DSC190: Machine Learning with Few Labels

Unsupervised Learning

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Lecture 17, November 6, 2024

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Outline

Unsupervised learning: Variational Inference

Presentations

- **So Hirota**: Mastering Chess with a Transformer Model
- **Jack Kai Lim**: GSM-Symbolic: Understanding the Limitations of Mathematical Reasoning in Large Language Models
- **Bingyan Liu**: REaLTabFormer: Generating Realistic Relational and Tabular Data using Transformers
- **Stephanie Wang**: Toolformer: Language Models Can Teach Themselves to Use Tools
- **Bobby Zhu**: Visualizing Data using t-SNE

Recap: EM and Variational Inference

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

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

$$= -F(q, \theta) + \mathrm{KL}\big(q(\boldsymbol{z}|\boldsymbol{x}) \,||\, p(\boldsymbol{z}|\boldsymbol{x}, \theta)\big)$$

Recap: EM and Variational Inference

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

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

Approximate $p(\boldsymbol{z}|\boldsymbol{x}, \theta^t)$:

- find a **tractable** $q(\boldsymbol{z}|\boldsymbol{x}, \boldsymbol{v}^*)$ that is closest to $p(\boldsymbol{z}|\boldsymbol{x}, \theta^t)$

$$q(\boldsymbol{z}|\boldsymbol{x}, \boldsymbol{v}^*) = \min_{\boldsymbol{v}} \mathrm{KL}\big(q(\boldsymbol{z}|\boldsymbol{x}, \boldsymbol{v}) \,||\, p(\boldsymbol{z}|\boldsymbol{x}, \theta^t)\big)$$

$$= \min_{\boldsymbol{v}} F(q(\boldsymbol{z}|\boldsymbol{x}, \boldsymbol{v}), \theta^t) + const.$$

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Question: what is the difference?

A: VI assume a simple form of q to ensure tractability

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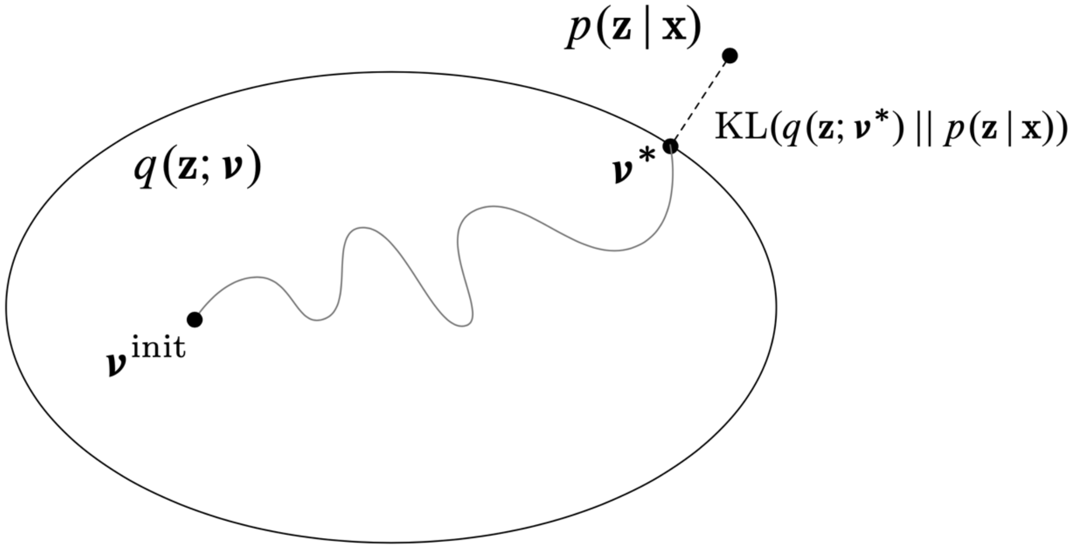

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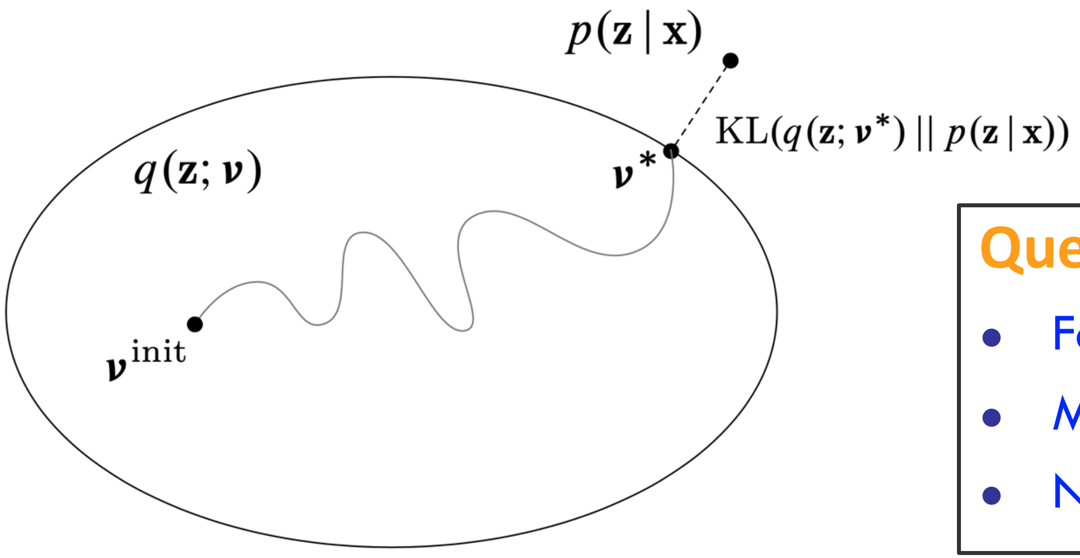

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Question: What forms of $q(\mathbf{z}|\mathbf{x}, \boldsymbol{\nu})$ shall we choose?

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

Black-box Variational Inference (BBVI)

- Probabilistic model: $\boldsymbol{x}$ -- observed variables, $\boldsymbol{z}$ -- latent variables
- Variational distribution $q_\lambda(\boldsymbol{z}|\boldsymbol{x})$ with parameters λ, e.g.,
  - Gaussian mixture distribution:
    - "A Gaussian mixture model is a universal approximator of densities, in the sense that any smooth density can be approximated with any specific nonzero amount of error by a Gaussian mixture model with enough components." (Deep Learning book, pp.65)
  - Deep neural networks
- ELBO:

$$\mathcal{L}(\lambda) = \mathbb{E}_{q(\boldsymbol{z}|\boldsymbol{\lambda})}[\log p(\boldsymbol{x}, \boldsymbol{z})] - \mathbb{E}_{q(\boldsymbol{z}|\boldsymbol{\lambda})}[\log q(\boldsymbol{z}|\lambda)]$$

- Want to compute the gradient w.r.t variational parameters λ

[Ranganath et al.,14]

The General Problem: Computing Gradients of Expectations

- When the objective function $\mathcal{L}$ is defined as an expectation of a (differentiable) test function $f_\lambda(\boldsymbol{z})$ w.r.t. a probability distribution $q_\lambda(\boldsymbol{z})$

$$\mathcal{L} = \mathbb{E}_{q_{\boldsymbol{\lambda}}(\boldsymbol{z})}[f_\lambda(\boldsymbol{z})]$$

- Computing exact gradients w.r.t. the parameters λ is often infeasible
- Need stochastic gradient estimates
  - The score function estimator (a.k.a log-derivative trick, REINFORCE)
  - The reparameterization trick (a.k.a the pathwise gradient estimator)

Computing Gradients of Expectations w/ score function

- Loss: $\mathcal{L} = \mathbb{E}_{q_\lambda(\boldsymbol{z})}[f_\lambda(\boldsymbol{z})]$

- Log-derivative trick: $\nabla_\lambda q_\lambda = q_\lambda \nabla_\lambda \log q_\lambda$
- **Question:** show that the gradient of $\mathcal{L}$ w.r.t. λ is:

$$\nabla_\lambda \mathcal{L} = \mathbb{E}_{q_\lambda(\boldsymbol{z})}[f_\lambda(\boldsymbol{z}) \nabla_\lambda \log q_\lambda(\boldsymbol{z}) + \nabla_\lambda f_\lambda(\boldsymbol{z})]$$

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  - score function: the gradient of the log of a probability distribution
- Monte Carlo estimation of the expectation:
  - Compute noisy unbiased gradients with Monte Carlo samples from q_λ

$$\nabla_\lambda \mathcal{L} \approx \frac{1}{S} \sum_{s=1}^{S} f_\lambda(\boldsymbol{z}_s) \nabla_\lambda \log q_\lambda(\boldsymbol{z}_s) + \nabla_\lambda f_\lambda(\boldsymbol{z}_s) \qquad \text{where } \boldsymbol{z}_s \sim q_\lambda(\boldsymbol{z})$$

