DSC291: Machine Learning with Few Labels

Unsupervised Learning

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EM Algorithm: Quick Recap

- Observed variables $\boldsymbol{x}$, latent variables $\boldsymbol{z}$
- To learn a model $p(\boldsymbol{x}, \boldsymbol{z}|\theta)$, we want to maximize the marginal log-likelihood
  - But it's too difficult

$$\ell(\theta; \boldsymbol{x}) = \log p(\boldsymbol{x}|\theta) = \log \sum_z p(\boldsymbol{x}, \boldsymbol{z}|\theta)$$

- EM algorithm:
  - maximize a lower bound of $\ell(\theta; \boldsymbol{x})$
- Key equation:

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

Evidence Lower Bound (ELBO)

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

Variational free energy

EM Algorithm: Quick Recap

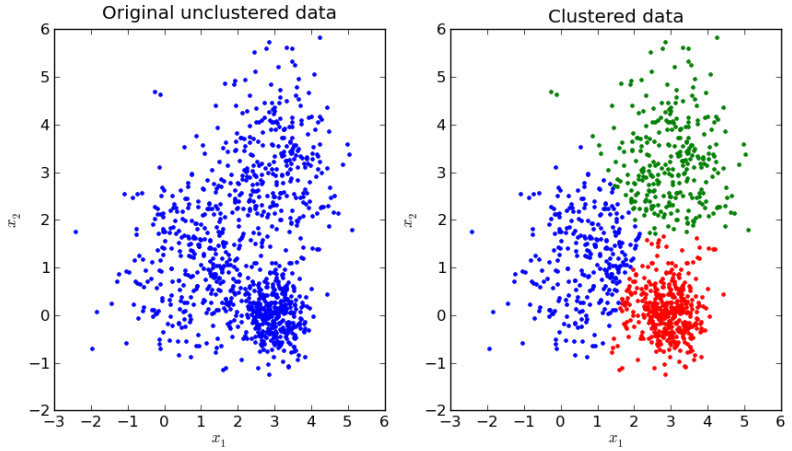
- The EM algorithm is coordinate-decent on $F(q, \theta)$
  - E-step: $q^{t+1} = \arg\min_q F\left(q, \theta^t\right) = p(\boldsymbol{z}|\boldsymbol{x}, \theta^t)$
    - the posterior distribution over the latent variables given the data and the current parameters
  - M-step: $\theta^{t+1} = \arg\min_\theta F\left(q^{t+1}, \theta^t\right) = \text{argmax}_\theta \sum_z q^{t+1}(\boldsymbol{z}|\boldsymbol{x}) \log p(\boldsymbol{x}, \boldsymbol{z}|\theta)$

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

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

Example: Gaussian Mixture Models

- Observed variables $\boldsymbol{x}$:
- Latent variables $\boldsymbol{z}$:
- Want to learn a model $p(\boldsymbol{x}, \boldsymbol{z}|\theta)$
  - Consider a mixture of K Gaussian components



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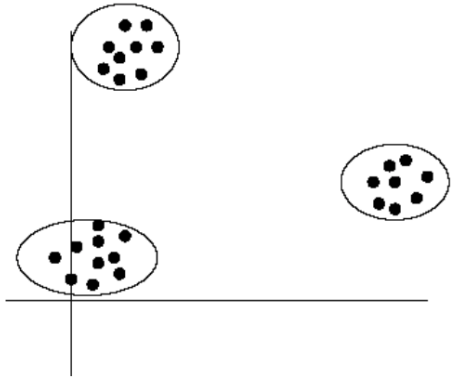

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- Latent variables $\boldsymbol{z}$:
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  - Consider a mixture of K Gaussian components
  - $p(\boldsymbol{x}, \boldsymbol{z}|\theta) =$
  - $p(\boldsymbol{x}|\theta) =$
  - The log likelihood of a sample $\boldsymbol{x}_n \in \{\boldsymbol{x}_i\}_{i=1}^N$:
    $\log p(\boldsymbol{x}_n|\theta) =$

$$q^{t+1} = \arg\min_{q} F\left(q, \theta^t\right) \quad = p(\boldsymbol{z}|\boldsymbol{x}, \theta^t)$$

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  - E-step: computing the posterior of $\boldsymbol{z}_n$ given the current estimate of the parameters (i.e., π , μ, Σ)

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$$p(z_n^k = 1 \mid x, \mu^{(t)}, \Sigma^{(t)}) = \frac{\pi_k^{(t)} N(x_n, \mid \mu_k^{(t)}, \Sigma_k^{(t)})}{\sum_i \pi_i^{(t)} N(x_n, \mid \mu_i^{(t)}, \Sigma_i^{(t)})}$$

$p(z_n^k = 1, x, \mu^{(t)}, \Sigma^{(t)})$

$p(x, \mu^{(t)}, \Sigma^{(t)})$

$$\theta^{t+1} = \arg\min_{\theta} F\left(q^{t+1}, \theta^{t}\right) = \text{argmax}_{\theta} \sum_{z} q^{t+1}(\boldsymbol{z}|\boldsymbol{x}) \log p(\boldsymbol{x}, \boldsymbol{z}|\theta)$$

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$$\mathbb{E}_{q(\boldsymbol{z}|\boldsymbol{x})}\left[\log p(\boldsymbol{x}, \boldsymbol{z}|\theta)\right] =$$

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$$\mathbb{E}_{q(\boldsymbol{z}|\boldsymbol{x})}\left[\log p(\boldsymbol{x}, \boldsymbol{z}|\theta)\right] = \sum_{n} \mathbb{E}_q\left[\log p\left(z_n \mid \pi\right)\right] + \sum_{n} \mathbb{E}_q\left[\log p\left(x_n \mid z_n, \mu, \Sigma\right)\right]$$

$$= \sum_{n}\sum_{k} \mathbb{E}_q\left[z_n^k\right] \log \pi_k - \frac{1}{2}\sum_{n}\sum_{k} \mathbb{E}_q\left[z_n^k\right]\left(\left(x_n - \mu_k\right)^T \Sigma_k^{-1}\left(x_n - \mu_k\right) + \log|\Sigma_k| + C\right)$$

$$\theta^{t+1} = \arg\min_{\theta} F\left(q^{t+1}, \theta^{t}\right) = \operatorname{argmax}_{\theta} \sum_{z} q^{t+1}(\boldsymbol{z}|\boldsymbol{x}) \log p(\boldsymbol{x}, \boldsymbol{z}|\theta)$$

Example: Gaussian Mixture Models

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$$\pi_k^* = \arg\max \langle l_c(\boldsymbol{\theta}) \rangle, \quad \Rightarrow \quad \frac{\partial}{\partial \pi_k} \langle l_c(\boldsymbol{\theta}) \rangle = 0, \forall k, \quad \text{s.t.} \sum_{\mathrm{k}} \pi_k = 1$$

$$\Rightarrow \quad \pi_k^* = \sum_n \left\langle z_n^k \right\rangle_{q^{(t)}} \Big/ N = \sum_n \tau_n^{k(t)} \Big/ N = \langle n_k \rangle \Big/ N$$

$$\mu_k^* = \arg\max \langle l(\boldsymbol{\theta}) \rangle, \quad \Rightarrow \quad \mu_k^{(t+1)} = \frac{\sum_n \tau_n^{k(t)} x_n}{\sum_n \tau_n^{k(t)}}$$

$$\Sigma_k^* = \arg\max \langle l(\boldsymbol{\theta}) \rangle, \quad \Rightarrow \quad \Sigma_k^{(t+1)} = \frac{\sum_n \tau_n^{k(t)} (x_n - \mu_k^{(t+1)})(x_n - \mu_k^{(t+1)})^T}{\sum_n \tau_n^{k(t)}}$$

