$ compute

$$\nu_{i\to j}^{(t+1)}(x_i) \;=\; \prod_{k\in\partial i\setminus j} \Big\{ \sum_{x_k} \psi_{ik}(x_i, x_k)\nu_{k\to i}^{(t)}(x_k) \Big\}$$

  3. for each $i \in V$ compute marginal

$$\nu_i(x_i) \;=\; \prod_{k\in\partial i} \Big\{ \sum_{x_k} \psi_{ik}(x_i, x_k)\nu_{k\to i}^{(t_{\max}+1)}(x_k) \Big\}$$

$$\mu_T(x_i) \;=\; \frac{\nu_i(x_i)}{\sum_{x_i} \nu_i(x_i)}$$

- computes 'approximate' marginals in $O(n|\mathcal{X}|^2 \cdot t_{\max})$ operations
- generally it does not converge; even if it does, it might be incorrect
- folklore about loopy BP
  - works better when G has few short loops
  - works better when $\psi_{ij}(x_i, x_j) = \psi_{ij,1}(x_i)\psi_{ij,2}(x_j) + \mathrm{small}(x_i, x_j)$
  - nonconvex variational principle

Exercise: partition function on trees

- using the recursion for messages:

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

$$\nu_i(x_i) = \prod_{k\in\partial i}\Big\{\sum_{x_k}\psi_{ik}(x_i,x_k)\nu_{k\to i}(x_k)\Big\}$$

it follows that we can easily compute the partition function as

$$Z(T) = \sum_{x_i}\nu_i(x_i)$$

- alternatively, if we had a black box that computes marginals for any tree, then we can use it to compute partition functions efficiently

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

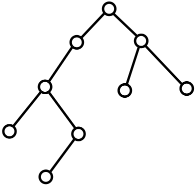
$$Z(T) = \sum_{x_i\in\mathcal{X}}\prod_{k\in\partial i}\Big\{\sum_{x_k\in\mathcal{X}}\psi_{ik}(x_i,x_k)\cdot Z(T_{k\to i})\cdot\mu_{k\to i}(x_k)\Big\}$$

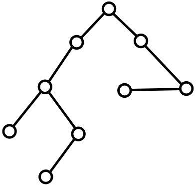
- this recursive algorithm naturally extends to general graphs

Why would one want to compute the partition function?
Suppose you observe

$$x = (+1, +1, +1, +1, +1, +1, +1, +1, +1)$$

and you know this comes from either of





$$\mu(x) = \frac{1}{Z(T)} \prod_{(i,j) \in E} \psi(x_i, x_j)$$

(e.g. coloring)

which one has highest likelihood?

Exercise: sampling on the tree

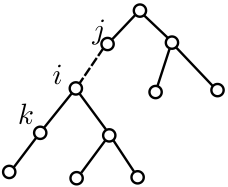
- if we have a black-box for computing marginals on any tree, we can use it to sample from any distribution on a tree

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

```
Choose a root o ∈ V;
Sample X_o ~ μ_o( · );
Recursively over i ∈ V (from root to leaves):
    Compute μ_{i|π(i)}(x_i|x_{π(i)});
    Sample X_i ~ μ_{i|π(i)}( · |x_{π(i)});
```

$\pi(i)$ is the parent of node i in the rooted tree T_o

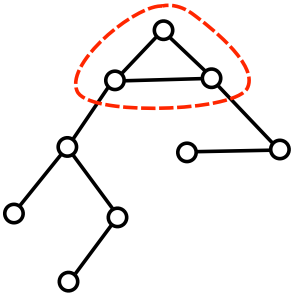
- we use the black-box to compute the conditional distribution



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

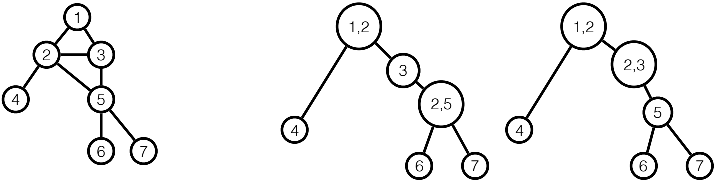
$$\mu_T(x_i|x_j) \propto \psi_{ij}(x_i x_j)\,\mu_{i\to j}(x_i)$$

Tree decomposition



- when we don't have a tree we can create an equivalent tree graph
- by enlarging the alphabet $\mathcal{X} \to \mathcal{X}^k$
- Treewidth$(G) \equiv$ Minimum such k
- it is NP-hard to determine the treewidth of a graph
- problem: in general Treewidth$(G) = \Theta(n)$

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.