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- Pros: generally applicable to any distribution $q(z|\lambda)$
- Cons: empirically has high variance → slow convergence

Computing Gradients of Expectations w/ reparametrization trick

- Loss: $\mathcal{L} = \mathbb{E}_{q_\lambda(\boldsymbol{z})}[f_\lambda(\boldsymbol{z})]$

- Assume that we can express the distribution $q_\lambda(\boldsymbol{z})$ with a transformation

$$\begin{aligned} \epsilon &\sim s(\epsilon) \\ z &= t(\epsilon, \lambda) \end{aligned} \quad \Leftrightarrow \quad z \sim q(z|\lambda)$$

  - E.g.,

$$\begin{aligned} \epsilon &\sim Normal(0, 1) \\ z &= \epsilon\sigma + \mu \end{aligned} \quad \Leftrightarrow \quad z \sim Normal(\mu, \sigma^2)$$

- Reparameterization gradient:

$$\mathcal{L} = \mathbb{E}_{\epsilon \sim s(\epsilon)}[f_\lambda(\boldsymbol{z}(\boldsymbol{\epsilon}, \lambda))]$$

  - **Question:** what's the gradient of $\mathcal{L}$ w.r.t. λ ?

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Computing Gradients of Expectations w/ reparametrization trick

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- Pros: empirically, lower variance of the gradient estimate
- Cons: Not all distributions can be reparameterized

Reparameterization trick

- Reparametrizing Gaussian distribution

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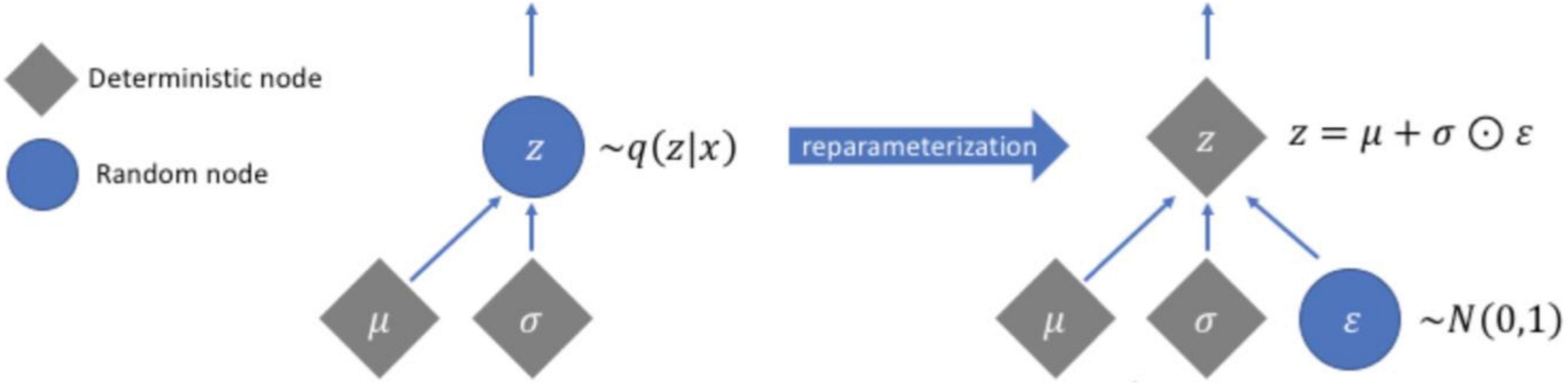

[Courtesy: Tansey, 2016]

Reparameterization trick

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- Other reparameterizable distributions:

$$\begin{array}{l}\epsilon \sim Uniform(\epsilon) \\ z = F^{-1}(\epsilon)\end{array} \Leftrightarrow \quad z \sim q(z)$$

  - Tractable inverse CDF F^{-1}:
    - Exponential, Cauchy, Logistic, Rayleigh, Pareto, Weibull, Reciprocal, Gompertz, Gumbel, Erlang
  - Location-scale:
    - Laplace, Elliptical, Student's t, Logistic, Uniform, Triangular, Gaussian
  - Composition:
    - Log-Normal (exponentiated normal) Gamma (sum of exponentials) Dirichlet (sum of Gammas) Beta, Chi-Squared, F

[Courtesy: Tansey, 2016]

Computing Gradients of Expectations: Summary

- Loss: $\mathcal{L} = \mathbb{E}_{q_\lambda(\boldsymbol{z})}[f_\lambda(\boldsymbol{z})]$
- **Score gradient**

$$\nabla_\lambda \mathcal{L} = \mathbb{E}_{q_\lambda(\boldsymbol{z})}[f_\lambda(\boldsymbol{z}) \nabla_\lambda \log q_\lambda(\boldsymbol{z}) + \nabla_\lambda f_\lambda(\boldsymbol{z})]$$

  - Pros: generally applicable to any distribution $q(z|\lambda)$
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- **Reparameterization gradient**

$$\nabla_\lambda \mathcal{L} = \mathbb{E}_{\epsilon \sim s(\epsilon)}[\nabla_{\boldsymbol{z}} f_\lambda(\boldsymbol{z})\, \nabla_\lambda t(\epsilon, \lambda)]$$

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Recall: Black-box Variational Inference (BBVI)

- Probabilistic model: $\boldsymbol{x}$ -- observed variables, $\boldsymbol{z}$ -- latent variables
- Variational distribution $q_\lambda(\boldsymbol{z}|\boldsymbol{x})$ with parameters λ, e.g.,
  - Gaussian mixture distribution:
    - "A Gaussian mixture model is a universal approximator of densities, in the sense that any smooth density can be approximated with any specific nonzero amount of error by a Gaussian mixture model with enough components." (Deep Learning book, pp.65)
  - Deep neural networks

$$\mathcal{L}(\lambda) \triangleq \mathrm{E}_{q_\lambda(z)}[\log p(x, z) - \log q(z)]$$

- ELBO to be maximized:

$$\mathcal{L}(\lambda) = \mathbb{E}_{q(\boldsymbol{z}|\boldsymbol{\lambda})}[\log p(\boldsymbol{x}, \boldsymbol{z})] - \mathbb{E}_{q(\boldsymbol{z}|\boldsymbol{\lambda})}[\log q(\boldsymbol{z}|\lambda)]$$

- Want to compute the gradient w.r.t variational parameters λ

[Ranganath et al.,14]

$$\mathcal{L} = \mathbb{E}_{q_{\boldsymbol{\lambda}}(\boldsymbol{z})}[f_\lambda(\boldsymbol{z})]$$

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BBVI with the score gradient

- ELBO:

$$\mathcal{L}(\lambda) = \mathbb{E}_{q(\boldsymbol{z}|\boldsymbol{\lambda})}[\log p(\boldsymbol{x}, \boldsymbol{z})] - \mathbb{E}_{q(\boldsymbol{z}|\boldsymbol{\lambda})}[\log q(\boldsymbol{z}|\lambda)]$$

- **Question:** what's the score gradient w.r.t. λ ?

$$\nabla_\lambda \mathcal{L} = \mathrm{E}_q[\nabla_\lambda \log q(z|\lambda)(\log p(x, z) - \log q(z|\lambda))]$$

BBVI with the score gradient

$$\mathcal{L} = \mathbb{E}_{q_\lambda(\boldsymbol{z})}[f_\lambda(\boldsymbol{z})]$$

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- Compute noisy unbiased gradients of the ELBO with Monte Carlo samples from the variational distribution

$$\nabla_\lambda \mathcal{L} \approx \frac{1}{S} \sum_{s=1}^{S} \nabla_\lambda \log q(z_s|\lambda)(\log p(x, z_s) - \log q(z_s|\lambda)),$$

$$\text{where } z_s \sim q(z|\lambda).$$

[Ranganath et al.,14]

BBVI with the reparameterization gradient

$$\mathcal{L} = \mathbb{E}_{q_{\boldsymbol{\lambda}}(\boldsymbol{z})}[f_\lambda(\boldsymbol{z})]$$

$$\nabla_\lambda \mathcal{L} = \mathbb{E}_{\boldsymbol{\epsilon}\sim \boldsymbol{s}(\boldsymbol{\epsilon})}[\nabla_{\boldsymbol{z}} f_\lambda(\boldsymbol{z})\ \nabla_\lambda t(\epsilon, \lambda)]$$

