School of Computer Science
Carnegie Mellon

Probabilistic Graphical Models

Variational Inference:
Loopy Belief Propagation

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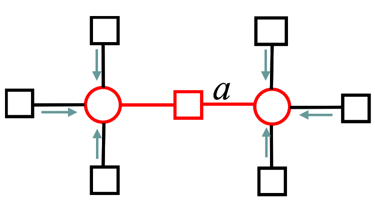
Lecture 12, February 27, 2017

Reading: See class website



Inference Problems

- Compute the likelihood of observed data
- Compute the marginal distribution $p(x_A)$ over a particular subset of nodes $A \subset V$
- Compute the conditional distribution $p(x_A | x_B)$ for disjoint subsets *A* and *B*
- Compute a mode of the density $\hat{x} = \arg \max_{x \in \mathcal{X}^m} p(x)$

- Methods we have

Brute force | **Elimination** → **Message Passing** (Forward-backward , Max-product /BP, Junction Tree)

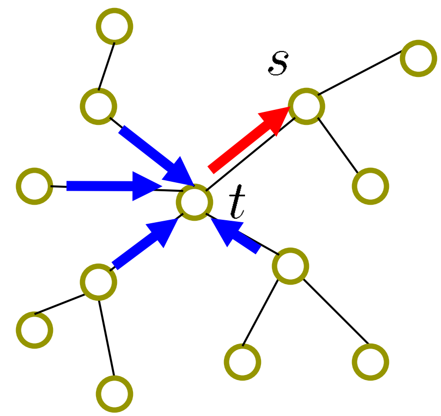
Individual computations independent

Sharing intermediate terms

Sum-Product Revisited

- Tree-structured GMs

$$p(x_1, \cdots, x_m) = \frac{1}{Z} \prod_{s \in V} \psi_s(x_s) \prod_{(s,t) \in E} \psi_{st}(x_s, x_t)$$



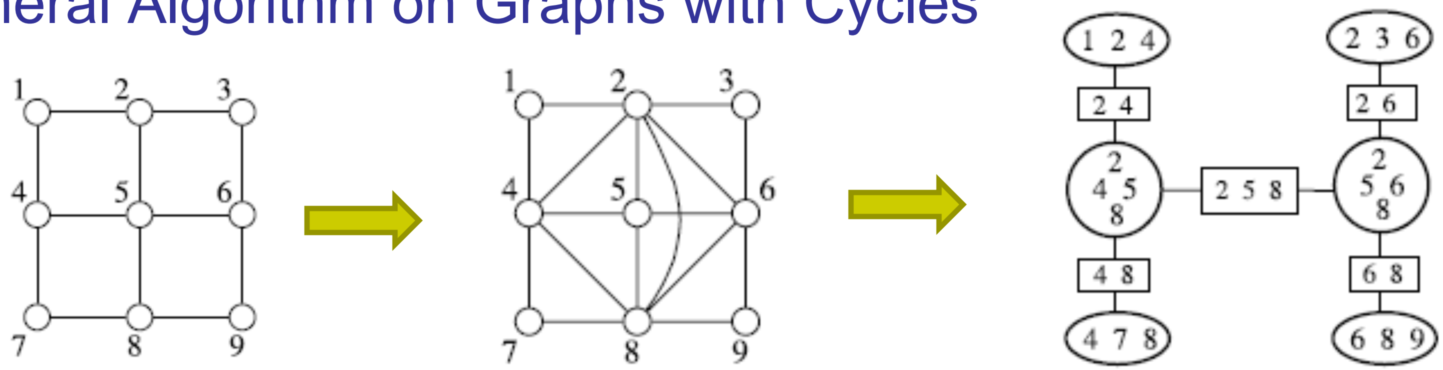
- Message Passing on Trees:

$$M_{t \to s}(x_s) \leftarrow \kappa \sum_{x'_t} \left\{ \psi_{st}(x_s, x'_t) \psi_t(x'_t) \prod_{u \in N(t) \setminus s} M_{u \to t}(x'_t) \right\}$$

  - On trees, converge to a unique fixed point after a finite number of iterations

Junction Tree Revisited

- General Algorithm on Graphs with Cycles

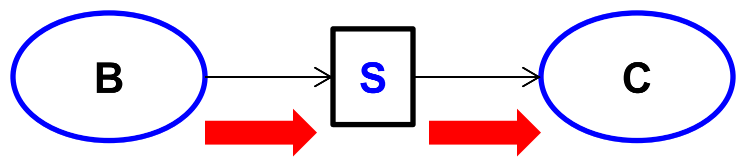


- Steps: **=> Triangularization** **=> Construct JTs**

=> Message Passing on Clique Trees

$$\widetilde{\phi}_S(x_S) \leftarrow \sum_{x_{B \setminus S}} \phi_B(x_B)$$

$$\phi_C(x_C) \leftarrow \frac{\widetilde{\phi}_S(x_S)}{\phi_S(x_S)} \phi_C(x_C)$$



Local Consistency

- Given a set of functions $\{\tau_C,\ C \in \mathcal{C}\}$ and $\{\tau_S,\ S \in \mathcal{S}\}$ associated with the cliques and separator sets

- They are locally consistent if:

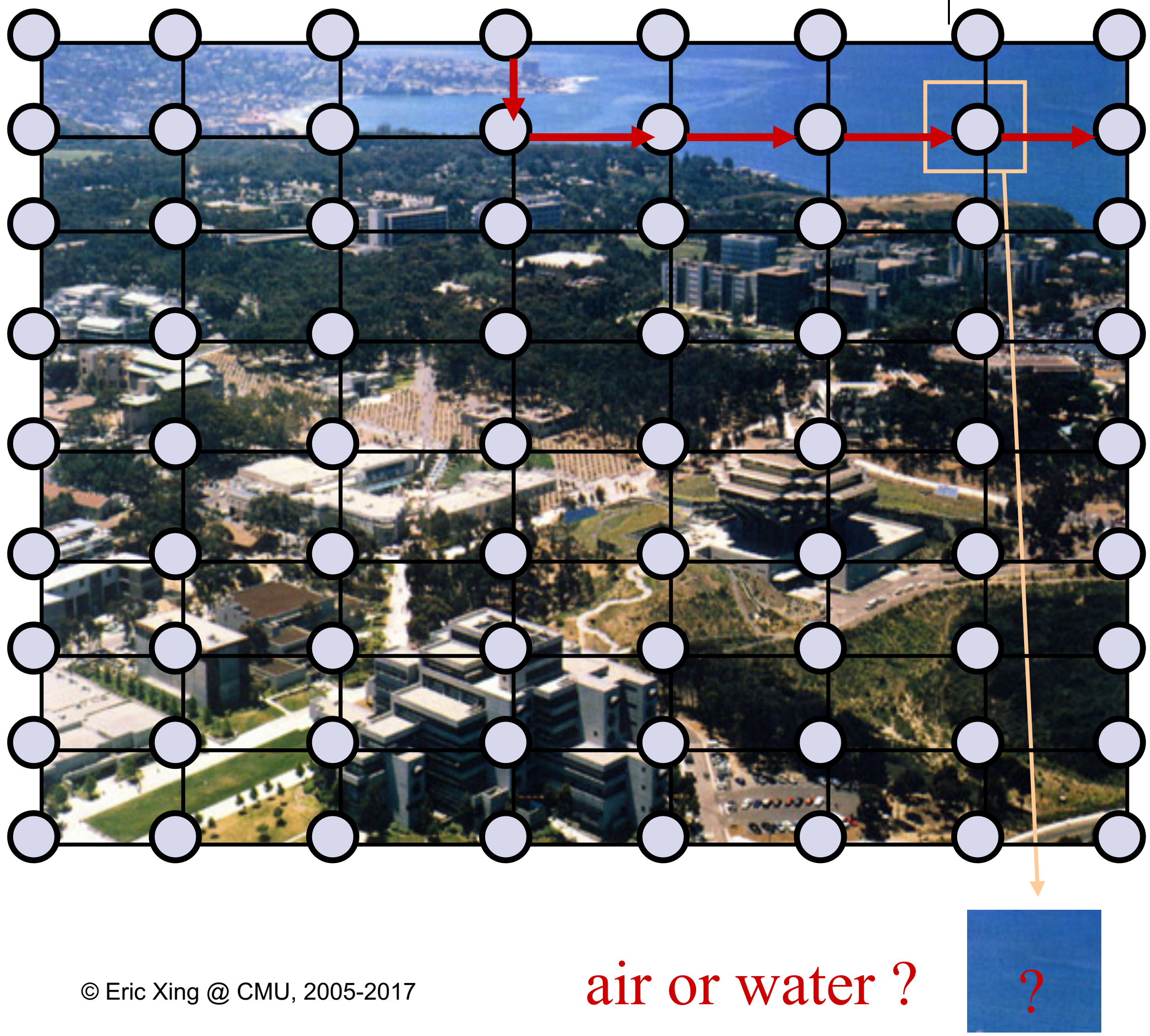
$$\sum_{x'_S} \tau_S(x'_S) = 1,\ \forall S \in \mathcal{S}$$

$$\sum_{x'_C | x'_S = x_S} \tau_C(x'_C) = \tau_S(x_S),\ \forall C \in \mathcal{C},\ S \subset C$$

- For junction trees, local consistency is equivalent to global consistency!

