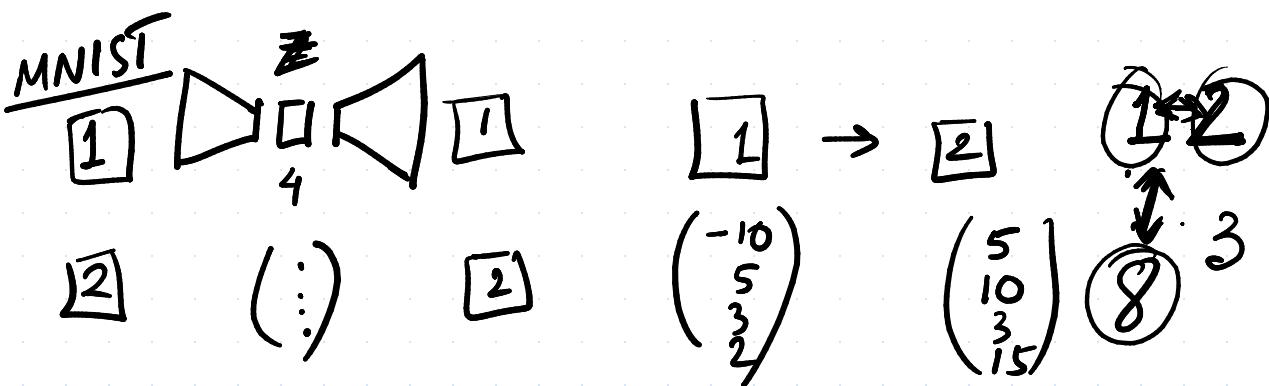
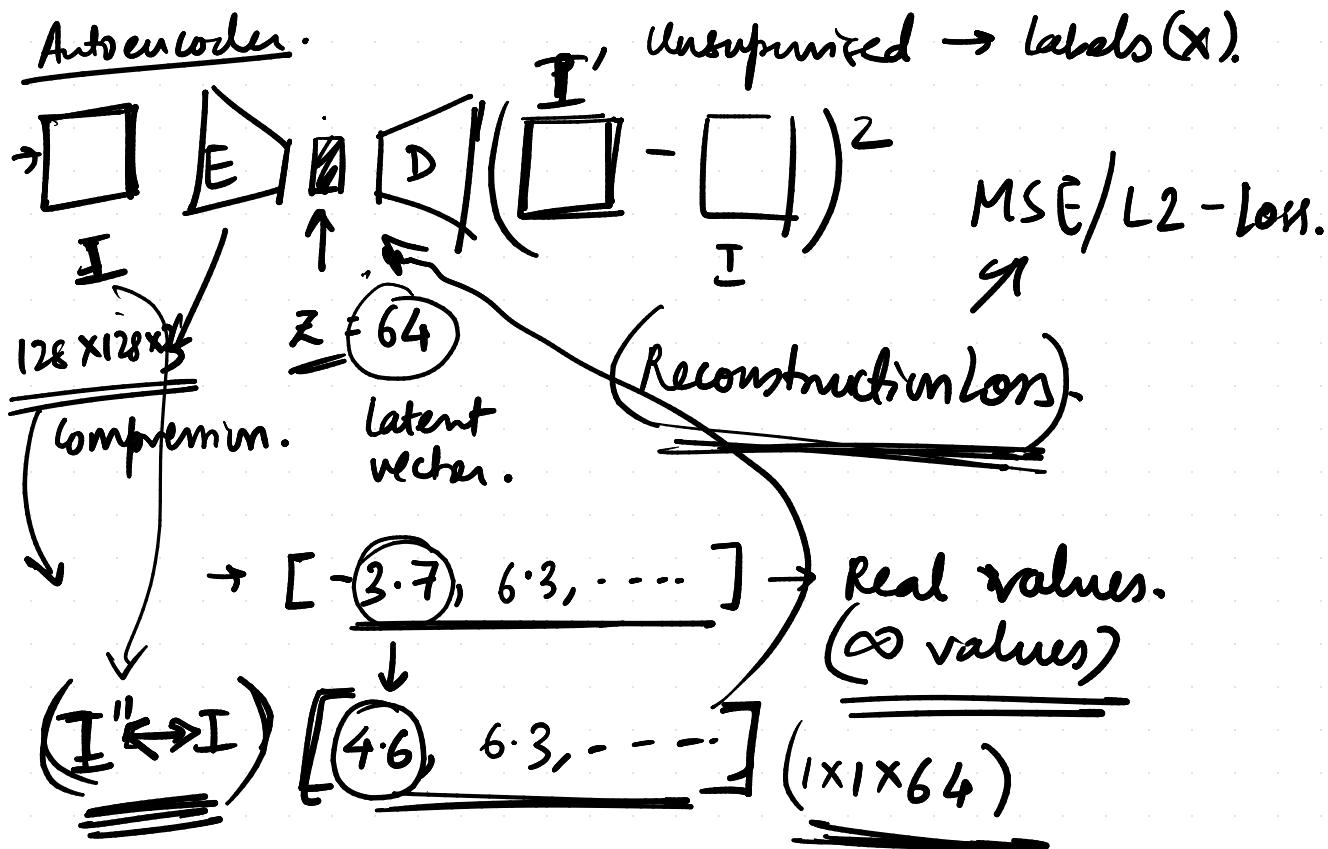


