CS 6347

Lecture 8

Variational Methods

Approximate Marginal Inference

- Last time: approximate MAP inference
  - Reparamaterizations
  - Linear programming over the local marginal polytope
- Approximate marginal inference (e.g., $p(y_i|x)$)
  - Sampling methods (MCMC, etc.)
  - Variational methods (loopy belief propagation, TRW, etc.)

KL Divergence

- In order to perform approximate marginal inference, we will try to find distributions that approximate the true distribution

  - Ideally, the marginals of the approximating distribution should be easy to compute

- For this, we need a notion of closeness of distributions

KL Divergence

$$D(p||q) = \sum_x p(x) \log \frac{p(x)}{q(x)}$$

- Called the Kullback-Leibler divergence
- $D(p||q) \geq 0$ with equality if and only if $p = q$
- Not symmetric, $D(p||q) \neq D(q||p)$

Jensen's Inequality

- Let $f(x)$ be a convex function and $a_i \geq 0$ such that $\sum_i a_i = 1$

$$\sum_i a_i f(x_i) \geq f\left(\sum_i a_i x_i\right)$$

- Useful inequality when dealing with convex/concave functions

- When does equality hold?

KL Divergence

$$D(p||q) = \sum_x p(x) \log \frac{p(x)}{q(x)}$$

- Suppose that we want to approximate the distribution p with some other distribution q in some family of distributions Q

- Could minimize KL divergence in one of two ways

  - $\arg\min_{q \in Q} D(p||q)$

  - $\arg\min_{q \in Q} D(q||p)$

KL Divergence

$$D(p||q) = \sum_x p(x) \log \frac{p(x)}{q(x)}$$

- Suppose that we want to approximate the distribution p with some other distribution q in some family of distributions Q

- Could minimize KL divergence in one of two ways

  - $\arg\min_{q \in Q} D(p||q)$ Called the M-projection

  - $\arg\min_{q \in Q} D(q||p)$ Called the I-projection

KL Divergence

$$D(p||q) = \sum_x p(x) \log \frac{p(x)}{q(x)}$$

- Suppose that we want to approximate the distribution p with some other distribution q in some family of distributions Q

- Could minimize KL divergence in one of two ways

  - $\arg\min_{q \in Q} D(p||q)$ As hard as the original inference problem

  - $\arg\min_{q \in Q} D(q||p)$ Potentially easier…

Variational Inference

- Let's let $p(x) = \frac{1}{Z}\prod_c \psi_c(x_c)$ be the distribution that we want to approximate with distribution q

$$D(q||p) = \sum_x q(x)\log\frac{q(x)}{p(x)}$$

$$= \sum_x q(x)\log q(x) - \sum_x q(x)\log p(x)$$

$$= -H(q) - \sum_x q(x)\log p(x)$$

$$= -H(q) + \log Z - \sum_x \sum_C q(x)\log \psi_c(x_c)$$

$$= -H(q) + \log Z - \sum_C \sum_{x_C} q_C(x_C)\log \psi_c(x_c)$$

Variational Inference

- Let's let $p(x) = \frac{1}{Z}\prod_c \psi_c(x_c)$ be the distribution that we want to approximate with distribution q

$$
\begin{aligned}
D(q||p) &= \sum_x q(x) \log \frac{q(x)}{p(x)} \\
&= \sum_x q(x) \log q(x) - \sum_x q(x) \log p(x) \\
&= -H(q) - \sum_x q(x) \log p(x) \\
&= -H(q) + \log Z - \sum_x \sum_C q(x) \log \psi_c(x_c) \\
&= -H(q) + \log Z - \sum_C \sum_{x_C} q_C(x_C) \log \psi_c(x_c)
\end{aligned}
$$

Where have we seen this before?

MAP Integer Program

$$\max_{\tau} \sum_{i \in V} \sum_{x_i} \tau_i(x_i) \log \phi_i(x_i) + \sum_{(i,j) \in E} \sum_{x_i, x_j} \tau_{ij}(x_i, x_j) \log \psi_{ij}(x_i, x_j)$$

such that

$$\sum_{x_i} \tau_i(x_i) = 1$$ For all $i \in V$

$$\sum_{x_j} \tau_{ij}(x_i, x_j) = \tau_i(x_i)$$ For all $(i,j) \in E, x_i$

$$\tau_i(x_i) \in \{0,1\}$$ For all $i \in V, x_i$

$$\tau_{ij}(x_i, x_j) \in \{0,1\}$$ For all $(i,j) \in E, x_i, x_j$

Variational Inference

- Let's let $p(x) = \frac{1}{Z}\prod_c \psi_c(x_c)$ be the distribution that we want to approximate with distribution q

$$D(q||p) = -H(q) + \log Z - \sum_C \sum_{x_C} q_C(x_C) \log \psi_c(x_c)$$

- Using the observation that the KL divergence is non-negative

$$\log Z \geq H(q) + \sum_C \sum_{x_C} q_C(x_C) \log \psi_c(x_c)$$

Variational Inference

- Let's let $p(x) = \frac{1}{Z}\prod_c \psi_c(x_c)$ be the distribution that we want to approximate with distribution q

$$D(q||p) = -H(q) + \log Z - \sum_C \sum_{x_C} q_C(x_C) \log \psi_c(x_c)$$

- Using the observation that the KL divergence is non-negative

$$\log Z \geq H(q) + \sum_C \sum_{x_C} q_C(x_C) \log \psi_c(x_c)$$

  - This lower bound holds for **any** q

Variational Inference

- Let's let $p(x) = \frac{1}{Z}\prod_c \psi_c(x_c)$ be the distribution that we want to approximate with distribution q