- ELBO:

$$\mathcal{L}(\lambda) = \mathbb{E}_{q(\boldsymbol{z}|\boldsymbol{\lambda})}[\log p(\boldsymbol{x}, \boldsymbol{z})] - \mathbb{E}_{q(\boldsymbol{z}|\boldsymbol{\lambda})}[\ \log q(\boldsymbol{z}|\lambda)\ ]$$

- **Question:** what's the reparamerization gradient w.r.t. λ ?

$$\begin{aligned} \epsilon &\sim s(\epsilon) \\ z &= t(\epsilon, \lambda) \end{aligned} \quad \Longleftrightarrow \quad z \sim q(z|\lambda)$$

$$\nabla_\lambda \mathcal{L} = \mathrm{E}_{\epsilon\sim s(\epsilon)}[\ \nabla_z[\log p(x, z) - \log q(z)]\ \nabla_\lambda t(\epsilon, \lambda)]$$

Variational Autoencoders (VAEs)

Variational Auto-Encoders (VAEs)

VAEs are a combination of the following ideas:

- Variational Inference
  - ELBO

- Variational distribution parametrized as neural networks

- Reparameterization trick

[Courtesy: Dhruv, CS 4803]

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:

$$\begin{aligned}\mathcal{L}(\boldsymbol{\theta}, \boldsymbol{\phi}; \boldsymbol{x}) &= \mathrm{E}_{q_\phi(\boldsymbol{z}|\boldsymbol{x})}[\log p_\theta(\boldsymbol{x}, \boldsymbol{z})] + \mathrm{H}(q_\phi(\boldsymbol{z}|\boldsymbol{x})) \\ &= \mathrm{E}_{q_\phi(\boldsymbol{z}|\boldsymbol{x})}[\log p_\theta(\boldsymbol{x}|\boldsymbol{z})] - \mathrm{KL}(q_\phi(\boldsymbol{z}|\boldsymbol{x}) \,||\, p(\boldsymbol{z}))\end{aligned}$$

Reconstruction

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

Variational Auto-Encoders (VAEs)

- ELBO:

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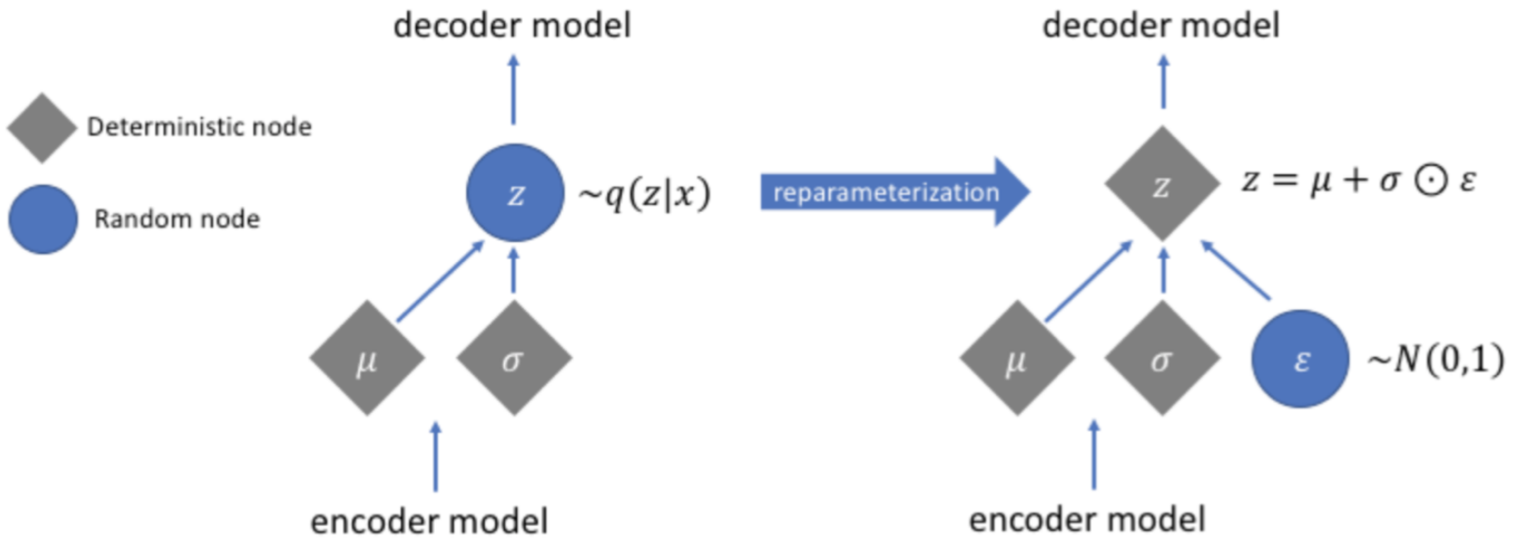
- Reparameterization:
  - $[\boldsymbol{\mu}; \boldsymbol{\sigma}] = f_\phi(\boldsymbol{x})$ (a neural network)
  - $\boldsymbol{z} = \boldsymbol{\mu} + \boldsymbol{\sigma} \odot \boldsymbol{\epsilon}, \quad \boldsymbol{\epsilon} \sim \boldsymbol{N}(\boldsymbol{0}, \boldsymbol{1})$



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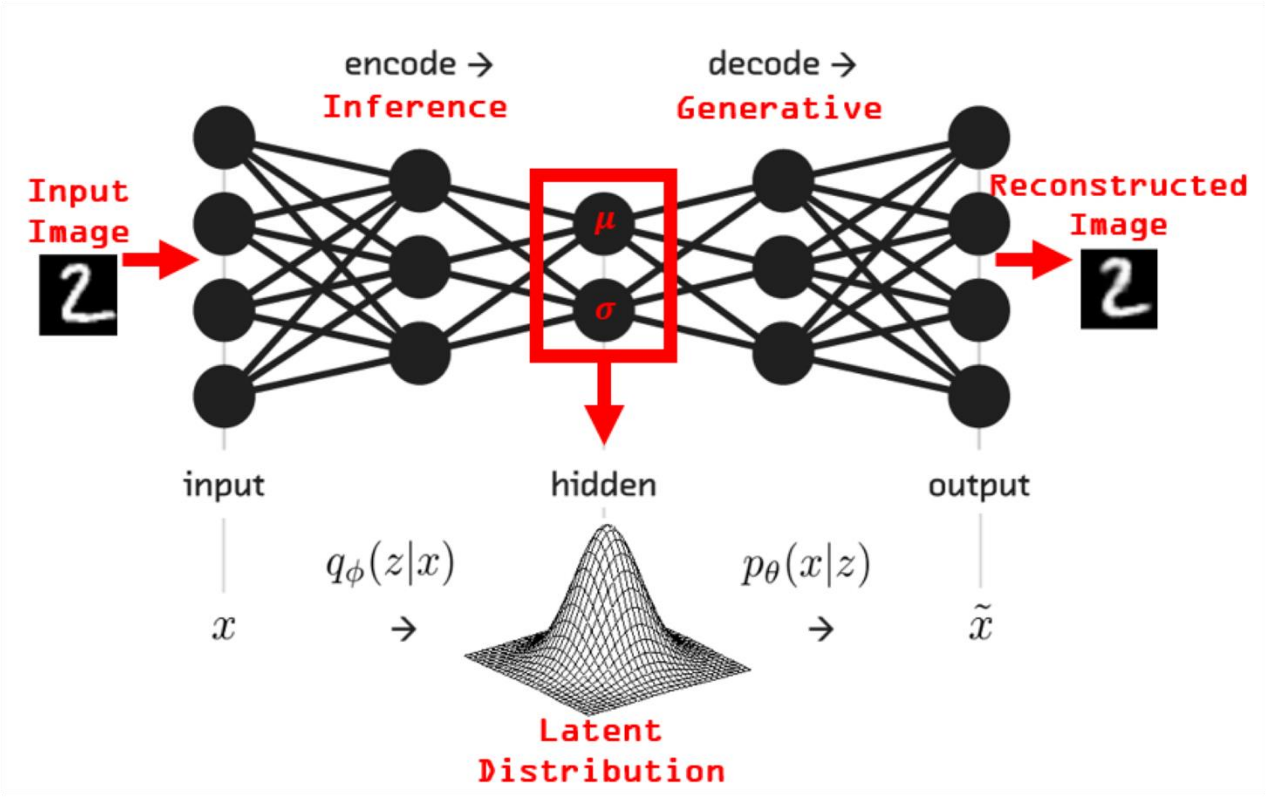
$$\nabla_{\boldsymbol{\phi}} \mathcal{L} = \mathrm{E}_{\epsilon \sim N(\mathbf{0},\mathbf{1})}[\, \nabla_{\boldsymbol{z}}[\log p_\theta(\boldsymbol{x}, \boldsymbol{z}) - \log q_\phi(\boldsymbol{z}|\boldsymbol{x})]\, \nabla_\phi z(\epsilon, \boldsymbol{\phi})]$$

