ITCS 6156/8156 Spring 2024
Machine Learning

Deep Generative Models

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Class Meeting: Mon & Wed, 4:00 PM – 5:15 PM, Denny 109

UNIVERSITY OF NORTH CAROLINA CHARLOTTE

Some content in the slides is based on Dr. Ruohan Gao's lectures

Supervised vs Unsupervised Learning

Supervised Learning

Data: (x, y)
x is data, y is label

Goal: Learn a *function* to map x -> y

Examples: Classification, regression, object detection, semantic segmentation, image captioning, etc.

Supervised vs Unsupervised Learning

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Cat

Classification

Supervised vs Unsupervised Learning

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A cat sitting on a suitcase on the floor

Image captioning

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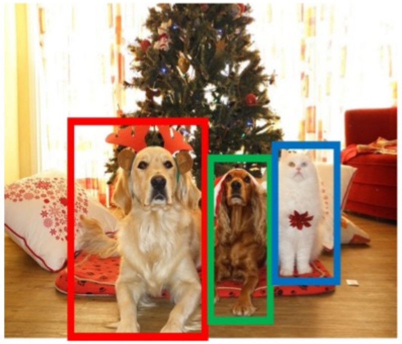

DOG, DOG, CAT

Object Detection

Supervised vs Unsupervised Learning

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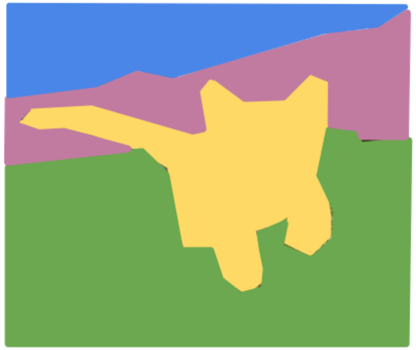

Semantic Segmentation

Supervised vs Unsupervised Learning

Unsupervised Learning

Data: x
Just data, **no labels!**

Goal: Learn some underlying hidden *structure* of the data

Examples: Clustering, dimensionality reduction, feature learning, density estimation, etc.

Supervised vs Unsupervised Learning

Unsupervised Learning

Data: x
Just data, no labels!

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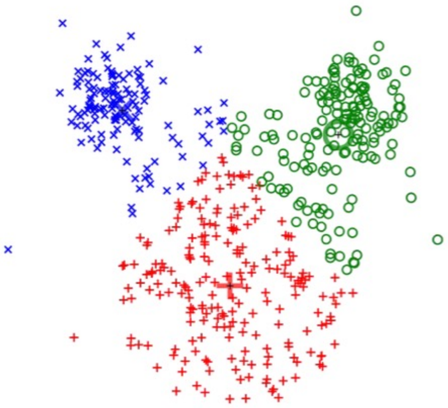
Examples: Clustering, dimensionality reduction, density estimation, etc.



K-means clustering

Supervised vs Unsupervised Learning

Unsupervised Learning

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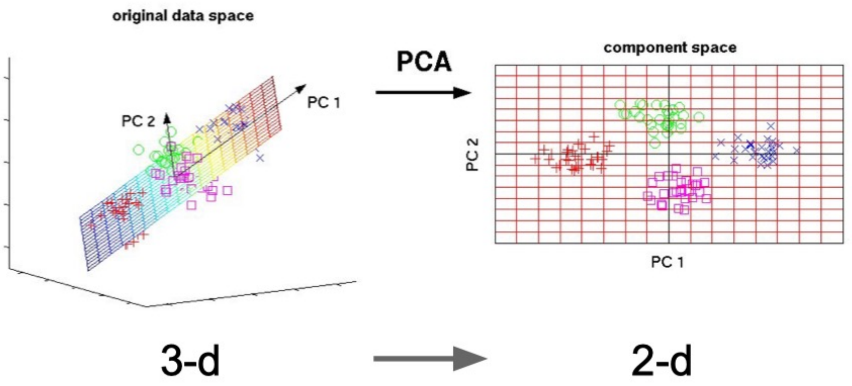
Just data, no labels!

Goal: Learn some underlying hidden *structure* of the data

Examples: Clustering, dimensionality reduction, density estimation, etc.



