EE512A – Advanced Inference in Graphical Models

— Fall Quarter, Lecture 13 —

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

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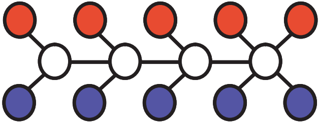

Announcements

- Wainwright and Jordan *Graphical Models, Exponential Families, and Variational Inference* `http://www.nowpublishers.com/product.aspx?product=MAL&doi=2200000001`
- Read chapters 1,2, and 3 in this book. Start reading chapter 4.
- Assignment due Wednesday (Nov 12th) night, 11:45pm. Non-binding final project proposals (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):
- L17 (11/26):
- L18 (12/1):
- L19 (12/3):
- Final Presentations: (12/10):

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

Mean Parameters, Convex Cores

- Consider quantities μ_α associated with statistic ϕ_α defined as:

$$\mu_\alpha = \mathbb{E}_p[\phi_\alpha(X)] = \int \phi_\alpha(x)p(x)\nu(dx) \tag{13.10}$$

- this defines a vector of "mean parameters" $(\mu_1, \mu_2, \dots, \mu_d)$ with $d = |\mathcal{I}|$.
- Define all possible such vectors, with $d = |\mathcal{I}|$,

$$\mathcal{M}(\phi) = \mathcal{M} \triangleq \left\{ \mu \in \mathbb{R}^d : \exists p \text{ s.t. } \forall \alpha \in \mathcal{I}, \mu_\alpha = \mathbb{E}_p[\phi_\alpha(X)] \right\} \tag{13.11}$$

- We don't say p was necessarily exponential family
- $\mathcal{M}$ is convex since expected value is a linear operator. So convex combinations of p and p' will lead to convex combinations of μ and μ'
- $\mathcal{M}$ is like a "convex core" of all distributions expressed via ϕ.

Mean Parameters and Marginal Polytopes

- Mean parameters are now true (fully specified) marginals, i.e., $\mu_v(j) = p(x_v = j)$ and $\mu_{st}(j,k) = p(x_s = j, x_t = k)$ since

$$\mu_{v,j} = \mathbb{E}_p[\mathbf{1}(x_v = j)] = p(x_v = j) \tag{13.20}$$
$$\mu_{st,jk} = \mathbb{E}_p[\mathbf{1}(x_s = j, x_t = k)] = p(x_s = j, x_t = k) \tag{13.21}$$

- Such an $\mathcal{M}$ is called the *marginal polytope* for discrete graphical models. Any μ must live in the polytope that corresponds to node and edge true marginals.
- We can also associate such a polytope with a graph G, where we take only $(s,t) \in E(G)$. Denote this as $\mathbb{M}(G)$.
- This polytope can help us to characterize when BP converges (there might be an outer bound of this polytope), or it might characterize the result of a mean-field approximation (an inner bound of this polytope) as we'll see.

Learning is the dual of Inference

- We can view the inference problem as moving from the canonical parameters θ to the point in the marginal polytope, called forward mapping, moving from $\theta \in \Omega$ to $\mu \in \mathcal{M}$.
- We can view the (maximum likelihood) learning problem as moving from a point in the polytope (given by the empirical distribution) to the canonical parameters. Called backwards mapping
- graph structure (e.g., tree-width) makes this easy or hard, and also characterizes the polytope (how complex it is in terms of number of faces).

Maximum entropy estimation

- Goal ("estimation", or "machine learning") is to find

$$p^* \in \operatorname*{argmax}_{p \in \mathcal{U}} H(p) \text{ s.t. } \mathbb{E}_p[\phi_\alpha(X)] = \hat{\mu}_\alpha \;\; \forall \alpha \in \mathcal{I} \tag{13.14}$$

where $H(p) = -\int p(x) \log p(x) \nu(dx)$, and $\forall \alpha \in \mathcal{I}$

$$\mathbb{E}_p[\phi_\alpha(X)] = \int_{\mathsf{D}_X} \phi_\alpha(x) p(x) \nu(dx). \tag{13.15}$$

