EE512A – Advanced Inference in Graphical Models

— Fall Quarter, Lecture 16 —

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

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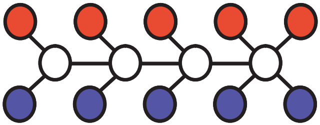
Nov 24th, 2014



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 1,2, 3, 4 in this book. Read chapter 5.
- Also should 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 (Nov 26th) night, 11:45pm. Final project proposal updates and progress report (one page max).

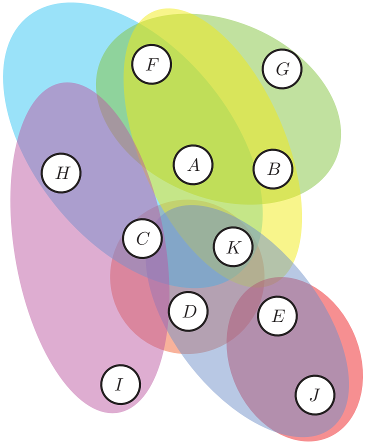
Class Road Map - EE512a

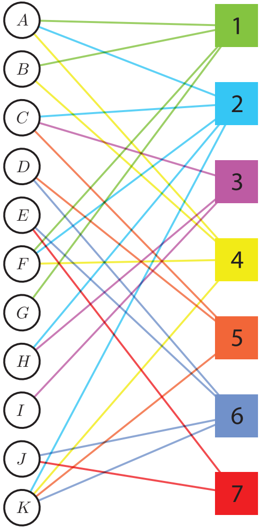
- L1 (9/29): Introduction, Families, Semantics
- L2 (10/1): MRFs, elimination, Inference on Trees
- L3 (10/6): Tree inference, message passing, more general queries, non-tree)
- L4 (10/8): Non-trees, perfect elimination, triangulated graphs
- L5 (10/13): triangulated graphs, k-trees, the triangulation 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):
- L19 (12/3):
- Final Presentations: (12/10):

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

Drawing/Visualizing Hypergraphs as Bipartite Graphs

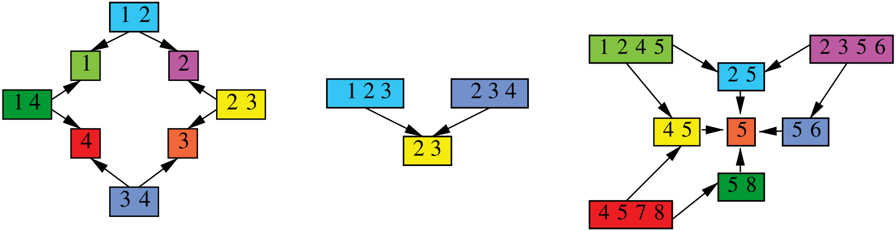
- Hypergraph (shaded regions) on left, while bipartite graph representation on the right.





Hypergraph, edge representations

- It is possible to represent hypergraphs by only showing their hyperedges.
- Here, we see graphical representations of three hypergraphs. Subsets of nodes corresponding to hyperedges are shown in rectangles, whereas the arrows represent inclusion relations among hyperedges.



(a) (b) (c)

- Which ones, if any, are in reduced representation?

Möbius Inversion Lemma and Inclusion-Exclusion

- For any $A \subseteq V$, define two functions $\Omega : 2^V \to \mathbb{R}$ and $\Upsilon : 2^V \to \mathbb{R}$.
- Then the above inclusion-exclusion principle is one instance of the more general Möbius Inversion lemma, namely that each of the below two equations implies the other.

$$\forall A \subseteq V : \Upsilon(A) = \sum_{B : B \subseteq A} \Omega(B) \tag{16.13}$$

$$\forall A \subseteq V : \Omega(A) = \sum_{B : B \subseteq A} (-1)^{|A \setminus B|} \Upsilon(B) \tag{16.14}$$

- Möbius Inversion lemma is also used to prove the Hammersley-Clifford theorem (that factorization and Markov property definitions of families are identical for positive distributions).
- We use it here to come up with alternative expressions for the entropy and for the marginal polytope.

