Variational Auto encoder(VAE)

Auto-Encoding Variational Bayes

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Abstract

How can we perform efficient inference and learning in directed probabilistic models, in the presence of continuous latent variables with intractable posterior

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박진수

Structure of Generative model

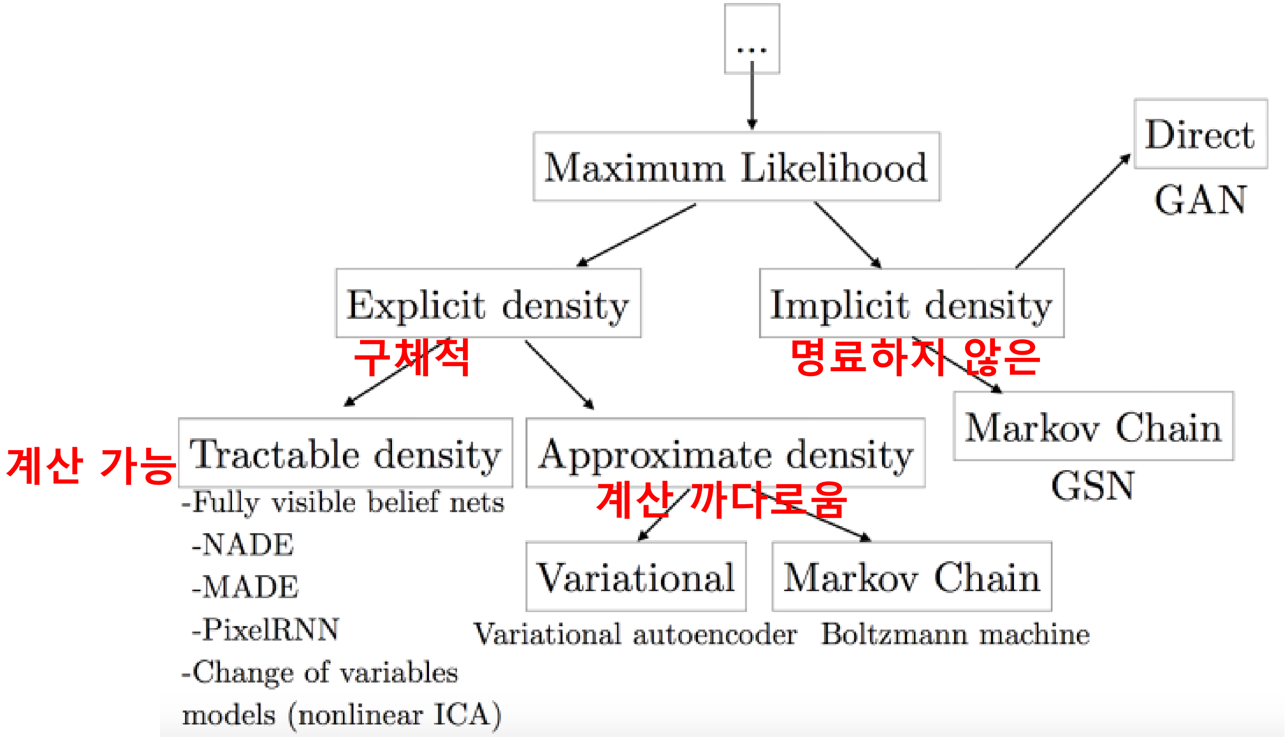
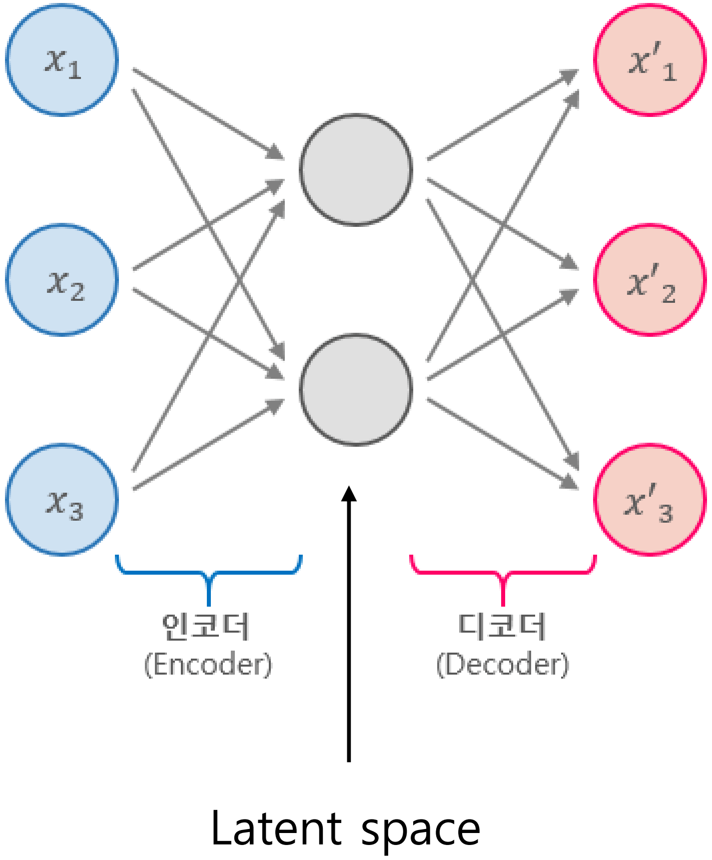