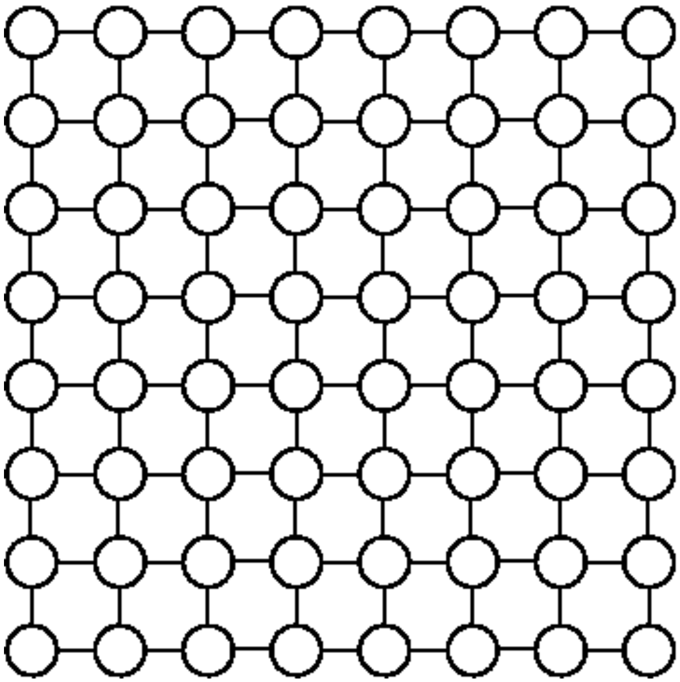
An Ising model on 2-D image

- Nodes encode hidden information (patch-identity).
- They receive local information from the image (brightness, color).
- Information is propagated though the graph over its edges.
- Edges encode 'compatibility' between nodes.



Why Approximate Inference?

- Why can't we just run junction tree on this graph?



$$p(X) = \frac{1}{Z}\exp\left\{\sum_{i<j}\theta_{ij}X_iX_j + \sum_i \theta_{i0}X_i\right\}$$

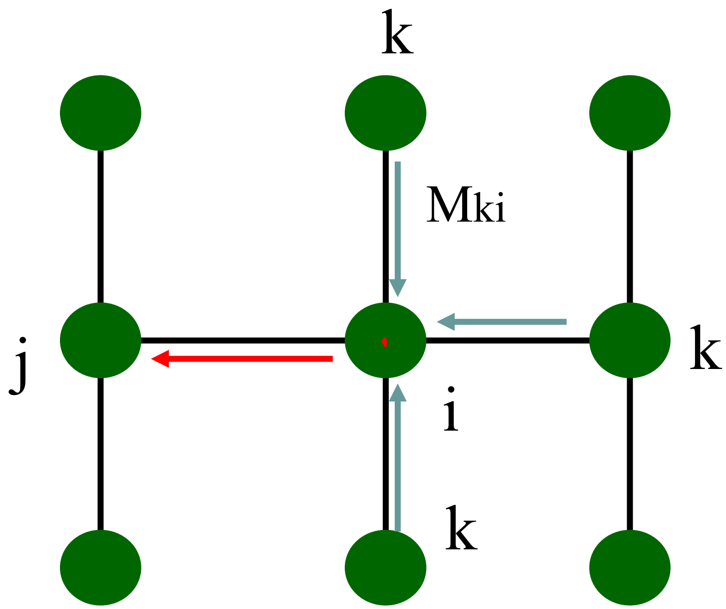
- If NxN grid, tree width at least N
- N can be a huge number(~1000s of pixels)
  - If N~O(1000), we have a clique with 2^{100} entries

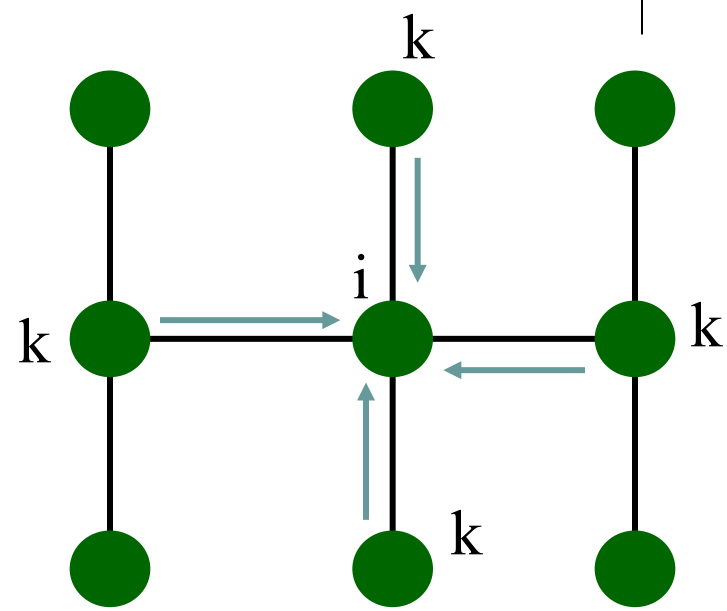
Approaches to inference

- Exact inference algorithms
  - The elimination algorithm
  - Message-passing algorithm (sum-product, belief propagation)
  - The junction tree algorithms
- Approximate inference techniques
  - Variational algorithms
    - Loopy belief propagation
    - Mean field approximation
  - Stochastic simulation / sampling methods
  - Markov chain Monte Carlo methods

Loopy Belief Propogation

Recap: Belief Propagation





- BP Message-update Rules

$$M_{i\to j}(x_j) \propto \sum_{x_i} \psi_{ij}(x_i, x_j)\psi_i(x_i)\prod_k M_{k\to i}(x_i)$$

external evidence

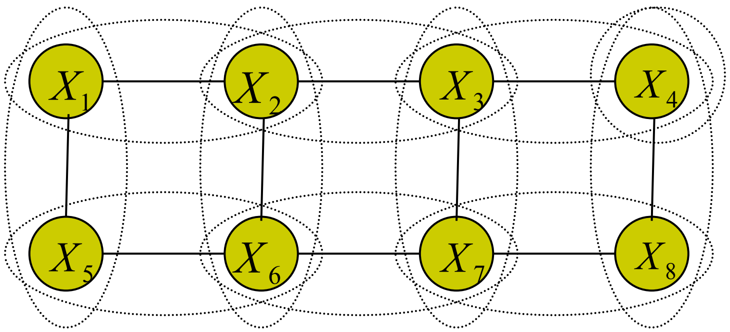
Compatibilities (interactions)

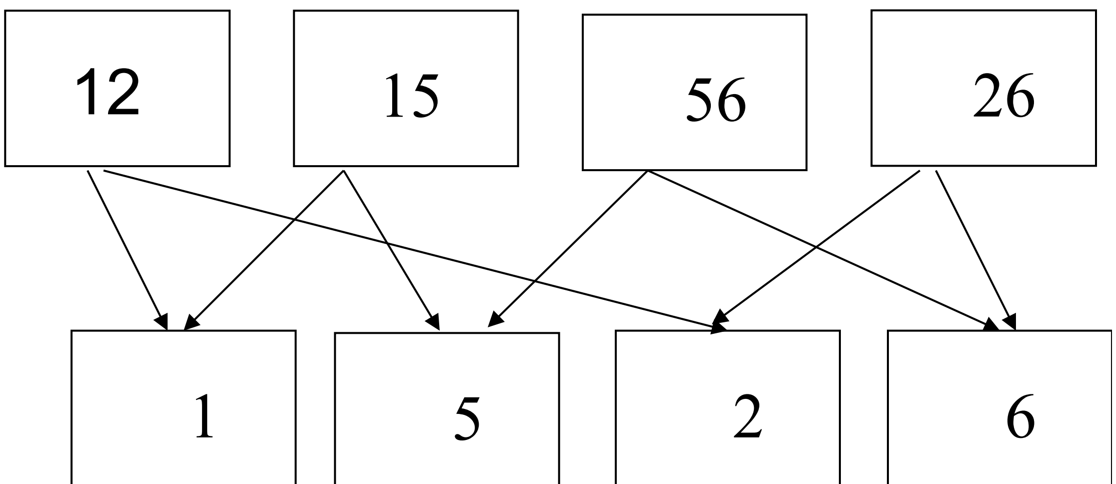
$$b_i(x_i) \propto \psi_i(x_i)\prod_k M_k(x_k)$$