Möbius Inversion Lemma for posets

- Let $\mathcal{P}$ be a partially ordered set with binary relation $\preceq$.
- A zeta function of a poset is a mapping $\zeta : \mathcal{P} \times \mathcal{P} \to \mathbb{R}$ defined by

$$\zeta(g,h) = \begin{cases} 1 & \text{if } g \preceq h, \\ 0 & \text{otherwise.} \end{cases} \tag{16.23}$$

- The Möbius function $\omega : \mathcal{P} \times \mathcal{P} \to \mathbb{R}$ is the multiplicative inverse of this function. It is defined recursively:
- $\omega(g,g) = 1$ for all $g \in \mathcal{P}$
- $\omega(g,h) = 0$ for all $h : h \not\preceq g$.
- Given $\omega(g,f)$ defined for f such that $g \preceq f \prec h$, we define

$$\omega(g,h) = - \sum_{\{f | g \preceq f \prec h\}} \omega(g,f) \tag{16.24}$$

- Then, ω and ζ are multiplicative inverses, in that

$$\sum_{f \in \mathcal{P}} \omega(g,f)\zeta(f,h) = \sum_{\{f | g \preceq f \preceq h\}} \omega(g,f) = \delta(g,h) \tag{16.25}$$

General Möbius Inversion Lemma for Posets

Lemma 16.2.8 (General Möbius Inversion Lemma)

Given real valued functions Υ and Ω defined on poset $\mathcal{P}$, then $\Omega(h)$ may be expressed via $\Upsilon(\cdot)$ via

$$\Omega(h) = \sum_{g \preceq h} \Upsilon(g) \quad \textit{for all } h \in \mathcal{P} \tag{16.23}$$

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When $\mathcal{P} = 2^V$ for some set V (so this means that the poset consists of sets and all subsets of an underlying set V) this can be simplified, where $\preceq$ becomes $\subseteq$; and $\succeq$ becomes $\supseteq$, like we saw above.
(see Stanley, "Enumerative Combinatorics" for more info.)

Back to Kikuchi: Möbius and expressions of factorization

- Suppose we are given marginals that factor w.r.t. a hypergraph $G = (V, E)$, so we have $\mu = (\mu_h, h \in E)$, then we can define new functions $\varphi = (\varphi_h, h \in E)$ via Möbius inversion lemma as follows

$$\log \varphi_h(x_h) \triangleq \sum_{g \preceq h} \omega(g, h) \log \mu_g(x_g) \tag{16.23}$$

- From Möbius inversion lemma, this then gives us a new way to write the log marginals, i.e., as

$$\log \mu_h(x_h) = \sum_{g \preceq h} \log \varphi_g(x_g) \tag{16.24}$$

- Key, when φ_h is defined as above, and G is a hypertree we have

$$p_\mu(x) = \prod_{h \in E} \varphi_h(x_h) \tag{16.25}$$

$\Rightarrow$ general way to factorize a distribution that factors w.r.t. a hypergraph.

multi-information decomposition

- Using Möbius, and Eqn. (**??**) we can write

$$I_h(\mu_h) = \sum_{x_h} \mu_h(x_h) \log \varphi_h(x_h) = \sum_{x_h} \mu_h(x_h) \left(\sum_{g \preceq h} \omega(g,h) \log \mu_g(x_g) \right)$$

$$= \sum_{g \preceq h} \omega(g,h) \left\{ \sum_{x_h} \mu_h(x_h) \log \mu_g(x_g) \right\}$$

$$= \sum_{f \preceq h} \sum_{e \succeq f} \omega(f,e) \left\{ \sum_{x_f} \mu_f(x_f) \log \mu_f(x_f) \right\} = -\sum_{f \preceq h} c(f) H_f(\mu_f)$$

where we define overcounting numbers ($\sim$ shattering coefficient)

$$c(f) \triangleq \sum_{e \succeq f} \omega(f,e) \tag{16.31}$$

- This gives us a new expression for the hypertree entropy

$$H_{\text{hyper}}(\mu) = \sum_{h \in E} c(h) H_h(\mu_h) \tag{16.32}$$

Usable to get Kikuchi variational approximation

- Sum to one constraint:

$$\sum_{x_h} \tau_h(x_h) = 1 \tag{16.33}$$

- Local agreement via the hypergraph constraint. For any $g \preceq h$ must have marginalization condition

$$\sum_{x_{h \setminus g}} \tau_h(x_h) = \tau_g(x_g) \tag{16.34}$$

- Define new polyhedral constraint set $\mathbb{L}_t(G)$

$$\mathbb{L}_t(G) = \{\tau \geq 0 | \text{ Equations } (\textbf{??}) \ \forall h, \text{ and } (\textbf{??}) \ \forall g \preceq h \text{ hold}\} \tag{16.35}$$

