Variational Inference: Scalability and Recent Advances

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Topics in Probabilistic Modeling and Inference (CS698X)

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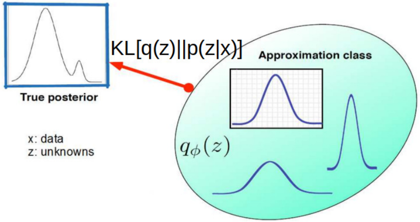
Recap: Variational Inference (VI)

- Approximate an intractable posterior $p(\mathbf{Z}|\mathbf{X})$ by another distribution $q(\mathbf{Z}|\phi)$ by solving

$$\phi^* = \arg\min_{\phi} \text{KL}[q_\phi(\mathbf{Z})||p(\mathbf{Z}|\mathbf{X})] \quad \text{or equivalently} \quad q^*(\mathbf{Z}) = \arg\min_{q \in \mathcal{Q}} \text{KL}[q(\mathbf{Z})||p(\mathbf{Z}|\mathbf{X})]$$



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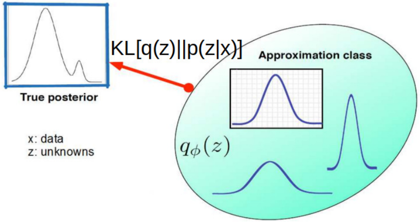

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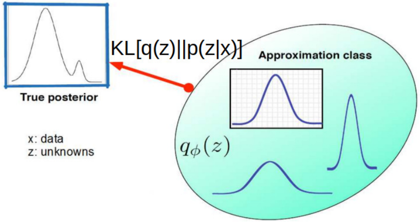

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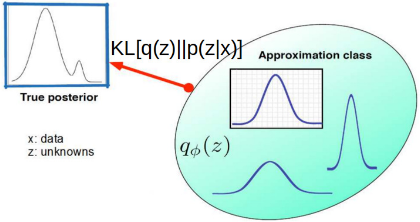

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- VI requires solving an **optimization problem** in general (but closed-form solution exists in some special cases, e.g., mean-field VI in locally-conjugate models)

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- For locally conjugate models, the CP $p(\mathbf{Z}_j|\mathbf{X},\mathbf{Z}_{-j})$ is easy to find, and usually an exp-fam dist.

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.. so its parameters $\phi_j = \mathbb{E}_{i\neq j}[\eta(\mathbf{X},\mathbf{Z}_{-j})]$, i.e., expectation of the natural params of the CP

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- Assume all the distributions in the above to be **exp-family distributions**

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- Note: Each update of global var. params requires waiting for all updates of local var. params

Advances in Variational Inference

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- Other divergences (recall that VI finds optimal q by minimizing the KL divergence $KL(q||p)$)

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- SVI makes the global params λ updates more efficient (note that λ depends on all ϕ_n's)

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6. Set $i = i + 1$. If ELBO not converged, go to Step 2

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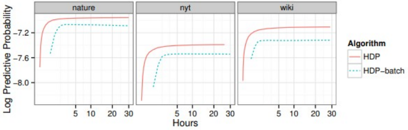

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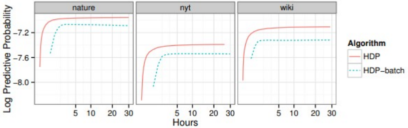

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- Learning rate (κ parameter) and minibatch size is also important (see Hoffman et al for details)

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VI for Non-conjugate Models

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$$-\mathbb{E}_q[\log(1 + \exp(-y_n \boldsymbol{w}^\top \boldsymbol{x}_n))] \geq \log \sigma(\xi_n) + \mathbb{E}_q\left[\frac{1}{2}(y_n \boldsymbol{w}^\top \boldsymbol{x}_n - \xi_n) - \lambda(\xi_n)(\boldsymbol{w}^\top \boldsymbol{x}_n \boldsymbol{x}_n^\top \boldsymbol{w} - \xi_n^2)\right]$$

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

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- Above is also called the "score function" based gradient (also REINFORCE method)

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- The ELBO gradient can be written as

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

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- Note that $\mathbb{E}_q[\nabla_\phi \log q(\mathbf{Z}|\phi)] = \mathbb{E}_q\left[\frac{\nabla_\phi q(\mathbf{Z}|\phi)}{q(\mathbf{Z}|\phi)}\right] = \int \nabla_\phi q(\mathbf{Z}|\phi) d\mathbf{Z} = \nabla_\phi \int q(\mathbf{Z}|\phi) d\mathbf{Z} = \nabla_\phi 1 = 0$
- Also note that $\nabla_\phi q(\mathbf{Z}|\phi) = \nabla_\phi [\log q(\mathbf{Z}|\phi)] q(\mathbf{Z}|\phi)$, using which

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Proof of BBVI Identity

- The ELBO gradient can be written as

$$\begin{aligned}
\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} \\
&= \int \nabla_\phi [(\log p(\mathbf{X},\mathbf{Z}) - \log q(\mathbf{Z}|\phi)) q(\mathbf{Z}|\phi)] d\mathbf{Z} \quad (\nabla \text{ and } \int \text{ interchangeable; dominated convergence theorem}) \\
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- Therefore $\nabla_\phi \mathcal{L}(q) = \mathbb{E}_q[\nabla_\phi \log q(\mathbf{Z}|\phi)(\log p(\mathbf{X},\mathbf{Z}) - \log q(\mathbf{Z}|\phi))]$

