Deep Learning:

Variational Autoencoders

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Deep Learning VO - WS 23/24

Lecture 9 - December 4th, 2023

Today

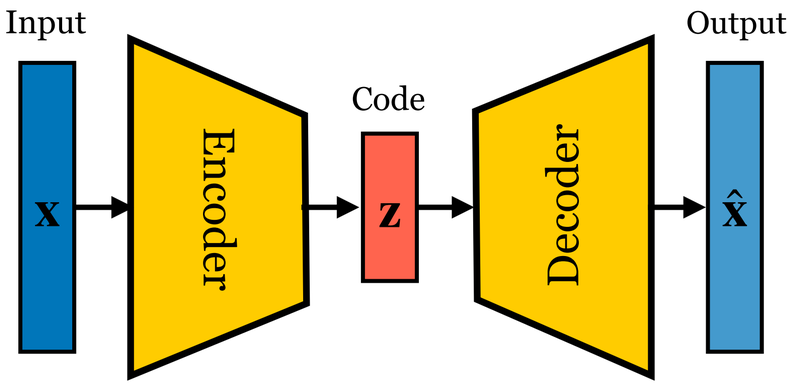
- [ ] Autoencoders
- [ ] Deep Generative Models
  - [ ] Variational Autoencoders
    - [ ] Architecture & Training
    - [ ] Variational Lower Bound
    - [ ] Experiments & Quantifying Performance

Autoencoders

An **autoencoder** is a neural network that gets as input some $\mathbf{x} \in \mathbb{R}^D$ and outputs a reconstruction $\hat{\mathbf{x}} \in \mathbb{R}^D$.

The neural network consists of an **encoder** $f_{\text{enc}} : \mathbb{R}^D \to \mathbb{R}^{d_z}$, and a **decoder** $f_{\text{dec}} : \mathbb{R}^{d_z} \to \mathbb{R}^D$, with a bottleneck layer with activations $\mathbf{z} \in \mathbb{R}^{d_z}$ where the information about the input is compressed.

The network is trained with gradient descent to minimize the reconstruction error (e.g., mean-squared error).



Autoencoders

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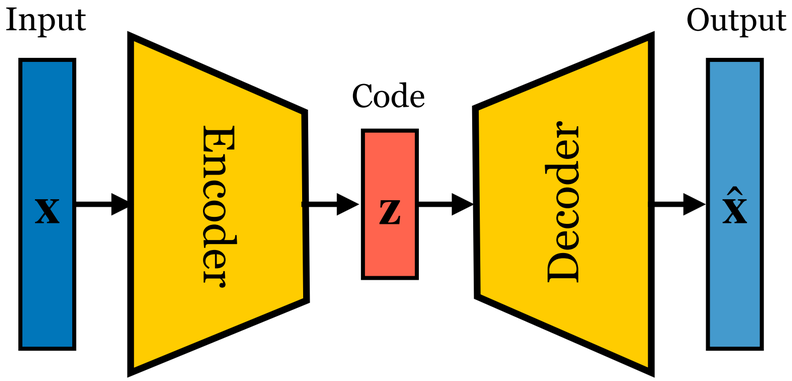
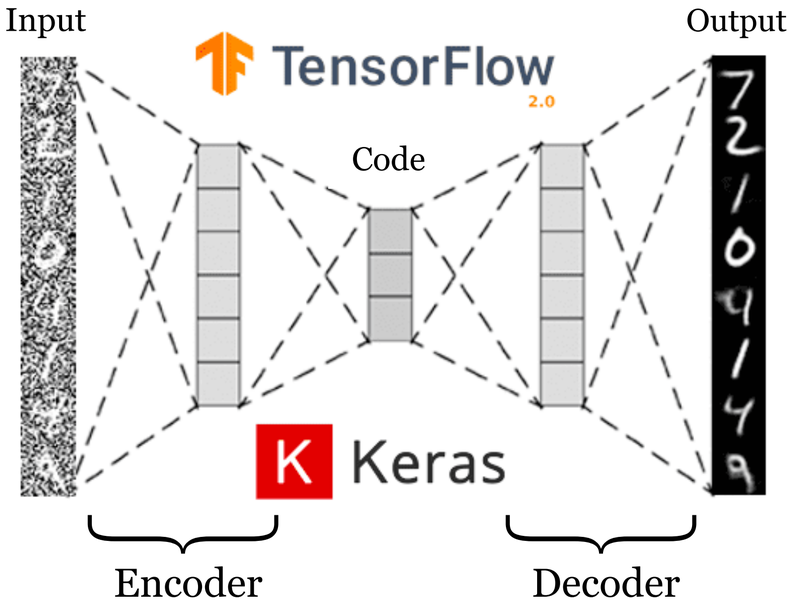


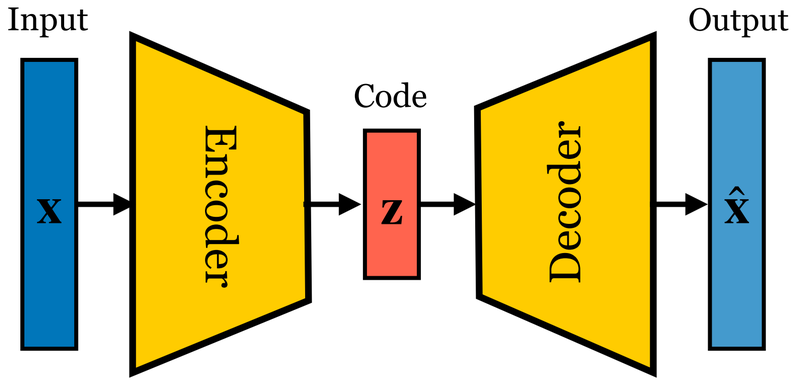


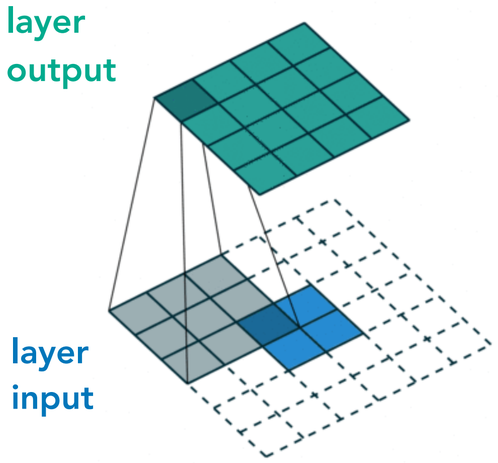
Applications:

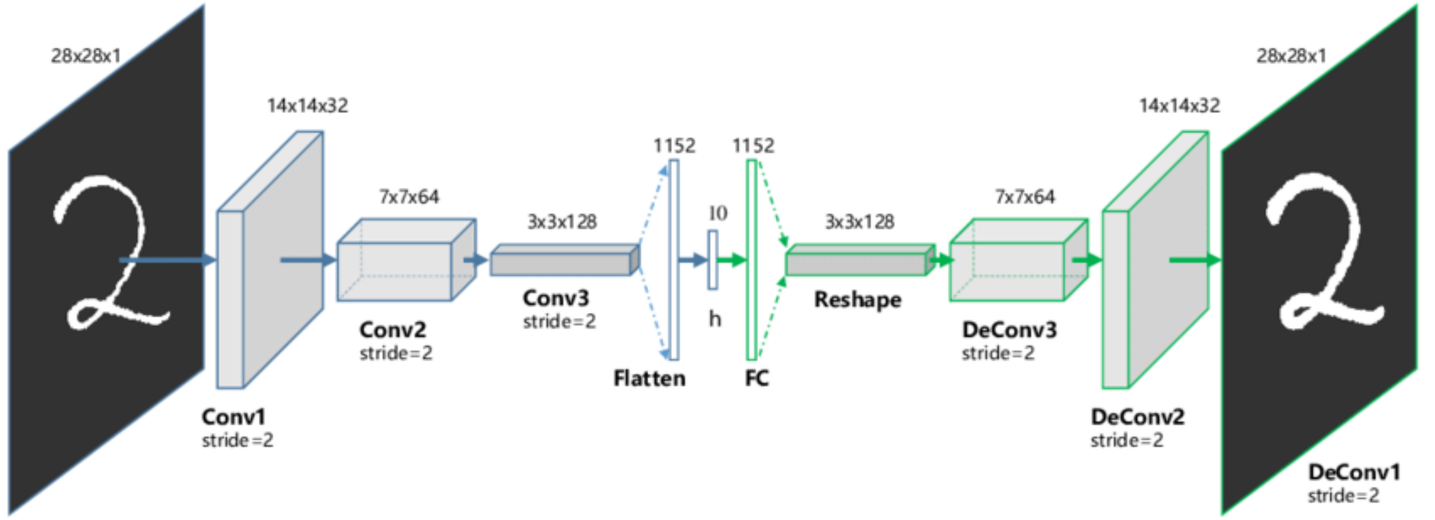
- Dimensionality reduction
- Feature extraction
- Denoising autoencoders → Training an autoencoder to reconstruct the original data from corrupted/noisy versions.

