Deep Generative Models

Lecture 4

Roman Isachenko

AI Masters

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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

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

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

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)

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

ELBO Derivation 2 (Equality)

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

Variational Decomposition

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

Recap of Previous Lecture

Variational Evidence Lower Bound (ELBO)

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

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

Log-likelihood Decomposition

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

- 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:

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

Recap of Previous Lecture

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

$$= \mathbb{E}_q \left[\log p_\theta(\mathbf{x}|\mathbf{z}) - \log \frac{q(\mathbf{z})}{p(\mathbf{z})}\right] d\mathbf{z} \to \max_{q,\theta}.$$

Variational Posterior

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

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

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

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

Recap of Previous Lecture

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

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

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

$$\approx \nabla_\theta \log p_\theta(\mathbf{x}|\mathbf{z}^*), \quad \mathbf{z}^* \sim q_\phi(\mathbf{z}|\mathbf{x}).$$

Gradient w.r.t. ϕ — Reparameterization Trick

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

$$\approx \nabla_\phi \log p_\theta(\mathbf{x}|\mathbf{g}_\phi(\mathbf{x}, \boldsymbol{\epsilon}^*)) - \nabla_\phi \mathrm{KL}$$

Variational Assumption

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

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

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):

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

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

- Update parameters via stochastic gradient steps with respect to $\boldsymbol{\phi}$ and $\boldsymbol{\theta}$.

