Prof. Jeff Bilmes

University of Washington, Seattle
Department of Electrical Engineering
http://melodi.ee.washington.edu/~bilmes

Dec 3rd, 2014
Announcements


- Should have read chapters 1 through 5 in our book. Read chapter 7

- Also read chapter 8 (integer/linear programming, although we cover only a bit of that chapter in class unfortunately).

- Also should have read “Divergence measures and message passing” by Thomas Minka, and “Structured Region Graphs: Morphing EP into GBP”, by Welling, Minka, and Teh.

- Assignment due Wednesday (Dec 3rd) night, 11:45pm. Final project proposal final progress report (one page max).

- Update: For status update, final writeup, and talk, use notation as close as possible to that used in class!
On Final Project

- Project update report due tonight, 11:45pm via canvas.
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- We have 21 presentations to give. 10 minutes each means 3.5 hours of presentation. 7 minutes each means 2.45 hours of presentation.
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- Final Exam time slot: Wednesday, December 10, 2014, 230-420 pm, PCAR 297 (two hours).
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- Final Exam time slot: Wednesday, December 10, 2014, 230-420 pm, PCAR 297 (two hours).
- Alternatively, you each do a 10-minute youtube presentation with at least screen capture and audio, can use perhaps http://tinytake.com/ or http://camstudio.org/, or post your favorite to canvas for others to discover. Then, it to an unlisted youtube link, send the link, and we all view it.
Class Road Map - EE512a

- L1 (9/29): Introduction, Families, Semantics
- L2 (10/1): MRFs, elimination, Inference on Trees
- L3 (10/6): Tree inference, message passing, more general queries, non-tree
- L4 (10/8): Non-trees, perfect elimination, triangulated graphs
- L5 (10/13): triangulated graphs, $k$-trees, the triangulation process/heuristics
- L6 (10/15): multiple queries, decomposable models, junction trees
- L7 (10/20): junction trees, begin intersection graphs
- L8 (10/22): intersection graphs, inference on junction trees
- L9 (10/27): inference on junction trees, semirings,
- L10 (11/3): conditioning, hardness, LBP
- L11 (11/5): LBP, exponential models,
- L12 (11/10): exponential models, mean params and polytopes,
- L13 (11/12): polytopes, tree outer bound, Bethe entropy approx.
- L14 (11/17): Bethe entropy approx, loop series correction
- L15 (11/19): Hypergraphs, posets, Mobius, Kikuchi
- L16 (11/24): Kikuchi, Expectation Propagation
- L17 (11/26): Expectation Propagation, Mean Field
- L18 (12/1): Structured mean field, Convex relaxations and upper bounds, tree reweighted case
- L19 (12/3): Variational MPE, Graph Cut MPE, LP Relaxations
- Final Presentations: (12/10):

Finals Week: Dec 8th-12th, 2014.
Theorem 19.2.3 (Relationship between $A$ and $A^*$)

(a) For any $\mu \in \mathcal{M}^\circ$, $\theta(\mu)$ unique canonical parameter sat. matching condition, then conj. dual takes form:

$$A^*(\mu) = \sup_{\theta \in \Omega} (\langle \theta, \mu \rangle - A(\theta)) = \begin{cases} -H(p_{\theta(\mu)}) & \text{if } \mu \in \mathcal{M}^\circ \\ +\infty & \text{if } \mu \notin \overline{\mathcal{M}} \end{cases}$$ (19.3)

(b) Partition function has variational representation (dual of dual)

$$A(\theta) = \sup_{\mu \in \mathcal{M}} \{\langle \theta, \mu \rangle - A^*(\mu)\}$$ (19.4)

(c) For $\theta \in \Omega$, sup occurs at $\mu \in \mathcal{M}^\circ$ of moment matching conditions

$$\mu = \int_{\mathbb{D}_X} \phi(x)p_{\theta}(x)\nu(dx) = \mathbb{E}_\theta[\phi(X)] = \nabla A(\theta)$$ (19.5)
Variational Approach Amenable to Approximation

- Original variational representation of log partition function

\[ A(\theta) = \sup_{\mu \in \mathcal{M}} \{ \langle \theta, \mu \rangle - A^*(\mu) \} \]  

(19.1)

where dual takes form:

\[ A^*(\mu) = \sup_{\theta \in \Omega} (\langle \theta, \mu \rangle - A(\theta)) = \begin{cases} -H(p_{\theta(\mu)}) & \text{if } \mu \in \mathcal{M}^o \\ +\infty & \text{if } \mu \notin \overline{\mathcal{M}} \end{cases} \]  

(19.2)

- Given efficient expression for \( A(\theta) \), we can compute marginals of interest.

- Above expression (dual of the dual) offers strategies to approximate or (upper or lower) bound \( A(\theta) \). We either approximate \( \mathcal{M} \) or \(-A^*(\mu)\) or (most likely) both.
Variational Approximations we cover

1. Set $\mathcal{M} \leftarrow \mathbb{L}$ and $-A^*(\mu) \leftarrow H_{\text{Bethe}}(\tau)$ to get Bethe variational approximation, LBP fixed point.

2. Set $\mathcal{M} \leftarrow \mathbb{L}_t(G)$ (hypergraph marginal polytope), $-A^*(\mu) \leftarrow H_{\text{app}}(\tau)$ where $H_{\text{app}} = \sum_{g \in E} c(g) H_g(\tau_g)$ (via Möbius) to get Kikuchi variational approximation, message passing on hypergraphs.

3. Partition $\tau$ into $(\tau, \tilde{\tau})$, and set $\mathcal{M} \leftarrow \mathcal{L}(\phi, \Phi)$ and set $-A^*(\mu) \leftarrow H_{\text{ep}}(\tau, \tilde{\tau})$ to get expectation propagation.

