16. Generative Model - VAE

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CSED515 - 2022 Spring

Announcement

- Assignment 4 has been released (final assignment, total score = 150)
  - Due: June 2 (Friday), 23:59
- Final exam: June 8 (Thursday), 11:00∼12:20
  - Off-line, closed book
  - Topics: 10. Evaluation ∼ 19. Reinforcement Learning

Examples of Unsupervised Learning

In fact, we've focused on supervised learning tasks, in particular, regression and classification. In next several lectures, we will study about unsupervised learning:

- Clustering, e.g., image segmentation
- Feature selection or dimensionality reduction, e.g., PCA
- **Generative model, e.g., VAE, GAN**

Generative Models

Training data ~ $p_{data}(x)$

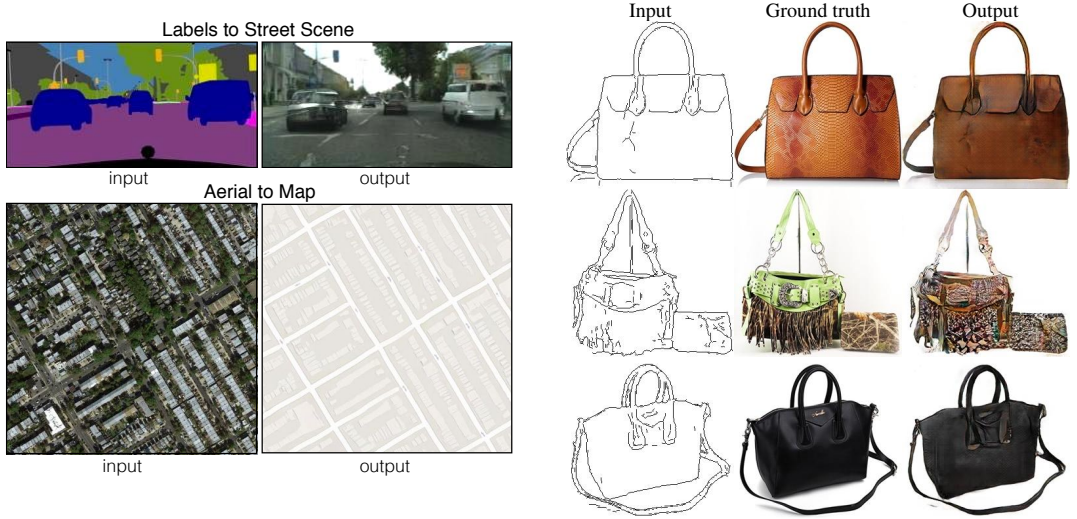
Generated samples ~ $p_{model}(x)$

Want to learn $p_{model}(x)$ similar to $p_{data}(x)$

- Given training dataset, we want to generate new samples from the same distribution
- In other words, we want to estimate density of data

Applications of Generative Model

- Generative model often provides useful approaches for other machine learning tasks, e.g., density estimation for regression, classification, out-of-distribution detection, ...
- Beside this, there are a number of interesting applications
  - e.g., Image-to-Image translation: super-resolution, style change, colorization, ...



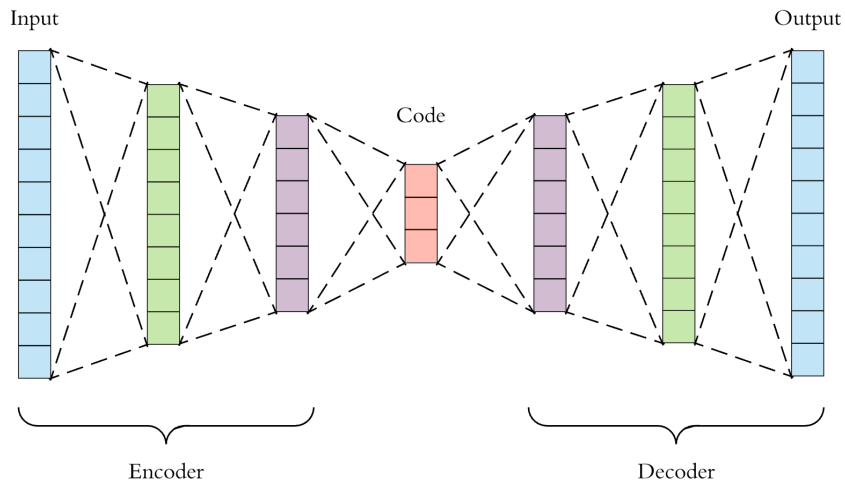
[Isola et al 16]

Applications of Generative Model

- Beside this, there are a number of interesting applications
  - e.g., POSCO steel plate with random pattern
  - More examples can be found at https://machinelearningmastery.com/impressive-applications-of-generative-adversarial-networks/

Ordinary Auto-encoder (AE) for Data Generation?

- We can use the ordinary autoencoder (in the previous lecture) to generate data
- However, we cannot control the shape of distribution of latent variable in AE
- Hence, it is hard to interpret or manipulate latent feature to generate desired data, i.e., we need some probabilistic approach



What we can do from manipulating latent feature?

