

Deep Generative Models

Lecture 3

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AI Masters

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Recap of Previous Lecture

Jacobian Matrix

Let $\mathbf{f} : \mathbb{R}^m \rightarrow \mathbb{R}^m$ 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)

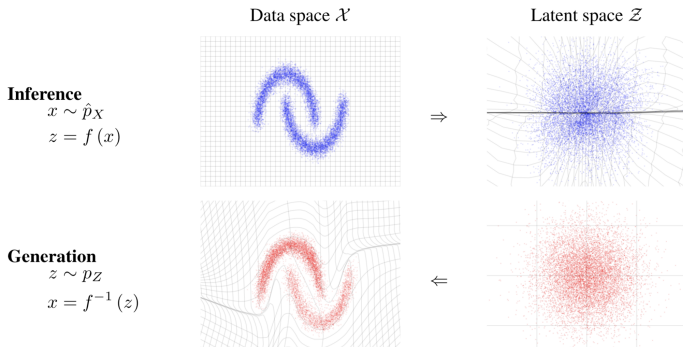
Let $\mathbf{x} \in \mathbb{R}^m$ be a random vector with density $p(\mathbf{x})$, and let $\mathbf{f} : \mathbb{R}^m \rightarrow \mathbb{R}^m$ be a C^1 -diffeomorphism (\mathbf{f} and \mathbf{f}^{-1} are continuously differentiable mappings). If $\mathbf{z} = \mathbf{f}(\mathbf{x})$, then

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

Recap of Previous Lecture

Definition

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



Log-Likelihood

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

Recap of Previous Lecture

Flow Log-Likelihood

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

One significant challenge is efficiently computing the Jacobian determinant.

Linear Flows

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

- ▶ 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.

Recap of Previous Lecture

Consider an autoregressive model:

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

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**.

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

$$\begin{cases} \mathbf{x}_1 = \mathbf{z}_1; \\ \mathbf{x}_2 = \mathbf{z}_2 \odot \sigma_{\theta}(\mathbf{z}_1) + \mu_{\theta}(\mathbf{z}_1). \end{cases} \quad \begin{cases} \mathbf{z}_1 = \mathbf{x}_1; \\ \mathbf{z}_2 = (\mathbf{x}_2 - \mu_{\theta}(\mathbf{x}_1)) \odot \frac{1}{\sigma_{\theta}(\mathbf{x}_1)}. \end{cases}$$

Both density estimation and sampling require just a single pass!

Jacobian

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

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

Recap of Previous Lecture

Posterior Distribution (Bayes' Theorem)

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

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

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)

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Latent Variable Models (LVM)

Maximum Likelihood Estimation (MLE) Problem

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

Latent Variable Models (LVM)

Maximum Likelihood Estimation (MLE) Problem

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The distribution $p_{\theta}(\mathbf{x})$ 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} :

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

Latent Variable Models (LVM)

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

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

Motivation

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

Latent Variable Models (LVM)

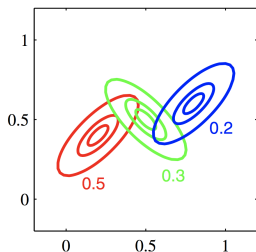
$$\log p_{\theta}(\mathbf{x}) = \log \int p_{\theta}(\mathbf{x}|\mathbf{z})p(\mathbf{z})d\mathbf{z} \rightarrow \max_{\theta}$$

Latent Variable Models (LVM)

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Examples

Mixture of Gaussians



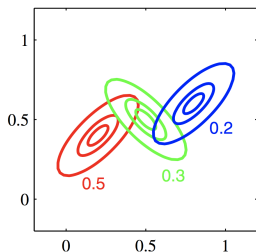
- ▶ $p_{\theta}(\mathbf{x}|\mathbf{z}) = \mathcal{N}(\boldsymbol{\mu}_{\mathbf{z}}, \boldsymbol{\Sigma}_{\mathbf{z}})$
- ▶ $p(\mathbf{z}) = \text{Cat}(\boldsymbol{\pi})$

Latent Variable Models (LVM)

