Deep Generative Models

Lecture 4

Roman Isachenko

Moscow Institute of Physics and Technology Yandex School of Data Analysis

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Forward KL for flow model

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

Reverse KL for flow model

$$\mathit{KL}(p||\pi) = \mathbb{E}_{p(\mathbf{z})} \left[\log p(\mathbf{z}) - \log |\det(\mathbf{J}_{\mathbf{g}})| - \log \pi(\mathbf{g}_{\boldsymbol{\theta}}(\mathbf{z})) \right]$$

Flow KL duality

$$\mathop{\arg\min}_{\boldsymbol{\theta}} \mathit{KL}(\pi(\mathbf{x})||p(\mathbf{x}|\boldsymbol{\theta})) = \mathop{\arg\min}_{\boldsymbol{\theta}} \mathit{KL}(p(\mathbf{z}|\boldsymbol{\theta})||p(\mathbf{z}))$$

- \triangleright $p(\mathbf{z})$ is a base distribution; $\pi(\mathbf{x})$ is a data distribution;
- ightharpoonup $\mathbf{z} \sim p(\mathbf{z}), \ \mathbf{x} = \mathbf{g}_{\boldsymbol{\theta}}(\mathbf{z}), \ \mathbf{x} \sim p(\mathbf{x}|\boldsymbol{\theta});$
- $ightharpoonup \mathbf{x} \sim \pi(\mathbf{x}), \ \mathbf{z} = \mathbf{f}_{\boldsymbol{\theta}}(\mathbf{x}), \ \mathbf{z} \sim p(\mathbf{z}|\boldsymbol{\theta}).$

Bayes theorem

$$p(\mathbf{t}|\mathbf{x}) = \frac{p(\mathbf{x}|\mathbf{t})p(\mathbf{t})}{p(\mathbf{x})} = \frac{p(\mathbf{x}|\mathbf{t})p(\mathbf{t})}{\int p(\mathbf{x}|\mathbf{t})p(\mathbf{t})d\mathbf{t}}$$

- x observed variables, t unobserved variables (latent variables/parameters);
- $p(\mathbf{x}|\mathbf{t})$ likelihood;
- $p(\mathbf{x}) = \int p(\mathbf{x}|\mathbf{t})p(\mathbf{t})d\mathbf{t}$ evidence;
- ho(t) prior distribution, p(t|x) posterior distribution.

Posterior distribution

$$p(\theta|\mathbf{X}) = \frac{p(\mathbf{X}|\theta)p(\theta)}{p(\mathbf{X})} = \frac{p(\mathbf{X}|\theta)p(\theta)}{\int p(\mathbf{X}|\theta)p(\theta)d\theta}$$

Latent variable models (LVM)

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

MLE problem for LVM

$$egin{aligned} m{ heta}^* &= rg\max_{m{ heta}} \log p(\mathbf{X}|m{ heta}) = rg\max_{m{ heta}} \sum_{i=1}^n \log p(\mathbf{x}_i|m{ heta}) = \ &= rg\max_{m{ heta}} \sum_{i=1}^n \log \int p(\mathbf{x}_i|\mathbf{z}_i,m{ heta}) p(\mathbf{z}_i) d\mathbf{z}_i. \end{aligned}$$

Naive Monte-Carlo estimation

$$p(\mathbf{x}|\boldsymbol{\theta}) = \int p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta}) p(\mathbf{z}) d\mathbf{z} = \mathbb{E}_{p(\mathbf{z})} p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta}) \approx \frac{1}{K} \sum_{k=1}^{K} p(\mathbf{x}|\mathbf{z}_k, \boldsymbol{\theta}),$$
 where $\mathbf{z}_k \sim p(\mathbf{z})$.

ELBO derivation 1 (inequality)

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

ELBO derivation 2 (equality)

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

Variational decomposition

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

Variational lower Bound (ELBO)

$$\log p(\mathbf{x}|oldsymbol{ heta}) = \mathcal{L}_{q,oldsymbol{ heta}}(\mathbf{x}) + \mathit{KL}(q(\mathbf{z})||p(\mathbf{z}|\mathbf{x},oldsymbol{ heta})) \geq \mathcal{L}_{q,oldsymbol{ heta}}(\mathbf{x}).$$