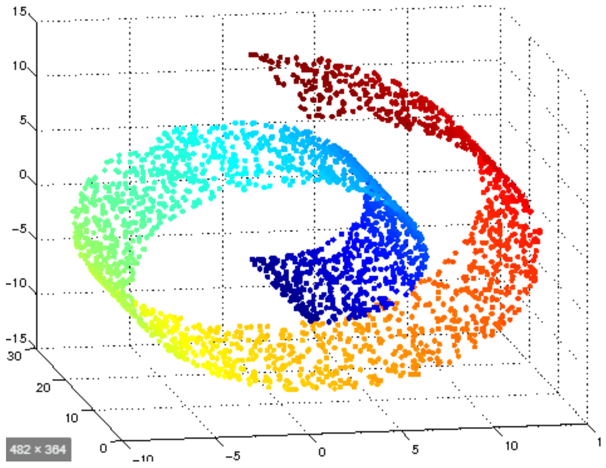
Figure is borrowed from Ian Goodfellow - NIPS 2016 Tutorial Generative Adversarial Networks

Auto encoder

Variational inference

Brief Intro. Autoencoder





1. Unsupervised learning -> like supervised learning
2. Manifold learning -> assume sub space
3. Dimensionality reduction -> important features
   (ex; PCA(linear activation))

Bayesian inference

<Bayes rule>

$$P(A|B) = \frac{P(B|A)P(A)}{P(B)}$$

Direct

- Calculate formula (using conjugate)

Indirect (Approximation)

- Sampling
- Variational inference

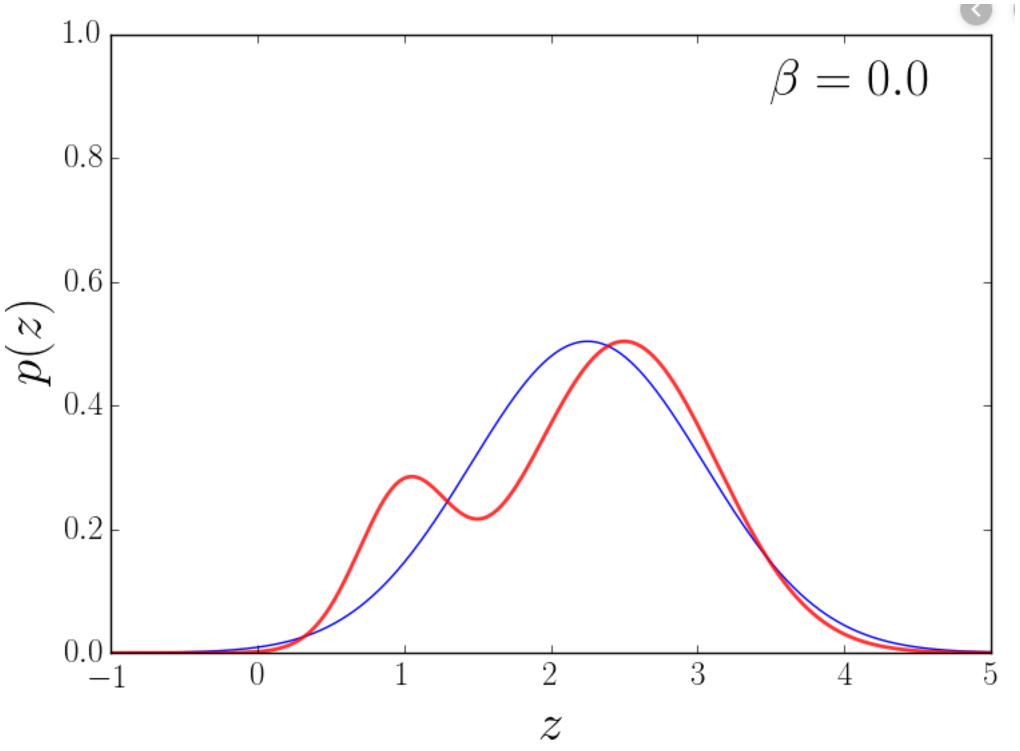
Variational Inference

$$P(\mathbf{Z} \mid \mathbf{X}) = \frac{P(\mathbf{X} \mid \mathbf{Z})P(\mathbf{Z})}{P(\mathbf{X})} = \frac{P(\mathbf{X} \mid \mathbf{Z})P(\mathbf{Z})}{\int_{\mathbf{Z}} P(\mathbf{X}, \mathbf{Z})\, d\mathbf{Z}}$$

