DSC291: Machine Learning with Few Labels

Self-supervised Learning

Zhiting Hu

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UC San Diego
HALICIOĞLU DATA SCIENCE INSTITUTE

Outline

- Variational Auto-Encoders (VAEs)
- Self-Supervised Learning (SSL)

Recap: EM and Variational Inference

- The EM algorithm:
  - E-step: $q^{t+1} = \arg\min_q F\left(q, \theta^t\right)$
  - M-step: $\theta^{t+1} = \arg\min_\theta F\left(q^{t+1}, \theta^t\right)$

Intractable when model $p(\boldsymbol{z}, \boldsymbol{x}|\theta)$ is complex

$$= p(\boldsymbol{z}|\boldsymbol{x}, \theta^t) = \frac{p(\boldsymbol{z}, \boldsymbol{x}|\theta^t)}{\sum_z p(\boldsymbol{z}, \boldsymbol{x}|\theta^t)}$$

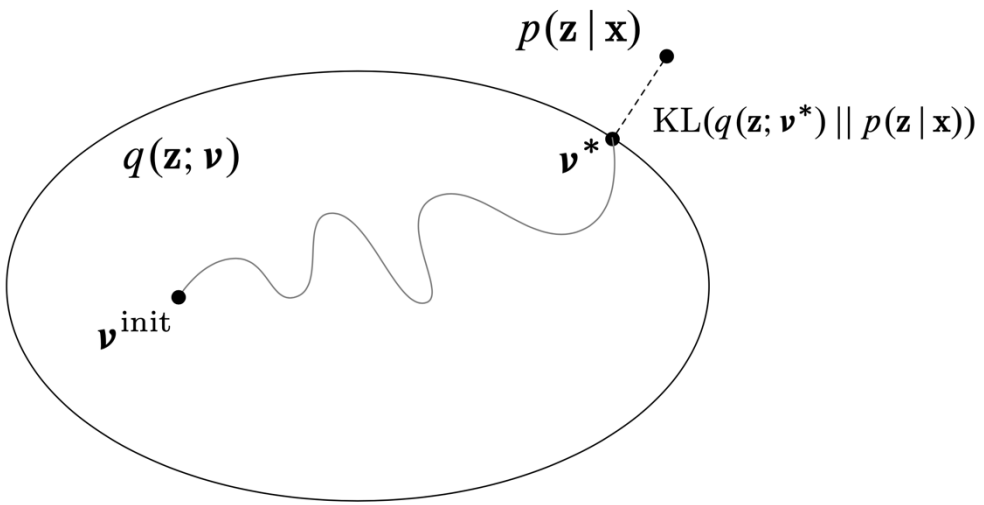
Need to approximate $p(\boldsymbol{z}|\boldsymbol{x}, \theta^t)$ with Variational Inference (VI)

$$\ell(\theta; \boldsymbol{x}) = \mathbb{E}_{q(\boldsymbol{z}|\boldsymbol{x})}\left[\log \frac{p(\boldsymbol{x}, \boldsymbol{z}|\theta)}{q(\boldsymbol{z}|\boldsymbol{x})}\right] + \mathrm{KL}\big(q(\boldsymbol{z}|\boldsymbol{x}) \,||\, p(\boldsymbol{z}|\boldsymbol{x}, \theta)\big)$$

Recap: Variational Inference

- Choose a family of distributions over the latent variables $\boldsymbol{z}$ with its own set of variational parameters ν , i.e. $q(\boldsymbol{z}|\boldsymbol{x}, \boldsymbol{\nu})$
- We maximize the ELBO over q to find an "optimal approximation" to $p(\boldsymbol{z}|\boldsymbol{x})$

$$\begin{aligned}
&\mathrm{argmax}_{\nu}\ \mathbb{E}_{q(\boldsymbol{z}|\boldsymbol{x},\boldsymbol{\nu})}\left[\log \frac{p(\boldsymbol{x}, \boldsymbol{z}|\theta)}{q(\boldsymbol{z}|\boldsymbol{x}, \boldsymbol{\nu})}\right] \\
&= \mathrm{argmax}_{\nu}\ \mathbb{E}_{q(\boldsymbol{z}|\boldsymbol{x},\boldsymbol{\nu})}[\log p(\boldsymbol{x}, \boldsymbol{z}|\theta)] - \mathbb{E}_{q(\boldsymbol{z}|\boldsymbol{x},\boldsymbol{\nu})}[\log q(\boldsymbol{z}|\boldsymbol{x}, \boldsymbol{\nu})]
\end{aligned}$$



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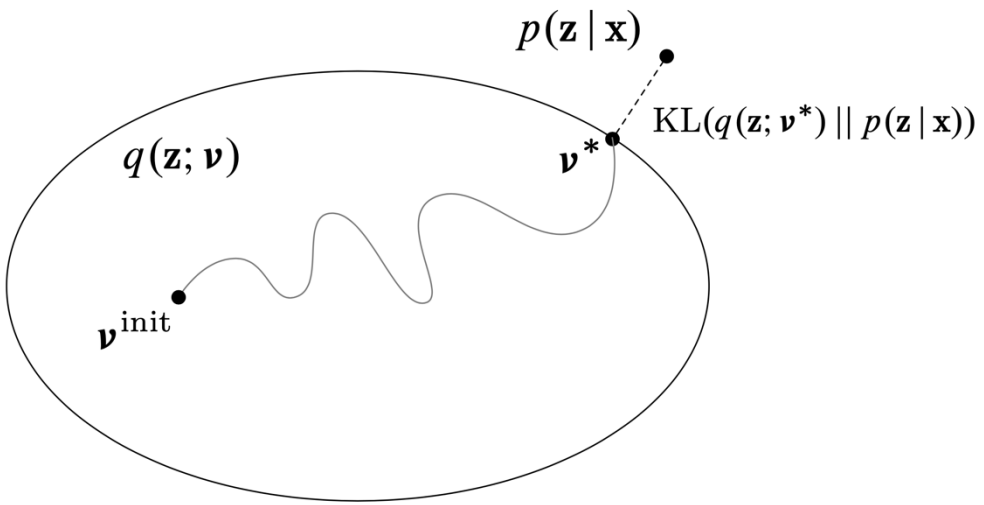

Question: How do we choose the variational family $q(\boldsymbol{z}|\boldsymbol{x}, \boldsymbol{\nu})$?