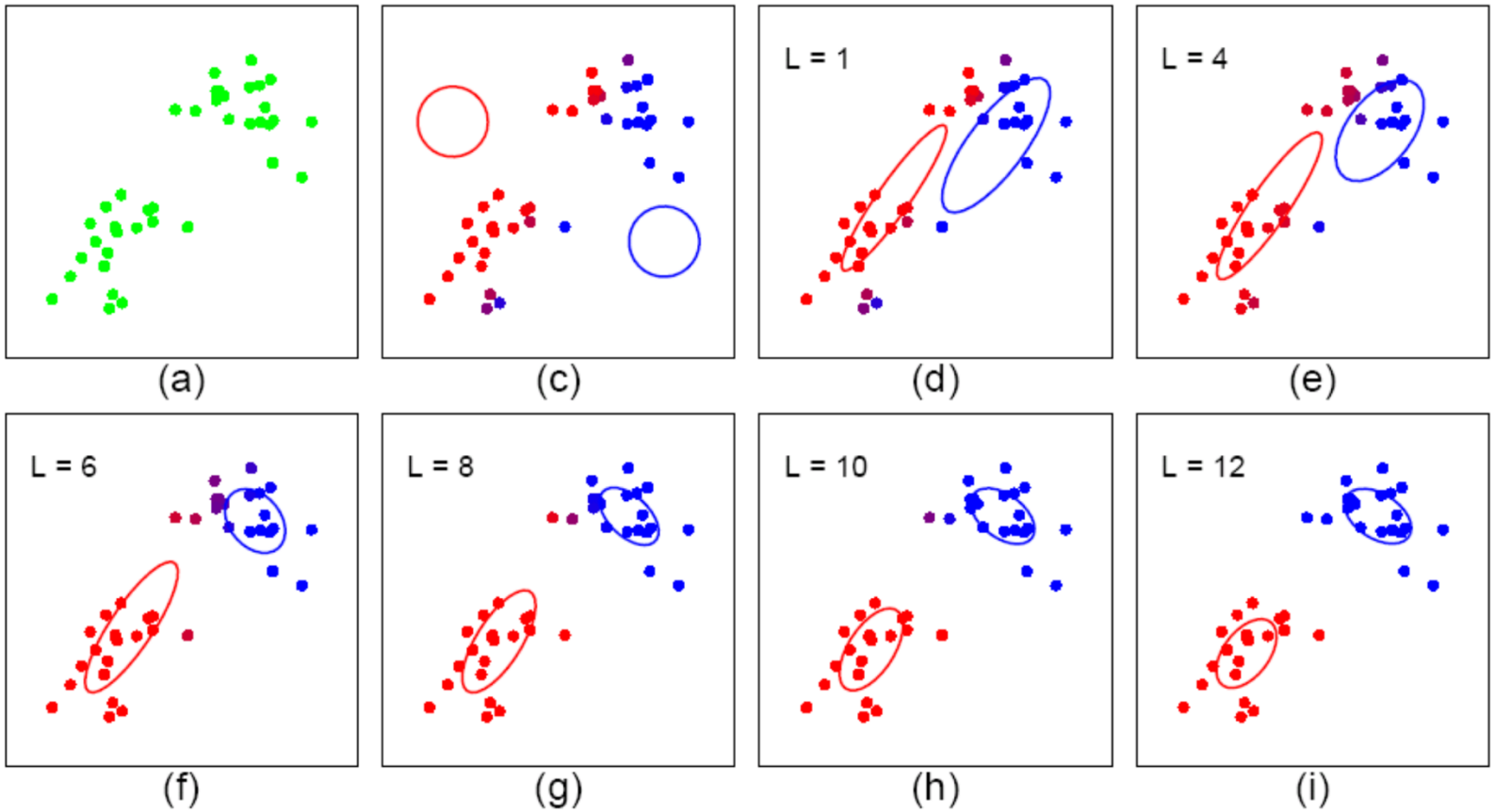
Fact:

$$\frac{\partial \log |\mathrm{A}^{-1}|}{\partial \mathrm{A}^{-1}} = \mathrm{A}^T$$

$$\frac{\partial \mathbf{x}^T \mathrm{A} \mathbf{x}}{\partial \mathrm{A}} = \mathbf{x}\mathbf{x}^T$$

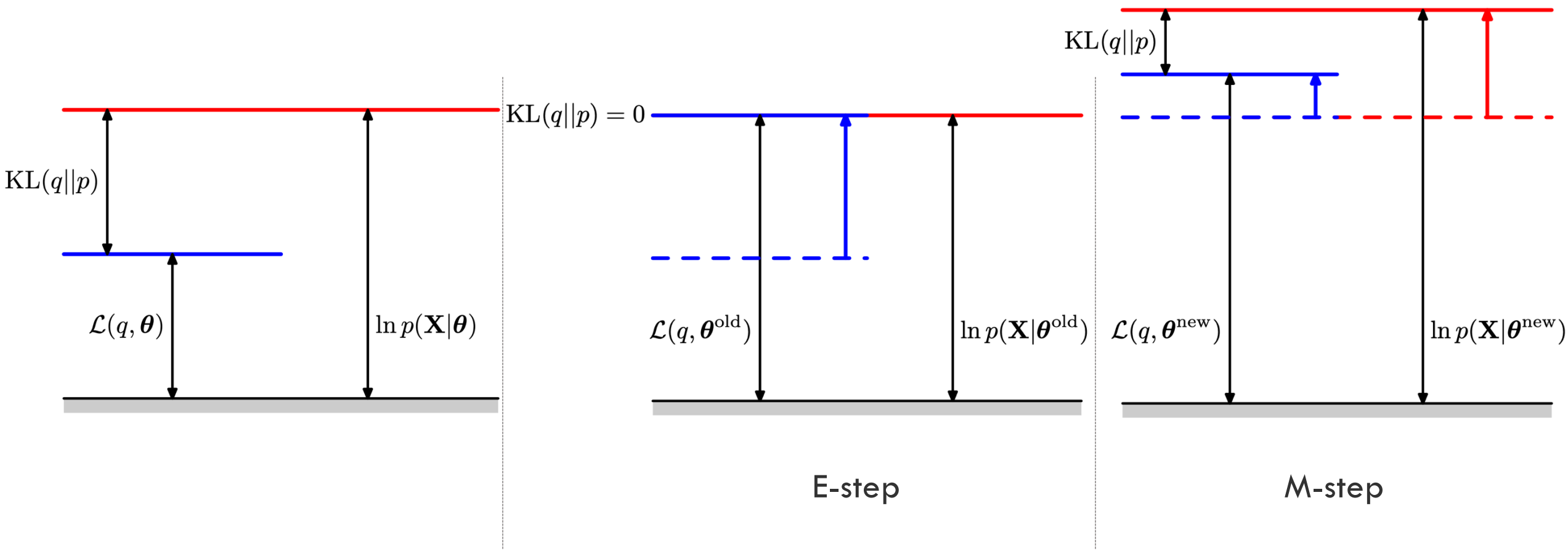
Example: Gaussian Mixture Models (GMMs)

- Start: "guess" the centroid μ_k and covariance Σ_k of each of the K clusters
- Loop:



Each EM iteration guarantees to improve the likelihood

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



[PRML, Chap 9.4]

Summary: EM Algorithm

- A way of maximizing likelihood function for latent variable models. Finds MLE of parameters when the original (hard) problem can be broken up into two (easy) pieces
  - Estimate some "missing" or "unobserved" data from observed data and current parameters.
  - Using this "complete" data, find the maximum likelihood parameter estimates.

- Alternate between filling in the latent variables using the best guess (posterior) and updating the parameters based on this guess:

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

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

Variational Inference / Variational Auto-Encoders (VAEs)

Content adapted from CMU 10-708 Spring 2017

Inference

- Given a model, the goals of inference can include:
  - Computing the likelihood of observed data $p(\boldsymbol{x}^*)$
  - Computing the marginal distribution over a given subset of variables in the model $p(\boldsymbol{x}_A)$
  - Computing the conditional distribution over a subsets of nodes given a disjoint subset of nodes $p(\boldsymbol{x}_A|\boldsymbol{x}_B)$
  - Computing a mode of the density (for the above distributions) $\text{argmax}_{\boldsymbol{x}}\, p(\boldsymbol{x})$
  - ….

Variational Inference

- Observed variables $\boldsymbol{x}$, latent variables $\boldsymbol{z}$
- Variational (Bayesian) inference, a.k.a. **variational Bayes,** is most often used to approximately infer the **posterior distribution** over the latent variables

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

- We cannot directly compute the posterior distribution for many interesting models
  - I.e. the posterior density is in an intractable form (often involving integrals) which cannot be easily analytically solved.

