Deep Generative Models

Lecture 6

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AI Masters

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Recap of previous lecture

EM-algorithm

- E-step

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

- M-step

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

Amortized variational inference

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

Variational Bayes

- E-step

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

- M-step

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

Recap of previous lecture

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

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

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

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

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

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

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

Variational assumption

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

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

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

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

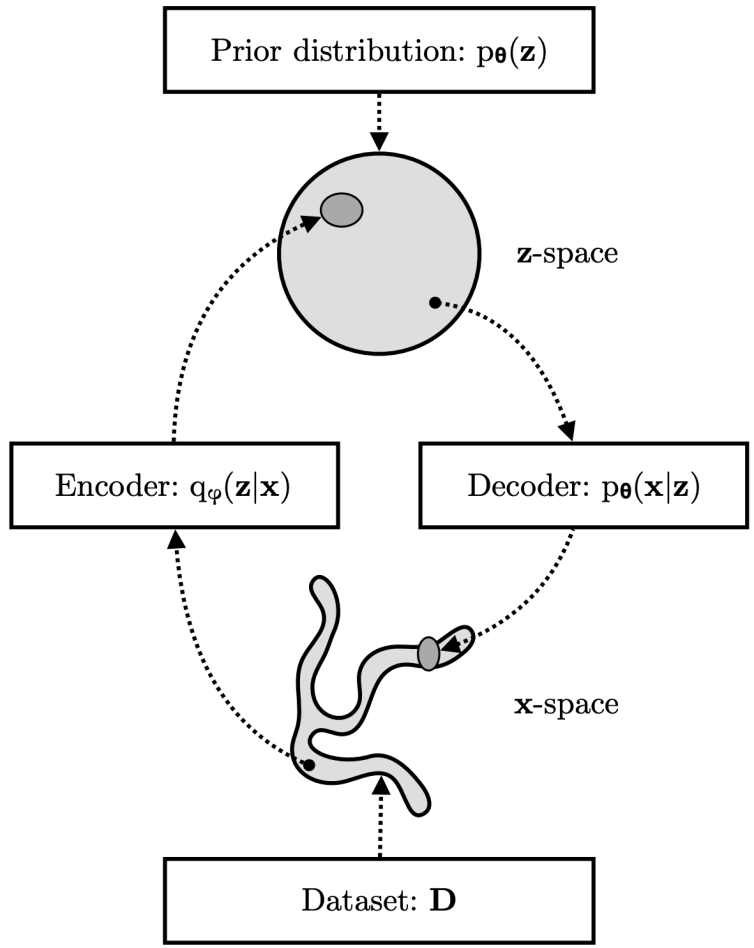
- update θ, ϕ according to the selected optimization method (SGD, Adam):

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

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 $p(\mathbf{x}, \mathbf{z}|\boldsymbol{\theta}) = p(\mathbf{z})p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta})$, with a prior distribution $p(\mathbf{z})$, and a stochastic decoder $p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta})$.
- The stochastic encoder $q(\mathbf{z}|\mathbf{x}, \boldsymbol{\phi})$ (inference model), approximates the true but intractable posterior $p(\mathbf{z}|\mathbf{x}, \boldsymbol{\theta})$.



Kingma D. P., Welling M. An introduction to variational autoencoders, 2019

Recap of previous lecture

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

- Use **discrete** model (e.x. $P(\mathbf{y}|\boldsymbol{\theta}) = \text{Cat}(\boldsymbol{\pi}(\boldsymbol{\theta}))$) 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 $p(\mathbf{x}|\boldsymbol{\theta})$ on uniformly dequantized data is equivalent to maximization of a lower bound on log-likelihood for a discrete model:

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

Outline

1. Normalizing flows as VAE model
2. ELBO surgery
3. Learnable VAE prior
4. Discrete VAE latent representations
   - Vector quantization
   - Gumbel-softmax for discrete VAE latents

