

# VARIATIONAL AUTOENCODER

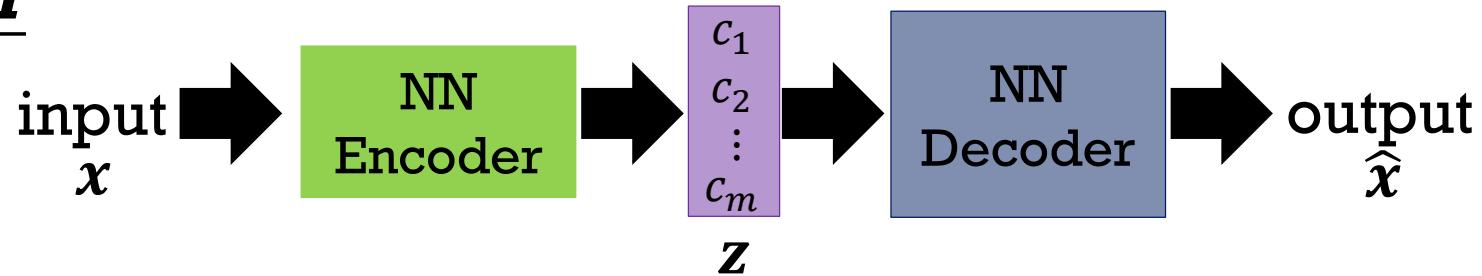
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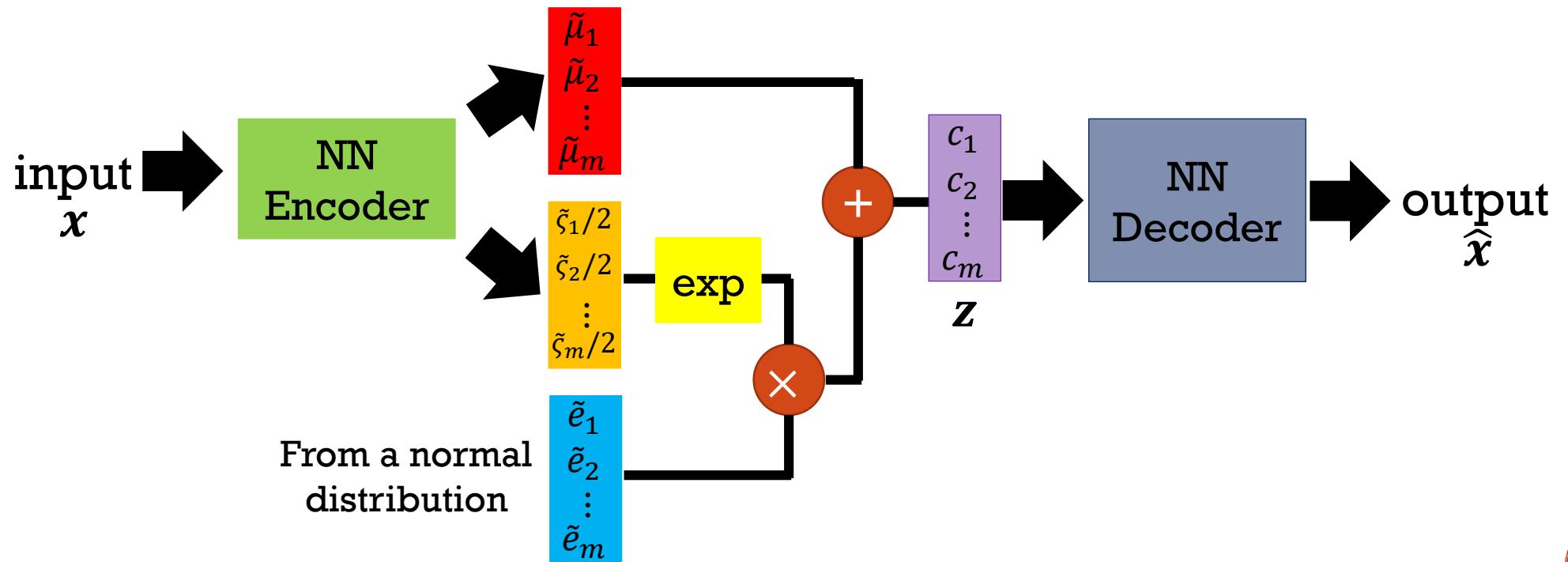
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# AUTO ENCODER V.S. VAE

## Auto-encoder

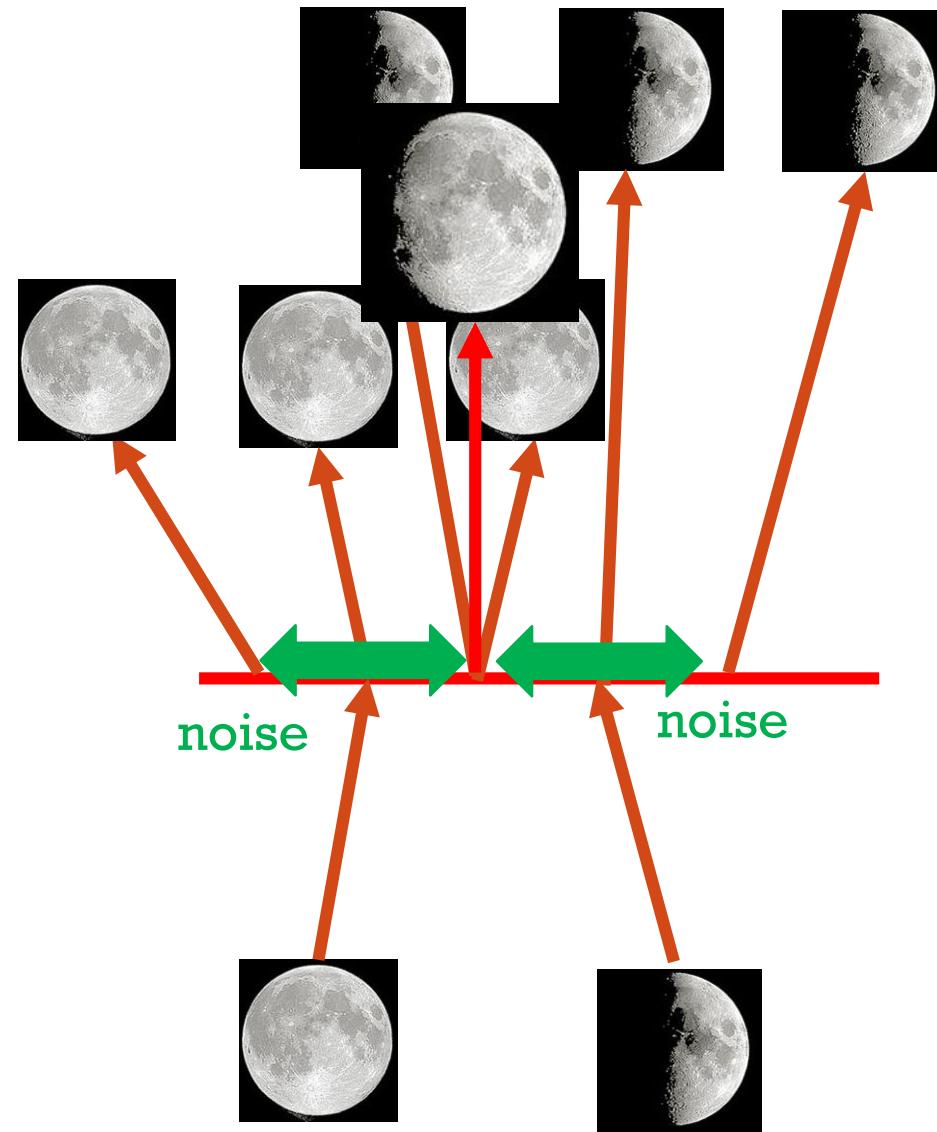
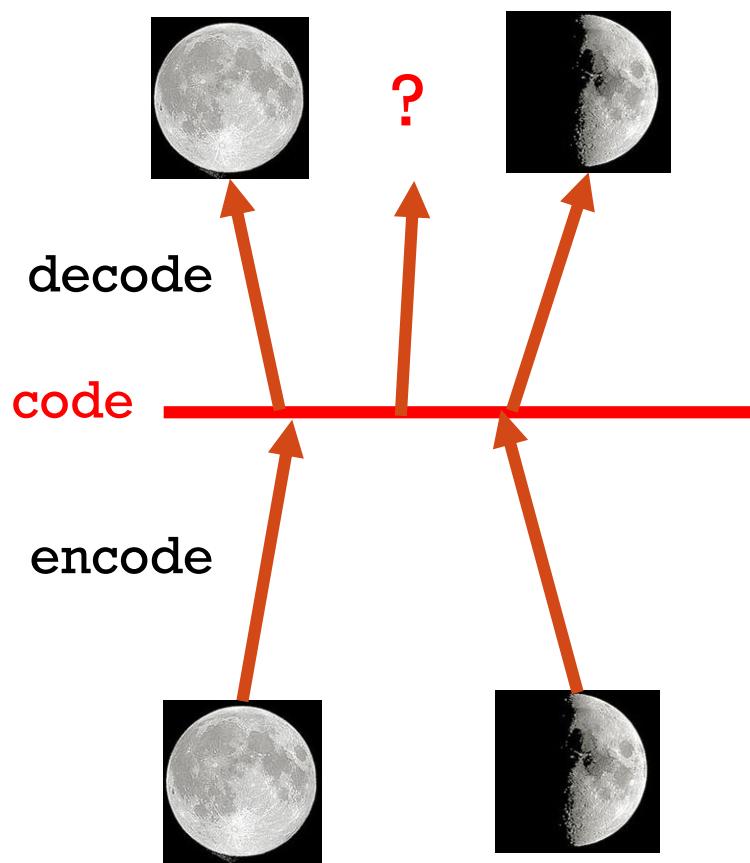


