EE512A – Advanced Inference in Graphical Models

— Fall Quarter, Lecture 19 —

http://j.ee.washington.edu/~bilmes/classes/ee512a_fall_2014/

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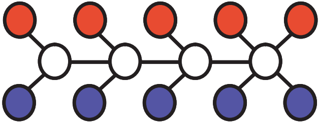
Dec 3rd, 2014



Announcements

- Wainwright and Jordan *Graphical Models, Exponential Families, and Variational Inference* http://www.nowpublishers.com/product.aspx?product=MAL&doi=2200000001
- 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!

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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/` 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.

Conjugate Duality, Maximum Likelihood, Negative Entropy

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:*

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

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

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

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

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

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 τ 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.**:

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

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.**:

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

with $\mathcal{L}(G; \mathfrak{D}) = \bigcap_{F \in \mathfrak{D}} \mathcal{M}(F)$

MPE - most probable explanation

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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.
- Can the variational approach help in this case as well?

MPE - most probable explanation

- MPE again

$$\operatorname*{argmax}_{x \in \mathsf{D}_{X^m}} p(x) = \{x \in \mathsf{D}_{X^m} : p_\theta(x) \geq p_\theta(y), \forall y \in \mathsf{D}_{X^m}\} \tag{19.1}$$

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- Since we are using exponential family models, we have

$$\operatorname*{argmax}_{x \in \mathsf{D}_{X^m}} p(x) = \operatorname*{argmax}_{x \in \mathsf{D}_{X^m}} \langle \theta, \phi(x) \rangle = \operatorname*{argmin}_{x \in \mathsf{D}_{X^m}} E[x] \tag{19.2}$$

i.e., cumulant function isn't required for computation. $E[x] = -\langle \theta, \phi(x) \rangle$ is seen as an "energy" function.

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- But it is related. Recall cumulant function

$$A(\theta) = \log \int \exp\{\langle \theta, \phi(x) \rangle\} d\nu(x) \tag{19.3}$$

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

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- If we substitute θ 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 $\beta \to \infty$.

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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

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

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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, theorem relating to MPE solution

Theorem 19.3.1 (MPE and variational)

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

$$\max_{x \in \mathsf{D}_{X^m}} \langle \theta, \phi(x) \rangle = \max_{\mu \in \bar{\mathcal{M}}} \langle \theta, \mu \rangle \,, \text{ and} \tag{19.6}$$

$$\max_{x \in \mathsf{D}_{X^m}} \langle \theta, \phi(x) \rangle = \lim_{\beta \to \infty} \frac{A(\beta\theta)}{\beta} \tag{19.7}$$

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- Intuition: We have $\mu = E_p[\phi(x)]$, so that $\max_{x \in \mathsf{D}_{X^m}} \langle \theta, \phi(x) \rangle = \max_{p \in \mathcal{P}} \langle \theta, E_p[\phi(x)] \rangle$ 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 $x \in \mathsf{D}_{X^m}$ with $p(x) = 1$.

$\int \phi(x) p(x) d\nu(x) = \int I(x=x^*) \phi(x) = \phi(x^*)$

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- Equation (19.6) says that max falls on extreme point of the mean parameter convex region $\bar{\mathcal{M}}$ (vertex of polytope, in polyhedral case).

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- 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).

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- 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 $\mathbb{M}(G)$.

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- Intution for Equation (19.7), repeated here:

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- Intuitively,

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

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

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- Due to convexity of A^* we can swap the $\lim$ and the $\sup$ and we get the result.

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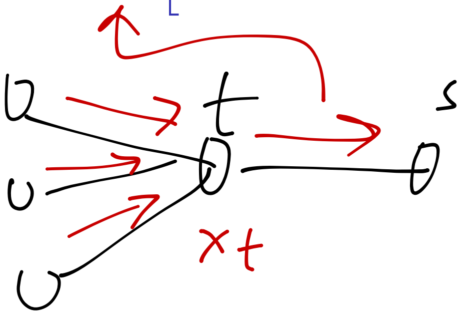
$$M_{t\to s}(x_s) \leftarrow \kappa \max_{x_t \in \mathsf{D}_{X_t}} \left[\exp\{\theta_{st}(x_s,x_t) + \theta_t(x_t)\} \prod_{u \in N(t)\backslash s} M_{u\to t}(x_t) \right] \tag{19.10}$$