Encoder-Decoder Architectures

- **Encoder** maps the input to a low-dimensional latent representation by using (often) a CNN.
- In that case it makes sense to use as **decoder** something like the inverse of a CNN.
- This can be done with **transposed convolutions** (i.e., de-convolution) in the decoder.

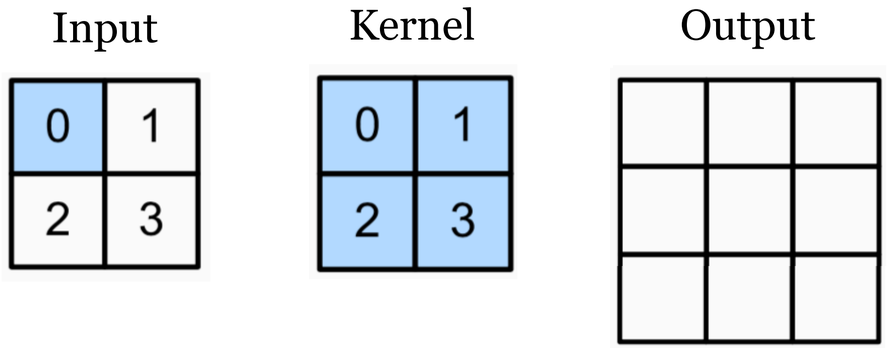






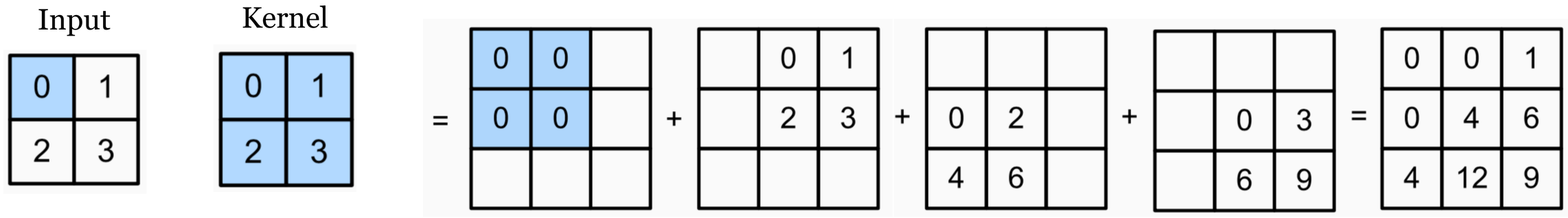
Learnable Upsampling: Transposed Convolution

- Consider a 2x2 feature map as **input.**
- We want to expand it to a 3x3 feature map **output,**
- By using a 2x2 **kernel** for transposed convolution.



Each element of the input is multiplied with the kernel and added to the output at the corresponding position.

Example: Transposed convolution with stride 1:



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Diederik P. Kingma & Max Welling, “Auto-Encoding Variational Bayes”, arXiv preprint arXiv:1312.6114 (2013).

Generative Models

- Given a list of data points $X = \langle \mathbf{x}^{(1)}, \ldots, \mathbf{x}^{(N)} \rangle$ coming from a data distribution $p(\mathbf{x})$.
- **Generative model:** a model for this distribution, from which we can sample.
- Notation: typically the model distribution is parameterized by θ and we write $p_\theta(\mathbf{x})$.

Simple example from previous lectures:

- Assume that data comes from a Gaussian distribution. Our model could then be: $p_\theta(\mathbf{x}) = N(\mu, \mathbf{\Sigma})$,
- … where the parameters $\theta = (\mu, \mathbf{\Sigma})$ are the mean and covariance matrix of the Gaussian.
- We have already seen how we can learn θ with maximum likelihood.

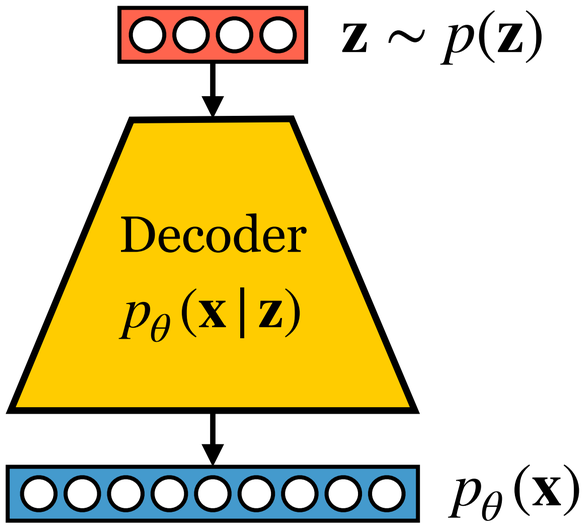
Variational Autoencoders (VAEs)

There are many ways to model more complex distributions.

Simple Idea:

- Draw latent variables $\mathbf{z}$ from a simple distribution $p(\mathbf{z})$.
- Use a model with parameters θ to transform $p(\mathbf{z})$ to a complex distribution:

$$p_\theta(\mathbf{x}) = \int p_\theta(\mathbf{x}\,|\,\mathbf{z})\, p(\mathbf{z})\, d\mathbf{z}$$

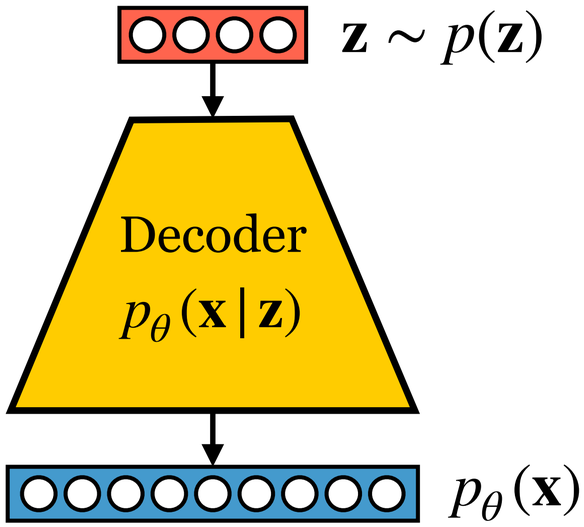


- To generate an $\mathbf{x}$:
  - We first sample $\mathbf{z} \sim p(\mathbf{z})$, then compute neural network output with $\mathbf{z}$ as input.
- In VAEs, we usually use as priors independent standard normal variables (zero mean, unit variance).

Variational Autoencoders: Training

How to train VAEs?

- For a dataset $X = \langle \mathbf{x}^{(1)}, \ldots, \mathbf{x}^{(N)} \rangle$ we want to maximize the likelihood that it is generated.
- If we would knew $\mathbf{z}$ for a given $\mathbf{x}$, we could simply optimize $p_\theta(\mathbf{x} \mid \mathbf{z})$, but $\mathbf{z}$ is latent.
- So we would need to compute $p_\theta(\mathbf{z} \mid \mathbf{x})$, which is intractable.



Variational Autoencoders: Training

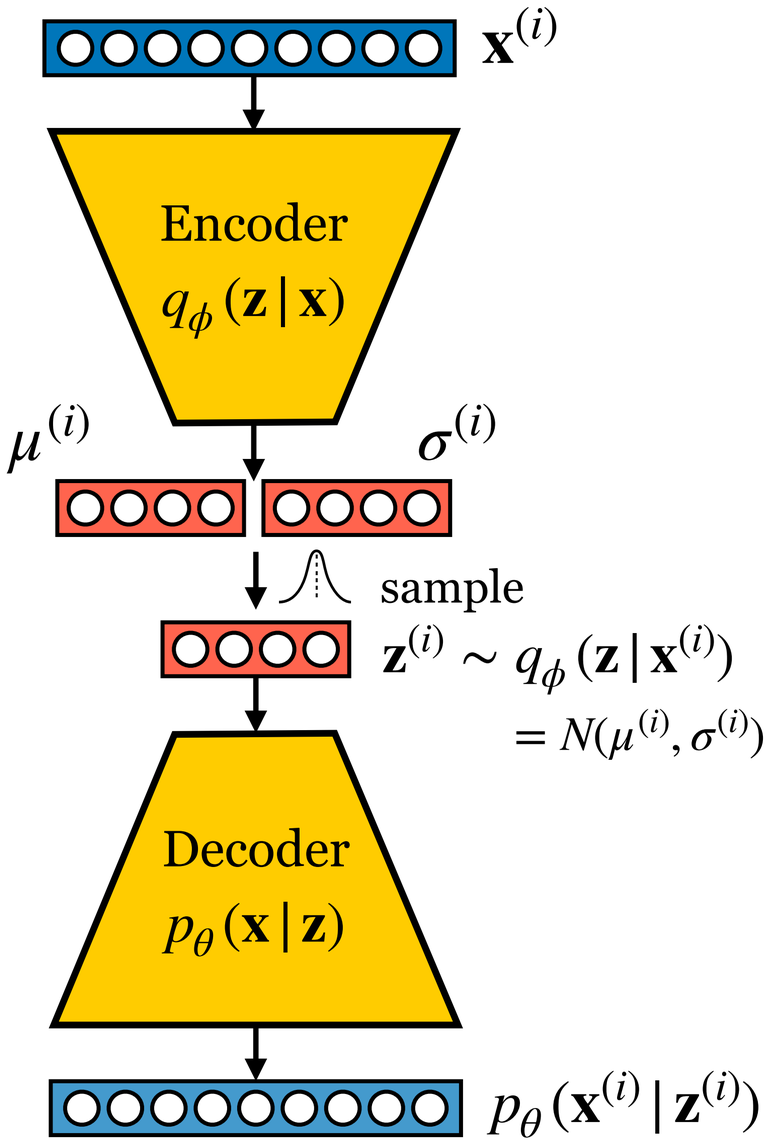
Solution of VAEs:

