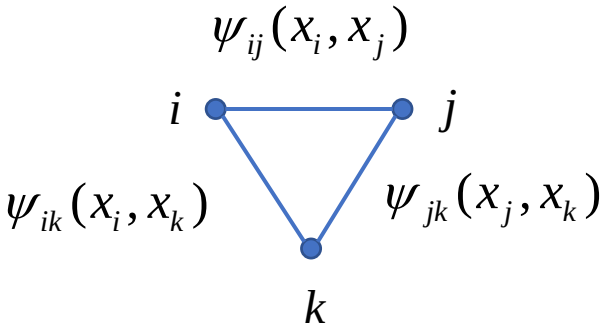
Deterministic Algorithms

$$P(\{x_i\}) = \frac{1}{Z}\prod_i \psi_i(x_i)\prod_{i,j}\psi_{ij}(x_i, x_j)$$ MRF



Suppose, we want to estimate the marginal distributions $\prod_i P_i(x_i)$

or $\mathbf{x}^* = \arg\max_{\{x_i\}} P(\{x_i\})$

If the graph is a polytree (i.e. no closed loops), then we can use dynamic programming

→ This cannot be applied if the graph has closed loops.

Here we describe a popular algorithm – **belief propagation** – that gives correct results on polytrees, and empirically good approximations most of time on graphs

And we will show the relation to MCMC

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Belief Propagation (BP)

proceeds by passing messages between the graph nodes

$m_{ij}(x_j : t)$:message that node i passes to node j to affect state x_j

The messages gets updated as follows:

$$m_{ij}(x_j : t+1) = \sum_{x_i} \psi_{ij}(x_i, x_j)\psi_i(x_i)\prod_{k \neq j} m_{ki}(x_i : t)$$ Sum-product rule

Alternative: the max-product

$$m_{ij}(x_j : t+1) = \max_{x_i} \left\{ \psi_{ij}(x_i, x_j)\psi_i(x_i)\prod_{k \neq j} m_{ki}(x_i : t) \right\}$$

If the algorithm converges (it may not), then we compute approximations to the marginals:

$$b_i(x_i) \propto \psi_i(x_i)\prod_k m_{ki}(x_i)$$

$$b_{ij}(x_i, x_j) \propto \psi_i(x_i)\psi_{ij}(x_i, x_j)\psi_j(x_j)\prod_{k \neq j} m_{ki}(x_i)\prod_{l \neq i} m_{lj}(x_j)$$

Belief Propagation

BP (sum-product) was first proposed by Judea Pearl (C.S. UCLA) for performing inference on polytrees

The max-product algorithm was proposed earlier by Gallagher

The application was developed in the 1990's for decoding problems
- goal was to achieve Shannon's bound on information transmission

Experimentally, it was shown that BP usually converges to reasonable approximations
- Full understanding of when & why it converges is an open problem

On polytree, it is similar to dynamic programming – so in a sense, it is the way to extend DP to graphs with closed loops

Example of BP (sum-product)

$$\mathbf{x} = (x_1, x_2, x_3, x_4)$$

$$P(\mathbf{x}) = \frac{1}{Z}\psi_{12}(x_1, x_2)\psi_{23}(x_2, x_3)\psi_{34}(x_3, x_4)$$

Messages:

$m_{12}(x_2)$, from node 1 to node 2

$m_{21}(x_1)$, from node 2 to node 1

$m_{23}(x_3)$, from node 2 to node 3

$m_{32}(x_2)$, from node 3 to node 2

$m_{34}(x_4)$, from node 3 to node 4

$m_{43}(x_3)$, from node 4 to node 3

Update rule (from message passing equation)

$$m_{12}(x_2 : t+1) = \sum_{x_1} \psi_{12}(x_1, x_2) \quad \rightarrow \text{boundary}$$

$$m_{21}(x_1 : t+1) = \sum_{x_2} \psi_{12}(x_1, x_2) m_{32}(x_2 : t)$$

$$m_{23}(x_3 : t+1) = \sum_{x_2} \psi_{23}(x_2, x_3) m_{12}(x_2 : t)$$

$$m_{32}(x_2 : t+1) = \sum_{x_3} \psi_{23}(x_2, x_3) m_{43}(x_3 : t)$$

$$m_{34}(x_4 : t+1) = \sum_{x_3} \psi_{34}(x_3, x_4) m_{23}(x_3 : t)$$

$$m_{43}(x_3 : t+1) = \sum_{x_4} \psi_{34}(x_3, x_4) \quad \rightarrow \text{boundary}$$