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

Log-likelihood decomposition

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

Instead of maximizing incomplete likelihood, maximize ELBO

$$\max_{\boldsymbol{\theta}} p(\mathbf{x}|\boldsymbol{\theta}) \quad \rightarrow \quad \max_{\boldsymbol{q},\boldsymbol{\theta}} \mathcal{L}_{\boldsymbol{q},\boldsymbol{\theta}}(\mathbf{x})$$

 Maximization of ELBO by variational distribution q is equivalent to minimization of KL

$$rg \max_{q} \mathcal{L}_{q, heta}(\mathbf{x}) \equiv rg \min_{q} \mathit{KL}(q(\mathbf{z}) || p(\mathbf{z} | \mathbf{x}, heta)).$$

Outline

- 1. ELBO gradients, reparametrization trick
- 2. Variational autoencoder (VAE)

- 3. Normalizing flows as VAE model
- 4. Discrete VAE latent representations

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Discrete VAE latent representations

ELBO gradients, (M-step, $\nabla_{\theta} \mathcal{L}_{\phi,\theta}(\mathbf{x})$)

$$\mathcal{L}_{\phi, oldsymbol{ heta}}(\mathbf{x}) = \mathbb{E}_{q(\mathbf{z}|\mathbf{x}, oldsymbol{\phi})} \left[\log p(\mathbf{x}|\mathbf{z}, oldsymbol{ heta}) - \log rac{q(\mathbf{z}|\mathbf{x}, oldsymbol{\phi})}{p(\mathbf{z})}
ight]
ightarrow \max_{\phi, oldsymbol{\phi}}.$$

M-step: $\nabla_{\theta} \mathcal{L}_{\phi,\theta}(\mathbf{x})$

$$egin{aligned}
abla_{m{ heta}} \mathcal{L}_{m{\phi},m{ heta}}(\mathbf{x}) &= \int q(\mathbf{z}|\mathbf{x},m{\phi})
abla_{m{ heta}} \log p(\mathbf{x}|\mathbf{z},m{ heta}) d\mathbf{z} pprox \\ &pprox
abla_{m{ heta}} \log p(\mathbf{x}|\mathbf{z}^*,m{ heta}), \quad \mathbf{z}^* \sim q(\mathbf{z}|\mathbf{x},m{\phi}). \end{aligned}$$

Naive Monte-Carlo estimation

$$p(\mathbf{x}|\boldsymbol{\theta}) = \int p(\mathbf{x}|\mathbf{z},\boldsymbol{\theta})p(\mathbf{z})d\mathbf{z} \approx \frac{1}{K} \sum_{k=1}^{K} p(\mathbf{x}|\mathbf{z}_{k},\boldsymbol{\theta}), \quad \mathbf{z}_{k} \sim p(\mathbf{z}).$$

The variational posterior $q(\mathbf{z}|\mathbf{x}, \phi)$ assigns typically more probability mass in a smaller region than the prior $p(\mathbf{z})$.

ELBO gradients, (E-step, $\nabla_{\phi} \mathcal{L}_{\phi,\theta}(\mathbf{x})$)

E-step:
$$\nabla_{\phi} \mathcal{L}_{\phi,\theta}(\mathbf{x})$$

Difference from M-step: density function $q(\mathbf{z}|\mathbf{x}, \phi)$ depends on the parameters ϕ , it is impossible to use the Monte-Carlo estimation:

$$\nabla_{\phi} \mathcal{L}_{\phi, \theta}(\mathbf{x}) = \nabla_{\phi} \int q(\mathbf{z}|\mathbf{x}, \phi) \left[\log p(\mathbf{x}|\mathbf{z}, \theta) - \log \frac{q(\mathbf{z}|\mathbf{x}, \phi)}{p(\mathbf{z})} \right] d\mathbf{z}$$

$$\neq \int q(\mathbf{z}|\mathbf{x}, \phi) \nabla_{\phi} \left[\log p(\mathbf{x}|\mathbf{z}, \theta) - \log \frac{q(\mathbf{z}|\mathbf{x}, \phi)}{p(\mathbf{z})} \right] d\mathbf{z}$$