- Factorized distribution -> mean field VI
- Mixture of Gaussian distribution -> black-box VI
- Neural-based distribution -> Variational Autoencoders (VAEs)

Variational Auto-Encoders (VAEs)

- Model $p_\theta(\boldsymbol{x}, \boldsymbol{z}) = p_\theta(\boldsymbol{x}|\boldsymbol{z})p(\boldsymbol{z})$
  - $p_\theta(\boldsymbol{x}|\boldsymbol{z})$: a.k.a., generative model, generator, (probabilistic) decoder, …
  - $p(\boldsymbol{z})$: prior, e.g., Gaussian
- Assume variational distribution $q_\phi(\boldsymbol{z}|\boldsymbol{x})$
  - E.g., a Gaussian distribution parameterized as **deep neural networks**
  - a.k.a, recognition model, inference network, (probabilistic) encoder, …
- ELBO:

$$\mathcal{L}(\boldsymbol{\theta}, \boldsymbol{\phi}; \boldsymbol{x}) = \mathrm{E}_{q_\phi(\boldsymbol{z}|\boldsymbol{x})}[\log p_\theta(\boldsymbol{x}, \boldsymbol{z})] + \mathrm{H}(q_\phi(\boldsymbol{z}|\boldsymbol{x}))$$
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Reconstruction

Divergence from prior
(KL divergence between two Gaussians has an analytic form)

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$\nabla_{\boldsymbol{\phi}} \mathcal{L} =$

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$$\nabla_\theta \mathcal{L} = \mathrm{E}_{q_\phi(\boldsymbol{z}|\boldsymbol{x})}[\nabla_\theta \log p_\theta(\boldsymbol{x}, \boldsymbol{z})]$$

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$$\nabla_{\boldsymbol{\phi}} \mathcal{L} =$$

  - Reparameterization:
    - $[\boldsymbol{\mu}; \boldsymbol{\sigma}] = f_\phi(\boldsymbol{x})$ (a neural network)
    - $\boldsymbol{z} = \boldsymbol{\mu} + \boldsymbol{\sigma} \odot \boldsymbol{\epsilon}, \quad \boldsymbol{\epsilon} \sim \boldsymbol{N}(\boldsymbol{0}, \boldsymbol{1})$

$$\nabla_\theta \mathcal{L} = \mathrm{E}_{q_\phi(\boldsymbol{z}|\boldsymbol{x})}[\nabla_\theta \log p_\theta(\boldsymbol{x}, \boldsymbol{z})]$$

Variational Auto-Encoders (VAEs)

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$$\nabla_{\boldsymbol{\phi}} \mathcal{L} = \mathrm{E}_{\epsilon \sim N(\mathbf{0},\mathbf{1})}\left[\nabla_{\boldsymbol{z}}\left[\log p_\theta(\boldsymbol{x}, \boldsymbol{z}) - \log q_\phi(\boldsymbol{z}|\boldsymbol{x})\right] \nabla_\phi z(\epsilon, \boldsymbol{\phi})\right]$$

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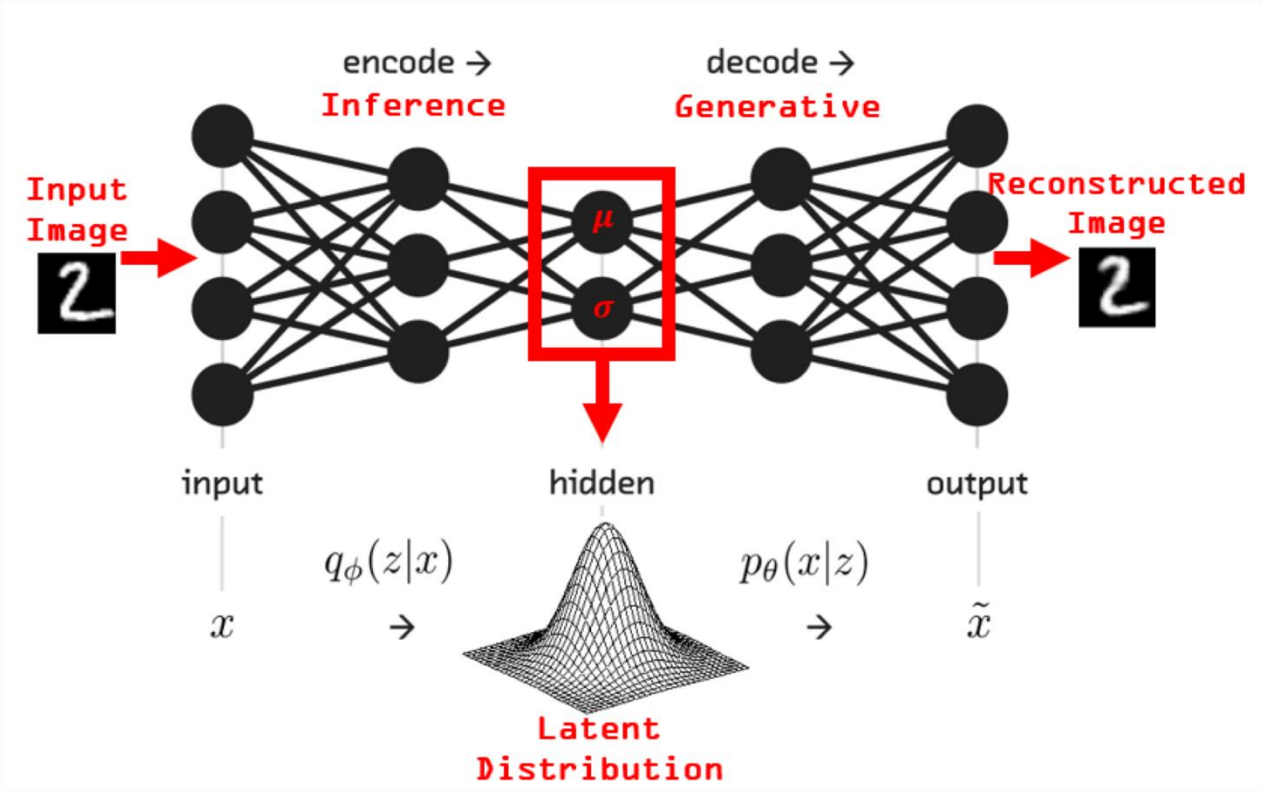
$$\nabla_\theta \mathcal{L} = \mathrm{E}_{q_\phi(\boldsymbol{z}|\boldsymbol{x})}[\nabla_\theta \log p_\theta(\boldsymbol{x}, \boldsymbol{z})]$$

Example: VAEs for images



[https://www.kaggle.com/rvislaywade/visualizing-mnist-using-a-variational-autoencoder]