- $\mathbb{E}_p[\phi_\alpha(X)]$ is mean value as measured by potential function, so above is a form of moment matching.
- Maximum entropy (MaxEnt) distribution is solved by taking distribution in form of $p_\theta(x) = \exp(\langle \theta, \phi(x) \rangle - A(\theta))$ and then by finding canonical parameters θ that solves

$$E_{p_\theta}[\phi_\alpha(X)] = \hat{\mu}_\alpha \text{ for all } \alpha \in \mathcal{I}. \tag{13.16}$$

Learning is the dual of Inference

- Ex: Estimate θ with $\hat{\theta}$ based on data $\mathbf{D} = \{\bar{x}^{(i)}\}_{i=1}^{M}$ of size M, likelihood function

$$\ell(\theta, \mathbf{D}) = \frac{1}{M}\sum_{i=1}^{M} \log p_\theta(\bar{x}^{(i)}) = \frac{1}{M}\sum_{i=1}^{M}\left(\left\langle \theta, \phi(\bar{x}^{(i)})\right\rangle - A(\theta)\right) \quad (13.20)$$

$$= \langle \theta, \hat{\mu}\rangle - A(\theta) \quad (13.21)$$

where empirical means are given by:

$$\hat{\mu} = \hat{\mathbb{E}}[\phi(X)] = \frac{1}{M}\sum_{i=1}^{M}\phi(\bar{x}^{(i)}) \quad (13.22)$$

- By taking derivatives of the above, it is easy to see that solution is the point $\hat{\theta} = \theta(\hat{\mu})$ such that empirical matches expected means, or what are called the moment matching conditions:

$$\mathbb{E}_{\hat{\theta}}[\phi(X)] = \hat{\mu} \quad (13.23)$$

this is the the backward mapping problem, going from μ to θ.

- Here, maximum likelihood is identical to maximum entropy problem.

Likelihood and negative entropy

- Entropy definition again: $H(p) = -\int p(x) \log p(x) \nu(dx)$
- Given data, $\mathbf{D} = \{\bar{x}^{(i)}\}_{i=1}^{M}$, defines an empirical distribution

$$\hat{p}(x) = \frac{1}{M} \sum_{i=1}^{M} \mathbf{1}(x = \bar{x}^{(i)}) \tag{13.20}$$

so that $\mathbb{E}_{\hat{p}}[\phi(X)] = \int \hat{p}(x)\phi(x)\nu(dx) = \frac{1}{M}\sum_{i=1}^{M} \phi(\bar{x}^{(i)}) = \hat{\mu}$

- Starting from maximum likelihood solution $\theta(\hat{u})$, meaning we are at moment matching conditions $\mathbb{E}_{p_{\theta(\hat{u})}}[\phi(X)] = \hat{\mu} = \mathbb{E}_{\hat{p}}[\phi(X)]$, we have

$$\ell(\theta(\hat{u}), \mathbf{D}) = \langle \theta(\hat{u}), \hat{\mu} \rangle - A(\theta(\hat{u})) = \frac{1}{M} \sum_{i=1}^{M} \log p_{\theta(\hat{u})}(\bar{x}^{(i)}) \tag{13.21}$$

$$= \int \hat{p}(x) \log p_{\theta(\hat{\mu})}(x) \nu(dx) = \mathbb{E}_{\hat{p}}[\log p_{\theta(\hat{\mu})}(x)] \tag{13.22}$$

$$= \mathbb{E}_{p_{\theta(\hat{\mu})}}[\log p_{\theta(\hat{\mu})}(x)] = -H_{p_{\theta(\hat{\mu})}}[p_{\theta(\hat{\mu})}(x)] \tag{13.23}$$

- Thus, maximum likelihood value and negative entropy are identical, at least for empirical $\hat{\mu}$ (which is $\in \mathcal{M}$).

Dual Mappings: Summary

Summarizing these relationships

- Forward mapping: moving from $\theta \in \Omega$ to $\mu \in \mathcal{M}$, this is the inference problem, getting the marginals.
- Backwards mapping: moving from $\mu \in \mathcal{M}$ to $\theta \in \Omega$, this is the learning problem, getting the parameters for a given set of empirical facts (means).
- In exponential family case, this is maximum entropy and is equivalent to maximum likelihood learning on an exponential family model.
- Turns out log partition function A, and its dual A^* can give us these mappings, and the mappings have interesting forms . . .

