Readings: K&F 11.1, 11.2, 11.3, 11.4

Approximate Inference II

Lecture 16 – May 18, 2011

CSE 515, Statistical Methods, Spring 2011

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Review: Metropolis-Hastings Algorithm

- Metropolis-Hastings algorithms
  - You decide the transition probability T^Q – based on the proposal distribution Q
  - Acceptance probability "corrects" for the discrepancy between Q and P

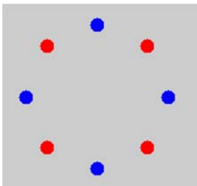
$$A(x \to x') = \min\left[1, \frac{P(x')T^Q(x' \to x)}{P(x)T^Q(x \to x')}\right]$$

  - Advantage: more "global" move from one state to another (compared to Gibbs sampling)
- The convergence of the M-H algorithm depends crucially on the proposal distribution Q
  - We need a proposal strategy that leads to a rapidly mixing Markov chains (i.e. one that converges quickly to the stationary distribution)
  - Let's see a toy example from Dellaert et al.*

* F. Dellaert, SM. Seitz, CE. Thorpe and S. Thrun. *EM, MCMC, and Chain Flipping for Structure from Motion with Unknown Correspondence.* Machine Learning 2003.

Revisit: Toy Model for Data Association

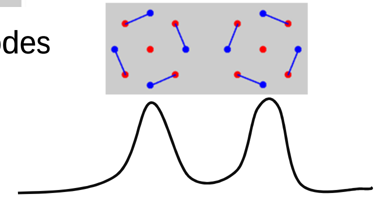
- Blue dots: variables, X_i (i=1,2,3,4)
- Red dots: observations (values that we assign to variables)



$$\mathbf{P}(\mathbf{X}) \propto \exp\Big(-\sum_{i=1}^{4} \Big\| \overbrace{\frac{x_i - x_i(value)}{\sigma}}^{\text{distance}} \Big\|^2\Big) \quad \text{if every } x_i \text{ has a different value}$$

$$\mathbf{P}(\mathbf{X}) = 0 \quad \text{otherwise}$$

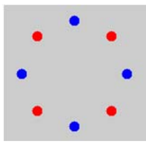
- Two modes



- We want to estimate $E_P(f)$ – Let's use M-H algorithm with three proposal distributions

Proposal distributions for M-H

- Proposal distribution 1 (flip proposal)
  - Simplest way of taking larger steps in moving over the state spaces (compared to Gibbs sampling)
  - Randomly pick two variables, flip their assignments

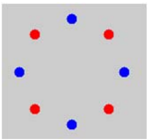


  - Attractive from a computational point of view, it has the severe disadvantage of leading to slowly mixing chains in many instances…

* F. Dellaert, SM. Seitz, CE. Thorpe and S. Thrun. *EM, MCMC, and Chain Flipping for Structure from Motion with Unknown Correspondence.* Machine Learning 2003.

Proposal distributions for M-H

- Proposal distribution 2 (augmenting path)
  - Suggest a move that is more likely to be accepted: recursively resolving the conflict
    - Improving the convergence properties of the chain:
  - 1. randomly pick one variable
  - 2. sample it pretending that all observations are available
  - 3. pick the variable X whose assignment was taken (conflict), goto step 2
  - 4. loop until step 2 creates no conflict



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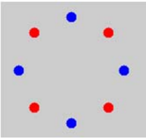
EM, MCMC, and Chain Flipping for Structure from Motion with Unknown Correspondence. Machine Learning 2003.

Proposal distributions for M-H

- Proposal distribution 3 (“smart” augmenting path)
  - More aggressive way of moving to different states
  - Same as the previous one except for the highlighted

  - 1. randomly pick one variable
  - 2. sample it pretending that all observations are available (excluding the current one)
  - 3. pick the variable whose assignment was taken (conflict), goto step 2
  - 4. loop until step 2 creates no conflict



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EM, MCMC, and Chain Flipping for Structure from Motion with Unknown Correspondence. Machine Learning 2003.

