

# Junction Tree, BP and Variational Methods

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MLSALT4 Lecture

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With thanks to David Sontag (MIT) and Tony Jebara (Columbia)  
for use of many slides and illustrations

For more information, see

<http://mlg.eng.cam.ac.uk/adrian/>

# High level overview of our 3 lectures

- 1. Directed and undirected graphical models (last Wed)
- 2. LP relaxations for MAP inference (last Friday)
- 3. Junction tree algorithm for exact inference, belief propagation, variational methods for approximate inference (today)

Further reading / viewing:

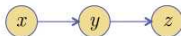
- Murphy, Machine Learning: a Probabilistic Perspective
- Barber, Bayesian Reasoning and Machine Learning
- Bishop, Pattern Recognition and Machine Learning
- Koller and Friedman, Probabilistic Graphical Models  
<https://www.coursera.org/course/pgm>
- Wainwright and Jordan, Graphical Models, Exponential Families, and Variational Inference

# Review: directed graphical models = Bayesian networks

- A **Bayesian network** is specified by a **directed acyclic graph** **DAG** =  $(V, \vec{E})$  with:
  - 1 One node  $i \in V$  for each random variable  $X_i$
  - 2 One conditional probability distribution (CPD) per node,  $p(x_i \mid \mathbf{x}_{\text{Pa}(i)})$ , specifying the variable's probability conditioned on its parents' values
- The DAG corresponds 1-1 with a particular factorization of the joint distribution:

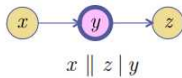
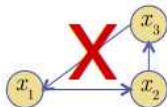
$$p(x_1, \dots, x_n) = \prod_{i \in V} p(x_i \mid \mathbf{x}_{\text{Pa}(i)})$$

Markov chain:



$$p(x, y, z) = p(x) p(y \mid x) p(z \mid y)$$

**Example binary events:**  
**x** = president says war  
**y** = general orders attack  
**z** = soldier shoots gun



$$p(x \mid y, z) = \frac{p(x, y, z)}{p(y, z)} = p(x \mid y)$$

## Review: undirected graphical models = MRFs

- As for directed models, we have one node for each random variable
- Rather than CPDs, we specify (non-negative) **potential functions** over sets of variables associated with (maximal) cliques  $C$  of the graph,

$$p(x_1, \dots, x_n) = \frac{1}{Z} \prod_{c \in C} \phi_c(\mathbf{x}_c)$$

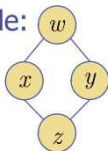
$Z$  is the **partition function** and normalizes the distribution:

$$Z = \sum_{\hat{x}_1, \dots, \hat{x}_n} \prod_{c \in C} \phi_c(\hat{\mathbf{x}}_c)$$

- Like a CPD,  $\phi_c(\mathbf{x}_c)$  can be represented as a table, but it is **not normalized**
- For both directed and undirected models, the joint probability is the **product of sub-functions of (small) subsets of variables**

# Directed and undirected models are different

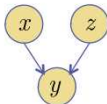
- Example:



$$x \parallel y \mid \{w, z\}$$

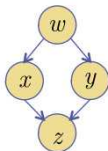
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- Example:



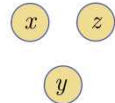
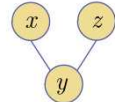
$$x \parallel z$$

$$x \not\parallel z \mid y$$



$$x \parallel y \mid \{w\}$$

$$x \not\parallel y \mid \{w, z\}$$



**Directed can't do it!**  
**Must be acyclic**  
**Will have at least one**  
**V structure and ball**  
**goes through**

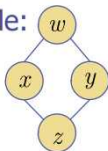
**With <3 edges,**  
**Undirected can't do it!**

$$x \parallel z \mid y$$

$$x \parallel z$$

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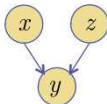
- Example:



$$x \perp\!\!\!\perp y \mid \{w, z\}$$

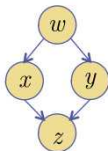
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- Example:



$$x \perp\!\!\!\perp z$$

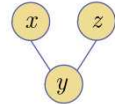
$$x \not\perp\!\!\!\perp z \mid y$$



$$x \perp\!\!\!\perp y \mid \{w\}$$

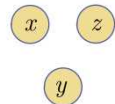
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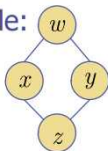


$$x \perp\!\!\!\perp z$$

$$p(x, y, z) = p(x)p(z)p(y|x, z)$$

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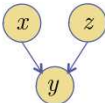
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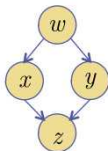
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- Example:



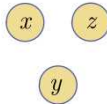
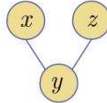
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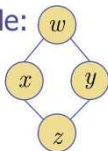
$$x \perp\!\!\!\perp z$$

$$p(x, y, z) = p(x)p(z)p(y|x, z) =: \phi_c(x, y, z), \quad c = \{x, y, z\}$$

$$p(x_1, \dots, x_n) = \frac{1}{Z} \prod_{c \in C} \phi_c(\mathbf{x}_c)$$

# Directed and undirected models are different

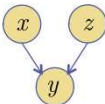
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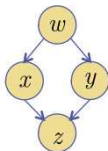
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- Example:



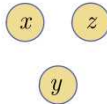
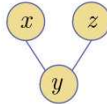
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$$p(x, y, z) = p(x)p(z)p(y|x, z) =: \phi_c(x, y, z), \quad c = \{x, y, z\}$$

$$p(x_1, \dots, x_n) = \frac{1}{Z} \prod_{c \in C} \phi_c(\mathbf{x}_c) \quad \text{What if we double } \phi_c?$$

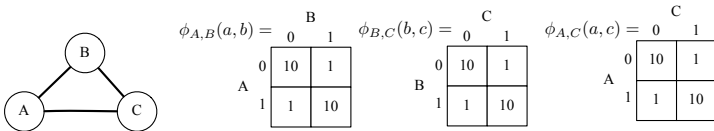


# Undirected graphical models / factor graphs

$$p(x_1, \dots, x_n) = \frac{1}{Z} \prod_{c \in C} \phi_c(\mathbf{x}_c),$$

$$Z = \sum_{\hat{x}_1, \dots, \hat{x}_n} \prod_{c \in C} \phi_c(\hat{\mathbf{x}}_c)$$

**Simple example** (each edge potential function encourages its variables to take the same value):



$$p(a, b, c) = \frac{1}{Z} \phi_{A,B}(a, b) \cdot \phi_{B,C}(b, c) \cdot \phi_{A,C}(a, c), \text{ where}$$

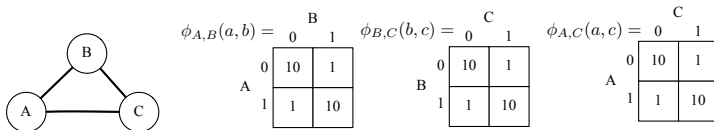
$$Z = \sum_{\hat{a}, \hat{b}, \hat{c} \in \{0,1\}^3} \phi_{A,B}(\hat{a}, \hat{b}) \cdot \phi_{B,C}(\hat{b}, \hat{c}) \cdot \phi_{A,C}(\hat{a}, \hat{c}) = 2 \cdot 1000 + 6 \cdot 10 = 2060.$$

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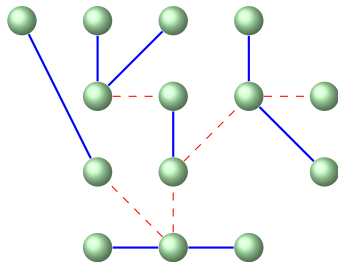


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With the max clique convention, this graph does not imply pairwise factorization: without further information, we must assume

$$p(a, b, c) = \frac{1}{Z} \phi_{A,B,C}(a, b, c)$$

# When is inference (relatively) easy?



Tree

## Basic idea: marginal inference for a chain

- Suppose we have a simple chain  $A \rightarrow B \rightarrow C \rightarrow D$ , and we want to compute  $p(D)$ , a **set** of values,  $\{p(D = d), d \in \text{Val}(D)\}$
- The joint distribution factorizes as

$$p(A, B, C, D) = p(A)p(B \mid A)p(C \mid B)p(D \mid C)$$

- In order to compute  $p(D)$ , we have to **marginalize over  $A, B, C$** :

$$p(D) = \sum_{a,b,c} p(A = a, B = b, C = c, D)$$

# How can we perform the sum efficiently?

- Our goal is to compute

$$\begin{aligned} p(D) &= \sum_{a,b,c} p(a, b, c, D) = \sum_{a,b,c} p(a)p(b|a)p(c|b)p(D|c) \\ &= \sum_c \sum_b \sum_a p(D|c)p(c|b)p(b|a)p(a) \end{aligned}$$

- We can push the summations inside to obtain:

$$p(D) = \sum_c p(D|c) \sum_b p(c|b) \underbrace{\sum_a p(b|a)p(a)}_{\tau_1(b) \text{ 'message about } b'}$$

