Variational Inference

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1 Set up

- As usual, we will assume that $x = x_{1:n}$ are observations and $z = z_{1:m}$ are hidden variables. We assume additional parameters α that are fixed.

- Note we are general—the hidden variables might include the "parameters," e.g., in a traditional inference setting. (In that case, α are the hyperparameters.)

- We are interested in the **posterior distribution**,

$$p(z \mid x, \alpha) = \frac{p(z, x \mid \alpha)}{\int_z p(z, x \mid \alpha)}. \tag{1}$$

- As we saw earlier, the posterior links the data and a model. It is used in all downstream analyses, such as for the predictive distribution.

- (Note: The problem of computing the posterior is an instance of a more general problem that variational inference solves.)

2 Motivation

- We can't compute the posterior for many interesting models.

- Consider the Bayesian mixture of Gaussians,

  1. Draw $\mu_k \sim \mathcal{N}(0, \tau^2)$ for $k = 1 \dots K$.
  2. For $i = 1 \dots n$:
     (a) Draw $z_i \sim \text{Mult}(\pi)$;

(b) Draw $x_i \sim \mathcal{N}(\mu_{z_i}, \sigma^2)$.

- Suppressing the fixed parameters, the posterior distribution is

$$p(\mu_{1:K}, z_{1:n} \mid x_{1:n}) = \frac{\prod_{k=1}^{K} p(\mu_k) \prod_{i=1}^{n} p(z_i) p(x_i \mid z_i, \mu_{1:K})}{\int_{\mu_{1:K}} \sum_{z_{1:n}} \prod_{k=1}^{K} p(\mu_k) \prod_{i=1}^{n} p(z_i) p(x_i \mid z_i, \mu_{1:K})}. \tag{2}$$

- The numerator is easy to compute for any configuration of the hidden variables. The problem is the denominator.

- Let's try to compute it. First, we can take advantage of the conditional independence of the z_i's given the cluster centers,

$$p(x_{1:n}) = \int_{\mu_{1:K}} \prod_{k=1}^{K} p(\mu_k) \prod_{i=1}^{n} \sum_{z_i} p(z_i) p(x_i \mid z_i, \mu_{1:K}). \tag{3}$$

  This leads to an integral that we can't (easily, anyway) compute.

- Alternatively, we can move the summation over the latent assignments to the outside,

$$p(x_{1:n}) = \int_{\mu_{1:K}} \prod_{k=1}^{K} p(\mu_k) \prod_{i=1}^{n} \sum_{z_i} p(z_i) p(x_i \mid z_i, \mu_{1:K}). \tag{4}$$

  It turns out that we can compute each term in this summation. (This is an exercise.) However, there are K^n terms. This is intractable when n is reasonably large.

- This situation arises in most interesting models. This is why approximate posterior inference is one of the central problems in Bayesian statistics.

3 Main idea

- We return to the general $\{x, z\}$ notation.

- The main idea behind variational methods is to pick a family of distributions over the latent variables with its own **variational parameters**,

$$q(z_{1:m} \mid \nu). \tag{5}$$

- Then, find the setting of the parameters that makes q close to the posterior of interest.

- Use q with the fitted parameters as a proxy for the posterior, e.g., to form predictions about future data or to investigate the posterior distribution of the hidden variables.

- Typically, the true posterior is not in the variational family. (Draw the picture from Wainwright and Jordan, 2008.)

4 Kullback-Leibler Divergence

- We measure the closeness of the two distributions with Kullback-Leibler (KL) divergence.

- This comes from **information theory**, a field that has deep links to statistics and machine learning. (See the books "Information Theory and Statistics" by Kullback and "Information Theory, Inference, and Learning Algorithms" by MacKay.)

- The KL divergence for variational inference is

$$\mathrm{KL}(q||p) = \mathrm{E}_q \left[\log \frac{q(Z)}{p(Z \mid x)} \right]. \tag{6}$$

- Intuitively, there are three cases
  - If q is high and p is high then we are happy.
  - If q is high and p is low then we pay a price.
  - If q is low then we don't care (because of the expectation).