- BP on trees always converges to exact marginals (cf. Junction tree algorithm)

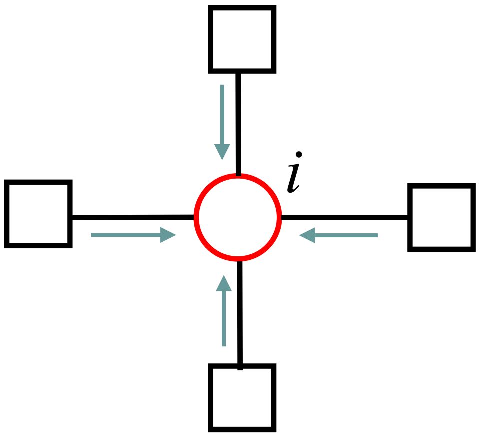
Region graphs (Factor Graph)

- It will be useful to look explicitly at the messages being passed
  - Messages from variable to factors
  - Messages from factors to variables
- Let us represent this graphically



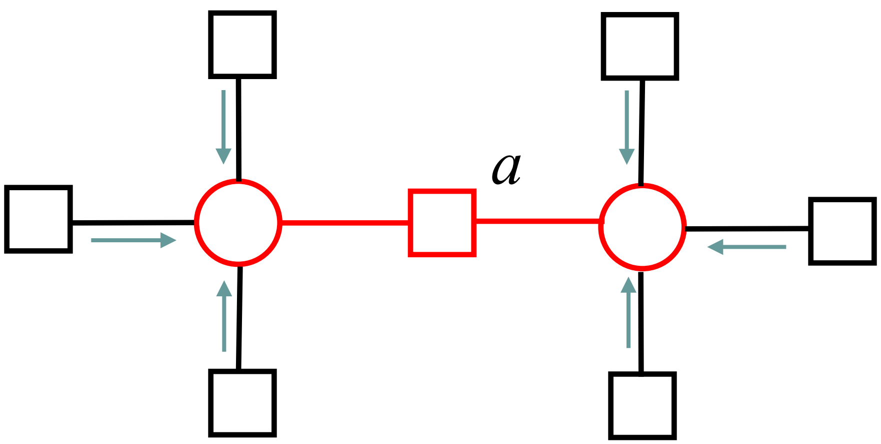


Beliefs and messages in FG



$$b_i(x_i) \propto f_i(x_i) \prod_{a \in N(i)} m_{a \to i}(x_i)$$

"beliefs" "messages"

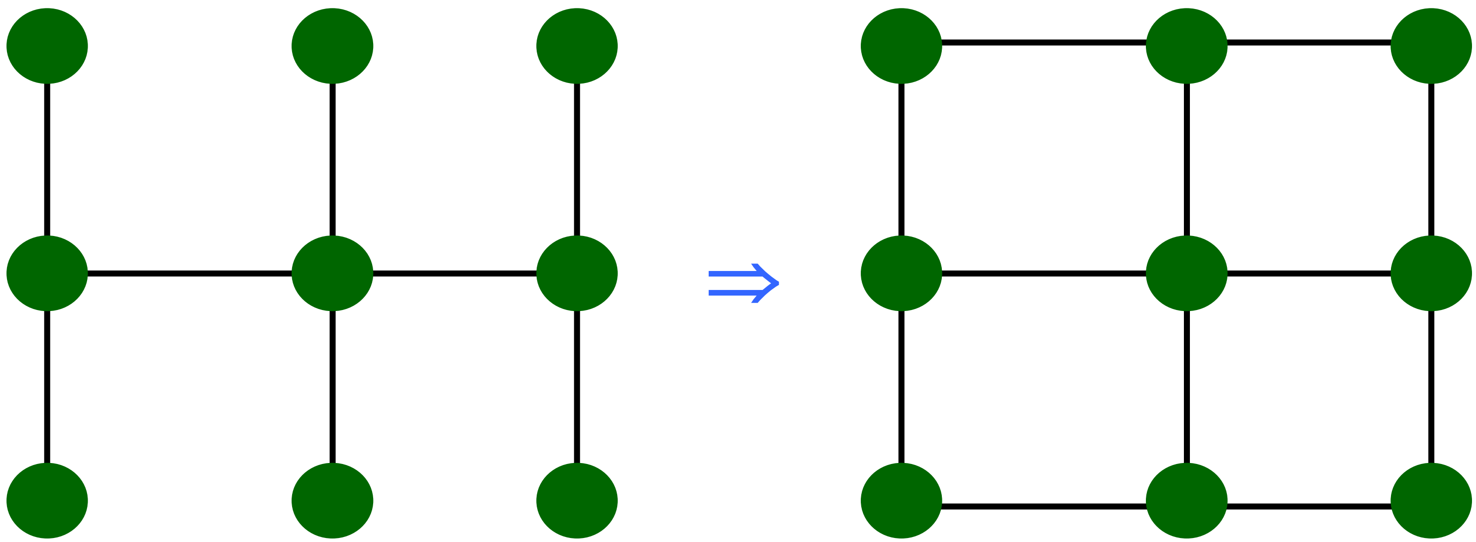


$$m_{i \to a}(x_i) = \prod_{c \in N(i) \backslash a} m_{c \to i}(x_i)$$

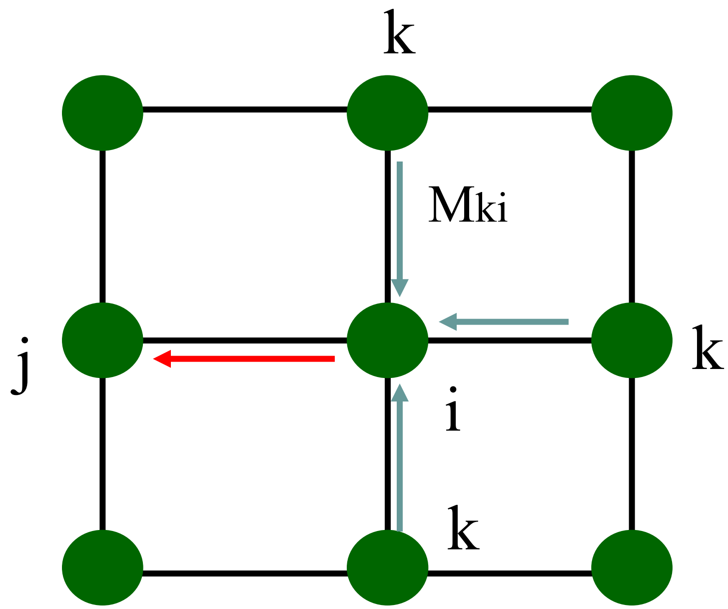
$$b_a(X_a) \propto f_a(X_a) \prod_{i \in N(a)} m_{i \to a}(x_i)$$

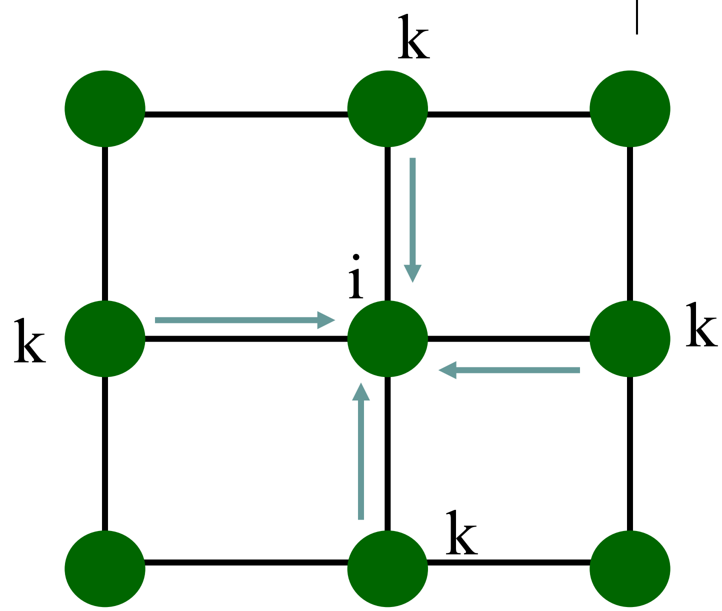
$$m_{a \to i}(x_i) = \sum_{X_a \backslash x_i} f_a(X_a) \prod_{j \in N(a) \backslash i} m_{j \to a}(x_j)$$

What if the graph is loopy?



