EE512A – Advanced Inference in Graphical Models

— Fall Quarter, Lecture 16 —

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

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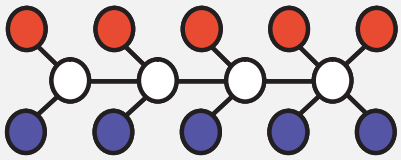


Announcements

- 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).

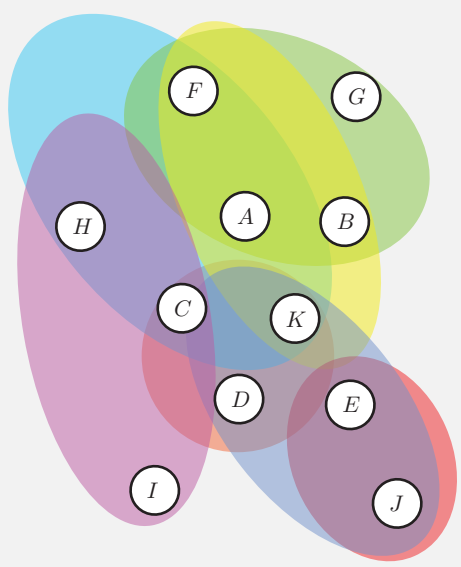
Class Road Map - EE512a

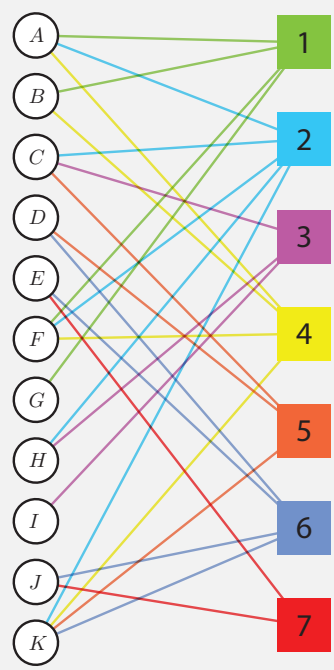
- L1 (9/29): Introduction, Families, Semantics
- L2 (10/1): MRFs, elimination, Inference on Trees
- L3 (10/6): Tree inference, message passing, more general queries, non-tree)
- L4 (10/8): Non-trees, perfect elimination, triangulated graphs
- L5 (10/13): triangulated graphs, k-trees, the triangulation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

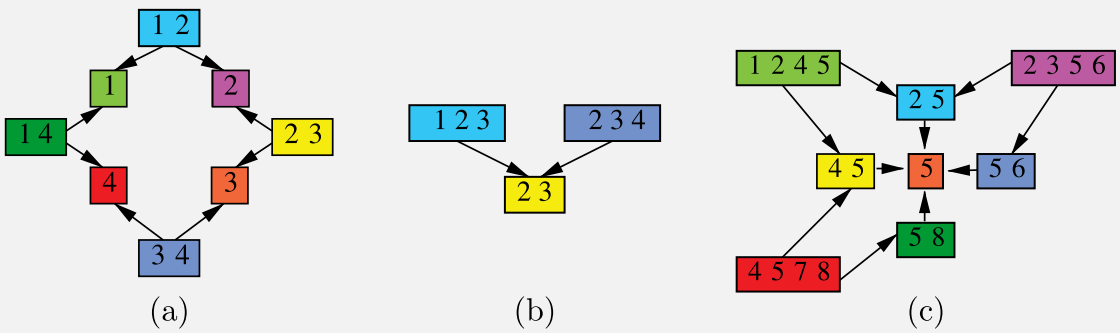
- Hypergraph (shaded regions) on left, while bipartite graph representation on the right.





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.



