

# EE512A – Advanced Inference in Graphical Models

— Fall Quarter, Lecture 18 —

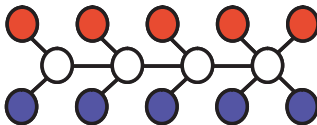
[http://j.ee.washington.edu/~bilmes/classes/ee512a\\_fall\\_2014/](http://j.ee.washington.edu/~bilmes/classes/ee512a_fall_2014/)

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Dec 1st, 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 programming, although we probably won't cover 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!**

# 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):
- Final Presentations: (12/10):

Finals Week: Dec 8th-12th, 2014.

# Conjugate Duality, Maximum Likelihood, Negative Entropy

## Theorem 18.2.3 (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:

$$A^*(\mu) = \sup_{\theta \in \Omega} (\langle \theta, \mu \rangle - A(\theta)) = \begin{cases} -H(p_{\theta(\mu)}) & \text{if } \mu \in \mathcal{M}^\circ \\ +\infty & \text{if } \mu \notin \overline{\mathcal{M}} \end{cases} \quad (18.3)$$

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

$$A(\theta) = \sup_{\mu \in \mathcal{M}} \{ \langle \theta, \mu \rangle - A^*(\mu) \} \quad (18.4)$$

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

$$\mu = \int_{\mathcal{D}_X} \phi(x) p_\theta(x) \nu(dx) = \mathbb{E}_\theta[\phi(X)] = \nabla A(\theta) \quad (18.5)$$

# Variational Approach Amenable to Approximation

- Original variational representation of log partition function

$$A(\theta) = \sup_{\mu \in \mathcal{M}} \{ \langle \theta, \mu \rangle - A^*(\mu) \} \quad (18.1)$$

where dual takes form:

$$A^*(\mu) = \sup_{\theta \in \Omega} (\langle \theta, \mu \rangle - A(\theta)) = \begin{cases} -H(p_{\theta(\mu)}) & \text{if } \mu \in \mathcal{M}^\circ \\ +\infty & \text{if } \mu \notin \overline{\mathcal{M}} \end{cases} \quad (18.2)$$

- 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  $\mathcal{M}_F(G) \subseteq \mathcal{M}$ ) **I.b.:**

$$A(\theta) \geq \max_{\mu \in \mathcal{M}_F(G)} \{ \langle \mu, \theta \rangle - A_F^*(\mu) \} = A_{\text{mf}}(\theta) \quad (18.1)$$

# EP as variational: Summary of key points

- Fixed points of EP exist assuming Lagrangian form has at least one optimum.
- No guarantees that EP will converge, but if it does it will be at a stationary point of the Lagrangian.
- EP can be seen to be based on variational framework, using Bethe-like entropy and convex outer bound for the mean parameters.
- When base distribution is unaries and  $\Phi^i$  is the edges of a graph, we in fact get standard Bethe approximation, and standard sum-product LBP.
- Moment matching of EP can be seen as striving for solution of associated Lagrangian.
- Lost of flexibility here, depending on what the base distribution is (e.g., could be a  $k$ -tree, clusters, or many other structures as well).
- Can also be done for Gaussian mixture and other distributions.
- Many more details, variations, and possible roads to new research. See text and also see Tom Minka's papers.

<http://research.microsoft.com/en-us/um/people/minka/papers/>

# Mean Field

- So far, we have been using an outer bound on  $\mathcal{M}$ .
- In mean-field methods, we use an “inner bound”, a subset of  $\mathcal{M}$  constructed so as to make the optimization of  $A(\theta)$  easier.
- Since subset, we get immediate bound on  $A(\theta)$ , all else (i.e., the entropy) being equal.
- Key: we based the inner bound on a “tractable family” like a 1-tree or even a 0-tree (all independent) so that the variational problem can be computed efficiently.
- Convexity of the optimization problem is often lost still, however, in the general case (due to the inner bound).
- Thus, in mean field, we will get a lower bound on  $A(\theta)$  but not a convex procedure to find it (both good and bad news).



