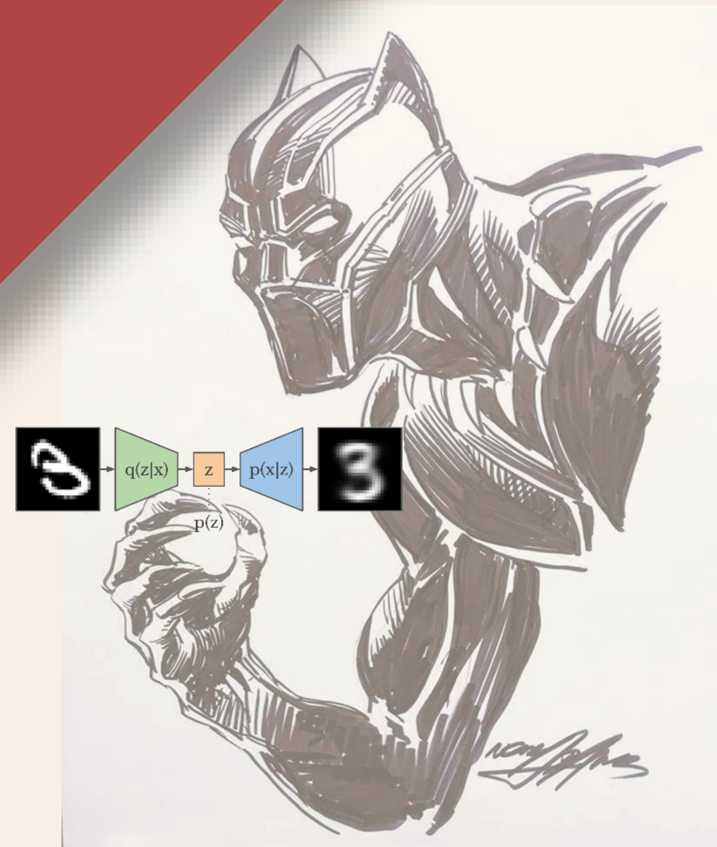
고려대학교
빅데이터 연구회

KU-BIG

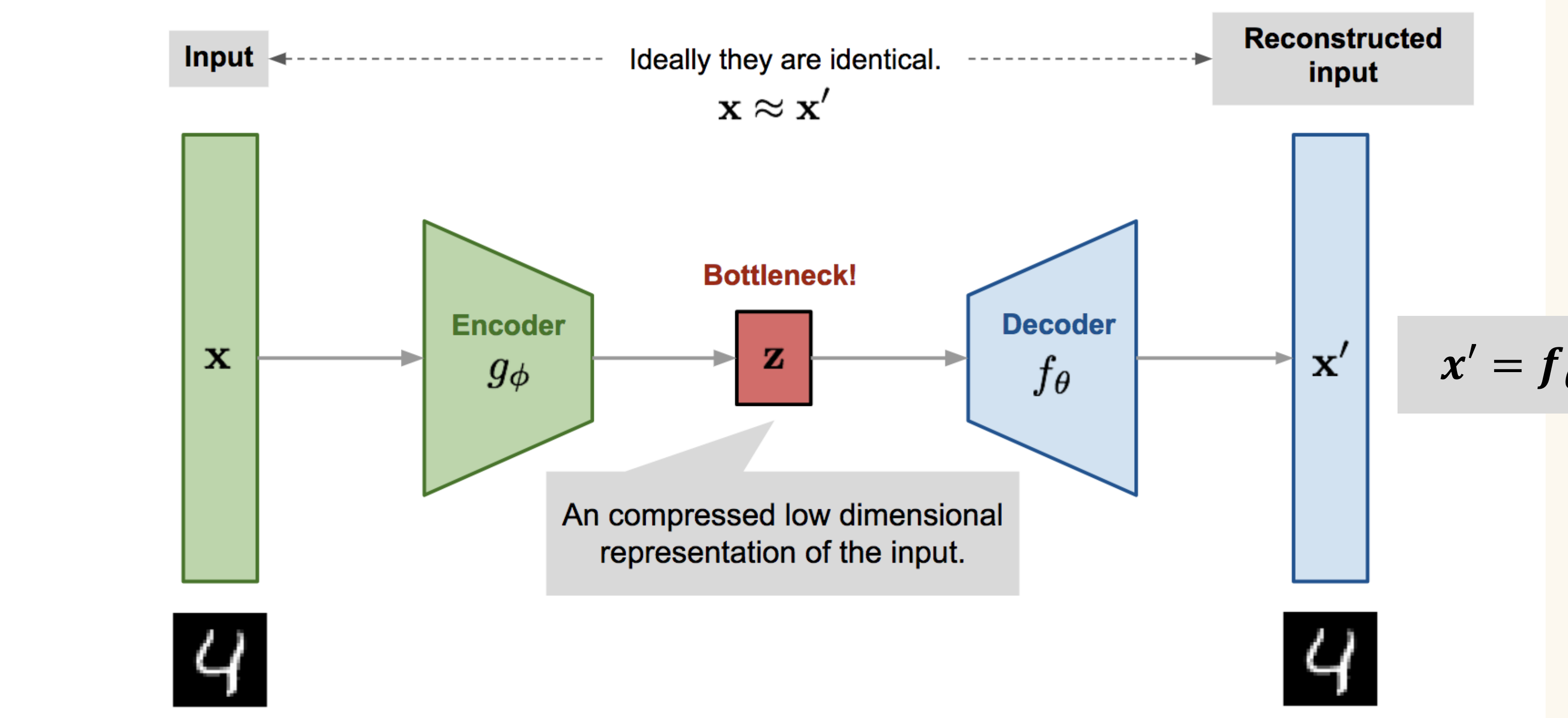
Credit Card Fraud Detection
- VAE algorithm

EBB



목 차

Autoencoder?