- Predict latent variables $\mathbf{z}$ using a neural network with parameters ϕ that computes the approximate posterior $q_\phi(\mathbf{z}|\mathbf{x}) \approx p_\theta(\mathbf{z}|\mathbf{x})$.

For a given $\mathbf{x}$,

- the **encoder** samples $\mathbf{z} \sim q_\phi(\mathbf{z}|\mathbf{x})$,
- the **decoder** takes $\mathbf{z}$ and computes $p_\theta(\mathbf{x}|\mathbf{z})$.

Now we have $\mathbf{z}$ and can optimize both ϕ and θ.



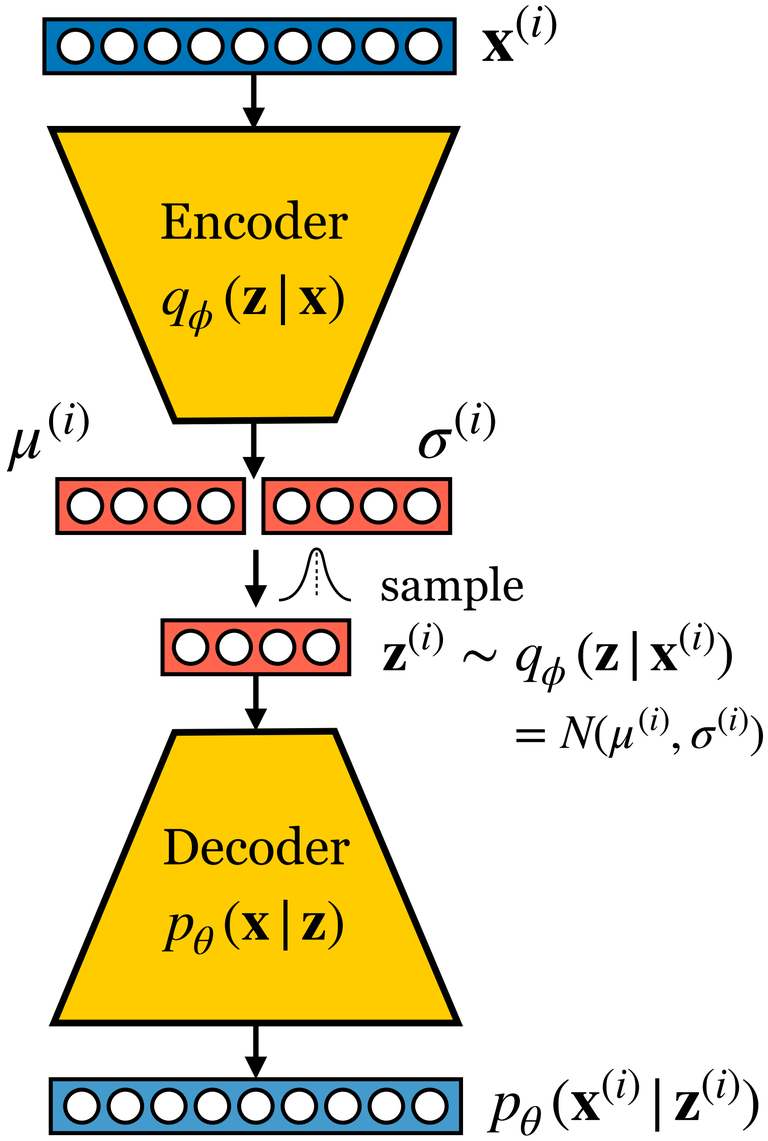
Variational Autoencoders: Training

Training objective

We want that:

1) The distribution $q_\phi(\mathbf{z}\,|\,\mathbf{x}^{(i)})$ is close to our prior distribution $p(\mathbf{z})$.

2) The decoder computes a good reconstruction of $\mathbf{x}^{(i)}$.



Variational Autoencoders: Training

1) The distribution $q_\phi(\mathbf{z}\,|\,\mathbf{x}^{(i)})$ is close to our prior distribution $p(\mathbf{z})$:

- We achieve this by minimizing the KL divergence between these distributions.

$$D_{KL}(q\|p) = \int q(x)\,\log\frac{q(x)}{p(x)}dx$$

- We will use a Gaussian prior with zero-mean independent variables of unit variance: $p(\mathbf{z}) = N(\mathbf{0}, \mathbf{I})$, i.e., $p(z_m) = N(0,1)$.
- For each latent variable z_m , the encoder produces a Gaussian distribution with mean μ_m and standard deviation σ_m, i.e.,

$$q_\phi(z_m\,|\,\mathbf{x}^{(i)}) = N\left(\mu_m(\mathbf{x}^{(i)}), \sigma_m(\mathbf{x}^{(i)})\right)$$

- The KL divergence in this case is: $D_{KL}(q_\phi\|p) = -\frac{1}{2}\sum_m\left(1 + \log\left(\sigma_m(\mathbf{x}^{(i)})^2\right) - \mu_m(\mathbf{x}^{(i)})^2 - \sigma_m(\mathbf{x}^{(i)})^2\right)$

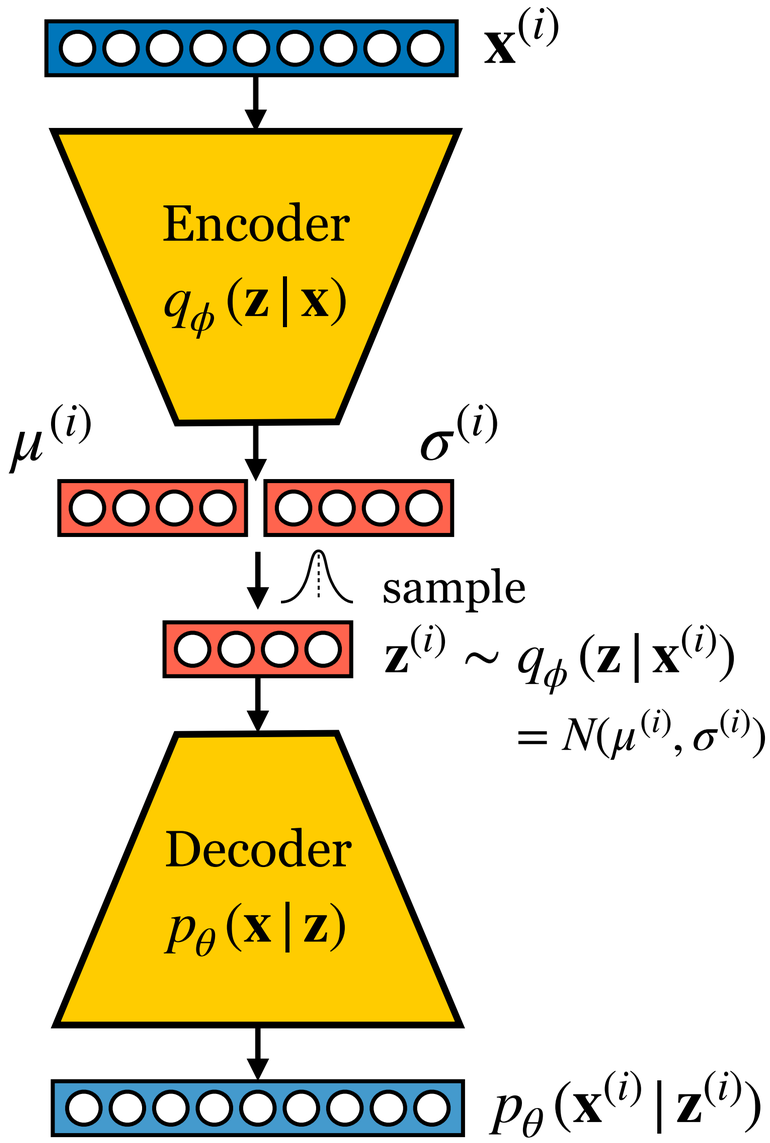
Variational Autoencoders: Training

1) The distribution $q_\phi(\mathbf{z} \mid \mathbf{x}^{(i)})$ is close to our prior distribution $p(\mathbf{z})$:

2) The decoder computes a good reconstruction of $\mathbf{x}^{(i)}$:

   - We achieve this by maximizing the likelihood on L drawn samples $\mathbf{z}^{(i,1)}, \ldots, \mathbf{z}^{(i,L)}$.

$$\frac{1}{L} \sum_{l=1}^{L} \log p_\theta \left(\mathbf{x}^{(i)} \mid \mathbf{z}^{(i,l)} \right)$$



Variational Autoencoders: Training

1) The distribution $q_\phi(\mathbf{z}\,|\,\mathbf{x}^{(i)})$ is close to our prior distribution $p(\mathbf{z})$:

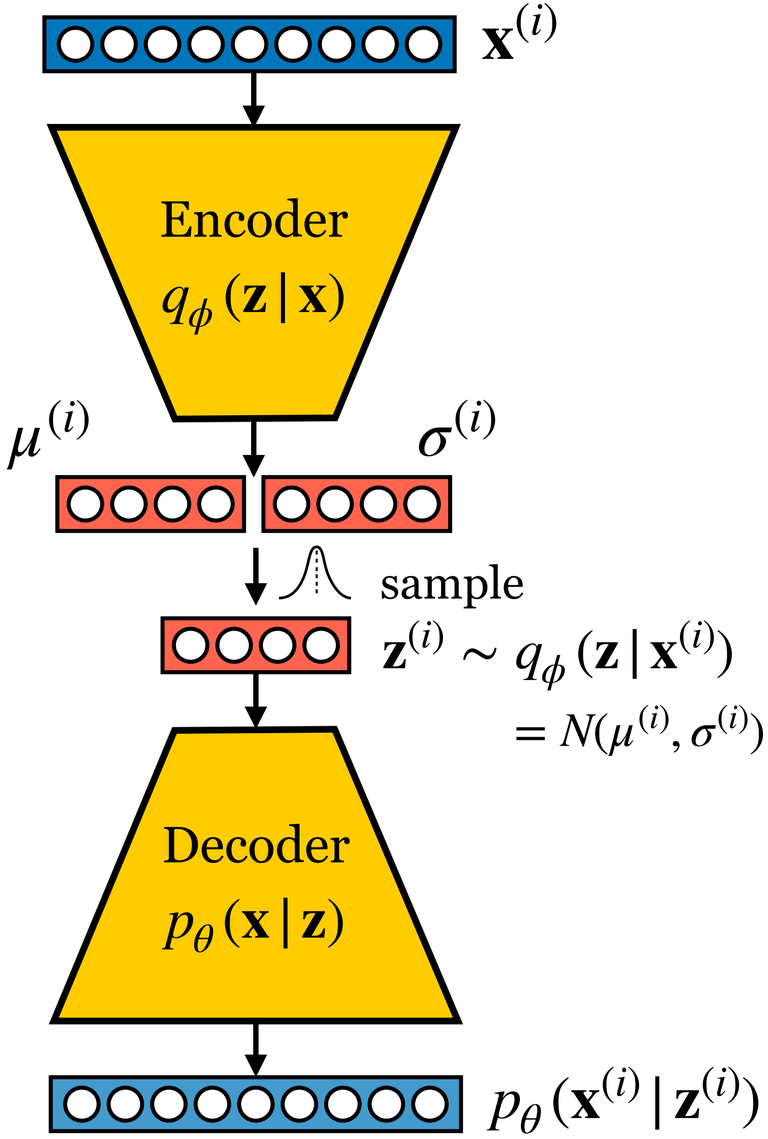
2) The decoder computes a good reconstruction of $\mathbf{x}^{(i)}$:

- Both parts together give rise to the loss to be minimized:

$$\mathscr{L}(\theta, \phi, X) = D_{KL}\left(q_\phi(\mathbf{z}\,|\,\mathbf{x}^{(i)}) \,\|\, p(\mathbf{z})\right) - \frac{1}{L}\sum_{l=1}^{L} \log p_\theta\left(\mathbf{x}^{(i)}\,|\,\mathbf{z}^{(i,l)}\right)$$

approx. posterior ≈ prior

"reconstruction" term



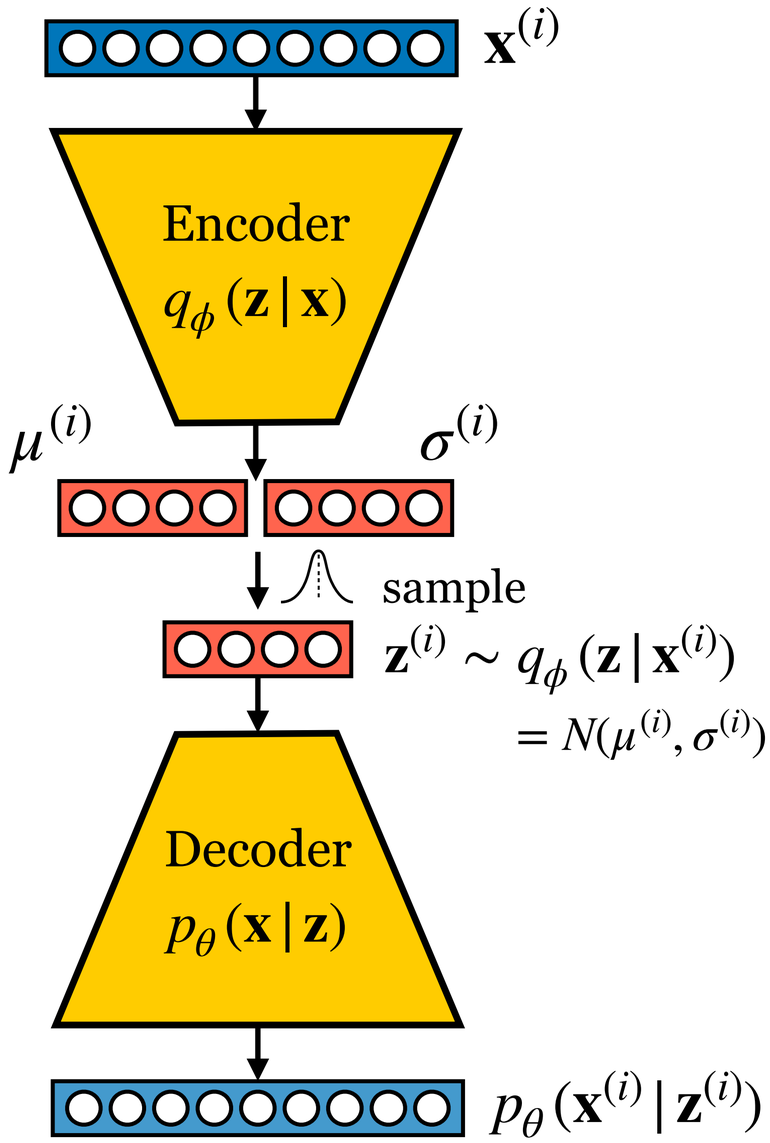
Variational Autoencoders: Training

1) The distribution $q_\phi(\mathbf{z}\,|\,\mathbf{x}^{(i)})$ is close to our prior distribution $p(\mathbf{z})$:

2) The decoder computes a good reconstruction of $\mathbf{x}^{(i)}$:

Note: Once the model is trained,

- The encoder is not needed for generation.
  - We just need to sample from the latent prior $p(\mathbf{z})$, and then use the decoder.
- The encoder can be used to extract the latent variables.
  - Low-dimensional representations of data.
  - For this we don't need the decoder.



