School of Computer Science
Carnegie Mellon

Probabilistic Graphical Models

Variational Inference:

Loopy Belief Propagation

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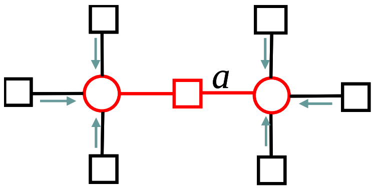
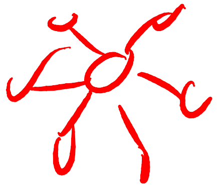
Lecture 12, February 23, 2015

Reading: See class website



Inference Problems

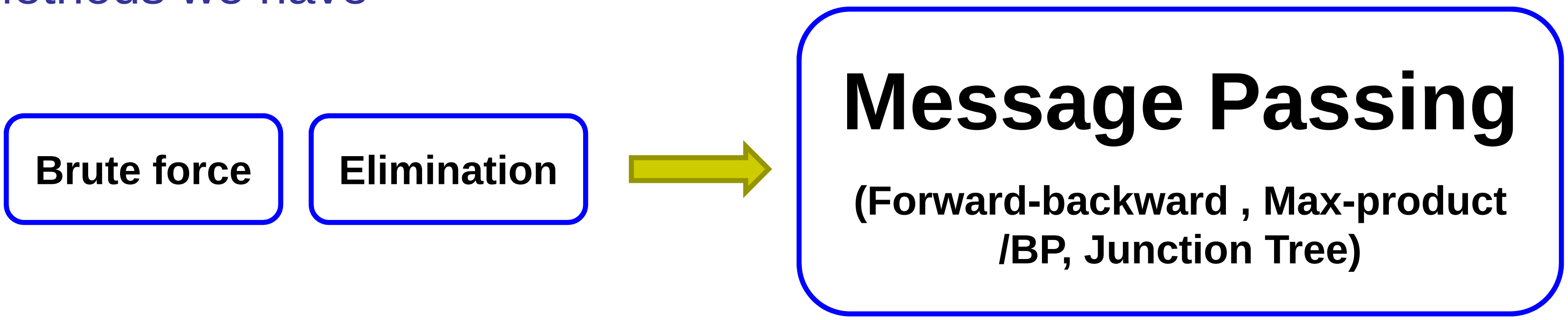


$p(x)$

$x = \{x_0, x_t\}$

- 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)

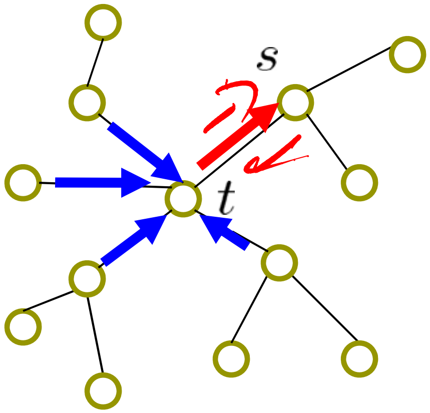
Individual computations independent

Sharing intermediate terms

Sum-Product Revisited

- Tree-structured GMs

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



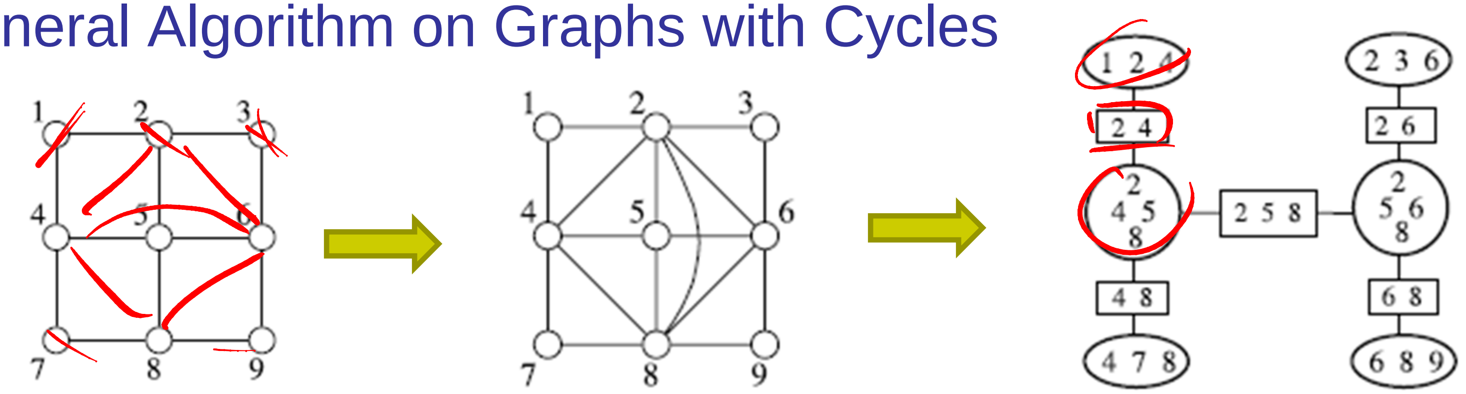
- Message Passing on Trees:

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

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

Junction Tree Revisited

- General Algorithm on Graphs with Cycles

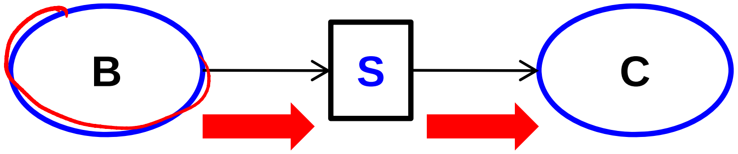


- Steps: **=> Triangularization** **=> Construct JTs**

=> Message Passing on Clique Trees

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

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



Local Consistency

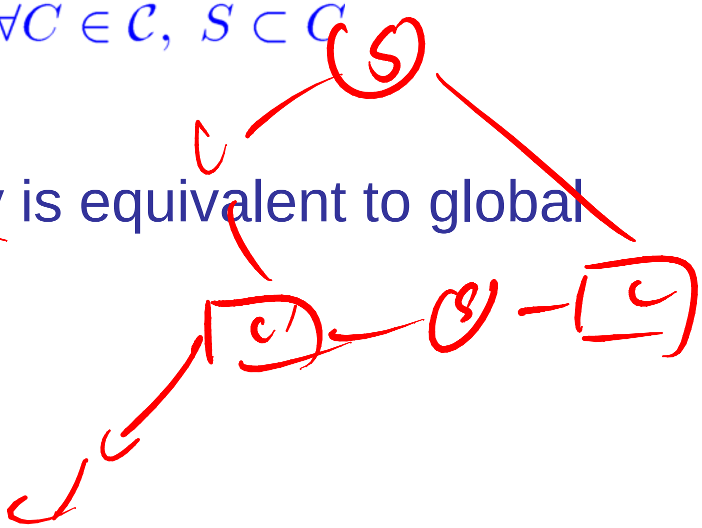
- Given a set of functions $\{\tau_C,\ C \in \mathcal{C}\}$ and $\{\tau_S,\ S \in \mathcal{S}\}$ associated with the cliques and separator sets ✓

- They are locally consistent if:

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

$\sum \phi(\ )$

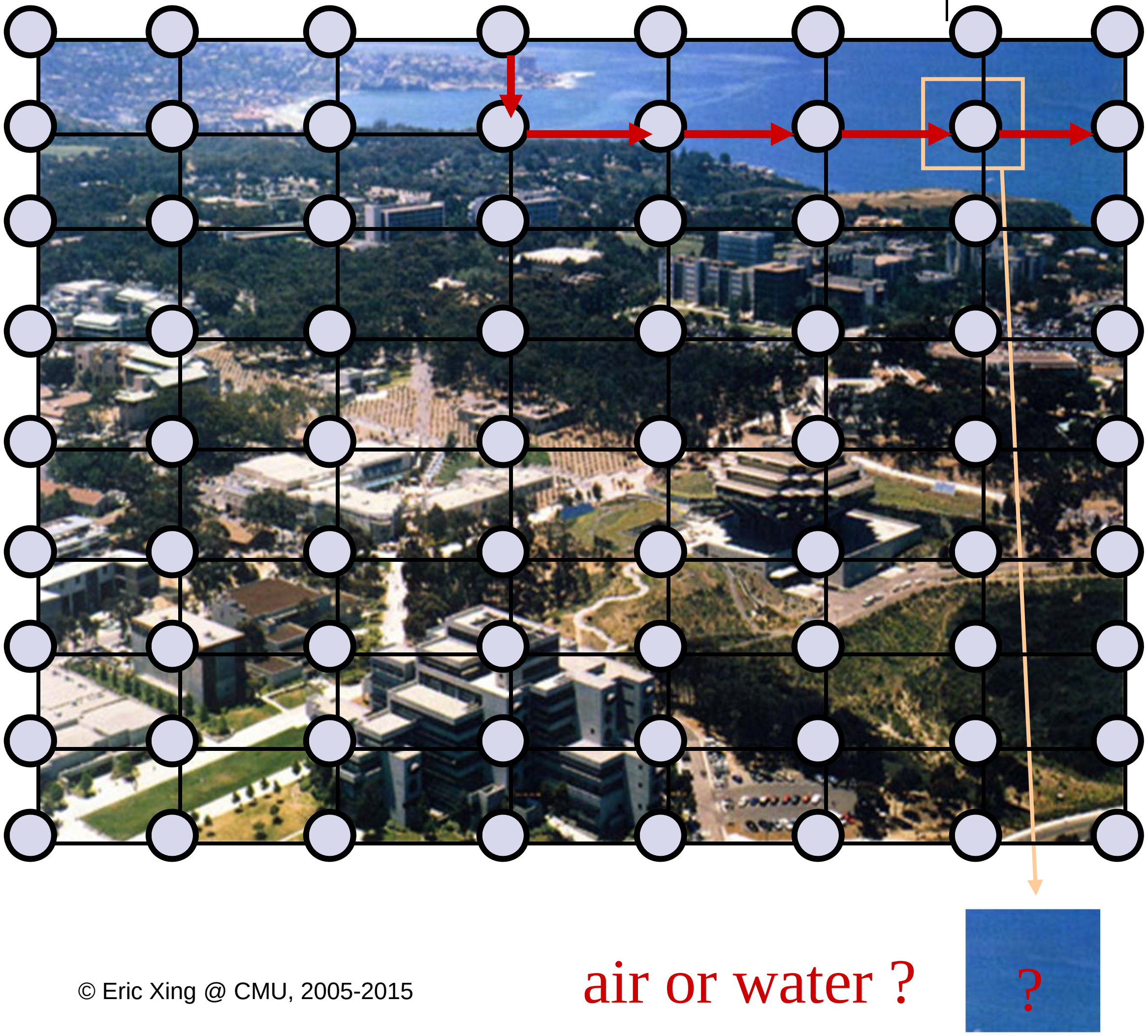
$$\underline{\sum_{x'_C | x'_S = x_S} \tau_C(x'_C) = \tau_S(x_S),\ \forall C \in \mathcal{C},\ S \subset C}$$



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

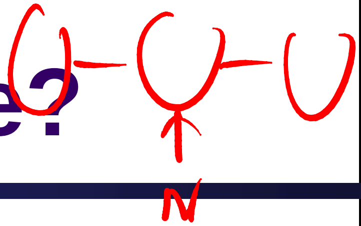
An Ising model on 2-D image

- 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.