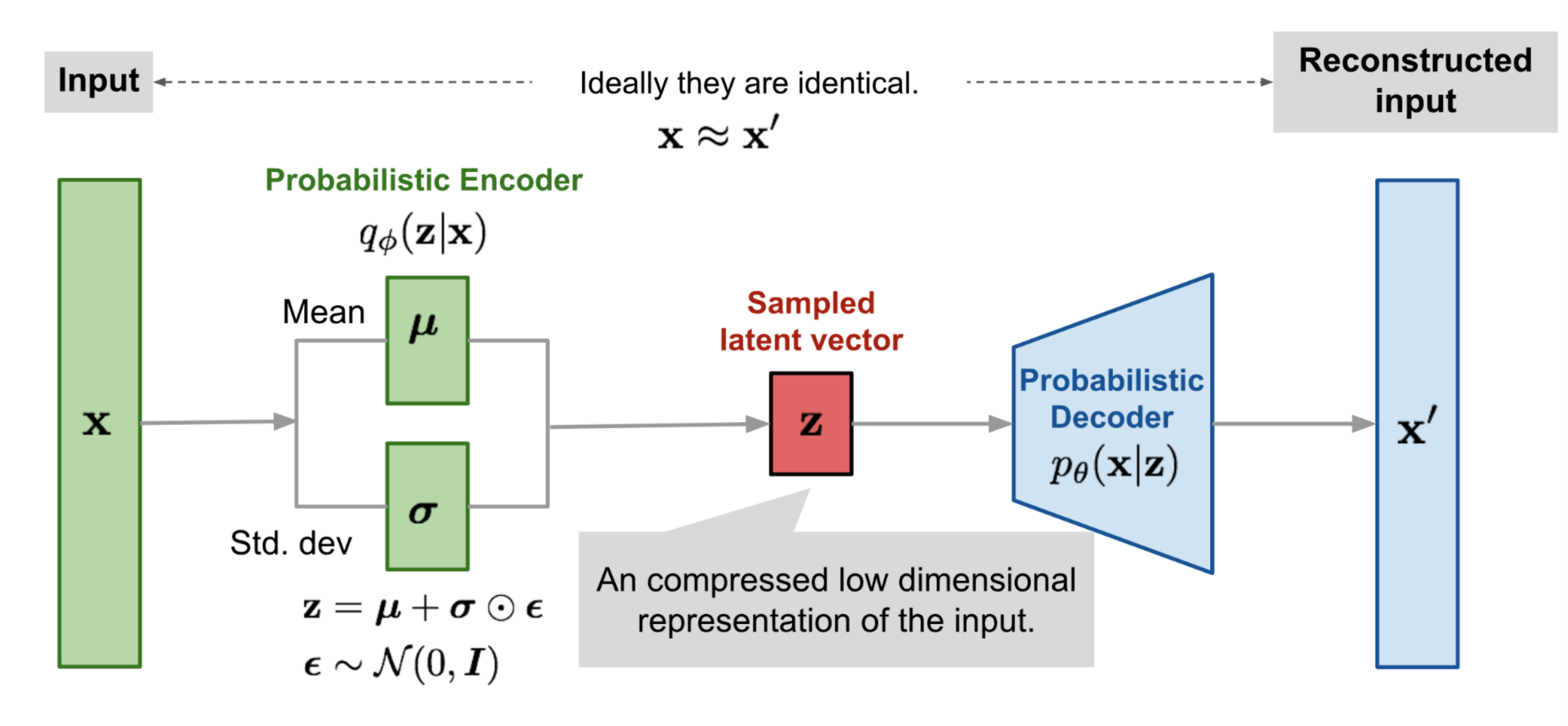


$$x' = f_\theta(g_\phi(x))$$

https://lilianweng.github.io/lil-log/2018/08/12/from-autoencoder-to-beta-vae.html

MSE loss function : $L_{AE}(\phi, \theta) = \frac{1}{n}\sum_{i=1}^{n} (x^{(i)} - f_\theta\left(g_\phi(x^{(i)})\right))^2$

Variational Autoencoder (VAE)?



