Deep Generative Models

Lecture 3

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AI Masters

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Recap of Previous Lecture

Jacobian Matrix

Let $\mathbf{f} : \mathbb{R}^m \to \mathbb{R}^m$ be a differentiable function.

$$\mathbf{z} = \mathbf{f}(\mathbf{x}), \quad \mathbf{J} = \frac{\partial \mathbf{z}}{\partial \mathbf{x}} = \begin{pmatrix} \frac{\partial z_1}{\partial x_1} & \cdots & \frac{\partial z_1}{\partial x_m} \\ \vdots & \ddots & \vdots \\ \frac{\partial z_m}{\partial x_1} & \cdots & \frac{\partial z_m}{\partial x_m} \end{pmatrix} \in \mathbb{R}^{m \times m}$$

Change of Variables Theorem (CoV)

Let $\mathbf{x} \in \mathbb{R}^m$ be a random vector with density $p(\mathbf{x})$, and let $\mathbf{f} : \mathbb{R}^m \to \mathbb{R}^m$ be a C^1-diffeomorphism ($\mathbf{f}$ and $\mathbf{f}^{-1}$ are continuously differentiable mappings). If $\mathbf{z} = \mathbf{f}(\mathbf{x})$, then

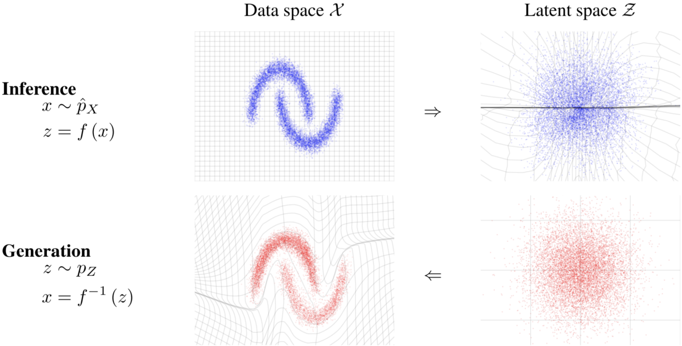
$$p(\mathbf{x}) = p(\mathbf{z}) |\det(\mathbf{J}_\mathbf{f})| = p(\mathbf{z}) \left| \det \left(\frac{\partial \mathbf{z}}{\partial \mathbf{x}} \right) \right| = p(\mathbf{f}(\mathbf{x})) \left| \det \left(\frac{\partial \mathbf{f}(\mathbf{x})}{\partial \mathbf{x}} \right) \right|$$

$$p(\mathbf{z}) = p(\mathbf{x}) |\det(\mathbf{J}_{\mathbf{f}^{-1}})| = p(\mathbf{x}) \left| \det \left(\frac{\partial \mathbf{x}}{\partial \mathbf{z}} \right) \right| = p(\mathbf{f}^{-1}(\mathbf{z})) \left| \det \left(\frac{\partial \mathbf{f}^{-1}(\mathbf{z})}{\partial \mathbf{z}} \right) \right|$$

Recap of Previous Lecture

Definition

A normalizing flow is a C^1-diffeomorphism that transforms data $\mathbf{x}$ to noise $\mathbf{z}$.



Log-Likelihood

$$\log p_{\boldsymbol{\theta}}(\mathbf{x}) = \log p(\mathbf{f}_K \circ \cdots \circ \mathbf{f}_1(\mathbf{x})) + \sum_{k=1}^{K} \log |\det(\mathbf{J}_{\mathbf{f}_k})|$$

Dinh L., Sohl-Dickstein J., Bengio S. Density Estimation Using Real NVP, 2016

Recap of Previous Lecture

Flow Log-Likelihood

$$\log p_{\boldsymbol{\theta}}(\mathbf{x}) = \log p(\mathbf{f}_{\boldsymbol{\theta}}(\mathbf{x})) + \log |\det(\mathbf{J}_{\mathbf{f}})|$$

One significant challenge is efficiently computing the Jacobian determinant.

Linear Flows

$$\mathbf{z} = \mathbf{f}_{\boldsymbol{\theta}}(\mathbf{x}) = \mathbf{W}\mathbf{x}, \quad \mathbf{W} \in \mathbb{R}^{m \times m}, \quad \boldsymbol{\theta} = \mathbf{W}, \quad \mathbf{J}_{\mathbf{f}} = \mathbf{W}^{\top}$$

- LU Decomposition:
$$\mathbf{W} = \mathbf{P}\mathbf{L}\mathbf{U}.$$
- QR Decomposition:
$$\mathbf{W} = \mathbf{Q}\mathbf{R}.$$

Decomposition is performed only once during initialization. Then the decomposed matrices ($\mathbf{P}, \mathbf{L}, \mathbf{U}$ or $\mathbf{Q}, \mathbf{R}$) are optimized.

Kingma D. P., et al. Glow: Generative Flow With Invertible 1x1 Convolutions, 2018
Hoogeboom E., et al. Emerging Convolutions for Generative Normalizing Flows, 2019

Recap of Previous Lecture

Consider an autoregressive model:

$$p_{\boldsymbol{\theta}}(\mathbf{x}) = \prod_{j=1}^{m} p_{\boldsymbol{\theta}}(x_j|\mathbf{x}_{1:j-1}), \quad p_{\boldsymbol{\theta}}(x_j|\mathbf{x}_{1:j-1}) = \mathcal{N}\left(\mu_{j,\boldsymbol{\theta}}(\mathbf{x}_{1:j-1}), \sigma^2_{j,\boldsymbol{\theta}}(\mathbf{x}_{1:j-1})\right).$$

Gaussian Autoregressive Normalizing Flow

$$\mathbf{x} = \mathbf{f}^{-1}_{\boldsymbol{\theta}}(\mathbf{z}) \quad \Rightarrow \quad x_j = \sigma_{j,\boldsymbol{\theta}}(\mathbf{x}_{1:j-1}) \cdot z_j + \mu_{j,\boldsymbol{\theta}}(\mathbf{x}_{1:j-1}).$$

$$\mathbf{z} = \mathbf{f}_{\boldsymbol{\theta}}(\mathbf{x}) \quad \Rightarrow \quad z_j = (x_j - \mu_{j,\boldsymbol{\theta}}(\mathbf{x}_{1:j-1})) \cdot \frac{1}{\sigma_{j,\boldsymbol{\theta}}(\mathbf{x}_{1:j-1})}.$$

- This transformation is both C^1-**diffeomorphism**, mapping $p(\mathbf{z})$ to $p_{\boldsymbol{\theta}}(\mathbf{x})$.
- The Jacobian matrix for this transformation is triangular.

The generative function $\mathbf{f}^{-1}_{\boldsymbol{\theta}}(\mathbf{z})$ is **sequential**, while the inference function $\mathbf{f}_{\boldsymbol{\theta}}(\mathbf{x})$ is **not sequential**.

Papamakarios G., Pavlakou T., Murray I. Masked Autoregressive Flow for Density Estimation, 2017

Recap of Previous Lecture

Let us partition $\mathbf{x}$ and $\mathbf{z}$ into two groups:

$$\mathbf{x} = [\mathbf{x}_1, \mathbf{x}_2] = [\mathbf{x}_{1:d}, \mathbf{x}_{d+1:m}]; \quad \mathbf{z} = [\mathbf{z}_1, \mathbf{z}_2] = [\mathbf{z}_{1:d}, \mathbf{z}_{d+1:m}].$$

Coupling Layer

$$\begin{cases} \mathbf{x}_1 = \mathbf{z}_1; \\ \mathbf{x}_2 = \mathbf{z}_2 \odot \boldsymbol{\sigma}_{\boldsymbol{\theta}}(\mathbf{z}_1) + \boldsymbol{\mu}_{\boldsymbol{\theta}}(\mathbf{z}_1). \end{cases} \qquad \begin{cases} \mathbf{z}_1 = \mathbf{x}_1; \\ \mathbf{z}_2 = (\mathbf{x}_2 - \boldsymbol{\mu}_{\boldsymbol{\theta}}(\mathbf{x}_1)) \odot \frac{1}{\boldsymbol{\sigma}_{\boldsymbol{\theta}}(\mathbf{x}_1)}. \end{cases}$$

Both density estimation and sampling require just a single pass!