Kikuchi variational approximation, entropy approx

- Generalized approximate (app) entropy for the hypergraph:

$$H_{\text{app}} = \sum_{g \in E} c(g) H_g(\tau_g) \tag{16.33}$$

where H_g is hyperedge entropy and overcounting number defined by:

$$c(g) = \sum_{f \succeq g} \omega(g, f) \tag{16.34}$$

Variational Approach Amenable to Approximation

- Original variational representation of log partition function

$$A(\theta) = \sup_{\mu \in \mathcal{M}} \{\langle \theta, \mu \rangle - A^*(\mu)\} \tag{16.1}$$

where dual takes form:

$$A^*(\mu) = \sup_{\theta \in \Omega} (\langle \theta, \mu \rangle - A(\theta)) = \begin{cases} -H(p_{\theta(\mu)}) & \text{if } \mu \in \mathcal{M}^\circ \\ +\infty & \text{if } \mu \notin \overline{\mathcal{M}} \end{cases} \tag{16.2}$$

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- 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.

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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.

Kikuchi variational approximation

- This at last gets the Kikuchi variational approximation

$$A_{\text{Kikuchi}}(\theta) = \max_{\tau \in \mathbb{L}_t(G)} \{\langle \theta, \tau \rangle + H_{\text{app}}(\tau)\} \tag{16.1}$$

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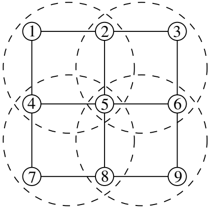
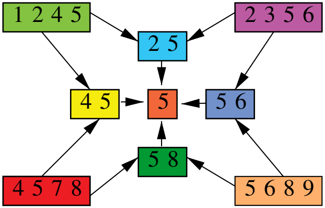
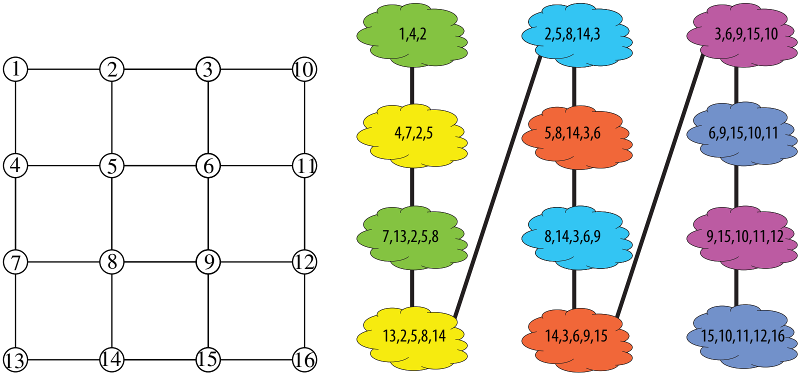
- Also, if hypergraph is junction tree (r.i.p. holds, tree-local consistency implies global consistency), then also exact (although expensive, exponential in the tree-width to compute H_{app}).
- We can define message passing algorithms on the hypertree, and show that if it converges, it is a fixed point of the associated Lagrangian.





Kikuchi variational approximation, 3x3 grid example

- Example, left is 3x3 grid, right is optimal junction tree cover.



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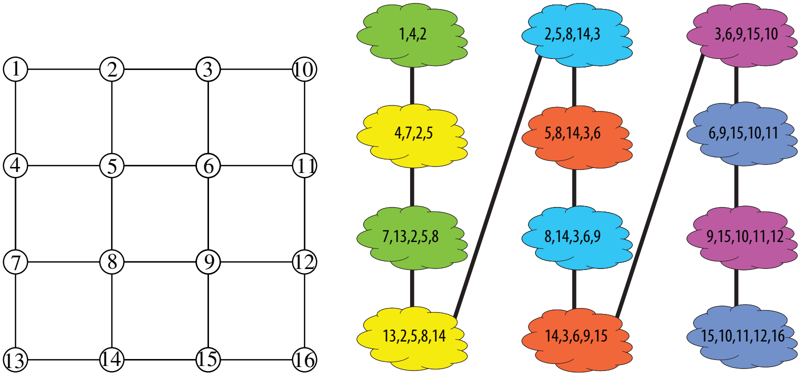

