Deep Generative Models

Lecture 3

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Recap of Previous Lecture

Jacobian Matrix

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

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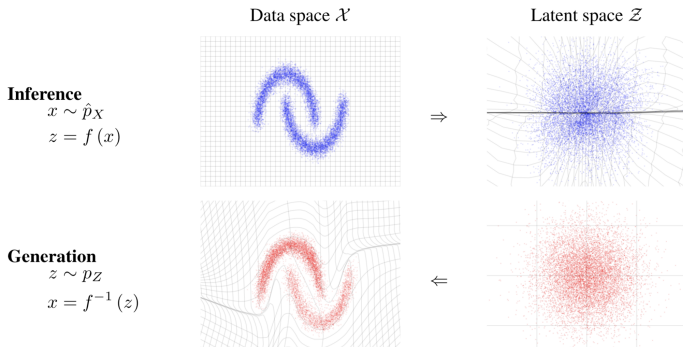
Change of Variables Theorem (CoV)

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

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

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

Recap of Previous Lecture

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

Data space $\mathcal{X}$ Latent space $\mathcal{Z}$

Inference
$x \sim \hat{p}_X$
$z = f(x)$
$\Rightarrow$

Generation
$z \sim p_Z$
$x = f^{-1}(z)$
$\Leftarrow$

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

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

One significant challenge is efficiently computing the Jacobian determinant.

Linear Flows

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

▶ LU Decomposition:

$$\mathbf{W} = \mathbf{PLU}.$$

▶ QR Decomposition:

$$\mathbf{W} = \mathbf{QR}.$$

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:

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

Gaussian Autoregressive Normalizing Flow

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

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

▶ This transformation is both C^1-**diffeomorphism**, mapping $p(\mathbf{z})$ to $p_{\theta}(\mathbf{x})$.

▶ The Jacobian matrix for this transformation is triangular.

The generative function $\mathbf{f}_{\theta}^{-1}(\mathbf{z})$ is **sequential**, while the inference function $\mathbf{f}_{\theta}(\mathbf{x})$ 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

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 $p_{\text{data}}(\mathbf{x})$).

Latent Variable Models (LVM)

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

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)

Maximum Likelihood Extimation (MLE) Problem

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

Latent Variable Models (LVM)

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

Extended Probabilistic Model

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 $p_{\boldsymbol{\theta}}(\mathbf{x})$.
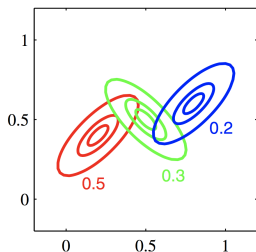
Latent Variable Models (LVM)

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

Bishop C. Pattern Recognition and Machine Learning, 2006

Latent Variable Models (LVM)

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Examples

Mixture of Gaussians

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

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Examples

Mixture of Gaussians   *PCA Model*

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

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

Bishop C. Pattern Recognition and Machine Learning, 2006
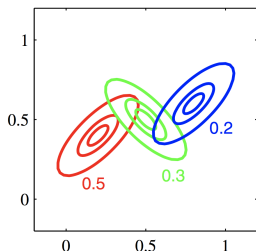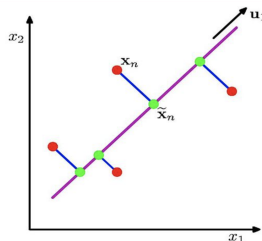
MLE for LVM