## VAE

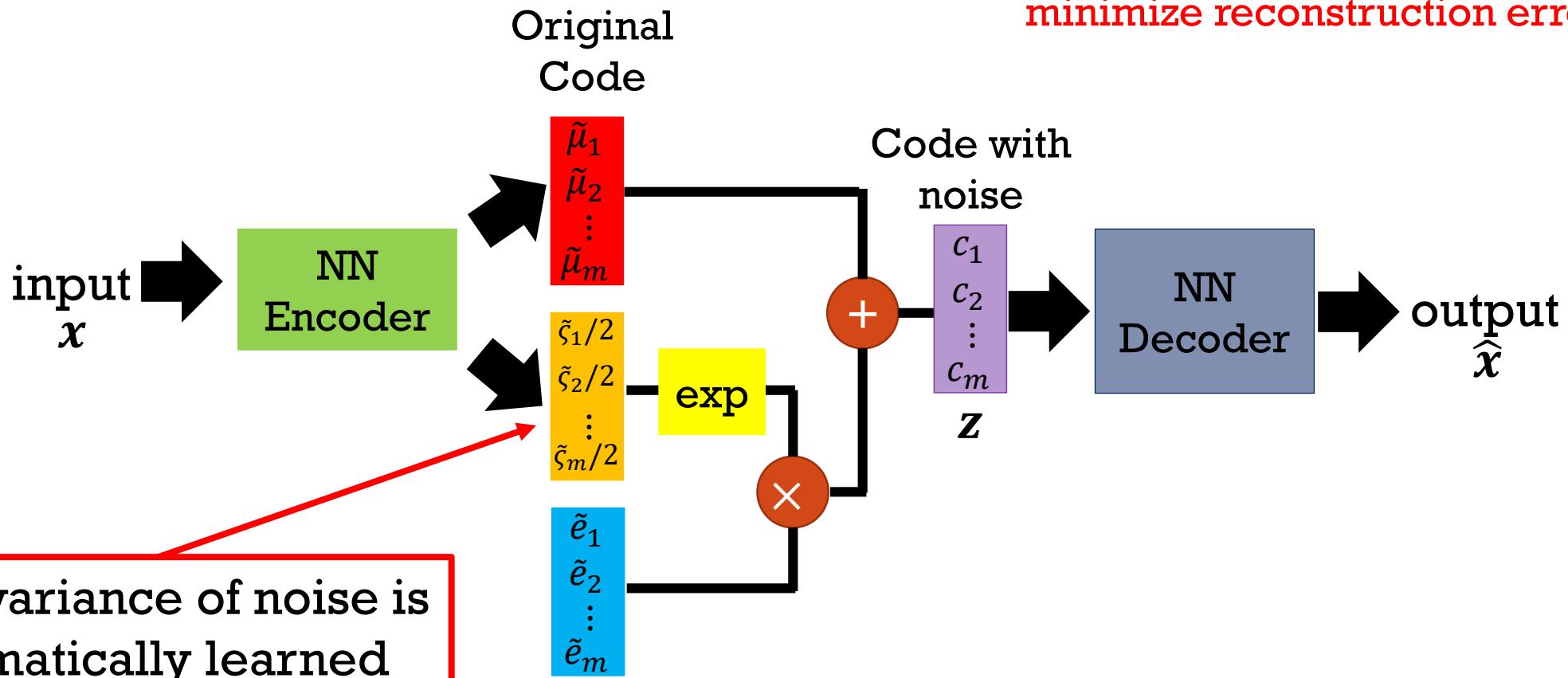


# WHY VAE?

## Intuitive Reason



# VAE LOSS FUNCTION



What will happen if we only minimize reconstruction error?