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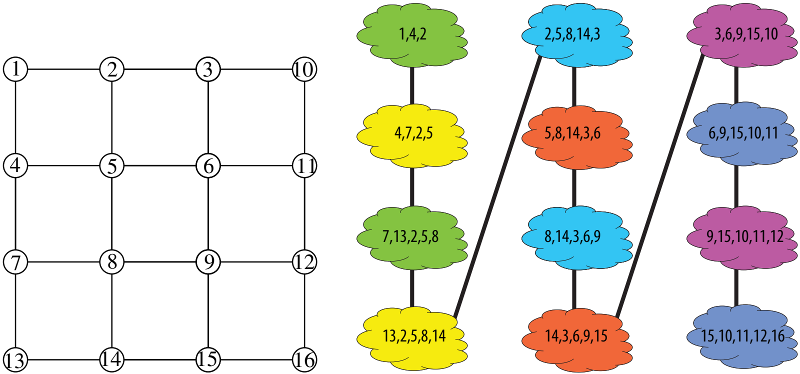

- Treewidth is 4, so complexity is $O(r^5)$.
- In general, for $n \times n$ grid strutured graph, treewidth is $O(n)$ (grows as the square root of the number of nodes).

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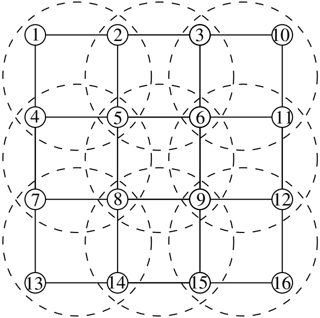
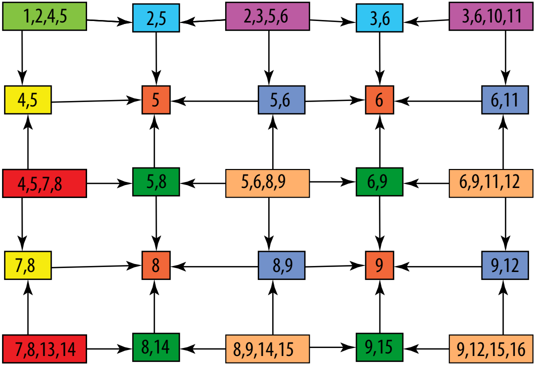
- Left is clustering of vertices in 3x3 grid, and right is hyperedge graph/region graph.





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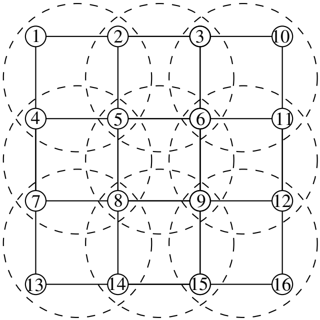

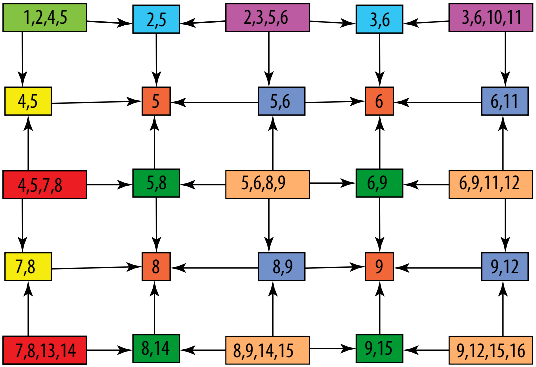

- Complexity is only $O(r^4)$ and will stay $O(r^4)$ even as n gets bigger (since clusters are at most size four).

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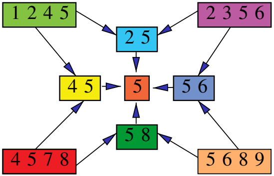
- Allows a trade-off between complexity for accuracy!
- In many cases, convergence of GBP will be at fixed points of the Lagrangian for the generalized variational approximation

$$A_{\text{Kikuchi}}(\theta) = \max_{\tau \in \mathbb{L}_t(G)} \{\langle \theta, \tau \rangle + H_{\text{app}}(\tau)\} \tag{16.2}$$

GBP examples: parent-to-child

- In hypergraph Hasse-like diagram, arrows point from parent (superset) to child (subset). Ex: on the right, set $\{1, 2, 4, 5\}$ is the parent of both $\{2, 5\}$ and $\{4, 5\}$.