⟨Decoder⟩

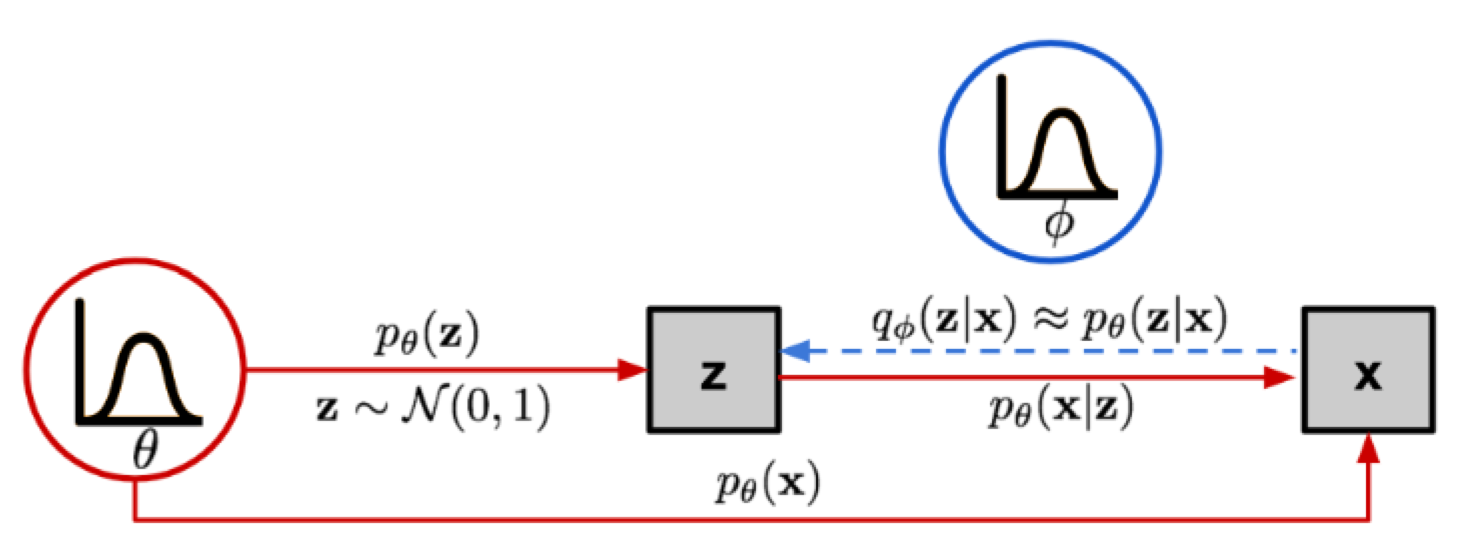
θ^* : true parameter

1. $p_{\theta^*}(\mathbf{z})$에서 $\mathbf{z}^{(i)}$ 추출.
2. $p_{\theta^*}(\mathbf{x}|\mathbf{z}^{(i)})$에서 $\mathbf{x}^{(i)}$생성

Optimal parameter : $\theta^* = \arg\max_\theta \sum_{i=1}^{n} \log \boxed{p_\theta(\mathbf{x}^{(i)})}$ → Intractable !!

https://lilianweng.github.io/lil-log/2018/08/12/from-autoencoder-to-beta-vae.html

Variational Autoencoder (VAE)?



z : latent variable

$p_\theta(\mathbf{z})$: prior

$p_\theta(\mathbf{x}|\mathbf{z})$: Likelihood

$p_\theta(\mathbf{z}|\mathbf{x})$: posterior

알려져 있는 분포 활용

$p_\theta(\mathbf{z})$를 추론하고자 $p_\theta(\mathbf{z}|\mathbf{x})$를 이용하고, $p_\theta(\mathbf{z}|\mathbf{x})$를 추론하고자 $q_\phi(\mathbf{z}|\mathbf{x})$를 활용한다.

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Variational Autoencoder (VAE)?

