Variational Autoencoder

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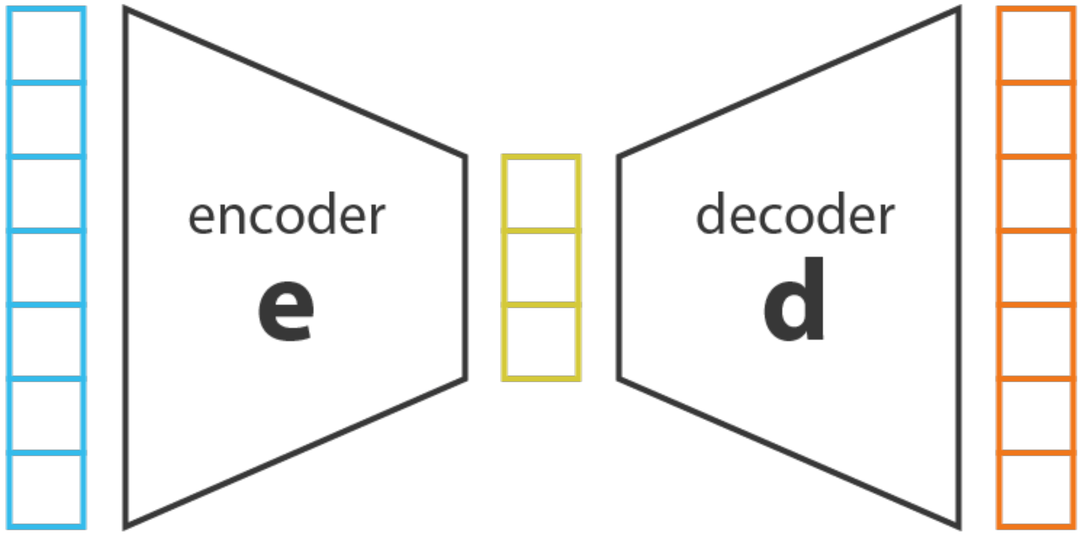
Encoder and Decoder



x

initial data
in space R^n

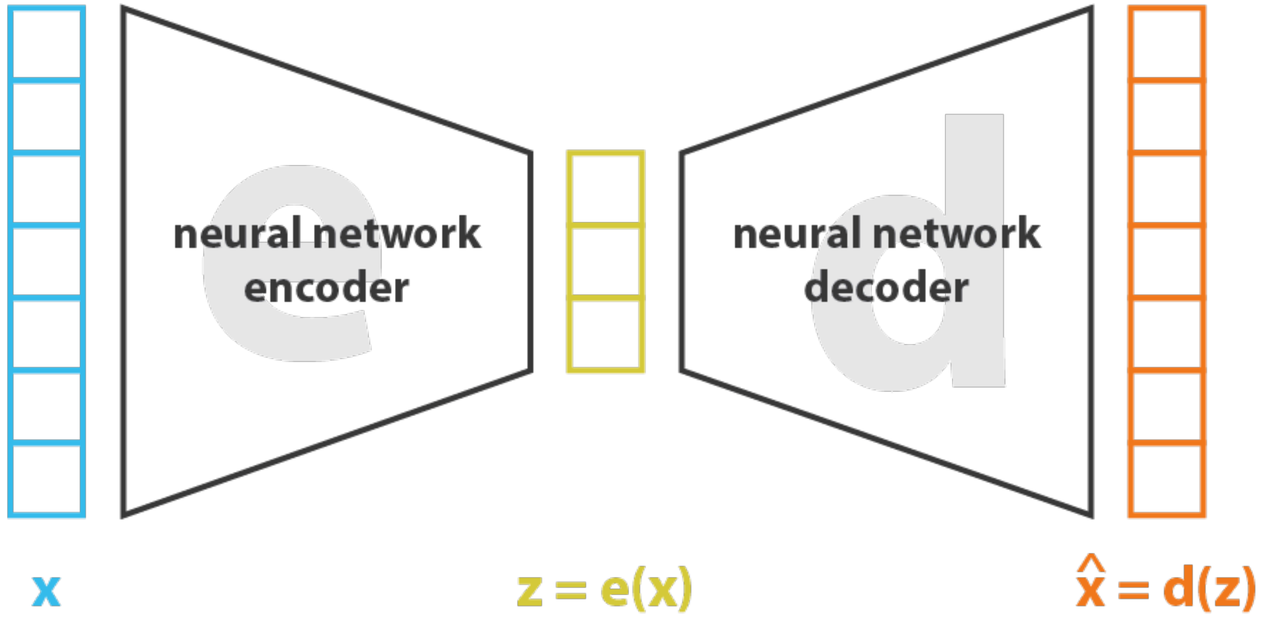
e(x)

encoded data
in latent space R^m (with m<n)

d(e(x))

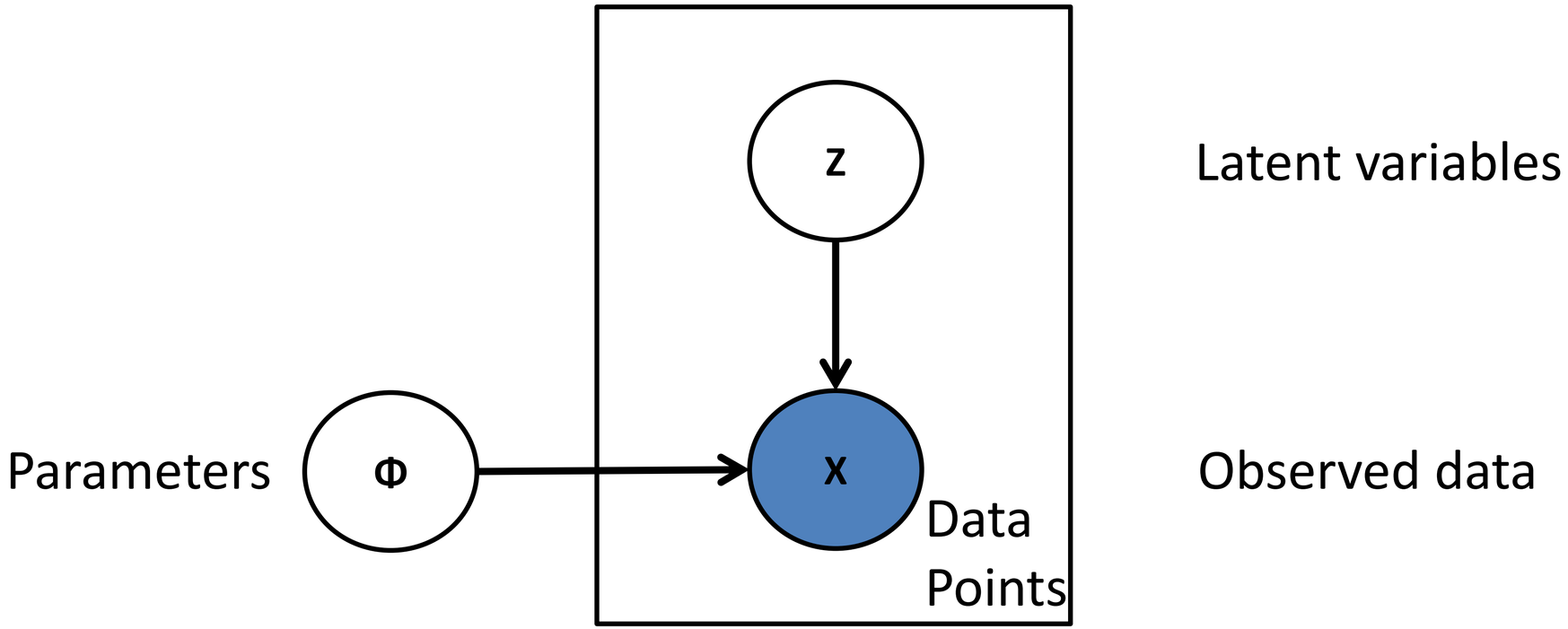
encoded-decoded data
back in the initial space R^n

