고려대학교 빅데이터 연구회

KU-BIG

Credit Card Fraud Detection

- VAE algorithm

**EBB** 

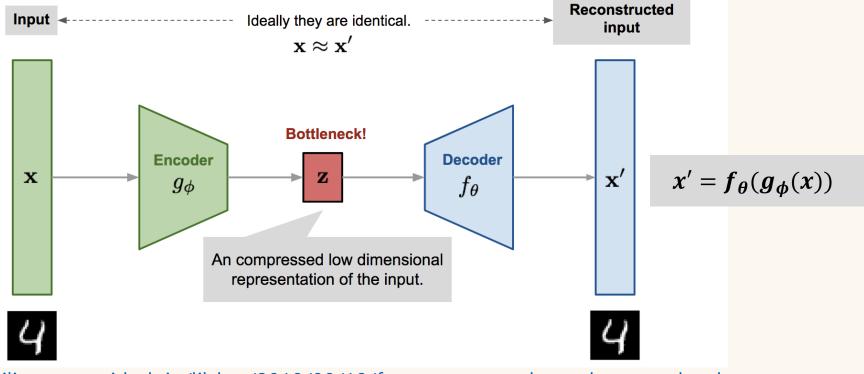


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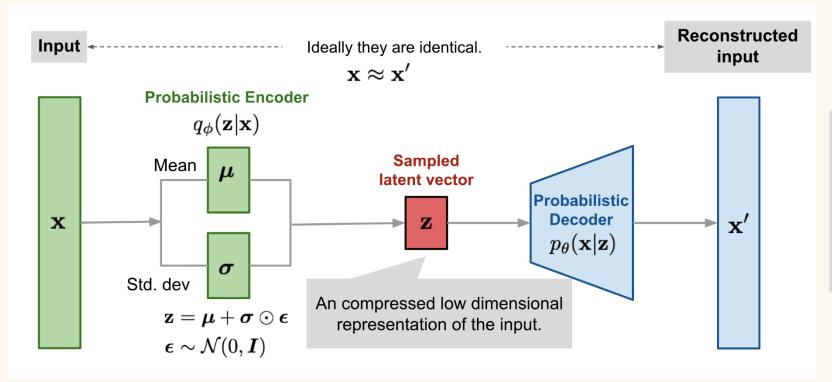
IV

#### Autoencoder?



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

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



#### (Decoder)

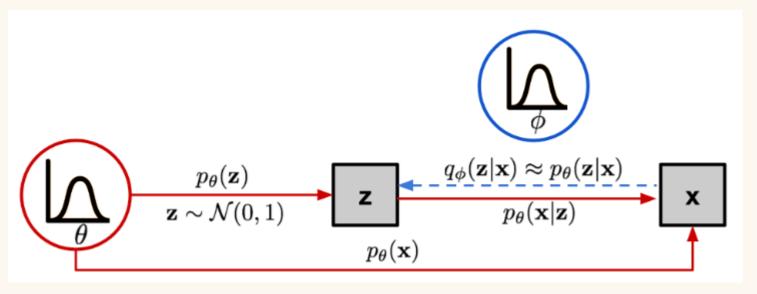
 $\theta^*$  : true parameter

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



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

## Variational Autoencoder (VAE)?



z: latent variable

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

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

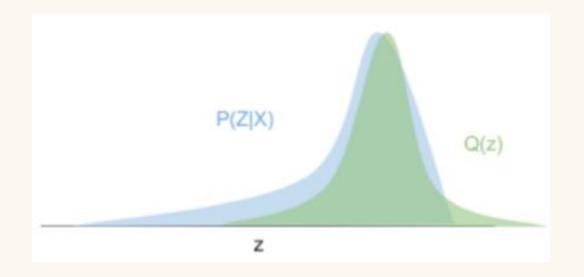
 $p_{\theta}(\mathbf{z}|\mathbf{x})$ : posterior

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

## Variational Autoencoder (VAE)?

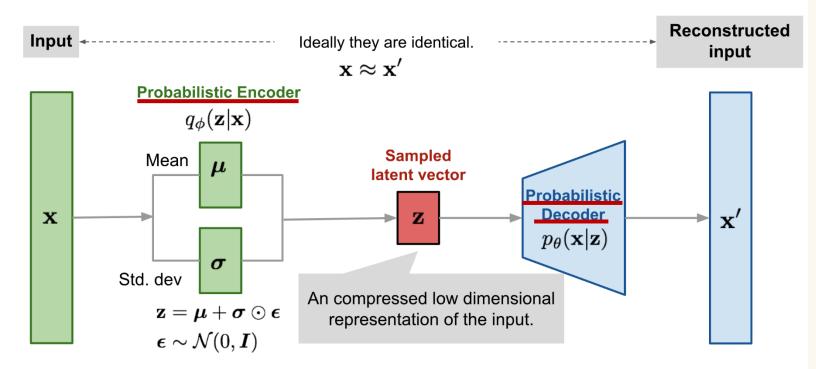
 $p_{\theta}(\mathbf{z})$ 를 추론하고자  $p_{\theta}(\mathbf{z}|\mathbf{x})$ 를 이용하고,  $p_{\theta}(\mathbf{z}|\mathbf{x})$ 를 추론하고자  $q_{\phi}(\mathbf{x}|\mathbf{z})$ 를 활용한다.

