Deep Generative Models

Lecture 4

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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.

Recap of Previous Lecture

Latent Variable Models (LVM)

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

MLE Problem for LVM

$$\begin{aligned}\boldsymbol{\theta}^* = \arg\max_{\boldsymbol{\theta}} \log p_{\boldsymbol{\theta}}(\mathbf{X}) = \arg\max_{\boldsymbol{\theta}} \sum_{i=1}^{n} \log p_{\boldsymbol{\theta}}(\mathbf{x}_i) = \\ = \arg\max_{\boldsymbol{\theta}} \sum_{i=1}^{n} \log \int p_{\boldsymbol{\theta}}(\mathbf{x}_i|\mathbf{z}_i) p(\mathbf{z}_i) d\mathbf{z}_i.\end{aligned}$$

Naive Monte Carlo Estimation

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

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

Recap of Previous Lecture

ELBO Derivation 1 (Inequality)

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

ELBO Derivation 2 (Equality)

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

Variational Decomposition

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

Recap of Previous Lecture

Variational Evidence Lower Bound (ELBO)

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

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

Log-likelihood Decomposition

$$\log p_{\boldsymbol{\theta}}(\mathbf{x}) = \mathbb{E}_q \log p_{\boldsymbol{\theta}}(\mathbf{x}|\mathbf{z}) - \mathrm{KL}(q(\mathbf{z}) \| p(\mathbf{z})) + \mathrm{KL}(q(\mathbf{z}) \| p_{\boldsymbol{\theta}}(\mathbf{z}|\mathbf{x})).$$

- Rather than maximizing 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:

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

Recap of Previous Lecture

$$
\begin{aligned}
\mathcal{L}_{q,\boldsymbol{\theta}}(\mathbf{x}) = \mathbb{E}_q \log p_{\boldsymbol{\theta}}(\mathbf{x}|\mathbf{z}) - \mathrm{KL}(q(\mathbf{z}) \| p(\mathbf{z})) = \\
= \mathbb{E}_q \left[\log p_{\boldsymbol{\theta}}(\mathbf{x}|\mathbf{z}) - \log \frac{q(\mathbf{z})}{p(\mathbf{z})} \right] d\mathbf{z} \rightarrow \max_{q,\boldsymbol{\theta}}.
\end{aligned}
$$

EM Algorithm (Block-Coordinate Optimization)

- Initialize $\boldsymbol{\theta}^*$;
- **E-step:** ($\mathcal{L}_{q,\boldsymbol{\theta}}(\mathbf{x}) \rightarrow \max_q$)

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

- **M-step:** ($\mathcal{L}_{q,\boldsymbol{\theta}}(\mathbf{x}) \rightarrow \max_{\boldsymbol{\theta}}$)

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

- Repeat E-step and M-step until convergence.

Recap of Previous Lecture

EM-Algorithm

- E-Step:

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

- M-Step:

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

Amortized Variational Inference

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

Variational Bayes

- E-Step:

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

- M-Step:

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

Outline

1. ELBO Gradients, Reparametrization Trick
2. Variational Autoencoder (VAE)
3. Discrete VAE Latent Representations

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1. ELBO Gradients, Reparametrization Trick

2. Variational Autoencoder (VAE)

3. Discrete VAE Latent Representations

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Naive Monte Carlo Estimation

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

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

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

Naive Monte Carlo Estimation

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

The variational posterior $q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x})$ 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: E-Step ($\nabla_\phi \mathcal{L}_{\phi,\theta}(\mathbf{x})$)

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

Unlike the M-step, 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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&\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}))
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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: E-Step ($\nabla_\phi \mathcal{L}_{\phi,\boldsymbol{\theta}}(\mathbf{x})$)

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\end{aligned}$$

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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 $p(\boldsymbol{\epsilon})$.

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

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

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

where $\boldsymbol{\epsilon}^* \sim p(\boldsymbol{\epsilon})$.

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

Reparametrization Trick (LOTUS Trick)

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

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

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

Variational Assumption

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

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

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

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

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

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

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Reconstruction Term

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

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

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

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

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

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

KL Term

$p(\mathbf{z})$ is the prior over latents $\mathbf{z}$, typically $p(\mathbf{z}) = \mathcal{N}(0, \mathbf{I})$.

$$\nabla_\phi \mathrm{KL}(q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x}) \| p(\mathbf{z})) = \nabla_\phi \mathrm{KL} \left(\mathcal{N}(\boldsymbol{\mu}_{\boldsymbol{\phi}}(\mathbf{x}), \boldsymbol{\sigma}^2_{\boldsymbol{\phi}}(\mathbf{x})) \| \mathcal{N}(0, \mathbf{I}) \right)$$