# Tractable Families (for mean field approach)

- We have graph  $G = (V, E)$  which is intractable and we find a **spanning subgraph** (recall, spanning = all nodes, subgraph = subset of edges), i.e.,  $F = (V, E_F)$  where  $E_F \subseteq E$ .
- Simplest example:  $F = (V, \emptyset)$  all independence model.
- Tree example:  $F = (V, E_T)$  where edges  $E_T \subset E$  constitute a spanning tree.
- Exponential family, sufficient statistics  $\phi = (\phi_\alpha, \alpha \in \mathcal{I})$  associated with this family  $\mathcal{I}(F) \subseteq \mathcal{I}$ . These are the statistics that need respect the Markov properties of only the subgraph  $F$ .
- $\Omega$  gets smaller too, canonical  $F$ -respecting parameters are of the form:

$$\mathbb{R}^{|\mathcal{I}|} \ni \Omega(F) \triangleq \{\theta \in \Omega \mid \theta_\alpha = 0 \quad \forall \alpha \in \mathcal{I} \setminus \mathcal{I}(F)\} \subseteq \Omega. \quad (18.14)$$

Notice, all parameters associated with sufficient statistic not in  $\mathcal{I}(F)$  are set to zero, those statistics are nonexistent in  $F$ .

- If parameter was not zero, model would not respect the family of  $F$ .

# Inner bound Approximate Polytope

- Before, we had  $\mathcal{M}(G; \phi)(= \mathcal{M}_G(G; \phi))$ , all possible mean parameters associated with  $G$  and associated set of sufficient statistics  $\phi$ .
- For a given subgraph  $F$ , we only consider those mean parameters possible under  $F$ -respecting models. I.e.,

$$\mathcal{M}_F(G; \phi) = \left\{ \mu \in \mathbb{R}^d \mid \mu = \mathbb{E}_\theta[\phi(x)] \text{ for some } \theta \in \Omega(F) \right\} \quad (18.18)$$

- Therefore, since  $\theta \in \Omega(F) \subseteq \Omega$ , we have that

$$\mathcal{M}_F^\circ(G; \phi) \subseteq \mathcal{M}^\circ(G; \phi) \quad (18.19)$$

and so  $\mathcal{M}_F^\circ(G; \phi)$  is an **inner approximation** of the set of realizable mean parameters.

- Shorthand notation:  $M_F^\circ(G) = M_F^\circ(G; \phi)$  and  $M^\circ(G) = M^\circ(G; \phi)$

# Tractable Dual

- Normally dual  $A^*(\mu) = \sup_{\theta \in \Omega} (\langle \theta, \mu \rangle - A(\theta))$  is intractable or unavailable, but key idea is that if  $\mu \in \mathcal{M}_F(G)$  it will be possible to compute easily.
- Thus, goal of mean field (from variational approximation perspective) is to form  $A_{MF}(\theta)$  where:

$$A(\theta) \geq \max_{\mu \in \mathcal{M}_F(G)} \{ \langle \mu, \theta \rangle - A_F^*(\mu) \} \triangleq A_{MF}(\theta) \quad (18.23)$$

where  $A_F^*(\mu)$  corresponds to dual function restricted to inner bound set  $\mathcal{F}(G)$ . I.e., when we expand  $A_F^*(\mu)$ , we can take advantage of the fact that  $\mu$  is restricted in all cases, so  $A_F^*(\mu)$  might be greatly simplified relative to  $A^*(\mu)$ .

- Note, for  $\mu \in \mathcal{M}_F(G)$  and since  $\mathcal{M}_F(G) \subseteq \mathcal{M}(G)$ ,  $A_F^*(\mu)$  is not an approximation, rather it is just easy to compute.

# Mean field, KL-Divergence, Exponential Model Families

- Thus, solving the mean-field variational problem (see Eqn. (??)) of:

$$\max_{\mu \in \mathcal{M}_F(G)} \{\langle \mu, \theta \rangle - A_F^*(\mu)\} = \max_{\mu \in \mathcal{M}_F(G)} \{\langle \mu, \theta \rangle - A^*(\mu)\} \quad (18.34)$$

is identical to minimizing KL Divergence  $D(\mu || \theta)$  subject to constraint  $\mu \in \mathcal{M}_F(G)$ .

- I.e., mean field can be seen as finding the best approximation, in terms of this particular KL-divergence, to  $p_\theta$ , over a family of “nice” distributions  $\mathcal{M}_F(G)$ .

# Naïve Mean field for Ising Model: optimization

- We get variational lower bound problem

$$A(\theta) \geq \max_{(\mu_1, \dots, \mu_m) \in [0, 1]^m} \left\{ \sum_{s \in V} \theta_s \mu_s + \sum_{(s, t) \in E} \theta_{st} \mu_s \mu_t + \sum_{s \in V} H_s(\mu_s) \right\} \quad (18.35)$$

- Have constrained form of edge mean parameters  $\mu_{st} = \mu_s \mu_t$
- $(\mu_1, \dots, \mu_m) \in [0, 1]^m$  is  $m$ -D hypercube.
- We have a non-convex problem, so while it is a bound, it might be hard to get as tight as possible.
- One way to optimize is to do coordinate ascent (given otherwise fixed vector, optimize one value at a time).
- If each coordinate optimization is optimal, we'll get a stationary point.
- Fortunately, each coordinate optimization is concave!

