Stochastic Gradients of ELBO

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Outline

1. Models with Latent Variables
2. Score Function Gradients of the ELBO
3. Pathwise Gradients of the ELBO
4. Amortized Inference

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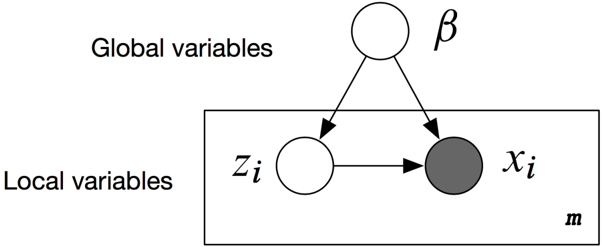
A Generic Class of Models



$$p(\beta, \mathbf{Z}, \mathbf{X}) = p(\beta) \prod_{i=1}^{m} p(\mathbf{z}_i, \mathbf{x}_i | \beta)$$

- The observations are $\mathbf{X} = \{\mathbf{x}_1, \ldots, \mathbf{x}_m\}$
- The local variables are $\mathbf{Z} = \{\mathbf{z}_1, \ldots, \mathbf{z}_m\}$
- The global variables are β
- The i-th data point $\mathbf{x}_i$ only depends on $\mathbf{z}_i$ and β
- Our aim:

$$\text{Compute } \; p(\beta, \mathbf{Z} | \mathbf{X})$$

- The observations are $\mathbf{X} = \{\mathbf{x}_1, \ldots, \mathbf{x}_m\}$
- The local variables are $\mathbf{Z} = \{\mathbf{z}_1, \ldots, \mathbf{z}_m\}$
- Example: GMM with
  - $\mathbf{X} = \{\mathbf{x}_1, \ldots, \mathbf{x}_m\}$ — observations from

$$p(\mathbf{x}) = \sum_{k=1}^{K} p(\mathbf{z} = k|\beta) \cdot p(\mathbf{x}|\mathbf{z} = k, \beta)$$

    with $p(\mathbf{x}|\mathbf{z} = k, \beta) = \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$
  - Unknown latent variables $\mathbf{Z} = \{\mathbf{z}_1, \ldots, \mathbf{z}_m\}$ with a distribution $p(\mathbf{z} = k|\beta) = \pi_k,\ k = 1, \ldots, K$
  - Unknown parameters $\beta = \{\pi_k, \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k\}_{k=1}^{K}$

$$p(\beta, \mathbf{Z}, \mathbf{X}) = p(\beta) \prod_{i=1}^{m} p(\mathbf{z}_i, \mathbf{x}_i|\beta)$$

- Not to overburden slides with notations we consider just

$$p(\mathbf{x}, \mathbf{z})$$

- Our model — joint distribution of
  - observations $\mathbf{x}$
  - and latent variables $\mathbf{z}$
- Out aim is to estimate $p(\mathbf{z}|\mathbf{x})$
- Variational Bayes

$$q^* = \arg\min_{q \in Q} KL(q(\cdot)||p(\cdot|\mathbf{x}))$$

- Variational Evidence Lower Bound (ELBO)

$$KL(q(\cdot)||p(\cdot|\mathbf{x})) =$$
$$= \log p(\mathbf{x}) - \underbrace{\int q(\mathbf{z}) \log \frac{p(\mathbf{x}, \mathbf{z})}{q(\mathbf{z})} d\mathbf{z}}_{\text{ELBO } \mathcal{L}(q)} \geq 0$$

- Thus $\log p(\mathbf{x}) \geq \mathcal{L}(q)$, and so we define

$$q^* = \arg\max_{q \in Q} \mathcal{L}(q)$$

- We start with a model $p(\mathbf{z}, \mathbf{x})$
- We choose a variational approximation $q(\mathbf{z}|\boldsymbol{\theta})$
- We write down the ELBO

$$\begin{aligned}\mathcal{L}(\boldsymbol{\theta}) &= \int q(\mathbf{z}|\boldsymbol{\theta}) \log \frac{p(\mathbf{x}, \mathbf{z})}{q(\mathbf{z}|\boldsymbol{\theta})} d\mathbf{z} \\ &= \mathbb{E}_{q(\mathbf{z}|\boldsymbol{\theta})}[\log p(\mathbf{x}, \mathbf{z}) - \log q(\mathbf{z}|\boldsymbol{\theta})] \to \max_{\boldsymbol{\theta}}\end{aligned}$$

- Data pairs $\{(\mathbf{x}_i, y_i)\}_{i=1}^m$
- Inputs $\mathbf{x}_i$
- Output labels y_i
- $\mathbf{z}$ is a regression coefficient
- Generative process

Step 1: $p(\mathbf{z}) \sim \mathcal{N}(0, 1)$

Step 2: $p(y_i|\mathbf{x}_i, \mathbf{z}) \sim \mathrm{Bernoulli}(\sigma(\mathbf{z}\mathbf{x}_i)),\ i = 1, \ldots, m$