- 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

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

iff $\Upsilon(h)$ may be expressed via $\Omega(\cdot)$ via

$$\Upsilon(h) = \sum_{g \preceq h} \Omega(g)\omega(g,h) \quad \textit{for all } h \in \mathcal{P} \tag{16.24}$$

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. (16.23) 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 $\mathbb{L}_t(G)$

$$\mathbb{L}_t(G) = \{\tau \geq 0 | \text{ Equations (16.3) } \forall h, \text{ and (16.34) } \forall g \preceq h \text{ hold}\} \tag{16.35}$$

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
Variational Approximations we cover

- 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:

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

- 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.

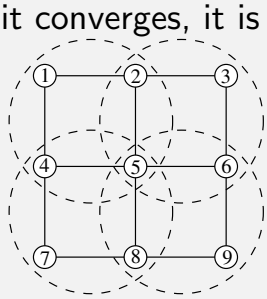
1. Set $\mathcal{M} \leftarrow \mathbb{L}$ and $-A^*(\mu) \leftarrow H_{\text{Bethe}}(\tau)$ to get Bethe variational approximation, LBP fixed point.
2. Set $\mathcal{M} \leftarrow \mathbb{L}_t(G)$ (hypergraph marginal polytope), $-A^*(\mu) \leftarrow H_{\text{app}}(\tau)$ where $H_{\text{app}} = \sum_{g \in E} c(g) H_g(\tau_g)$ (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.

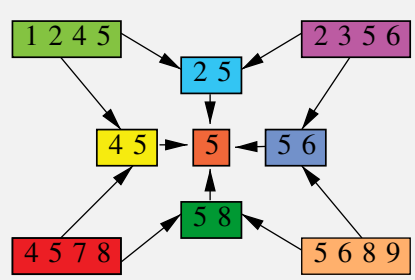
Kikuchi variational approximation

- This at last gets the Kikuchi variational approximation

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

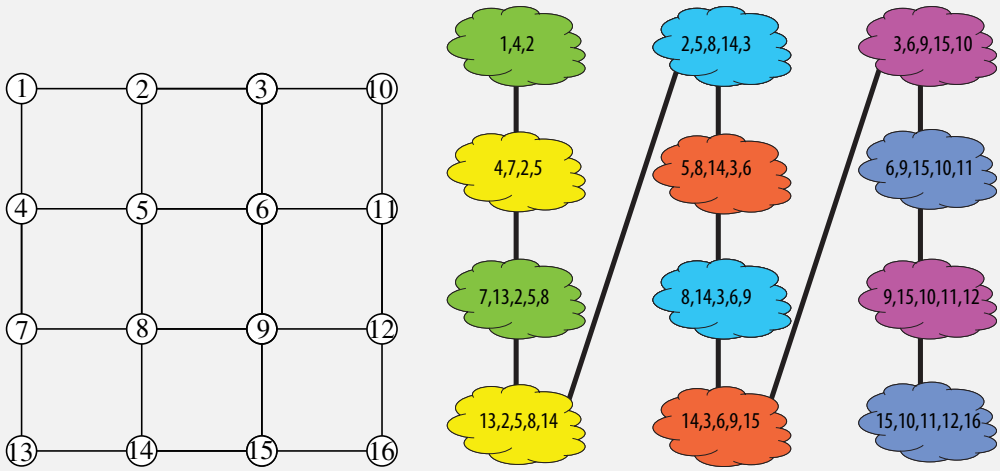
- For a graph, this is exactly $A_{\text{Bethe}}(\theta)$.
- Also, if hypergraph is junction tree (r.i.p. holds, tree-local consistency implies global consistency), then also exact (although expensive, exponential in the tree-width to compute H_{app}).
- We can define message passing algorithms on the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