Given data set  $x_1, \dots, x_N$ , minimize

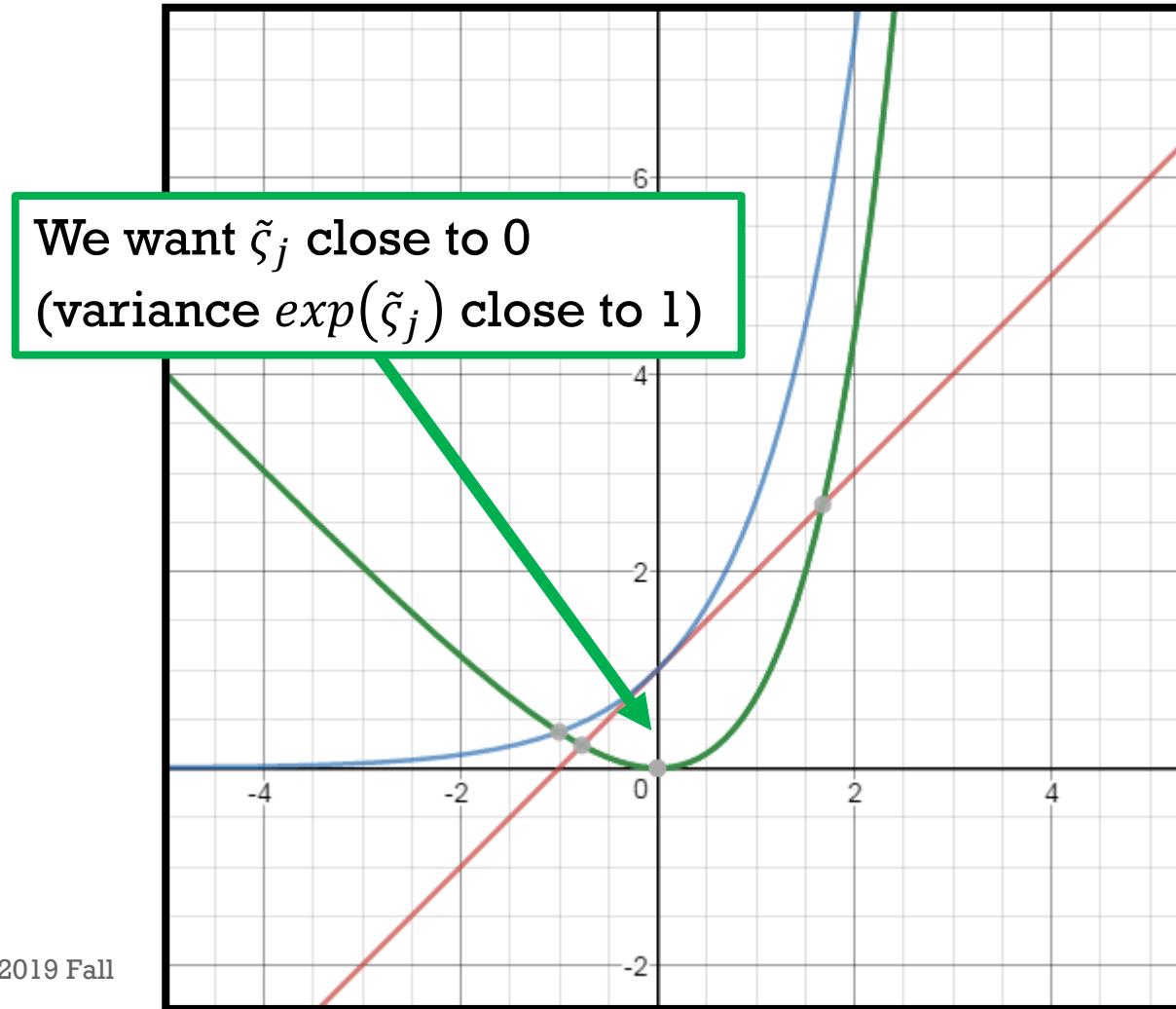
$$L_{VAE} = \sum_{i=1}^N \left( \|x_i - \hat{x}_i\|^2 + \sum_{j=1}^m \left( \|\tilde{\mu}_j(x_i)\|^2 + \exp(\tilde{\xi}_j(x_i)) - (1 + \tilde{\xi}_j(x_i)) \right) \right)$$

Reconstruction loss

Regularization loss

# WHY VAE REGULARIZATION?

**Intuitive Reason:** Want the code to have zero mean and unit variance



Regularization loss  
$$\|\tilde{\mu}_j(x_i)\|^2 + \exp(\tilde{\zeta}_j(x_i)) - (1 + \tilde{\zeta}_j(x_i))$$

# VAE GENERATIVE MODEL AND MLE

- We have data set  $\mathcal{X} = \{x_1, \dots, x_N\}$ , and assume each data point  $x_i$  is generated according to generative model

$$p_\theta(x) = \int p_\theta(x|z)p_\theta(z)dz$$

- Goal: Maximum log-likelihood parameter estimation:

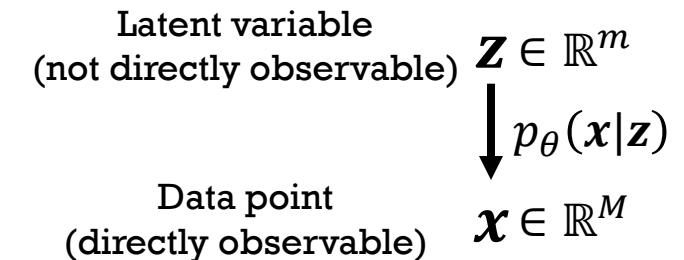
$$\theta^* = \max_{\theta \in \Theta} p_\theta(\mathcal{X}) = \max_{\theta \in \Theta} \log p_\theta(\mathcal{X})$$

- If each data point  $x_i$  is generated independently, then

$$\log p_\theta(\mathcal{X}) = \log \left( \prod_{i=1}^N p_\theta(x_i) \right) = \sum_{i=1}^N \log p_\theta(x_i)$$

$$p_\theta(x_i) = \int p_\theta(x_i|z_i)p_\theta(z_i)dz_i$$

- Introduce latent variables  $Z = \{z_1, \dots, z_N\}$ , where  $z_i$  indicates the latent code of  $x_i$ .



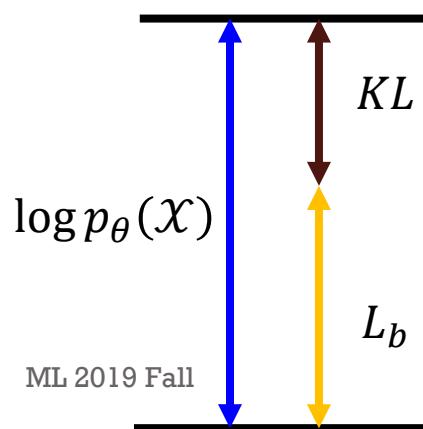
# LOG-LIKELIHOOD LOWER BOUND

$$\begin{aligned}\log p_\theta(\mathcal{X}) &= \int q_\phi(Z|\mathcal{X}) \log p_\theta(\mathcal{X}) dZ \\ &= \int q_\phi(Z|\mathcal{X}) \left( \log \frac{p_\theta(Z, \mathcal{X})}{q_\phi(Z|\mathcal{X})} - \log \frac{p_\theta(Z|\mathcal{X})}{q_\phi(Z|\mathcal{X})} \right) dZ \\ &= \int q_\phi(Z|\mathcal{X}) \log \frac{p_\theta(Z, \mathcal{X})}{q_\phi(Z|\mathcal{X})} dZ + KL(q_\phi(\cdot|\mathcal{X}), p_\theta(\cdot|\mathcal{X}))\end{aligned}$$