Benefits of BBVI

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

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

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- 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)

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* Autoencoding Variational Bayes - Kingma and Welling (2013)

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- Such gradients are called pathwise gradients (we took a "path" from ϵ to $\mathbf{Z}$)

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- Suppose our variational distribution is $q_\phi(\boldsymbol{w}) = \mathcal{N}(\boldsymbol{w}|\mu, \Sigma)$, so $\phi = \{\mu, \Sigma\}$

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$$\nabla_\mu \mathbb{E}_{\mathcal{N}(\boldsymbol{w}|\mu,\Sigma)}[f(\boldsymbol{w})] = \mathbb{E}_{\mathcal{N}(\boldsymbol{v}|0,\mathbf{I})}[\nabla_\mu f(\mu + \mathbf{L}\boldsymbol{v})] \approx \nabla_\mu f(\mu + \mathbf{L}\boldsymbol{v}_s)$$

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Reparametrization Trick: An Example

- Suppose our variational distribution is $q_\phi(\boldsymbol{w}) = \mathcal{N}(\boldsymbol{w}|\mu, \Sigma)$, so $\phi = \{\mu, \Sigma\}$
- Suppose our ELBO has a difficult term $\mathbb{E}_q[f(\boldsymbol{w})]$ (due to the expectation being intractable)
- We are actually interested in its gradient $\nabla_\phi \mathbb{E}_q[f(\boldsymbol{w})]$. Let's use the reparametrization trick
- Reparametrize $\boldsymbol{w}$ as $\boldsymbol{w} = \mu + \mathbf{L}\boldsymbol{v}$ where $\mathbf{L} = \text{chol}(\Sigma)$ and $\boldsymbol{v} \sim \mathcal{N}(0, \mathbf{I})$, and write

$$\nabla_{\mu,\mathbf{L}} \mathbb{E}_{\mathcal{N}(\boldsymbol{w}|\mu,\Sigma)}[f(\boldsymbol{w})] = \nabla_{\mu,\mathbf{L}} \mathbb{E}_{\mathcal{N}(\boldsymbol{v}|0,\mathbf{I})}[f(\mu + \mathbf{L}\boldsymbol{v})] = \mathbb{E}_{\mathcal{N}(\boldsymbol{v}|0,\mathbf{I})}[\nabla_{\mu,\mathbf{L}} f(\mu + \mathbf{L}\boldsymbol{v})]$$

- Now easy to take derivatives w.r.t. variational params $\mu, \mathbf{L}$ using Monte Carlo sampling
- In practice, even one random sample $\boldsymbol{v}_s \sim \mathcal{N}(\boldsymbol{v}|0, \mathbf{I})$ suffices*. So the above gradients will be

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- Note: Std. reparam. trick assumes differentiability but recent work on removing this limitation

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- Standard Reparametrization Trick assumes the model to be differentiable

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- Very active area of research in VI right now!

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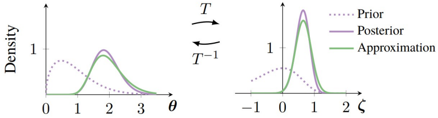
- If we can somehow transform our distributions to unconstrained ones, we can use AD for VI



(a) Latent variable space **(b)** Real coordinate space

$$T : \text{supp}(p(\boldsymbol{\theta})) \to \mathbb{R}^K$$

$$\boldsymbol{\zeta} = T(\boldsymbol{\theta})$$

$$p(\mathbf{x}, \boldsymbol{\zeta}) = p\left(\mathbf{x}, T^{-1}(\boldsymbol{\zeta})\right) \left| \det J_{T^{-1}}(\boldsymbol{\zeta}) \right|$$

Transformed density | Original density | Jacobian of inverse of T

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- Popular in deep probabilistic models such as variational autoencoders, deep Gaussian Processes, etc

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- An even more general form of divergece is f-Divergence

$$D_f(p(\boldsymbol{x})||q(\boldsymbol{x})) = \int q(\boldsymbol{x}) f\left(\frac{p(\boldsymbol{x})}{q(\boldsymbol{x})}\right) d\boldsymbol{x}$$

Other Divergence Measures

- VI minimizes $KL(q||p)$ but other divergences can be minimized as well
- A general form of divergence is Renyi's α-divergence defined as

$$D_\alpha^R(p(\boldsymbol{x})||q(\boldsymbol{x})) = \frac{1}{\alpha - 1}\log\int p(\boldsymbol{x})^\alpha q(\boldsymbol{x})^{1-\alpha}d\boldsymbol{x}$$

- $KL(p||q)$ is a special case with $\alpha \to 1$ (can verify using L'Hopital rule of taking limits)
- An even more general form of divergece is f-Divergence

$$D_f(p(\boldsymbol{x})||q(\boldsymbol{x})) = \int q(\boldsymbol{x})f\left(\frac{p(\boldsymbol{x})}{q(\boldsymbol{x})}\right)d\boldsymbol{x}$$

- Many recent inference algorithms are based on minimizing such divergences

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- Many VI and advanced VI algorithms are implemented in probabilistic programming packages (e.g., Stan, Tensorflow Probability, etc), making VI a painless exercise even for complex models
- Still a very active area of research, especially for doing VI in complex models
  - Models with discrete latent variables
  - Reducing the variance in Monte-Carlo estimate of ELBO gradients