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

$$\max_{x \in \mathsf{D}_{X^m}} \left[\sum_{s \in V} \theta_s(x_s) + \sum_{(s,t) \in E} \theta_{st}(x_s, x_t) \right] = \max_{\mu \in \mathbb{L}(T)} \langle \mu, \theta \rangle \tag{19.11}$$

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

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

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

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

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

Max-Product and LP Duality

Theorem 19.3.2 (Max-product and LP Duality)

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

$$\mathcal{Q}(\lambda) = \max_{\mu \in \mathbb{N}} \mathcal{L}(\mu; \lambda), \text{ where} \tag{19.14}$$

$$L(\mu; \lambda) = \langle \theta, \mu \rangle + \sum_{(s,t) \in E(T)} \left[\sum_{x_s} \lambda_{ts}(x_s) C_{ts}(x_s) + \sum_{x_t} \lambda_{st}(x_t) C_{st}(x_t) \right] \tag{19.15}$$

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 $\min_\lambda Q(\lambda)$.

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$$-\log p(x) = \sum_{v \in V(G)} e_v(x_v) + \sum_{(i,j) \in E(G)} e_{ij}(x_i, x_j) + \text{const.} \tag{19.17}$$

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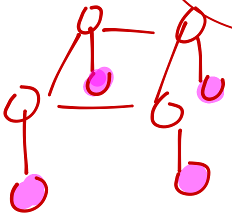
$$-\log p(x) \propto \sum_{v \in V(G)} e_v(x_v) + \sum_{(i,j) \in E(G)} e_{ij}(x_i, x_j) \tag{19.17}$$

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

$$E(x) = \sum_{v \in V(G)} e_v(x_v) + \sum_{(i,j) \in E(G)} e_{ij}(x_i, x_j) \tag{19.18}$$



$$e_v(x_v) = e_v(x_v, \bar{y}_v)$$

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- Further, say that $\mathrm{D}_{X_v} = \{0, 1\}$ (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.,

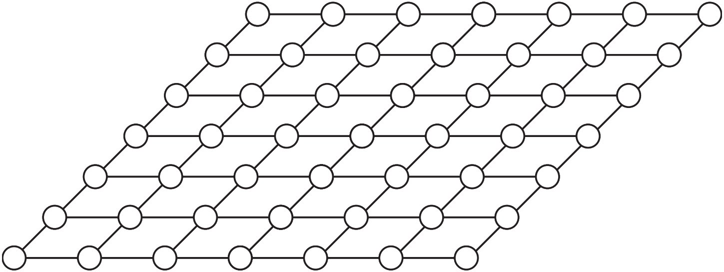
$$\min_{x \in \{0,1\}^V} E(x) \tag{19.19}$$

MRF example

Markov random field

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

When G is a 2D grid graph, we have

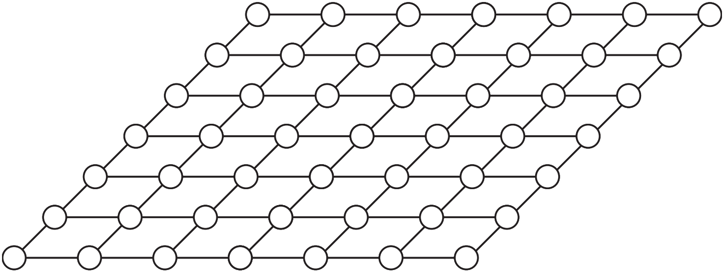


Create an auxiliary graph

- 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 amonst the vertices $v \in V$, we connect each of s and t to all of the original nodes.
- I.e., we form $G_a = (V \cup \{s,t\}, E + \cup_{v \in V}((s,v) \cup (v,t)))$.