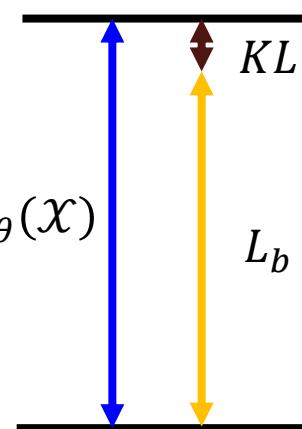
Tractable lower bound

$$L_b(p_\theta, q_\phi, \mathcal{X})$$

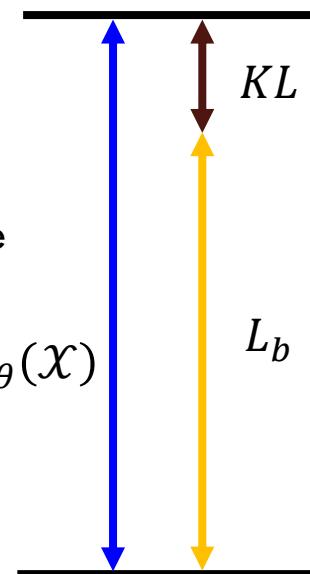
Intractable but always  $\geq 0$



Fix  $p_\theta$  and increase  
 $L_b$  by adjusting  $q_\phi$



Fix  $q_\phi$  and increase  
 $L_b$  by adjusting  $p_\theta$



# VAE V.S. EM ALGORITHM

- Randomly initialize parameters  $\theta^{(1)}$ .
- Iterate through step  $t=1, 2, \dots$

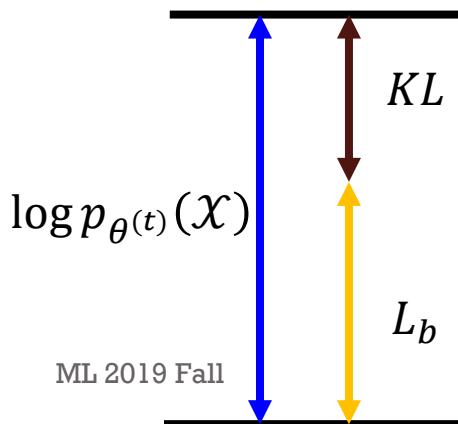
➤ Expectation Step (E-step): Compute

$$Q(\theta|\theta^{(t)}) = \sum_Z p(Z|\mathcal{X}; \theta^{(t)}) \log p(\mathcal{X}, Z; \theta)$$

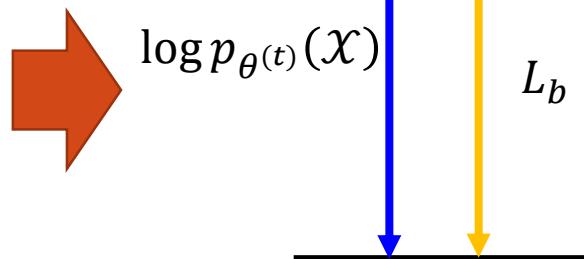
➤ Maximization Step (M-step): Choose

$$\theta^{(t+1)} = \operatorname{argmax}_{\theta \in \Theta} Q(\theta|\theta^{(t)})$$

Adjust  $q_\phi$  to decrease  $KL(q_\phi(\cdot|\mathcal{X}), p_{\theta^{(t)}}(\cdot|\mathcal{X}))$   
will make  $q_\phi(\cdot|\mathcal{X}) \approx p_{\theta^{(t)}}(\cdot|\mathcal{X})$



Fix  $p_\theta$  and increase  
 $L_b$  by adjusting  $q_\phi$



Fix  $q_\phi$  and adjust  $p_\theta$  to maximize

$$L_b(p_\theta, q_\phi, \mathcal{X}) = \mathbb{E}_{Z \sim q_\phi(\cdot|\mathcal{X})} \left[ \log \frac{p_\theta(\mathcal{X}, Z)}{q_\phi(Z|\mathcal{X})} \right]$$

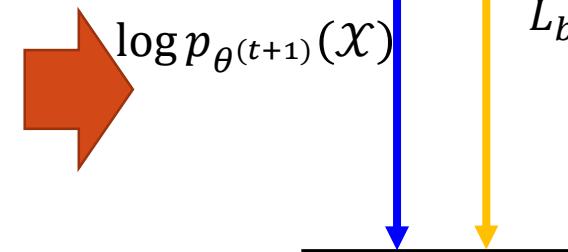
is equivalent to maximizing

$$\mathbb{E}_{Z \sim q_\phi(\cdot|\mathcal{X})} [\log p_\theta(\mathcal{X}, Z)] \approx Q(\theta|\theta^{(t)})$$

approx.  $p_{\theta^{(t)}}(\cdot|\mathcal{X})$

**EM Algorithm**

Fix  $q_\phi$  and increase  
 $L_b$  by adjusting  $p_\theta$



# VAE WITH INDEPENDENT SAMPLES

- Goal: Adjust  $p_\theta$  and  $q_\phi$  to maximize

$$\begin{aligned} L_b(p_\theta, q_\phi, \mathcal{X}) &= \mathbb{E}_{Z \sim q_\phi(\cdot | \mathcal{X})} \left[ \log \frac{p_\theta(\mathcal{X}, Z)}{q_\phi(Z | \mathcal{X})} \right] \\ &= \mathbb{E}_{Z \sim q_\phi(\cdot | \mathcal{X})} \left[ \log \frac{p_\theta(\mathcal{X} | Z)}{q_\phi(Z | \mathcal{X})} \right] + \mathbb{E}_{Z \sim q_\phi(\cdot | \mathcal{X})} [\log p_\theta(Z)] \end{aligned}$$

- Assume  $(x_1, z_1), \dots, (x_N, z_N)$  are independent w.r.t.  $p_\theta$  and  $q_\phi$ , then