$$D(q||p) = -H(q) + \log Z - \sum_C \sum_{x_C} q_C(x_C) \log \psi_c(x_c)$$

- Using the observation that the KL divergence is non-negative

$$\log Z \geq H(q) + \sum_C \sum_{x_C} q_C(x_C) \log \psi_c(x_c)$$

Maximizing this over all probability distributions q gives equality

Variational Inference

$$\log Z \geq H(q) + \sum_{C} \sum_{x_C} q_C(x_C) \log \psi_c(x_c)$$

- The right hand side is a concave function of q
- Despite that, this optimization problem is **hard**! (surprised?)
  - Exponentially many distributions, $q(x)$
    We need a more compact way to express them
  - Computing the entropy is non-trivial

Variational Inference

$$\log Z \geq H(q) + \sum_{C} \sum_{x_C} q_C(x_C) \log \psi_c(x_c)$$

- Two kinds of methods that are used to deal with these difficulties
  - Mean-field methods: assume that the approximating distribution factorizes as $q(x) \propto \prod_{i \in V} q_i(x_i)$
  - Relaxation based methods: replace hard pieces of the optimization with easier optimization problems
    - Similar to the MAP IP -> MAP LP relaxation

Relaxation Approach

$$\log Z \geq H(q) + \sum_C \sum_{x_C} q_C(x_C) \log \psi_c(x_c)$$

- To handle the representation problem, we can use the same LP relaxation trick that we did before

- For each τ in the marginal polytope, we can rewrite the RHS as

$$\log Z \geq H(\tau) + \sum_C \sum_{x_C} \tau_C(x_C) \log \psi_c(x_c)$$

Relaxation Approach

$$\log Z \geq H(q) + \sum_{C} \sum_{x_C} q_C(x_C) \log \psi_c(x_c)$$

- To handle the representation problem, we can use the same LP relaxation trick that we did before
- For each τ in the marginal polytope, we can rewrite the RHS as

$$\log Z \geq H^*(\tau) + \sum_{C} \sum_{x_C} \tau_C(x_C) \log \psi_c(x_c)$$

Maximum entropy over all τ with these marginals

Relaxation Approach

$$\max_{\tau \in \mathrm{M}} H^*(\tau) + \sum_C \sum_{x_C} \tau_C(x_C) \log \psi_c(x_c)$$

- Marginal polytope, M, is intractable to optimize over
- Use the local polytope, T

$$\sum_{x_{C \setminus i}} \tau_C(x_C) = \tau_i(x_i) \;\; for\ all\ C, i \in V$$

$$\sum_{x_i} \tau_i(x_i) = 1\ for\ all\ i \in V$$

Relaxation Approach

$$\max_{\tau \in \mathbf{T}} H^*(\tau) + \sum_C \sum_{x_C} \tau_C(x_C) \log \psi_c(x_c)$$

- Even with the polytope relaxation, the optimization problem still remains challenging as computing the entropy remains nontrivial
  - We will need to approximate the entropy as well
  - For which distributions is it easy to compute the entropy?

Tree Reparameterization

- On a tree, the joint distribution factorizes in a special way

$$p(x_1, \dots, x_n) = \prod_{i \in V} p_i(x_i) \prod_{(i,j) \in E} \frac{p_{ij}(x_i, x_j)}{p_i(x_i) p_j(x_j)}$$

- p_i is the marginal distribution of the i^{th} variable and p_{ij} is the max-marginal distribution for the edge $(i,j) \in E$

- This applies to tree-structured factor graphs as well

Tree Reparameterization

- On a tree, the joint distribution factorizes in a special way

$$p(x_1, \dots, x_n) = \prod_{i \in V} p_i(x_i) \prod_{C} \frac{p_C(x_C)}{\prod_{i \in C} p_i(x_i)}$$

- p_i is the marginal distribution of the i^{th} variable and p_{ij} is the max-marginal distribution for the edge $(i, j) \in E$

- This applies to tree-structured factor graphs as well

Entropy of a Tree

- Given this factorization, we can easily compute the entropy of a tree structured distribution

$$H_{Tree} = -\sum_{i \in V} \sum_{x_i} p_i\,(x_i) \log p_i(x_i) - \sum_{C} \sum_{x_C} p_C(x_C) \log \frac{p_C(x_C)}{\prod_{i \in C} p_i(x_i)}$$

- This only depends on the marginals

- Use this as an approximation for general distributions!

Bethe Free Energy

- Combining these two approximations gives us the so-called Bethe free energy approximation

$$\max_{\tau \in \mathbf{T}} H_B(\tau) + \sum_C \sum_{x_C} \tau_C(x_C) \log \psi_c(x_c)$$

where

$$H_B(\tau) = -\sum_{i \in \mathrm{V}} \sum_{x_i} \tau_i(x_i) \log \tau_i(x_i) - \sum_C \sum_{x_C} \tau_C(x_C) \log \frac{\tau_C(x_C)}{\prod_{i \in C} \tau_i(x_i)}$$

Bethe Free Energy

$$\max_{\tau \in \mathbf{T}} H_B(\tau) + \sum_C \sum_{x_C} \tau_C(x_C) \log \psi_c(x_c)$$

- This is not a concave optimization problem for general graphs
  - It is still difficult to maximize
  - Fixed points of loopy belief propagation, i.e., BP on a graph with cycles, correspond to saddle points of this objective over the local marginal polytope