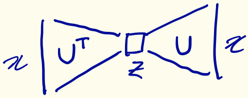
[Variational Auto-encoder, information metric] 18. 06. 23.

[Auto-encoder]



※ PCA

$x \in \mathbb{R}^d$,

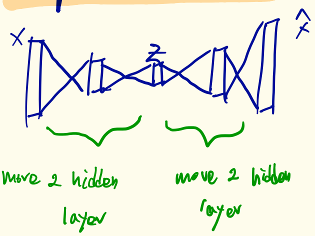
$y = U^T x$

$\hat{x} = U^T U x$

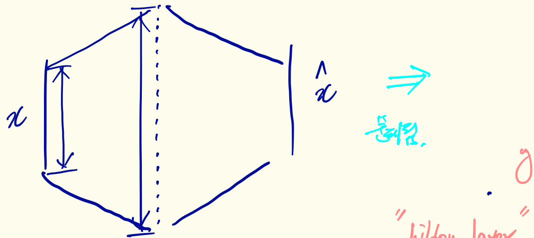
objective : $\min |x - \hat{x}|$

$\min_U |X - U^T U X|$

[Deep Auto-encoder]



※ Over-complete Auto encoder

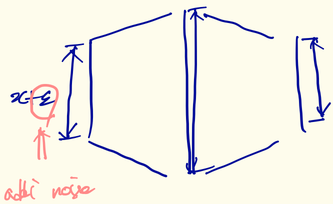


⇒ 문제점.

"hidden layer"

· trivial solution : x의 정보를 그대로 copy해서 가지고 있다가 output에서 보내는 방식

↳ 매우 useless 한 방법이다.

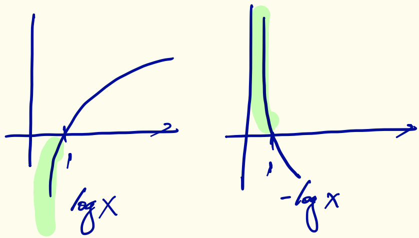


noise가 들어가게 되면, 위 방식의 trivial solution이 정확하게 작동하지 않는다.

[information]

$I : -\log p(x)$

where x : event



high probability : low information

low probability : high information

[Entropy]

$H : -\sum p(x) \log p(x)$

where x : event

↳ expectation of information

※ 두 분포의 entropy의 차 :

$$-\sum q(x) \log q(x) + \sum p(x) \log p(x)$$

[KLD]

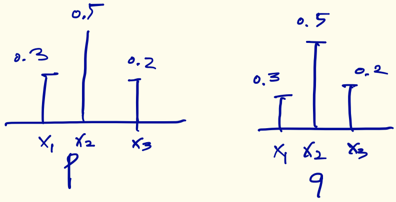
상대적 두 분포의 차이 : KLD w.r.t $p(x)$

$$KL(p \| q) = -\sum p(x) \log q(x) + \sum p(x) \log p(x)$$

$$= \sum p(x) \log \frac{p(x)}{q(x)}$$

$$= -\sum p(x) \log \frac{q(x)}{p(x)}$$

※ example of KLD



$$KLD(p \| q) = \left(0.3 \cdot \log \frac{0.3}{0.3}\right) + \left(0.5 \cdot \log \frac{0.5}{0.5}\right) + \left(0.2 \cdot \log \frac{0.2}{0.2}\right)$$

$\therefore KLD(q \| p) = 0$

※ KLD Property

① $KLD \geq 0$

② $KL(p \| q) \neq KL(q \| p)$

but, distance 정의에 의해, $D(p \| q) = D(q \| p)$ 이고

$\therefore$ KLD은 distance가 아니다.

[Graphical Model]의 적용이 어려운점.

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

※ 문제점 : evaluating marginal distribution

$$p(x) = \int p(x,z)\,dz \longrightarrow \int\!\!\int\!\!\int\!\!\int\!\!\int \cdots p(x,z)\,dz_1 \cdots dz_n$$

z : high dimension

∴ marginal distribution을 구하기가 매우 어렵다.