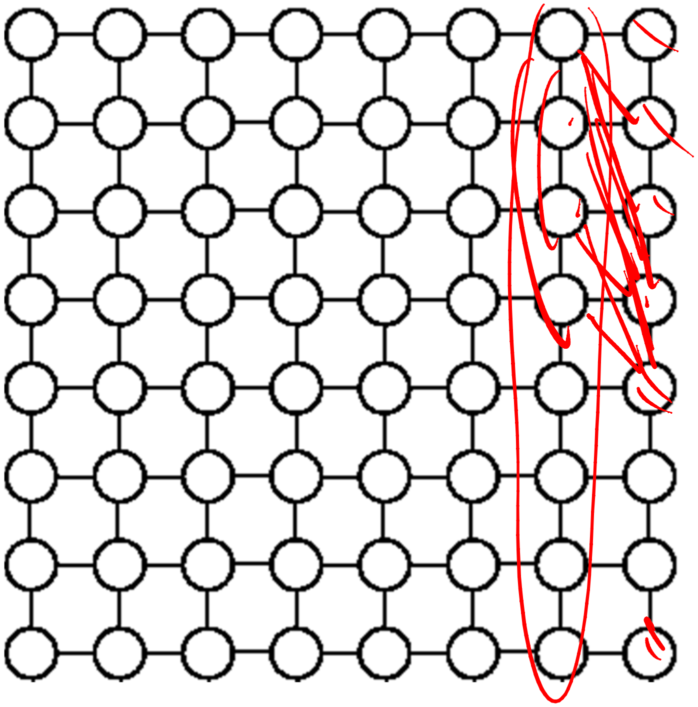


air or water ?

Why Approximate Inference?



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



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

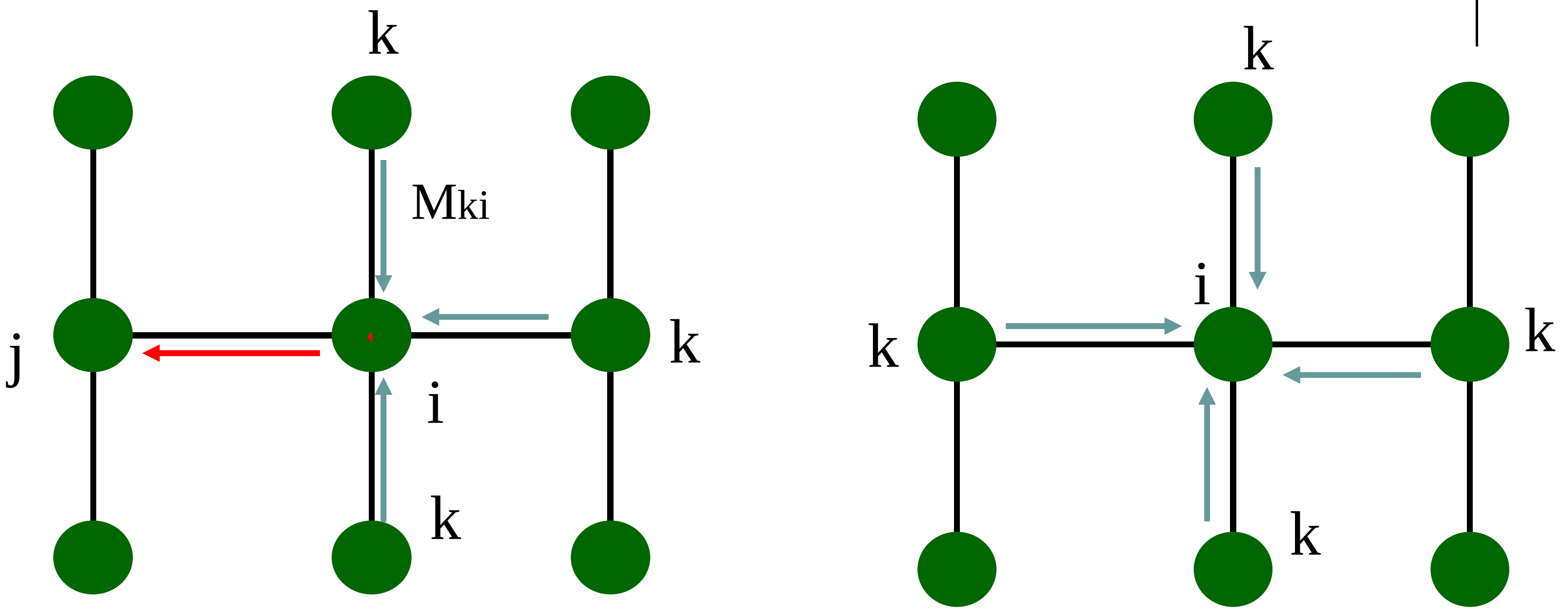
- If NxN grid, tree width at least N
- N can be a huge number(~1000s of pixels)
  - If N~O(1000), we have a clique with 2^{100} entries

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

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

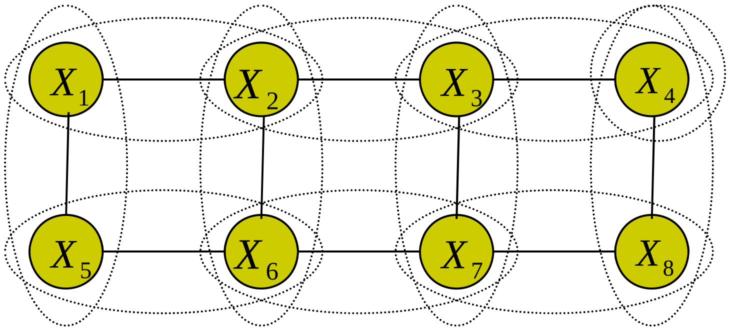
external evidence

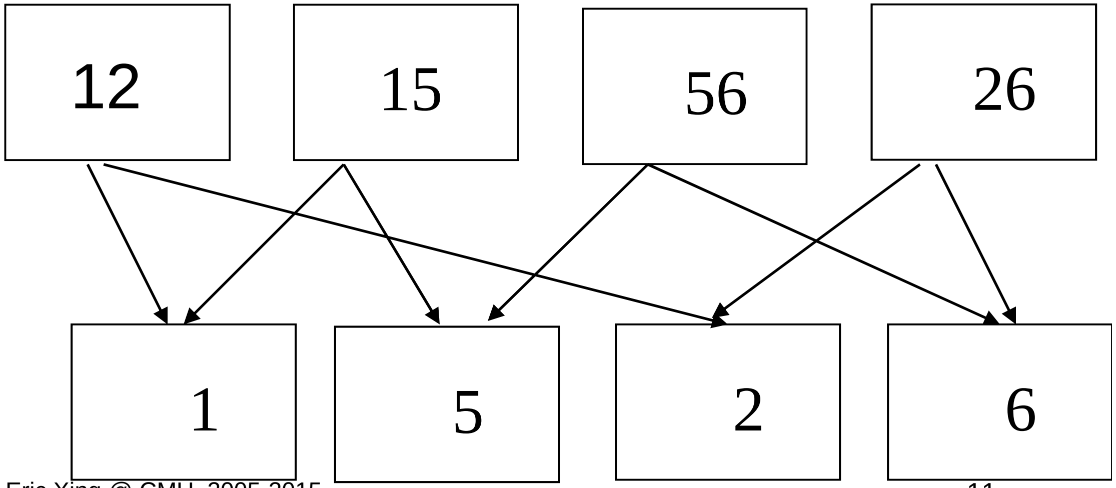
Compatibilities (interactions)

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

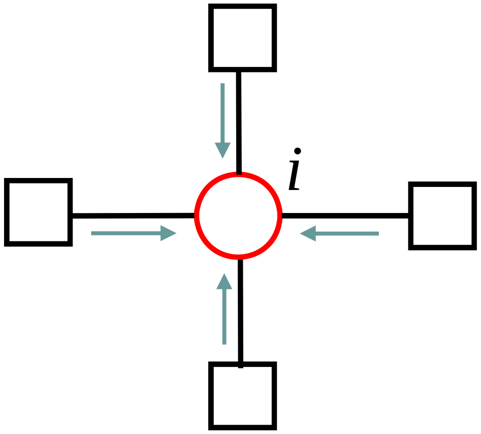
Region graphs (Factor Graph)

- 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





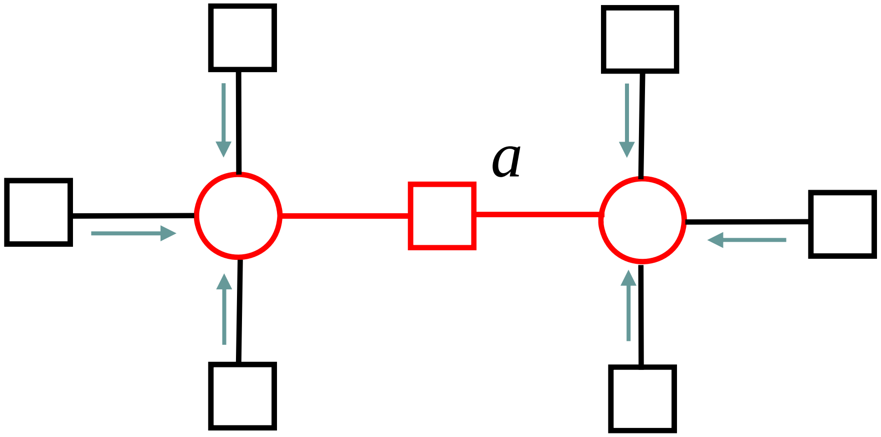
Beliefs and messages in FG



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

“beliefs”

“messages”

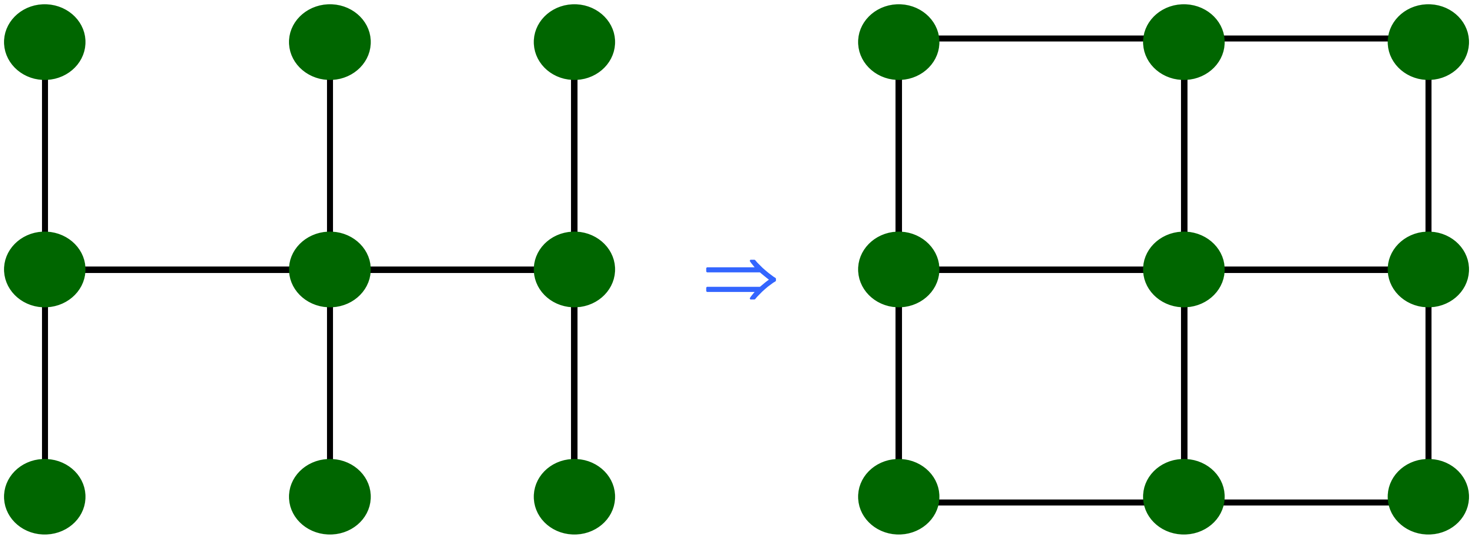


$$m_{i\to a}(x_i) = \prod_{c\in N(i)\backslash a} m_{c\to i}(x_i)$$

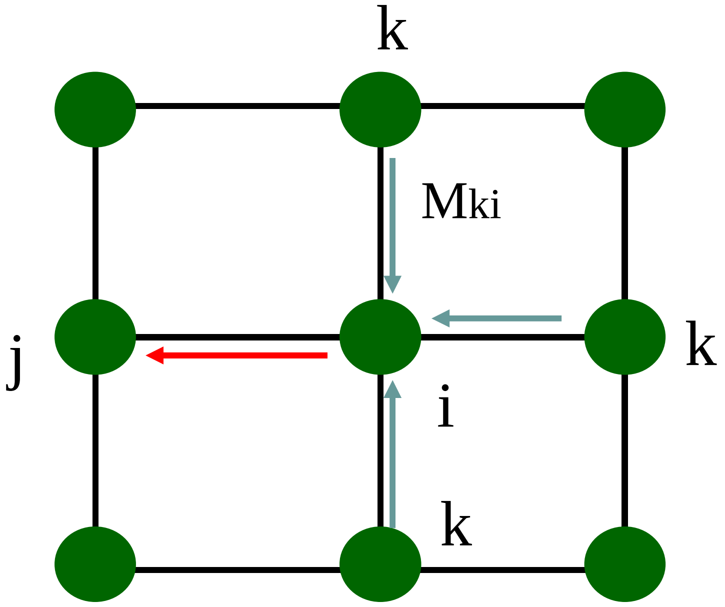
$$b_a(X_a) \propto f_a(X_a) \prod_{i\in N(a)} m_{i\to a}(x_i)$$