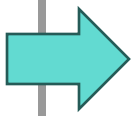
EM and Variational Inference

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

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

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

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



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

Variational Inference

Recall that in EM, we assume $q(z|x)$ can be any distribution. E-step shows the optimal $q(z|x)$ is the posterior distribution.

Variational Inference

Recall that in EM, we assume $q(z|x)$ can be any distribution. E-step shows the optimal $q(z|x)$ is the posterior distribution.

The main idea behind variational inference:

- Choose a family of distributions over the latent variables $z_{1:m}$ with its own set of variational parameters ν , i.e.

$$q(z_{1:m}|\nu)$$

- Then, we find the setting of the parameters that makes our approximation q closest to the posterior distribution.
  - This is where optimization algorithms come in.

- Then we can use q with the fitted parameters in place of the posterior.
  - E.g. to form predictions about future data, or to investigate the posterior distribution over the hidden variables, find modes, etc.

Variational Inference

- We want to minimize the KL divergence between our approximation $q(\boldsymbol{z}|\boldsymbol{x},\boldsymbol{\nu})$ and our posterior $p(\boldsymbol{z}|\boldsymbol{x})$

$$\mathrm{KL}(q(\boldsymbol{z}|\boldsymbol{x},\boldsymbol{\nu}) \,||\, p(\boldsymbol{z}|\boldsymbol{x}))$$

  - But we can't actually minimize this quantity w.r.t q because $p(\boldsymbol{z}|\boldsymbol{x})$ is unknown

- **Question:** how can we minimize the KL divergence?
  - **Hint**: recall the equation that holds for any q:

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

Variational Inference

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Evidence Lower Bound (ELBO)

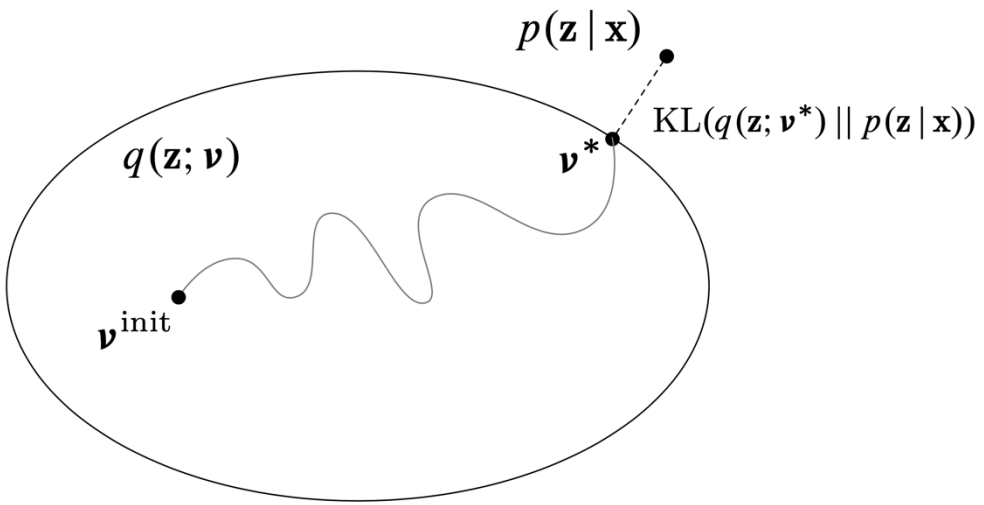
- The ELBO is equal to the negative KL divergence up to a constant $\ell(\theta;\boldsymbol{x})$
- We maximize the ELBO over q to find an "optimal approximation" to $p(\boldsymbol{z}|\boldsymbol{x})$

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 $p(\boldsymbol{z}|\boldsymbol{x})$

$$\text{argmax}_{\nu}\ \mathbb{E}_{q(\boldsymbol{z}|\boldsymbol{x},\boldsymbol{\nu})}\left[\log \frac{p(\boldsymbol{x},\boldsymbol{z}|\theta)}{q(\boldsymbol{z}|\boldsymbol{x},\boldsymbol{\nu})}\right]$$

$$= \text{argmax}_{\nu}\ \mathbb{E}_{q(\boldsymbol{z}|\boldsymbol{x},\boldsymbol{\nu})}[\log p(\boldsymbol{x},\boldsymbol{z}|\theta)] - \mathbb{E}_{q(\boldsymbol{z}|\boldsymbol{x},\boldsymbol{\nu})}[\log q(\boldsymbol{z}|\boldsymbol{x},\boldsymbol{\nu})]$$



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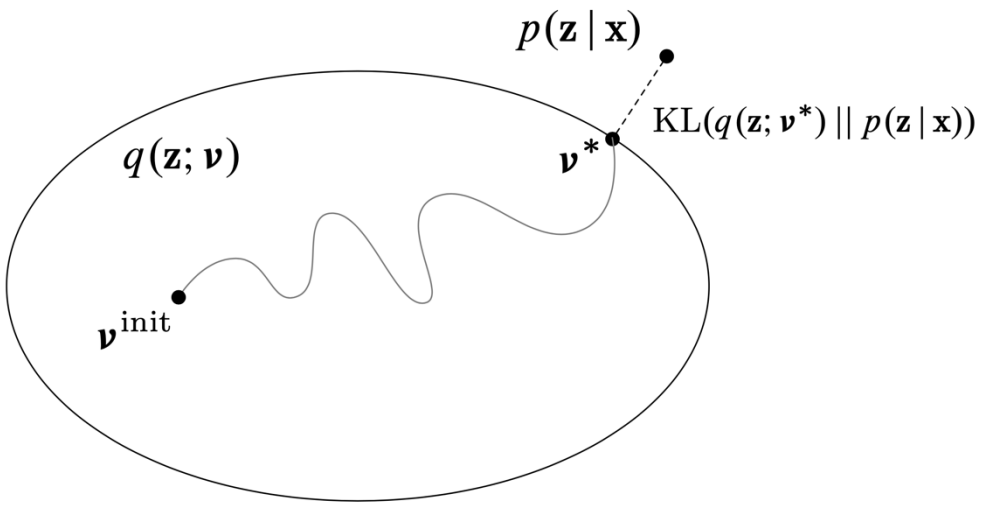

Question: How do we choose the variational family $q(\boldsymbol{z}|\boldsymbol{x},\boldsymbol{\nu})$?

Variational Inference

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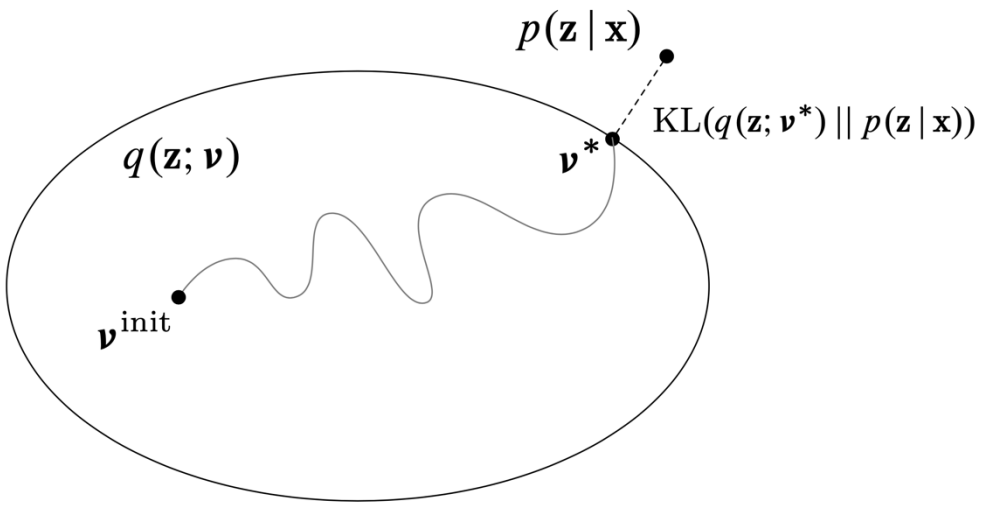

Question: How do we choose the variational family $q(\boldsymbol{z}|\boldsymbol{x},\boldsymbol{\nu})$?