- Assume:
  - We have one data point $(y, \mathbf{x})$ $(m = 1)$
  - $\mathbf{x}$ is a scalar
  - The approximating family q is the normal, i.e.

$$q(\mathbf{z}|\boldsymbol{\theta}) = \mathcal{N}(\mathbf{z}|\mu, \sigma^2),\ \boldsymbol{\theta} = (\mu, \sigma)$$

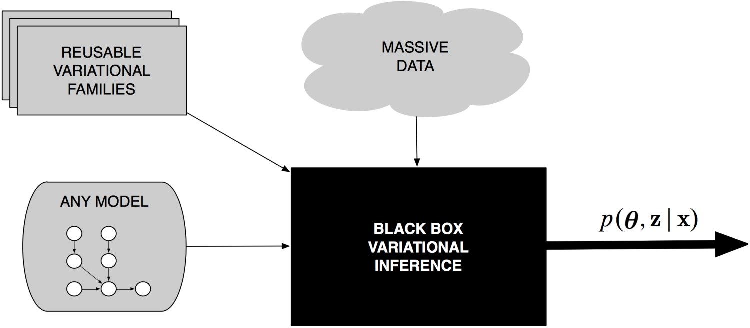
- The ELBO is

$$\begin{aligned}\mathcal{L}(\mu, \sigma^2) &= \mathbb{E}_{\mathbf{z}\sim q}\left[\log p(y, \mathbf{z}|\mathbf{x}) - \log q(\mathbf{z})\right] \\ &= \mathbb{E}_q\left[\log p(\mathbf{z}) + \log p(y|\mathbf{x}, \mathbf{z}) - \log q(\mathbf{z})\right]\end{aligned}$$

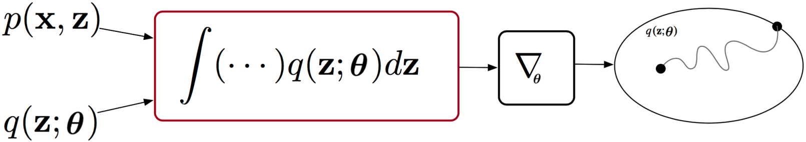
$$
\begin{aligned}
&\mathcal{L}(\mu, \sigma^2) = \\
&= \mathbb{E}_{\mathbf{z}\sim q}[\log p(\mathbf{z}) - \log q(\mathbf{z}) + \log p(y|\mathbf{x}, \mathbf{z})] \\
&= -\frac{1}{2}(\mu^2 + \sigma^2) + \frac{1}{2}\log \sigma^2 + \mathbb{E}_{\mathbf{z}\sim q}[\log p(y|\mathbf{x}, \mathbf{z})] + \mathrm{const} \\
&= -\frac{1}{2}(\mu^2 + \sigma^2) + \frac{1}{2}\log \sigma^2 + \mathbb{E}_{\mathbf{z}\sim q}[y\mathbf{x}\mathbf{z} - \log(1 + \exp(\mathbf{x}\mathbf{z}))] + \mathrm{const} \\
&= -\frac{1}{2}(\mu^2 + \sigma^2) + \frac{1}{2}\log \sigma^2 + y\mathbf{x}\mu - \mathbb{E}_{\mathbf{z}\sim q(\cdot|\boldsymbol{\theta})}[\log(1 + \exp(\mathbf{x}\mathbf{z}))] + \mathrm{const}
\end{aligned}
$$

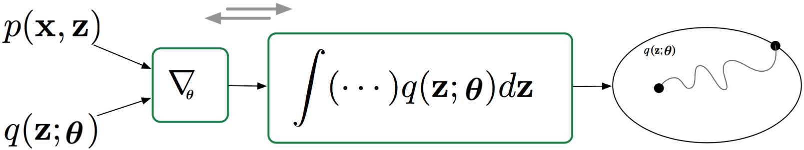
- We cannot analytically take that expectation
- The expectation hides the objectives dependence on the variational parameters $\boldsymbol{\theta} = (\mu, \sigma)$. This makes it hard to directly optimize

Black Box Variational Inference (BBVI)



The Problem in the Classical VI Recipe





Use stochastic optimization!