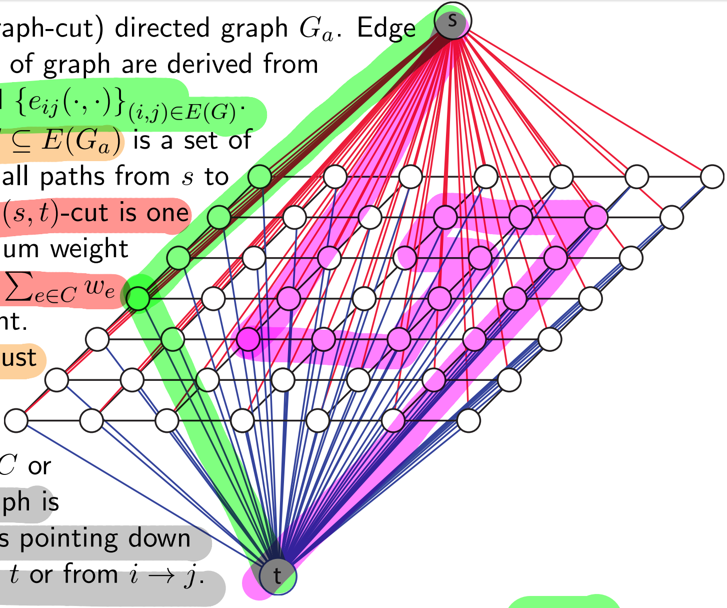
Transformation from graphical model to auxiliary graph

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 $O(\sqrt{|V|})$.



Transformation from graphical model to auxiliary graph

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 $i \to j$.



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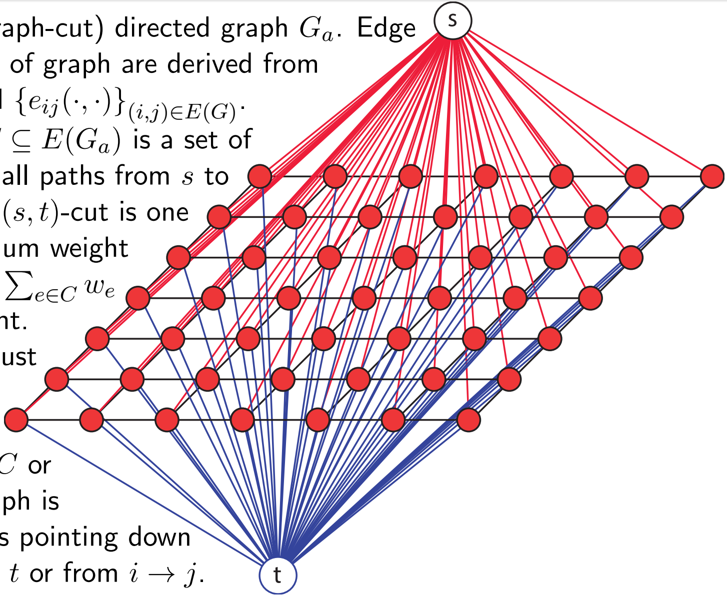
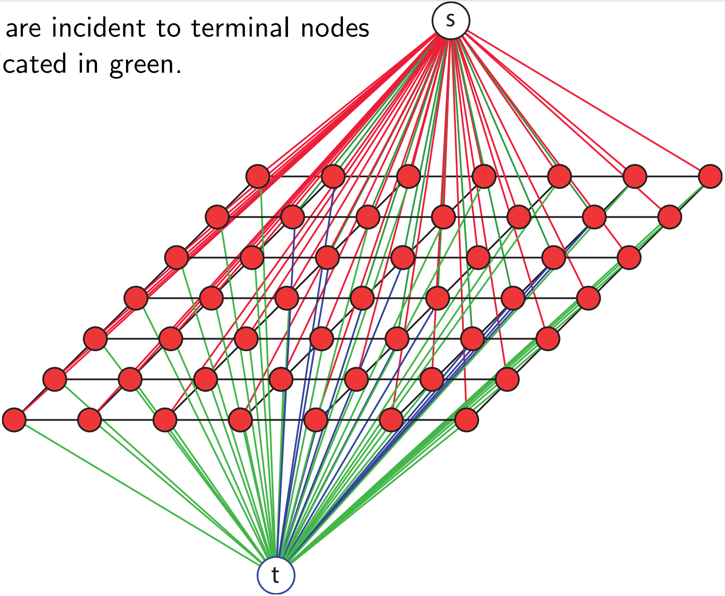