Let's "See" How They Work

- Which proposal strategy is the most "aggressive" in moving over the states??
  - Converges the fastest to the stationary distribution

- Run the following Matlab scripts:

  VisualMCMC2(10000, 0.7, 0.05);

  % live animation of sampling

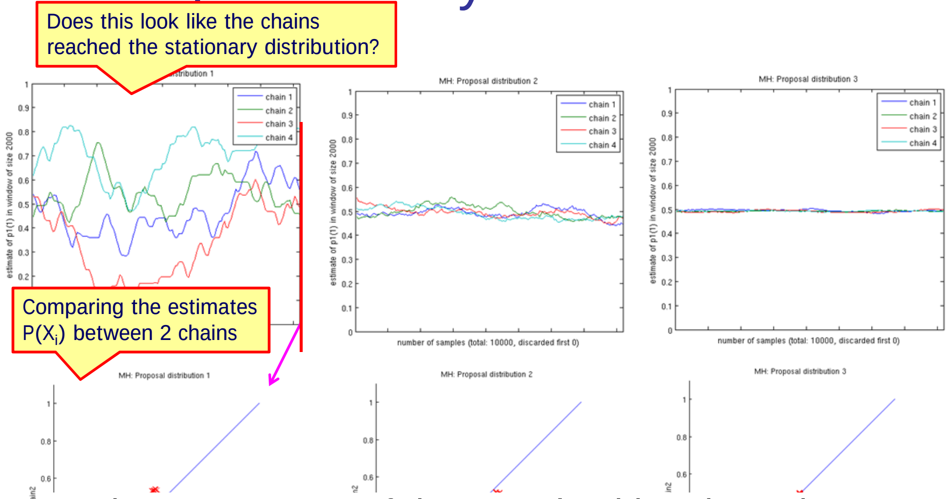
  % parameters: num of samples, sigma, pause time after each sample

  Plot2;

  % the first few lines of Plot2.m contain the parameters you may want to play around with

- How to evaluate the convergence performance?
  - Compare between multiple Markov chains, in terms of $E_p(f)$, $P(\mathbf{Y}=\mathbf{y})$, etc

Plots generated by "Plot2"



- The convergence of the M-H algorithm depends crucially on the proposal distribution Q
  - We need a proposal strategy that leads to a rapidly mixing Markov chains

Review: Particle-based Inference

- General framework:
  - Estimate $E_P(f)$ from particles x[1],…,x[M] from P (target distribution) or Q (proposal distribution)

- Full particle methods
  - Sampling methods
    - Forward sampling, Likelihood weighting
    - (Un-normalized/normalized) Importance sampling
    - Markov chain Monte Carlo
      - Gibbs sampling
      - Metropolis-Hastings algorithm
  - Deterministic particle generation
    - Upper/lower bounds of $E_P(f)$

- Distributional (Collapsed) particles

Let's now talk about a different kind of approximate inference algorithm that views inference as optimization…

GLOBAL APPROXIMATE INFERENCE

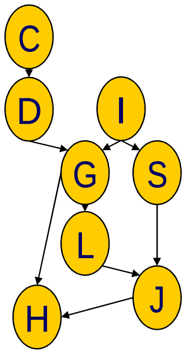
General Approximate Inference

- Again, in many real-life applications using large and dense networks, exact inference is infeasible...
- Strategy
  - Define a class of simpler distributions **Q**
  - Search for a particular instance in **Q** that is "close" to P
    - All methods we will discuss optimize the same target function for measuring the similarity between Q and P
  - Answer queries using inference in Q rather than P
- Before considering approximate inference methods, let's revisit exact inference based on message passing algorithms