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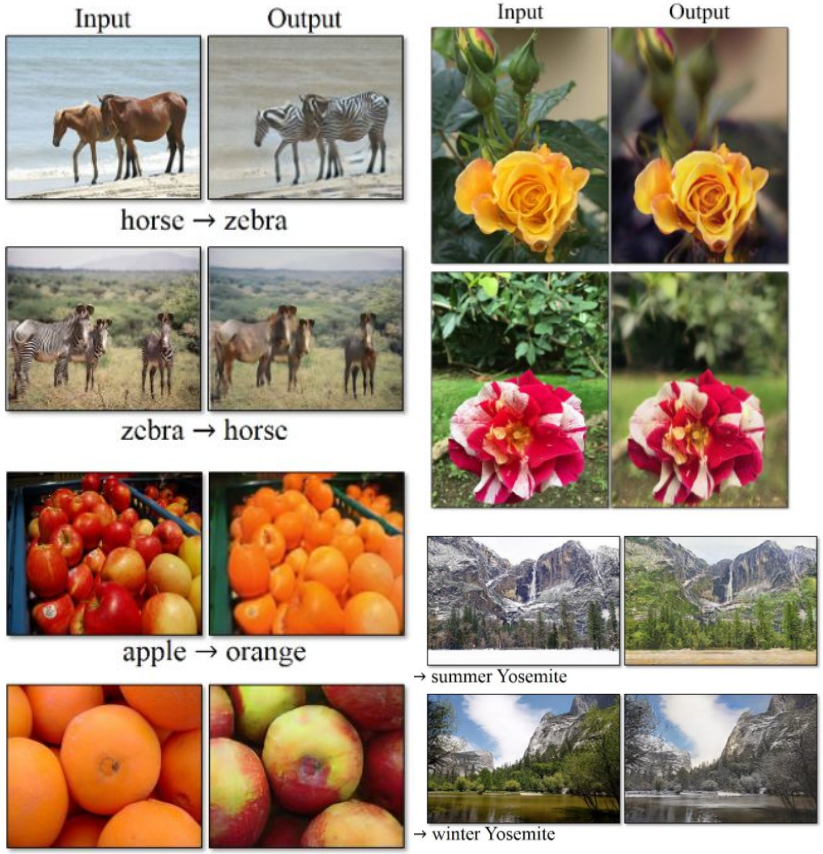
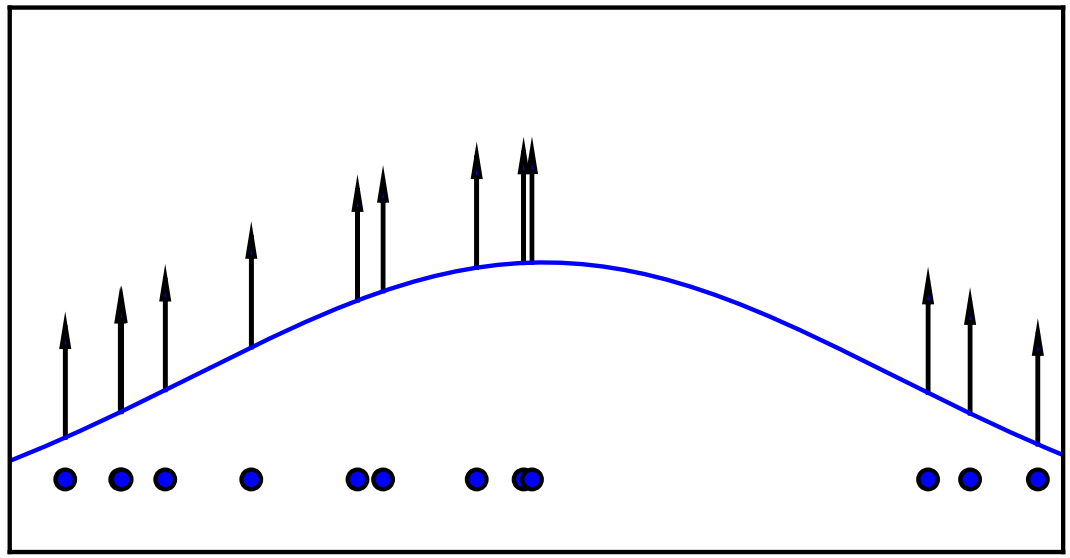
Source->Target domain transfer