Belief Propagation on loopy graphs





- BP Message-update Rules

$$M_{i\to j}(x_j) \propto \sum_{x_i} \psi_{ij}(x_i, x_j)\psi_i(x_i)\prod_k M_{k\to i}(x_i)$$

$$b_i(x_i) \propto \psi_i(x_i)\prod_k M_k(x_k)$$

Compatibilities (interactions)

external evidence

- May not converge or converge to a wrong solution

Loopy Belief Propagation

- A fixed point iteration procedure that tries to minimize F_{bethe}
- Start with random initialization of messages and beliefs
  - While not converged do

$$b_i(x_i) \propto \prod_{a \in N(i)} m_{a \to i}(x_i) \qquad b_a(X_a) \propto f_a(X_a) \prod_{i \in N(a)} m_{i \to a}(x_i)$$

$$m_{i \to a}^{new}(x_i) = \prod_{c \in N(i) \backslash a} m_{c \to i}(x_i) \qquad m_{a \to i}^{new}(x_i) = \sum_{X_a \backslash x_i} f_a(X_a) \prod_{j \in N(a) \backslash i} m_{j \to a}(x_j)$$

  - At convergence, stationarity properties are guaranteed
  - However, not guaranteed to converge!

Loopy Belief Propagation

- If BP is used on graphs with loops, messages may circulate indefinitely

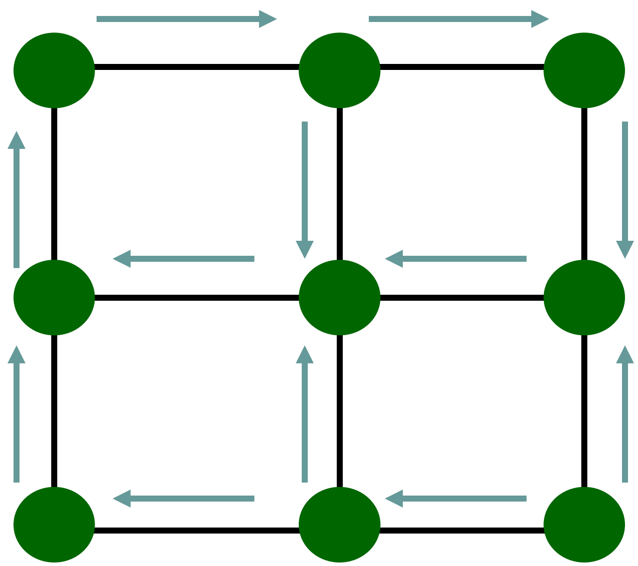
- But let's run it anyway and hope for the best … ☺

- Empirically, a good approximation is still achievable
  - Stop after fixed # of iterations
  - Stop when no significant change in beliefs
  - If solution is not oscillatory but converges, it usually is a good approximation

[Loopy-belief Propagation for Approximate Inference: An Empirical Study](#)
Kevin Murphy, Yair Weiss, and Michael Jordan.
***UAI '99 (Uncertainty in AI).*]**

So what is going on?

- Is it a dirty hack that you bet your luck?



Approximate Inference

- Let us call the actual distribution P

$$P(X) = 1/Z \prod_{f_a \in F} f_a(X_a)$$

- We wish to find a distribution Q such that Q is a "good" approximation to P
- Recall the definition of KL-divergence

$$KL(Q_1 \| Q_2) = \sum_X Q_1(X) \log\left(\frac{Q_1(X)}{Q_2(X)}\right)$$

  - $KL(Q_1||Q_2) >= 0$
  - $KL(Q_1||Q_2) = 0$ iff $Q_1 = Q_2$
  - We can therefore use KL as a scoring function to decide a good Q
  - But, $KL(Q_1||Q_2) \neq KL(Q_2||Q_1)$

Which KL?

- Computing KL(P||Q) requires inference!
- But KL(Q||P) can be computed without performing inference on P

$$KL(Q \| P) = \sum_X Q(X) \log\left(\frac{Q(X)}{P(X)}\right)$$
$$= \sum_X Q(X) \log Q(X) - \sum_X Q(X) \log P(X)$$
$$= -H_Q(X) - E_Q \log P(X)$$

- Using $P(X) = 1/Z \prod_{f_a \in F} f_a(X_a)$

$$KL(Q \| P) = -H_Q(X) - E_Q \log(1/Z \prod_{f_a \in F} f_a(X_a))$$
$$= -H_Q(X) - \log 1/Z - \sum_{f_a \in F} E_Q \log f_a(X_a)$$

Optimization function

$$KL(Q\|P) = \underbrace{\boxed{-H_Q(X) - \sum_{f_a \in F} E_Q \log f_a(X_a)}}_{F(P,Q)} + \log Z$$

- We will call $F(P,Q)$ the "Free energy" *
- $F(P,P)$ =?

- F(P,Q) >= F(P,P)

*Gibbs Free Energy

The Energy Functional

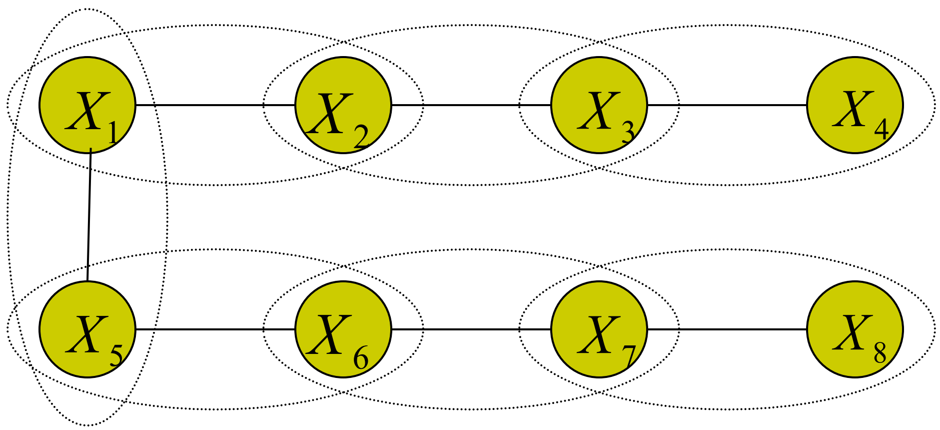
- Let us look at the functional

$$F(P,Q) = -H_Q(X) - \sum_{f_a \in F} E_Q \log f_a(X_a)$$

- $\sum_{f_a \in F} E_Q \log f_a(X_a)$ can be computed if we have marginals over each f_a
- $H_Q = -\sum_X Q(X) \log Q(X)$ is harder! Requires summation over all possible values
- Computing F, is therefore hard in general.
- Approach 1: Approximate $F(P,Q)$ with easy to compute $\hat{F}(P,Q)$

Tree Energy Functionals

- Consider a tree-structured distribution



- The probability can be written as: $b(\mathbf{x}) = \prod_a b_a(\mathbf{x}_a) \prod_i b_i(x_i)^{1-d_i}$
- $$H_{tree} = -\sum_a \sum_{\mathbf{x}_a} b_a(\mathbf{x}_a) \ln b_a(\mathbf{x}_a) + \sum_i (d_i - 1) \sum_{\mathbf{x}_i} b_i(\mathbf{x}_i) \ln b_i(\mathbf{x}_i)$$
- $$F_{Tree} = \sum_a \sum_{\mathbf{x}_a} b_a(\mathbf{x}_a) \ln \frac{b_a(\mathbf{x}_a)}{f_a(\mathbf{x}_a)} + \sum_i (1 - d_i) \sum_{\mathbf{x}_i} b_i(\mathbf{x}_i) \ln b_i(\mathbf{x}_i)$$
  $$= F_{12} + F_{23} + .. + F_{67} + F_{78} - F_1 - F_5 - F_2 - F_6 - F_3 - F_7$$
  - involves summation over edges and vertices and is therefore easy to compute

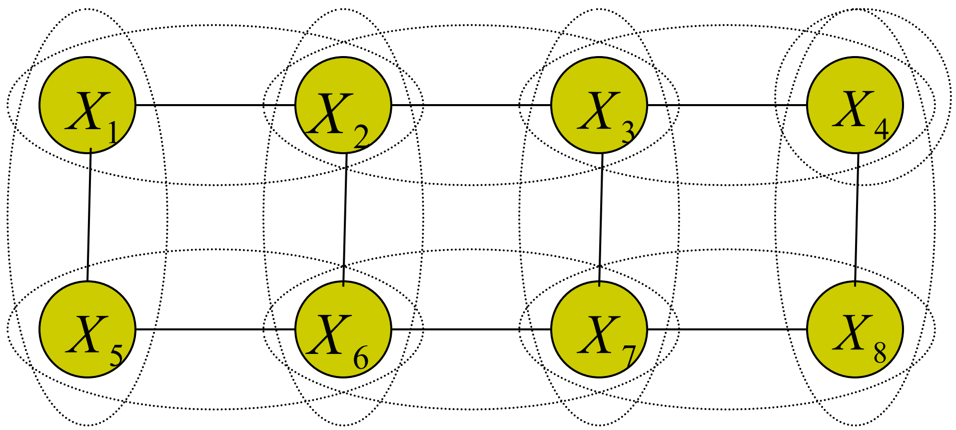
Bethe Approximation to Gibbs Free Energy