Log partition (or cumulant) function: derivative offerings

$$A(\theta) = \log \int_{\mathsf{D}_X} \exp \langle \theta, \phi(x) \rangle \, \nu(dx) \tag{13.20}$$

- If we know the log partition function, we know a lot for an exponential family model. In particular, we know
- $A(\theta)$ is convex in θ (strictly so if minimal representation).
- It yields cumulants of the random vector $\phi(X)$

$$\frac{\partial A}{\partial \theta_\alpha}(\theta) = \mathbb{E}_\theta[\phi_\alpha(X)] = \int \phi_\alpha(X) p_\theta(x) \nu(dx) = \mu_\alpha \tag{13.21}$$

  in general, derivative of log part. function is expected value of feature
- Also, we get

$$\frac{\partial^2 A}{\partial \theta_{\alpha_1} \partial \theta_{\alpha_2}}(\theta) = \mathbb{E}_\theta[\phi_{\alpha_1}(X)\phi_{\alpha_2}(X)] - \mathbb{E}_\theta[\phi_{\alpha_1}(X)]\mathbb{E}_\theta[\phi_{\alpha_2}(X)] \tag{13.22}$$

- Proof given in book (Proposition 3.1, page 62).

Log partition function: properties

- So derivative of log partition function w.r.t. θ is equal to our mean parameter μ in the discrete case.
- Given $A(\theta)$, we can recover the marginals for each potential function $\phi_\alpha, \alpha \in \mathcal{I}$ (when mean parameters lie in the marginal polytope).
- If we can approximate $A(\theta)$ with $\tilde{A}(\theta)$ then we can get approximate marginals. Perhaps we can bound it without inordinate compute resources. Why do we want bounds? We shall soon see.
- The Bethe approximation (as we'll also see) is such an approximation and corresponds to fixed points of loopy belief propagation.
- In some rarer cases, we can bound the approximation (current research trend).

Exponential Family: Recap

- Exponential Family

$$p_\theta(x) = \exp(\langle \theta, \phi(x) \rangle - A(\theta)) \tag{13.1}$$

with

$$A(\theta) = \log \int_{\mathsf{D}_X} \langle \theta, \phi(x) \rangle \, \nu(dx) \tag{13.2}$$

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- Backwards mapping, learning: from $\mu \in \mathcal{M}$ to $\theta \in \Omega$, getting best parameters associated with empirical facts (means).
- So learning is dual of inference.

Log partition function: Properties

- So $\nabla A : \Omega \to \mathcal{M}'$, where $\mathcal{M}' \subseteq \mathcal{M}$, and where $\mathcal{M} = \left\{\mu \in \mathbb{R}^d | \exists p \text{ s.t. } \mathbb{E}_p[\phi(X)] = \mu\right\}$.

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- Key point: all mean parameters that are realizable by some dist. are also realizable by member of exp. family.

Mappings - one-to-one

Expanding on one of the previous properties, . . .

Theorem 13.3.1

The gradient map ∇A is one-to-one iff the exponential representation is minimal.

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- Proof basically uses property that if representation is non-minimal, and $\langle a, \phi(x) \rangle = c$ for all x, then we can form an affine set of equivalent parameters $\theta + \gamma a$.
- Other direction, uses strict convexity of $A(\theta)$

Mappings - onto

Theorem 13.3.2

In a minimal exponential family, the gradient map ∇A is onto the interior of $\mathcal{M}$ (denoted $\mathcal{M}^\circ$). Consequently, for each $\mu \in \mathcal{M}^\circ$, there exists some $\theta = \theta(\mu) \in \Omega$ such that $\mathbb{E}_\theta[\phi(X)] = \mu$.

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- The theorem here is more general and applies for any set of sufficient statistics.

Conjugate Duality

- Consider maximum likelihood problem for exp. family

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- Key: when $\mu \in \mathcal{M}$, dual is negative entropy of exponential model $p_{\theta(\mu)}$ where $\theta(\mu)$ is the unique set of canonical parameters satisfying this *matching condition*

$$\mathbb{E}_{\theta(\mu)}[\phi(X)] = \nabla A(\theta(\mu)) = \mu \tag{13.5}$$

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$$\mathbb{E}_{\theta(\mu)}[\phi(X)] = \nabla A(\theta(\mu)) = \mu \tag{13.5}$$

- When $\mu \notin \mathcal{M}$, then $A^*(\mu) = +\infty$, optimization with dual need consider points only in $\mathcal{M}$.