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

Example: VAEs for images



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

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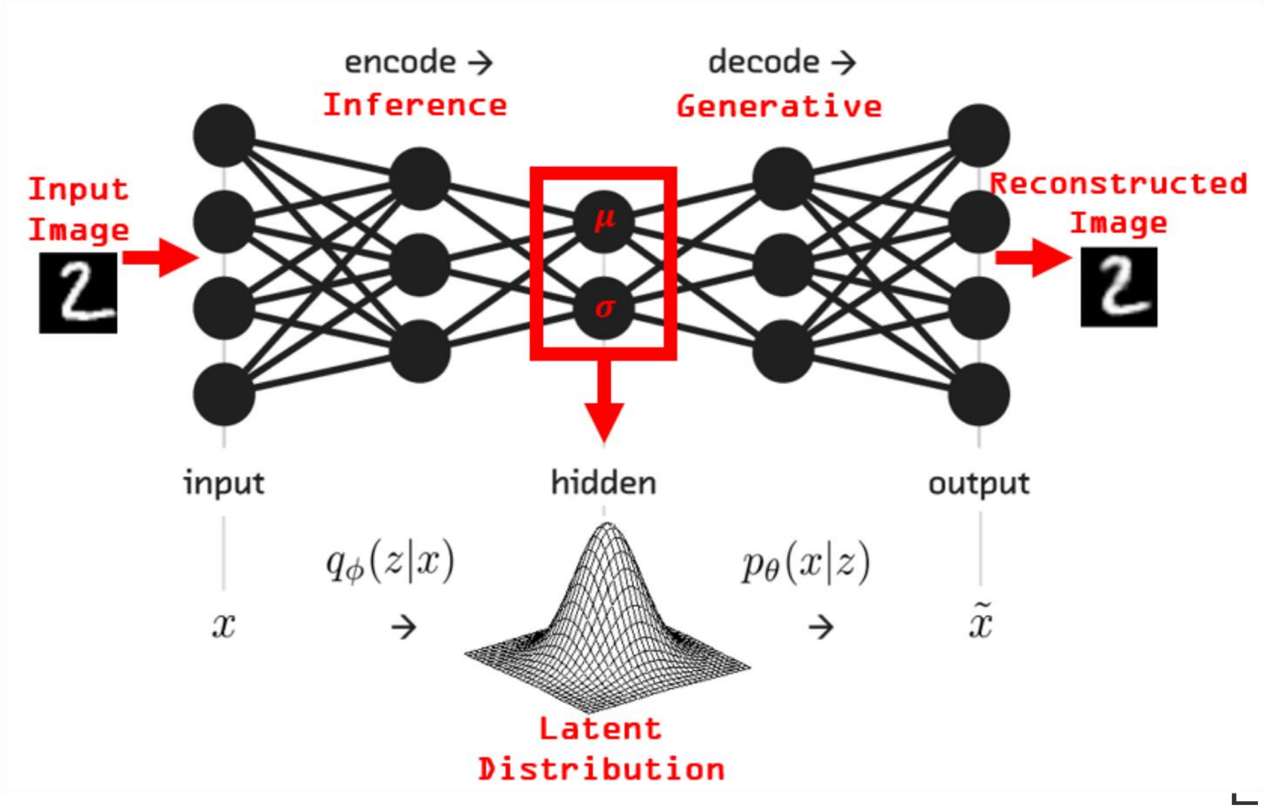

[Courtesy: Fei-Fei Li, Justin Johnson, Serena Yeung, CS 231n]

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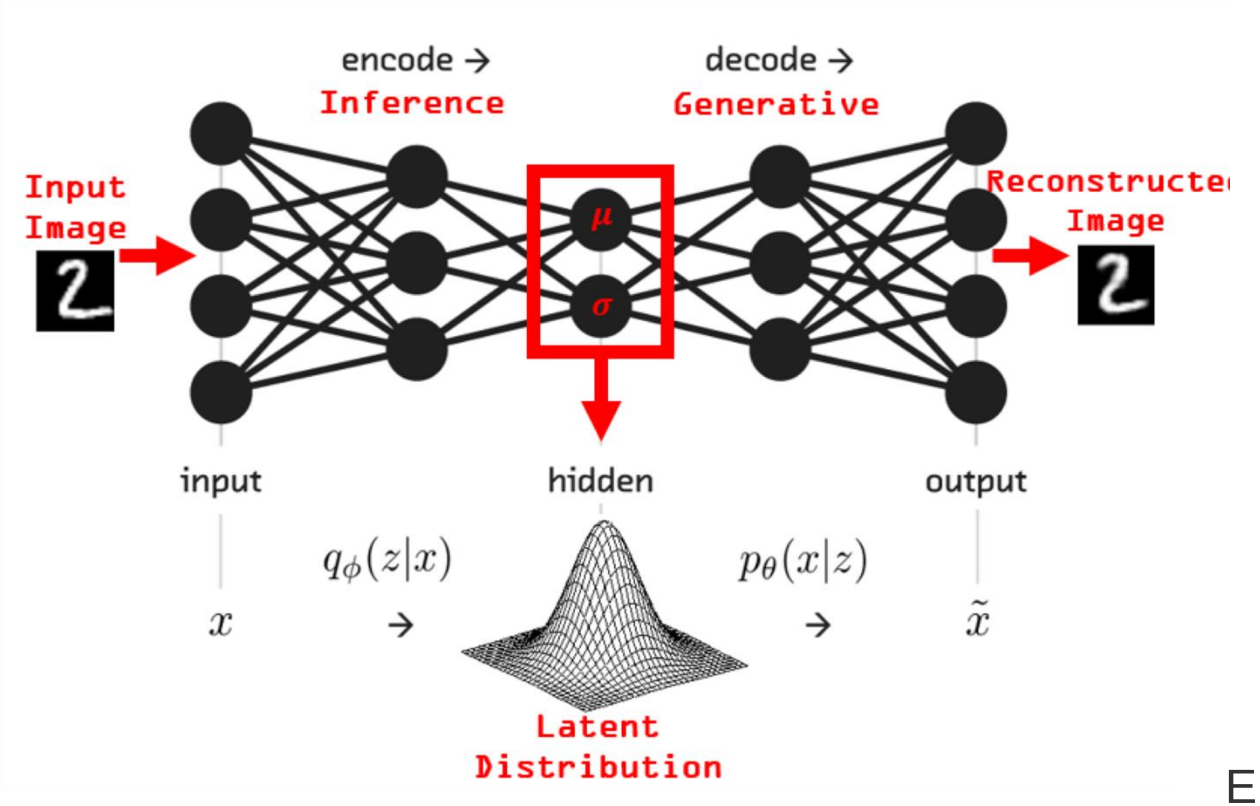

