Deep Generative Models

Lecture 4

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Recap of previous lecture

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

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

Flow KL duality

$$\arg\min_{\boldsymbol{\theta}} KL(\pi(\mathbf{x})||p(\mathbf{x}|\boldsymbol{\theta})) = \arg\min_{\boldsymbol{\theta}} KL(p(\mathbf{z}|\boldsymbol{\theta})||p(\mathbf{z}))$$

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

Papamakarios G. et al. Normalizing flows for probabilistic modeling and inference, 2019

Recap of previous lecture

Bayes theorem

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

- $\mathbf{x}$ – observed variables, $\mathbf{t}$ – 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;
- $p(\mathbf{t})$ – prior distribution, $p(\mathbf{t}|\mathbf{x})$ – posterior distribution.

Posterior distribution

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

Recap of previous lecture

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

$$\begin{aligned} \boldsymbol{\theta}^* = \arg\max_{\boldsymbol{\theta}} \log p(\mathbf{X}|\boldsymbol{\theta}) = \arg\max_{\boldsymbol{\theta}} \sum_{i=1}^{n} \log p(\mathbf{x}_i|\boldsymbol{\theta}) = \\ = \arg\max_{\boldsymbol{\theta}} \sum_{i=1}^{n} \log \int p(\mathbf{x}_i|\mathbf{z}_i, \boldsymbol{\theta}) p(\mathbf{z}_i) d\mathbf{z}_i. \end{aligned}$$

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 $\mathbf{z}_k \sim p(\mathbf{z})$.

Recap of previous lecture

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)

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

Variational decomposition

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

Recap of previous lecture

Variational lower Bound (ELBO)

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

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

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

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

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

$$\arg\max_q \mathcal{L}_{q,\boldsymbol{\theta}}(\mathbf{x}) \equiv \arg\min_q KL(q(\mathbf{z})||p(\mathbf{z}|\mathbf{x}, \boldsymbol{\theta})).$$

Outline

EM-algorithm
Amortized inference
ELBO gradients, reparametrization trick

1. Variational autoencoder (VAE)

2. Normalizing flows as VAE model

3. Discrete VAE latent representations

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Amortized variational inference

E-step

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

- $q(\mathbf{z})$ approximates true posterior distribution $p(\mathbf{z}|\mathbf{x}, \boldsymbol{\theta}^*)$, that is why it is called **variational posterior**;
- $p(\mathbf{z}|\mathbf{x}, \boldsymbol{\theta}^*)$ could be **intractable**;
- $q(\mathbf{z})$ is different for each object $\mathbf{x}$.

Idea

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

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

- M-step

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

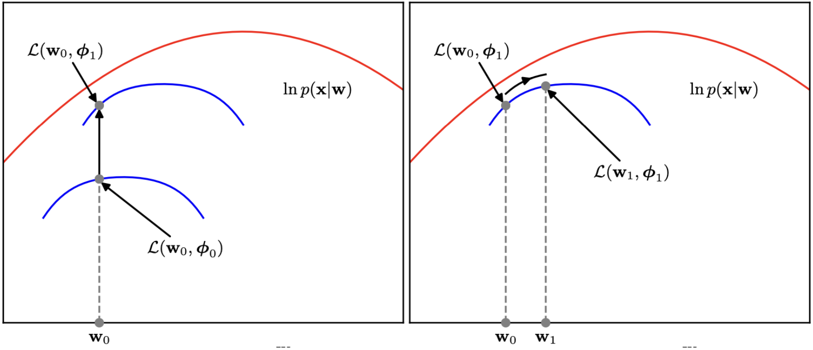
Variational EM illustration

- E-step

$$\phi_k = \phi_{k-1} + \eta \nabla_{\phi} \mathcal{L}_{\phi, \boldsymbol{\theta}_{k-1}}(\mathbf{x})\Big|_{\phi=\phi_{k-1}}$$

- M-step

$$\boldsymbol{\theta}_k = \boldsymbol{\theta}_{k-1} + \eta \nabla_{\boldsymbol{\theta}} \mathcal{L}_{\phi_k, \boldsymbol{\theta}}(\mathbf{x})\Big|_{\boldsymbol{\theta}=\boldsymbol{\theta}_{k-1}}$$



Bishop C. Deep Learning: Foundations and Concepts, 2024

Variational EM-algorithm

ELBO

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

- **E-step**

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

  where $\boldsymbol{\phi}$ – parameters of variational posterior distribution $q(\mathbf{z}|\mathbf{x},\boldsymbol{\phi})$.

- **M-step**

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

  where $\boldsymbol{\theta}$ – parameters of the generative distribution $p(\mathbf{x}|\mathbf{z},\boldsymbol{\theta})$.

