

Deep Generative Models

Lecture 4

Roman Isachenko

Moscow Institute of Physics and Technology
Yandex School of Data Analysis

2025, Autumn

Recap of Previous Lecture

Latent Variable Models (LVM)

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

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

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

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

Recap of Previous Lecture

ELBO Derivation 1 (Inequality)

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

ELBO Derivation 2 (Equality)

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

Variational Decomposition

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

Recap of Previous Lecture

Variational Evidence Lower Bound (ELBO)

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

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

Log-likelihood Decomposition

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

- ▶ Rather than maximizing likelihood, maximize the ELBO:

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

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

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

Recap of Previous Lecture

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

Variational Posterior

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

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 .

Gradient Update

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

Recap of Previous Lecture

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

Gradient w.r.t. θ — Monte Carlo Estimation

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

Gradient w.r.t. ϕ — Reparameterization Trick

$$\begin{aligned}\nabla_{\phi} \mathcal{L}_{\phi, \theta}(\mathbf{x}) &= \int p(\epsilon) \nabla_{\phi} \log p_{\theta}(\mathbf{x}|\mathbf{g}_{\phi}(\mathbf{x}, \epsilon)) d\epsilon - \nabla_{\phi} \text{KL} \\ &\approx \nabla_{\phi} \log p_{\theta}(\mathbf{x}|\mathbf{g}_{\phi}(\mathbf{x}, \epsilon^*)) - \nabla_{\phi} \text{KL}\end{aligned}$$

Variational Assumption

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

$$\mathbf{z} = \mathbf{g}_{\phi}(\mathbf{x}, \epsilon) = \boldsymbol{\sigma}_{\phi}(\mathbf{x}) \odot \epsilon + \boldsymbol{\mu}_{\phi}(\mathbf{x}).$$

Recap of Previous Lecture

Training

- ▶ Pick a batch of samples $\{\mathbf{x}_i\}_{i=1}^B$ (here we use Monte Carlo technique).
- ▶ Compute the objective for each sample (apply the reparametrization trick):

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

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

- ▶ Update parameters via stochastic gradient steps with respect to ϕ and θ .

Inference

- ▶ Sample \mathbf{z}^* from the prior $p(\mathbf{z}) (\mathcal{N}(0, \mathbf{I}))$;
- ▶ Generate data from the decoder $p_\theta(\mathbf{x}|\mathbf{z}^*)$.

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

Recap of Previous Lecture

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

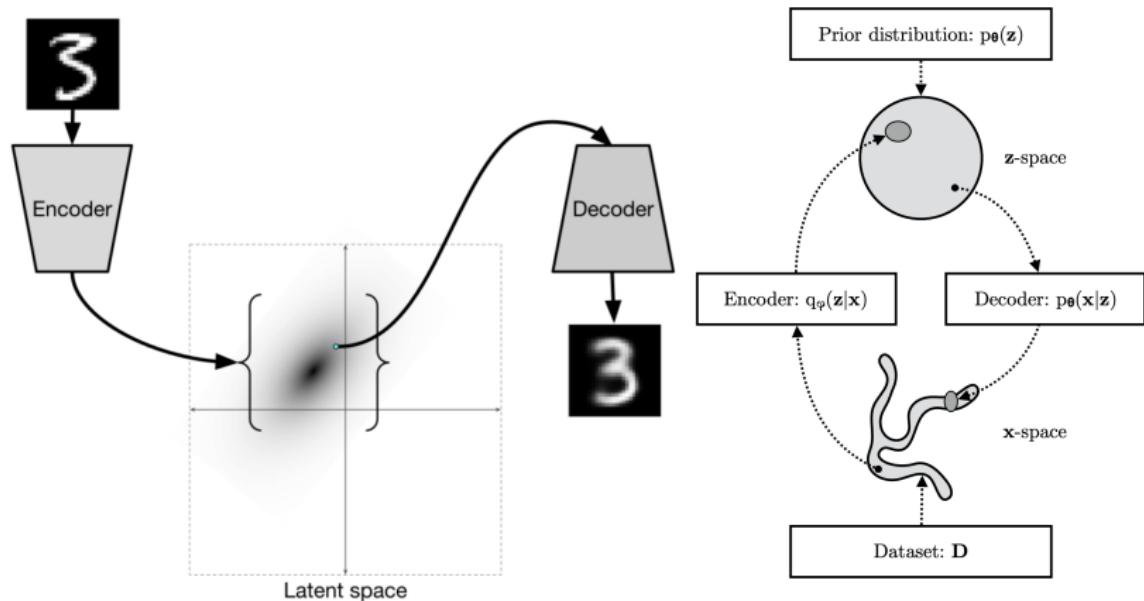


image credit: <http://ijdykeman.github.io/ml/2016/12/21/cvae.html>

Kingma D. P., Welling M. An Introduction to Variational Autoencoders, 2019

Outline

1. Discrete VAE Latent Representations
2. Vector Quantized VAE
3. ELBO Surgery
4. Learnable VAE Prior

Outline

1. Discrete VAE Latent Representations
2. Vector Quantized VAE
3. ELBO Surgery
4. Learnable VAE Prior

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.

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.

ELBO

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

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.

ELBO

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

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

Discrete VAE Latents

Assumptions

- ▶ Let $c \sim \text{Categorical}(\boldsymbol{\pi})$, where

$$\boldsymbol{\pi} = (\pi_1, \dots, \pi_K), \quad \pi_k = P(c = k), \quad \sum_{k=1}^K \pi_k = 1.$$

- ▶ Suppose the VAE adopts a discrete latent variable c with prior $p(c) = \text{Uniform}\{1, \dots, K\}$.

Discrete VAE Latents

Assumptions

- ▶ Let $c \sim \text{Categorical}(\boldsymbol{\pi})$, where

$$\boldsymbol{\pi} = (\pi_1, \dots, \pi_K), \quad \pi_k = P(c = k), \quad \sum_{k=1}^K \pi_k = 1.$$

- ▶ Suppose the VAE adopts a discrete latent variable c with prior $p(c) = \text{Uniform}\{1, \dots, K\}$.

ELBO

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

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

Discrete VAE Latents

Assumptions

- ▶ Let $c \sim \text{Categorical}(\boldsymbol{\pi})$, where

$$\boldsymbol{\pi} = (\pi_1, \dots, \pi_K), \quad \pi_k = P(c = k), \quad \sum_{k=1}^K \pi_k = 1.$$

- ▶ Suppose the VAE adopts a discrete latent variable c with prior $p(c) = \text{Uniform}\{1, \dots, K\}$.

ELBO

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

$$\begin{aligned} \text{KL}(q_\phi(c|\mathbf{x}) \| p(c)) &= \sum_{k=1}^K q_\phi(k|\mathbf{x}) \log \frac{q_\phi(k|\mathbf{x})}{p(k)} = \\ &= \sum_{k=1}^K q_\phi(k|\mathbf{x}) \log q_\phi(k|\mathbf{x}) - \sum_{k=1}^K q_\phi(k|\mathbf{x}) \log p(k) \end{aligned}$$

Discrete VAE Latents

Assumptions

- ▶ Let $c \sim \text{Categorical}(\boldsymbol{\pi})$, where

$$\boldsymbol{\pi} = (\pi_1, \dots, \pi_K), \quad \pi_k = P(c = k), \quad \sum_{k=1}^K \pi_k = 1.$$

- ▶ Suppose the VAE adopts a discrete latent variable c with prior $p(c) = \text{Uniform}\{1, \dots, K\}$.