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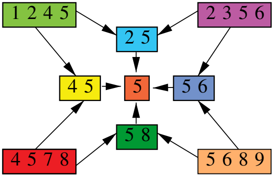

- For $h \in E$, let Par(h) be the set of parents. Also define descendants as $\mathcal{D}(h) = \{g \in E | g \prec h\}$ and ancestors as $\mathcal{A}(h) = \{g \in E | g \succ h\}$.

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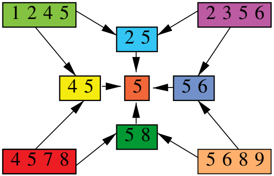

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- Also define $\mathcal{D}^+(h) = \mathcal{D}(h) \cup \{h\}$ and $\mathcal{A}^+(h) = \mathcal{A}(h) \cup \{h\}$

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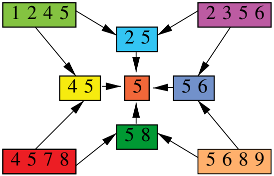

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- Also define $\mathcal{D}^+(h) = \mathcal{D}(h) \cup \{h\}$ and $\mathcal{A}^+(h) = \mathcal{A}(h) \cup \{h\}$
- If $f \succ g$ then x_f has more variables than x_g and one can perform a message of the form $M_{f \to g}(x_g) = \sum_{f \setminus g} \tau(x_f) = \sum_{f \setminus g} \tau(x_g, x_{f \setminus g})$

GBP examples: parent-to-child message

- Then parent-to-child message passing takes the form:

$$\tau_h(x_h) \propto \left[\prod_{g \in \mathcal{D}^+(h)} \exp(\theta(x_g)) \right] \left[\prod_{g \in \mathcal{D}^+(h)} \prod_{f \in \mathsf{Par}(g) \setminus \mathcal{D}^+(h)} M_{f \to g}(x_g) \right] \tag{16.3}$$

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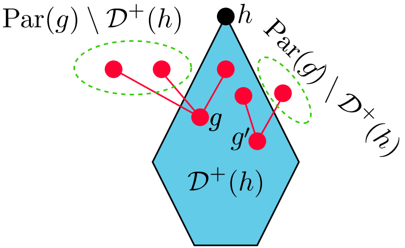
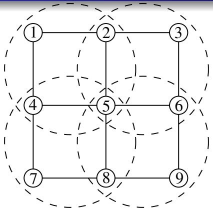
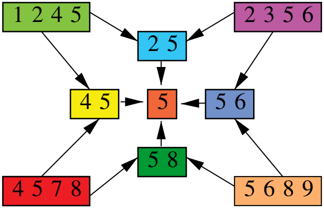
- We form marginal at h from the factors associated with each hyperedge, namely $\exp(\theta(x_g))$, and by the messages sent to h and h's descendants from other parents.



GBP examples: parent-to-child message, grid graph





- Consider message for hyperedge $h = \{1, 2, 4, 5\}$, which has factors ψ' associated with (regular graph) edges $\{1, 2\}$, $\{2, 5\}$, $\{4, 5\}$, and $\{1, 4\}$ and also unary factors for each of the nodes 1, 2, 4, and 5 (eg., to associate evidence into the model).

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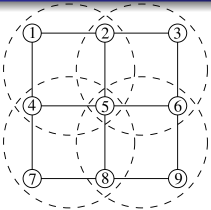

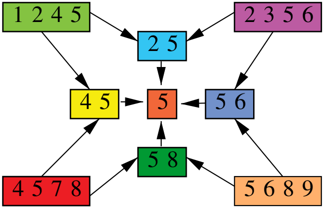

- Consider message for hyperedge $h = \{1, 2, 4, 5\}$, which has factors ψ' associated with (regular graph) edges $\{1, 2\}$, $\{2, 5\}$, $\{4, 5\}$, and $\{1, 4\}$ and also unary factors for each of the nodes 1, 2, 4, and 5 (eg., to associate evidence into the model).
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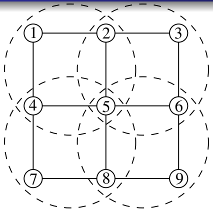

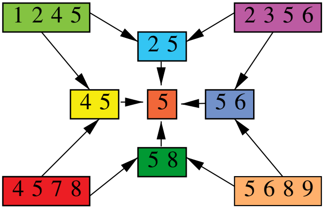

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- We get and expression for the marginal at h using the above formula.