Jacobian

$$\det \left(\frac{\partial \mathbf{z}}{\partial \mathbf{x}} \right) = \det \begin{pmatrix} \mathbf{I}_d & 0_{d \times (m-d)} \\ \frac{\partial \mathbf{z}_2}{\partial \mathbf{x}_1} & \frac{\partial \mathbf{z}_2}{\partial \mathbf{x}_2} \end{pmatrix} = \prod_{j=1}^{m-d} \frac{1}{\sigma_{j,\boldsymbol{\theta}}(\mathbf{x}_1)}.$$

A coupling layer is a special instance of an gaussian autoregressive normalizing flow.

Dinh L., Sohl-Dickstein J., Bengio S. Density Estimation Using Real NVP, 2016

Recap of Previous Lecture

Posterior Distribution (Bayes' Theorem)

$$p(\boldsymbol{\theta}|\mathbf{x}) = \frac{p(\mathbf{x}|\boldsymbol{\theta})p(\boldsymbol{\theta})}{p(\mathbf{x})} = \frac{p(\mathbf{x}|\boldsymbol{\theta})p(\boldsymbol{\theta})}{\int p(\mathbf{x}|\boldsymbol{\theta})p(\boldsymbol{\theta})d\boldsymbol{\theta}}$$

- $\mathbf{x}$ – observed variables;
- $\boldsymbol{\theta}$ – unobserved variables (latent parameters);
- $p_{\boldsymbol{\theta}}(\mathbf{x}) = p(\mathbf{x}|\boldsymbol{\theta})$ – likelihood;
- $p(\mathbf{x}) = \int p(\mathbf{x}|\boldsymbol{\theta})p(\boldsymbol{\theta})d\boldsymbol{\theta}$ – evidence;
- $p(\boldsymbol{\theta})$ – prior distribution;
- $p(\boldsymbol{\theta}|\mathbf{x})$ – posterior distribution.

Outline

Outline

1. Latent Variable Models (LVM) (continued)
2. Variational Evidence Lower Bound (ELBO)
3. Amortized Inference
4. ELBO Gradients, Reparametrization Trick
5. Variational Autoencoder (VAE)

Latent Variable Models (LVM)

Maximum Likelihood Extimation (MLE) Problem

$$\boldsymbol{\theta}^* = \arg\max_{\boldsymbol{\theta}} p_{\boldsymbol{\theta}}(\mathbf{X}) = \arg\max_{\boldsymbol{\theta}} \prod_{i=1}^{n} p_{\boldsymbol{\theta}}(\mathbf{x}_i) = \arg\max_{\boldsymbol{\theta}} \sum_{i=1}^{n} \log p_{\boldsymbol{\theta}}(\mathbf{x}_i).$$

Latent Variable Models (LVM)

Maximum Likelihood Extimation (MLE) Problem

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The distribution $p_{\boldsymbol{\theta}}(\mathbf{x})$ can be highly complex and often intractable (just like the true data distribution $p_{\text{data}}(\mathbf{x})$).

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Extended Probabilistic Model

Introduce a latent variable $\mathbf{z}$ for each observed sample $\mathbf{x}$:

$$p_{\boldsymbol{\theta}}(\mathbf{x}, \mathbf{z}) = p_{\boldsymbol{\theta}}(\mathbf{x}|\mathbf{z})p(\mathbf{z}); \quad \log p_{\boldsymbol{\theta}}(\mathbf{x}, \mathbf{z}) = \log p_{\boldsymbol{\theta}}(\mathbf{x}|\mathbf{z}) + \log p(\mathbf{z}).$$

Latent Variable Models (LVM)

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$$p_{\boldsymbol{\theta}}(\mathbf{x}) = \int p_{\boldsymbol{\theta}}(\mathbf{x}, \mathbf{z}) d\mathbf{z} = \int p_{\boldsymbol{\theta}}(\mathbf{x}|\mathbf{z})p(\mathbf{z}) d\mathbf{z}.$$

Latent Variable Models (LVM)

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Introduce a latent variable $\mathbf{z}$ for each observed sample $\mathbf{x}$:

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$$p_{\boldsymbol{\theta}}(\mathbf{x}) = \int p_{\boldsymbol{\theta}}(\mathbf{x}, \mathbf{z}) d\mathbf{z} = \int p_{\boldsymbol{\theta}}(\mathbf{x}|\mathbf{z})p(\mathbf{z}) d\mathbf{z}.$$

Motivation

Both $p_{\boldsymbol{\theta}}(\mathbf{x}|\mathbf{z})$ and $p(\mathbf{z})$ are usually much simpler than $p_{\boldsymbol{\theta}}(\mathbf{x})$.

Latent Variable Models (LVM)

$$\log p_{\boldsymbol{\theta}}(\mathbf{x}) = \log \int p_{\boldsymbol{\theta}}(\mathbf{x}|\mathbf{z}) p(\mathbf{z}) d\mathbf{z} \to \max_{\boldsymbol{\theta}}$$

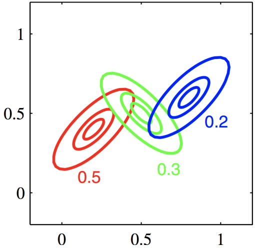
Bishop C. Pattern Recognition and Machine Learning, 2006

Latent Variable Models (LVM)

$$\log p_{\boldsymbol{\theta}}(\mathbf{x}) = \log \int p_{\boldsymbol{\theta}}(\mathbf{x}|\mathbf{z})p(\mathbf{z})d\mathbf{z} \to \max_{\boldsymbol{\theta}}$$

Examples

Mixture of Gaussians



- $p_{\boldsymbol{\theta}}(\mathbf{x}|z) = \mathcal{N}(\boldsymbol{\mu}_z, \boldsymbol{\Sigma}_z)$
- $p(z) = \mathrm{Cat}(\boldsymbol{\pi})$

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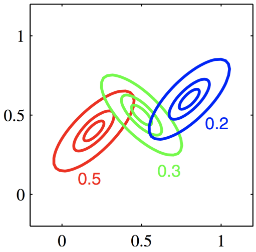
Latent Variable Models (LVM)

$$\log p_{\theta}(\mathbf{x}) = \log \int p_{\theta}(\mathbf{x}|\mathbf{z})p(\mathbf{z})d\mathbf{z} \to \max_{\theta}$$

Examples

Mixture of Gaussians



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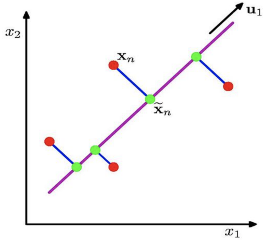
PCA Model



- $p_{\theta}(\mathbf{x}|\mathbf{z}) = \mathcal{N}(\mathbf{W}\mathbf{z} + \boldsymbol{\mu}, \sigma^2\mathbf{I})$
- $p(\mathbf{z}) = \mathcal{N}(0, \mathbf{I})$

Bishop C. Pattern Recognition and Machine Learning, 2006

MLE for LVM

$$\sum_{i=1}^{n} \log p_{\boldsymbol{\theta}}(\mathbf{x}_i) = \sum_{i=1}^{n} \log \int p_{\boldsymbol{\theta}}(\mathbf{x}_i|\mathbf{z}_i)p(\mathbf{z}_i)d\mathbf{z}_i \to \max_{\boldsymbol{\theta}}.$$

image credit: https://jmtomczak.github.io/blog/4/4_VAE.html

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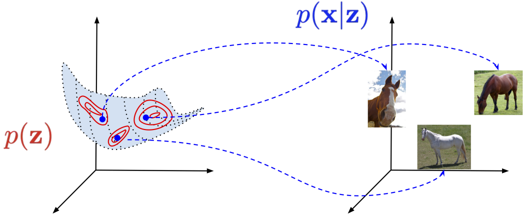

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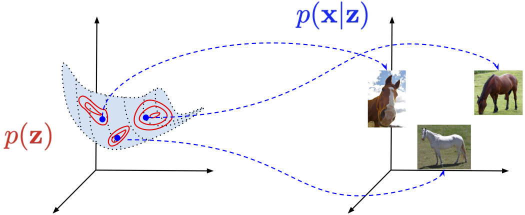

Naive Monte Carlo Estimation

$$\log p_{\boldsymbol{\theta}}(\mathbf{x}) = \log \mathbb{E}_{p(\mathbf{z})} p_{\boldsymbol{\theta}}(\mathbf{x}|\mathbf{z}) \geq \mathbb{E}_{p(\mathbf{z})} \log p_{\boldsymbol{\theta}}(\mathbf{x}|\mathbf{z}) \approx \frac{1}{K} \sum_{k=1}^{K} \log p_{\boldsymbol{\theta}}(\mathbf{x}|\mathbf{z}_k),$$

where $\mathbf{z}_k \sim p(\mathbf{z})$.