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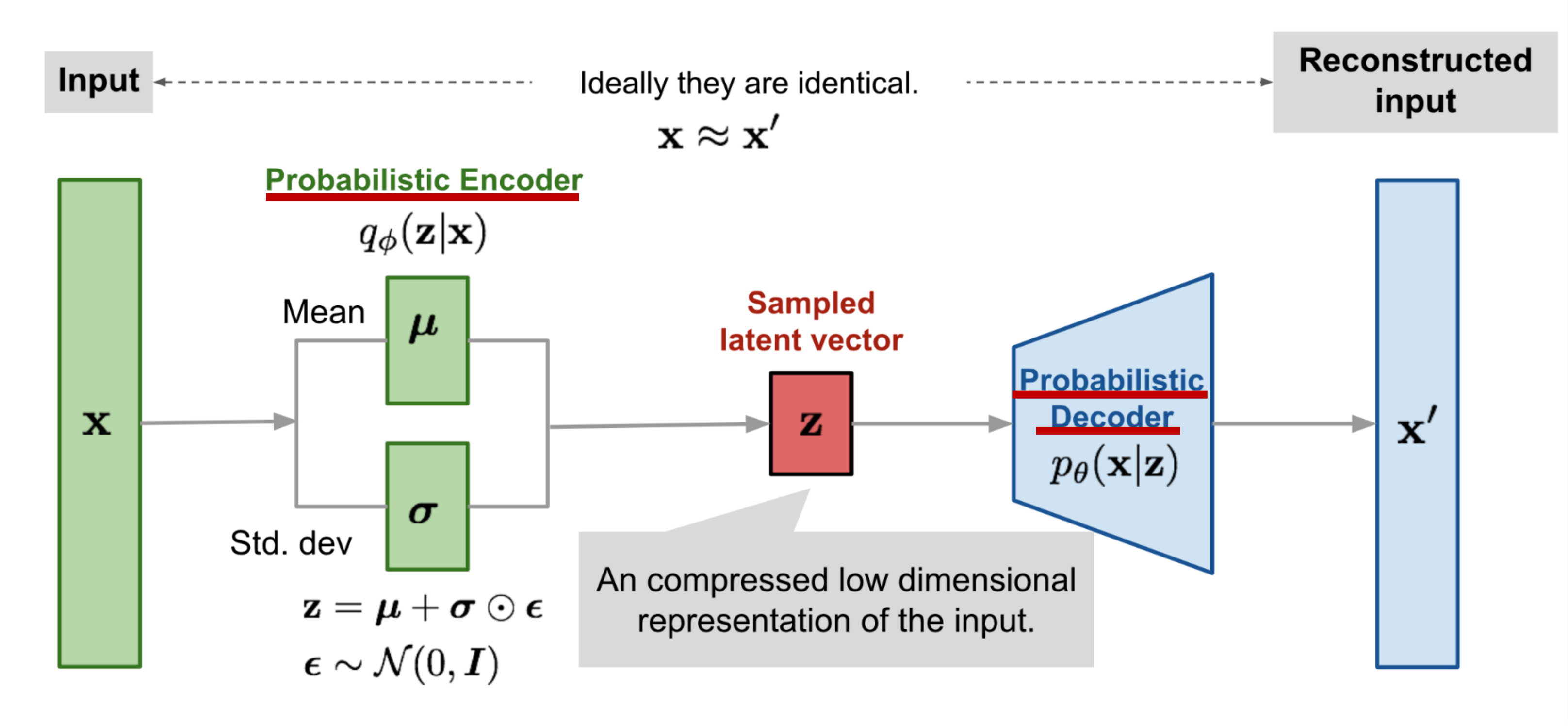
Variational Inference

1. $p_\theta(\mathbf{x})$를 계산하기 힘든 경우
2. $p_\theta(\mathbf{z})$, $p_\theta(\mathbf{x}|\mathbf{z})$ 를 더 복잡하게 모델링하고 싶은 경우

https://ratsgo.github.io/generative%20model/2017/12/19/vi/

Variational Autoencoder (VAE)?



Loss function :

$$
\begin{aligned}
L_{\mathrm{VAE}}(\theta, \phi) &= -\log p_\theta(\mathbf{x}) + D_{\mathrm{KL}}(q_\phi(\mathbf{z}|\mathbf{x}) \| p_\theta(\mathbf{z}|\mathbf{x})) \\
&= -\mathbb{E}_{\mathbf{z}\sim q_\phi(\mathbf{z}|\mathbf{x})} p_\theta(\mathbf{x}|\mathbf{z}) + D_{\mathrm{KL}}(q_\phi(\mathbf{z}|\mathbf{x}) \| p_\theta(\mathbf{z})) \\
\theta^*, \phi^* &= \arg\min_{\theta,\phi} L_{\mathrm{VAE}}
\end{aligned}
$$

https://lilianweng.github.io/lil-log/2018/08/12/from-autoencoder-to-beta-vae.html

$L_{VAE}(\theta,\phi)$ 뜯어보기.

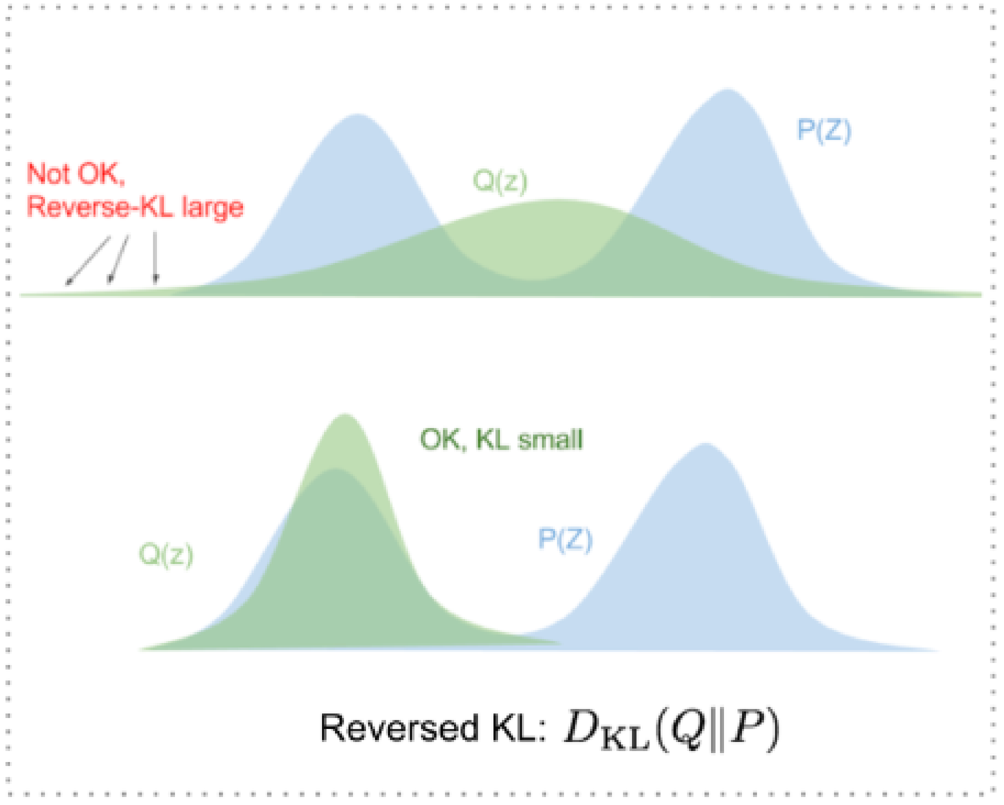
$$L_{\mathrm{VAE}}(\theta,\phi) = -\log p_\theta(\mathbf{x}) + D_{\mathrm{KL}}(q_\phi(\mathbf{z}|\mathbf{x})\|p_\theta(\mathbf{z}|\mathbf{x}))$$
$$= -\mathbb{E}_{\mathbf{z}\sim q_\phi(\mathbf{z}|\mathbf{x})} p_\theta(\mathbf{x}|\mathbf{z}) + D_{\mathrm{KL}}(q_\phi(\mathbf{z}|\mathbf{x})\|p_\theta(\mathbf{z}))$$
$$\theta^*, \phi^* = \arg\min_{\theta,\phi} L_{\mathrm{VAE}}$$