Conjugate Duality, Maximum Likelihood, Negative Entropy

Theorem 13.3.3 (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:*

$$A^*(\mu) = \sup_{\theta \in \Omega} (\langle \theta, \mu \rangle - A(\theta)) = \begin{cases} -H(p_{\theta(\mu)}) & \text{if } \mu \in \mathcal{M}^\circ \\ +\infty & \text{if } \mu \notin \overline{\mathcal{M}} \end{cases} \tag{13.6}$$

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

$$A(\theta) = \sup_{\mu \in \mathcal{M}} \{\langle \theta, \mu \rangle - A^*(\mu)\} \tag{13.7}$$

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

$$\mu = \int_{\mathsf{D}_X} \phi(x) p_\theta(x) \nu(dx) = \mathbb{E}_\theta[\phi(X)] = \nabla A(\theta) \tag{13.8}$$

Conjugate Duality, and Inference

- Note that $A*$ isn't exactly entropy, only entropy sometimes, and depends on matching parameters to μ via the matching mapping $\theta(\mu)$ which achieves

$$\mathbb{E}_{\theta(\mu)}[\phi(X)] = \mu \tag{13.9}$$

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- $A(\theta)$ in Equation 13.7 is the "inference" problem (dual of the dual) for a given θ, since computing it involves computing the desired node/edge marginals.

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- $A(\theta)$ in Equation 13.7 is the "inference" problem (dual of the dual) for a given θ, since computing it involves computing the desired node/edge marginals.
- Whenever $\mu \notin \mathcal{M}$, then $A^*(\mu)$ returns ∞ which can't be the resulting sup in Equation 13.7, so Equation 13.7 need only consider $\mathcal{M}$.

Conjugate Duality, Good and Bad News

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- Key: **we compute the log partition function simultaneously with solving inference, given the dual.**
- Good news: problem is concave objective over a convex set. Should be easy. In simple examples, indeed, it is easy. ☺

Conjugate Duality, Good and Bad News

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- Computing $A(\theta)$ in this way corresponds to the inference problem (finding mean parameters, or node and edge marginals).
- Key: **we compute the log partition function simultaneously with solving inference, given the dual.**
- Good news: problem is concave objective over a convex set. Should be easy. In simple examples, indeed, it is easy. ☺
- Bad news: $\mathcal{M}$ is quite complicated to characterize, depends on the complexity of the graphical model. ☹

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- Bad news: $\mathcal{M}$ is quite complicated to characterize, depends on the complexity of the graphical model. ☹
- More bad news: A^* not given explicitly in general and hard to compute. ☹

Conjugate Duality, Avenues to Approximation

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- Surprisingly, this is strongly related to belief propagation (i.e., the sum-product commutative semiring). ☺☺
- Much of the rest of the class will be above approaches to the above — giving not only to junction tree algorithm (that we've seen) but also to well-known approximation methods (LBP, mean-field, Bethe, expectation-propagation (EP), Kikuchi methods, linear programming relaxations, and semidefnite relaxations, some of which we will cover).

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- We'll see: LBP (sum-product alg.) has much to do with an approximation to the aforementioned variational problems.
- Recall: dealing only with pairwise interactions (natural for image processing) – If not pairwise, we can convert from factor graph to factor graph with factor-width 2 factors.
- Exponential overcomplete family model of form

$$p_\theta(x) = \frac{1}{Z(\theta)} \exp \left\{ \sum_{v \in V(G)} \theta_v(x_v) + \sum_{(s,t) \in E(G)} \theta_{st}(x_s, x_t) \right\}$$

with simple new shorthand notation functions θ_v and θ_{st}.

$$\theta_v(x_v) \triangleq \sum_i \theta_{v,i} \mathbf{1}(x_v = i) \text{ and } \tag{13.10}$$

$$\theta_{s,t}(x_s, x_t) \triangleq \sum_{i,j} \theta_{st,ij} \mathbf{1}(x_s = i, x_t = j) \tag{13.11}$$