Cluster Graph

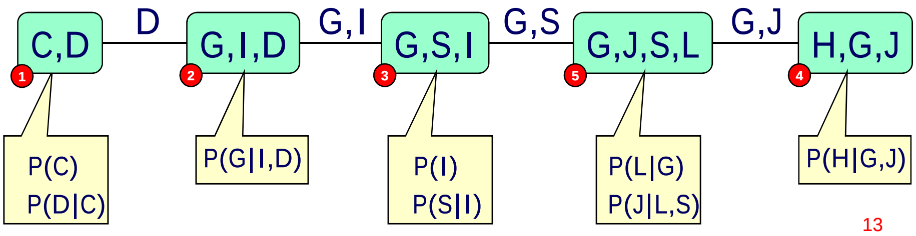
- A cluster graph K for factors F is an undirected graph
  - Nodes are associated with a subset of variables $\mathbf{C}_i \subseteq \mathbf{U}$
  - The graph is family preserving: each factor $\phi \in F$ is associated with one node $\mathbf{C}_i$ such that Scope[ϕ]$\subseteq \mathbf{C}_i$
  - Each edge $\mathbf{C}_i$–$\mathbf{C}_j$ is associated with a sepset $\mathbf{S}_{i,j} = \mathbf{C}_i \cap \mathbf{C}_j$
- Clique tree: a cluster graph over factors F that forms a tree and satisfies the running intersection property

Clique Tree Inference



Verify:

- Tree and family preserving
- Running intersection property



Message Passing: Belief Propagation

- Initialize the clique tree
  - For each clique C_i set $\pi_i \leftarrow \prod_{\phi:\alpha(\phi)=i} \phi$
  - For each edge C_i—C_j set $\mu_{i,j} \leftarrow 1$

- While unset cliques exist (clique tree is calibrated)
  - Select C_i—C_j
  - Send message from C_i to C_j
    - Marginalize the clique over the sepset $\sigma_{i\to j} \leftarrow \sum_{C_i - S_{i,j}} \pi_i$
    - Update the belief at C_j $\pi_j \leftarrow \pi_j \dfrac{\sigma_{i\to j}}{\mu_{i,j}}$
    - Update the sepset at C_i–C_j $\mu_{i,j} \leftarrow \sigma_{i\to j}$

Clique Tree Invariant

- Belief propagation can be viewed as reparameterizing the joint distribution
  - Upon calibration we showed $P(U) = \dfrac{\prod_{C_i \in T} \pi_i[C_i]}{\prod_{(C_i \leftrightarrow C_j) \in T} \mu_{i,j}(S_{i,j})}$
  - Initially this invariant holds since $\dfrac{\prod_{C_i \in T} \pi_i[C_i]}{\prod_{(C_i \leftrightarrow C_j) \in T} \mu_{i,j}(S_{i,j})} = \dfrac{\prod_{\phi \in F} \phi}{1} = P(U)$
  - At each update step invariant is also maintained
    - Message only changes π_i and $\mu_{i,j}$ so most terms remain unchanged
    - We need to show $\dfrac{\pi'_i}{\mu'_{i,j}} = \dfrac{\pi_i}{\mu_{i,j}}$
    - But this is exactly the message passing step $\pi'_i = \dfrac{\mu'_{i,j}\,\pi_i}{\mu_{i,j}}$

→ Belief propagation re-parameterizes P at each step

Global Approximate Inference

- Inference as optimization
- Generalized Belief Propagation (GBP)
  - Define algorithm
  - Constructing cluster graphs
  - Analyze approximation guarantees
  - GBP as optimization
- Propagation with approximate messages (EP)
  - Factorized messages
  - Approximate message propagation
- Structured variational approximations

The Energy Functional

- Suppose we want to approximate P with Q
  - Represent P by factors F $P_F(\mathbf{U}) = \frac{1}{Z}\prod_{\phi\in F}\phi(\mathbf{U}_\phi)$
  - Distance metric? – Many ways, but let's use relative entropy (aka KL-divergence)

$$D(Q\,\|\,P_F) = E_Q\left[\ln\frac{Q}{P_F}\right]$$

Unwieldy for direct optimization: an explicit summation over all possible assignments of **U**