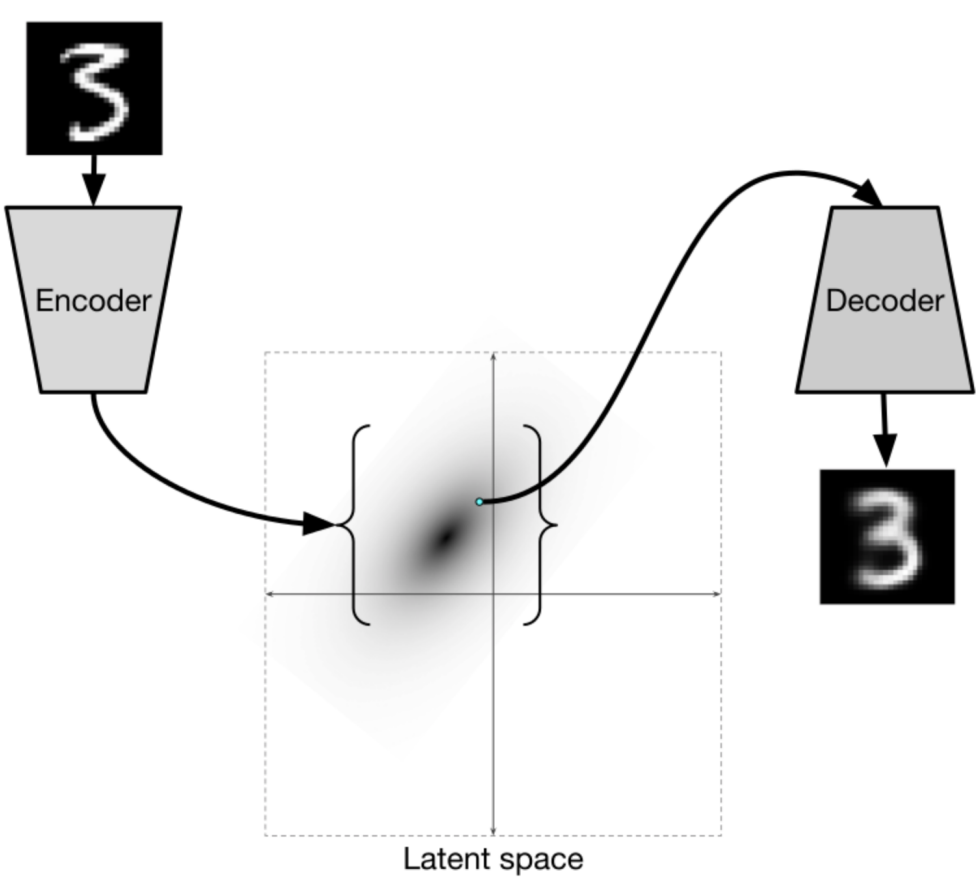
Inference

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

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

Recap of Previous Lecture

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



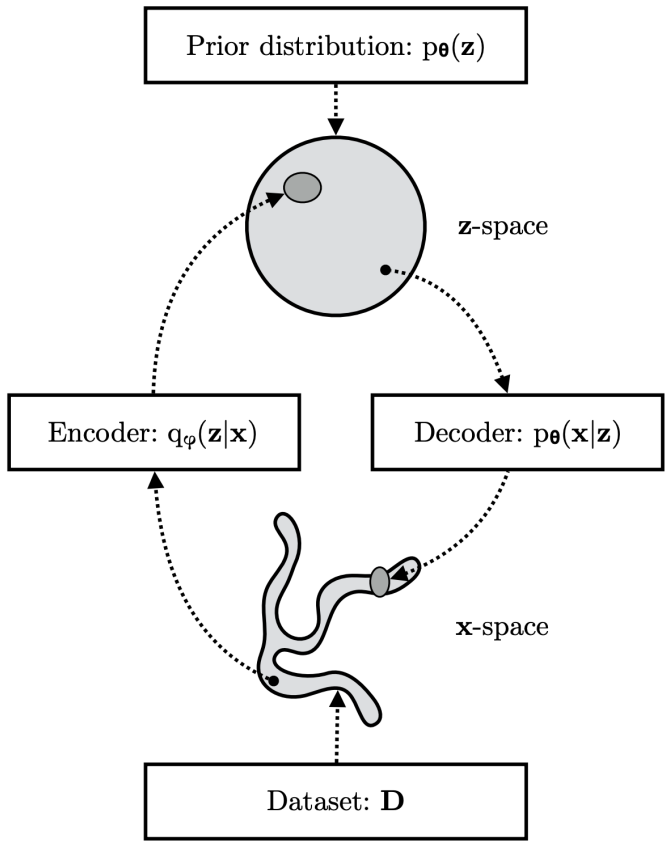


image credit: http://ijdykeman.github.io/ml/2016/12/21/cvae.html
Kingma D. P., Welling M. An Introduction to Variational Autoencoders, 2019

Outline

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

Outline

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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- 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 $c \sim \text{Cat}(\boldsymbol{\pi})$, 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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$$D_{\text{KL}}(q_\phi(c|\mathbf{x}) \| p(c)) = \sum_{k=1}^{K} q_\phi(k|\mathbf{x}) \log \frac{q_\phi(k|\mathbf{x})}{p(k)}$$

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

Discrete VAE Latents

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

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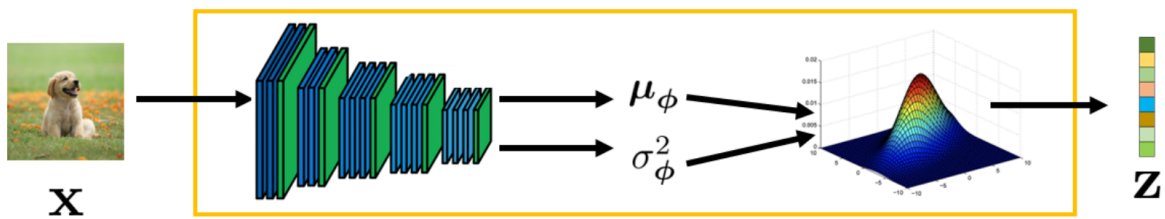
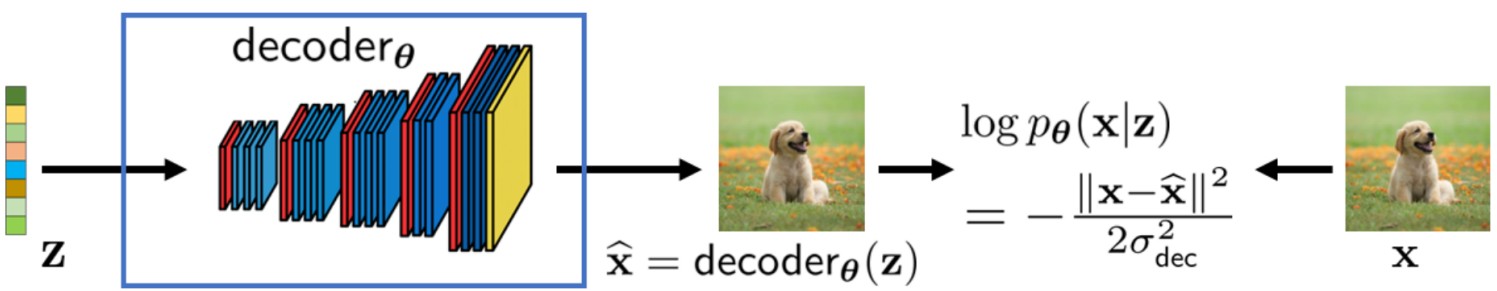
- The encoder should output a discrete distribution $q_\phi(c|\mathbf{x})$.
- We need an analogue of the reparametrization trick for discrete $q_\phi(c|\mathbf{x})$.
- The decoder $p_\theta(\mathbf{x}|c)$ must take a discrete random variable c as input.





Outline

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.