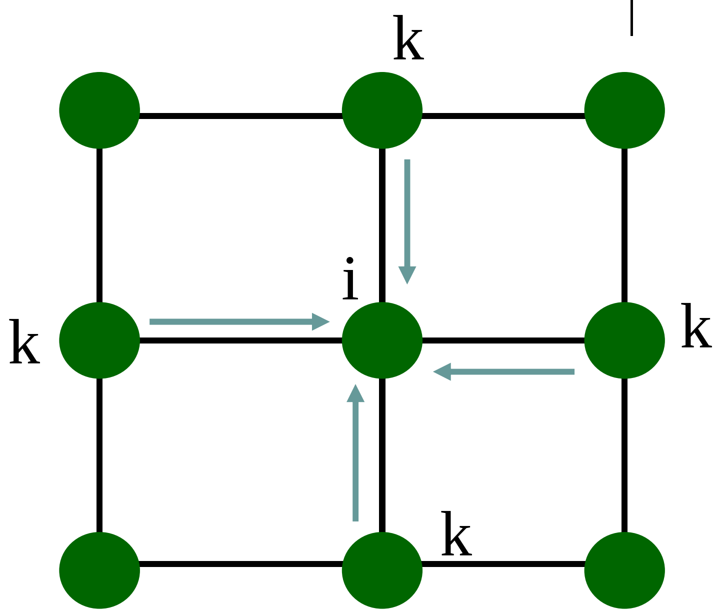
$$m_{a\to i}(x_i) = \sum_{X_a\backslash x_i} f_a(X_a) \prod_{j\in N(a)\backslash i} m_{j\to a}(x_j)$$

What if the graph is loopy?



Belief Propagation on loopy graphs





- BP Message-update Rules

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

external evidence

Compatibilities (interactions)

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

- 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

$p(x_i)$

$\hat{p}(x_i)$

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

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

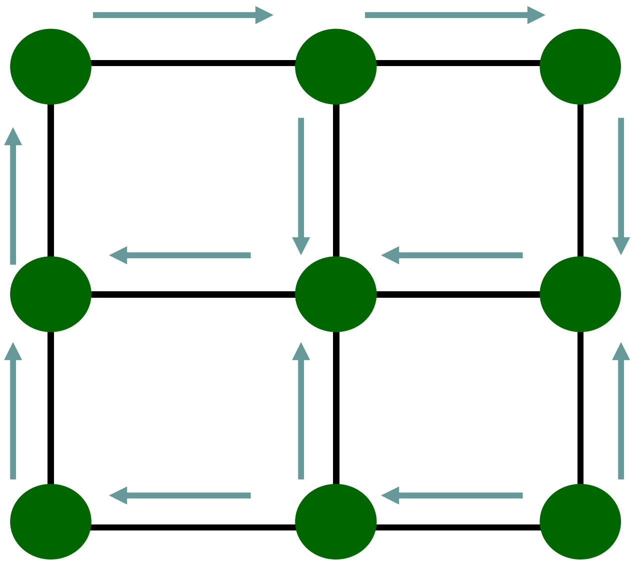
- Empirically, a good approximation is still achievable
  - Stop after fixed # of iterations
  - Stop when no significant change in beliefs
  - If solution is not oscillatory but converges, it usually is a good approximation

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?

LBP



Approximate Inference

- Let us call the actual distribution P

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

P(x) = diff

Q(x) = easy

- 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?

KL(P||Q) KL(Q||P)

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

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

$$= \sum_X Q(X)\log Q(X) - \sum_X Q(X)\log P(X)$$

$$= -H_Q(X) - E_Q \log P(X)$$

$P(X) = \frac{1}{Z}\prod \phi(x_i)$

$Q(X) = \prod q(x_i)$

$= \sum H(q_i)$

- 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" *
- $F(P,P)$ =? $-\log Z$

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

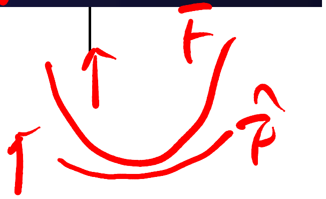
*Gibbs Free Energy

$\sum_{\alpha} \sum_{x_\alpha} F(x_\alpha)$ $\sum_{x} F(x)$

The Energy Functional

$Q(x_\alpha)$

$\sum E_{Q_\alpha} \log f_\alpha$



- 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 $\hat{F}(P,Q)$

$Q^* = \arg\max F.$

$F \sim$ hard!

$Q^* = \arg\max \hat{F}$

$F \leftarrow \tilde{F}$

$\hat{F}$

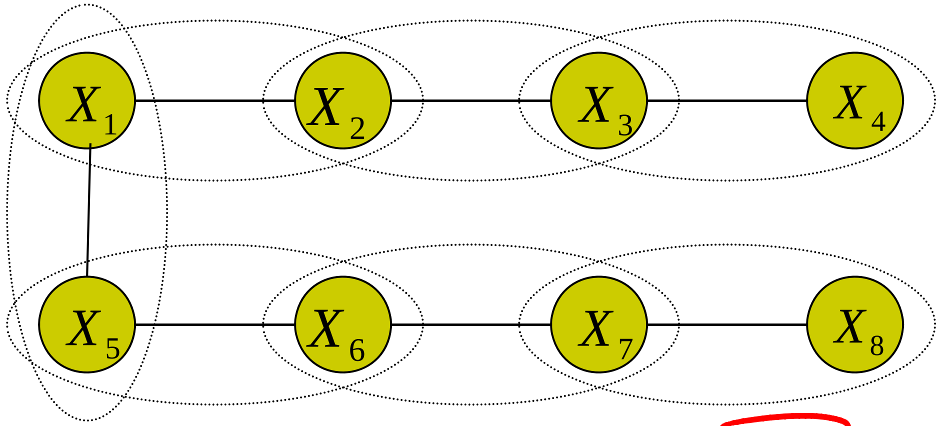
$p(\quad) = P(x|x_2)P(x_2|\ldots)$

$P(X_1 \ldots X_8) = P(x_8 . x_7) P(X_7 . X_6) P(X_6 . X_5) P(X_5 \; X_4) P(X_1 X_2) P(X_2)$ $P(X_1 \; X_4)$

Tree Energy Functionals

$P(X_1)P(X_6)P(X_5)P_1 \quad P_2 P_3 .$

- Consider a tree-structured distribution



$F_q = H + \sum G \log b(x)$

- The probability can be written as: $\underline{b(\mathbf{x}) = \prod_a \boxed{b_a(\mathbf{x}_a)} \prod_i b_i(x_i)^{1-d_i}}$

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

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

$$= F_{12} + F_{23} + .. + F_{67} + F_{78} - F_1 - F_5 - F_2 - F_6 - F_3 - F_7$$

  - involves summation over edges and vertices and is therefore easy to compute

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Bethe Approximation to Gibbs Free Energy

$F = H_\omega + \sum Q \log f(x_a)?$

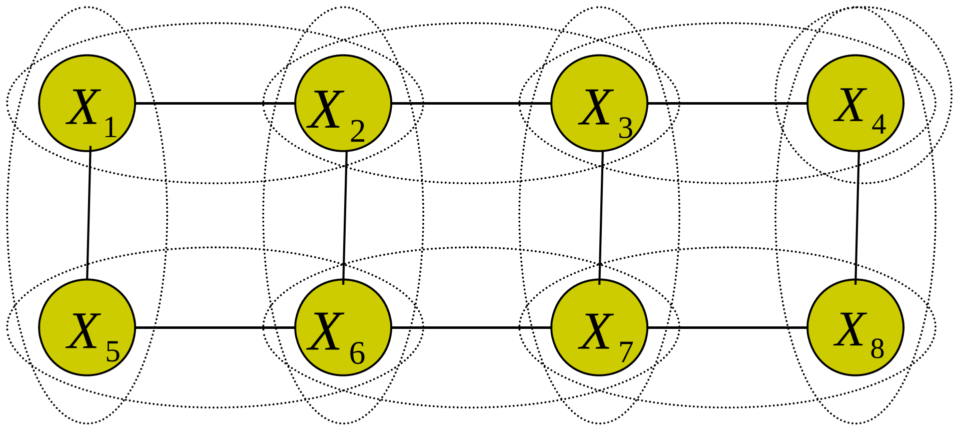
- For a general graph, choose $\hat{F}(P,Q) = F_{Betha}$

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

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

$$P \neq \prod b(x_a) \prod b(x_i)^{-d+1}$$

- Called “Bethe approximation” after the physicist Hans Bethe



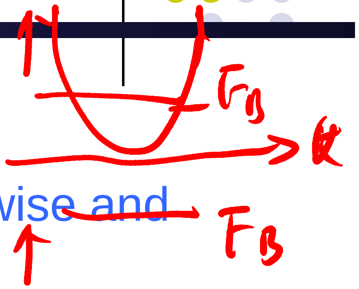
$$F_{bethe} = F_{12} + F_{23} + .. + F_{67} + F_{78} - F_1 - F_5 - 2F_2 - 2F_6 .. - F_8$$

- 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

$F_{bethe} \neq F_G$

$\gtrless$

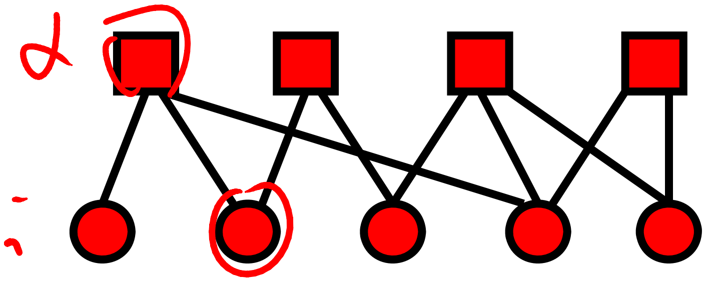


- Pros:
  - Easy to compute, since entropy term involves sum over pairwise and single variables
- Cons:
  - $\hat{F}(P,Q) = \underline{F_{bethe}}$ **may or may not** be well connected to $\underline{F(P,Q)}$
  - It could, in general, be greater, equal or less than $F(P,Q)$
- Optimize each $b(\mathbf{x}_a)$'s.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