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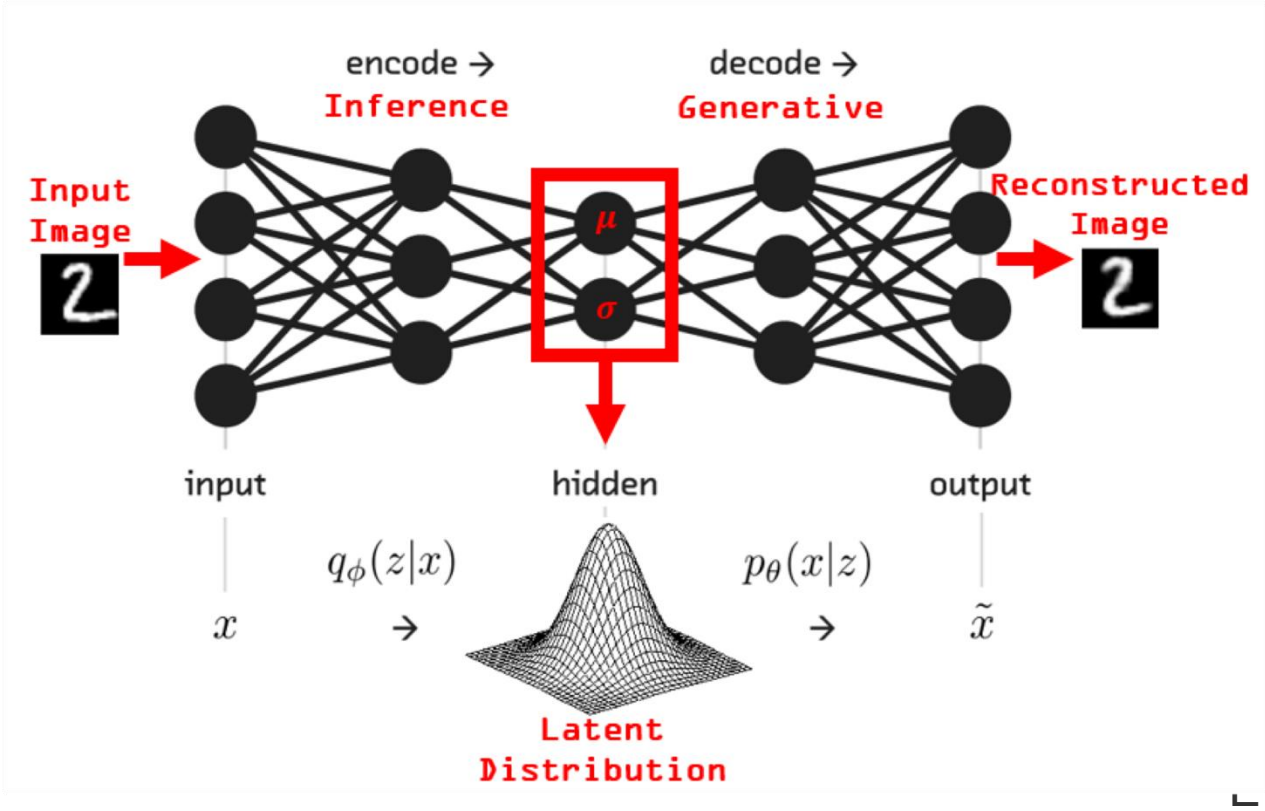

Input Data x

[Courtesy: Fei-Fei Li, Justin Johnson, Serena Yeung, CS 231n]

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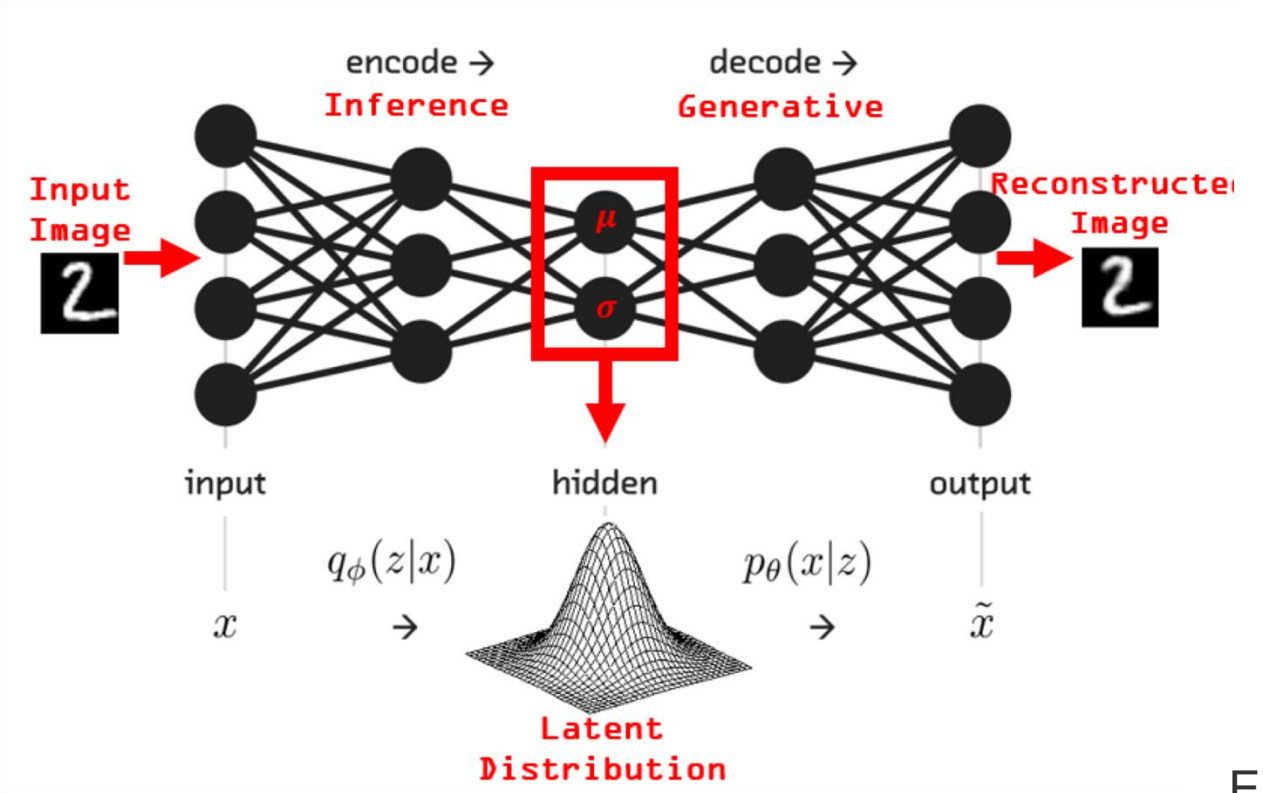
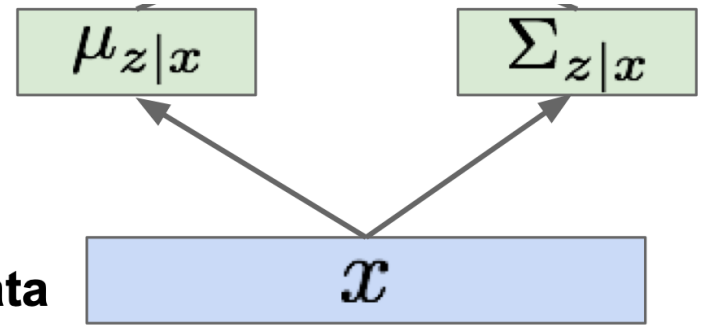


