School of Computer Science
Carnegie Mellon

Probabilistic Graphical Models

Theory of Variational Inference: Inner and Outer Approximation

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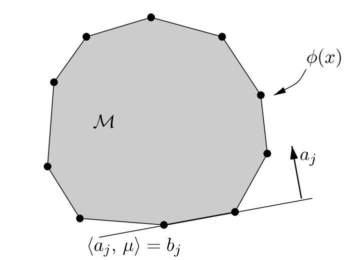


Reading: W & J Book Chapters

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

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

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:

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

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:

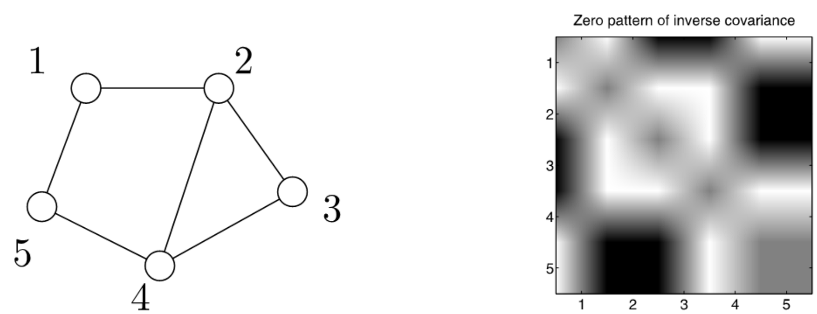
$$p(\mathbf{x};\theta) = \exp\left\{ \sum_{C \in \mathcal{C}} \log \psi(\mathbf{x}_C;\theta_C) - \log Z(\theta) \right\}$$

  - $\log \psi(\mathbf{x}_C;\theta_C)$ 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 also respects the graph structure

$$\Lambda = \Sigma^{-1}$$



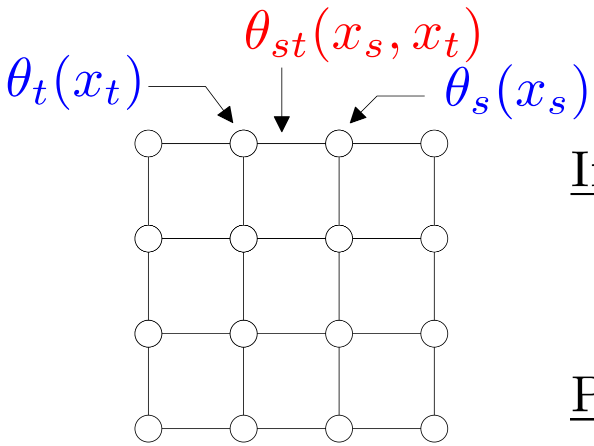
(a) (b)

- Gaussian MRF in the exponential form

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

  - 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

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

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

- 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

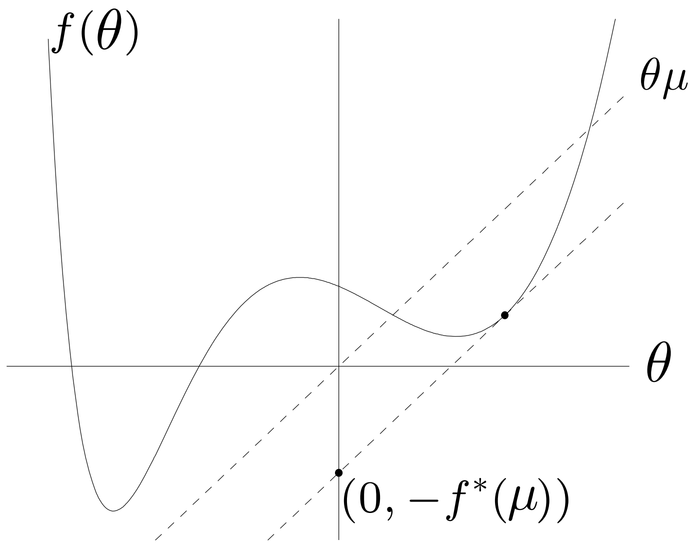
$$\mu(\theta) = \mathbb{E}_{\theta}[X] = 1 \cdot p(X=1;\theta) + 0 \cdot p(X=0;\theta) = \frac{e^{\theta}}{1+e^{\theta}}$$

- 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 $\mu = \dfrac{e^\theta}{1 + e^\theta} \quad (\mu = \nabla A(\theta))$
- If $\mu \in (0,1),\ \theta(\mu) = \log\left(\dfrac{\mu}{1-\mu}\right),\ A^*(\mu) = \mu \log(\mu) + (1-\mu)\log(1-\mu)$
- 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 $\mu(\theta) = \dfrac{e^\theta}{1 + e^\theta}$. This is the mean!