- (Draw a multi-modal posterior and consider various possibilities for single modes.)

- Note that we could try to reverse these arguments. In a way, that makes more intuitive sense. However, we choose q so that we can take expectations.

- That said, reversing the arguments leads to a different kind of variational inference than we are discussing. It is called "expectation propagation." (In general, it's more computationally expensive than the algorithms we will study.)

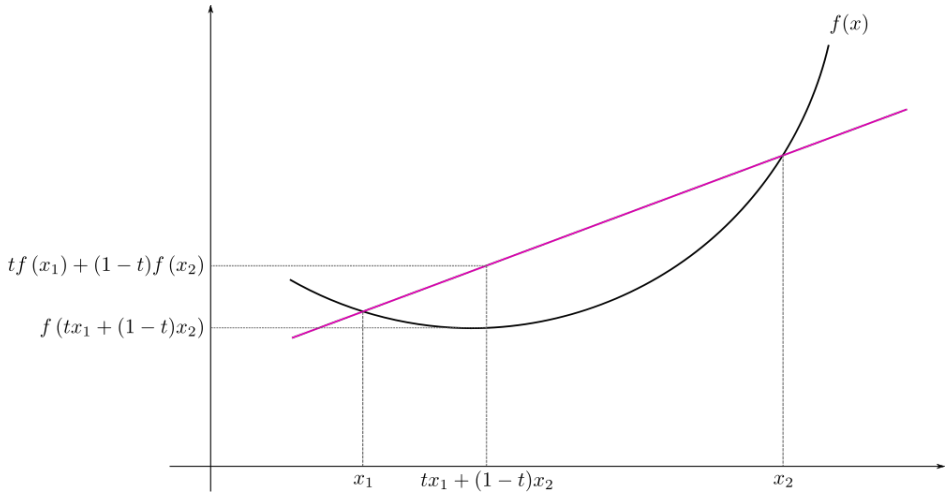
5 The evidence lower bound

- 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,

$$f(\mathrm{E}[X]) \geq \mathrm{E}[f(X)]. \tag{7}$$

- If you haven't seen Jensen's inequality, spend 15 minutes to learn about it.



(This figure is from Wikipedia.)

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

$$\begin{aligned}
\log p(x) &= \log \int_z p(x,z) && (8)\\
&= \log \int_z p(x,z)\frac{q(z)}{q(z)} && (9)\\
&= \log \left(\mathrm{E}_q \left[\frac{p(x,Z)}{q(z)} \right] \right) && (10)\\
&\geq \mathrm{E}_q[\log p(x,Z)] - \mathrm{E}_q[\log q(Z)]. && (11)
\end{aligned}$$

This is the ELBO. (Note: This is the same bound used in deriving the expectation-maximization algorithm.)

- We choose a family of variational distributions (i.e., a parameterization of a distribution of the latent variables) such that the expectations are computable.

- Then, we maximize the ELBO to find the parameters that gives as tight a bound as possible on the marginal probability of x.

- Note that the second term is the entropy, another quantity from information theory.

- What does this have to do with the KL divergence to the posterior?
  - First, note that
$$p(z \mid x) = \frac{p(z, x)}{p(x)}. \tag{12}$$
  - Now use this in the KL divergence,
$$\begin{aligned} \mathrm{KL}(q(z)||p(z \mid x)) &= \mathrm{E}_q\left[\log \frac{q(Z)}{p(Z \mid x)}\right] && (13)\\ &= \mathrm{E}_q[\log q(Z)] - \mathrm{E}_q[\log p(Z \mid x)] && (14)\\ &= \mathrm{E}_q[\log q(Z)] - \mathrm{E}_q[\log p(Z, x)] + \log p(x) && (15)\\ &= -(\mathrm{E}_q[\log p(Z, x)] - \mathrm{E}_q[\log q(Z)]) + \log p(x) && (16) \end{aligned}$$
    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.

- And, the difference between the ELBO and the KL divergence is the log normalizer—which is what the ELBO bounds.