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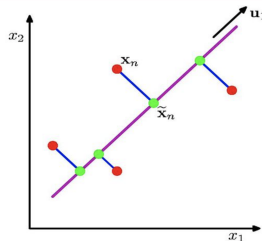
Examples

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- ▶ $p_{\theta}(\mathbf{x}|\mathbf{z}) = \mathcal{N}(\boldsymbol{\mu}_{\mathbf{z}}, \boldsymbol{\Sigma}_{\mathbf{z}})$
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PCA Model



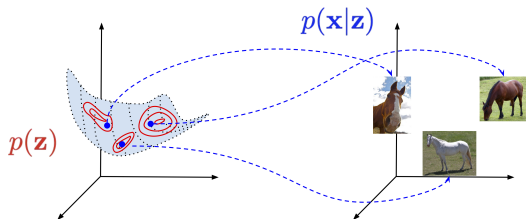
- ▶ $p_{\theta}(\mathbf{x}|\mathbf{z}) = \mathcal{N}(\mathbf{W}\mathbf{z} + \boldsymbol{\mu}, \sigma^2\mathbf{I})$
- ▶ $p(\mathbf{z}) = \mathcal{N}(0, \mathbf{I})$

MLE for LVM

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

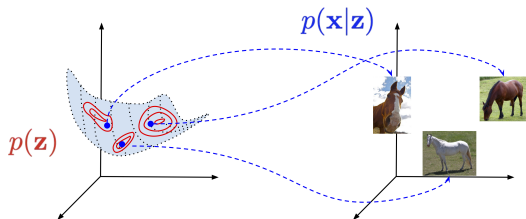
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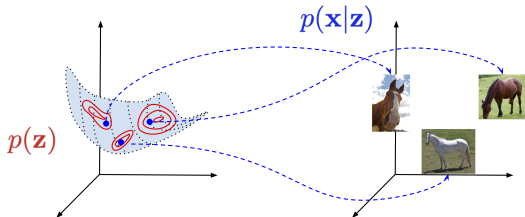
Naive Monte Carlo Estimation

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

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

MLE for LVM

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



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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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ELBO Derivation I

Inequality Derivation

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

ELBO Derivation I

Inequality Derivation

$$\begin{aligned}\log p_{\theta}(\mathbf{x}) &= \log \int p_{\theta}(\mathbf{x}, \mathbf{z}) d\mathbf{z} = \log \int \frac{q(\mathbf{z})}{q(\mathbf{z})} p_{\theta}(\mathbf{x}, \mathbf{z}) d\mathbf{z} = \\ &= \log \mathbb{E}_q \left[\frac{p_{\theta}(\mathbf{x}, \mathbf{z})}{q(\mathbf{z})} \right]\end{aligned}$$

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

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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

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

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Variational Decomposition

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

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

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

Variational Evidence Lower Bound (ELBO)

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

Variational Evidence Lower Bound (ELBO)

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

Log-Likelihood Decomposition

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

Variational Evidence Lower Bound (ELBO)

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Log-Likelihood Decomposition

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

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- Instead of maximizing the likelihood, maximize the ELBO:

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

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- Instead of maximizing the likelihood, maximize the ELBO:

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

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

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

Variational Posterior

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

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

Variational Posterior

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

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$$\begin{aligned} q^*(\mathbf{z}) &= \arg \max_q \mathcal{L}_{q,\theta^*}(\mathbf{x}) = \\ &= \arg \min_q \text{KL}(q(\mathbf{z})\|p_{\theta^*}(\mathbf{z}|\mathbf{x})) = p_{\theta^*}(\mathbf{z}|\mathbf{x}). \end{aligned}$$

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

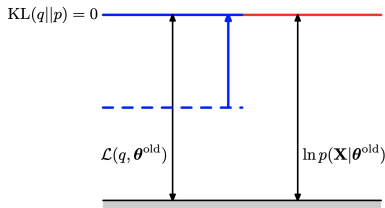
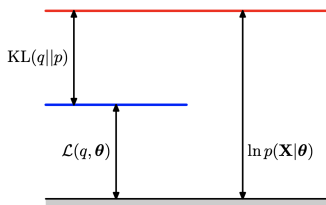
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Outline