- 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:

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

Reconstruction

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

Variational Auto-Encoders (VAEs)

- ELBO:

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

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

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

Variational Auto-Encoders (VAEs)

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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)

- ELBO:

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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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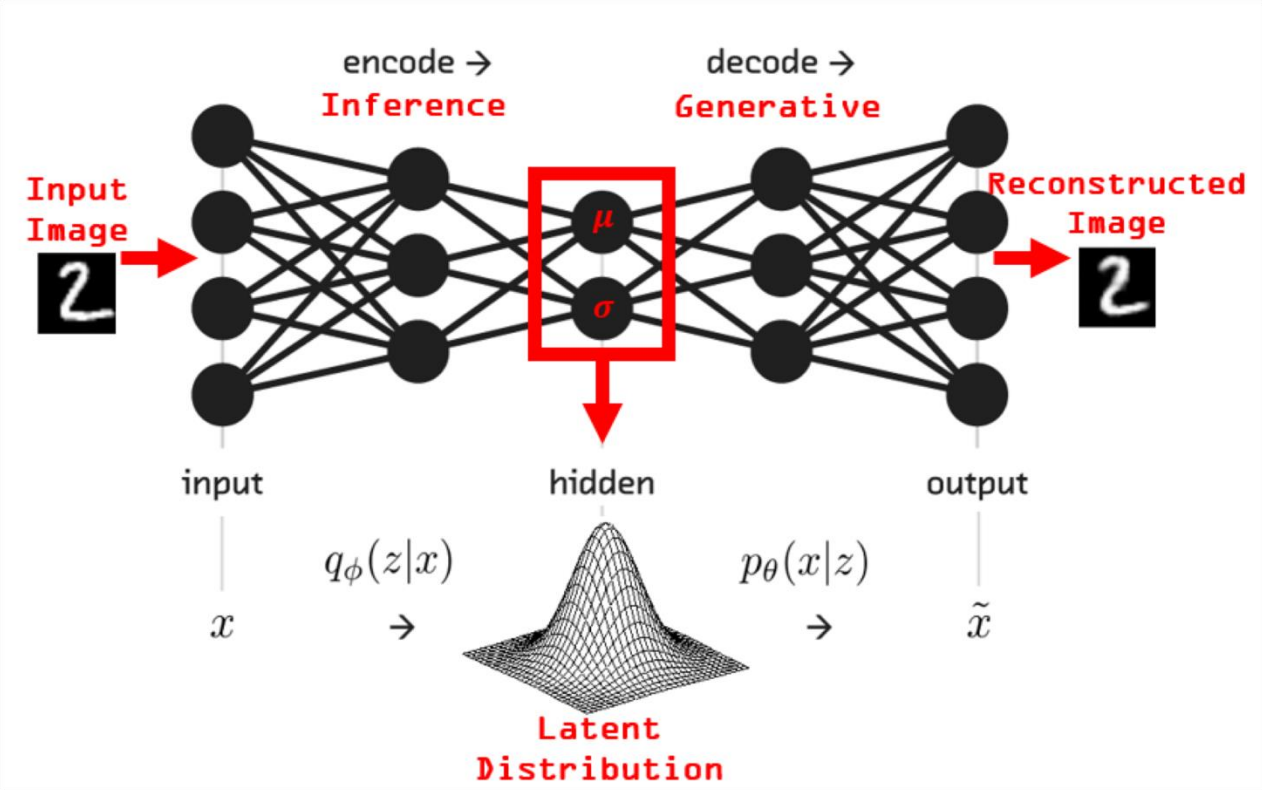
Example: VAEs for images



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

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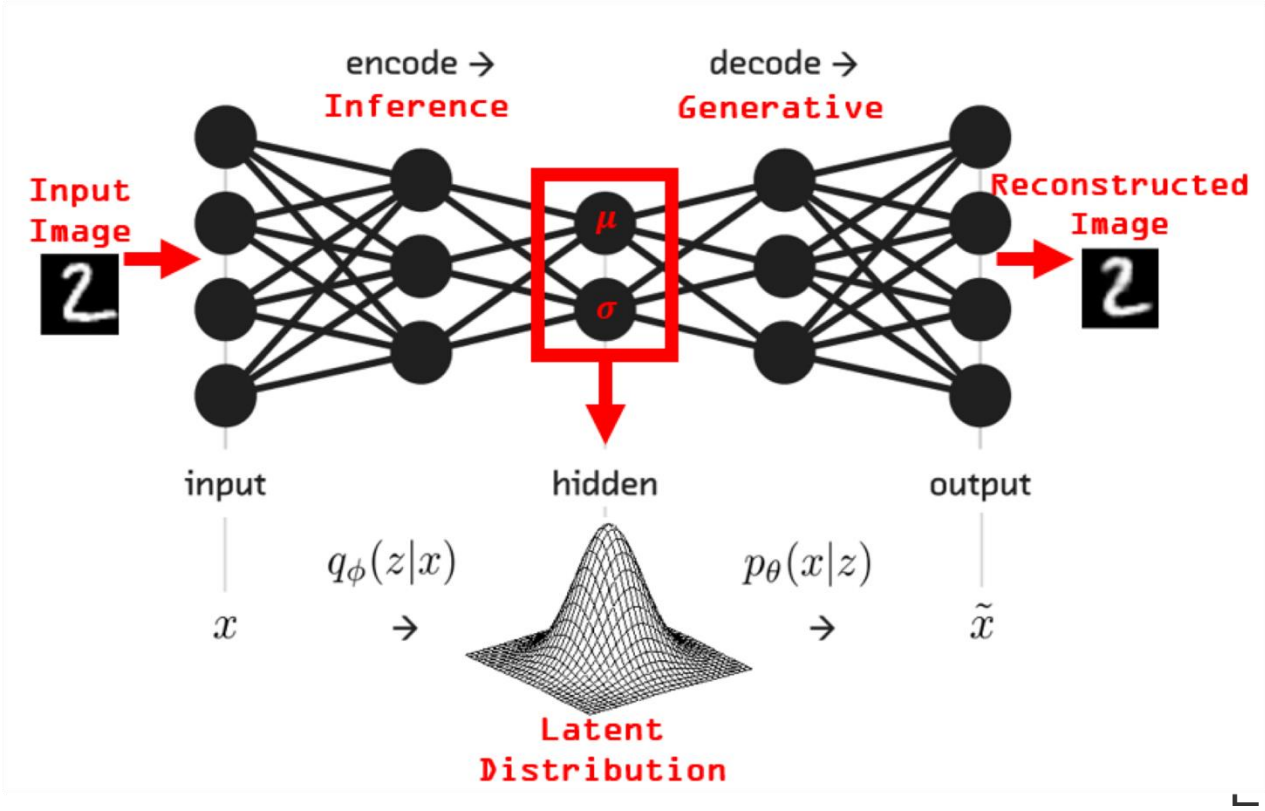