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VAE vs Normalizing flows

	VAE	**NF**
Objective	ELBO $\mathcal{L}$	Forward KL/MLE
Encoder	stochastic $\mathbf{z} \sim q(\mathbf{z}\|\mathbf{x}, \boldsymbol{\phi})$	deterministic $\mathbf{z} = \mathbf{f}_{\boldsymbol{\theta}}(\mathbf{x})$ $q(\mathbf{z}\|\mathbf{x}, \boldsymbol{\theta}) = \delta(\mathbf{z} - \mathbf{f}_{\boldsymbol{\theta}}(\mathbf{x}))$
Decoder	stochastic $\mathbf{x} \sim p(\mathbf{x}\|\mathbf{z}, \boldsymbol{\theta})$	deterministic $\mathbf{x} = \mathbf{g}_{\boldsymbol{\theta}}(\mathbf{z})$ $p(\mathbf{x}\|\mathbf{z}, \boldsymbol{\theta}) = \delta(\mathbf{x} - \mathbf{g}_{\boldsymbol{\theta}}(\mathbf{z}))$
Parameters	$\boldsymbol{\phi}, \boldsymbol{\theta}$	$\boldsymbol{\theta} \equiv \boldsymbol{\phi}$

Theorem

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

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

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

Nielsen D., et al. SurVAE Flows: Surjections to Bridge the Gap between VAEs and Flows, 2020

Normalizing flow as VAE

Proof

1. Dirac delta function property

$$\mathbb{E}_{\delta(\mathbf{x}-\mathbf{y})}\mathbf{f}(\mathbf{x}) = \int \delta(\mathbf{x}-\mathbf{y})\mathbf{f}(\mathbf{x})d\mathbf{x} = \mathbf{f}(\mathbf{y}).$$

2. CoV theorem and Bayes theorem:

$$p(\mathbf{x}|\boldsymbol{\theta}) = p(\mathbf{z})|\det(\mathbf{J}_\mathbf{f})|;$$

$$p(\mathbf{z}|\mathbf{x},\boldsymbol{\theta}) = \frac{p(\mathbf{x}|\mathbf{z},\boldsymbol{\theta})p(\mathbf{z})}{p(\mathbf{x}|\boldsymbol{\theta})}; \quad \Rightarrow \quad p(\mathbf{x}|\mathbf{z},\boldsymbol{\theta}) = p(\mathbf{z}|\mathbf{x},\boldsymbol{\theta})|\det(\mathbf{J}_\mathbf{f})|.$$

3. Log-likelihood decomposition

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

Nielsen D., et al. SurVAE Flows: Surjections to Bridge the Gap between VAEs and Flows, 2020

Normalizing flow as VAE

Proof

ELBO objective:

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

$$= \mathbb{E}_{q(\mathbf{z}|\mathbf{x},\boldsymbol{\theta})}\left[\log \frac{p(\mathbf{x}|\mathbf{z},\boldsymbol{\theta})}{q(\mathbf{z}|\mathbf{x},\boldsymbol{\theta})} + \log p(\mathbf{z})\right].$$

1. Dirac delta function property:

$$\mathbb{E}_{q(\mathbf{z}|\mathbf{x},\boldsymbol{\theta})} \log p(\mathbf{z}) = \int \delta(\mathbf{z} - \mathbf{f}_{\boldsymbol{\theta}}(\mathbf{x})) \log p(\mathbf{z}) d\mathbf{z} = \log p(f_{\boldsymbol{\theta}}(\mathbf{x})).$$

2. CoV theorem and Bayes theorem:

$$\mathbb{E}_{q(\mathbf{z}|\mathbf{x},\boldsymbol{\theta})} \log \frac{p(\mathbf{x}|\mathbf{z},\boldsymbol{\theta})}{q(\mathbf{z}|\mathbf{x},\boldsymbol{\theta})} = \mathbb{E}_{q(\mathbf{z}|\mathbf{x},\boldsymbol{\theta})} \log \frac{p(\mathbf{z}|\mathbf{x},\boldsymbol{\theta})|\det(\mathbf{J}_{\mathbf{f}})|}{q(\mathbf{z}|\mathbf{x},\boldsymbol{\theta})} = \log|\det \mathbf{J}_{\mathbf{f}}|.$$

3. Log-likelihood decomposition

$$\log p(\mathbf{x}|\boldsymbol{\theta}) = \mathcal{L}(\boldsymbol{\theta}) = \log p(f_{\boldsymbol{\theta}}(\mathbf{x})) + \log|\det \mathbf{J}_{\mathbf{f}}|.$$

Nielsen D., et al. SurVAE Flows: Surjections to Bridge the Gap between VAEs and Flows, 2020