- Let's call  $\psi_1(A, B) = P(A)P(B|A)$ . Then,  $\tau_1(B) = \sum_a \psi_1(a, B)$
- Similarly, let  $\psi_2(B, C) = \tau_1(B)P(C|B)$ . Then,  $\tau_2(C) = \sum_b \psi_2(b, C)$
- This procedure is **dynamic programming**: efficient 'inside out' computation instead of 'outside in'

# Marginal inference in a chain

- Generalizing the previous example, suppose we have a chain  $X_1 \rightarrow X_2 \rightarrow \cdots \rightarrow X_n$ , where each variable has  $k$  states
- For  $i = 1$  up to  $n - 1$ , compute (and cache)

$$p(X_{i+1}) = \sum_{x_i} p(X_{i+1} \mid x_i) p(x_i)$$

- Each update takes  $\mathcal{O}(k^2)$  time
- The total running time is  $\mathcal{O}(nk^2)$
- In comparison, naively marginalizing over all latent variables has time complexity  $\mathcal{O}(k^n)$
- Great! We performed marginal inference over the joint distribution without ever explicitly constructing it

# How far can we extend the chain approach?

Can we extend the chain idea to do something similar for:

- More complex graphs with many branches?
- Can we get marginals of **all** variables efficiently?
- With cycles?

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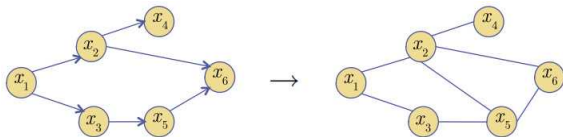
- More complex graphs with many branches?
- Can we get marginals of **all** variables efficiently?
- With cycles?
- The **junction tree algorithm** does all these
- But it's not magic: in the worst case, the problem is NP-hard (even to approximate)
- Junction tree achieves time linear in the number of **bags** = **maximal cliques**, **exponential in the treewidth** ← **key point**





# Recipe **guaranteed** to build a junction tree

- 1 Moralize (if directed)

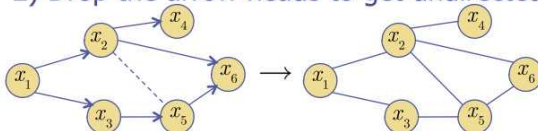


- 2 Triangulate
- 3 Identify maximal cliques
- 4 Build a max weight spanning tree

Then we can propagate probabilities: **junction tree algorithm**

# Moralize

- Converts directed graph into undirected graph
- By **moralization**, marrying the parents:
  - 1) Connect nodes that have common children
  - 2) Drop the arrow heads to get undirected



$$p(x_1)p(x_2|x_1)p(x_3|x_1)p(x_4|x_2)p(x_5|x_3)p(x_6|x_2, x_5) \\ \rightarrow \frac{1}{Z} \psi(x_1, x_2) \psi(x_1, x_3) \psi(x_2, x_4) \psi(x_3, x_5) \psi(x_2, x_5, x_6)$$

$$p(x_1)p(x_2|x_1) \\ \rightarrow \psi(x_1, x_2)$$

$$p(x_4|x_2) \\ \rightarrow \psi(x_2, x_4)$$

$$Z \rightarrow 1$$

- Note: moralization resolves *coupling* due to marginalizing
- **moral graph** is more general (loses some independencies)

**most  
specific**



...



...



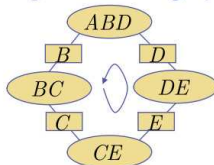
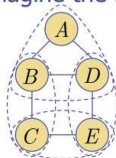
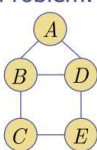
**most  
general**

- Each  $\psi$  is different based on its arguments, don't get confused
- Ok to put the  $p(x_1)$  term into **either**  $\psi_{12}(x_1, x_2)$  **or**  $\psi_{13}(x_1, x_3)$

# Triangulate

- We want to build a tree of **maximal cliques** = bags
- Notation here: an **oval** is a **maximal clique**,  
a **rectangle** is a **separator**

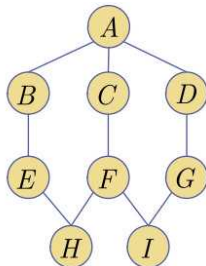
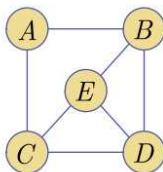
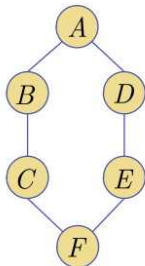
- Problem: imagine the following undirected graph