Input Data x

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

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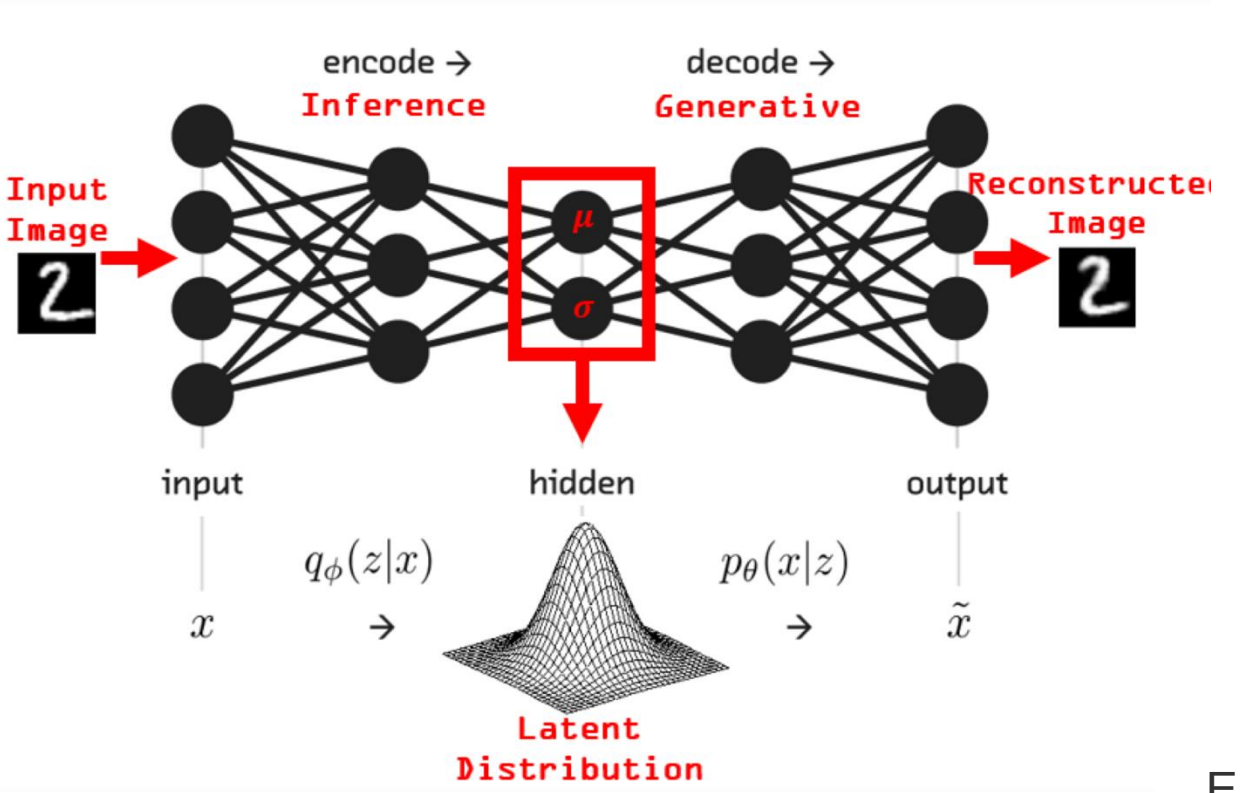
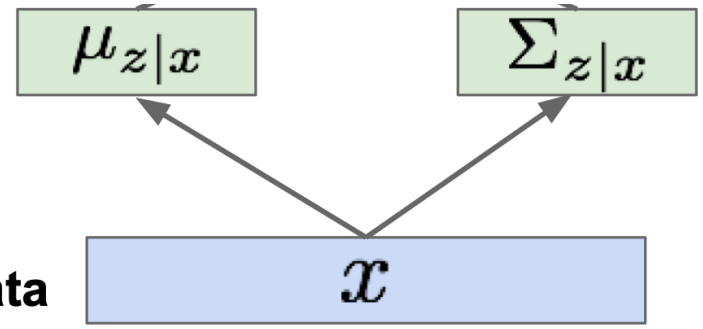