ELBO

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

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

$$= \sum_{k=1}^K q_\phi(k|\mathbf{x}) \log q_\phi(k|\mathbf{x}) - \sum_{k=1}^K q_\phi(k|\mathbf{x}) \log p(k) =$$

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

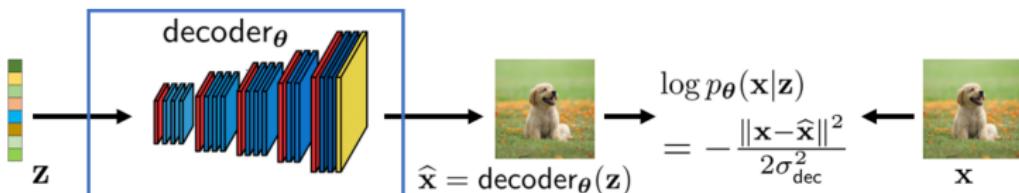
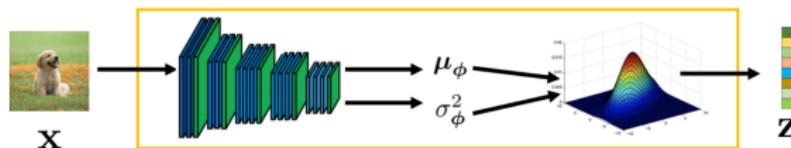
Discrete VAE Latents

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

Discrete VAE Latents

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

- ▶ 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.



Outline

1. Discrete VAE Latent Representations
2. Vector Quantized VAE
3. ELBO Surgery
4. Learnable VAE Prior

Vector Quantization

Define the codebook (dictionary) space $\{\mathbf{e}_k\}_{k=1}^K$ with $\mathbf{e}_k \in \mathbb{R}^L$ and K the number of codebook entries.

Vector Quantization

Define the codebook (dictionary) space $\{\mathbf{e}_k\}_{k=1}^K$ with $\mathbf{e}_k \in \mathbb{R}^L$ and K the number of codebook entries.

Quantized Representation

A quantized vector $\mathbf{z}_q \in \mathbb{R}^L$, for any $\mathbf{z} \in \mathbb{R}^L$, is defined via nearest-neighbor lookup in the codebook:

$$\mathbf{z}_q = \mathbf{q}(\mathbf{z}) = \mathbf{e}_{k^*}, \quad \text{where } k^* = \arg \min_k \|\mathbf{z} - \mathbf{e}_k\|.$$

Vector Quantization

Define the codebook (dictionary) space $\{\mathbf{e}_k\}_{k=1}^K$ with $\mathbf{e}_k \in \mathbb{R}^L$ and K the number of codebook entries.

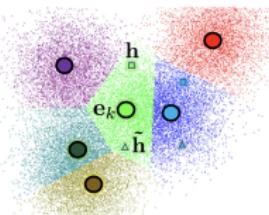
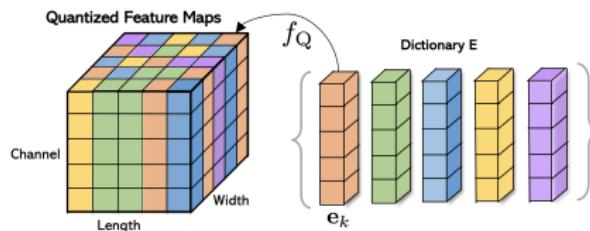
Quantized Representation

A quantized vector $\mathbf{z}_q \in \mathbb{R}^L$, for any $\mathbf{z} \in \mathbb{R}^L$, is defined via nearest-neighbor lookup in the codebook:

$$\mathbf{z}_q = \mathbf{q}(\mathbf{z}) = \mathbf{e}_{k^*}, \quad \text{where } k^* = \arg \min_k \|\mathbf{z} - \mathbf{e}_k\|.$$

Quantization Procedure

If the encoded tensor has spatial dimensions, quantization is independently applied to each of the $W \times H$ locations.



Vector Quantized VAE (VQ-VAE)

- ▶ The encoder outputs a continuous vector $\mathbf{z}_e = \text{NN}_{\mathbf{e}, \phi}(\mathbf{x}) \in \mathbb{R}^L$.
- ▶ Quantization deterministically maps \mathbf{z}_e to its quantized codebook vector \mathbf{z}_q .
- ▶ The decoder is conditioned on codebook entries \mathbf{e}_c , i.e., via $p_{\theta}(\mathbf{x}|\mathbf{e}_c)$ (instead of $p_{\theta}(\mathbf{x}|c)$).

Vector Quantized VAE (VQ-VAE)

- ▶ The encoder outputs a continuous vector $\mathbf{z}_e = \text{NN}_{\mathbf{e}, \phi}(\mathbf{x}) \in \mathbb{R}^L$.
- ▶ Quantization deterministically maps \mathbf{z}_e to its quantized codebook vector \mathbf{z}_q .
- ▶ The decoder is conditioned on codebook entries \mathbf{e}_c , i.e., via $p_{\theta}(\mathbf{x}|\mathbf{e}_c)$ (instead of $p_{\theta}(\mathbf{x}|c)$).

Deterministic Variational Posterior

$$q_{\phi}(c = k^* | \mathbf{x}) = \begin{cases} 1, & \text{for } k^* = \arg \min_k \|\mathbf{z}_e - \mathbf{e}_k\|; \\ 0, & \text{otherwise.} \end{cases}$$

Vector Quantized VAE (VQ-VAE)

- ▶ The encoder outputs a continuous vector $\mathbf{z}_e = \text{NN}_{\mathbf{e}, \phi}(\mathbf{x}) \in \mathbb{R}^L$.
- ▶ Quantization deterministically maps \mathbf{z}_e to its quantized codebook vector \mathbf{z}_q .
- ▶ The decoder is conditioned on codebook entries \mathbf{e}_c , i.e., via $p_{\theta}(\mathbf{x}|\mathbf{e}_c)$ (instead of $p_{\theta}(\mathbf{x}|c)$).

Deterministic Variational Posterior

$$q_{\phi}(c = k^* | \mathbf{x}) = \begin{cases} 1, & \text{for } k^* = \arg \min_k \|\mathbf{z}_e - \mathbf{e}_k\|; \\ 0, & \text{otherwise.} \end{cases}$$

$$\text{KL}(q_{\phi}(c|\mathbf{x}) \| p(c)) = - \underbrace{\mathbb{H}(q_{\phi}(c|\mathbf{x}))}_{=0} + \log K = \log K.$$

Vector Quantized VAE (VQ-VAE)

- ▶ The encoder outputs a continuous vector $\mathbf{z}_e = \text{NN}_{\mathbf{e}, \phi}(\mathbf{x}) \in \mathbb{R}^L$.
- ▶ Quantization deterministically maps \mathbf{z}_e to its quantized codebook vector \mathbf{z}_q .
- ▶ The decoder is conditioned on codebook entries \mathbf{e}_c , i.e., via $p_{\theta}(\mathbf{x}|\mathbf{e}_c)$ (instead of $p_{\theta}(\mathbf{x}|c)$).