$q_\phi(\mathbf{z}|\mathbf{x})$는 $p_\theta(\mathbf{z}|\mathbf{x})$에 최대한 비슷해야 한다.

→ KL-Divergence

$$D_{\mathrm{KL}}(Q\|P) = \mathbb{E}_{z\sim Q(z)} \log \frac{Q(z)}{P(z)} \geq 0$$

→ Minimize $D_{\mathrm{KL}}(Q||P)$



https://lilianweng.github.io/lil-log/2018/08/12/from-autoencoder-to-beta-vae.html

$$D_{\mathrm{KL}}(Q\|P) = \mathbb{E}_{z\sim Q(z)} \log \frac{Q(z)}{P(z)}$$

$$
\begin{aligned}
& D_{\mathrm{KL}}(q_\phi(\mathbf{z}|\mathbf{x})\|p_\theta(\mathbf{z}|\mathbf{x})) \\
&= \int q_\phi(\mathbf{z}|\mathbf{x}) \log \frac{q_\phi(\mathbf{z}|\mathbf{x})}{p_\theta(\mathbf{z}|\mathbf{x})} d\mathbf{z} \\
&= \int q_\phi(\mathbf{z}|\mathbf{x}) \log \frac{q_\phi(\mathbf{z}|\mathbf{x}) p_\theta(\mathbf{x})}{p_\theta(\mathbf{z},\mathbf{x})} d\mathbf{z} && \text{; Because } p(z|x)=p(z,x)/p(x) \\
&= \int q_\phi(\mathbf{z}|\mathbf{x}) \big(\log p_\theta(\mathbf{x}) + \log \frac{q_\phi(\mathbf{z}|\mathbf{x})}{p_\theta(\mathbf{z},\mathbf{x})} \big) d\mathbf{z} \\
&= \log p_\theta(\mathbf{x}) + \int q_\phi(\mathbf{z}|\mathbf{x}) \log \frac{q_\phi(\mathbf{z}|\mathbf{x})}{p_\theta(\mathbf{z},\mathbf{x})} d\mathbf{z} && \text{; Because } \textstyle\int q(z|x)dz=1 \\
&= \log p_\theta(\mathbf{x}) + \int q_\phi(\mathbf{z}|\mathbf{x}) \underbrace{\boxed{\log \frac{q_\phi(\mathbf{z}|\mathbf{x})}{p_\theta(\mathbf{x}|\mathbf{z}) p_\theta(\mathbf{z})}}}_{g(\mathbf{z})} d\mathbf{z} && \text{; Because } p(z,x)=p(x|z)p(z) \\
&= \underbrace{\log p_\theta(\mathbf{x}) + \mathbb{E}_{\mathbf{z}\sim q_\phi(\mathbf{z}|\mathbf{x})} [\log \frac{q_\phi(\mathbf{z}|\mathbf{x})}{p_\theta(\mathbf{z})} - \log p_\theta(\mathbf{x}|\mathbf{z})]}_{\mathbb{E}_{z\sim q_\phi(\mathbf{z}|\mathbf{x})}[g(\mathbf{z})]} \\
&= \log p_\theta(\mathbf{x}) + D_{\mathrm{KL}}(q_\phi(\mathbf{z}|\mathbf{x})\|p_\theta(\mathbf{z})) - \mathbb{E}_{\mathbf{z}\sim q_\phi(\mathbf{z}|\mathbf{x})} \log p_\theta(\mathbf{x}|\mathbf{z})
\end{aligned}
$$

https://lilianweng.github.io/lil-log/2018/08/12/from-autoencoder-to-beta-vae.html

$$D_{\mathrm{KL}}(q_\phi(\mathbf{z}|\mathbf{x})\|p_\theta(\mathbf{z}|\mathbf{x})) = \log p_\theta(\mathbf{x}) + D_{\mathrm{KL}}(q_\phi(\mathbf{z}|\mathbf{x})\|p_\theta(\mathbf{z})) - \mathbb{E}_{\mathbf{z}\sim q_\phi(\mathbf{z}|\mathbf{x})}\log p_\theta(\mathbf{x}|\mathbf{z})$$