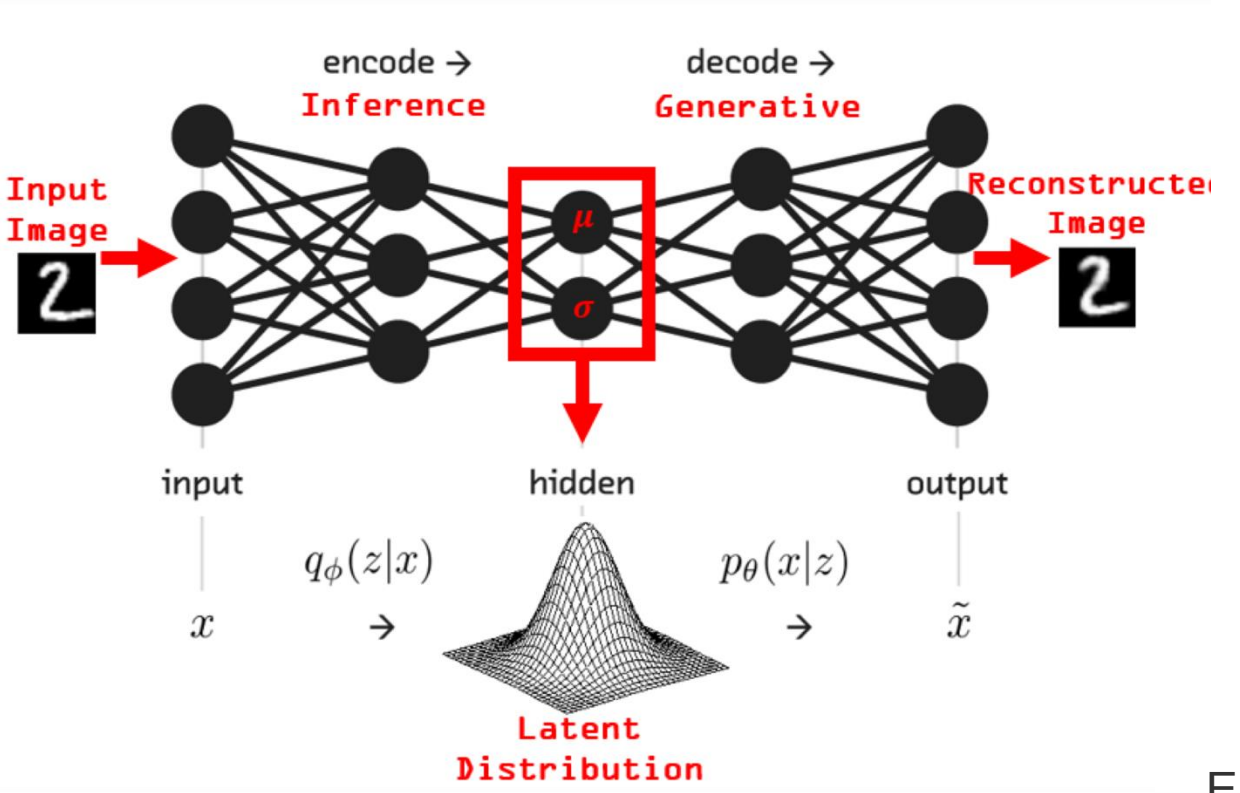
Encoder network

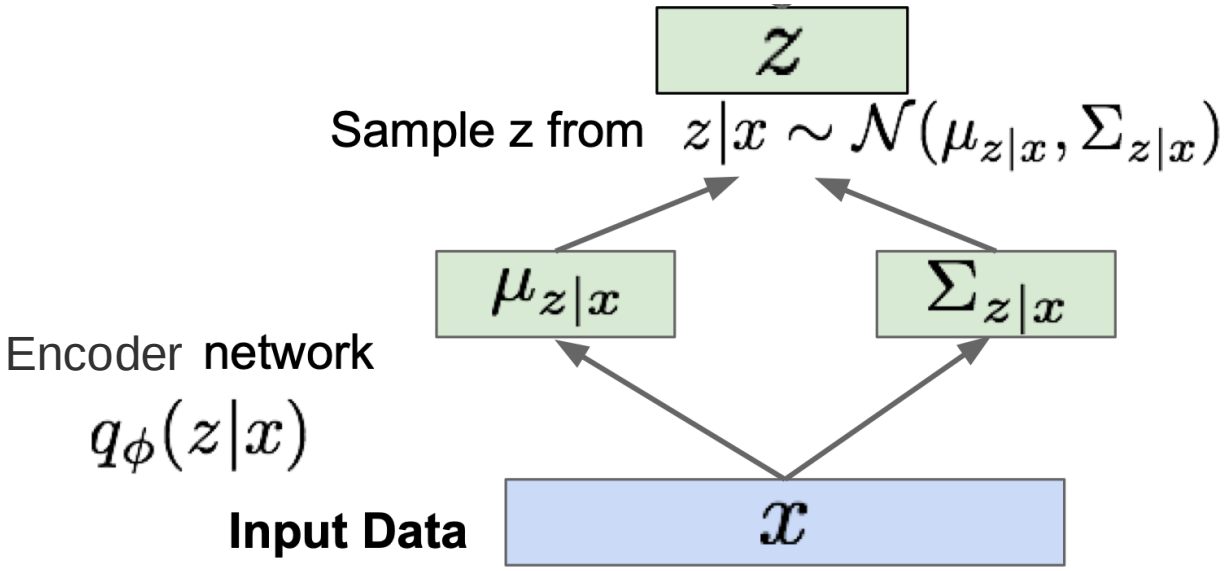
$q_\phi(z|x)$



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

Example: VAEs for images





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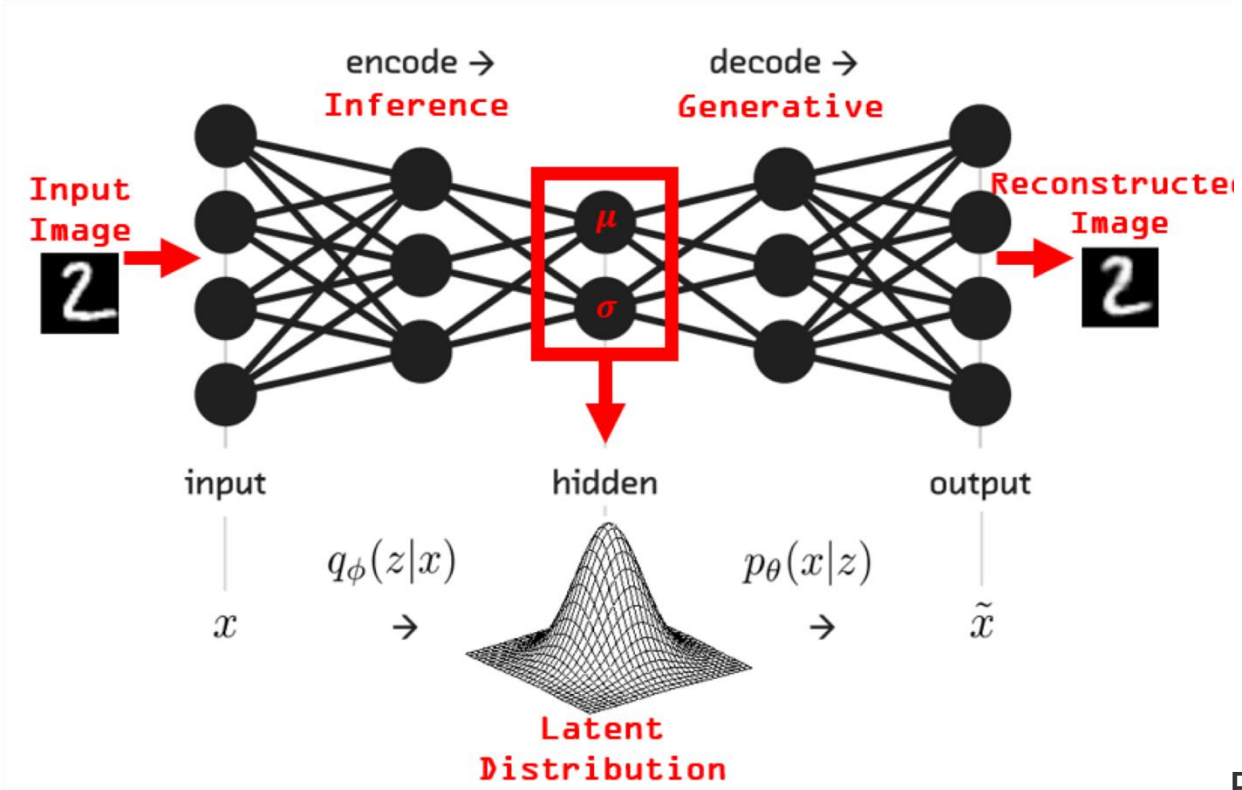
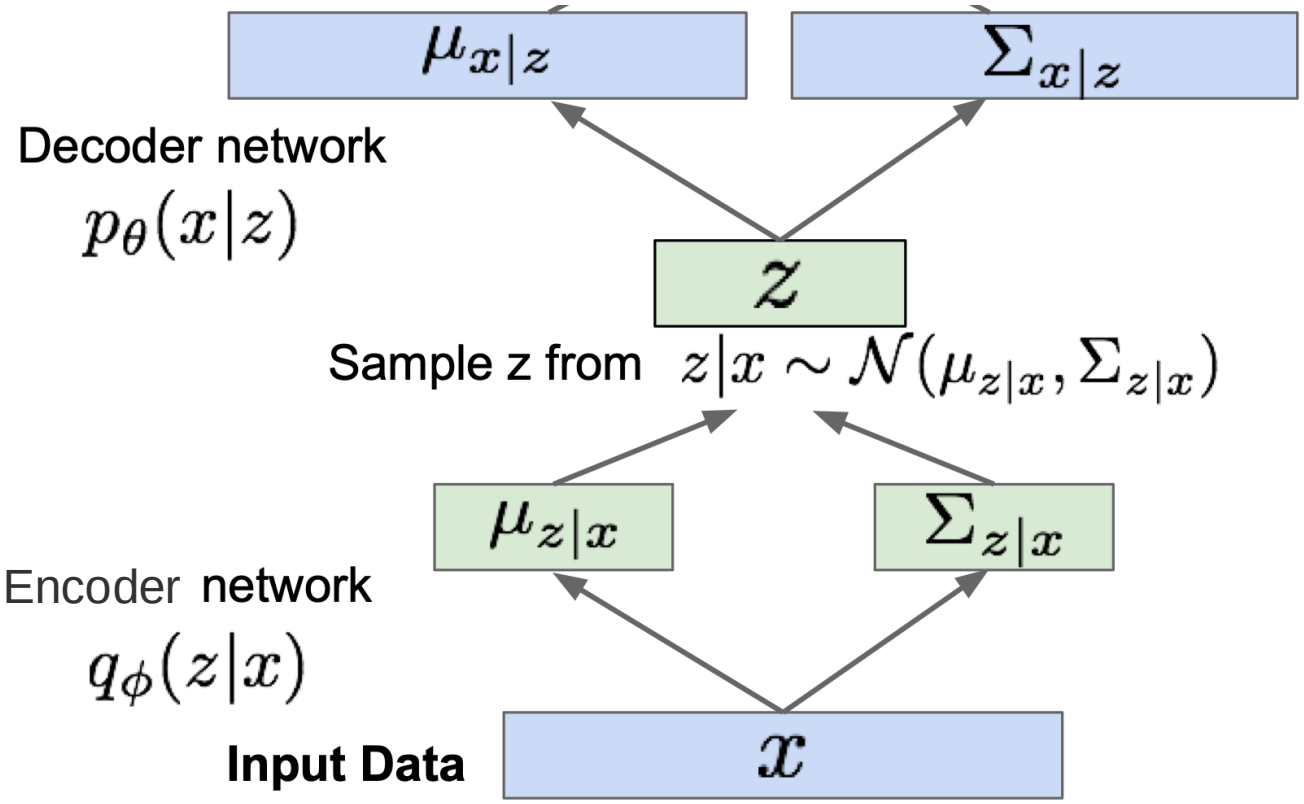
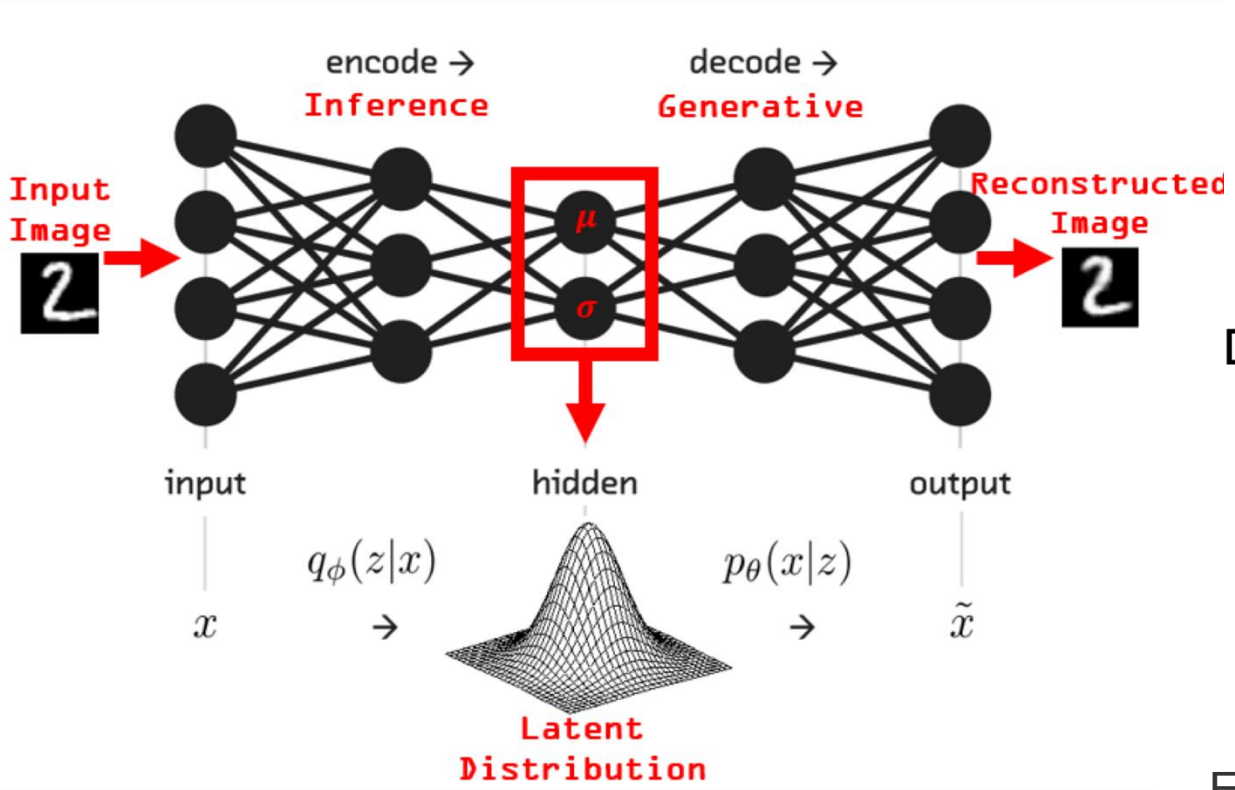
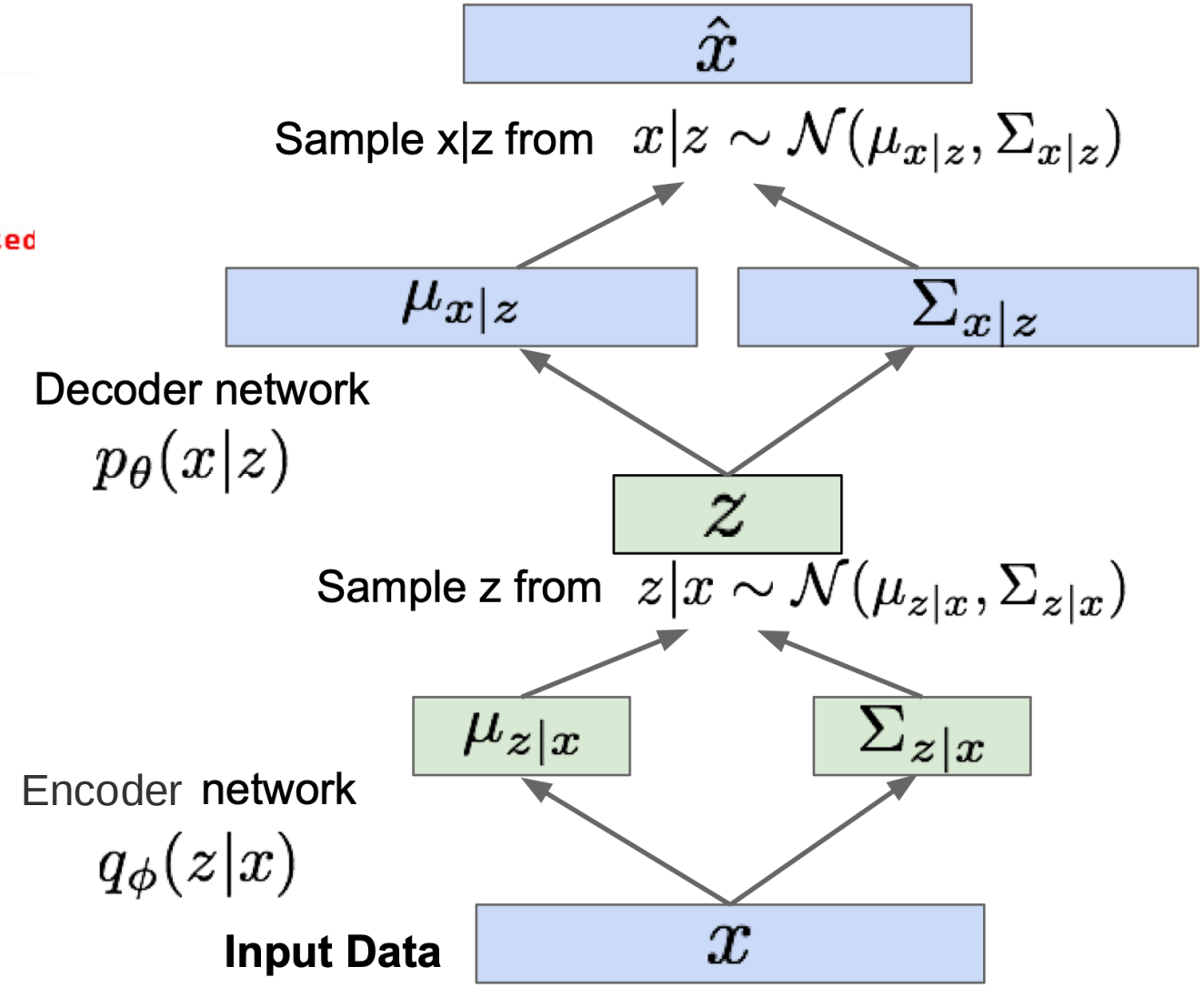