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

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

Reconstruction Term

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

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KL Term

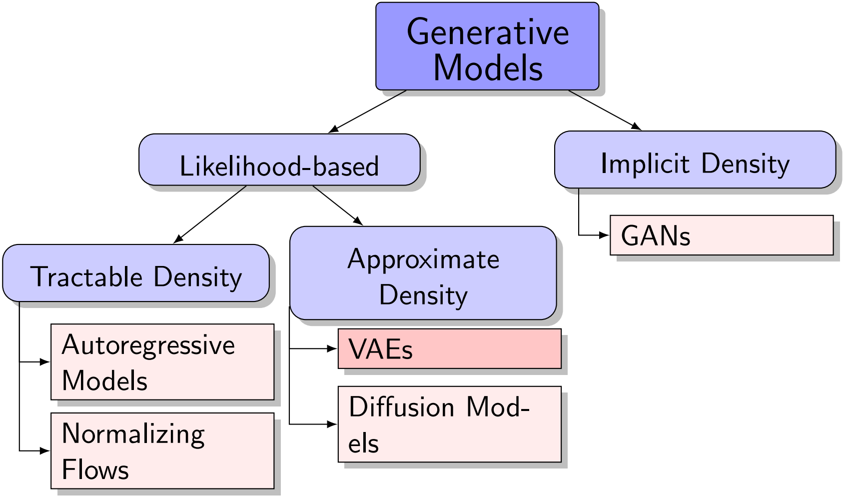
$p(\mathbf{z})$ is the prior over latents $\mathbf{z}$, typically $p(\mathbf{z}) = \mathcal{N}(0, \mathbf{I})$.

$$\nabla_{\phi}\mathrm{KL}(q_{\phi}(\mathbf{z}|\mathbf{x}) \| p(\mathbf{z})) = \nabla_{\phi}\mathrm{KL}\left(\mathcal{N}(\boldsymbol{\mu}_{\phi}(\mathbf{x}), \boldsymbol{\sigma}^2_{\phi}(\mathbf{x})) \| \mathcal{N}(0, \mathbf{I})\right)$$

This expression admits a closed-form analytic solution.

Outline

Generative Models Zoo



Variational Autoencoder (VAE)

Training (EM Algorithm)

- Select a random sample $\mathbf{x}_i, i \sim \text{Uniform}\{1, n\}$ (or a batch).

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- Compute the objective (apply the reparametrization trick):

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

$$\mathcal{L}_{\boldsymbol{\phi},\boldsymbol{\theta}}(\mathbf{x}) \approx \log p_{\boldsymbol{\theta}}(\mathbf{x}|\mathbf{z}^*) - \mathrm{KL}(q_{\boldsymbol{\phi}}(\mathbf{z}^*|\mathbf{x}) \| p(\mathbf{z}^*)).$$

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- Update parameters via stochastic gradient steps with respect to $\boldsymbol{\phi}$ and $\boldsymbol{\theta}$ (as in autograd).

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

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- Update parameters via stochastic gradient steps with respect to $\boldsymbol{\phi}$ and $\boldsymbol{\theta}$ (as in autograd).

Inference

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Variational Autoencoder (VAE)

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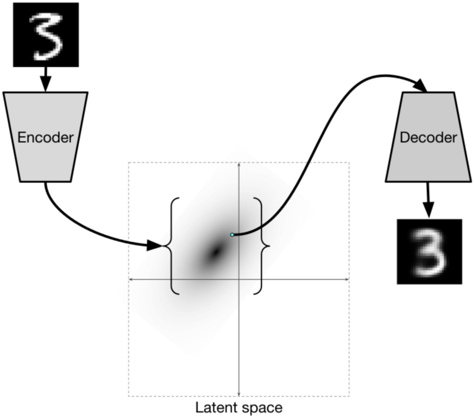
Note: The encoder $q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x})$ isn't needed during generation.

Variational Autoencoder

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



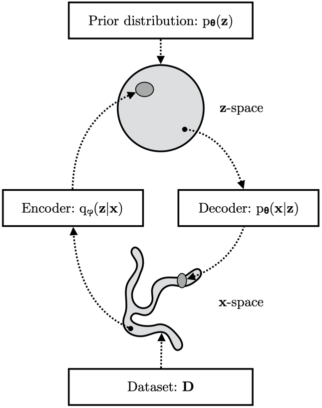
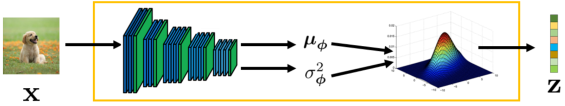
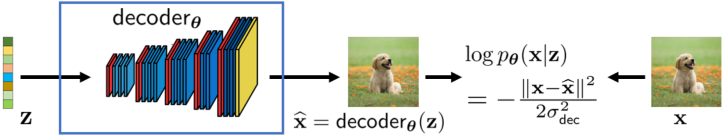


image credit: http://ijdykeman.github.io/ml/2016/12/21/cvae.html
Kingma D. P., Welling M., An Introduction to Variational Autoencoders, 2019