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ELBO surgery

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

Theorem

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

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

Theorem

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

Proof

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

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

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

Without proof:

$$\mathbb{I}_q[\mathbf{x}, \mathbf{z}] = \frac{1}{n}\sum_{i=1}^{n} KL(q(\mathbf{z}|\mathbf{x}_i)||q_{\text{agg}}(\mathbf{z})) \in [0, \log n].$$

Hoffman M. D., Johnson M. J. ELBO surgery: yet another way to carve up the variational evidence lower bound, 2016

ELBO surgery

ELBO revisiting

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

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

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

Optimal VAE prior

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

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

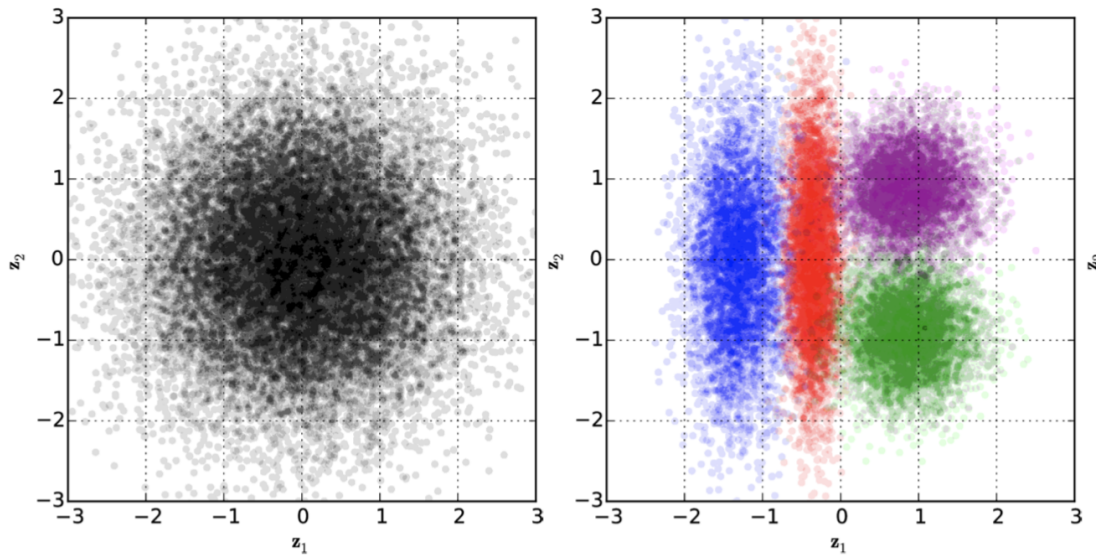
Hoffman M. D., Johnson M. J. ELBO surgery: yet another way to carve up the variational evidence lower bound, 2016

Variational posterior

ELBO decomposition

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

- $q(\mathbf{z}|\mathbf{x}, \boldsymbol{\phi}) = \mathcal{N}(\boldsymbol{\mu}_{\boldsymbol{\phi}}(\mathbf{x}), \boldsymbol{\sigma}^2_{\boldsymbol{\phi}}(\mathbf{x}))$ is a unimodal distribution.
- The optimal prior $p(\mathbf{z})$ is the aggregated posterior $q_{\text{agg}}(\mathbf{z})$.



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

It is widely believed that **mismatch between $p(\mathbf{z})$ and $q_{\text{agg}}(\mathbf{z})$ is the main reason of blurry images of VAE**.

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

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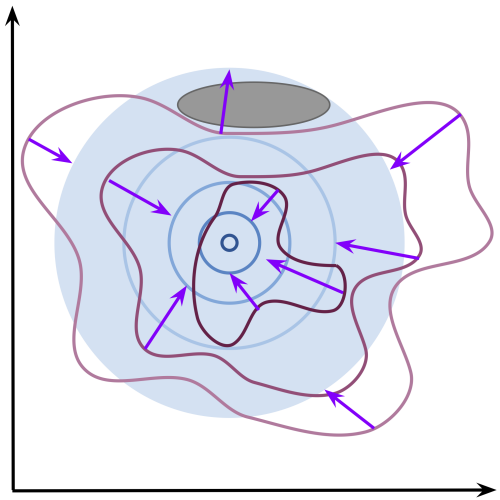
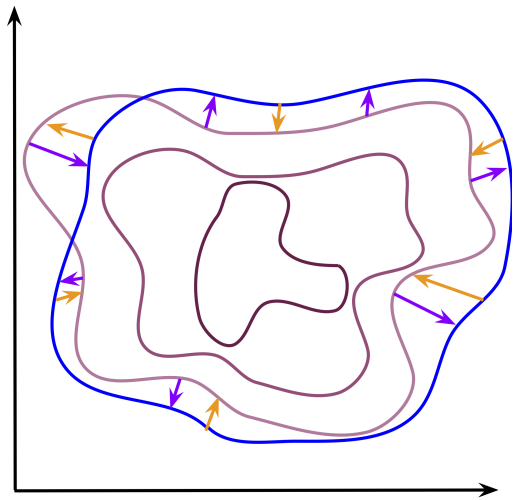
Optimal VAE prior