Encoder network

$q_\phi(z|x)$



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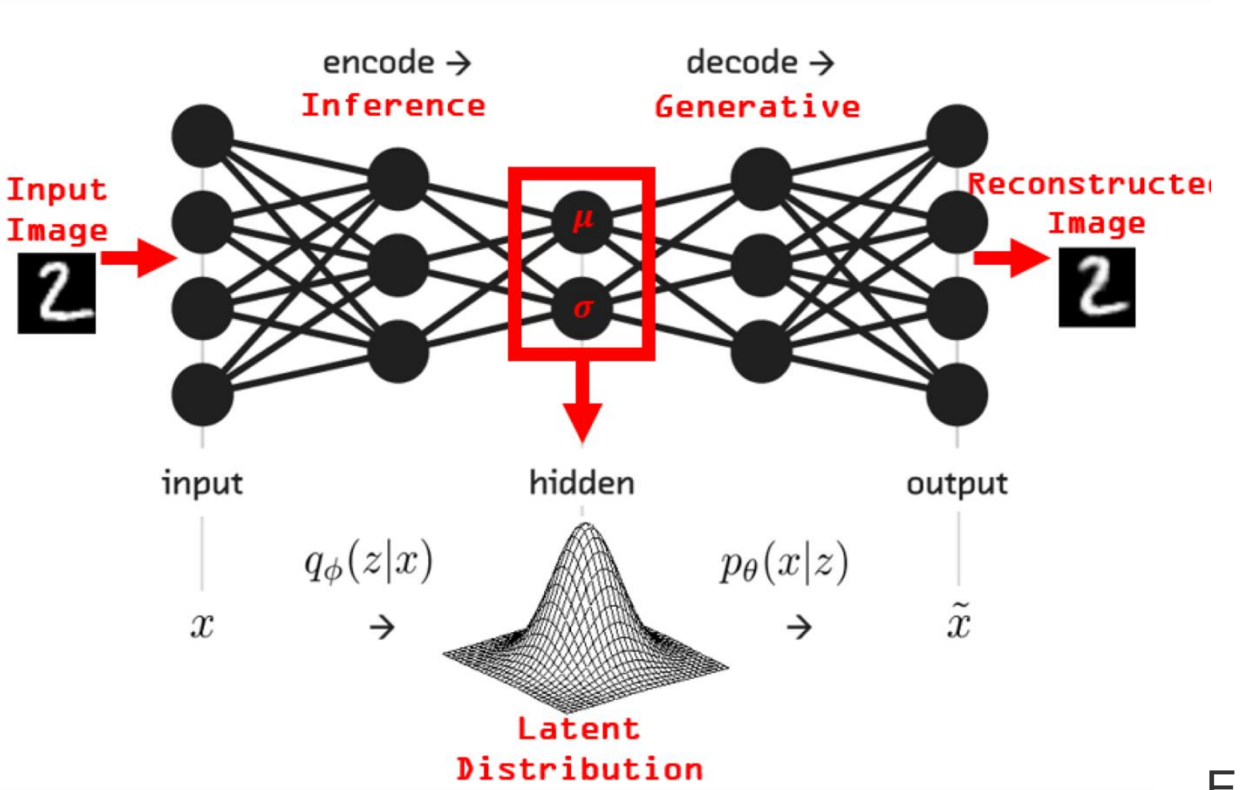