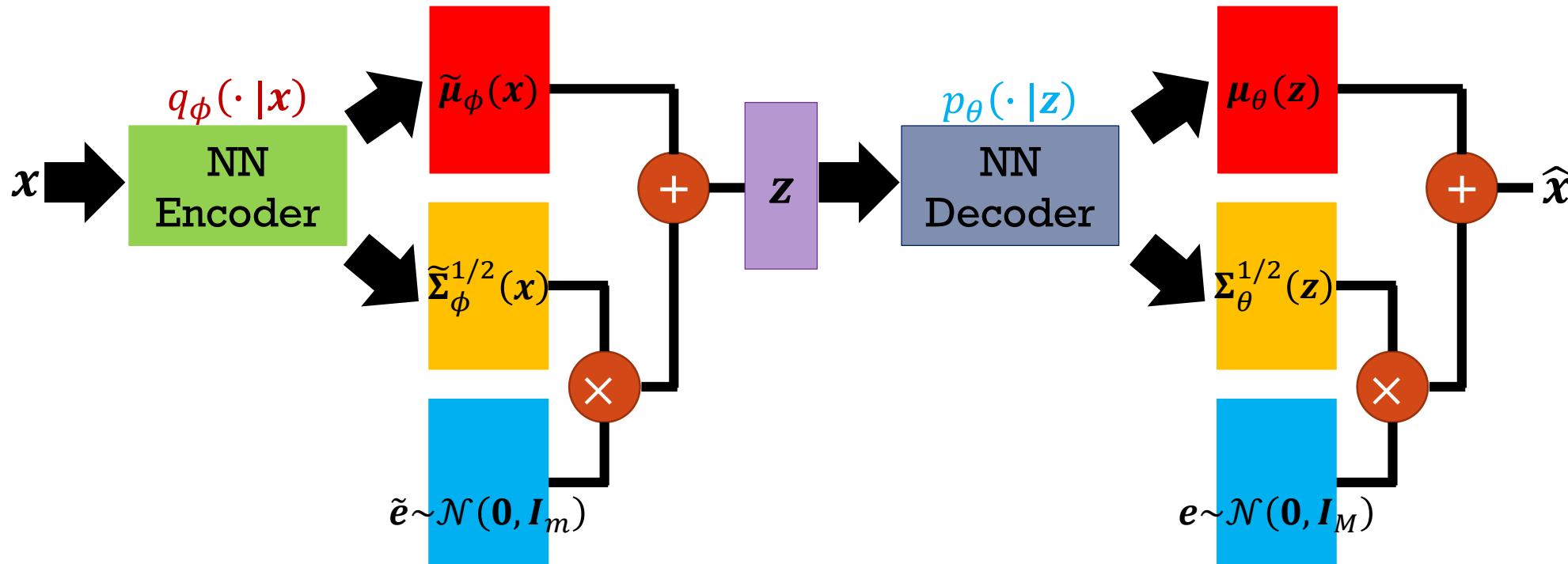
$$\begin{aligned} q_\phi(Z | \mathcal{X}) &= \prod_{i=1}^N q_\phi(z_i | x_i), p_\theta(\mathcal{X} | Z) = \prod_{i=1}^N p_\theta(x_i | z_i), p_\theta(Z) = \prod_{i=1}^N p_\theta(z_i) \\ \mathbb{E}_{Z \sim q_\phi(\cdot | \mathcal{X})} \left[ \log \frac{p_\theta(\mathcal{X} | Z)}{q_\phi(Z | \mathcal{X})} \right] &= \sum_{i=1}^N \mathbb{E}_{Z \sim q_\phi(\cdot | \mathcal{X})} \left[ \log \frac{p_\theta(x_i | z_i)}{q_\phi(z_i | x_i)} \right] = \sum_{i=1}^N \mathbb{E}_{z_i \sim q_\phi(\cdot | x_i)} \left[ \log \frac{p_\theta(x_i | z_i)}{q_\phi(z_i | x_i)} \right] \\ \mathbb{E}_{Z \sim q_\phi(\cdot | \mathcal{X})} [\log p_\theta(Z)] &= \sum_{i=1}^N \mathbb{E}_{Z \sim q_\phi(\cdot | \mathcal{X})} [\log p_\theta(z_i)] = \sum_{i=1}^N \mathbb{E}_{z_i \sim q_\phi(\cdot | x_i)} [\log p_\theta(z_i)] \end{aligned}$$

Hence

$$L_b(p_\theta, q_\phi, \mathcal{X}) = \sum_{i=1}^N \mathbb{E}_{z_i \sim q_\phi(\cdot | x_i)} \left[ \log \frac{p_\theta(x_i | z_i)}{q_\phi(z_i | x_i)} + \log p_\theta(z_i) \right]$$

# VAE AND GAUSSIAN DISTRIBUTION

- Assume latent code has Gaussian prior, and both encoder/decoder described by Gaussian distributions:  $p_\theta(z) = \mathcal{N}(z; \mathbf{0}, I)$ ,  $p_\theta(x|z) = \mathcal{N}(x; \mu_\theta(z), \Sigma_\theta(z))$ ,  $q_\phi(z|x) = \mathcal{N}(z; \tilde{\mu}_\phi(x), \tilde{\Sigma}_\phi(x))$ .



# CLOSE FORM OF $L_b$

- Assume latent code has Gaussian prior, and both encoder/decoder described by Gaussian distributions:  $p_\theta(\mathbf{z}) = \mathcal{N}(\mathbf{z}; \mathbf{0}, \mathbf{I})$ ,  $p_\theta(\mathbf{x}|\mathbf{z}) = \mathcal{N}(\mathbf{x}; \boldsymbol{\mu}_\theta(\mathbf{z}), \boldsymbol{\Sigma}_\theta(\mathbf{z}))$ ,  $q_\phi(\mathbf{z}|\mathbf{x}) = \mathcal{N}(\mathbf{z}; \tilde{\boldsymbol{\mu}}_\phi(\mathbf{x}), \tilde{\boldsymbol{\Sigma}}_\phi(\mathbf{x}))$ . Then

$$\begin{aligned}
& \mathbb{E}_{\mathbf{z}_i \sim q_\phi(\cdot|\mathbf{x}_i)} \left[ \log \frac{p_\theta(\mathbf{x}_i|\mathbf{z}_i)}{q_\phi(\mathbf{z}_i|\mathbf{x}_i)} + \log p_\theta(\mathbf{z}_i) \right] = \mathbb{E}_{\mathbf{z}_i \sim \mathcal{N}(\tilde{\boldsymbol{\mu}}_\phi(\mathbf{x}_i), \tilde{\boldsymbol{\Sigma}}_\phi(\mathbf{x}_i))} \left[ \log \frac{\mathcal{N}(\mathbf{x}_i; \boldsymbol{\mu}_\theta(\mathbf{z}_i), \boldsymbol{\Sigma}_\theta(\mathbf{z}_i))}{\mathcal{N}(\mathbf{z}_i; \tilde{\boldsymbol{\mu}}_\phi(\mathbf{x}_i), \tilde{\boldsymbol{\Sigma}}_\phi(\mathbf{x}_i))} + \log \mathcal{N}(\mathbf{z}_i; \mathbf{0}, \mathbf{I}) \right] \\
&= \mathbb{E}_{\mathbf{z}_i \sim \mathcal{N}(\tilde{\boldsymbol{\mu}}_\phi(\mathbf{x}_i), \tilde{\boldsymbol{\Sigma}}_\phi(\mathbf{x}_i))} [\log \mathcal{N}(\mathbf{x}_i; \boldsymbol{\mu}_\theta(\mathbf{z}_i), \boldsymbol{\Sigma}_\theta(\mathbf{z}_i))] + \log \frac{\mathcal{N}(\tilde{\boldsymbol{\mu}}_\phi(\mathbf{x}_i); \mathbf{0}, \mathbf{I})}{\mathcal{N}(\tilde{\boldsymbol{\mu}}_\phi(\mathbf{x}_i); \tilde{\boldsymbol{\mu}}_\phi(\mathbf{x}_i), \tilde{\boldsymbol{\Sigma}}_\phi(\mathbf{x}_i))} - \frac{\text{Tr}(\tilde{\boldsymbol{\Sigma}}_\phi(\mathbf{x}_i) - \mathbf{I})}{2} \\
&= \mathbb{E}_{\mathbf{z}_i \sim \mathcal{N}(\tilde{\boldsymbol{\mu}}_\phi(\mathbf{x}_i), \tilde{\boldsymbol{\Sigma}}_\phi(\mathbf{x}_i))} \left[ \log \left( \frac{1}{\sqrt{(2\pi)^M |\boldsymbol{\Sigma}_\theta(\mathbf{z}_i)|}} \exp \left( -\frac{1}{2} (\mathbf{x}_i - \boldsymbol{\mu}_\theta(\mathbf{z}_i))^T \boldsymbol{\Sigma}_\theta(\mathbf{z}_i)^{-1} (\mathbf{x}_i - \boldsymbol{\mu}_\theta(\mathbf{z}_i)) \right) \right) \right] \\
&\quad + \log \left( \frac{\frac{1}{\sqrt{(2\pi)^m}} \exp \left( -\frac{1}{2} \|\tilde{\boldsymbol{\mu}}_\phi(\mathbf{x}_i)\|^2 \right)}{1/\sqrt{(2\pi)^m |\tilde{\boldsymbol{\Sigma}}_\phi(\mathbf{x}_i)|}} \right) - \frac{\text{Tr}(\tilde{\boldsymbol{\Sigma}}_\phi(\mathbf{x}_i) - \mathbf{I})}{2} \\
&= \mathbb{E}_{\mathbf{z}_i \sim \mathcal{N}(\tilde{\boldsymbol{\mu}}_\phi(\mathbf{x}_i), \tilde{\boldsymbol{\Sigma}}_\phi(\mathbf{x}_i))} \left[ \log \frac{1}{\sqrt{(2\pi)^M |\boldsymbol{\Sigma}_\theta(\mathbf{z}_i)|}} - \frac{1}{2} (\mathbf{x}_i - \boldsymbol{\mu}_\theta(\mathbf{z}_i))^T \boldsymbol{\Sigma}_\theta(\mathbf{z}_i)^{-1} (\mathbf{x}_i - \boldsymbol{\mu}_\theta(\mathbf{z}_i)) \right] + \frac{1}{2} \log |\boldsymbol{\Sigma}_\theta(\mathbf{z}_i)| \\
&\quad - \frac{1}{2} \|\tilde{\boldsymbol{\mu}}_\phi(\mathbf{x}_i)\|^2 - \frac{\text{Tr}(\tilde{\boldsymbol{\Sigma}}_\phi(\mathbf{x}_i) - \mathbf{I})}{2}
\end{aligned}$$