Autoencoder



$$\text{loss} = \| x - \hat{x} \|^2 = \| x - d(z) \|^2 = \| x - d(e(x)) \|^2$$

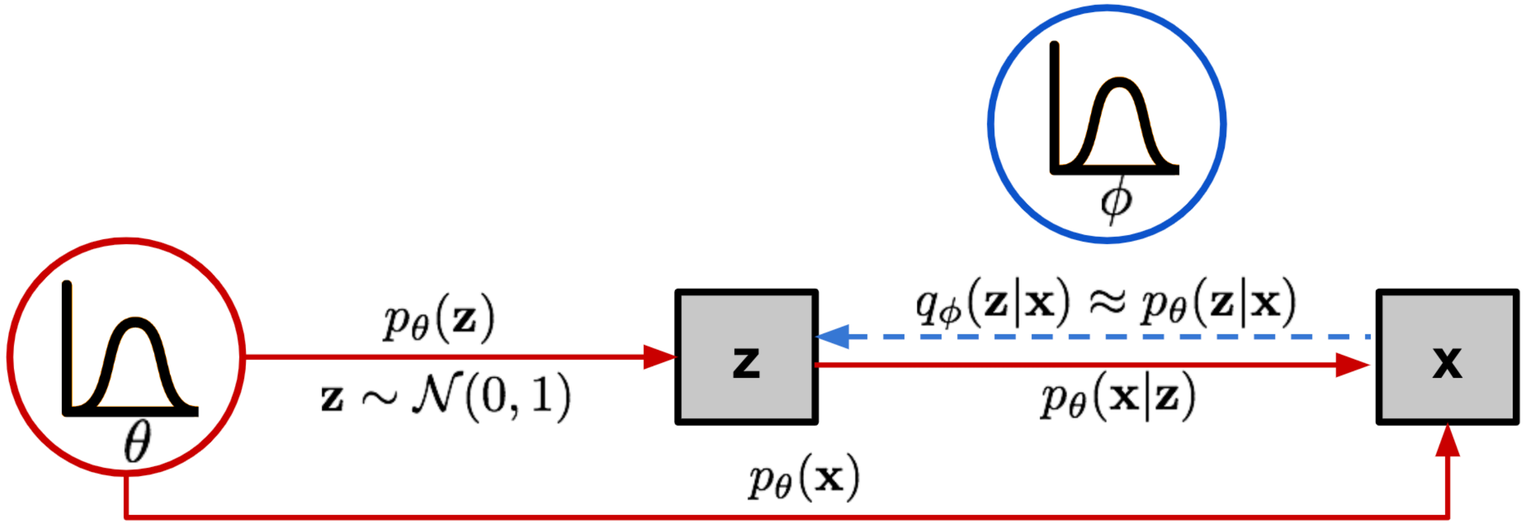
Latent Variable Models

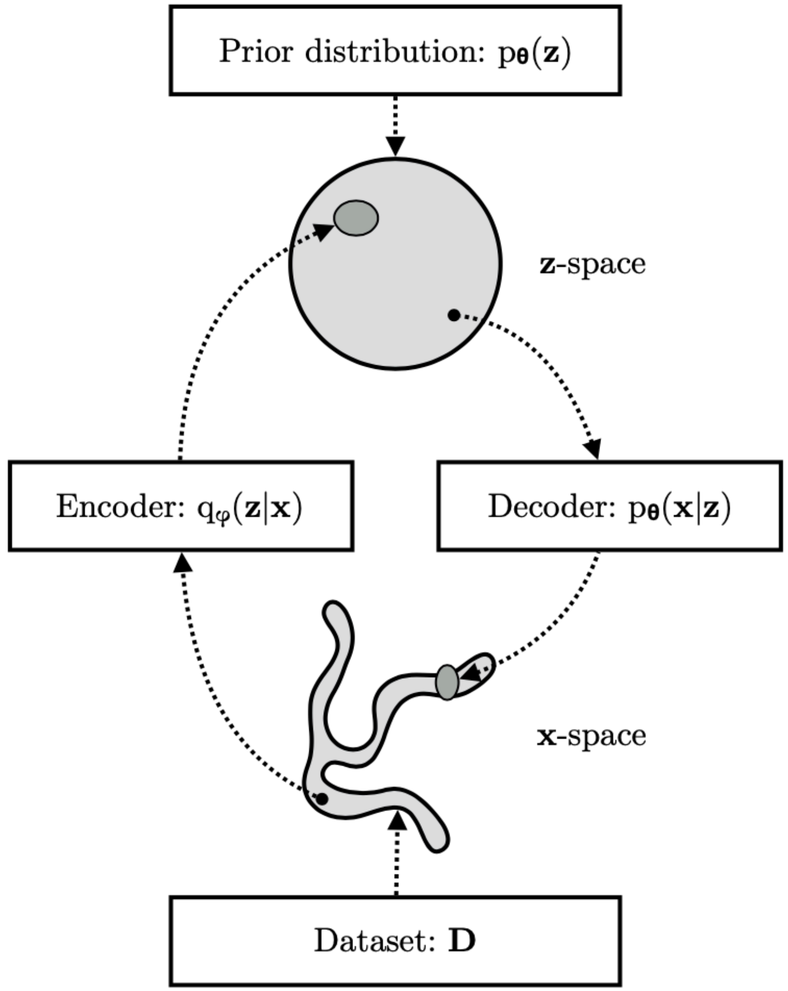


Dimensionality(X) >> dimensionality(Z)

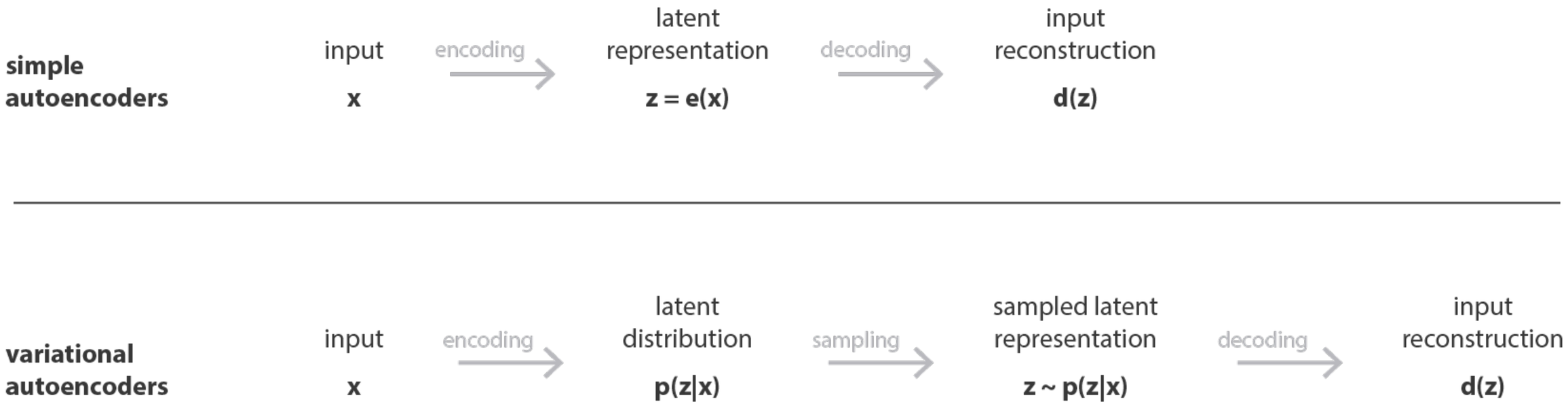
Z is a **bottleneck**, which finds a **compressed**, **low-dimensional representation** of X

Variational Autoencoder (VAE)