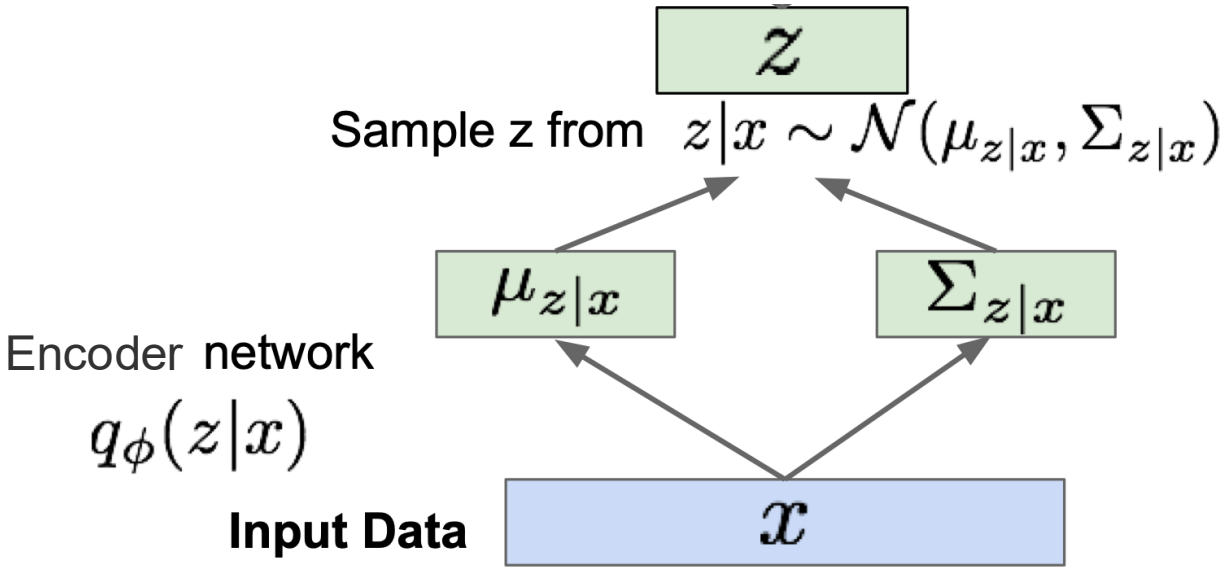

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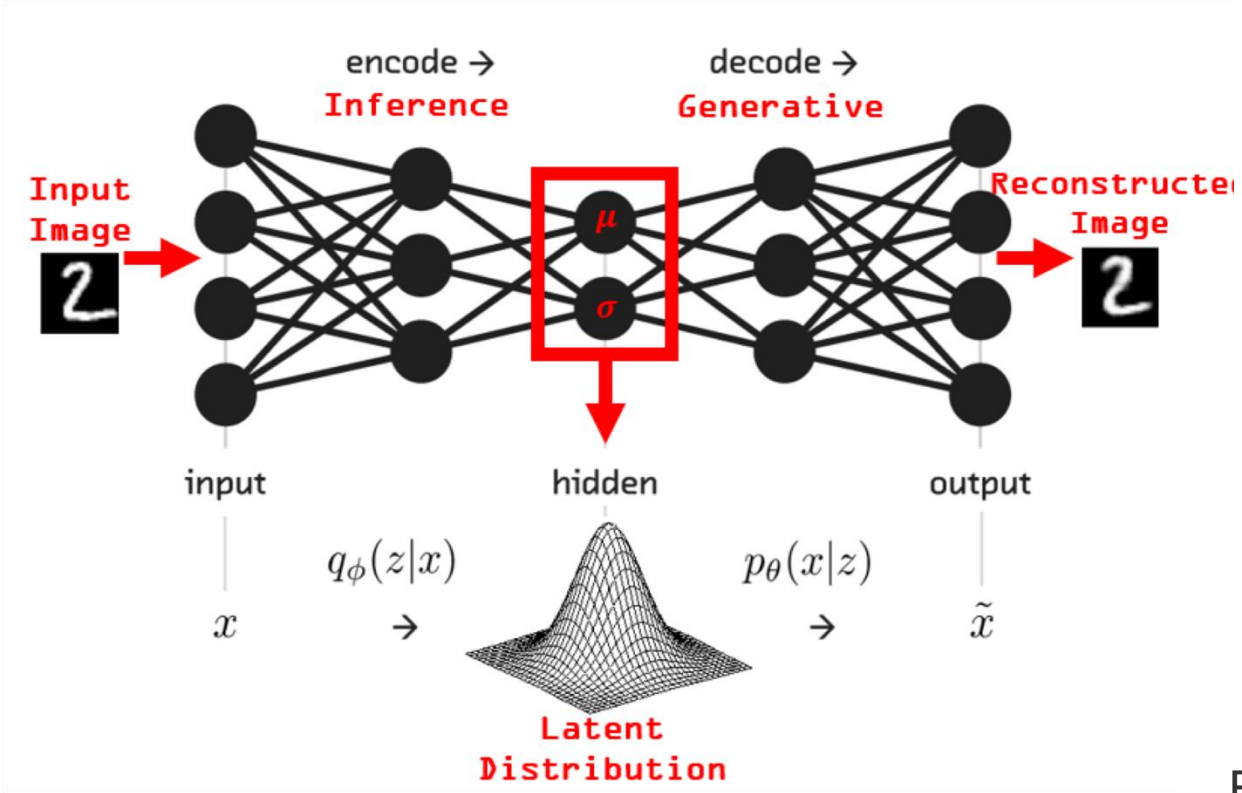