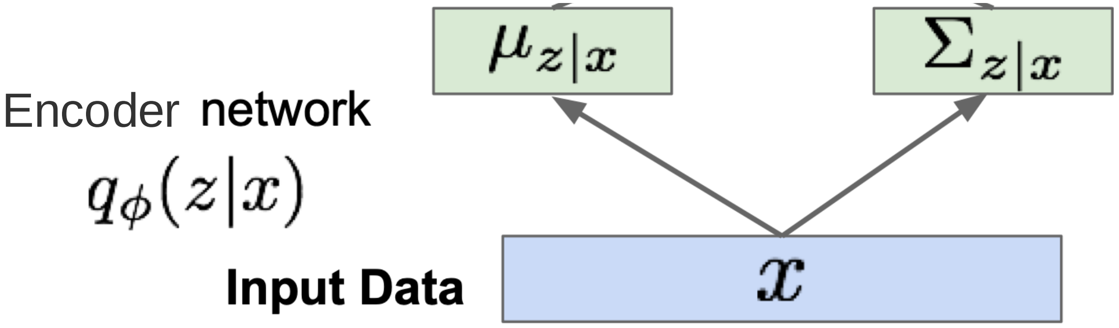

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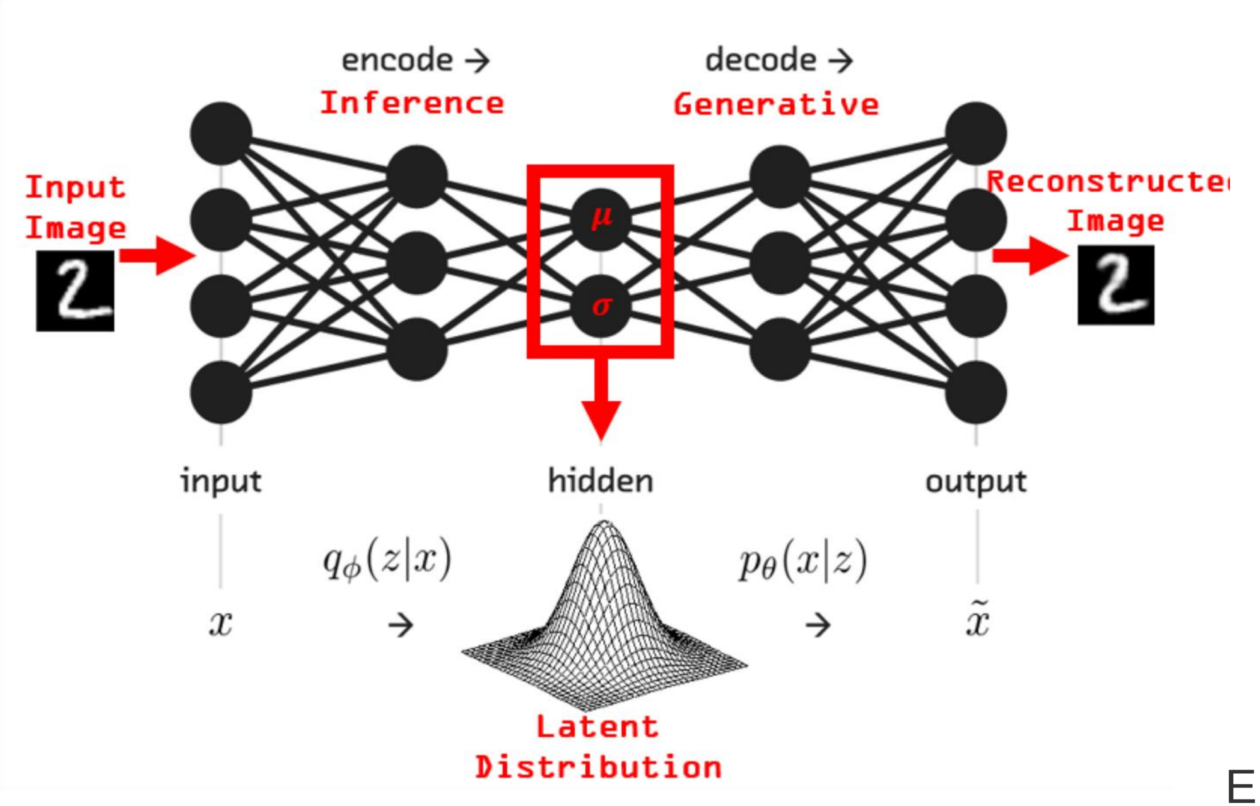
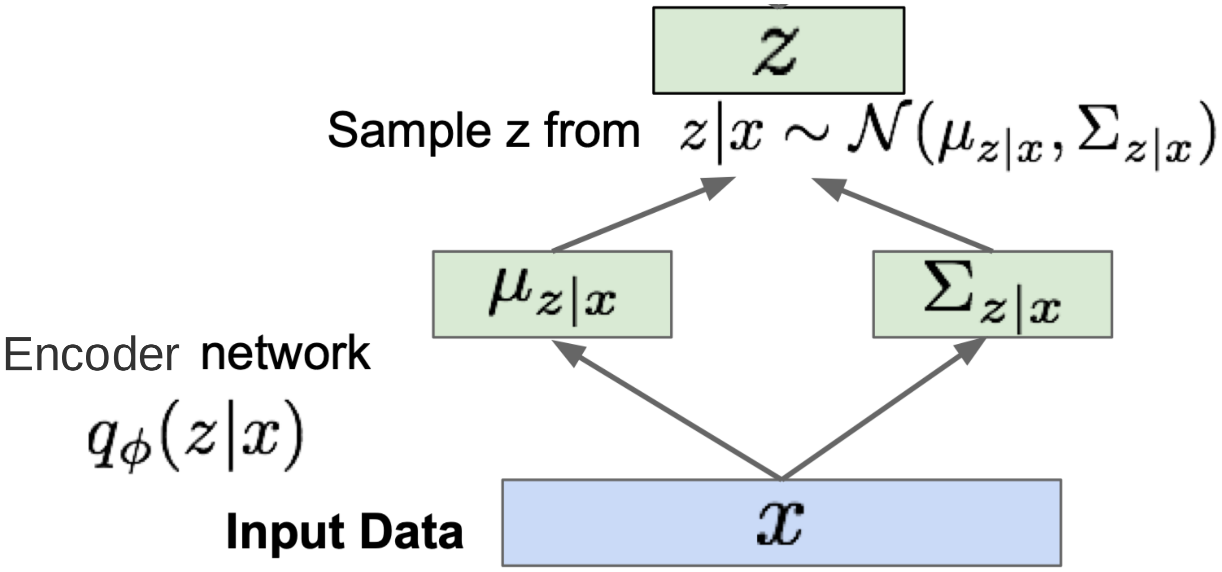
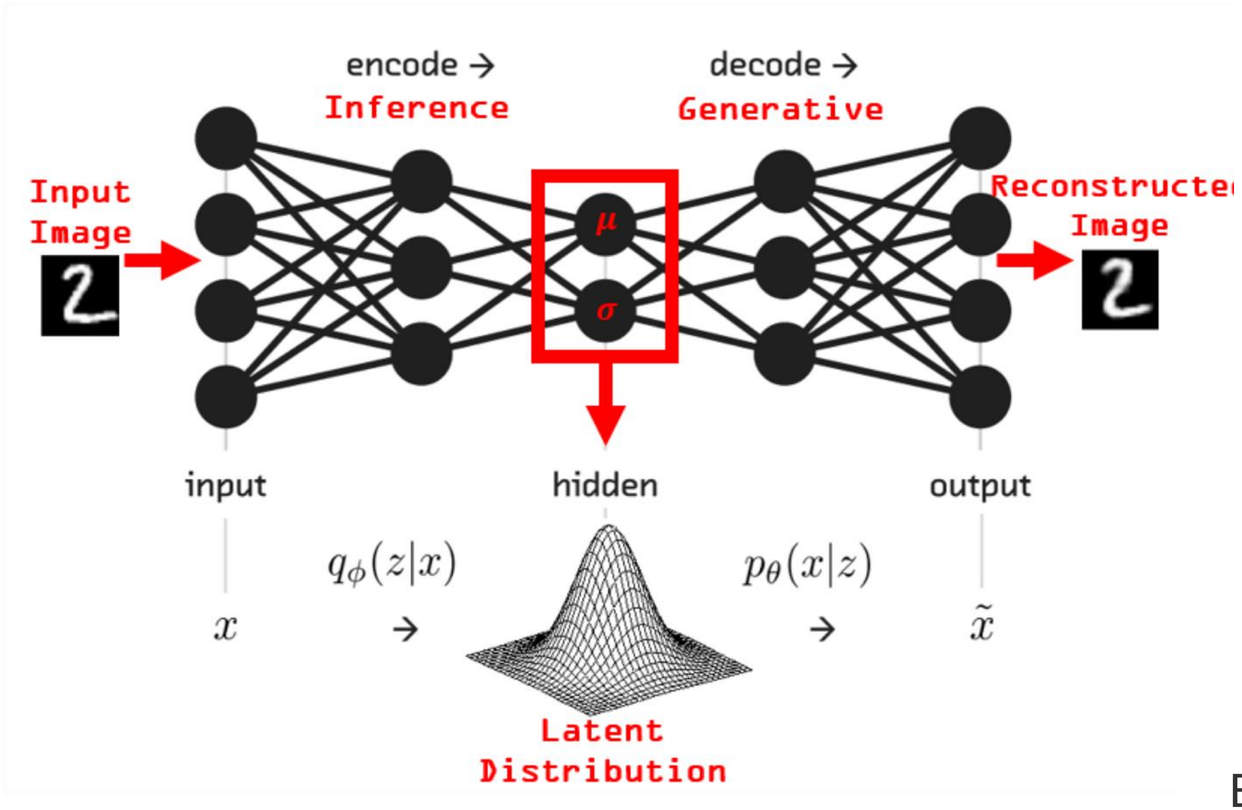
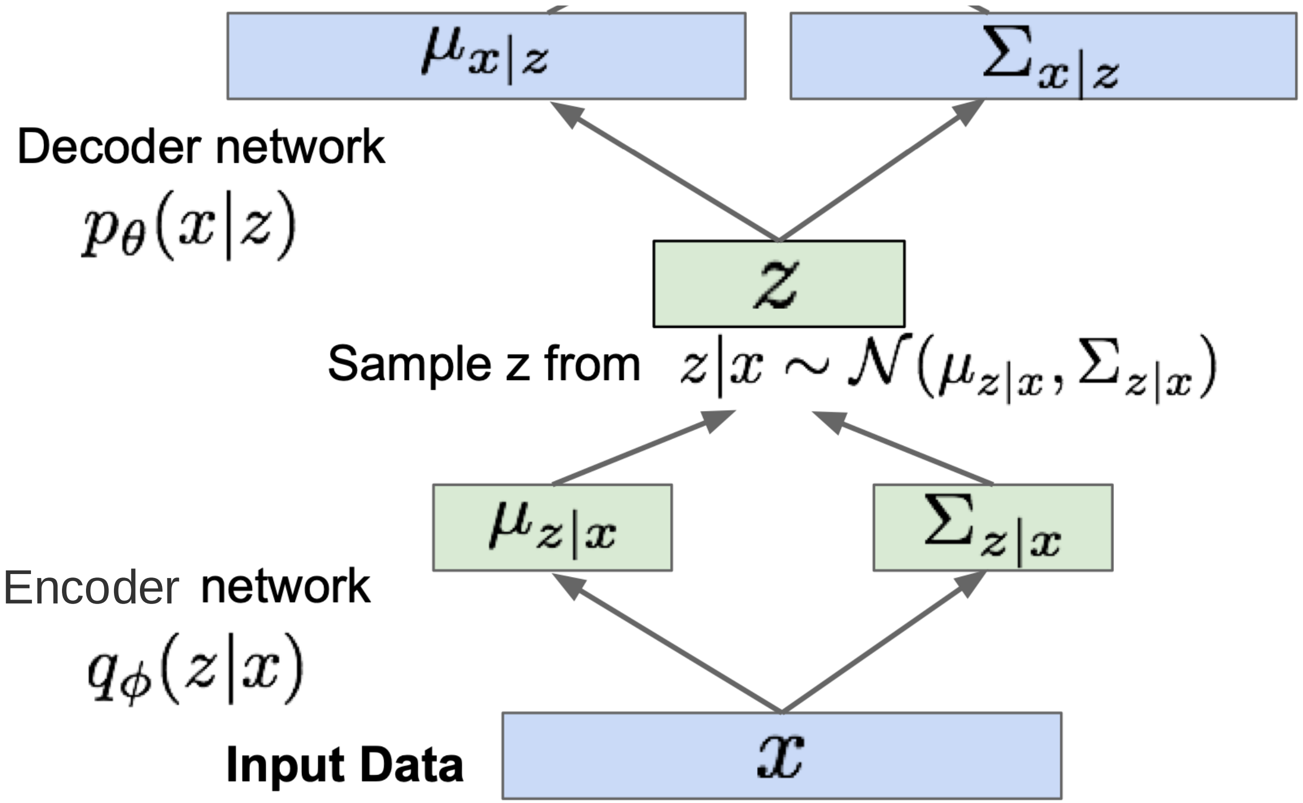