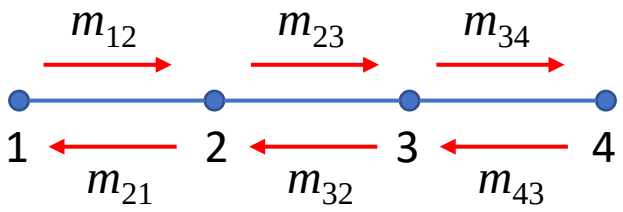
Many ways to run BP

(1) Update all messages in parallel

Note: BP can be parallelized but Dynamic Programming cannot)

(2) Start at boundaries

i.e.,



Calculate $m_{12}(x_2)$, then $m_{23}(x_3)$, then $m_{34}(x_4)$

➔ Forward pass (like Dynamic Programming)

$m_{43}(x_3)$, then $m_{32}(x_2)$, then $m_{21}(x_1)$

➔ Backward pass (like backward pass of DP)

Then read off estimates of unary marginals

$$b_1(x_1) = \frac{1}{Z_1} m_{21}(x_1), \quad Z_1 = \sum_{x_1} m_{21}(x_1) \text{ :normalization}$$

$$b_2(x_2) = \frac{1}{Z_2} m_{12}(x_2) m_{32}(x_2), \quad Z_2 \text{ :normalization}$$

$$b_3(x_3) = \frac{1}{Z_3} m_{23}(x_3) m_{43}(x_3), \quad Z_3 \text{ :normalization}$$

$$b_4(x_4) = \frac{1}{Z_4} m_{34}(x_4), \quad Z_4 \text{ :normalization}$$

$$b_{12}(x_1, x_2) = \frac{1}{Z_{12}} \psi_{12}(x_1, x_2) m_{32}(x_2), \quad \text{and so on}$$

Many ways to run BP

Alternatively, initialize the m's to take
- an initial value – e.g. $m_{ij}(x_j)=1$ for all i, j
- and update the messages in any order
  - will still converge for graph with no closed loops
- Then estimates (beliefs) will be the true marginals

$$\text{e.g.} \quad b_1(x_1) = \sum_{x_2,x_3,x_4} P(x_1, x_2, x_3, x_4)$$

$$b_{12}(x_1, x_2) = \sum_{x_3,x_4} P(x_1, x_2, x_3, x_4)$$

But, BP will often converge to a good approximation to the marginals for graphs which do not have closed loops
- This was discovered in the late 1980's

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Advantages of BP over DP

(1) BP will converges (approximates) for many graphs with closed loops

(2) BP is parallelizable (nice if you have a parallel computer or GPU)

An alternative way to consider BP

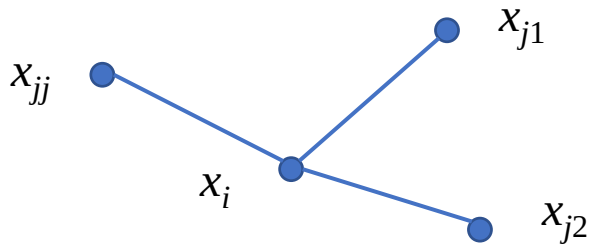
Make local approximations to the local distribution (BP w/o messages)

$$B(x_i, \mathbf{x}_{N(i)}) = \frac{1}{Z} b_i(x_i) \prod_{j \in N(i)} \frac{b_{ij}(x_i, x_j)}{b_i(x_i)}$$

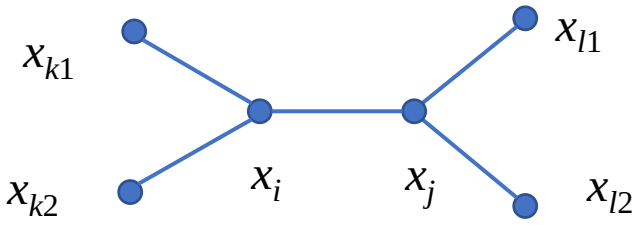
If the $b_{ij}(x_i, x_j)$ & $b_i(x_i)$ are the true marginal distribution, then $\frac{b_{ij}(x_i, x_j)}{b_i(x_i)} = b(x_j \mid x_i)$