- Standard Gaussian $p(\mathbf{z}) = \mathcal{N}(0, \mathbf{I}) \Rightarrow$ 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

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

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

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

NF-based VAE prior

NF model in latent space

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

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

- RealNVP with coupling layers.
- Autoregressive NF (fast $\mathbf{f}_{\boldsymbol{\lambda}}(\mathbf{z})$, slow $\mathbf{g}_{\boldsymbol{\lambda}}(\mathbf{z}^*)$).

ELBO with NF-based VAE prior

$$\mathcal{L}(\phi, \theta) = \mathbb{E}_{q(\mathbf{z}|\mathbf{x},\phi)} \left[\log p(\mathbf{x}|\mathbf{z}, \theta) + \log p(\mathbf{z}|\boldsymbol{\lambda}) - \log q(\mathbf{z}|\mathbf{x}, \phi) \right]$$

$$= \mathbb{E}_{q(\mathbf{z}|\mathbf{x},\phi)} \Big[\log p(\mathbf{x}|\mathbf{z}, \theta) + \underbrace{\Big(\log p(f_{\boldsymbol{\lambda}}(\mathbf{z})) + \log |\det(\mathbf{J_f})| \Big)}_{\text{NF-based prior}} - \log q(\mathbf{z}|\mathbf{x}, \phi) \Big]$$

Chen X. et al. Variational Lossy Autoencoder, 2016

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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

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

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

Discrete VAE latents

ELBO

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

KL term

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

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

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

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

Outline

Vector quantization

Quantized representation

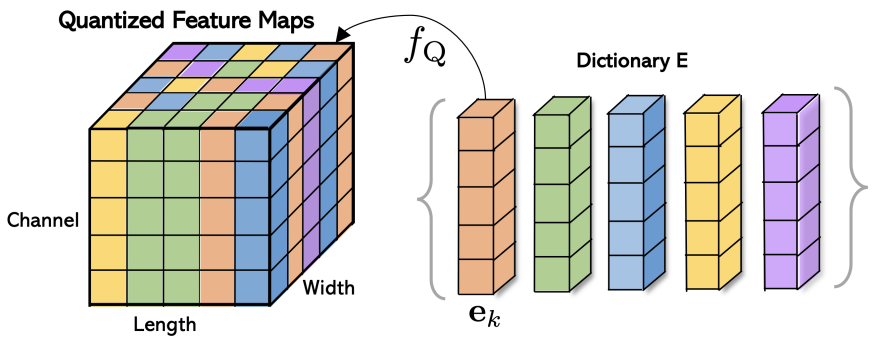
$\mathbf{z}_q \in \mathbb{R}^C$ for $\mathbf{z} \in \mathbb{R}^C$ is defined by a nearest neighbor look-up using the shared dictionary space

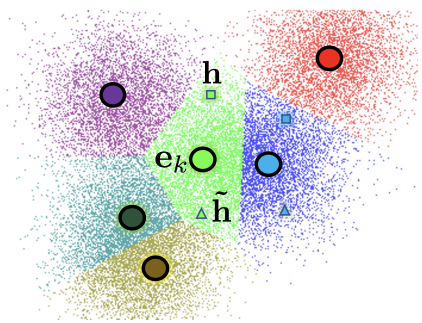
$$\mathbf{z}_q = \mathbf{e}_{k^*}, \quad \text{where } k^* = \arg\min_k \|\mathbf{z} - \mathbf{e}_k\|.$$

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

Quantization procedure

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





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

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.