Zhao Y. et al. Feature Quantization Improves GAN Training, 2020

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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:

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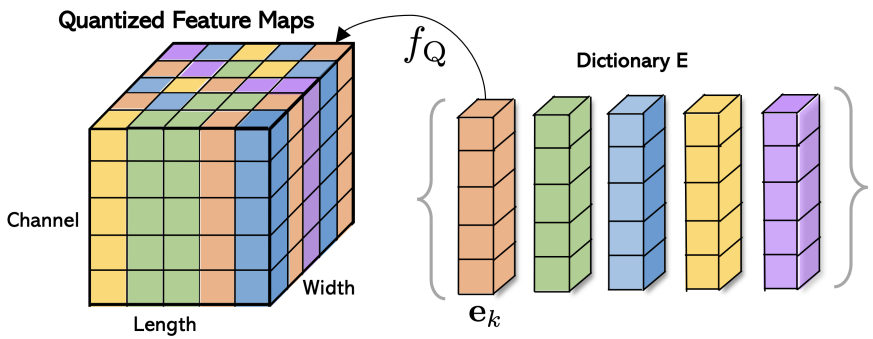
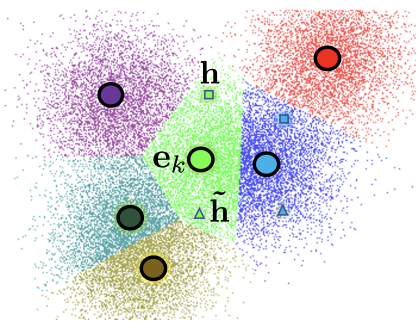
Quantization Procedure

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





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Vector Quantized VAE (VQ-VAE)

- The encoder outputs a continuous vector $\mathbf{z}_e = \mathrm{NN}_{e,\phi}(\mathbf{x}) \in \mathbb{R}^L$.
- 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 $p_\theta(\mathbf{x}|c)$).

Oord A., Vinyals O., Kavukcuoglu K. Neural Discrete Representation Learning, 2017

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Deterministic Variational Posterior

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

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

Oord A., Vinyals O., Kavukcuoglu K. Neural Discrete Representation Learning, 2017

Vector Quantized VAE (VQ-VAE): Forward

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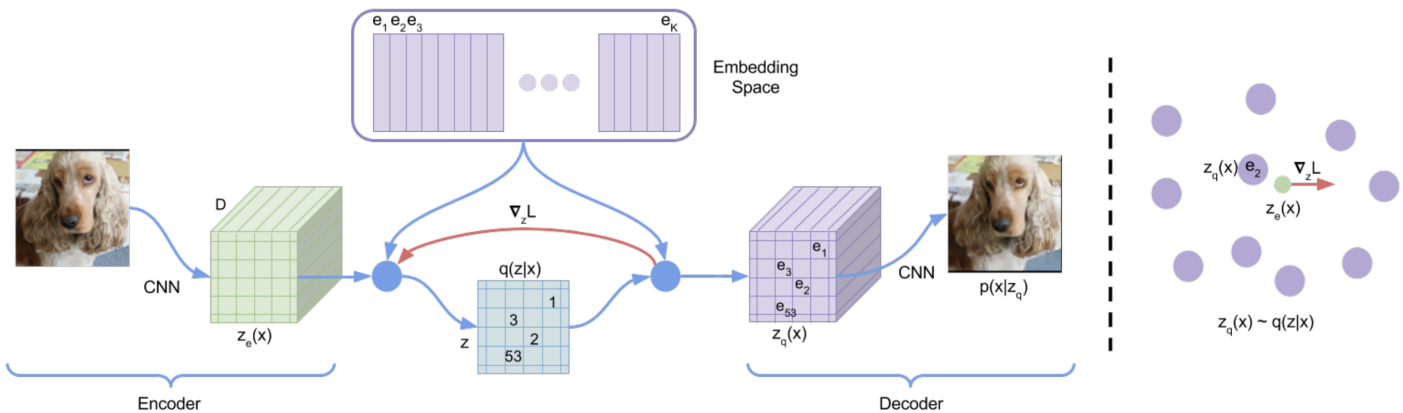