  - Define the energy functional $F[P_F', Q] = \sum_{\phi\in F} E_Q[\ln\phi] + H_Q(\mathbf{U})$
- Then, we can show that $D(Q\,\|\,P_F) = \ln Z - F[P_F', Q]$
  - Proof in K&F (page 385)
- Minimizing $D(Q||P_F)$ is equivalent to maximizing $F[P_F',Q]$
- $\ln Z \geq F[P_F',Q]$ (since $D(Q||P_F)\geq 0$)

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Inference as Optimization

- Basic idea: We can show that inference can be viewed as maximizing the energy functional $F[P_F',Q]$
  - Define a distribution Q over clique potentials
  - Transform $F[P_F',Q]$ to an equivalent factored form $F'[P_F',Q]$
  - Show that if **Q** maximizes $F'[P_F',\mathbf{Q}]$ subject to constraints in which **Q** represents calibrated potentials, then there exists factors (messages) that satisfy the inference message passing equations
    - Equivalent to belief propagation!

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Defining Q

- Recall that throughout BP $P(U) = \frac{\prod_{C_i \in T} \pi_i[C_i]}{\prod_{(C_i \leftrightarrow C_j) \in T} \mu_{i,j}(S_{i,j})}$

- Define Q as re-parameterization of P such that

$$\mathbf{Q} = \{\pi_i\} \cup \{\mu_{i,j} : (C_i - C_j) \in \text{clique tree } T\}$$

$$Q_T(\mathbf{U}) = \frac{\prod_{C_i \in T} \pi_i[C_i]}{\prod_{(C_i \leftrightarrow C_j) \in T} \mu_{i,j}(S_{i,j})}$$

- If T is calibrated, $D(Q||P_F)=0$ and so $F[P_F',Q]$ is maximized.

Factored Energy Functional

- Recall that the energy functional is defined as

$$F[P_F',Q] = \sum_{\phi \in F} E_Q[\ln \phi] + H_Q(\mathbf{U})$$

Q is defined as: $Q(\mathbf{U}) = \frac{\prod_{C_i \in T} \pi_i[C_i]}{\prod_{(C_i \leftrightarrow C_j) \in T} \mu_{i,j}(S_{i,j})}$

- Define the factored energy functional as

$$F'[P_F',\mathbf{Q}] = \sum_i E_{\pi_i}[\ln \pi_i^0] + \sum_{C_i \in T} H_{\pi_i}(C_i) - \sum_{(C_i - C_j) \in T} H_{\mu_{i,j}}(S_{i,j})$$

$$\boxed{\mathbf{Q} = \{\pi_i\} \cup \{\mu_{i,j} : (C_i - C_j) \in \text{clique tree } T\}}$$

- Theorem: if **Q** is a set of calibrated potentials for T, then $F[P_F',Q] = F'[P_F',\mathbf{Q}]$ (K&F page 387)

Inference as Optimization

$\mathbf{Q} = \{\pi_i\} \cup \{\mu_{i,j} : (C_i - C_j) \in \text{clique tree } T\}$

- Optimization task
  - Find **Q** that maximizes F'[P_F',**Q**] subject to

$$\mu_{i,j} = \sum_{C_i - S_{i,j}} \pi_i \quad \forall (C_i - C_j) \in \text{clique tree } T$$

$$\sum_{C_i} \pi_i = 1 \quad \forall C_i \in T$$

General optimization tool based on Lagrange multipliers

- The solution of the above optimization problem satisfies (if exists)

$$\begin{aligned} \delta_{i\to j} &\propto \sum\nolimits_{C_i - S_{i,j}} \pi_i^0 \left(\prod\nolimits_{k \in N_{C_i} - \{j\}} \delta_{k \to i} \right) \\ \pi_i &\propto \pi_i^0 \left(\prod\nolimits_{j \in N_{C_i}} \delta_{j \to i} \right) \\ \mu_{i,j} &= \delta_{i \to j} \times \delta_{j \to i} \end{aligned}$$

  - Suggests iterative procedure
  - Identical to belief propagation!