Lecture - 10

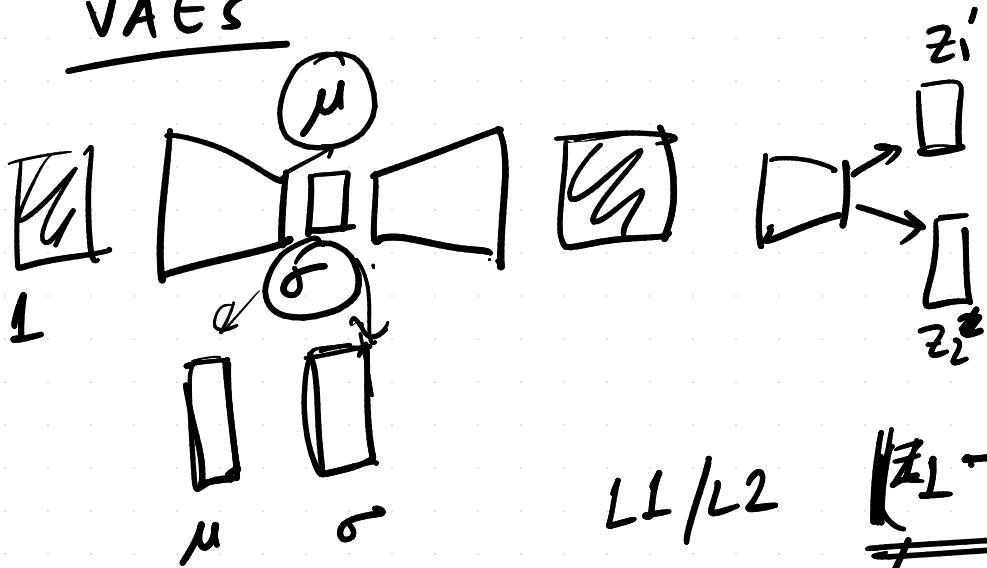
10/03/24

VAE - Theory Derivations & Insights.



$z \left([1] + [2] \right) \times (\dots) \times$ Autoencoder

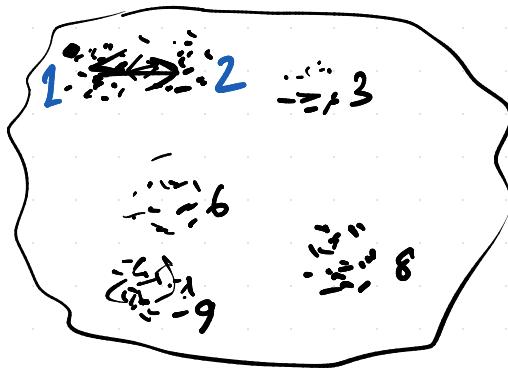
VAE's



$$L1/L2 \frac{||z_1 - z_2||}{\sqrt{\sigma}} = -$$

$$z_1 (z_1^{(1)}) (z_2^{(0)})$$

z_2

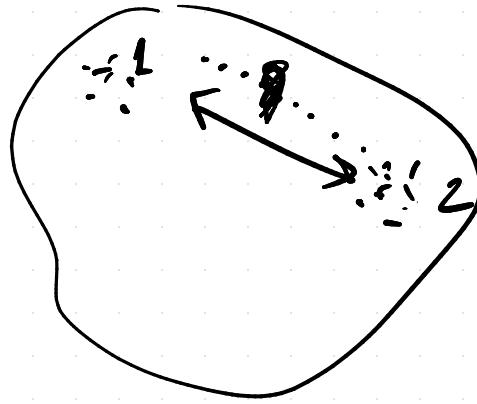


$$28 \times 28 \rightarrow 4$$

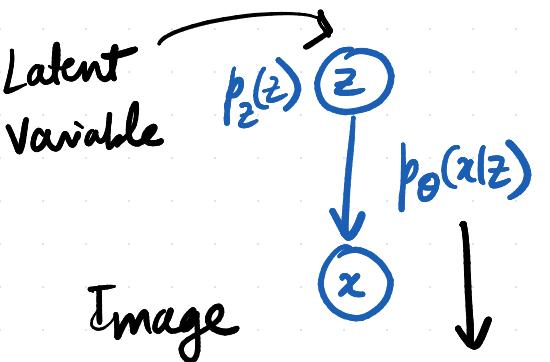
$$1 \rightarrow 2$$

1	1	1	2	2	2
---	---	---	---	---	---

$$\begin{matrix} 4 \\ 4 \end{matrix} =$$



$$\begin{aligned} z &\sim p_z(z) \\ x &\sim p_{\theta}(x|z) \end{aligned} \quad \left. \right\} \text{Sample.}$$