$$P(\mathbf{Z} \mid \mathbf{X}) \approx Q(\mathbf{Z}).$$

$$D_{\mathrm{KL}}(Q \parallel P) \triangleq \sum_{\mathbf{Z}} Q(\mathbf{Z}) \log \frac{Q(\mathbf{Z})}{P(\mathbf{Z} \mid \mathbf{X})}.$$

- 단순 선형 방정식이라도 3개의 모수가 필요
; 기울기, 절편, 오차



Variational Auto Encoder

VAE = Generative model

- X가 생성될 수 있게 분포 p(X)에 대해서 학습한다면 어떨까?

Variational Auto Encoder

$\mathbf{x}$: data we want to model

$\mathbf{z}$: *latent variables*

$p(\mathbf{x})$: probability distribution of the data $\mathbf{x}$

$p(\mathbf{z})$: probability distribution of the latent variables $\mathbf{z}$

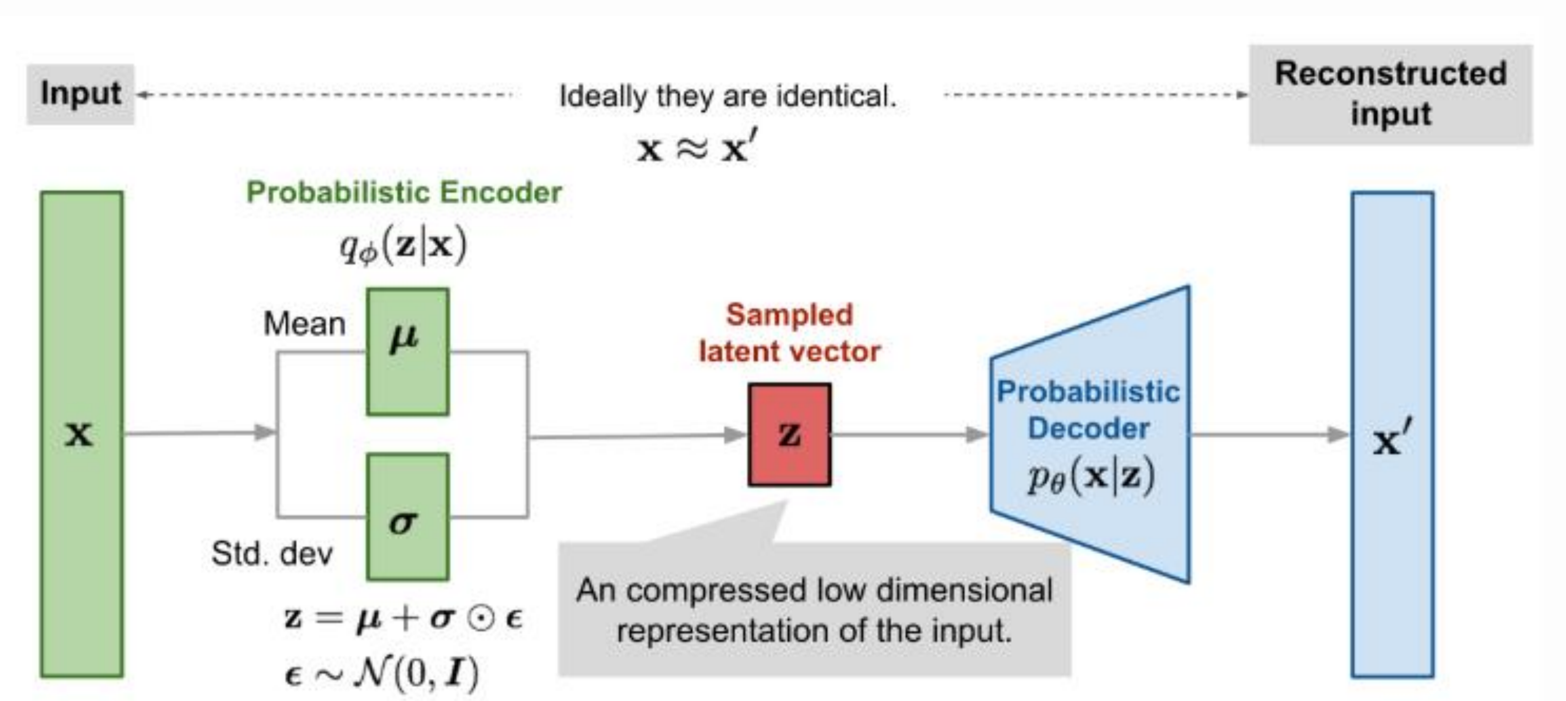
$p(\mathbf{x}|\mathbf{z})$: conditional probability distribution of the data given latent variables