Marginal notation, and graph
Marginal polytope

- We also have mean parameters that constitute the marginal polytope.

$$\mu_v(x_v) \triangleq \sum_{i \in \mathsf{D}_{X_v}} \mu_{v,i} \mathbf{1}(x_v = i), \text{ for } u \in V(G) \tag{13.12}$$

$$\mu_{st}(x_s, x_t) \triangleq \sum_{(j,k) \in \mathsf{D}_{X_{\{s,t\}}}} \mu_{st,jk} \mathbf{1}(x_s = j, x_t = k), \text{ for } (s,t) \in E(G) \tag{13.13}$$

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- And $\mathbb{M}(G)$ corresponds to the set of all singleton and pairwise marginals that can be jointly realized by some underlying probability distribution $p \in \mathcal{F}(G, \mathcal{M}^{(\mathrm{f})})$ that contains only pairwise interactions.

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- And $\mathbb{M}(G)$ corresponds to the set of all singleton and pairwise marginals that can be jointly realized by some underlying probability distribution $p \in \mathcal{F}(G, \mathcal{M}^{(\mathrm{f})})$ that contains only pairwise interactions.
- Note, $\mathbb{M}(G)$ is respect to a graph G.
- Recall, $\mathbb{M}$ can be represented as a convex hull of a set of points, or by a set of linear inequality constraints.

Local consistency (tree outer bound) polytope

- An "outer bound" of $\mathbb{M}$ consists of a set that contains $\mathbb{M}$. If formed from a **subset** of the linear inequalities (subset of the rows of matrix module (A, b)), then it is a polyhedral outer bound.

Local consistency (tree outer bound) polytope

- An "outer bound" of $\mathbb{M}$ consists of a set that contains $\mathbb{M}$. If formed from a **subset** of the linear inequalities (subset of the rows of matrix module (A, b)), then it is a polyhedral outer bound.
- A simple way to form outer bound: require only local consistency, i.e., consider set $\{\tau_v, v \in V(G)\} \cup \{\tau_{s,t}, (s,t) \in E(G)\}$ that is, always non-negative , and that satisfies normalization

$$\sum_{x_v} \tau_v(x_v) = 1 \tag{13.14}$$

and pair-node marginal consistency constraints

$$\sum_{x'_t} \tau_{s,t}(x_s, x'_t) = \tau_s(x_s) \tag{13.15a}$$

$$\sum_{x'_s} \tau_{s,t}(x'_s, x_t) = \tau_t(x_t) \tag{13.15b}$$

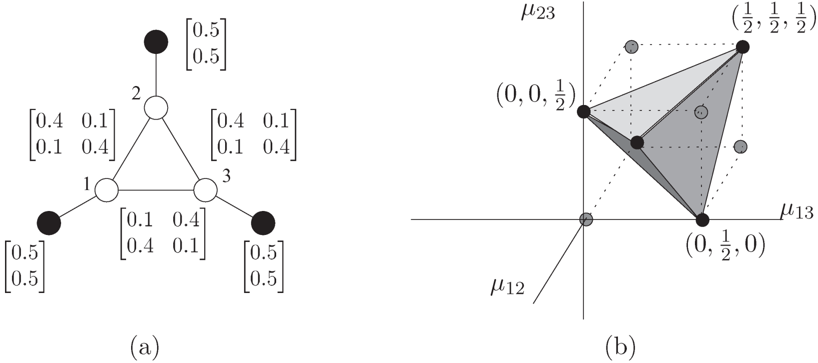
Local consistency (tree outer bound) polytope: properties

- Define $\mathbb{L}(G)$ to be the (locally consistent) polytope that obeys the constraints in Equations 13.14 and 13.15.
- Recall: local consistency was the necessary conditions for potentials being marginals that, it turned out, for junction tree that also guaranteed global consistency.
- Clearly $\mathbb{M} \subseteq \mathbb{L}(G)$ since any member of $\mathbb{M}$ (true marginals) will be locally consistent.
- When G is a tree, we say that local consistency implies global consistency, so for any tree T, we have $\mathbb{M}(T) = \mathbb{L}(T)$
- When G has cycles, however, $\mathbb{M}(G) \subset \mathbb{L}(G)$ strictly. We refer to members of $\mathbb{L}(G)$ as **pseudo-marginals**
- Key problem is that members of $\mathbb{L}$ might not be true possible marginals for any distribution.