Deterministic Variational Posterior

$$q_{\phi}(c = k^* | \mathbf{x}) = \begin{cases} 1, & \text{for } k^* = \arg \min_k \|\mathbf{z}_e - \mathbf{e}_k\|; \\ 0, & \text{otherwise.} \end{cases}$$

$$\text{KL}(q_{\phi}(c|\mathbf{x}) \| p(c)) = - \underbrace{\mathbb{H}(q_{\phi}(c|\mathbf{x}))}_{=0} + \log K = \log K.$$

Note: The KL regularizer becomes constant and has no direct effect on the ELBO objective in this case.

Vector Quantized VAE (VQ-VAE): Forward

Deterministic Variational Posterior

$$q_{\phi}(c = k^* | \mathbf{x}) = \begin{cases} 1, & \text{if } k^* = \arg \min_k \|\mathbf{z}_e - \mathbf{e}_k\|; \\ 0, & \text{otherwise.} \end{cases}$$

Vector Quantized VAE (VQ-VAE): Forward

Deterministic Variational Posterior

$$q_{\phi}(c = k^* | \mathbf{x}) = \begin{cases} 1, & \text{if } k^* = \arg \min_k \|\mathbf{z}_e - \mathbf{e}_k\|; \\ 0, & \text{otherwise.} \end{cases}$$

ELBO

$$\mathcal{L}_{\phi, \theta}(\mathbf{x}) = \mathbb{E}_{q_{\phi}(c | \mathbf{x})} \log p_{\theta}(\mathbf{x} | \mathbf{e}_c) - \log K$$

Vector Quantized VAE (VQ-VAE): Forward

Deterministic Variational Posterior

$$q_{\phi}(c = k^* | \mathbf{x}) = \begin{cases} 1, & \text{if } k^* = \arg \min_k \|\mathbf{z}_e - \mathbf{e}_k\|; \\ 0, & \text{otherwise.} \end{cases}$$

ELBO

$$\mathcal{L}_{\phi, \theta}(\mathbf{x}) = \mathbb{E}_{q_{\phi}(c | \mathbf{x})} \log p_{\theta}(\mathbf{x} | \mathbf{e}_c) - \log K = \log p_{\theta}(\mathbf{x} | \mathbf{z}_q) - \log K,$$

where $\mathbf{z}_q = \mathbf{e}_{k^*}$, $k^* = \arg \min_k \|\mathbf{z}_e - \mathbf{e}_k\|$.

Vector Quantized VAE (VQ-VAE): Forward

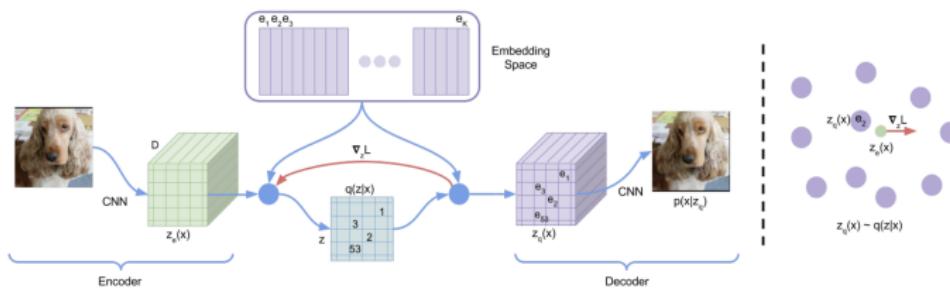
Deterministic Variational Posterior

$$q_{\phi}(c = k^* | \mathbf{x}) = \begin{cases} 1, & \text{if } k^* = \arg \min_k \|\mathbf{z}_e - \mathbf{e}_k\|; \\ 0, & \text{otherwise.} \end{cases}$$

ELBO

$$\mathcal{L}_{\phi, \theta}(\mathbf{x}) = \mathbb{E}_{q_{\phi}(c|\mathbf{x})} \log p_{\theta}(\mathbf{x}|\mathbf{e}_c) - \log K = \log p_{\theta}(\mathbf{x}|\mathbf{z}_q) - \log K,$$

where $\mathbf{z}_q = \mathbf{e}_{k^*}$, $k^* = \arg \min_k \|\mathbf{z}_e - \mathbf{e}_k\|$.



Vector Quantized VAE (VQ-VAE): Forward

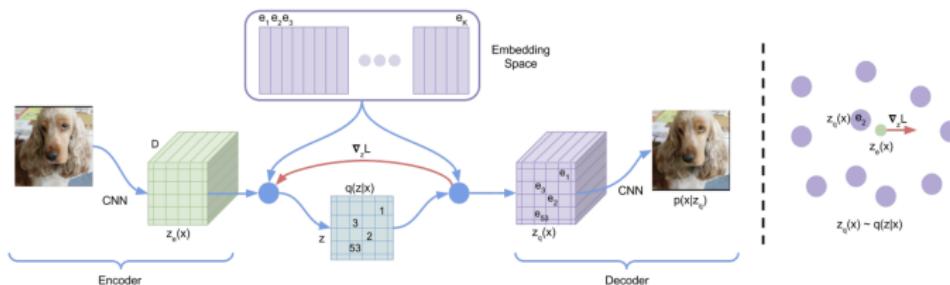
Deterministic Variational Posterior

$$q_{\phi}(c = k^* | \mathbf{x}) = \begin{cases} 1, & \text{if } k^* = \arg \min_k \|\mathbf{z}_e - \mathbf{e}_k\|; \\ 0, & \text{otherwise.} \end{cases}$$

ELBO

$$\mathcal{L}_{\phi, \theta}(\mathbf{x}) = \mathbb{E}_{q_{\phi}(c|\mathbf{x})} \log p_{\theta}(\mathbf{x}|\mathbf{e}_c) - \log K = \log p_{\theta}(\mathbf{x}|\mathbf{z}_q) - \log K,$$

where $\mathbf{z}_q = \mathbf{e}_{k^*}$, $k^* = \arg \min_k \|\mathbf{z}_e - \mathbf{e}_k\|$.



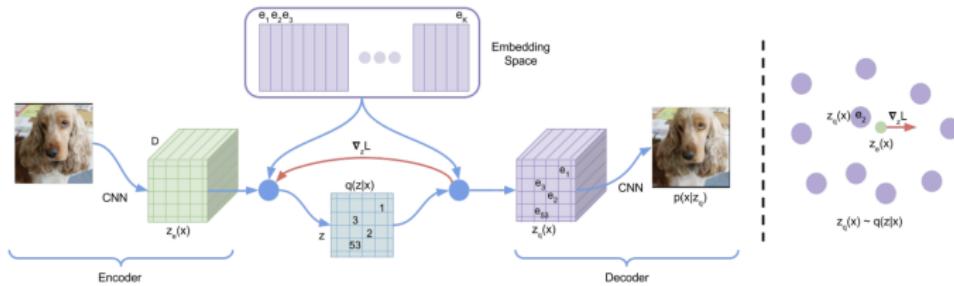
Challenge: The $\arg \min$ operation is non-differentiable.