$$p(\mathbf{x}) = \int p(\mathbf{x}, \mathbf{z}) \mathrm{d}\mathbf{z} = \int p(\mathbf{x}|\mathbf{z}) p(\mathbf{z}) \mathrm{d}\mathbf{z}$$

- 목표는 **P(X)**를 구하는 것이다.
- P(X)를 구하기 위해서는 모수Z를 구해야 한다.**(P(X|Z)**
  -> **P(Z)**도 알아야한다.
- P(Z)를 구하기 위해선 데이터에 대한 정보가 있어야 한다.**P(Z|X)**

P(X) -> P(Z|X) -> Z -> P(X|Z) -> P(X')

Variational Auto Encoder



P(X) P(Z|X) ≒ q(Z|X) Z P(X|Z) P(X)

우리가 prior로 선택할 p(z)는 최대한 직관적이고 간단한 것이 좋다.
-> 분석자의 통제력이 커진다.

Variational Auto Encoder

Data likelihood: $p_\theta(x) = \int p_\theta(z)p_\theta(x|z)dz$

Posterior density also intractable: $p_\theta(z|x) = p_\theta(x|z)p_\theta(z)/p_\theta(x)$

Solution: In addition to decoder network modeling $p_\theta(x|z)$, define additional encoder network $q_\phi(z|x)$ that approximates $p_\theta(z|x)$

Will see that this allows us to derive a lower bound on the data likelihood that is tractable, which we can optimize

Variational Auto Encoder

$$p(\mathbf{z}|\mathbf{x}) = \frac{p(\mathbf{x}|\mathbf{z})p(\mathbf{z})}{p(\mathbf{x})} \quad ≒ \quad q(z|x)$$

"복잡한 posterior를 q(z|x)로 근사"

Variational Auto Encoder

$$D_{KL}[q_\lambda(\mathbf{z}|\mathbf{x})||p(\mathbf{z}|\mathbf{x})] = \mathbb{E}_{q_\lambda}\left[\log \frac{q_\lambda(\mathbf{z}|\mathbf{x})}{p(\mathbf{z}|\mathbf{x})}\right] = \mathbb{E}_{q_\lambda}\left[\log q_\lambda(\mathbf{z}|\mathbf{x}) - \log p(\mathbf{z}|\mathbf{x})\right]$$

$$\begin{aligned} D_{KL}[q_\lambda(\mathbf{z}|\mathbf{x})||p(\mathbf{z}|\mathbf{x})] &= \mathbb{E}_{q_\lambda}\left[\log q_\lambda(\mathbf{z}|\mathbf{x}) - \log p(\mathbf{z}|\mathbf{x})\right] \\ &= \mathbb{E}_{q_\lambda}\left[\log q_\lambda(\mathbf{z}|\mathbf{x}) - \log \frac{p(\mathbf{x},\mathbf{z})}{p(\mathbf{x})}\right] \\ &= \mathbb{E}_{q_\lambda}\left[\log q_\lambda(\mathbf{z}|\mathbf{x}) - \log p(\mathbf{x},\mathbf{z}) + \log p(\mathbf{x})\right] \\ &= \mathbb{E}_{q_\lambda}\left[\log q_\lambda(\mathbf{z}|\mathbf{x}) - \log p(\mathbf{x},\mathbf{z})\right] + \log p(\mathbf{x}) \end{aligned}$$

"KL divergency가 최소화 되게 하는 q(z|x)를 선택해야 한다"