6 Mean field variational inference

- In mean field variational inference, we assume that the variational family **factorizes**,
$$q(z_1, \ldots, z_m) = \prod_{j=1}^{m} q(z_j). \tag{17}$$
  Each variable is independent. (We are suppressing the parameters ν_j.)

- This is more general that it initially appears—the hidden variables can be grouped and the distribution of each group factorizes.

- Typically, this family does not contain the true posterior because the hidden variables are dependent.
  - E.g., in the Gaussian mixture model all of the cluster assignments z_i are dependent on each other and the cluster locations $\mu_{1:K}$ given the data $x_{1:n}$.
  - These dependencies are often what makes the posterior difficult to work with.

– (Again, look at the picture from Wainwright and Jordan.)

- 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.

- We emphasize that this is not the only possible optimization algorithm. Later, we'll see one based on the natural gradient.

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

$$p(z_{1:m}, x_{1:n}) = p(x_{1:n}) \prod_{j=1}^{m} p(z_j \mid z_{1:(j-1)}, x_{1:n}) \tag{18}$$

  Notice that the z variables can occur in any order in this chain. The indexing from 1 to m is arbitrary. (This will be important later.)

- Second, decompose the entropy of the variational distribution,

$$\mathrm{E}[\log q(z_{1:m})] = \sum_{j=1}^{m} \mathrm{E}_j[\log q(z_j)], \tag{19}$$

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

- Third, with these two facts, decompose the the ELBO,

$$\mathcal{L} = \log p(x_{1:n}) + \sum_{j=1}^{m} \mathrm{E}[\log p(z_j \mid z_{1:(j-1)}, x_{1:n})] - \mathrm{E}_j[\log q(z_j)]. \tag{20}$$

- Consider the ELBO as a function of $q(z_k)$.
  - Employ the chain rule with the variable z_k as the last variable in the list.
  - This leads to the objective function

$$\mathcal{L} = \mathrm{E}[\log p(z_k \mid z_{-k}, x)] - \mathrm{E}_j[\log q(z_k)] + \text{const.} \tag{21}$$

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

$$\mathcal{L}_k = \int q(z_k) \mathrm{E}_{-k}[\log p(z_k \mid z_{-k}, x)] dz_k - \int q(z_k) \log q(z_k) dz_k. \tag{22}$$

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

$$\frac{d\mathcal{L}_j}{dq(z_k)} = \mathrm{E}_{-k}[\log p(z_k \mid z_{-k}, x)] - \log q(z_k) - 1 = 0 \tag{23}$$

– This (and Lagrange multipliers) leads to the coordinate ascent update for $q(z_k)$

$$q^*(z_k) \propto \exp\{\mathrm{E}_{-k}[\log p(z_k \mid Z_{-k}, x)]\} \tag{24}$$

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

$$q^*(z_k) \propto \exp\{\mathrm{E}_{-k}[\log p(z_k, Z_{-k}, x)]\} \tag{25}$$

– Either of these perspectives might be helpful in deriving variational inference algorithms.

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

- Notice
  - The RHS only depends on $q(z_j)$ for $j \neq k$ (because of factorization).
  - This determines the form of the optimal $q(z_k)$. We didn't specify the form in advance, only the factorization.
  - Depending on that form, the optimal $q(z_k)$ might not be easy to work with. However, for many models it is. (Stay tuned.)

- There is a strong relationship between this algorithm and Gibbs sampling.
  - In Gibbs sampling we sample from the conditional.
  - In coordinate ascent variational inference, we iteratively set each factor to

$$\text{distribution of } z_k \propto \exp\{\mathrm{E}[\log(\text{conditional})]\}. \tag{26}$$

- Easy example: Multinomial conditionals
  - Suppose the conditional is multinomial

$$p(z_j \mid z_{-j}, x_{1:n}) := \pi(z_{-j}, x_{1:n}) \tag{27}$$

  - Then the optimal $q(z_j)$ is also a multinomial,

$$q^*(z_j) \propto \exp\{\mathrm{E}[\log \pi(z_{-j}, x)]\} \tag{28}$$

7 Exponential family conditionals

- Suppose each conditional is in the exponential family

$$p(z_j \mid z_{-j}, x) = h(z_j) \exp\{\eta(z_{-j}, x)^\top t(z_j) - a(\eta(z_{-j}, x))\} \tag{29}$$