Vector Quantized VAE (VQ-VAE): Backward ELBO

$$\mathcal{L}_{\phi, \theta}(\mathbf{x}) = \log p_{\theta}(\mathbf{x}|\mathbf{z}_q) - \log K, \quad \mathbf{z}_q = \mathbf{e}_{k^*}, \quad k^* = \arg \min_k \|\mathbf{z}_e - \mathbf{e}_k\|.$$

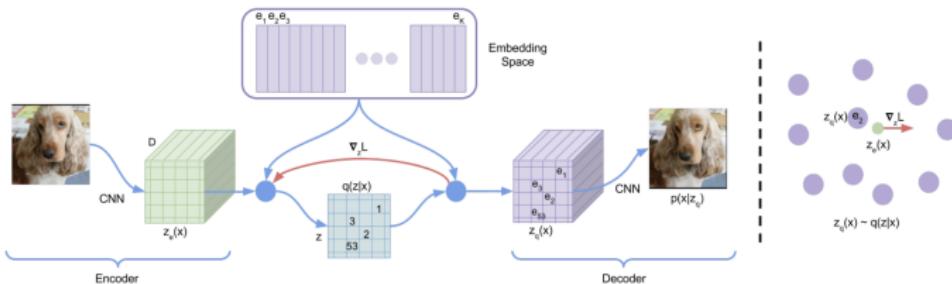
Vector Quantized VAE (VQ-VAE): Backward ELBO

$$\mathcal{L}_{\phi, \theta}(x) = \log p_{\theta}(x|z_q) - \log K, \quad z_q = \mathbf{e}_{k^*}, \quad k^* = \arg \min_k \|\mathbf{z}_e - \mathbf{e}_k\|.$$



Vector Quantized VAE (VQ-VAE): Backward ELBO

$$\mathcal{L}_{\phi, \theta}(x) = \log p_{\theta}(x|z_q) - \log K, \quad z_q = e_{k^*}, \quad k^* = \arg \min_k \|z_e - e_k\|.$$

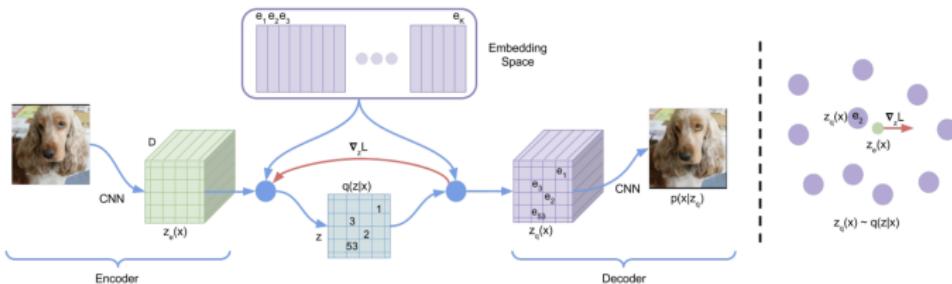


Straight-Through Gradient Estimator

$$\frac{\partial \log p(x|z_q, \theta)}{\partial \phi} = \frac{\partial \log p_{\theta}(x|z_q)}{\partial z_q} \cdot \frac{\partial z_q}{\partial \phi} =$$

Vector Quantized VAE (VQ-VAE): Backward ELBO

$$\mathcal{L}_{\phi, \theta}(x) = \log p_{\theta}(x|z_q) - \log K, \quad z_q = e_{k^*}, \quad k^* = \arg \min_k \|z_e - e_k\|.$$

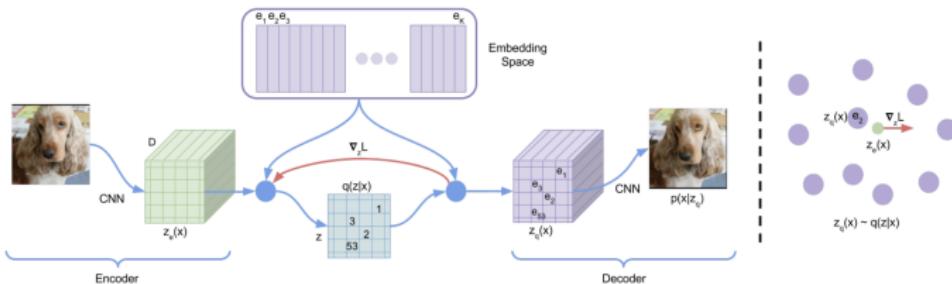


Straight-Through Gradient Estimator

$$\begin{aligned} \frac{\partial \log p(x|z_q, \theta)}{\partial \phi} &= \frac{\partial \log p_{\theta}(x|z_q)}{\partial z_q} \cdot \frac{\partial z_q}{\partial \phi} = \\ &= \frac{\partial \log p_{\theta}(x|z_q)}{\partial z_q} \cdot \frac{\partial z_q}{\partial z_e} \cdot \frac{\partial z_e}{\partial \phi} \end{aligned}$$

Vector Quantized VAE (VQ-VAE): Backward ELBO

$$\mathcal{L}_{\phi, \theta}(x) = \log p_{\theta}(x|z_q) - \log K, \quad z_q = e_{k^*}, \quad k^* = \arg \min_k \|z_e - e_k\|.$$



Straight-Through Gradient Estimator

$$\begin{aligned} \frac{\partial \log p(x|z_q, \theta)}{\partial \phi} &= \frac{\partial \log p_{\theta}(x|z_q)}{\partial z_q} \cdot \frac{\partial z_q}{\partial \phi} = \\ &= \frac{\partial \log p_{\theta}(x|z_q)}{\partial z_q} \cdot \frac{\partial z_q}{\partial z_e} \cdot \frac{\partial z_e}{\partial \phi} \approx \frac{\partial \log p_{\theta}(x|z_q)}{\partial z_q} \cdot \frac{\partial z_e}{\partial \phi} \end{aligned}$$

Vector Quantized VAE-2 (VQ-VAE-2)

Extension to the spatial domain: $\mathbf{c} \in \{1, \dots, K\}^{W \times H}$

$$q_{\phi}(\mathbf{c}|\mathbf{x}) = \prod_{i=1}^W \prod_{j=1}^H q(c_{ij}|\mathbf{x}, \phi); \quad p(\mathbf{c}) = \prod_{i=1}^W \prod_{j=1}^H \text{Uniform}\{1, \dots, K\}.$$

Sample Diversity



VQ-VAE (Proposed)

BigGAN deep

Outline

1. Discrete VAE Latent Representations
2. Vector Quantized VAE
3. ELBO Surgery
4. Learnable VAE Prior

ELBO Surgery

$$\frac{1}{n} \sum_{i=1}^n \mathcal{L}_{\phi, \theta}(\mathbf{x}_i) = \frac{1}{n} \sum_{i=1}^n \left[\mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x}_i)} \log p_\theta(\mathbf{x}_i|\mathbf{z}) - \text{KL}(q_\phi(\mathbf{z}|\mathbf{x}_i) \| p(\mathbf{z})) \right].$$

ELBO Surgery

$$\frac{1}{n} \sum_{i=1}^n \mathcal{L}_{\phi, \theta}(\mathbf{x}_i) = \frac{1}{n} \sum_{i=1}^n \left[\mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x}_i)} \log p_\theta(\mathbf{x}_i|\mathbf{z}) - \text{KL}(q_\phi(\mathbf{z}|\mathbf{x}_i) \| p(\mathbf{z})) \right].$$

