

Deep Generative Models

Lecture 6

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Recap of previous lecture

$$\mathcal{L}(\phi, \theta) = \mathbb{E}_{q(z|x, \phi)} \left[\log p(x|z, \theta) - \log \frac{q(z|x, \phi)}{p(z)} \right] \rightarrow \max_{\phi, \theta}.$$

M-step: $\nabla_{\theta} \mathcal{L}(\phi, \theta)$, Monte Carlo estimation

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

E-step: $\nabla_{\phi} \mathcal{L}(\phi, \theta)$, reparametrization trick

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

Variational assumption

$$r(\epsilon) = \mathcal{N}(0, \mathbf{I}); \quad q(z|x, \phi) = \mathcal{N}(\mu_{\phi}(x), \sigma_{\phi}^2(x)).$$

$$z = g_{\phi}(x, \epsilon) = \sigma_{\phi}(x) \cdot \epsilon + \mu_{\phi}(x).$$

Recap of previous lecture

Final EM-algorithm

- ▶ pick random sample $\mathbf{x}_i, i \sim U[1, n]$.
- ▶ compute the objective:

$$\epsilon^* \sim r(\epsilon); \quad \mathbf{z}^* = g_\phi(\mathbf{x}, \epsilon^*);$$

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

- ▶ compute a stochastic gradients w.r.t. ϕ and θ

$$\nabla_\phi \mathcal{L}(\phi, \theta) \approx \nabla_\phi \log p(\mathbf{x}|g_\phi(\mathbf{x}, \epsilon^*), \theta) - \nabla_\phi KL(q(\mathbf{z}|\mathbf{x}, \phi)||p(\mathbf{z}));$$

$$\nabla_\theta \mathcal{L}(\phi, \theta) \approx \nabla_\theta \log p(\mathbf{x}|\mathbf{z}^*, \theta).$$

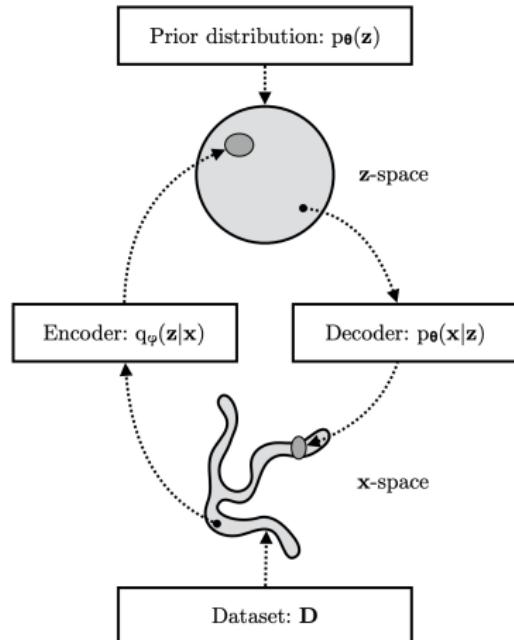
- ▶ update θ, ϕ according to the selected optimization method (SGD, Adam, RMSProp):

$$\begin{aligned}\phi &:= \phi + \eta \nabla_\phi \mathcal{L}(\phi, \theta), \\ \theta &:= \theta + \eta \nabla_\theta \mathcal{L}(\phi, \theta).\end{aligned}$$

Recap of previous lecture

Variational autoencoder (VAE)

- ▶ VAE learns stochastic mapping between \mathbf{x} -space, from $\pi(\mathbf{x})$, and a latent \mathbf{z} -space, with simple distribution.
- ▶ The generative model learns distribution $p(\mathbf{x}, \mathbf{z}|\theta) = p(\mathbf{z})p(\mathbf{x}|\mathbf{z}, \theta)$, with a prior distribution $p(\mathbf{z})$, and a stochastic decoder $p(\mathbf{x}|\mathbf{z}, \theta)$.
- ▶ The stochastic encoder $q(\mathbf{z}|\mathbf{x}, \phi)$ (inference model), approximates the true but intractable posterior $p(\mathbf{z}|\mathbf{x}, \theta)$.



Recap of previous lecture

Let our data \mathbf{y} comes from discrete distribution $\Pi(\mathbf{y})$.