$$\sum_{i=1}^{n} \log p_{\boldsymbol{\theta}}(\mathbf{x}_i) = \sum_{i=1}^{n} \log \int p_{\boldsymbol{\theta}}(\mathbf{x}_i|\mathbf{z}_i)p(\mathbf{z}_i)d\mathbf{z}_i \to \max_{\boldsymbol{\theta}}.$$
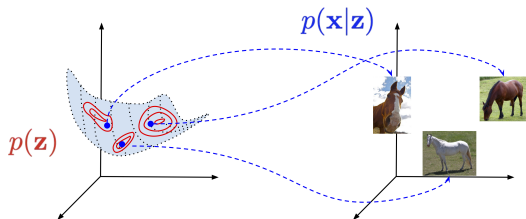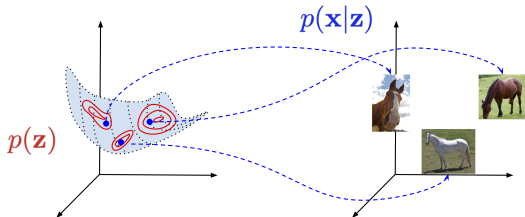
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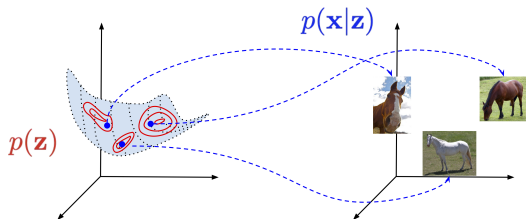
image credit: https://jmtomczak.github.io/blog/4/4_VAE.html

MLE for LVM

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

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

MLE for LVM

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

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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.

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

Outline

ELBO Derivation I

Inequality Derivation

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

ELBO Derivation I

Inequality Derivation

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

ELBO Derivation I

Inequality Derivation

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

ELBO Derivation I

Inequality Derivation

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▶ Here, $q(\mathbf{z})$ is any distribution such that $\int q(\mathbf{z}) d\mathbf{z} = 1$.

▶ We assume that $\mathrm{supp}(q(\mathbf{z})) = \mathrm{supp}(p_\theta(\mathbf{z}|\mathbf{x})) = \mathbb{R}^d$.

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Variational Evidence Lower Bound (ELBO)

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

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

ELBO Derivation II

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

Equality Derivation

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

ELBO Derivation II

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

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

Variational Decomposition

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

ELBO Derivation II

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Equality Derivation

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

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

Variational Decomposition

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

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

Variational Evidence Lower Bound (ELBO)

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

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Variational Evidence Lower Bound (ELBO)

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$$= \int q(\mathbf{z}) \log p_\theta(\mathbf{x}|\mathbf{z}) d\mathbf{z} + \int q(\mathbf{z}) \log \frac{p(\mathbf{z})}{q(\mathbf{z})} d\mathbf{z}$$

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Log-Likelihood Decomposition

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▶ Instead of maximizing the likelihood, maximize the ELBO:

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

$$\arg\max_q \mathcal{L}_{q,\theta}(\mathbf{x}) \equiv \arg\min_q \mathrm{KL}(q(\mathbf{z})\|p_\theta(\mathbf{z}|\mathbf{x})).$$
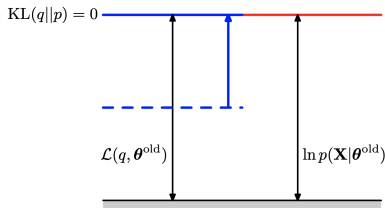
Variational Posterior

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

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

Variational Posterior

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

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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

Variational Posterior

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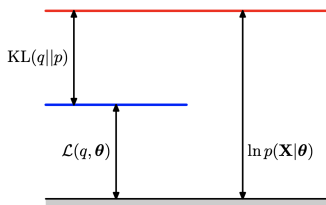

Bishop C. Pattern Recognition and Machine Learning, 2006

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

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

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

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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.

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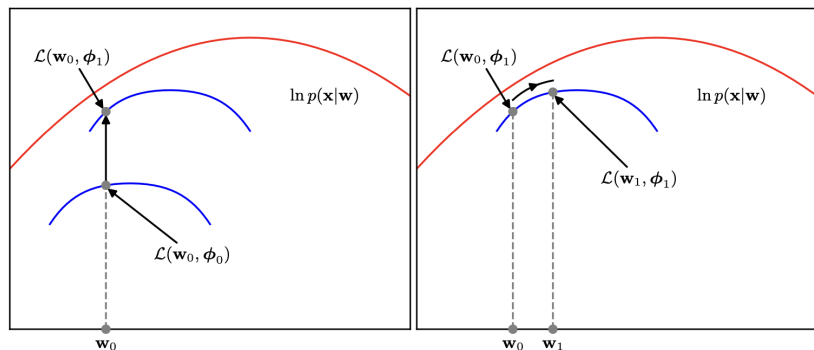
Gradient Update

