

Deep Generative Models

Lecture 6

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Recap of previous lecture

EM-algorithm

- ▶ E-step

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

- ▶ M-step

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

Amortized variational inference

Restrict a family of all possible distributions $q(\mathbf{z})$ to a parametric class $q(\mathbf{z}|\mathbf{x}, \phi)$ conditioned on samples \mathbf{x} with parameters ϕ .

Variational Bayes

- ▶ E-step

$$\phi_k = \phi_{k-1} + \eta \cdot \nabla_{\phi} \mathcal{L}(\phi, \theta_{k-1})|_{\phi=\phi_{k-1}}$$

- ▶ M-step

$$\theta_k = \theta_{k-1} + \eta \cdot \nabla_{\theta} \mathcal{L}(\phi_k, \theta)|_{\theta=\theta_{k-1}}$$

Recap of previous lecture

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

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

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

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

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

Variational assumption

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

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

Recap of previous lecture

Final EM-algorithm

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

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

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

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

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

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

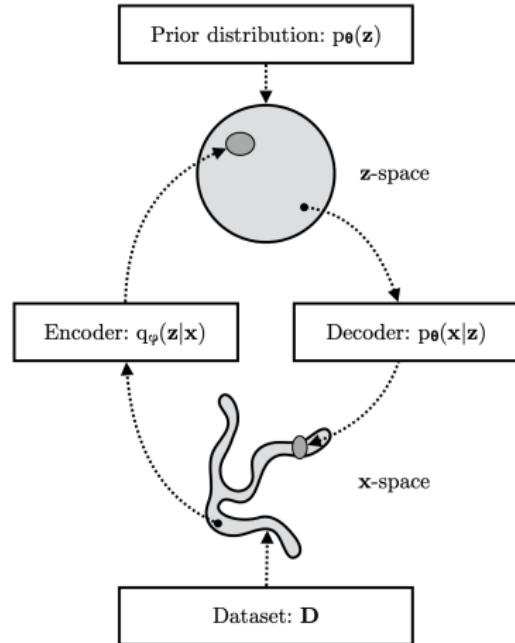
- ▶ update θ, ϕ according to the selected optimization method (SGD, Adam):

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

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

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

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

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

Outline

1. Discrete VAE latent representations

Vector quantization

Gumbel-softmax for discrete VAE latents

2. ELBO surgery

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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

- ▶ 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 $p(c) = \text{Uniform}\{1, \dots, K\}$.

ELBO

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

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

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

Discrete VAE latents

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

- ▶ Our encoder should output discrete distribution $q(c|x, \phi)$.
- ▶ We need the analogue of the reparametrization trick for the discrete distribution $q(c|x, \phi)$.
- ▶ Our decoder $p(x|c, \theta)$ should input discrete random variable c .

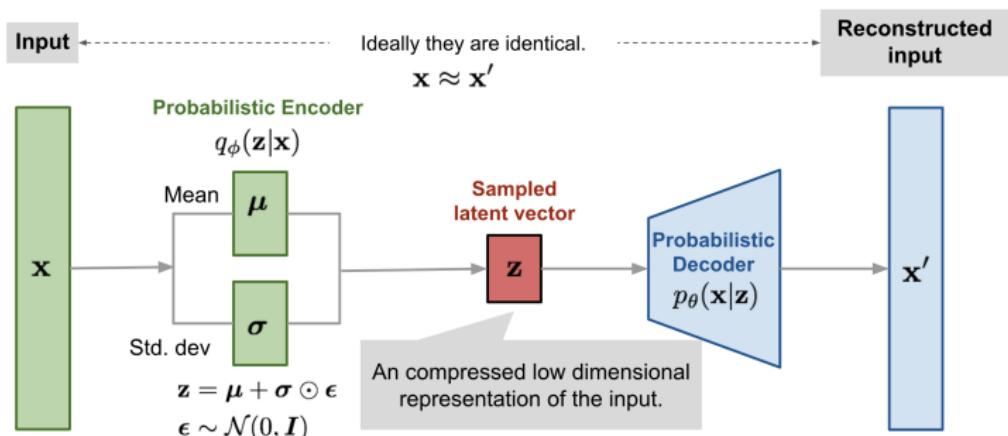


image credit:

<https://lilianweng.github.io/lil-log/2018/08/12/from-autoencoder-to-beta-vae.html>

Outline

1. Discrete VAE latent representations

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Vector quantization

Define the dictionary space $\{\mathbf{e}_k\}_{k=1}^K$, where $\mathbf{e}_k \in \mathbb{R}^C$, K is the size of the dictionary.