- ▶ Use **discrete** model (e.x. $P(\mathbf{y}|\theta) = \text{Cat}(\pi(\theta))$) and minimize any suitable divergence measure $D(\Pi, P)$.
- ▶ Use **continuous** model, but **dequantize** data (make the data continuous): transform $\Pi(\mathbf{y})$ to $\pi(\mathbf{x})$.

Uniform dequantization bound

Let dequantize discrete distribution $\Pi(\mathbf{y})$ to continuous distribution $\pi(\mathbf{x})$ in the following way: $\mathbf{x} = \mathbf{y} + \mathbf{u}$, where $\mathbf{u} \sim U[0, 1]$.

Theorem

Fitting continuous model $p(\mathbf{x}|\theta)$ on uniformly dequantized data is equivalent to maximization of a lower bound on log-likelihood for a discrete model:

$$P(\mathbf{y}|\theta) = \int_{U[0,1]} p(\mathbf{y} + \mathbf{u}|\theta) d\mathbf{u}$$

Recap of previous lecture

	VAE	NF
Objective	ELBO \mathcal{L}	Forward KL/MLE
Encoder	stochastic $\mathbf{z} \sim q(\mathbf{z} \mathbf{x}, \phi)$	deterministic $\mathbf{z} = f_{\theta}(\mathbf{x})$ $q(\mathbf{z} \mathbf{x}, \theta) = \delta(\mathbf{z} - f_{\theta}(\mathbf{x}))$
Decoder	stochastic $\mathbf{x} \sim p(\mathbf{x} \mathbf{z}, \theta)$	deterministic $\mathbf{x} = g_{\theta}(\mathbf{z})$ $p(\mathbf{x} \mathbf{z}, \theta) = \delta(\mathbf{x} - g_{\theta}(\mathbf{z}))$
Parameters	ϕ, θ	$\theta \equiv \phi$

Theorem

MLE for normalizing flow is equivalent to maximization of ELBO for VAE model with deterministic encoder and decoder:

$$p(\mathbf{x}|\mathbf{z}, \theta) = \delta(\mathbf{x} - f^{-1}(\mathbf{z}, \theta)) = \delta(\mathbf{x} - g_{\theta}(\mathbf{z}));$$

$$q(\mathbf{z}|\mathbf{x}, \theta) = p(\mathbf{z}|\mathbf{x}, \theta) = \delta(\mathbf{z} - f_{\theta}(\mathbf{x})).$$

Recap of previous lecture

Theorem

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

ELBO surgery

$$\frac{1}{n} \sum_{i=1}^n \mathcal{L}_i(q, \theta) = \underbrace{\frac{1}{n} \sum_{i=1}^n \mathbb{E}_{q(\mathbf{z}|\mathbf{x}_i)} \log p(\mathbf{x}_i|\mathbf{z}, \theta)}_{\text{Reconstruction loss}} - \underbrace{\mathbb{I}_q[\mathbf{x}, \mathbf{z}]}_{\text{MI}} - \underbrace{KL(q_{\text{agg}}(\mathbf{z}) || p(\mathbf{z}))}_{\text{Marginal KL}}$$

Optimal prior

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

The optimal prior distribution $p(\mathbf{z})$ is aggregated posterior $q(\mathbf{z})$.

Outline

1. Learnable VAE prior
2. Discrete VAE latent representations
 - Vector quantization
 - Gumbel-softmax for discrete VAE latents

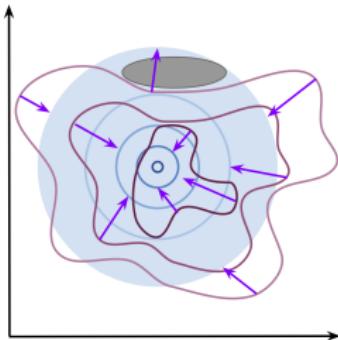
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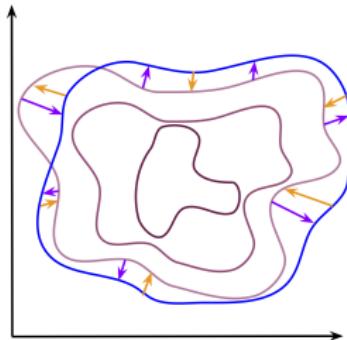
Optimal VAE prior

- ▶ Standard Gaussian $p(\mathbf{z}) = \mathcal{N}(0, I) \Rightarrow$ over-regularization;
- ▶ $p(\mathbf{z}) = q_{\text{agg}}(\mathbf{z}) = \frac{1}{n} \sum_{i=1}^n q(\mathbf{z}|\mathbf{x}_i) \Rightarrow$ overfitting and highly expensive.