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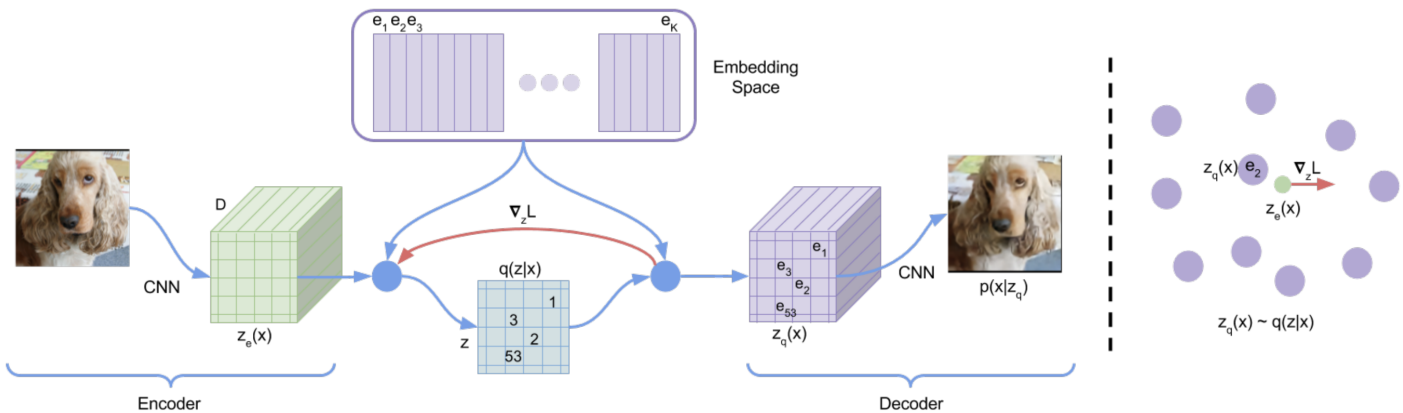

Challenge: The arg min operation is non-differentiable.

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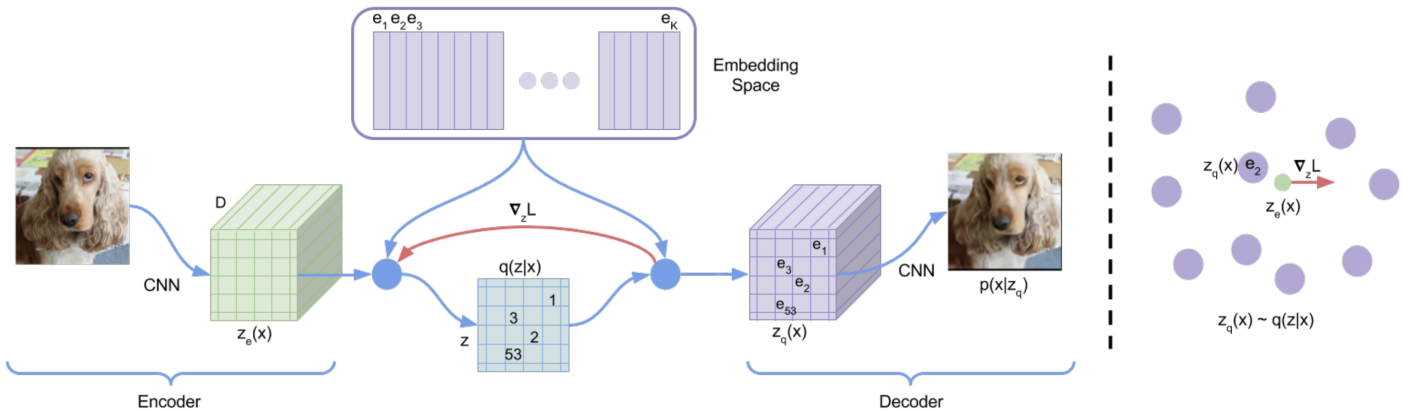
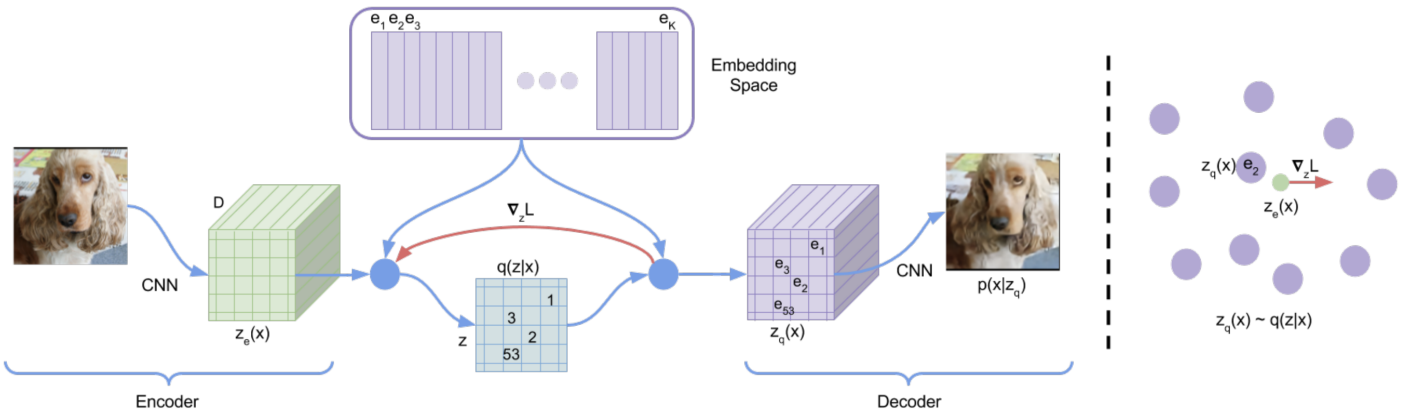


