

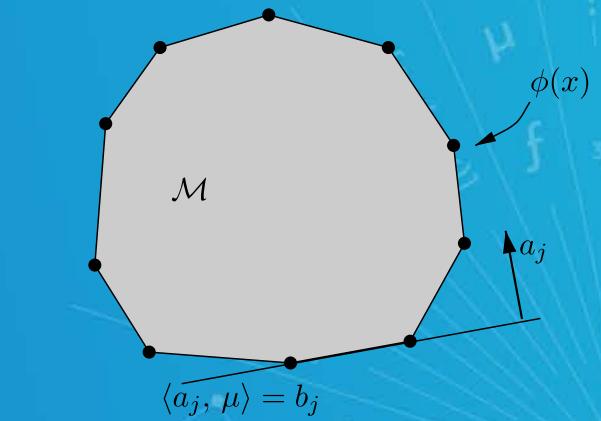
Probabilistic Graphical Models

Theory of Variational Inference: Marginal Polytope, Inner and Outer Approximation

Eric Xing

Lecture 12, February 25, 2019

Reading: see class homepage





Roadmap

- ❑ Two families of approximate inference algorithms
 - ❑ Loopy belief propagation (sum-product)
 - ❑ Mean-field approximation
- ❑ Are there some connections of these two approaches?
- ❑ We will re-exam them from a **unified** point of view based on the variational principle:
 - ❑ Loop BP: **outer** approximation
 - ❑ Mean-field: **inner** approximation





Variational Methods

- “Variational”: fancy name for optimization-based formulations
 - i.e., represent the quantity of interest as the solution to an optimization problem
 - *approximate* the desired solution by *relaxing/approximating* the *intractable* optimization problem

- Examples:

- Courant-Fischer for eigenvalues: $\lambda_{\max}(A) = \max_{\|x\|_2=1} x^T A x$

- Linear system of equations: $Ax = b, A \succ 0, x^* = A^{-1}b$
 - **variational formulation:**

$$x^* = \arg \min_x \left\{ \frac{1}{2} x^T A x - b^T x \right\}$$

- for large system, apply conjugate gradient method





Inference Problems in Graphical Models

- Undirected graphical model (MRF):

$$p(x) = \frac{1}{Z} \prod_{C \in \mathcal{C}} \psi_C(x_C)$$

- The quantities of interest:

- marginal distributions:

$$p(x_i) = \sum_{x_j, j \neq i} p(x)$$

- normalization constant (partition function): Z

- Question: how to represent these quantities in a variational form?

- Use tools from (1) **exponential families**; (2) **convex analysis**





Exponential Families

- Canonical parameterization

$$p_{\theta}(x_1, \dots, x_m) = \exp \left\{ \theta^{\top} \phi(x) - A(\theta) \right\}$$

Canonical Parameters **Sufficient Statistics** **Log partition Function**



- Log normalization constant:

$$A(\theta) = \log \int \exp\{\theta^T \phi(x)\} dx$$

it is a **convex** function (Prop 3.1)

- Effective canonical parameters:

$$\Omega := \left\{ \theta \in \mathbb{R}^d \mid A(\theta) < +\infty \right\}$$





Graphical Models as Exponential Families

- Undirected graphical model (MRF):

$$p(\mathbf{x}; \theta) = \frac{1}{Z(\theta)} \prod_{C \in \mathcal{C}} \psi(\mathbf{x}_C; \theta_C)$$

- MRF in an exponential form:

$$p(\mathbf{x}; \theta) = \exp \left\{ \sum_{C \in \mathcal{C}} \log \psi(\mathbf{x}_C; \theta_C) - \log Z(\theta) \right\}$$

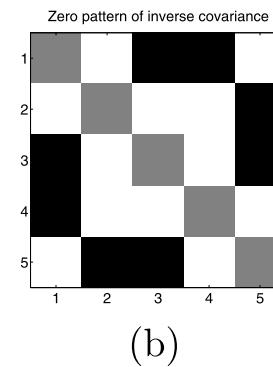
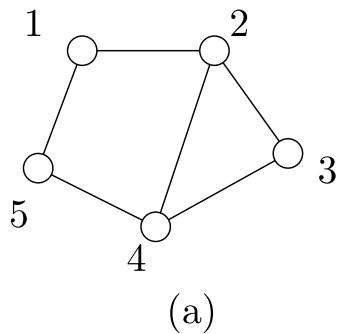
- $\log \psi(\mathbf{x}_C; \theta_C)$ can be written in a *linear* form after some parameterization





Example: Gaussian MRF

- Consider a zero-mean multivariate Gaussian distribution that respects the Markov property of a graph
 - **Hammersley-Clifford theorem** states that the precision matrix $\Lambda = \Sigma^{-1}$ also respects the graph structure



- Gaussian MRF in the exponential form

$$p(\mathbf{x}) = \exp \left\{ \frac{1}{2} \langle \Theta, \mathbf{x} \mathbf{x}^T \rangle - A(\Theta) \right\}, \text{ where } \Theta = -\Lambda$$

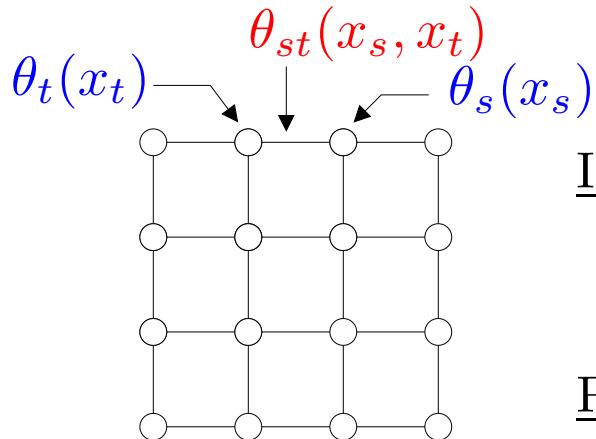
- Sufficient statistics are

$$\{x_s^2, s \in V; x_s x_t, (s, t) \in E\}$$





Example: Discrete MRF



Indicators:

$$\mathbb{I}_j(x_s) = \begin{cases} 1 & \text{if } x_s = j \\ 0 & \text{otherwise} \end{cases}$$