- Define

$$g(\mathbf{z}, \boldsymbol{\theta}) = \log p(\mathbf{x}, \mathbf{z}) - \log q(\mathbf{z}|\boldsymbol{\theta})$$

- Gradient?

$$\begin{aligned}
\nabla_{\boldsymbol{\theta}} \mathcal{L} &= \nabla_{\boldsymbol{\theta}} \int q(\mathbf{z}|\boldsymbol{\theta}) g(\mathbf{z}, \boldsymbol{\theta}) d\mathbf{z} \\
&= \int \left[\nabla_{\boldsymbol{\theta}} q(\mathbf{z}|\boldsymbol{\theta}) \cdot g(\mathbf{z}, \boldsymbol{\theta}) + q(\mathbf{z}|\boldsymbol{\theta}) \nabla_{\boldsymbol{\theta}} g(\mathbf{z}, \boldsymbol{\theta})\right] d\mathbf{z} \\
&= \int \left[q(\mathbf{z}|\boldsymbol{\theta}) \frac{\nabla_{\boldsymbol{\theta}} q(\mathbf{z}|\boldsymbol{\theta})}{q(\mathbf{z}|\boldsymbol{\theta})} \cdot g(\mathbf{z}|\boldsymbol{\theta}) + q(\mathbf{z}|\boldsymbol{\theta}) \nabla_{\boldsymbol{\theta}} g(\mathbf{z}, \boldsymbol{\theta})\right] d\mathbf{z} \\
&= \int \left[q(\mathbf{z}|\boldsymbol{\theta}) \nabla_{\boldsymbol{\theta}} \log q(\mathbf{z}|\boldsymbol{\theta}) \cdot g(\mathbf{z}|\boldsymbol{\theta}) + q(\mathbf{z}|\boldsymbol{\theta}) \nabla_{\boldsymbol{\theta}} g(\mathbf{z}, \boldsymbol{\theta})\right] d\mathbf{z} \\
&= \int q(\mathbf{z}|\boldsymbol{\theta}) \left[\nabla_{\boldsymbol{\theta}} \log q(\mathbf{z}|\boldsymbol{\theta}) \cdot g(\mathbf{z}|\boldsymbol{\theta}) + \nabla_{\boldsymbol{\theta}} g(\mathbf{z}, \boldsymbol{\theta})\right] d\mathbf{z} \\
&= \mathbb{E}_{q(\mathbf{z}|\boldsymbol{\theta})} \left[\nabla_{\boldsymbol{\theta}} \log q(\mathbf{z}|\boldsymbol{\theta}) \cdot g(\mathbf{z}|\boldsymbol{\theta}) + \nabla_{\boldsymbol{\theta}} g(\mathbf{z}, \boldsymbol{\theta})\right]
\end{aligned}$$

Approaches

- Score Function Gradients
- Pathwise Gradients
- Amortized Inference

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- Recall

$$\nabla_{\boldsymbol{\theta}} \mathcal{L} = \mathbb{E}_{q(\mathbf{z}|\boldsymbol{\theta})}[\nabla_{\boldsymbol{\theta}} \log q(\mathbf{z}|\boldsymbol{\theta}) g(\mathbf{z}, \boldsymbol{\theta}) + \nabla_{\boldsymbol{\theta}} g(\mathbf{z}, \boldsymbol{\theta})]$$

- We get that

$$\int q(\mathbf{z}|\boldsymbol{\theta}) d\mathbf{z} = 1 \Rightarrow \nabla_{\boldsymbol{\theta}} \int q(\mathbf{z}|\boldsymbol{\theta}) d\mathbf{z} = 0 \Rightarrow \int \nabla_{\boldsymbol{\theta}} q(\mathbf{z}|\boldsymbol{\theta}) d\mathbf{z} = 0$$

$$\int \frac{\nabla_{\boldsymbol{\theta}} q(\mathbf{z}|\boldsymbol{\theta})}{q(\mathbf{z}|\boldsymbol{\theta})} \cdot q(\mathbf{z}|\boldsymbol{\theta}) d\mathbf{z} = 0 \Rightarrow \int [\nabla_{\boldsymbol{\theta}} \log q(\mathbf{z}|\boldsymbol{\theta})] \cdot q(\mathbf{z}|\boldsymbol{\theta}) d\mathbf{z} = 0$$

$$\mathbb{E}_q[\nabla_{\boldsymbol{\theta}} \log q(\mathbf{z}|\boldsymbol{\theta})] = 0$$

- Since $g(\mathbf{z}, \boldsymbol{\theta}) = \log p(\mathbf{x}, \mathbf{z}) - \log q(\mathbf{z}|\boldsymbol{\theta})$, then

$$\nabla_{\boldsymbol{\theta}} g(\mathbf{z}, \boldsymbol{\theta}) = -\nabla_{\boldsymbol{\theta}} \log q(\mathbf{z}|\boldsymbol{\theta})$$

$$\mathbb{E}_q[\nabla_{\boldsymbol{\theta}} g(\mathbf{z}, \boldsymbol{\theta})] = -\mathbb{E}_q[\nabla_{\boldsymbol{\theta}} \log q(\mathbf{z}|\boldsymbol{\theta})] = 0$$