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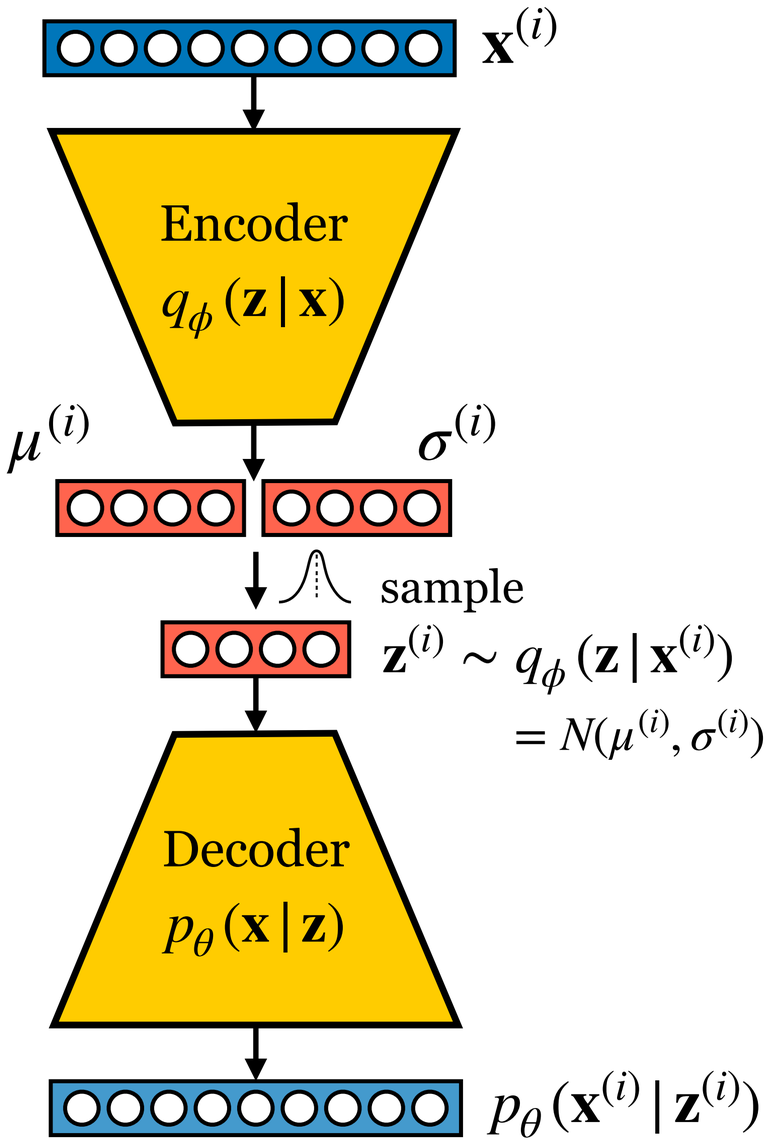
approx. posterior ≈ prior

"reconstruction" term

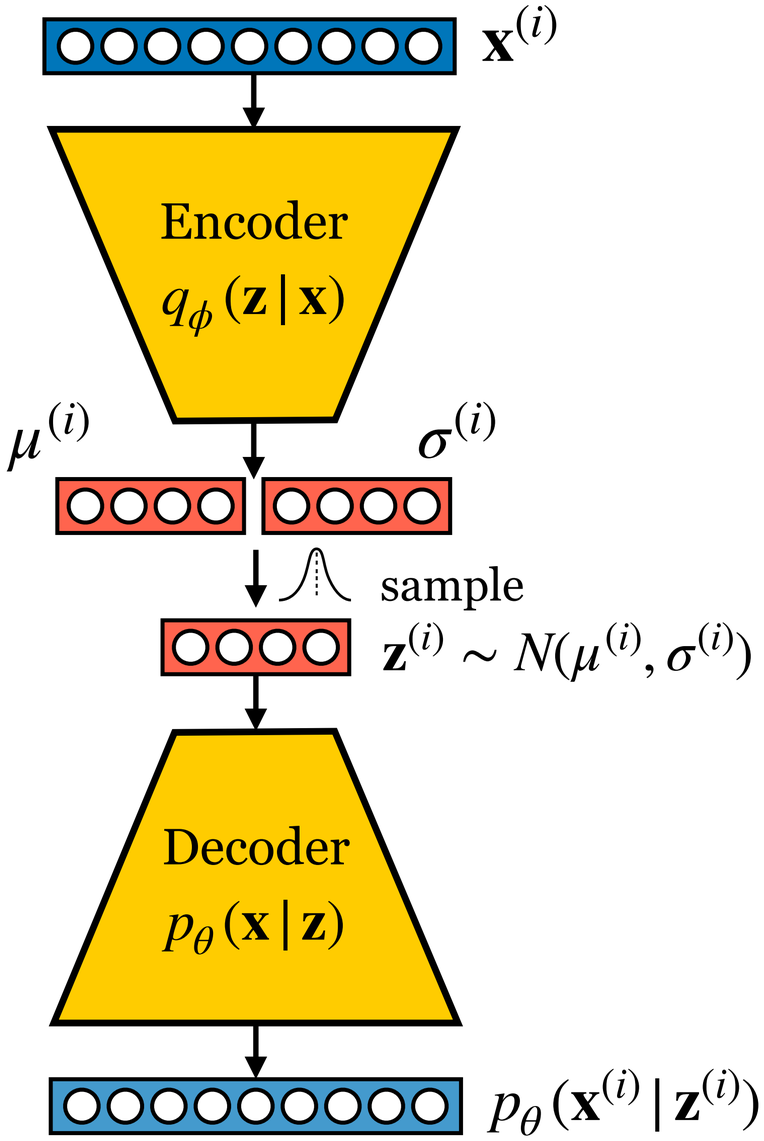
  - We want to use gradient descent on mini-batches, **backpropagating** loss gradients through both networks.



Reparametrization Trick

Problem: $\mathbf{z}$ is a sampled variable.

- We can compute $\frac{\partial \mathscr{L}}{\partial \mathbf{z}}$, but not $\frac{\partial \mathbf{z}}{\partial \mu}$ and $\frac{\partial \mathbf{z}}{\partial \sigma}$ because the sampler is not differentiable.



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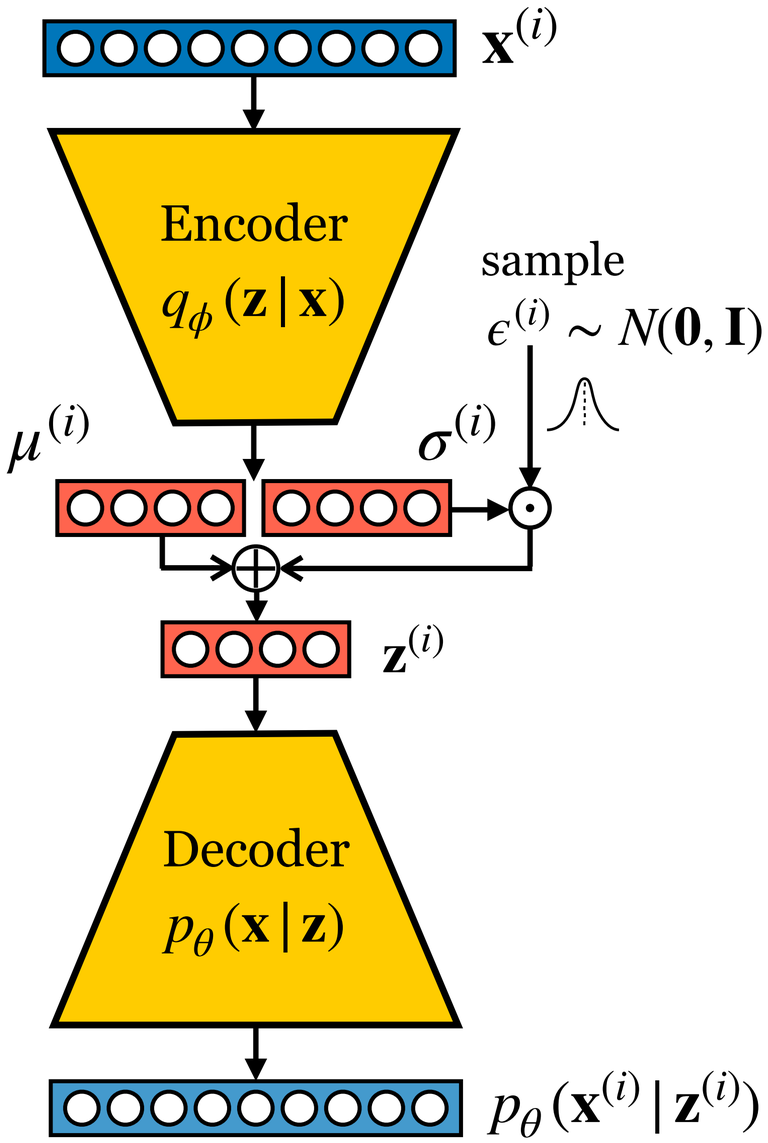
Reparametrization trick:

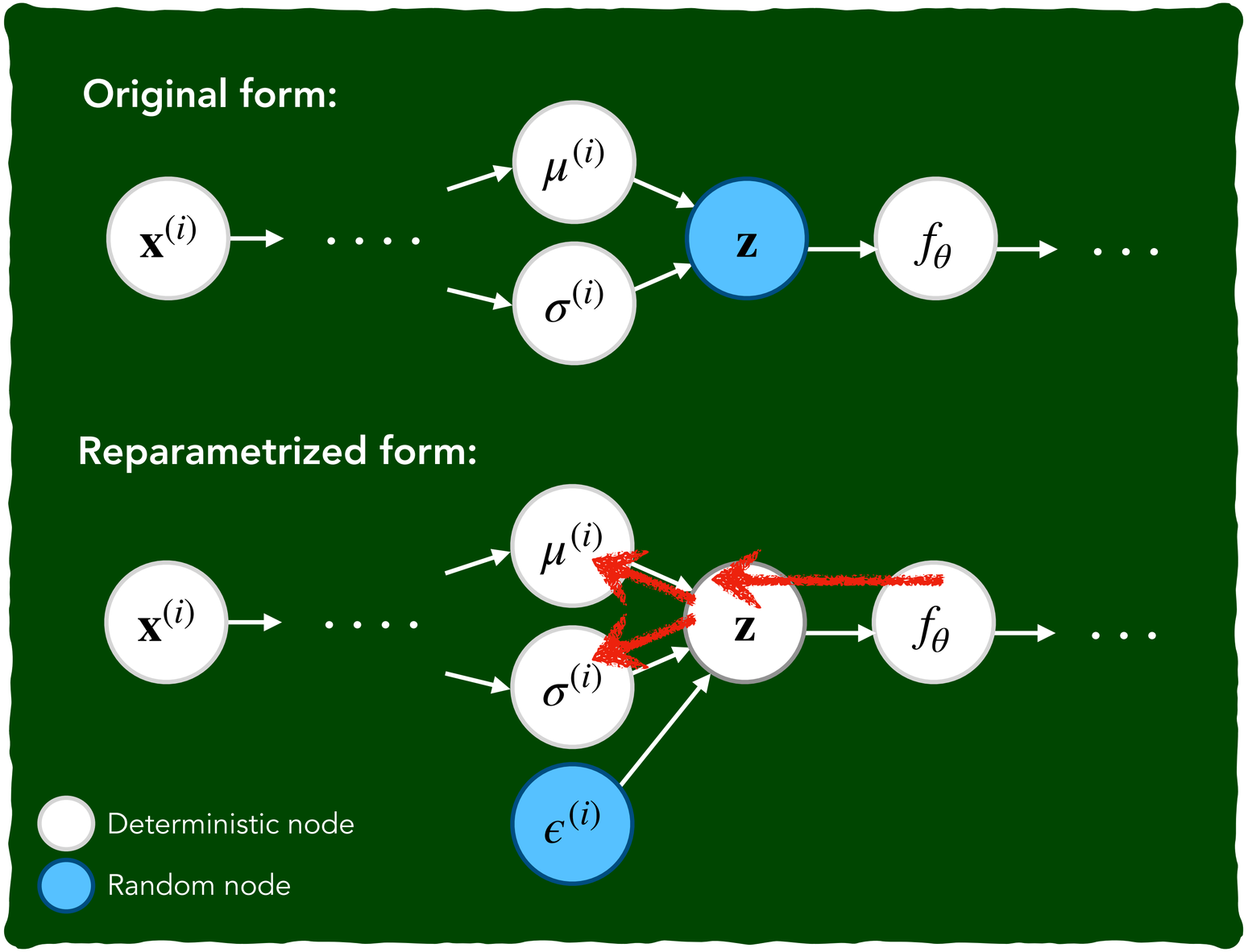
- For many distributions (e.g., for independent Gaussians) we can obtain the same distribution over $\mathbf{z}$ by including an auxiliary random variable ϵ.
- For univariate Gaussian:

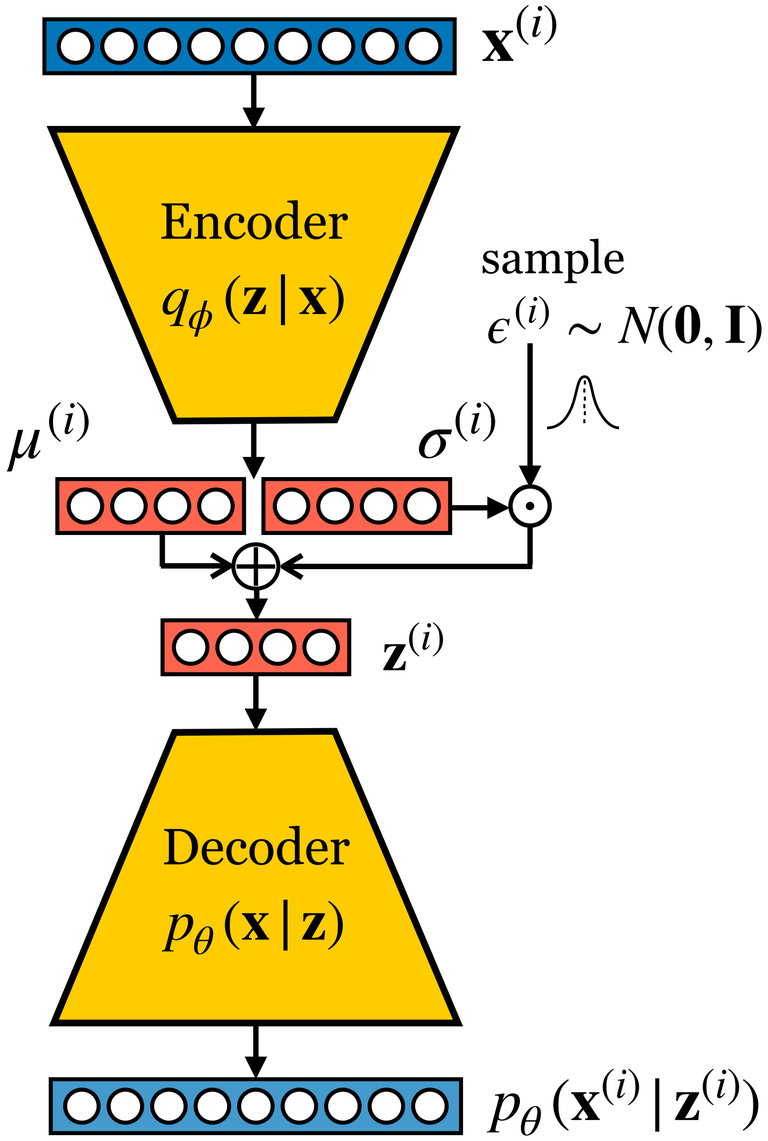
$$z^{(i,l)} = \mu\left(\mathbf{x}^{(i)}\right) + \sigma\left(\mathbf{x}^{(i)}\right)\epsilon^{(i,l)} \quad \text{with} \quad \epsilon^{(i,l)} \sim N(0,1)$$

In this case, we get $\frac{\partial \mathbf{z}}{\partial \mu} = 1$ and $\frac{\partial \mathbf{z}}{\partial \sigma} = \epsilon$