Parameters:

$$\theta_s = \{\theta_{s;j}, j \in \mathcal{X}_s\}$$

$$\theta_{st} = \{\theta_{st;jk}, (j, k) \in \mathcal{X}_s \times \mathcal{X}_t\}$$

- In exponential form

$$p(x; \theta) \propto \exp \left\{ \sum_{s \in V} \sum_j \theta_{s;j} \mathbb{I}_j(x_s) + \sum_{(s,t) \in E} \theta_{st;jk} \mathbb{I}_j(x_s) \mathbb{I}_k(x_t) \right\}$$





Why Exponential Families?

- Computing the expectation of sufficient statistics (**mean parameters**) given the **canonical parameters** yields the marginals

$$\mu_{s;j} = \mathbb{E}_p[\mathbb{I}_j(X_s)] = \mathbb{P}[X_s = j] \quad \forall j \in \mathcal{X}_s,$$

$$\mu_{st;jk} = \mathbb{E}_p[\mathbb{I}_{st;jk}(X_s, X_t)] = \mathbb{P}[X_s = j, X_t = k] \quad \forall (j, k) \in \mathcal{X}_s \times \mathcal{X}_t.$$

- Computing the normalizer yields the log partition function (or log likelihood function)

$$\log Z(\theta) = A(\theta)$$





Computing Mean Parameter: Bernoulli

- ❑ A single Bernoulli random variable

$$X \quad \theta$$

$$p(x; \theta) = \exp\{\theta x - A(\theta)\}, x \in \{0, 1\}, A(\theta) = \log(1 + e^\theta)$$

- ❑ Inference = Computing the mean parameter

$$\mu(\theta) = \mathbb{E}_\theta[X] = 1 \cdot p(X = 1; \theta) + 0 \cdot p(X = 0; \theta) = \frac{e^\theta}{1 + e^\theta}$$

- ❑ Want to do it in a **variational** manner: cast the procedure of computing mean (summation) in an optimization-based formulation

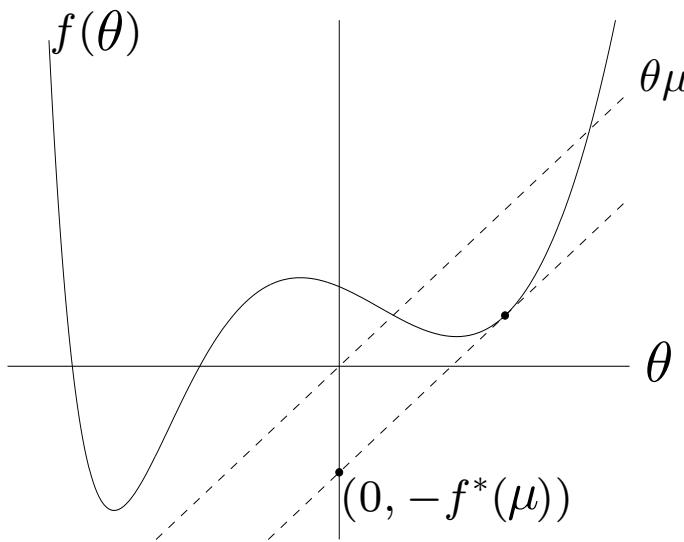




Conjugate Dual Function

- Given any function $f(\theta)$, its conjugate dual function is:

$$f^*(\mu) = \sup_{\theta} \{ \langle \theta, \mu \rangle - f(\theta) \}$$



- Conjugate dual is always a **convex** function: point-wise supremum of a class of linear functions





Dual of the Dual is the Original

- Under some technical condition on f (convex and lower semi-continuous), the dual of dual is itself:

$$f = (f^*)^*$$

$$f(\theta) = \sup_{\mu} \{ \langle \theta, \mu \rangle - f^*(\mu) \}$$

- For log partition function

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

- The dual variable μ has a natural interpretation as the mean parameters





Computing Mean Parameter: Bernoulli

- The conjugate

$$A^*(\mu) := \sup_{\theta \in \mathbb{R}} \{\mu\theta - \log[1 + \exp(\theta)]\}$$

- Stationary condition

$$\mu = \frac{e^\theta}{1 + e^\theta} \quad (\mu = \nabla A(\theta))$$

- If $\mu \in (0, 1)$, $\theta(\mu) = \log\left(\frac{\mu}{1 - \mu}\right)$, $A^*(\mu) = \mu \log(\mu) + (1 - \mu) \log(1 - \mu)$

- If $\mu \notin [0, 1]$, $A^*(\mu) = +\infty$

- We have

$$A^*(\mu) = \begin{cases} \mu \log \mu + (1 - \mu) \log(1 - \mu) & \text{if } \mu \in [0, 1] \\ +\infty & \text{otherwise.} \end{cases}.$$

- The variational form: $A(\theta) = \max_{\mu \in [0, 1]} \{\mu \cdot \theta - A^*(\mu)\}.$

- The optimum is achieved at $\mu(\theta) = \frac{e^\theta}{1 + e^\theta}$. This is the mean!





Computation of Conjugate Dual

- Given an exponential family

$$p(x_1, \dots, x_m; \theta) = \exp \left\{ \sum_{i=1}^d \theta_i \phi_i(x) - A(\theta) \right\}$$

- The dual function

$$A^*(\mu) := \sup_{\theta \in \Omega} \{ \langle \mu, \theta \rangle - A(\theta) \}$$

- The stationary condition:

$$\mu - \nabla A(\theta) = 0$$

- Derivatives of A yields mean parameters

$$\frac{\partial A}{\partial \theta_i}(\theta) = \mathbb{E}_\theta[\phi_i(X)] = \int \phi_i(x)p(x; \theta) dx$$

- The stationary condition becomes

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

- Question: for which $\mu \in \mathbb{R}^d$ does it have a solution $\theta(\mu)$?





