Approximate Inference: Variational Bayes Inference (2)

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Probabilistic Machine Learning (CS772A)

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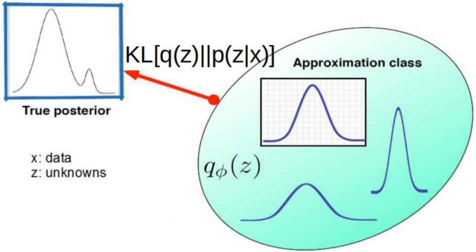
Recap

Variational Bayes (VB) or Variational Inference (VI)

- Assume an approximation class of distributions $\{q(\boldsymbol{z}|\phi)\}$ parameterized by free parameters ϕ
- Approximate the true distribution $p(\boldsymbol{z}|\boldsymbol{x})$ by finding the "closest" $q(\boldsymbol{z}|\phi)$ from this class



Picture courtesy: Modified from the original pic by Shakir Mohamed

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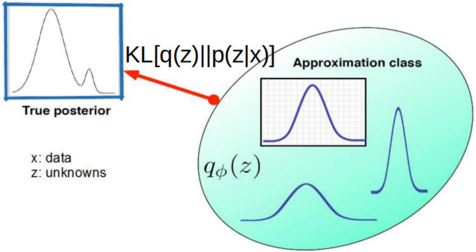

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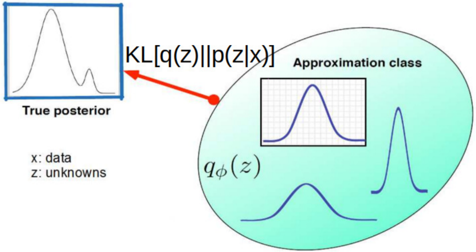

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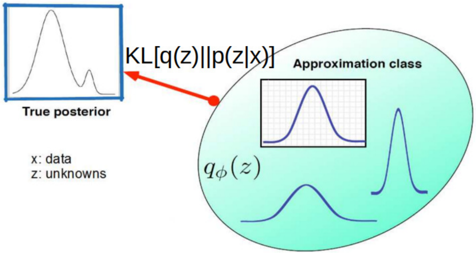

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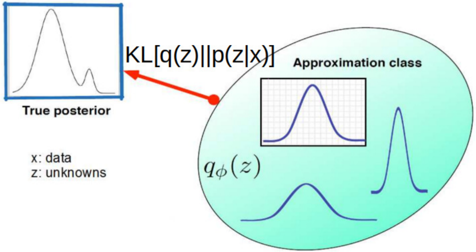

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- Even though we don't know $p(\boldsymbol{z}|\boldsymbol{x})$, we can solve the above problem by maximizing the **ELBO**

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Variational Bayes (VB) Inference

- The key identity central to VB inference is the following (holds for any choice of q)

$$\ln p(\mathbf{X}) = \mathcal{L}(q) + \mathrm{KL}(q\|p)$$

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

VB by Maximizing the ELBO

- VB finds the q distribution that maximizes the ELBO

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  2. Using Monte-Carlo approximation of the expectation/gradient of the ELBO

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- For both cases, deriving mean-field VB updates is easy if the model has local conjugacy

Some Properties of VB

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

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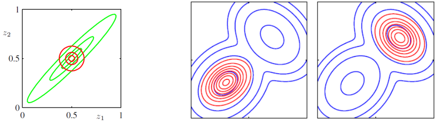
- Underestimates the variances of the true posterior
- For multimodal posteriors, VB locks onto one of the modes



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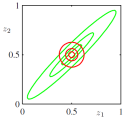

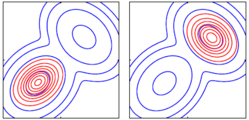

Figure: (Left) Zero-Forcing Property of VB, (Right) For multi-modal posterior, VB locks onto one of the models

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

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  - Based on the idea of Monte-Carlo approximation of the ELBO gradient
- Scaling up VB for large datasets (Stochastic/Online VB)
  - Based on the idea of stochastic optimization techniques

Variational Inference for Non-Conjugate Models

Mean-Field VB for Non-Conjugate Models

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*Black Box Variational Inference - Ranganath et al (2014)