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

Parametric Variable Posterior

Variational Posterior

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

Parametric Variable Posterior

Variational Posterior

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

- ▶ $p_{\theta^*}(\mathbf{z} | \mathbf{x})$ 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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Variational Posterior

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

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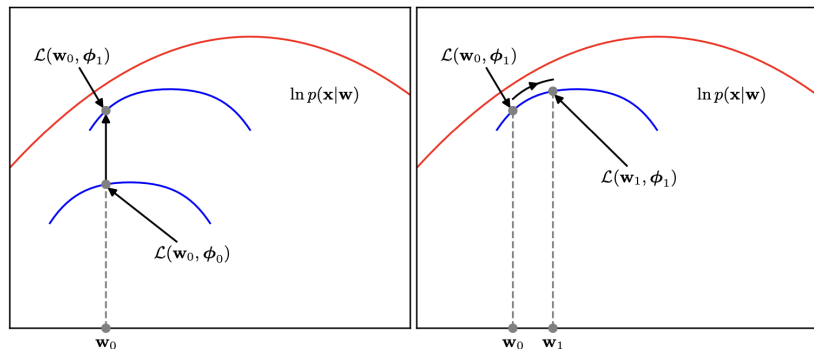
Gradient Update

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

ELBO optimization

Gradient Update

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



ELBO optimization

ELBO

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

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

ELBO optimization

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

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

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

Outline

1. Latent Variable Models (LVM) (continued)
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ELBO Gradients: $\nabla_{\theta} \mathcal{L}_{\phi, \theta}(\mathbf{x})$

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

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

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

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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 $p(\mathbf{z})$.

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:

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

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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,

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

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

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

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

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

Variational Assumption

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

$$q_{\phi}(\mathbf{z}|\mathbf{x}) = \mathcal{N}(\mu_{\phi}(\mathbf{x}), \sigma_{\phi}^2(\mathbf{x})).$$

Here, $\mu_{\phi}(\cdot)$ and $\sigma_{\phi}(\cdot)$ 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: $\nabla_{\phi} \mathcal{L}_{\phi, \theta}(\mathbf{x})$

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

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

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

Reconstruction Term

$$\begin{aligned} \nabla_{\phi} \int q_{\phi}(\mathbf{z}|\mathbf{x}) \log p_{\theta}(\mathbf{x}|\mathbf{z}) d\mathbf{z} &= \int p(\epsilon) \nabla_{\phi} \log p_{\theta}(\mathbf{x} | \mathbf{g}_{\phi}(\mathbf{x}, \epsilon)) d\epsilon \approx \\ &\approx \nabla_{\phi} \log p_{\theta}(\mathbf{x} | \sigma_{\phi}(\mathbf{x}) \odot \epsilon^* + \mu_{\phi}(\mathbf{x})), \quad \text{where } \epsilon^* \sim \mathcal{N}(0, \mathbf{I}) \end{aligned}$$

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

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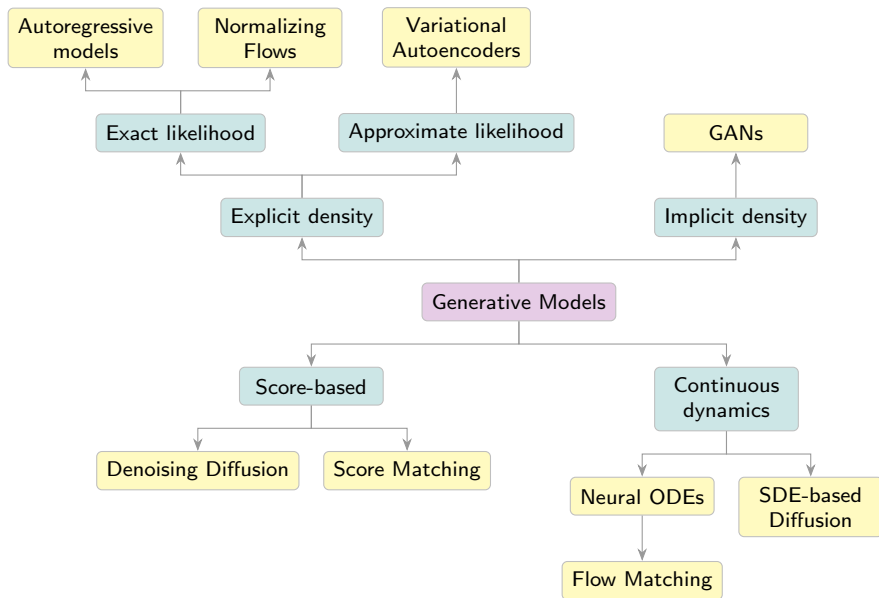
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This expression admits a closed-form analytic solution.