Computation of Conjugate Dual

- Let's assume there is a solution $\theta(\mu)$ such that $\mu = \mathbb{E}_{\theta(u)}[\phi(X)]$
- The dual has the form

$$\begin{aligned} A^*(\mu) &= \langle \theta(\mu), \mu \rangle - A(\theta(\mu)) \\ &= \mathbb{E}_{\theta(\mu)} [\langle \theta(\mu), \phi(X) \rangle - A(\theta(\mu))] \\ &= \mathbb{E}_{\theta(\mu)} [\log p(X; \theta(\mu))] \end{aligned}$$

- The entropy is defined as

$$H(p(x)) = - \int p(x) \log p(x) dx$$

- So the dual is $A^*(\mu) = -H(p(x; \theta(\mu)))$ when there is a solution $\theta(\mu)$





Remark

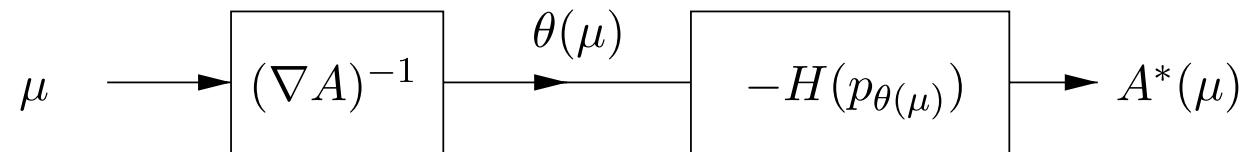
- ❑ The last few identities are not coincidental but rely on a deep theory in general exponential family.
 - ❑ The dual function is the negative **entropy** function
 - ❑ The mean parameter is **restricted**
 - ❑ Solving the optimization returns the mean parameter and log partition function
- ❑ Next step: develop this framework for general exponential families/graphical models.
- ❑ However,
 - ❑ Computing the conjugate dual (**entropy**) is in general intractable
 - ❑ The **constrain set** of mean parameter is hard to characterize
 - ❑ Hence we need approximation





Complexity of Computing Conjugate Dual

- The dual function is **implicitly** defined:



- Solving the inverse mapping $\mu = \mathbb{E}_\theta[\phi(X)]$ for canonical parameters $\theta(\mu)$ is nontrivial
- Evaluating the negative entropy requires **high-dimensional** integration (summation)
- Question: for which $\mu \in \mathbb{R}^d$ does it have a solution $\theta(\mu)$? i.e., the **domain** of $A^*(\mu)$.
 - the ones in marginal polytope!





Marginal Polytope

- For any distribution $p(x)$ and a set of sufficient statistics $\phi(x)$, define a vector of **mean parameters**

$$\mu_i = \mathbb{E}_p[\phi_i(X)] = \int \phi_i(x)p(x) dx$$

- $p(x)$ is **not** necessarily an exponential family
- The set of all realizable mean parameters

$$\mathcal{M} := \{\mu \in \mathbb{R}^d \mid \exists p \text{ s.t. } \mathbb{E}_p[\phi(X)] = \mu\}.$$

- It is a **convex** set
- For discrete exponential families, this is called **marginal polytope**





Convex Polytope

- Convex hull representation

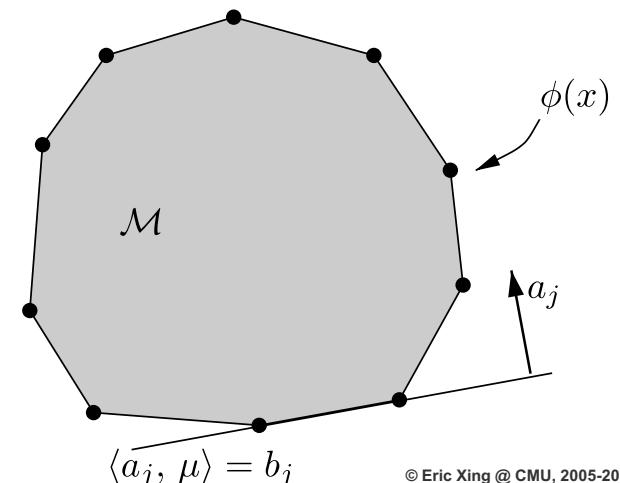
$$\mathcal{M} = \left\{ \mu \in \mathbb{R}^d \mid \sum_{x \in \mathcal{X}^m} \phi(x)p(x) = \mu, \text{ for some } p(x) \geq 0, \sum_{x \in \mathcal{X}^m} p(x) = 1 \right\}$$
$$\triangleq \text{conv}\left\{ \phi(x), x \in \mathcal{X}^m \right\}$$

- Half-plane representation

- **Minkowski-Weyl Theorem**: any non-empty convex polytope can be characterized by a **finite** collection of linear inequality constraints

$$\mathcal{M} = \left\{ \mu \in \mathbb{R}^d \mid a_j^\top \mu \geq b_j, \forall j \in \mathcal{J} \right\},$$

where $|\mathcal{J}|$ is finite.