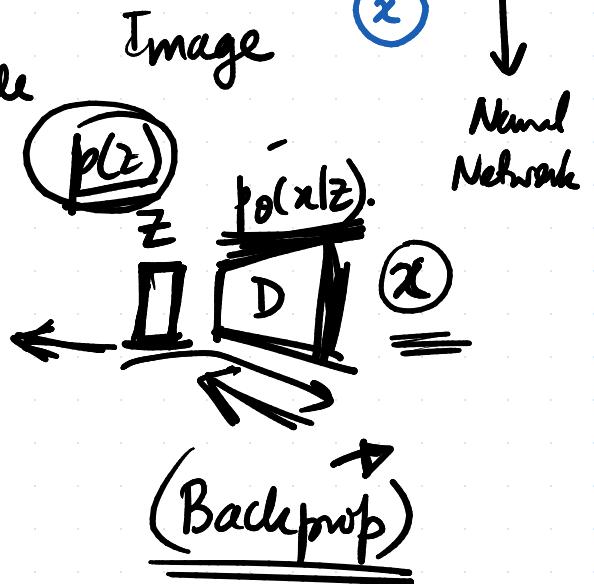


Likelihood.

$$p_{\theta}(x) = \sum_z p_z(z) p_{\theta}(x|z)$$

\rightarrow easy to sample from

Marginalization



Training objective

$$\max_{\theta} \sum_i \log p_{\theta}(x^{(i)})$$

$$= \sum_i \log \sum_z p_z(z) p_{\theta}(x^{(i)}|z)$$

$z \rightarrow$ can take many values.

Hard to sample z that leads to

meaningful terms.

$$\sum_i \log \sum_z p_z(z) p_{\theta}(x^{(i)} | z)$$

$$\approx \sum_i \log \frac{1}{k} \sum_{k=1}^k p_{\theta}(x^{(i)} | z_k^{(i)})$$

$z_k^{(i)} \sim p_z(z)$

$z \rightarrow$ takes many values, hard to select samples that leads to meaningful func.

Importance Weighted VAE (IWVAE)

$$z \rightarrow x$$

$z = \text{discrete R.V.}$
(small domain)

But in general

exact objective
is tractable.

$z \rightarrow \text{CRV.}$ & hence
the objective is not
tractable.

$$\{ p_z(z=A) = p_z(z=B) = p_z(z=C) = \frac{1}{3}$$

May send
(endsem)

$$p_{\theta}(x|z=k) = \frac{1}{(2\pi)^{n/2} |\Sigma_k|^{1/2}} \exp \left(-\frac{1}{2} (x - \mu_k)^T \Sigma_k^{-1} (x - \mu_k) \right)$$

Training objective :-

$$\max_{\theta} \sum_i \log p_{\theta}(x^{(i)})$$

$$= \sum_i \log \sum_z p_z(z=z) p_{\theta}(x|z=z)$$

$$= \underbrace{p_z(z=A)}_{1/3} \underbrace{p_{\theta}(x|z=A)}_{1/3} + \underbrace{p_z(z=B)}_{1/3} \underbrace{p_{\theta}(x|z=B)}_{1/3} + \underbrace{p_z(z=C)}_{1/3} \underbrace{p_{\theta}(x|z=C)}_{1/3}$$

$$= \max_{\mu, \Sigma} \sum_i \log \left[\frac{1}{3} \frac{1}{(2\pi)^{n/2}} \frac{1}{|\Sigma_A|^{1/2}} \exp \left(-\frac{1}{2} (x^{(i)} - \mu_A)^T \cdot \Sigma_A^{-1} \cdot (x^{(i)} - \mu_A) \right) \right]$$

$$+ \frac{1}{3} \frac{1}{(2\pi)^{n/2}} \frac{1}{|\Sigma_B|^{1/2}} \exp \left(-\frac{1}{2} (x^{(i)} - \mu_B)^T \Sigma_B^{-1} (x^{(i)} - \mu_B) \right)$$

$$+ \frac{1}{3} \frac{1}{(2\pi)^{n/2}} \cdot \frac{1}{|\Sigma_C|^{1/2}} \exp \left(-\frac{1}{2} (x^{(i)} - \mu_C)^T \Sigma_C^{-1} (x^{(i)} - \mu_C) \right)$$



Importance Sampling

$$\mathbb{E}_{z \sim p_z(z)} [f(z)] = \sum_z p_z(z) f(z)$$

$$= \sum_z \frac{q(z)}{q(z)} \cdot p_z(z) \cdot f(z).$$

$$= \mathbb{E}_{z \sim q(z)} \left[\frac{p_z(z) f(z)}{q(z)} \right]$$

Here we will sample from $q(z)$ rather than $p(z)$, sample based expectations

$$\approx \frac{1}{K} \sum_{k=1}^K \frac{p_z(z^{(k)})}{q(z^{(k)})} f(z^{(k)}) \quad \text{with} \\ \underbrace{\qquad\qquad\qquad}_{z^{(k)} \sim q(z)}$$

We can sample from q to compute expectations w.r.t p .

Train objective (New) :-

$$\max_{\theta} \sum_i \log p_{\theta}(x^{(i)}) = \sum_i \log \sum_z p_z(z) \frac{p_{\theta}(x^{(i)}|z)}{p_{\theta}(x^{(i)})}$$

\uparrow \downarrow

$$\approx \sum_i \log \frac{1}{k} \sum_{k=1}^K \frac{p_z(z_k^{(i)})}{q(z_k^{(i)})} p_{\theta}(x^{(i)}|z_k^{(i)})$$

$f(z)$

hence, we use
importance sampling.

$$z_k^{(i)} \sim q(z_k^{(i)})$$

$$q(z) = p_{\theta}(z|x^{(i)}) = \frac{p_{\theta}(x^{(i)}|z) p_z(z)}{p_{\theta}(x^{(i)})}$$

Not easy to sample from.