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MLE for LVM

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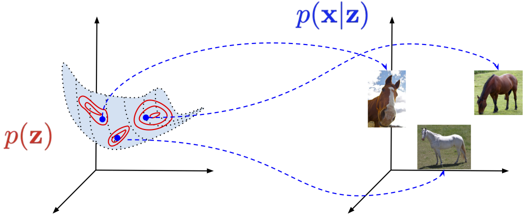

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where $\mathbf{z}_k \sim p(\mathbf{z})$.

Challenge: As the dimensionality of $\mathbf{z}$ increases, the number of samples needed to adequately cover the latent space grows exponentially.

image credit: https://jmtomczak.github.io/blog/4/4_VAE.html

Outline

ELBO Derivation I

Inequality Derivation

$$\log p_{\boldsymbol{\theta}}(\mathbf{x}) = \log \int p_{\boldsymbol{\theta}}(\mathbf{x}, \mathbf{z}) d\mathbf{z}$$

ELBO Derivation I

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$$\log p_{\boldsymbol{\theta}}(\mathbf{x}) = \log \int p_{\boldsymbol{\theta}}(\mathbf{x}, \mathbf{z}) d\mathbf{z} = \log \int \frac{q(\mathbf{z})}{q(\mathbf{z})} p_{\boldsymbol{\theta}}(\mathbf{x}, \mathbf{z}) d\mathbf{z}$$

ELBO Derivation I

Inequality Derivation

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$$= \log \mathbb{E}_q \left[\frac{p_{\boldsymbol{\theta}}(\mathbf{x}, \mathbf{z})}{q(\mathbf{z})} \right]$$

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- Here, $q(\mathbf{z})$ is any distribution such that $\int q(\mathbf{z}) d\mathbf{z} = 1$.
- We assume that $\text{supp}(q(\mathbf{z})) = \text{supp}(p_{\boldsymbol{\theta}}(\mathbf{z}|\mathbf{x})) = \mathbb{R}^d$.

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Variational Evidence Lower Bound (ELBO)

$$\mathcal{L}_{q,\boldsymbol{\theta}}(\mathbf{x}) = \mathbb{E}_q \log \frac{p_{\boldsymbol{\theta}}(\mathbf{x}, \mathbf{z})}{q(\mathbf{z})} \leq \log p_{\boldsymbol{\theta}}(\mathbf{x})$$

ELBO Derivation I

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This inequality holds for any choice of $q(\mathbf{z})$.

ELBO Derivation II

$$p_{\boldsymbol{\theta}}(\mathbf{z}|\mathbf{x}) = \frac{p_{\boldsymbol{\theta}}(\mathbf{x}, \mathbf{z})}{p_{\boldsymbol{\theta}}(\mathbf{x})}$$

Equality Derivation

$$\mathcal{L}_{q,\boldsymbol{\theta}}(\mathbf{x}) = \int q(\mathbf{z}) \log \frac{p_{\boldsymbol{\theta}}(\mathbf{x}, \mathbf{z})}{q(\mathbf{z})} d\mathbf{z}$$

ELBO Derivation II

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\mathcal{L}_{q,\boldsymbol{\theta}}(\mathbf{x}) = \int q(\mathbf{z}) \log \frac{p_{\boldsymbol{\theta}}(\mathbf{x}, \mathbf{z})}{q(\mathbf{z})} d\mathbf{z} = \\
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= \int q(\mathbf{z}) \log p_{\boldsymbol{\theta}}(\mathbf{x}) d\mathbf{z} + \int q(\mathbf{z}) \log \frac{p_{\boldsymbol{\theta}}(\mathbf{z}|\mathbf{x})}{q(\mathbf{z})} d\mathbf{z}
\end{aligned}$$

ELBO Derivation II

$$p_{\boldsymbol{\theta}}(\mathbf{z}|\mathbf{x}) = \frac{p_{\boldsymbol{\theta}}(\mathbf{x}, \mathbf{z})}{p_{\boldsymbol{\theta}}(\mathbf{x})}$$

Equality Derivation

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= \log p_{\boldsymbol{\theta}}(\mathbf{x}) - \mathrm{KL}(q(\mathbf{z}) \| p_{\boldsymbol{\theta}}(\mathbf{z}|\mathbf{x}))
\end{aligned}$$

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Equality Derivation

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\end{aligned}$$

Variational Decomposition

$$\log p_{\boldsymbol{\theta}}(\mathbf{x}) = \mathcal{L}_{q,\boldsymbol{\theta}}(\mathbf{x}) + \mathrm{KL}(q(\mathbf{z}) \| p_{\boldsymbol{\theta}}(\mathbf{z}|\mathbf{x})) \geq \mathcal{L}_{q,\boldsymbol{\theta}}(\mathbf{x}).$$

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\mathcal{L}_{q,\boldsymbol{\theta}}(\mathbf{x}) = \int q(\mathbf{z}) \log \frac{p_{\boldsymbol{\theta}}(\mathbf{x}, \mathbf{z})}{q(\mathbf{z})} d\mathbf{z} = \\
= \int q(\mathbf{z}) \log \frac{p_{\boldsymbol{\theta}}(\mathbf{z}|\mathbf{x}) p_{\boldsymbol{\theta}}(\mathbf{x})}{q(\mathbf{z})} d\mathbf{z} = \\
= \int q(\mathbf{z}) \log p_{\boldsymbol{\theta}}(\mathbf{x}) d\mathbf{z} + \int q(\mathbf{z}) \log \frac{p_{\boldsymbol{\theta}}(\mathbf{z}|\mathbf{x})}{q(\mathbf{z})} d\mathbf{z} = \\
= \log p_{\boldsymbol{\theta}}(\mathbf{x}) - \mathrm{KL}(q(\mathbf{z}) \| p_{\boldsymbol{\theta}}(\mathbf{z}|\mathbf{x}))
\end{aligned}$$

Variational Decomposition

$$\log p_{\boldsymbol{\theta}}(\mathbf{x}) = \mathcal{L}_{q,\boldsymbol{\theta}}(\mathbf{x}) + \mathrm{KL}(q(\mathbf{z}) \| p_{\boldsymbol{\theta}}(\mathbf{z}|\mathbf{x})) \geq \mathcal{L}_{q,\boldsymbol{\theta}}(\mathbf{x}).$$

Here, $\mathrm{KL}(q(\mathbf{z}) \| p_{\boldsymbol{\theta}}(\mathbf{z}|\mathbf{x})) \geq 0$.

Variational Evidence Lower Bound (ELBO)

$$\mathcal{L}_{q,\boldsymbol{\theta}}(\mathbf{x}) = \int q(\mathbf{z}) \log \frac{p_{\boldsymbol{\theta}}(\mathbf{x}, \mathbf{z})}{q(\mathbf{z})} d\mathbf{z}$$

Variational Evidence Lower Bound (ELBO)

$$\begin{aligned}\mathcal{L}_{q,\boldsymbol{\theta}}(\mathbf{x}) &= \int q(\mathbf{z}) \log \frac{p_{\boldsymbol{\theta}}(\mathbf{x}, \mathbf{z})}{q(\mathbf{z})} d\mathbf{z} \\ &= \int q(\mathbf{z}) \log p_{\boldsymbol{\theta}}(\mathbf{x}|\mathbf{z}) d\mathbf{z} + \int q(\mathbf{z}) \log \frac{p(\mathbf{z})}{q(\mathbf{z})} d\mathbf{z}\end{aligned}$$

