EE512A – Advanced Inference in Graphical Models

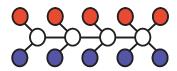
— Fall Quarter, Lecture 15 —

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

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Nov 19th, 2014



Logistics Review

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 Friday (Nov 21st) morning, 9:amr. Final project proposals (one page max).

Logistics

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
- \bullet 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.

EE512a/Fall 2014/Graphical Models - Lecture 15 - Nov 19th, 2014

Review

Bethe Variational Problem and LBP

Original variational representation of log partition function

$$A(\theta) = \sup_{\mu \in \mathcal{M}} \{ \langle \theta, \mu \rangle \mid A^*(\mu) \}$$
 (15.14)

Approximate variational representation of log partition function

$$A_{\mathsf{Bethe}}(\theta) = \sup_{\tau \in \mathbb{L}} \left\{ \langle \theta, \tau \rangle + H_{\mathsf{Bethe}}(\tau) \right\} \tag{15.15}$$

$$= \sup_{\tau \in \mathbb{N}} \left\{ \langle \theta, \tau \rangle + \sum_{v \in V(G)} H_v(\tau_v) - \sum_{(s,t) \in E(G)} I_{st}(\tau_{st}) \right\} \quad (15.16)$$

- 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.

Comparison of A and A_{Bethe} : loop series expansion

Proposition 15.2.2

Consider a pairwise MRF with binary variables, with $A_{\text{Bethe}}(\theta)$ being the optimized free energy evaluated at a LBP fixed point $\tau = (\tau_s, s \in V; \tau_{st}, (s,t) \in E(G))$. Then we have the following relationship with the cumulant function $A(\theta)$.

$$A(\theta) = A_{Bethe}(\theta) + \log \left\{ 1 + \sum_{\emptyset \neq \tilde{E} \subseteq E} \beta_{\tilde{E}} \prod_{s \in V} \mathbb{E}_{\tau_s} \left[(X_s - \tau_s)^{d_s(\tilde{E})} \right] \right\}$$
 (15.6)

- For any \tilde{E} such that $\exists s$ with $d_s(\tilde{E})=1$, inner term is zero and vanishes. why? Since $E_{\tau_s}\left[(X_s-\tau_s)^d\right]$ is the d^{th} central moment. Thus, terms in the sum only exists for generalized loops.
- The generalized loops give the correction!
- For trees, there are no generalized loops, and so if G is a tree then we have an equality between $A(\theta)$ and $A_{\text{Bethe}}(\theta)$ (recall both defs recoil).

Review

General idea of Kikuchi

Variational representation of log partition function

$$A(\theta) = \sup_{\mu \in \mathbb{M}(G)} \{ \langle \theta, \mu \rangle - A^*(\mu) \}$$
 (15.14)

- ullet So far, we used a replacement for $-A^*(\mu)$ and $\mathbb{M}(G)$ inspired by trees.
- A tree is just a 1-tree, so one simple generalization would be to use a k-tree, for constant k, where k is not too large.
- More generally still, why not some other structure, like junction tree (embedable into a k-tree for k not too large).
- Junction trees are hypertrees (to be defined) that satisfy r.i.p. (special case of hypergraphs). Every clique need not be of size k + 1.
- So approach is the following: 1) derive expression for $-A^*(\mu)$ associated with a hypertree/junction tree; 2) generalize this expression for any hypergraph; 3) consider local consistency properties of hypertrees/junction tree; 4) use hypertrees local consistency property for generalized polytope associated with any hypergraph.
- → Kikuchi variational approach ("clustered variational approximation")

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A hypergraph H=(V,E) is a set of vertices V and a collection of hyperedges E, where each element $e\in E$ is a subset of V, so $\forall e\in E, e\subseteq V$.

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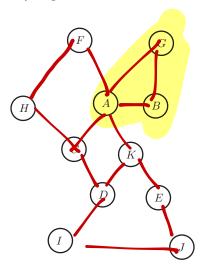
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- In a graph, |e| = 2. Thus, a graph is a (restricted) hypergraph, but not vice verse.

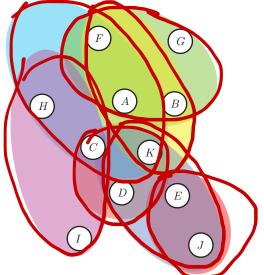
Drawing/Visualizing Hypergraphs

A set of vertices, normally edges connect two nodes.