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

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

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

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

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

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

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- ▶ ϕ denotes the parameters of the variational posterior $q_\phi(\mathbf{z}|\mathbf{x})$.
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The remaining step is to obtain **unbiased** Monte Carlo estimates of the gradients: $\nabla_\phi \mathcal{L}_{\phi,\boldsymbol{\theta}}(\mathbf{x})$ and $\nabla_{\boldsymbol{\theta}} \mathcal{L}_{\phi,\boldsymbol{\theta}}(\mathbf{x})$.

Outline

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

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

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

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

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

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

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

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Naive Monte Carlo Estimation

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

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

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

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:

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

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Reparametrization Trick (LOTUS Trick)

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

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

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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 $p(\epsilon)$.

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

Reparametrization Trick (LOTUS Trick)

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

,

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

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where $\epsilon^* \sim p(\epsilon)$.

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$$= \int p(\epsilon)\nabla_\phi \mathbf{f}(\mathbf{g}_\phi(\mathbf{x},\epsilon))d\epsilon \approx \nabla_\phi \mathbf{f}(\mathbf{g}_\phi(\mathbf{x},\epsilon^*)),$$

where $\epsilon^* \sim p(\epsilon)$.

Variational Assumption

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

$$q_\phi(\mathbf{z}|\mathbf{x}) = \mathcal{N}(\boldsymbol{\mu}_\phi(\mathbf{x}), \boldsymbol{\sigma}_\phi^2(\mathbf{x})).$$

Here, $\boldsymbol{\mu}_\phi(\cdot)$ and $\boldsymbol{\sigma}_\phi(\cdot)$ are parameterized functions (outputs of a neural network).

Thus, we can write $q_\phi(\mathbf{z}|\mathbf{x}) = \mathrm{NN}_{e,\phi}(\mathbf{x})$, the **encoder**.

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

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

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Reconstruction Term

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

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

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The generative distribution $p_\theta(\mathbf{x}|\mathbf{z})$ can be implemented as a neural network.
We may write $p_\theta(\mathbf{x}|\mathbf{z}) = \mathrm{NN}_{d,\theta}(\mathbf{z})$, called the **decoder**.

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

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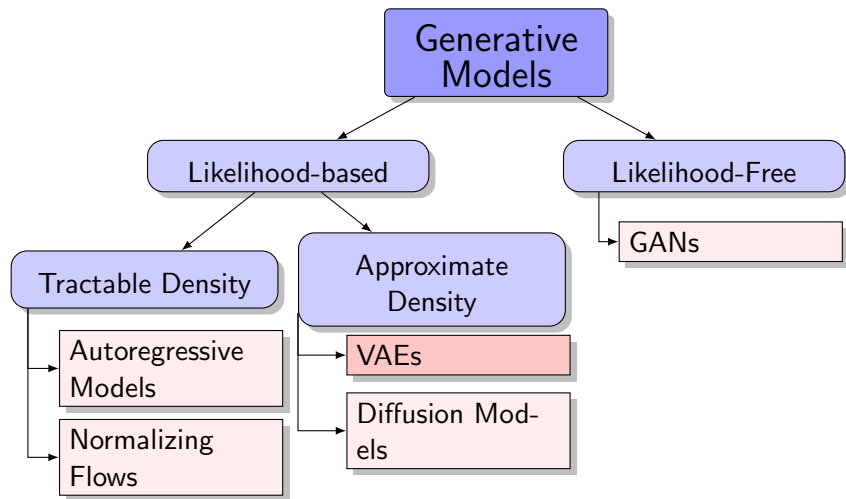
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This expression admits a closed-form analytic solution.