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- Thus ELBO gradient can be written in terms of expectation of gradient of $\log q(\mathbf{Z}|\phi)$
- Given S samples $\{\mathbf{Z}_s\}_{s=1}^S$ from $q(\mathbf{Z}|\phi)$, we can get (noisy) gradient $\nabla_\phi \mathcal{L}(q)$ as follows

$$
\nabla_\phi \mathcal{L}(q) \approx \frac{1}{S} \sum_{s=1}^{S} \nabla_\phi \log q(\mathbf{Z}_s|\phi)(\log p(\mathbf{X}, \mathbf{Z}_s) - \log q(\mathbf{Z}_s|\phi))
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Proof of BBVI Identity

- The ELBO gradient can be written as

$$\nabla_\phi \mathcal{L}(q) = \nabla_\phi \int (\log p(\mathbf{X}, \mathbf{Z}) - \log q(\mathbf{Z}|\phi)) q(\mathbf{Z}|\phi) d\mathbf{Z}$$

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- Recall that BBVI approximates the ELBO gradients by the Monte Carlo expectations

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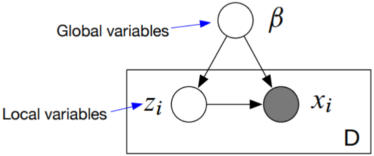
- Some tricks needed to control the variance in the Monte Carlo estimate of the ELBO gradient (if interested in the details, please refer to the BBVI paper)

Scalable (Online) Variational Inference

A Generic Probabilistic Model

- Assume D data points $\mathbf{X} = \{\boldsymbol{x}_1, \ldots, \boldsymbol{x}_D\}$ generated via a probabilistic model



- Assume local latent variables $\mathbf{Z} = \{\boldsymbol{z}_1, \ldots, \boldsymbol{z}_D\}$, one per data point ($\boldsymbol{z}_i$ for $\boldsymbol{x}_i$, $i = 1, \ldots, D$)
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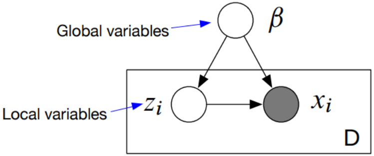

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- The joint distribution for this model admits the following factorization

$$p(\mathbf{X}, \mathbf{Z}, \beta) = p(\beta) \prod_{i=1}^{D} p(x_i, z_i | \beta)$$

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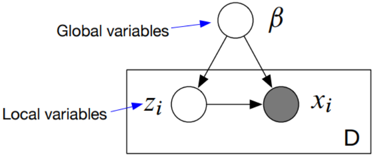

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- Our goal is to infer the posterior distribution $p(\mathbf{Z}, \beta|\mathbf{X})$. Intractable in general.
- Let's approximate $p(\mathbf{Z}, \beta|\mathbf{X})$ using a mean-field distribution $q(\mathbf{Z}, \beta)$

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- Can now do mean-field VB by optimizing w.r.t. $q(\boldsymbol{z}_i)$, $\forall i$, and $q(\beta)$, until convergence

Mean-Field VB

- The basic mean-field VB is a batch algorithm (each iteration operates on all the data)
- Each iteration has to look at every data point $\boldsymbol{x}_i$ and infer the corresponding $q(\boldsymbol{z}_i)$, $\forall i$

Batch variational inference

1. For $i = 1, \ldots, D$, optimize $q(z_i)$
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- This can be very slow is the number of data points D is very large
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- This can be very slow is the number of data points D is very large
  - Before updating the global variables β, we must update all the local variables $\boldsymbol{z}_i$'s
- Would like to have a faster inference algorithm that scales nicely with number of data points

Stochastic Variational Inference (SVI)

- Based on the well-known idea of stochastic optimization

Stochastic Variational Inference - Hoffman et al (2013)

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Stochastic variational inference

1. Randomly select a subset of local data, $S_t \subset \{1, \ldots, D\}$
2. Construct the scaled variational objective function

$$\mathcal{L}_t = \frac{D}{|S_t|} \sum_{i \in S_t} \mathbb{E}_q \left[\ln \frac{p(x_i, z_i | \beta)}{q(z_i)} \right] + \mathbb{E}_q \left[\ln \frac{p(\beta)}{q(\beta)} \right]$$

3. Optimize each $q(z_i)$ in $\mathcal{L}_t$ *only*
4. Update the parameters of $q(\beta|\psi)$ using a gradient step

$$q(\beta|\psi) \quad \rightarrow \quad \psi_t = \psi_{t-1} + \rho_t M_t \nabla_\psi \mathcal{L}_t$$