**Lemma:** Let  $\xi \sim \mathcal{N}(\tilde{\mu}, \tilde{\Sigma})$  be a Gaussian-distributed r.v. in  $\mathbb{R}^m$ , then

$$\begin{aligned}\mathbb{E}_{\xi \sim \mathcal{N}(\tilde{\mu}, \tilde{\Sigma})} [\log \mathcal{N}(\xi; \mu, \Sigma)] &= \log \frac{1}{\sqrt{(2\pi)^m |\Sigma|}} - \frac{1}{2} \left( (\tilde{\mu} - \mu)^T \Sigma^{-1} (\tilde{\mu} - \mu) + \text{Tr}(\tilde{\Sigma} \Sigma^{-1}) \right) \\ &= \log \mathcal{N}(\tilde{\mu}; \mu, \Sigma) - \text{Tr}(\tilde{\Sigma} \Sigma^{-1}) / 2\end{aligned}$$

In particular, if  $\tilde{\mu} = \mu$ ,  $\tilde{\Sigma} = \Sigma$ , then

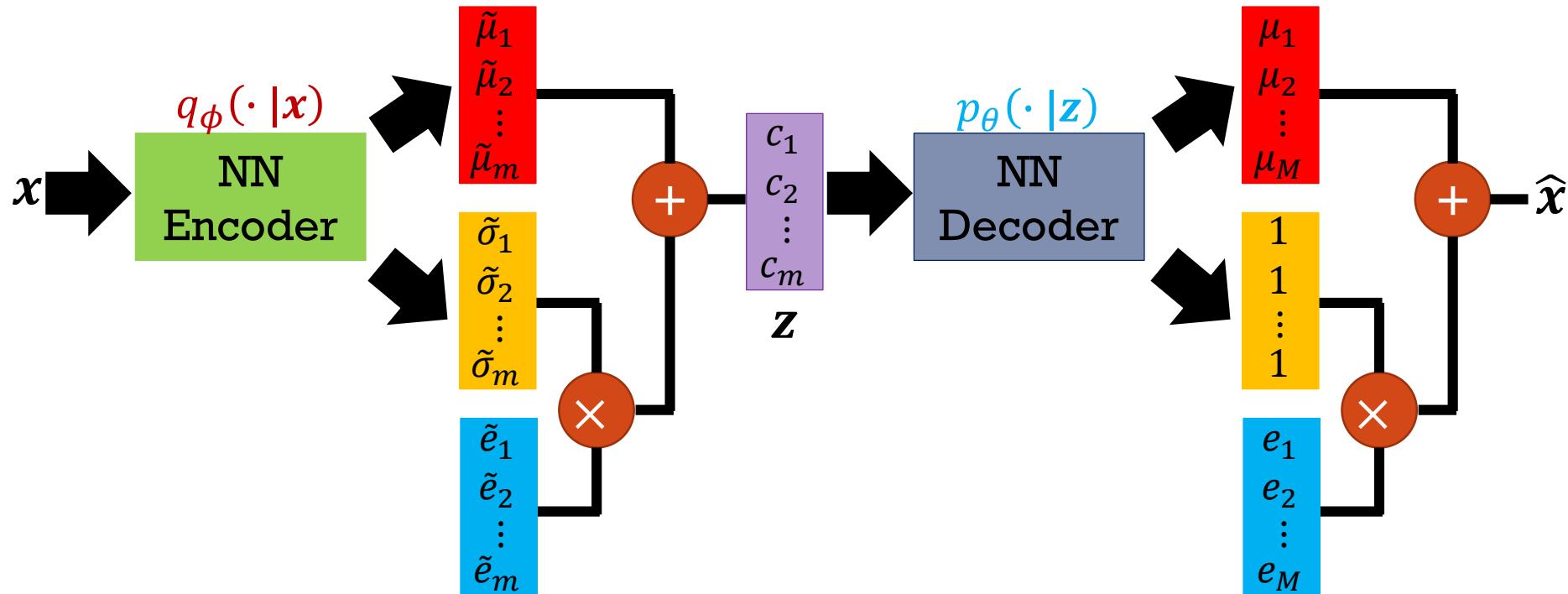
$$\mathbb{E}_{\xi \sim \mathcal{N}(\mu, \Sigma)} [\log \mathcal{N}(\xi; \mu, \Sigma)] = -\frac{m}{2} \log(2\pi e |\Sigma|^{1/m})$$

