Approximate Inference: Variational Bayes Inference (1)

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Probabilistic Machine Learning (CS772A)

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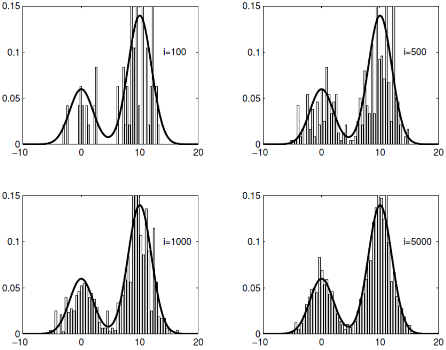
Sampling based Methods

- Approximate a distribution by a set of randomly drawn samples



Target distribution and histogram of the MCMC samples at different iteration points.

Picture courtesy: An Introduction to MCMC for Machine Learning (Andrieu et al, 2003)

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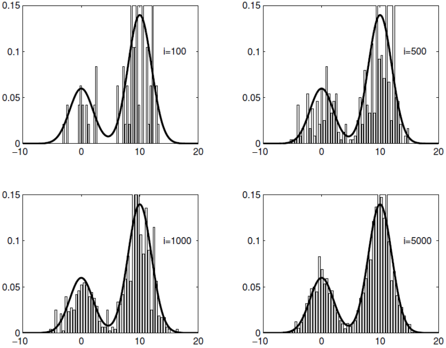

Target distribution and histogram of the MCMC samples at different iteration points.

- Compute quantities that depend on this distribution by averaging using these samples

$$p(y_*|\boldsymbol{x}_*) = \mathbb{E}_{p(\boldsymbol{w}|\mathbf{X},\boldsymbol{y})}[p(y_*|\boldsymbol{x}_*, \boldsymbol{w})] = \int p(y_*|\boldsymbol{x}_*, \boldsymbol{w})p(\boldsymbol{w}|\mathbf{X}, \boldsymbol{y})d\boldsymbol{w} \approx \frac{1}{L}\sum_{\ell=1}^{L} p(y_*|\boldsymbol{x}_*, \boldsymbol{w}^{(\ell)})$$

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  - Expensive storage-wise (need to store samples) and also at prediction-time (e.g., we need to average using the collected samples)

Variational Bayes (VB) or Variational Inference (VI)

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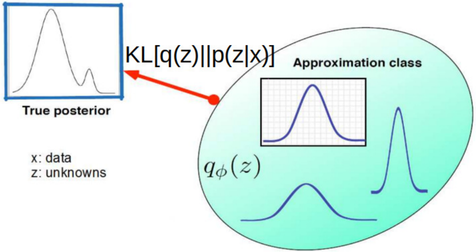

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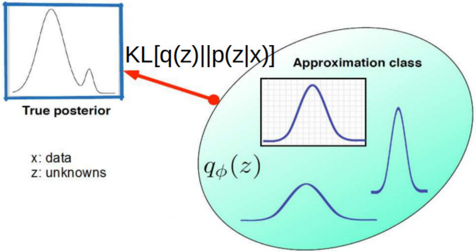

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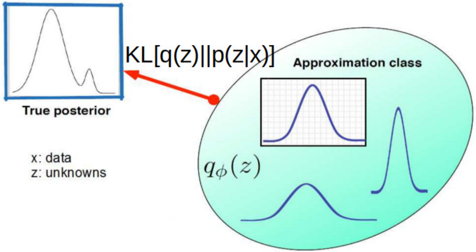

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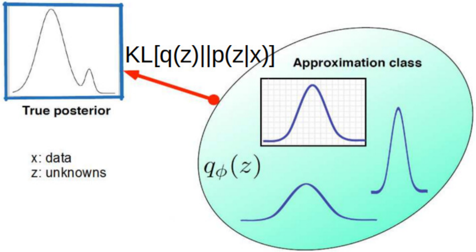

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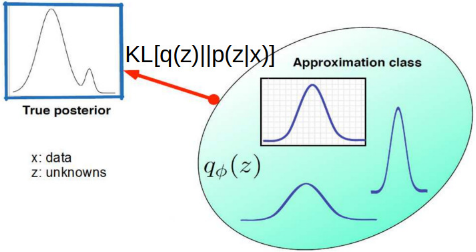

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- **But wait!** We don't know the true distribution $p(\boldsymbol{z}|\boldsymbol{x})$. How to solve the above problem then?