#### Variational Inference



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

### Variational Autoencoder (VAE)?



#### Loss function:

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

$$L_{\text{VAE}}(\theta, \phi) = -\log p_{\theta}(\mathbf{x}) + \underline{D_{\text{KL}}(q_{\phi}(\mathbf{z}|\mathbf{x})||p_{\theta}(\mathbf{z}|\mathbf{x}))}$$

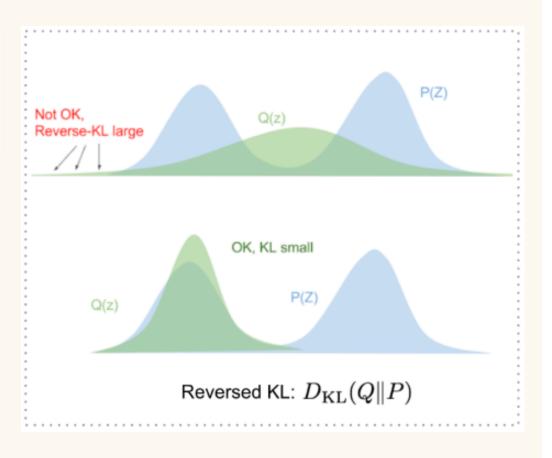
$$= -\mathbb{E}_{\mathbf{z} \sim q_{\phi}(\mathbf{z}|\mathbf{x})} p_{\theta}(\mathbf{x}|\mathbf{z}) + D_{\text{KL}}(q_{\phi}(\mathbf{z}|\mathbf{x})||p_{\theta}(\mathbf{z}))$$

$$\theta^*, \phi^* = \arg \min_{\theta, \phi} L_{\text{VAE}}$$

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

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

 $\rightarrow$  Minimize  $D_{\mathrm{KL}}(Q||P)$ 



$$D_{\mathrm{KL}}(q_{\phi}(\mathbf{z}|\mathbf{x})||p_{\theta}(\mathbf{z}|\mathbf{x})) \qquad D_{\mathrm{KL}}(Q||P) = \mathbb{E}_{z \sim Q(z)} \log \frac{Q(z)}{P(z)}$$

$$= \int q_{\phi}(\mathbf{z}|\mathbf{x}) \log \frac{q_{\phi}(\mathbf{z}|\mathbf{x})}{p_{\theta}(\mathbf{z}|\mathbf{x})} d\mathbf{z} \qquad ; \text{Because } p(z|x) = p(z,x)/p(x)$$

$$= \int q_{\phi}(\mathbf{z}|\mathbf{x}) \left(\log p_{\theta}(\mathbf{x}) + \log \frac{q_{\phi}(\mathbf{z}|\mathbf{x})}{p_{\theta}(\mathbf{z},\mathbf{x})}\right) d\mathbf{z}$$

$$= \log p_{\theta}(\mathbf{x}) + \int q_{\phi}(\mathbf{z}|\mathbf{x}) \log \frac{q_{\phi}(\mathbf{z}|\mathbf{x})}{p_{\theta}(\mathbf{z},\mathbf{x})} d\mathbf{z} \qquad ; \text{Because } \int q(z|x) dz = 1$$

$$= \log p_{\theta}(\mathbf{x}) + \int q_{\phi}(\mathbf{z}|\mathbf{x}) \log \frac{q_{\phi}(\mathbf{z}|\mathbf{x})}{p_{\theta}(\mathbf{x}|\mathbf{z})p_{\theta}(\mathbf{z})} d\mathbf{z} \qquad ; \text{Because } p(z,x) = p(x|z)p(z)$$

$$= \log p_{\theta}(\mathbf{x}) + \mathbb{E}_{\mathbf{z} \sim q_{\phi}(\mathbf{z}|\mathbf{x})} \left[\log \frac{q_{\phi}(\mathbf{z}|\mathbf{x})}{p_{\theta}(\mathbf{z})} - \log p_{\theta}(\mathbf{x}|\mathbf{z})\right] \qquad \mathbb{E}_{z \sim q_{\phi}(\mathbf{z}|\mathbf{x})} [g(z)]$$

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

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

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

$$\log p_{\theta}(\mathbf{x}) \geq \underbrace{\mathbb{E}_{\mathbf{z} \sim q_{\phi}(\mathbf{z}|\mathbf{x})} \log p_{\theta}(\mathbf{x}|\mathbf{z}) - D_{\mathrm{KL}}(q_{\phi}(\mathbf{z}|\mathbf{x}) \| p_{\theta}(\mathbf{z}))}_{\text{Lower bound of } \log p_{\theta}(\mathbf{x})} \longrightarrow \text{Maximize}$$

$$L_{\text{VAE}}(\theta, \phi) = -\log p_{\theta}(\mathbf{x}) + \underline{D_{\text{KL}}(q_{\phi}(\mathbf{z}|\mathbf{x}) \| p_{\theta}(\mathbf{z}|\mathbf{x}))}$$