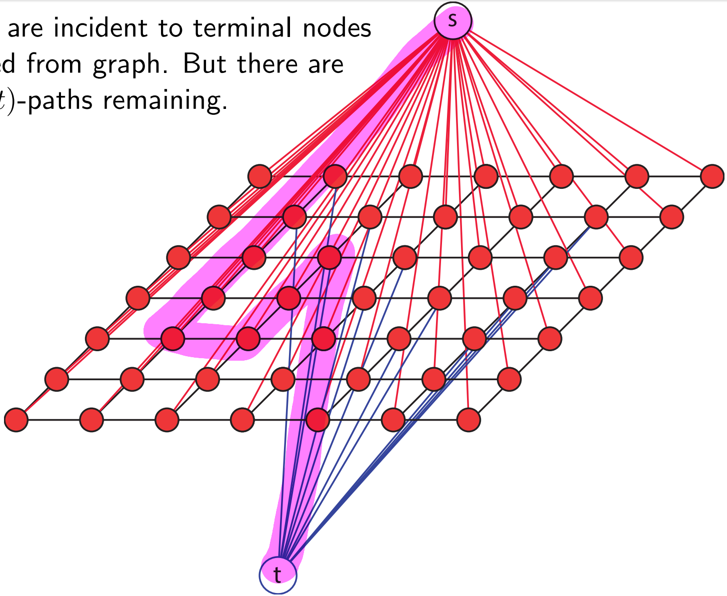
Transformation from graphical model to auxiliary graph

Cut edges that are incident to terminal nodes s and t are indicated in green.



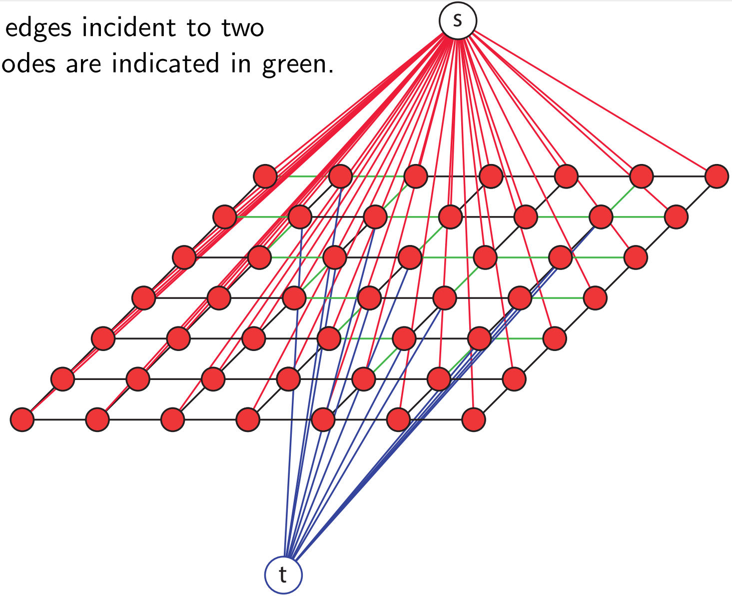
Transformation from graphical model to auxiliary graph

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



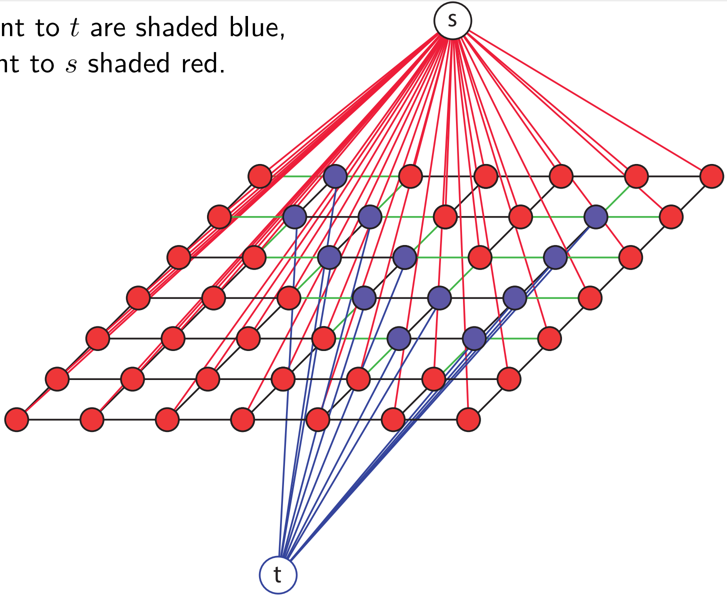
Transformation from graphical model to auxiliary graph

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.



