Linear Regression & MLE

$*$ Assumption : x, y in linear relationship (only 1 feature for each data x)

$$y = ax + b + \epsilon \qquad (\epsilon \sim N(0, \delta^2),\ \delta \text{ is constant})$$

(Vector version for single data $\mathbb{x}$: $y = W^T \mathbb{x} + \epsilon$
where $\mathbb{x} = [1\ x_1\ x_2 \cdots x_n]$)

$*$ Linear Regression Model

$$\hat{y} = Wx + b \quad \text{where } W, b \text{ are parameters}$$

(Vector version : $\hat{y} = W^T \mathbb{x}$)

$*$ MLE in Linear Regression? (For a single data y given x)

$$\epsilon = y - \hat{y} \sim N(0, \delta^2) \quad (\text{where } \delta \text{ is constant})$$

$$y \sim N(y; \hat{y}, \delta) \Longleftrightarrow y \sim p(y \mid x; W, b) \quad (\delta \text{ is constant})$$

δ가 constant라서 parameter로 넣지 않음.

$$\log P_\theta(y) = \log P(y \mid x; W, b) = \log N(y; \hat{y}, \delta)$$

$$= \log\left(\frac{1}{\sqrt{2\pi\delta^2}} e^{-\frac{(y-\hat{y})^2}{2\delta^2}}\right)$$

$$= \log \frac{1}{\sqrt{2\pi\delta^2}} + \log e^{-\frac{(y-\hat{y})^2}{2\delta^2}}$$

$$= -\frac{1}{2\delta^2}(y-\hat{y})^2 + \log \frac{1}{\sqrt{2\pi\delta^2}}$$

$$= -\frac{1}{2\delta^2}(y - Wx - b)^2 + \cancel{\log \frac{1}{\sqrt{2\pi\delta^2}}}$$

does not change (Since parameters are only W, b)

$$\underset{W,b}{\operatorname{argmax}} \log N(y; \hat{y}, \delta)$$

$$\Leftrightarrow \underset{W,b}{\operatorname{argmax}} \log P(y \mid x; W, b)$$

$$\Leftrightarrow \underset{W,b}{\operatorname{argmax}} -\frac{1}{2\delta^2}(y - Wx - b)^2$$

$$\Leftrightarrow \underset{W,b}{\operatorname{argmax}} -(y - Wx - b)^2$$

$$\Leftrightarrow \underset{W,b}{\operatorname{argmin}} (y - Wx - b)^2$$

$$\Leftrightarrow \underset{W,b}{\operatorname{argmin}} (y - (Wx + b))^2 \quad (\text{square of residual!})$$

⇝ This is why objective function for Linear Regression leads to MSE Loss.

For n datas?

$$L(W, b) = \frac{1}{N} \sum_{n=1}^{N} (y^{(n)} - (Wx^{(n)} + b))^2 \quad (\text{MSE})$$

object function

VAE : Variational Autoencoder

→ 학습하는 data에 따라 유연하게 그 형태가 결정되는 확률분포 ($P_\theta(x)$를 신경망으로 구현)

purpose of generative models

*** Review**

- Single normal distribution (Multivariate)

$$P_\theta(x) = N(x;\theta) \quad \text{where } \theta = \{u, \Sigma\}$$

MLE for D

$D = \{x^{(1)}, x^{(2)} \cdots x^{(N)}\}$

$$L(D;\theta)$$
$$= \log P_\theta(D)$$
$$= \log\left(\prod_{n=1}^{N} P_\theta(x^{(n)})\right)$$
$$= \sum_{n=1}^{N} \log P_\theta(x^{(n)})$$

Solve : $\frac{\partial}{\partial\theta} L(D;\theta) = 0$

- GMM : Gaussian Mixture Model

$\frac{\partial}{\partial\theta} \log_\theta(D) = 0$ → 해석적으로 풀 수 X ($p(x,z)$에서 $p(x)$를 도출하기 때문에 $\sum_z$ marginalization이 필요하고 이는 log-sum을 유발)

use ELBO,

$$ELBO(D; q, \theta) \leq \log P_\theta(D)$$

$$\Longleftrightarrow \sum_{n=1}^{N} \sum_{z^{(n)}} q^{(n)}(z^{(n)}) \log \frac{P_\theta(x^{(n)}, z^{(n)})}{q^{(n)}(z^{(n)})} \leq \log P_\theta(D)$$

E-M with ELBO (θ, q update stepwisely)

E: $q^{(n)}(z^{(n)}) = P_\theta(z^{(n)} | x^{(n)})$ (for all n datas & for all K latent variables), ELBO log-likelihood approx.