Variational Evidence Lower Bound (ELBO)

$$
\begin{aligned}
\mathcal{L}_{q,\boldsymbol{\theta}}(\mathbf{x}) &= \int q(\mathbf{z}) \log \frac{p_{\boldsymbol{\theta}}(\mathbf{x}, \mathbf{z})}{q(\mathbf{z})} d\mathbf{z} \\
&= \int q(\mathbf{z}) \log p_{\boldsymbol{\theta}}(\mathbf{x}|\mathbf{z}) d\mathbf{z} + \int q(\mathbf{z}) \log \frac{p(\mathbf{z})}{q(\mathbf{z})} d\mathbf{z} \\
&= \mathbb{E}_q \log p_{\boldsymbol{\theta}}(\mathbf{x}|\mathbf{z}) - \mathrm{KL}(q(\mathbf{z}) \| p(\mathbf{z}))
\end{aligned}
$$

Variational Evidence Lower Bound (ELBO)

$$\begin{aligned}
\mathcal{L}_{q,\boldsymbol{\theta}}(\mathbf{x}) &= \int q(\mathbf{z}) \log \frac{p_{\boldsymbol{\theta}}(\mathbf{x}, \mathbf{z})}{q(\mathbf{z})} d\mathbf{z} \\
&= \int q(\mathbf{z}) \log p_{\boldsymbol{\theta}}(\mathbf{x}|\mathbf{z}) d\mathbf{z} + \int q(\mathbf{z}) \log \frac{p(\mathbf{z})}{q(\mathbf{z})} d\mathbf{z} \\
&= \mathbb{E}_q \log p_{\boldsymbol{\theta}}(\mathbf{x}|\mathbf{z}) - \mathrm{KL}(q(\mathbf{z}) \| p(\mathbf{z}))
\end{aligned}$$

Log-Likelihood Decomposition

$$\log p_{\boldsymbol{\theta}}(\mathbf{x}) = \mathcal{L}_{q,\boldsymbol{\theta}}(\mathbf{x}) + \mathrm{KL}(q(\mathbf{z}) \| p_{\boldsymbol{\theta}}(\mathbf{z}|\mathbf{x}))$$

Variational Evidence Lower Bound (ELBO)

$$\begin{aligned}\mathcal{L}_{q,\boldsymbol{\theta}}(\mathbf{x}) &= \int q(\mathbf{z}) \log \frac{p_{\boldsymbol{\theta}}(\mathbf{x}, \mathbf{z})}{q(\mathbf{z})} d\mathbf{z} \\ &= \int q(\mathbf{z}) \log p_{\boldsymbol{\theta}}(\mathbf{x}|\mathbf{z}) d\mathbf{z} + \int q(\mathbf{z}) \log \frac{p(\mathbf{z})}{q(\mathbf{z})} d\mathbf{z} \\ &= \mathbb{E}_q \log p_{\boldsymbol{\theta}}(\mathbf{x}|\mathbf{z}) - \mathrm{KL}(q(\mathbf{z}) \| p(\mathbf{z}))\end{aligned}$$

Log-Likelihood Decomposition

$$\begin{aligned}\log p_{\boldsymbol{\theta}}(\mathbf{x}) &= \mathcal{L}_{q,\boldsymbol{\theta}}(\mathbf{x}) + \mathrm{KL}(q(\mathbf{z}) \| p_{\boldsymbol{\theta}}(\mathbf{z}|\mathbf{x})) = \\ &= \mathbb{E}_q \log p_{\boldsymbol{\theta}}(\mathbf{x}|\mathbf{z}) - \mathrm{KL}(q(\mathbf{z}) \| p(\mathbf{z})) + \mathrm{KL}(q(\mathbf{z}) \| p_{\boldsymbol{\theta}}(\mathbf{z}|\mathbf{x})).\end{aligned}$$

Variational Evidence Lower Bound (ELBO)

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- Instead of maximizing the likelihood, maximize the ELBO:

$$\max_{\boldsymbol{\theta}} p_{\boldsymbol{\theta}}(\mathbf{x}) \quad \rightarrow \quad \max_{q,\boldsymbol{\theta}} \mathcal{L}_{q,\boldsymbol{\theta}}(\mathbf{x})$$

Variational Evidence Lower Bound (ELBO)

$$\begin{aligned}
\mathcal{L}_{q,\boldsymbol{\theta}}(\mathbf{x}) &= \int q(\mathbf{z}) \log \frac{p_{\boldsymbol{\theta}}(\mathbf{x}, \mathbf{z})}{q(\mathbf{z})} d\mathbf{z} \\
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\end{aligned}$$

- Instead of maximizing the likelihood, maximize the ELBO:

$$\max_{\boldsymbol{\theta}} p_{\boldsymbol{\theta}}(\mathbf{x}) \quad \rightarrow \quad \max_{q,\boldsymbol{\theta}} \mathcal{L}_{q,\boldsymbol{\theta}}(\mathbf{x})$$

- Maximizing the ELBO with respect to the **variational** distribution q is equivalent to minimizing the KL divergence:

$$\arg\max_{q} \mathcal{L}_{q,\boldsymbol{\theta}}(\mathbf{x}) \equiv \arg\min_{q} \mathrm{KL}(q(\mathbf{z}) \| p_{\boldsymbol{\theta}}(\mathbf{z}|\mathbf{x})).$$

Variational Posterior

$$\mathcal{L}_{q,\boldsymbol{\theta}}(\mathbf{x}) = \mathbb{E}_q \log p_{\boldsymbol{\theta}}(\mathbf{x}|\mathbf{z}) - \mathrm{KL}(q(\mathbf{z}) \| p(\mathbf{z})) \to \max_{q,\boldsymbol{\theta}}.$$

What is the optimal distribution $q^*(\mathbf{z})$ given fixed $\boldsymbol{\theta}^*$?

Bishop C. Pattern Recognition and Machine Learning, 2006

Variational Posterior

$$\mathcal{L}_{q,\boldsymbol{\theta}}(\mathbf{x}) = \mathbb{E}_q \log p_{\boldsymbol{\theta}}(\mathbf{x}|\mathbf{z}) - \mathrm{KL}(q(\mathbf{z})\|p(\mathbf{z})) \rightarrow \max_{q,\boldsymbol{\theta}}.$$

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$$q^*(\mathbf{z}) = \arg\max_q \mathcal{L}_{q,\boldsymbol{\theta}^*}(\mathbf{x}) =$$

$$= \arg\min_q \mathrm{KL}(q(\mathbf{z})\|p_{\boldsymbol{\theta}^*}(\mathbf{z}|\mathbf{x})) = p_{\boldsymbol{\theta}^*}(\mathbf{z}|\mathbf{x}).$$

Here we got the intuition about $q(\mathbf{z})$ – it estimates the posterior $p_{\boldsymbol{\theta}^*}(\mathbf{z}|\mathbf{x})$.

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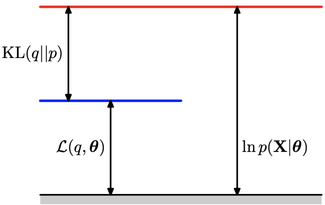
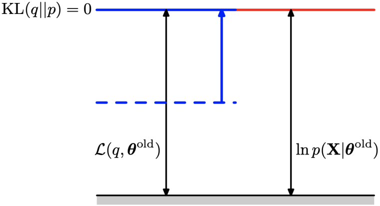
Here we got the intuition about $q(\mathbf{z})$ – it estimates the posterior $p_{\boldsymbol{\theta}^*}(\mathbf{z}|\mathbf{x})$.





Bishop C. Pattern Recognition and Machine Learning, 2006

Outline

Parametric Variable Posterior

Variational Posterior

$$q(\mathbf{z}) = \arg\max_q \mathcal{L}_{q,\boldsymbol{\theta}^*}(\mathbf{x}) = \arg\min_q \mathrm{KL}(q\|p) = p_{\boldsymbol{\theta}^*}(\mathbf{z}|\mathbf{x}).$$

Parametric Variable Posterior

Variational Posterior

$$q(\mathbf{z}) = \arg\max_q \mathcal{L}_{q,\boldsymbol{\theta}^*}(\mathbf{x}) = \arg\min_q \mathrm{KL}(q\|p) = p_{\boldsymbol{\theta}^*}(\mathbf{z}|\mathbf{x}).$$

- $p_{\boldsymbol{\theta}^*}(\mathbf{z}|\mathbf{x})$ may be **intractable**;
- $q(\mathbf{z})$ is individual for each data point $\mathbf{x}$.