Example: Two-node Ising Model

- Sufficient statistics:

$$\phi(x) := (x_1, x_2, x_1 x_2)$$

- Mean parameters:

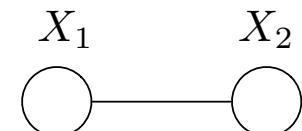
$$\mu_1 = \mathbb{P}(X_1 = 1), \mu_2 = \mathbb{P}(X_2 = 1)$$

- Two-node Ising model

- Convex hull representation

$$\text{conv}\{(0,0,0), (1,0,0), (0,1,0), (1,1,1)\}$$

$$\mu_{12} = \mathbb{P}(X_1 = 1, X_2 = 1)$$



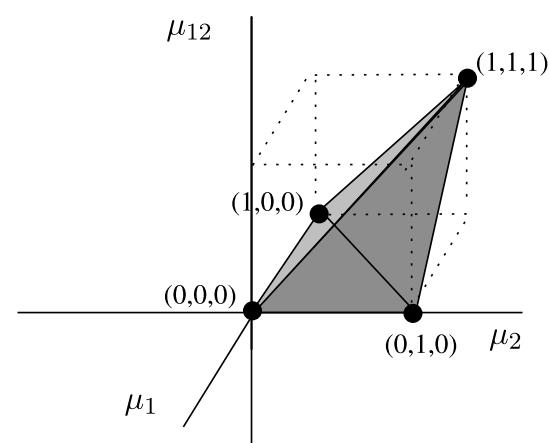
- Half-plane representation

$$\mu_1 \geq \mu_{12}$$

$$\mu_2 \geq \mu_{12}$$

$$\mu_{12} \geq 0$$

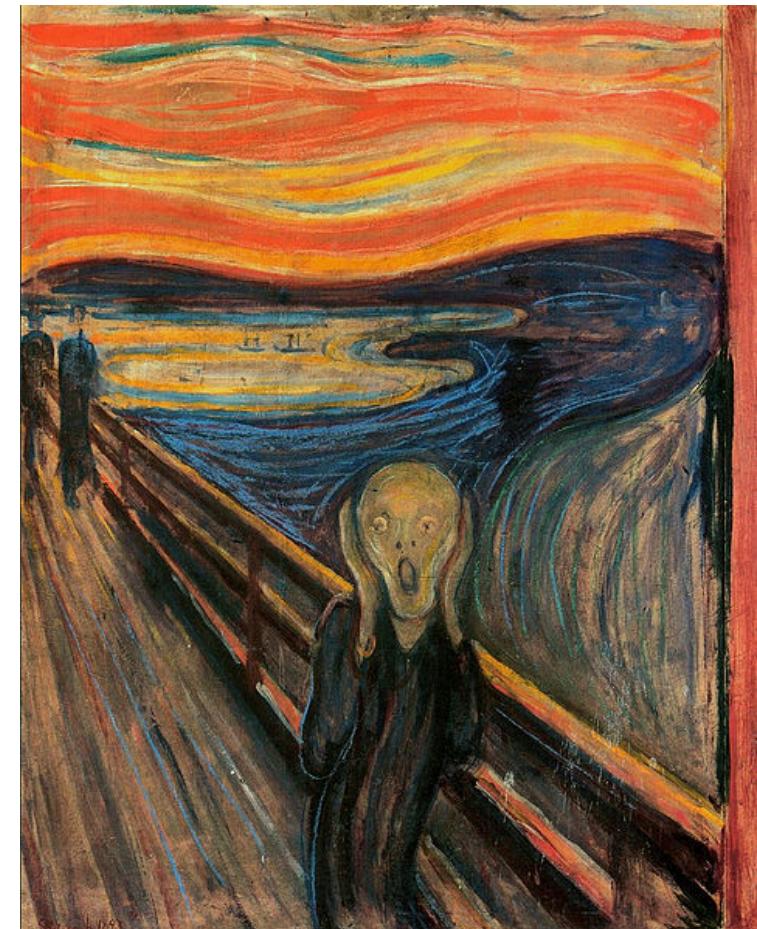
$$1 + \mu_{12} \geq \mu_1 + \mu_2$$





Marginal Polytope for General Graphs

- ❑ Still doable for connected binary graphs with 3 nodes: 16 constraints
- ❑ For tree graphical models, the number of half-planes (**facet complexity**) grows only *linearly* in the graph size
- ❑ General graphs?
 - ❑ extremely hard to characterize the marginal polytope





Variational Principle (Theorem 3.4)

- The dual function takes the form

$$A^*(\mu) = \begin{cases} -H(p_{\theta(\mu)}) & \text{if } \mu \in \mathcal{M}^\circ \\ +\infty & \text{if } \mu \notin \overline{\mathcal{M}}. \end{cases}$$

- $\theta(\mu)$ satisfies $\mu = \mathbb{E}_{\theta(u)}[\phi(X)]$
- The log partition function has the variational form

$$A(\theta) = \sup_{\mu \in \mathcal{M}} \{\theta^T \mu - A^*(\mu)\}$$

- For all $\theta \in \Omega$, the above optimization problem is attained uniquely at that satisfies $\mu(\theta) \in \mathcal{M}^\circ$

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

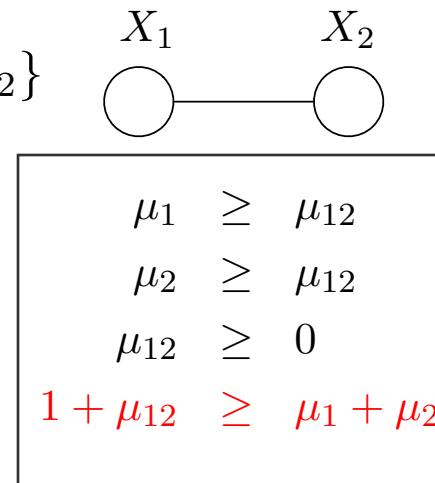




Example: Two-node Ising Model

- The distribution
 - Sufficient statistics
- The marginal polytope is characterized by
- The dual has an explicit form

$$p(x; \theta) \propto \exp\{\theta_1 x_1 + \theta_2 x_2 + \theta_{12} x_{12}\}$$
$$\phi(x) = \{x_1, x_2, x_1 x_2\}$$



$$A^*(\mu) = \mu_{12} \log \mu_{12} + (\mu_1 - \mu_{12}) \log(\mu_1 - \mu_{12}) + (\mu_2 - \mu_{12}) \log(\mu_2 - \mu_{12})$$
$$+ (1 + \mu_{12} - \mu_1 - \mu_2) \log(1 + \mu_{12} - \mu_1 - \mu_2)$$