4. Mean field (from variational perspective) is (with $\mathcal{M}_F(G) \subseteq \mathcal{M}$) l.b.:

$$A(\theta) \geq \max_{\mu \in \mathcal{M}_F(G)} \{ \langle \mu, \theta \rangle - A^*_F(\mu) \} = A_{\text{mf}}(\theta) \quad (19.1)$$

5. Upper bound Convexified/tree reweighted LBP, entropy upper bounds $H(\tau(F))$ for all members $F \in \mathcal{D}$ of tractable substructures. Get U.b.:

$$A(\theta) \leq B_\mathcal{D}(\theta; \rho) \triangleq \sup_{\tau \in \mathcal{L}(G; \mathcal{D})} \left\{ \langle \tau, \theta \rangle + \sum_{F \in \mathcal{D}} \rho(F) H(\tau(F)) \right\} \quad (19.2)$$

with $\mathcal{L}(G; \mathcal{D}) = \bigcap_{F \in \mathcal{D}} \mathcal{M}(F)$
In many cases, we care not to sum over $x$ in $\sum_x p(x)$ but instead to compute $x^* \in \arg\max_{x \in D_X} p(x)$. This is called the "Viterbi assignment", or the "most probable explanation" (MPE), or the "most probable configuration" or the "mode", or a few other names.

From the perspective of semirings, we are only changing the semiring (from sum-product to max-product). Can do exactly same form of exact inference algorithms (e.g., trees, $k$-trees, junction trees) using different semiring, to get answer. To get $n$-best answers, can also be seen as a semiring. Equally difficult when tree-width is large. Can the variational approach help in this case as well?
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Equally difficult when tree-width is large.

Can the variational approach help in this case as well?
MPE - most probable explanation

MPE again

\[
\arg\max_{x \in \mathcal{D}_{X^m}} p(x) = \{ x \in \mathcal{D}_{X^m} : p_{\theta}(x) \geq p_{\theta}(y), \forall y \in \mathcal{D}_{X^m} \} \quad (19.1)
\]
MPE - most probable explanation

- MPE again

\[
\arg\max_{x \in D_X^m} p(x) = \{ x \in D_X^m : p_\theta(x) \geq p_\theta(y), \forall y \in D_X^m \} \tag{19.1}
\]

- Since we are using exponential family models, we have

\[
\arg\max_{x \in D_X^m} p(x) = \arg\max_{x \in D_X^m} \langle \theta, \phi(x) \rangle = \arg\min_{x \in D_X^m} E[x] \tag{19.2}
\]

i.e., cumulant function isn’t required for computation.

\( E[x] = -\langle \theta, \phi(x) \rangle \) is seen as an “energy” function.
MPE - most probable explanation

- MPE again

\[
\arg\max_{x \in D_{X^m}} p(x) = \left\{ x \in D_{X^m} : p_\theta(x) \geq p_\theta(y), \forall y \in D_{X^m} \right\} \quad (19.1)
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- Since we are using exponential family models, we have

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\]

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\[E[x] = -\langle \theta, \phi(x) \rangle\] is seen as an “energy” function.

- But it is related. Recall cumulant function

\[
A(\theta) = \log \int \exp \{ \langle \theta, \phi(x) \rangle \} d\nu(x) \quad (19.3)
\]

\[= \sup_{\mu \in \mathcal{M}} \{ \langle \theta, \mu \rangle - A^*(\mu) \} \quad (19.4)\]
MPE - and variational

- Considering $p_\theta(x) = \exp\{\langle \theta, \phi(x) \rangle - A(\theta)\}$. 

Let $\beta \in \mathbb{R}^+_{\text{+}}$ be a positive scalar.

If we substitute $\theta$ with $\beta \theta$ (i.e., $p_\theta(x)$ with $p_{\beta \theta}(x)$), and when $\beta \theta \in \Omega$, then $p_{\beta \theta}(x)$ becomes more concentrated (relatively) around MPE solutions as $\beta \to \infty$.

Ex: Let $p_\theta(x^\ast) > p_\theta(y)$ for all $y \neq x^\ast$, so $x^\ast$ is the unique maximum.

Then $\langle \theta, \phi(x^\ast) \rangle > \langle \theta, \phi(y) \rangle$ and $h(\beta) \triangleq \langle \beta \theta, \phi(x^\ast) \rangle - \langle \beta \theta, \phi(y) \rangle = \beta \langle \theta, \phi(x^\ast) \rangle - \langle \theta, \phi(y) \rangle \quad (19.5)$ grows unboundedly large as $\beta \to \infty$.

Since $A(\beta \theta)$ keeps things normalized, $A(\beta \theta)$ somehow must counteract the otherwise unbounded increase in $h(\beta)$. This suggests $A(\beta \theta)/\beta$ might tell us something.
MPE - and variational

- Considering $p_\theta(x) = \exp \{\langle \theta, \phi(x) \rangle - A(\theta) \}$.
- Let $\beta \in \mathbb{R}_+$ be a positive scalar.
Variational MPE

Graph Cut MPE

LP Relaxations

Class Recap

Refs

MPE - and variational

- Considering \( p_\theta(x) = \exp\{\langle \theta, \phi(x) \rangle - A(\theta)\} \).

- Let \( \beta \in \mathbb{R}_+ \) be a positive scalar.

- If we substitute \( \theta \) with \( \beta \theta \) (i.e., \( p_\theta(x) \) with \( p_{\beta \theta}(x) \)), and when \( \beta \theta \in \Omega \), then \( p_{\beta \theta}(x) \) becomes more concentrated (relatively) around MPE solutions as \( \beta \to \infty \).
MPE - and variational

- Considering \( p_\theta(x) = \exp \{ \langle \theta, \phi(x) \rangle - A(\theta) \} \).
- Let \( \beta \in \mathbb{R}_+ \) be a positive scalar.
- If we substitute \( \theta \) with \( \beta \theta \) (i.e., \( p_\theta(x) \) with \( p_{\beta \theta}(x) \)), and when \( \beta \theta \in \Omega \), then \( p_{\beta \theta}(x) \) becomes more concentrated (relatively) around MPE solutions as \( \beta \to \infty \).
- Ex: Let \( p_\theta(x^*) > p_\theta(y) \) for all \( y \neq x^* \), so \( x^* \) is the unique maximum. Then \( \langle \theta, \phi(x^*) \rangle > \langle \theta, \phi(y) \rangle \) and

\[
\begin{align*}
    h(\beta) &\triangleq \langle \beta \theta, \phi(x^*) \rangle - \langle \beta \theta, \phi(y) \rangle = \beta (\langle \theta, \phi(x^*) \rangle - \langle \theta, \phi(y) \rangle) \\
    &\text{grows unboundedly large as } \beta \to \infty.
\end{align*}
\]
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Let $\beta \in \mathbb{R}_+$ be a positive scalar.