- This describes *a lot* of complicated models
  - Bayesian mixtures of exponential families with conjugate priors
  - Switching Kalman filters
  - Hierarchical HMMs
  - Mixed-membership models of exponential families
  - Factorial mixtures/HMMs of exponential families
  - Bayesian linear regression

- Notice that any model containing conjugate pairs and multinomials has this property.

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

$$\log p(z_j \mid z_{-j}, x) = \log h(z_j) + \eta(z_{-j}, x)^\top t(z_j) - a(\eta(z_{-j}, x)) \tag{30}$$

  - Compute the expectation with respect to $q(z_{-j})$

$$\mathrm{E}[\log p(z_j \mid z_{-j}, x)] = \log h(z_j) + \mathrm{E}[\eta(z_{-j}, x)]^\top t(z_j) - \mathrm{E}[a(\eta(z_{-j}, x))] \tag{31}$$

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

$$q^*(z_j) \propto h(z_j) \exp\{\mathrm{E}[\eta(z_{-j}, x)]^\top t(z_j)\} \tag{32}$$

    and the normalizing constant is $a(\mathrm{E}[\eta(z_{-j}, x)])$.

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

- Coordinate ascent algorithm
  - Give each hidden variable a variational parameter ν_j, and put each one in the same exponential family as its model conditional,

$$q(z_{1:m} \mid \nu) = \prod_{j=1}^{m} q(z_j \mid \nu_j) \tag{33}$$

– The coordinate ascent algorithm iteratively sets each natural variational parameter ν_j equal to the expectation of the natural conditional parameter for variable z_j given all the other variables and the observations,

$$\nu_j^* = \mathrm{E}[\eta(z_{-j}, x)]. \tag{34}$$

8 Example: Bayesian mixtures of Gaussians

- Let's go back to the Bayesian mixture of Gaussians. For simplicity, assume that the data generating variance is one.

- The latent variables are cluster assignments z_i and cluster means μ_k.

- The mean field family is

$$q(\mu_{1:K}, z_{1:n}) = \prod_{k=1}^{K} q(\mu_k \mid \tilde{\mu}_k, \tilde{\sigma}_k^2) \prod_{i=1}^{n} q(z_i \mid \phi_i), \tag{35}$$

  where $(\tilde{\mu}_k, \tilde{\sigma}_k)$ are Gaussian parameters and ϕ_i are multinomial parameters (i.e., positive K-vectors that sum to one.)

- (Draw the graphical model and draw the graphical model with the mean-field family.)

- We compute the update for $q(z_i)$.
  - Recall that
  $$q^*(z_i) \propto \exp\{\mathrm{E}_{-i}[\log p(\mu_{1:K}, z_i, z_{-i}, x_{1:n})]\}. \tag{36}$$
  - Because z_i is a multinomial, this has to be one too.
  - The log joint distribution is

$$\begin{aligned}&\log p(\mu_{1:K}, z_i, z_{-i}, x_{1:n}) = \\ &\quad \log p(\mu_{1:k}) + \left(\textstyle\sum_{j \neq i} \log p(z_j) + \log p(x_j \mid z_j)\right) + \log p(z_i) + \log p(x_i \mid z_i).\end{aligned} \tag{37}$$

  - Restricting to terms that are a function of z_i,

$$q^*(z_i) \propto \exp\{\log \pi_{z_i} + \mathrm{E}[\log p(x_i \mid \mu_{z_i})]\}. \tag{38}$$

  - Let's compute the expectation,

$$\mathrm{E}[\log p(x_i \mid \mu_i)]\} = -(1/2)\log 2\pi - x_i^2/2 + x_i \mathrm{E}[\mu_{z_i}] - \mathrm{E}[\mu_{z_i}^2]/2. \tag{39}$$