Oord A., Vinyals O., Kavukcuoglu K. Neural Discrete Representation Learning, 2017

Vector Quantized VAE (VQ-VAE): Backward

ELBO

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



Straight-Through Gradient Estimator

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

Oord A., Vinyals O., Kavukcuoglu K. Neural Discrete Representation Learning, 2017

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ELBO

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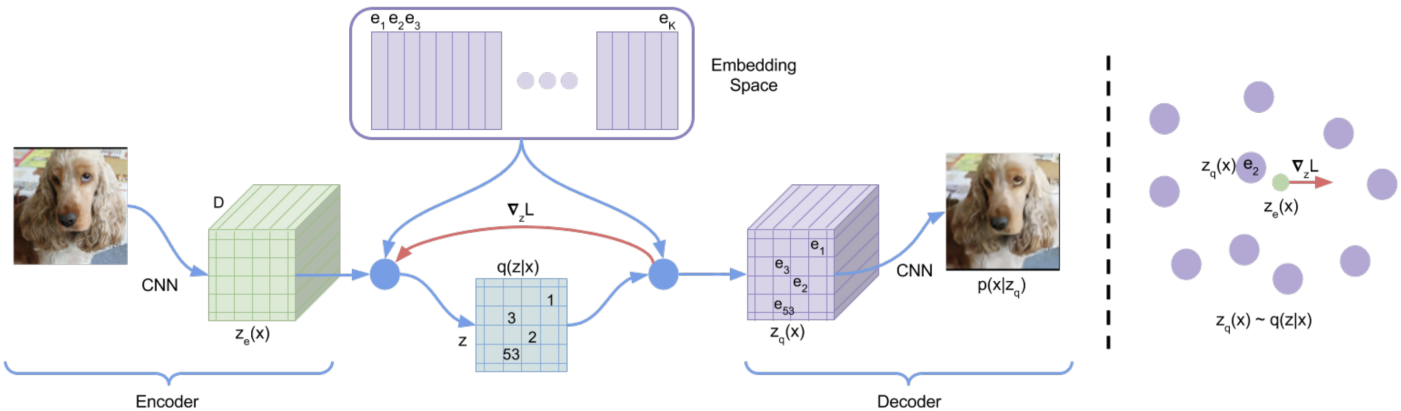

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$$= \frac{\partial \log p_\theta(\mathbf{x}|\mathbf{z}_q)}{\partial \mathbf{z}_q} \cdot \frac{\partial \mathbf{z}_q}{\partial \mathbf{z}_e} \cdot \frac{\partial \mathbf{z}_e}{\partial \phi}$$

Oord A., Vinyals O., Kavukcuoglu K. Neural Discrete Representation Learning, 2017

Vector Quantized VAE (VQ-VAE): Backward

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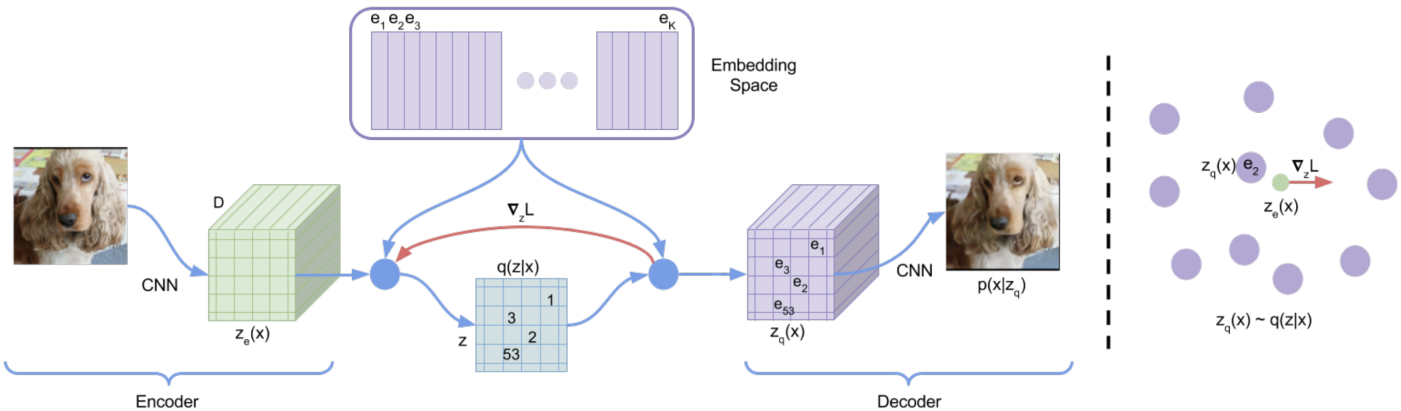