If we substitute $\theta$ with $\beta \theta$ (i.e., $p_\theta(x)$ with $p_{\beta \theta}(x)$), and when $\beta \theta \in \Omega$, then $p_{\beta \theta}(x)$ becomes more concentrated (relatively) around MPE solutions as $\beta \to \infty$.

Ex: Let $p_\theta(x^*) > p_\theta(y)$ for all $y \neq x^*$, so $x^*$ is the unique maximum. Then $\langle \theta, \phi(x^*) \rangle > \langle \theta, \phi(y) \rangle$ and

$$h(\beta) \triangleq \langle \beta \theta, \phi(x^*) \rangle - \langle \beta \theta, \phi(y) \rangle = \beta (\langle \theta, \phi(x^*) \rangle - \langle \theta, \phi(y) \rangle) \quad (19.5)$$

grows unboundedly large as $\beta \to \infty$.

Since $A(\beta \theta)$ keeps things normalized, $A(\beta \theta)$ somehow must counteract the otherwise unbounded increase in $h(\beta)$. This suggests $A(\beta \theta)/\beta$ might tell us something.
Theorem 19.3.1 (MPE and variational)

For all $\theta \in \Omega$, the problem of mode computation has the following alternative representations:

\[
\max_{x \in D_X^m} \langle \theta, \phi(x) \rangle = \max_{\mu \in \bar{M}} \langle \theta, \mu \rangle, \quad \text{and} \quad (19.6)
\]

\[
\max_{x \in D_X^m} \langle \theta, \phi(x) \rangle = \lim_{\beta \to \infty} \frac{A(\beta \theta)}{\beta} \quad (19.7)
\]

Intuition: We have $\mu = \mathbb{E}_p[\phi(x)]$, so that

\[
\max_{x \in D_X^m} \langle \theta, \phi(x) \rangle = \max_{p \in P} \langle \theta, \mathbb{E}_p[\phi(x)] \rangle
\]

where $P$ is a set of zero entropy distributions with point mass on some point in $D_X^m$. I.e., for each $p \in P$, there exists $x \in D_X^m$ with $p(x) = 1$. Equation (19.6) says that max falls on extreme point of the mean parameter convex region (vertex of polytope, in polyhedral case).
Theorem 19.3.1 (MPE and variational)

For all $\theta \in \Omega$, the problem of mode computation has the following alternative representations:

$$\max_{x \in D_{X^m}} \langle \theta, \phi(x) \rangle = \max_{\mu \in M} \langle \theta, \mu \rangle,$$

(19.6)

$$\max_{x \in D_{X^m}} \langle \theta, \phi(x) \rangle = \lim_{\beta \to \infty} \frac{A(\beta \theta)}{\beta}$$

(19.7)

- Intuition: We have $\mu = E_p[\phi(x)]$, so that
  $$\max_{x \in D_{X^m}} \langle \theta, \phi(x) \rangle = \max_{p \in P} \langle \theta, E_p[\phi(x)] \rangle$$
  where $P$ is a set of zero entropy distributions with point mass on some point in $D_{X^m}$. I.e., for each $p \in P$, there exists $x \in D_{X^m}$ with $p(x) = 1$. 

Prof. Jeff Bilmes
Theorem 19.3.1 (MPE and variational)

For all $\theta \in \Omega$, the problem of mode computation has the following alternative representations:

$$\max_{x \in D_{X_m}} \langle \theta, \phi(x) \rangle = \max_{\mu \in \bar{M}} \langle \theta, \mu \rangle, \text{ and}$$

$$\max_{x \in D_{X_m}} \langle \theta, \phi(x) \rangle = \lim_{\beta \to \infty} \frac{A(\beta \theta)}{\beta}$$

- **Intuition:** We have $\mu = E_p[\phi(x)]$, so that
  $$\max_{x \in D_{X_m}} \langle \theta, \phi(x) \rangle = \max_{p \in \mathcal{P}} \langle \theta, E_p[\phi(x)] \rangle$$
  where $\mathcal{P}$ is a set of zero entropy distributions with point mass on some point in $D_{X_m}$. I.e., for each $p \in \mathcal{P}$, there exists $x \in D_{X_m}$ with $p(x) = 1$.

- **Equation (19.6)** says that max falls on extreme point of the mean parameter convex region $\bar{M}$ (vertex of polytope, in polyhedral case).
Also, Equation (19.6) shows how MPE can be seen as a linear optimization over a convex set $\mathcal{M}$. 
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For discrete distributions, we have $\mathcal{M} = \mathcal{M}(G)$ for graph $G$, so this is a linear objective with polyhedral constraints, i.e., a linear program (LP).
Also, Equation (19.6) shows how MPE can be seen as a linear optimization over a convex set $\mathcal{M}$.

For discrete distributions, we have $\mathcal{M} = \mathbb{M}(G)$ for graph $G$, so this is a linear objective with polyhedral constraints, i.e., a linear program (LP).