AE vs. VAE

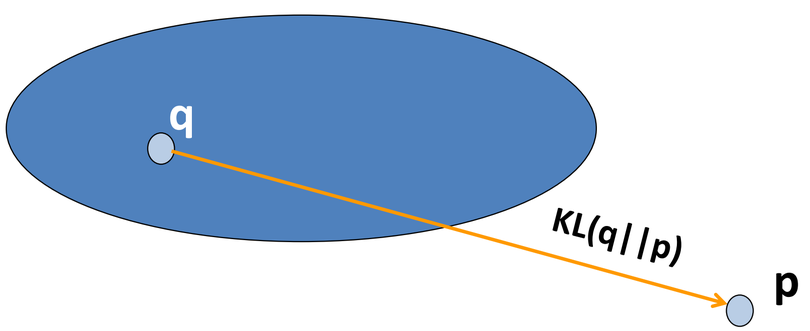

simple autoencoders
input
x
encoding
latent representation
z = e(x)
decoding
input reconstruction
d(z)
variational autoencoders
input
x
encoding
latent distribution
p(z|x)
sampling
sampled latent representation
z ~ p(z|x)
decoding
input reconstruction
d(z)

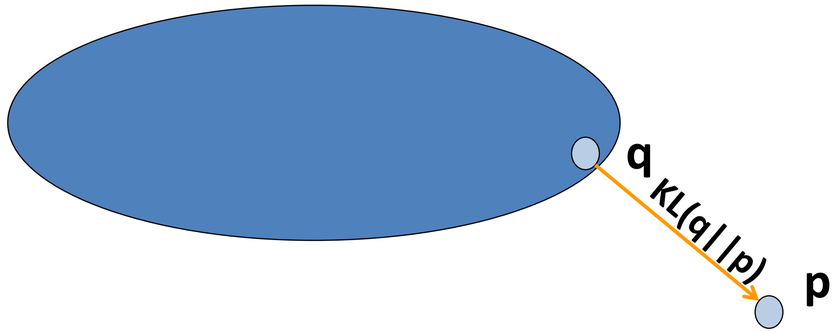
Approximate Inference

- **Optimization approaches**
  - EM
  - Variational inference
    - Variational Bayes
    - Message passing
  - Laplace approximation
- **Simulation approches** (Monte Carlo methods)
  - MCMC: Gibbs sampling, etc
  - ...

Variational Inference

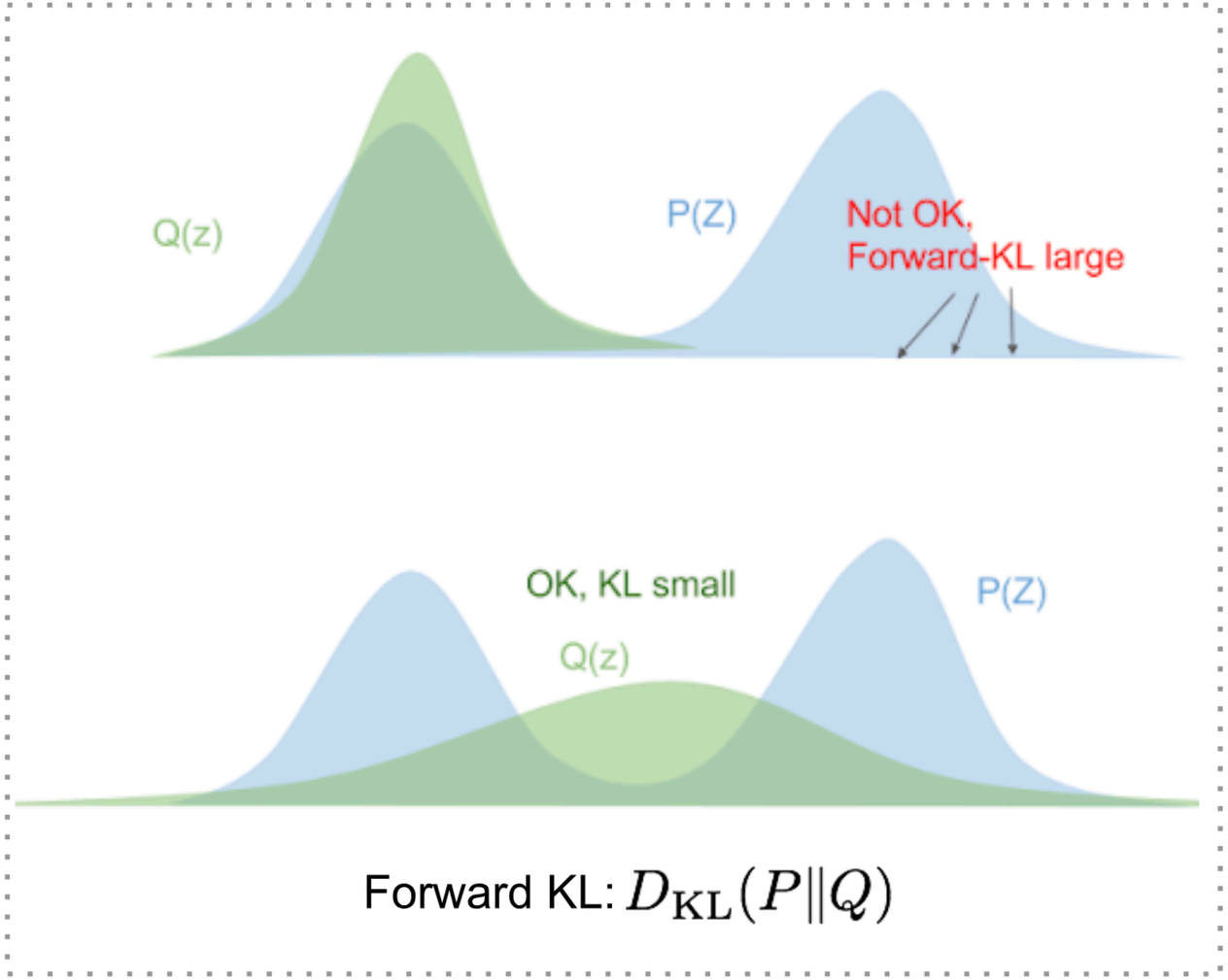
- Approximate p(z) with q(z)
- Make q(z) tractable to work with
- Solve an optimization problem, e.g. KL(q(z)||p(z))