- Not a Tree!
- To ensure Junction Tree is a tree (no loops, etc.)  
before forming it must first **Triangulate** moral graph  
before finding the cliques...
- Triangulating gives more general graph (like moralization)
- Adds links to get rid of cycles or loops
- Triangulation: Connect nodes in moral graph until  
no chordless cycle of 4 or more nodes remains in the graph

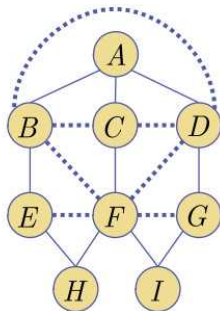
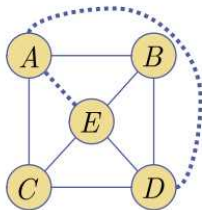
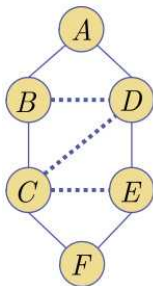
Actually, often we enforce a tree, in which case triangulation and other steps  $\Rightarrow$  **running intersection property**

# Triangulate



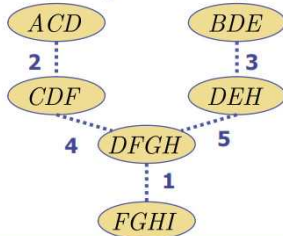
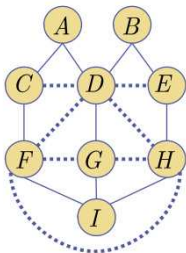
- Cycle:** A closed (simple) path, with no repeated vertices other than the starting and ending vertices
- Chordless Cycle:** a cycle where no two non-adjacent vertices on the cycle are joined by an edge.
- Triangulated Graph:** a graph that contains no chordless cycle of four or more vertices (aka a **Chordal Graph**).

# Triangulation examples



# Identify maximal cliques, build a max weight spanning tree

- For edge weights, use *separator*
- For max weight spanning tree, several algorithms e.g. Kruskal's
- Start with unconnected cliques (after triangulation)



	ACD	BDE	CDF	DEH	DFGH	FGHI
ACD	-	1	2	1	1	0
BDE		-	1	2	1	0
CDF			-	1	2	1
DEH				-	2	1
DFGH					-	3
FGHI						-

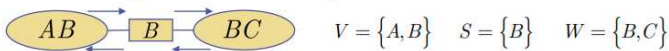
# We now have a valid junction tree!

- We had  $p(x_1, \dots, x_n) = \frac{1}{Z} \prod_c \psi_c(x_c)$
- Think of our junction tree as composed of **maximal cliques**  $c$  = **bags** with  $\psi_c(x_c)$  terms
- And **separators**  $s$  with  $\phi_s(x_s)$  terms, initialize all  $\phi_s(x_s) = 1$
- Write  $p(x_1, \dots, x_n) = \frac{1}{Z} \frac{\prod_c \psi_c(x_c)}{\prod_s \phi_s(x_s)}$
- **Now let the message passing begin!**
- At every step, we update some  $\psi'_c(x_c)$  and  $\phi'_s(x_s)$  functions but we **always preserve**  $p(x_1, \dots, x_n) = \frac{1}{Z} \frac{\prod_c \psi'_c(x_c)}{\prod_s \phi'_s(x_s)}$
- This is called Hugin propagation, can interpret updates as reparameterizations 'moving score around between functions' (may be used as a theoretical proof technique)



# Message passing for just 2 maximal cliques (Hugin)

- Send message from each clique *to* its separators of what it thinks the submarginal on the separator is.
- Normalize each clique by incoming message *from* its separators so it agrees with them



**If agree:**  $\sum_{V \setminus S} \psi_V = \phi_S = p(S) = \phi_S = \sum_{W \setminus S} \psi_W \quad \dots \text{Done!}$

**Else: Send message  
From V to W...**

$$\begin{aligned} \phi_S^* &= \sum_{V \setminus S} \psi_V \\ \psi_W^* &= \frac{\phi_S^*}{\phi_S} \psi_W \\ \psi_V^* &= \psi_V \end{aligned}$$