- For a general graph, choose $\hat{F}(P,Q) = F_{Betha}$

$$H_{Bethe} = -\sum_{a}\sum_{\mathbf{x}_a} b_a(\mathbf{x}_a)\ln b_a(\mathbf{x}_a) + \sum_{i}(d_i - 1)\sum_{\mathbf{x}_i} b_i(\mathbf{x}_i)\ln b_i(\mathbf{x}_i)$$

$$F_{Bethe} = \sum_{a}\sum_{\mathbf{x}_a} b_a(\mathbf{x}_a)\ln\frac{b_a(\mathbf{x}_a)}{f_a(\mathbf{x}_a)} + \sum_{i}(1 - d_i)\sum_{\mathbf{x}_i} b_i(\mathbf{x}_i)\ln b_i(\mathbf{x}_i) = -\langle f_a(\mathbf{x}_a)\rangle - H_{betha}$$

  - Called “Bethe approximation” after the physicist Hans Bethe



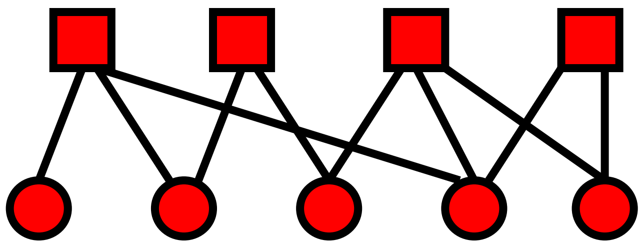
$$F_{bethe} = F_{12} + F_{23} + .. + F_{67} + F_{78} - F_1 - F_5 - 2F_2 - 2F_6 .. - F_8$$

  - Equal to the exact Gibbs free energy when the factor graph is a tree
  - In general, H_{Bethe} is **not** the same as the H of a tree

Bethe Approximation

- Pros:
  - Easy to compute, since entropy term involves sum over pairwise and single variables
- Cons:
  - $\hat{F}(P,Q) = F_{bethe}$ **may or may not** be well connected to $F(P,Q)$
  - It could, in general, be greater, equal or less than $F(P,Q)$
- Optimize each $b(\mathbf{x}_a)$'s.
  - For discrete belief, constrained opt. with *Lagrangian* multiplier
  - For continuous belief, not yet a general formula
  - Not always converge

Bethe Free Energy for FG



$$F_{Betha} = \sum_a \sum_{\mathbf{x}_a} b_a(\mathbf{x}_a) \ln \frac{b_a(\mathbf{x}_a)}{f_a(\mathbf{x}_a)} + \sum_i (1 - d_i) \sum_{\mathbf{x}_i} b_i(\mathbf{x}_i) \ln b_i(\mathbf{x}_i)$$

$$H_{Bethe} = -\sum_a \sum_{\mathbf{x}_a} b_a(\mathbf{x}_a) \ln b_a(\mathbf{x}_a) + \sum_i (d_i - 1) \sum_{\mathbf{x}_i} b_i(\mathbf{x}_i) \ln b_i(\mathbf{x}_i)$$

$$F_{Bethe} = -\langle f_a(\mathbf{x}_a) \rangle - H_{betha}$$

Minimizing the Bethe Free Energy

- $$L = F_{Bethe} + \sum_i \gamma_i \{1 - \sum_{x_i} b_i(x_i)\}$$
$$+ \sum_a \sum_{i \in N(a)} \sum_{x_i} \lambda_{ai}(x_i) \left\{ b_i(x_i) - \sum_{X_a \setminus x_i} b_a(X_a) \right\}$$

- Set derivative to zero

Constrained Minimization of the Bethe Free Energy

$$L = F_{Bethe} + \sum_i \gamma_i \{\sum_{x_i} b_i(x_i) - 1\}$$

$$+ \sum_a \sum_{i \in N(a)} \sum_{x_i} \lambda_{ai}(x_i) \left\{ \sum_{X_a \setminus x_i} b_a(X_a) - b_i(x_i) \right\}$$

$$\frac{\partial L}{\partial b_i(x_i)} = 0 \quad \Longrightarrow \quad b_i(x_i) \propto \exp\left(\frac{1}{d_i - 1} \sum_{a \in N(i)} \lambda_{ai}(x_i) \right)$$

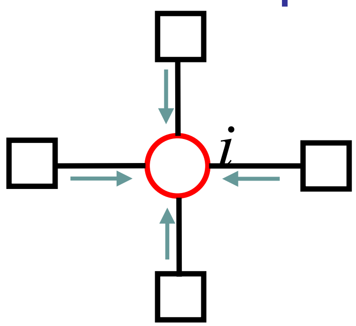
$$\frac{\partial L}{\partial b_a(X_a)} = 0 \quad \Longrightarrow \quad b_a(X_a) \propto \exp\left(-E_a(X_a) + \sum_{i \in N(a)} \lambda_{ai}(x_i) \right)$$

Bethe = BP on FG

- We had:

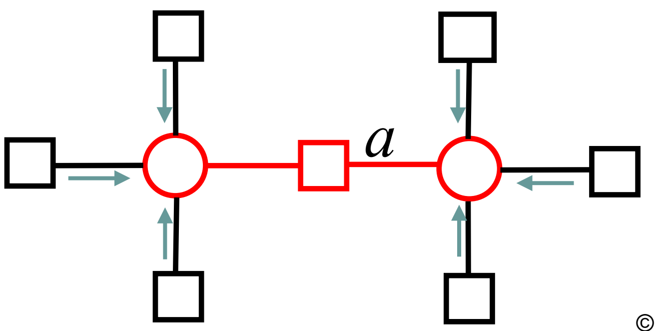
$$b_i(x_i) \propto \exp\left(\frac{1}{d_i - 1}\sum_{a\in N(i)}\lambda_{ai}(x_i)\right) \quad b_a(X_a) \propto \exp\left(-\log f_a(X_a) + \sum_{i\in N(a)}\lambda_{ai}(x_i)\right)$$

- Identify $\lambda_{ai}(x_i) = \log(m_{i\to a}(x_i)) = \log \prod_{b\in N(i)\neq a} m_{b\to i}(x_i)$
- to obtain BP equations:



$$b_i(x_i) \propto f_i(x_i) \prod_{a\in N(i)} m_{a\to i}(x_i)$$

"beliefs" "messages"



$$b_a(X_a) \propto f_a(X_a) \prod_{i\in N(a)} \prod_{c\in N(i)\backslash a} m_{c\to i}(x_i)$$

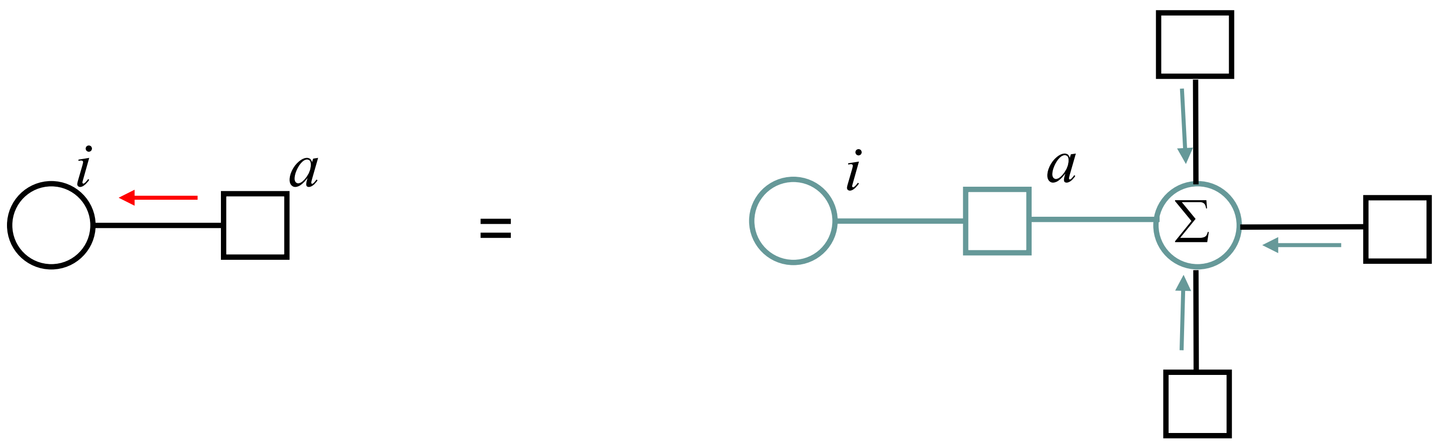
The "belief" is the BP approximation of the marginal probability.