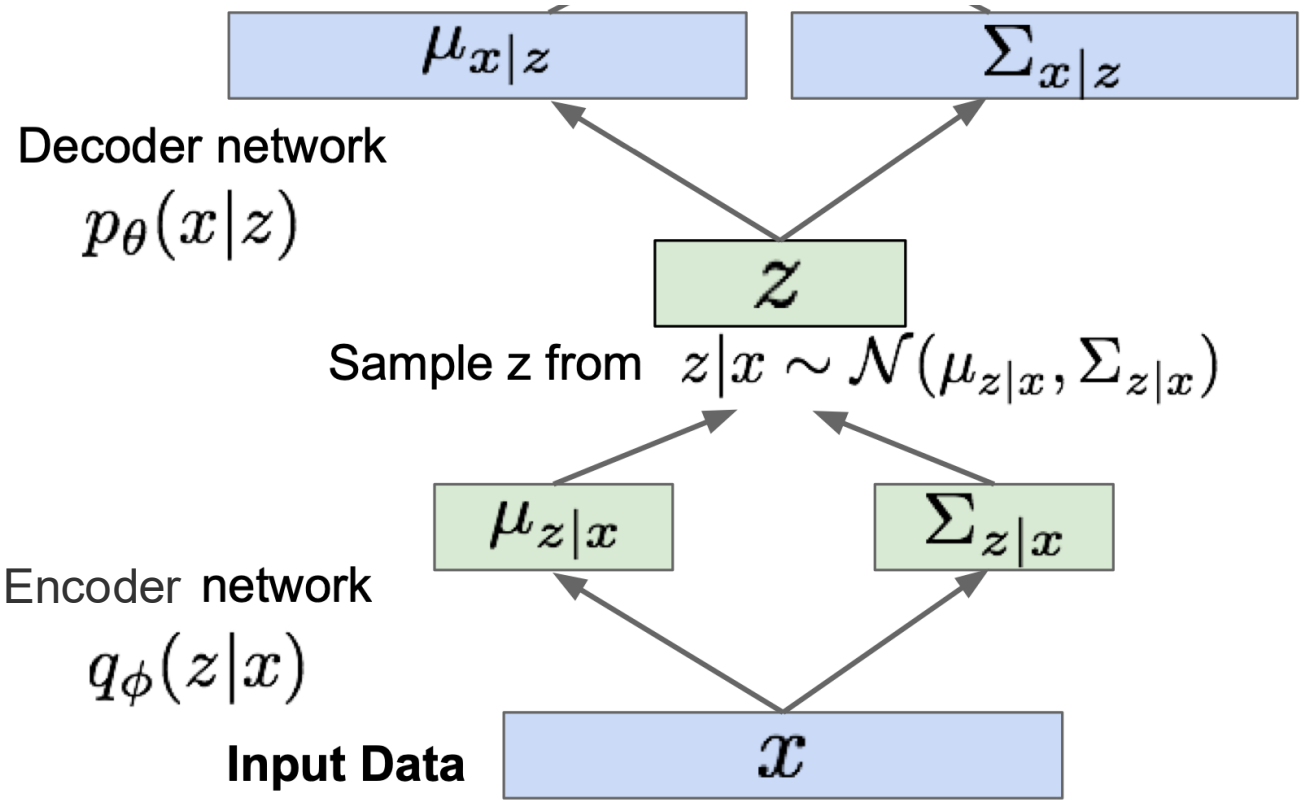

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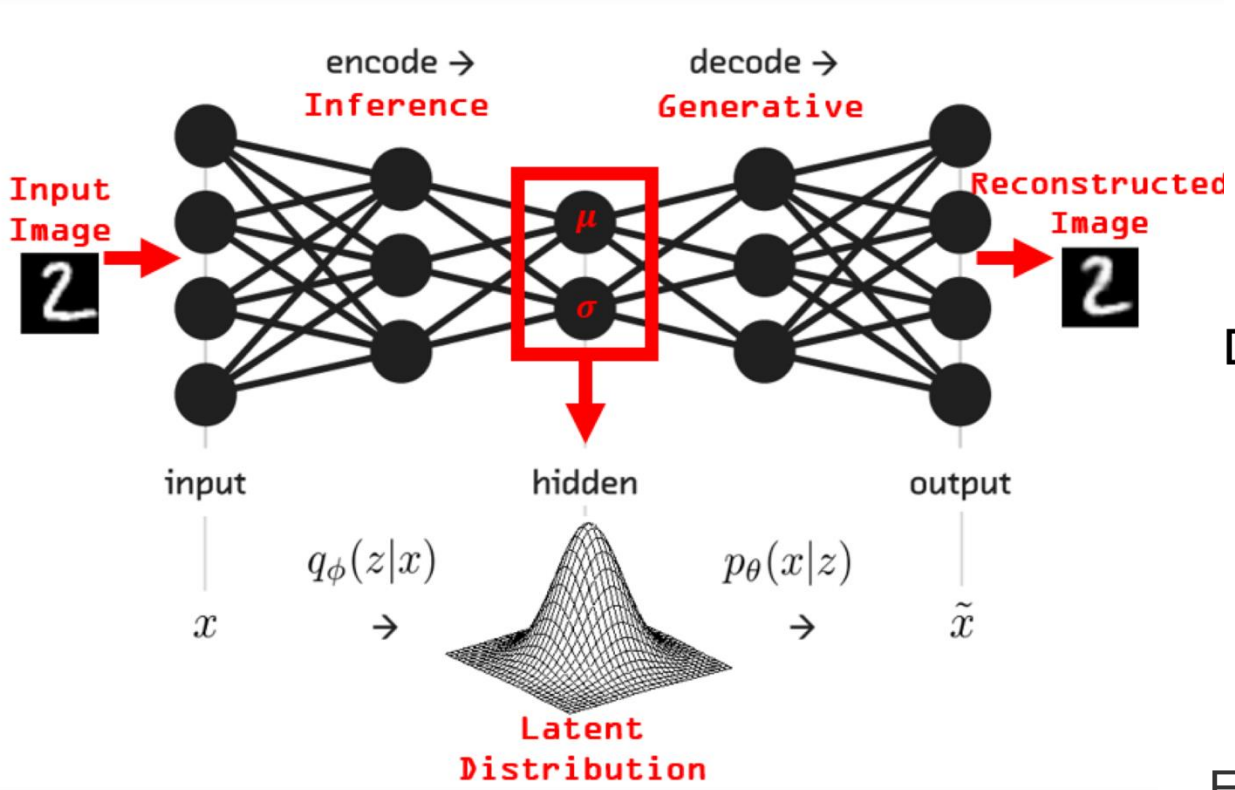