Reparametrization trick (LOTUS trick)

$$ightharpoonup r(x) = \mathcal{N}(0,1), \ y = \sigma \cdot x + \mu, \ p(y|\theta) = \mathcal{N}(\mu,\sigma^2), \ \theta = [\mu,\sigma].$$

$$ightharpoonup \epsilon^* \sim r(\epsilon), \quad \mathsf{z} = \mathsf{g}_\phi(\mathsf{x},\epsilon), \quad \mathsf{z} \sim q(\mathsf{z}|\mathsf{x},\phi)$$

$$egin{aligned}
abla_{\phi} \int q(\mathbf{z}|\mathbf{x},\phi)\mathbf{f}(\mathbf{z})d\mathbf{z} &= \left.
abla_{\phi} \int r(\epsilon)\mathbf{f}(\mathbf{z})d\epsilon \right|_{\mathbf{z}=\mathbf{g}_{\phi}(\mathbf{x},\epsilon)} \ &= \int r(\epsilon)
abla_{\phi}\mathbf{f}(\mathbf{g}_{\phi}(\mathbf{x},\epsilon))d\epsilon pprox
abla_{\phi}\mathbf{f}(\mathbf{g}_{\phi}(\mathbf{x},\epsilon^*)) \end{aligned}$$

ELBO gradient (E-step, $\nabla_{\phi} \mathcal{L}_{\phi,\theta}(\mathbf{x})$)

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

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

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

Variational assumption

$$egin{aligned} r(\epsilon) &= \mathcal{N}(0, \mathbf{I}); \quad q(\mathbf{z}|\mathbf{x}, \phi) = \mathcal{N}(\mu_{\phi}(\mathbf{x}), \sigma_{\phi}^2(\mathbf{x})). \ \mathbf{z} &= \mathbf{g}_{\phi}(\mathbf{x}, \epsilon) = \sigma_{\phi}(\mathbf{x}) \odot \epsilon + \mu_{\phi}(\mathbf{x}). \end{aligned}$$

Here $\mu_{\phi}(\cdot), \sigma_{\phi}(\cdot)$ are parameterized functions (outputs of neural network).

- p(z) prior distribution on latent variables z. We could specify any distribution that we want. Let say $p(z) = \mathcal{N}(0, \mathbf{I})$.
- $p(\mathbf{x}|\mathbf{z}, \theta)$ generative distibution. Since it is a parameterized function let it be neural network with parameters θ .

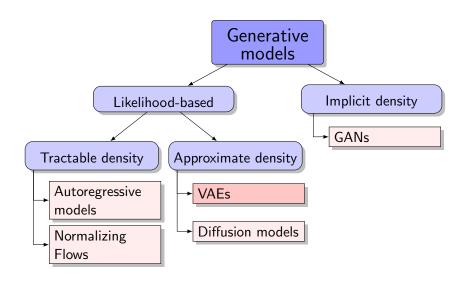
Outline

- 1. ELBO gradients, reparametrization trick
- 2. Variational autoencoder (VAE)

Normalizing flows as VAE model

4. Discrete VAE latent representations

Generative models zoo



Variational autoencoder (VAE)

Final EM-algorithm

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

$$egin{aligned} oldsymbol{\epsilon}^* &\sim r(oldsymbol{\epsilon}); & \mathbf{z}^* = \mathbf{g}_{oldsymbol{\phi}}(\mathbf{x}, oldsymbol{\epsilon}^*); \end{aligned}$$
 $\mathcal{L}_{oldsymbol{\phi}, oldsymbol{ heta}}(\mathbf{x}) &pprox \log p(\mathbf{x}|\mathbf{z}^*, oldsymbol{ heta}) - \mathit{KL}(q(\mathbf{z}^*|\mathbf{x}, oldsymbol{\phi})||p(\mathbf{z}^*)). \end{aligned}$

ightharpoonup compute a stochastic gradients w.r.t. ϕ and heta

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

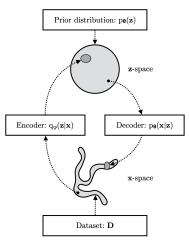
• update θ , ϕ according to the selected optimization method (SGD, Adam, etc):

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

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

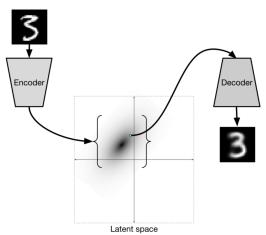
Variational autoencoder (VAE)

- ▶ VAE learns stochastic mapping between **x**-space, from complicated distribution $\pi(\mathbf{x})$, and a latent **z**-space, with simple distribution.
- The generative model learns a joint 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 $p(\mathbf{z}|\mathbf{x}, \theta)$ of the generative model.