# Structured Mean Field

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- “structured” in general means that it is not a monolithic single variable, but is a vector with some decomposability properties.
- In Structured mean field, we exploit this and it again can be seen in our variational framework.
- We first see a nice way that we can use fixed points of the mean field primal/dual equations to derive a general form of the mean field update.

# Structured Mean Field

- Again,  $\mathcal{I}(F)$  is set of suff. stats. corresponding to  $F$ , and we have corresponding mean vector  $\mu(F) = (\mu_\alpha, \alpha \in \mathcal{I}(F))$ .

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- Again,  $\mathcal{I}(F)$  is set of suff. stats. corresponding to  $F$ , and we have corresponding mean vector  $\mu(F) = (\mu_\alpha, \alpha \in \mathcal{I}(F))$ .
- Define new quantity  $\mathcal{M}(F)$ , the set of realizable mean parameters associated with  $F$ , so that  $\mu(F) \in \mathcal{M}(F)$ . Thus,  $\mathcal{M}(F) \subseteq \mathbb{R}^{|\mathcal{I}(F)|}$ .

$$\mathcal{M}_F(\sigma)$$

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- Ex: mean field Ising, edges  $(s, t) \in E$ , get  $\mu_{st} = g_{st}(\mu(F)) = \mu_s \mu_t$ .



# Structured Mean Field

- The mean field optimization problem becomes

$$\max_{\mu \in \mathcal{M}_F(G)} \{ \langle \mu, \theta \rangle - A_F^*(\mu) \} \quad (18.1)$$

$$= \max_{\mu(F) \in \mathcal{M}(F)} \left\{ \underbrace{\sum_{\alpha \in \mathcal{I}(F)} \theta_\alpha \mu_\alpha + \sum_{\alpha \in \mathcal{I}^c(F)} \theta_\alpha g_\alpha(\mu(F)) - A_F^*(\mu(F))}_{f(\mu(F))} \right\} \quad (18.2)$$

$$\mathcal{I}^c(F) = \mathcal{I} \setminus \mathcal{I}(F)$$

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- With this, we can recover our sigmoid mean field coordinate update process by iterating fixed point equations of  $f$ , i.e., for  $\beta \in \mathcal{I}(F)$ ,

$$\frac{\partial f}{\partial \mu_\beta}(\mu(F)) = \theta_\beta + \sum_{\alpha \in \mathcal{I}(G) \setminus \mathcal{I}(F)} \theta_\alpha \frac{\partial g_\alpha}{\partial \mu_\beta}(\mu(F)) - \frac{\partial A_F^*}{\partial \mu_\beta}(\mu(F)) \quad (18.3)$$

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- Setting this to zero, and then aggregating/concating over  $\beta \in \mathcal{I}(F)$ , vector fix point condition is:

$$\nabla A_F^*(\mu(F)) = \theta + \sum_{\alpha \in \mathcal{I}(G) \setminus \mathcal{I}(F)} \theta_\alpha \nabla g_\alpha(\mu(F)) \quad (18.4)$$

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- $\nabla A$  is the forward mapping, maps from canonical to mean parameters, and  $\nabla A^*$  does the reverse. Hence, naming  $\gamma(F) = \nabla A(\mu(F))$ , gives a parameter update equation for  $\beta \in \mathcal{I}(F)$

$$\gamma_\beta(F) \leftarrow \theta_\beta + \sum_{\alpha \in \mathcal{I}(G) \setminus \mathcal{I}(F)} \theta_\alpha \frac{\partial g_\alpha}{\partial \mu_\beta}(\mu(F)) \quad (18.5)$$

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- Above is the mean field update, mapping from canonical parameters ( $\theta_\beta$ , and  $\theta_\alpha$  for  $\alpha \in \mathcal{I}(G) \setminus \mathcal{I}(F)$ ) and using the mean parameters  $\mu(F)$  to new updated canonical parameters  $\gamma_\beta(F)$  for  $\beta \in \mathcal{I}(F)$ ). It is to be repeated over and over.

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- After each update of Eqn. (18.5), a mean parameter, say  $\mu(F)_\delta$ , that depends on any of the updated canonical parameter also needs to be updated before doing the next update.