↳ 해결책

- sampling method :
- variational inference : introduce $q(z)$ which is tractable
  - ↳ e.x) exponential family

[KLD와 Variational inference]

$$\min KL(q\|p) = -\sum q(x)\log\frac{p(x)}{q(x)} \Rightarrow \min KL(q(z)\|p(z|x)) = -\sum q(z)\log\frac{p(z|x)}{q(z)}$$

$$-\sum q(z)\log\frac{\frac{p(x,z)}{p(x)}}{q(z)} = -\sum q(z)\log\frac{p(x,z)}{q(z)}\cdot\frac{1}{p(x)} = -\sum q(z)\left[\log\frac{p(x,z)}{q(z)} - \log p(x)\right]$$

$$= -\sum_z q(z)\log\frac{p(x,z)}{q(z)} + \underbrace{\sum_z q(z)\log p(x)}_{\log p(x)\underbrace{\sum_z q(z)}_{=1} = \log p(x)}$$

Given $X \Rightarrow \log p(x)$: constant

$$\therefore \log p(x) = \underbrace{KLD(q(z)\|p(z|x))}_{\text{minimize KLD}} + \underbrace{\sum q(x)\log\frac{p(x,z)}{q(z)}}_{L\Uparrow}$$

$$\because \underbrace{L}_{\text{Lower bound.}} \le \log p(x) \longrightarrow \sum q(z)\log\frac{p(x,z)}{q(z)} \le \underbrace{\log p(x)}$$

variational lower bound.

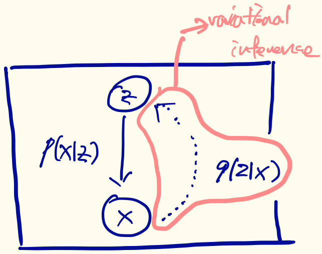
$$\cdot \ \sum q(z) \log \frac{p(x,z)}{q(z)} = \sum q(z) \log \frac{p(x|z)p(z)}{q(z)} = \sum q(z) \left[\log p(z|x) + \log \frac{p(z)}{q(z)} \right]$$

$$= \underbrace{\sum q(z) \log p(x|z)}_{\text{expectation } \log p(z|x) \text{ w.r.t } q(z)} + \underbrace{\sum q(z) \log \frac{p(z)}{q(z)}}_{-KL(q(z) \| p(z))}$$

$$= \mathbb{E}_{q(z)} \left[p(x|z) \right] - KL(q(z) \| p(z))$$

maximize $\mathbb{E}[p(x|z)]$, minimize $KL(q(z) \| p(z))$

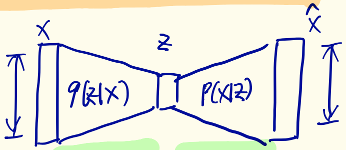
objective function for VAE.



$p(z|x)$를 구하기가 어려우니,

$q(z|x)$를

[Variational Auto encoder]



ANN. "ANN" structure -

⟹ ANN 구조이므로

complete deterministic 이므로.

여기서 한번 likelihood 관점으로
objective function을 결정해보면? ⟹ $p(x|\hat{x}) = |x - \hat{x}|$

∴ 만약 gaussian form 이면

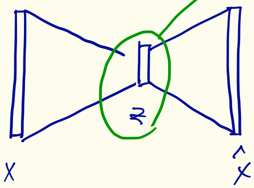
$$p(x|\hat{x}) = \exp(-|x-\hat{x}|^2)$$

log 값을 취해주는 것이면 $p(x|\hat{x}) = -|x-\hat{x}|^2$

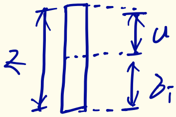
[AE와 VAE의 objective function의 차이]

- Auto-encoder의 objective : $\min |x-\hat{x}|^2$
- variational auto-encoder의 objective : $\min |x-\hat{x}|^2 + KL(q(z) \| p(z))$

[VAE의 구조]



· classical VAE에서는
diagonal multivariate normal을 가정한다.



$$\sigma_i \rightarrow \begin{bmatrix} \sigma_1 & & \\ & \ddots & \\ & & \sigma_z \end{bmatrix} = \Sigma$$