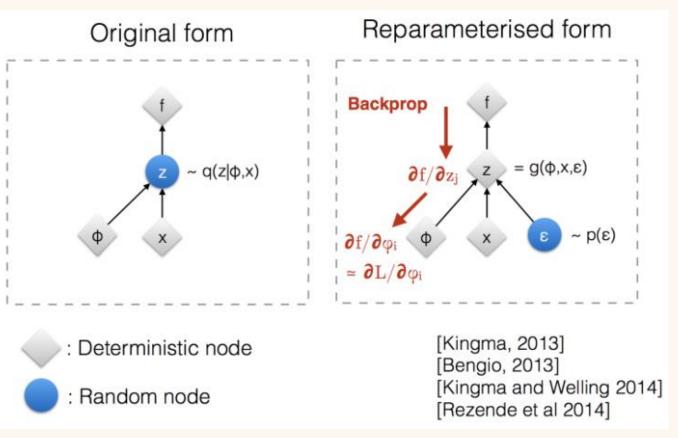
$$= -\mathbb{E}_{\mathbf{z} \sim q_{\phi}(\mathbf{z}|\mathbf{x})} p_{\theta}(\mathbf{x}|\mathbf{z}) + D_{\text{KL}}(q_{\phi}(\mathbf{z}|\mathbf{x}) \| p_{\theta}(\mathbf{z}))$$

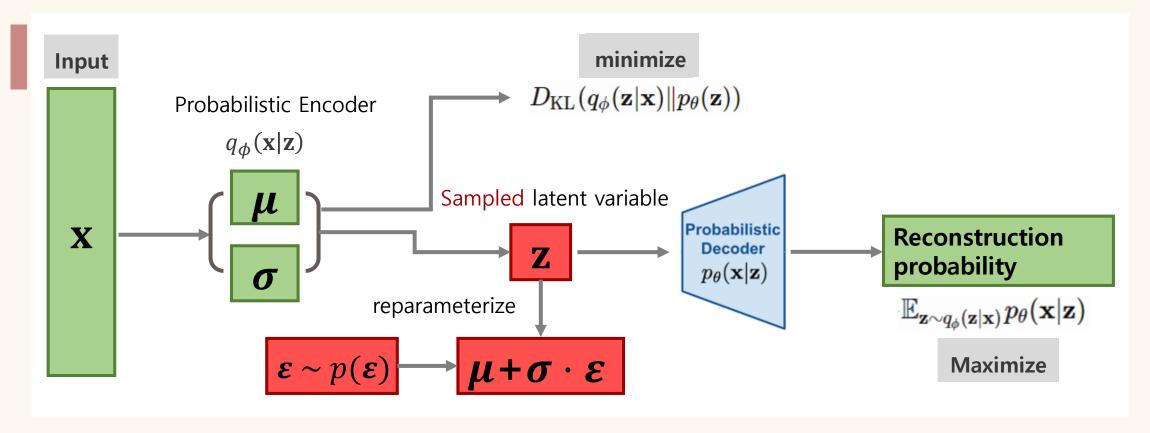
$$\theta^*, \phi^* = \arg \min_{\theta, \phi} L_{\text{VAE}}$$
Reconstruction probability

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

### Reparameterization trick

$$\mathbf{z} \sim q_{\phi}(\mathbf{z}|\mathbf{x}^{(i)}) = \mathcal{N}(\mathbf{z}; \boldsymbol{\mu}^{(i)}, \boldsymbol{\sigma}^{2(i)}\boldsymbol{I})$$
  
 $\mathbf{z} = \boldsymbol{\mu} + \boldsymbol{\sigma} \odot \boldsymbol{\epsilon}$ , where  $\boldsymbol{\epsilon} \sim \mathcal{N}(0, \boldsymbol{I})$   
 $\odot$  refers to element-wise product.





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

```
Algorithm 3 Variational autoencoder training algorithm

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

OUTPUT: probabilistic encoder f_{\phi}, probabilistic decoder g_{\theta}

\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)}) 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)}))

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

until convergence of parameters \phi, \theta
```

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

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

```
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) =
                                                           Encoder
        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)
                                                           Decoder
    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)
```

z\_dim: parameter쌍의 개수 fc2, fc3는 mu와 sigma를 도출함. fc2, fc3 중에 어느 것이 mu인지, sigma인지는 알 수 없음.

fc2가 mu가 되도록, fc3이 sigma가 되도록 최적화 시킬 뿐임.
(맞는지 모르겠음돠 ㅠㅠ)

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