BP Message-update Rules

Using $b_{a\to i}(x_i)=\sum_{X_a\setminus x_i} b_a(X_a)$, we get

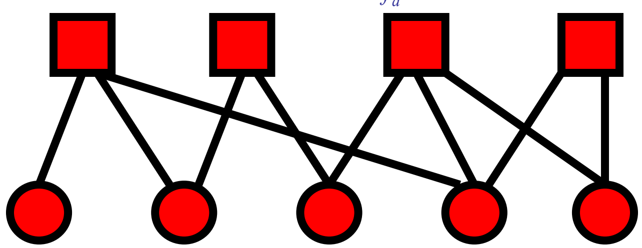
$$\boxed{m_{a\to i}(x_i)=\sum_{X_a\setminus x_i} f_a(X_a)\prod_{j\in N(a)\setminus i}\;\prod_{b\in N(j)\setminus a} m_{b\to j}(x_j)}$$

(A sum product algorithm)



Summary so far

- $P(X) = 1/Z \prod_{f_a \in F} f_a(X_a)$

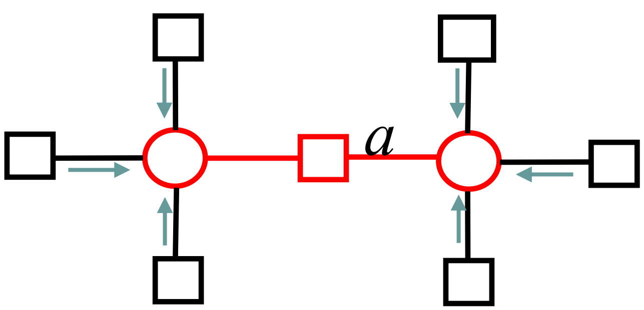


$$F(P,Q) = -H_Q(X) - \sum_{f_a \in F} E_Q \log f_a(X_a)$$

$$\hat{F}(P,Q) = \sum_a \sum_{\mathbf{x}_a} b_a(\mathbf{x}_a) \log \frac{f_a(\mathbf{x}_a)}{b_a(\mathbf{x}_a)} + \sum_i (1-d_i) \sum_{\mathbf{x}_i} b_i(\mathbf{x}_i) \log b_i(\mathbf{x}_i)$$

$$b_a(X_a) \propto \exp\left(-\log f_a(X_a) + \sum_{i \in N(a)} \lambda_{ai}(x_i) \right)$$

$$b_i(x_i) \propto \exp\left(\frac{1}{d_i - 1} \sum_{a \in N(i)} \lambda_{ai}(x_i) \right)$$



The Theory Behind LBP

- For a distribution $p(X|\theta)$ associated with a complex graph, computing the marginal (or conditional) probability of arbitrary random variable(s) is intractable

- Variational methods
  - formulating probabilistic inference as an optimization problem:

$$q^* = \arg\min_{q \in S} \left\{ F_{Betha}(p,q) \right\}$$

$$F_{Bethe} = \sum_a \sum_{\mathbf{x}_a} b_a(\mathbf{x}_a) \ln \frac{b_a(\mathbf{x}_a)}{f_a(\mathbf{x}_a)} + \sum_i (1-d_i) \sum_{\mathbf{x}_i} b_i(\mathbf{x}_i) \ln b_i(\mathbf{x}_i) = -\langle f_a(\mathbf{x}_a) \rangle - H_{bethe}$$

q : a (tractable) probability distribution

The Theory Behind LBP

- But we do not optimize $q(\mathbf{X})$ explicitly, focus on the set of beliefs
  - $e.g., \quad b = \{b_{i,j} = \tau(x_i, x_j), \ \ b_i = \tau(x_i)\}$
- Relax the optimization problem
  - approximate objective: $H_q \approx F(b)$
  - relaxed feasible set: $\mathcal{M} \rightarrow \mathcal{M}_o \quad (\mathcal{M}_o \supseteq \mathcal{M})$

$$b^* = \arg\min_{b \in \mathcal{M}_o} \left\{ \left\langle E \right\rangle_b + F(b) \right\}$$

- The loopy BP algorithm:
  - a fixed point iteration procedure that tries to solve b^*

The Theory Behind LBP

- But we do not optimize $q(\mathbf{X})$ explicitly, focus on the set of beliefs
  - $e.g., \quad b = \{b_{i,j} = \tau(x_i, x_j), \ \ b_i = \tau(x_i)\}$
- Relax the optimization problem
  - approximate objective: $H_{Betha} = H(b_{i,j}, b_i)$
  - relaxed feasible set: $\mathcal{M}_o = \left\{ \ \tau \geq 0 \mid \sum_{x_i} \tau(x_i) = 1, \sum_{x_i} \tau(x_i, x_j) = \tau(x_j) \ \right\}$

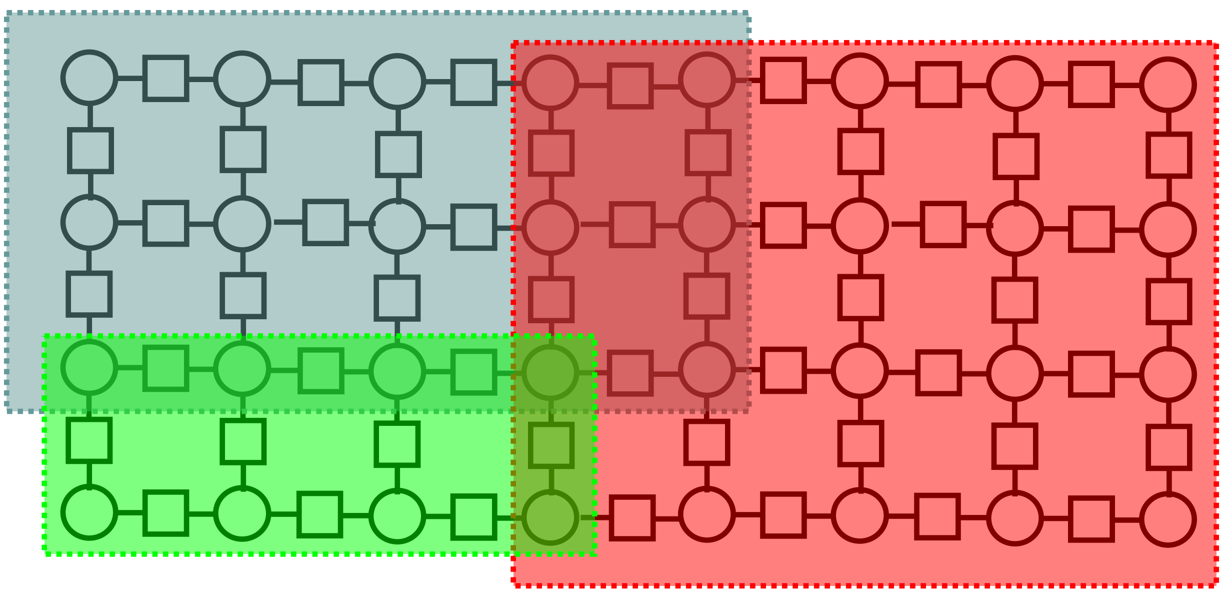
$$b^* = \arg\min_{b \in \mathcal{M}_o} \left\{ \ \langle E \rangle_b + F(b) \ \right\}$$

- The loopy BP algorithm:
  - a fixed point iteration procedure that tries to solve b^*

Region-based Approximations to the Gibbs Free Energy (Kikuchi, 1951)