- We get the gradient

$$\nabla_{\boldsymbol{\theta}} \mathcal{L} = \mathbb{E}_{q(\mathbf{z}|\boldsymbol{\theta})}[\{\nabla_{\boldsymbol{\theta}} \log q(\mathbf{z}|\boldsymbol{\theta})\} \cdot g(\mathbf{z}, \boldsymbol{\theta})]$$

$$\nabla_{\boldsymbol{\theta}} \mathcal{L} = \mathbb{E}_{q(\mathbf{z}|\boldsymbol{\theta})}[\nabla_{\boldsymbol{\theta}} \{\log q(\mathbf{z}|\boldsymbol{\theta})\} \cdot (\log p(\mathbf{x}, \mathbf{z}) - \log q(\mathbf{z}|\boldsymbol{\theta}))]$$

Sometimes called likelihood ratio or REINFORCE gradients

- Gradient

$$\mathbb{E}_{q(\mathbf{z}|\boldsymbol{\theta})}[\nabla_{\boldsymbol{\theta}} \log q(\mathbf{z}|\boldsymbol{\theta}) \cdot (\log p(\mathbf{x}, \mathbf{z}) - \log q(\mathbf{z}|\boldsymbol{\theta}))]$$

- Noisy unbiased gradients with Monte Carlo!

$$\frac{1}{S} \sum_{s=1}^{S} \nabla_{\boldsymbol{\theta}} \log q(\mathbf{z}_s|\boldsymbol{\theta}) \cdot (\log p(\mathbf{x}, \mathbf{z}_s) - \log q(\mathbf{z}_s|\boldsymbol{\theta})),$$

where $\mathbf{z}_s \sim q(\mathbf{z}|\boldsymbol{\theta})$

Basic Black Box Variational Inference

- **Input**: Model $\log p(\mathbf{x}, \mathbf{z})$, variational approximation $q(\mathbf{z}|\boldsymbol{\theta})$
- **Output**: Variational Parameters $\boldsymbol{\theta}$
- **while** not converged **do**
- $\mathbf{z}_s \sim q(\cdot|\boldsymbol{\theta})$ — Draw S samples from q
- $\rho = t$-th value of a Robbins Monro sequence
- We update

$$\boldsymbol{\theta} \Leftarrow \boldsymbol{\theta} + \rho \frac{1}{S} \sum_{s=1}^{S} \nabla_{\boldsymbol{\theta}} \log q(\mathbf{z}_s|\boldsymbol{\theta}) \cdot (\log p(\mathbf{x}, \mathbf{z}_s) - \log q(\mathbf{z}_s|\boldsymbol{\theta}))$$

- **end**

- The noisy gradient:

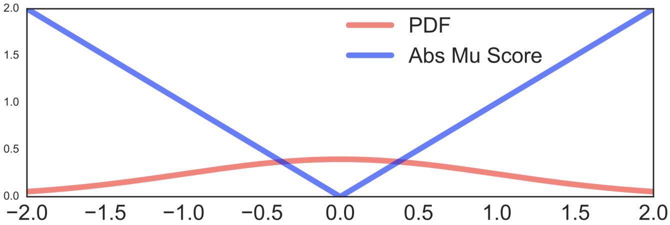
$$\frac{1}{S}\sum_{s=1}^{S} \nabla_{\boldsymbol{\theta}} \log q(\mathbf{z}_s|\boldsymbol{\theta})(\log p(\mathbf{x}, \mathbf{z}_s) - \log q(\mathbf{z}_s|\boldsymbol{\theta})),$$

where $\mathbf{z}_s \sim q(\mathbf{z}|\boldsymbol{\theta})$

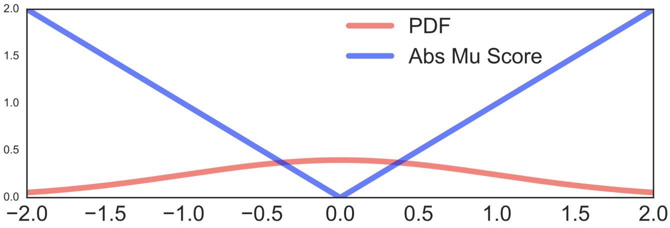
- To compute the noisy gradient of the ELBO we need
  - Sampling from $q(\mathbf{z}|\boldsymbol{\theta})$
  - Evaluating $\nabla_{\boldsymbol{\theta}} \log q(\mathbf{z}|\boldsymbol{\theta})$
  - Evaluating $\log p(\mathbf{x}, \mathbf{z})$ and $\log q(\mathbf{z}|\boldsymbol{\theta})$
- There is no model specific work: black box criteria are satisfied!