Variational Auto Encoder

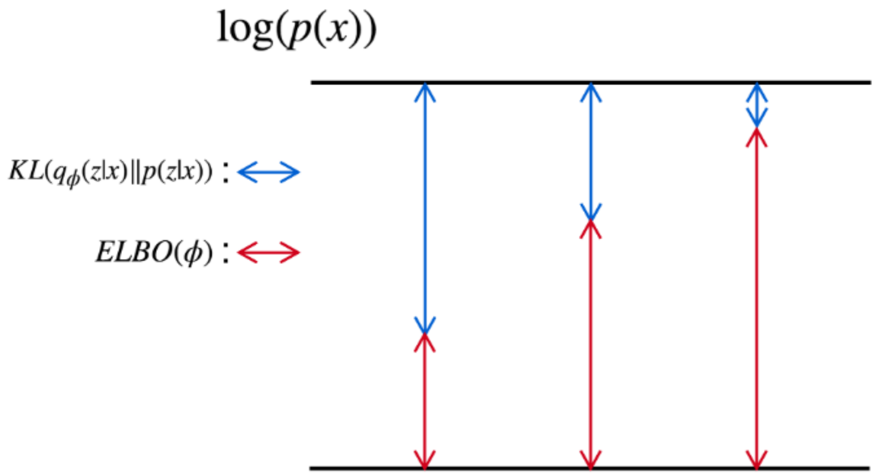
$$
\begin{aligned}
q_\lambda^*(\mathbf{z}|\mathbf{x}) &= \arg\min_\lambda D_{KL}(q_\lambda(\mathbf{z}|\mathbf{x})||p(\mathbf{z}|\mathbf{x})) \\
&= \arg\min_\lambda \mathbb{E}_q \left[\log q_\lambda(\mathbf{z}|\mathbf{x}) - \log p(\mathbf{x}, \mathbf{z})\right] + \log p(\mathbf{x})
\end{aligned}
$$

ELBO를 다음과 같이 가정하면,

$$
\mathrm{ELBO}(\lambda) = \mathbb{E}_{q_\lambda}\left[\log p(\mathbf{x}, \mathbf{z})\right] - \mathbb{E}_{q_\lambda}\left[\log q_\lambda(\mathbf{z}|\mathbf{x})\right]
$$

$$
\log p(\mathbf{x}) = \mathrm{ELBO}(\lambda) + D_{KL}(q_\lambda(\mathbf{z}|\mathbf{x})||p(\mathbf{z}|\mathbf{x}))
$$

Variational Auto Encoder



$$\log p(\mathbf{x}) = \mathrm{ELBO}(\lambda) + D_{KL}(q_\lambda(\mathbf{z}|\mathbf{x})||p(\mathbf{z}|\mathbf{x}))$$

$$\log p(\mathbf{x}) \geq \mathrm{ELBO}(\lambda) = \mathbb{E}_{q_\lambda}\left[\log p(\mathbf{x}, \mathbf{z})\right] - \mathbb{E}_{q_\lambda}\left[\log q_\lambda(\mathbf{z}|\mathbf{x})\right]$$

Always $D_{KL} \geq 0$

Minimizing KL divergence is equivalent maximizing ELBO

Variational Auto Encoder

$$
\begin{aligned}
\mathrm{ELBO}(\lambda) &= \mathbb{E}_{q_\lambda}\left[\log p(\mathbf{x},\mathbf{z})\right] - \mathbb{E}_{q_\lambda}\left[\log q_\lambda(\mathbf{z}|\mathbf{x})\right] \\
&= \mathbb{E}_{q_\lambda}\left[\log p(\mathbf{x},\mathbf{z}) - \log q_\lambda(\mathbf{z}|\mathbf{x})\right] \\
&= \mathbb{E}_{q_\lambda}\left[\log p(\mathbf{x}|\mathbf{z})p(\mathbf{z}) - \log q_\lambda(\mathbf{z}|\mathbf{x})\right] \\
&= \mathbb{E}_{q_\lambda}\left[\log p(\mathbf{x}|\mathbf{z}) + \log p(\mathbf{z}) - \log q_\lambda(\mathbf{z}|\mathbf{x})\right] \\
&= \mathbb{E}_{q_\lambda}\left[\log p(\mathbf{x}|\mathbf{z}) - (\log q_\lambda(\mathbf{z}|\mathbf{x}) - \log p(\mathbf{z}))\right] \\
&= \mathbb{E}_{q_\lambda}\left[\log p(\mathbf{x}|\mathbf{z})\right] - D_{KL}\left[q_\lambda(\mathbf{z}|\mathbf{x})||p(\mathbf{z})\right]
\end{aligned}
$$

Variational Auto Encoder

Loss : 1) Reconstruction loss + 2) regularization loss

```
generation_loss = mean(square(generated_image - real_image))
latent_loss = KL-Divergence(latent_variable, unit_gaussian)
loss = generation_loss + latent_loss
```

1) Reconstruction loss

$$\mathbb{E}_{q_\lambda(\mathbf{z}|\mathbf{x})}[\log p(\mathbf{x}|\mathbf{z})]$$

- Latent variable(z)가 주어졌을 때 디코더가 얼마나 효과적으로 데이터(x)를 잘 recon 하는지
- loss function L(x−x^) ; x(input), x^(recon)

2) Regularization loss

$$D_{KL}[q_\lambda(\mathbf{z}|\mathbf{x})||p(\mathbf{z})]$$

- 인코더에서 근사한 함수 q와 다루기 쉬운 함수로 우리가 선택한 p와의 거리
- 생성한 변수들을 잘 다루기 위해 P는 단순하면 좋다.