**Send message  
From W to V...**

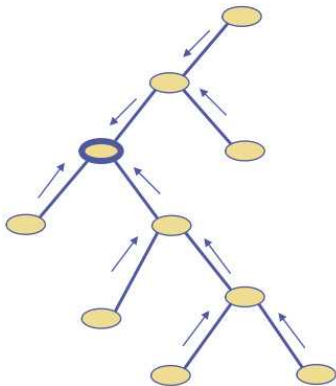
$$\begin{aligned} \phi_S^{**} &= \sum_{W \setminus S} \psi_W^* \\ \psi_V^{**} &= \frac{\phi_S^{**}}{\phi_S^*} \psi_V^* \\ \psi_W^{**} &= \psi_W^* \end{aligned}$$

**Now they  
Agree...Done!**

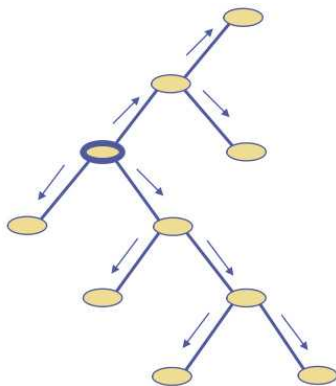
$$\begin{aligned} \sum_{V \setminus S} \psi_V^{**} &= \sum_{V \setminus S} \frac{\phi_S^{**}}{\phi_S^*} \psi_V^* \\ &= \frac{\phi_S^{**}}{\phi_S^*} \sum_{V \setminus S} \psi_V^* \\ &= \phi_S^{**} = \sum_{W \setminus S} \psi_W^{**} \end{aligned}$$

# Message passing for a general junction tree

1. Collect



2. Distribute



Then done!  
(may need to normalize)

## A different idea: belief propagation (Pearl)

- If the initial graph is a tree, inference is simple
- If there are cycles, we can form a **junction tree** of **maximal cliques** 'super-nodes'...
- Or just pretend the graph is a tree! Pass messages until convergence (we hope)
- This is **loopy belief propagation (LBP)**, an **approximate method**
- Perhaps surprisingly, it is **often very accurate** (e.g. error correcting codes, see McEliece, MacKay and Cheng, 1998, *Turbo Decoding as an Instance of Pearl's "Belief Propagation" Algorithm*)
- Prompted much work to try to understand **why**
- First we need some background on **variational inference** (**you should know**: almost all approximate marginal inference approaches are either **variational** or **sampling** methods)

# Variational approach for marginal inference

- We want to find the true distribution  $p$  but this is hard
- Idea: Approximate  $p$  by  $q$  for which computation is easy, with  $q$  'close' to  $p$
- How should we measure 'closeness' of probability distributions?

# Variational approach for marginal inference

- We want to find the true distribution  $p$  but this is hard
- Idea: Approximate  $p$  by  $q$  for which computation is easy, with  $q$  'close' to  $p$
- How should we measure 'closeness' of probability distributions?
- A very common approach: **Kullback-Leibler (KL) divergence**
- The ' $qp$ ' **KL-divergence** between two probability distributions  $q$  and  $p$  is defined as

$$D(q\|p) = \sum_{\mathbf{x}} q(\mathbf{x}) \log \frac{q(\mathbf{x})}{p(\mathbf{x})}$$

(measures the expected number of extra bits required to describe *samples from*  $q(\mathbf{x})$  using a code based on  $p$  instead of  $q$ )

- $D(q\|p) \geq 0$  for all  $q, p$ , with equality iff  $q = p$  (a.e.)
- **KL-divergence is not symmetric**

# Variational approach for marginal inference

- Suppose that we have an arbitrary graphical model:

$$p(\mathbf{x}; \theta) = \frac{1}{Z(\theta)} \prod_{\mathbf{c} \in \mathcal{C}} \psi_{\mathbf{c}}(\mathbf{x}_{\mathbf{c}}) = \exp \left( \sum_{\mathbf{c} \in \mathcal{C}} \theta_{\mathbf{c}}(\mathbf{x}_{\mathbf{c}}) - \log Z(\theta) \right)$$

- Rewrite the KL-divergence as follows:

$$\begin{aligned} D(q \| p) &= \sum_{\mathbf{x}} q(\mathbf{x}) \log \frac{q(\mathbf{x})}{p(\mathbf{x})} \\ &= - \sum_{\mathbf{x}} q(\mathbf{x}) \log p(\mathbf{x}) - \sum_{\mathbf{x}} q(\mathbf{x}) \log \frac{1}{q(\mathbf{x})} \\ &= - \sum_{\mathbf{x}} q(\mathbf{x}) \left( \sum_{\mathbf{c} \in \mathcal{C}} \theta_{\mathbf{c}}(\mathbf{x}_{\mathbf{c}}) - \log Z(\theta) \right) - H(q(\mathbf{x})) \\ &= - \sum_{\mathbf{c} \in \mathcal{C}} \sum_{\mathbf{x}} q(\mathbf{x}) \theta_{\mathbf{c}}(\mathbf{x}_{\mathbf{c}}) + \sum_{\mathbf{x}} q(\mathbf{x}) \log Z(\theta) - H(q(\mathbf{x})) \\ &= \underbrace{- \sum_{\mathbf{c} \in \mathcal{C}} E_q[\theta_{\mathbf{c}}(\mathbf{x}_{\mathbf{c}})]}_{\text{expected score}} + \log Z(\theta) - \underbrace{H(q(\mathbf{x}))}_{\text{entropy}} \end{aligned}$$

# The log-partition function $\log Z$

- Since  $D(q\|p) \geq 0$ , we have

$$-\sum_{\mathbf{c} \in \mathcal{C}} E_q[\theta_{\mathbf{c}}(\mathbf{x}_{\mathbf{c}})] + \log Z(\theta) - H(q(\mathbf{x})) \geq 0,$$

which implies that

$$\log Z(\theta) \geq \sum_{\mathbf{c} \in \mathcal{C}} E_q[\theta_{\mathbf{c}}(\mathbf{x}_{\mathbf{c}})] + H(q(\mathbf{x}))$$

- Thus, **any** approximating distribution  $q(\mathbf{x})$  gives a **lower bound** on the log-partition function (for a Bayesian network, this is the probability of the evidence)
- Recall that  $D(q\|p) = 0$  iff  $q = p$ . Thus, if we optimize over **all** distributions, we have:

$$\log Z(\theta) = \max_q \sum_{\mathbf{c} \in \mathcal{C}} E_q[\theta_{\mathbf{c}}(\mathbf{x}_{\mathbf{c}})] + H(q(\mathbf{x}))$$

# Variational inference: Naive Mean Field

$$\log Z(\theta) = \max_{q \in \mathbb{M}} \underbrace{\sum_{\mathbf{c} \in \mathcal{C}} E_q[\theta_{\mathbf{c}}(\mathbf{x}_{\mathbf{c}})] + H(q(\mathbf{x}))}_{\text{concave}} \leftarrow H \text{ of global distn}$$

- The space of **all** valid marginals for  $q$  is the **marginal polytope**
- The **naive mean field** approximation **restricts**  $q$  to a simple factorized distribution:

$$q(\mathbf{x}) = \prod_{i \in V} q_i(x_i)$$

- Corresponds to optimizing over a **non-convex inner bound** on the marginal polytope  $\Rightarrow$  **global optimum hard to find**

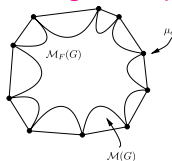
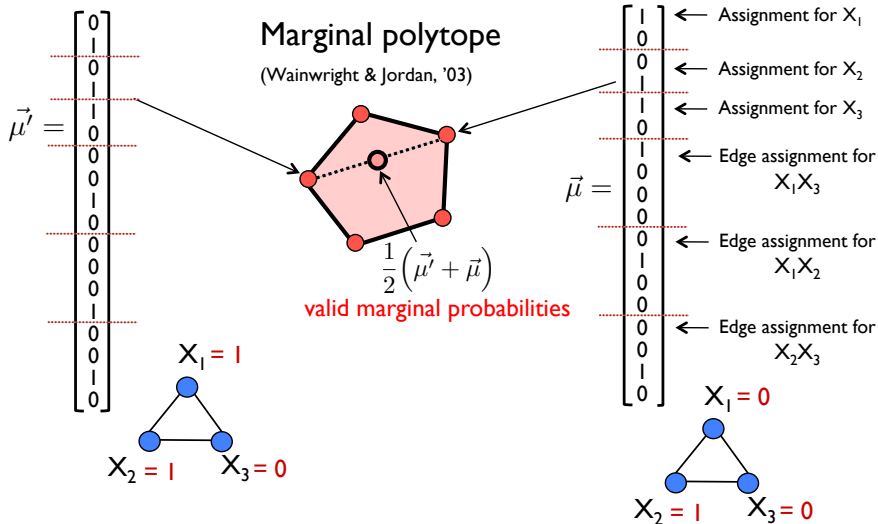


Figure from Martin Wainwright

- Hence, always attains a **lower bound** on  **$\log Z$**



# Background: *the marginal polytope* $\mathbb{M}$ (all valid marginals)



Entropy?