$F_B(\underline{b_\alpha}\ \underline{b_i})$

Bethe Free Energy for FG

$\{\underline{b_i}\ \underline{b_\alpha}\} = \arg\max F_B$



$\sum_{x_i} b_i(x_i) = 1$

$\sum_{x_\alpha} b_\alpha(x_\alpha) = 1$

$\sum_{x_\alpha \backslash i} b(x_\alpha) = b(x_i)$

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

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

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

$\{b_i^* \quad b_\alpha^*\} = \arg\max(F_B)$

Minimizing the Bethe Free Energy

- $$L = F_{Bethe} + \sum_i \gamma_i \{1 - \sum_{x_i} \underline{b_i(x_i)}\}$$ $\boxed{\frac{\gamma_i}{\lambda_{x}}}$

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

田

- Set derivative to zero

$$\frac{\partial L}{\partial b_i} = 0$$

$$\frac{\partial L}{\partial b_\alpha} = 0$$

Constrained Minimization of the Bethe Free Energy

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

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

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

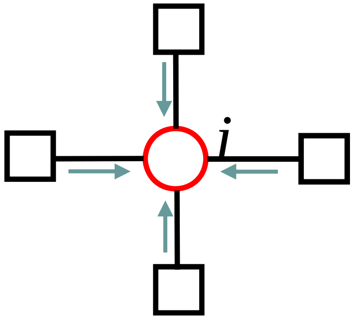
$$\frac{\partial L}{\partial b_a(X_a)} = 0 \quad \Longrightarrow \quad b_a(X_a) \propto \exp\left(-E_a(X_a) + \sum_{i \in N(a)} \lambda_{ai}(x_i) \right)$$

Bethe = BP on FG

- We had:

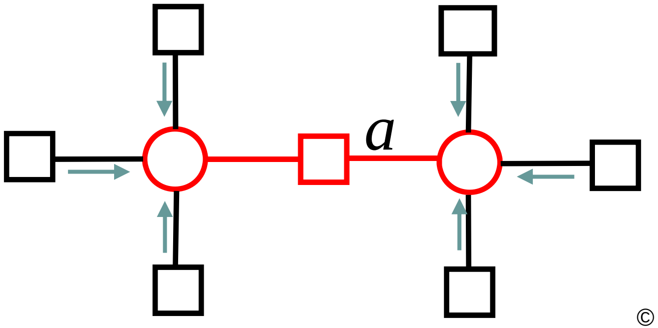
$$\underline{b_i(x_i)} \propto \exp\left(\frac{1}{d_i - 1} \sum_{a \in N(i)} \lambda_{ai}(x_i) \right) \qquad \underline{b_a(X_a)} \propto \exp\left(-\log f_a(X_a) + \sum_{i \in N(a)} \lambda_{ai}(x_i) \right)$$

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



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

“beliefs” “messages”



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

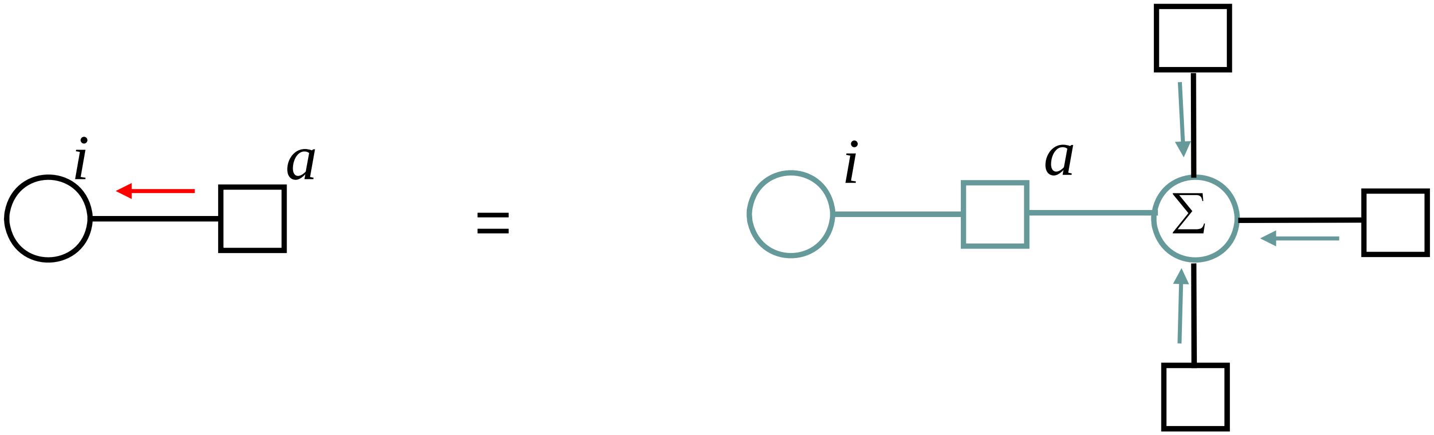
The “belief” is the BP approximation of the marginal probability.

BP Message-update Rules

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

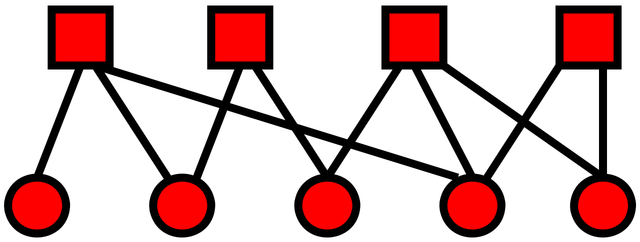
$$\boxed{m_{a\to i}(x_i) = \sum_{X_a \backslash x_i} f_a(X_a) \prod_{j\in N(a)\backslash i} \prod_{b\in N(j)\backslash a} m_{b\to j}(x_j)}$$

(A sum product algorithm)



Summary so far

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

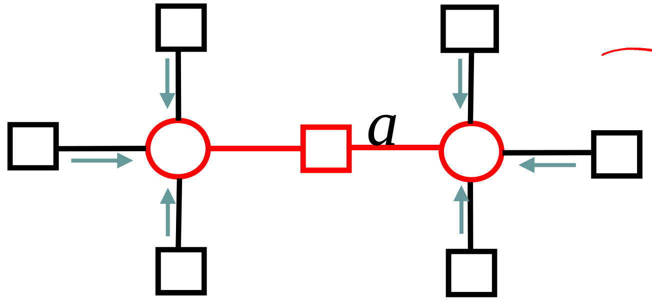


$$F(P,Q) = -H_Q(X) - \sum_{f_a \in F} E_Q \log f_a(X_a)$$

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

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

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



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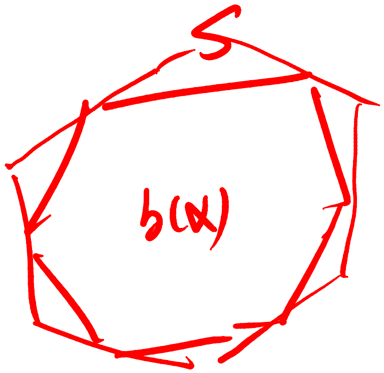
The Theory Behind LBP

$Q \Rightarrow P$

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

h_i

h_α



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

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

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

q : a (tractable) probability distribution

The Theory Behind LBP

- But we do not optimize *q*(**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: $\mathcal{M} \to \mathcal{M}_o \quad (\mathcal{M}_o \supseteq \mathcal{M})$

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

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

The Theory Behind LBP

- But we do not optimize *q*(**X**) explicitly, focus on the set of beliefs
  - $e.g., \quad b = \{ b_{i,j} = \tau(x_i, x_j), \quad b_i = \tau(x_i) \}$
- 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)