Proof:

$$\begin{aligned}\mathbb{E}_{\xi \sim \mathcal{N}(\tilde{\mu}, \tilde{\Sigma})} [\log \mathcal{N}(\xi; \mu, \Sigma)] &= \mathbb{E}_{\xi \sim \mathcal{N}(\tilde{\mu}, \tilde{\Sigma})} \left[ \log \frac{1}{\sqrt{(2\pi)^m |\Sigma|}} - \frac{1}{2} (\xi - \mu)^T \Sigma^{-1} (\xi - \mu) \right] \\ &= \log \frac{1}{\sqrt{(2\pi)^m |\Sigma|}} - \frac{1}{2} \mathbb{E}_{\xi \sim \mathcal{N}(\tilde{\mu}, \tilde{\Sigma})} [\text{Tr}((\xi - \mu)^T \Sigma^{-1} (\xi - \mu))] \\ &= \log \frac{1}{\sqrt{(2\pi)^m |\Sigma|}} - \frac{1}{2} \text{Tr} \left( \mathbb{E}_{\xi \sim \mathcal{N}(\tilde{\mu}, \tilde{\Sigma})} [(\xi - \mu)(\xi - \mu)^T \Sigma^{-1}] \right) \\ &= \log \frac{1}{\sqrt{(2\pi)^m |\Sigma|}} - \frac{1}{2} \text{Tr} \left( \mathbb{E}_{\xi \sim \mathcal{N}(\tilde{\mu}, \tilde{\Sigma})} [(\xi - \mu)(\xi - \mu)^T \Sigma^{-1}] \right) \\ &= \log \frac{1}{\sqrt{(2\pi)^m |\Sigma|}} - \frac{1}{2} \text{Tr} \left( \mathbb{E}_{\xi' \sim \mathcal{N}(\mathbf{0}, \tilde{\Sigma})} [(\xi' + \tilde{\mu} - \mu)(\xi' + \tilde{\mu} - \mu)^T \Sigma^{-1}] \right) \\ &= \log \frac{1}{\sqrt{(2\pi)^m |\Sigma|}} - \frac{1}{2} \text{Tr} \left( (\tilde{\Sigma} + (\tilde{\mu} - \mu)(\tilde{\mu} - \mu)^T) \Sigma^{-1} \right) = \log \frac{1}{\sqrt{(2\pi)^m |\Sigma|}} - \frac{1}{2} \left( (\tilde{\mu} - \mu)^T \Sigma^{-1} (\tilde{\mu} - \mu) + \text{Tr}(\tilde{\Sigma} \Sigma^{-1}) \right)\end{aligned}$$

# SIMPLER CLOSE FORM OF $L_b$

- For simplicity, assume  $\Sigma_\theta(z_i) = I$ ,  $\tilde{\Sigma}_\phi(x) = \text{diag}(\tilde{\sigma}_{\phi,1}^2(x), \dots, \tilde{\sigma}_{\phi,m}^2(x))$ .



# VAE LOSS FUNCTION

- For simplicity, assume  $\Sigma_\theta(\mathbf{z}_i) = \mathbf{I}$ ,  $\tilde{\Sigma}_\phi(\mathbf{x}) = \text{diag}(\tilde{\sigma}_{\phi,1}^2(\mathbf{x}), \dots, \tilde{\sigma}_{\phi,m}^2(\mathbf{x}))$ , then

$$\begin{aligned} & \mathbb{E}_{\mathbf{z}_i \sim q_\phi(\cdot | \mathbf{x}_i)} \left[ \log \frac{p_\theta(\mathbf{x}_i | \mathbf{z}_i)}{q_\phi(\mathbf{z}_i | \mathbf{x}_i)} + \log p_\theta(\mathbf{z}_i) \right] \\ &= \mathbb{E}_{\mathbf{z}_i \sim \mathcal{N}(\tilde{\mu}_\phi(\mathbf{x}_i), \tilde{\Sigma}_\phi(\mathbf{x}_i))} \left[ \log \frac{1}{\sqrt{(2\pi)^M |\Sigma_\theta(\mathbf{z}_i)|}} - \frac{1}{2} (\mathbf{x}_i - \boldsymbol{\mu}_\theta(\mathbf{z}_i))^T \Sigma_\theta(\mathbf{z}_i)^{-1} (\mathbf{x}_i - \boldsymbol{\mu}_\theta(\mathbf{z}_i)) \right] + \frac{1}{2} \log |\Sigma_\theta(\mathbf{z}_i)| - \frac{1}{2} \|\tilde{\boldsymbol{\mu}}_\phi(\mathbf{x}_i)\|^2 \\ & - \frac{1}{2} \text{Tr}(\tilde{\Sigma}_\phi(\mathbf{x}_i) - \mathbf{I}) = \log \frac{1}{\sqrt{(2\pi)^M}} - \frac{1}{2} \left( \mathbb{E}_{\mathbf{z}_i \sim \mathcal{N}(\tilde{\mu}_\phi(\mathbf{x}_i), \tilde{\Sigma}_\phi(\mathbf{x}_i))} [\|\mathbf{x}_i - \boldsymbol{\mu}_\theta(\mathbf{z}_i)\|^2] + \|\tilde{\boldsymbol{\mu}}_\phi(\mathbf{x}_i)\|^2 + \sum_{j=1}^m (\tilde{\sigma}_{\phi,j}^2(\mathbf{x}_i) - \log \tilde{\sigma}_{\phi,j}^2(\mathbf{x}_i) - 1) \right) \end{aligned}$$

Hence maximizing

$$L_b(p_\theta, q_\phi, \mathcal{X}) = N \log \frac{1}{\sqrt{(2\pi)^M}} - \frac{1}{2} \sum_{i=1}^N \left( \mathbb{E}_{\mathbf{z}_i \sim \mathcal{N}(\tilde{\mu}_\phi(\mathbf{x}_i), \tilde{\Sigma}_\phi(\mathbf{x}_i))} [\|\mathbf{x}_i - \boldsymbol{\mu}_\theta(\mathbf{z}_i)\|^2] + \|\tilde{\boldsymbol{\mu}}_\phi(\mathbf{x}_i)\|^2 + \sum_{j=1}^m (\tilde{\sigma}_{\phi,j}^2(\mathbf{x}_i) - \log \tilde{\sigma}_{\phi,j}^2(\mathbf{x}_i) - 1) \right)$$