Theorem

$$\frac{1}{n} \sum_{i=1}^n \text{KL}(q_\phi(\mathbf{z}|\mathbf{x}_i) \| p(\mathbf{z})) = \text{KL}(q_{\text{agg}, \phi}(\mathbf{z}) \| p(\mathbf{z})) + \mathbb{I}_q[\mathbf{x}, \mathbf{z}];$$

ELBO Surgery

$$\frac{1}{n} \sum_{i=1}^n \mathcal{L}_{\phi, \theta}(\mathbf{x}_i) = \frac{1}{n} \sum_{i=1}^n \left[\mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x}_i)} \log p_\theta(\mathbf{x}_i|\mathbf{z}) - \text{KL}(q_\phi(\mathbf{z}|\mathbf{x}_i) \| p(\mathbf{z})) \right].$$

Theorem

$$\frac{1}{n} \sum_{i=1}^n \text{KL}(q_\phi(\mathbf{z}|\mathbf{x}_i) \| p(\mathbf{z})) = \text{KL}(q_{\text{agg}, \phi}(\mathbf{z}) \| p(\mathbf{z})) + \mathbb{I}_q[\mathbf{x}, \mathbf{z}];$$

- ▶ $q_{\text{agg}, \phi}(\mathbf{z}) = \frac{1}{n} \sum_{i=1}^n q_\phi(\mathbf{z}|\mathbf{x}_i)$ denotes the **aggregated** variational posterior.
- ▶ $\mathbb{I}_q[\mathbf{x}, \mathbf{z}]$ is the mutual information between \mathbf{x} and \mathbf{z} under the data distribution $p_{\text{data}}(\mathbf{x})$ and $q_\phi(\mathbf{z}|\mathbf{x})$.
- ▶ The first term encourages $q_{\text{agg}, \phi}(\mathbf{z})$ to match the prior $p(\mathbf{z})$.
- ▶ The second term reduces the information about \mathbf{x} encoded in \mathbf{z} .

ELBO Surgery

$$\frac{1}{n} \sum_{i=1}^n \text{KL}(q_\phi(\mathbf{z}|\mathbf{x}_i) \| p(\mathbf{z})) = \text{KL}(q_{\text{agg},\phi}(\mathbf{z}) \| p(\mathbf{z})) + \mathbb{I}_q[\mathbf{x}, \mathbf{z}].$$

Proof

$$\frac{1}{n} \sum_{i=1}^n \text{KL}(q_\phi(\mathbf{z}|\mathbf{x}_i) \| p(\mathbf{z})) = \frac{1}{n} \sum_{i=1}^n \int q_\phi(\mathbf{z}|\mathbf{x}_i) \log \frac{q_\phi(\mathbf{z}|\mathbf{x}_i)}{p(\mathbf{z})} d\mathbf{z}$$

ELBO Surgery

$$\frac{1}{n} \sum_{i=1}^n \text{KL}(q_\phi(\mathbf{z}|\mathbf{x}_i) \| p(\mathbf{z})) = \text{KL}(q_{\text{agg},\phi}(\mathbf{z}) \| p(\mathbf{z})) + \mathbb{I}_q[\mathbf{x}, \mathbf{z}].$$

Proof

$$\begin{aligned}\frac{1}{n} \sum_{i=1}^n \text{KL}(q_\phi(\mathbf{z}|\mathbf{x}_i) \| p(\mathbf{z})) &= \frac{1}{n} \sum_{i=1}^n \int q_\phi(\mathbf{z}|\mathbf{x}_i) \log \frac{q_\phi(\mathbf{z}|\mathbf{x}_i)}{p(\mathbf{z})} d\mathbf{z} = \\ &= \frac{1}{n} \sum_{i=1}^n \int q_\phi(\mathbf{z}|\mathbf{x}_i) \log \frac{q_{\text{agg},\phi}(\mathbf{z}) q_\phi(\mathbf{z}|\mathbf{x}_i)}{p(\mathbf{z}) q_{\text{agg},\phi}(\mathbf{z})} d\mathbf{z}\end{aligned}$$

ELBO Surgery

$$\frac{1}{n} \sum_{i=1}^n \text{KL}(q_\phi(\mathbf{z}|\mathbf{x}_i) \| p(\mathbf{z})) = \text{KL}(q_{\text{agg},\phi}(\mathbf{z}) \| p(\mathbf{z})) + \mathbb{I}_q[\mathbf{x}, \mathbf{z}].$$

Proof

$$\begin{aligned} \frac{1}{n} \sum_{i=1}^n \text{KL}(q_\phi(\mathbf{z}|\mathbf{x}_i) \| p(\mathbf{z})) &= \frac{1}{n} \sum_{i=1}^n \int q_\phi(\mathbf{z}|\mathbf{x}_i) \log \frac{q_\phi(\mathbf{z}|\mathbf{x}_i)}{p(\mathbf{z})} d\mathbf{z} = \\ &= \frac{1}{n} \sum_{i=1}^n \int q_\phi(\mathbf{z}|\mathbf{x}_i) \log \frac{q_{\text{agg},\phi}(\mathbf{z}) q_\phi(\mathbf{z}|\mathbf{x}_i)}{p(\mathbf{z}) q_{\text{agg},\phi}(\mathbf{z})} d\mathbf{z} = \\ &= \int \frac{1}{n} \sum_{i=1}^n q_\phi(\mathbf{z}|\mathbf{x}_i) \log \frac{q_{\text{agg},\phi}(\mathbf{z})}{p(\mathbf{z})} d\mathbf{z} + \frac{1}{n} \sum_{i=1}^n \int q_\phi(\mathbf{z}|\mathbf{x}_i) \log \frac{q_\phi(\mathbf{z}|\mathbf{x}_i)}{q_{\text{agg},\phi}(\mathbf{z})} d\mathbf{z} \end{aligned}$$

ELBO Surgery

$$\frac{1}{n} \sum_{i=1}^n \text{KL}(q_\phi(\mathbf{z}|\mathbf{x}_i) \| p(\mathbf{z})) = \text{KL}(q_{\text{agg},\phi}(\mathbf{z}) \| p(\mathbf{z})) + \mathbb{I}_q[\mathbf{x}, \mathbf{z}].$$

Proof

$$\begin{aligned} \frac{1}{n} \sum_{i=1}^n \text{KL}(q_\phi(\mathbf{z}|\mathbf{x}_i) \| p(\mathbf{z})) &= \frac{1}{n} \sum_{i=1}^n \int q_\phi(\mathbf{z}|\mathbf{x}_i) \log \frac{q_\phi(\mathbf{z}|\mathbf{x}_i)}{p(\mathbf{z})} d\mathbf{z} = \\ &= \frac{1}{n} \sum_{i=1}^n \int q_\phi(\mathbf{z}|\mathbf{x}_i) \log \frac{q_{\text{agg},\phi}(\mathbf{z}) q_\phi(\mathbf{z}|\mathbf{x}_i)}{p(\mathbf{z}) q_{\text{agg},\phi}(\mathbf{z})} d\mathbf{z} = \\ &= \int \frac{1}{n} \sum_{i=1}^n q_\phi(\mathbf{z}|\mathbf{x}_i) \log \frac{q_{\text{agg},\phi}(\mathbf{z})}{p(\mathbf{z})} d\mathbf{z} + \frac{1}{n} \sum_{i=1}^n \int q_\phi(\mathbf{z}|\mathbf{x}_i) \log \frac{q_\phi(\mathbf{z}|\mathbf{x}_i)}{q_{\text{agg},\phi}(\mathbf{z})} d\mathbf{z} = \\ &= \text{KL}(q_{\text{agg},\phi}(\mathbf{z}) \| p(\mathbf{z})) + \frac{1}{n} \sum_{i=1}^n \text{KL}(q_\phi(\mathbf{z}|\mathbf{x}_i) \| q_{\text{agg},\phi}(\mathbf{z})) \end{aligned}$$