$$\log p_\theta(\mathbf{x}) - \underbrace{D_{\mathrm{KL}}(q_\phi(\mathbf{z}|\mathbf{x})\|p_\theta(\mathbf{z}|\mathbf{x}))}_{\geq 0} = \mathbb{E}_{\mathbf{z}\sim q_\phi(\mathbf{z}|\mathbf{x})}\log p_\theta(\mathbf{x}|\mathbf{z}) - D_{\mathrm{KL}}(q_\phi(\mathbf{z}|\mathbf{x})\|p_\theta(\mathbf{z}))$$

$$\log p_\theta(\mathbf{x}) \geq \underbrace{\mathbb{E}_{\mathbf{z}\sim q_\phi(\mathbf{z}|\mathbf{x})}\log p_\theta(\mathbf{x}|\mathbf{z}) - D_{\mathrm{KL}}(q_\phi(\mathbf{z}|\mathbf{x})\|p_\theta(\mathbf{z})) = -L_{\mathrm{VAE}}}$$

Lower bound of $\log p_\theta(\mathbf{x})$ → Maximize

$$L_{\mathrm{VAE}}(\theta,\phi) = -\log p_\theta(\mathbf{x}) + D_{\mathrm{KL}}(q_\phi(\mathbf{z}|\mathbf{x})\|p_\theta(\mathbf{z}|\mathbf{x}))$$
$$= -\mathbb{E}_{\mathbf{z}\sim q_\phi(\mathbf{z}|\mathbf{x})}p_\theta(\mathbf{x}|\mathbf{z}) + D_{\mathrm{KL}}(q_\phi(\mathbf{z}|\mathbf{x})\|p_\theta(\mathbf{z}))$$
$$\theta^*,\phi^* = \arg\min_{\theta,\phi} L_{\mathrm{VAE}}$$

→ Reconstruction probability

Minimize Loss -> Maximize real data sample을 생성하는 확률의 lower bound

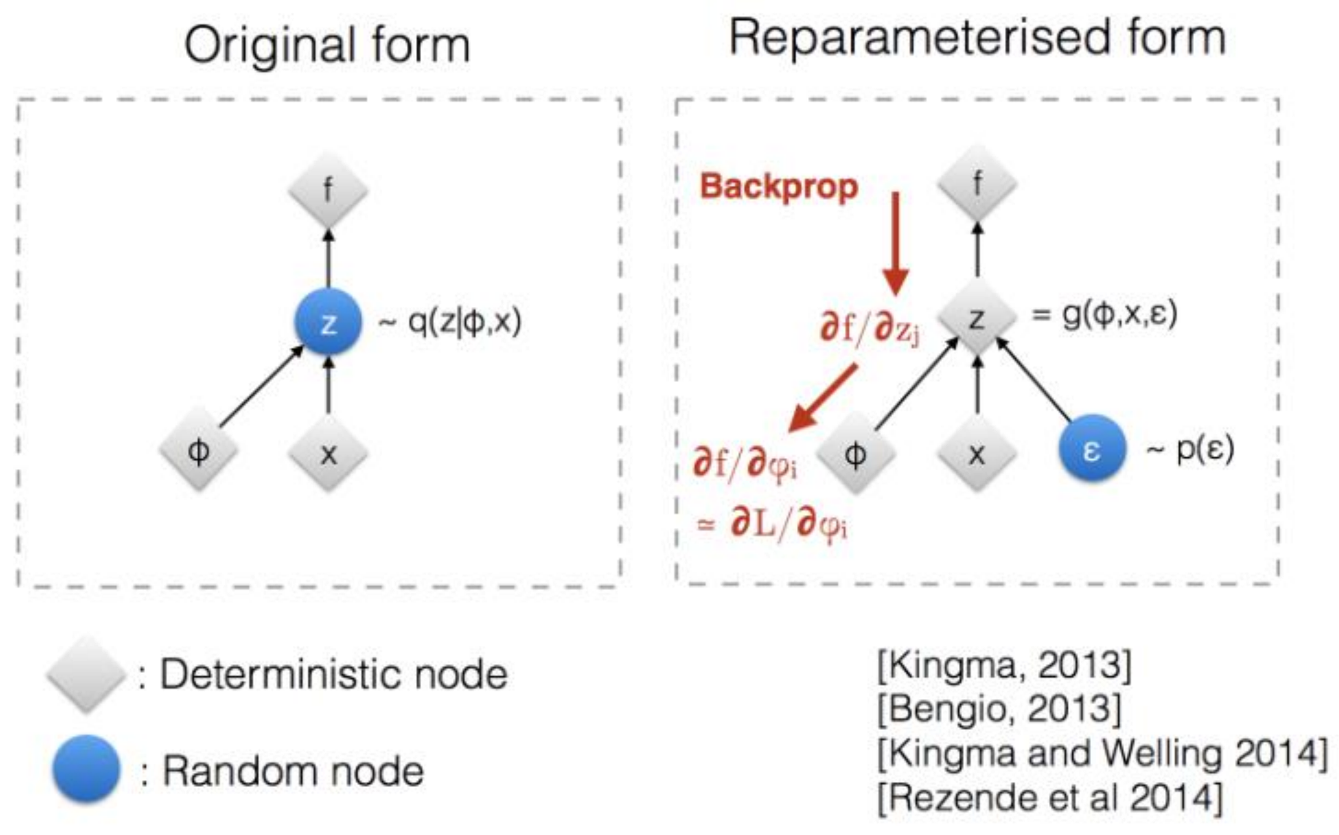
https://lilianweng.github.io/lil-log/2018/08/12/from-autoencoder-to-beta-vae.html