[Courtesy: Fei-Fei Li, Justin Johnson, Serena Yeung, CS 231n]

Example: VAEs for images





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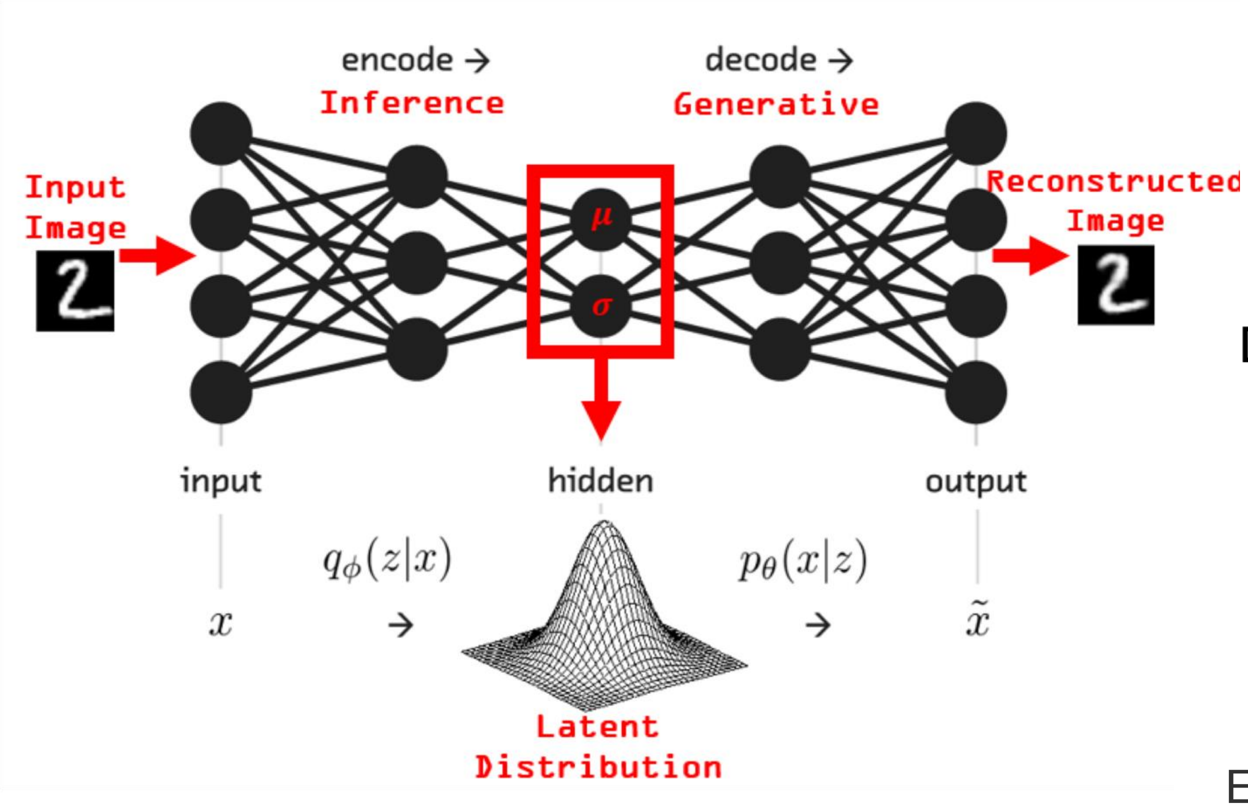
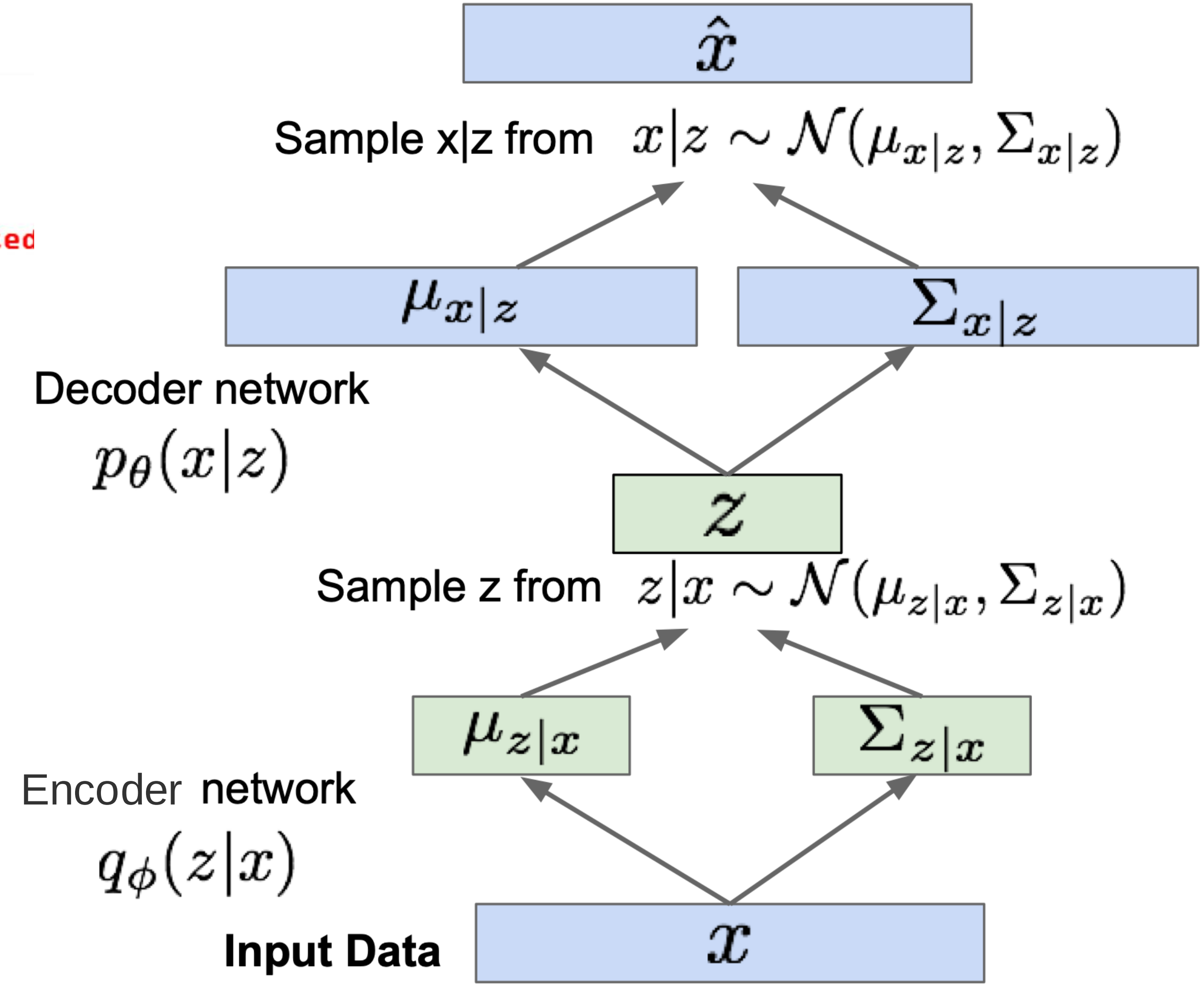
Example: VAEs for images