Drawing/Visualizing Hypergraphs

• Hypergraph: hyperedges are shaded regions, each region a vertex cluster



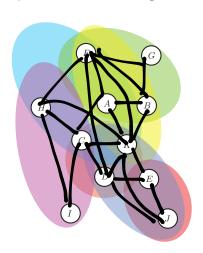
Hypergraphs and bipartite graphs

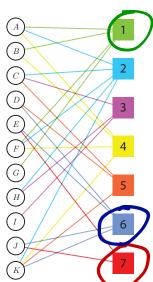
Hypergraphs can be represented by a bipartite G=(V,F,E) graphs where V is a set of left-nodes, F is a set of right nodes, and E is a set of size-two edges. Right nodes are hyperedges in the hypergraphs.

Next slide shows an example.

Drawing/Visualizing Hypergraphs as Bipartite Graphs

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





• Let H = (V, E) be a hypergraph with vertex set V and edge set E.

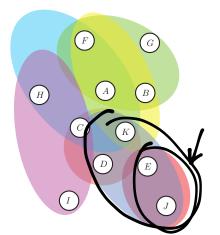
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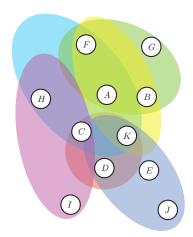
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- ullet A hypergraph H is acyclic if H is conformal and G(H) is chordal/triangulated.

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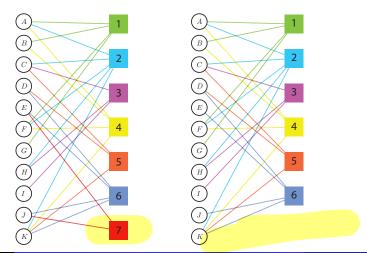
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- Hypergraph (as shaded regions) on left, reduced hypergraph on the right (i.e., hyper edge $\{E,J\}\subset\{E,J,D,K\}$ is removed).



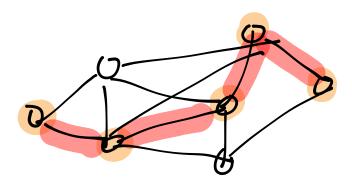


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• A hypergraph path from $s \in V$ to $t \in V$ is a sequence of $k \ge 1$ edges (e_1, e_2, \ldots, e_k) such that $s \in e_1$, $t \in e_k$, and $e_i \cap e_{i+1} \ne \emptyset$ for $1 \le i < k$.



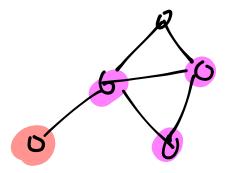
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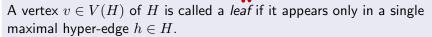
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- In fact, a junction tree is a hypertree where the cliques (which are clusters of original graph nodes) in the junction tree are the edges of the hypertree.

Definition 15.3.2 (leaf)

A vertex $v \in V(H)$ of H is called a *leaf* if it appears only in a single maximal hyper-edge $h \in H$.

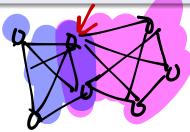


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Definition 15.3.3 (acyclic)

A hypergraph H is called *acyclic* if it is empty, or if it contains a **leaf** v such that induced hypergraph $H(V-\{v\})$ is acyclic (note, generalization of perfect elimination order in a triangulated graph, junction tree).



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Definition 15.3.5 (hypertree)

A hypergraph H that is acyclic is called a *hypertree*.

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 which can be read as "is contained in" or "is part of" or "is less than or equal to".

$$A = \{1, 1, 3, 4\} \subset \{4, 5\}$$

 $B = \{1, 4\} \subset A$
 $A \preceq B$

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| For all $x, x \leq x$. | (Reflexive) | (P1.) |
|--|-----------------|-------|
| If $x \leq y$ and $y \leq x$, then $x = y$ | (Antisymmetriy) | (P2.) |
| If $x \leq y$ and $y \leq z$, then $x \leq z$. | (Transitivity) | (P3.) |

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• We can use the above to get other operators as well such as "less than" via $x \leq y$ and $x \neq y$ implies $x \prec y$. And $x \succeq y$ is read "x contains y". And so on.

• Given two elements, we need not have either $x \leq y$ or $y \leq x$ be true, i.e., these elements might not be comparable. If for all $x, y \in V$ we have $x \leq y$ or $y \leq x$ then the poset is **totally ordered**.