Non learnable prior $p(\mathbf{z})$



Learnable prior $p(\mathbf{z}|\boldsymbol{\lambda})$



ELBO revisiting

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

It is Forward KL with respect to $p(\mathbf{z}|\boldsymbol{\lambda})$.

NF-based VAE prior

NF model in latent space

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

$$\mathbf{z} = g_{\boldsymbol{\lambda}}(\mathbf{z}^*) = f_{\boldsymbol{\lambda}}^{-1}(\mathbf{z}^*)$$

- ▶ RealNVP with coupling layers.
- ▶ Autoregressive NF (fast $f_{\boldsymbol{\lambda}}(\mathbf{z})$, slow $g_{\boldsymbol{\lambda}}(\mathbf{z}^*)$).

ELBO with NF-based VAE prior

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

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Discrete VAE latents

Motivation

- ▶ Previous VAE models had **continuous** latent variables \mathbf{z} .
- ▶ **Discrete** representations \mathbf{z} are potentially a more natural fit for many of the modalities.
- ▶ Powerful autoregressive models (like PixelCNN) have been developed for modelling distributions over discrete variables.
- ▶ All cool transformer-like models work with discrete tokens.

ELBO

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

- ▶ Reparametrization trick to get unbiased gradients.
- ▶ Normal assumptions for $q(\mathbf{z}|\mathbf{x}, \phi)$ and $p(\mathbf{z})$ to compute KL analytically.

Discrete VAE latents

Assumptions

- ▶ Define dictionary (word book) space $\{\mathbf{e}_k\}_{k=1}^K$, where $\mathbf{e}_k \in \mathbb{R}^C$, K is the size of the dictionary.
- ▶ Let $c \sim \text{Categorical}(\boldsymbol{\pi})$, where
$$\boldsymbol{\pi} = (\pi_1, \dots, \pi_K), \quad \pi_k = P(c = k), \quad \sum_{k=1}^K \pi_k = 1.$$
- ▶ Let VAE model has discrete latent representation c with prior $p(c) = \text{Uniform}\{1, \dots, K\}$.

How it should work?

- ▶ Our variational posterior $q(c|\mathbf{x}, \phi) = \text{Categorical}(\boldsymbol{\pi}_\phi(\mathbf{x}))$ (encoder) outputs discrete probabilities vector.
- ▶ We sample c^* from $q(c|\mathbf{x}, \phi)$ (reparametrization trick analogue).
- ▶ Our generative distribution $p(\mathbf{x}|\mathbf{e}_{c^*}, \theta)$ (decoder).

Discrete VAE latents

ELBO

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

KL term

$$\begin{aligned} KL(q(c|\mathbf{x}, \phi)||p(c)) &= \sum_{k=1}^K q(k|\mathbf{x}, \phi) \log \frac{q(k|\mathbf{x}, \phi)}{p(k)} = \\ &= \sum_{k=1}^K q(k|\mathbf{x}, \phi) \log q(k|\mathbf{x}, \phi) - \sum_{k=1}^K q(k|\mathbf{x}, \phi) \log p(k) = \\ &= -H(q(c|\mathbf{x}, \phi)) + \log K. \end{aligned}$$

- ▶ Is it possible to make reparametrization trick? (we sample from discrete distribution now!).
- ▶ Entropy term should be estimated.

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Vector quantization

Gumbel-softmax for discrete VAE latents

Vector quantization

Quantized representation

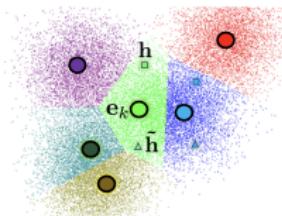
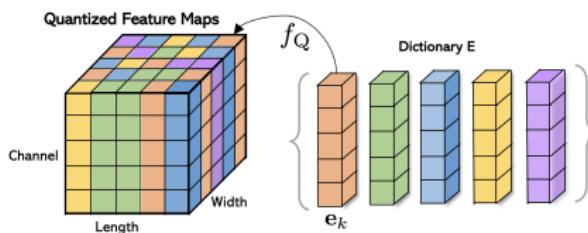
$\mathbf{z}_q \in \mathbb{R}^C$ for $\mathbf{z} \in \mathbb{R}^C$ is defined by a nearest neighbor look-up using the shared dictionary space

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

- ▶ Let our encoder outputs continuous representation \mathbf{z} .
- ▶ Quantization will give us the discrete distribution $q(c|x, \phi)$.