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

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

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

- 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 $\theta(\mu)$

Complexity of Computing Conjugate Dual

- The dual function is implicitly defined:

$$\mu \longrightarrow \boxed{(\nabla A)^{-1}} \xrightarrow{\theta(\mu)} \boxed{-H(p_{\theta(\mu)})} \longrightarrow A^*(\mu)$$

  - 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

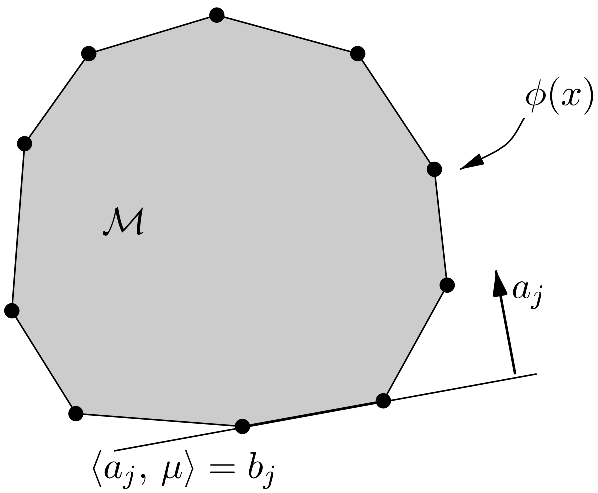
Convex Polytope

- Convex hull representation

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

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

$$\mathcal{M} = \left\{ \mu \in \mathbb{R}^d \,|\, a_j^\top \mu \geq b_j, \ \forall j \in \mathcal{J} \right\},$$
where $|\mathcal{J}|$ is finite.



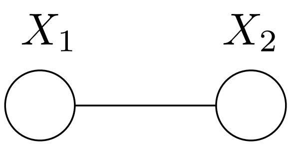
Example: Two-node Ising Model

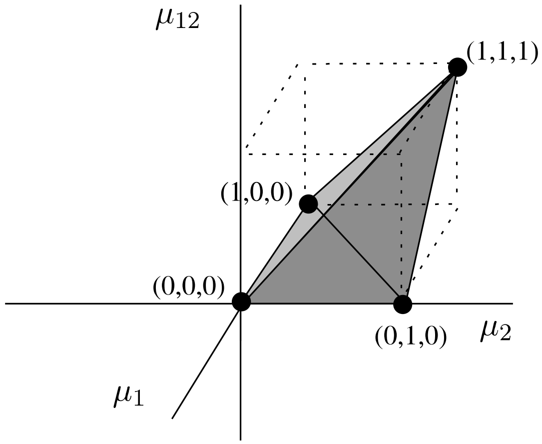
- Sufficient statistics: $$\phi(x) := (x_1, x_2, x_1 x_2)$$
- Mean parameters: $$\mu_1 = \mathbb{P}(X_1 = 1), \mu_2 = \mathbb{P}(X_2 = 1)$$ $$\mu_{12} = \mathbb{P}(X_1 = 1, X_2 = 1)$$
- Two-node Ising model
  - Convex hull representation