Variance of the gradient can be a problem

$$\mathrm{Var}_{q(\mathbf{x}|\boldsymbol{\theta})} = \mathbb{E}_{q(\mathbf{z}|\boldsymbol{\theta})}[(\nabla_{\boldsymbol{\theta}} \log q(\mathbf{z}|\boldsymbol{\theta})(\log p(\mathbf{x},\mathbf{z}) - \log q(\mathbf{z}|\boldsymbol{\theta})) - \nabla_{\boldsymbol{\theta}}\mathcal{L})^2]$$



Intuition: Sampling rare values can lead to large scores and thus high variance



Replace f with $\widehat{f}$ where $\mathbb{E}[\widehat{f}(\mathbf{z})] = \mathbb{E}[f(\mathbf{z})]$. General class

$$\widehat{f}(\mathbf{z}) = f(\mathbf{z}) - a(h(\mathbf{z}) - \mathbb{E}[h(\mathbf{z})])$$

- For variational inference we need functions with known q expectation
- Set h as $\nabla_{\boldsymbol{\theta}} \log q(\mathbf{z}|\boldsymbol{\theta})$
- Simple as $\mathbb{E}_q[\nabla_{\boldsymbol{\theta}} \log q(\mathbf{z}|\boldsymbol{\theta})] = 0$ for any q

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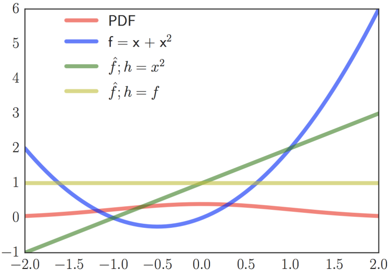
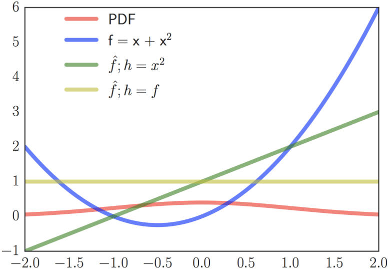


- h is a function of our choice
- a is chosen to minimize the variance
- Good h have high correlation with the original function f

Replace f with $\widehat{f}$ where $EE[\widehat{f}(\mathbf{z})] = \mathbb{E}[f(\mathbf{z})]$. General class

$$\widehat{f}(\mathbf{z}) = f(\mathbf{z}) - a(h(\mathbf{z}) - \mathbb{E}[h(\mathbf{z})])$$

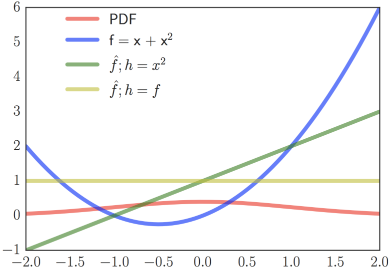


Many of the other techniques from Monte Carlo can help:

- For variational inference we need functions with known q expectation
- Set h as $\nabla_{\boldsymbol{\theta}} \log q(\mathbf{z}|\boldsymbol{\theta})$
- Simple as $\mathbb{E}_q[\nabla_{\boldsymbol{\theta}} \log q(\mathbf{z}|\boldsymbol{\theta})] = 0$ for any q

Replace f with $\widehat{f}$ where $\mathbb{E}[\widehat{f}(\mathbf{z})] = \mathbb{E}[f(\mathbf{z})]$. General class

$$\widehat{f}(\mathbf{z}) = f(\mathbf{z}) - a(h(\mathbf{z}) - \mathbb{E}[h(\mathbf{z})])$$



Many of the other techniques from Monte Carlo can help:

- Importance Sampling, Quasi Monte Carlo, Rao-Blackwellization

- The current black box criteria
  - Sampling from $q(\mathbf{z}|\boldsymbol{\theta})$
  - Evaluating $\nabla_{\boldsymbol{\theta}} \log q(\mathbf{z}|\boldsymbol{\theta})$
  - Evaluating $\log p(\mathbf{x}, \mathbf{z})$ and $\log q(\mathbf{z}|\boldsymbol{\theta})$
- Can we make additional assumptions that are not too restrictive?

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Assume

1. Let $\mathbf{z} \sim q(\mathbf{z}|\boldsymbol{\theta})$ can be realized as $\mathbf{z} = t(\boldsymbol{\epsilon}, \boldsymbol{\theta})$ for some r.v. $\boldsymbol{\epsilon} \sim s(\boldsymbol{\epsilon})$. Example:

$$
\begin{aligned}
&\epsilon \sim \mathcal{N}(0, 1) \\
&z = \epsilon\sigma + \mu \quad \Rightarrow z \sim \mathcal{N}(z|\mu, \sigma^2)
\end{aligned}
$$

2. $\log p(\mathbf{x}, \mathbf{z})$ and $\log q(\mathbf{z}|\boldsymbol{\theta})$ are differentiable with respect to $\mathbf{z}$

- Let us for $\boldsymbol{\mu} \in \mathbb{R}^p$, $\boldsymbol{\Sigma} = \operatorname{diag}(\sigma_1^2, \dots, \sigma_p^2)$ set

$$q(\mathbf{z}|\boldsymbol{\theta}) = \mathcal{N}(\mathbf{z}|\boldsymbol{\mu}, \boldsymbol{\Sigma}),\ \boldsymbol{\theta} = (\boldsymbol{\mu}, \boldsymbol{\Sigma})$$