Quantization procedure

If we have tensor with the spatial dimensions we apply the quantization for each of $W \times H$ locations.



Vector Quantized VAE (VQ-VAE)

Let VAE latent variable $\mathbf{c} \in \{1, \dots, K\}^{W \times H}$ is the discrete with spatial-independent variational posterior and prior distributions

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

Let $\mathbf{z}_e = \text{NN}_{e, \phi}(\mathbf{x}) \in \mathbb{R}^{W \times H \times C}$ is the encoder output.

Deterministic variational posterior

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

$KL(q(c|\mathbf{x}, \phi)||p(c))$ term in ELBO is constant, entropy of the posterior is zero.

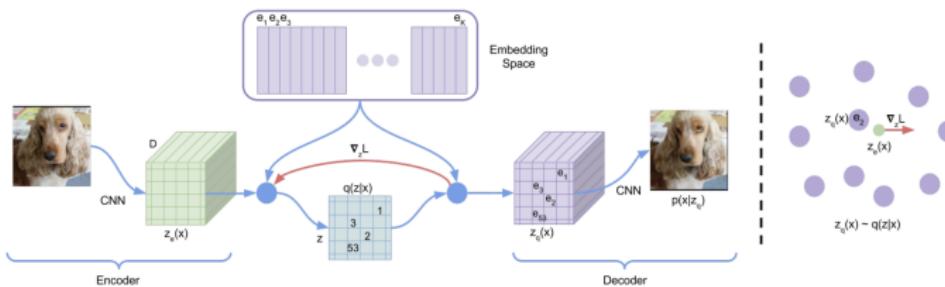
$$KL(q(c|\mathbf{x}, \phi)||p(c)) = -H(q(c|\mathbf{x}, \phi)) + \log K = \log K.$$

Vector Quantized VAE (VQ-VAE)

ELBO

$$\mathcal{L}(\phi, \theta) = \mathbb{E}_{q(c|x, \phi)} \log p(x|e_c, \theta) - \log K = \log p(x|z_q, \theta) - \log K,$$

where $z_q = e_{k^*}$, $k^* = \arg \min_k \|z_e - e_k\|$.



Problem: $\arg \min$ is not differentiable.

Straight-through gradient estimation

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

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

Samples 1024x1024



Samples diversity



VQ-VAE (Proposed)

BigGAN deep

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

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Gumbel-softmax trick

- ▶ VQ-VAE has deterministic variational posterior (it allows to get rid of discrete sampling and reparametrization trick).
- ▶ There is no uncertainty in the encoder output.

Gumbel-max trick

Let $g_k \sim \text{Gumbel}(0, 1)$ for $k = 1, \dots, K$, i.e. $g = -\log(-\log u)$, $u \sim \text{Uniform}[0, 1]$. Then a discrete random variable

$$c = \arg \max_k [\log \pi_k + g_k],$$

has a categorical distribution $c \sim \text{Categorical}(\pi)$.

- ▶ Let our encoder $q(c|\mathbf{x}, \phi) = \text{Categorical}(\pi_\phi(\mathbf{x}))$ outputs logits of $\pi_\phi(\mathbf{x})$.
- ▶ We could sample from the discrete distribution using Gumbel-max reparametrization.

Maddison C. J., Mnih A., Teh Y. W. The Concrete distribution: A continuous relaxation of discrete random variables, 2016

Jang E., Gu S., Poole B. Categorical reparameterization with Gumbel-Softmax, 2016

Gumbel-softmax trick

Reparametrization trick (LOTUS)

$$\nabla_{\phi} \mathbb{E}_{q(c|\mathbf{x}, \phi)} \log p(\mathbf{x}|\mathbf{e}_c, \theta) = \mathbb{E}_{\text{Gumbel}(0,1)} \nabla_{\phi} \log p(\mathbf{x}|\mathbf{e}_{k^*}, \theta),$$

where $k^* = \arg \max_k [\log q(k|\mathbf{x}, \phi) + g_k]$.