Variational Auto Encoder

***Reparameterization trick*

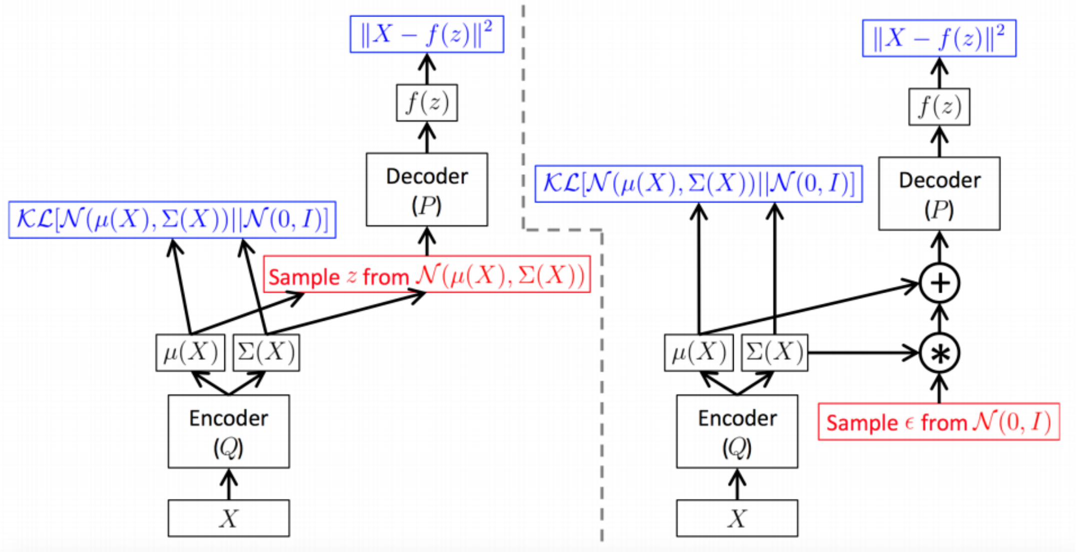
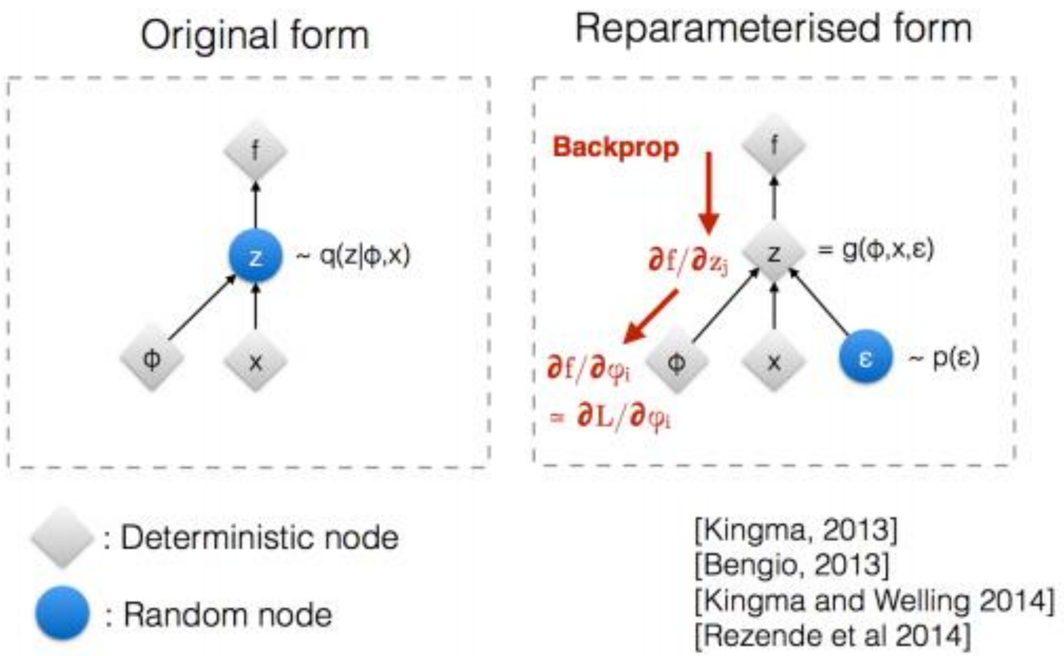