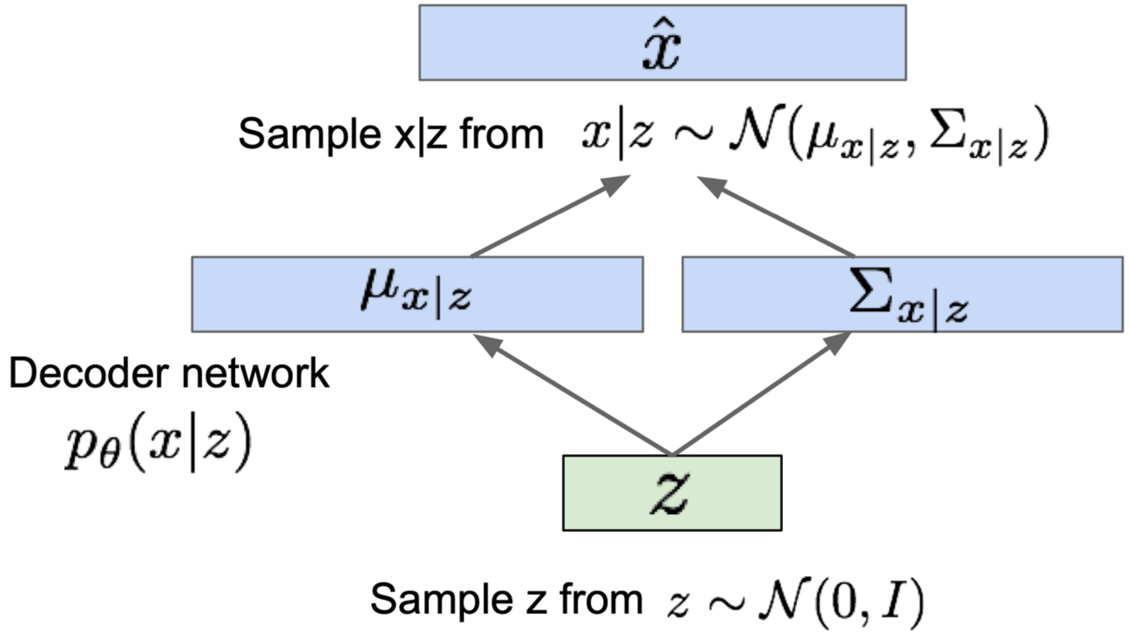


[Courtesy: Fei-Fei Li, Justin Johnson, Serena Yeung, CS 231n]

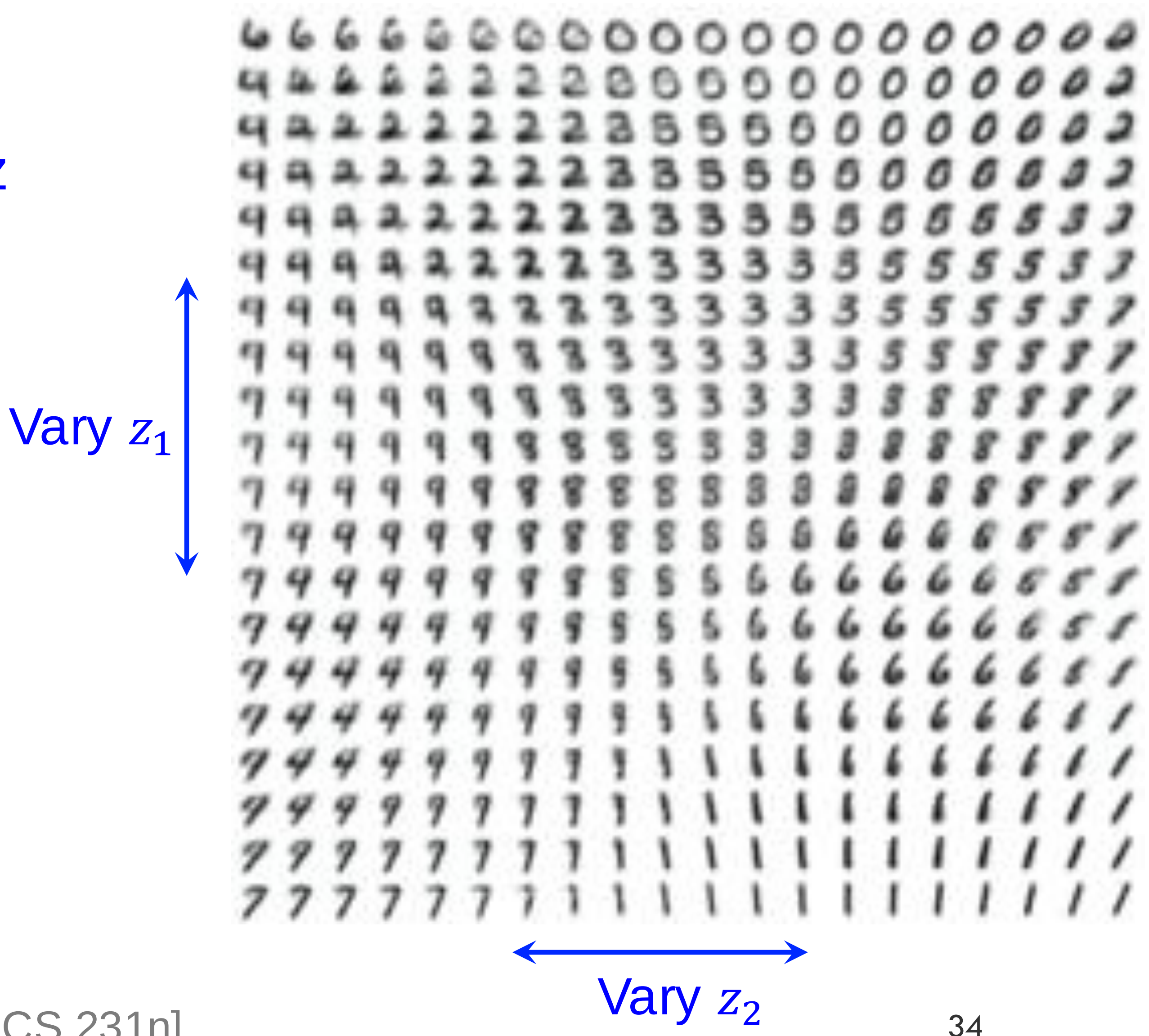
Example: VAEs for images

Generating samples:

- Use decoder network. Now sample z from prior!