Since l.h.s. of Equation (19.6) is integer program, this shows the difficulty of $\mathbb{M}(G)$. 
MPE - and variational

- Intuition for Equation (19.7), repeated here:

\[
\max_{x \in D_X^m} \langle \theta, \phi(x) \rangle = \lim_{\beta \to \infty} \frac{A(\beta \theta)}{\beta}
\]  

(19.7)
MPE - and variational

- Intuition for Equation (19.7), repeated here:

\[
\max_{x \in \mathcal{D}_X} \langle \theta, \phi(x) \rangle = \lim_{\beta \to \infty} \frac{A(\beta \theta)}{\beta} = \frac{1}{\beta} \sup_{\mu \in \mathcal{M}} \left\{ \langle \beta \theta, \mu \rangle - A^*(\mu) \right\}.
\]  

- Intuitively,

\[
\lim_{\beta \to +\infty} \frac{A(\beta \theta)}{\beta} = \lim_{\beta \to +\infty} \sup_{\mu \in \mathcal{M}} \left\{ \langle \beta \theta, \mu \rangle - A^*(\mu) \right\}.
\]
MPE - and variational

- Intuition for Equation (19.7), repeated here:

\[
\max_{x \in D_X} \langle \theta, \phi(x) \rangle = \lim_{\beta \to \infty} \frac{A(\beta \theta)}{\beta}
\] (19.7)

- Intuitively,

\[
\lim_{\beta \to +\infty} \frac{A(\beta \theta)}{\beta} = \lim_{\beta \to +\infty} \frac{1}{\beta} \sup_{\mu \in \mathcal{M}} \{ \langle \beta \theta, \mu \rangle - A^*(\mu) \}
\] (19.8)

\[
= \lim_{\beta \to +\infty} \sup_{\mu \in \mathcal{M}} \left\{ \langle \theta, \mu \rangle - \frac{1}{\beta} A^*(\mu) \right\}
\] (19.9)

- Due to convexity of $A^*$ we can swap the lim and the sup and we get the result.
When graph is a tree, we can find an interesting connection between the max-product form of messages and a particular Lagrangian.
MPE - and variational for trees

- When graph is a tree, we can find an interesting connection between the max-product form of messages and a particular Lagrangian.

- Maxproduct updates take the form:

\[
M_{t \rightarrow s}(x_s) \leftarrow \kappa \max_{x_t \in \mathcal{D}_X} \left[ \exp \left\{ \theta_{st}(x_s, x_t) + \theta_t(x_t) \right\} \prod_{u \in N(t) \setminus s} M_{u \rightarrow t}(x_t) \right]
\]

(19.10)
MPE - and variational for trees

- When graph is a tree, we can find an interesting connection between the max-product form of messages and a particular Lagrangian.

\[ M_{t\rightarrow s}(x_s) \leftarrow \kappa \max_{x_t \in \mathcal{D}_{X_t}} \left[ \exp \left\{ \theta_{st}(x_s, x_t) + \theta_t(x_t) \right\} \prod_{u \in N(t) \setminus s} M_{u\rightarrow t}(x_t) \right] \]

(19.10)

- Maxproduct updates take the form:

\[ \max_{x \in \mathcal{D}_{X^m}} \left[ \sum_{s \in V} \theta_s(x_s) + \sum_{(s,t) \in E} \theta_{st}(x_s, x_t) \right] = \max_{\mu \in \mathcal{L}(T)} \langle \mu, \theta \rangle \]

(19.11)

- Using the Theorem 19.3.1, we get (in the case of a tree \(T\))
When graph is a tree, we can find an interesting connection between the max-product form of messages and a particular Lagrangian.

Maxproduct updates take the form:

\[
M_{t \rightarrow s}(x_s) \leftarrow \kappa \max_{x_t \in D_{X_t}} \left[ \exp \{ \theta_{st}(x_s, x_t) + \theta_t(x_t) \} \prod_{u \in N(t) \setminus s} M_{u \rightarrow t}(x_t) \right]
\]

Using the Theorem 19.3.1, we get (in the case of a tree \( T \))

\[
\max_{x \in D_{X^m}} \left[ \sum_{s \in V} \theta_s(x_s) + \sum_{(s,t) \in E} \theta_{st}(x_s, x_t) \right] = \max_{\mu \in \mathbb{L}(T)} \langle \mu, \theta \rangle
\]

Right hand side is a LP over a simple polytope, the marginal polytope for trees \( \mathbb{L}(T) \).
MPE, relationship between max-product algorithm and linear program

It turns out that: the max-product updates are a Lagrangian method for solving the dual of the above linear program, i.e., $\max_{\mu \in \mathbb{L}(T)} \langle \mu, \theta \rangle$. 

$$
C_{ts}(x_s) = \mu_s(x_s) - \sum_{x_t} \mu_{st}(x_s, x_t)
$$

and associated Lagrange multiplier $\lambda_{st}(x_s)$.

Also define a (non-negative and normalized) mean parameter space $\mathbb{N} \subseteq \mathbb{R}^d$ as follows:

$$
\mathbb{N} = \left\{ \mu \in \mathbb{R}^d \mid \mu \geq 0, \sum_{x_s} \mu_s(x_s) = 1, \sum_{x_s, x_t} \mu_{st}(x_s, x_t) = 1 \right\}
$$
It turns out that: the max-product updates are a Lagrangian method for solving the dual of the above linear program, i.e., \( \max_{\mu \in \mathbb{L}(T)} \langle \mu, \theta \rangle \).