- The variational problem
- The optimum is attained at

$$\mu_1(\theta) = \frac{\exp\{\theta_1\} + \exp\{\theta_1 + \theta_2 + \theta_{12}\}}{1 + \exp\{\theta_1\} + \exp\{\theta_2\} + \exp\{\theta_1 + \theta_2 + \theta_{12}\}}$$





Variational Principle

- ❑ Exact variational formulation

$$A(\theta) = \sup_{\mu \in \mathcal{M}} \{\theta^T \mu - A^*(\mu)\}$$

- ❑ \mathcal{M} : the marginal polytope, difficult to characterize
- ❑ A^* : the negative entropy function, no explicit form
- ❑ Mean field method: non-convex inner bound and exact form of entropy
- ❑ Bethe approximation and loopy belief propagation: polyhedral outer bound and non-convex Bethe approximation





Mean Field Approximation



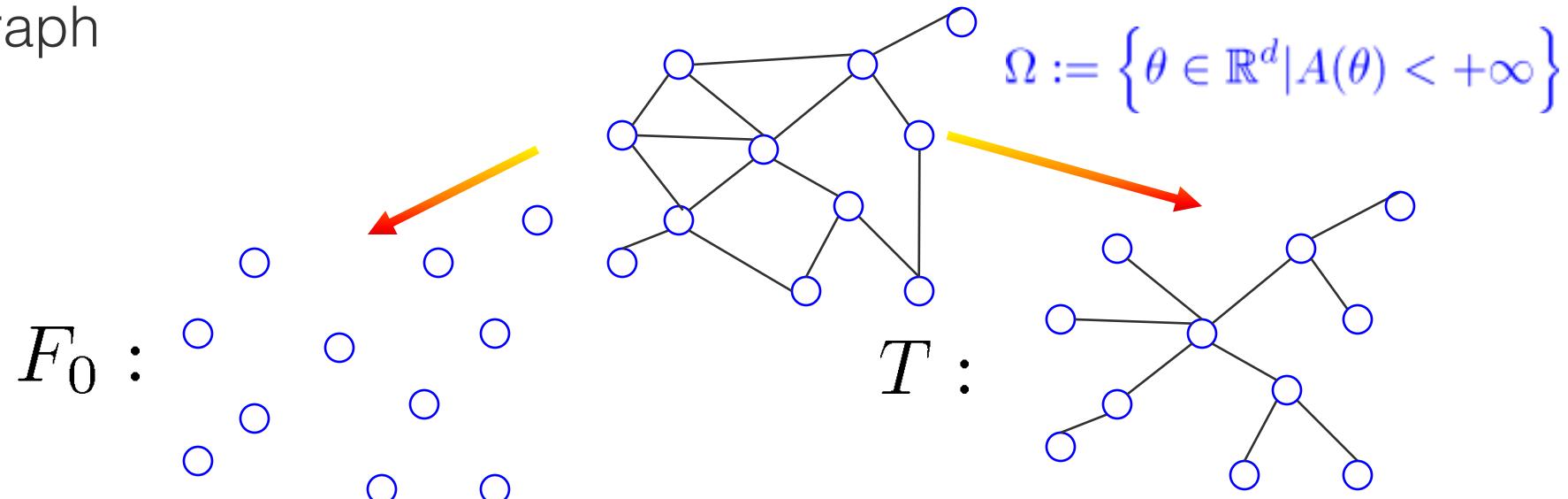


Tractable Subgraphs

- For an exponential family with sufficient statistics ϕ defined on graph G , the set of realizable mean parameter set

$$\mathcal{M}(G; \phi) := \{\mu \in \mathbb{R}^d \mid \exists p \text{ s.t. } \mathbb{E}_p[\phi(X)] = \mu\}$$

- Idea: restrict p to a subset of distributions associated with a **tractable** subgraph





Mean Field Methods

- For a given tractable subgraph F , a **subset** of canonical parameters is

$$\mathcal{M}(F; \phi) := \{\tau \in \mathbb{R}^d \mid \tau = \mathbb{E}_\theta[\phi(X)] \text{ for some } \theta \in \Omega(F)\}$$

- Inner approximation

$$\mathcal{M}(F; \phi)^o \subseteq \mathcal{M}(G; \phi)^o$$

- Mean field solves the relaxed problem

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

$A_F^* = A^*|_{\mathcal{M}_F(G)}$ is the **exact** dual function restricted to $\mathcal{M}_F(G)$





Example: Naïve Mean Field for Ising Model

- Ising model in $\{0,1\}$ representation

$$p(x) \propto \exp \left\{ \sum_{s \in V} x_s \theta_s + \sum_{(s,t) \in E} x_s x_t \theta_{st} \right\}$$

- Mean parameters

$$\mu_s = \mathbb{E}_p[X_s] = \mathbb{P}[X_s = 1] \quad \text{for all } s \in V, \text{ and}$$

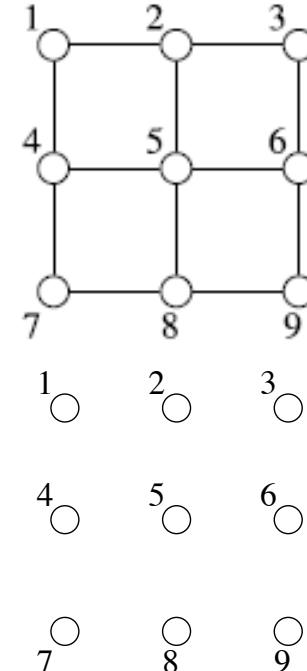
$$\mu_{st} = \mathbb{E}_p[X_s X_t] = \mathbb{P}[(X_s, X_t) = (1, 1)] \quad \text{for all } (s, t) \in E.$$