Kikuchi variational approximation, 3x3 grid example

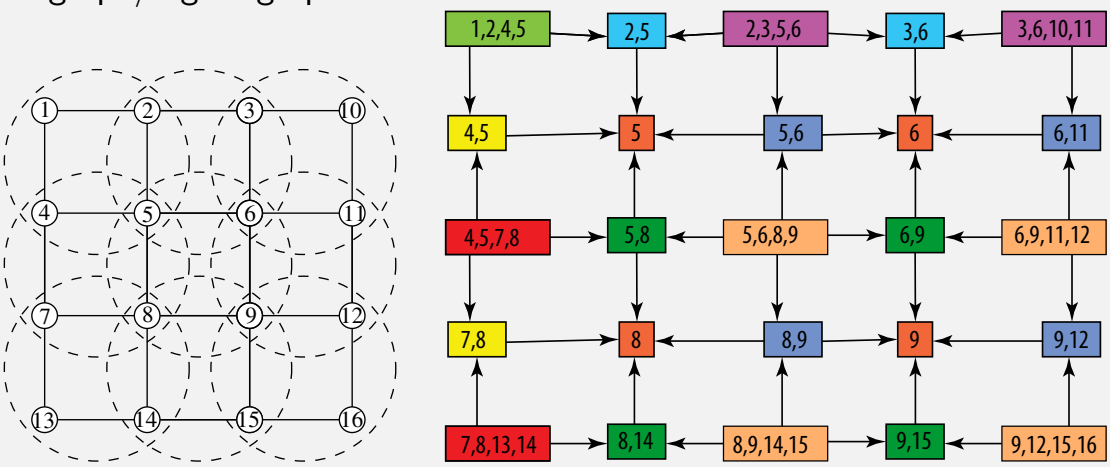
- Example, left is 3x3 grid, right is optimal junction tree cover.



- 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).

Kikuchi variational approximation, 3x3 grid example

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



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

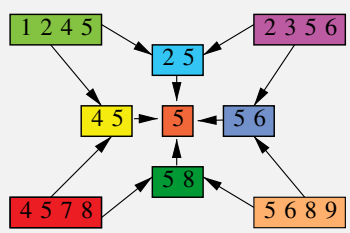
Generalized BP (GBP): Key idea

- Key idea: sets of nodes send messages to other sets of nodes.
- The node sets that communicate with each other represented using hypergraph (hyperedges are the ndoe sets)
- Standard LBP algorithm is merely a special case of GBP
- Different choices of node sets/hyperedges and message passings give different GBP algorithms.
- This gives the user a gradual tradeoff between the most expensive, intractable, and accurate junction tree algorithm, and the least expensive but possibly quite inaccurate LBP algorithm.
- 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 $\{4, 5\}$.



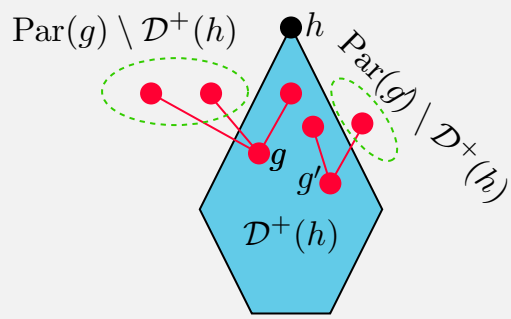
- For $h \in E$, let Par(h) be the set of parents. Also define descendants as $\mathcal{D}(h) = \{g \in E | g \prec h\}$ and ancestors as $\mathcal{A}(h) = \{g \in E | g \succ h\}$.
- Also define $\mathcal{D}^+(h) = \mathcal{D}(h) \cup \{h\}$ and $\mathcal{A}^+(h) = \mathcal{A}(h) \cup \{h\}$
- If $f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

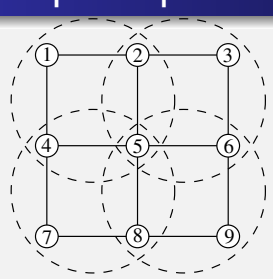
- Then parent-to-child message passing takes the form:

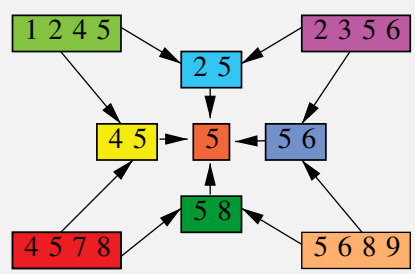
$$\tau_h(x_h) \propto \left[\prod_{g\in\mathcal{D}^+(h)} \exp(\theta(x_g))\right]\left[\prod_{g\in\mathcal{D}^+(h)}\prod_{f\in\mathsf{Par}(g)\setminus\mathcal{D}^+(h)} M_{f\to g}(x_g)\right] \tag{16.3}$$

- 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).
- Then $\mathcal{D}^+(h) = \{\{1,2,4,5\},\{4,5\},\{2,5\},\{5\}\}$.
- We get and expression for the marginal at h using the above formula.