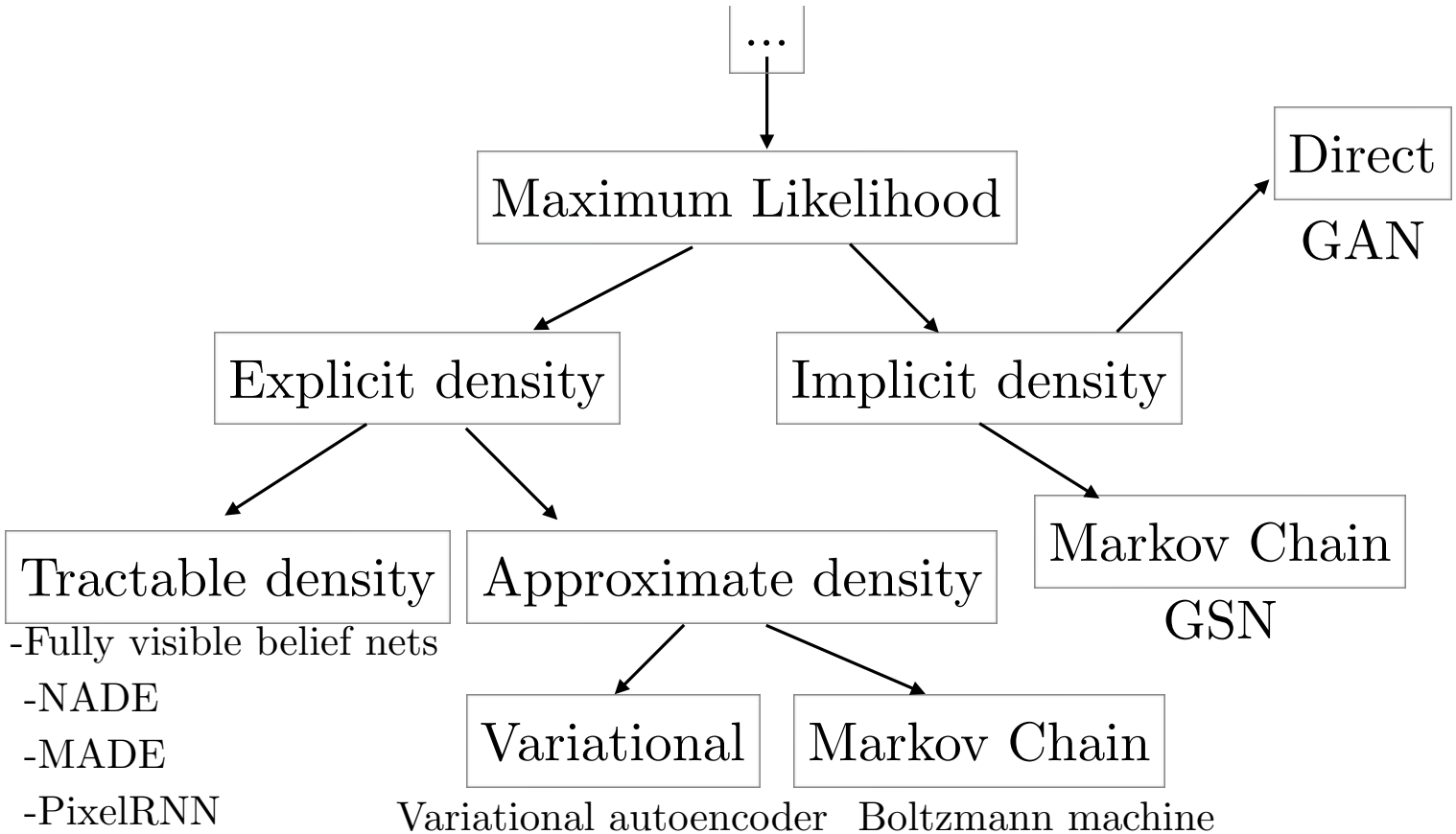
CycleGAN. Zhu et al. 2017.

A General Approach: Maximum Likelihood



$$\boldsymbol{\theta}^* = \arg\max_{\boldsymbol{\theta}} \mathbb{E}_{x \sim p_{\text{data}}} \log p_{\text{model}}(\boldsymbol{x} \mid \boldsymbol{\theta})$$

Taxonomy of Generative Models



(Goodfellow 2016)

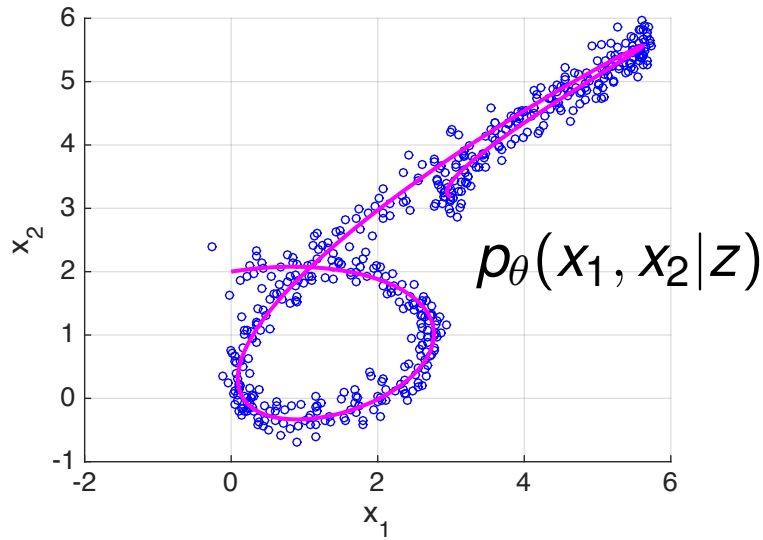
Outline

- Variational Auto-Encoder (VAE) [Kingma & Welling 14]
- Generative Adversarial Network (GAN) [Goodfellow et al 14]