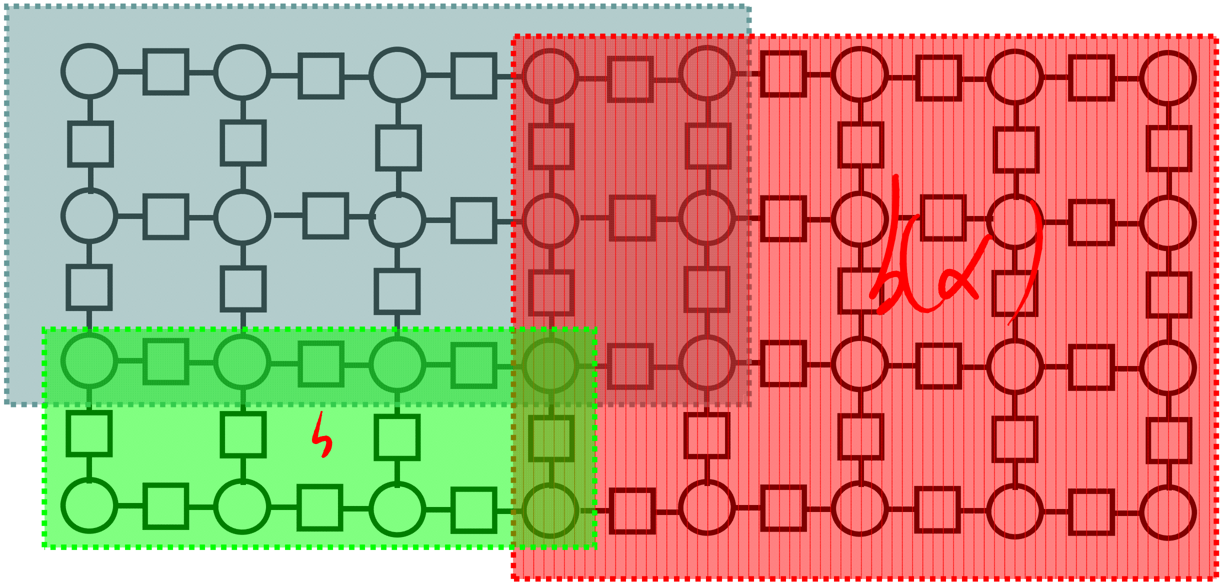
$\theta_m \leftarrow b_i$

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

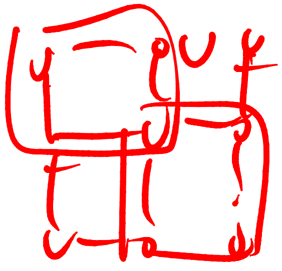
Regions: $G[\{b_r(X_r)\}]$

Q_B b_α

b_i



Q_C

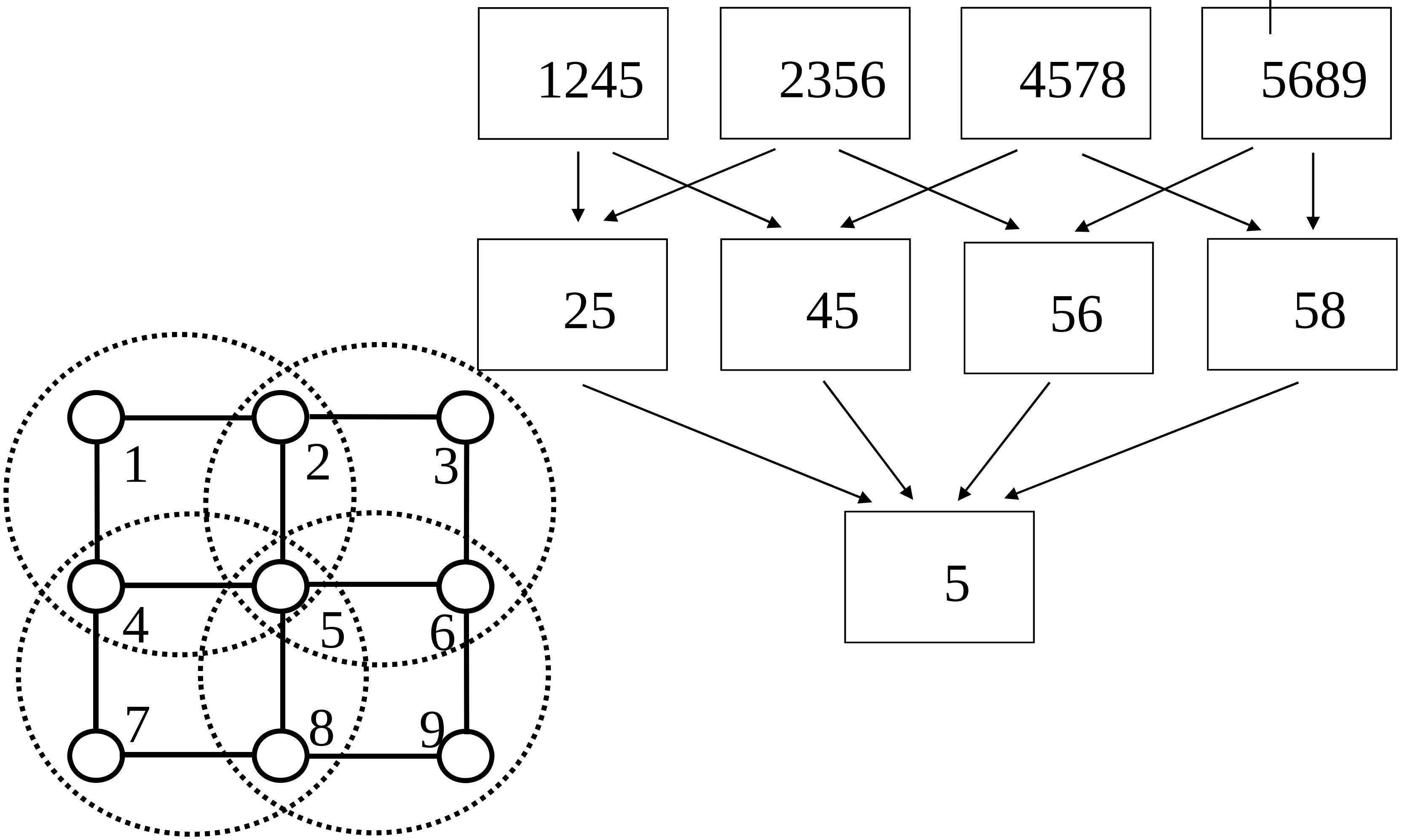


$b_{\hat{\alpha}}$

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

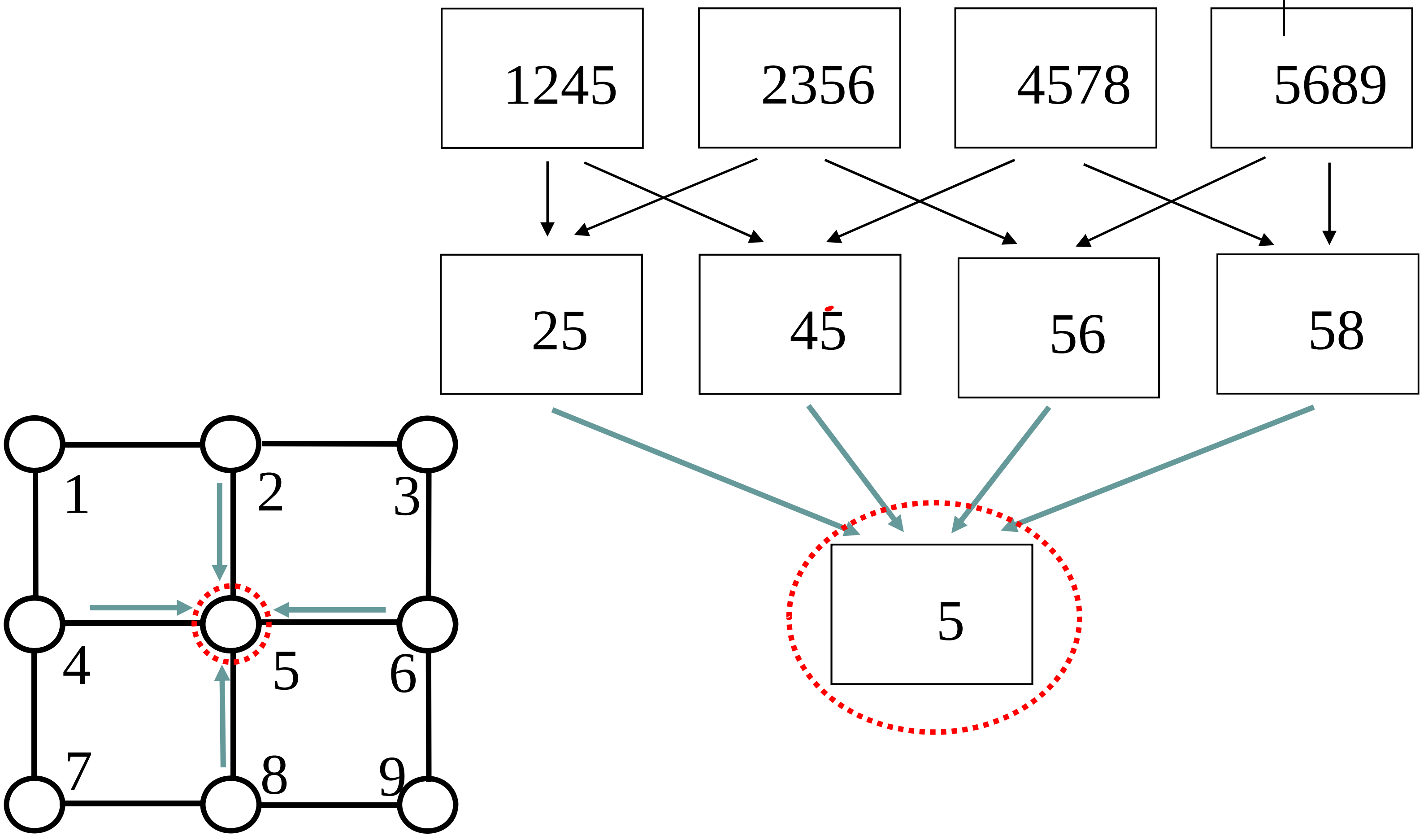


1245 2356 4578 5689

25 45 56 58

5

Generalized Belief Propagation



1245

2356

4578

5689

25

45

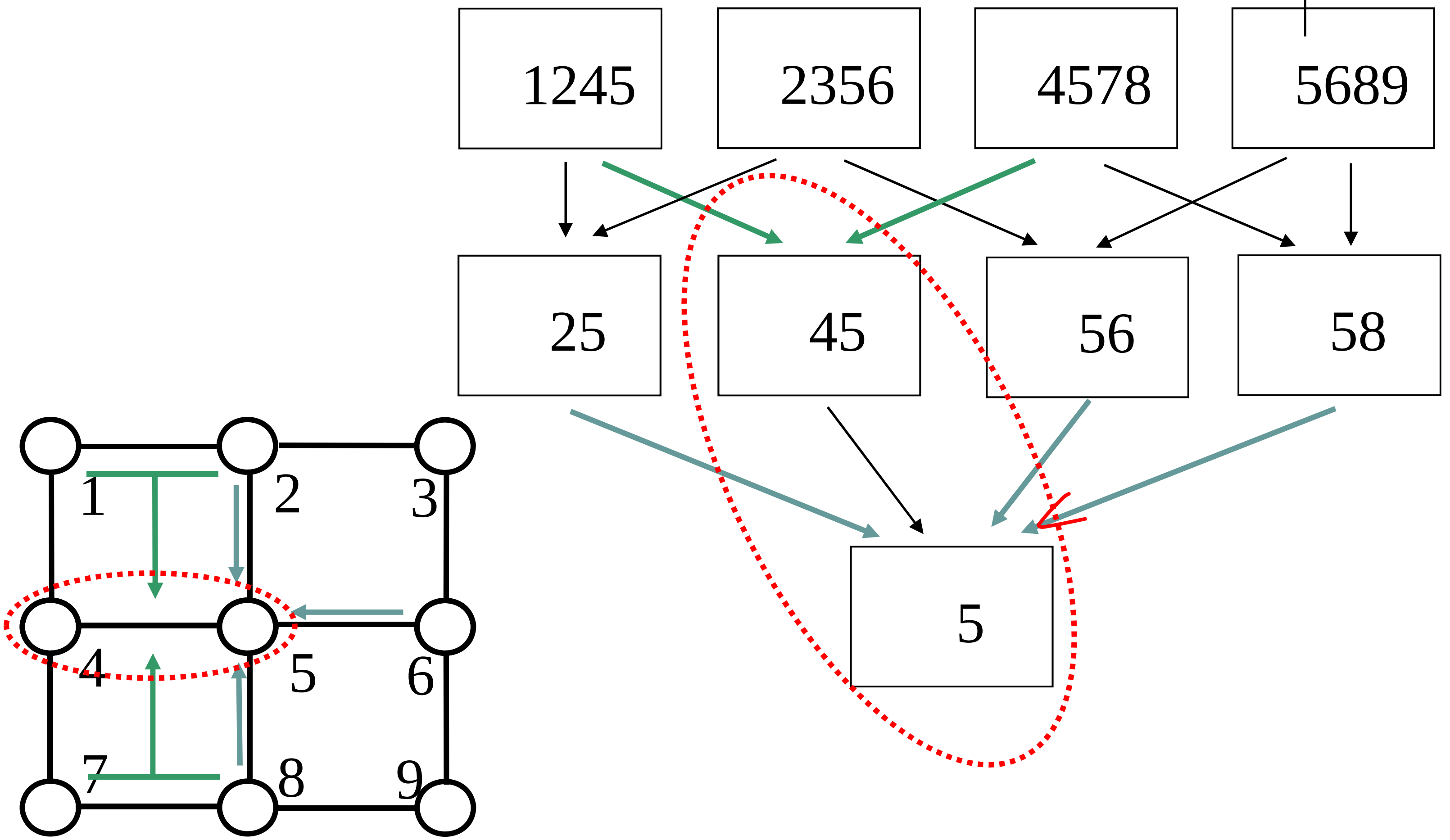
56

58

5

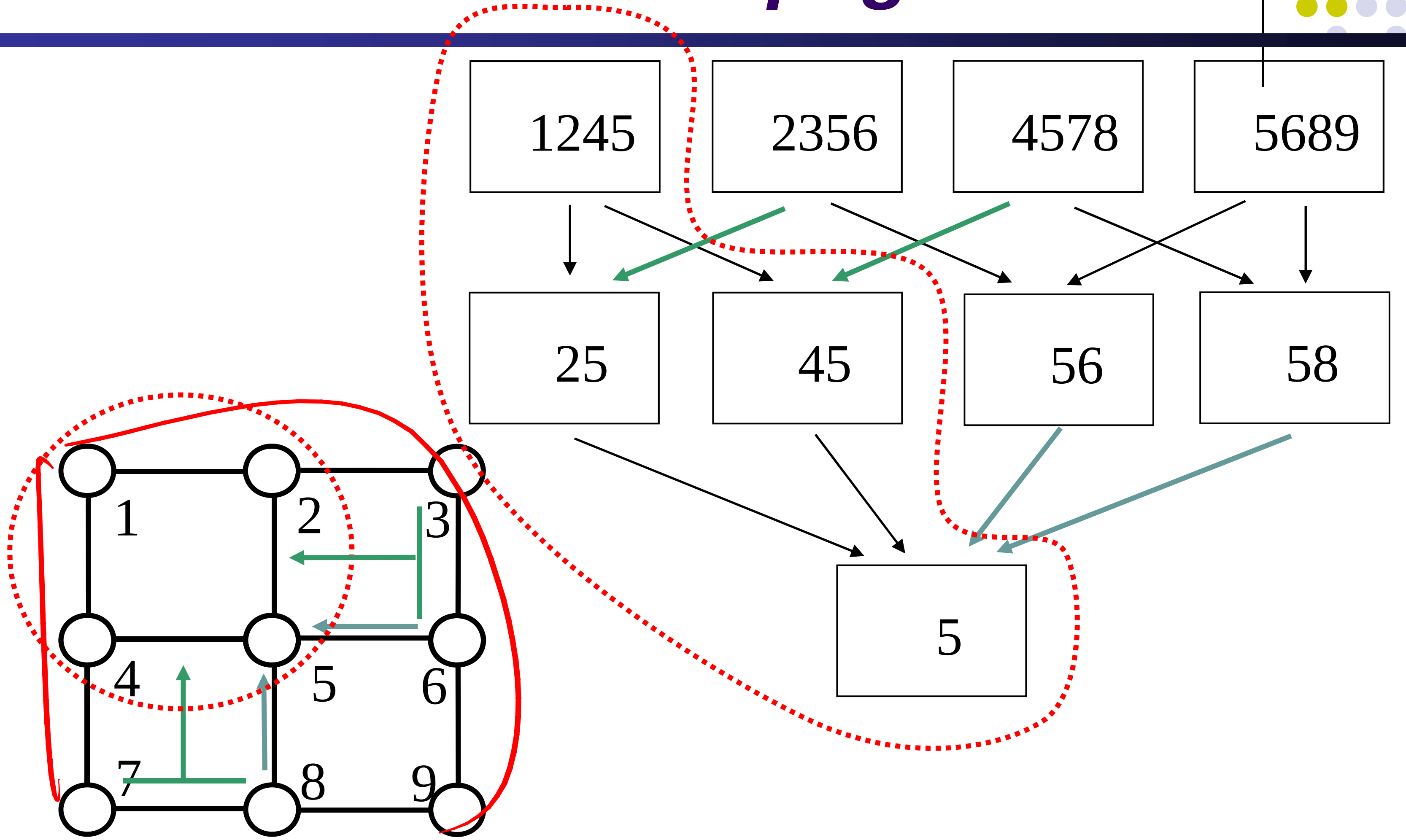
$$b_5 \propto m_{2\to5} m_{4\to5} m_{6\to5} m_{8\to5}$$

