School of Computer Science
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Probabilistic Graphical Models

Variational Inference III:
Variational Principle I

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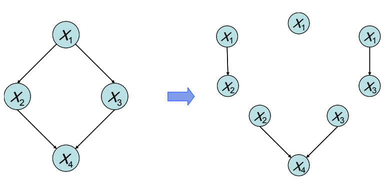
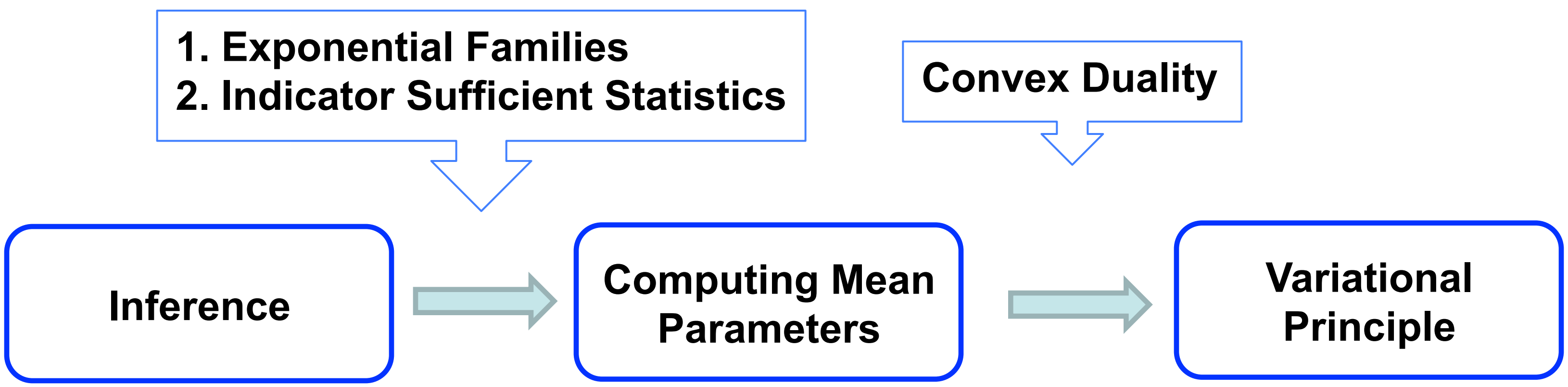


Reading:

What have we learned so far

- Free energy based approaches
  - Direct approximation of Gibbs free energy: Bethe free energy and loop BP
  - Restricting the family of approximation distribution: mean field method

- Convex duality based approaches



Computing Mean Parameter: Bernoulli

- A single Bernoulli random variable

X θ

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

- Inference = Computing the mean parameter

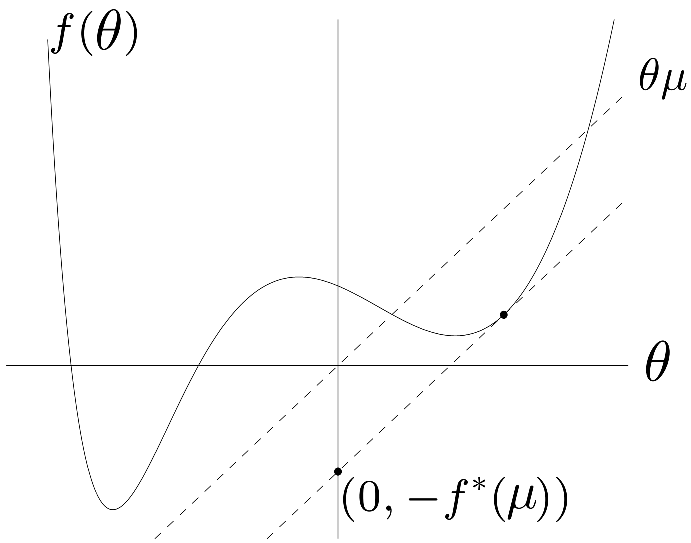
$$\mu(\theta) = \mathbb{E}_{\theta}[X] = p(X=1;\theta) = \frac{e^{\theta}}{1+e^{\theta}}$$

- 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: pointwise 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 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!