ELBO Surgery

$$\frac{1}{n} \sum_{i=1}^n \text{KL}(q_\phi(\mathbf{z}|\mathbf{x}_i) \| p(\mathbf{z})) = \text{KL}(q_{\text{agg},\phi}(\mathbf{z}) \| p(\mathbf{z})) + \mathbb{I}_q[\mathbf{x}, \mathbf{z}].$$

Proof

$$\begin{aligned}\frac{1}{n} \sum_{i=1}^n \text{KL}(q_\phi(\mathbf{z}|\mathbf{x}_i) \| p(\mathbf{z})) &= \frac{1}{n} \sum_{i=1}^n \int q_\phi(\mathbf{z}|\mathbf{x}_i) \log \frac{q_\phi(\mathbf{z}|\mathbf{x}_i)}{p(\mathbf{z})} d\mathbf{z} = \\ &= \frac{1}{n} \sum_{i=1}^n \int q_\phi(\mathbf{z}|\mathbf{x}_i) \log \frac{q_{\text{agg},\phi}(\mathbf{z}) q_\phi(\mathbf{z}|\mathbf{x}_i)}{p(\mathbf{z}) q_{\text{agg},\phi}(\mathbf{z})} d\mathbf{z} = \\ &= \int \frac{1}{n} \sum_{i=1}^n q_\phi(\mathbf{z}|\mathbf{x}_i) \log \frac{q_{\text{agg},\phi}(\mathbf{z})}{p(\mathbf{z})} d\mathbf{z} + \frac{1}{n} \sum_{i=1}^n \int q_\phi(\mathbf{z}|\mathbf{x}_i) \log \frac{q_\phi(\mathbf{z}|\mathbf{x}_i)}{q_{\text{agg},\phi}(\mathbf{z})} d\mathbf{z} = \\ &= \text{KL}(q_{\text{agg},\phi}(\mathbf{z}) \| p(\mathbf{z})) + \frac{1}{n} \sum_{i=1}^n \text{KL}(q_\phi(\mathbf{z}|\mathbf{x}_i) \| q_{\text{agg},\phi}(\mathbf{z})) \\ \mathbb{I}_q[\mathbf{x}, \mathbf{z}] &= \frac{1}{n} \sum_{i=1}^n \text{KL}(q_\phi(\mathbf{z}|\mathbf{x}_i) \| q_{\text{agg},\phi}(\mathbf{z})).\end{aligned}$$

ELBO Surgery

Revisiting the ELBO

$$\frac{1}{n} \sum_{i=1}^n \mathcal{L}_{\phi, \theta}(\mathbf{x}_i) = \frac{1}{n} \sum_{i=1}^n [\mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x}_i)} \log p_\theta(\mathbf{x}_i|\mathbf{z}) - \text{KL}(q_\phi(\mathbf{z}|\mathbf{x}_i) \| p(\mathbf{z}))]$$

ELBO Surgery

Revisiting the ELBO

$$\begin{aligned} \frac{1}{n} \sum_{i=1}^n \mathcal{L}_{\phi, \theta}(\mathbf{x}_i) &= \frac{1}{n} \sum_{i=1}^n [\mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x}_i)} \log p_\theta(\mathbf{x}_i|\mathbf{z}) - \text{KL}(q_\phi(\mathbf{z}|\mathbf{x}_i)\|p(\mathbf{z}))] = \\ &= \underbrace{\frac{1}{n} \sum_{i=1}^n \mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x}_i)} \log p_\theta(\mathbf{x}_i|\mathbf{z})}_{\text{Reconstruction Loss}} - \underbrace{\mathbb{I}_q[\mathbf{x}, \mathbf{z}]}_{\text{Mutual Information}} - \underbrace{\text{KL}(q_{\text{agg}, \phi}(\mathbf{z})\|p(\mathbf{z}))}_{\text{Marginal KL}} \end{aligned}$$

ELBO Surgery

Revisiting the ELBO

$$\begin{aligned} \frac{1}{n} \sum_{i=1}^n \mathcal{L}_{\phi, \theta}(\mathbf{x}_i) &= \frac{1}{n} \sum_{i=1}^n [\mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x}_i)} \log p_\theta(\mathbf{x}_i|\mathbf{z}) - \text{KL}(q_\phi(\mathbf{z}|\mathbf{x}_i)\|p(\mathbf{z}))] = \\ &= \underbrace{\frac{1}{n} \sum_{i=1}^n \mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x}_i)} \log p_\theta(\mathbf{x}_i|\mathbf{z})}_{\text{Reconstruction Loss}} - \underbrace{\mathbb{I}_q[\mathbf{x}, \mathbf{z}]}_{\text{Mutual Information}} - \underbrace{\text{KL}(q_{\text{agg}, \phi}(\mathbf{z})\|p(\mathbf{z}))}_{\text{Marginal KL}} \end{aligned}$$

The prior distribution $p(\mathbf{z})$ only appears in the last term.

ELBO Surgery

Revisiting the ELBO

$$\begin{aligned}\frac{1}{n} \sum_{i=1}^n \mathcal{L}_{\phi, \theta}(\mathbf{x}_i) &= \frac{1}{n} \sum_{i=1}^n [\mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x}_i)} \log p_\theta(\mathbf{x}_i|\mathbf{z}) - \text{KL}(q_\phi(\mathbf{z}|\mathbf{x}_i)\|p(\mathbf{z}))] = \\ &= \underbrace{\frac{1}{n} \sum_{i=1}^n \mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x}_i)} \log p_\theta(\mathbf{x}_i|\mathbf{z})}_{\text{Reconstruction Loss}} - \underbrace{\mathbb{I}_q[\mathbf{x}, \mathbf{z}]}_{\text{Mutual Information}} - \underbrace{\text{KL}(q_{\text{agg}, \phi}(\mathbf{z})\|p(\mathbf{z}))}_{\text{Marginal KL}}\end{aligned}$$

The prior distribution $p(\mathbf{z})$ only appears in the last term.