Variational Autoencoder

- The encoder $q_\phi(\mathbf{z}|\mathbf{x}) = \text{NN}_e(\mathbf{x}, \phi)$ outputs $\boldsymbol{\mu}_\phi(\mathbf{x})$ and $\boldsymbol{\sigma}_\phi(\mathbf{x})$.
- The decoder $p_{\boldsymbol{\theta}}(\mathbf{x}|\mathbf{z}) = \text{NN}_d(\mathbf{z}, \boldsymbol{\theta})$ 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 $\mathbf{z} = \mathbf{f}_{\boldsymbol{\theta}}(\mathbf{x})$ $q_{\boldsymbol{\theta}}(\mathbf{z}\|\mathbf{x}) = \delta(\mathbf{z} - \mathbf{f}_{\boldsymbol{\theta}}(\mathbf{x}))$
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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Outline

1. ELBO Gradients, Reparametrization Trick
2. Variational Autoencoder (VAE)
3. Discrete VAE Latent Representations

Discrete VAE Latents

Motivation

- Previous VAE models have used **continuous** latent variables $\mathbf{z}$.
- For some modalities, **discrete** representations $\mathbf{z}$ may be a more natural choice.
- Advanced autoregressive models (e.g., PixelCNN) are highly effective for distributions over discrete variables.
- Current transformer-like models process discrete tokens.

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ELBO

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- Apply the reparametrization trick to obtain unbiased gradients.
- Use Gaussian distributions for $q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x})$ and $p(\mathbf{z})$ to compute the KL analytically.

Discrete VAE Latents

Assumptions

- Let $c \sim \mathrm{Categorical}(\boldsymbol{\pi})$, where
$$\boldsymbol{\pi} = (\pi_1, \ldots, \pi_K), \quad \pi_k = P(c = k), \quad \sum_{k=1}^{K} \pi_k = 1.$$
- Suppose the VAE adopts a discrete latent variable c with prior $p(c) = \text{Uniform}\{1, \ldots, K\}$.

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$$\mathrm{KL}(q_\phi(c|\mathbf{x}) \| p(c)) = \sum_{k=1}^{K} q_\phi(k|\mathbf{x}) \log \frac{q_\phi(k|\mathbf{x})}{p(k)}$$

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$$= -\mathrm{H}(q_{\boldsymbol{\phi}}(c|\mathbf{x})) + \log K.$$

Discrete VAE Latents

$$\mathcal{L}_{\boldsymbol{\phi},\boldsymbol{\theta}}(\mathbf{x}) = \mathbb{E}_{q_{\boldsymbol{\phi}}(c|\mathbf{x})} \log p_{\boldsymbol{\theta}}(\mathbf{x}|c) + \mathrm{H}(q_{\boldsymbol{\phi}}(c|\mathbf{x})) - \log K \to \max_{\boldsymbol{\phi},\boldsymbol{\theta}}.$$

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

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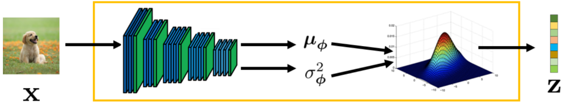
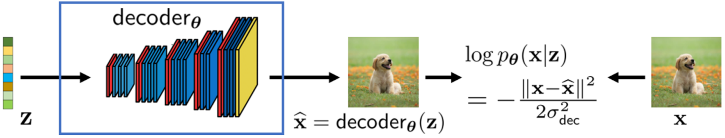
$$\mathcal{L}_{\phi,\theta}(\mathbf{x}) = \mathbb{E}_{q_\phi(c|\mathbf{x})} \log p_\theta(\mathbf{x}|c) + \mathrm{H}(q_\phi(c|\mathbf{x})) - \log K \to \max_{\phi,\theta}.$$

- The encoder should output a discrete distribution $q_\phi(c|\mathbf{x})$.
- We need an analogue of the reparametrization trick for discrete $q_\phi(c|\mathbf{x})$.
- The decoder $p_\theta(\mathbf{x}|c)$ must take a discrete random variable c as input.





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Summary

- 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 $p_{\boldsymbol{\theta}}(\mathbf{x}|\mathbf{z})$.
- NF models can be interpreted as VAEs with deterministic encoder and decoder functions.
- Discrete VAE latents offer a natural class of latent variable models.