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Variational Bayes (VB) Inference

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- Therefore $\mathcal{L}(q)$ is also known as the **Evidence Lower Bound (ELBO)**

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- Option (1) becomes especially easy if $p(\mathbf{X}|\mathbf{Z})$ and $p(\mathbf{Z})$ are exponential family distributions or if the model is locally conjugate

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- As a short-hand, sometimes we write $q = \prod_{i=1}^{M} q_i$ where $q_i = q(\mathbf{Z}_i|\phi_i)$

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- Under the mean-field assumption, the ELBO simplifies to

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\begin{aligned}
\mathcal{L}(q) &= \int q(\mathbf{Z}) \ln \left\{ \frac{p(\mathbf{X}, \mathbf{Z})}{q(\mathbf{Z})} \right\} \mathrm{d}\mathbf{Z} \\
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- Suppose we have N obs. $\mathcal{D} = \{x_1, \ldots, x_N\}$ from a 1-D Gaussian $\mathcal{N}(\mu, \tau)$

$$p(\mathcal{D}|\mu,\tau) = \left(\frac{\tau}{2\pi}\right)^{N/2} \exp\left\{-\frac{\tau}{2}\sum_{n=1}^{N}(x_n-\mu)^2\right\}$$

- Assume the following priors on the mean μ and precision τ

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- Assuming shape-rate parameterization of gamma prior on the precision τ, the variational distribution for the Gaussian's precision (verify):

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The Full Algorithm

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2. Update μ_N, λ_N as follows (depends on a_N, b_N)

$$\begin{aligned}\mu_N &= \frac{\lambda_0\mu_0 + N\bar{x}}{\lambda_0 + N} \\ \lambda_N &= (\lambda_0 + N)\mathbb{E}[\tau]\end{aligned}$$

3. Update a_N, b_N as follows (depends on μ_N, λ_N)

$$\begin{aligned}a_N &= a_0 + \frac{N}{2} \\ b_N &= b_0 + \frac{1}{2}\mathbb{E}_\mu\left[\sum_{n=1}^{N}(x_n - \mu)^2 + \lambda_0(\mu - \mu_0)^2\right]\end{aligned}$$

4. Go to step 2 if not converged

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  - Note: Each ϕ_j usually depends on the other ϕ_i's ($i \neq j$). Co-ordinate ascent/descent like procedure

An Example of Mean-Field VB via ELBO Derivatives

- Let's revisit the Gaussian parameter estimation via explicitly taking derivatives of ELBO
- Suppose $q_\mu(\mu) = \mathcal{N}(\mu|\mu_N, \lambda_N)$ and $q_\tau(\tau) = \text{Gamma}(\tau|a_N, b_N)$
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- Can plug these into Eq 1 and take expectations w.r.t. $q(\mathbf{Z}) = q_\mu(\mu)q_\tau(\tau)$
- Expectations simplify due to the factored form of q (do it as an exercise)
- Finally take derivatives w.r.t. each variational parameter $\mu_N, \lambda_N, a_N, b_N$

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  - Usually considered to be the more direct method
  - The value of $\mathcal{L}$ can be readily calculated (since we have written its full expression in terms of ϕ_i's)
  - Can use the current value of $\mathcal{L}$ (ELBO) to easily check for convergence