Outline

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

Generative Models Taxonomy



Variational Autoencoder (VAE)

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

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

Variational Autoencoder

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

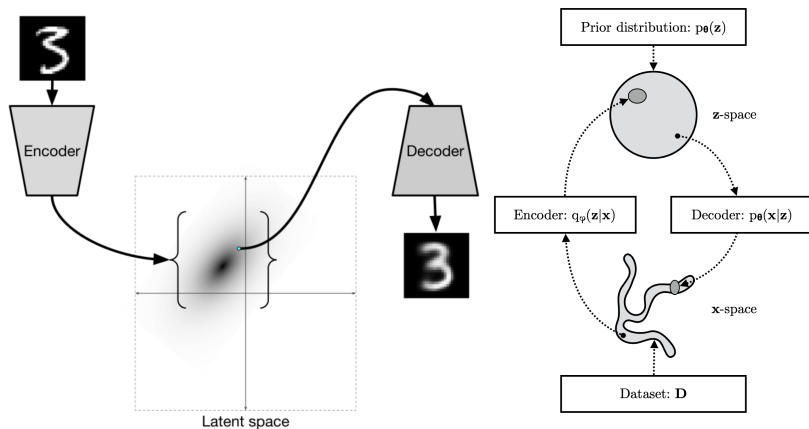
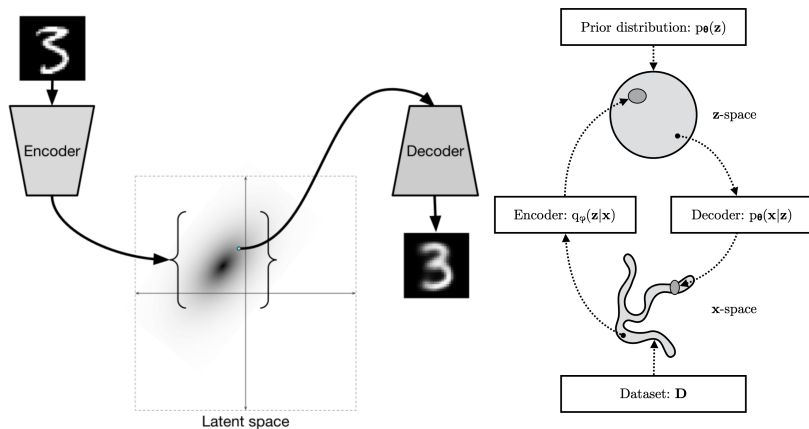


image credit: <http://ijdykeman.github.io/ml/2016/12/21/cvae.html>
Kingma D. P., Welling M., *An Introduction to Variational Autoencoders*, 2019

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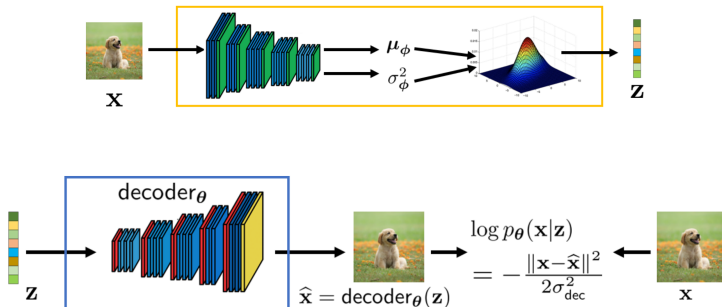


VAEs are widely used as a preliminary stage of projecting data onto low-dimensional space.

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

Variational Autoencoder

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



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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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.