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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- Final writeup: 4-pages, 10 point font, 8.5x11 inch pages, 1 inch margins on all four sides.
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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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- **Alternatively,** you each do a **10-minute** youtube presentation with at least screen capture and audio, can use perhaps [http://tinytake.com/](http://tinytake.com/) or [http://camstudio.org/](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.
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:

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

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

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

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

$$\mu = \int_{D_X} \phi(x)p_{\theta}(x)\nu(dx) = \mathbb{E}_\theta[\phi(X)] = \nabla A(\theta) \quad (19.5)$$
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 $H_{\text{app}} = \sum_{g \in \mathcal{E}} c(g) H_g(\tau_g)$ (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.:

\[ A(\theta) \geq \max_{\mu \in \mathcal{M}_F(G)} \{ \langle \mu, \theta \rangle - A^*_F(\mu) \} = A_{\text{mf}}(\theta) \]  \hspace{1cm} (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.:

\[ A(\theta) \leq B_{\mathcal{D}}(\theta; \rho) \overset{\Delta}{=} \sup_{\tau \in \mathcal{L}(G; \mathcal{D})} \left\{ \langle \tau, \theta \rangle + \sum_{F \in \mathcal{D}} \rho(F) H(\tau(F)) \right\} \]  \hspace{1cm} (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 $x^* \in \arg\max_{x \in \mathcal{D}_X} p(x)$. 

MPE - most probable explanation
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.
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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.
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Equally difficult when tree-width is large.
In many cases, we care not to sum over $x$ in $\sum_x p(x)$ but instead to compute $x^* \in \text{argmax}_{x \in D_X} p(x)$.

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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

\[
\arg\max_{x \in D_{X^m}} p(x) = \left\{ x \in D_{X^m} : p_\theta(x) \geq p_\theta(y), \forall y \in D_{X^m} \right\} \tag{19.1}
\]
MPE - most probable explanation

- MPE again

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

(19.1)

- Since we are using exponential family models, we have

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

(19.2)

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

- MPE again

\[
\text{argmax } p(x) = \{x \in \mathbb{D}_{X^m} : p_\theta(x) \geq p_\theta(y), \forall y \in \mathbb{D}_{X^m}\} \quad (19.1)
\]

- Since we are using exponential family models, we have

\[
\text{argmax } p(x) = \text{argmax } \langle \theta, \phi(x) \rangle = \text{argmin } E[x] \quad (19.2)
\]

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

\[E[x] = -\langle \theta, \phi(x) \rangle\] 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 \( p_\theta(x) = \exp \{ \langle \theta, \phi(x) \rangle - A(\theta) \} \).
MPE - and variational

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

Let's consider $p_\theta(x) > p_\theta(y)$ for all $y \neq x^*$, so $x^*$ is the unique maximum. Then $\langle \theta, \phi(x^*) \rangle > \langle \theta, \phi(y) \rangle$ and $h(\beta) \equiv \langle \beta \theta, \phi(x^*) \rangle - \langle \beta \theta, \phi(y) \rangle = \beta(\langle \theta, \phi(x^*) \rangle - \langle \theta, \phi(y) \rangle)$ (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.
- 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

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

(19.5)

grows unboundedly large as $\beta \to \infty$. 
Considering $p_\theta(x) = \exp \{ \langle \theta, \phi(x) \rangle - A(\theta) \}$.

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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

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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:

$$\max_{x \in D_X^m} \langle \theta, \phi(x) \rangle = \max_{\mu \in \mathcal{M}} \langle \theta, \mu \rangle, \quad \text{and}$$

$$\max_{x \in D_X^m} \langle \theta, \phi(x) \rangle = \lim_{\beta \to \infty} \frac{A(\beta \theta)}{\beta} \quad (19.7)$$
Theorem 19.3.1 (MPE and variational)

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

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

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

- Intuition: We have $\mu = E_p[\phi(x)]$, so that
  \[
  \max_{x \in \mathcal{D}_X^m} \langle \theta, \phi(x) \rangle = \max_{\mathcal{P}} \langle \theta, E_p[\phi(x)] \rangle \quad \text{where } \mathcal{P} \text{ is a set of zero entropy distributions with point mass on some point in } \mathcal{D}_X^m. \text{ I.e., for each } p \in \mathcal{P}, \text{ there exists } x \in \mathcal{D}_X^m \text{ with } p(x) = 1.
Theorem 19.3.1 (MPE and variational)

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

\[
\max_{x \in D_{Xm}} \langle \theta, \phi(x) \rangle = \max_{\mu \in \bar{M}} \langle \theta, \mu \rangle, \quad \text{and}
\]

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

\[\text{(19.6)}\]

\[\text{(19.7)}\]

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

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

(19.7)
MPE - and variational

- Intuition for Equation (19.7), repeated here:

\[
\max_{x \in \mathcal{D}_X^m} \langle \theta, \phi(x) \rangle = \lim_{\beta \to \infty} \frac{A(\beta \theta)}{\beta} = \lim_{\beta \to \infty} \frac{1}{\beta} \sup_{\mu \in \mathcal{M}} \{ \langle \beta \theta, \mu \rangle - A^*(\mu) \} \quad (19.7)
\]

- Intuitively,

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

- Intuition for Equation (19.7), repeated here:

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

(19.7)

- Intuitively,

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

(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:

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

(19.10)
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\[
M_{t \rightarrow s}(x_s) \leftarrow \kappa \max_{x_t \in D_{X_t}} \exp \left\{ \theta_{st}(x_s, x_t) + \theta_t(x_t) \right\} \prod_{u \in N(t) \setminus s} M_{u \rightarrow t}(x_t)
\]

(19.10)