M: $\frac{\partial}{\partial\theta} ELBO = 0$ → maximize latent variable (z) generation model

* Sampling (or generating) data with VAE (Decoder)

Parameter is fixed!

① Sample latent variable z from "fixed" normal distribution $(P(z) = N(z; 0, I))$

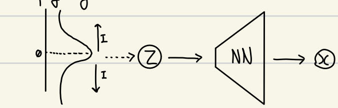
② Transform latent variable z to observed data x using neural network (Decoder)

Zero vector　　Identity Matrix

where $z \in D^H$, fixed params are $\{0, I\}$

* ···> : sampling

· Sampling figure



① $\therefore p(z) = N(z; 0, I)$

· In GMM z follows categorical distribution where z is discrete variable. In VAE, z is sampled from gaussian distribution $(N(z; 0, I))$ where z is continuous variable which makes representation broader.

더 다양하고 풍부한 대상 표현가능

population

· VAE is also a generative model which estimates the observed variable x's distribution $P(x)$ based on sample.

Since VAE transforms z to x, this models probability $P(x|z)$

Since VAE decoder outputs $\hat{x}$ from sampled z, define the x's distribution as..

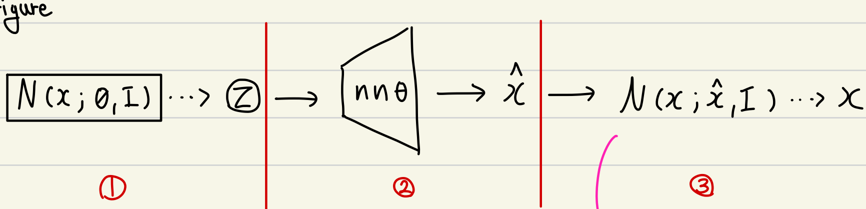
vector

② $\hat{x} = NeuralNet(z; \theta)$

Identity matrix

③ $P_\theta(x|z) = N(x; \hat{x}, I)$　　$(x \sim N(x; \hat{x}, I))$

* figure



If the observed data is binary $\{0, 1\}$

$P_\theta(x|z)$ can be modeled as Bernoulli dist.

* Limitation of EM in VAE (Difficulty in E-step)

- ELBO EM Estep for n datas.

  renew $q^{(n)}(z^{(n)}) = P_\theta(z^{(n)} \mid x^{(n)})$

Review) latent variable model $p(x,z)$ 에서 x에 대한 주도 $p(x) = \int p(x,z)\,dz$ 이다.

$$p(x) = \int p(x,z)\,dz$$
$$= \int p(z)\,p(x \mid z)\,dz$$

for VAE, $P_\theta(z^{(n)} \mid x^{(n)}) = \dfrac{P_\theta(x^{(n)}, z^{(n)})}{P_\theta(x^{(n)})}$

$$= \frac{P_\theta(x^{(n)}, z^{(n)})}{\int P_\theta(x^{(n)}, z^{(n)})\,dz} \rightarrow \text{marginalization}$$

$\int P_\theta(x, z)\,dz$ is easily countable in GMM since latent variable z is discrete.

$\Leftrightarrow \sum_z P_\theta(x, z)\,dz$

But in VAE z is continuous and z is vector $\rightarrow \int P_\theta(x,z)\,dz$ is impossible (or very hard)

∴ VAE에서는 EM의 E-step을 direct하게 적용할 수 X. → Needs improvement in EM algorithm.

"How To Solve?"

* VAE training by improving EM algorithm (Encoder)

• Review : Derive ELBO from $\log P_\theta(x)$ using $q(z)$!