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

  - Half-plane representation

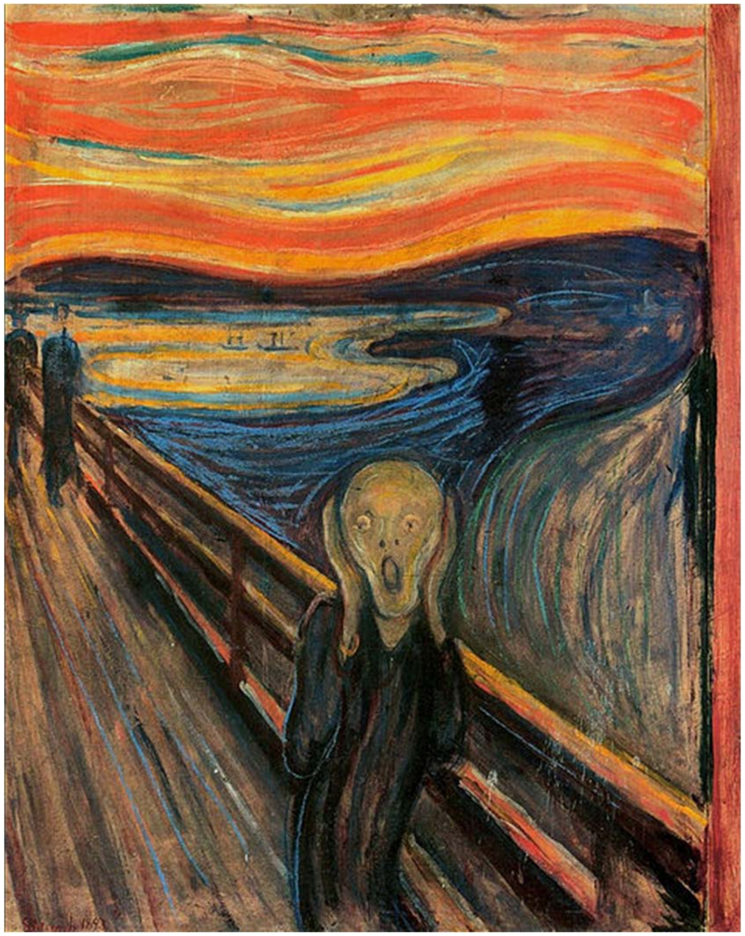
$$\begin{aligned} \mu_1 &\geq \mu_{12} \\ \mu_2 &\geq \mu_{12} \\ \mu_{12} &\geq 0 \\ 1 + \mu_{12} &\geq \mu_1 + \mu_2 \end{aligned}$$





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

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

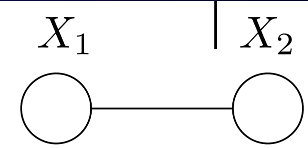
  - $\theta(\mu)$ satisfies $\mu = \mathbb{E}_{\theta(u)}[\phi(X)]$
- The log partition function has the variational form

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

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

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

Example: Two-node Ising Model



- The distribution $p(x;\theta) \propto \exp\{\theta_1 x_1 + \theta_2 x_2 + \theta_{12} x_{12}\}$
  - Sufficient statistics $\phi(x) = \{x_1, x_2, x_1 x_2\}$
- The marginal polytope is characterized by

$$\begin{aligned} \mu_1 &\geq \mu_{12} \\ \mu_2 &\geq \mu_{12} \\ \mu_{12} &\geq 0 \\ 1+\mu_{12} &\geq \mu_1 + \mu_2 \end{aligned}$$

- The dual has an explicit form

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

- The variational problem $A(\theta) = \max_{\{\mu_1,\mu_2,\mu_{12}\}\in\mathcal{M}} \{\theta_1\mu_1 + \theta_2\mu_2 + \theta_{12}\mu_{12} - A^*(\mu)\}$
- 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

