Variational Inference and Mean Field Method

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Introduction

We are interested in the **posterior distribution**

$$p(z|x) \propto p(x|z)p(z)$$

However, we can't compute the posterior for many models. (Example:GMM)

Other methods: Integrated Nested Laplace Approximations(INLA), Monte Carlo Method...

Introduction

The basic idea of **Variational Inference** is, to pick an approximation $q(z)$ to the distribution from some tractable families, approximation should be as close as possible to the true posterior, $p^*(z) = p(z|x)$. This reduces inference to an optimization problem.

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Kullback-Leibler Divergence

We measure the closeness of the two distributions with Kullback-Leibler (KL) divergence.
The KL divergence for variational inference is

$$KL(q||p) = E_q \left[\log \frac{q(z)}{p(z|x)} \right]$$

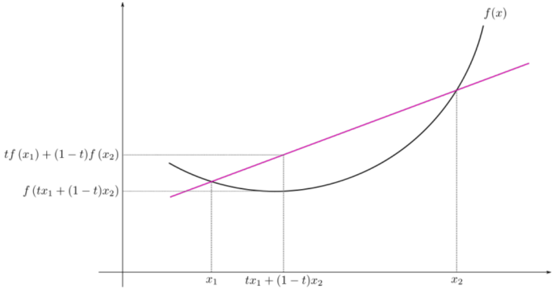
Note:reversing the arguments leads to a different kind of variational inference than we are discussing. In general, it's more computationally expensive than the algorithms we will study. We choose q so that we can take expectations.

The evidence lower bound

We actually can't minimize the KL divergence exactly, but we can minimize a function that is equal to it up to a constant. This is the **evidence lower bound (ELBO)**.

Recall Jensen's inequality as applied to probability distributions. When f is concave

$$f(E[X]) \geq E(f(X))$$



The evidence lower bound

We use Jensen's inequality on the log probability of the observations x

$$
\begin{aligned}
\log p(x) &= \log \int_z p(x, z) \\
&= \log \int_z p(x, z) \frac{q(z)}{q(z)} \\
&= \log \left(E_q \left[\frac{p(x, z)}{q(z)} \right] \right) \\
&\geq E_q[\log p(x, z)] - E_q[\log q(z)]
\end{aligned}
$$

We define $ELBO(q) = E_q[\log \frac{p(x,z)}{q(z)}]$.

The evidence lower bound

First, note that

$$p(z|x) = \frac{p(z,x)}{p(x)}$$

Now use the K-L divergence,

$$\begin{aligned}
KL(q(z)||p(z|x)) &= E_q\left[\log \frac{q(z)}{p(z|x)}\right] \\
&= E_q[\log q(z)] - E_q[\log p(z|x)] \\
&= E_q[\log q(z)] - E_q[\log p(z,x)] + \log p(x) \\
&= -(E_q[\log p(z,x)] - E_q[\log q(z)]) + \log p(x) \\
KL(q(z)||p(z|x)) + ELBO &= \log p(x)
\end{aligned}$$

This is the negative ELBO plus the log marginal probability of x. Notice that $\log p(x)$ does not depend on q. So, as a function of the variational distribution, minimizing the KL divergence is the same as maximizing the ELBO.

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Mean field variational inference

In mean field variational inference, we assume that the variational family factorizes,

$$q(z_1, \cdots, z_m) = \prod_{j=i}^{m} q(z_j)$$

Each variable is independent.

Mean field variational inference

We now turn to optimizing the ELBO for this factorized distribution.
We will use **coordinate ascent inference**, interatively optimizing each variational distribution holding the others fixed.

Mean field variational inference

First, recall the chain rule and use it to decompose the joint,

$$p(z_{1:m}, x_{1:n}) = p(x_{1:n}) \prod_{j=i}^{m} p(z_j | z_{1:(j-1)}, x_{1:n})$$

Notice that the z variables can occur in any order in this chain.
The indexing from 1 to m is arbitrary.
Second, decompose the entropy of the variational distribution,

$$E[\log q(z_{1:m})] = \sum_{j=1}^{m} E_j[\log q(z_j)]$$

where E_j denotes an expectation with respect to $q(z_j)$.