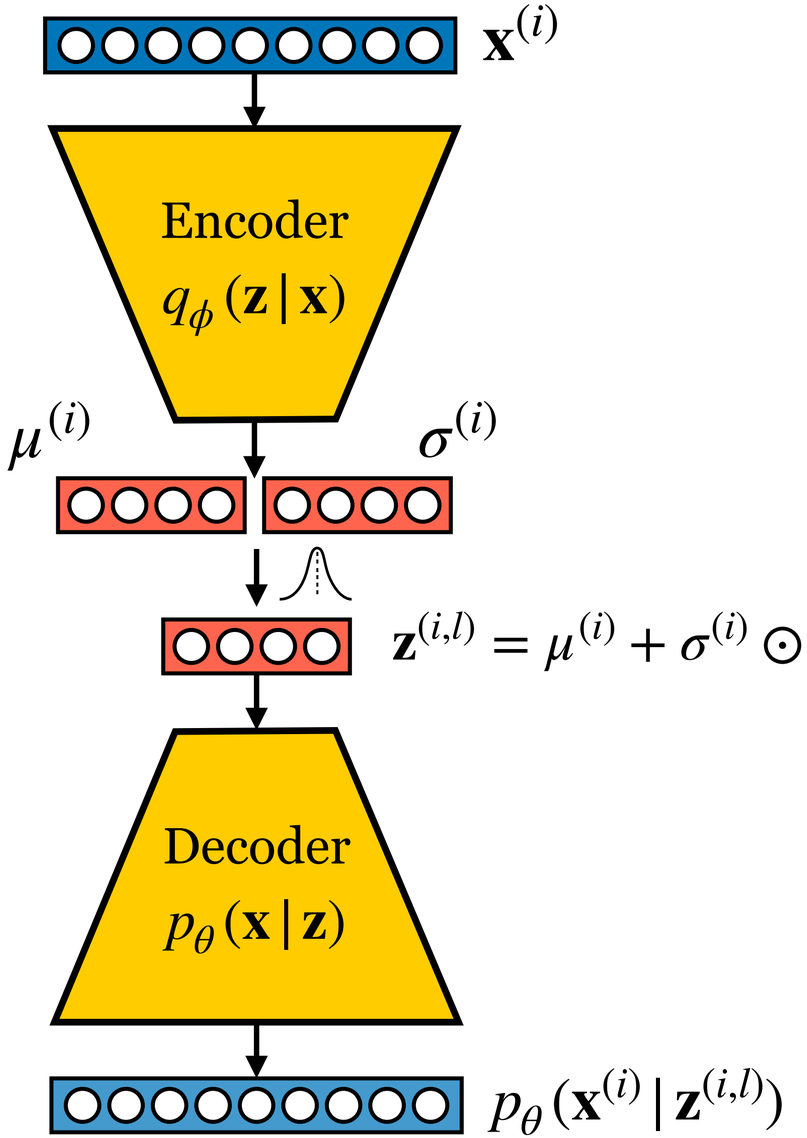


Reparametrization Trick





Variational Autoencoders: Final Model



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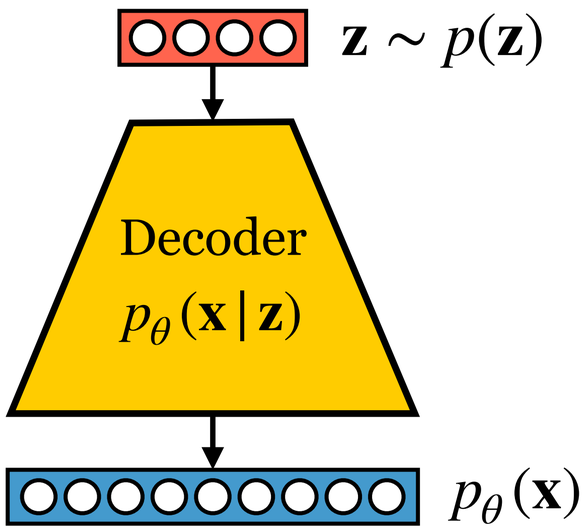
Variational Lower Bound

Our posterior is only an approximation to $p_\theta(\mathbf{z}\,|\,\mathbf{x})$.



Background on variational inference:

The problem to invert a directed graphical model is a general problem.

- Given: A model for $p_\theta(\mathbf{x}\,|\,\mathbf{z})$
- What we want: $p_\theta(\mathbf{z}\,|\,\mathbf{x})$

Suppose we are given an intractable probability distribution p.

Variational techniques try to solve an optimization problem over a class of tractable distributions Q in order to find a $q \in Q$ that is most similar to p. We will then query q (rather than p) in order to get an approximate solution.

Variational Lower Bound

Justification for our approach:

- Mainly we want to maximize $\log p_\theta(\mathbf{x})$. We can write this log-likelihood as:

$$\log p_\theta(\mathbf{x}) = D_{KL}\left(q_\phi(\mathbf{z}\,|\,\mathbf{x}) \,\|\, p_\theta(\mathbf{z}\,|\,\mathbf{x})\right) + \mathscr{L}(\theta, \phi, \mathbf{x})$$

with $\mathscr{L}(\theta, \phi, X)$ being the **"variational lower bound"** as the (negated) loss objective from before:

$$\mathscr{L}(\theta, \phi, X) = -D_{KL}\left(q_\phi(\mathbf{z}\,|\,\mathbf{x}) \,\|\, p(\mathbf{z})\right) + \mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x})}\left[\log p_\theta(\mathbf{x}\,|\,\mathbf{z})\right]$$

sometimes also called:
"evidence lower bound" (ELBO)

Variational Lower Bound

$$\log p_\theta(\mathbf{x}) = D_{KL}\left(q_\phi(\mathbf{z}|\mathbf{x}) \,\|\, p_\theta(\mathbf{z}|\mathbf{x})\right) + \mathscr{L}(\theta, \phi, \mathbf{x}) \qquad \mathscr{L}(\theta, \phi, X) = -D_{KL}\left(q_\phi(\mathbf{z}|\mathbf{x}) \,\|\, p(\mathbf{z})\right) + \mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x})}\left[\log p_\theta(\mathbf{x}|\mathbf{z})\right]$$

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

$$= \int q_\phi(\mathbf{z}|\mathbf{x}) \log \frac{q_\phi(\mathbf{z}|\mathbf{x})}{p_\theta(\mathbf{z}|\mathbf{x})} dz - \int q_\phi(\mathbf{z}|\mathbf{x}) \log \frac{q_\phi(\mathbf{z}|\mathbf{x})}{p(\mathbf{z})} dz + \int q_\phi(\mathbf{z}|\mathbf{x}) \log p_\theta(\mathbf{x}|\mathbf{z}) dz$$

$$= \int q_\phi(\mathbf{z}|\mathbf{x}) \left[\log q_\phi(\mathbf{z}|\mathbf{x}) - \log p_\theta(\mathbf{z}|\mathbf{x}) - \log q_\phi(\mathbf{z}|\mathbf{x}) + \log p(\mathbf{z}) + \log p_\theta(\mathbf{x}|\mathbf{z})\right] dz$$

$$= \int q_\phi(\mathbf{z}|\mathbf{x}) \left[\log \frac{p_\theta(\mathbf{x}|\mathbf{z}) p(\mathbf{z})}{p_\theta(\mathbf{z}|\mathbf{x})}\right] dz = \int q_\phi(\mathbf{z}|\mathbf{x}) \log p_\theta(\mathbf{x}) \, dz = \log p_\theta(\mathbf{x}) \int q_\phi(\mathbf{z}|\mathbf{x}) \, dz = \log p_\theta(\mathbf{x}) \quad \square$$

Variational Lower Bound

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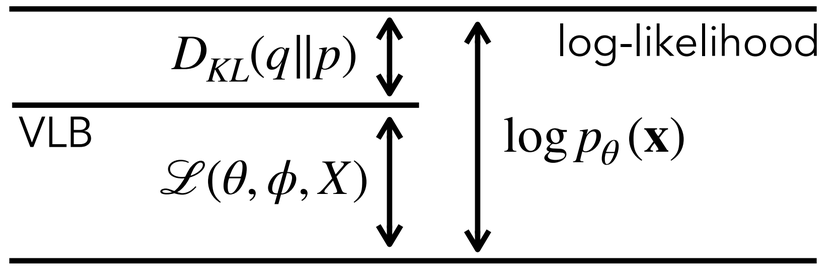
- By optimizing this, we actually maximize a variational lower bound on $\log p_\theta(\mathbf{x})$ because $D_{KL}(q_\phi(\mathbf{z}\,|\,\mathbf{x})\,||\,p_\theta(\mathbf{z}\,|\,\mathbf{x}))$ is always non-negative, i.e., $\log p_\theta(\mathbf{x}) \geq \mathscr{L}(\theta, \phi, X)$



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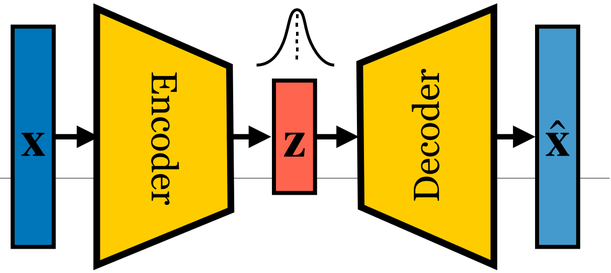
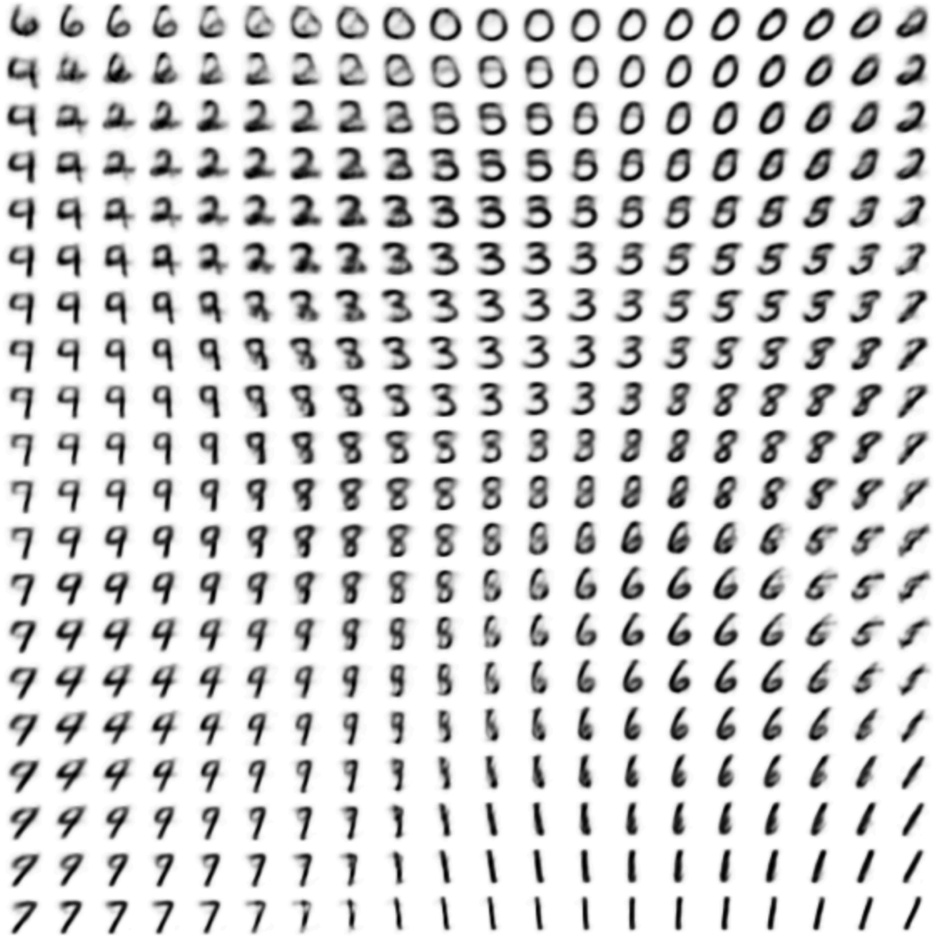
Experiments