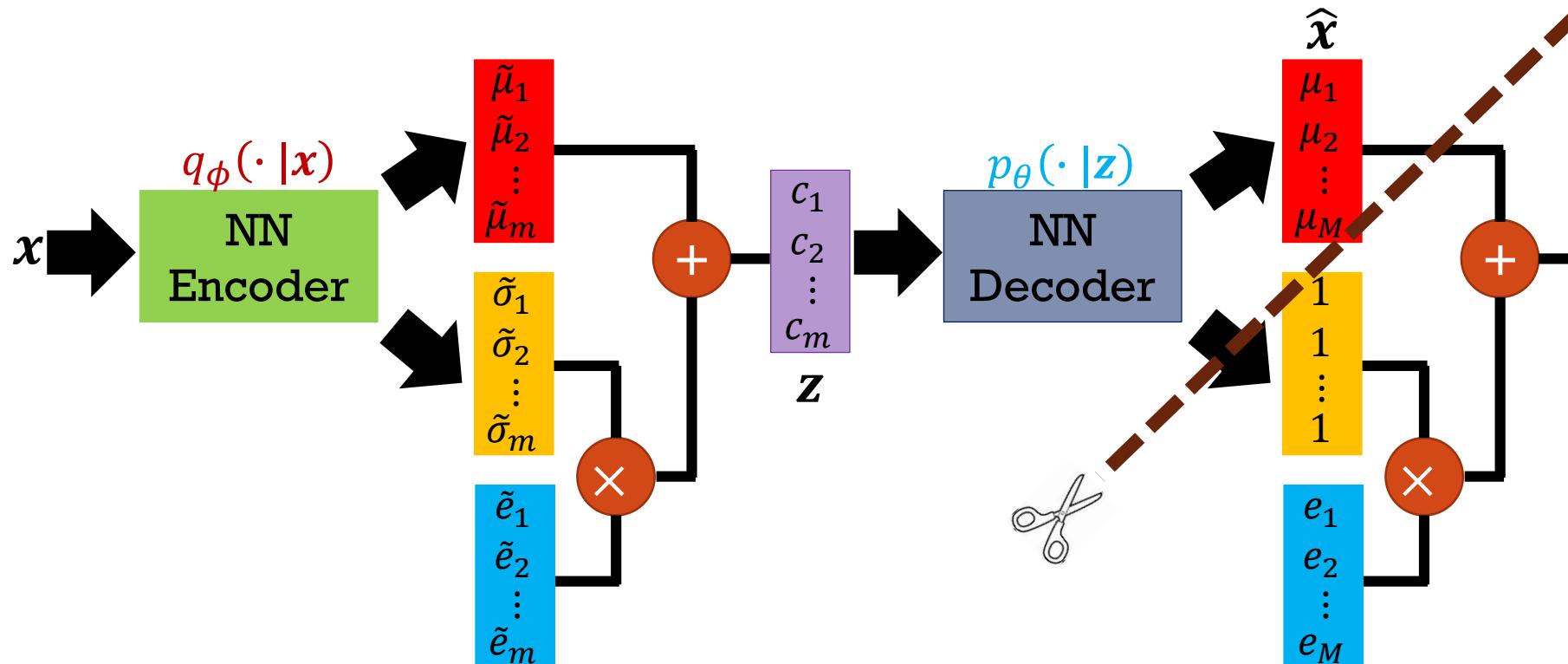
Is equivalent to minimizing

$$\sum_{i=1}^N \left( \mathbb{E}_{\mathbf{z}_i \sim \mathcal{N}(\tilde{\mu}_\phi(\mathbf{x}_i), \tilde{\Sigma}_\phi(\mathbf{x}_i))} [\|\mathbf{x}_i - \boldsymbol{\mu}_\theta(\mathbf{z}_i)\|^2] + \|\tilde{\boldsymbol{\mu}}_\phi(\mathbf{x}_i)\|^2 + \sum_{j=1}^m (\tilde{\sigma}_{\phi,j}^2(\mathbf{x}_i) - (1 + \log \tilde{\sigma}_{\phi,j}^2(\mathbf{x}_i))) \right)$$

Approx. expectation by sample mean

# VAE LOSS FUNCTION

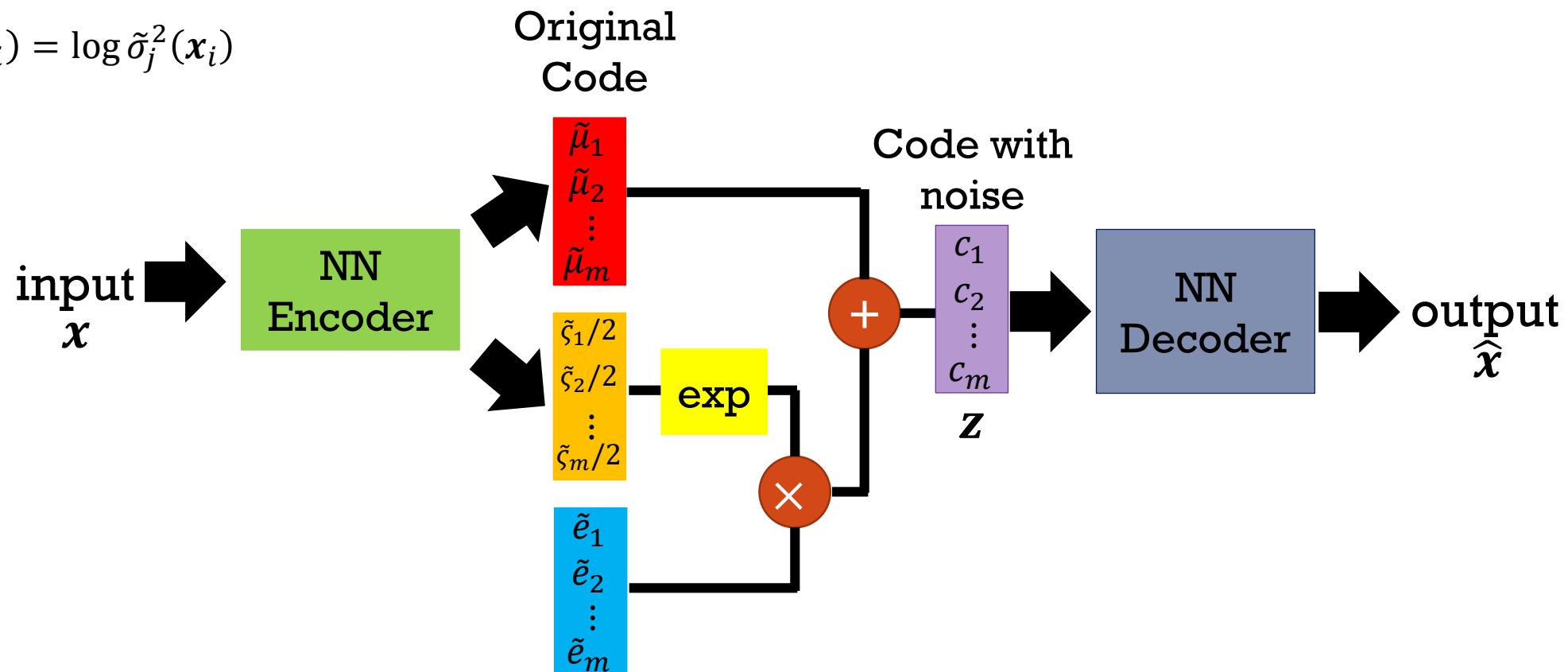
- For simplicity, assume  $\Sigma_\theta(z_i) = I$ ,  $\tilde{\Sigma}_\phi(x) = \text{diag}(\tilde{\sigma}_{\phi,1}^2(x), \dots, \tilde{\sigma}_{\phi,m}^2(x))$ .



$$L_{VAE} = \sum_{i=1}^N \left( \|x_i - \hat{x}_i\|^2 + \sum_{j=1}^m \left( \|\tilde{\mu}_j(x_i)\|^2 + \tilde{\sigma}_j^2(x_i) - (1 + \log \tilde{\sigma}_j^2(x_i)) \right) \right)$$

# VAE LOSS FUNCTION

Take  $\tilde{\zeta}_j(x_i) = \log \tilde{\sigma}_j^2(x_i)$



Minimize

$$L_{VAE} = \sum_{i=1}^N \left( \|x_i - \hat{x}_i\|^2 + \sum_{j=1}^m \left( \|\tilde{\mu}_j(x_i)\|^2 + \exp(\tilde{\zeta}_j(x_i)) - (1 + \tilde{\zeta}_j(x_i)) \right) \right)$$

