CS281A/Stat241A Lecture 23

Variational Methods

Peter Bartlett
Key ideas of this lecture

- Variational versus sampling methods
- Examples of algorithms:
  - Loopy belief propagation
  - Mean field algorithm
- Graphical model exponential families
  - Examples: Ising model; Gaussian MRF.
  - Mean parameters, marginal polytope.
  - Mean ↔ natural parameters
  - Conjugate duality
  - Variational representation
- Mean field algorithm
Inference

Consider a graphical model (say undirected):

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

The inference problem:

Given observations \( x_E \)

of variables in an evidence set, \( E \subset V \),

and a set of variables \( F \subset V \),

\[ \text{find } p(x_F|x_E = \bar{x}_E). \]
Maximizing \textit{a posteriori} Probability

Consider a graphical model (say undirected):

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

- Maximize \textit{a posteriori} probability:

  Given observations \( x_E \) of variables in an evidence set, \( E \subset V \),

  \[ \ldots \text{find } \arg \max_x p(x|x_E = \bar{x}_E). \]
Variational Methods

- Represent quantity of interest as solution to (or value of) an optimization problem.
- Then approximate the optimization problem:
  - Approximate the constraint set.
  - Approximate the criterion.
Sampling versus Variational Methods

Sampling Methods:
- Are asymptotically exact.
- But mixing can be slow.

Variational Methods:
- Are deterministic, and typically fast.
- But are approximations, and the approximation might be poor.
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Examples: Loopy Belief Propagation

Recall Belief Propagation for trees:

1. Incorporate the evidence through an evidence potential:

   \[ \psi^E(x_i) = \begin{cases} 
   \delta(x_i, \bar{x}_i) & \text{if } i \in E, \\
   1 & \text{otherwise}. 
   \end{cases} \]

2. Pass messages (potentials) along the edge from \( j \) to \( i \) of the form

   \[ m_{j,i}(x_i) = \sum_{x_j} \left( \psi^E(x_j) \psi(x_i, x_j) \prod_{k \in N(j) \setminus \{i\}} m_{k,j}(x_j) \right), \]

   where \( N(j) = \{k : \{k, j\} \in E\} \).
Examples: Loopy Belief Propagation

3. Pass messages (potentials) along the edge from \( j \) to \( i \) of the form

\[
m_{j,i}(x_i) = \sum_{x_j} \left( \psi^E(x_j) \psi(x_i, x_j) \prod_{k \in N(j) \setminus \{i\}} m_{k,j}(x_j) \right),
\]

where \( N(j) = \{k : \{k, j\} \in \mathcal{E}\} \). This corresponds to the potential obtained from eliminating the subtree rooted at \( j \) and away from \( i \).

4. Follow the protocol:
Node \( j \) sends message \( m_{j,i} \) to node \( i \) iff it has received all messages \( m_{k,j} \) for \( k \in N(j) \setminus \{i\} \).
Examples: Loopy Belief Propagation

5. Calculate

\[ p(x_i | \bar{x}_E) = \frac{1}{Z} \psi^E(x_i) \prod_{k \in N(i)} m_{k,i}(x_i). \]
Examples: Loopy Belief Propagation

Instead of the protocol:

Node $j$ sends message $m_{j,i}$ to node $i$ iff it has received all messages $m_{k,j}$ for $k \in N(j) \setminus \{i\}$

Consider:

1. $m_{j,i}^{(0)}(x_i) = 1$ for all $\{i, j\} \in E$.

2. At iteration $t = 1, 2, \ldots$,

$$m_{j,i}^{(t)}(x_i) = \sum_{x_j} \left( \psi^E(x_j) \psi(x_i, x_j) \prod_{k \in N(j) \setminus \{i\}} m_{k,j}^{(t-1)}(x_j) \right).$$
Examples: Loopy Belief Propagation

Node $j$ sends message $m_{j,i}$ to node $i$ iff it has received all messages $m_{k,j}$ for $k \in N(j) \setminus \{i\}$

$$m_{j,i}^{(t)}(x_i) = \sum_{x_j} \left( \psi^E(x_j) \psi(x_i, x_j) \prod_{k \in N(j) \setminus \{i\}} m_{k,j}^{(t-1)}(x_j) \right).$$

These protocols are equivalent for trees:

- By induction (working inwards from the leaves), we can see that, for $t$ at least as large as the depth of the subtree rooted at $j$ and away from $i$,

$$m_{j,i}^{(t)}(x_i) = m_{j,i}(x_i).$$
Examples: Loopy Belief Propagation

1. $m_{j,i}^{(0)}(x_i) = 1$ for all $\{i, j\} \in \mathcal{E}$.