Parametric Variable Posterior

Variational Posterior

$$q(\mathbf{z}) = \arg\max_q \mathcal{L}_{q,\boldsymbol{\theta}^*}(\mathbf{x}) = \arg\min_q \mathrm{KL}(q\|p) = p_{\boldsymbol{\theta}^*}(\mathbf{z}|\mathbf{x}).$$

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Amortized Variational Inference

We restrict the family of possible distributions $q(\mathbf{z})$ to a parametric class $q_{\phi}(\mathbf{z}|\mathbf{x})$, conditioned on data $\mathbf{x}$ and parameterized by ϕ.

Parametric Variable Posterior

Variational Posterior

$$q(\mathbf{z}) = \arg\max_{q} \mathcal{L}_{q,\boldsymbol{\theta}^*}(\mathbf{x}) = \arg\min_{q} \mathrm{KL}(q \| p) = p_{\boldsymbol{\theta}^*}(\mathbf{z}|\mathbf{x}).$$

- $p_{\boldsymbol{\theta}^*}(\mathbf{z}|\mathbf{x})$ may be **intractable**;
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Amortized Variational Inference

We restrict the family of possible distributions $q(\mathbf{z})$ to a parametric class $q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x})$, conditioned on data $\mathbf{x}$ and parameterized by $\boldsymbol{\phi}$.

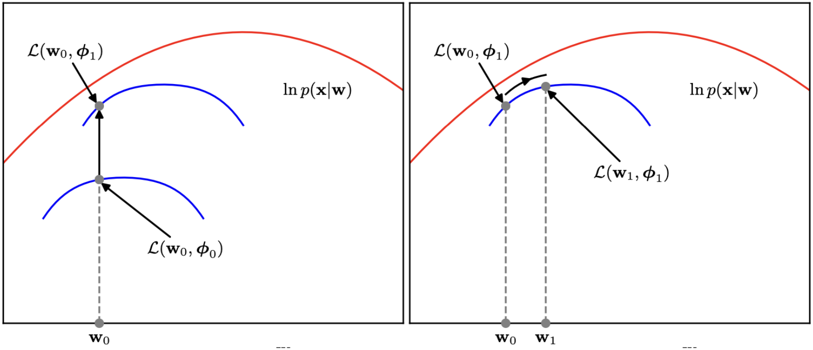
Gradient Update

$$\begin{bmatrix} \boldsymbol{\phi}_k \\ \boldsymbol{\theta}_k \end{bmatrix} = \left.\begin{bmatrix} \boldsymbol{\phi}_{k-1} + \eta \cdot \nabla_{\boldsymbol{\phi}} \mathcal{L}_{\boldsymbol{\phi},\boldsymbol{\theta}}(\mathbf{x}) \\ \boldsymbol{\theta}_{k-1} + \eta \cdot \nabla_{\boldsymbol{\theta}} \mathcal{L}_{\boldsymbol{\phi},\boldsymbol{\theta}}(\mathbf{x}) \end{bmatrix}\right|_{(\boldsymbol{\phi}_{k-1}, \boldsymbol{\theta}_{k-1})}$$

ELBO optimization

Gradient Update

$$\begin{bmatrix} \phi_k \\ \boldsymbol{\theta}_k \end{bmatrix} = \begin{bmatrix} \phi_{k-1} + \eta \cdot \nabla_{\phi} \mathcal{L}_{\phi,\boldsymbol{\theta}}(\mathbf{x}) \\ \boldsymbol{\theta}_{k-1} + \eta \cdot \nabla_{\boldsymbol{\theta}} \mathcal{L}_{\phi,\boldsymbol{\theta}}(\mathbf{x}) \end{bmatrix} \Bigg|_{(\phi_{k-1},\boldsymbol{\theta}_{k-1})}$$



Bishop C., Deep Learning: Foundations and Concepts, 2024

ELBO optimization

ELBO

$$\log p_{\boldsymbol{\theta}}(\mathbf{x}) = \mathcal{L}_{\boldsymbol{\phi},\boldsymbol{\theta}}(\mathbf{x}) + \mathrm{KL}(q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x}) \| p_{\boldsymbol{\theta}}(\mathbf{z}|\mathbf{x})) \geq \mathcal{L}_{\boldsymbol{\phi},\boldsymbol{\theta}}(\mathbf{x}).$$

$$\mathcal{L}_{q,\boldsymbol{\theta}}(\mathbf{x}) = \mathbb{E}_q \log p_{\boldsymbol{\theta}}(\mathbf{x}|\mathbf{z}) - \mathrm{KL}(q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x}) \| p(\mathbf{z}))$$

ELBO optimization

ELBO

$$\log p_{\boldsymbol\theta}(\mathbf{x}) = \mathcal{L}_{\boldsymbol\phi,\boldsymbol\theta}(\mathbf{x}) + \mathrm{KL}(q_{\boldsymbol\phi}(\mathbf{z}|\mathbf{x}) \| p_{\boldsymbol\theta}(\mathbf{z}|\mathbf{x})) \geq \mathcal{L}_{\boldsymbol\phi,\boldsymbol\theta}(\mathbf{x}).$$

$$\mathcal{L}_{q,\boldsymbol\theta}(\mathbf{x}) = \mathbb{E}_q \log p_{\boldsymbol\theta}(\mathbf{x}|\mathbf{z}) - \mathrm{KL}(q_{\boldsymbol\phi}(\mathbf{z}|\mathbf{x}) \| p(\mathbf{z}))$$

Gradient Update

$$\begin{bmatrix} \boldsymbol\phi_k \\ \boldsymbol\theta_k \end{bmatrix} = \left.\begin{bmatrix} \boldsymbol\phi_{k-1} + \eta \cdot \nabla_{\boldsymbol\phi} \mathcal{L}_{\boldsymbol\phi,\boldsymbol\theta}(\mathbf{x}) \\ \boldsymbol\theta_{k-1} + \eta \cdot \nabla_{\boldsymbol\theta} \mathcal{L}_{\boldsymbol\phi,\boldsymbol\theta}(\mathbf{x}) \end{bmatrix}\right|_{(\boldsymbol\phi_{k-1}, \boldsymbol\theta_{k-1})}$$

- $\boldsymbol\phi$ denotes the parameters of the variational posterior $q_{\boldsymbol\phi}(\mathbf{z}|\mathbf{x})$.
- $\boldsymbol\theta$ represents the parameters of the generative model $p_{\boldsymbol\theta}(\mathbf{x}|\mathbf{z})$.

ELBO optimization

ELBO

$$\log p_{\boldsymbol{\theta}}(\mathbf{x}) = \mathcal{L}_{\boldsymbol{\phi},\boldsymbol{\theta}}(\mathbf{x}) + \mathrm{KL}(q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x}) \| p_{\boldsymbol{\theta}}(\mathbf{z}|\mathbf{x})) \geq \mathcal{L}_{\boldsymbol{\phi},\boldsymbol{\theta}}(\mathbf{x}).$$

$$\mathcal{L}_{q,\boldsymbol{\theta}}(\mathbf{x}) = \mathbb{E}_q \log p_{\boldsymbol{\theta}}(\mathbf{x}|\mathbf{z}) - \mathrm{KL}(q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x}) \| p(\mathbf{z}))$$

Gradient Update

$$\begin{bmatrix} \boldsymbol{\phi}_k \\ \boldsymbol{\theta}_k \end{bmatrix} = \left.\begin{bmatrix} \boldsymbol{\phi}_{k-1} + \eta \cdot \nabla_{\boldsymbol{\phi}} \mathcal{L}_{\boldsymbol{\phi},\boldsymbol{\theta}}(\mathbf{x}) \\ \boldsymbol{\theta}_{k-1} + \eta \cdot \nabla_{\boldsymbol{\theta}} \mathcal{L}_{\boldsymbol{\phi},\boldsymbol{\theta}}(\mathbf{x}) \end{bmatrix}\right|_{(\boldsymbol{\phi}_{k-1}, \boldsymbol{\theta}_{k-1})}$$

- $\boldsymbol{\phi}$ denotes the parameters of the variational posterior $q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x})$.
- $\boldsymbol{\theta}$ represents the parameters of the generative model $p_{\boldsymbol{\theta}}(\mathbf{x}|\mathbf{z})$.