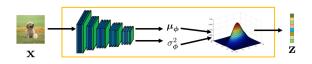
Variational Autoencoder

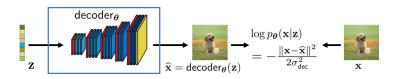
$$\mathcal{L}_{\phi, oldsymbol{ heta}}(\mathbf{x}) = \mathbb{E}_{q(\mathbf{z}|\mathbf{x}, oldsymbol{\phi})} \left[\log p(\mathbf{x}|\mathbf{z}, oldsymbol{ heta}) - \log rac{q(\mathbf{z}|\mathbf{x}, oldsymbol{\phi})}{p(\mathbf{z})}
ight]
ightarrow \max_{\phi, oldsymbol{\phi}}.$$



Variational autoencoder (VAE)

- lacksquare Encoder $q(\mathbf{z}|\mathbf{x},\phi) = \mathsf{NN}_{\mathsf{e}}(\mathbf{x},\phi)$ outputs $\mu_{\phi}(\mathbf{x})$ and $\sigma_{\phi}(\mathbf{x})$.
- ▶ Decoder $p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta}) = \mathsf{NN}_d(\mathbf{z}, \boldsymbol{\theta})$ outputs parameters of the sample distribution.





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VAE vs Normalizing flows

	VAE	NF
Objective	ELBO $\mathcal L$	Forward KL/MLE
Encoder	$\begin{array}{c} stochastic \\ z \sim q(z x, \phi) \end{array}$	$\begin{aligned} deterministic \\ \mathbf{z} &= \mathbf{f}_{\boldsymbol{\theta}}(\mathbf{x}) \\ q(\mathbf{z} \mathbf{x}, \boldsymbol{\theta}) &= \delta(\mathbf{z} - \mathbf{f}_{\boldsymbol{\theta}}(\mathbf{x})) \end{aligned}$
Decoder	$ \begin{array}{c} stochastic \\ x \sim p(x z,\theta) \end{array} $	$\begin{aligned} deterministic \\ \mathbf{x} &= \mathbf{g}_{\boldsymbol{\theta}}(\mathbf{z}) \\ p(\mathbf{x} \mathbf{z}, \boldsymbol{\theta}) &= \delta(\mathbf{x} - \mathbf{g}_{\boldsymbol{\theta}}(\mathbf{z})) \end{aligned}$
Parameters	$oldsymbol{\phi}, oldsymbol{ heta}$	$ heta \equiv \phi$

Theorem

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

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

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

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:

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

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

3. Log-likelihood decomposition

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

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:

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

3. Log-likelihood decomposition

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

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Discrete VAE latents

Motivation

- Previous VAE models had continuous latent variables z.
- ▶ **Discrete** representations **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

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

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

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

Let VAE model has discrete latent representation c with prior $p(c) = \text{Uniform}\{1, \dots, K\}.$

ELBO

$$\mathcal{L}_{\phi, oldsymbol{ heta}}(\mathbf{x}) = \mathbb{E}_{q(c|\mathbf{x}, \phi)} \log p(\mathbf{x}|c, oldsymbol{ heta}) - rac{ extsf{KL}(q(c|\mathbf{x}, \phi)||p(c))}{\phi, oldsymbol{ heta}}
ightarrow \max_{\phi, oldsymbol{ heta}}.$$

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

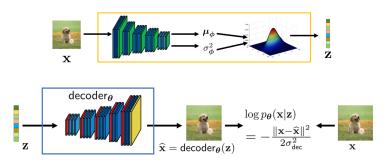
$$= \sum_{k=1}^{K} q(k|\mathbf{x}, \phi) \log q(k|\mathbf{x}, \phi) - \sum_{k=1}^{K} q(k|\mathbf{x}, \phi) \log p(k) =$$

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

Discrete VAE latents

$$\mathcal{L}_{\phi, oldsymbol{ heta}}(\mathbf{x}) = \mathbb{E}_{q(c|\mathbf{x}, \phi)} \log p(\mathbf{x}|c, oldsymbol{ heta}) + H(q(c|\mathbf{x}, \phi)) - \log K
ightarrow \max_{\phi, oldsymbol{ heta}}.$$

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



Summary

- The reparametrization trick gets unbiased gradients w.r.t to the variational posterior distribution $q(\mathbf{z}|\mathbf{x}, \phi)$.
- ► The VAE model is an LVM with two neural network: stochastic encoder $q(\mathbf{z}|\mathbf{x}, \phi)$ and stochastic decoder $p(\mathbf{x}|\mathbf{z}, \theta)$.
- ▶ NF models could be treated as VAE model with deterministic encoder and decoder.

Discrete VAE representations is a natural form of latent variables.