$\log P_\theta(x)$ (log likelihood for single data x)

$$= \int q(z)dz \log P_\theta(x) \quad \left(\int q(z)dz = 1\right)$$

$$= \int q(z) \log P_\theta(x)\, dz$$

$$= \int q(z) \log \frac{P_\theta(x,z)}{P_\theta(z|x)}\, dz$$

$$= \int q(z) \log \frac{P_\theta(x,z)}{P_\theta(z|x)} \frac{q(z)}{q(z)}\, dz \quad \left(\frac{q(z)}{q(z)} = 1\right)$$

$$= \int q(z) \left(\log \frac{P_\theta(x,z)}{q(z)} + \log \frac{q(z)}{P_\theta(z|x)}\right) dz$$

$$= \underbrace{\int q(z) \log \frac{P_\theta(x,z)}{q(z)}\, dz}_{\text{ELBO}(x;\, q,\, \theta)} + \underbrace{\int q(z) \log \frac{q(z)}{P_\theta(z|x)}\, dz}_{D_{KL}(q(z)\,\|\,P_\theta(z|x))}$$

$$\therefore \log P_\theta(x) = \int q(z) \log \frac{P_\theta(x,z)}{q(z)}\, dz + D_{KL}(q(z)\,\|\,P_\theta(z|x)) \quad (D_{KL} \geq 0)$$

$$\geq \int q(z) \log \frac{P_\theta(x,z)}{q(z)}\, dz \quad (\text{ELBO})$$

According to EM algorithm, E fixes θ and renews $q(z) = P_\theta(z|x)$, but according to previous page it is hard to get $P_\theta(z|x)$ since z is continual vector.

☆ $P(z)$ VS $q(z)$ ($= q(z|x)$)

for generative model $p(x,z)$ (with latent variable)

$$p(x) = \int p(x,z)\,dz = \int p(z)\,p(x|z)\,dz \quad \cdots Ⓐ$$

Since Ⓐ is not easily calculable and optimze (for D)

we use $q(z|x)$ (or $q(z)$) to approximate $p(z|x)$

Comparison?

$p(z)$

- 사전 분포 (Prior)
- 모델이 가정하는 z에 대한 분포
- z에 대한 가정 / Generation시 이용되는 z 분포
- 모델이 정의
- $\log P(x) = \log \int p(z)\,p(x|z)\,dz$ 구성

$q(z|x)$

- 근사 후분포 (Variational Posterior)
- 데이터 x에 대해 조건부로 정의된 분포
- 모델 훈련 시, ELBO 계산을 위한 계산 가능한 분포, $p(z|x)$를 근사하기 위해
- 사용자가 도입
- $\text{ELBO} = E_{q(z|x)}[\log p(x|z)] - D_{KL}[q(z|x) \,||\, p(z)]$를 구성
- VAE에서는 Encoder에 의해 구현됨

* Solution

① $q(z)$를 정규분포로 제한 Ⓐ, 제한한 $q(z)$의 매개변수 $\psi = \{u, \Sigma\} \Leftrightarrow q_\psi(z) = \mathcal{N}(z; u, \Sigma)$

② $q(z)$를 정규분포로 제한한 상태에서 ELBO를 최대화한다.

$$\log P_\theta(x) = \underbrace{\int q_\psi(z) \log \frac{P_\theta(x,z)}{q_\psi(z)} dz}_{\text{ELBO}} + D_{KL}(q_\psi(z) \,\|\, p_\theta(z|x)) \quad \cdots ①$$

$$\theta, \psi = \underset{\theta,\psi}{\operatorname{argmax}} \ \mathrm{ELBO}(x; \theta, \psi) = \underset{\theta,\psi}{\operatorname{argmax}} \int q_\psi(z) \log \frac{P_\theta(x,z)}{q_\psi(z)} dz$$

In VAE, cannot find $P_\theta(z|x)$ for $q_\psi(z) = P_\theta(z|x)$ with ψ

But can fit $q_\psi(z) = P_\theta(z|x)$ by maximizing ELBO (명시적으로 E step을 수행하지 않아도, ELBO를 maximize 하는 과정에서 $q_\psi(z)$가 $P_\theta(z|x)$에 fit된다)

Why? ①에서 좌항 $\log P_\theta(x)$는 ψ를 가지고 있지 않음

$\therefore$ ψ가 변해도 ELBO와 KL의 총합인 $\log P_\theta(x)$는 변하지 X

$\Leftrightarrow$ ψ에 대해 ELBO가 최대가 되면, KL항은 최소가 됨.