[Courtesy: Fei-Fei Li, Justin Johnson, Serena Yeung, CS 231n]

Example: VAEs for images



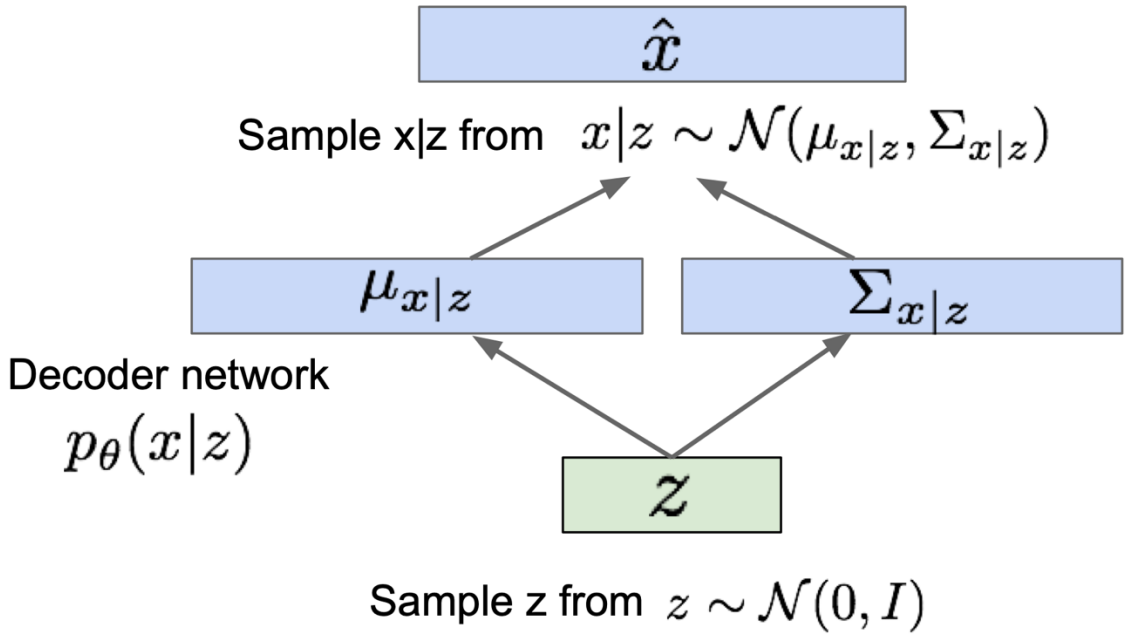


[Courtesy: Fei-Fei Li, Justin Johnson, Serena Yeung, CS 231n]