The remaining step is to obtain **unbiased** Monte Carlo estimates of the gradients: $\nabla_{\boldsymbol{\phi}} \mathcal{L}_{\boldsymbol{\phi},\boldsymbol{\theta}}(\mathbf{x})$ and $\nabla_{\boldsymbol{\theta}} \mathcal{L}_{\boldsymbol{\phi},\boldsymbol{\theta}}(\mathbf{x})$.

Outline

ELBO Gradients: $\nabla_{\theta}\mathcal{L}_{\phi,\theta}(\mathbf{x})$

$$\mathcal{L}_{q,\boldsymbol{\theta}}(\mathbf{x}) = \mathbb{E}_q \log p_{\boldsymbol{\theta}}(\mathbf{x}|\mathbf{z}) - \mathrm{KL}(q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x})\|p(\mathbf{z}))$$

image credit: https://jmtomczak.github.io/blog/4/4_VAE.html

ELBO Gradients: $\nabla_{\boldsymbol{\theta}} \mathcal{L}_{\phi,\boldsymbol{\theta}}(\mathbf{x})$

$$\mathcal{L}_{q,\boldsymbol{\theta}}(\mathbf{x}) = \mathbb{E}_q \log p_{\boldsymbol{\theta}}(\mathbf{x}|\mathbf{z}) - \mathrm{KL}(q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x}) \| p(\mathbf{z}))$$

Gradient $\nabla_{\boldsymbol{\theta}} \mathcal{L}_{\phi,\boldsymbol{\theta}}(\mathbf{x})$

$$\nabla_{\boldsymbol{\theta}} \mathcal{L}_{\boldsymbol{\phi},\boldsymbol{\theta}}(\mathbf{x}) = \nabla_{\boldsymbol{\theta}} \int q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x}) \log p_{\boldsymbol{\theta}}(\mathbf{x}|\mathbf{z}) d\mathbf{z}$$

image credit: https://jmtomczak.github.io/blog/4/4_VAE.html

ELBO Gradients: $\nabla_{\boldsymbol{\theta}} \mathcal{L}_{\phi,\boldsymbol{\theta}}(\mathbf{x})$

$$\mathcal{L}_{q,\boldsymbol{\theta}}(\mathbf{x}) = \mathbb{E}_q \log p_{\boldsymbol{\theta}}(\mathbf{x}|\mathbf{z}) - \mathrm{KL}(q_{\phi}(\mathbf{z}|\mathbf{x}) \| p(\mathbf{z}))$$

Gradient $\nabla_{\boldsymbol{\theta}} \mathcal{L}_{\phi,\boldsymbol{\theta}}(\mathbf{x})$

$$\begin{aligned}
\nabla_{\boldsymbol{\theta}} \mathcal{L}_{\phi,\boldsymbol{\theta}}(\mathbf{x}) &= \nabla_{\boldsymbol{\theta}} \int q_{\phi}(\mathbf{z}|\mathbf{x}) \log p_{\boldsymbol{\theta}}(\mathbf{x}|\mathbf{z}) d\mathbf{z} \\
&= \int q_{\phi}(\mathbf{z}|\mathbf{x}) \nabla_{\boldsymbol{\theta}} \log p_{\boldsymbol{\theta}}(\mathbf{x}|\mathbf{z}) d\mathbf{z}
\end{aligned}$$

image credit: https://jmtomczak.github.io/blog/4/4_VAE.html

ELBO Gradients: $\nabla_{\boldsymbol{\theta}} \mathcal{L}_{\phi,\boldsymbol{\theta}}(\mathbf{x})$

$$\mathcal{L}_{q,\boldsymbol{\theta}}(\mathbf{x}) = \mathbb{E}_q \log p_{\boldsymbol{\theta}}(\mathbf{x}|\mathbf{z}) - \mathrm{KL}(q_\phi(\mathbf{z}|\mathbf{x}) \| p(\mathbf{z}))$$

Gradient $\nabla_{\boldsymbol{\theta}} \mathcal{L}_{\phi,\boldsymbol{\theta}}(\mathbf{x})$

$$\begin{aligned}
\nabla_{\boldsymbol{\theta}} \mathcal{L}_{\phi,\boldsymbol{\theta}}(\mathbf{x}) &= \nabla_{\boldsymbol{\theta}} \int q_\phi(\mathbf{z}|\mathbf{x}) \log p_{\boldsymbol{\theta}}(\mathbf{x}|\mathbf{z}) d\mathbf{z} \\
&= \int q_\phi(\mathbf{z}|\mathbf{x}) \nabla_{\boldsymbol{\theta}} \log p_{\boldsymbol{\theta}}(\mathbf{x}|\mathbf{z}) d\mathbf{z} \\
&\approx \nabla_{\boldsymbol{\theta}} \log p_{\boldsymbol{\theta}}(\mathbf{x}|\mathbf{z}^*), \quad \mathbf{z}^* \sim q_\phi(\mathbf{z}|\mathbf{x}).
\end{aligned}$$

image credit: https://jmtomczak.github.io/blog/4/4_VAE.html

ELBO Gradients: $\nabla_{\boldsymbol{\theta}} \mathcal{L}_{\phi,\boldsymbol{\theta}}(\mathbf{x})$

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\end{aligned}$$

Naive Monte Carlo Estimation

$$\log p_{\boldsymbol{\theta}}(\mathbf{x}) \geq \int \log p_{\boldsymbol{\theta}}(\mathbf{x}|\mathbf{z}) p(\mathbf{z}) d\mathbf{z} \approx \frac{1}{K} \sum_{k=1}^{K} \log p_{\boldsymbol{\theta}}(\mathbf{x}|\mathbf{z}_k), \quad \mathbf{z}_k \sim p(\mathbf{z}).$$

image credit: https://jmtomczak.github.io/blog/4/4_VAE.html

ELBO Gradients: $\nabla_{\boldsymbol{\theta}} \mathcal{L}_{\phi,\boldsymbol{\theta}}(\mathbf{x})$

$$\mathcal{L}_{q,\boldsymbol{\theta}}(\mathbf{x}) = \mathbb{E}_q \log p_{\boldsymbol{\theta}}(\mathbf{x}|\mathbf{z}) - \mathrm{KL}(q_{\phi}(\mathbf{z}|\mathbf{x}) \| p(\mathbf{z}))$$

Gradient $\nabla_{\boldsymbol{\theta}} \mathcal{L}_{\phi,\boldsymbol{\theta}}(\mathbf{x})$

$$\begin{aligned}
\nabla_{\boldsymbol{\theta}} \mathcal{L}_{\phi,\boldsymbol{\theta}}(\mathbf{x}) &= \nabla_{\boldsymbol{\theta}} \int q_{\phi}(\mathbf{z}|\mathbf{x}) \log p_{\boldsymbol{\theta}}(\mathbf{x}|\mathbf{z}) d\mathbf{z} \\
&= \int q_{\phi}(\mathbf{z}|\mathbf{x}) \nabla_{\boldsymbol{\theta}} \log p_{\boldsymbol{\theta}}(\mathbf{x}|\mathbf{z}) d\mathbf{z} \\
&\approx \nabla_{\boldsymbol{\theta}} \log p_{\boldsymbol{\theta}}(\mathbf{x}|\mathbf{z}^*), \quad \mathbf{z}^* \sim q_{\phi}(\mathbf{z}|\mathbf{x}).
\end{aligned}$$

Naive Monte Carlo Estimation

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The variational posterior $q_{\phi}(\mathbf{z}|\mathbf{x})$ typically concentrates more probability mass in a much smaller region than the prior $p(\mathbf{z})$.