$\Leftrightarrow$ $q_\psi(z) \approx P_\theta(z|x)$에 가까워짐. (E step 수행가능)

(간단한 확률분포 $q_\psi(z)$를 이용해 계산이 불가능한 $P_\theta(z|x)$를 근사시킴. 이를 Variational approximation 또는 Variational bayes 라고함.)
변분 근사

* For n datas?

$$\sum_{n=1}^{N} \mathrm{ELBO}(x^{(n)}; \theta, \psi^{(n)}) = \sum_{n=1}^{N} \int q_{\psi^{(n)}}(z) \log \frac{p_\theta(x^{(n)}, z)}{q_{\psi^{(n)}}(z)} dz$$

- prepare $q_{\psi^{(n)}}(z)$ for each $x^{(n)}$ where $\psi^{(n)} = \{u^{(n)}, \Sigma^{(n)}\}$ … ①

- $\underset{\psi^{(n)}}{\mathrm{argmax}}\, \mathrm{ELBO}(x^{(n)}; \theta, \psi^{(n)}) \Longleftrightarrow q_{\psi^{(n)}}(z) \approx p_\theta(z \mid x^{(n)})$ (각각 $\psi^{(n)}$에 대해 ELBO 최대화)

"Prepare $\psi^{(n)}$ for each data $x^{(n)}$? what if n=1 billion?"

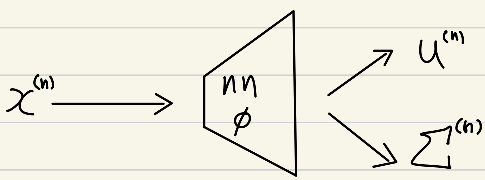
$\downarrow$

"Use Neural Network for extracting $\psi^{(n)} = \{u^{(n)}, \Sigma^{(n)}\}$ for each $x^{(n)}$"

$\downarrow$

"The role of Encoder in VAE"

* Encoder in VAE



분할 상환 추론

- 근사사후 분포 $q(z)$의 매개변수를 nn으로 출력하는 기법을 amortized inference라고함.

$z^{(n)} \in D^{H} \longrightarrow u^{(n)} \in D^{H},\ \Sigma^{(n)} \in D^{H \times H}$

Refine Σ to diagonal matrix

$$\Leftrightarrow \Sigma = \begin{bmatrix} \delta_1^2 & & O \\ & \delta_2^2 & \\ O & & \ddots \ \delta_H^2 \end{bmatrix}$$

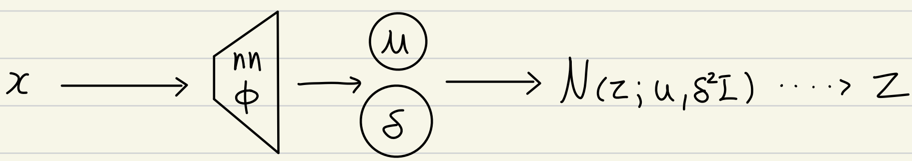
elements are standard deviation of each feature

$\Leftrightarrow$ Σ is expressible as $\delta^2 I$ where $\delta \in D^{H}$, $I = I_H$

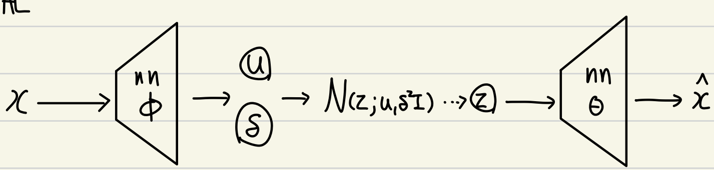
$$\therefore\ u, \delta = \text{NeuralNetEncoder}(x; \phi)$$
$$q_\phi(z|x) = N(z; u, \delta^2 I)$$

※ EM에서는 $x^{(n)}$에 대한 $q^{(n)}(z)$이고, VAE에서는 $q^{(n)}(z)$의 parameter를 x로부터 파라미터 ϕ로 이루어진 신경망을 통해 얻어내기에, $q_\phi(z|x)$로 표현

- Encoder



- VAE



* ELBO Optimization in VAE

- Decoder

$$p(z) = \mathcal{N}(z; 0, I)$$
$$\hat{x} = \text{NeuralNet}(z; \theta)$$
$$p_\theta(x|z) = \mathcal{N}(x; \hat{x}, I)$$ where θ is decoder parameter