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- Since we're using a tractable sub-structure  $F$ , we can then update the out-of-date mean parameters using any exact inference algorithm (e.g., junction tree, possible since sub-structure is tractable), and then repeat Eqn. (18.5).

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- This generalizes our mean field coordinate ascent update from before, where in that case we would get  $\frac{\partial A_F}{\partial \gamma_\beta}$  as being the sigmoid mapping.

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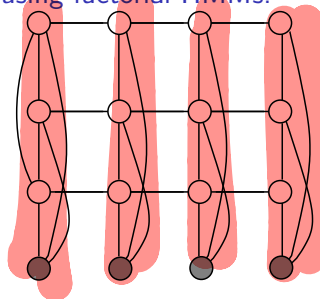
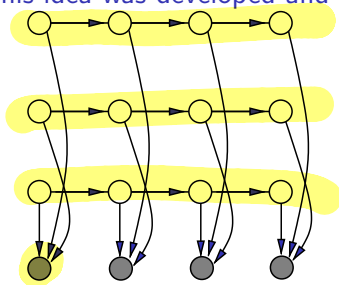
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- This generalizes our mean field coordinate ascent update from before, where in that case we would get  $\frac{\partial A_F}{\partial \gamma_\beta}$  as being the sigmoid mapping.
- But here, we can use this for any tractable substructure (e.g., trees or chains or collections thereof).

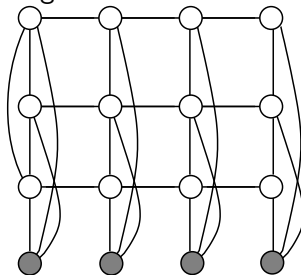
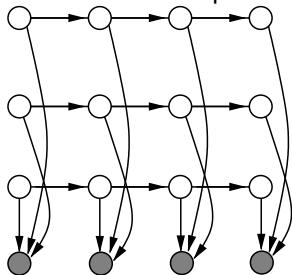
# Structured Mean Field Factorial HMMs

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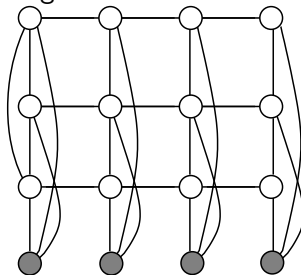
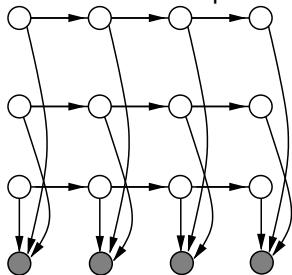
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- Graph consists of  $M$  1st-order Markov chains  $x_{1:T}^i$  for  $i \in [M]$ , coupled together at each time via factor  $p(\bar{y}_t | x_t^1, x_t^2, \dots, x_t^M)$ .

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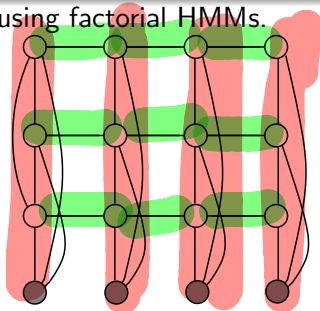
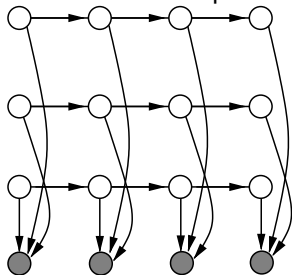
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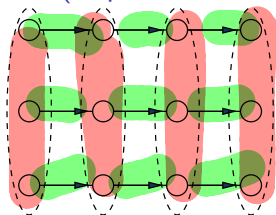


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- After moralization, covering hypergraph consists of tractable sub-substructure hyperedges  $F = \{\{x_t^i, x_{t+1}^i\} : i \in [M], t \in [T]\}$  and remaining structure  $E \setminus F = \{\{x_t^1, x_t^2, \dots, x_t^M\} : t \in [T]\}$ .