# Variational inference: Tree-reweighted (TRW)

$$\log Z(\theta) = \max_{q \in \mathbb{M}} \sum_{\mathbf{c} \in C} E_q[\theta_{\mathbf{c}}(\mathbf{x}_{\mathbf{c}})] + H(q(\mathbf{x}))$$

- TRW makes 2 pairwise approximations:

- Relaxes marginal polytope  $\mathbb{M}$  to local polytope  $\mathbb{L}$ , convex outer bound
- Uses a tree-reweighted upper bound  $H_T(q(\mathbf{x})) \geq H(q(\mathbf{x}))$

The exact entropy on any spanning tree is easily computed from single and pairwise marginals, and yields an upper bound on the true entropy, then  $H_T$  takes a convex combination

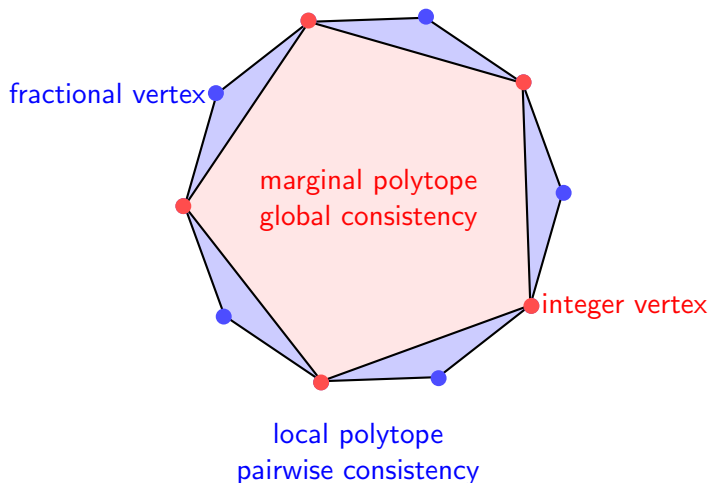
$$\log Z_T(\theta) = \max_{q \in \mathbb{L}} \underbrace{\sum_{\mathbf{c} \in C} E_q[\theta_{\mathbf{c}}(\mathbf{x}_{\mathbf{c}})] + H_T(q(\mathbf{x}))}_{\text{concave}}$$

- Hence, always attains an upper bound on  $\log Z$

$$Z_{MF} \leq Z \leq Z_T$$

# The local polytope $\mathbb{L}$ has extra fractional vertices

The **local polytope** is a **convex outer bound** on the **marginal polytope**





$$\log Z(\theta) = \max_{q \in \mathbb{M}} \sum_{\mathbf{c} \in \mathcal{C}} E_q[\theta_{\mathbf{c}}(\mathbf{x}_{\mathbf{c}})] + H(q(\mathbf{x}))$$

- Bethe makes 2 pairwise approximations:
  - Relaxes marginal polytope  $\mathbb{M}$  to local polytope  $\mathbb{L}$
  - Uses the Bethe entropy approximation  $H_B(q(\mathbf{x})) \approx H(q(\mathbf{x}))$

The Bethe entropy is exact for a tree. Loosely, it calculates an approximation **pretending** the model is a tree.

$$\log Z_B(\theta) = \max_{q \in \mathbb{L}} \underbrace{\sum_{\mathbf{c} \in \mathcal{C}} E_q[\theta_{\mathbf{c}}(\mathbf{x}_{\mathbf{c}})] + H_B(q(\mathbf{x}))}_{\text{not concave in general}}$$

- In general, is neither an upper nor a lower bound on  $\log Z$ , though is **often very accurate** (bounds are known for some cases)
- There is a neat relationship between the approximate methods

$$Z_{MF} \leq Z_B \leq Z_T$$



$$\log Z(\theta) = \max_{q \in \mathbb{M}} \sum_{\mathbf{c} \in \mathcal{C}} E_q[\theta_{\mathbf{c}}(\mathbf{x}_{\mathbf{c}})] + H(q(\mathbf{x}))$$

- Bethe makes 2 pairwise approximations:

- Relaxes **marginal polytope**  $\mathbb{M}$  to **local polytope**  $\mathbb{L}$
- Uses the **Bethe entropy** approximation  $H_B(q(\mathbf{x})) \approx H(q(\mathbf{x}))$

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$$\log Z_B(\theta) = \max_{q \in \mathbb{L}} \underbrace{\sum_{\mathbf{c} \in \mathcal{C}} E_q[\theta_{\mathbf{c}}(\mathbf{x}_{\mathbf{c}})] + H_B(q(\mathbf{x}))}_{\text{not concave in general}}$$