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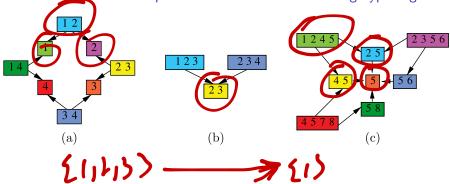
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- The length of a chain of n elements is n-1.

Hypergraph, edge representations

 It is possible to represent hypergraphs by only showing their hyperedges.

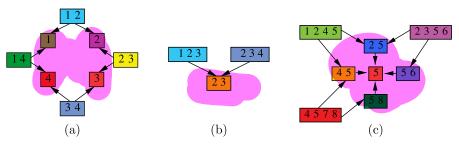
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- Here, we see graphical representations of three hypergraphs. Subsets
 of nodes corresponding to hyperedges are shown in rectangles,
 whereas the arrows represent inclusion relations among hyperedges.



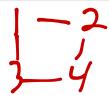
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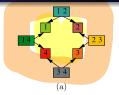


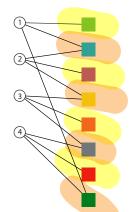
• Which ones, if any, are in reduced representation?

Hypergraph, edge representations, bipartite graphs



Edge-representations of hypergraphs and their corresponding bipartite graph representation.
An ordinary single 4-cycle graph represented as a

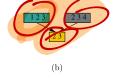




hypergraph.

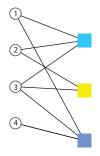
Hypergraph, edge representations, bipartite graphs





Edge-representations of hypergraphs and their corresponding bipartite graph representation.

A simple hypertree of "width" two.

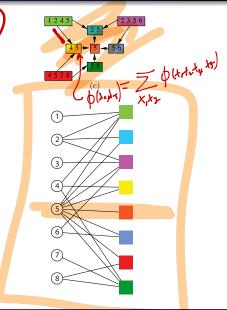


Hypergraph, edge representations, bipartite graphs



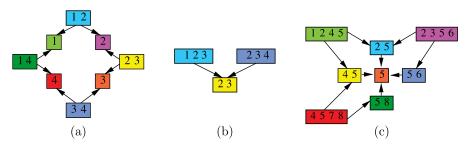
Edge-representations of hypergraphs and their corresponding bipartite graph representation.

A more complex hypertree of "width" three.



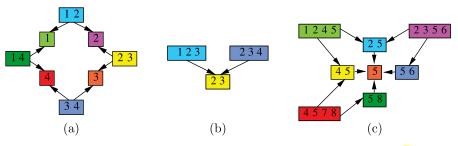
Hypergraph, edge representations, and posets

Hypergraphs and edge representations.



Hypergraph, edge representations, and posets

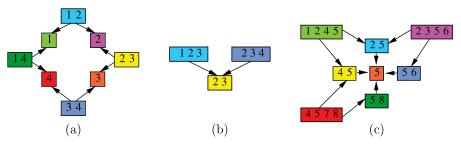
Hypergraphs and edge representations.



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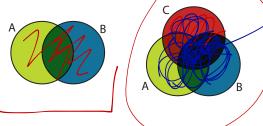


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- Hence, the edges of a hypergraph form a partially ordered set.

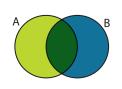
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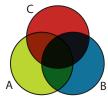
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Start by including, then excluding, and then including again.



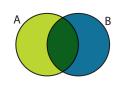
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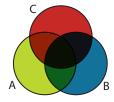




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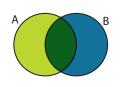
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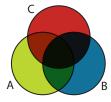




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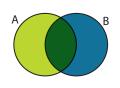
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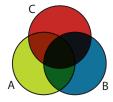




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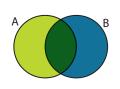
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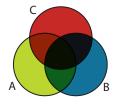




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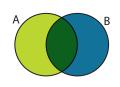
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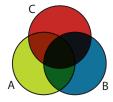




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Kikuchi and Hypertree-based Methods

• In general, inclusion-exclusion refers to measuring a quantity by, first "adding" some other quantities and overshooting, then "subtracting" off some more quantities and undershooting, then "adding" some still other quantities and again overshooting, then "subtracting" off some still more quantities and again undershooting, and so on, until we reach the right answer. "adding" might mean "multiplying", etc.

Entropic Inclusion-Exclusion

• Inclusion/exclusion also applies to entropy.