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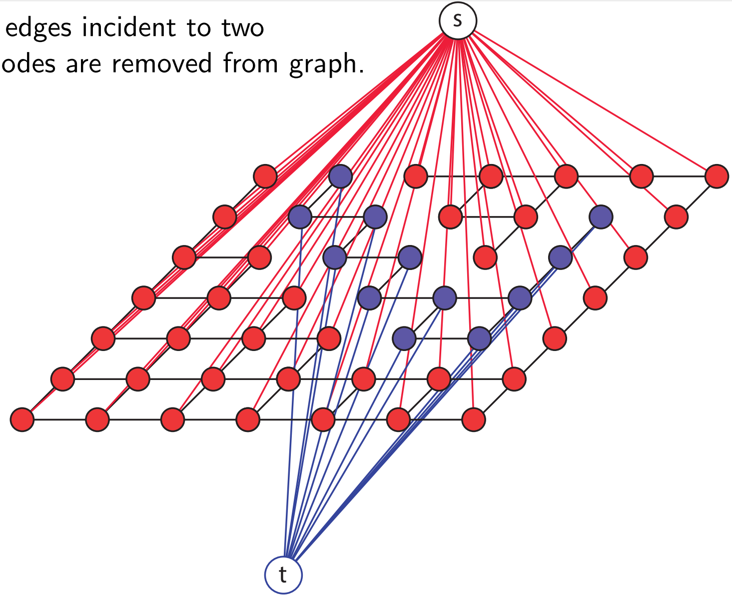
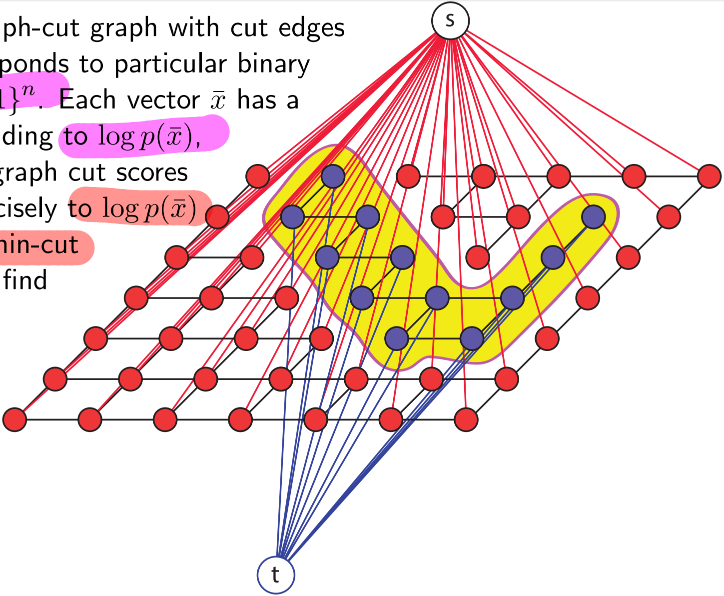


Transformation from graphical model to auxiliary graph

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

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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

$$w_{s,v} = (e_v(1) - e_v(0))\mathbf{1}(e_v(1) > e_v(0)) \tag{19.21}$$

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

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

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

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

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

and analogous increments if inequalities are flipped.

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 $e_{ij}(1,0) > e_{ij}(0,0)$.

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- 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:

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- As a set function, this is the same as:

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

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which is submodular if each of the $f_{i,j}$'s are submodular!
- 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

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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 □

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- image segmentation problems can use such a model.

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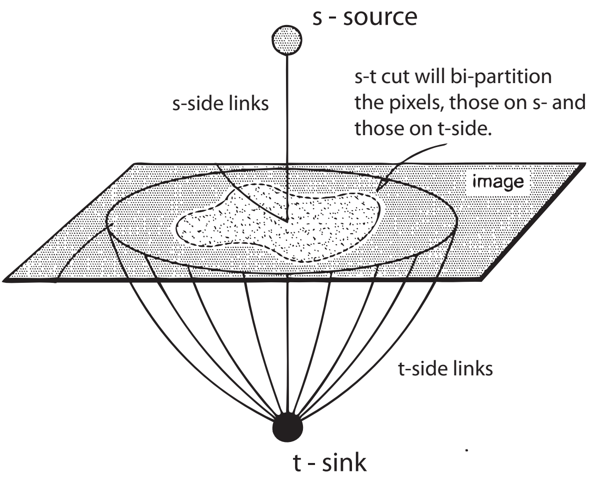
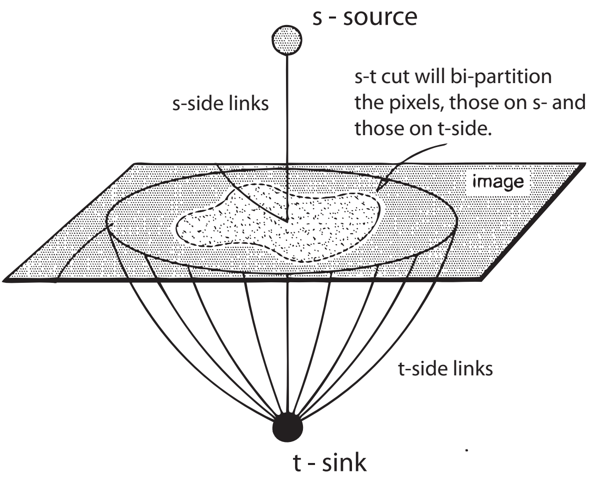
- Consider a 2D image, with a MRF to encode "smoothness" (i.e., spatial locality means things are likely to be similar).