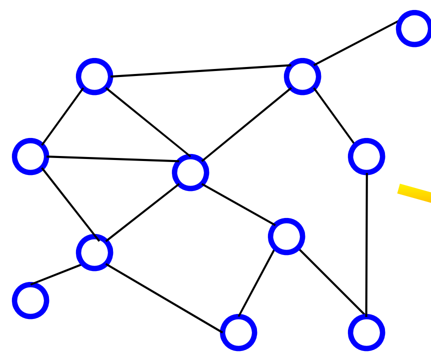
Mean Field Approximation

Tractable Subgraphs

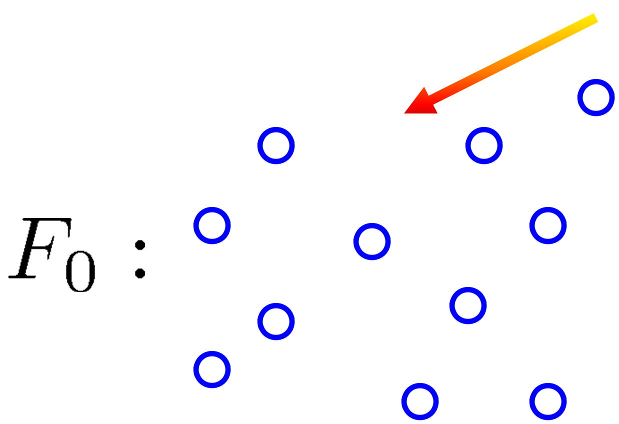
- For an exponential family with sufficient statistics ϕ defined on graph G, the set of realizable mean parameter set

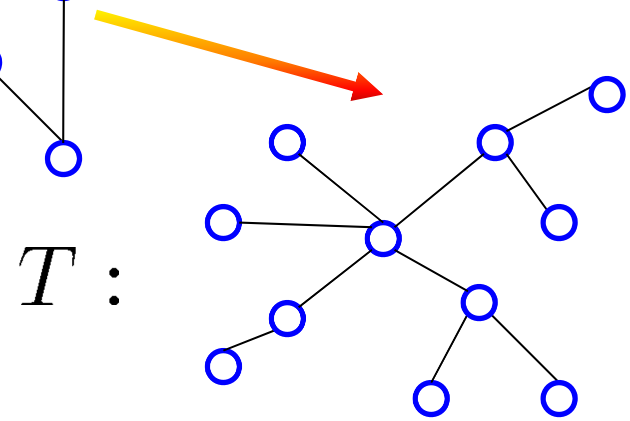
$$\mathcal{M}(G;\phi) := \{\mu \in \mathbb{R}^d \mid \exists p \text{ s.t. } \mathbb{E}_p[\phi(X)] = \mu\}$$

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



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





$$\Omega(F_0) := \left\{\theta \in \Omega \mid \theta_{(s,t)} = 0 \;\forall\, (s,t) \in E\right\}. \quad \Omega(T) := \left\{\theta \in \Omega \mid \theta_{(s,t)} = 0 \;\; \forall\, (s,t) \notin E(T)\right\}.$$

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

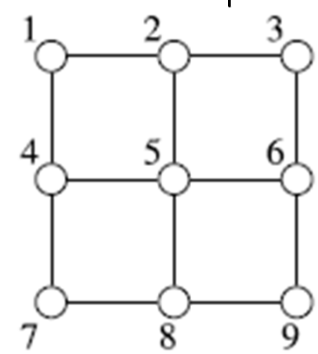
$$\mathcal{M}(F;\phi)^o \subseteq \mathcal{M}(G;\phi)^o$$

- Mean field solves the relaxed problem

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

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

Example: Naïve Mean Field for Ising Model



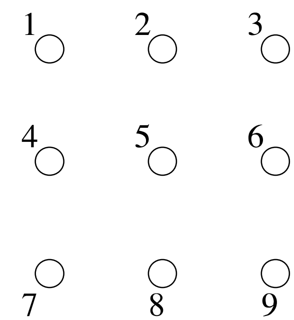
- Ising model in {0,1} representation

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

- Mean parameters

$\mu_s = E_p[X_s] = P[X_s = 1]$ for all s □ V, and

$\mu_{st} = E_p[X_s X_t] = P[(X_s, X_t) = (1,1)]$ for all (s,t) □ 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

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

- The same objective function as in free energy based approach

- The naïve mean field update equations

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

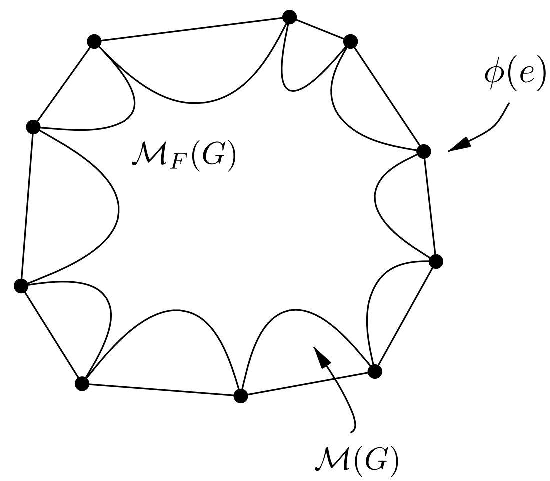
- Also yields lower bound on log partition function