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

- Next step: develop this framework for general exponential families/graphical models

Computation of Conjugate Dual

- Given an exponential family

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

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

Marginal Polytope

- For any distribution $p(x)$ and a set of sufficient statistics ,
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

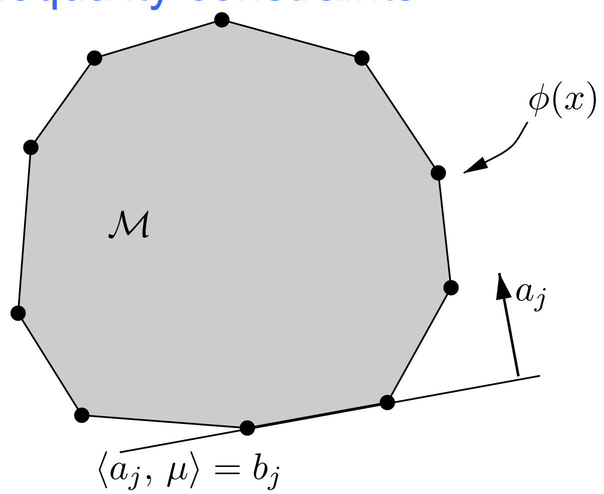
Convex Polytope

- Convex hull representation

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

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

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



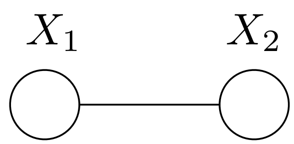
Example: Ising Model

- Sufficient statistics: $\phi(x) := \big(x_s, s \in V;\ x_s x_t,\ (s,t) \in E\big) \in \mathbb{R}^{|V|+|E|}$.
- Mean parameters:

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

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

- Two-node Ising model

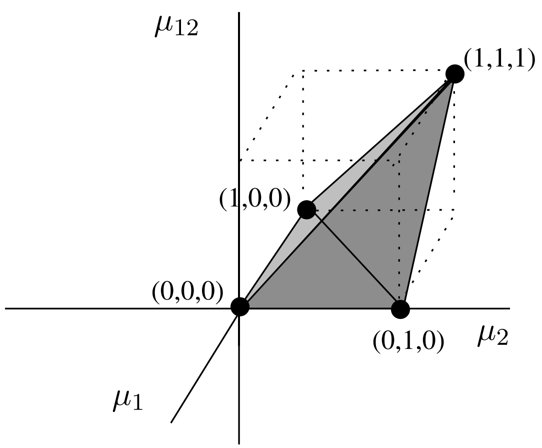


  - Convex hull representation

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

  - Half-plane representation

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



- Exercise: three-node Ising model

Example: Discrete MRF

- Sufficient statistics:
$$\begin{array}{lll} \mathbb{I}_j(x_s) & \text{for } s = 1, \ldots n, & j \in \mathcal{X}_s \\ \mathbb{I}_{jk}(x_s, x_t) & \text{for}(s,t) \in E, & (j,k) \in \mathcal{X}_s \times \mathcal{X}_t \end{array}$$

- Mean parameters are marginal probabilities:

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

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

- Marginal Polytope

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

- For tree graphical models, the number of half-planes (facet complexity) grows only *linearly* in the graph size

- For general graphs, it is extremely difficult 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 $\mu = \mathbb{E}_{\theta(u)}[\phi(X)]$

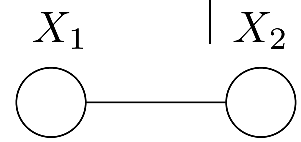
- The log partition function has the variational form

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

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

- The marginal polytope is characterized by

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

- 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

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

Challenges

- In general graphical models, the marginal polytope can be very difficult to characterize explicitly

- The dual function is implicitly defined:

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

  - Inverse mapping is nontrivial
  - Evaluating the entropy requires high-dimensional integration (summation)

Variational Inference

- Variational formulation

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

- General idea of variational inference for graphical models:
  - Approximate the function to be optimized, i.e., the entropy term (Bethe-Kikuchi, sum-product)
  - Restrict the set over which the optimization takes place to a subset, i.e., the marginal polytope (mean field methods)