Generalized Belief Propagation



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

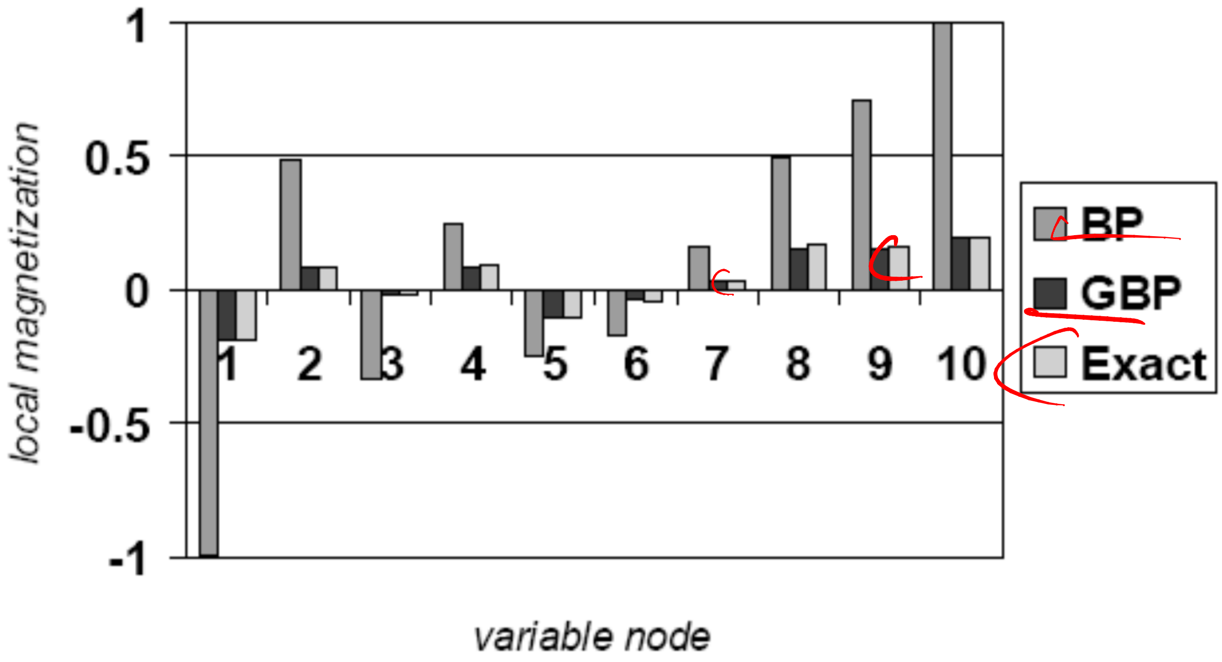
Generalized Belief Propagation



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

Some results

-



LBP ?

Summary

$$\begin{tikzcd} F \arrow[d] \\ F_\alpha \arrow[d] \\ b_i. \quad b_\alpha \end{tikzcd}$$

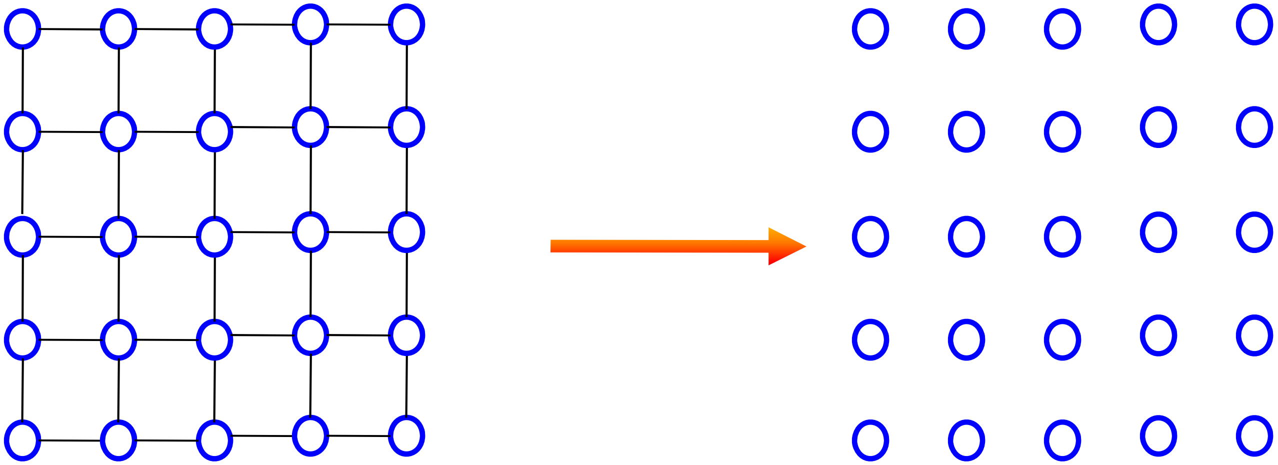
- We defined an objective function (F) for approximate inference
- However, we found that optimizing this function was hard
- We first approximated objective function F to simpler F_{bethe}
  - Minima of F_{bethe} turned out to be fixed points of BP
- Then we extended this to more complicated approximations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

Mean Field Approximation

Naïve Mean Field

- Fully factorized variational distribution

$$q(x) = \prod_{s \in V} q(x_s)$$



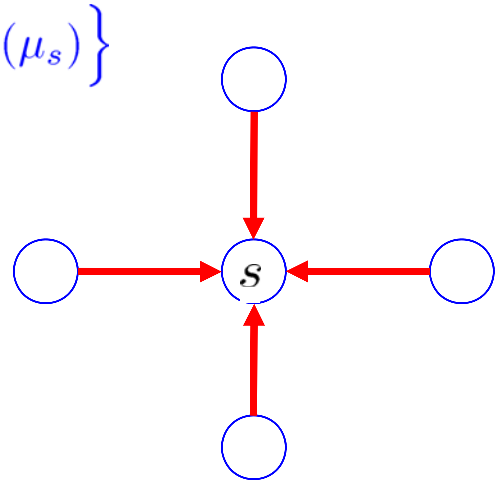
Naïve Mean Field for Ising Model

- Optimization Problem

$$\max_{\mu \in [0,1]^m} \left\{ \sum_{s \in V} \theta_s \mu_s + \sum_{(s,t) \in E} \theta_{st} \mu_s \mu_t + \sum_{s \in V} H_s(\mu_s) \right\}$$

- Update Rule

$$\mu_s \leftarrow \sigma\left(\theta_s + \sum_{t \in N(s)} \theta_{st} \mu_t \right)$$



- $\mu_t = p(X_t = 1) = \mathbb{E}_p[X_t]$ resembles "message" sent from node t to s

- $\{\mathbb{E}_p[X_t], t \in N(s)\}$ forms the "mean field" applied to s from its neighborhood

Mean field methods

- Optimize $q(\mathbf{X}_H)$ in the space of tractable families
  - *i.e.*, subgraph of G_p over which exact computation of H_q is feasible

- Tightening the optimization space
  - exact objective: H_q
  - tightened feasible set: $\mathcal{Q} \rightarrow \mathcal{T} \quad (\mathcal{T} \subseteq \mathcal{Q})$

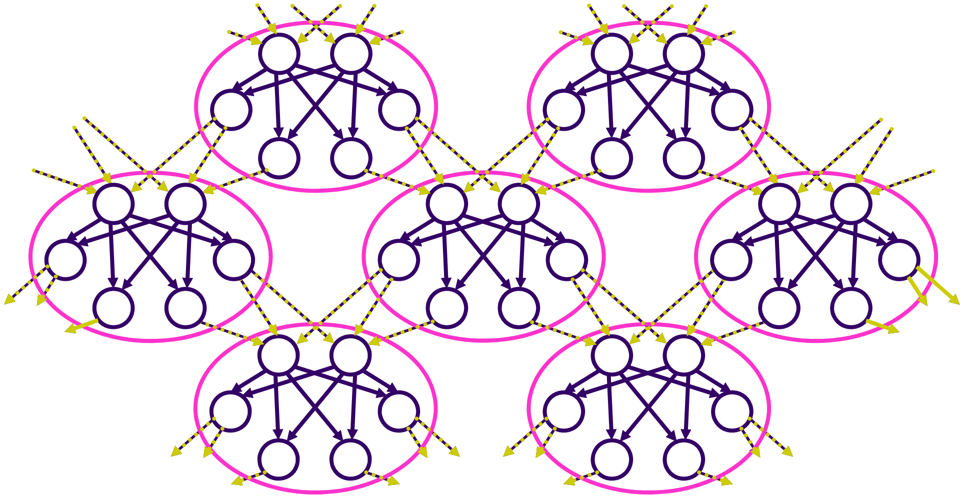
$$q^* = \arg\min_{q \in \mathcal{T}} \langle E \rangle_q - H_q$$

Cluster-based approx. to the Gibbs free energy

(Wiegerinck 2001, Xing *et al* 03,04)

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

Clusters: $G[\{q_c(X_c)\}]$



Mean field approx. to Gibbs free energy

- Given a disjoint clustering, {C$_1$, … , C$_l$}, of all variables
- Let
$$q(\mathbf{X}) = \prod_i q_i(\mathbf{X}_{C\,i}),$$
- Mean-field free energy

$$G_{\mathrm{MF}} = \sum_i \sum_{\mathbf{x}_{C_i}} \prod_i q_i(\mathbf{x}_{C_i}) E(\mathbf{x}_{C_i}) + \sum_i \sum_{\mathbf{x}_{C_i}} q_i(\mathbf{x}_{C_i}) \ln q_i(\mathbf{x}_{C_i})$$

e.g., $$G_{\mathrm{MF}} = \sum_{i<j} \sum_{x_i x_j} q(x_i) q(x_j) \phi(x_i x_j) + \sum_i \sum_{x_i} q(x_i) \phi(x_i) + \sum_i \sum_{x_i} q(x_i) \ln q(x_i)$$ (naïve mean field)

  - Will **never** equal to the exact Gibbs free energy no matter what clustering is used, but it does **always** define a lower bound of the likelihood