5. Repeat

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- Note: In step-4, instead of solving for $q(\beta|\psi)$ analytically, we are using a gradient method

Stochastic Variational Inference - Hoffman et al (2013)

ELBO on the Mini-Batch

- The ELBO on the full data

$$\mathcal{L} = \sum_{i=1}^{D} \mathbb{E}_q \left[\ln \frac{p(x_i, z_i|\beta)}{q(z_i)} \right] + \mathbb{E}_q \left[\ln \frac{p(\beta)}{q(\beta)} \right]$$

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- The (scaled) ELBO on the random subset (mini-batch) of the data chosen in iteration t

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- The expectation of the mini-batch ELBO (expectation w.r.t. the random selection of mini-batch)

$$\mathbb{E}_P[\mathcal{L}_t] = \frac{D}{|S_t|}\sum_{i=1}^{D} \underbrace{\mathbb{E}_P[\mathbb{1}(d \in S_t)]}_{P(d\in S_t)}\mathbb{E}_q\left[\ln \frac{p(x_i, z_i|\beta)}{q(z_i)}\right] + \mathbb{E}_q\left[\ln \frac{p(\beta)}{q(\beta)}\right]$$

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- Note that $P(d \in S_t) = \frac{|S_t|}{D}$. Therefore $\mathbb{E}_P[\mathcal{L}_t] = \mathcal{L}$ (this is good news!)

Stochastic Updates for SVI

- For our stochastic update of ψ for updating $q(\beta|\psi)$, i.e., $\psi_t = \psi_{t-1} + \rho_t M_t \nabla_\psi \mathcal{L}_t$

$$\mathbb{E}_P[\psi_t] = \psi_{t-1} + \rho_t M_t \nabla_\psi \mathbb{E}_P[\mathcal{L}_t] (= \psi_{t-1} + \rho_t M_t \nabla_\psi \mathcal{L})$$

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  - Setting $\rho_t = \frac{1}{(t_0+t)^\kappa}$ with $\kappa \in (0.5, 1)$ ensures this. t_0 is some positive number.
- Note that SVI also gives us all the "local" $q(\boldsymbol{z}_i)$ distributions in the normal way. It's only the $q(\beta)$ distribution (which depends on the local distributions) that is inferred in an online fashion

SVI for Exponential Family Distributions

- Assuming the joint distribution of data $\boldsymbol{x}_i$ and local latent var. $\boldsymbol{z}_i$ to be exponential family dist.

$$p(\mathbf{X}, \mathbf{Z}|\beta) = \prod_{i=1}^{D} p(x_i, z_i|\beta) = \left[\prod_{i=1}^{D} h(x_i, z_i)\right] e^{\beta^T \sum_{i=1}^{D} t(x_i, z_i) - DA(\beta)}$$

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$$p(\beta) = f(\xi, \nu) e^{\beta^\top \xi - \nu A(\beta)}$$

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- SVI will basically do stochastic optimization to learn the parameters ξ', ν' of variational distribution
- We will now look at the general form of these updates for a generic model with exp. family dist.

SVI for Exponential Family Distributions

- If we were doing full batch updates for $q(\beta|\psi)$ (where $\psi = [\xi, \nu]$) using gradient methods then

$$\begin{bmatrix} \xi' \\ \nu' \end{bmatrix} \leftarrow \begin{bmatrix} \xi' \\ \nu' \end{bmatrix} + \rho_t M_t \nabla_{(\xi', \nu')} \mathcal{L}$$

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- Plugging in the expressions for exponential family distributions (given on the previous slide)

$$\mathcal{L}_\beta = \mathbb{E}_q[\beta]^T \left(\sum_{i=1}^{D} \mathbb{E}[t(x_i, z_i)] + \xi - \xi' \right) - \mathbb{E}_q[A(\beta)](D + \nu - \nu') + \ln f(\xi', \nu') + \text{const.}$$

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- Note that it requires computing two expectations $\mathbb{E}_q[\beta]$ and $\mathbb{E}_q[A(\beta)]$

SVI for Exponential Family Distributions

- The expectations $\mathbb{E}_q[\beta]$ and $\mathbb{E}_q[A(\beta)]$ can be computed as follows

$$q(\beta) = f(\xi', \nu')\mathrm{e}^{\beta^T \xi' - \nu' A(\beta)}$$

$$\int \nabla_{\xi'} q(\beta) d\beta = 0, \qquad \int \frac{\partial}{\partial \nu'} q(\beta) d\beta = 0$$

$$\mathbb{E}_q[\beta] = -\nabla_{\xi'} \ln f(\xi', \nu'), \qquad \mathbb{E}_q[A(\beta)] = \frac{\partial \ln f(\xi', \nu')}{\partial \nu'}$$

- Exercise: Verify the above (using the fact that $q(\beta)$ is an exp-family dist.)