- Thus

$$\mathbf{z} = \boldsymbol{\mu} + \boldsymbol{\Sigma}^{1/2}\boldsymbol{\epsilon},\ \boldsymbol{\epsilon} \sim \mathcal{N}(\boldsymbol{\epsilon}|\mathbf{0}, \mathrm{I})$$

- Since

$$\begin{aligned}
\log q(\mathbf{z}|\boldsymbol{\theta}) &= -\frac{1}{2}\log\det\boldsymbol{\Sigma} - \frac{1}{2}(\mathbf{z}-\boldsymbol{\mu})\boldsymbol{\Sigma}^{-1}(\mathbf{z}-\boldsymbol{\mu})^\top + \mathrm{const} \\
&= -\frac{1}{2}\log\prod_{i=1}^{p}\sigma_i^2 - \frac{1}{2}\sum_{i=1}^{p}\frac{(z_i-\mu_i)^2}{\sigma_i^2} + \mathrm{const} \\
&= -\sum_{i=1}^{p}\log\sigma_i - \frac{1}{2}\sum_{i=1}^{p}\frac{(z_i-\mu_i)^2}{\sigma_i^2} + \mathrm{const} \\
&= -\sum_{i=1}^{p}\log\sigma_i - \frac{1}{2}\sum_{i=1}^{p}\epsilon_i^2 + \mathrm{const}
\end{aligned}$$

- We would like to calculate $\nabla_{\boldsymbol{\theta}} \mathbb{E}_{q(\mathbf{z}|\boldsymbol{\theta})}[\log p(\mathbf{x}, \mathbf{z}) - \log q(\mathbf{z}|\boldsymbol{\theta})]$
- We set $\mathbf{z} = \boldsymbol{\mu} + \boldsymbol{\Sigma}^{1/2}\boldsymbol{\epsilon}$ and

$$\log q(\mathbf{z}|\boldsymbol{\theta}) = -\sum_{i=1}^{p} \log \sigma_i - \frac{1}{2}\sum_{i=1}^{p} \epsilon_i^2 + \mathrm{const}$$

- E.g. for $\nabla_{\mu_j}\mathcal{L}(\boldsymbol{\theta})$ we get that

$$\begin{aligned}
\nabla_{\mu_j}\mathcal{L}(\boldsymbol{\theta}) &= \nabla_{\mu_j}\mathbb{E}_{\boldsymbol{\epsilon}}\left[\log p(\mathbf{x}, \boldsymbol{\mu} + \boldsymbol{\Sigma}^{1/2}\boldsymbol{\epsilon}) + \sum_{i=1}^{p} \log \sigma_i + \frac{1}{2}\sum_{i=1}^{p} \epsilon_i^2\right] \\
&= \mathbb{E}_{\boldsymbol{\epsilon}}\left[\nabla_{z_j} \log p(\mathbf{x}, \mathbf{z})\Big|_{\mathbf{z}=\boldsymbol{\mu}+\boldsymbol{\Sigma}^{1/2}\boldsymbol{\epsilon}} \cdot \nabla_{\mu_j}\left(\boldsymbol{\mu} + \boldsymbol{\Sigma}^{1/2}\boldsymbol{\epsilon}\right)\right] \\
&= \mathbb{E}_{\boldsymbol{\epsilon}}\left[\nabla_{z_j} \log p(\mathbf{x}, \mathbf{z})\Big|_{\mathbf{z}=\boldsymbol{\mu}+\boldsymbol{\Sigma}^{1/2}\boldsymbol{\epsilon}}\right] \\
&\approx \frac{1}{S}\sum_{s=1}^{S}\left[\nabla_{z_j} \log p(\mathbf{x}, \mathbf{z})\Big|_{\mathbf{z}_s=\boldsymbol{\mu}+\boldsymbol{\Sigma}^{1/2}\boldsymbol{\epsilon}_s}\right],
\end{aligned}$$

where $\boldsymbol{\epsilon}_s \sim \mathcal{N}(\boldsymbol{\epsilon}|\mathbf{0}, \mathrm{I})$

- Recall that for $g(\mathbf{z}, \boldsymbol{\theta}) = \log p(\mathbf{x}, \mathbf{z}) - \log q(\mathbf{z}|\boldsymbol{\theta})$ we have

$$\nabla_{\boldsymbol{\theta}} \mathcal{L} = \nabla_{\boldsymbol{\theta}} \mathbb{E}_{q(\mathbf{z}|\boldsymbol{\theta})}[g(\mathbf{z}, \boldsymbol{\theta})]$$

