# ELBO and KL-Divergence 

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## Problem Formulation



Figure: Graphical model to be considered for the latent variable $\mathbf{z}$ and observed variable $\mathbf{x}$. Solid lines denote the generative (decoding) model $p_{\theta}(\mathbf{x}, \mathbf{z})=p_{\theta}(\mathbf{x} \mid \mathbf{z}) p_{\theta}(\mathbf{z})$, while the dashed lines denote the variational approximation (encoding) model $q_{\phi}(\mathbf{z} \mid \mathbf{x})$.

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- Consider a dataset $\mathbf{X}=\left\{\mathbf{x}_{i}\right\}_{i=1}^{N}$ of $N$ i.i.d. samples of some continuous/discrete random variable $\mathbf{x}$.


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## Problem Formulation

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- We assume that the random variable $\mathbf{x}$ is generated from some unobserved/latent continuous random variable $\mathbf{z}$, as shown in Fig 1.


Figure: Graphical model to be considered for the latent variable $\mathbf{z}$ and observed variable $\mathbf{x}$. Solid lines denote the generative (decoding) model $p_{\theta}(\mathbf{x}, \mathbf{z})=p_{\theta}(\mathbf{x} \mid \mathbf{z}) p_{\theta}(\mathbf{z})$, while the dashed lines denote the variational approximation (encoding) model $q_{\phi}(\mathbf{z} \mid \mathbf{x})$.


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We wish to calculate the posterior distribution $p_{\theta}(\mathbf{z} \mid \mathbf{x})$.

## Calculating $p_{\theta}(\mathbf{x})$ is hard

Although we can assume that $p_{\theta}(\mathbf{z})$ and $p_{\theta}(\mathbf{x} \mid \mathbf{z})$ are from some parametric family, getting the posterior distribution $p_{\theta}(\mathbf{z} \mid \mathbf{x})$ is generally intractable due to the integration of the marginal $p_{\theta}(\mathbf{x})=\int p_{\theta}(\mathbf{x} \mid \mathbf{z}) p_{\theta}(\mathbf{z}) d \mathbf{z}$


## Proposed solution



## Proposed solution

In variational inference, we propose a posterior $q_{\phi}(\mathbf{z} \mid \mathbf{x})$ of some parametric form to approximate the generally intractable true posterior $p_{\theta}(\mathbf{z} \mid \mathbf{x})$.


## Methodology

$$
\begin{equation*}
\log p_{\theta}(x)=\mathbb{E}_{\mathbf{z} \sim q_{\phi}\left(\mathbf{z} \mid \mathbf{x}_{i}\right)}\left[\log p_{\theta}(x)\right] \tag{1}
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& =\mathbb{E}_{\mathbf{z} \sim q_{\phi}\left(\mathbf{z} \mid \mathbf{x}_{i}\right)}\left[\log \frac{p_{\theta}(x, z)}{p_{\theta}(z \mid x)}\right] \tag{2}
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& =\mathbb{E}_{\mathbf{z} \sim q_{\phi}\left(\mathbf{z} \mid \mathbf{x}_{i}\right)}\left[\log p_{\theta}(x, z)-\log p_{\theta}(z \mid x)-\log q_{\phi}(z \mid x)+\log q_{\phi}(z \mid x)\right] \tag{3}
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& =\mathbb{E}_{\mathbf{z} \sim q_{\phi}\left(\mathbf{z} \mid x_{i}\right)}\left[\log \frac{p_{\theta}(x, z)}{q_{\phi}(z \mid x)}+\log \frac{q_{\phi}(z \mid x)}{p_{\theta}(z \mid x)}\right] \tag{4}
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& =\mathbb{E}_{\mathbf{z} \sim q_{\phi}\left(\mathbf{z} \mid \mathbf{x}_{i}\right)}\left[\log \frac{p_{\theta}(x, z)}{q_{\phi}(z \mid x)}\right]+K L\left[q_{\phi}(z \mid x) \| p_{\theta}(z \mid x)\right] \tag{5}
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& =\mathbb{E}_{\mathbf{z} \sim q_{\phi}\left(z \mid x_{i}\right)}\left[\log \frac{p_{\theta}(x, z)}{q_{\phi}(z \mid x)}\right]+\operatorname{KL}\left[q_{\phi}(z \mid x) \| p_{\theta}(z \mid x)\right]  \tag{5}\\
& \geq \mathbb{E}_{\mathbf{z} \sim q_{\phi}\left(z \mid x_{i}\right)}\left[\log \frac{p_{\theta}(x, z)}{q_{\phi}(z \mid x)}\right]=\operatorname{ELBO}\left(\phi, \theta ; x_{i}\right) \tag{6}
\end{align*}
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## Note:

Maximum value of $\operatorname{ELBO}\left(\phi, \theta ; x_{i}\right)$ is the best possible estimate of $\log p_{\theta}(x)$ with variational posterrior.