- Optimize each $q_i(x_c)$'s.
  - Variational calculus …
  - Do inference in each $q_i(x_c)$ using any tractable algorithm

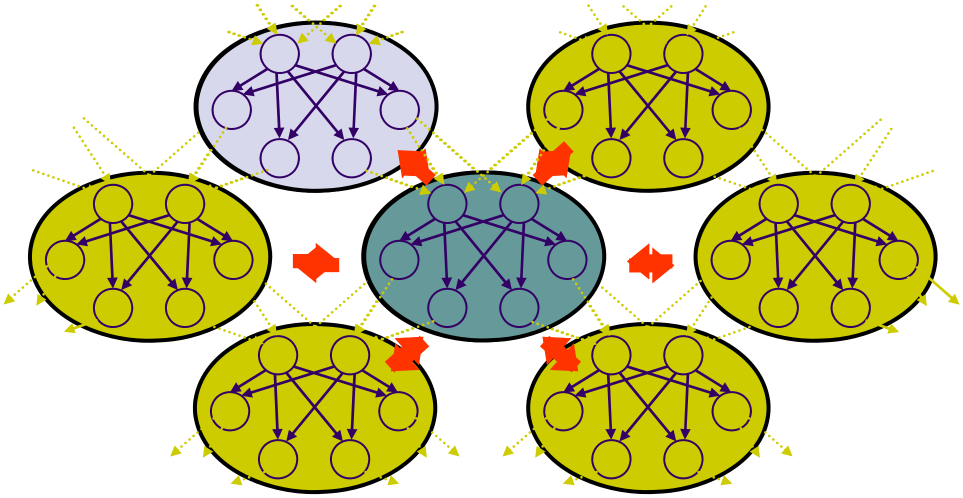
The Generalized Mean Field theorem

Theorem: The optimum GMF approximation to the cluster marginal is isomorphic to the cluster posterior of the original distribution given internal evidence and its generalized mean fields:

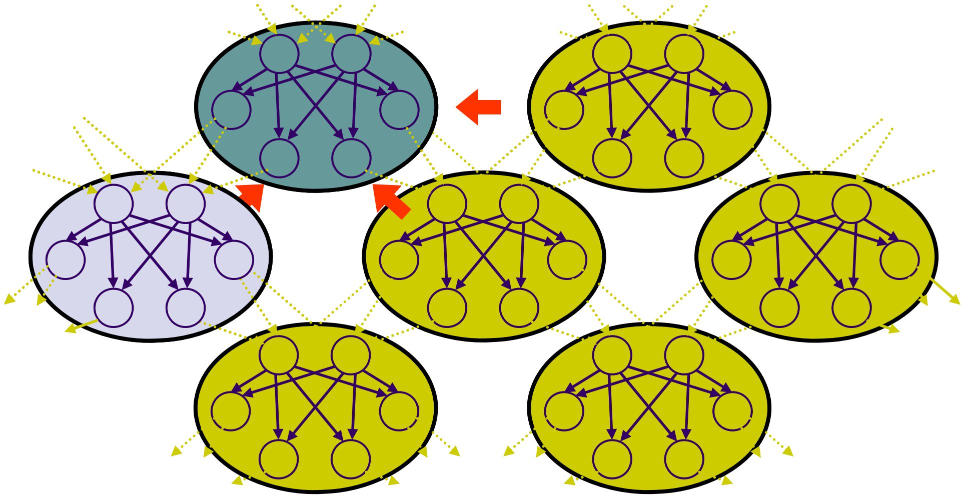
$$q_i^*(\mathbf{X}_{H,C_i}) = p(\mathbf{X}_{H,C_i} \mid \mathbf{x}_{E,C_i}, \langle \mathbf{X}_{H,MB_i} \rangle_{q_{j \neq i}})$$

GMF algorithm: Iterate over each q_i

A generalized mean field algorithm [xing *et al*. UAI 2003]



A generalized mean field algorithm [xing *et al*. UAI 2003]



Convergence theorem

Theorem: The GMF algorithm is guaranteed to converge to a local optimum, and provides a lower bound for the likelihood of evidence (or partition function) the model.

The naive mean field approximation

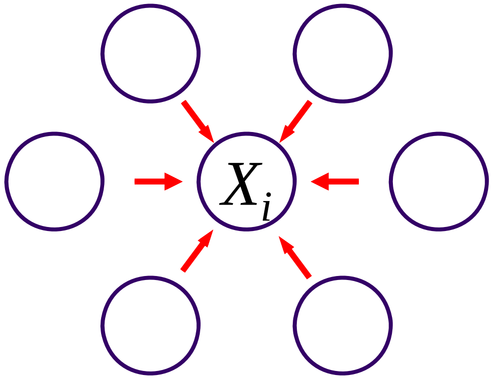
- Approximate $p(\mathbf{X})$ by fully factorized $q(\mathbf{X})=\mathrm{P}_i q_i(X_i)$

- For Boltzmann distribution $p(X)=\exp\{\sum_{i<j} q_{ij}X_iX_j+q_{io}X_i\}/Z$:

mean field equation:

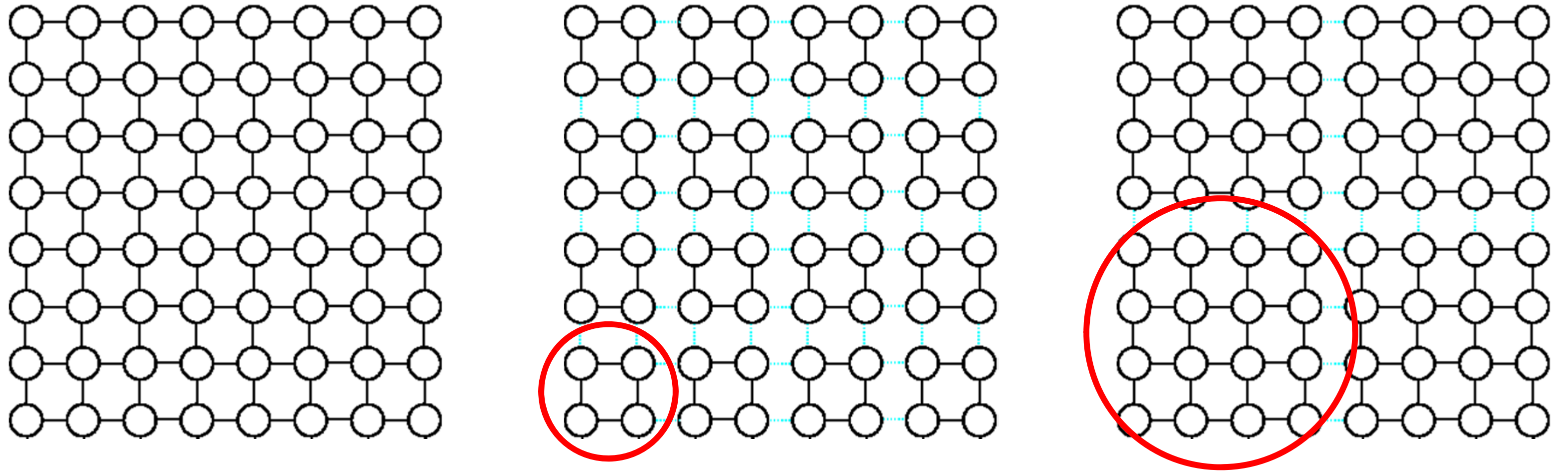
$$q_i(X_i)=\exp\left\{\theta_{i0}X_i+\sum_{j\in\mathcal{N}_i}\theta_{ij}X_i\left\langle X_j\right\rangle_{q_j}+A_i\right\}$$

$$=p(X_i\,|\,\{\langle X_j\rangle_{q_j}:j\in\mathcal{N}_i\})$$



- $\left\langle X_j\right\rangle_{q_j}$ resembles a "message" sent from node j to i
- $\{\langle X_j\rangle_{q_j}:j\in\mathcal{N}_i\}$ forms the "mean field" applied to X_i from its neighborhood

Example 1: Generalized MF approximations to Ising models

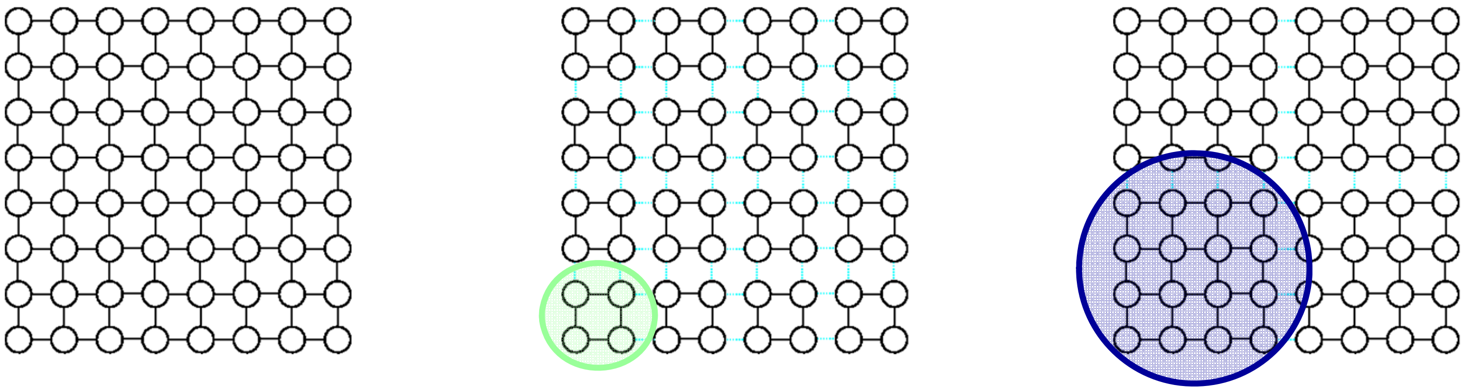


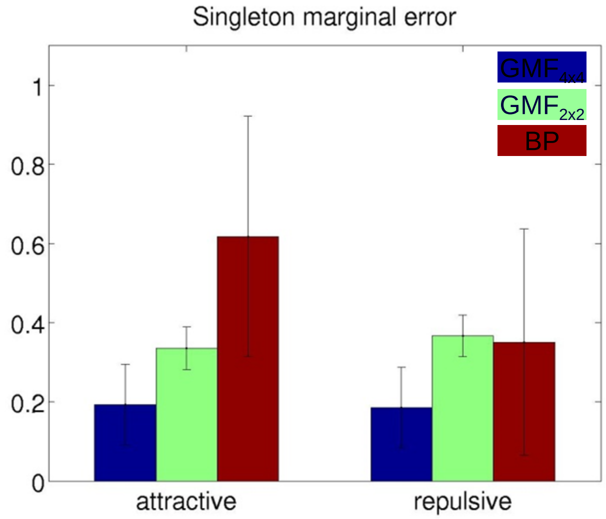
Cluster marginal of a square block C_k:

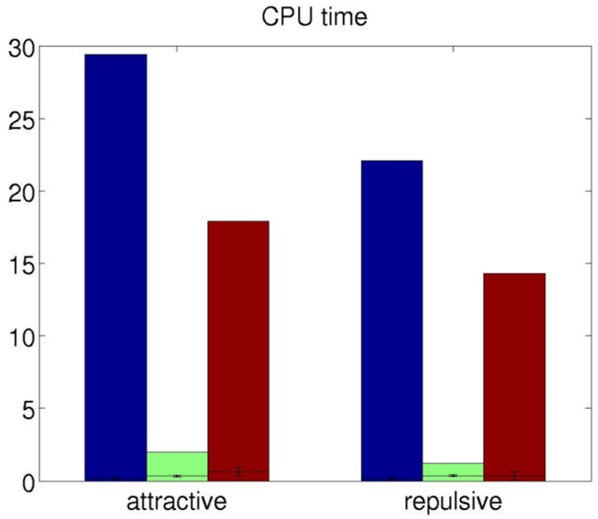
$$q(X_{C_k}) \propto \exp\left\{ \sum_{i,j\in C_k} \theta_{ij} X_i X_j + \sum_{i\in C_k} \theta_{i0} X_i + \sum_{\substack{i\in C_k,\, j\in MB_k,\\ k'\in MBC_k}} \theta_{ij} X_i \left\langle X_j \right\rangle_{q(X_{C_{k'}})} \right\}$$

Virtually a reparameterized Ising model of small size.