Manifold Hypothesis

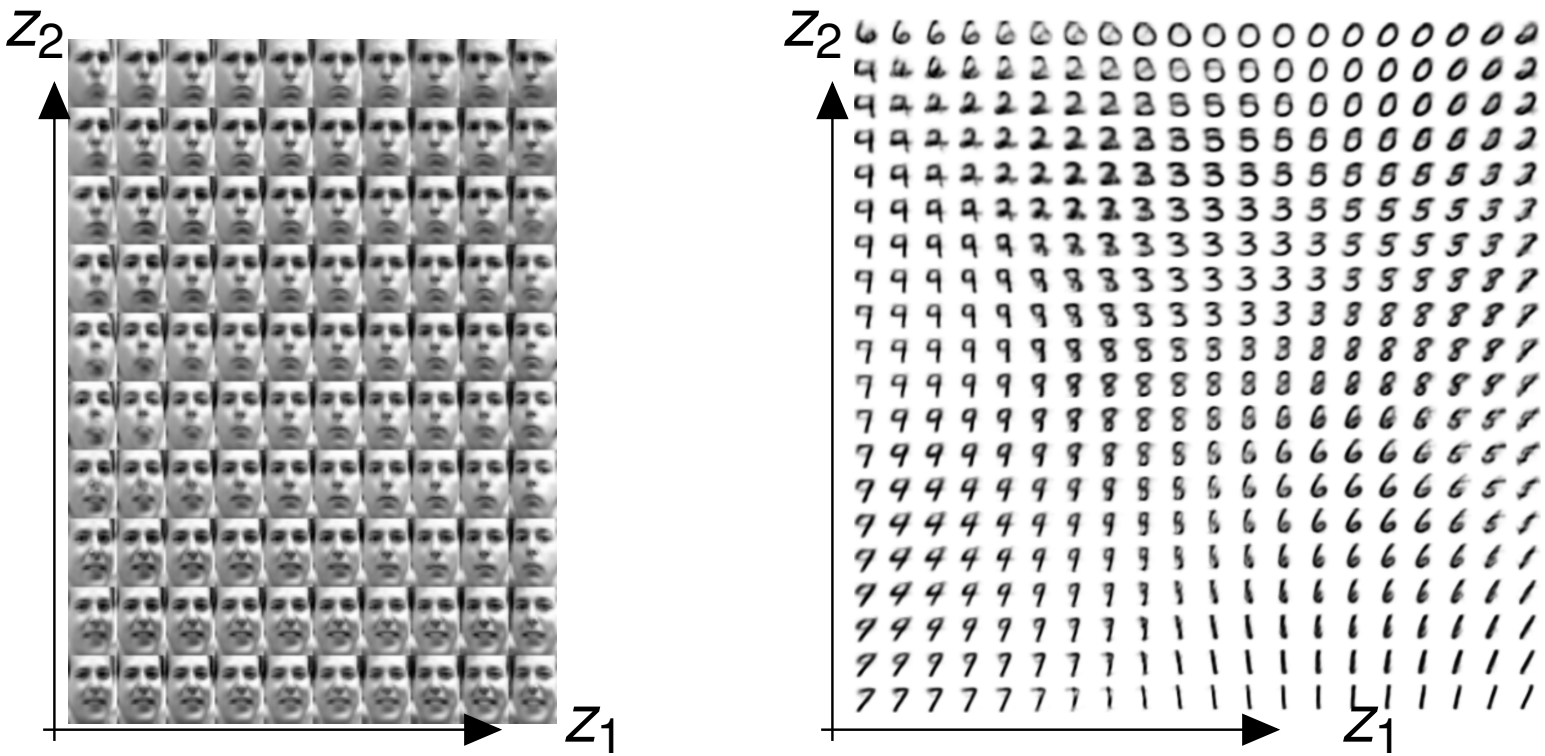
- x is a high dimensional vector
- Data is concentrated around a low dimensional manifold

$$z \in [0, 1] \quad \rightarrow$$



Manifold Hypothesis

- $x \in \mathbb{R}^D$ is a high dimensional vector
- Data is concentrated around a low dimensional manifold ($z \in \mathbb{R}^M$ with $M \ll D$)



[Kingma and Welling 14]

A Probabilistic Approach for Generative Model

Recalling MLE, our objective is maximizing

$$p_\theta(x) = \int p(z) p_\theta(x \mid z) dz$$

where generative model is $p_\theta(x \mid z)$

- Recalling manifold hypothesis, choose prior $p(z)$ to be simple, e.g., Gaussian distribution of reasonable latent attributes z, e.g., pose, degree of smile, ...
- As conditional $p_\theta(x \mid z)$ is anticipated to be complex, neural network is widely selected