- Rewrite using $\mathbf{z} = t(\boldsymbol{\epsilon}, \boldsymbol{\theta})$

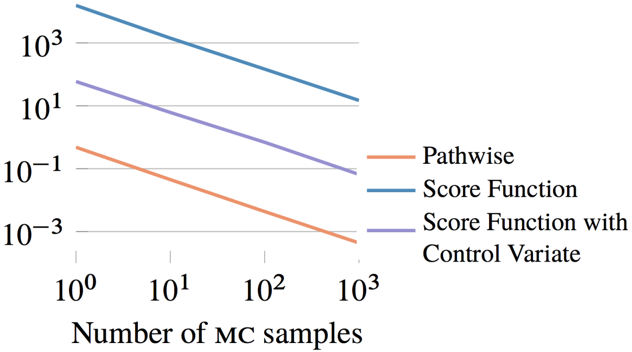
$$\nabla_{\boldsymbol{\theta}} \mathcal{L} = \nabla_{\boldsymbol{\theta}} \mathbb{E}_{\boldsymbol{\epsilon} \sim s(\boldsymbol{\epsilon})}[g(t(\boldsymbol{\epsilon}, \boldsymbol{\theta}), \boldsymbol{\theta})] = \mathbb{E}_{\boldsymbol{\epsilon} \sim s(\boldsymbol{\epsilon})}[\nabla_{\boldsymbol{\theta}} g(t(\boldsymbol{\epsilon}, \boldsymbol{\theta}), \boldsymbol{\theta})]$$

- We get that

$$\begin{aligned}
&\nabla_{\boldsymbol{\theta}} \mathcal{L}(\boldsymbol{\theta}) = \mathbb{E}_{s(\boldsymbol{\epsilon})}[\nabla_{\boldsymbol{\theta}} g(t(\boldsymbol{\epsilon}, \boldsymbol{\theta}), \boldsymbol{\theta})] \\
&= \mathbb{E}_{s(\boldsymbol{\epsilon})} \left[\nabla_{\mathbf{z}} g(\mathbf{z}, \boldsymbol{\theta}) \Big|_{\mathbf{z}=t(\boldsymbol{\epsilon}, \boldsymbol{\theta})} \cdot \nabla_{\boldsymbol{\theta}} t(\boldsymbol{\epsilon}, \boldsymbol{\theta}) + \nabla_{\boldsymbol{\theta}} g(\mathbf{z}, \boldsymbol{\theta}) \Big|_{\mathbf{z}=t(\boldsymbol{\epsilon}, \boldsymbol{\theta})} \right] \\
&= \mathbb{E}_{s(\boldsymbol{\epsilon})} \left[\nabla_{\mathbf{z}} [\log p(\mathbf{x}, \mathbf{z}) - \log q(\mathbf{z}|\boldsymbol{\theta})] \Big|_{\mathbf{z}=t(\boldsymbol{\epsilon}, \boldsymbol{\theta})} \cdot \nabla_{\boldsymbol{\theta}} t(\boldsymbol{\epsilon}, \boldsymbol{\theta}) - \nabla_{\boldsymbol{\theta}} \log q(\mathbf{z}|\boldsymbol{\theta}) \right] \\
&= \mathbb{E}_{s(\boldsymbol{\epsilon})} \left[\nabla_{\mathbf{z}} [\log p(\mathbf{x}, \mathbf{z}) - \log q(\mathbf{z}|\boldsymbol{\theta})] \Big|_{\mathbf{z}=t(\boldsymbol{\epsilon}, \boldsymbol{\theta})} \cdot \nabla_{\boldsymbol{\theta}} t(\boldsymbol{\epsilon}, \boldsymbol{\theta}) \right]
\end{aligned}$$

This is also known as the reparameterization gradient

Variance Comparison



[Kucukelbir+ 2016]

Score Function

- Differentiates the density $\nabla_{\boldsymbol{\theta}} q(\mathbf{z}|\boldsymbol{\theta})$
- Works for discrete and continuous models
- Works for large class of variational approximations
- Variance can be a big problem

Pathwise

- Differentiates the function $\nabla_{\mathbf{z}}[\log p(\mathbf{x}, \mathbf{z}) - \log q(\mathbf{z}|\boldsymbol{\theta})]$
- Requires differentiable models
- Requires variational approximation to have the form $\mathbf{z} = t(\boldsymbol{\epsilon}, \boldsymbol{\theta})$
- Generally better behaved variance