GMF approximation to Ising models

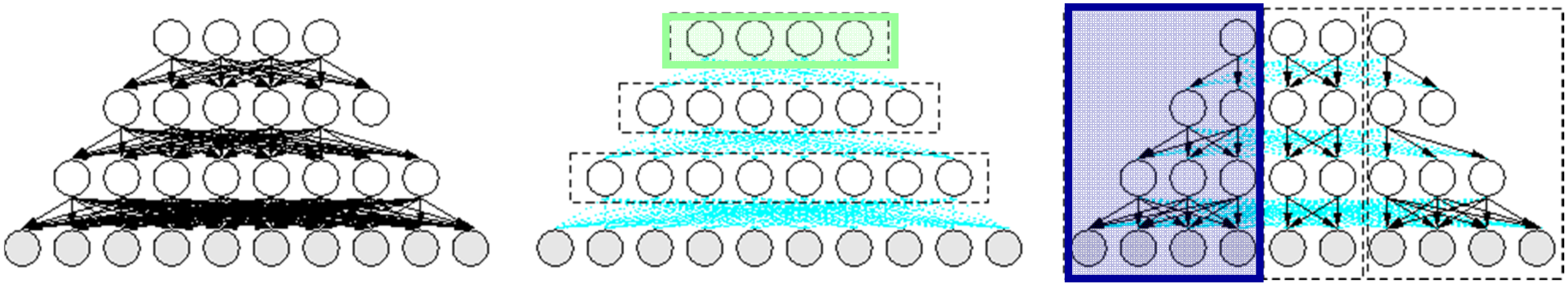


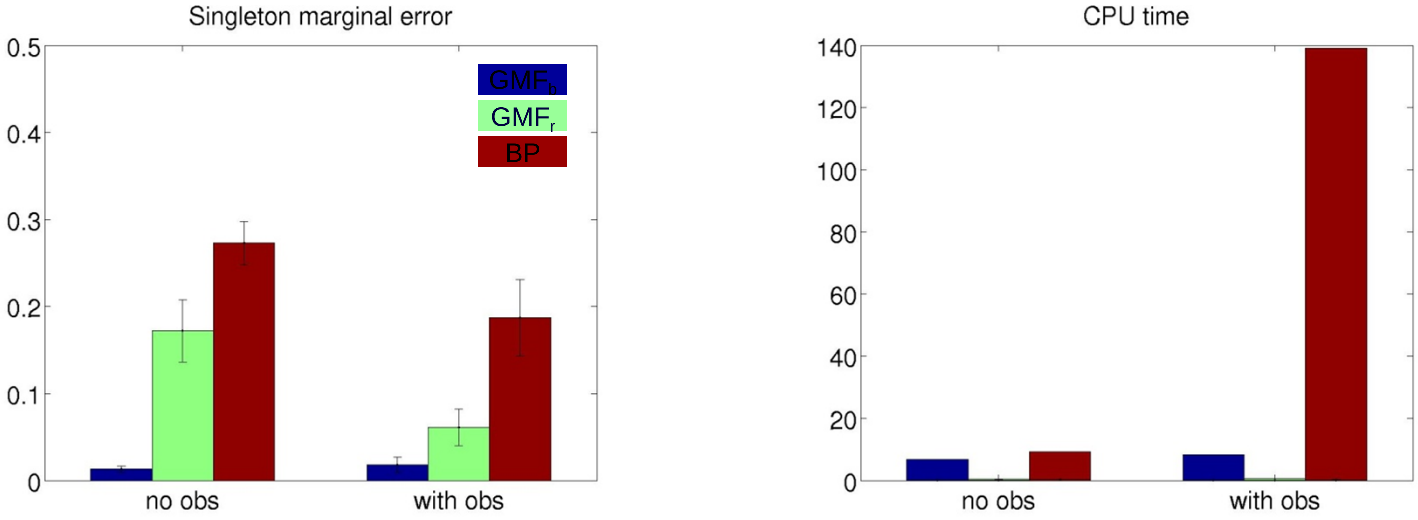




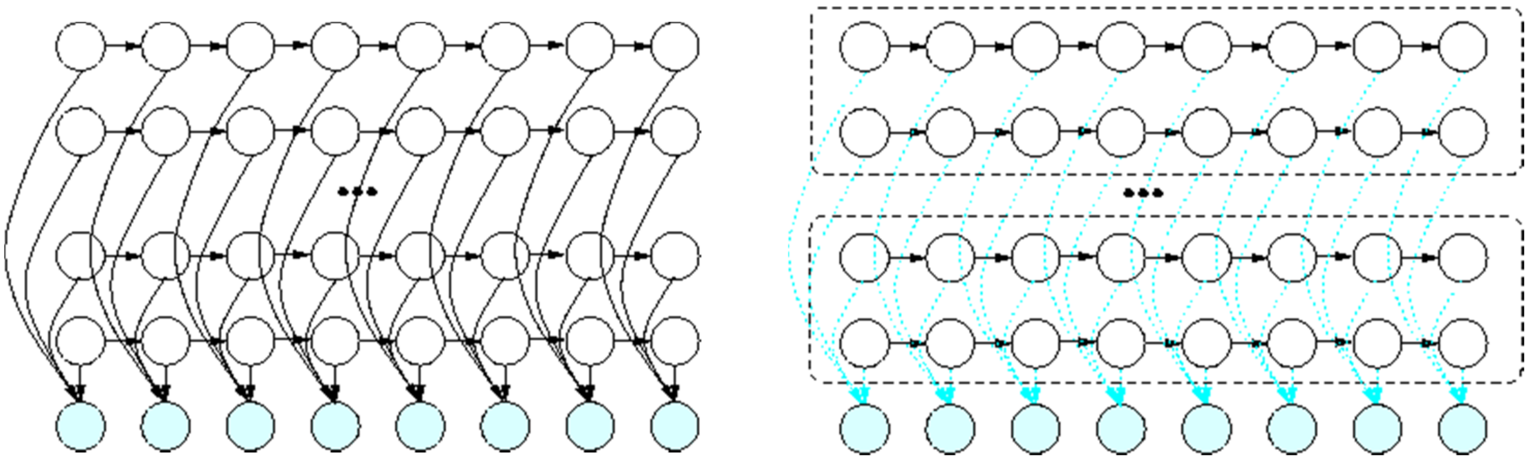
Attractive coupling: positively weighted
Repulsive coupling: negatively weighted

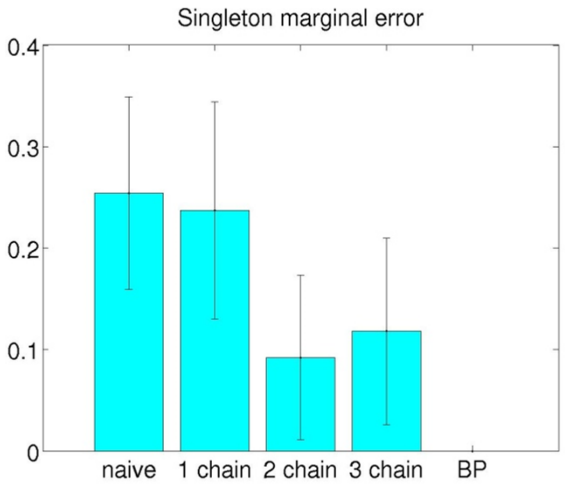
Example 2: Sigmoid belief network

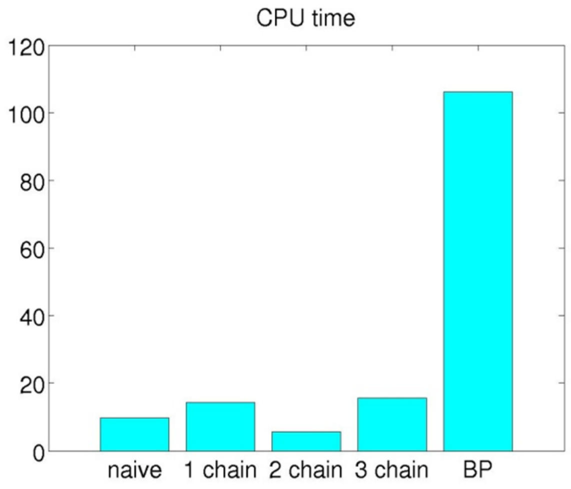




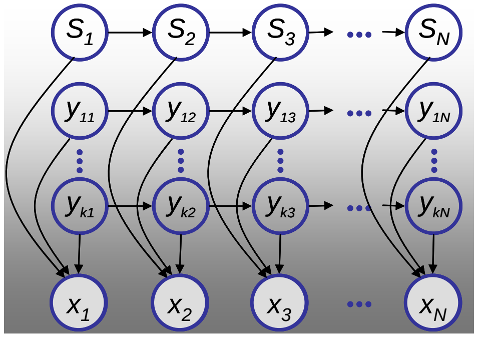
Example 3: Factorial HMM



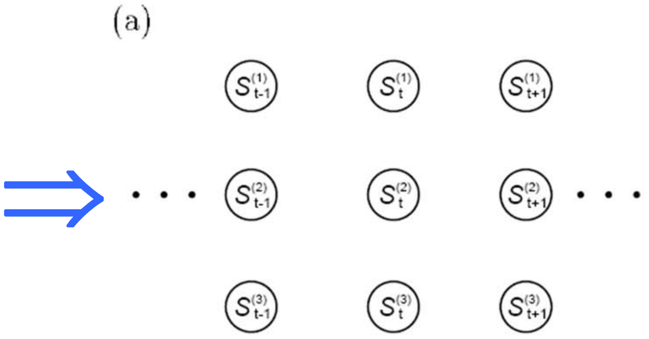




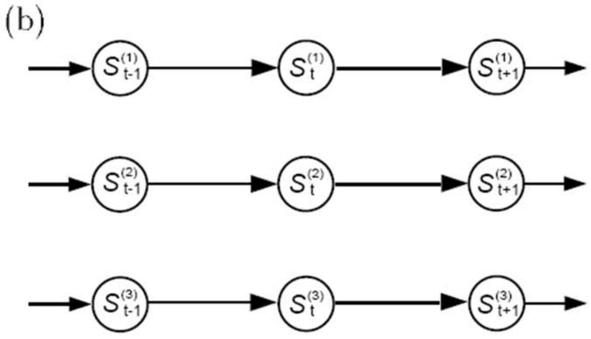
Automatic Variational Inference



fHMM


(a)
S(1) t-1, S(1) t, S(1) t+1
S(2) t-1, S(2) t, S(2) t+1
S(3) t-1, S(3) t, S(3) t+1

Mean field approx.


(b)
S(1) t-1, S(1) t, S(1) t+1
S(2) t-1, S(2) t, S(2) t+1
S(3) t-1, S(3) t, S(3) t+1

Structured variational approx.

- Currently for each new model we have to
  - derive the variational update equations
  - write application-specific code to find the solution
- Each can be time consuming and error prone
- Can we build a general-purpose inference engine which automates these procedures?

Cluster-based MF (e.g., GMF)

- a general, iterative message passing algorithm
- clustering completely defines approximation
  - preserves dependencies
  - flexible performance/cost trade-off
  - clustering automatable
- recovers model-specific structured VI algorithms, including:
  - fHMM, LDA
  - variational Bayesian learning algorithms
- easily provides new structured VI approximations to complex models