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

- 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:*

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

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

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

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

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

Expectation Propagation: basic idea

- Came from a method called "assumed density filtering" (ADF).
- Doing full inference involves exponential computation.
- We do a bit of inference, involving reasonable computation, and getting us a new distribution that is a bit more complex but not too much more complex.
- Before going further, we "project" this new distribution back down to a class of simple distributions.
- We then repeat the above step with a bit more of inference, different than what we did above.
- We keep repeating: do a bit of inference, and project, until all inference has been done.
- The difference between ADF and EP is that, with ADF at this stage we're done. With EP we can keep repeating the process of inference, projection.
- EP can be seen as a generalization of BP.
- Interestingly, EP is instance of our variational framework, Equation 16.7

Term Decoupling in EP

- Partition the d sufficient statistics into two parts, the tractable ones (of which there are d_T) and the intracxtable ones (of which there are d_I). Thus, $d = d_T + d_I$.
- Tractable component

$$\phi \triangleq (\phi_1, \phi_2, \ldots, \phi_{d_T}) \tag{16.5}$$

- Intractable component

$$\Phi \triangleq (\Phi^1, \Phi^2, \ldots, \Phi^{d_I}) \tag{16.6}$$

- ϕ_i are typically univariate, while Φ^i are typically multivariate (b-dimensional we'll assume), although this need not always be the case (but will be for our exposition).
- Consider exponential families associated with subcollection (ϕ, Φ).

Tractable component

- Tractable component

$$\phi \triangleq (\phi_1, \phi_2, \ldots, \phi_{d_T}) \tag{16.7}$$

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

Intractable component

- Intractable component

$$\Phi \triangleq (\Phi_1, \Phi_2, \ldots, \Phi_{d_I}) \tag{16.8}$$

- Each $\Phi_i : \mathcal{X}^m \to \mathbb{R}^b$.
- $\Phi : \mathcal{X}^m \to \mathbb{R}^{b \times d_I}$.
- Parameters $\tilde{\theta} \in \mathbb{R}^{b \times d_I}$.

Associated Distributions: base and i-augmented

- The associated exponential family

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

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

- Base model is tractable

$$p(x; \theta, \vec{0}) \propto \exp\left(\langle \theta, \phi(x) \rangle\right) \tag{16.11}$$

- Φ^i-augmented model

$$p(x; \theta, \tilde{\theta}^i) \propto \exp\left(\langle \theta, \phi(x) \rangle\right) \exp\left(\left\langle \tilde{\theta}^i, \Phi^i(x) \right\rangle\right) \tag{16.12}$$

Associated Distributions: key points

The basic premises in the tractable-intractable partitioning between ϕ and Φ are:

- It is possible to compute marginals exactly in polynomial time for distributions of the base form (any member of the ϕ-exponential family).
- For each $i = 1, \ldots, d_I$, exact polynomial-time computation is still possible for any Φ^i-augmented form (any member of the (ϕ, Φ^i)-exponential family).
- Intractable to perform exact computations with the full (ϕ, Φ)-exponential family.