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Global Approximate Inference

- Inference as optimization
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  - Define algorithm
  - Constructing cluster graphs
  - Analyze approximation guarantees
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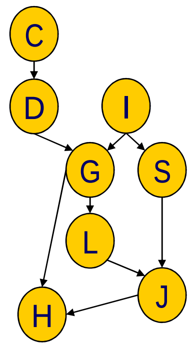
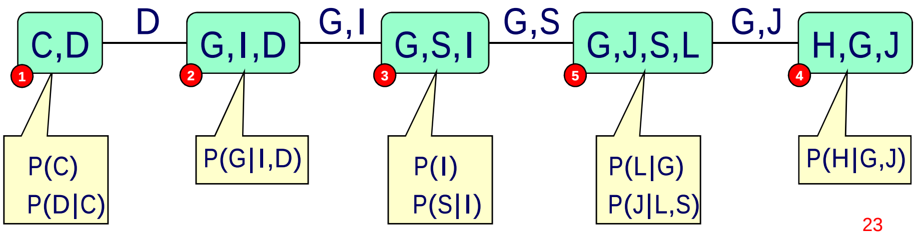
Revisit: Clique Tree Inference



Verify:

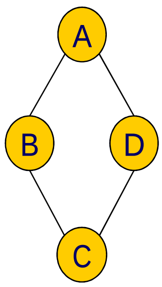
- ~~Tree~~ and family preserving
- Running intersection property → ***Modify***



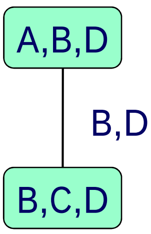
Generalized Belief Propagation

Strategy:

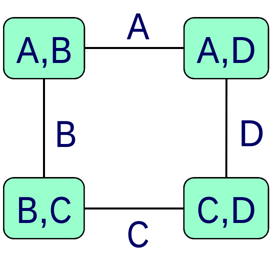
Perform belief propagation in a cluster graph with loops



Simple network



Clique tree



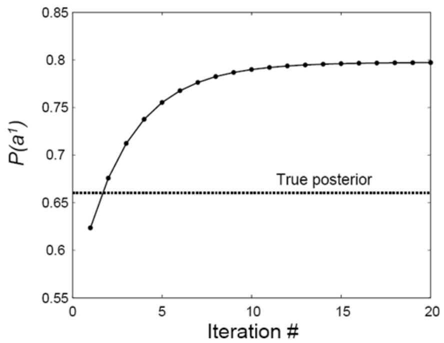
Cluster graph

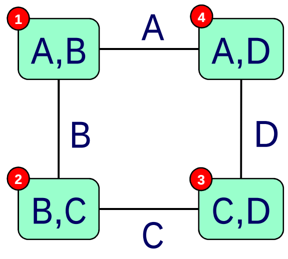
Generalized Belief Propagation

Strategy:

Perform belief propagation in a cluster graph with loops

- Inference may be incorrect: double counting evidence





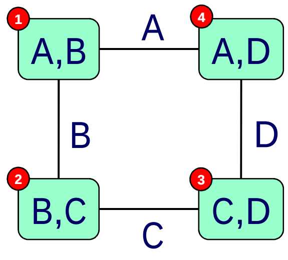
Cluster graph

Generalized Belief Propagation

Strategy:

Perform belief propagation in a cluster graph with loops

- Inference may be incorrect: double counting evidence
- Unlike in BP on trees:
  - Convergence is not guaranteed
  - Potentials in calibrated tree are not guaranteed to be marginals in P



Cluster graph

Generalized Cluster Graph

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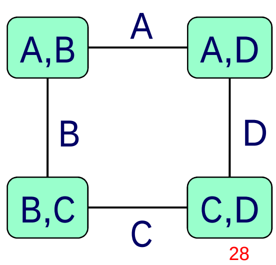
  - Each edge $\mathbf{C_i}$–$\mathbf{C_j}$ is associated with a subset $\mathbf{S_{i,j}} \subseteq \mathbf{C_i} \cap \mathbf{C_j}$