- Encoder

$$u, \delta = \text{NeuralNet}(x; \phi)$$
$$q_\phi(z|x) = \mathcal{N}(z; u, \delta^2 I)$$ where ϕ is encoder parameter

- ELBO

Single Sample x : $\text{ELBO}(x; \theta, \phi) = \int q_\phi(z|x) \log \frac{p_\theta(x,z)}{q_\phi(z|x)} dz$

$$= \int q_\phi(z|x) \log \frac{p_\theta(x|z) p(z)}{q_\phi(z|x)} dz$$

$$= \int q_\phi(z|x) \log p_\theta(x|z) dz + \int q_\phi(z|x) \log \frac{p(z)}{q_\phi(z|x)} dz$$

$$= \int q_\phi(z|x) \log p_\theta(x|z) dz - \int q_\phi(z|x) \log \frac{q_\phi(z|x)}{p(z)} dz$$

$$= \underbrace{E_{q_\phi(z|x)}[\log p_\theta(x|z)]}_{J_1} - \underbrace{D_{KL}(q_\phi(z|x) \,||\, p(z))}_{J_2}$$

$D = \{x^{(1)}, x^{(2)} \cdots x^{(N)}\}$: $\text{ELBO}(D; \theta, \phi) = \sum_{n=1}^{N} \text{ELBO}(x^{(n)}; \theta, \phi) = \sum_{n=1}^{N} \int q_\phi(z|x) \log \frac{p_\theta(x,z)}{q_\phi(z|x)} dz$

$$\mathrm{ELBO}(x;\theta,\phi) = \underbrace{E_{q_\phi(z|x)}[\log P_\theta(x|z)]}_{J_1} - \underbrace{D_{KL}(q_\phi(z|x) \,||\, p(z))}_{J_2}$$

→ ϕ, θ에 대해 J_1은 최대화 J_2는 최소화 해야함

• J_1

J_1은 $q_\phi(z|x)$를 따르는 z에 대한 $\log P_\theta(x|z)$의 Expectation

Monte carlo approximation으로 $q_\phi(z|x)$에서 z를 "1"개만 sampling해서 근사

$$u, \delta = \mathrm{NeuralNet}(x;\phi)$$

$$z \sim N(z; u, \delta^2 I) \quad \text{(sample only 1)}$$

$$\hat{x} = \mathrm{NeuralNet}(z;\theta)$$

$$J_1 \approx \log P_\theta(x|z)$$

$$\Leftrightarrow J_1 \approx \log N(x; \hat{x}, I)$$

$$= \log\left(\frac{1}{\sqrt{(2\pi)^D |I|}} \exp\left(-\frac{1}{2}(x-\hat{x})^T I^{-1} (x-\hat{x})\right)\right)$$

$$= -\frac{1}{2}(x-\hat{x})^T(x-\hat{x}) + \log\frac{1}{\sqrt{(2\pi)^D}} \quad (I^{-1} = I, \ |I| = 1)$$

$$= \underbrace{-\frac{1}{2}\sum_{d=1}^{D}(x_d-\hat{x}_d)^2}_{\text{defined by } \theta, \phi} + \underbrace{\log\frac{1}{\sqrt{(2\pi)^D}}}_{\text{constant}}$$

$$\underset{\theta,\phi}{\mathrm{argmax}}\, J_1 = \underset{\theta,\phi}{\mathrm{argmax}} -\frac{1}{2}\sum_{d=1}^{D}(x_d-\hat{x}_d)^2$$

$$= \underset{\theta,\phi}{\mathrm{argmin}} \sum_{d=1}^{D}(x_d-\hat{x}_d)^2$$: reconstruction error

· J_2

– minimize J_2 for maximizing $\mathrm{ELBO}(x;\phi,\theta)$

$$q_\phi(z|x) : \mathcal{N}(z; u, \delta^2 I)$$
$$p(z) : \mathcal{N}(z; 0, I)$$

why Ⓐ? : $D_{KL}(q_\phi(z|x) \| p(z))$ 값을 해석적으로 구하기 위함.