Example: Mixture models

- Let $X \in \mathbb{R}^m$ be Gaussian with distribution $N(0, \Sigma)$.
- Let $\varphi(y; \mu, \Lambda)$ be Gaussian with mean μ covariance Λ.
- Suppose y conditioned on x is a two-component Gaussian mixture model taking the form:

$$p(y|X = x) = (1 - \alpha)\varphi(y; 0, \sigma_0^2 I) + \alpha\varphi(y; x, \sigma_1^2 I) \tag{16.13}$$

- Assume we have obtained n i.i.d. samples $y^1, \ldots, y^n$ from mixture density, and goal is to produce posterior $p(x|y^1, \ldots, y^n)$, similar to Bayes-rule inverting a Naive-Bayes model.
- Using Bayes rule, we get mixture model with 2^n components!

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

$$= \exp\left(-\frac{1}{2}x^\intercal \Sigma^{-1} x\right) \exp\left\{\sum_{i=1}^{n} \log p(y^i|X = x)\right\} \tag{16.15}$$

Example: Mixture models

- We equate $\exp\left(-\frac{1}{2}x^\intercal\Sigma^{-1}x\right)$ with $\exp(\langle\theta,\phi(x)\rangle)$, with $d_T = m$.
- Such a distribution is multivariate Gaussian, and getting marginals (say $p(x_A)$ for $A \subseteq [m]$) from it is relatively "cheap" $O(m^3)$.
- $\exp\left\{\sum_{i=1}^n \log p(y^i|X=x)\right\}$ equates to $\prod_{i=1}^{d_I}\exp\left(\left\langle\tilde{\theta}^i,\Phi^i(x)\right\rangle\right)$, with $b=1$. These are the intractable factors.
- Base distribution $p(x;\theta,\vec{0}) \propto \exp\left(-\frac{1}{2}x^\intercal\Sigma^{-1}x\right)$ which is a Gaussian and easy as mentioned above.
- If we multiply in only one intractable term, complexity to produce marginal still not so bad (quite easy in fact).
- I.e., Φ^i-augmented distribution is proportional to

$$\exp\left(-\frac{1}{2}x^\intercal\Sigma^{-1}x\right)\left[(1-\alpha)\varphi(y^i;0,\sigma_0^2 I)+\alpha\varphi(y^i;x,\sigma_1^2 I)\right] \quad (16.16)$$

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

Polytope and Base case

- We can partition the mean parameters $(\mu,\tilde{\mu}) \in \mathbb{R}^{d_T+d_I\times b}$
- Marginal polytope associated with these means

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

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

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

- Thus, any such mean parameters has instance for associated exponential family, and also $H(\mu, \tilde{\mu}^i)$ is easy to compute.
- 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 $\tilde{\tau}$.
- Define outer bound on true means $\mathcal{M}(\phi, \Phi)$ (which is still convex)

$$\mathcal{L}(\phi, \Phi) = \left\{ (\tau, \tilde{\tau}) | \tau \in \mathcal{M}(\phi), \Pi^i(\tau, \tilde{\tau}) \in \mathcal{M}(\phi, \Phi^i), \ \forall i \right\} \tag{16.21}$$

- Note, based on a set of projections onto $\mathcal{M}(\phi, \Phi^i)$.
- Outer bound, i.e., $\mathcal{M}(\phi, \Phi) \subseteq \mathcal{L}(\phi, \Phi)$, since:

$$\tau \in \mathcal{M}(\phi) \Leftrightarrow \exists p \text{ s.t. } \tau = E_p[\phi(X)] \tag{16.22}$$

$$(\tau, \tilde{\tau}) \in \mathcal{L}(\phi, \Phi) \Leftrightarrow \tau \in \mathcal{M}(\phi) \ \& \ \exists p \text{ s.t. } (\tau, \tilde{\tau}^i) = E_p[\phi(X), \Phi^i(X)] \tag{16.23}$$

$$(\tau, \tilde{\tau}) \in \mathcal{M}(\phi, \Phi) \Leftrightarrow \exists p \text{ s.t. } (\tau, \tilde{\tau}) = E_p[\phi(X), \Phi(X)] \tag{16.24}$$