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

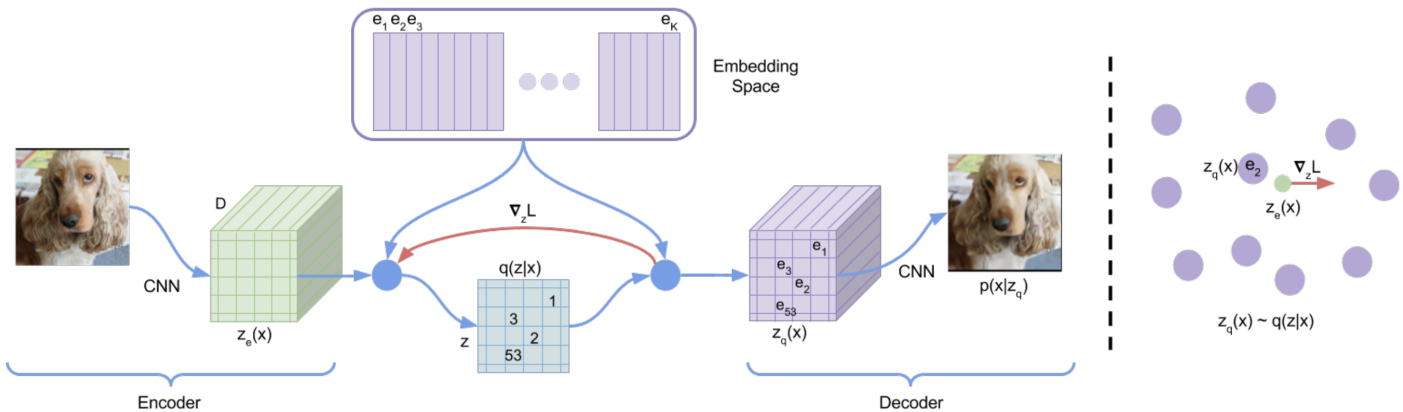
Oord A., Vinyals O., Kavukcuoglu K. Neural Discrete Representation Learning, 2017

Vector Quantized VAE (VQ-VAE)

ELBO

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

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



Problem: arg min is not differentiable.

Straight-through gradient estimation

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

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

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

Outline

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 $k = 1, \ldots, K$, 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 $c \sim \text{Categorical}(\boldsymbol{\pi})$.

- Let our encoder $q(c|\mathbf{x}, \phi) = \text{Categorical}(\boldsymbol{\pi}_\phi(\mathbf{x}))$ outputs logits of $\boldsymbol{\pi}_\phi(\mathbf{x})$.
- 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)

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

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 = **con**tinuous + dis**crete**

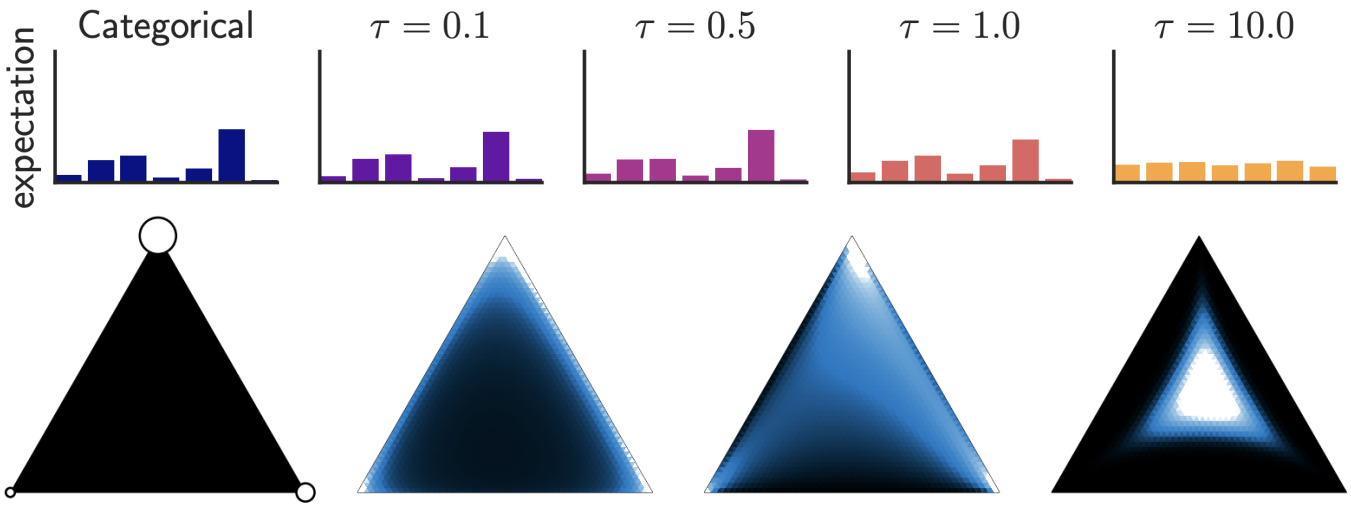
$$\hat{c}_k = \frac{\exp\left(\frac{\log q(k|\mathbf{x},\phi)+g_k}{\tau}\right)}{\sum_{j=1}^{K} \exp\left(\frac{\log q(j|\mathbf{x},\phi)+g_j}{\tau}\right)}, \quad k = 1, \ldots, K.$$