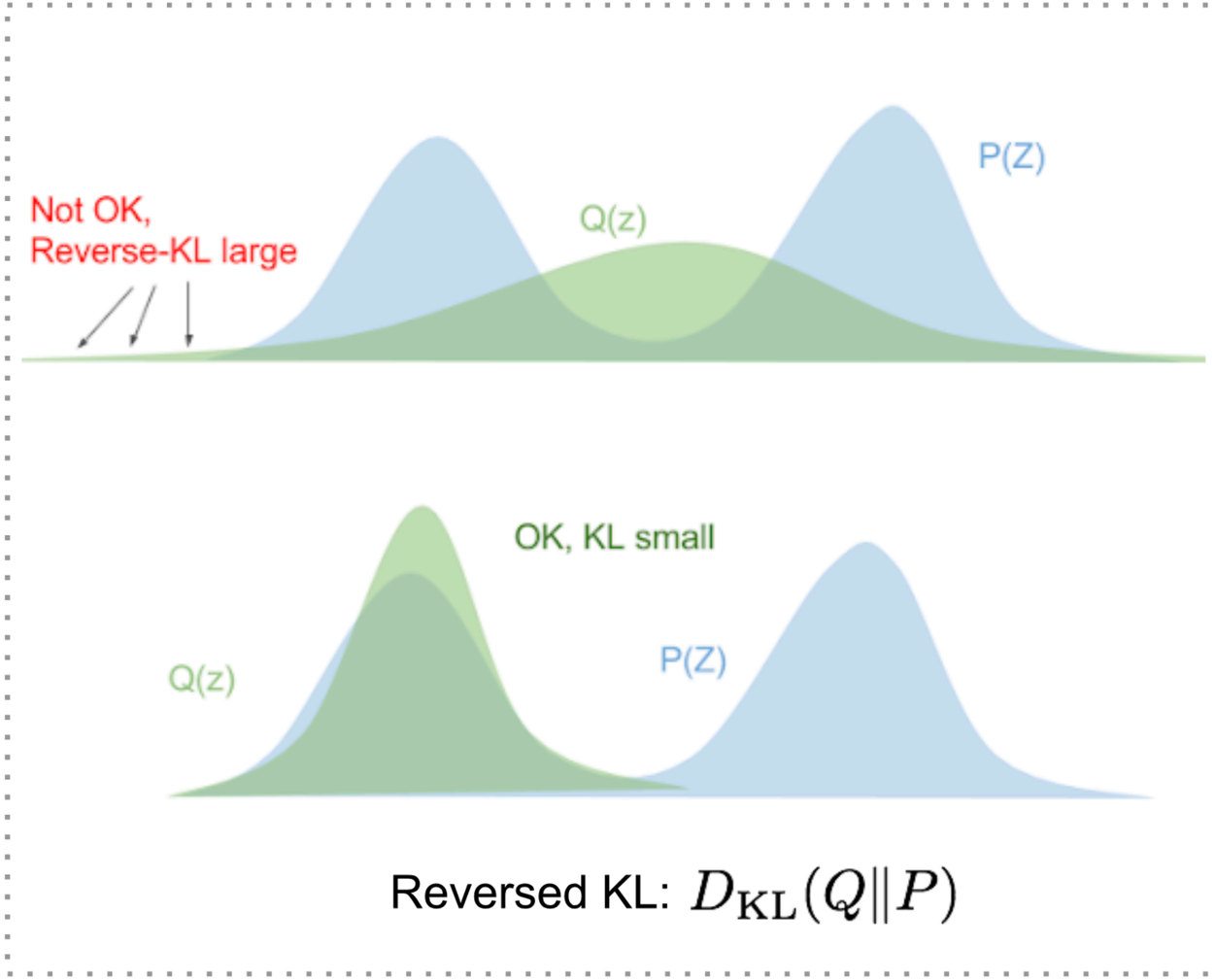


Variational Inference

$$KL(P||Q) = \sum_z p(z) \log \frac{p(z)}{q(z)}$$
$$= \mathbb{E}_{p(z)} \left[\log \frac{p(z)}{q(z)} \right]$$



Forward KL: $D_{\mathrm{KL}}(P\|Q)$



Reversed KL: $D_{\mathrm{KL}}(Q\|P)$

Monte Carlo Methods

$$E_{P(\mathbf{x})}[f(\mathbf{x})] \approx \frac{1}{S}\sum_{i=1}^{S} f(\mathbf{x}^{(i)}), \mathbf{x}^{(i)} \sim P(\mathbf{x})$$

- This suggests the procedure:
  - Draw S samples from P(x)
  - Compute f(x) for each of the samples
  - Approximate E[f(x)] by the sample average

Evidence Lower BOund (ELBO)

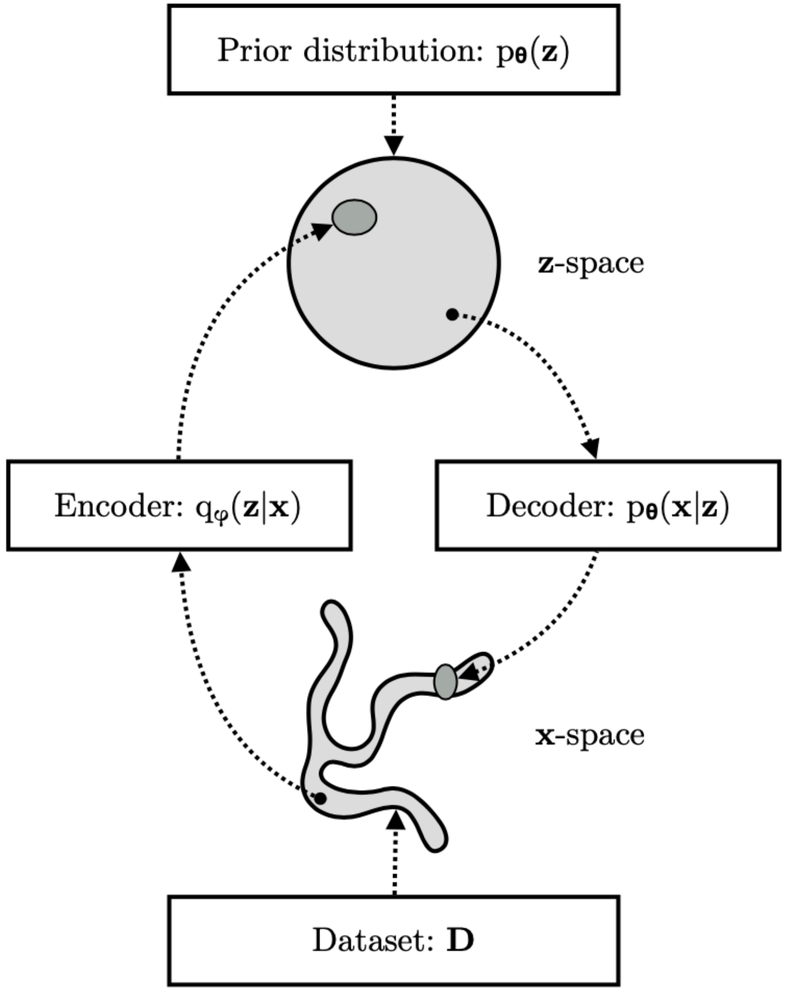
$$\log p_{\boldsymbol{\theta}}(\mathbf{x}) = \mathbb{E}_{q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x})}\left[\log p_{\boldsymbol{\theta}}(\mathbf{x})\right] \tag{2.5}$$

$$= \mathbb{E}_{q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x})}\left[\log\left[\frac{p_{\boldsymbol{\theta}}(\mathbf{x},\mathbf{z})}{p_{\boldsymbol{\theta}}(\mathbf{z}|\mathbf{x})}\right]\right] \tag{2.6}$$

$$= \mathbb{E}_{q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x})}\left[\log\left[\frac{p_{\boldsymbol{\theta}}(\mathbf{x},\mathbf{z})}{q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x})}\frac{q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x})}{p_{\boldsymbol{\theta}}(\mathbf{z}|\mathbf{x})}\right]\right] \tag{2.7}$$

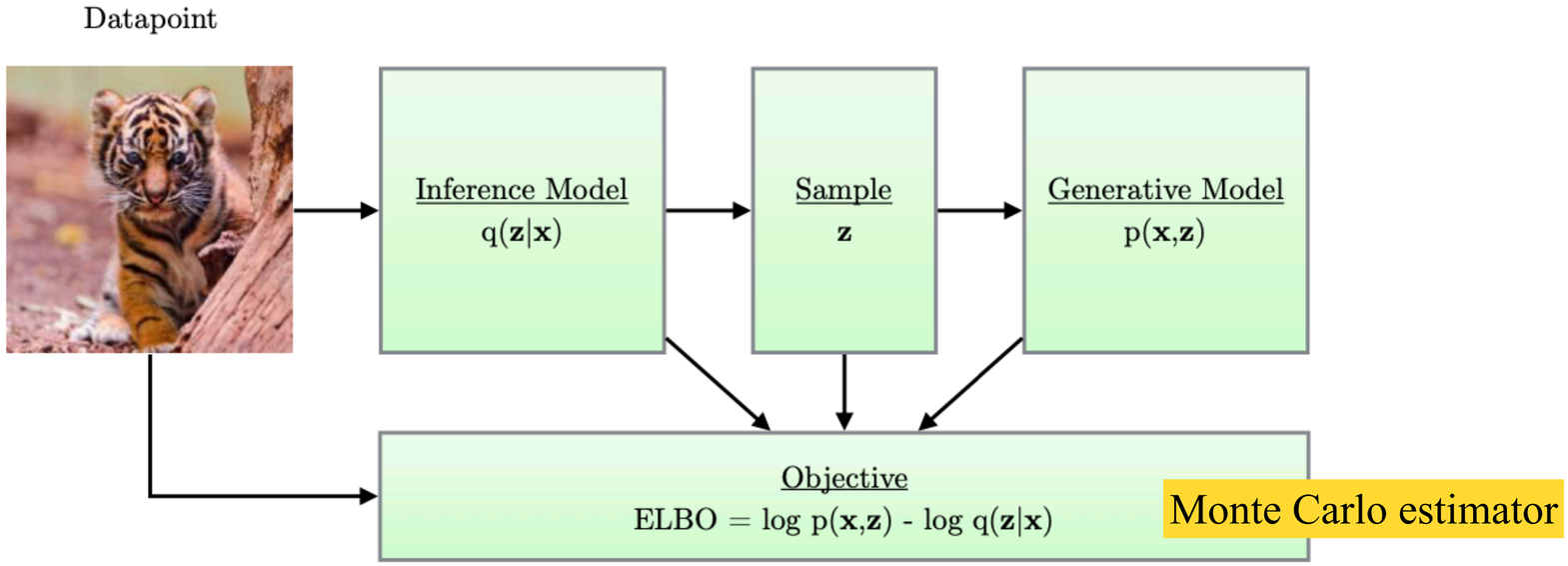
$$= \underbrace{\mathbb{E}_{q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x})}\left[\log\left[\frac{p_{\boldsymbol{\theta}}(\mathbf{x},\mathbf{z})}{q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x})}\right]\right]}_{=\mathcal{L}_{\boldsymbol{\theta},\boldsymbol{\phi}}(\mathbf{x})\ \text{(ELBO)}} + \underbrace{\mathbb{E}_{q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x})}\left[\log\left[\frac{q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x})}{p_{\boldsymbol{\theta}}(\mathbf{z}|\mathbf{x})}\right]\right]}_{=D_{KL}(q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x})||p_{\boldsymbol{\theta}}(\mathbf{z}|\mathbf{x}))} \tag{2.8}$$