Mean field variational inference

Third, define $\mathcal{L} := ELBO$, with these two facts, decompose $\mathcal{L}$,

$$\mathcal{L} = \log p(x_{1:n}) + \sum_{j=1}^{m} (E_j[\log p(z_j | z_{1:(j-1)}, x_{1:n})] - E_j[\log q(z_j)])$$

Employ the chain rule with the variable z_k as the last variable in the list.This leads to the objective function

$$\mathcal{L} = E[\log p(z_k | z_{-k}, x)] - E_j[\log q(z_k)] + \mathrm{const}$$

Write this objective as a function of $q(z_k)$:

$$\mathcal{L}_k = \int q(z_k) E_{-k}[\log p(z_k | z_{-k}, x)] dz_k - \int q(z_k) \log q(z_k) dz_k$$

Mean field variational inference

Take the derivative with respect to $q(z_k)$

$$\frac{d\mathcal{L}_k}{dq(z_k)} = E_{-k}[\log p(z_k|z_{-k}, x)] - \log q(z_k) - 1 = 0$$

This leads to the coordinate ascent update for $q(z_k)$

$$q^*(z_k) \propto \exp\{E_{-k}[\log p(z_k|z_{-k}, x)]\}$$

But the denominator of the posterior does not depend on z_j, so

$$q^*(z_k) \propto \exp\{E_{-k}[\log p(z_k, z_{-k}, x)]\}$$

The coordinate ascent algorithm is to iteratively update each $q(z_k)$. The ELBO converges to a local optimum. Use the resulting q is as a proxy for the true posterior

Exponential family conditionals

Suppose each conditional is in the exponential family

$$p(z_j|z_{-j}, x) = h(z_j)\exp\{\eta(z_{-j}, x)^T t(z_j) - a(\eta(z_{-j}, x))\}$$

This describes a lot of complicated models
-Bayesian mixtures of exponential families with conjugate priors
-Hierarchical HMMs
-Bayesian linear regression

Exponential family conditionals

Mean field variational inference is straightforward.
Compute the log of the conditional

$$\log p(z_j | z_{-j}, x) = \log h(z_j) + \eta(z_{-j}, x)^T t(z_j) - a(\eta(z_{-j}, x))$$

Compute the expectation with respect to $q(z_j)$

$$E[\log p(z_j | z_{-j}, x)] = \log h(z_j) + E[\eta(z_{-j}, x)]^T t(z_j) - E[a(\eta(z_{-j}, x))]$$

Noting that the last term does not depend on q_j, this means that

$$q^*(z_j) \propto h(z_j) \exp\{E[\eta(z_{-j}, x)]^T t(z_j)\}$$

So, the optimal $q(z_j)$ is in the same exponential family as the conditional.

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Connection between VI and EM

In EM algorithm, we compute

$$\theta^{(n+1)} = \arg\max_{\theta} E_{z|x,\theta_n} \log p(x, z|\theta)$$

until it converges. So this gives rise to two steps. The E-step calculates the conditional expectation $E_{z|x,\theta_n} \log p(x, z|\theta)$, and the M-step maximizes the expectation.

Connection between VI and EM

When variational methods used in parameter estimation, notice that the ELBO is a function of the approximate distribution q and the unknown parameter θ,

$$ELBO(q, \theta) = \sum_z q(z|x) \log \frac{p(z, x|\theta)}{q(z|x)}$$

It is easy to prove that $p(z|x, \theta^{(k)}) = \arg\max_q ELBO(q, \theta^{(k)})$.

Connection between VI and EM

Procedure:

step1: $q^{(k+1)} = \arg\max_q ELBO(q, \theta^{(k)})$
step2: $\theta^{(k+1)} = \arg\max_\theta ELBO(q^{(k+1)}, \theta)$

Let's fix the approximate distribution $q(z|x)$ to be $p(z|x, \theta^{(k)})$.
Originally, we need to calculate $\theta^{(k+1)}$ as

$$\theta^{(k+1)} = \arg\max_\theta \sum \int p(z|x_i, \theta) \log p(x_i, z, \theta) dz - \int p(z|x_i, \theta) \log p(z|x_i, \theta) dz$$

However, we actually use

$$\theta^{(k+1)} = \arg\max_\theta \sum \int p(z|x_i, \theta^{(k)}) \log p(x_i, z, \theta) dz$$

Since after we set $\theta^{(k)}$ fixed, we can safely omit the terms in ELBO that don't contain θ.