2. At iteration $t = 1, 2, \ldots$,

$$m_{j,i}^{(t)}(x_i) = \sum_{x_j} \left( \psi^E(x_j) \psi(x_i, x_j) \prod_{k \in N(j) \setminus \{i\}} m_{k,j}^{(t-1)}(x_j) \right).$$

- This protocol makes sense for arbitrary graphs: pretend that the graph is a tree.
- If there are a few long cycles, we might expect this to work well.
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Examples: Mean Field Algorithm

Consider a discrete undirected model (Markov random field):

\[ x_u \in \mathcal{X}_u \quad |\mathcal{X}_u| < \infty, \]

\[
\ln \psi_{u,v}(x_u, x_v) = \sum_{i,j} \theta_{u,i;v,j} \mathbf{1}[x_u = i] \mathbf{1}[x_v = j]
\]

\[ = \theta_{u;v}(x_u, x_v), \]

\[
\ln \psi_v(x_v) = \sum_i \theta_{v,i} \mathbf{1}[x_v = i]
\]

\[ = \theta_v(x_v). \]

\[
p(x) \propto \exp \left( \sum_{v \in V} \theta_v(x_v) + \sum_{\{u,v\} \in E} \theta_{u,v}(x_u, x_v) \right). \]
Examples: Mean Field Algorithm

Consider Gibbs sampling in the Ising model, a discrete MRF with $x_v \in \{0, 1\}$:

$$X_v^{(t+1)} = \begin{cases} 1 & \text{if } U \leq 1 / \left( 1 + \exp \left( -\theta_v - \sum_{u \in N(v)} \theta_{v,u} X_u^{(t)} \right) \right), \\ 0 & \text{otherwise,} \end{cases}$$

where $U$ is chosen uniformly from $[0, 1]$. 
Examples: Mean Field Algorithm

- Suppose that \( \sum_{u \in N(v)} \theta_{v,u} X_u^{(t)} \) is close to its expectation.

- For example, if the set \( N(v) \) is large, this is true with high probability.

- Then we could replace the random \( X_v^{(t)} \) values with their expectations, \( \mu_v \), to obtain

\[
\mu_v := \frac{1}{1 + \exp \left( -\theta_v - \sum_{u \in N(v)} \theta_{v,u} \mu_u \right)}.
\]

- This is called the naive mean field algorithm for the Ising model.

- It can also be viewed as message passing.
Issues to Consider

For message passing algorithms like loopy belief propagation or the mean field algorithm,

- Do these message passing updates have a fixed point?
- Is it (close to) the desired conditional probability?
- Do the updates converge to the fixed point?

We’ll see that these algorithms can be viewed as methods for solving approximate versions of variational formulations of the inference problem.
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Example: Ising Model \((x_v \in \{0, 1\})\).

\[
p(x) = \exp \left( \sum_{v \in V} \theta_v x_v + \sum_{\{u,v\} \in E} \theta_{u,v} x_u x_v - A(\theta) \right).
\]

for \(\theta \in \Omega = \{\theta : A(\theta) < \infty\} = \mathbb{R}^{\vert V \vert + \vert E \vert} .

- Regular (\(\Omega\) is open.)
- Minimal (no \(p\)-invariant subspace of \(\Omega\).)
Generalization of Ising: pairwise MRF

\( (x_v \in \{0, 1, \ldots, r - 1\}) \).

\[
p(x) = \exp \left( \sum_{v \in V} \sum_i \theta_{v,i} 1[x_v = i] + \sum_{\{u,v\} \in E} \sum_{i,j} \theta_{u,i;v,j} 1[x_u = i] 1[x_v = j] - A(\theta) \right),
\]

for \( \theta \in \Omega = \{ \theta : A(\theta) < \infty \} = \mathbb{R}^{|V|+r^2|E|} \).

- Regular (\( \Omega \) is open.)
- Non-minimal or overcomplete.
Special case: Hidden Markov model with $y$ observed.