$q(z) = \mathcal{N}(z; u_1, \delta_1^2 I)$, $p(z) = \mathcal{N}(z; u_2, \delta_2^2 I)$ (두 정규분포가 Normal distribution일때)

$D_{KL}(q \| p) = -\frac{1}{2}\sum_{h=1}^{H}\left(1 + \log\frac{\delta_{1,h}^2}{\delta_{2,h}^2} - \frac{(u_{1,h}-u_{2,h})^2}{\delta_{2,h}^2} - \frac{\delta_{1,h}^2}{\delta_{2,h}^2}\right)$ ($D_{KL}(p \| q)$를 해석적으로 구할 수 있음) ··· ①

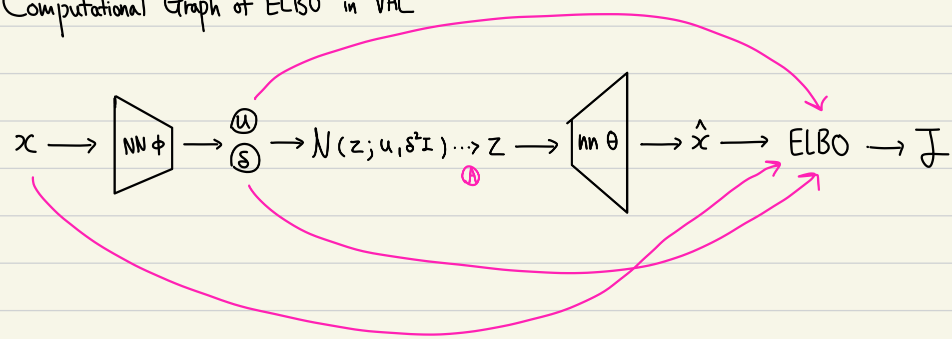
$$J_2 = D_{KL}(q_\phi(z|x) \| p(z))$$

$$= -\frac{1}{2}\sum_{h=1}^{H}(1 + \log\delta_h^2 - u_h^2 - \delta_h^2)$$

minimize J_2 ?$\Leftrightarrow$ $q_\phi(z|x) = p(z)$ (consistency / regularization term)

$$\therefore \mathrm{ELBO}(x,\theta,\phi) \approx \underbrace{-\frac{1}{2}\sum_{d=1}^{D}(x_d - \hat{x}_d)^2}_{\text{reconstruction loss}} + \underbrace{\frac{1}{2}\sum_{h=1}^{H}(1 + \log\delta_h^2 - u_h^2 - \delta_h^2)}_{\text{regularization term}} + \text{const}$$

– Computational Graph of ELBO in VAE



– update θ, ϕ simultaneously with G.D for maximizing ELBO

↳ 원래 두 단계로 나누어 θ, ϕ를 차례로 갱신했음 (EM algorithm)

– issue : Gradient flow is unavailabe in Ⓐ

* Reparameterization trick for solving issue

– Make sampling to enable gradient flow

$$Z \sim N(Z; u, \delta^2 I) \text{ sampling} \iff \epsilon \sim N(\epsilon; 0, I)$$

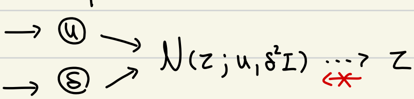
$$Z = u + \delta \odot \epsilon$$ where $\odot$ is elementwise multiplication

$$Z = u + \delta \odot \epsilon$$

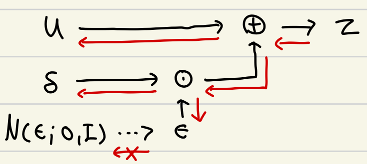
$$= \begin{bmatrix} u_1 \\ u_2 \\ \vdots \\ u_H \end{bmatrix} + \begin{bmatrix} \delta_1 \\ \delta_2 \\ \vdots \\ \delta_H \end{bmatrix} \odot \begin{bmatrix} \epsilon_1 \\ \epsilon_2 \\ \vdots \\ \epsilon_H \end{bmatrix}$$

$$= \begin{bmatrix} u_1 + \delta_1 \epsilon_1 \\ u_2 + \delta_2 \epsilon_2 \\ \vdots \\ u_H + \delta_H \epsilon_H \end{bmatrix}$$

- Without reparameterization trick



- With reparameterization trick



"Gradient flow available for Encoder"