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## Alternatively, KL - ELBO relation

$K L\left[q_{\phi}(z \mid x) \| p_{\theta}(z \mid x)\right]=\log p_{\theta}(x)-E L B O\left(\phi, \theta ; x_{i}\right)$ Thus, maximizing $\operatorname{ELBO}\left(\phi, \theta ; x_{i}\right)$ is same as minimizing $K L\left[q_{\phi}(z \mid x) \| p_{\theta}(z \mid x)\right]$

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& =\mathbb{E}_{\mathbf{z} \sim q_{\phi}\left(\mathbf{z} \mid \mathbf{x}_{i}\right)}\left[\log p_{\theta}(x \mid z)\right]-K L\left[q_{\phi}(z \mid x) \| p_{\theta}(z)\right] \tag{9}
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- In Eqn.9, we will differentiate and optimize the ELBO w.r.t. the encoder parameter $\phi$ and decoder parameter $\theta$.


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- While $\nabla_{\theta} E L B O$ is trivial, $\nabla_{\phi} E L B O$ is problematic due to the expected value over $\mathbf{z}$.


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To estimate the gradient of the form $\nabla_{\phi} \mathbb{E}_{\mathbf{z} \sim q_{\phi}(\mathbf{z})}[f(\mathbf{z})]$, we derive a score function $\hat{I}_{1}(\phi)$.

## Maximizing ELBO

$$
\begin{equation*}
\nabla_{\phi} \mathbb{E}_{z \sim q_{\phi}(\mathrm{z})}[f(\mathrm{z})]=\int \nabla_{\phi} q_{\phi}(\mathrm{z}) f(\mathrm{z}) d \mathrm{z} \tag{10}
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& =\mathbb{E}_{\mathbf{z} \sim q_{\phi}(\mathbf{z})}\left[\nabla_{\phi} \log q_{\phi}(\mathbf{z}) f(\mathbf{z})\right]=\mathbb{E}_{\mathbf{z} \sim q_{\phi}(\mathbf{z})}\left[\hat{I}_{1}(\phi)\right] \tag{13}
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& \hat{l}_{1}(\phi)=f(\mathbf{z}) \frac{\partial \log q_{\phi}(\mathbf{z})}{\partial \phi}, \tag{14}
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\end{align*}
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The gradient can be approximated by MC Sampling from $\mathbf{z}_{i} \sim q_{\phi}(\mathbf{z})$.

$$
\begin{equation*}
\nabla_{\phi} \mathbb{E}_{\mathbf{z} \sim q_{\phi}(\mathbf{z})}[f(\mathbf{z})] \approx \frac{1}{M} \sum_{l=1}^{M} f\left(\mathbf{z}_{l}\right) \frac{\partial \log q_{\phi}\left(\mathbf{z}_{l}\right)}{\partial \phi} \tag{15}
\end{equation*}
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- Assuming that we can re-parameterize the random variable $\mathbf{z} \sim q_{\phi}\left(\mathbf{z} \mid \mathbf{x}_{i}\right)$ with a deterministic differentiable transformation $\left(g_{\phi}\right)$ of some parameter-free auxiliary variable $\epsilon$ :


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z=g_{\phi}\left(\mathbf{x}_{i}, \epsilon\right) \text { with } \quad \epsilon \sim p(\epsilon) \tag{16}
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We can estimate with the gradient with the pathwise derivative estimator

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\begin{equation*}
\hat{\imath}_{2}(\phi)=f^{\prime}\left(g_{\phi}\left(\mathbf{x}_{i}, \epsilon\right)\right) \frac{\partial g_{\phi}\left(\mathbf{x}_{i}, \epsilon\right)}{\partial \phi} \tag{17}
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and the gradient can be approximated by

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\begin{equation*}
\nabla_{\phi} \mathbb{E}_{\mathbf{z} \sim q_{\phi}\left(\mathbf{z} \mid \mathbf{x}_{i}\right)}[f(\mathbf{z})] \approx \frac{1}{M} \sum_{l=1}^{M} f^{\prime}\left(g_{\phi}\left(\mathbf{x}_{i}, \epsilon_{l}\right)\right) \frac{\partial g_{\phi}\left(\mathbf{x}_{i}, \epsilon_{l}\right)}{\partial \phi} \tag{18}
\end{equation*}
$$

with $\epsilon_{I} \sim p(\epsilon)$.

## The End