$$\tau_{1,2,4,5} \propto \psi'_{1,2}\psi'_{1,4}\psi'_{2,5}\psi'_{4,5}\psi'_1\psi'_2\psi'_4\psi'_5 \times M_{\{2,3,5,6\}\to\{2,5\}} M_{\{4,5,7,8\}\to\{4,5\}} M_{\{5,6\}\to\{5\}} M_{\{5,8\}\to\{5\}} \tag{16.4}$$

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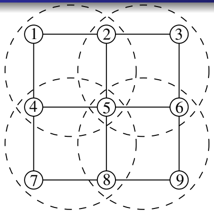

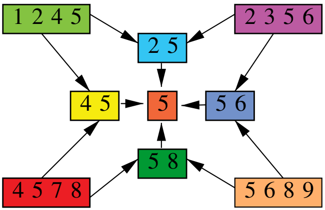

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- This could repeat for each of the largest clusters, until convergence.

Conjugate Duality, Maximum Likelihood, Negative Entropy

Theorem 16.4.3 (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:*

$$A^*(\mu) = \sup_{\theta \in \Omega} \left(\langle \theta, \mu \rangle - A(\theta) \right) = \begin{cases} -H(p_{\theta(\mu)}) & \text{if } \mu \in \mathcal{M}^\circ \\ +\infty & \text{if } \mu \notin \overline{\mathcal{M}} \end{cases} \tag{16.3}$$

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

$$A(\theta) = \sup_{\mu \in \mathcal{M}} \left\{ \langle \theta, \mu \rangle - A^*(\mu) \right\} \tag{16.4}$$

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

$$\mu = \int_{\mathsf{D}_X} \phi(x) p_\theta(x) \nu(dx) = \mathbb{E}_\theta[\phi(X)] = \nabla A(\theta) \tag{16.5}$$

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- Interestingly, EP is instance of our variational framework, Equation

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- Consider exponential families associated with subcollection (ϕ, Φ).

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- So $\phi : \mathcal{X}^m \rightarrow \mathbb{R}^{d_T}$ with vector of parameters $\theta \in \mathbb{R}^{d_T}$.
- Could instantiate model based only on this subcomponent, called the base model

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- Parameters $\tilde{\theta} \in \mathbb{R}^{b \times d_I}$.

Associated Distributions: base and i-augmented

- The associated exponential family

$$p(x;\theta,\tilde{\theta}) \propto \exp\left(\langle\theta,\phi(x)\rangle\right)\exp\left(\left\langle\tilde{\theta},\Phi(x)\right\rangle\right) \tag{16.9}$$

$$= \exp\left(\langle\theta,\phi(x)\rangle\right)\prod_{i=1}^{d_I}\exp\left(\left\langle\tilde{\theta}^i,\Phi^i(x)\right\rangle\right) \tag{16.10}$$

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- Intractable to perform exact computations with the full (ϕ, Φ)-exponential family.

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- Using Bayes rule, we get mixture model with 2^n components!

$$p(x|y^1, \ldots, y^n) \propto \exp\left(-\frac{1}{2}x^\intercal \Sigma^{-1} x\right) \prod_{i=1}^n p(y^i|X = x) \tag{16.14}$$

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- If we multiply in all Φ^i, becomes intractable (2^n potentially distinct components each of which requires marginalization).

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- We also have polytope associated with only base distribution

$$\mathcal{M}(\phi) = \left\{ \mu \in \mathbb{R}^{d_T} | \mu = \mathbb{E}_p(\phi(X)) \right\} \quad (16.18)$$

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$$\mathcal{M}(\phi, \Phi) = \{(\mu, \tilde{\mu}) | (\mu, \tilde{\mu}) = \mathbb{E}_p[(\phi(X), \Phi(X))] \text{ for some } p\} \quad (16.17)$$

along with negative dual of cumulant, or entropy $H(\mu, \tilde{\mu}) = -A^*(\mu, \tilde{\mu})$.

- We also have polytope associated with only base distribution

$$\mathcal{M}(\phi) = \left\{ \mu \in \mathbb{R}^{d_T} | \mu = \mathbb{E}_p(\phi(X)) \right\} \quad (16.18)$$

- Recall thm: any mean in the interior is realizable via an exponential family model, and associated entropy $H(\mu)$ is tractable.