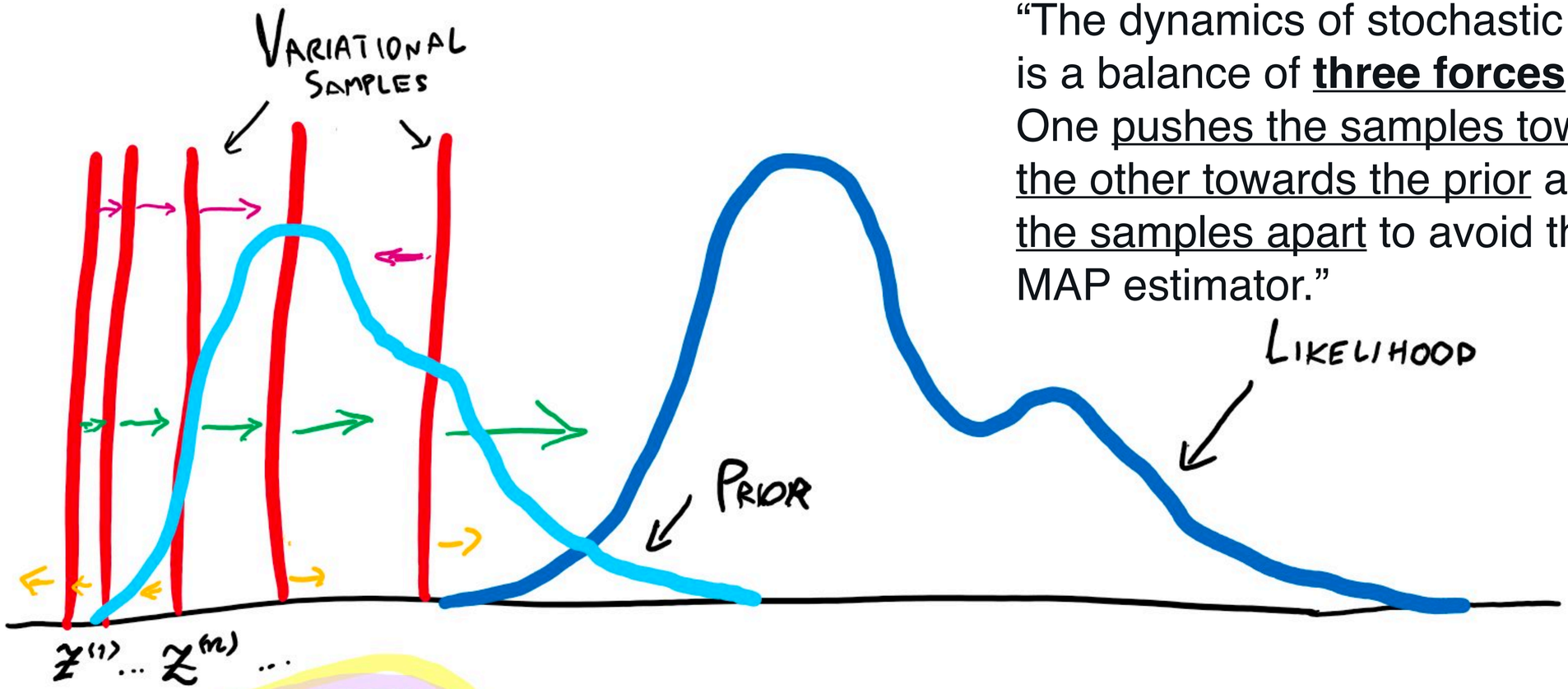
$$\mathcal{L}_{\boldsymbol{\theta},\boldsymbol{\phi}}(\mathbf{x}) = \log p_{\boldsymbol{\theta}}(\mathbf{x}) - D_{KL}(q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x})||p_{\boldsymbol{\theta}}(\mathbf{z}|\mathbf{x}))$$
$$\leq \log p_{\boldsymbol{\theta}}(\mathbf{x})$$



ELBO

$$
\begin{aligned}
\mathcal{L}_{\theta,\phi}(\mathbf{x}) &= \log p_\theta(\mathbf{x}) - D_{KL}(q_\phi(\mathbf{z}|\mathbf{x})||p_\theta(\mathbf{z}|\mathbf{x})) \\
&= \int q_\phi(\mathbf{z}|\mathbf{x}) \log p_\theta(\mathbf{x}) d\mathbf{z} + \int q_\phi(\mathbf{z}|\mathbf{x}) \log p_\theta(\mathbf{z}|\mathbf{x}) d\mathbf{z} - \int q_\phi(\mathbf{z}|\mathbf{x}) \log q_\phi(\mathbf{z}|\mathbf{x}) d\mathbf{z} \\
&= \mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x})}[\log p_\theta(\mathbf{x}, \mathbf{z}) - \log q_\phi(\mathbf{z}|\mathbf{x})] \\
&= \mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x})}[\log p_\theta(\mathbf{x}|\mathbf{z}) + \log p_\theta(\mathbf{z}) - \log q_\phi(\mathbf{z}|\mathbf{x})]
\end{aligned}
$$





"The dynamics of stochastic variational inference is a balance of **three forces**.
One pushes the samples towards the likelihood, the other towards the prior and the third pushes the samples apart to avoid the collapse into the MAP estimator."