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



(a) $\lambda = 0$ (b) $\lambda = 1/2$ (c) $\lambda = 1$ (d) $\lambda = 2$

Reparametrization trick

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

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

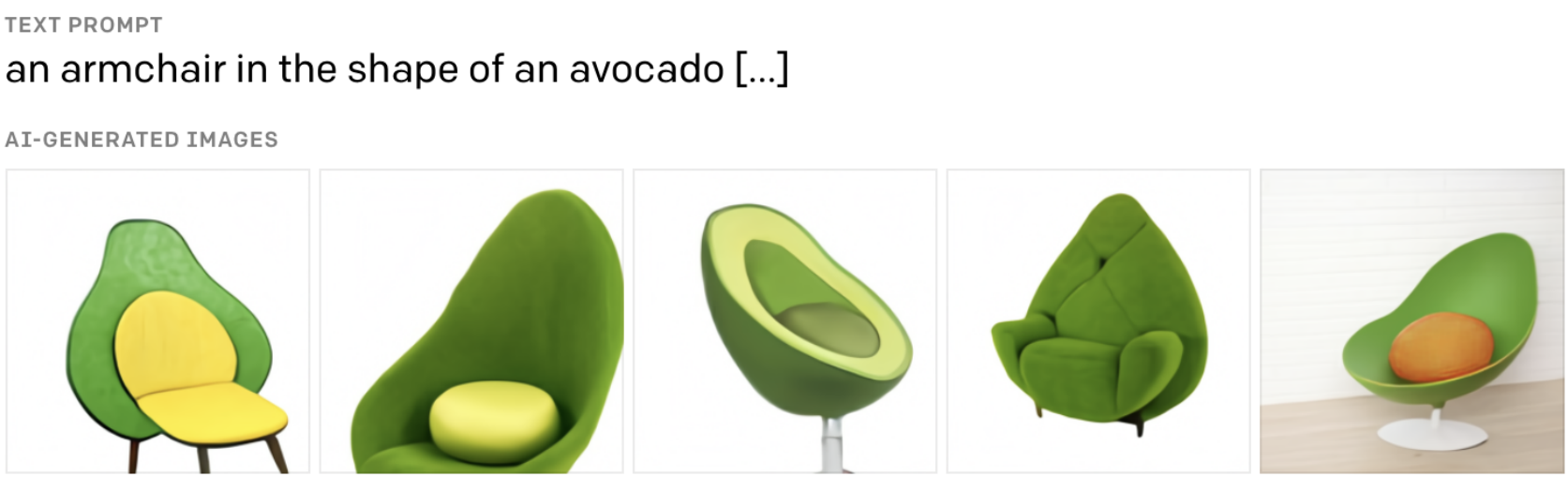
Maddison C. J., Mnih A., Teh Y. W. The Concrete distribution: A continuous relaxation of discrete random variables, 2016
Jang E., Gu S., Poole B. Categorical reparameterization with Gumbel-Softmax, 2016

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.



Ramesh A. et al. Zero-shot text-to-image generation, 2021

Summary

- NF models could be treated as VAE model with deterministic encoder and decoder.
- The ELBO surgery reveals insights about a prior distribution in VAE. The optimal prior is the aggregated posterior. It is widely believed that mismatch between $p(\mathbf{z})$ and $q_{\text{agg}}(\mathbf{z})$ is the main reason of blurry images of VAE.
- 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.