$q(z) = N(z; \mu, \sigma^2) \rightarrow$ easy to sample from.

Importance sampling \rightarrow proposal Distribution

$$\Rightarrow \min_{q(z)} \text{KL}(q(z) \parallel p_\theta(z|x^{(i)})) \quad \begin{matrix} \leftarrow \text{Distance} \\ \text{b/w 2 dist.} \end{matrix}$$

$$\Rightarrow \min_{q(z)} \sum_i q(z) \circ \log \left(\frac{q(z)}{p_\theta(z|x^{(i)})} \right)$$

$$\Rightarrow \min_{q(z)} \mathbb{E}_{z \sim q(z)} \underbrace{\log \left(\frac{q(z)}{p_\theta(z|x^{(i)})} \right)}$$

$q \rightarrow \text{gaussian}$

$$\Rightarrow \min_{q(z)} \mathbb{E}_{z \sim q(z)} \log \left(\frac{q(z)}{p_\theta(z|x^{(i)})} \frac{p_z(z)}{p_\theta(x^{(i)})} \right)$$

$$\Rightarrow \min_{q(z)} \mathbb{E}_{z \sim q(z)} [\log q(z) - \log p_z(z) - \log p_\theta(x^{(i)}|z)]$$

constant independent of z .

$\underbrace{\quad\quad\quad}_{+ \log p_\theta(x^{(i)})}$
 doesn't
 depends on z

$$\Rightarrow \min_{q(z)} \mathbb{E}_{z \sim q(z)} [\underbrace{\log q(z)}_{\text{sample from } q \text{ by design.}} - \underbrace{\log p_z(z)}_{\text{optimize to find } q} - \underbrace{\log p_\theta(x^{(i)}|z)}_{\text{easy to work with}}]$$

\downarrow
Neural Network.
(SAD)

Amortized Inference

$x^{(i)} \rightarrow$ want to solve.

$$\min_{q(z)} \text{KL}(q(z) \parallel p_\theta(z|x^{(i)}))$$

for all $x^{(i)}$, we want to solve.

$$\phi: x^{(i)} \rightarrow \mu^{(i)}, \sigma^{(i)}$$

Amortized formulation

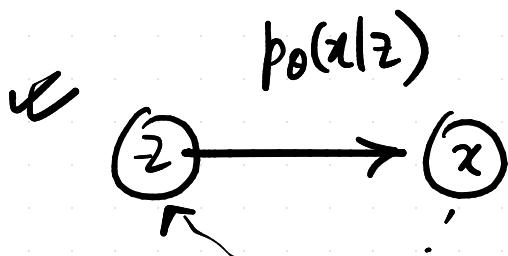
$$\min_{\phi} \sum_i \text{KL}(q_{\phi}(z|x^{(i)}) || p_{\theta}(z|x^{(i)}))$$

faster, regularization (not as precise).

Gaussian

$$\min_{\phi} \sum_i \text{KL}(q_{\phi}(z|x^{(i)}) || p_{\theta}(z|x^{(i)}))$$

↑
multiple posteriors.



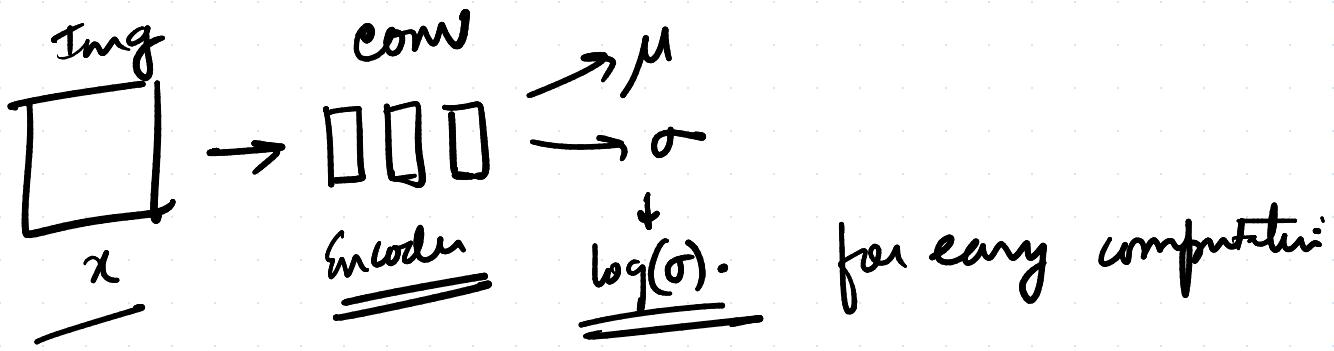
$$q_{\phi}(z|x)$$

→ part of our inference model, not a part of generative model.

$$q_{\phi}(z|x) = N(\mu_{\phi}(x), \sigma_{\phi}^2(x))$$

$$\underline{z} = \mu_{\phi} + \varepsilon \sigma_{\phi}(x) \quad \text{with } (\varepsilon \sim \mathcal{N}(0, I))$$

$$z \sim q(z|x) = N(z; \mu_{\phi}^{(x)}, \sigma_{\phi}^{(x)})$$



Importance - Weighted A.E. (IWAE)

$$\text{objective} \sum_i \log \frac{1}{K} \sum_{k=1}^K \frac{p_z(z_k^{(i)})}{q(z_k^{(i)})} p_{\theta}(x^{(i)}|z_k^{(i)})$$

$$\text{with } z_k^{(i)} \sim q(z_k^{(i)})$$

$$\min_{\phi} \sum_i \text{KL}(q_\phi(z|x^{(i)}) || p_\theta(z|x^{(i)}))$$

maximize $(\text{term 1} - \text{term 2}) = L_k$ - Likelihood.
 θ, ϕ

for all k , the lower bounds satisfy :-

real objective $\leftarrow \log p(x) \geq L_{k+1} \geq L_k$.