@LucaAmb

$$q(z) \quad \text{ELBO} = E\Big[\log P(D|z) + \log P(z) - \log q(z)\Big]$$

GRADIENT FLOWS THROUGH THE SAMPLER

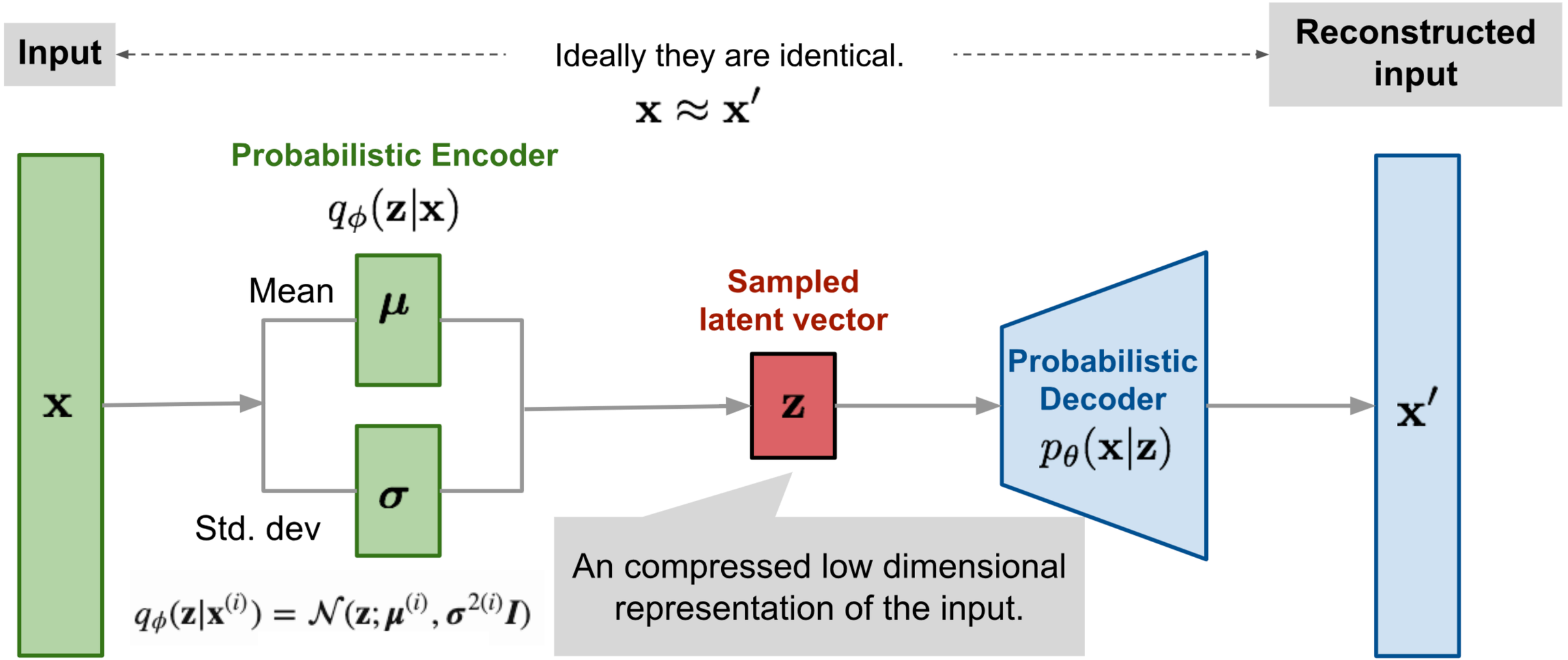
FIT LIKELIHOOD

FIT PRIOR

PROMOTE SAMPLER ENTROPY

$$\mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x})}[\log p_\theta(\mathbf{x}|\mathbf{z}) + \log p_\theta(\mathbf{z}) - \log q_\phi(\mathbf{z}|\mathbf{x})]$$

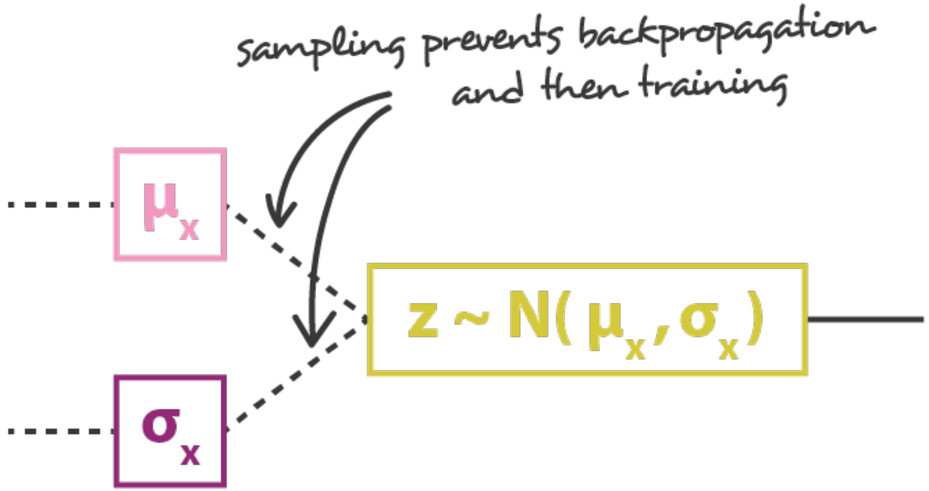
(vanilla) VAE


Input
Ideally they are identical.
$\mathbf{x} \approx \mathbf{x}'$
Reconstructed input
Probabilistic Encoder
$q_\phi(\mathbf{z}|\mathbf{x})$
Mean
μ
σ
Std. dev
$\mathbf{x}$
Sampled latent vector
$\mathbf{z}$
Probabilistic Decoder
$p_\theta(\mathbf{x}|\mathbf{z})$
$\mathbf{x}'$
$q_\phi(\mathbf{z}|\mathbf{x}^{(i)}) = \mathcal{N}(\mathbf{z}; \boldsymbol{\mu}^{(i)}, \boldsymbol{\sigma}^{2(i)}\boldsymbol{I})$
An compressed low dimensional representation of the input.