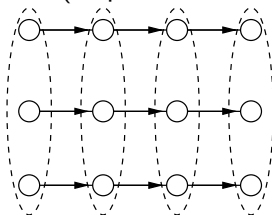
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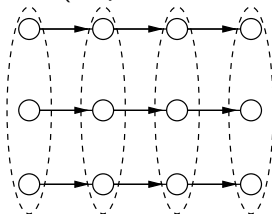
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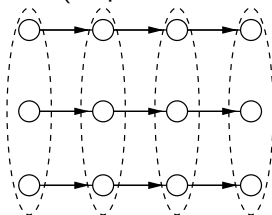
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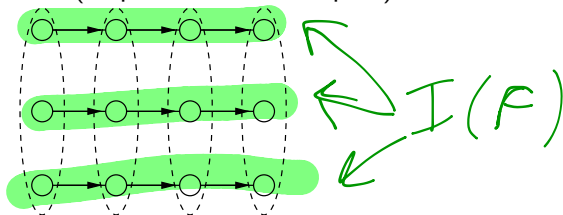
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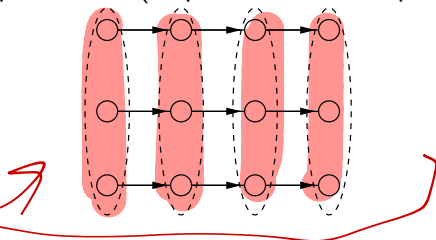
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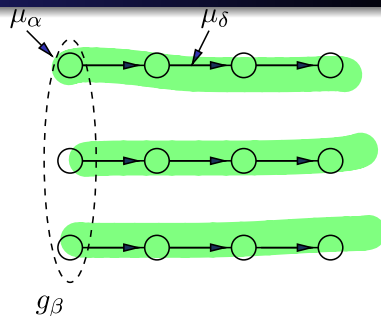
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- Each  $\beta \in \mathcal{I} \setminus \mathcal{I}(F)$  corresponds to one of the size  $M$  cliques (dotted ellipses above) corresponding to the v-structure moralizations, each costing  $O(r^M)$ .

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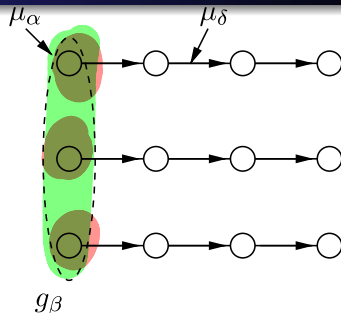
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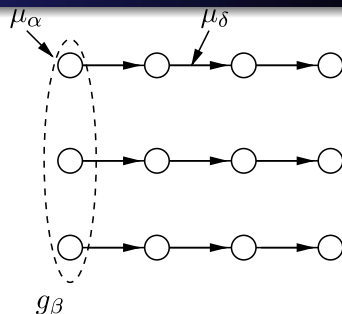
- Under this independent chains case, we have that for each  $\beta \in \mathcal{I} \setminus \mathcal{I}(F)$ , derivable functions have form  $g_\beta(\mu(F)) = \prod_{i=1}^M f_i(\{\mu_i(F)\})$ , for some functions  $f_i$ . This is fully factored, so is easy to work with, maintains separate chains.



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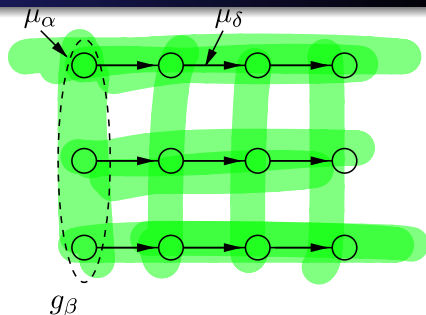
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- Each update of form Eqn. (18.5) updates parameters for  $\beta \in \mathcal{I}(F)$ , corresponds to all edges of all  $M$  Markov chains.
- To recover mean parameters (or do Eqn. (18.6)), need only forward-backward procedure on each chain separately,  $O(MTr^2)$ .

# Convex Relaxations and Upper Bounds

$$A(\theta) = \sup_{\mu \in \mathcal{M}} \{ \langle \theta, \mu \rangle - A^*(\mu) \} \quad (18.7)$$

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- In this next chapter (Chap 7), we will “convexify”  $H(\mu)$  and at the same time produce upper bounds.

# Convex Relaxations and Upper Bounds - Relaxed Entropy

- Recall sufficient stats  $\phi = (\phi_\alpha, \alpha \in \mathcal{I})$  and canonical parameters  $\theta = (\theta_\alpha, \alpha \in \mathcal{I})$ .