- $\theta_{t,i}$ corresponds to $\log p(y_t | x_t = i)$.
- $\theta_{t,i; t+1, j}$ corresponds to $\log p(x_{t+1} = j | x_t = i)$.

Another generalization: Higher order interactions, that is, $k$-cliques, with $k > 2$. 
Example: Gaussian Markov random field.

For an undirected graph \((V, E)\), define the sufficient statistics \(x_v, x_v^2, x_u x_v\) for \(v \in V\) and \({u, v}\) \(\in E\).

\[
p(x) = \exp \left( \langle \theta, x \rangle + \frac{1}{2} \langle \Theta, xx' \rangle - A(\theta, \Theta) \right),
\]

where the second inner product is

\[
\langle \Theta, xx' \rangle = \text{tr}(\Theta xx').
\]
Example: Gaussian Markov random field.

Here, the natural parameters are a vector $\theta \in \mathbb{R}^{|V|}$ and a symmetric positive definite matrix $\Theta \in \mathbb{R}^{|V| \times |V|}$, with $\Theta_{u,v} = 0$ if $\{u, v\} \not\in E$.

The natural parameters corresponding to $x^2_v$ and $x_u x_v$ correspond to the non-zero entries of the precision matrix $\Theta$.

In this case, the parameters are restricted to

$$
\Omega = \{(\theta, \Theta) : A(\theta, \Theta) < \infty\} = \{(\theta, \Theta) : \Theta < 0\},
$$

where the $\Theta$ are symmetric matrices with zero entries where edges are missing.
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Mean Parameters

Fix a density \( p \) defined with respect to a reference distribution \( h \).
For a sufficient statistic \( \phi_\alpha \), define the mean parameter \( \mu_\alpha \) as

\[
\mu_\alpha = \mathbb{E}_p[\phi_\alpha(X)] = \int \phi_\alpha(x) p(x) h(dx).
\]

For \( d \) sufficient statistics, we can define the \( d \)-vector of mean parameters, \( \mu = (\mu_1, \ldots, \mu_d) \).
Define the set \( M \) of realizable mean parameters as

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

if \( \mathcal{X} \) is finite:

\[
\overset{\text{co}}{=} \{ \phi(x) : x \in \mathcal{X} \},
\]

where \( \text{co} \) represents the convex hull.
Mean Parameters: Ising Model

\[ p(x) = \exp \left( \sum_{v \in V} \theta_v x_v + \sum_{\{u,v\} \in E} \theta_{u,v} x_u x_v - A(\theta) \right). \]

The vector of sufficient statistics is

\[ \phi(x) = (x_v : v \in V, x_u x_v : \{u,v\} \in E). \]

and the mean parameters are

\[ \mu_v = \Pr(X_v = 1), \]
\[ \mu_{u,v} = \Pr(X_u = X_v = 1). \]
Mean Parameters: Ising Model

The vector of sufficient statistics is

$$\phi(x) = (x_v : v \in V, x_u x_v : \{u, v\} \in E).$$

Then $\mathcal{M}$ is the *marginal polytope*,

$$\mathcal{M} = \text{co}\{\phi(x) : x \in \{0, 1\}^{|V|}\},$$

the convex hull of the sufficient statistic values. It is the set of achievable singleton and pairwise marginal probabilities.
Mean Parameters: Gaussian MRF

\[ p(x) = \exp \left( \langle \theta, x \rangle + \frac{1}{2} \langle \Theta, xx' \rangle - A(\theta, \Theta) \right). \]

The mean parameters are \((\mu, \Sigma)\), where

\[ \mu = \mathbb{E}[X], \quad \Sigma = \mathbb{E}[XX']. \]

Easy to check that \(\Sigma - \mu \mu' \geq 0\) is necessary and sufficient. That is,

\[ \mathcal{M} = \{ (\mu, \Sigma) : \Sigma - \mu \mu' \geq 0 \}. \]

Notice that \(\mathcal{M}\) is again convex.
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Mean $\leftrightarrow$ Natural Parameters

Recall:

1. 

$$\nabla A(\eta) = \mathbb{E}\phi(x),$$

$$\nabla^2 A(\eta) = \text{Var}\phi(x).$$

2. For a regular family, the gradient mapping

$$\nabla A : \Omega \rightarrow \mathcal{M}$$

is one-to-one iff the representation is minimal.
3. The forward mapping, $\theta \mapsto \mu$, corresponds to computing expectations of sufficient statistics.