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Oord A., Vinyals O., Kavukcuoglu K. Neural Discrete Representation Learning, 2017

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

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

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

Sample Diversity

VQ-VAE (Proposed) **BigGAN deep**

Razavi A., Oord A., Vinyals O. Generating Diverse High-Fidelity Images with VQ-VAE-2, 2019

Vector Quantized VAE (VQ-VAE): Final algorithm

Training

- Vector-quantize (per spatial location if applicable):

$$k^* = \arg\min_k \|\mathbf{z}_e - \mathbf{e}_k\|_2, \quad \mathbf{z}_q = \mathbf{e}_{k^*}, \quad \mathbf{z}_e = \mathrm{NN}_{e,\phi}(\mathbf{x}).$$

- Compute ELBO objective:

$$\mathcal{L}_{\phi,\theta}(\mathbf{x}) = \log p_\theta(\mathbf{x}|\mathbf{z}_q) - \log K.$$

- Compute total loss with codebook and commitment losses (with stop-gradient sg[·]):

$$\mathcal{L} = -\mathcal{L}_{\phi,\theta}(\mathbf{x}) + \left\|\mathrm{sg}[\mathbf{z}_e] - \mathbf{e}_{k^*}\right\|_2^2 + \beta\left\|\mathbf{z}_e - \mathrm{sg}[\mathbf{e}_{k^*}]\right\|_2^2$$

- Use straight-through gradient estimation for encoder.

Vector Quantized VAE (VQ-VAE): Final algorithm

Training

- Vector-quantize (per spatial location if applicable):

$$k^* = \arg\min_k \|\mathbf{z}_e - \mathbf{e}_k\|_2, \quad \mathbf{z}_q = \mathbf{e}_{k^*}, \quad \mathbf{z}_e = \mathrm{NN}_{e,\phi}(\mathbf{x}).$$

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- Use straight-through gradient estimation for encoder.

Sampling

- Sample $c \sim p(c) = \mathrm{Uniform}\{1, \ldots, K\}$.
- Generate $\mathbf{x} \sim p_\theta(\mathbf{x}|\mathbf{e}_c)$.

Outline

ELBO Surgery

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

Hoffman M. D., Johnson M. J. ELBO Surgery: Yet Another Way to Carve Up the Variational Evidence Lower Bound, 2016

ELBO Surgery

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

Theorem

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

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ELBO Surgery

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- $q_{\mathrm{agg},\phi}(\mathbf{z}) = \frac{1}{n}\sum_{i=1}^{n} q_\phi(\mathbf{z}|\mathbf{x}_i)$ 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 $p_{\mathrm{data}}(\mathbf{x})$ and $q_\phi(\mathbf{z}|\mathbf{x})$.
- The first term encourages $q_{\mathrm{agg},\phi}(\mathbf{z})$ to match the prior $p(\mathbf{z})$.
- The second term reduces the information about $\mathbf{x}$ encoded in $\mathbf{z}$.

Hoffman M. D., Johnson M. J. ELBO Surgery: Yet Another Way to Carve Up the Variational Evidence Lower Bound, 2016

ELBO Surgery

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Proof

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

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ELBO Surgery

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

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

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

$$= D_{\mathrm{KL}}(q_{\mathrm{agg},\phi}(\mathbf{z})\|p(\mathbf{z})) + \frac{1}{n}\sum_{i=1}^{n} D_{\mathrm{KL}}(q_\phi(\mathbf{z}|\mathbf{x}_i)\|q_{\mathrm{agg},\phi}(\mathbf{z}))$$

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$$= D_{\mathrm{KL}}(q_{\mathrm{agg},\phi}(\mathbf{z})\|p(\mathbf{z})) + \frac{1}{n}\sum_{i=1}^{n} D_{\mathrm{KL}}(q_\phi(\mathbf{z}|\mathbf{x}_i)\|q_{\mathrm{agg},\phi}(\mathbf{z}))$$

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

Hoffman M. D., Johnson M. J. ELBO Surgery: Yet Another Way to Carve Up the Variational Evidence Lower Bound, 2016

ELBO Surgery

Revisiting the ELBO

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

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

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

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

Optimal VAE Prior

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

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

Hoffman M. D., Johnson M. J. ELBO Surgery: Yet Another Way to Carve Up the Variational Evidence Lower Bound, 2016