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- As conditional $p_\theta(x \mid z)$ is anticipated to be complex, neural network is widely selected
- The marginalization $\int$ is intractable $\rightarrow$ variational inference

Intractability

- Data likelihood is intractable due to the integral:

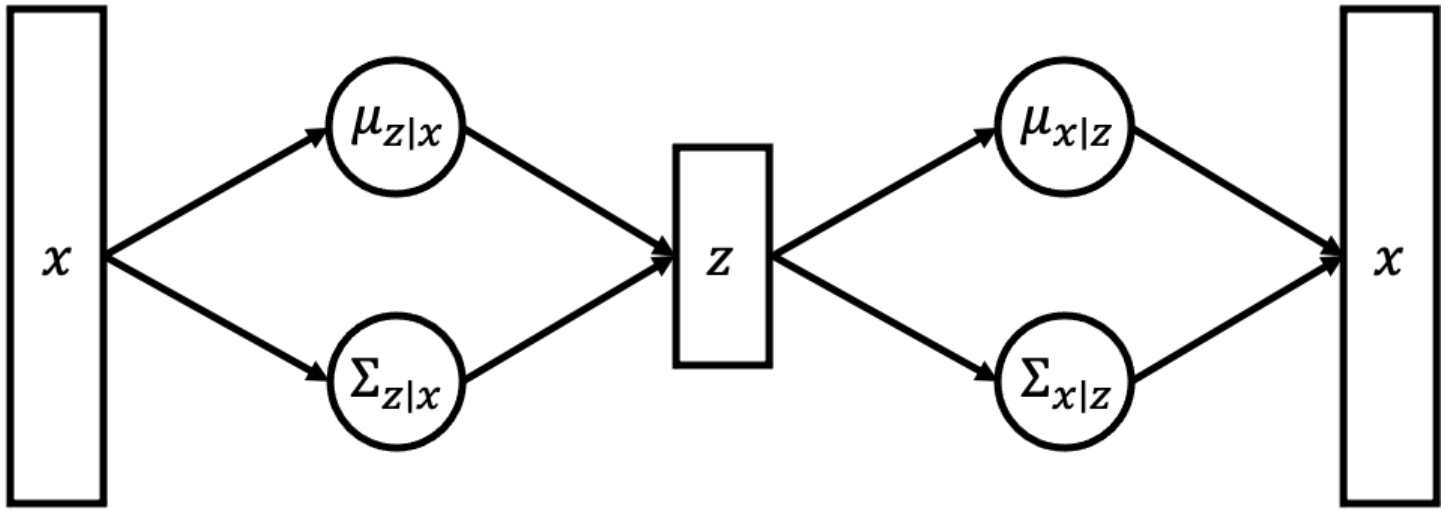
$$p_\theta(x) = \int p(z) p_\theta(x \mid z) dz$$

- Posterior density is also intractable due to the data likelihood:

$$p_\theta(z \mid x) = \frac{p_\theta(x \mid z) p(z)}{p_\theta(x)}$$

- A solution: approximate the posterior $p_\theta(z \mid x)$ using another (encoder) network $q_\phi(z \mid x)$

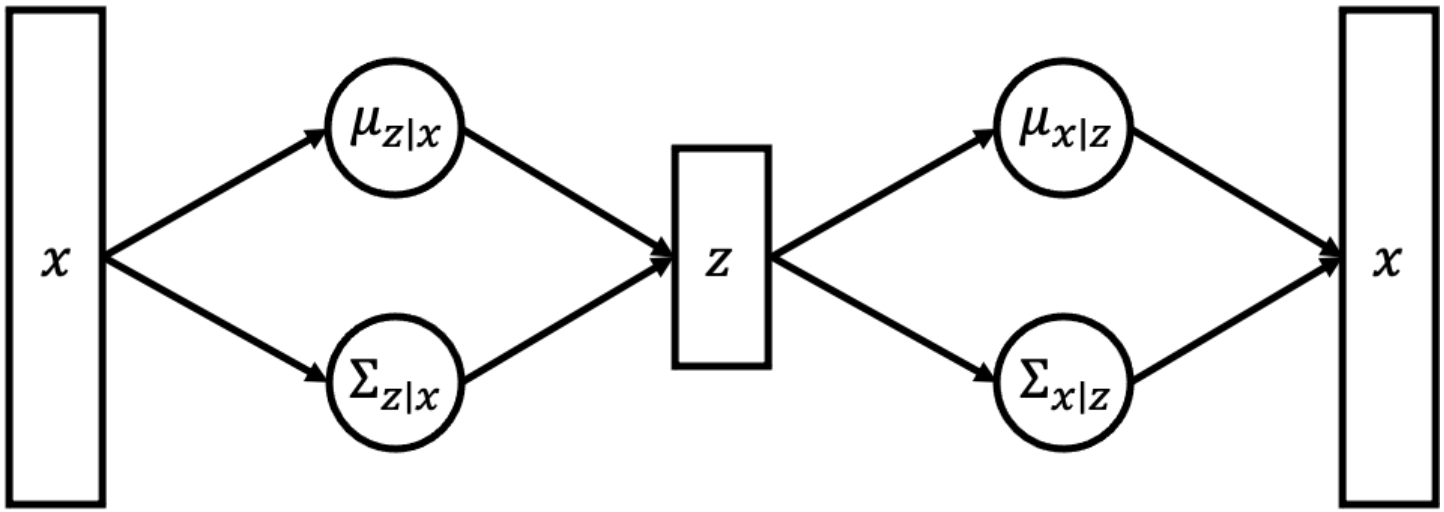
A Probabilistic Framework of Auto-encoder