Exact: $G[q(X)]$ *(intractable)*

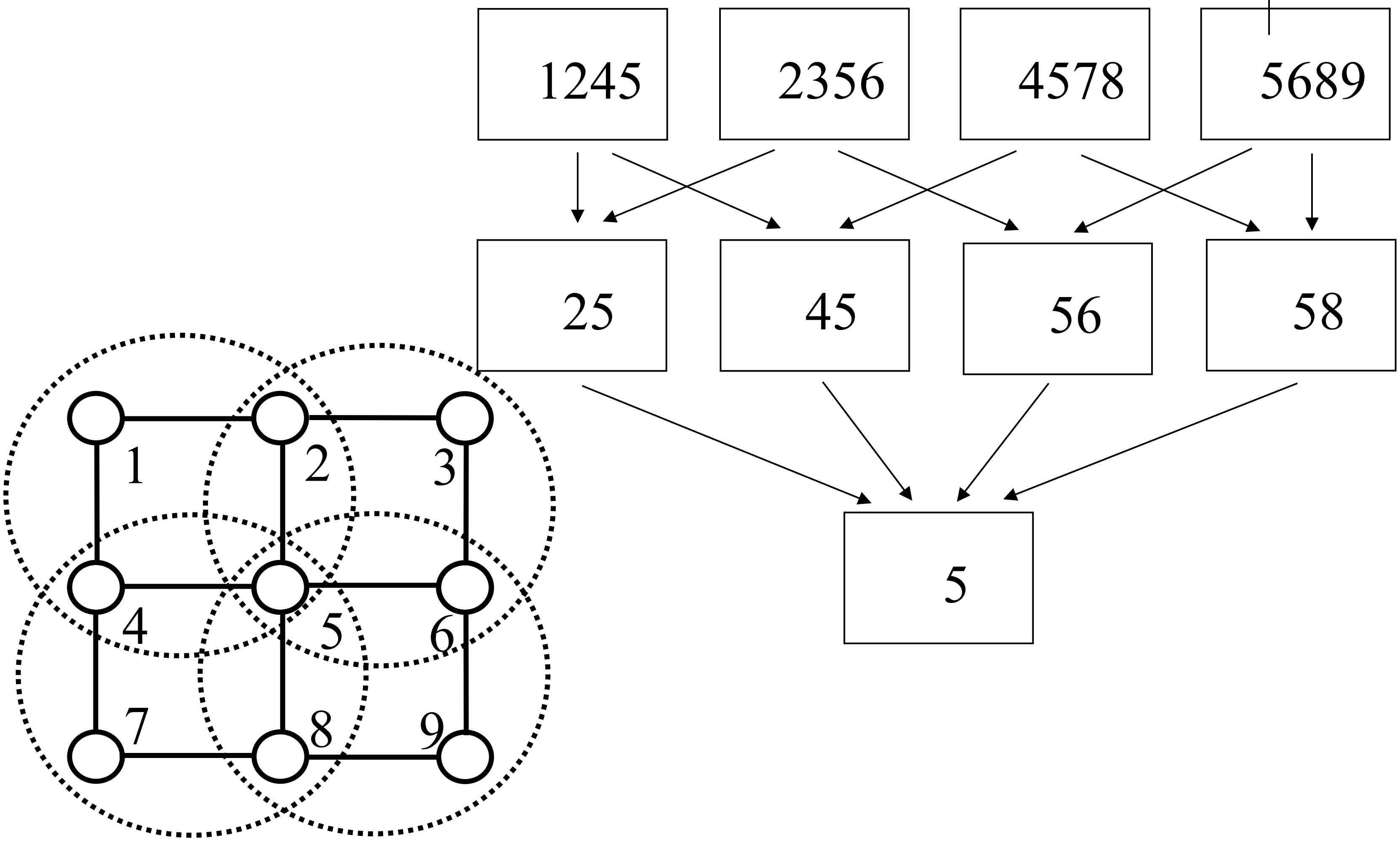
Regions: $G[\{b_r(X_r)\}]$



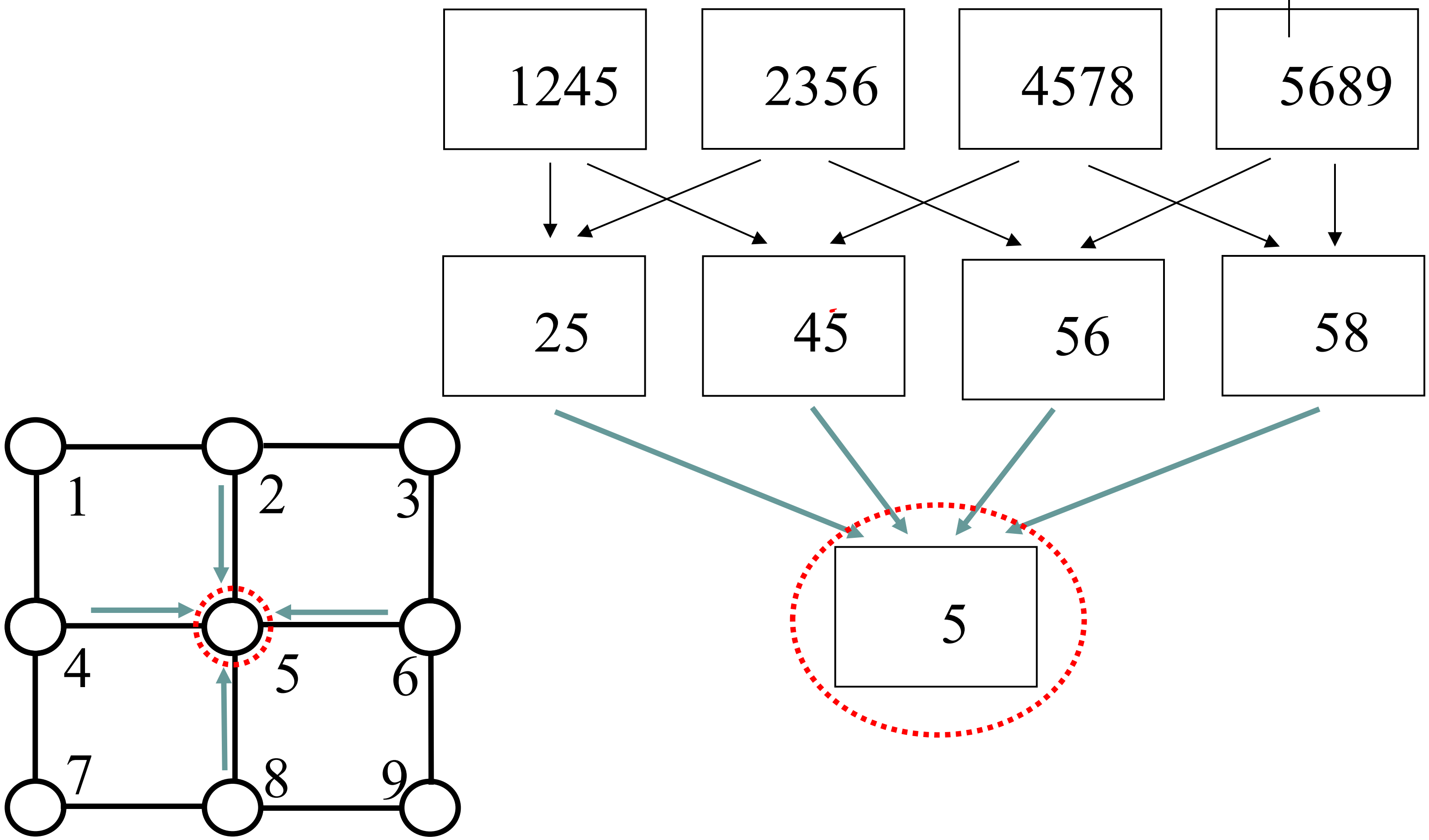
Generalized Belief Propagation

- Belief in a region is the product of:
  - Local information (factors in region)
  - Messages from parent regions
  - Messages into descendant regions from parents who are not descendants.
- Message-update rules obtained by enforcing marginalization constraints.