- For fully disconnected graph F ,

$$\mathcal{M}_F(G) := \{\tau \in \mathbb{R}^{|V|+|E|} \mid 0 \leq \tau_s \leq 1, \forall s \in V, \tau_{st} = \tau_s \tau_t, \forall (s, t) \in E\}$$

- The dual decomposes into sum, one for each node

$$A_F^*(\tau) = \sum_{s \in V} [\tau_s \log \tau_s + (1 - \tau_s) \log(1 - \tau_s)]$$





Example: Naïve Mean Field for Ising Model

- Mean field problem

$$A(\theta) \geq \max_{(\tau_1, \dots, \tau_m) \in [0,1]^m} \left\{ \sum_{s \in V} \theta_s \tau_s + \sum_{(s,t) \in E} \theta_{st} \tau_s \tau_t - A_F^*(\tau) \right\}$$

- The same objective function as in free energy based approach
- The naïve mean field update equations

$$\tau_s \leftarrow \sigma \left(\theta_s + \sum_{t \in N(s)} \theta_s \tau_t \right)$$

- Also yields lower bound on log partition function



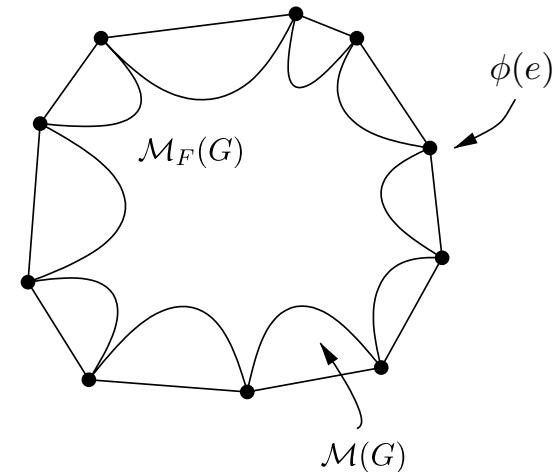


Geometry of Mean Field

- Mean field optimization is always **non-convex** for any exponential family in which the state space \mathcal{X}^m is finite
- Recall the marginal polytope is a convex hull
$$\mathcal{M}(G) = \text{conv}\{\phi(e); e \in \mathcal{X}^m\}$$
- $\mathcal{M}_F(G)$ contains all the extreme points
 - If it is a **strict** subset, then it must be non-convex
- Example: two-node Ising model

$$\mathcal{M}_F(G) = \{0 \leq \tau_1 \leq 1, 0 \leq \tau_2 \leq 1, \tau_{12} = \tau_1 \tau_2\}$$

- It has a parabolic cross section along $\tau_1 = \tau_2$, hence non-convex





Bethe Approximation and Sum-Product





Sum-Product/Belief Propagation Algorithm

- Message passing rule:

$$M_{ts}(x_s) \leftarrow \kappa \sum_{x'_t} \left\{ \psi_{st}(x_s, x'_t) \psi_t(x'_t) \prod_{u \in N(t)/s} M_{ut}(x'_t) \right\}$$

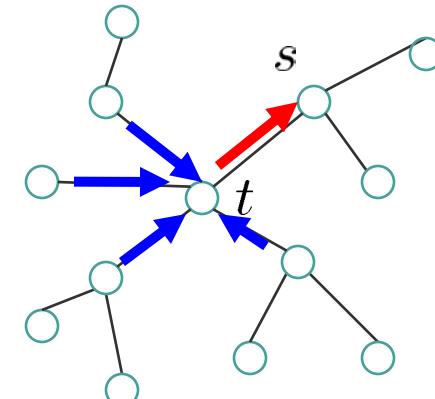
- Marginals:

$$\mu_s(x_s) = \kappa \psi_s(x_s) \prod_{t \in N(s)} M_{ts}^*(x_s)$$

- Exact for trees, but approximate for loopy graphs (so called loopy belief propagation)

- Question:

- How is the algorithm on trees related to variational principle?
- What is the algorithm doing for graphs with cycles?





Tree Graphical Models

- Discrete variables $X_s \in \{0, 1, \dots, m_s - 1\}$ on a tree $T = (V, E)$
- Sufficient statistics:
 $\mathbb{I}_j(x_s) \quad \text{for } s = 1, \dots, n, \quad j \in \mathcal{X}_s$
 $\mathbb{I}_{jk}(x_s, x_t) \quad \text{for } (s, t) \in E, \quad (j, k) \in \mathcal{X}_s \times \mathcal{X}_t$
- Exponential representation of distribution:

$$p(\mathbf{x}; \theta) \propto \exp \left\{ \sum_{s \in V} \theta_s(x_s) + \sum_{(s, t) \in E} \theta_{st}(x_s, x_t) \right\}$$

where

$$\theta_s(x_s) := \sum_{j \in \mathcal{X}_s} \theta_{s;j} \mathbb{I}_j(x_s) \quad (\text{and similarly for } \theta_{st}(x_s, x_t))$$

- Mean parameters are marginal probabilities:

$$\mu_{s;j} = \mathbb{E}_p[\mathbb{I}_j(X_s)] = \mathbb{P}[X_s = j] \quad \forall j \in \mathcal{X}_s, \quad \mu_s(x_s) = \sum_{j \in \mathcal{X}_s} \mu_{s;j} \mathbb{I}_j(x_s) = \mathbb{P}(X_s = x_s)$$

$$\mu_{st;jk} = \mathbb{E}_p[\mathbb{I}_{st;jk}(X_s, X_t)] = \mathbb{P}[X_s = j, X_t = k] \quad \forall (j, k) \in \mathcal{X}_s \times \mathcal{X}_t.$$

$$\mu_{st}(x_s, x_t) = \sum_{(j, k) \in \mathcal{X}_s \times \mathcal{X}_t} \mu_{st;jk} \mathbb{I}_{jk}(x_s, x_t) = \mathbb{P}(X_s = x_s, X_t = x_t)$$