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- Exercise: Verify the above (using the fact that $q(\beta)$ is an exp-family dist.)
- These can then be plugged into the expression of $\mathcal{L}_\beta$

SVI for Exponential Family Distributions

- ELBO gradient (batch case)

$$\nabla_{(\xi',\nu')}\mathcal{L}_\beta = \begin{bmatrix} \nabla_{\xi'}\mathcal{L}_\beta \\ \frac{\partial}{\partial\nu'}\mathcal{L}_\beta \end{bmatrix} = -\begin{bmatrix} \nabla^2_{\xi'}\ln f(\xi',\nu') & \frac{\partial^2 \ln f(\xi',\nu')}{\partial\nu'\partial\xi} \\ \frac{\partial^2 \ln f(\xi',\nu')}{\partial\nu'\partial\xi'^T} & \frac{\partial^2 \ln f(\xi',\nu')}{\partial\nu'^2} \end{bmatrix} \begin{bmatrix} \sum_{i=1}^D \mathbb{E}_q[t(x_i,z_i)] + \xi - \xi' \\ D + \nu - \nu' \end{bmatrix}$$

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- Since preconditioning matrix is p.s.d., setting gradient to zero gives closed-form batch VB update

$$\xi' = \xi + \sum_{i=1}^D \mathbb{E}[t(x_i,z_i)], \qquad \nu' = \nu + D$$

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- M_t can be set to $\mathbf{I}$. However we can choose M_t sensibly to get a clean update.

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- Our stochastic gradient updates had the form

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$$\begin{bmatrix} \xi'_t \\ \nu'_t \end{bmatrix} = \begin{bmatrix} \xi'_{t-1} \\ \nu'_{t-1} \end{bmatrix} - \rho_t M_t \begin{bmatrix} \nabla^2_{\xi'} \ln f(\xi', \nu') & \frac{\partial^2 \ln f(\xi',\nu')}{\partial \nu' \partial \xi} \\ \frac{\partial^2 \ln f(\xi',\nu')}{\partial \nu' \partial \xi'^T} & \frac{\partial^2 \ln f(\xi',\nu')}{\partial \nu'^2} \end{bmatrix} \begin{bmatrix} \frac{D}{|S_t|} \sum_{i \in S_t} \mathbb{E}[t(x_i, z_i)] + \xi - \xi'_{t-1} \\ D + \nu - \nu'_{t-1} \end{bmatrix}$$

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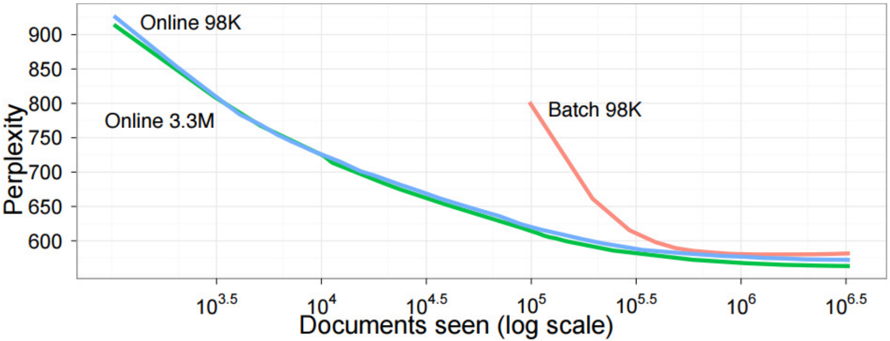
  - This choice makes our stochastic gradient a "natural gradient" (considered to be good direction)

SVI vs Batch Inference

- Online inference methods (e.g., SVI) usually have a faster convergence than batch inference
- Shown below is a plot comparing batch and online inference for topic model (LDA)



(Pic courtesy: David Blei)

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- Implementations of many classic/advanced VB methods available in Stan, Edward, etc.