Marginalization constraint \( C_{ts}(x_s) = 0 \) for edge \( t, s \)

\[
C_{ts}(x_s) = \mu_s(x_s) - \sum_{x_t} \mu_{st}(x_s, x_t)
\]  

(19.12)

and associated Lagrange multiplier \( \lambda_{st}(x_s) \).
MPE, relationship between max-product algorithm and linear program

- It turns out that: the max-product updates are a Lagrangian method for solving the dual of the above linear program, i.e., $\max_{\mu \in \mathbb{L}(T)} \langle \mu, \theta \rangle$.
- Marginalization constraint $C_{ts}(x_s) = 0$ for edge $t, s$

$$C_{ts}(x_s) = \mu_s(x_s) - \sum_{x_t} \mu_{st}(x_s, x_t) \quad (19.12)$$

and associated Lagrange multiplier $\lambda_{st}(x_s)$.
- Also define a (non-negative and normalized) mean parameter space $N \subseteq \mathbb{R}^d$ as follows:

$$N = \left\{ \mu \in \mathbb{R}^d | \mu \geq 0, \sum_{x_s} \mu_s(x_s) = 1, \sum_{x_s, x_t} \mu_{st}(x_s, x_t) = 1 \right\} \quad (19.13)$$
Theorem 19.3.2 (Max-product and LP Duality)

Consider the dual function $Q$ defined by the following partial Lagrangian formulation of the tree-structured LP:

$$Q(\lambda) = \max_{\mu \in \mathbb{N}} L(\mu; \lambda), \text{ where}$$

$$L(\mu; \lambda) = \langle \theta, \mu \rangle + \sum_{(s,t) \in E(T)} \left[ \sum_{x_s} \lambda_{ts}(x_s) C_{ts}(x_s) + \sum_{x_t} \lambda_{st}(x_t) C_{st}(x_t) \right]$$

(19.14)

For any fixed point $M^*$ of the max-product updates, the vector $\lambda^* = \log M^*$, where the logarithm is taken elementwise, is an optimal solution of the dual problem $\min_{\lambda} Q(\lambda)$. 

(19.15)
Restricted clique functions

- Here we don’t restrict $G$ but restrict clique functions.
Restricted clique functions

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- Given $G$ let $p \in \mathcal{F}(G, \mathcal{M}(f))$ such that we can write
Restricted clique functions

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- Given $G$ let $p \in \mathcal{F}(G, M^f)$ such that we can write

$$\log p(x) = \prod_{v \in V(G)} \psi_v(x_v) \prod_{(i,j) \in E(G)} \psi_{ij}(x_i, x_j)$$  \hspace{1cm} (19.16)
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$$\log p(x) = \prod_{v \in V(G)} \psi_v(x_v) \prod_{(i,j) \in E(G)} \psi_{ij}(x_i, x_j)$$  \hspace{1cm} (19.16)

or equivalently

$$-\log p(x) \propto \sum_{v \in V(G)} e_v(x_v) + \sum_{(i,j) \in E(G)} e_{ij}(x_i, x_j)$$ \hspace{1cm} (19.17)
Restricted clique functions

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- Given $G$ let $p \in \mathcal{F}(G, \mathcal{M}(f))$ such that we can write

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\log p(x) = \prod_{v \in V(G)} \psi_v(x_v) \prod_{(i,j) \in E(G)} \psi_{ij}(x_i, x_j) \quad (19.16)
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or equivalently

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- \log p(x) \propto \sum_{v \in V(G)} e_v(x_v) + \sum_{(i,j) \in E(G)} e_{ij}(x_i, x_j) \quad (19.17)
$$

- $e_v(x_v)$ and $e_{ij}(x_i, x_j)$ are like local energy potentials, the smaller they are, the higher the probability. E.g., $e_{ij}(x_i, x_j) = -\theta_{ij} \phi_{ij}(x_i, x_j)$
Restricted clique functions

Given $G$ let $p \in \mathcal{F}(G, M^{(f)})$ such that we can write the global energy $E(x)$ as a sum of unary and pairwise potentials:

$$E(x) = \sum_{v \in V(G)} e_v(x_v) + \sum_{(i, j) \in E(G)} e_{ij}(x_i, x_j)$$  \hspace{1cm} (19.18)
Restricted clique functions

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- $e_v(x_v)$ and $e_{ij}(x_i, x_j)$ are like local energy potentials.

- Since $\log p(x) = -E(x) + \text{const.}$, the smaller $e_v(x_v)$ or $e_{ij}(x_i, x_j)$ become, the higher the probability becomes.
Restricted clique functions

- Given \( G \) let \( p \in \mathcal{F}(G, \mathcal{M}^{(f)}) \) such that we can write the global energy \( E(x) \) as a sum of \textit{unary} and \textit{pairwise} potentials:

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- Further, say that \( D_{X_v} = \{0, 1\} \) (binary), so we have binary random vectors distributed according to \( p(x) \).
Restricted clique functions

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- $e_v(x_v)$ and $e_{ij}(x_i, x_j)$ are like local energy potentials.
- Since $\log p(x) = -E(x) + \text{const.}$, the smaller $e_v(x_v)$ or $e_{ij}(x_i, x_j)$ become, the higher the probability becomes.
- Further, say that $\mathcal{D}_{X_v} = \{0, 1\}$ (binary), so we have binary random vectors distributed according to $p(x)$.
- Thus, $x \in \{0, 1\}^V$, and finding MPE solution is setting some of the variables to 0 and some to 1, i.e.,

$$\min_{x \in \{0,1\}^V} E(x)$$  \hspace{1cm} (19.19)
Markov random field

$$\log p(x) \propto \sum_{v \in V(G)} e_v(x_v) + \sum_{(i,j) \in E(G)} e_{ij}(x_i, x_j) \quad (19.20)$$

When $G$ is a 2D grid graph, we have
Create an auxiliary graph

- We can create auxiliary graph $G_a$ that involves two new “terminal” nodes $s$ and $t$ and all of the original “non-terminal” nodes $v \in V(G)$.
- The non-terminal nodes represent the original random variables $x_v, v \in V$.
- Starting with the original grid-graph among the vertices $v \in V$, we connect each of $s$ and $t$ to all of the original nodes.
- I.e., we form $G_a = (V \cup \{s, t\}, E + \bigcup_{v \in V} ((s, v) \cup (v, t)))$. 
Transformation from graphical model to auxiliary graph

Original 2D-grid graphical model $G$ and energy function

$$E(x) = \sum_{v \in V(G)} e_v(x_v) + \sum_{(i,j) \in E(G)} e_{ij}(x_i, x_j)$$

needing to be minimized over $x \in \{0, 1\}^V$. Recall, tree-width is $O(\sqrt{|V|})$. 
Augmented (graph-cut) directed graph $G_a$. Edge weights (TBD) of graph are derived from
$\{e_v(\cdot)\}_{v \in V}$ and $\{e_{ij}(\cdot, \cdot)\}_{(i,j) \in E(G)}$.