Figure is borrowed from Carl Doersch. Tutorial on Variational Autoencoders

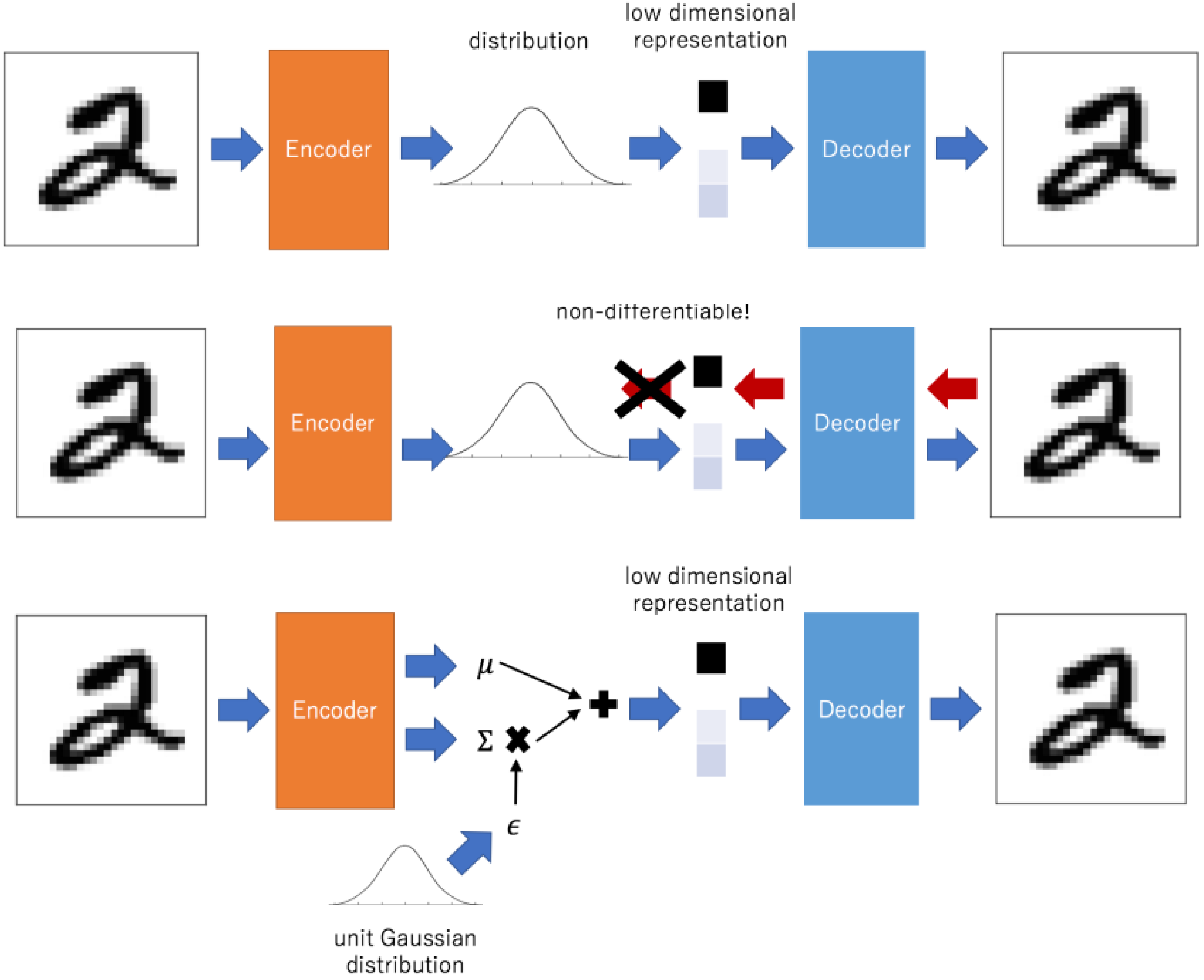


- Left: sampling operations ($\mathbf{z}$ from $\mathcal{N}(\mu(\mathbf{x}), \Sigma(\mathbf{x}))$) are *non-differentiable*
- Right: reparameterization trick allows us to be able to do BP operations

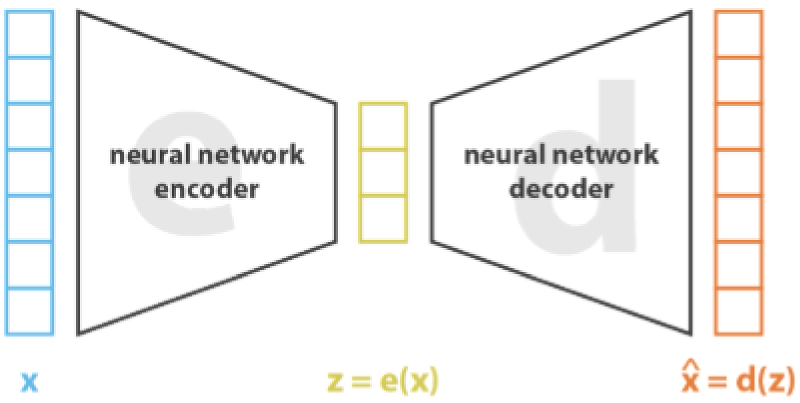
$$z = \mu(\mathbf{x}) + \Sigma^{1/2}(\mathbf{x})\ \varepsilon$$