Reparameterization trick

$$\mathbf{z} \sim q_\phi(\mathbf{z}|\mathbf{x}^{(i)}) = \mathcal{N}(\mathbf{z}; \boldsymbol{\mu}^{(i)}, \boldsymbol{\sigma}^{2(i)}\boldsymbol{I})$$
$$\mathbf{z} = \boldsymbol{\mu} + \boldsymbol{\sigma} \odot \boldsymbol{\epsilon}, \text{ where } \boldsymbol{\epsilon} \sim \mathcal{N}(0, \boldsymbol{I})$$

$\odot$ refers to element-wise product.

Stochastic process(확률과정)라
Backprop이 불가능한 z를
미분 가능하게 만들어서 (수식화하여)
Backprop을 가능하게 만든다!!!!!!!!!!!!!!!



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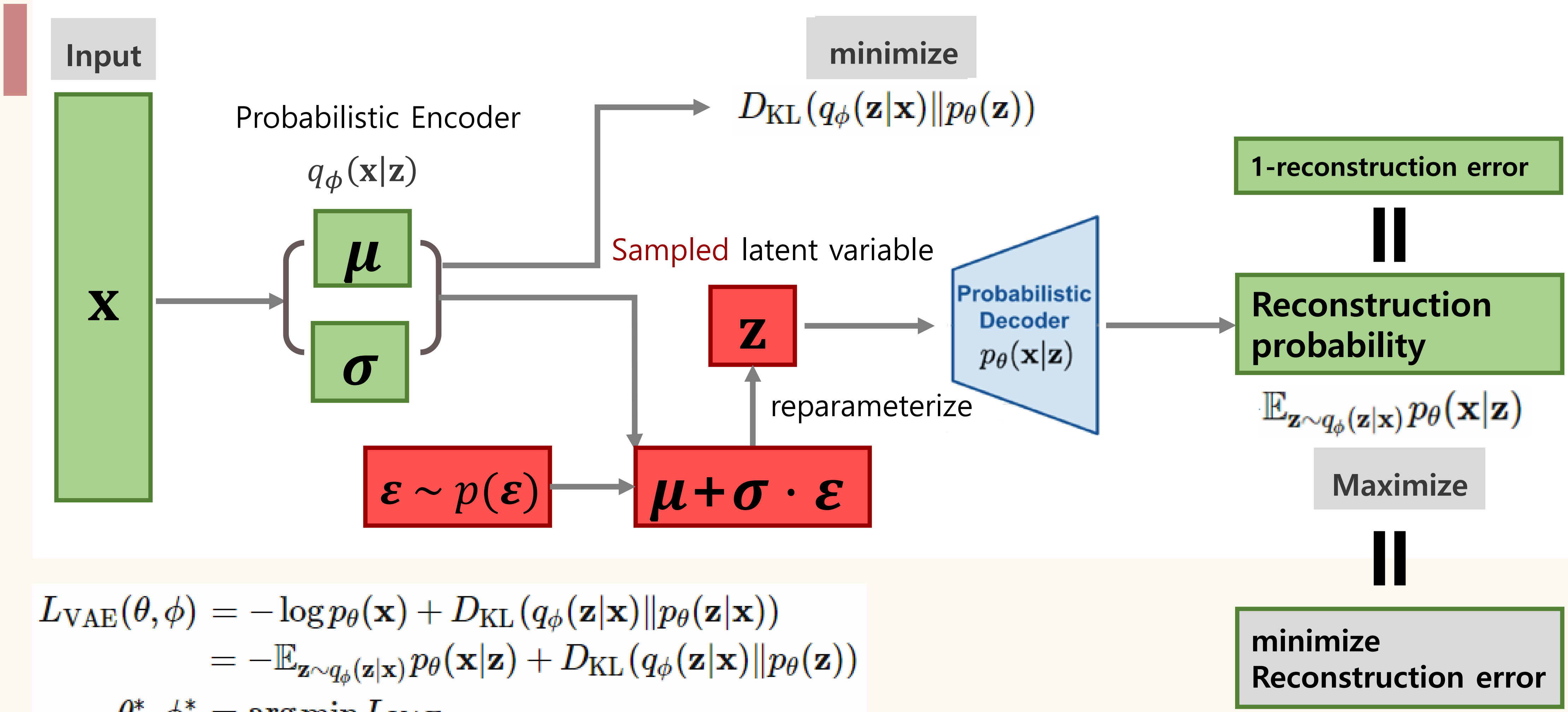

$$
\begin{aligned}
L_{\mathrm{VAE}}(\theta,\phi) &= -\log p_\theta(\mathbf{x}) + D_{\mathrm{KL}}(q_\phi(\mathbf{z}|\mathbf{x})\|p_\theta(\mathbf{z}|\mathbf{x})) \\
&= -\mathbb{E}_{\mathbf{z}\sim q_\phi(\mathbf{z}|\mathbf{x})}p_\theta(\mathbf{x}|\mathbf{z}) + D_{\mathrm{KL}}(q_\phi(\mathbf{z}|\mathbf{x})\|p_\theta(\mathbf{z})) \\
\theta^*,\phi^* &= \arg\min_{\theta,\phi} L_{\mathrm{VAE}}
\end{aligned}
$$