Generalized Cluster Graph

- A generalized cluster graph obeys the running intersection property if for each $X \in C_i$ and $X \in C_j$, there is exactly one path between C_i and C_j for which $X \in \mathbf{S}$ for each subset S along the path

- → All edges associated with X form a tree that spans all the clusters that contain X
  - Note: some of these clusters may be connected with more than one path



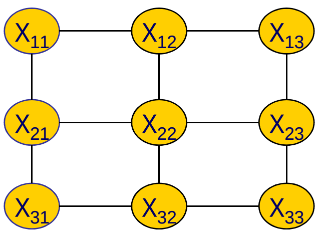
Calibrated Cluster Graph

- A generalized cluster graph is calibrated if for each edge C_i – C_j we have:

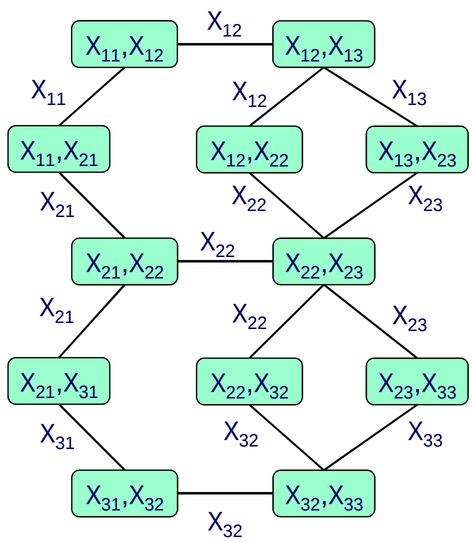
$$\sum_{C_i - S_{i,j}} \pi_i[C_i] = \sum_{C_j - S_{i,j}} \pi_j[C_j]$$

  - Weaker than in clique trees, since $S_{i,j}$ is a subset of the intersection between C_i and C_j
  - If a cluster graph satisfies the running intersection property, then the marginal on any variable X is the same in every cluster that contains X

GBP is Efficient



Markov grid network



Note: clique tree in a n x n grid is exponential in n

Round of GBP is O(n)

Cluster graph

Global Approximate Inference

- Inference as optimization
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  - Define algorithm
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Constructing Cluster Graphs

- When constructing clique trees, all constructions give the same result, but differ in computational complexity

- In GBP, different cluster graphs can vary in both computational complexity and approximation quality (accuracy)

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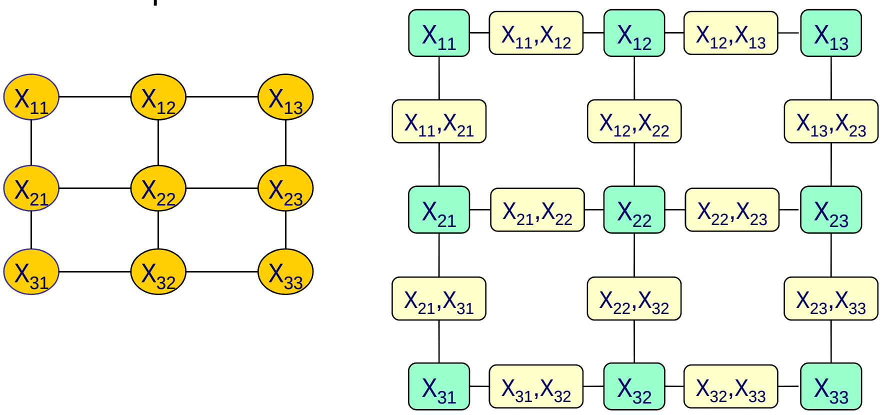
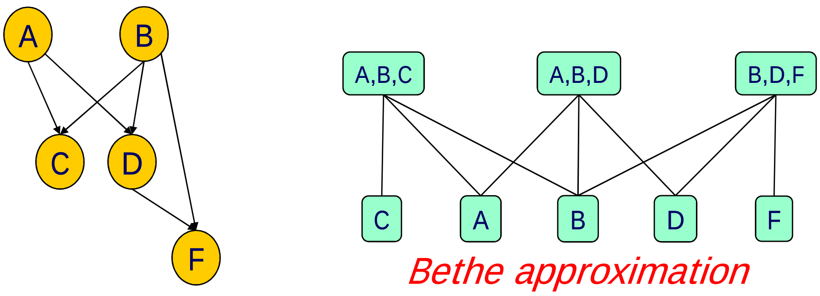
Transforming Pairwise MNs