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- As before,  $\mathcal{M}(F)$  is set of realizable mean parameters associated with  $F$ , and  $\mu(F) \in \mathcal{M}(F)$ . Thus,  $\mathcal{M}(F) \subseteq \mathbb{R}^{|\mathcal{I}(F)|}$ , and

$$\mathcal{M}(F) = \left\{ \mu \in \mathbb{R}^{|\mathcal{I}(F)|} \mid \exists p \text{ s.t. } \mu_\alpha = \mathbb{E}_p[\phi_\alpha(X)] \forall \alpha \in \mathcal{I}(F) \right\} \quad (18.8)$$

Note  $\mathcal{M}_F(G) \neq \mathcal{M}(F)$ .

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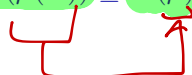


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- Critically, we have that  $H(\mu(F)) \geq H(\mu) = H(p_\mu)$ , as we show next.



# Convex Relaxations and Upper Bounds - Relaxed Entropy

## Proposition 18.4.1 (Maximum Entropy Bounds)

*Given any mean parameter  $\mu \in \mathcal{M}$  and its projection  $\mu(F)$  onto any subgraph  $F$ , we have the bound*

$$A^*(\mu(F)) \leq A^*(\mu) \quad (18.9)$$

*or alternatively stated,  $H(\mu(F)) \geq H(\mu)$ , entropy of projection is higher.*

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Proof.

- Dual problem

$$A^*(\mu) = \sup_{\theta \in \mathbb{R}^d} \{ \langle \mu, \theta \rangle - A(\theta) \} \quad (18.10)$$

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- This will be our **convexified upper bound on entropy** (lower bound on the dual).

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# Convex Relaxations and Upper Bounds - Relaxed Entropy

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- compared to mean field, we are not choosing only one structure, but many of them, and mixing them together in a certain way.
- This so far gives us an upper bound on  $A(\theta)$ , but we still need an outer bound. The combination will give us our upper bound on  $A(\theta)$ .



# Convex Relaxations and Upper Bounds - Outer bound

- When we form mixture of entropies (which really are duals), we make sure any given  $\mu(F)$  can be evaluated for any dual (i.e., each component can properly evaluate any possible  $\mu(F)$ ).

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- Also note,  $\mathcal{L}(G; \mathcal{D})$  is convex since it is the intersection of a set of convex sets.

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- Combining the upper bound on entropy, and the outer bound on  $\mathcal{M}$ , we get a new variational approximation to the cumulant function.

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- Evaluating the objective (optimization) is concave, so possible to get!
- Also,  $\mathcal{L}(G; \mathcal{D})$  is a convex outer bound on  $\mathcal{M}(G)$
- Thus  $B_{\mathcal{D}}(\theta; \rho)$  is convex, has a global optimal solution, it approximates  $A(\theta)$ , and best of all is an upper bound,  $A(\theta) \leq B_{\mathcal{D}}(\theta; \rho)$

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- We want to use this to see what happens when we take the expected value w.r.t. distribution  $\rho$ .



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Note right hand sum is over **all**  $E$  (not just a given spanning tree) and terms are weighted by probability of the given edge  $\rho_{st}$ .

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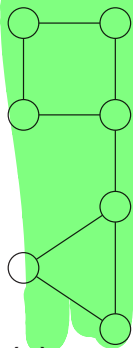
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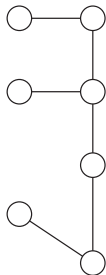
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- $\rho_{st}$  is edge appearance probability,  $\rho = (\rho_{st}, (s, t) \in E)$  is spanning tree polytope.

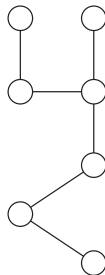
# Edge appearance probabilities example



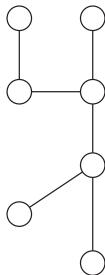
(a)



(b)



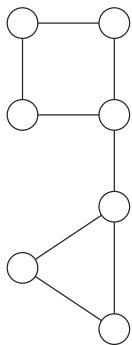
(c)



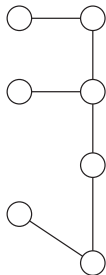
(d)

- (a) a graph  $G = (V, E)$  with  $m = |V| = 7$

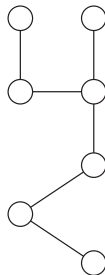
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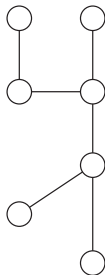
(a)



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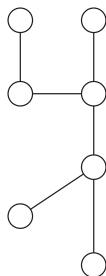
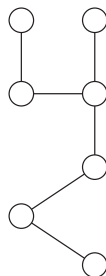
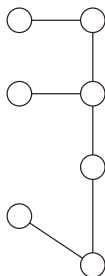
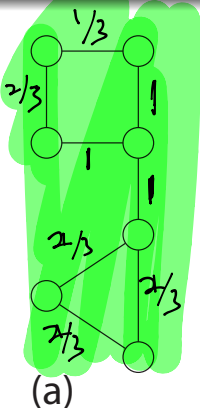
(c)



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- (a) a graph  $G = (V, E)$  with  $m = |V| = 7$
- (b), (c), and (d) various spanning trees, each with probability  $1/3$ .