4. The reverse mapping, $\mu \mapsto \theta$, corresponds to computing a maximum likelihood estimate of $\theta$ for sample average $\mu$.

5. The maximum entropy $p$ satisfying a constraint on $\mu$ is in the exponential family. In particular, $\nabla A : \Omega \to \mathcal{M}$ is onto the interior of $\mathcal{M}$. 
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Conjugate Duality: Definition

Given a function $A : \Omega \rightarrow \mathbb{R}$, the conjugate dual is

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

where $\mu \in \mathbb{R}^d$ for $\Omega \subseteq \mathbb{R}^d$.

- $A^*$ is convex (a maximum of linear functions).
- Think of $A^* : \mathbb{R}^d \rightarrow \mathbb{R} \cup \{\infty\}$.
- If $A$ is convex ($+\ldots$), $A^{**} = A$. We can think of $A^*$ as capturing the shape of a convex $A$ through the locations of the tangent planes to its epigraph.
- If $A$ is log normalization for an exponential family, $\langle \mu, \theta \rangle - A(\theta)$ is (constant plus) log likelihood with sample average $\mu$ and natural parameter $\theta$. 
Conjugate Duality

Theorem:

1. For $\mu$ in the interior of $\mathcal{M}$, let $\theta(\mu)$ satisfy

$$E_{p_\theta(\mu)}[\phi(X)] = \nabla A(\theta(\mu)) = \mu.$$

Then

$$A^*(\mu) = -H(p_{\theta(\mu)}) = \int_{\mathcal{X}} \log p_{\theta(\mu)}(x)p_{\theta(\mu)}(x)h(dx).$$

2. For $\mu$ outside the closure of $\mathcal{M}$,

$$A^*(\mu) = \infty.$$
3. For $\theta \in \Omega$, we have the variational representation

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

4. For $\theta \in \Omega$, 

$$A(\theta) = \langle \theta, \mu(\theta) \rangle - A^*(\mu(\theta)),$$

where

$$\mu(\theta) := \mathbb{E}_{p_\theta}[\phi(X)] = \nabla A(\theta).$$
Conjugate Duality

- $-A^*(\mu)$ is the value of the maximum entropy problem for mean parameter $\mu$.
- $-A^*(\mu) = -\infty$ for infeasible $\mu$.
- Forward mapping: $\nabla A : \Omega \rightarrow M$.
- Backward mapping: $\nabla A^* : \text{int}(M) \rightarrow \Omega$. 
Conjugate Duality: Bernoulli

\[ X \in \{0, 1\}, \]
\[ \phi(x) = x, \]
\[ p(x) = \exp(\theta x - A(\theta)), \]
\[ A(\theta) = \log(\exp(0) + \exp(\theta)) = \log(1 + \exp(\theta)), \]
\[ \Omega = \{\theta \in \mathbb{R} : A(\theta) < \infty\} = \mathbb{R}. \]
Conjugate Duality: Bernoulli

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

Solving for the maximizing \( \theta \) gives

\[ \mu = \frac{\exp(\theta)}{1 + \exp(\theta)} \]
\[ \theta = \log \frac{\mu}{1 - \mu} \quad \text{for} \quad \mu \in (0, 1), \]
\[ A^*(\mu) = \mu \log \frac{\mu}{1 - \mu} - \log \frac{1}{1 - \mu} \]
\[ = \mu \log \mu + (1 - \mu) \log(1 - \mu) = -H(p_{\theta(\mu)}). \]
And if $\mu$ is outside $[0, 1]$?

$$\frac{d}{d\theta} \mu \theta = \mu,$$

$$\frac{d}{d\theta} \log(1 + \exp(\theta)) = \frac{\exp(\theta)}{1 + \exp(\theta)} \in (0, 1).$$

So for $\mu$ outside $[0, 1]$,

$$A^*(\mu) = \sup_{\theta \in \mathbb{R}} (\theta \mu - \log(1 + \exp(\theta))) = \infty.$$
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Variational Representation of $A(\theta)$

For $\theta \in \Omega$,

$$A(\theta) = \sup_{\mu \in M} \left( \langle \theta, \mu \rangle - A^*(\mu) \right)$$

$$= \sup_{\mu \in M} \left( \langle \theta, \mu \rangle + H(p_{\theta(\mu)}) \right).$$

- Solving this optimization problem gives the value $A(\theta)$ and the mean parameters $\mu = \mathbb{E}_{\theta}[\phi(X)]$.