Generalized Belief Propagation

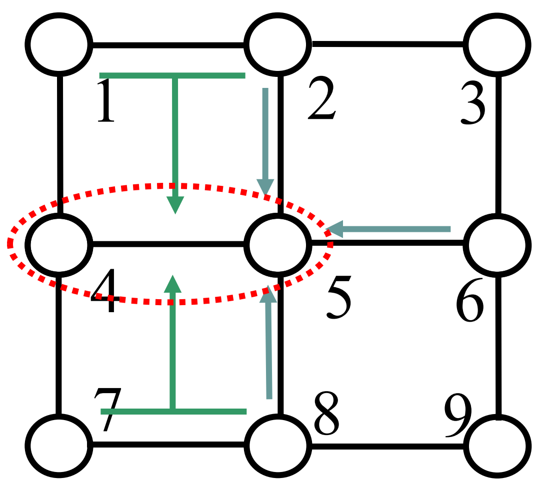


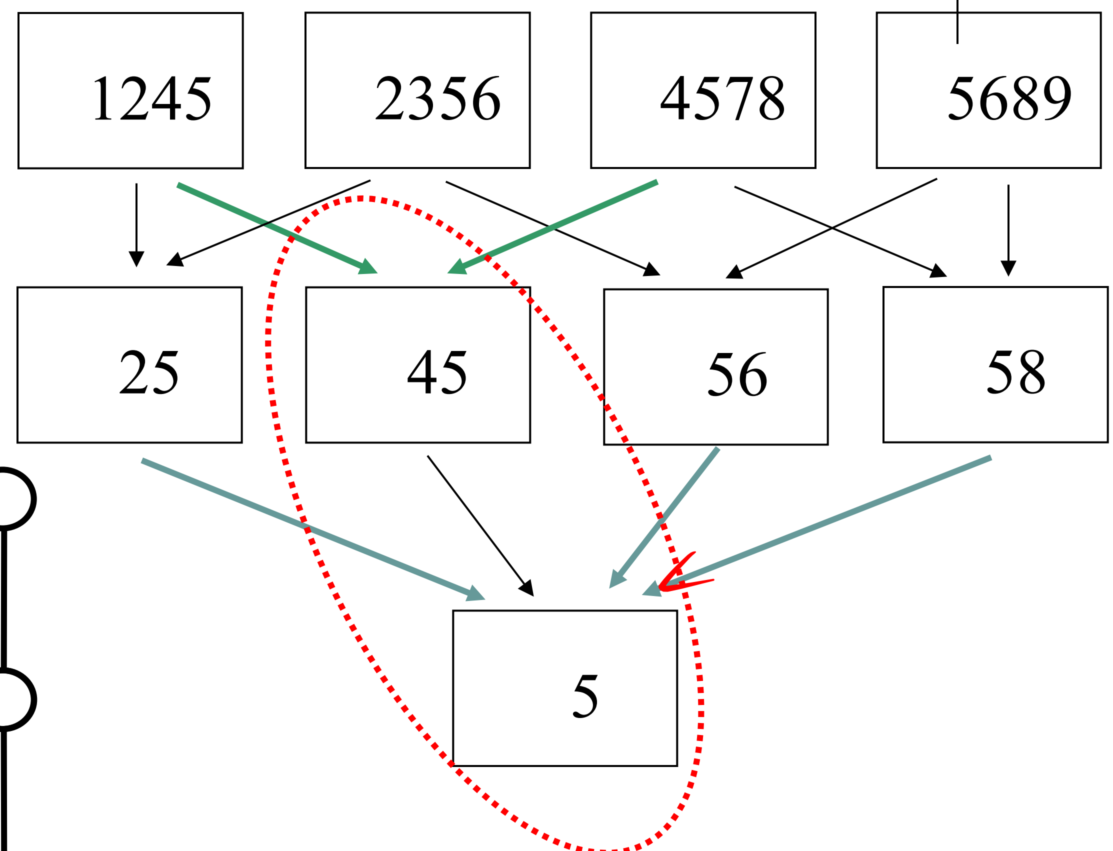
Generalized Belief Propagation



$$b_5 \propto m_{2\to 5} m_{4\to 5} m_{6\to 5} m_{8\to 5}$$

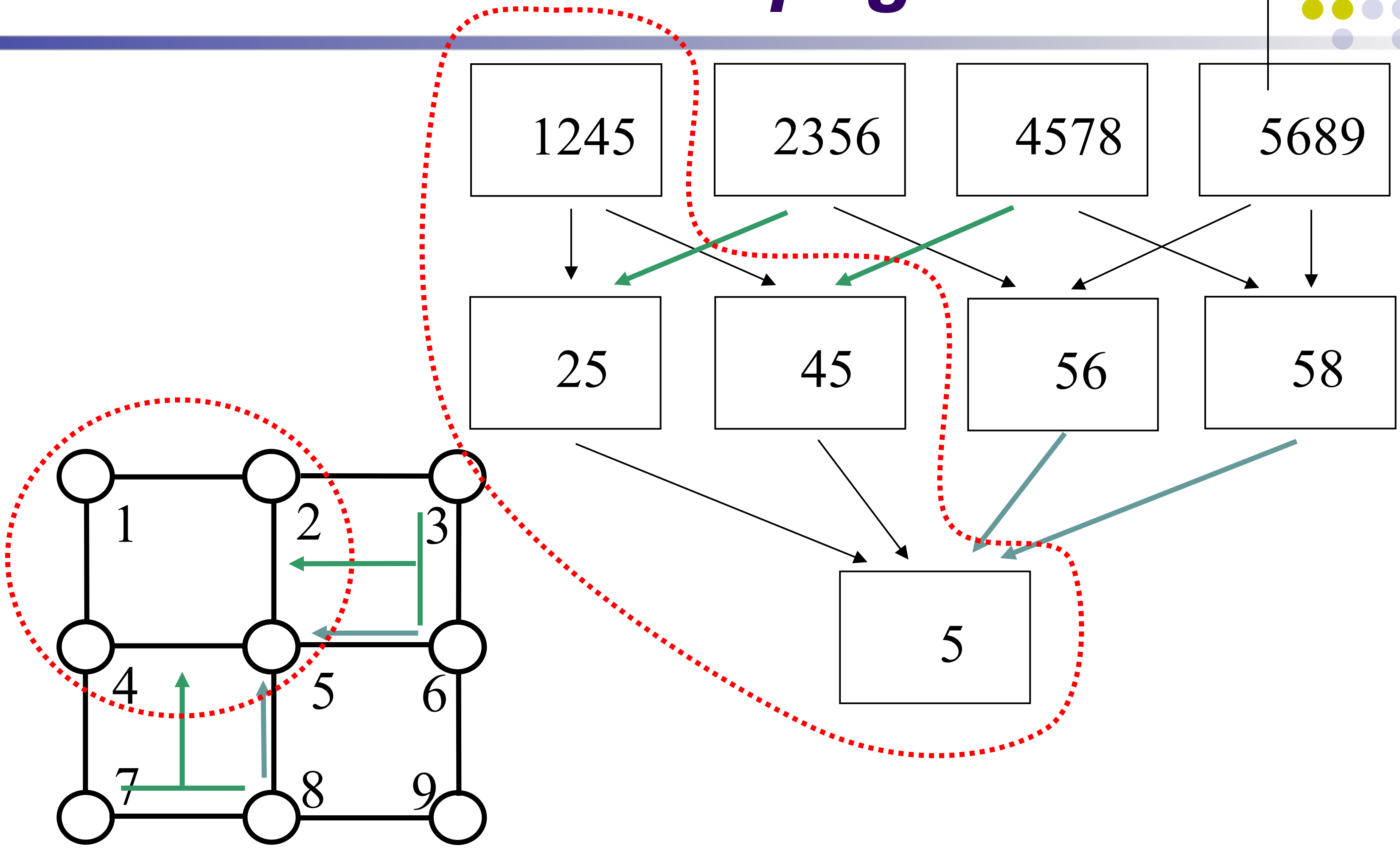
Generalized Belief Propagation





$$b_{45} \propto [f_{45}][m_{12\to45} m_{78\to45} m_{2\to5} m_{6\to5} m_{8\to5}]$$

Generalized Belief Propagation



$$b_{1245} \propto [f_{12} f_{14} f_{25} f_{45}][m_{36\to 25} m_{78\to 45} m_{6\to 5} m_{8\to 5}]$$

Some results

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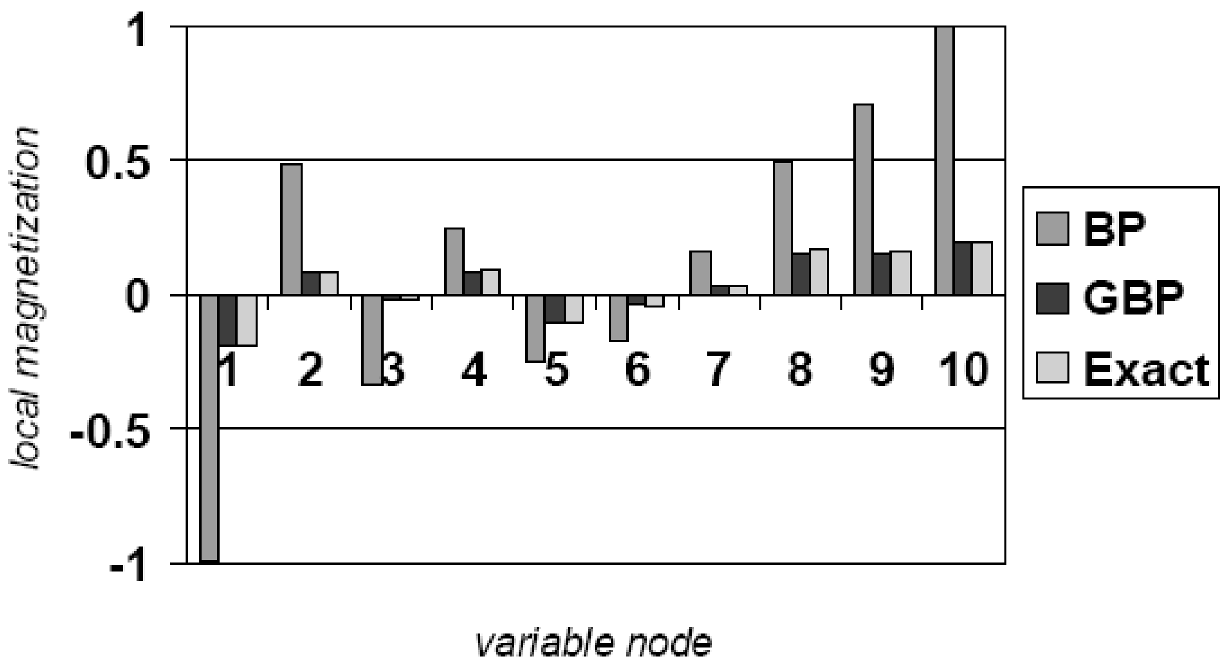

Summary

- We defined an objective function (F) for approximate inference
- However, we found that optimizing this function was hard
- We first approximated objective function F to simpler F_{bethe}
  - Minima of F_{bethe} turned out to be fixed points of BP
- Then we extended this to more complicated approximations
  - The resulting algorithms come under a family called Generalized Belief Propagation
- Next class, we will cover other methods of approximations