Marginal Polytope for Trees

- Recall marginal polytope for general graphs

$$\mathcal{M}(G) = \{\mu \in \mathbb{R}^d \mid \exists p \text{ with marginals } \mu_{s;j}, \mu_{st;jk}\}$$

- By junction tree theorem (see Prop. 2.1 & Prop. 4.1)

$$\mathcal{M}(T) = \left\{ \mu \geq 0 \mid \sum_{x_s} \mu_s(x_s) = 1, \sum_{x_t} \mu_{st}(x_s, x_t) = \mu_s(x_s) \right\}$$

- In particular, if $\mu \in \mathcal{M}(T)$ then

has the corresponding marginals $p_\mu(x) := \prod_{s \in V} \mu_s(x_s) \prod_{(s,t) \in E} \frac{\mu_{st}(x_s, x_t)}{\mu_s(x_s) \mu_t(x_t)}$.





Decomposition of Entropy for Trees

- For trees, the entropy decomposes as

$$\begin{aligned} H(p(x; \mu)) &= - \sum_x p(x; \mu) \log p(x; \mu) \\ &= \sum_{s \in V} \left(\underbrace{- \sum_{x_s} \mu_s(x_s) \log \mu_s(x_s)}_{H_s(\mu_s)} \right) - \\ &\quad - \sum_{(s,t) \in E} \left(\underbrace{\sum_{x_s, x_t} \mu_{st}(x_s, x_t) \log \frac{\mu_{st}(x_s, x_t)}{\mu_s(x_s) \mu_t(x_t)}}_{I_{st}(\mu_{st}), \text{KL-Divergence}} \right) \\ &= \sum_{s \in V} H_s(\mu_s) - \sum_{(s,t) \in E} I_{st}(\mu_{st}) \end{aligned}$$

- The dual function has an explicit form $A^*(\mu) = -H(p(x; \mu))$





Exact Variational Principle for Trees

- Variational formulation

$$A(\theta) = \max_{\mu \in \mathcal{M}(T)} \left\{ \langle \theta, \mu \rangle + \sum_{s \in V} H_s(\mu_s) - \sum_{(s,t) \in E} I_{st}(\mu_{st}) \right\}$$

- Assign Lagrange multiplier λ_{ss} for the normalization constraint $C_{ss}(\mu) := 1 - \sum_{x_s} \mu_s(x_s) = 0$; and $\lambda_{ts}(x_s)$ for each marginalization constraint

$$C_{ts}(x_s; \mu) := \mu_s(x_s) - \sum_{x_t} \mu_{st}(x_s, x_t) = 0$$

- The Lagrangian has the form

$$\begin{aligned} \mathcal{L}(\mu, \lambda) &= \langle \theta, \mu \rangle + \sum_{s \in V} H_s(\mu_s) - \sum_{(s,t) \in E} I_{st}(\mu_{st}) + \sum_{s \in V} \lambda_{ss} C_{ss}(\mu) \\ &\quad + \sum_{(s,t) \in E} \left[\sum_{x_t} \lambda_{st}(x_t) C_{st}(x_t) + \sum_{x_s} \lambda_{ts}(x_s) C_{ts}(x_s) \right] \end{aligned}$$





Lagrangian Derivation

- Taking the derivatives of the Lagrangian w.r.t. μ_s and μ_{st}

$$\begin{aligned}\frac{\partial \mathcal{L}}{\partial \mu_s(x_s)} &= \theta_s(x_s) - \log \mu_s(x_s) + \sum_{t \in \mathcal{N}(s)} \lambda_{ts}(x_s) + C \\ \frac{\partial \mathcal{L}}{\partial \mu_{st}(x_s, x_t)} &= \theta_{st}(x_s, x_t) - \log \frac{\mu_{st}(x_s, x_t)}{\mu_s(x_s) \mu_t(x_t)} - \lambda_{ts}(x_s) - \lambda_{st}(x_t) + C'\end{aligned}$$

- Setting them to zeros yields

$$\mu_s(x_s) \propto \exp\{\theta_s(x_s)\} \prod_{t \in \mathcal{N}(s)} \underbrace{\exp\{\lambda_{ts}(x_s)\}}_{M_{ts}(x_s)}$$

$$\begin{aligned}\mu_s(x_s, x_t) &\propto \exp\{\theta_s(x_s) + \theta_t(x_t) + \theta_{st}(x_s, x_t)\} \times \\ &\quad \prod_{u \in \mathcal{N}(s) \setminus t} \exp\{\lambda_{us}(x_s)\} \prod_{v \in \mathcal{N}(t) \setminus s} \exp\{\lambda_{vt}(x_t)\}\end{aligned}$$





Lagrangian Derivation (continued)

- Adjusting the Lagrange multipliers or messages to enforce

$$C_{ts}(x_s; \mu) := \mu_s(x_s) - \sum_{x_t} \mu_{st}(x_s, x_t) = 0$$

yields

$$M_{ts}(x_s) \leftarrow \sum_{x_t} \exp \{ \theta_t(x_t) + \theta_{st}(x_s, x_t) \} \prod_{u \in \mathcal{N}(t) \setminus s} M_{ut}(x_t)$$

- Conclusion: the message passing updates are a Lagrange method to solve the stationary condition of the variational formulation





BP on Arbitrary Graphs

- Two main difficulties of the variational formulation

$$A(\theta) = \sup_{\mu \in \mathcal{M}} \{\theta^T \mu - A^*(\mu)\}$$

- The marginal polytope \mathcal{M} is hard to characterize, so let's use the tree-based **outer** bound

$$\mathbb{L}(G) = \left\{ \tau \geq 0 \mid \sum_{x_s} \tau_s(x_s) = 1, \sum_{x_t} \tau_{st}(x_s, x_t) = \tau_s(x_s) \right\}$$

These locally consistent vectors τ are called **pseudo-marginals**.