You can imagine that there is a neural network f_ϕ for encoder, so that

$$f_\phi(x) = \begin{bmatrix} \mu_{z|x} \\ \sigma_{z|x} \end{bmatrix}, \quad \text{and} \quad q_\phi(z|x) = \mathcal{N}\left(f_\phi(x)_1, (f_\phi(x)_2)^2\right)$$

A Probabilistic Framework of Auto-encoder



For decoder p_θ,

$$g_\theta(z) = \begin{bmatrix} \mu_{x|z} \\ \sigma_{x|z} \end{bmatrix}, \quad \text{and} \quad p_\theta(x|z) = \mathcal{N}\left(g_\theta(z)_1, (g_\theta(z)_2)^2\right)$$

Variational Autoencoder

Recalling we aim at MLE: for given x [1],

$$
\begin{aligned}
\log p_\theta(x) &= \mathbb{E}_{z\sim q_\phi(\cdot|x)}\left[\log p_\theta(x)\right] \\
&= \mathbb{E}_z\left[\log \frac{p_\theta(x \mid z)p(z)}{p_\theta(z \mid x)}\right] \\
&= \mathbb{E}_z\left[\log \frac{p_\theta(x \mid z)p(z)}{p_\theta(z \mid x)}\frac{q_\phi(z \mid x)}{q_\phi(z \mid x)}\right] \\
&= \mathbb{E}_z\left[\log p_\theta(x \mid z)\right] - \mathbb{E}_z\left[\log \frac{q_\phi(z \mid x)}{p(z)}\right] + \mathbb{E}_z\left[\log \frac{q_\phi(z \mid x)}{p_\theta(z \mid x)}\right] \\
&= \mathbb{E}_z\left[\log p_\theta(x \mid z)\right] - \mathrm{KL}(q_\phi(z \mid x)\|p(z)) + \mathrm{KL}(q_\phi(z \mid x)\|p_\theta(z \mid x))
\end{aligned}
$$

where the KL divergences take the expectation w.r.t. $z \sim q_\phi(\cdot \mid x)$.

[1] $p(x)p(z \mid x) = p(x \mid z)p(z)$

Variational Autoencoder

Recalling we aim at MLE: for given x,

$$\log p_\theta(x) = \underbrace{\mathbb{E}_z\left[\log p_\theta(x \mid z)\right]}_{\text{(A)}} - \underbrace{\mathrm{KL}(q_\phi(z \mid x) \| p(z))}_{\text{(B)}} + \underbrace{\mathrm{KL}(q_\phi(z \mid x) \| p_\theta(z \mid x))}_{\text{(C)}}$$

- Term (A) is tractable as we can sample $z \sim q_\phi(\cdot \mid x)$ from the encoder, and compute $p_\theta(x \mid z)$ from the decoder.
- Term (B) is tractable as the KL divergence between Gaussians has a closed-form
- Term (C) is intractable, while we know it is non-negative thanks to Gibbs' inequality ($KL \geq 0$)
- Hence, define (A)+(B) as variational lower bound $\mathcal{L}(x, \theta, \phi)$ (ELBO: Evidence Lower BOund [2]) and maximize it

[2] c.f. EM slides p. 12

Training VAE

Training VAE:

$$\arg\max_{\theta,\phi} \sum_{i=1}^{N} \mathcal{L}(x^{(i)}, \theta, \phi)$$

Understanding ELBO:

$$\begin{aligned}\log p_\theta(x) &\geq \mathcal{L}(x, \theta, \phi) \\ &= \mathbb{E}_z \left[\log p_\theta(x \mid z)\right] - \mathrm{KL}(q_\phi(z \mid x) \| p_\theta(z))\end{aligned}$$

- $\mathbb{E}_z \left[\log p_\theta(x \mid z)\right]$ for reconstruction
- $\mathrm{KL}(q_\phi(z \mid x) \| p(z))$ for regularization to make the approximate posterior close to the prior

Training VAE: Monte Carlo Method

Let's simplify the model by assuming $x, z \in \mathbb{R}$,

$$q_\phi(z|x) \sim \mathcal{N}(z \mid f_\phi(x), \sigma_z^2) \quad \text{and} \quad p_\theta(x|z) \sim \mathcal{N}(x|g_\theta(z), \sigma_x^2)$$

where $f_\phi(x)$ is a function of x parameterized by ϕ, and $g_\theta(z)$ is a function of z parameterized by θ.