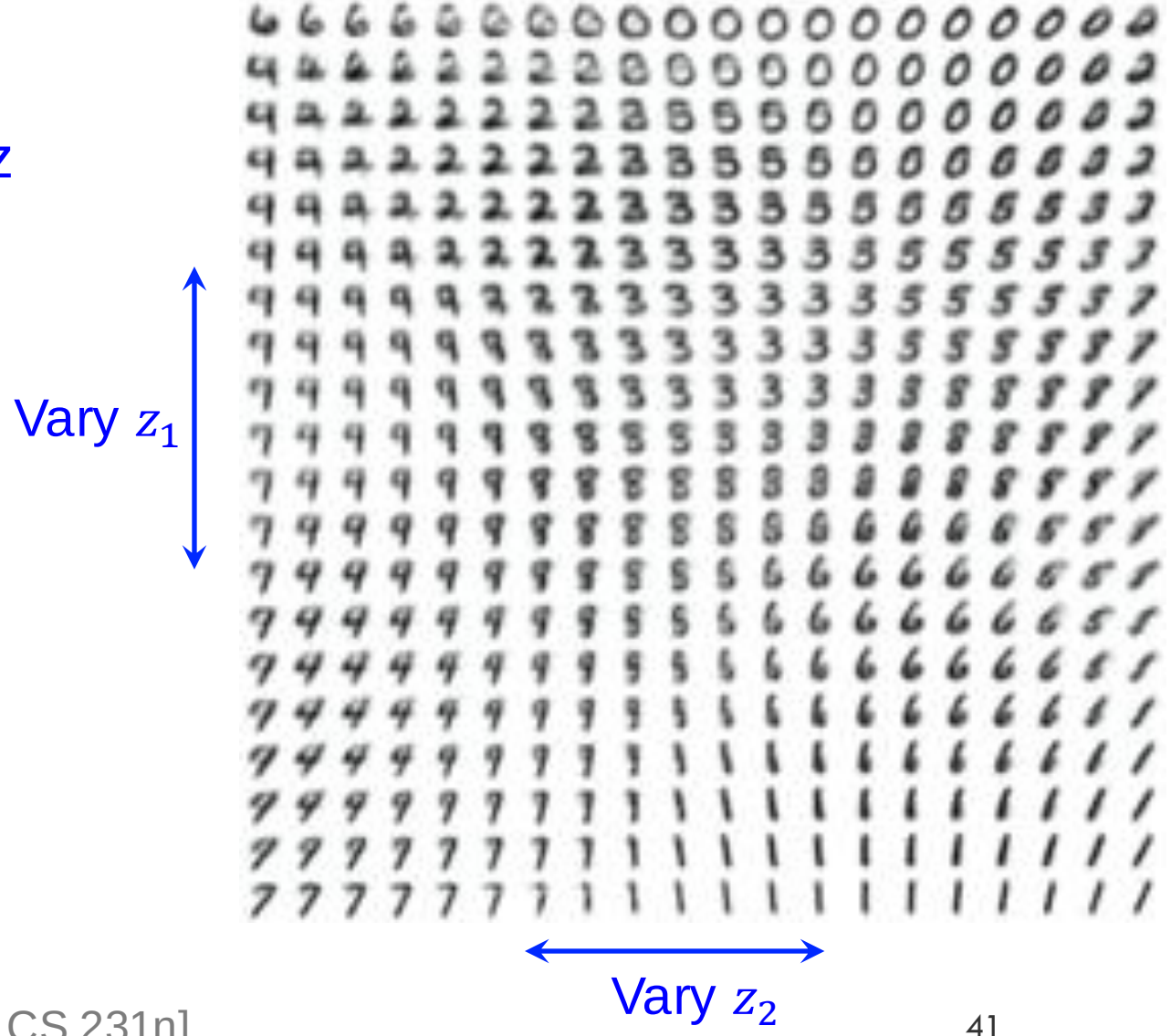
Example: VAEs for images

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

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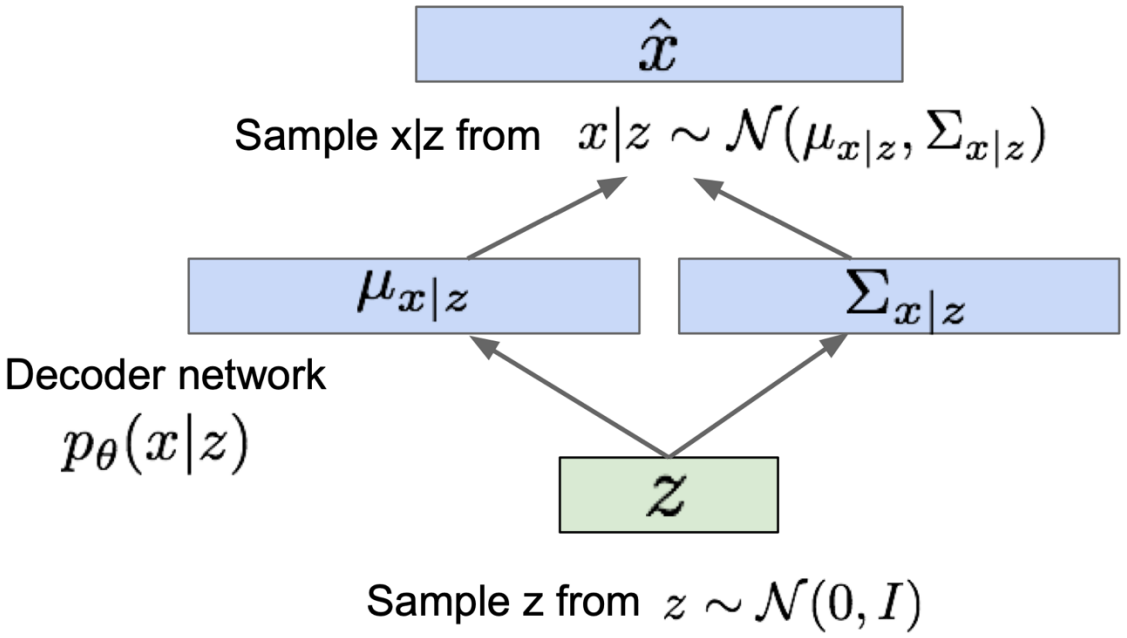


Data manifold for 2-d **z**

[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

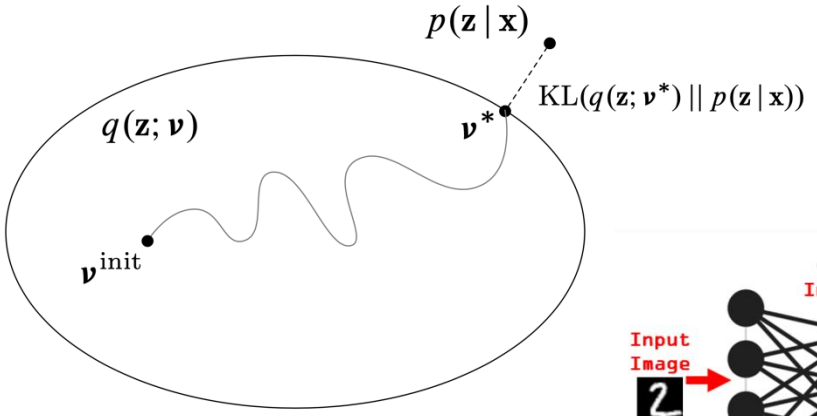
(Razavi et al., 2019)

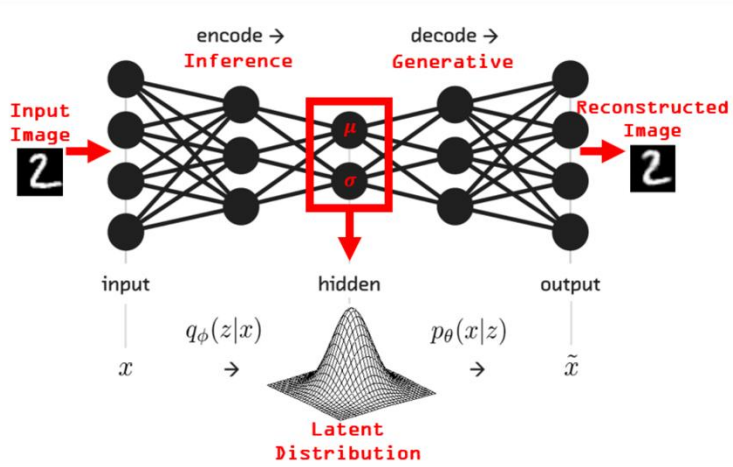
- Pros:
  - Principled approach to generative models
  - Allows inference of $q(z|x)$, can be useful feature representation for other tasks
- Cons:
  - Samples blurrier and lower quality compared to GANs
  - Tend to collapse on text data

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?