Entropic Inclusion-Exclusion

- Inclusion/exclusion also applies to entropy.
- That is, we have

$$H(X,Y) = H(X) + H(Y) - I(X;Y)$$
(15.1)

$$H(X,Y,Z) = H(X) + H(Y) + H(Z)$$
(15.2)

$$-I(X;Y) - I(X;Z) - I(Y;Z)$$
 (15.3)

$$+I(X;Y;Z). \tag{15.4}$$

and so on (see Yeung's book on information theory, the chapter on information measures).

 \bullet Given $X_1, X_2, \ldots, X_n \subseteq U$,

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(15.5)

$$+ \sum_{1 \le i < j < k \le n} \mu(X_i \cup X_j \cup X_k) + \dots$$
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• A "dual" form has the form:

$$\mu(\bigcup_{i=1}^{n} X_i) = \sum_{i=1}^{n} \mu(X_i) - \sum_{1 \le i < j \le n} \mu(X_i \cap X_j)$$
 (15.8)

$$+\sum_{1 \le i < j < k \le n} \mu(X_i \cap X_j \cap X_k) + \dots \tag{15.9}$$

$$+(-1)^{n-1}\mu(X_1\cap X_2\cap\ldots\cap X_n)$$
 (15.10)

• Another (easier, shorter) way of writing these is as:

$$\mu(\cap_{i=1}^{n} X_{i}) = \sum_{k=1}^{n} (-1)^{k+1} \left(\sum_{1 \leq i_{1} < i_{2} < \dots < i_{k} \leq n} \mu(X_{i_{1}} \cup \dots \cup X_{i_{k}}) \right)$$
(15.11)

and

$$\mu(\cup_{i=1}^{n} X_i) = \sum_{k=1}^{n} (-1)^{k+1} \left(\sum_{1 \le i_1 < i_2 < \dots < i_k \le n} \mu(X_{i_1} \cap \dots \cap X_{i_k}) \right)$$
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$$\forall A \subseteq V : \Upsilon(A) = \sum_{B:B \subseteq A} \Omega(B)$$
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- 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.

Hammersley Clifford Theorem

Theorem 15.3.6

(Hammersley and Clifford) Let \mathcal{F}^+ be the family of distributions with positive (and continuous in the continuous case) density (i.e., p(x) > 0 for all $p \in \mathcal{F}^+$). Then $\mathcal{F}^+ \cap \mathcal{F}(G, \mathcal{M}^{(f)}) = \mathcal{F}^+ \cap \mathcal{F}(G, \mathcal{M}^{(p)})$. In other words the four above rules define the same family of distributions over a graph G when the distributions are restricted to be everywhere positive.

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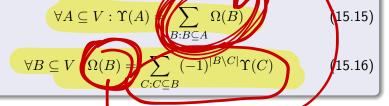
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- In fact, $\mathcal{F}(G, \mathcal{M}^{(p)}) \supseteq \mathcal{F}(G, \mathcal{M}^{(f)})$. always holds. Hammersley and \mathcal{F}^+ nord theorem (which uses Möbius inversion lemma) shows that $\mathcal{F}^+(G, R^{(p)}) \subseteq \mathcal{F}^+(G, R^{(f)})$, where $\mathcal{F}^+(G, \mathcal{M}) = \mathcal{F}^+ \cap \mathcal{F}(G, \mathcal{M})$.

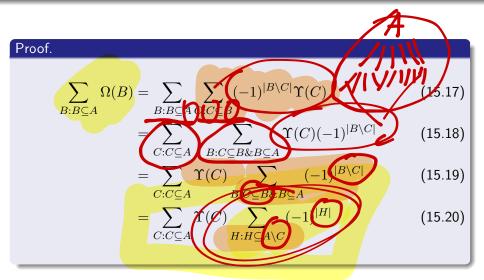
Möbius Inversion Lemma

Lemma 15.3.7 (Möbius Inversion Lemma (for sets))

Let Υ and Ω be functions defined on the set of all subsets of a finite set V, taking values in an Abelian group (i.e., a set and an operator having properties closure, associativity, identity, and inverse, and for which the elements also commute, the real numbers being just one example). The following two equations imply each other.



Proof of Möbius Inversion Lemma



Proof of Möbius Inversion Lemma

Proof Cont.