---

image credit: https://jmtomczak.github.io/blog/4/4_VAE.html

ELBO Gradients: $\nabla_{\phi} \mathcal{L}_{\phi,\boldsymbol{\theta}}(\mathbf{x})$

Gradient $\nabla_{\phi} \mathcal{L}_{\phi,\boldsymbol{\theta}}(\mathbf{x})$

Unlike the $\boldsymbol{\theta}$-gradient, the density $q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x})$ now depends on ϕ, so standard Monte Carlo estimation can't be applied:

$$\nabla_{\boldsymbol{\phi}} \mathcal{L}_{\boldsymbol{\phi},\boldsymbol{\theta}}(\mathbf{x}) = \nabla_{\boldsymbol{\phi}} \int q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x}) \log p_{\boldsymbol{\theta}}(\mathbf{x}|\mathbf{z}) d\mathbf{z} - \nabla_{\boldsymbol{\phi}} \mathrm{KL}(q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x}) \| p(\mathbf{z}))$$

ELBO Gradients: $\nabla_\phi \mathcal{L}_{\phi,\theta}(\mathbf{x})$

Gradient $\nabla_\phi \mathcal{L}_{\phi,\theta}(\mathbf{x})$

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&\neq \int q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x}) \nabla_{\phi} \log p_{\boldsymbol{\theta}}(\mathbf{x}|\mathbf{z}) d\mathbf{z} - \nabla_{\boldsymbol{\phi}} \mathrm{KL}(q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x}) \| p(\mathbf{z}))
\end{aligned}$$

ELBO Gradients: $\nabla_\phi \mathcal{L}_{\phi,\boldsymbol{\theta}}(\mathbf{x})$

Gradient $\nabla_\phi \mathcal{L}_{\phi,\boldsymbol{\theta}}(\mathbf{x})$

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$$\begin{aligned}\nabla_\phi \mathcal{L}_{\phi,\boldsymbol{\theta}}(\mathbf{x}) &= \nabla_\phi \int q_\phi(\mathbf{z}|\mathbf{x}) \log p_{\boldsymbol{\theta}}(\mathbf{x}|\mathbf{z}) d\mathbf{z} - \nabla_\phi \mathrm{KL}(q_\phi(\mathbf{z}|\mathbf{x}) \| p(\mathbf{z})) \\ &\neq \int q_\phi(\mathbf{z}|\mathbf{x}) \nabla_\phi \log p_{\boldsymbol{\theta}}(\mathbf{x}|\mathbf{z}) d\mathbf{z} - \nabla_\phi \mathrm{KL}(q_\phi(\mathbf{z}|\mathbf{x}) \| p(\mathbf{z}))\end{aligned}$$

Reparametrization Trick (LOTUS Trick)

Assume $\mathbf{z} \sim q_\phi(\mathbf{z}|\mathbf{x})$ is generated by a random variable $\boldsymbol{\epsilon} \sim p(\boldsymbol{\epsilon})$ via a deterministic mapping $\mathbf{z} = \mathbf{g}_\phi(\mathbf{x}, \boldsymbol{\epsilon})$. Then,

$$\mathbb{E}_{\mathbf{z} \sim q_\phi(\mathbf{z}|\mathbf{x})} \mathbf{f}(\mathbf{z}) = \mathbb{E}_{\boldsymbol{\epsilon} \sim p(\boldsymbol{\epsilon})} \mathbf{f}(\mathbf{g}_\phi(\mathbf{x}, \boldsymbol{\epsilon}))$$

ELBO Gradients: $\nabla_{\phi}\mathcal{L}_{\phi,\theta}(\mathbf{x})$

Gradient $\nabla_{\phi}\mathcal{L}_{\phi,\theta}(\mathbf{x})$

Unlike the θ-gradient, the density $q_{\phi}(\mathbf{z}|\mathbf{x})$ now depends on ϕ, so standard Monte Carlo estimation can't be applied:

$$\begin{aligned}\nabla_{\phi}\mathcal{L}_{\phi,\theta}(\mathbf{x}) &= \nabla_{\phi}\int q_{\phi}(\mathbf{z}|\mathbf{x})\log p_{\theta}(\mathbf{x}|\mathbf{z})d\mathbf{z} - \nabla_{\phi}\mathrm{KL}(q_{\phi}(\mathbf{z}|\mathbf{x})\|p(\mathbf{z})) \\ &\neq \int q_{\phi}(\mathbf{z}|\mathbf{x})\nabla_{\phi}\log p_{\theta}(\mathbf{x}|\mathbf{z})d\mathbf{z} - \nabla_{\phi}\mathrm{KL}(q_{\phi}(\mathbf{z}|\mathbf{x})\|p(\mathbf{z}))\end{aligned}$$

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$$\mathbb{E}_{\mathbf{z}\sim q_{\phi}(\mathbf{z}|\mathbf{x})}\mathbf{f}(\mathbf{z}) = \mathbb{E}_{\boldsymbol{\epsilon}\sim p(\boldsymbol{\epsilon})}\mathbf{f}(\mathbf{g}_{\phi}(\mathbf{x}, \boldsymbol{\epsilon}))$$

Note: The LHS expectation is with respect to the parametric distribution $q_{\phi}(\mathbf{z}|\mathbf{x})$, while the RHS is for the non-parametric $p(\boldsymbol{\epsilon})$.

ELBO Gradients: $\nabla_\phi \mathcal{L}_{\phi,\theta}(\mathbf{x})$

Reparametrization Trick (LOTUS Trick)

$$\nabla_\phi \int q_\phi(\mathbf{z}|\mathbf{x})\mathbf{f}(\mathbf{z})d\mathbf{z} = \nabla_\phi \int p(\epsilon)\mathbf{f}(\mathbf{g}_\phi(\mathbf{x},\epsilon))d\epsilon$$

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Variational Assumption

$$p(\epsilon) = \mathcal{N}(0, \mathbf{I}); \quad \mathbf{z} = \mathbf{g}_\phi(\mathbf{x},\epsilon) = \boldsymbol{\sigma}_\phi(\mathbf{x}) \odot \epsilon + \boldsymbol{\mu}_\phi(\mathbf{x});$$
$$q_\phi(\mathbf{z}|\mathbf{x}) = \mathcal{N}(\boldsymbol{\mu}_\phi(\mathbf{x}), \boldsymbol{\sigma}^2_\phi(\mathbf{x})).$$

Here, $\boldsymbol{\mu}_\phi(\cdot)$ and $\boldsymbol{\sigma}_\phi(\cdot)$ are parameterized functions (outputs of a neural network).
Thus, we can write $q_\phi(\mathbf{z}|\mathbf{x}) = \text{NN}_{e,\phi}(\mathbf{x})$, the **encoder**.

ELBO Gradient: $\nabla_\phi \mathcal{L}_{\phi,\theta}(\mathbf{x})$

$$\nabla_{\boldsymbol{\phi}} \mathcal{L}_{\boldsymbol{\phi},\boldsymbol{\theta}}(\mathbf{x}) = \nabla_\phi \int q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x}) \log p_{\boldsymbol{\theta}}(\mathbf{x}|\mathbf{z}) d\mathbf{z} - \nabla_\phi \mathrm{KL}(q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x}) \| p(\mathbf{z}))$$

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Reconstruction Term

$$\nabla_\phi \int q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x}) \log p_{\boldsymbol{\theta}}(\mathbf{x}|\mathbf{z}) d\mathbf{z} = \int p(\boldsymbol{\epsilon}) \nabla_{\boldsymbol{\phi}} \log p_{\boldsymbol{\theta}}(\mathbf{x}|\mathbf{g}_{\boldsymbol{\phi}}(\mathbf{x}, \boldsymbol{\epsilon})) d\boldsymbol{\epsilon} \approx$$

$$\approx \nabla_{\boldsymbol{\phi}} \log p_{\boldsymbol{\theta}} \left(\mathbf{x}|\boldsymbol{\sigma}_{\boldsymbol{\phi}}(\mathbf{x}) \odot \boldsymbol{\epsilon}^* + \boldsymbol{\mu}_{\boldsymbol{\phi}}(\mathbf{x})\right), \quad \text{where } \boldsymbol{\epsilon}^* \sim \mathcal{N}(0, \mathbf{I})$$

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The generative distribution $p_{\boldsymbol{\theta}}(\mathbf{x}|\mathbf{z})$ can be implemented as a neural network.

We may write $p_{\boldsymbol{\theta}}(\mathbf{x}|\mathbf{z}) = \mathrm{NN}_{d,\boldsymbol{\theta}}(\mathbf{z})$, called the **decoder**.