Moreover, if $p(z|x)/q(z|x)$ is bounded

then $L_k \rightarrow \log p(x)$ (approaches)

as $k \rightarrow \infty$.

As we have more terms inside the importance sampling, we will do better.

$$L_k = \mathbb{E}_{h_1, h_2, \dots, h_k} \left[\log \frac{1}{k} \sum_{i=1}^k \frac{p(x|h_i)}{q(h_i|x)} \right]$$

$$= \mathbb{E}_{h_1, h_2, \dots, h_K} \left[\log \mathbb{E}_{I = \{i_1, i_2, \dots, i_m\}} \left[\frac{1}{m} \sum_{j=1}^m \frac{p(x, h_{ij})}{q_V(h_{ij}|x)} \right] \right]$$

$$\geq \mathbb{E}_{h_1, h_2, \dots, h_K} \left[\mathbb{E}_{I = \{i_1, i_2, \dots, i_m\}} \left[\log \frac{1}{m} \sum_{j=1}^m \frac{p(x, h_{ij})}{q_V(h_{ij}|x)} \right] \right]$$

$$= \mathbb{E}_{h_1, h_2, \dots, h_m} \left[\log \frac{1}{m} \sum_{i=1}^m \frac{p(x_i, h_i)}{q(h_i|x)} \right] = dm$$

Variational Lower Bound Derivation \Rightarrow

(ELBO)

(Using Jensen)

$$\max_{\theta} \sum_i \log p_{\theta}(x^{(i)})$$

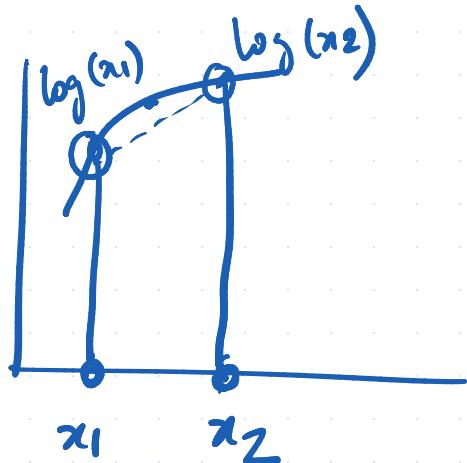
$$= \max_{\theta} \sum_i \log \left(\sum_z p_z(z) \cdot p_{\theta}(x^{(i)}|z) \right)$$

$$= \max_{\theta} \sum_i \log \left(\sum_z \frac{q(z)}{q(z)} \underbrace{p_z(z) \cdot p_{\theta}(x^{(i)}|z)}_{\text{Importance Sampling}} \right)$$

$$= \max_{\theta} \sum_i \log E_{z \sim q(z)} \frac{p_z(z)}{q(z)} p_{\theta}(x^{(i)}|z).$$

$$\geq \max_{\theta} \sum_i E_{z \sim q(z)} \left\{ \log \frac{p_z(z)}{q(z)} \cdot p_{\theta}(x^{(i)}|z) \right\}$$

↙
constant, then Equality



$$\log E_z(w) \geq E_z(\log(w))$$

$$= \max_{\theta} \sum_i \mathbb{E}_{z \sim q(z)} \log p_z(z) +$$

$$\mathbb{E}_{z \sim q(z)} \log p_{\theta}(x^{(i)}|z)$$

$$- \mathbb{E}_{z \sim q(z)} \log q(z).$$

$q \rightarrow$ something we can choose,

$$q(z) \propto p_z(z) p_{\theta}(x^{(i)}|z)$$

↳ un-normalized dist.

$p_{\theta}(z|x^{(i)}) \rightarrow$ normalized.



$$\Rightarrow \max_{\theta, q} \sum_i \mathbb{E}_{z \sim q(z)} \log p_z(z) +$$

$$\mathbb{E}_{z \sim q(z)} \log p_\theta(x^{(i)}|z)$$

$$\mathbb{E}_{z \sim q(z)} \log q(z).$$

Evidence Lower Bound (ELBO)

Variational Lower Bound (VLB).