Also, note that for any set D,

$$\sum_{H:H\subseteq D} (-1)^{|H|} = \sum_{i=0}^{|D|} {|D| \choose i} - 1)^{i} \neq \sum_{i=0}^{|D|} {|D| \choose i} (-1)^{i} (1)^{|D|-i}$$

$$= (1-1)^{|D|} = \begin{cases} 1 & \text{if } |D| = 0 \\ 0 & \text{otherwise} \end{cases}$$
(15.22)

which means that when we take $D = A \setminus C$, with $C \subseteq A$, we get

$$\sum_{H:H\subseteq A\setminus C} (-1)^{|H|} = \begin{cases} 1 & \text{if } A = C \\ 0 & \text{otherwise} \end{cases}$$
 (15.23)

Proof of Möbius Inversion Lemma

Proof Cont.

This gives

$$\sum_{B:B\subseteq A} \Omega(B) = \sum_{C:C\subseteq A} \Upsilon(C) \mathbf{1}\{A = C\} = \Upsilon(A)$$
 (15.24)

thus proving one direction. The other direction is very similar.



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- Given $\omega(g, f)$ defined for f such that $g \leq f < h$, we define

$$(15.26)$$

$$\omega(g,h) \neq -\sum_{\{f|g \leq f(h)\}} \omega(g,f)$$

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- Given $\omega(g, f)$ defined for f such that $g \leq f < h$, we define

$$\omega(g,h) = -\sum_{\{f|g \preceq f \prec h\}} \omega(g,f) \tag{15.26}$$

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

$$\sum_{f \in \mathcal{P}} \omega(g, f) \zeta(f, h) = \sum_{\{f \mid g \preceq f \preceq h\}} \omega(g, f) = \delta(g, h)$$
 (15.27)

General Möbius Inversion Lemma

Lemma 15.3.8 (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

$$\Omega(h) = \sum_{g \leq h} \Upsilon(g)$$
 for all $h \in \mathcal{P}$ (15.28)

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

$$\Upsilon(h) = \sum_{g \leq h} \Omega(g)\omega(g, h)$$
 for all $h \in \mathcal{P}$ (15.29)

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

$$\log \varphi_h(x_h) \triangleq \sum_{g \leq h} \omega(g, h) \log \mu_g(x_g)$$
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$$\log \mu_h(x_h) = \sum_{g \prec h} \log \varphi_g(x_g) \tag{15.31}$$

ullet Key, when $arphi_h$ is defined as above, and G is a hypertree we have

$$p_{\mu}(x) = \prod_{h \in E} \varphi_h(x_h) \tag{15.32}$$

⇒ general way to factorize a distribution that factors w.r.t. a hypergraph.

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- In such case, from Equation (15.31), we have that for all $s \in V$, $\varphi_s(x_s) = \mu_s(x_s)$ and for all $(s, v) = e \in E$, we have:

$$\varphi_{st}(x_s, x_t) = \frac{\mu_{st}(x_s, x_t)}{\mu_s(x_s)\mu_t(x_t)}$$
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• Gives us the tree factorization we saw early in this course, namely:

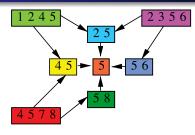
$$p(x) = \prod_{h \in E} \varphi_h(x_h) = \prod_{s \in V} \mu_s(x_s) \prod_{(s,t) = e \in E} \frac{\mu_{st}(x_s, x_t)}{\mu_s(x_s)\mu_t(x_t)}$$
(15.34)