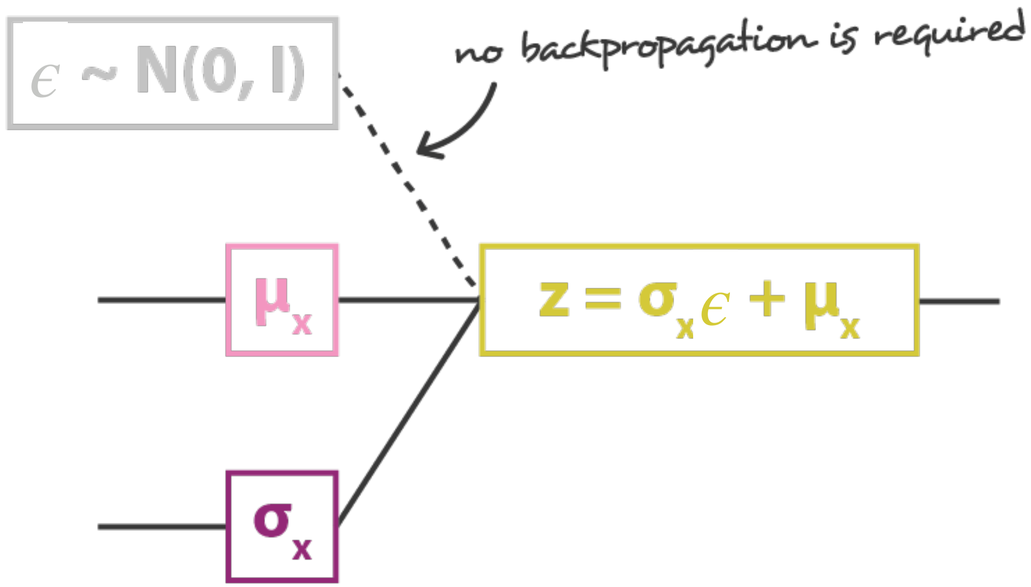
Reparameterization trick

no problem for backpropagation

backpropagation is not possible due to sampling

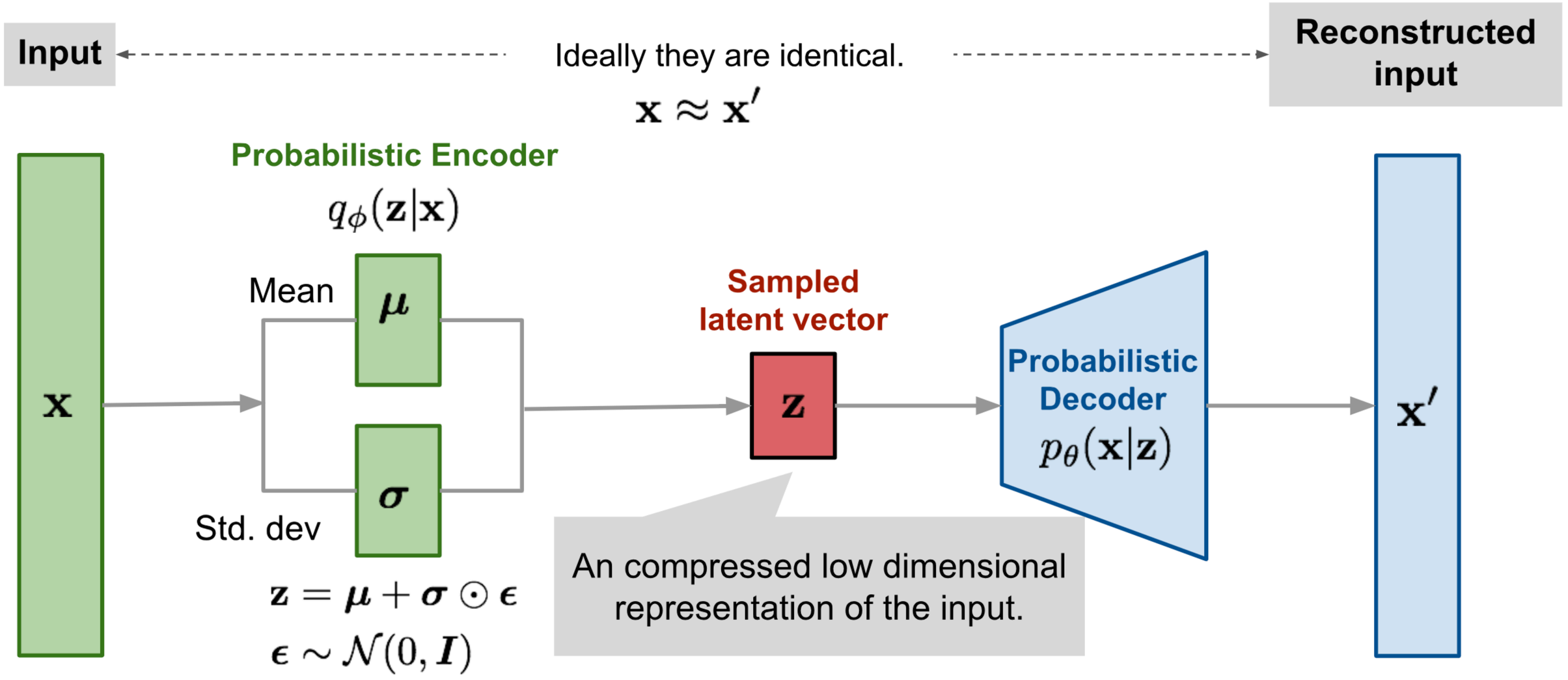


sampling without reparametrisation trick



sampling with reparametrisation trick

(vanilla) VAE


Input
Ideally they are identical.
$\mathbf{x} \approx \mathbf{x}'$
Reconstructed input
Probabilistic Encoder
$q_\phi(\mathbf{z}|\mathbf{x})$
Mean
μ
σ
Std. dev
$\mathbf{x}$
$\mathbf{z} = \mu + \sigma \odot \epsilon$
$\epsilon \sim \mathcal{N}(0, I)$
Sampled latent vector
$\mathbf{z}$
An compressed low dimensional representation of the input.
Probabilistic Decoder
$p_\theta(\mathbf{x}|\mathbf{z})$
$\mathbf{x}'$

ELBO

$$
\begin{aligned}
\mathcal{L}_{\theta,\phi}(\mathbf{x}) &= \log p_\theta(\mathbf{x}) - D_{KL}(q_\phi(\mathbf{z}|\mathbf{x})||p_\theta(\mathbf{z}|\mathbf{x})) \\
&= \int q_\phi(\mathbf{z}|\mathbf{x}) \log p_\theta(\mathbf{x}) d\mathbf{z} + \int q_\phi(\mathbf{z}|\mathbf{x}) \log p_\theta(\mathbf{z}|\mathbf{x}) d\mathbf{z} - \int q_\phi(\mathbf{z}|\mathbf{x}) \log q_\phi(\mathbf{z}|\mathbf{x}) d\mathbf{z} \\
&= \mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x})}[\log p_\theta(\mathbf{x}, \mathbf{z}) - \log q_\phi(\mathbf{z}|\mathbf{x})] \\
&= \mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x})}[\log p_\theta(\mathbf{x}|\mathbf{z}) + \log p_\theta(\mathbf{z}) - \log q_\phi(\mathbf{z}|\mathbf{x})] \\
&= \mathbb{E}_{p(\epsilon)}[\log p_\theta(\mathbf{x}|\mathbf{z}) + \log p_\theta(\mathbf{z}) - \log q_\phi(\mathbf{z}|\mathbf{x})], \text{where } \mathbf{z} = \boldsymbol{\sigma} \odot \boldsymbol{\epsilon} + \boldsymbol{\mu}
\end{aligned}
$$

ELBO

$$\mathcal{L}_{\theta,\phi}(\mathbf{x}) = \mathbb{E}_{p(\epsilon)}[\log p_\theta(\mathbf{x}|\mathbf{z}) + \log p_\theta(\mathbf{z}) - \log q_\phi(\mathbf{z}|\mathbf{x})], \text{ where } \mathbf{z} = \boldsymbol{\sigma} \odot \boldsymbol{\epsilon} + \boldsymbol{\mu}$$

Assuming a Gaussian likelihood for the decoder, i.e. $\mathbf{x}|\mathbf{z} = z \sim \mathcal{N}(\boldsymbol{\mu}_{\theta,z}, \boldsymbol{\Sigma}_{\theta,z})$, we have

$$\begin{aligned}
\log p_\theta(\mathbf{x}|\mathbf{z}) &= \log \left[(2\pi)^{-\frac{J}{2}} |\boldsymbol{\Sigma}_{\theta,z}|^{-\frac{1}{2}} \exp(-\frac{1}{2}(\mathbf{x} - \boldsymbol{\mu}_{\theta,z})^T \boldsymbol{\Sigma}_{\theta,z}^{-1}(\mathbf{x} - \boldsymbol{\mu}_{\theta,z})) \right] \\
&= -\frac{1}{2} \left[(\mathbf{x} - \boldsymbol{\mu}_{\theta,z})^T \boldsymbol{\Sigma}_{\theta,z}^{-1}(\mathbf{x} - \boldsymbol{\mu}_{\theta,z}) + J \log(2\pi) + \log |\boldsymbol{\Sigma}_{\theta,z}| \right]
\end{aligned}$$

In the isotropic Gaussian case, this reduces to

$$\begin{aligned}
\log p_\theta(\mathbf{x}|\mathbf{z}) &= \sum_{i=1}^{J} \log \left[(2\pi)^{-\frac{1}{2}} \sigma_i^{-1} e^{-\frac{1}{2\sigma_i^2}(x_i - \mu_{\theta,z,i})^2} \right] \\
&= -\frac{1}{2} \sum_{i=1}^{J} \left[\frac{(x_i - \mu_{\theta,z,i})^2}{\sigma_i^2} + \log(2\pi) + \log \sigma_i^2 \right],
\end{aligned}$$

where $\mu_{\theta,z,i}$ is the i^{th} element of $\boldsymbol{\mu}_{\theta,z}$, and σ_i^2 is the i^{th} diagonal entry of $\boldsymbol{\Sigma}_{\theta,z}$.