- In general, is neither an upper nor a lower bound on  $\log Z$ , though is **often very accurate** (bounds are known for some cases)
- Does this remind you of anything?



$$\log Z(\theta) = \max_{q \in \mathbb{M}} \sum_{c \in C} E_q[\theta_c(\mathbf{x}_c)] + H(q(\mathbf{x}))$$

- Bethe makes 2 pairwise approximations:

- Relaxes **marginal polytope**  $\mathbb{M}$  to **local polytope**  $\mathbb{L}$
- Uses the **Bethe entropy** approximation  $H_B(q(\mathbf{x})) \approx H(q(\mathbf{x}))$   
The Bethe entropy is exact for a tree. Loosely, it calculates an approximation **pretending** the model is a tree.

$$\log Z_B(\theta) = \max_{q \in \mathbb{L}} \underbrace{\sum_{c \in C} E_q[\theta_c(\mathbf{x}_c)] + H_B(q(\mathbf{x}))}_{\text{stationary points correspond 1-1 with fixed points of LBP!}}$$

- Hence, LBP may be considered a heuristic to optimize the Bethe approximation
- This connection was revealed by Yedidia, Freeman and Weiss, NIPS 2000, *Generalized Belief Propagation*

## ① libDAI

- <http://www.libdai.org>
- Mean-field, loopy sum-product BP, tree-reweighted BP, double-loop GBP

## ② Infer.NET

- <http://research.microsoft.com/en-us/um/cambridge/projects/infernet/>
- Mean-field, loopy sum-product BP
- Also handles continuous variables

Extra slides for questions or further explanation



# ML learning in Bayesian networks

- Maximum likelihood learning:  $\max_{\theta} \ell(\theta; \mathcal{D})$ , where

$$\begin{aligned}\ell(\theta; \mathcal{D}) = \log p(\mathcal{D}; \theta) &= \sum_{\mathbf{x} \in \mathcal{D}} \log p(\mathbf{x}; \theta) \\ &= \sum_i \sum_{\hat{\mathbf{x}}_{pa(i)}} \sum_{\substack{\mathbf{x} \in \mathcal{D}: \\ \mathbf{x}_{pa(i)} = \hat{\mathbf{x}}_{pa(i)}}} \log p(x_i \mid \hat{\mathbf{x}}_{pa(i)})\end{aligned}$$

- In Bayesian networks, we have the closed form ML solution:

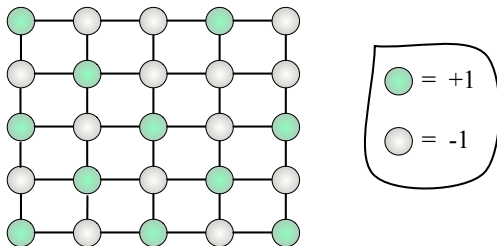
$$\theta_{x_i | \mathbf{x}_{pa(i)}}^{ML} = \frac{N_{x_i, \mathbf{x}_{pa(i)}}}{\sum_{\hat{x}_i} N_{\hat{x}_i, \mathbf{x}_{pa(i)}}}$$

where  $N_{x_i, \mathbf{x}_{pa(i)}}$  is the number of times that the (partial) assignment  $x_i, \mathbf{x}_{pa(i)}$  is observed in the training data

- We can estimate each CPD independently because the objective **decomposes** by variable and parent assignment

# Parameter learning in Markov networks

- How do we learn the parameters of an Ising model?



$$p(x_1, \dots, x_n) = \frac{1}{Z} \exp \left( \sum_{i < j} w_{i,j} x_i x_j + \sum_i \theta_i x_i \right)$$

# Bad news for Markov networks

- The global normalization constant  $Z(\theta)$  kills decomposability:

$$\begin{aligned}\theta^{ML} &= \arg \max_{\theta} \log \prod_{\mathbf{x} \in \mathcal{D}} p(\mathbf{x}; \theta) \\ &= \arg \max_{\theta} \sum_{\mathbf{x} \in \mathcal{D}} \left( \sum_c \log \phi_c(\mathbf{x}_c; \theta) - \log Z(\theta) \right) \\ &= \arg \max_{\theta} \left( \sum_{\mathbf{x} \in \mathcal{D}} \sum_c \log \phi_c(\mathbf{x}_c; \theta) \right) - |\mathcal{D}| \log Z(\theta)\end{aligned}$$

- The log-partition function prevents us from decomposing the objective into a sum over terms for each potential
- Solving for the parameters becomes much more complicated