Pseudo-marginals

$$\tau_v(x_v) = [0.5, 0.5], \text{ and } \tau_{s,t}(x_s, x_t) = \begin{bmatrix} \beta_{st} & .5 - \beta_{st} \\ .5 - \beta_{st} & \beta_{st} \end{bmatrix} \tag{13.16}$$

- Consider on 3-cycle C_3, satisfies local consistency.
- But for this won't give us a marginal. Below shows $\mathbb{M}(C_3)$ for $\mu_1 = \mu_2 = \mu_3 = 1/2$ and the $\mathbb{L}(C_3)$ outer bound (dotted).



Bethe Entropy Approximation

$$A(\theta) = \sup_{\mu \in \mathcal{M}} \{\langle \theta, \mu \rangle - A^*(\mu)\} \tag{13.7}$$

- So inference corresponds to Equation 13.7, and we have two difficulties $\mathcal{M}$ and $A^*(\mu)$.

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- Maybe it is hard to compute $A^*(\mu)$ but perhaps we can reasonably approximate it.
- In case when $-A^*(\mu)$ is the entropy, lets use an approximate entropy based on $\mathbb{L}$ being those distributions that factor w.r.t. a tree.
- When $p \in \mathcal{F}(G, \mathcal{M}^{(\mathrm{f})})$ and G is a tree T, then we can write p as:

$$p(x_1, \dots, x_N) = \frac{\prod_{(i,j) \in E(T)} p_{ij}(x_i, x_j)}{\prod_{v \in V(T)} p_v(x_v)^{d(v)-1}} \tag{13.17}$$

$$= \prod_{v \in V(T)} p_v(x_v) \prod_{(i,j) \in E(T)} \frac{p_{ij}(x_i, x_j)}{p_i(x_i) p_j(x_j)} \tag{13.18}$$

where $d(v)$ is the degree of v (shattering coefficient of v as separator)

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- In terms of current notation, we can let $\mu \in \mathbb{L}(T)$, the pseudo marginals associated with T. Since local consistency requires global consistency, for a tree, any $\mu \in \mathbb{L}(T)$ is such that $\mu \in \mathbb{M}(T)$, thus

$$p_\mu(x) = \prod_{s \in V(T)} \mu_s(x_s) \prod_{(s,t) \in E(T)} \frac{\mu_{st}(x_s, x_t)}{\mu_s(x_s)\mu_t(x_t)} \tag{13.19}$$

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- When $G = T$ is a tree, and $\mu \in \mathbb{L}(T) = \mathbb{M}(T)$ we have

$$-A^*(\mu) = H(p_\mu) = \sum_{v \in V(T)} H(X_v) - \sum_{(s,t) \in E(T)} I(X_s; X_t) \tag{13.20}$$

$$= \sum_{v \in V(T)} H_v(\mu_v) - \sum_{(s,t) \in E(T)} I_{st}(\mu_{st}) \tag{13.21}$$

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- That is, for $G = T$, $-A^*(\mu)$ is very easy to compute (only need to compute entropy and mutual information over at most pairs).

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- We can perhaps just use this as an approximation, i.e., say that for **any** graph $G = (V, E)$ not nec. a tree.

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- That is, assuming that the distribution is structured over pairwise potential functions w.r.t. a graph G, we can make an approximation to $-A^*(\tau)$ based on equation that has same form, i.e.,

$$-A^*(\tau) \approx H_{\text{Bethe}}(\tau) \triangleq \sum_{v \in V(G)} H_v(\tau_v) - \sum_{(s,t) \in E(G)} I_{st}(\tau_{st}) \qquad (13.22)$$

$$= \sum_{v \in V(G)} (d(v) - 1) H_v(\tau_v) + \sum_{(i,j) \in E(G)} H_{st}(\tau_s, \tau_t) \qquad (13.23)$$