An $(s, t)$-cut $C \subseteq E(G_a)$ is a set of edges that cut all paths from $s$ to $t$. A minimum $(s, t)$-cut is one that has minimum weight where $w(C) = \sum_{e \in C} w_e$ is the cut weight.

To be a cut, must have that, for every $v \in V$, either $(s, v) \in C$ or $(v, t) \in C$. Graph is directed, arrows pointing down from $s$ towards $t$ or from $i \rightarrow j$. 
Augmented (graph-cut) directed graph $G_a$. Edge weights (TBD) of graph are derived from 
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Transformation from graphical model to auxiliary graph

Cut edges that are incident to terminal nodes $s$ and $t$ are indicated in green.
Transformation from graphical model to auxiliary graph

Cut edges that are incident to terminal nodes $s$ and $t$ removed from graph. But there are still un-cut $(s, t)$-paths remaining.
Transformation from graphical model to auxiliary graph

Additional cut edges incident to two non-terminal nodes are indicated in green.
Transformation from graphical model to auxiliary graph

Vertices adjacent to $t$ are shaded blue, vertices adjacent to $s$ shaded red.
Transformation from graphical model to auxiliary graph

Additional cut edges incident to two non-terminal nodes are removed from graph.
Transformation from graphical model to auxiliary graph

Augmented graph-cut graph with cut edges removed corresponds to particular binary vector $\bar{x} \in \{0, 1\}^n$. Each vector $\bar{x}$ has a score corresponding to $\log p(\bar{x})$, but when can graph cut scores correspond precisely to $\log p(\bar{x})$ in a way that min-cut algorithms can find minimum of energy $E(x)$?
Setting of the weights in the auxiliary cut graph

- Any graph cut corresponds to a vector $\bar{x} \in \{0, 1\}^n$. 
Setting of the weights in the auxiliary cut graph

- Any graph cut corresponds to a vector $\bar{x} \in \{0, 1\}^n$.
- If weights of all edges, except those involving terminals $s$ and $t$, are non-negative, graph cut computable in polynomial time via max-flow (many algorithms, e.g., Edmonds&Karp $O(nm^2)$ or $O(n^2m \log(nC))$; Goldberg&Tarjan $O(nm \log(n^2/m))$, see Schrijver, page 161).
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- If weights are set correctly in the cut graph, and if edge functions \( e_{ij} \) satisfy certain properties, then graph-cut score corresponding to \( \bar{x} \) can be made equivalent to \( E(x) = \log p(\bar{x}) + \text{const} \).
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- Hence, poly time graph cut, can find the optimal MPE assignment, regardless of the graphical model’s tree-width!
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- Hence, poly time graph cut, can find the optimal MPE assignment, regardless of the graphical model’s tree-width!
- In general, finding MPE is an NP-hard optimization problem.
Setting of the weights in the auxiliary cut graph

Edge weight assignments. Start with all weights set to zero.

- For \((s, v)\) with \(v \in V(G)\), set edge
  
  \[
  w_{s,v} = (e_v(1) - e_v(0))1(e_v(1) > e_v(0))
  \]  
  (19.21)
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  \[
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  (19.22)

- For original edge \((i, j)\) \(\in E\), \(i, j \in V\), set weight
  \[ w_{i,j} = e_{ij}(1,0) + e_{ij}(0,1) - e_{ij}(1,1) - e_{ij}(0,0) \]  
  (19.23)
Setting of the weights in the auxiliary cut graph

Edge weight assignments. Start with all weights set to zero.

- For \((s, v)\) with \(v \in V(G)\), set edge

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\[
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- For original edge \((i, j)\) \(\in E\), \(i, j \in V\), set weight

\[
w_{i,j} = e_{ij}(1, 0) + e_{ij}(0, 1) - e_{ij}(1, 1) - e_{ij}(0, 0)
\]  (19.23)

and if \(e_{ij}(1, 0) > e_{ij}(0, 0)\), and \(e_{ij}(1, 1) > e_{ij}(0, 1)\),

\[
w_{s,i} \leftarrow w_{s,i} + (e_{ij}(1, 0) - e_{ij}(0, 0))
\]  (19.24)

\[
w_{j,t} \leftarrow w_{j,t} + (e_{ij}(1, 1) - e_{ij}(0, 1))
\]  (19.25)

and analogous increments if inequalities are flipped.
Non-negative edge weights

The inequalities ensure that we are adding non-negative weights to each of the edges. I.e., we do $w_{s,i} ← w_{s,i} + (e_{ij}(1, 0) - e_{ij}(0, 0))$ only if $e_{ij}(1, 0) > e_{ij}(0, 0)$.
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- For $(i, j)$ edge weight, it takes the form:

  $$w_{i,j} = e_{ij}(1, 0) + e_{ij}(0, 1) - e_{ij}(1, 1) - e_{ij}(0, 0) \quad (19.26)$$
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- For this to be non-negative, we need:

$$e_{ij}(1,0) + e_{ij}(0,1) \geq e_{ij}(1,1) - e_{ij}(0,0) \quad (19.27)$$
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For this to be non-negative, we need:

\[
    e_{ij}(1,0) + e_{ij}(0,1) \geq e_{ij}(1,1) - e_{ij}(0,0) \tag{19.27}
\]

Thus weights \( w_{ij} \) in \( s,t \)-graph above are always non-negative, so graph-cut solvable exactly.
Submodular potentials

Edge functions must be **submodular** (in the binary case, equivalent to "associative", "attractive", "regular", "Potts", or "ferromagnetic"): for all \((i, j) \in E(G)\), must have:

\[
e_{ij}(0, 1) + e_{ij}(1, 0) \geq e_{ij}(1, 1) + e_{ij}(0, 0)
\]