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

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

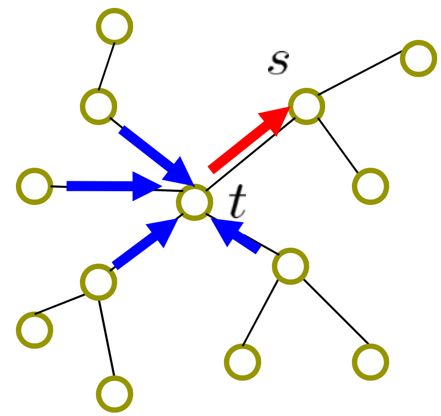
  - It has a parabolic cross section along $\tau_1 = \tau_2$, hence non-convex

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

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

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

- Mean parameters are marginal probabilities:

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

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

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

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

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

has the corresponding marginals

Decomposition of Entropy for Trees

- For trees, the entropy decomposes as

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

- 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

$$\mathcal{L}(\mu, \lambda) = \langle \theta, \mu \rangle + \sum_{s \in V} H_s(\mu_s) - \sum_{(s,t) \in E} I_{st}(\mu_{st}) + \sum_{s \in V} \lambda_{ss} C_{ss}(\mu)$$

$$+ \sum_{(s,t) \in E} \Big[\sum_{x_t} \lambda_{st}(x_t) C_{st}(x_t) + \sum_{x_s} \lambda_{ts}(x_s) C_{ts}(x_s) \Big]$$

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

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

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

Lagrangian Derivation (continued)

- Adjusting the Lagrange multipliers or messages to enforce

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

  yields

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

- 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)

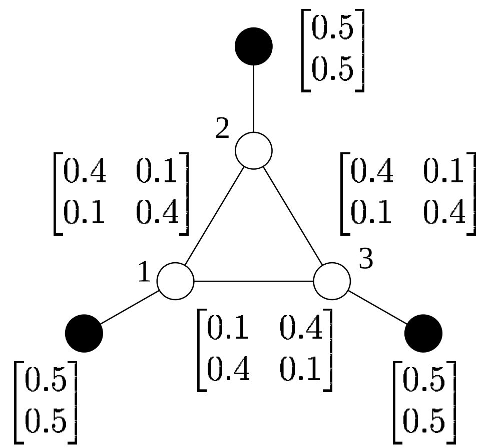
- Combining these two ingredient leads to the Bethe variational problem (BVP):

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

  - 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

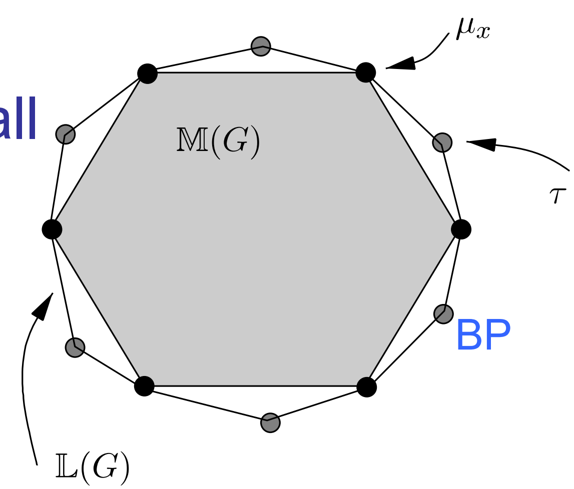
Geometry of BP

- 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 fixed point (Wainwright et. al. 2003)

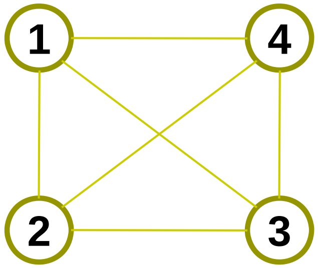


Inexactness of Bethe Entropy Approximation

- Consider a fully connected graph with

$$\mu_s(x_s) = \begin{bmatrix} 0.5 & 0.5 \end{bmatrix} \quad \text{for } s = 1, 2, 3, 4$$

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



- 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)