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For the more general hypertree, consider edge set E = \{(12345), (2356), (4578), (25), (45), (56), (58), (5)\}. Check: is this a junction tree of cliques?
```

- For the more general hypertree, consider edge set $E = \{(12345), (2356), (4578), (25), (45), (56), (58), (5)\}$. Check: is this a junction tree of cliques?
- Then, from Eqn. (15.31), we get unaries $\varphi_s(x_s) = \mu_s(x_s)$ and pairwise (e.g., $\varphi_{25} = \mu_{25}/\mu_5$, etc.) and

$$\varphi_{1245} = \frac{\mu_{1245}}{\varphi_{25}\varphi_{45}\varphi_5} = \frac{\mu_{1245}}{\frac{\mu_{25}}{\mu_5}\frac{\mu_{45}}{\mu_5}\mu_5} = \frac{\mu_{1245}\mu_5}{\mu_{25}\mu_{45}}$$
(15.35)

expressions of factorization and Möbius



 Doing this for all maxcliques of the figure, we get a factorization of the form:

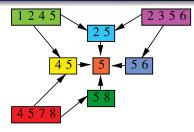
$$p_{\mu} = \frac{\mu_{1245}\mu_{5}}{\mu_{25}\mu_{45}} \frac{\mu_{2356}\mu_{5}}{\mu_{25}\mu_{56}} \frac{\mu_{4578}\mu_{5}}{\mu_{45}\mu_{58}} \frac{\mu_{25}}{\mu_{5}} \frac{\mu_{45}}{\mu_{5}} \frac{\mu_{56}}{\mu_{5}} \frac{\mu_{58}}{\mu_{5}} \mu_{5}$$

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$$= \frac{\mu_{1245}\mu_{2356}\mu_{4578}}{\mu_{25}\mu_{45}}$$
(15.36)

• This is the same as the junction tree factorization with max cliques $\{1245\}$, $\{4578\}$, and $\{2356\}$ and separators $\{25\}$ and $\{45\}$.

• Can express entropic quantities as well, such as the hyperedge entropy

$$H_h(\mu_h) = -\sum_{x_h} \mu_h(x_h) \log \mu_h(x_h)$$
 (15.38)

and the "multi-information" function

$$I_h(\mu_h) = \sum_{x_h} \mu_h(x_h) \log \varphi_h(x_h)$$
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- mutual information (= $H(X_s) + H(X_t) H(X_s, X_t)$).
- By Eqn (15.32), overall entropy of any hypertree distribution becomes

$$H_{\mathsf{hyper}}(\mu) = -\sum_{h \in E} I_h(\mu_h) \tag{15.40}$$

multi-information decomposition

• Using Möbius, and Eqn. (15.30) we can write

Using Mobius, and Eqn. (13.50) we can write
$$I_h(\mu_h) = \sum_{x_h} \mu_h(x_h) \log \varphi_h(x_h) = \sum_{x_h} \mu_h(x_h) \left(\sum_{g \leq h} \omega(g, h) \log \mu_g(x_g) \right)$$

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

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

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$$= \sum_{g \leq h} \omega(g, h) \left\{\sum_{x_h} \mu_h(x_h) \log \mu_g(x_g)\right\}$$
$$= \sum_{f \leq h} \sum_{e \succeq f} \omega(f, e) \left\{\sum_{x_f} \mu_f(x_f) \log \mu_f(x_f)\right\} = -\sum_{f \leq h} c(f) H_f(\mu_f)$$

where we define overcounting numbers (~ shattering coefficient)

$$c(f) \triangleq \sum_{e \succeq f} \omega(f, e) \tag{15.41}$$

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• This gives us a new expression for the hypertree entropy

$$H_{\mathsf{hyper}}(\mu) = \sum_{h \in E} c(h) H_h(\mu_h) \tag{15.42}$$

• Given arbitrary hypergraph now, we can generalize the hypertree-specific expressions above to this arbitrary hypergraph. This will give us a variational expression that approximates cumulant.

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• Hypergraph will give us local marginal constraints on hypergraph pseudo marginals, i.e., for each $h \in E$, we form marginal $\tau_h(x_h)$ and define constraints, non-negative, and

$$\sum \tau_h(x_h) = 1 \tag{15.44}$$

• Sum to one constraint:

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

$$\mathbb{L}_t(G) = \{ \tau \ge 0 | \text{ Equations (15.45) } \forall h, \text{ and (15.46) } \forall g \le h \text{ hold} \}$$

$$(15.47)$$

• Generalized approximate (app) entropy for the hypergraph:

$$H_{\mathsf{app}} = \sum_{g \in E} c(g) H_g(\tau_g) \tag{15.48}$$

where H_q is hyperedge entropy and overcounting number defined by:

$$c(g) = \sum_{f \succeq g} \omega(g, f) \tag{15.49}$$

This at last gets the Kikuchi variational approximation

$$A_{\mathsf{Kikuchi}}(\theta) = \max_{\tau \in \mathbb{L}_t(G)} \left\{ \langle \theta, \tau \rangle + H_{\mathsf{app}}(\tau) \right\}$$
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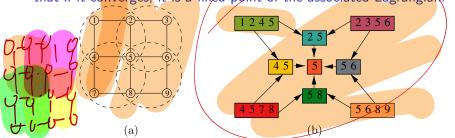
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- Also, if hypergraph is junction tree (r.i.p. holds, tree-local consistency implies global consistency), then also exact (although expensive, exponential in the tree-width to compute $H_{\rm app}$).

 We can define message passing algorithms on the hypertree, and show that if it converges, it is a fixed point of the associated Lagrangian.



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