# Edge appearance probabilities example



- (a) a graph  $G = (V, E)$  with  $m = |V| = 7$
- (b), (c), and (d) various spanning trees, each with probability  $1/3$ .
- What are the edge appearance probabilities  $\rho_{st}$ ?



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- In Bethe case, however, we did not have a bound on entropy, only an outer bound on the marginal polytope. Now, however, we also have a (convexification based) bound on entropy.

# Tree-reweighted sum-product and Bethe

## Theorem 18.5.1 (Tree-Reweighted Bethe and Sum-Product)

- (a) For any choice of edge appearance vector  $\rho = (\rho_{st}, (s, t) \in E)$  in the spanning tree polytope, the cumulant function  $A(\theta)$  evaluated at  $\theta$  is upper bounded by the solution of the tree reweighted Bethe variational problem (BVP):

$$B_{\tilde{\tau}}(\theta; \rho) = \max_{\tau \in \mathbb{L}(G)} \left\{ \langle \tau, \theta \rangle + \sum_{s \in V} H_s(\tau_s) - \sum_{(s,t) \in E} \rho_{st} I_{st}(\tau_{st}) \right\} \quad (18.20)$$

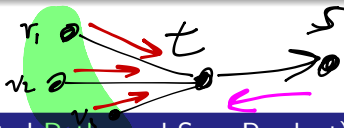
$$\geq A(\theta) \quad (18.21)$$

For any edge appearance vector such that  $\rho_{st} > 0$  for all edges  $(s, t)$ , this problem is strictly convex with a unique optimum.

...



# Tree-reweighted sum-product and Bethe



## Theorem 18.5.1 (Tree-Reweighted Bethe and Sum-Product)

(b) *The tree-reweighted BVP can be solved using the tree-reweighted sum-product updates*

$$M_{t \rightarrow s}(x_s) \leftarrow \kappa \sum_{x'_t \in \mathcal{X}_t} \varphi_{st}(x_s, x'_t) \frac{\prod_{v \in N(t) \setminus \{s\}} [M_{v \rightarrow t}(x'_t)]^{\rho_{vt}}}{[M_{s \rightarrow t}(x'_t)]^{(1 - \rho_{ts})}} \quad (18.22)$$

where  $\varphi_{st}(x_s, x'_t) = \exp\left(\frac{1}{\rho_{st}} \phi_{st}(x_s, x'_t) + \theta_t(x'_t)\right)$ . The updates have a unique fixed point under assumptions given in (a).

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- Thus, this is a true convex generalization, when  $\rho_{st} < 1$  for many  $s, t$ .

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$$\rho \in \text{conv}(\{\mathbf{1}_T : T \in \mathfrak{T}\}) \quad (18.23)$$

where  $\text{conv}(\cdot)$  is the convex hull of its argument.

# More on spanning tree polytope

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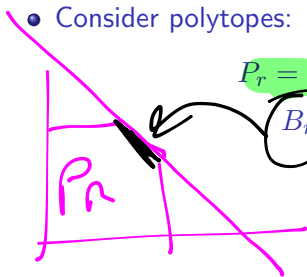
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- Consider polytopes:

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- Then if  $T$  is a spanning tree,  $\mathbf{1}_T \in B_r$ , and  $B_r = \text{conv}(\{\mathbf{1}_T : T \in \mathfrak{T}\})$ .
- Edmonds showed that a simple fast greedy procedure will maximize a linear function over this polytope, and this can be useful for finding good points in the spanning tree polytope.

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- In above case, we have both a convexification of the cumulant and an upper bound property.
- It should be pointed out that these are not mutual requirements: one can have convex without upper bound and vice versa.