- $\varepsilon \sim \mathcal{N}(\mathbf{0}, \mathbf{1})$

Variational Auto Encoder

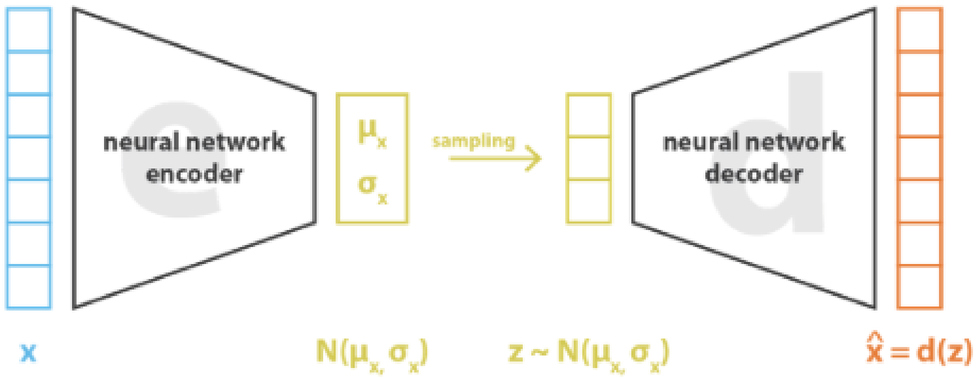


Summary



$$\text{loss} = \| x - \hat{x} \|^2 = \| x - d(z) \|^2 = \| x - d(e(x)) \|^2$$

Auto encoder



$$\text{loss} = \| x - \hat{x} \|^2 + KL[\, N(\mu_x, \sigma_x), N(0, I) \,] = \| x - d(z) \|^2 + KL[\, N(\mu_x, \sigma_x), N(0, I) \,]$$

Variational Auto encoder

reference

https://www.youtube.com/watch?v=KYA-GEhObIs
https://www.youtube.com/watch?v=o_peo6U7IRM
https://lilianweng.github.io/lil-log/2018/08/12/from-autoencoder-to-beta-vae.html#autoencoder

$$\int q(z|x) = 1$$

$$p(x) = \frac{p(z,x)}{p(z|x)}$$

$$E[x] = \int x * f(x)$$

$$D_{KL}(p||q) = \int p(x) * \log(\frac{p(x)}{q(x)}$$

$$
\begin{aligned}
\log p_\theta(x^{(i)}) &= \mathbf{E}_{z\sim q_\phi(z|x^{(i)})}\left[\log p_\theta(x^{(i)})\right] \quad (p_\theta(x^{(i)}) \text{ Does not depend on } z) \\
&= \mathbf{E}_z\left[\log \frac{p_\theta(x^{(i)} \mid z)p_\theta(z)}{p_\theta(z \mid x^{(i)})}\right] \quad (\text{Bayes' Rule}) \\
&= \mathbf{E}_z\left[\log \frac{p_\theta(x^{(i)} \mid z)p_\theta(z)}{p_\theta(z \mid x^{(i)})} \frac{q_\phi(z \mid x^{(i)})}{q_\phi(z \mid x^{(i)})}\right] \quad (\text{Multiply by constant}) \\
&= \mathbf{E}_z\left[\log p_\theta(x^{(i)} \mid z)\right] - \mathbf{E}_z\left[\log \frac{q_\phi(z \mid x^{(i)})}{p_\theta(z)}\right] + \mathbf{E}_z\left[\log \frac{q_\phi(z \mid x^{(i)})}{p_\theta(z \mid x^{(i)})}\right] \quad (\text{Logarithms}) \\
&= \boxed{\underbrace{\mathbf{E}_z\left[\log p_\theta(x^{(i)} \mid z)\right] - D_{KL}(q_\phi(z \mid x^{(i)}) \,||\, p_\theta(z))}_{\mathcal{L}(x^{(i)},\theta,\phi)}} + \underbrace{D_{KL}(q_\phi(z \mid x^{(i)}) \,||\, p_\theta(z \mid x^{(i)}))}_{\boxed{\geq 0}}
\end{aligned}
$$

Tractable lower bound which we can take gradient of and optimize! ($p_\theta(x|z)$ differentiable, KL term differentiable)