Now all that is left is to obtain gradients: $\nabla_{\boldsymbol{\phi}} \mathcal{L}_{\boldsymbol{\phi},\boldsymbol{\theta}}(\mathbf{x})$, $\nabla_{\boldsymbol{\theta}} \mathcal{L}_{\boldsymbol{\phi},\boldsymbol{\theta}}(\mathbf{x})$.
Challenge: Number of samples n could be huge (we need derive the **unbiased** stochastic gradients).

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

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

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

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

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

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 $p(\mathbf{z})$.

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image credit: https://jmtomczak.github.io/blog/4/4_VAE.html

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

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

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:

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

Reparametrization trick (LOTUS trick)

- $r(x) = \mathcal{N}(0,1)$, $y = \sigma\cdot x + \mu$, $p(y|\boldsymbol{\theta}) = \mathcal{N}(\mu,\sigma^2)$, $\boldsymbol{\theta} = [\mu,\sigma]$.
- $\boldsymbol{\epsilon}^* \sim r(\boldsymbol{\epsilon})$, $\quad \mathbf{z} = \mathbf{g}_{\phi}(\mathbf{x},\boldsymbol{\epsilon})$, $\quad \mathbf{z}\sim q(\mathbf{z}|\mathbf{x},\phi)$

$$
\begin{aligned}
\nabla_{\phi}\int q(\mathbf{z}|\mathbf{x},\phi)\mathbf{f}(\mathbf{z})d\mathbf{z} &= \nabla_{\phi}\int r(\boldsymbol{\epsilon})\mathbf{f}(\mathbf{z})d\boldsymbol{\epsilon}\Big|_{\mathbf{z}=\mathbf{g}_{\phi}(\mathbf{x},\boldsymbol{\epsilon})} \\
&= \int r(\boldsymbol{\epsilon})\nabla_{\phi}\mathbf{f}(\mathbf{g}_{\phi}(\mathbf{x},\boldsymbol{\epsilon}))d\boldsymbol{\epsilon} \approx \nabla_{\phi}\mathbf{f}(\mathbf{g}_{\phi}(\mathbf{x},\boldsymbol{\epsilon}^*))
\end{aligned}
$$

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

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

Variational assumption

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

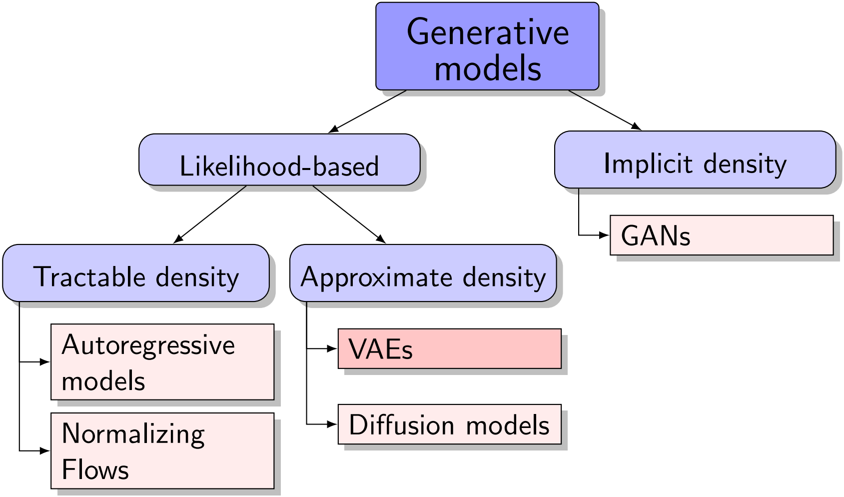
$$
\mathbf{z} = \mathbf{g}_{\phi}(\mathbf{x},\boldsymbol{\epsilon}) = \boldsymbol{\sigma}_{\phi}(\mathbf{x})\odot\boldsymbol{\epsilon} + \boldsymbol{\mu}_{\phi}(\mathbf{x}).
$$

Here $\boldsymbol{\mu}_{\phi}(\cdot),\boldsymbol{\sigma}_{\phi}(\cdot)$ are parameterized functions (outputs of neural network).