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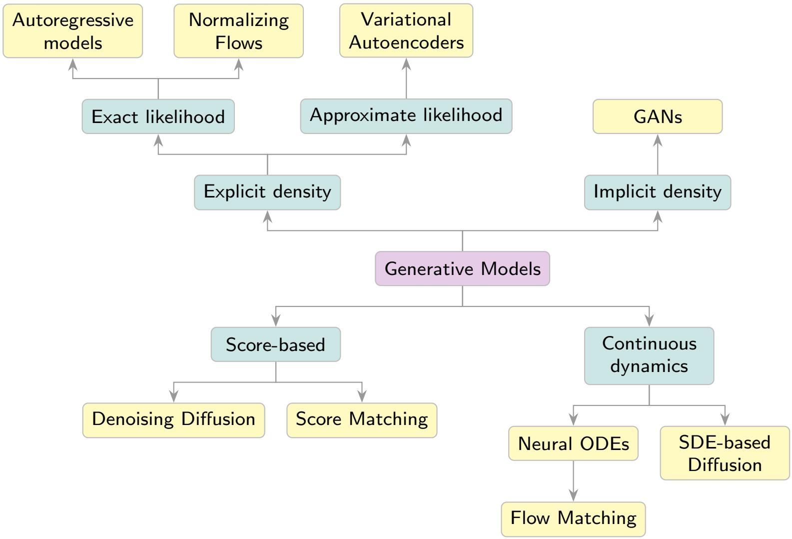
This expression admits a closed-form analytic solution.

Outline

Generative Models Taxonomy



Variational Autoencoder (VAE)

Training

- Pick a batch of samples $\{\mathbf{x}_i\}_{i=1}^{B}$ (here we use Monte Carlo technique).

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$$\boldsymbol{\epsilon}^* \sim p(\boldsymbol{\epsilon}); \quad \mathbf{z}^* = \mathbf{g}_{\phi}(\mathbf{x}, \boldsymbol{\epsilon}^*);$$

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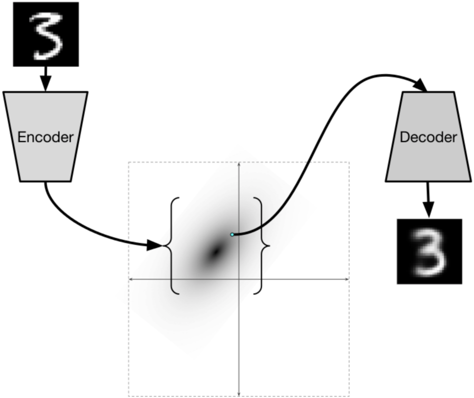
Note: The encoder $q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x})$ isn't needed during generation.

Variational Autoencoder

$$\mathcal{L}_{q,\boldsymbol{\theta}}(\mathbf{x}) = \mathbb{E}_q \log p_{\boldsymbol{\theta}}(\mathbf{x}|\mathbf{z}) - \mathrm{KL}(q_\phi(\mathbf{z}|\mathbf{x}) \| p(\mathbf{z}))$$



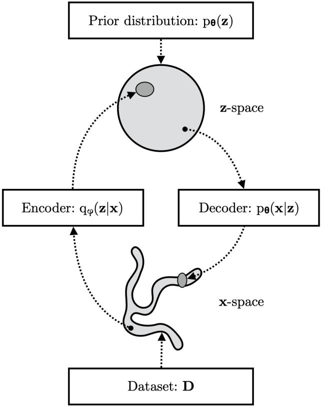


image credit: http://ijdykeman.github.io/ml/2016/12/21/cvae.html
Kingma D. P., Welling M., An Introduction to Variational Autoencoders, 2019

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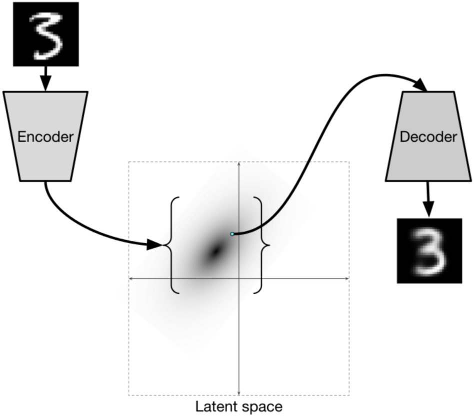

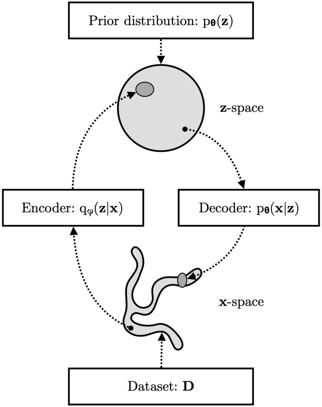

VAEs are widely used as a preliminary stage of projecting data onto low-dimensional space.

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image credit: http://ijdykeman.github.io/ml/2016/12/21/cvae.html
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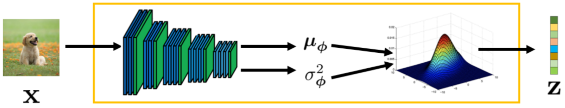
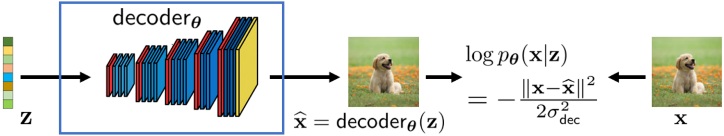
Variational Autoencoder

- The encoder $q_\phi(\mathbf{z}|\mathbf{x}) = \text{NN}_{e,\phi}(\mathbf{x})$ outputs $\boldsymbol{\mu}_\phi(\mathbf{x})$ and $\boldsymbol{\sigma}_\phi(\mathbf{x})$.
- The decoder $p_{\boldsymbol{\theta}}(\mathbf{x}|\mathbf{z}) = \text{NN}_{d,\boldsymbol{\theta}}(\mathbf{z})$ outputs parameters of the observed data distribution.





Chan S., Tutorial on Diffusion Models for Imaging and Vision, 2024

VAE vs Normalizing Flows

	VAE	**NF**
Objective	ELBO $\mathcal{L}$	Forward KL/MLE
Encoder	stochastic $\mathbf{z} \sim q_{\boldsymbol{\phi}}(\mathbf{z}\|\mathbf{x})$	deterministic $\mathbf{z} = \mathbf{f}_{\boldsymbol{\theta}}(\mathbf{x})$ $q_{\boldsymbol{\theta}}(\mathbf{z}\|\mathbf{x}) = \delta(\mathbf{z} - \mathbf{f}_{\boldsymbol{\theta}}(\mathbf{x}))$
Decoder	stochastic $\mathbf{x} \sim p_{\boldsymbol{\theta}}(\mathbf{x}\|\mathbf{z})$	deterministic $\mathbf{x} = \mathbf{g}_{\boldsymbol{\theta}}(\mathbf{z})$ $p_{\boldsymbol{\theta}}(\mathbf{x}\|\mathbf{z}) = \delta(\mathbf{x} - \mathbf{g}_{\boldsymbol{\theta}}(\mathbf{z}))$
Parameters	$\boldsymbol{\phi}, \boldsymbol{\theta}$	$\boldsymbol{\theta} \equiv \boldsymbol{\phi}$

Nielsen D., et al., SurVAE Flows: Surjections to Bridge the Gap Between VAEs and Flows, 2020

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Theorem

MLE for a normalizing flow is equivalent to maximizing the ELBO for a VAE where:

$$p_{\boldsymbol{\theta}}(\mathbf{x}|\mathbf{z}) = \delta(\mathbf{x} - \mathbf{f}_{\boldsymbol{\theta}}^{-1}(\mathbf{z})) = \delta(\mathbf{x} - \mathbf{g}_{\boldsymbol{\theta}}(\mathbf{z}));$$

$$q_{\boldsymbol{\theta}}(\mathbf{z}|\mathbf{x}) = \delta(\mathbf{z} - \mathbf{f}_{\boldsymbol{\theta}}(\mathbf{x})).$$

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Summary

- LVMs introduce latent representations for observed data, enabling more interpretable models.
- LVMs maximize the variational evidence lower bound (ELBO) to obtain maximum likelihood estimates for the parameters.
- Parametric posterior distribution $q_\phi(\mathbf{z}|\mathbf{x})$ makes the method scalable.
- The reparametrization trick provides unbiased gradients with respect to the variational posterior $q_\phi(\mathbf{z}|\mathbf{x})$.
- The VAE model is a latent variable model parameterized by two neural networks: a stochastic encoder $q_\phi(\mathbf{z}|\mathbf{x})$ and a stochastic decoder $p_\theta(\mathbf{x}|\mathbf{z})$.
- Nowadays, the main role of VAEs is to project data into low-dimensional latent space.