(19.28)
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- This means: on average, preservation is preferred over change.
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- Actual probability are of the form \(p(x) \propto \prod \psi\), so this means

\[
\psi_{ij}(1, 0)\psi_{ij}(0, 1) \leq \psi_{ij}(0, 0)\psi_{ij}(1, 1):
\]

geometric mean of factor scores higher when neighboring pixels have the same value - a reasonable assumption about natural scenes and signals.
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- As a set function, this is the same as:

\[
f(X) = \sum_{\{i, j\} \in E(G)} f_{i,j}(X \cap \{i, j\}) \tag{19.29}
\]

which is submodular if each of the \(f_{i,j}\)'s are submodular!
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- A special case of more general submodular functions – unconstrained submodular function minimization is solvable in polytime.
Submodular potentials

**Theorem 19.4.1**

*If the edge functions are submodular and the edge weights in the s, t-graph are set as above, then finding the minimum s, t-cut in the auxiliary graph will yield a variable assignment having maximum probability.*
Submodular potentials

**Theorem 19.4.1**

*If the edge functions are submodular and the edge weights in the $s,t$-graph are set as above, then finding the minimum $s,t$-cut in the auxiliary graph will yield a variable assignment having maximum probability.*

**Theorem 19.4.2**

*Submodular pairwise potentials is a necessary and sufficient condition for an energy function like the above $E(x)$ to be graph representable, meaning that we can set up a graph cut based MPE inference algorithm and the resulting graph cut solves the MPE problem, $\min_{x \in \{0,1\}^V} E(x) = \max_{x \in \{0,1\}^V} p(x)$, exactly in polytime in $n = |V|$.***

**Proof.**

See Kolmogorov 2004
Useful for computer vision

- image segmentation problems can use such a model.
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Consider a 2D image, with a MRF to encode “smoothness” (i.e., spatial locality means things are likely to be similar).
Useful for computer vision

- Image segmentation problems can use such a model.
- Consider a 2D image, with a MRF to encode “smoothness” (i.e., spatial locality means things are likely to be similar).
- On average, similar neighbors have lower energy (higher probability) via
  \[ e_{ij}(0, 1) + e_{ij}(1, 0) \geq e_{ij}(1, 1) + e_{ij}(0, 0) \]
Graph Cut Marginalization

- What to do when potentials are not submodular?
What to do when potentials are not submodular? QPBO, quadratic pseudo Boolean optimization (computes only a partial solution).
Graph Cut Marginalization

- What to do when potentials are not submodular? QPBO, quadratic pseudo Boolean optimization (computes only a partial solution).
- For non-binary, use move making algorithms ($\alpha - \beta$-swaps, $\alpha$-expansions, fusion moves, etc.)
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- Is submodularity sufficient to make standard marginalization possible?
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- Unfortunately, even in submodular case, computing partition function is a $\#P$-complete problem (if it was possible to do it in poly time, that would require $P = NP$).
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- On the other hand, for pairwise MRFs, computing partition function in submodular potential case is approximable (has low error with high probability).
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Is submodularity sufficient to make standard marginalization possible?

Unfortunately, even in submodular case, computing partition function is a $\#P$-complete problem (if it was possible to do it in poly time, that would require $P = NP$).

On the other hand, for pairwise MRFs, computing partition function in submodular potential case is approximable (has low error with high probability).

Attractive potentials (generalization of submodular to non-binary case) leads to bound in Bethe, as we saw.
Bounds on inner product

- We know $\mathbb{L}(G) \supseteq \mathbb{M}(G)$ with equality only when $G = T$. 

\[\text{r.h.s. is called a first-order LP relaxation (i.e., due to 1-tree), with only linear number of constraints and can be solved exactly.} \]

\[\text{Note, middle case means that solution lies on integral extremal point of polytope } \mathbb{M}(G) (\text{always at least one extremal point in solution set of any LP over a polytope).} \]

\[\text{I.e., solution is some point } \phi(y) = \mu \text{ for solution vector } y \in \{0, 1\}^n.\]
Bounds on inner product

- We know $\mathbb{L}(G) \supseteq \mathbb{M}(G)$ with equality only when $G = T$.
- Thus,

$$\max_{x \in D_X^m} \langle \theta, \phi(x) \rangle = \max_{\mu \in \mathbb{M}(G)} \langle \theta, \mu \rangle \leq \max_{\tau \in \mathbb{L}(G)} \langle \theta, \tau \rangle \quad (19.30)$$
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\[
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Prof. Jeff Bilmes
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- We can relate extreme points of $\mathbb{M}(G)$ and $\mathbb{L}(G)$. 

Extreme points

Proposition 19.5.1

The extreme points of $\mathbb{L}(G)$ and $\mathbb{M}(G)$ are related in the following way:

(a) All extreme points of $\mathbb{M}(G)$ are integral, each one is also an extreme point of $\mathbb{L}(G)$.

(b) For graphs with cycles, $\mathbb{L}(G)$ also includes additional extreme points with fractional elements that lie strictly outside of $\mathbb{M}(G)$.

If the relaxation works or not, depends on the tightness. If we end up with integral point, we are tight and have an exact solution.
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- In such case, we could potentially round the nonintegral values back down to integers.
Fractional solutions

- Perhaps fractional solutions have at least some information about the optimal solution.
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- We get:

  \[ \text{Definition 19.5.2} \]
  
  Given a fractional solution \( \tau \) to the LP relaxation, let \( I \subset V \) represent the subset of vertices for which \( \tau \) has only integral elements, say fixing \( x_s = x^*_s \) for all \( s \in I \). The fractional solution is said to be strongly persistent if any optimal integral solution \( y^* \) satisfies \( y^*_s = x^*_s \) for all \( s \in I \). The fractional solution is weakly persistent if there exists at least one optimal \( y^* \) such that \( y^*_s = x^*_s \) for all \( s \in I \).