The first term of ELBO has no analytic solution:

$$\mathbb{E}_z \left[\log p_\theta(x \mid z)\right] = \int q_\phi(z|x) \log p_\theta(x \mid z) dz$$

We can approximate the expectation with Monte-Carlo method:

$$\mathbb{E}_z \left[\log p_\theta(x \mid z)\right] \approx \frac{1}{N} \sum_{i=1}^{N} \log p_\theta(x \mid z^{(i)})$$

where $z^{(1)}, z^{(2)}, ..., z^{(N)}$ are samples drawn from $q_\phi(z|x)$.

Training Decoder p

Given the Monte Carlo approximation

$$\mathbb{E}_z \left[\log p_\theta(x \mid z)\right] \approx \frac{1}{N} \sum_{i=1}^{N} \log p_\theta(x \mid z^{(i)})$$

$$= -\log \sigma_x^2 \sqrt{2\pi} - \frac{1}{2N} \sum_{i=1}^{N} \frac{(x - g_\theta(z^{(i)}))^2}{\sigma_x^2}$$

we can approximate the derivative w.r.t θ[3].

For example, if $g_\theta(z) = \theta_1 z + \theta_0$ where $\theta_1, \theta_0 \in \mathbb{R}$,

$$\frac{\partial \, \mathbb{E}_z \left[\log p_\theta(x \mid z)\right]}{\partial \theta_1} \approx \frac{1}{N} \sum_{i=1}^{N} \frac{(x - g_\theta(z^{(i)}))z^{(i)}}{\sigma_x^2}$$

[3] The same procedure can be applied if g_θ is a NN parameterized by θ.

Training Encoder q

Again, given the Monte Carlo approximation

$$\mathbb{E}_z \left[\log p_\theta(x \mid z)\right] \approx \frac{1}{N} \sum_{i=1}^{N} \log p_\theta(x \mid z^{(i)})$$

$$= -\log \sigma_x^2 \sqrt{2\pi} - \frac{1}{2N} \sum_{i=1}^{N} \frac{(x - g_\theta(z^{(i)}))^2}{\sigma_x^2}$$

we cannot approximate the derivative w.r.t ϕ in this case.

Why? the distribution q is replaced by its samples!

$\Rightarrow$ Reparameterization is a key trick to train VAE!

Reparameterization Trick

Some random variables can be represented as a function of another variable.

For example, assume $Z \sim \mathcal{N}(\mu, \sigma^2)$.

The distribution of Z can be explained by the standard normal distribution as

$$Z = \sigma\epsilon + \mu, \quad \text{where} \quad \epsilon \sim \mathcal{N}(0, 1)$$

We can also take a sample of Z using the sample from $\mathcal{N}(0, 1)$ via $z^{(i)} = \sigma\epsilon^{(i)} + \mu$

Training Encoder with Reparameterization

Recall $q_\phi(z|x) \sim \mathcal{N}(z \mid f_\phi(x), \sigma_z^2)$.

Using reparam $z^{(i)} = \epsilon^{(i)}\sigma_z + f_\phi(x)$, the expectation can be rewritten as

$$\begin{aligned}
\mathbb{E}_z\left[\log p_\theta(x \mid z)\right] &\approx \frac{1}{N}\sum_{i=1}^{N} \log p_\theta(x \mid z^{(i)}) \\
&= -\log \sigma_x^2\sqrt{2\pi} - \frac{1}{2N}\sum_{i=1}^{N}\frac{(x - g_\theta(z^{(i)}))^2}{\sigma_x^2} \\
&= -\log \sigma_x^2\sqrt{2\pi} - \frac{1}{2N}\sum_{i=1}^{N}\frac{(x - g_\theta(\epsilon^{(i)}\sigma_z + f_\phi(x)))}{\sigma_x^2}
\end{aligned}$$

Then the partial derivative w.r.t. ϕ can be computed via

$$\frac{\partial\, \mathbb{E}_z\left[\log p_\theta(x \mid z)\right]}{\partial \phi} \approx \frac{1}{N}\sum_{i=1}^{N}\frac{(x - g_\theta(z^{(i)}))}{\sigma_x^2}\frac{\partial g_\theta}{\partial \phi}$$

KL Divergence

The second term in ELBO, i.e., $\mathrm{KL}(q_\phi(z \mid x) \| p(z))$, has an analytic solution if both q and p follows the normal distribution:

$$\int q_\theta(z|x) \log p(z) dz = \int \mathcal{N}(z; \mu, \sigma^2) \log \mathcal{N}(z; 0, I) dz$$
$$= -\frac{J}{2} \log 2\pi - \frac{1}{2} \sum_{j=1}^{J} (\mu_j^2 + \sigma_j^2)$$

where J is a dimensionality of z, μ and σ is a function of x.

We can easily compute the derivatives w.r.t μ and σ.