An alternative way to consider BP

Cut
the rest of
the graph



$$B(x_i, x_j, \mathbf{x}_{N(i)}, \mathbf{x}_{N(j)}) = \frac{1}{Z_{ij}} b_{ij}(x_i, x_j) \prod_{k \in N(i)/j} \frac{b_{ik}(x_i, x_k)}{b_i(x_i)} \prod_{l \in N(j)/i} \frac{b_{jl}(x_j, x_l)}{b_j(x_j)}$$



Update Rule: Marginalization

$$b_{ij}(x_i, x_j : t+1) = \sum_{\mathbf{x}_{N(i,j)}} B(x_i, x_j, \mathbf{x}_{N(i)}, \mathbf{x}_{N(j)} : t)$$

$$b_{ij}(x_i : t+1) = \sum_{\mathbf{x}_{N(i)}} B(x_i, \mathbf{x}_{N(i)} : t)$$

Provably equivalent to BP

How does this relate to MCMC?

Chapman-Kolmogorov ⟵A deterministic form of Gibbs sampling

$$M_{t+1}(\mathbf{x}) = \sum_{\mathbf{x}'} K(\mathbf{x} \mid \mathbf{x}')\mu_t(\mathbf{x}') \qquad (K\text{: Transition kernel})$$

This converges to fixed point distribution $\Pi(\mathbf{x})$ s.t $\sum_{\mathbf{x}'} K(\mathbf{x} \mid \mathbf{x}')\mu(\mathbf{x}') = \Pi(\mathbf{x})$

MCMC estimates $\Pi(\mathbf{x})$ by repeatedly sampling from $K(\mathbf{x}, \mathbf{x}')$

Recall that Gibbs Sampler $K_\gamma(\mathbf{x} \mid \mathbf{x}') = P(x_\gamma \mid x'_{N(\gamma)})S_{\mathbf{x}/\gamma, \mathbf{x}'/\gamma}$

Substituting the Gibbs sampler into the Chapman-Kolmogorov equation

$$\mu_{t+1}(\mathbf{x}_\gamma) = \sum_{\mathbf{x}_{N(\gamma)}} P(\mathbf{x}_r \mid \mathbf{x}'_{N(\gamma)})\mu_t(\mathbf{x}_{N(\gamma)})$$

Replace $\mu_{t+1}(\mathbf{x}_\gamma)$ by $\sum_{x_i} B(x_i, x_{N(\gamma)}), \quad \mathbf{x}_r = y_i$

or $\sum_{x_i, x_j} B(x_i, x_j, x_{N(i,j)}), \quad \mathbf{x}_\gamma = (x_i, x_j)$

Bethe Free Energy

It can be shown that the fixed point of BP correspond to extreme of the Bethe Free Energy

$$F[b] = \sum_{ij} \sum_{x_i, x_j} b_{ij}(x_i, x_j) \ln \frac{b_{ij}(x_i, x_j)}{\psi_i(x_i)\psi_j(x_j)\psi_{ij}(x_i, x_j)} - \sum_i (n_i - 1) \sum_{x_i} b_i(x_i) \ln \frac{b_i(x_i)}{\psi_i(x_i)}$$

This leads an alternative class of algorithm which seek to directly minimize $F[b]$

These algorithms are more complex than BP, more time consuming, and do not always give better results

Note M. Wainwright defines a class of convex free energies similar to Bethe

Note Junction trees allows DP to be applied to same graphs with closed loops (see Lauritzen and Spiegelhalter).

A range of alternative algorithms

The original is meanfield (MFT)

Kulback-Leibler: Define $B(\mathbf{x}) = \prod_i b_i(x_i)$ $KL(B) = \sum_{\mathbf{x}} B(\mathbf{x}) \ln \frac{B(\mathbf{x})}{P(\mathbf{x})}$

Seek to find the $B(\mathbf{x})$ that minimizes $KL(B)$

Equivalent to $\sum_{i,j} \sum_{x_i, x_j} b_i(x_i) b_j(x_j) \ln \frac{b_i(x_i) b_j(x_j)}{\psi_i(x_i) \psi_{ij}(x_i, x_j) \psi_j(x_j)} - \sum_i (n_i - 1) \sum_{x_i} b_i(x_i) \ln \frac{b_i(x_i)}{\psi_i(x_i)}$

Compare to Bethe Free Energy: $b_{ij}(x_i, x_j) \rightarrow b_i(x_i) b_j(x_j)$

Minimizing KL(B) is not straightforward, but it is straightforward to find a local minima

- These approaches are significantly faster than MCMC, but MCMC works when these do not.