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Algorithm 3 Variational autoencoder training algorithm

INPUT: Dataset $x^{(1)}, \cdots, x^{(N)}$

OUTPUT: probabilistic encoder f_ϕ, probabilistic decoder g_θ

$\phi, \theta \leftarrow$ Initialize parameters

repeat

for i=1 **to** N **do**

Draw L samples from $\epsilon \sim \mathcal{N}(0,1)$

$z^{(i,l)} = h_\phi(\epsilon^{(i)}, x^{(i)}) \quad i = 1, \cdots, N$ ← Reparameterization trick

end for

$E = \sum_{i=1}^{N} -D_{KL}(q_\phi(z|x^{(i)})||p_\theta(z)) + \frac{1}{L}\sum_{l=1}^{L}(\log p_\theta(x^{(i)}|z^{(i,l)}))$ ← loss

$\phi, \theta \leftarrow$ Update parameters using gradients of E (e.g. Stochastic Gradient Descent)

until convergence of parameters ϕ, θ

Jinwon An, Sungzoon Cho, (2015). Variational Autoencoder based Anomaly Detection using Reconstruction Probability

Algorithm 4 Variational autoencoder based anomaly detection algorithm

INPUT: Normal dataset X, Anomalous dataset $x^{(i)}$ $i = 1, \cdots, N$, threshold α

OUTPUT: reconstruction probability $p_\theta(x|\hat{x})$

$\phi, \theta \leftarrow$ train a variational autoencoder using the normal dataset X

for i=1 **to** N **do**

$\boldsymbol{\mu}_{z^{(i)}}, \boldsymbol{\sigma}_{z^{(i)}} = f_\theta(z|x^{(i)})$

draw L samples from $z \sim \mathcal{N}(\boldsymbol{\mu}_{z^{(i)}}, \boldsymbol{\sigma}_{z^{(i)}})$

for l=1 **to** L **do**

$\boldsymbol{\mu}_{\hat{x}^{(i,l)}}, \boldsymbol{\sigma}_{\hat{x}^{(i,l)}} = g_\phi(x|z^{(i,l)})$

end for

$\textit{reconstruction probability}(i) = \frac{1}{L}\sum_{l=1}^{L} p_\theta(x^{(i)}|\boldsymbol{\mu}_{\hat{x}^{(i,l)}}, \boldsymbol{\sigma}_{\hat{x}^{(i,l)}})$

if $\textit{reconstruction probability}(i) < \alpha$ **then**

$x^{(i)}$ is an anomaly

else

$x^{(i)}$ is not an anomaly

end if

end for

Encoder로부터 z분포에 대한
parameter 추출

Decoder로부터 $\hat{\mathbf{x}}$분포에 대한
(reconstruction) parameter 추출

reconstruction parameter가 주어졌을 때,
original input x가 생성될 확률의 평균
Reconstruction error = 1- reconstruction probability

Jinwon An, Sungzoon Cho, (2015). Variational Autoencoder based Anomaly Detection using Reconstruction Probability

```python
class VAE(nn.Module):
    def __init__(self, image_size = 784, h_dim = 400, z_dim = 20):
        super(VAE, self).__init__()
        self.fc1 = nn.Linear(image_size, h_dim)
        self.fc2 = nn.Linear(h_dim, z_dim)
        self.fc3 = nn.Linear(h_dim, z_dim)
        self.fc4 = nn.Linear(z_dim, h_dim)
        self.fc5 = nn.Linear(h_dim, image_size)

    def encode(self, x):
        h = F.relu(self.fc1(x))
        return self.fc2(h), self.fc3(h)
    def reparameterize(self, mu, log_var):
        std = torch.exp(log_var/2)
        eps = torch.randn_like(std)
        return mu+eps*std
    def decode(self, z):
        h = F.relu(self.fc4(z))
        return self.fc5(h)

    def forward(self, x):
        mu, log_var = self.encode(x)
        z = self.reparameterize(mu, log_var)
        x_reconst = self.decode(z)
        return x_reconst, mu, log_var

model = VAE().to(device)
optimizer = torch.optim.Adam(model.parameters(), lr = learning_rate)
```

Encoder

Decoder

z_dim : parameter쌍의 개수

fc2, fc3는 mu와 sigma를 도출함.

fc2, fc3 중에 어느 것이 mu인지, sigma인지는 알 수 없음.

빛희정 님의 은혜로운 코드. https://github.com/KU-BIG/novelty-detection/blob/master/novelty_detection_pytorch.ipynb


Q&A
Time!
Thank you
for your attention.