Augmented Base case

- For each $i = 1 \dots d_I$ we have a Φ^i-augmented exp. model and polytope

$$\mathcal{M}(\phi, \Phi^i) = \left\{ (\mu, \tilde{\mu}^i) \in \mathbb{R}^{d_T + b} | (\mu, \tilde{\mu}^i) = \mathbb{E}_p[(\phi(X), \Phi^i(X))] \text{ for some } p \right\} \tag{16.19}$$

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- Goal, variational approximation: Need outer bounds on $\mathcal{M}(\phi, \Phi)$ and expression for entropy (as is now normal).
- Turns out we can do this, and an iterative algorithm to find fixed points of associated Lagrangian, that correspond to EP.

New EP-based outer bound

- For any mean parms $(\tau, \tilde{\tau})$ where $\tilde{\tau} = (\tilde{\tau}^1, \tilde{\tau}^2, \ldots, \tilde{\tau}^{d_I})$, define coordinate "projection operation"

$$\Pi^i(\tau, \tilde{\tau}) \to (\tau, \tilde{\tau}^i) \tag{16.20}$$

This operator simply removes all but $\tilde{\tau}^i$ from $\tilde{\tau}$.

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- If Φ^i are edges of a graph (i.e. local consistency) then we get standard $\mathbb{L}$ outer bound we saw before with Bethe approximation

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$$\max_{(\tau,\tilde{\tau}) \in \mathcal{L}(\phi,\Phi)} \left\{ \langle \tau, \theta \rangle + \left\langle \tilde{\tau}, \tilde{\theta} \right\rangle + H_{\text{ep}}(\tau, \tilde{\tau}) \right\} \tag{16.26}$$

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- This characterizes the EP algorithms.
- Given graph $G = (V, E)$ when we take ϕ to be unaries V and Φ to be edges E, we exactly recover Bethe approximation.

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subject to $\tau \in \mathcal{M}(\phi)$, and for all i that $\tau = \eta^i$ and that $(\eta^i, \tilde{\tau}^i) \in \mathcal{M}(\phi, \Phi^i)$.

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  subject to $\tau \in \mathcal{M}(\phi)$, and for all i that $\tau = \eta^i$ and that $(\eta^i, \tilde{\tau}^i) \in \mathcal{M}(\phi, \Phi^i)$.
- Use Lagrange multipliers to impose constraint $\eta^i = \tau$ for all i, and for the rest of the constraints too.

To Lagrangian optimization

- We get a Lagrangian version of the objective

$$L(\tau;\lambda) = \langle \tau, \theta \rangle + \sum_{i=1}^{d_I} \left\langle \tilde{\tau}^i, \tilde{\theta}^i \right\rangle + F(\tau; (\eta^i, \tilde{\tau}^i)) + \sum_{i=1}^{d_I} \langle \lambda^i, \tau - \eta^i \rangle + \dots \tag{16.29}$$

where

$$F(\tau; (\eta^i, \tilde{\tau}^i)) = H(\tau) + \sum_{i=1}^{d_I} \left[H(\eta^i, \tilde{\tau}^i) - H(\eta^i) \right] \tag{16.30}$$

and where λ^i are the Lagrange multipliers assocaited with the constraint $\eta^i = \tau$ for all i (other multipliers not shown).

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- First condition means we're a member of the ϕ-exponential family, and (it can be shown) has form:

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- Second condition means we're a member of the (ϕ, Φ^i)-exponential family, and (it can be shown) has form:

$$q^i(x, \theta, \tilde{\theta}^i, \lambda) \propto \exp\left(\left\langle \theta + \sum_{\ell \neq i} \lambda^\ell, \phi(x) \right\rangle + \left\langle \tilde{\theta}^i, \Phi^i(x) \right\rangle\right) \tag{16.32}$$

To Lagrangian optimization to Moment Matching

- Thid condiiton is a form of moment-matching. I.e., we have $\tau = E_q[\phi(X)]$ and $\eta^i = E_{q^i}[\phi(X)]$, so equating these gives:

$$\int q(x;\theta,\lambda)\phi(x)\nu(dx) = \int q^i(x;\theta,\tilde{\theta}^i)\phi(x)\nu(dx) \tag{16.33}$$

fro $i \in [d_I]$.

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5. This is a KL-divergence minimization step, but done w. exponential family models which thus corresponds to moment-matching.

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`