- 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

EP outer bound entropy and opt

- For any mean parms $(\tau, \tilde{\tau}) \in \mathcal{L}(\phi, \Phi)$: A) There is a member of the ϕ-exponential family which mean parameters τ with entropy $H(\tau)$; B) Also, for $i = 1 \ldots d_I$, there is a member of the (ϕ, Φ^i)-exponential family with mean parameters $(\tau, \tilde{\tau}^i)$ with entropy $H(\tau, \tilde{\tau}^i)$.
- Both entropy forms are easy to compute, and so is a new entropy approximation:

$$H(\tau, \tilde{\tau}) \approx H_{\text{ep}}(\tau, \tilde{\tau}) \triangleq H(\tau) + \sum_{\ell=1}^{d_I} \Big[H(\tau, \tilde{\tau}^l) - H(\tau) \Big] \tag{16.25}$$

- With outer bound and entropy expression, we get new variational form

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

- 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.

Lagrangian optimization setup

- Make d_I duplicates of vector $\tau \in \mathbb{R}^{d_T}$, call them $\eta^i \in \mathbb{R}^{d_T}$ for $i \in [d_T]$.
- This gives large set of pseudo-mean parameters

$$\big\{ \tau, (\eta^i, \tilde{\tau}^i), i \in [d_I] \big\} \in \mathbb{R}^{d_T} \times (\mathbb{R}^{d_T} \times \mathbb{R}^b)^{d_I} \tag{16.27}$$

- We arrive at the optimization:

$$\max_{\{\tau, \{(\eta^i, \tilde{\tau}^i)\}_i\}} \left\{ \langle \tau, \theta \rangle + \sum_{i=1}^{d_I} \Big\langle \tilde{\tau}^i, \tilde{\theta}^i \Big\rangle + H(\tau) + \sum_{i=1}^{d_I} \big[H(\eta^i, \tilde{\tau}^i) - H(\eta^i) \big] \right\} \tag{16.28}$$

  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).

To Lagrangian optimization to Moment Matching

- Considering optimality conditions on what must hold for a solution $\{\tau, (\eta^i, \tilde{\tau}^i), i \in [d_I]\}$ to the above Lagrangian, must have properties:
  1. τ belongs to relative interior, i.e., $\tau \in \mathcal{M}^\circ(\theta)$ of the base model.
  2. $(\eta^i, \tilde{\tau}^i)$ belongs to relative interior of extended model, so $(\eta^i, \tilde{\tau}^i) \in \mathcal{M}^\circ(\phi, \Phi^i)$.
  3. Means must agree, i.e., $\tau = \eta^i$ for all i.
- First condition means we're a member of the ϕ-exponential family, and (it can be shown) has form:

$$q(x;\theta,\lambda) \propto \exp\left\{ \left\langle \theta + \sum_{i=1}^{d_I} \lambda^i, \phi(x) \right\rangle \right\} \tag{16.31}$$

- 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 $i \in [d_I]$.

Moment Matching $\rightarrow$ Expectation Propagation Updates

1. At iteration $n = 0$, initialize the Lagrange multiplier vectors $(\lambda^1, \ldots, \lambda^{d_I})$
2. At each iteration $n = 1, 2, \ldots$ choose some index $i(n) \in \{1, \ldots, d_I\}$.
3. Under the following augmented distribution

$$q^i(x;\theta,\tilde{\theta}^i,\lambda) \propto \exp\left(\left\langle \theta + \sum_{\ell \neq i} \lambda^l, \phi(x) \right\rangle + \left\langle \tilde{\theta}^i, \Phi^i(x) \right\rangle\right), \tag{16.34}$$

compute the mean parameters η^i as follows:

$$\eta^{i(n)} = \int q^{i(n)}(x)\phi(x)\nu(dx) = \mathbb{E}_{q^{i(n)}}[\phi(X)] \tag{16.35}$$

4. Form base distribution q using Equation 16.31 and adjust $\lambda^{i(n)}$ to satisfy the moment-matching condition

$$\mathbb{E}_q[\phi(X)] = \eta^{i(n)} \tag{16.36}$$

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`