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

Outline

Generative models zoo



Variational autoencoder (VAE)

Final EM-algorithm

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

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

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

- compute a stochastic gradients w.r.t. $\boldsymbol{\phi}$ and $\boldsymbol{\theta}$

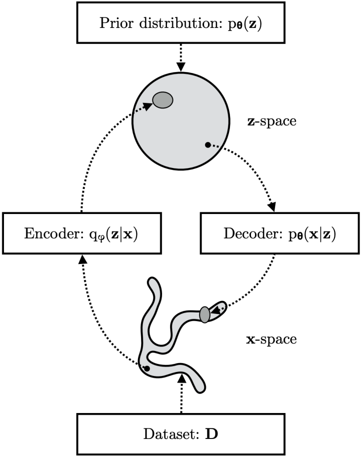
$$\nabla_{\boldsymbol{\phi}}\mathcal{L}_{\boldsymbol{\phi},\boldsymbol{\theta}}(\mathbf{x}) \approx \nabla_{\boldsymbol{\phi}} \log p(\mathbf{x}|\mathbf{g}_{\boldsymbol{\phi}}(\mathbf{x}, \boldsymbol{\epsilon}^*), \boldsymbol{\theta}) - \nabla_{\boldsymbol{\phi}}\mathrm{KL}(q(\mathbf{z}|\mathbf{x}, \boldsymbol{\phi})||p(\mathbf{z}));$$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

- update $\boldsymbol{\theta}, \boldsymbol{\phi}$ according to the selected optimization method (SGD, Adam, etc):

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

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



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

Variational Autoencoder

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

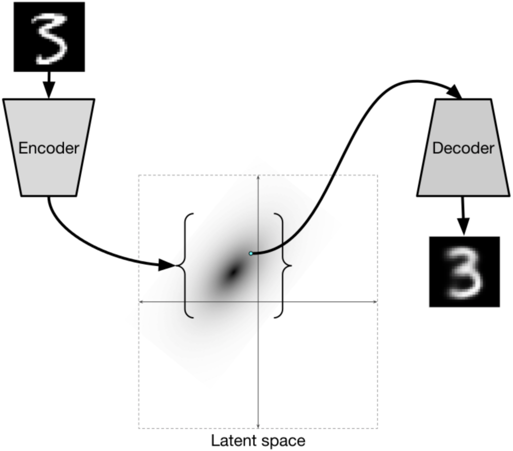
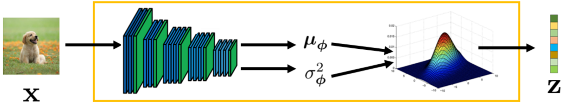
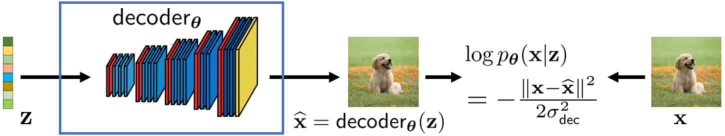


image credit: http://ijdykeman.github.io/ml/2016/12/21/cvae.html

Variational autoencoder (VAE)

- Encoder $q(\mathbf{z}|\mathbf{x}, \phi) = \mathrm{NN}_e(\mathbf{x}, \phi)$ outputs $\boldsymbol{\mu}_\phi(\mathbf{x})$ and $\boldsymbol{\sigma}_\phi(\mathbf{x})$.
- Decoder $p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta}) = \mathrm{NN}_d(\mathbf{z}, \boldsymbol{\theta})$ outputs parameters of the sample distribution.





Chan S. Tutorial on Diffusion Models for Imaging and Vision, 2024

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VAE vs Normalizing flows

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

Theorem

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

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

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

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:

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

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

3. Log-likelihood decomposition

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

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

Normalizing flow as VAE

Proof

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

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

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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

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

- 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

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

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

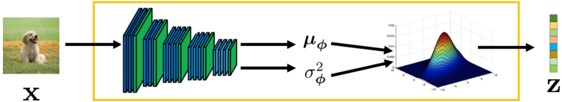
$$= \sum_{k=1}^{K} q(k|\mathbf{x}, \phi) \log q(k|\mathbf{x}, \phi) - \sum_{k=1}^{K} q(k|\mathbf{x}, \phi) \log p(k) =$$

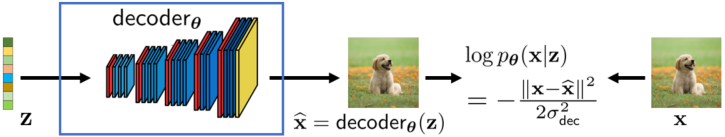
$$= -H(q(c|\mathbf{x}, \phi)) + \log K.$$

Discrete VAE latents

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

- 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 $p(\mathbf{x}|c, \boldsymbol{\theta})$ should input discrete random variable c.





Chan S. Tutorial on Diffusion Models for Imaging and Vision, 2024

Summary

- Amortized variational inference allows to efficiently compute the stochastic gradients for ELBO using Monte-Carlo estimation.

- 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 $p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta})$.

- NF models could be treated as VAE model with deterministic encoder and decoder.

- Discrete VAE representations is a natural form of latent variables.