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

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

(19.11)
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:

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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]
\]

(19.10)

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\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
\]

(19.11)

- Right hand side is a LP over a simple polytope, the marginal polytope for trees \( \mathbb{L}(T) \).
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 $t,s$

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:

$N = \{ \mu \in \mathbb{R}^d | \mu \geq 0, \sum x_s \mu_s(x_s) = 1, \sum x_s, x_t \mu_{st}(x_s, x_t) = 1 \}$

(19.13)
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 \( t, s \)

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

(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 \( t, s \)

\[
C_{ts}(x_s) = \mu_s(x_s) - \sum_{x_t} \mu_{st}(x_s, x_t) \tag{19.12}
\]

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:

\[
\mathbb{N} = \left\{ \mu \in \mathbb{R}^d | \mu \geq 0, \sum_{x_s} \mu_s(x_s) = 1, \sum_{x_s, x_t} \mu_{st}(x_s, x_t) = 1 \right\} \tag{19.13}
\]
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

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

$$\log p(x) = \prod_{v \in V(G)} \psi_v(x_v) \prod_{(i,j) \in E(G)} \psi_{ij}(x_i, x_j) \quad (19.16)$$
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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) \tag{19.17}
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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)
$$

- $e_v(x_v)$ 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 $p \in \mathcal{F}(G, \mathcal{M}^{(f)})$ 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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- 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.
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- Further, say that $D_{X_v} = \{0, 1\}$ (binary), so we have binary random vectors distributed according to $p(x)$. 
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- 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 $D_{X_v} = \{0, 1\}$ (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.,

$$\min_{x \in \{0,1\}^V} E(x) \quad (19.19)$$
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 amongst the vertices $v \in V$, we connect each of $s$ and $t$ to all of the original nodes.
- I.e., we form $G_a = (V \cup \{s, t\}, E + \cup_{v \in V}((s, v) \cup (v, t)))$. 
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 $O(\sqrt{|V|})$. 

![Graphical Model Diagram](image-url)
Augmented (graph-cut) directed graph $G_a$. Edge weights (TBD) of graph are derived from
\[ \{ e_v(\cdot) \}_{v \in V} \text{ and } \{ e_{ij}(\cdot, \cdot) \}_{(i,j) \in E(G)} \cdot \]
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
\[ w(C) = \sum_{e \in C} w_e \]
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 $i \rightarrow j$. 
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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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  w_{v,t} = (e_v(0) - e_v(1)) \mathbf{1}(e_v(0) \geq e_v(1))
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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)
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  w_{i,j} = e_{ij}(1, 0) + e_{ij}(0, 1) - e_{ij}(1, 1) - e_{ij}(0, 0)
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  (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 $w_{s,i} \leftarrow w_{s,i} + (e_{ij}(1,0) - e_{ij}(0,0))$ 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) \tag{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)
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Non-negative edge weights

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

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- For this to be non-negative, we need:

  $$e_{ij}(1, 0) + e_{ij}(0, 1) \geq e_{ij}(1, 1) - e_{ij}(0, 0) \quad (19.27)$$

- 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:

\[ e_{ij}(0, 1) + e_{ij}(1, 0) \geq e_{ij}(1, 1) + e_{ij}(0, 0) \quad (19.28) \]
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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:

\[
f(X) = \sum_{\{i,j\} \in E(G)} f_{i,j}(X \cap \{i, j\})
\]  \hspace{1cm} (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.*

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, $\min_{x \in \{0,1\}^V} E(x) = \max_{x \in \{0,1\}^V} V_p(x)$, exactly in polytime in $n = |V|$.*

Proof.

See Kolmogorov 2004
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.

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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?

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.).

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.
What to do when potentials are not submodular? QPBO, quadratic pseudo Boolean optimization (computes only a partial solution).
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- Attractive potentials (generalization of submodular to non-binary case) leads to bound in Bethe, as we saw.
We know $\mathbb{L}(G) \supseteq \mathbb{M}(G)$ with equality only when $G = T$. 

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

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We can relate extreme points of $\mathbb{M}(G)$ and $\mathbb{L}(G)$.
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 \( \mathbb{M}(G) \).

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- In such case, we could potentially round the nonintegral values back down to integers.
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We get:

- Definition 19.5.2
  Given a fractional solution $\tau$ to the LP relaxation, let $I \subset V$ represent the subset of vertices for which $\tau_s$ 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 $y^*_s$ satisfies $y^*_s = x^*_s$ for all $s \in I$. The fractional solution is weakly persistent if there exists at least one optimal $y^*_s$ 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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- 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

$$\max_{x \in \{0,1\}^m} \left\{ \sum_{s \in V} \theta_s x_s + \sum_{(s,t) \in E} \theta_{st} x_s x_t \right\}$$  \hspace{1cm} (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?).
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Graphical Model Inference

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- 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
Approximation: Two general approaches

- exact solution to approximate problem - approximate problem

- approximate solution to exact problem - approximate inference

- Message or other form of propagation, variational approaches, LP relaxations, loopy belief propagation (LBP)

- Sampling (Monte Carlo, MCMC, importance sampling) and pruning (e.g., search based A*, score based, number of hypothesis based) procedures

Both methods only guaranteed approximate quality solutions. No longer in the achievable region in time-space tradeoff graph, new set of time/space tradeoffs to achieve a particular accuracy.
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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:

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

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

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

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

$$\mu = \int_{\mathcal{D}_X} \phi(x)p_{\theta}(x)\nu(dx) = \mathbb{E}_\theta[\phi(X)] = \nabla A(\theta) \quad (19.5)$$
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:

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

(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.:

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

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.:

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

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


- Earlier lectures of this class.