- We will see that $q(\mu_i)$ is Gaussian, so these expectations are easy to compute.
- Thus the coordinate update for $q(z_i)$ is

$$q^*(z_i = k) \propto \exp\{\log \pi_k + x_i \mathrm{E}[\mu_k] - \mathrm{E}[\mu_k^2]/2\}. \tag{40}$$

- Now we turn to the update for $q(\mu_k)$.
  - Here, we are going to use our reasoning around the exponential family and conditional distributions.
  - What is the conditional distribution of μ_k given $x_{1:n}$ and $z_{1:n}$?
  - Intuitively, this is the posterior Gaussian mean with the data being the observations that were assigned (in $z_{1:n}$) to the kth cluster.
  - Let's put the prior and posterior, which are Gaussians, in their canonical form. The parameters are

$$\hat{\lambda}_1 = \lambda_1 + \textstyle\sum_{i=1}^n z_i^k x_i \tag{41}$$
$$\hat{\lambda}_2 = \lambda_2 + \textstyle\sum_{i=1}^n z_i^k). \tag{42}$$

  - Note that z_i^k is the indicator of whether the ith data point is assigned to the kth cluster. (This is because z_i is an indicator vector.)
  - See how we sum the data in cluster k with $\sum_{i=1}^n z_i^k x_i$ and how $\sum_{i=1}^n z_i^k$ counts the number of data in cluster k.
  - So, the optimal variational family is going to be a Gaussian with natural parameters

$$\tilde{\lambda}_1 = \lambda_1 + \textstyle\sum_{i=1}^n \mathrm{E}[z_i^k] x_i \tag{43}$$
$$\tilde{\lambda}_2 = \lambda_2 + \textstyle\sum_{i=1}^n \mathrm{E}[z_i^k] \tag{44}$$

  - Finally, because z_i^k is an indicator, its expectation is its probability, i.e., $q(z_i = k)$.

- It's convenient to specify the Gaussian prior in its mean parameterization, and we need the expectations of the variational posterior for the updates on z_i.
  - The mapping from natural parameters to mean parameters is

$$\mathrm{E}[X] = \eta_1/\eta_2 \tag{45}$$
$$\mathrm{Var}(X) = 1/\eta_2 \tag{46}$$

    (Note: this is an alternative parameterization of the Gaussian, appropriate for the conjugate prior of the unit-variance likelihood. See the exponential family lecture.)
  - So, the variational posterior mean and variance of the cluster component k is

$$\mathrm{E}[\mu_k] = \frac{\lambda_1 + \sum_{i=1}^n \mathrm{E}[z_i^k] x_i}{\lambda_2 + \sum_{i=1}^n \mathrm{E}[z_i^k]} \tag{47}$$
$$\mathrm{Var}(\mu_k) = 1/(\lambda_2 + \textstyle\sum_{i=1}^n \mathrm{E}[z_i^k]) \tag{48}$$

- We'd rather specify a prior mean and variance.
  - For the Gaussian conjugate prior, we map

$$\eta = \langle \mu/\sigma^2, 1/\sigma^2 \rangle. \tag{49}$$

  - This gives the variational update in mean parameter form,

$$\begin{aligned} \mathrm{E}[\mu_k] &= \frac{\mu_0/\sigma_0^2 + \sum_{i=1}^n \mathrm{E}[z_i^k] x_i}{1/\sigma_0^2 + \sum_{i=1}^n \mathrm{E}[z_i^k]} && (50) \\ \mathrm{Var}(\mu_k) &= 1/(1/\sigma_0^2 + \textstyle\sum_{i=1}^n \mathrm{E}[z_i^k]). && (51) \end{aligned}$$

    These are the usual Bayesian updates with the data weighted by its variational probability of being assigned to cluster k.