- A pairwise Markov network over a graph H has:
  - A set of node potentials $\{\pi[X_i]:i=1,\ldots n\}$
  - A set of edge potentials $\{\pi[X_i,X_j]: X_i,X_j \in H\}$
  - Example:



Transforming Bayesian Networks

- Example:



- "Large" cluster per each CPD
- Single nodes for each variable
- Connect node and large cluster if node in CPD
- → Graph obeys running intersection property

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Generalized Belief Propagation

- GBP maintains distribution invariance

$$P_F(\mathbf{U}) = \frac{\prod_{C_i \in K} \pi_i[C_i]}{\prod_{(C_i \leftrightarrow C_j) \in K} \mu_{i,j}(S_{i,j})}$$

  - (since message passing maintains invariance)

Generalized Belief Propagation

- If GBP converges (K is calibrated)
  - Each subtree T is calibrated with edge potentials corresponding to marginals of $P_T(\mathbf{U})$

$$P_T(\mathbf{U}) = \frac{\prod_{C_i \in T} \pi_i[C_i]}{\prod_{(C_i \leftrightarrow C_j) \in T} \mu_{i,j}(S_{i,j})}$$

  - (since $P_T(\mathbf{U})$ is a calibrated tree)

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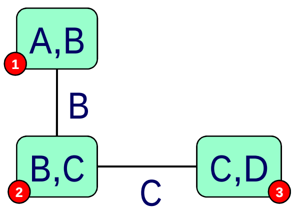
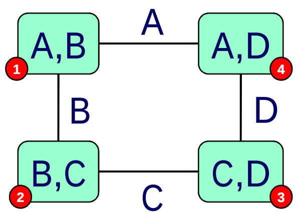
Generalized Belief Propagation

- → Calibrated graph potentials are not $P_F(\mathbf{U})$ marginals





$$P_T(A,B,C,D) \propto \frac{\pi_1[A,B]\pi_2[B,C]\pi_3[C,D]}{\mu_{1,2}[B]\mu_{2,3}[C]}$$

$$P_F(A,B,C,D) \propto \frac{\pi_1[A,B]\pi_2[B,C]\pi_3[C,D]\pi_4[A,D]}{\mu_{1,2}[B]\mu_{2,3}[C]\mu_{3,4}[D]\mu_{4,1}[A]}$$

$$\pi_4[A,D] \neq \mu_{3,4}[D]\mu_{1,4}[A]$$

$$\Downarrow$$

$$P_T \neq P_F \rightarrow \pi_1[A,B] \neq P_F(A,B)$$

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Inference as Optimization

$\mathbf{Q} = \{\pi_i\} \cup \{\mu_{i,j} : (C_i - C_j) \in \text{clique tree } T\}$

- Optimization task
  - Find **Q** that maximizes F'[P_F',**Q**] subject to

$$\mu_{i,j} = \sum_{C_i - S_{i,j}} \pi_i \quad \forall (C_i - C_j) \in \text{clique tree } T$$

$$\sum_{C_i} \pi_i = 1 \quad \forall C_i \in T$$

General optimization tool based on Lagrange multipliers

- The solution of the above optimization problem satisfies

$$\begin{aligned} \delta_{i \to j} &\propto \sum\nolimits_{C_i - S_{i,j}} \pi_i^0 \left(\prod\nolimits_{k \in N_{C_i} - \{j\}} \delta_{k \to i} \right) \\ \pi_i &\propto \pi_i^0 \left(\prod\nolimits_{j \in N_{C_i}} \delta_{j \to i} \right) \\ \mu_{i,j} &= \delta_{i \to j} \times \delta_{j \to i} \end{aligned}$$

  - Suggests iterative procedure
  - Identical to belief propagation!