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- Key: $H_{\text{Bethe}}(\tau)$ is not necessarily concave as it is not a real entropy.
- MI equation is not hard to compute $O(r^2)$.

$$I_{st}(\tau_{st}) = I_{st}(\tau_{st}(x_s, x_t)) \quad (13.24)$$

$$= \sum_{x_s, x_t} \tau_{st}(x_s, x_t) \log \frac{\tau_{st}(x_s, x_t)}{\tau_s(x_s)\tau_t(x_t)} \quad (13.25)$$

Bethe Variational Problem and LBP

Original variational representation of log partition function

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- Exact when $G = T$ but we do this for any G, still commutable
- we get an approximate log partition function, and approximate (pseudo) marginals (in $\mathbb{L}$), but this is perhaps much easier to compute.
- We can optimize this directly using a Lagrangian formulation.

Bethe Variational Problem and LBP

- Lagrangian constraints for summing to unity at nodes

$$C_{vv}(\tau) = 1 - \sum_{x_v} \tau_v(x_v) \tag{13.29}$$

- Lagrangian constraints for local consistency

$$C_{ts}(x_s;\tau) = \tau_s(x_s) - \sum_{x_t} \tau_{st}(x_s, x_t) \tag{13.30}$$

- Yields following Lagrangian

$$\mathcal{L}(\tau,\lambda;\theta) = \langle \theta, \tau \rangle + H_{\text{Bethe}}(\tau) + \sum_{v \in V} \lambda_{vv} C_{vv}(\tau) \tag{13.31}$$

$$+ \sum_{(s,t)\in E(G)} \left[\sum_{x_s} \lambda_{ts}(x_s) C_{ts}(x_s;\tau) + \sum_{x_t} \lambda_{st}(x_t) C_{st}(x_t;\tau) \right] \tag{13.32}$$

Fixed points: Variational Problem and LBP

Theorem 13.5.1

LBP updates are Lagrangian method for attempting to solve Bethe variational problem:
(a) *For any G, any LBP fixed point specifies a pair (τ^*, λ^*) s.t.*

$$\nabla_\tau \mathcal{L}(\tau^*, \lambda^*; \theta) = 0 \text{ and } \nabla_\lambda \mathcal{L}(\tau^*, \lambda^*; \theta) = 0 \tag{13.33}$$

(b) *For tree MRFs, Lagrangian equations have unique solution (τ^*, λ^*) where τ^* are exact node and edge marginals for the tree and the optimal value obtained is the true log partition function.*

- Not guaranteed convex optimization, but is if graph is tree.
- Remarkably, this means if we run loopy belief propagation, and we reach a point where we have converged, then we will have achieved a fixed-point of the above Lagrangian, and thus a (perhaps reasonable) local optimum of the underlying variational problem.

Fixed points: Variational Problem and LBP

- The resulting Lagrange multipliers λ_{st} end up being exactly the messages that we have defined. I.e., we get

$$\lambda_{st}(x_t) = \mu_{s\to t}(x_t) = \sum_{x_s} \psi_{s,t}(x_s, x_t) \prod_{k\in\delta(s)\setminus\{t\}} \mu_{k\to s}(x_s) \tag{13.34}$$

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- Proof: take derivatives of Lagrangian, set equal to zero, use Lagrangian constraints, do a bit of algebra, and amazingly, the BP messages suddenly pop out!!! (see page 86 in book).

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- So we can now (at least) characterize any stable point of LBP.
- This does not mean that it will converge.
- For trees, we'll get $A_{\text{Bethe}}(\theta) = A(\theta)$, results of previous lectures (parallel or MPP-based message passing).

Bounds on A: why would we want them?

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- For certain "attractive" potential functions, we get $A_{\text{Bethe}}(\theta) \leq A(\theta)$, these are common in computer vision and are related to graph cuts.

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  we would like both upper and lower bounds on A depending on if we want to upper or lower bound probability estimates.
- Perhaps more importantly, $\exp(A(\theta))$ is a marginal in and of itself (recall it is marginalization over everything). If we can bound $A(\theta)$, we can come up with other forms of bounds over other marginals.

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- True $-A^*(\mu) = \log 2 > 0$.

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`