# Tree-reweighted sum-product fixed point

The fixed point we ultimately reach has following form:

$$\tau_s^*(x_s) = \kappa \exp \{ \theta_s(x_s) \} \prod_{v \in N(s)} [M_{v \rightarrow s}^*(x_s)]^{\rho_{vs}} \quad (18.27)$$

$$\tau_{st}^*(x_s, x_t) = \kappa \varphi_{st}(x_s, x_t) \frac{\prod_{v \in N(s) \setminus t} [M_{vs}^*(x_s)]^{\rho_{vs}} \prod_{v \in N(t) \setminus s} [M_{vt}^*(x_t)]^{\rho_{vt}}}{[M_{ts}^*(x_s)]^{(1-\rho_{st})} [M_{st}^*(x_t)]^{(1-\rho_{ts})}} \quad (18.28)$$

with  $\varphi_{st}(x_s, x_t) = \exp \left\{ \frac{1}{\rho_{st}} \theta_{st}(x_s, x_t) + \theta_s(x_s) + \theta_t(x_t) \right\}$  where the  $*$  versions are the final (convergent) messages.

- In practice: damping of messages  $M$  appears in practice to help reach convergence, where each new message is a convex mixture of the previous version of itself and the new message according to the equations.

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$$H(\mu) \leq E_{\rho}[H(\mu(T))] = \sum_{T \in \mathfrak{T}(t)} \rho(T) H(\mu(T)) \quad (18.29)$$

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- This leads to a convexified Kikuchi variational problem

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- Optimizing  $\rho$  over hypertree polytope is hard, unfortunately.

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- In this case, reweighted entropy is concave!
- Lagrangian formulation leads to solutions that are a form of “reweighted” EP, ideas which also are sometimes called “power EP” (blending the above reweighted sum-product ideas and EP).



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  - use of conditional entropy, various forms of use of polyhedral approximations.
- This is still an active research area!

# 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  $\mathcal{M}_F(G) \subseteq \mathcal{M}$ ) **I.b.:**

$$A(\theta) \geq \max_{\mu \in \mathcal{M}_F(G)} \{ \langle \mu, \theta \rangle - A_F^*(\mu) \} = A_{\text{mf}}(\theta) \quad (18.1)$$

- 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.:**

$$A(\theta) \leq B_{\mathcal{D}}(\theta; \rho) \triangleq \sup_{\tau \in \mathcal{L}(G; \mathcal{D})} \left\{ \langle \tau, \theta \rangle + \sum_{F \in \mathcal{D}} \rho(F) H(\tau(F)) \right\} \quad (18.2)$$

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

# 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?

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- MPE again

$$\operatorname{argmax}_{x \in \mathcal{D}_{X^m}} p(x) = \{x \in \mathcal{D}_{X^m} : p_{\theta}(x) \geq p_{\theta}(y), \forall y \in \mathcal{D}_{X^m}\} \quad (18.32)$$

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- But it is related. Recall cumulant function

$$A(\theta) = \log \int \exp \{ \langle \theta, \phi(x) \rangle \} d\nu(x) \quad (18.34)$$

$$= \sup_{\mu \in \mathcal{M}} \{ \langle \theta, \mu \rangle - A^*(\mu) \} \quad (18.35)$$

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- This should have some influence on the cumulant. I.e., if we look at  $A(\beta\theta)/\beta$  and let  $\beta$  get large.
- Moreover, with respect to mean parameters, the maximum mean should (intuitively) fall on a vertex.

# MPE - and variational

We have following theorem.

## Theorem 18.6.1

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

$$\max_{x \in \mathcal{D}_{X^m}} \langle \theta, \phi(x) \rangle = \max_{\mu \in \mathcal{M}} \langle \theta, \mu \rangle, \text{ and} \quad (18.36)$$

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- Since l.h.s. is IP, this shows the difficulty of  $\mathbb{M}(G)$ .

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- It turns out that: the max-product updates are a Lagrangian method for solving dual of the above linear program.
- **Maxproduct updates take the form:**

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

# Max-Product and LP Duality

## Theorem 18.6.2

*Max-product and LP Duality Consider the dual function  $Q$  defined by the following partial Lagrangian formulation of the tree-structured LP:*

$$Q(\lambda) = \max_{\mu \in \mathbb{N}} \mathcal{L}(\mu; \lambda), \text{ where} \quad (18.40)$$

$$L(\mu; \lambda) = \langle \theta, \mu \rangle + \sum_{(s,t) \in E(T)} \left[ \sum_{x_s} \lambda_{ts}(x_s) C_{ts}(x_s) + \sum_{x_t} \lambda_{st}(x_t) C_{st}(x_t) \right] \quad (18.41)$$

*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  $\min_{\lambda} Q(\lambda)$ .*

# Sources for Today's Lecture

- Wainwright and Jordan *Graphical Models, Exponential Families, and Variational Inference* <http://www.nowpublishers.com/product.aspx?product=MAL&doi=22000000001>