Derivation using KL

$$D_{KL} [q_x(z) \parallel p(z|x)] = \mathbb{E}_{z \sim q(z)} [\log q_x(z) - \text{conditional}] \downarrow \log p(z|x)$$

$$= \mathbb{E}_{z \sim q_x(z)} [\log q_x(z) - \log \frac{p(z|x)}{p(x)}]$$

$$= \mathbb{E}_{z \sim q_{\pi}(z)} \left[\log q_{\pi}(z) - \log p(z) - \log p(x|z) + \log p(x) \right]$$

$$= \mathbb{E}_{z \sim q_{\pi}(z)} \left[\log q_{\pi}(z) - \log p(z) - \log p(x|z) \right]$$

Only this part depends
on z , (VLB) $+ \log p(x)$

$$D_{KL} [q_{\pi}(z) \parallel p(z|x)] = \mathbb{E}_{z \sim q_{\pi}(z)} \left[\log q_{\pi}(z) - \log p(z) - \log p(x|z) \right] + \log p(x)$$

$$\log p(x) = \mathbb{E}_{z \sim q_{\pi}(z)} [-\log q_{\pi}(z) + \log p(z)]$$

$$\underline{\text{VLB}} \left\{ + \log p(x|z) \right\} + \underbrace{D_{KL} [q_{\pi}(z) \parallel p(z|x)]}_{\geq 0}$$

Same with Jensen's, but now we know
the gap = KL .

Stochastic Optimization (Objective amenable
 to this)

$$\log p(x) = - \mathbb{E}_{z \sim q_x(z)} [\log q_x(z) - \log p(z) \\ - \log p(x|z)]$$

$$+ D_{KL} [q_x(z) \parallel p(z|x)]$$

$$= \overbrace{\mathbb{E}_{z \sim q_x(z)} [\log p(z) + \log p(x|z) \\ - \log q_x(z)]} +$$

$$D_{KL} [q_x(z) \parallel p(z|x)]$$

$$= 0, \text{ we set} \\ \text{this to } 0.$$

only work with this

$q_x(z) \rightarrow$ optimal of VLB is $p(z|x)$ at which point, VLB is tight, $\log p(x)$.

$x \sim p_{\text{data}}$, we can now train the generative model by maximizing the VLB under data distribution.

$$\begin{aligned} \text{VLB} &= \mathbb{E}_{x \sim p_{\text{data}}} \left[\mathbb{E}_{z \sim q_x(z)} \left[\log p(z) + \log p(x|z) - \log q_x(z) \right] \right] \\ &\leq \mathbb{E}_{x \sim p_{\text{data}}} [\log p(x)] + \end{aligned}$$

Likelihood Ratio Gradient

$$\max_{\phi} \mathbb{E}_{z \sim q_{\phi}(z)} [\underline{f(z)}]$$

$$z^{(i)} \sim q_{\phi}(z)$$

~~$$\nabla_{\phi} \times \sum_{i=1}^k f(z^{(i)}) \cdot z^{(i)}$$~~

Empirical expectation

$$\max_{\phi} \sum_z q_{\phi}(z) f(z).$$

$$\Rightarrow \nabla_{\phi} \left(\sum_z q_{\phi}(z) f(z) \right)$$

$$\Rightarrow \sum_z \nabla_{\phi} q_{\phi}(z) f(z).$$

$$\Rightarrow \sum_z \frac{q_{\phi}(z)}{\bar{q}_{\phi}(z)} \nabla_{\phi} q_{\phi}(z) f(z)$$

$$\mathbb{E}_{z \sim q_{\phi}(z)} \frac{\nabla_{\phi} q_{\phi}(z)}{q_{\phi}(z)} f(z)$$


$$\Rightarrow \mathbb{E}_{z \sim q_{\phi}(z)} \left[\underline{\nabla_{\phi} \log q_{\phi}(z) f(z)} \right]$$

$$\approx \mathbb{E}_{z \sim q_{\phi}(z)} \left[\underline{\nabla_{\phi} \log q_{\phi}(z) f(z)} \right]$$

$$\approx \frac{1}{k} \sum_{i=1}^K \nabla_{\phi} \log q_{\phi}(z^{(i)}) f(z^{(i)})$$

↗ ↘ gradient

↓
 change dist q_{ϕ}
 the expectation
 will change
for most $f(z)$

Increasing the log probability of something we sampled higher.

This leads to perfect gradient when we pick only many samples, hence, we do a reparameterization trick.

Reparameterization trick

Pathwise Derivative

$$\mathbb{E}_{z \sim q_\phi(z)} [f(z)] \quad q_\phi(z) = N(\mu, \sigma^2)$$

$$\downarrow$$

$$z = \mu + \epsilon \cdot \sigma$$

$$= \mathbb{E}_{\epsilon \sim N(0, I)} [f(\mu + \epsilon \sigma)] \quad \epsilon \sim N(0, I).$$

↑
no, & here

$$= \frac{1}{K} \sum_{i=1}^K f(\mu + \epsilon^{(i)} \sigma)$$

$\nabla_{\mu, \sigma} (\longrightarrow)$

\hookrightarrow much lower
variance

$$\max_{\theta, \phi} \mathbb{E}_{z \sim q_\phi(z|x^{(i)})} [\log p_z(z) + \log p_\theta(x^{(i)}|z) - \log q_\phi(z|x^{(i)})]$$