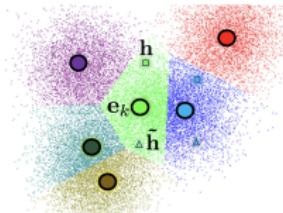
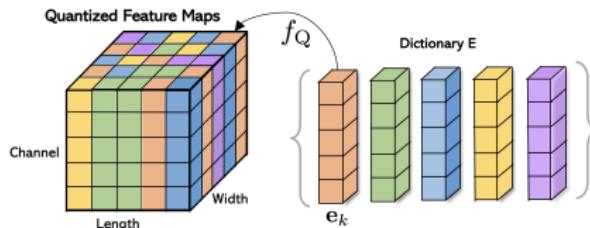
Quantized representation

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

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

Quantization procedure

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



Vector Quantized VAE (VQ-VAE)

- ▶ Let our encoder outputs continuous representation $\mathbf{z}_e = \text{NN}_{e,\phi}(\mathbf{x}) \in \mathbb{R}^C$.
- ▶ Quantization will give us the deterministic mapping from the encoder output \mathbf{z}_e to its quantized representation \mathbf{z}_q .
- ▶ Let use the dictionary elements \mathbf{e}_c in the generative distribution $p(\mathbf{x}|\mathbf{e}_c, \theta)$ (decoder).

Deterministic variational posterior

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

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

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

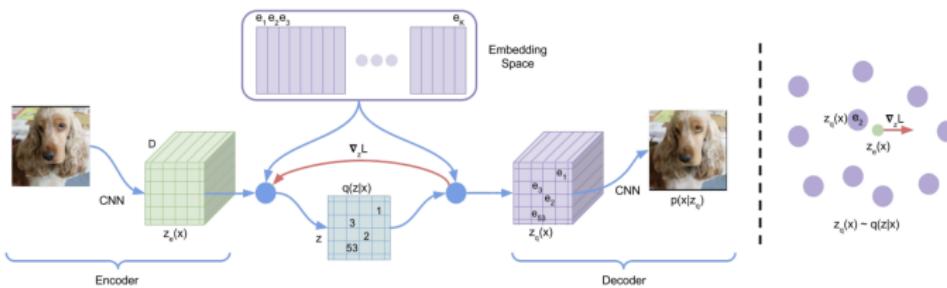
$$q(\mathbf{c}|\mathbf{x}, \phi) = \prod_{i=1}^W \prod_{j=1}^H q(c_{ij}|\mathbf{x}, \phi); \quad p(\mathbf{c}) = \prod_{i=1}^W \prod_{j=1}^H \text{Uniform}\{1, \dots, K\}.$$

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



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

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Discrete probabilistic VAE encoder

- ▶ 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.

How to make the model with probabilistic encoder?

- ▶ Variational posterior $q(c|\mathbf{x}, \phi) = \text{Categorical}(\pi_\phi(\mathbf{x}))$ (encoder) outputs discrete probabilities vector $\pi_\phi(\mathbf{x}) = \text{Softmax}(\text{NN}_{e,\phi}(\mathbf{x}))$.
- ▶ We sample c^* from $q(c|\mathbf{x}, \phi)$ (reparametrization trick analogue).
- ▶ We use \mathbf{e}_{c^*} in the generative distribution $p(\mathbf{x}|\mathbf{e}_{c^*}, \theta)$ (decoder).

Problem: Reparametrization trick does not work in this case. Non-differentiable sampling operation depends on the parameters $\pi_\phi(\mathbf{x})$.

Gumbel-max trick

Gumbel distribution

$$g \sim \text{Gumbel}(0, 1) \Leftrightarrow g = -\log(-\log u), u \sim \text{Uniform}[0, 1]$$

Theorem

Let $g_k \sim \text{Gumbel}(0, 1)$ for $k = 1, \dots, K$. Then a discrete random variable

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

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

- ▶ We could sample from the discrete distribution using Gumbel-max reparametrization.
- ▶ Here **parameters** and **random variable sampling** are separated (reparametrization trick). We could apply LOTUS trick.

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)

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

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

$$\hat{\mathbf{c}} = \text{Softmax} \left(\frac{\log q(\mathbf{c}|\mathbf{x}, \phi) + \mathbf{g}}{\tau} \right)$$