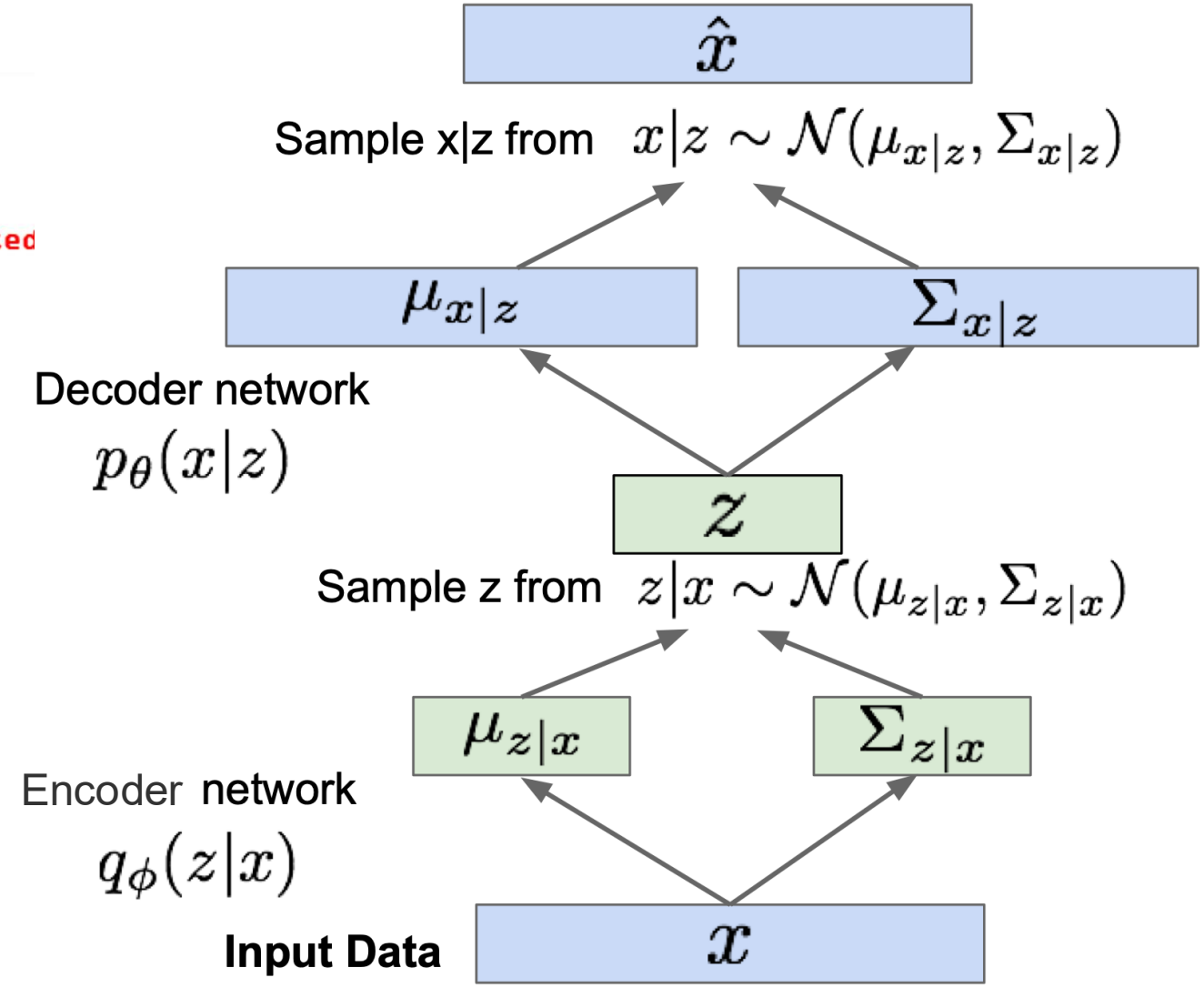

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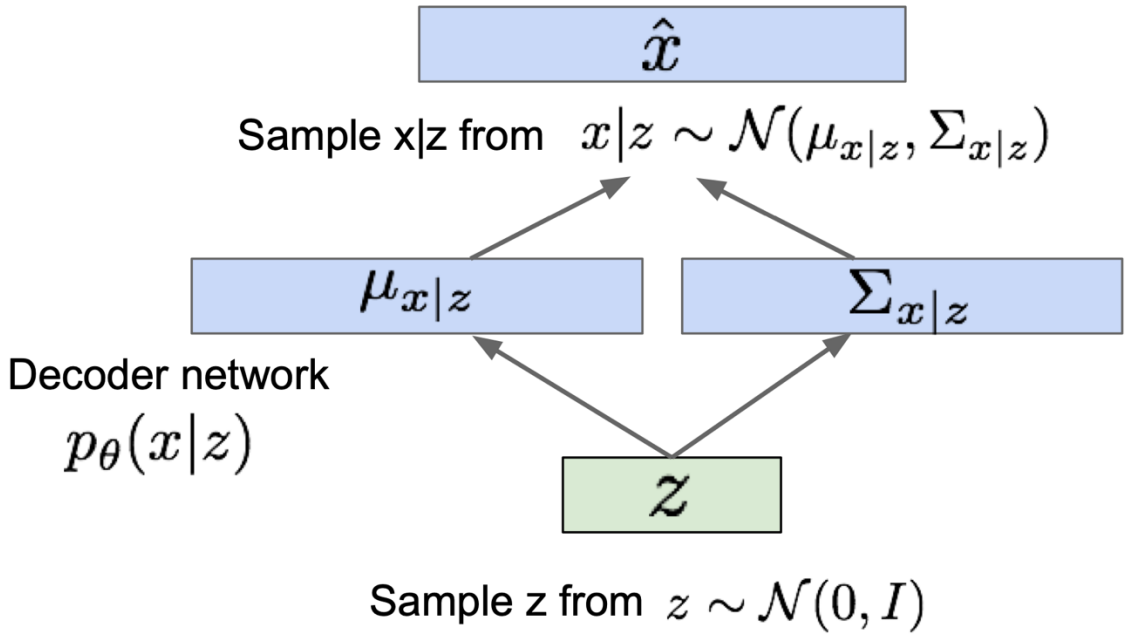
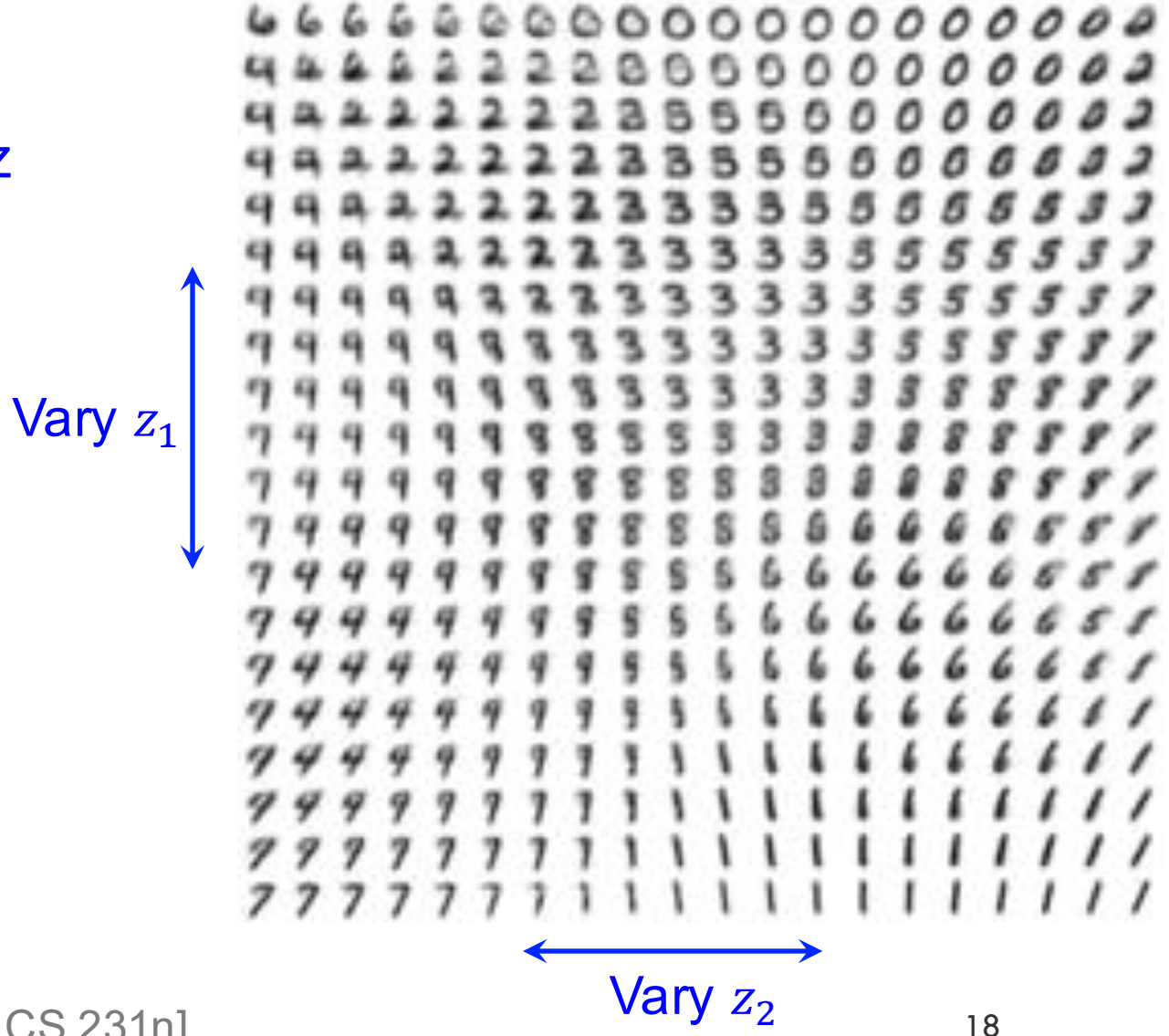
Example: VAEs for images

Generating samples:

- Use decoder network. Now sample z from prior!