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?

Graph Cut Marginalization

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

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- I.e., solution is some point $\phi(y) = \mu_y \in \mathbb{M}(G)$ for solution vector $y \in \{0, 1\}^n$.
- 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 $\mathbb{M}(G)$.*

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

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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 $s \in I$.

Persistent solutions in LP relaxation binary case

Proposition 19.5.3

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

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

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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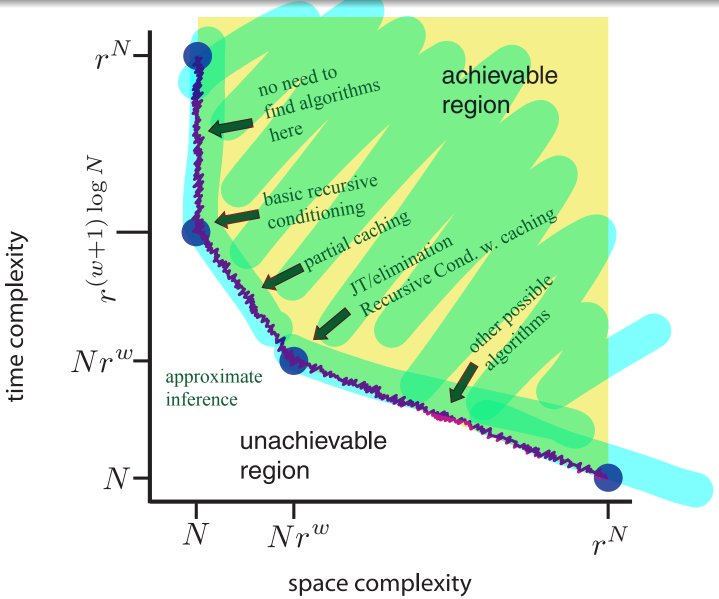
- Once done we can convert to junction tree and run message passing (equivalent to eliminating on the hypertree).
- Often, slimmest possible tree (even if we could find it) is not slim enough, need approximation.

Time-Space Tradeoffs in Exact and Approximate Inference



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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.

Conjugate Duality, Maximum Likelihood, Negative Entropy

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:*

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

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

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

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

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

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 τ 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.**:
$$A(\theta) \geq \max_{\mu \in \mathcal{M}_F(G)} \{\langle \mu, \theta \rangle - A_F^*(\mu)\} = A_{\text{mf}}(\theta) \tag{19.1}$$
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.**:
$$A(\theta) \leq B_{\mathfrak{D}}(\theta; \rho) \triangleq \sup_{\tau \in \mathcal{L}(G; \mathfrak{D})} \left\{ \langle \tau, \theta \rangle + \sum_{F \in \mathfrak{D}} \rho(F) H(\tau(F)) \right\} \tag{19.2}$$
with $\mathcal{L}(G; \mathfrak{D}) = \bigcap_{F \in \mathfrak{D}} \mathcal{M}(F)$

Sources for Today's Lecture

- Wainwright and Jordan *Graphical Models, Exponential Families, and Variational Inference* http://www.nowpublishers.com/product.aspx?product=MAL&doi=2200000001
- *Markov Random Fields for Vision and Image Processing* http://mitpress.mit.edu/catalog/item/default.asp?ttype=2&tid=12668 edited by Andrew Blake, Pushmeet Kohli and Carsten Rother
- Earlier lectures of this class.