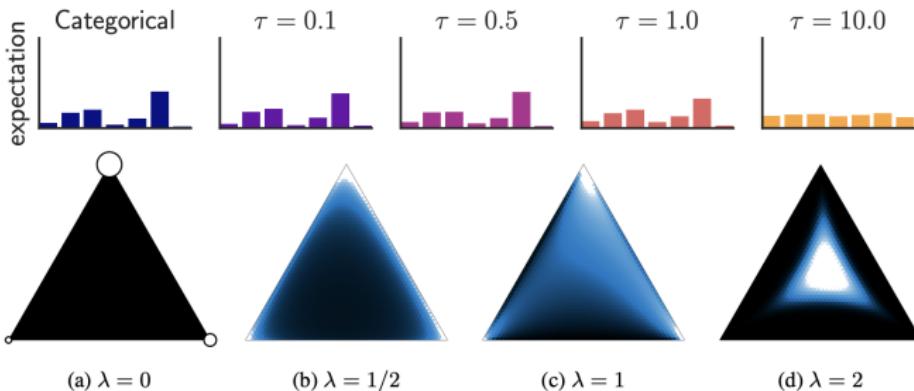
Here τ is a temperature parameter. Now we have differentiable operation, but the gradient estimator is biased now.

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

$$\hat{\mathbf{c}} = \text{Softmax} \left(\frac{\log q(\mathbf{c}|\mathbf{x}, \phi) + \mathbf{g}}{\tau} \right)$$



Reparametrization trick

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

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



Outline

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Gumbel-softmax for discrete VAE latents

2. ELBO surgery

ELBO surgery

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

Theorem

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

- ▶ $q_{\text{agg}}(\mathbf{z}|\phi) = \frac{1}{n} \sum_{i=1}^n q(\mathbf{z}|\mathbf{x}_i, \phi)$ – **aggregated** variational posterior distribution.
- ▶ $\mathbb{I}_q[\mathbf{x}, \mathbf{z}]$ – mutual information between \mathbf{x} and \mathbf{z} under empirical data distribution and distribution $q(\mathbf{z}|\mathbf{x}, \phi)$.
- ▶ **First term** pushes $q_{\text{agg}}(\mathbf{z}|\phi)$ towards the prior $p(\mathbf{z})$.
- ▶ **Second term** reduces the amount of information about \mathbf{x} stored in \mathbf{z} .

ELBO surgery

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

Proof

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

ELBO surgery

ELBO revisiting

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

Prior distribution $p(\mathbf{z})$ is only in the last term.

Optimal VAE prior

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

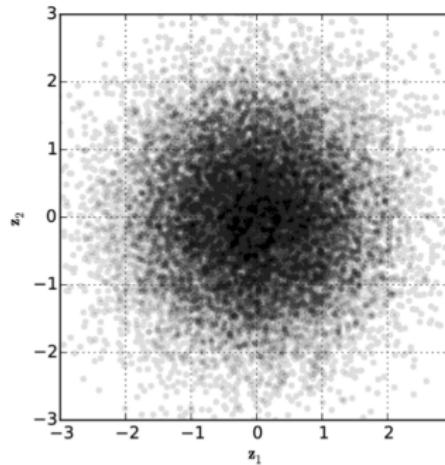
The optimal prior $p(\mathbf{z})$ is the aggregated variational posterior distribution $q_{\text{agg}}(\mathbf{z}|\phi)$!

Variational posterior

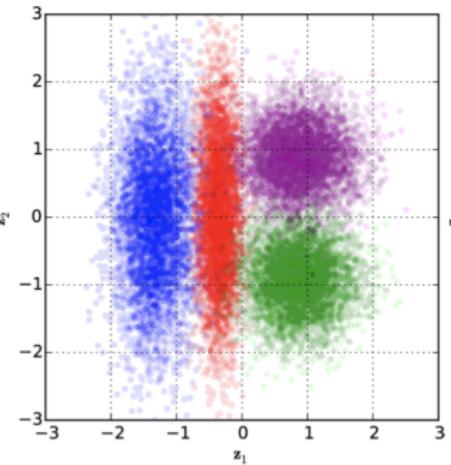
ELBO decomposition

$$\log p(\mathbf{x}|\theta) = \mathcal{L}(\phi, \theta) + KL(q(\mathbf{z}|\mathbf{x}, \phi) || p(\mathbf{z}|\mathbf{x}, \theta)).$$

- ▶ $q(\mathbf{z}|\mathbf{x}, \phi) = \mathcal{N}(\mu_\phi(\mathbf{x}), \sigma_\phi^2(\mathbf{x}))$ is a unimodal distribution.
- ▶ It is widely believed that **mismatch between $p(\mathbf{z})$ and $q_{\text{agg}}(\mathbf{z}|\phi)$ is the main reason of blurry images of VAE.**



(a) Prior distribution



(b) Posteriors in standard VAE

Summary

- ▶ 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.
- ▶ The ELBO surgery reveals insights about a prior distribution in VAE. The optimal prior is the aggregated variational posterior distribution.
- ▶ It is widely believed that mismatch between $p(\mathbf{z})$ and $q_{\text{agg}}(\mathbf{z}|\phi)$ is the main reason of blurry images of VAE.