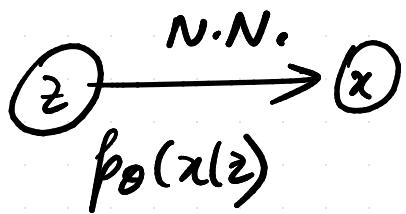
Differentiate
w.r.t. θ

$$\nabla_\theta = \nabla_\theta \mathbb{E}_{z \sim q_\phi} [\log p_\theta(x^{(i)}|z)]$$

$$= \nabla_\theta \sum_{k=1}^K \log p_\theta(x^{(i)}|z^{(k)})$$

$$z^{(k)} \sim q_\phi(z|x^{(i)})$$

(optimizing)



$$\nabla_{\phi} = \nabla_{\phi} q_{\phi}(z^{(k)}) \left[\log p_z(z^{(k)}) + \log p_0(x^{(i)}|z^{(k)}) - \log q_{\phi}(z^{(k)}|x^{(i)}) \right]$$

$$\Rightarrow \mathbb{E}_{z \sim q_{\phi}(z|x^{(i)})} \left[-\nabla_{\phi} \log q_{\phi}(z|x^{(i)}) \right]$$

$$\Rightarrow \mathbb{E}_{z \sim q_{\phi}} - \frac{\nabla_{\phi} q_{\phi}(z|x^{(i)})}{q_{\phi}(z|x^{(i)})}$$

$$\Rightarrow \sum_z \cancel{q_{\phi}(z|x^{(i)})} \quad \frac{\nabla_{\phi} q_{\phi}(z|x^{(i)})}{\cancel{q_{\phi}(z|x^{(i)})}}$$

$$\Rightarrow \nabla_{\phi} \left(\sum_z q_{\phi}(z|x^{(i)}) \right) = 0 \rightarrow \text{distribution, hence the gradient contribution is 0.}$$

Likelihood Ratio Estimator.

We are interested in :-

$$\arg \max_{\phi} \mathbb{E}_{z \sim q_{\phi}(z|x)} [f(z)]$$

How do we compute ,

$$\nabla_{\phi} \mathbb{E}_{z \sim q_{\phi}(z|x)} [f(z)]$$

$$\nabla_{\phi} \sum_z q_{\phi}(z|x) f(z) = \sum_z \nabla_{\phi} q_{\phi}(z|x) f(z)$$

$$= \sum_z \frac{\nabla_{\phi} q_{\phi}(z|x)}{q_{\phi}(z|x)} f(z) q_{\phi}(z|x)$$

$$= \nabla_{\phi} \mathbb{E}_{z \sim q_{\phi}(z|x)} [f(z)]$$

$$\Rightarrow \sum_z (\nabla_{\phi} \log q_{\phi}(z|x) f(z)) q_{\phi}(z|x)$$

if you derivative, then
this will be the (reverse).

$$\Rightarrow \sum_z (\nabla_{\phi} \log q_{\phi}(z|x) f(z)) q_{\phi}(z|x)$$

$$\Rightarrow \mathbb{E}_{z \sim q_{\phi}(\cdot|x)} [\nabla_{\phi} \log q_{\phi}(z|x) f(z)]$$

$$\phi \leftarrow \phi + \alpha \nabla_{\phi} \mathbb{E}_{z \sim q_{\phi}(\cdot|x)} [\nabla_{\phi} \log q_{\phi}(z|x) f(z)]$$

= 

pathwise derivative \underline{g}

z ~ continuous \rightarrow cast z as a function
of a sample fixed noise, such as a
standard Gaussian.

$$z = g(\varepsilon, \phi) \Rightarrow \varepsilon \sim N(0, I)$$

$$\mathbb{E}_{z \sim q_{\phi}(\cdot|x)} [f(z)] = \mathbb{E}_{\varepsilon \sim N(0,I)} [f(g(\varepsilon, \phi))]$$

When f is differentiable :-

$$\nabla_{\phi} \mathbb{E}_{z \sim q_{\phi}(z|x)} [f(z)] = \mathbb{E}_{\epsilon \sim N(0, I)} [\nabla_{\phi} f(g(\epsilon; \phi))]$$

Pathwise derivative applied to

Variational Inference \rightarrow Variational A-E.

$q_{\phi}(z|x) \rightarrow$ modelled as a Gaussian

with params μ & σ a DNN encoder
(param ϕ) of x . DNN decoder $p_{\theta}(x|z)$
is differentiable.

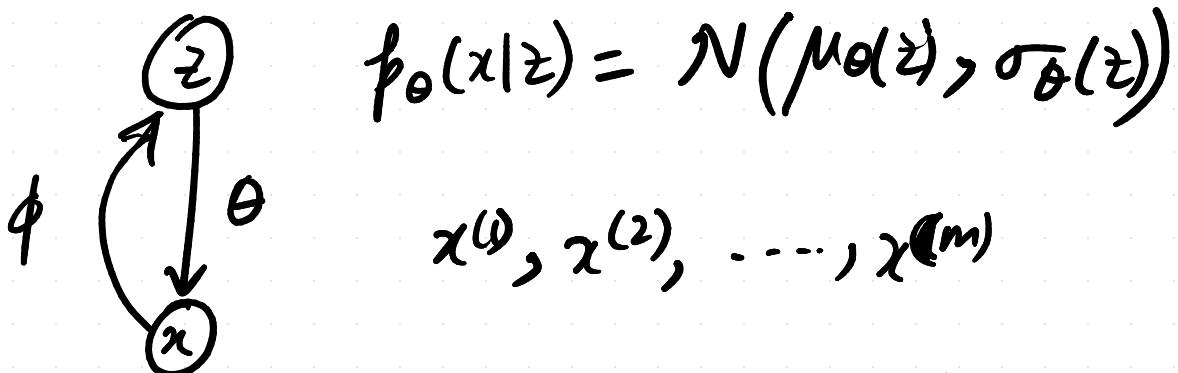
$$z = \sum^{\frac{1}{2}} (x; \phi) \epsilon + \mu(x; \phi).$$