Marginal KL

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

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

Rezende D. J., Mohamed S. Variational Inference with Normalizing Flows, 2015

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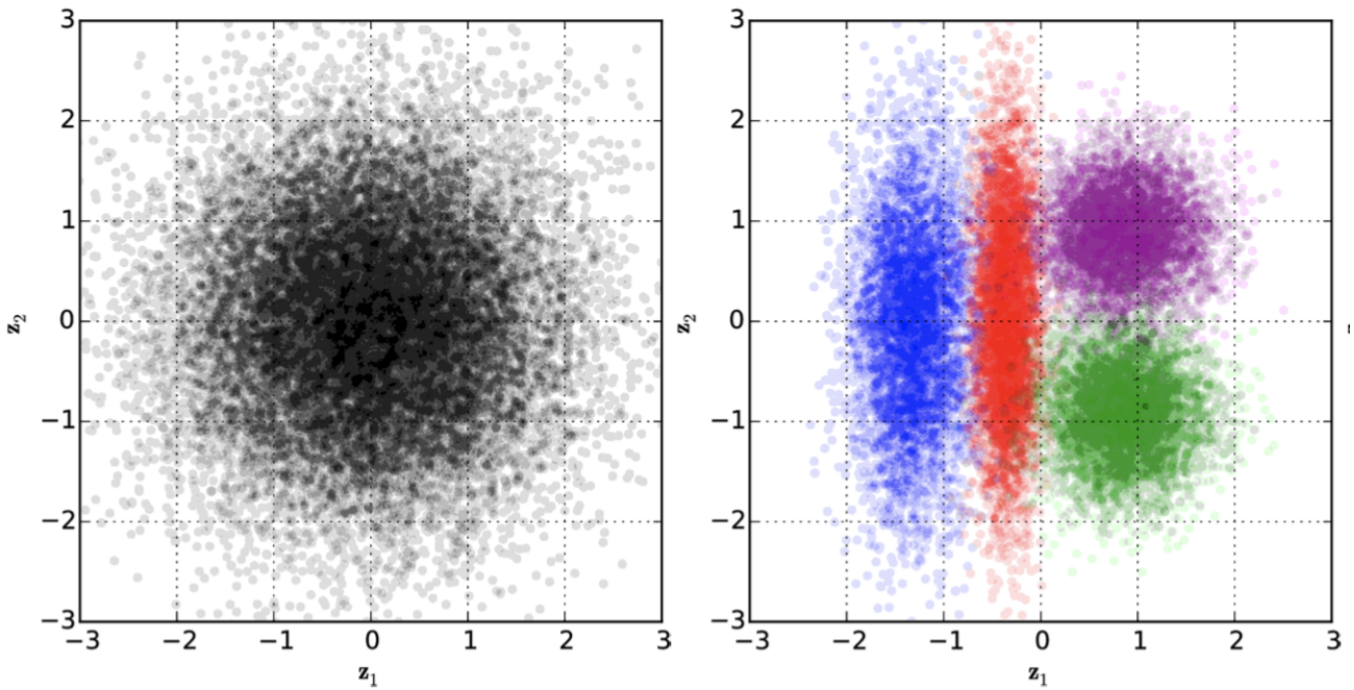

(a) Prior distribution (b) Posteriors in standard VAE

Rezende D. J., Mohamed S. Variational Inference with Normalizing Flows, 2015

Why are VAE Generations Blurry?

Consider a Gaussian decoder $p_{\boldsymbol{\theta}}(\mathbf{x}|\mathbf{z}) = \mathcal{N}(\boldsymbol{\mu}_{\boldsymbol{\theta}}(\mathbf{z}), \sigma^2\mathbf{I})$.

Lai C. H. et al. The principles of diffusion models, 2025.

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ELBO Optimization

With **fixed** encoder $q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x})$, optimizing ELBO reduces to

$$\arg\min_{\boldsymbol{\theta}} \mathbb{E}_{p_{\text{data}}(\mathbf{x})q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x})} \|\mathbf{x} - \boldsymbol{\mu}_{\boldsymbol{\theta}}(\mathbf{z})\|^2$$

The optimal decoder mean is the **conditional expectation**:

$$\boldsymbol{\mu}^*(\mathbf{z}) = \mathbb{E}_{q_{\boldsymbol{\phi}}(\mathbf{x}|\mathbf{z})}[\mathbf{x}] = \frac{\mathbb{E}_{p_{\text{data}}(\mathbf{x})}[q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x}) \cdot \mathbf{x}]}{\mathbb{E}_{p_{\text{data}}(\mathbf{x})}[q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x})]}$$

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Blurriness from Averaging

- $p_{\text{data}}(\mathbf{x})$ and $q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x})$ give us the aggregated posterior $q_{\text{agg},\boldsymbol{\phi}}(\mathbf{z})$.
- If $\mathbf{x} \neq \mathbf{x}'$ map to overlapping latent regions, $\boldsymbol{\mu}^*(\mathbf{z})$ averages over unrelated inputs.
- This leads to **blurry, non-distinct outputs**.