  So if either of these are true, we'd get some sort of partial solution. Strongly persistent ensures that no solutions are eliminated by sticking with the integral values of \( x_s \) for \( s \in I \).
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- So if either of these are true, we’d get some sort of partial solution.
- **Strongly persistent** ensures that no solutions are eliminated by sticking with the integral values of $x_s$ for $s \in I$. 
Proposition 19.5.3

Suppose that the first-order LP relaxation is applied to the binary quadratic program

\[
\max_{x \in \{0,1\}^m} \left\{ \sum_{s \in V} \theta_s x_s + \sum_{(s,t) \in E} \theta_{st} x_s x_t \right\}
\] (19.31)

Then any fractional solution is strongly persistent!
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- Important to generalize to discrete non-binary case, so far little is known (much work here done in the graph cut case, in terms of move-making algorithms).
- Can move-making algorithms be seen in the variational framework (i.e., is there a variational approximation such that move making algorithms correspond to fixed point of some Lagrangian?).
We started by marginalizing variables, the elimination algorithm.
Graphical Model Inference

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Once done we can convert to junction tree and run message passing (equivalent to eliminating on the hypertree).

Often, slimmest possible tree (even if we could find it) is not slim enough, need approximation.
Time-Space Tradeoffs in Exact and Approximate Inference

- Variational MPE
- Graph Cut MPE
- LP Relaxations
- Class Recap
- Refs

Prof. Jeff Bilmes
EE512a/Fall 2014/Graphical Models - Lecture 19 - Dec 3rd, 2014
F35/40 (pg.124/136)
Approximation: Two general approaches

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  - learning with or using a model with a structural restriction, **structure learning**, using a $k$-tree for a lower $k$ than one knows is true. Make sure $k$ is small enough so that exact inference can be performed, and make sure that, in that low tree-width model, one has best possible graph
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  2. Functional restrictions to the model (i.e., use factors or potential functions that obey certain properties). Then certain fast algorithms (e.g., graph-cut) can be performed.
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- Both methods only guaranteed approximate quality solutions.
- No longer in the achievable region in time-space tradoff graph, new set of time/space tradeoffs to achieve a particular accuracy.
Theorem 19.6.3 (Relationship between $A$ and $A^*$)

(a) For any $\mu \in \mathcal{M}^\circ$, $\theta(\mu)$ unique canonical parameter sat. matching condition, then conj. dual takes form:

$$A^*(\mu) = \sup_{\theta \in \Omega} (\langle \theta, \mu \rangle - A(\theta)) = \begin{cases} -H(p_{\theta(\mu)}) & \text{if } \mu \in \mathcal{M}^\circ \\ +\infty & \text{if } \mu \notin \overline{\mathcal{M}} \end{cases}$$ (19.3)

(b) Partition function has variational representation (dual of dual)

$$A(\theta) = \sup_{\mu \in \mathcal{M}} \{\langle \theta, \mu \rangle - A^*(\mu)\}$$ (19.4)

(c) For $\theta \in \Omega$, sup occurs at $\mu \in \mathcal{M}^\circ$ of moment matching conditions

$$\mu = \int_{D_X} \phi(x)p_{\theta}(x)\nu(dx) = \mathbb{E}_\theta[\phi(X)] = \nabla A(\theta)$$ (19.5)
Variational Approach Amenable to Approximation

- Original variational representation of log partition function

\[
A(\theta) = \sup_{\mu \in \mathcal{M}} \{ \langle \theta, \mu \rangle - A^*(\mu) \} \tag{19.1}
\]

where dual takes form:

\[
A^*(\mu) = \sup_{\theta \in \Omega} (\langle \theta, \mu \rangle - A(\theta)) = \begin{cases} 
-H(p_{\theta(\mu)}) & \text{if } \mu \in \mathcal{M}^\circ \\
+\infty & \text{if } \mu \notin \overline{\mathcal{M}} 
\end{cases} \tag{19.2}
\]

- Given efficient expression for \( A(\theta) \), we can compute marginals of interest.

- Above expression (dual of the dual) offers strategies to approximate or (upper or lower) bound \( A(\theta) \). We either approximate \( \mathcal{M} \) or \(-A^*(\mu)\) or (most likely) both.
Variational Approximations we cover

1. Set $\mathcal{M} \leftarrow \mathbb{L}$ and $-A^*(\mu) \leftarrow H_{\text{Bethe}}(\tau)$ to get Bethe variational approximation, LBP fixed point.

2. Set $\mathcal{M} \leftarrow \mathbb{L}_t(G)$ (hypergraph marginal polytope), $-A^*(\mu) \leftarrow H_{\text{app}}(\tau)$ where $H_{\text{app}} = \sum_{g \in E} c(g) H_g(\tau_g)$ (via Möbius) to get Kikuchi variational approximation, message passing on hypergraphs.

3. Partition $\tau$ into $(\tau, \tilde{\tau})$, and set $\mathcal{M} \leftarrow \mathcal{L}(\phi, \Phi)$ and set $-A^*(\mu) \leftarrow H_{\text{ep}}(\tau, \tilde{\tau})$ to get expectation propagation.

4. Mean field (from variational perspective) is (with $\mathcal{M}_F(G) \subseteq \mathcal{M}$) l.b.:

   $$A(\theta) \geq \max_{\mu \in \mathcal{M}_F(G)} \{ \langle \mu, \theta \rangle - A^*_F(\mu) \} = A_{\text{mf}}(\theta) \quad (19.1)$$

5. Upper bound Convexified/tree reweighted LBP, entropy upper bounds $H(\tau(F))$ for all members $F \in \mathfrak{D}$ of tractable substructures. Get u.b.:

   $$A(\theta) \leq B_\mathfrak{D}(\theta; \rho) := \sup_{\tau \in \mathcal{L}(G; \mathfrak{D})} \left\{ \langle \tau, \theta \rangle + \sum_{F \in \mathfrak{D}} \rho(F) H(\tau(F)) \right\} \quad (19.2)$$

   with $\mathcal{L}(G; \mathfrak{D}) = \bigcap_{F \in \mathfrak{D}} \mathcal{M}(F)$.
Sources for Today’s Lecture


- Earlier lectures of this class.