Problem: We still have non-differentiable $\arg \max$ operation.

Gumbel-softmax relaxation

Concrete distribution = continuous + discrete

$$\hat{c}_k = \frac{\exp\left(\frac{\log q(k|\mathbf{x}, \phi) + g_k}{\tau}\right)}{\sum_{j=1}^K \exp\left(\frac{\log q(j|\mathbf{x}, \phi) + g_j}{\tau}\right)}, \quad k = 1, \dots, K.$$

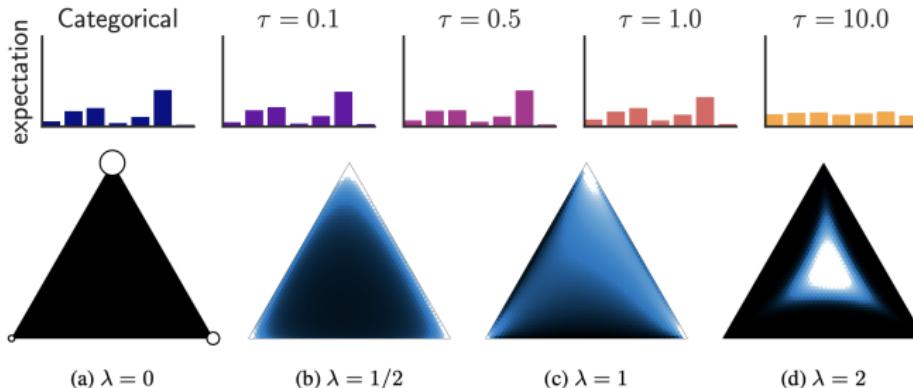
Here τ is a temperature parameter. Now we have differentiable operation, but the gradient estimate is biased now.

Maddison C. J., Mnih A., Teh Y. W. *The Concrete distribution: A continuous relaxation of discrete random variables*, 2016

Jang E., Gu S., Poole B. *Categorical reparameterization with Gumbel-Softmax*, 2016

Gumbel-softmax trick

Concrete distribution



Reparametrization trick

$$\nabla_{\phi} \mathbb{E}_{q(c|x, \phi)} \log p(\mathbf{x}|\mathbf{e}_c, \theta) = \mathbb{E}_{\text{Gumbel}(0,1)} \nabla_{\phi} \log p(\mathbf{x}|\mathbf{z}, \theta),$$

where $\mathbf{z} = \sum_{k=1}^K \hat{c}_k \mathbf{e}_k$ (all operations are differentiable now).

Maddison C. J., Mnih A., Teh Y. W. *The Concrete distribution: A continuous relaxation of discrete random variables*, 2016

Jang E., Gu S., Poole B. *Categorical reparameterization with Gumbel-Softmax*, 2016

DALL-E/dVAE

Deterministic VQ-VAE posterior

$$q(\hat{z}_{ij} = k^* | \mathbf{x}) = \begin{cases} 1, & \text{for } k^* = \arg \min_k \|[\mathbf{z}_e]_{ij} - \mathbf{e}_k\| \\ 0, & \text{otherwise.} \end{cases}$$

- ▶ Gumbel-Softmax trick allows to make true categorical distribution and sample from it.
- ▶ Since latent space is discrete we could train autoregressive transformers in it.
- ▶ It is a natural way to incorporate text and image token spaces.

TEXT PROMPT

an armchair in the shape of an avocado [...]

AI-GENERATED IMAGES



Summary

- ▶ We could use NF-based prior in VAE (even autoregressive).
- ▶ Discrete VAE latents is a natural idea, but we have to avoid non-differentiable sampling operation.
- ▶ Vector Quantization is the way to create VAE with discrete latent space and deterministic variational posterior.
- ▶ Straight-through gradient ignores quantize operation in backprop.
- ▶ Gumbel-softmax trick relaxes discrete problem to continuous one using Gumbel-max reparametrization trick.
- ▶ It becomes more and more popular to use discrete latent spaces in the fields of image/video/music generation.