Optimal VAE Prior

$$\text{KL}(q_{\text{agg}, \phi}(\mathbf{z})\|p(\mathbf{z})) = 0 \Leftrightarrow p(\mathbf{z}) = q_{\text{agg}, \phi}(\mathbf{z}) = \frac{1}{n} \sum_{i=1}^n q_\phi(\mathbf{z}|\mathbf{x}_i).$$

ELBO Surgery

Revisiting the ELBO

$$\begin{aligned}\frac{1}{n} \sum_{i=1}^n \mathcal{L}_{\phi, \theta}(\mathbf{x}_i) &= \frac{1}{n} \sum_{i=1}^n [\mathbb{E}_{q_{\phi}(\mathbf{z}|\mathbf{x}_i)} \log p_{\theta}(\mathbf{x}_i|\mathbf{z}) - \text{KL}(q_{\phi}(\mathbf{z}|\mathbf{x}_i)\|p(\mathbf{z}))] = \\ &= \underbrace{\frac{1}{n} \sum_{i=1}^n \mathbb{E}_{q_{\phi}(\mathbf{z}|\mathbf{x}_i)} \log p_{\theta}(\mathbf{x}_i|\mathbf{z})}_{\text{Reconstruction Loss}} - \underbrace{\mathbb{I}_q[\mathbf{x}, \mathbf{z}]}_{\text{Mutual Information}} - \underbrace{\text{KL}(q_{\text{agg}, \phi}(\mathbf{z})\|p(\mathbf{z}))}_{\text{Marginal KL}}\end{aligned}$$

The prior distribution $p(\mathbf{z})$ only appears in the last term.

Optimal VAE Prior

$$\text{KL}(q_{\text{agg}, \phi}(\mathbf{z})\|p(\mathbf{z})) = 0 \Leftrightarrow p(\mathbf{z}) = q_{\text{agg}, \phi}(\mathbf{z}) = \frac{1}{n} \sum_{i=1}^n q_{\phi}(\mathbf{z}|\mathbf{x}_i).$$

Hence, the optimal prior $p(\mathbf{z})$ is the aggregated variational posterior $q_{\text{agg}, \phi}(\mathbf{z})$.

Marginal KL

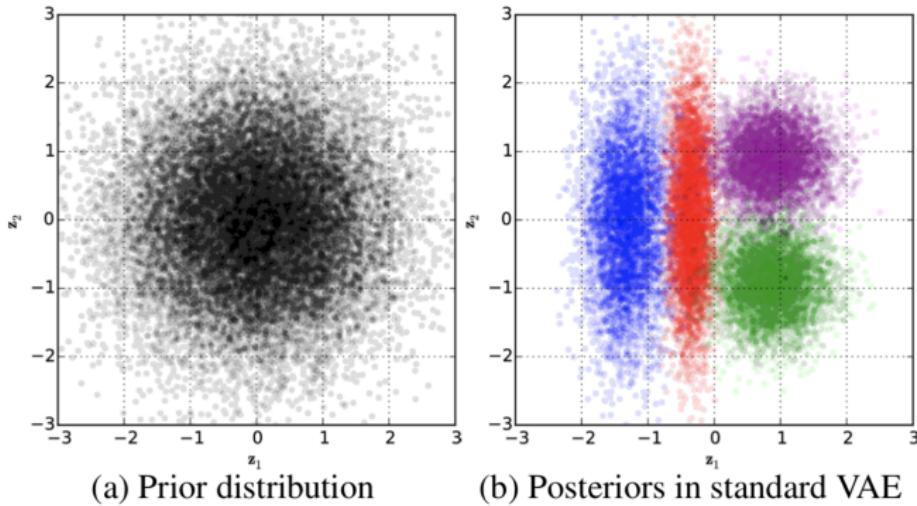
$$\text{KL}(q_{\text{agg}, \phi}(\mathbf{z}) \| p(\mathbf{z}))$$

- ▶ $q_\phi(\mathbf{z}|\mathbf{x}) = \mathcal{N}(\boldsymbol{\mu}_\phi(\mathbf{x}), \boldsymbol{\sigma}_\phi^2(\mathbf{x}))$ is unimodal.
- ▶ It is generally believed that the **mismatch between $p(\mathbf{z})$ and $q_{\text{agg}, \phi}(\mathbf{z})$** is the primary explanation for blurry VAE-generated images.

Marginal KL

$$\text{KL}(q_{\text{agg}, \phi}(\mathbf{z}) \| p(\mathbf{z}))$$

- ▶ $q_\phi(\mathbf{z}|\mathbf{x}) = \mathcal{N}(\boldsymbol{\mu}_\phi(\mathbf{x}), \boldsymbol{\sigma}_\phi^2(\mathbf{x}))$ is unimodal.
- ▶ It is generally believed that the **mismatch between $p(\mathbf{z})$ and $q_{\text{agg}, \phi}(\mathbf{z})$** is the primary explanation for blurry VAE-generated images.



Outline

1. Discrete VAE Latent Representations
2. Vector Quantized VAE
3. ELBO Surgery
4. Learnable VAE Prior

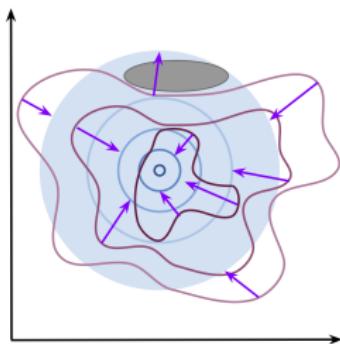
Optimal VAE Prior

- ▶ Standard Gaussian $p(\mathbf{z}) = \mathcal{N}(0, \mathbf{I})$ often leads to over-regularization.
- ▶ $p(\mathbf{z}) = q_{\text{agg}, \phi}(\mathbf{z}) = \frac{1}{n} \sum_{i=1}^n q_\phi(\mathbf{z} | \mathbf{x}_i)$ risks overfitting and incurs high computational cost.

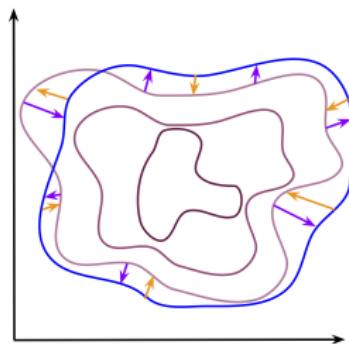
Optimal VAE Prior

- ▶ Standard Gaussian $p(\mathbf{z}) = \mathcal{N}(0, \mathbf{I})$ often leads to over-regularization.
- ▶ $p(\mathbf{z}) = q_{\text{agg}, \phi}(\mathbf{z}) = \frac{1}{n} \sum_{i=1}^n q_\phi(\mathbf{z} | \mathbf{x}_i)$ risks overfitting and incurs high computational cost.

Non-Learnable Prior $p(\mathbf{z})$



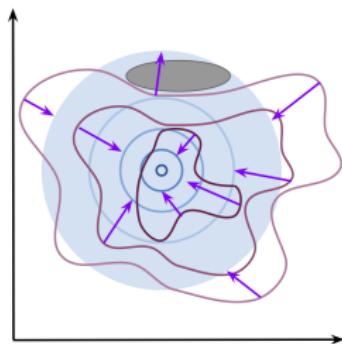
Learnable Prior $p_\lambda(\mathbf{z})$



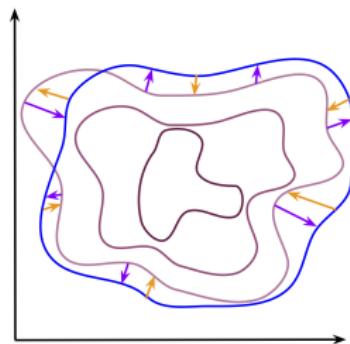
Optimal VAE Prior

- ▶ Standard Gaussian $p(\mathbf{z}) = \mathcal{N}(0, \mathbf{I})$ often leads to over-regularization.
- ▶ $p(\mathbf{z}) = q_{\text{agg}, \phi}(\mathbf{z}) = \frac{1}{n} \sum_{i=1}^n q_\phi(\mathbf{z} | \mathbf{x}_i)$ risks overfitting and incurs high computational cost.