Another Example: VB for Linear Regression via ELBO Derivatives

- Consider a Bayesian linear regression model with unknown noise variance α^{-1} (assume λ known)

$$y_i \sim \text{Normal}(x_i^T w, \alpha^{-1}), \quad w \sim \text{Normal}(0, \lambda^{-1} I), \quad \alpha \sim \text{Gamma}(a, b)$$

$$p(y, w, \alpha | x) = p(\alpha) p(w) \prod_{i=1}^{N} p(y_i | x_i, w, \alpha)$$

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- The ELBO $\mathcal{L}(q) = \int q(\mathbf{Z}) \log p(\mathbf{X}, \mathbf{Z}) d\mathbf{Z} - \int q(\mathbf{Z}) \log q(\mathbf{Z}) d\mathbf{Z}$ is

$$\begin{aligned}
\mathcal{L}(a', b', \mu', \Sigma') \quad = \quad & \int q(\alpha) \ln p(\alpha) d\alpha + \int q(w) \ln p(w) dw \\
& + \sum_{i=1}^{N} \int \int q(\alpha) q(w) \ln p(y_i | x_i, w, \alpha) dw d\alpha \\
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- ELBO is now a function of the variational parameters a', b', μ', Σ'

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\mathcal{L}(a', b', \mu', \Sigma') &= (a-1)(\psi(a') - \ln b') - b\frac{a'}{b'} + \text{constant} \\
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- ψ is the digamma function (derivative of log of gamma function)
- Can now take gradients w.r.t. each of a', b', μ', Σ' and estimate these in an alternating fashion

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$$
\begin{aligned}
\mathcal{L}(a', b', \mu', \Sigma') \quad = \quad & (a-1)(\psi(a') - \ln b') - b\frac{a'}{b'} + \text{constant} \\
& -\frac{\lambda}{2}(\mu'^T\mu' + \text{tr}(\Sigma')) + \text{constant} \\
& +\frac{N}{2}(\psi(a') - \ln b') - \sum_{i=1}^{N} \frac{1}{2}\frac{a'}{b'}\left((y_i - x_i^T\mu')^2 + x_i^T\Sigma' x_i\right) + \text{constant} \\
& +a' - \ln b' + \ln\Gamma(a') + (1-a')\psi(a') \\
& +\frac{1}{2}\ln|\Sigma'| + \text{constant}
\end{aligned}
$$

- ψ is the digamma function (derivative of log of gamma function)
- Can now take gradients w.r.t. each of a', b', μ', Σ' and estimate these in an alternating fashion
- This will give us $q(\boldsymbol{w}, \alpha) = \text{Normal}(\boldsymbol{w}|\mu', \Sigma')\text{Gamma}(\alpha|a', b')$

Another Example: VB for Linear Regression via ELBO Derivatives

Inputs: Data and definitions $q(\alpha) = \text{Gamma}(\alpha|a', b')$ and $q(w) = \text{Normal}(w|\mu', \Sigma')$

Output: Values for a', b', μ' and Σ'

1. Initialize a'_0, b'_0, μ'_0 and Σ'_0 in some way
2. For iteration $t = 1, \ldots, T$
   - Update $q(\alpha)$ by setting

$$
\begin{aligned}
a'_t &= a + \frac{N}{2} \\
b'_t &= b + \frac{1}{2}\sum_{i=1}^{N}(y_i - x_i^T\mu'_{t-1})^2 + x_i^T\Sigma'_{t-1}x_i
\end{aligned}
$$

   - Update $q(w)$ by setting

$$
\begin{aligned}
\Sigma'_t &= \left(\lambda I + \frac{a'_t}{b'_t}\sum_{i=1}^{N} x_i x_i^T\right)^{-1} \\
\mu'_t &= \Sigma'_t\left(\frac{a'_t}{b'_t}\sum_{i=1}^{N} y_i x_i\right)
\end{aligned}
$$

   - Evaluate $\mathcal{L}(a'_t, b'_t, \mu'_t, \Sigma'_t)$ to assess convergence (i.e., decide T).