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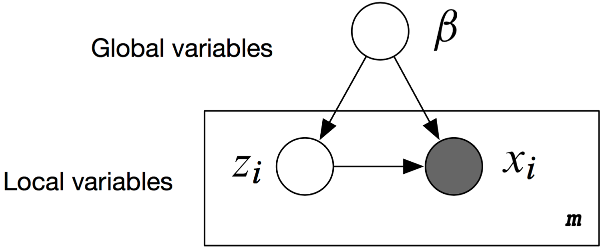
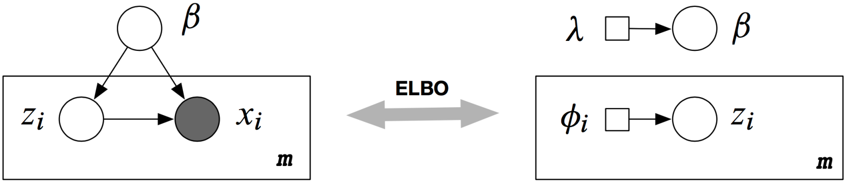


$$p(\beta, \mathbf{Z}, \mathbf{X}) = p(\beta) \prod_{i=1}^{m} p(\mathbf{z}_i, \mathbf{x}_i | \beta)$$

- The observations are $\mathbf{X} = \{\mathbf{x}_1, \dots, \mathbf{x}_m\}$
- The local variables are $\mathbf{Z} = \{\mathbf{z}_1, \dots, \mathbf{z}_m\}$
- The global variables are β


β
z_i
x_i
m
ELBO
λ
β
ϕ_i
z_i
m

- **Input**: data $\mathbf{X}$, model $p(\beta, \mathbf{Z}, \mathbf{X})$
- **Aim**: approximate the posterior $p(\beta, \mathbf{Z}|\mathbf{X})$
- The mean-field family for $\boldsymbol{\theta} = (\lambda, \phi_{1\ldots m})$

$$q(\beta, \mathbf{Z}|\boldsymbol{\theta}) = q(\beta|\lambda)\prod_{i=1}^{m} q(\mathbf{z}_i|\phi_i)$$

- The ELBO has the form

$$\begin{aligned}\mathcal{L}(\boldsymbol{\theta}) &= \mathbb{E}_{q(\beta,\mathbf{Z}|\boldsymbol{\theta})}[\log p(\beta, \mathbf{Z}, \mathbf{X}) - \log q(\beta, \mathbf{Z}|\boldsymbol{\theta})] \\ &= \mathbb{E}_q[\log p(\beta, \mathbf{Z}, \mathbf{X})] - \mathbb{E}_q\left[\log q(\beta|\lambda) + \sum_{i=1}^{m}\log q(\mathbf{z}_i|\phi_i)\right]\end{aligned}$$

- These expectations are no longer tractable
- Inner stochastic optimization needed for each data point
- **Idea**: Learn a mapping f from $\mathbf{x}_i$ to ϕ_i!!!

- ELBO

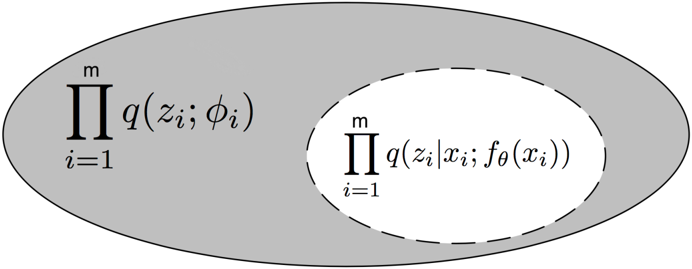
$$\mathcal{L}(\boldsymbol{\theta}) = \mathbb{E}_q[\log p(\beta, \mathbf{Z}, \mathbf{X})] - \mathbb{E}_q\left[\log q(\beta|\lambda) + \sum_{i=1}^{m} q(\mathbf{z}_i|\phi_i)\right]$$

- Amortizing the ELBO with inference network f:

$$\begin{aligned}\mathcal{L}(\boldsymbol{\theta}) = {} & \mathbb{E}_q[\log p(\beta, \mathbf{Z}, \mathbf{X})] - \\ & - \mathbb{E}_q\left[\log q(\beta|\lambda) + \sum_{i=1}^{m} \log q(\mathbf{z}_i|\mathbf{x}_i; \phi_i = f_\theta(\mathbf{x}_i))\right],\end{aligned}$$

here $\boldsymbol{\theta} = (\lambda, \theta)$

- Amortized inference is faster, but admits a smaller class of approximations
- The size of the smaller class depends on the flexibility of f



- If $\log p(\mathbf{x}, \mathbf{z})$ is differentiable w.r.t. $\mathbf{z}$
  - Try out an approximation q that is reparameterizable
- If $\log p(\mathbf{x}, \mathbf{z})$ is not differentiable w.r.t. $\mathbf{z}$
  - Use score function estimator with control variates
  - Add further variance reductions based on experimental evidence
- General Advice:
  - Use coordinate specific learning rates (e.g. RMSProp, AdaGrad)
  - Annealing + Tempering
  - Consider parallelizing across samples from q

- Systems with Variational Inference:
  - Venture, WebPPL, Edward, Stan, PyMC3, Infer.net, Anglican
    Good for trying out lots of models
- Differentiation Tools:
  - Theano, Torch, Tensorflow, Stan Math, Caffe

  Can lead to more scalable implementations of individual models