- The ELBO is the sum of two terms,

$$\left(\sum_{k=1}^K \mathrm{E}[\log p(\mu_k)] + \mathrm{H}(q(\mu_k)) \right) + \left(\sum_{i=1}^n \mathrm{E}[\log p(z_i)] + \mathrm{E}[\log p(x_i \mid z_i, \mu_{1:K})] + \mathrm{H}(q(z_i)) \right).$$

- The expectations in these terms are the following.
  - The expected log prior over mixture locations is

$$\mathrm{E}[\log p(\mu_k)] = -(1/2) \log 2\pi\sigma_0^2 - \mathrm{E}[\mu_k^2]/2\sigma_0^2 + \mathrm{E}[\mu_k]\mu_0/\sigma_0^2 - \mu_0^2/2\sigma_0^2, \tag{52}$$

    where $\mathrm{E}[\mu_k] = \tilde{\mu}_k$ and $\mathrm{E}[\mu_k^2] = \tilde{\sigma}_k^2 + \tilde{\mu}_k^2$.
  - The expected log prior over mixture assignments is not random,

$$\mathrm{E}[\log p(z_i)] = \log(1/K) \tag{53}$$

  - The entropy of each variational location posterior is

$$\mathrm{H}(q(\mu_k)) = (1/2) \log 2\pi\tilde{\sigma}_k^2 + 1/2. \tag{54}$$

    If you haven't seen this, work it out at home by computing $-\mathrm{E}[\log q(\mu_k)]$.
  - The entropy of each variational assignment posterior is

$$\mathrm{H}(q(z_i)) = -\sum_{k=1}^K \phi_{ij} \log \phi_{ij} \tag{55}$$

- Now we can describe the coordinate ascent algorithm.
  - We are given data $x_{1:n}$, hyperparameters μ_0 and σ_0^2, and a number of groups K.

- The variational distributions are
  - n variational multinomials $q(z_i)$
  - K variational Gaussians $q(\mu_k \mid \tilde{\mu}_k, \tilde{\sigma}_k^2)$.
- Repeat until the ELBO converges:
  1. For each data point x_i
     - Update the variational multinomial $q(z_i)$ from Equation 40.
  2. For each cluster $k = 1 \dots K$
     - Update the mean and variance from Equation 50 and Equation 51.

- We can obtain a posterior decomposition of the data.
  - Points are assigned to $\arg\max_k \phi_{i,k}$.
  - Cluster means are estimated as $\tilde{\mu}_k$.

- We can approximate the predictive distribution with a mixture of Gaussians, each at the expected cluster mean. This is

$$p(x_{\text{new}} \mid x_{1:n}) \approx \frac{1}{K} \sum_{k=1}^{K} p(x_{\text{new}} \mid \tilde{\mu_k}), \tag{56}$$

  where $p(x \mid \tilde{\mu_k})$ is a Gaussian with mean $\tilde{\mu_k}$ and unit variance.

9 Multivariate mixtures of Gaussians

- We adjust the algorithm (slightly) when the data are multivariate. Assume the observations $x_{1:n}$ are p-dimensional and, thus, so are the mixture locations $\mu_{1:K}$.

- The multinomial update on Z_i is

$$q^*(z_i = k) \propto \exp\{\log \pi_k + x_i \mathrm{E}[\mu_k] - \mathrm{E}[\mu_k^\top \mu_k]/2\}. \tag{57}$$

- The expected log prior over mixture locations is

$$\mathrm{E}[\log p(\mu_k)] = -(p/2) \log 2\pi\sigma_0^2 - \mathrm{E}[\mu_k^\top \mu_k]/2\sigma_0^2 + \mathrm{E}[\mu_k]^\top \mu_0/\sigma_0^2 - \mu_0^\top \mu_0/2\sigma_0^2, \tag{58}$$

  where $\mathrm{E}[\mu_k] = \tilde{\mu}_k$ and $\mathrm{E}[\mu_k^\top \mu_k] = p\tilde{\sigma}_k^2 + \tilde{\mu}_k^\top \tilde{\mu}_k$.

- The entropy of the Gaussian is

$$\mathrm{H}(q(\mu_k)) = (p/2) \log 2\pi\tilde{\sigma}_k^2 + p/2. \tag{59}$$