Data manifold for 2-d **z**



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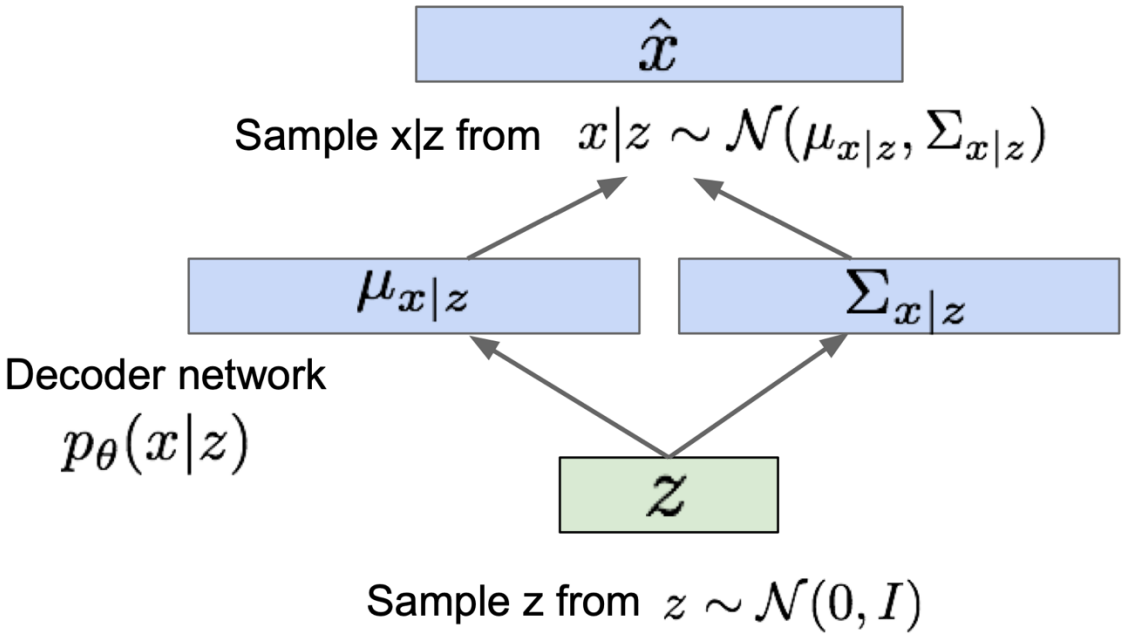


Data manifold for 2-d **z**

[Courtesy: Fei-Fei Li, Justin Johnson, Serena Yeung, CS 231n]

Example: VAEs for text

- Latent code interpolation and sentences generation from VAEs [Bowman et al., 2015].

“ i want to talk to you . ”

“i want to be with you . ”

“i do n’t want to be with you . ”

i do n’t want to be with you .

she did n’t want to be with him .

Variational Auto-encoders: Summary

- A combination of the following ideas:
  - Variational Inference: ELBO
  - Variational distribution parametrized as neural networks
  - Reparameterization trick

$$\mathcal{L}(\boldsymbol{\theta}, \boldsymbol{\phi}; \boldsymbol{x}) = [\log p_\theta(\boldsymbol{x}|\boldsymbol{z})] - \mathrm{KL}(q_\phi(\boldsymbol{z}|\boldsymbol{x}) \,||\, p(\boldsymbol{z}))$$

Reconstruction

Divergence from prior

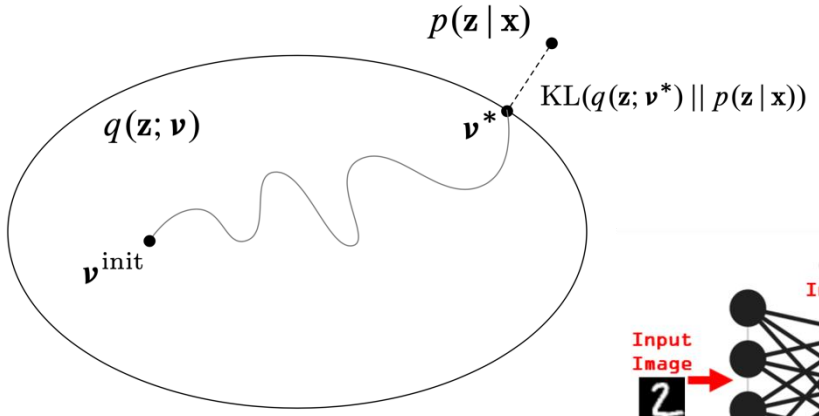
(Razavi et al., 2019)

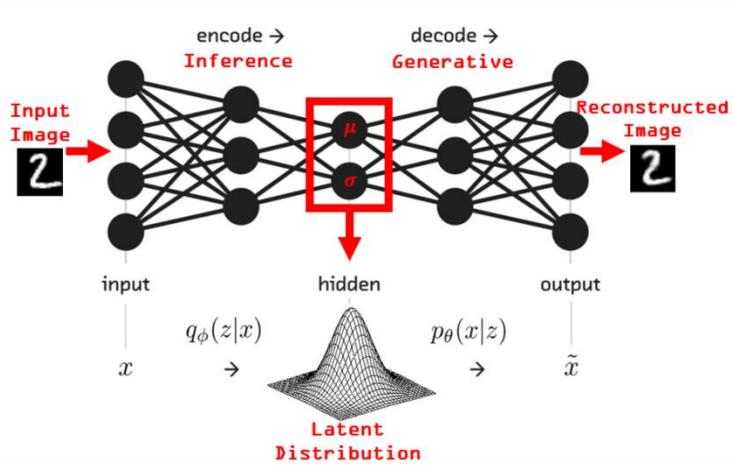
- Pros:
  - Principled approach to generative models
  - Allows inference of $q(z|x)$, can be useful feature representation for other tasks
- Cons:
  - Samples blurrier and lower quality compared to GANs
  - Tend to collapse on text data

Summary: Supervised / Unsupervised Learning

- Supervised Learning
  - Maximum likelihood estimation (MLE)

- Unsupervised learning
  - Maximum likelihood estimation (MLE) with latent variables
    - Marginal log-likelihood
  - EM algorithm for MLE
    - ELBO / Variational free energy
  - Variational Inference
    - ELBO / Variational free energy
    - Variational distributions
      - Factorized (mean-field VI)
      - Mixture of Gaussians (Black-box VI)
      - Neural-based (VAEs)





Questions?