GBP as Optimization

$\mathbf{Q} = \{\pi_i\} \cup \{\mu_{i,j} : (C_i - C_j) \in \text{clique tree } T\}$

- Optimization task
  - Find **Q** that maximizes F'[P_F',**Q**] subject to

$$\mu_{i,j} = \sum_{C_i - S_{i,j}} \pi_i \quad \forall (C_i - C_j) \in K$$

$$\sum_{C_i} \pi_i = 1 \quad \forall C_i \in K$$

- The solution of the above optimization problem satisfies

$$\begin{aligned} \delta_{i \to j} &\propto \sum\nolimits_{C_i - S_{i,j}} \pi_i^0 \left(\prod\nolimits_{k \in N_{C_i} - \{j\}} \delta_{k \to i} \right) \\ \pi_i &\propto \pi_i^0 \left(\prod\nolimits_{j \in N_{C_i}} \delta_{j \to i} \right) \\ \mu_{i,j} &= \delta_{i \to j} \times \delta_{j \to i} \end{aligned}$$

  - Note: $S_{i,j}$ is only a subset of intersection between C_i and C_j
  - Iterative optimization procedure is GBP

GBP as Optimization

- Clique trees
  - $F[P_F,Q]=F'[P_F,Q]$
  - Iterative procedure (BP) guaranteed to converge
  - Convergence point represents marginal distributions of P_F
- Cluster graphs
  - $F[P_F,Q]=F'[P_F,Q]$ does not hold!
  - Iterative procedure (GBP) not guaranteed to converge
  - Convergence point does not represent marginal distributions of P_F

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GBP in Practice

- Dealing with non-convergence
  - Often small portions of the network do not converge
    - → stop inference and use current beliefs
  - Use intelligent message passing scheduling
    - Tree reparameterization (TRP) selects entire trees, and calibrates them while keeping all other beliefs fixed
    - Focus attention on uncalibrated regions of the graph

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Global Approximate Inference

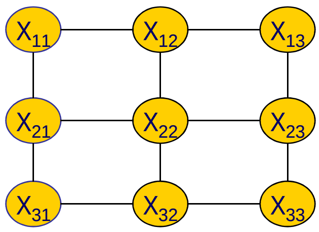
- Inference as optimization
- Generalized Belief Propagation
  - Define algorithm
  - Constructing cluster graphs
  - Analyze approximation guarantees
- Propagation with approximate messages
  - Factorized messages
  - Approximate message propagation
- Structured variational approximations

Propagation w. Approximate Msgs

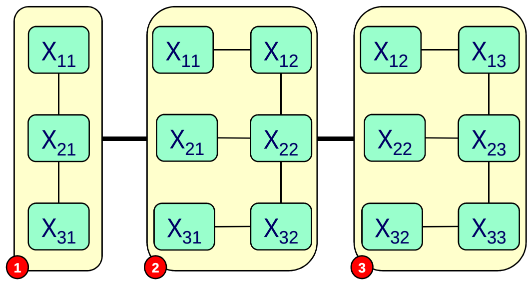
- General idea
  - Perform BP (or GBP) as before, but propagate messages that are only approximate
  - Modular approach
    - General inference scheme remains the same
    - Can plug in many different approximate message computations

Factorized Messages

- Keep internal structure of the clique tree cliques
- Calibration involves sending messages that are joint over three variables
- Idea: simplify messages using factored representation
  - Example: $\tilde{\delta}_{1\to2}[X_{11}, X_{21}, X_{31}] = \tilde{\delta}_{1\to2}[X_{11}]\tilde{\delta}_{1\to2}[X_{21}]\tilde{\delta}_{1\to2}[X_{31}]$



Markov network



Clique tree

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