- Exact entropy $-A^*(\mu)$ lacks explicit form, so let's approximate it by the exact expression for trees

$$-A^*(\tau) \approx H_{\text{Bethe}}(\tau) := \sum_{s \in V} H_s(\tau_s) - \sum_{(s,t) \in E} I_{st}(\tau_{st}).$$





Bethe Variational Problem (BVP)

- Combining these two ingredient leads to the Bethe variational problem (BVP):

$$\max_{\tau \in \mathbb{L}(G)} \left\{ \langle \theta, \tau \rangle + \sum_{s \in V} H_s(\tau_s) - \sum_{(s,t) \in E} I_{st}(\tau_{st}) \right\}.$$

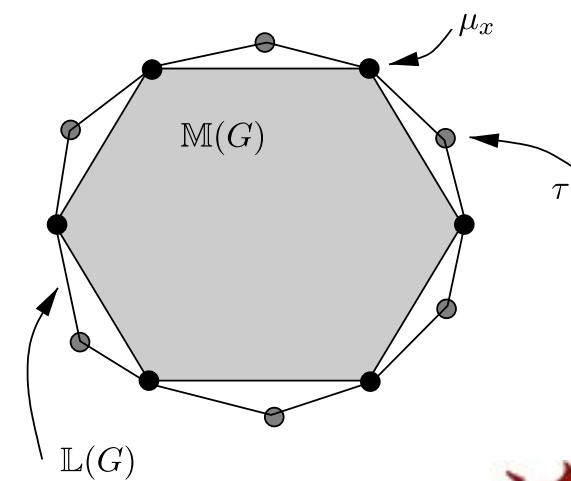
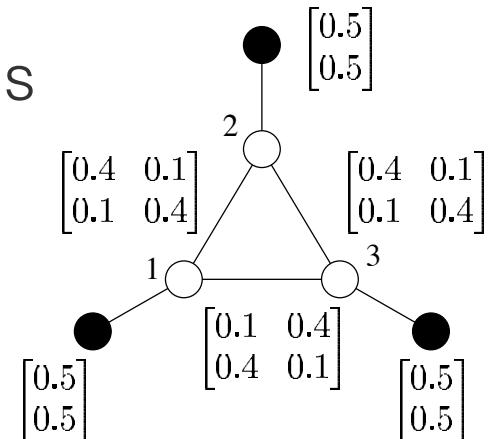
- A simple structured problem (**differentiable & constraint set is a simple convex polytope**)
- Loopy BP can be derived as am iterative method for solving a Lagrangian formulation of the BVP (Theorem 4.2); similar proof as for tree graphs
- A set of pseudo-marginals given by Loopy BP fixed point in **any** graph if and only if they are local stationary points of BVP





Geometry of BP

- Consider the following assignment of pseudo-marginals
 - Can easily verify $\tau \in \mathbb{L}(G)$
 - However, $\tau \notin \mathcal{M}(G)$ (need a bit more work)
- Tree-based outer bound
 - For any graph, $\mathcal{M}(G) \subseteq \mathbb{L}(G)$
 - Equality holds if and only if the graph is a tree
- Question: does solution to the BVP ever fall into the gap?
 - Yes, for any element of outer bound $\mathbb{L}(G)$, it is possible to construct a distribution with it as a BP fixed point (Wainwright et. al. 2003)



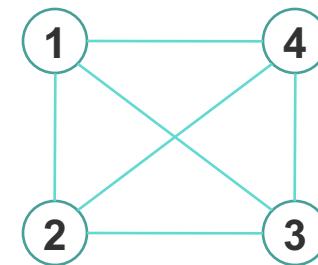


Inexactness of Bethe Entropy Approximation

- Consider a fully connected graph with

$$\mu_s(x_s) = [0.5 \quad 0.5] \quad \text{for } s = 1, 2, 3, 4$$

$$\mu_{st}(x_s, x_t) = \begin{bmatrix} 0.5 & 0 \\ 0 & 0.5 \end{bmatrix} \quad \forall (s, t) \in E.$$



- It is **globally** valid: $\tau \in \mathcal{M}(G)$ realized by the distribution that places mass 1/2 on each of configuration (0,0,0,0) and (1,1,1,1)
- $H_{\text{Bethe}}(\mu) = 4\log 2 - 6\log 2 = -2\log 2 < 0,$
- $-A^*(\mu) = \log 2 > 0.$





Remark

- ❑ This connection provides a **principled basis** for applying the sum-product algorithm for loopy graphs
- ❑ However,
 - ❑ Although there is always **a fixed point of loopy BP**, there is **no guarantees** on the convergence of the algorithm on loopy graphs
 - ❑ The Bethe variational problem is usually **non-convex**. Therefore, there are **no guarantees** on the **global optimum**
 - ❑ Generally, **no guarantees** that $A_{\text{Bethe}}(\theta)$ is a lower bound of $A(\theta)$
- ❑ Nevertheless,
 - ❑ The connection and understanding suggest a number of **avenues for improving upon the ordinary sum-product algorithm**, via progressively better approximations to the entropy function and outer bounds on the marginal polytope (Kikuchi clustering)





Summary

- ❑ Variational methods in general turn inference into an optimization problem via **exponential families** and **convex duality**
- ❑ The exact variational principle is intractable to solve; there are two distinct components for approximations:
 - ❑ Either **inner** or **outer** bound to the marginal polytope
 - ❑ Various approximation to the entropy function
- ❑ Mean field: **non-convex inner bound** and **exact form of entropy**
- ❑ BP: **polyhedral outer bound** and **non-convex Bethe approximation**
- ❑ Kikuchi and variants: tighter polyhedral outer bounds and better entropy approximations (Yedidia et. al. 2002)