Outline

Generative Models Zoo

Variational Autoencoder (VAE)

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

Variational Autoencoder

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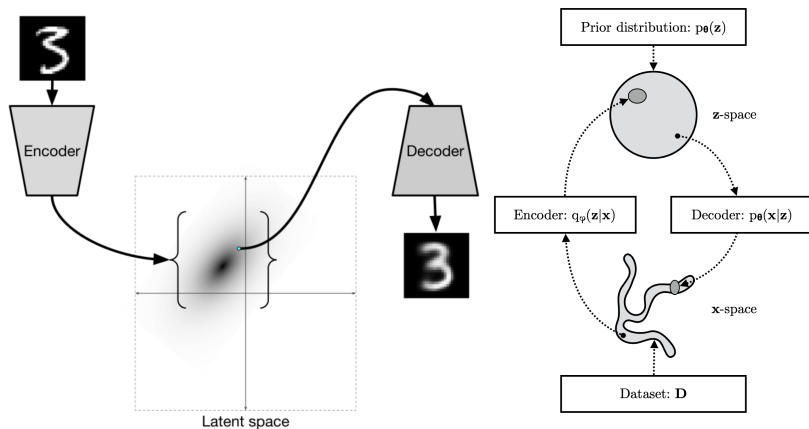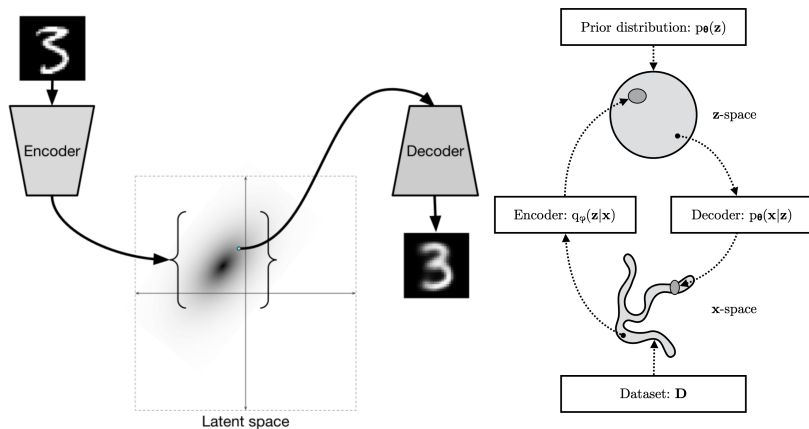

image credit: http://ijdykeman.github.io/ml/2016/12/21/cvae.html
Kingma D. P., Welling M., An Introduction to Variational Autoencoders, 2019

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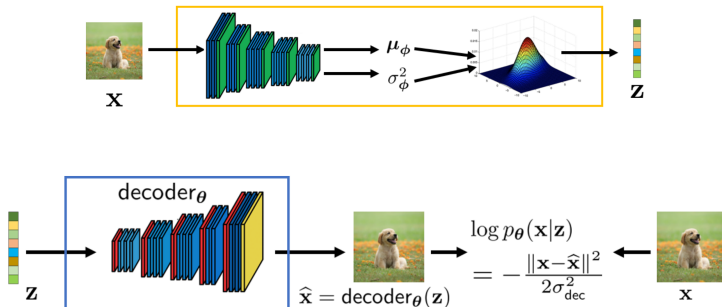

VAEs are widely used as a preliminary stage of projecting data onto low-dimensional space.

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 $p_\theta(\mathbf{x}|\mathbf{z}) = \text{NN}_{d,\theta}(\mathbf{z})$ 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 $\mathbf{z} \sim q_\phi(\mathbf{z}\|\mathbf{x})$	deterministic $\mathbf{z} = \mathbf{f}_\theta(\mathbf{x})$ $q_\theta(\mathbf{z}\|\mathbf{x}) = \delta(\mathbf{z} - \mathbf{f}_\theta(\mathbf{x}))$
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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:

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

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

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

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.