Training VAE: Summary

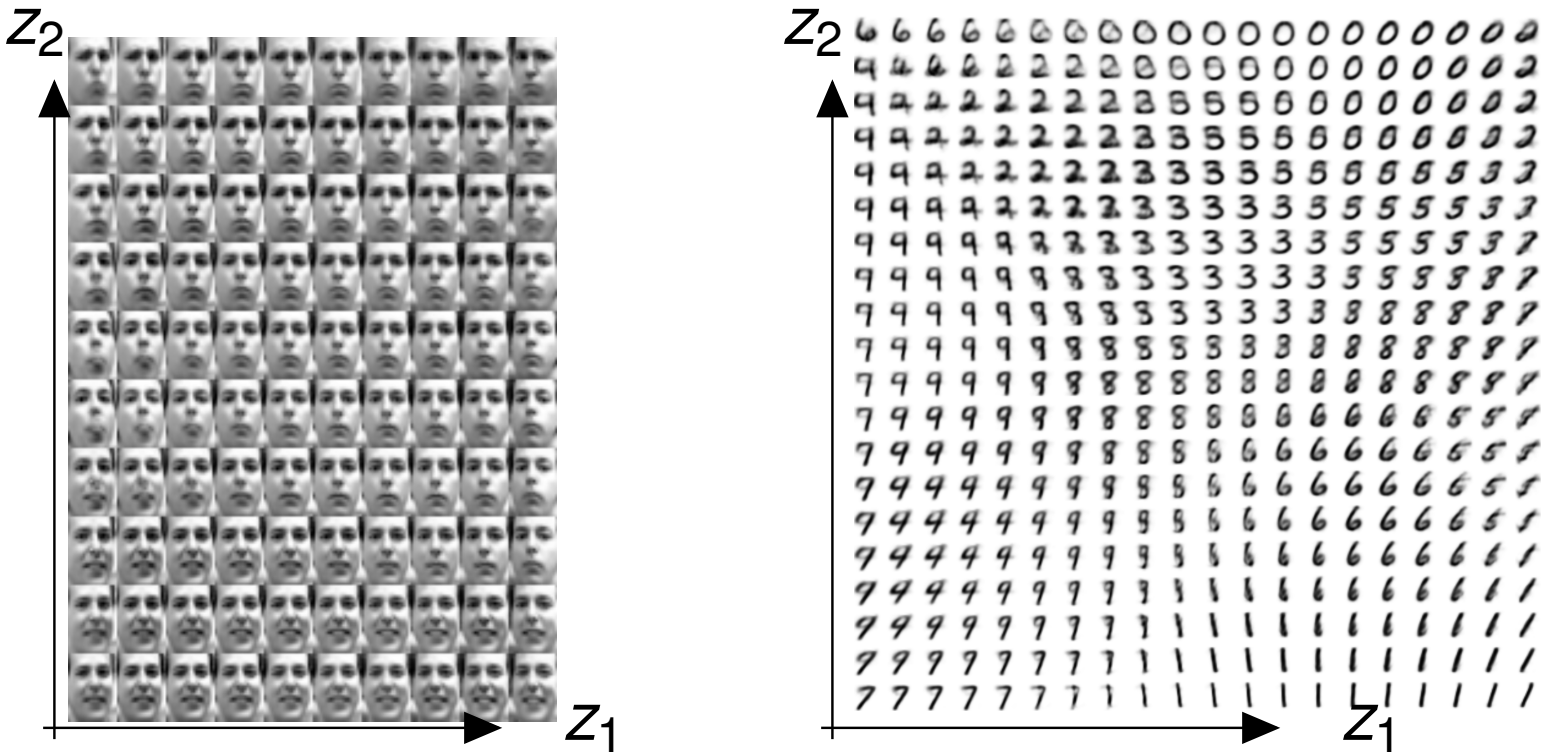
Training VAE via ELBO:

$$\begin{aligned}\log p_\theta(x) &\geq \mathcal{L}(x, \theta, \phi) \\ &= \mathbb{E}_z \left[\log p_\theta(x \mid z)\right] - \mathrm{KL}(q_\phi(z \mid x) \| p(z)) \\ &\approx \frac{1}{N} \sum_{n=1}^{N} \left[\log p_\theta(x \mid z^{(n)})\right] - \mathrm{KL}\left(q_\phi(z^{(n)} \mid x) \| p(z^{(n)})\right)\end{aligned}$$

- $\partial \mathcal{L}(x, \theta, \phi)/\partial \theta$ is simple given samples from $q(z|x)$
- $\partial \mathcal{L}(x, \theta, \phi)/\partial \phi$ requires reparameterization trick.

Generating Data from VAE

Use the decoder network with z sampled from prior $\mathcal{N}(0, I)$



[Kingma and Welling 14]

- Similar z implies similar output x
- It is interesting to see that in the left, $z_1 \approx$ head pose, and $z_2 \approx$ degree of smile

Pros and Cons of VAE

Pros:

- A principled approach to generative models
- Encoder $q_\theta(z \mid x)$, which can be useful for other tasks, e.g., semisupervised learning

Cons:

- A variational inference (approximating likelihood using ELBO)
- Blurry and low quality generations compared to state-of-the-art, e.g., GANs