Lai C. H. et al. The principles of diffusion models, 2025.

Outline

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.

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

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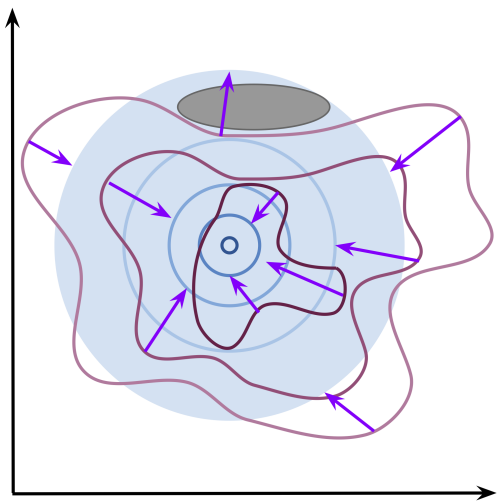
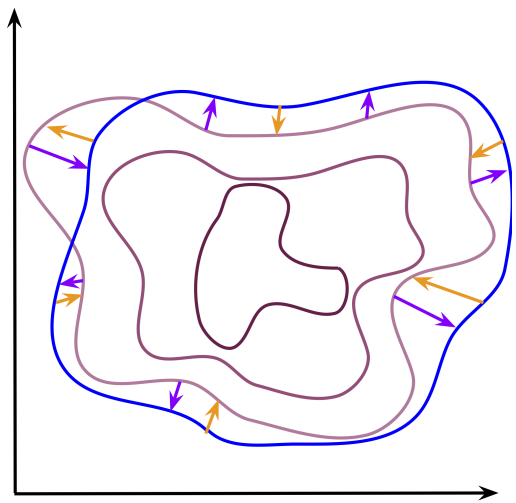
Non-Learnable Prior $p(\mathbf{z})$



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



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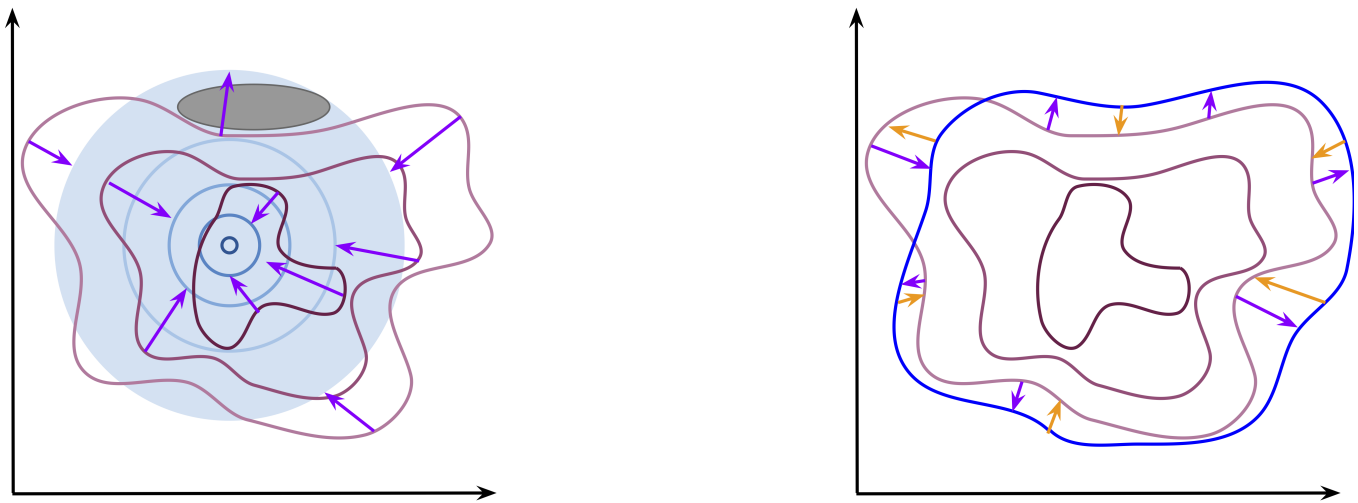
Non-Learnable Prior $p(\mathbf{z})$ Learnable Prior $p_\lambda(\mathbf{z})$



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

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

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NF-Based VAE Prior

NF Model in Latent Space

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

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

Chen X. et al. Variational Lossy Autoencoder, 2016

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

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ELBO with NF-Based VAE Prior

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

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ELBO with NF-Based VAE Prior

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

Chen X. et al. Variational Lossy Autoencoder, 2016

NF-Based VAE Prior

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ELBO with NF-Based VAE Prior

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

Chen X. et al. Variational Lossy Autoencoder, 2016

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.