Non-Learnable Prior $p(\mathbf{z})$



Learnable Prior $p_\lambda(\mathbf{z})$



$$\frac{1}{n} \sum_{i=1}^n \mathcal{L}_{\phi, \theta}(\mathbf{x}_i) = \text{RL} - \text{MI} - \text{KL}(q_{\text{agg}, \phi}(\mathbf{z}) \| p_\lambda(\mathbf{z}))$$

This is the forward KL divergence with respect to $p_\lambda(\mathbf{z})$.

image credit: https://jmtomczak.github.io/blog/7/7_priors.html

NF-Based VAE Prior

NF Model in Latent Space

$$\log p_{\lambda}(\mathbf{z}) = \log p(\mathbf{z}^*) + \log \left| \det \left(\frac{d\mathbf{z}^*}{d\mathbf{z}} \right) \right| = \log p(\mathbf{f}_{\lambda}(\mathbf{z})) + \log |\det(\mathbf{J}_f)|$$

$$\mathbf{z} = \mathbf{g}_{\lambda}(\mathbf{z}^*) = \mathbf{f}_{\lambda}^{-1}(\mathbf{z}^*)$$

NF-Based VAE Prior

NF Model in Latent Space

$$\log p_{\lambda}(\mathbf{z}) = \log p(\mathbf{z}^*) + \log \left| \det \left(\frac{d\mathbf{z}^*}{d\mathbf{z}} \right) \right| = \log p(\mathbf{f}_{\lambda}(\mathbf{z})) + \log |\det(\mathbf{J}_f)|$$

$$\mathbf{z} = \mathbf{g}_{\lambda}(\mathbf{z}^*) = \mathbf{f}_{\lambda}^{-1}(\mathbf{z}^*)$$

- ▶ RealNVP with coupling layers,
- ▶ Autoregressive normalizing flows (efficient $\mathbf{f}_{\lambda}(\mathbf{z})$, but $\mathbf{g}_{\lambda}(\mathbf{z}^*)$ can be slow).

NF-Based VAE Prior

NF Model in Latent Space

$$\log p_{\lambda}(\mathbf{z}) = \log p(\mathbf{z}^*) + \log \left| \det \left(\frac{d\mathbf{z}^*}{d\mathbf{z}} \right) \right| = \log p(\mathbf{f}_{\lambda}(\mathbf{z})) + \log |\det(\mathbf{J}_f)|$$

$$\mathbf{z} = \mathbf{g}_{\lambda}(\mathbf{z}^*) = \mathbf{f}_{\lambda}^{-1}(\mathbf{z}^*)$$

- ▶ RealNVP with coupling layers,
- ▶ Autoregressive normalizing flows (efficient $\mathbf{f}_{\lambda}(\mathbf{z})$, but $\mathbf{g}_{\lambda}(\mathbf{z}^*)$ can be slow).

ELBO with NF-Based VAE Prior

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

NF-Based VAE Prior

NF Model in Latent Space

$$\log p_{\lambda}(\mathbf{z}) = \log p(\mathbf{z}^*) + \log \left| \det \left(\frac{d\mathbf{z}^*}{d\mathbf{z}} \right) \right| = \log p(\mathbf{f}_{\lambda}(\mathbf{z})) + \log |\det(\mathbf{J}_f)|$$

$$\mathbf{z} = \mathbf{g}_{\lambda}(\mathbf{z}^*) = \mathbf{f}_{\lambda}^{-1}(\mathbf{z}^*)$$

- ▶ RealNVP with coupling layers,
- ▶ Autoregressive normalizing flows (efficient $\mathbf{f}_{\lambda}(\mathbf{z})$, but $\mathbf{g}_{\lambda}(\mathbf{z}^*)$ can be slow).

ELBO with NF-Based VAE Prior

$$\begin{aligned}\mathcal{L}_{\phi, \theta}(\mathbf{x}) &= \mathbb{E}_{q_{\phi}(\mathbf{z}|\mathbf{x})} \log p_{\theta}(\mathbf{x}|\mathbf{z}) - \text{KL}(q_{\phi}(\mathbf{z}|\mathbf{x}) \| p(\mathbf{z})) = \\ &= \mathbb{E}_{q_{\phi}(\mathbf{z}|\mathbf{x})} [\log p_{\theta}(\mathbf{x}|\mathbf{z}) + \log p_{\lambda}(\mathbf{z}) - \log q_{\phi}(\mathbf{z}|\mathbf{x})]\end{aligned}$$

NF-Based VAE Prior

NF Model in Latent Space

$$\log p_{\lambda}(\mathbf{z}) = \log p(\mathbf{z}^*) + \log \left| \det \left(\frac{d\mathbf{z}^*}{d\mathbf{z}} \right) \right| = \log p(\mathbf{f}_{\lambda}(\mathbf{z})) + \log |\det(\mathbf{J}_f)|$$

$$\mathbf{z} = \mathbf{g}_{\lambda}(\mathbf{z}^*) = \mathbf{f}_{\lambda}^{-1}(\mathbf{z}^*)$$

- ▶ RealNVP with coupling layers,
- ▶ Autoregressive normalizing flows (efficient $\mathbf{f}_{\lambda}(\mathbf{z})$, but $\mathbf{g}_{\lambda}(\mathbf{z}^*)$ can be slow).

ELBO with NF-Based VAE Prior

$$\begin{aligned}\mathcal{L}_{\phi, \theta}(\mathbf{x}) &= \mathbb{E}_{q_{\phi}(\mathbf{z}|\mathbf{x})} \log p_{\theta}(\mathbf{x}|\mathbf{z}) - \text{KL}(q_{\phi}(\mathbf{z}|\mathbf{x}) \| p(\mathbf{z})) = \\ &= \mathbb{E}_{q_{\phi}(\mathbf{z}|\mathbf{x})} [\log p_{\theta}(\mathbf{x}|\mathbf{z}) + \log p_{\lambda}(\mathbf{z}) - \log q_{\phi}(\mathbf{z}|\mathbf{x})] = \\ &= \mathbb{E}_{q_{\phi}(\mathbf{z}|\mathbf{x})} \left[\log p_{\theta}(\mathbf{x}|\mathbf{z}) + \underbrace{\left(\log p(\mathbf{f}_{\lambda}(\mathbf{z})) + \log |\det(\mathbf{J}_f)| \right)}_{\text{NF-based prior}} - \log q_{\phi}(\mathbf{z}|\mathbf{x}) \right]\end{aligned}$$

Summary

- ▶ Discrete VAE latents offer a natural class of latent variable models.
- ▶ Vector quantization provides a way to construct VAEs with discrete latents and deterministic variational posteriors.
- ▶ The straight-through gradient estimator allows gradients to pass as if quantization were an identity operation during backpropagation.
- ▶ ELBO surgery gives insights into the prior's influence in VAEs; the optimal prior is the aggregated variational posterior.
- ▶ The mismatch between $p(\mathbf{z})$ and $q_{\text{agg},\phi}(\mathbf{z})$ is widely regarded as the principal reason for VAE-generated image blurriness.
- ▶ Normalizing flow-based priors, including autoregressive flows, can be incorporated directly into VAEs.