Latent manifold representation for two-dimensional latent space:

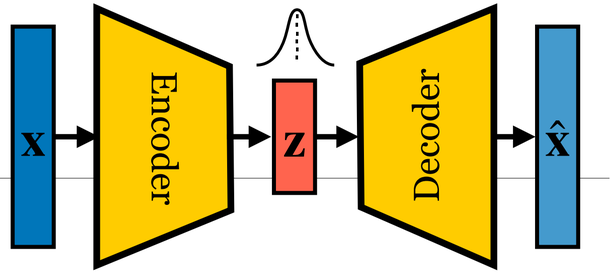
(a) Learned Frey Face manifold



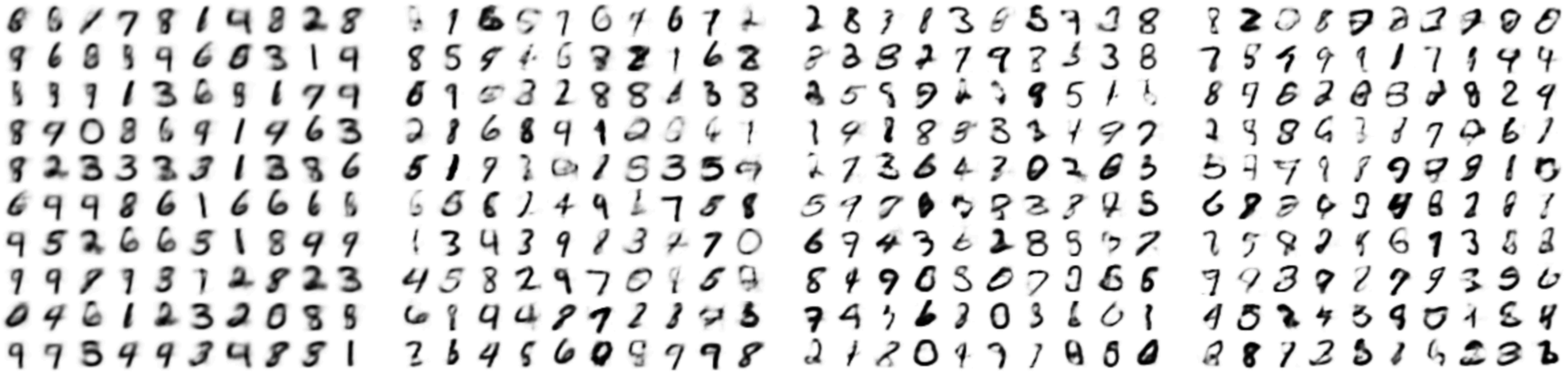
(b) Learned MNIST manifold

[Diederik P. Kingma & Max Welling, "Auto-Encoding Variational Bayes", arXiv preprint arXiv:1312.6114 (2013).]

Experiments



Samples from generative model trained on MNIST:



(a) 2-D latent space (b) 5-D latent space (c) 10-D latent space (d) 20-D latent space

[Diederik P. Kingma & Max Welling, "Auto-Encoding Variational Bayes", arXiv preprint arXiv:1312.6114 (2013).]

Quantifying Performance

Quantitative measures for success of generative models.

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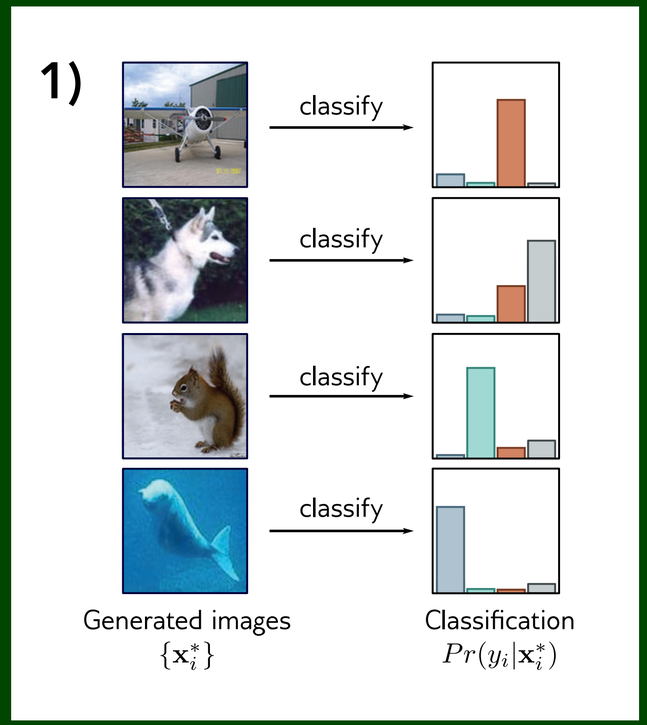

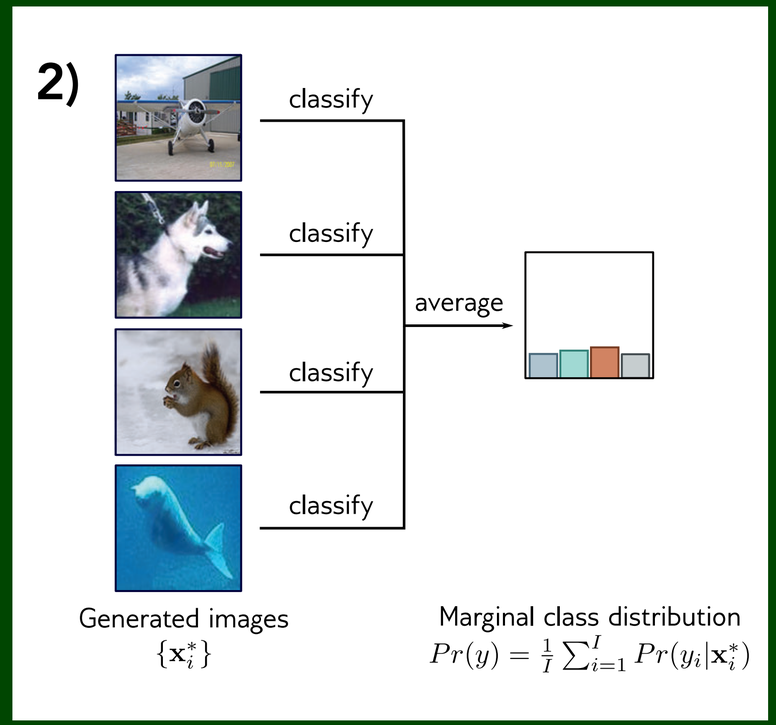

Inception Score: $$\mathbf{IS} = \exp\left(\frac{1}{I}\sum_{i=1}^{I} D_{KL}\left[Pr(y_i \mid \mathbf{x}_i^*) \parallel Pr(y)\right]\right)$$

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- **Fréchet Inception Distance (FID):** Measures similarities between the feature representations (learned by a pre-trained classifier) for generated samples and a test dataset.
- …

Summary

- Variational autoencoders are encoder-decoder architectures.
- Training is performed by maximizing a variational lower bound on the log-likelihood.
- VAEs can be used as generative models or as feature extractors.
- Individual features of the latent space often encode specific parameters of the input.
  - e.g. facial expression, object rotation, etc.
  - By changing the latent variable, one can transform images (e.g., make a person smile).
- Often, encoders are CNNs and decoders use transposed convolutions.
- Some (indirect) measures to quantify performance exist (e.g., Inception score).
- VAEs are easier to train, but Generative Adversarial Networks are usually better generators.

[Ian Goodfellow et al. “Generative Adversarial Nets.” NIPS 2014.]

Today

- ☑ Autoencoders
- ☐ Deep Generative Models
  - ☑ Variational Autoencoders
    - ☑ Architecture & Training
    - ☑ Variational Lower Bound
    - ☑ Experiments & Quantifying Performance

Questions?