ELBO

$$\mathcal{L}_{\theta,\phi}(\mathbf{x}) = \mathbb{E}_{p(\epsilon)}[\log p_\theta(\mathbf{x}|\mathbf{z}) + \log p_\theta(\mathbf{z}) - \log q_\phi(\mathbf{z}|\mathbf{x})], \text{ where } \mathbf{z} = \boldsymbol{\sigma} \odot \boldsymbol{\epsilon} + \boldsymbol{\mu}$$

$$\begin{aligned}
\log p_\theta(\mathbf{z}) &= \sum_{i=1}^{J} \log \mathcal{N}(z_i; 0, 1) \\
&= \sum_{i=1}^{J} \log \left[(2\pi)^{-\frac{1}{2}} e^{-\frac{1}{2} z_i^2} \right] \\
&= -\sum_{i=1}^{J} \frac{1}{2} (z_i^2 + \log(2\pi))
\end{aligned}$$

ELBO

$$\mathcal{L}_{\theta,\phi}(\mathbf{x}) = \mathbb{E}_{p(\epsilon)}[\log p_\theta(\mathbf{x}|\mathbf{z}) + \log p_\theta(\mathbf{z}) - \log q_\phi(\mathbf{z}|\mathbf{x})], \text{ where } \mathbf{z} = \boldsymbol{\sigma} \odot \boldsymbol{\epsilon} + \boldsymbol{\mu}$$

Reparameterization

ϵ-> z:

Change of variables formula (vector case):

$$p(\boldsymbol{\epsilon}) = q_{\boldsymbol{\phi}}(\mathbf{g}(\boldsymbol{\epsilon}))\left|\det\left[\frac{\partial \mathbf{g}(\boldsymbol{\epsilon})}{\partial \boldsymbol{\epsilon}}\right]\right|$$

$$\log p(\boldsymbol{\epsilon}) = \log q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x}) + \log\left|\det\left[\frac{\partial \mathbf{z}}{\partial \boldsymbol{\epsilon}}\right]\right|$$

$$\log q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x}) = \log p(\boldsymbol{\epsilon}) - \log\left|\det\left[\frac{\partial \mathbf{z}}{\partial \boldsymbol{\epsilon}}\right]\right|$$

$$\log\left|\det\left[\frac{\partial \mathbf{z}}{\partial \boldsymbol{\epsilon}}\right]\right| = \sum_{i=1}^{J} \log \sigma_i = \frac{1}{2}\sum_{i=1}^{J} \log \sigma_i^2$$

ELBO

$$\mathcal{L}_{\theta,\phi}(\mathbf{x}) = \mathbb{E}_{p(\epsilon)}[\log p_\theta(\mathbf{x}|\mathbf{z}) + \log p_\theta(\mathbf{z}) - \log q_\phi(\mathbf{z}|\mathbf{x})], \text{ where } \mathbf{z} = \boldsymbol{\sigma} \odot \boldsymbol{\epsilon} + \boldsymbol{\mu}$$

$$\begin{aligned}
\mathbb{E}_{p(\epsilon)}[\log p_\theta(\mathbf{z})] &= \mathbb{E}_{p(\epsilon)}\left[-\frac{1}{2}\sum_{i=1}^{J}(z_i^2 + \log(2\pi))\right] \\
&= -\frac{1}{2}\sum_{i=1}^{J}\mathbb{E}_{p(\epsilon)}[(\mu_i + \sigma_i \cdot \epsilon_i)^2] - \frac{1}{2}\sum_{i=1}^{J}\log(2\pi) \\
&= -\frac{1}{2}\sum_{i=1}^{J}(\mathbb{E}_{p(\epsilon)}[\mu_i^2] + \mathbb{E}_{p(\epsilon)}[\sigma_i^2\epsilon_i^2] + \mathbb{E}_{p(\epsilon)}[2\mu_i\sigma_i\epsilon_i]) - \frac{J}{2}\log(2\pi) \\
&= -\frac{1}{2}\sum_{i=1}^{J}(\mu_i^2 + \sigma_i^2\mathbb{E}_{p(\epsilon)}[\epsilon_i^2] + 2\mu_i\sigma_i\mathbb{E}_{p(\epsilon)}[\epsilon_i]) - \frac{J}{2}\log(2\pi) \\
&= -\frac{1}{2}\sum_{i=1}^{J}(\mu_i^2 + \sigma_i^2 + 2\mu_i\sigma_i \cdot 0) - \frac{J}{2}\log(2\pi) \\
&= -\frac{J}{2}\log(2\pi) - \frac{1}{2}\sum_{i=1}^{J}(\mu_i^2 + \sigma_i^2)
\end{aligned}$$

ELBO

$$\mathcal{L}_{\theta,\phi}(\mathbf{x}) = \mathbb{E}_{p(\epsilon)}[\log p_\theta(\mathbf{x}|\mathbf{z}) + \log p_\theta(\mathbf{z}) - \log q_\phi(\mathbf{z}|\mathbf{x})], \text{ where } \mathbf{z} = \boldsymbol{\sigma} \odot \boldsymbol{\epsilon} + \boldsymbol{\mu}$$

$$\begin{aligned}
\mathbb{E}_{p(\epsilon)}[\log q_\phi(\mathbf{z}|\mathbf{x})] &= \mathbb{E}_{p(\epsilon)}\left[-\frac{1}{2}\sum_{i=1}^{J}(\epsilon_i^2 + \log(2\pi) + \log\sigma_i^2)\right] \\
&= -\frac{1}{2}\sum_{i=1}^{J}\mathbb{E}_{p(\epsilon)}[\epsilon_i^2] - \frac{1}{2}\sum_{i=1}^{J}\log(2\pi) - \frac{1}{2}\sum_{i=1}^{J}\log\sigma_i^2 \\
&= -\frac{J}{2}\log(2\pi) - \frac{1}{2}\sum_{i=1}^{J}(1 + \log\sigma_i^2).
\end{aligned}$$

ELBO

$$\mathcal{L}_{\theta,\phi}(\mathbf{x}) = \mathbb{E}_{p(\epsilon)}[\log p_\theta(\mathbf{x}|\mathbf{z}) + \log p_\theta(\mathbf{z}) - \log q_\phi(\mathbf{z}|\mathbf{x})], \text{ where } \mathbf{z} = \boldsymbol{\sigma} \odot \boldsymbol{\epsilon} + \boldsymbol{\mu}$$

$$\mathcal{L}_{\theta,\phi}(x_j) \simeq \frac{1}{2}\sum_{i=1}^{J}(1 + \log((\sigma_i^{(j)})^2) - (\mu_i^{(j)})^2 - (\sigma_i^{(j)})^2) + \mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x})}\left[\log p_\theta(x_j|z_j)\right]$$

ELBO: full covariance

- Reparameterization

$$\boldsymbol{\epsilon} \sim \mathcal{N}(0, \mathbf{I})$$
$$\mathbf{z} = \boldsymbol{\mu} + \mathbf{L}\boldsymbol{\epsilon}$$

$$\frac{\partial \mathbf{z}}{\partial \boldsymbol{\epsilon}} = \mathbf{L}$$

$$\log|\det(\frac{\partial \mathbf{z}}{\partial \boldsymbol{\epsilon}})| = \sum_i \log|L_{ii}|$$

$$\begin{aligned}\boldsymbol{\Sigma} &= \mathbb{E}\left[(\mathbf{z} - \mathbb{E}\left[\mathbf{z}|\right])(\mathbf{z} - \mathbb{E}\left[\mathbf{z}|\right])^T\right] \\ &= \mathbb{E}\left[\mathbf{L}\boldsymbol{\epsilon}(\mathbf{L}\boldsymbol{\epsilon})^T\right] = \mathbf{L}\mathbb{E}\left[\boldsymbol{\epsilon}\boldsymbol{\epsilon}^T\right]\mathbf{L}^T \\ &= \mathbf{L}\mathbf{L}^T\end{aligned}$$

$$(\boldsymbol{\mu}, \log\boldsymbol{\sigma}, \mathbf{L}') \leftarrow \text{EncoderNeuralNet}_{\boldsymbol{\phi}}(\mathbf{x})$$
$$\mathbf{L} \leftarrow \mathbf{L}_{mask} \odot \mathbf{L}' + \text{diag}(\boldsymbol{\sigma})$$

$$\log\left|\det\left(\frac{\partial \mathbf{z}}{\partial \boldsymbol{\epsilon}}\right)\right| = \sum_i \log\sigma_i$$

Note that σ_i here is not standard deviation