- These correspond to the expectation of the sufficient statistics. (conditional expectation, if evidence has been incorporated into $\theta$).

- For example, for discrete pairwise MRFs, they give the marginal singleton and pairwise distributions.
Variational Representation of $A(\theta)$

$$A(\theta) = \sup_{\mu \in \mathcal{M}} \left( \langle \theta, \mu \rangle + H(p_{\theta(\mu)}) \right).$$

We can approximate this optimization problem to obtain a simpler problem:

- Approximate $\mathcal{M}$ by a simpler set $\hat{\mathcal{M}}$.
  - $\hat{\mathcal{M}} \subset \mathcal{M}$ gives a lower bound.
  - $\mathcal{M} \subset \hat{\mathcal{M}}$ gives an upper bound.
- Approximate $H(p_{\theta(\mu)})$ by something simpler.
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Examples: Mean Field Algorithm

Consider an Ising model (binary pairwise Markov random field):

\[ x_u \in \{0, 1\}, \]
\[ \psi_{u,v}(x_u, x_v) = \theta_{u,v}x_u x_v, \]
\[ \psi_v(x_v) = \theta_v x_v. \]

\[ p(x) \propto \exp \left( \sum_{v \in V} \theta_v x_v + \sum_{\{u,v\} \in E} \theta_{u,v} x_u x_v \right). \]

\[ \mu_{u,v} = \Pr(x_u = x_v = 1), \]
\[ \mu_v = \Pr(x_v = 1). \]
Mean Field Algorithm

- We approximate $\mathcal{M}$ with a smaller set:
  \[ \hat{\mathcal{M}} = \{ \mu : \mu_{u,v} = \mu_u \mu_v \} \].

- This adds independence, so $\hat{\mathcal{M}} \subset \mathcal{M}$.

- Thus, we can represent the distribution as
  \[ p(x; \theta) = \prod_{v \in V} p_v(x_v; \theta). \]

- Hence, the entropy is
  \begin{align*}
  H(p_{\theta(\mu)}) &= \mathbb{E} \log p(X; \theta) = \sum_{v \in V} \mathbb{E} \log p_v(X_v; \theta) \\
  &= \sum_{v \in V} (\mu_v \log \mu_v + (1 - \mu_v) \log(1 - \mu_v)).
  \end{align*}
So we have

\[ A(\theta) = \sup_{\mu \in \hat{\mathcal{M}}} \left( \langle \theta, \mu \rangle + H(p_{\theta(\mu)}) \right) \]

\[ = \sup_{\mu \in \hat{\mathcal{M}}} \left( \sum_{v \in V} \theta_v \mu_v + \sum_{\{u,v\} \in E} \theta_{u,v} \mu_u \mu_v \right. \]

\[ \left. - \sum_{v \in V} (\mu_v \log \mu_v + (1 - \mu_v) \log(1 - \mu_v)) \right) . \]
Mean Field Algorithm

We can solve this with coordinate maximization:
Calculate gradient of criterion w.r.t. $\mu_v$:

$$\theta_v + \sum_{u \in N(v)} \theta_{u,v} \mu_u - (1 + \log \mu_v - 1 - \log(1 - \mu_v))$$

$$= \theta_v + \sum_{u \in N(v)} \theta_{u,v} \mu_u - \log \frac{\mu_v}{1 - \mu_v}.$$ 

Setting to zero gives

$$\mu_v = \frac{1}{1 + \exp \left( -\theta_v - \sum_{u \in N(v)} \theta_{u,v} \mu_u \right)},$$

which is the mean field update.
Mean Field Algorithm

Summary:

- We approximate $\mathcal{M}$ with a smaller set:

$$\hat{\mathcal{M}} = \{ \mu : \mu_{u,v} = \mu_u \mu_v \}.$$

- Solve for $A(\theta)$ and $\mu$ with coordinate maximization:

$$\mu_v := \frac{1}{1 + \exp \left( -\theta_v - \sum_{u \in N(v)} \theta_{u,v} \mu_u \right)}.$$
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Announcements

My office hours:
Thursday Nov 19 (today), 1-2pm, in 723 SD Hall.