$$\text{VLB} = \mathbb{E}_{\epsilon \sim N(0, I)} [\log p_{\theta}(x|z) - \log q_{\phi}(z|x) + \log p(z)]$$

$$= \mathbb{E}_{z \sim N(0, I)} [\log p_\theta(x|z)] - KL(q_\phi(z|x) || p(z))$$

$\nabla_\theta [VLB]$ & $\nabla_\phi [VLB]$ \rightarrow effectively
computed using SGD.

$$q(z|x) = N(\mu_\phi(x), \sigma_\phi(x))$$



$$\underline{q_\phi(z|x^{(t)}) \rightarrow z^{(t)}}$$

$ELBO(z^{(t)}) \rightarrow$ do a gradient descent
using that, update & repeat.

Why is it called Auto-Encoder?

Gaussian Prior $\rightarrow p(z)$.

Approximate posterior $\rightarrow q_\phi(z|x)$.
reconstruction loss.

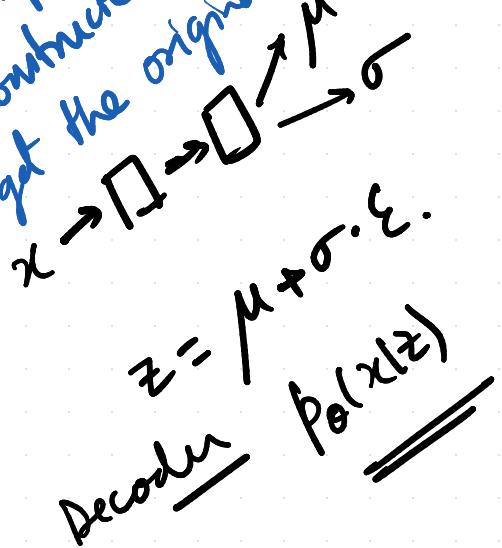
$$\log p_\theta(x) \geq \left(E_{z \sim q_\phi(z)} \log p_\theta(x|z) \right)$$

$$- \text{KL} \left(q_\phi(z|x) \parallel p(z) \right)$$

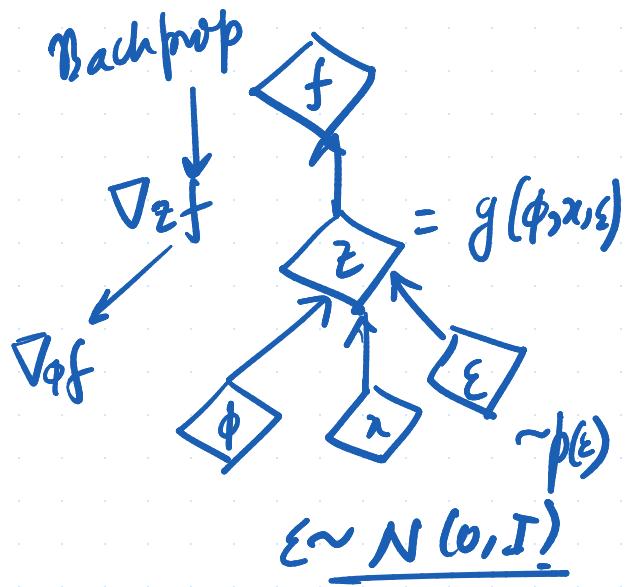
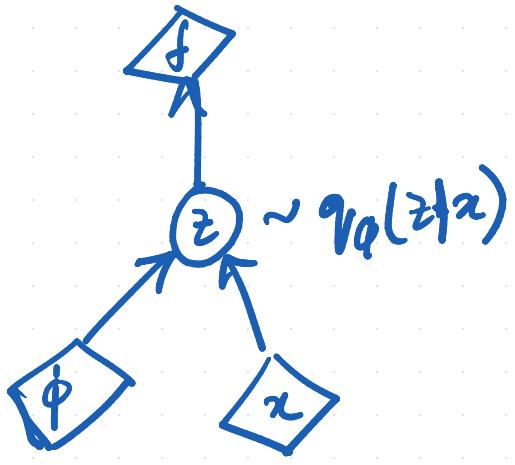
Auto-encoder
part.

Regularization

How likely
 $p_\theta(x|z)$ to
sample the x &
reconstructed, we will
get the original one back.
 $\mathcal{L}(\theta, \phi)$ - VAE objective



My posterior of $z|x$ has
to be some-what close
to $p(z)$.



The variational parameter ϕ affects the objective f through the R.V. $z \sim q_\phi(z|x)$, we wish to compute gradients $\nabla_{\phi} f$ to optimize the objective with SGD.

Original form (left) we cannot differentiate f w.r.t. ϕ , because we cannot directly backprop gradients through R.V. (z).

Externalize the randomness in z by re-parameterizing the variable as a

deterministic and differentiable function ϕ , and a newly introduced L-V-E.

This allows us to backprop through
 z & compute $\nabla \phi f$.