Data manifold for 2-d **z**

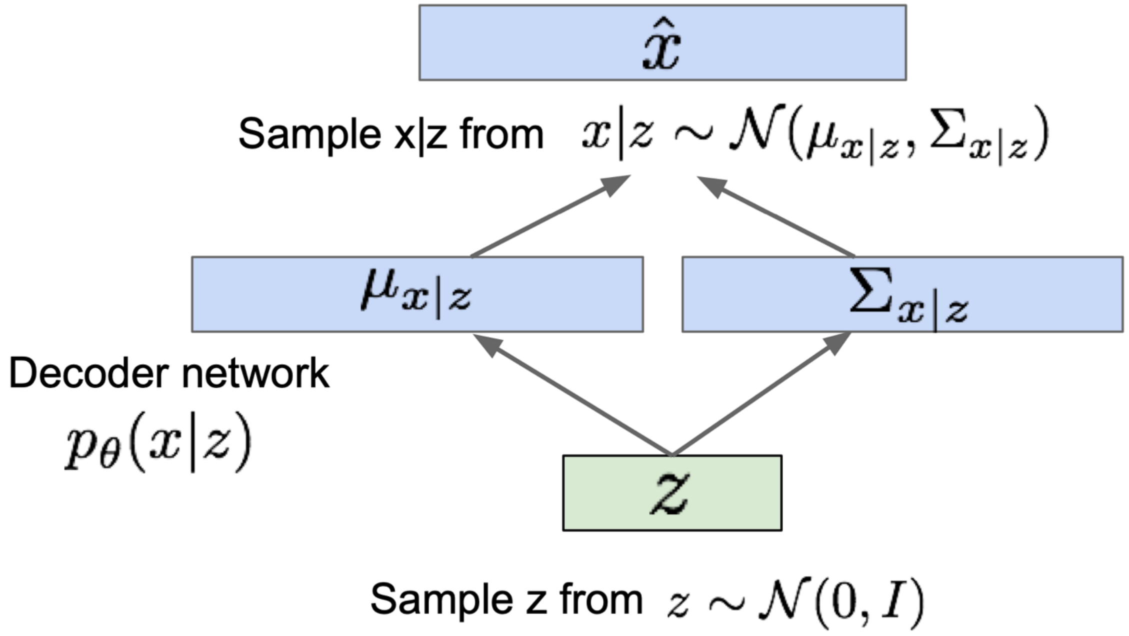


[Courtesy: Fei-Fei Li, Justin Johnson, Serena Yeung, CS 231n]

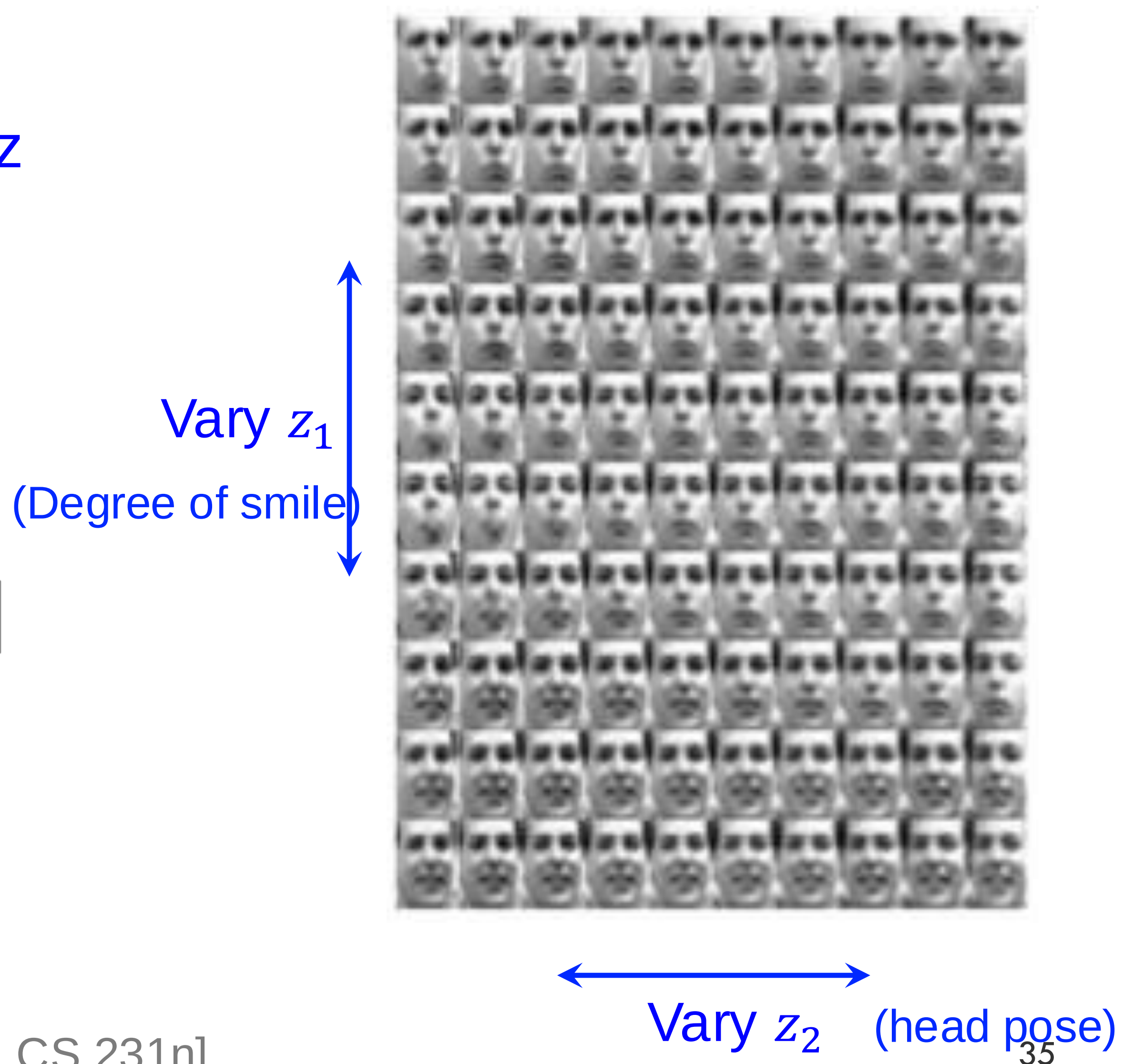
Example: VAEs for images

Generating samples:

- Use decoder network. Now sample z from prior!



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 .

Note: Amortized Variational Inference

- Variational distribution as an inference model $q_\phi(\boldsymbol{z}|\boldsymbol{x})$ with parameters $\boldsymbol{\phi}$ (which was traditionally factored over samples)
- Amortize the cost of inference by learning a **single** data-dependent inference model
- The trained inference model can be used for quick inference on new data

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

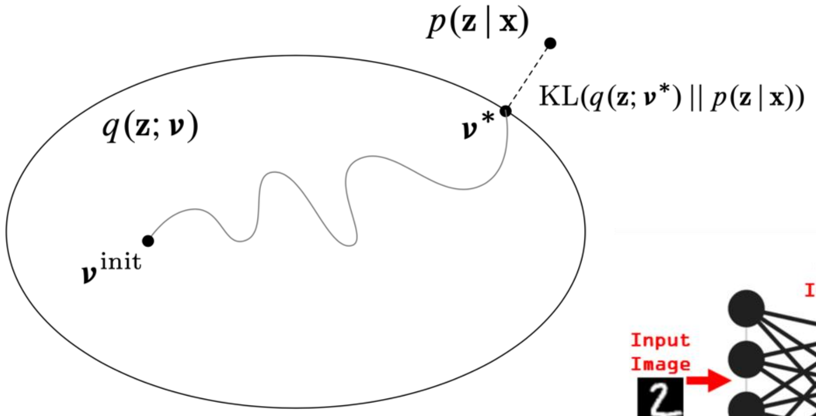
(Razavi et al., 2019)

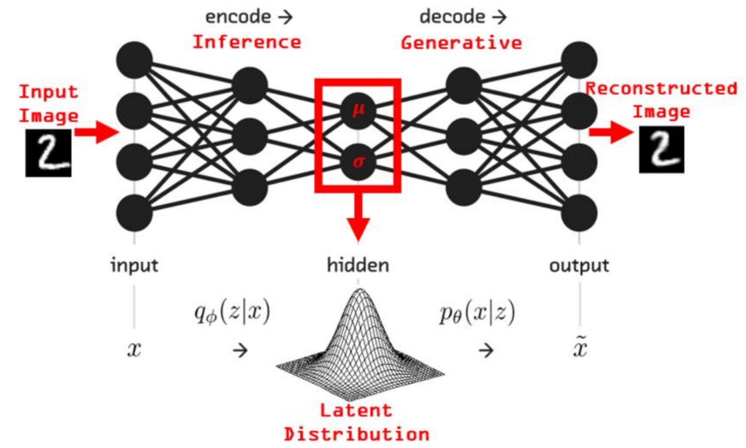
- Pros:
  - Principled approach to generative models
  - Allows inference of $q(z|x)$, can be useful feature representation for other tasks
- Cons:
  - Samples blurrier and lower quality compared to GANs
  - Tend to collapse on text data

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)





Presentations

Questions?