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Mean-Field VB for Exponential Family

- Using method 1, variational post'r for **Z** can be written (only keeping terms that depend on **Z**)

$$\begin{aligned}\ln q^\star(\mathbf{Z}) &= \mathbb{E}_\eta[\ln p(\mathbf{X},\mathbf{Z}|\boldsymbol{\eta})] + \text{const} \\ &= \sum_{n=1}^{N}\left\{\ln h(\mathbf{x}_n,\mathbf{z}_n) + \mathbb{E}[\boldsymbol{\eta}^{\mathrm{T}}]\mathbf{u}(\mathbf{x}_n,\mathbf{z}_n)\right\} + \text{const}\end{aligned}$$

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$$\begin{aligned}\nu_N &= \nu_0 + N \\ \boldsymbol{\chi}_N &= \boldsymbol{\chi}_0 + \sum_{n=1}^{N}\mathbb{E}_{\mathbf{z}_n}[\mathbf{u}(\mathbf{x}_n,\mathbf{z}_n)]\end{aligned}$$

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- Again note that updates of $q(\mathbf{Z})$ and $q(\boldsymbol{\eta})$ are coupled

VB and Expectation Maximization (EM)

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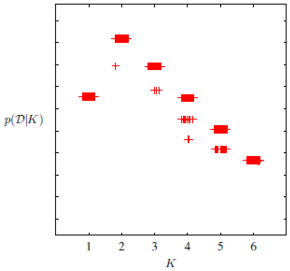
- VB treats all unknowns of the model as latent variables and calls them $\mathbf{Z}$
- Since there is no notion of "parameters", VB is like EM without the "M step"
- VB can be used within an EM algorithm if the E step is intractable
    - This is known as Variational EM algorithm

ELBO for Model Selection

- ELBO can also be used for model selection
- We can compute ELBO for each model and then choose the one with largest value of ELBO
- An Example: The ELBO plot for a Gaussian Mixture Model with different K values

Plot of the variational lower bound $\mathcal{L}$ versus the number K of components in the Gaussian mixture model, for the Old Faithful data, showing a distinct peak at $K = 2$ components. For each value of K, the model is trained from 100 different random starts, and the results shown as '+' symbols plotted with small random horizontal perturbations so that they can be distinguished. Note that some solutions find suboptimal local maxima, but that this happens infrequently.



- Note that unlike likelihood, ELBO doesn't monotonically increase with K (penalizes large K)

Figure courtesy: PRML (Bishop, 2006)

Some Properties of VB

Recall that VB is equivalent to finding q by minimizing $\text{KL}(q||p)$

$$\text{KL}(q\|p) = -\int q(\mathbf{Z}) \ln \left\{ \frac{p(\mathbf{Z})}{q(\mathbf{Z})} \right\} \mathrm{d}\mathbf{Z}$$

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- Underestimates the variances of the true posterior
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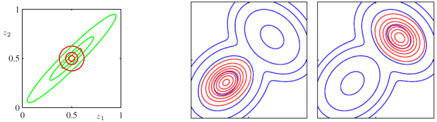

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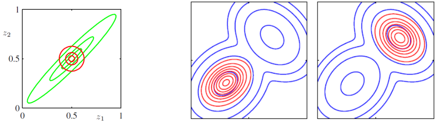

Figure: (Left) Zero-Forcing Property of VB, (Right) For multi-modal posterior, VB locks onto one of the models

Note: Some other inference methods, e.g., Expectation Propagation (EP) can avoid this behavior

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- Implementations of many classic/advanced VB methods available in Stan, Edward, etc.
- VB can be a very useful inference method to apply Bayesian models for large-scale data. A lot of recent work on stochastic (i.e., online) variational inference algorithms that work with small randomly chosen minibatches of data and can easily scale to massive-scale data sets