Principal Component Analysis
(Dimensionality reduction)

Supervised vs Unsupervised Learning

Unsupervised Learning

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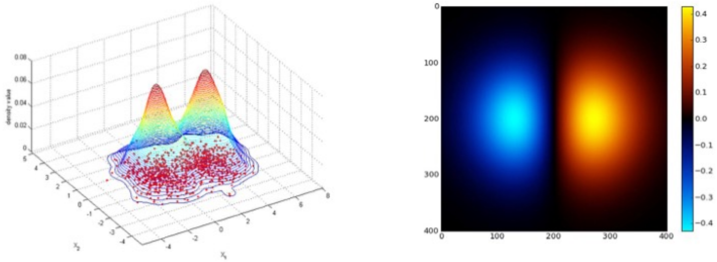
Just data, no labels!

Goal: Learn some underlying hidden *structure* of the data

Examples: Clustering, dimensionality reduction, density estimation, etc.

1-d density estimation



2-d density estimation

Modeling p(x)

Supervised vs Unsupervised Learning

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Unsupervised Learning

Data: x
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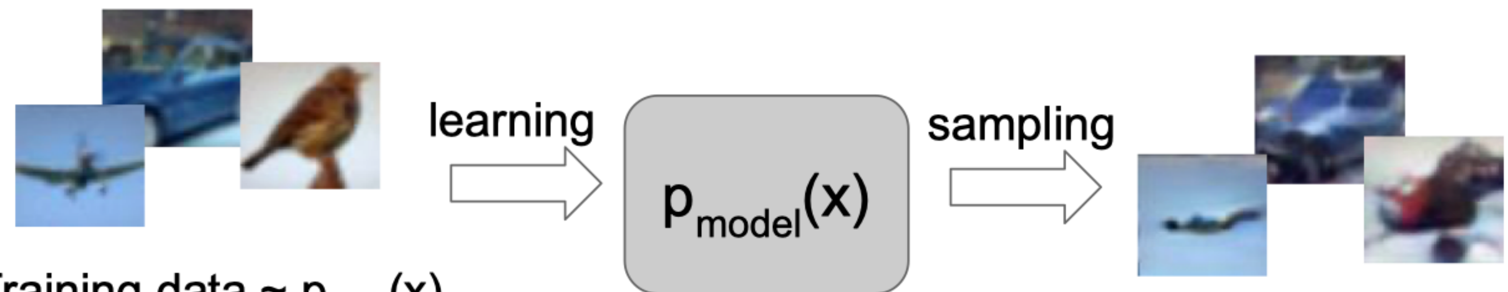
Goal: Learn some underlying hidden *structure* of the data

Examples: Clustering, dimensionality reduction, density estimation, etc.

Generative Modeling

Given training data, generate new samples from same distribution



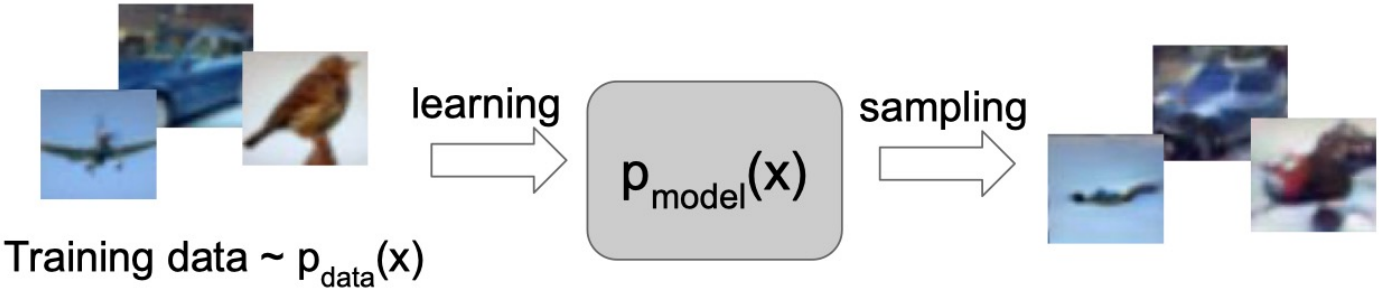
Training data ~ $p_{data}(x)$

Objectives:

1. Learn $p_{model}(x)$ that approximates $p_{data}(x)$
2. **Sampling new x from $p_{model}(x)$**

Generative Modeling

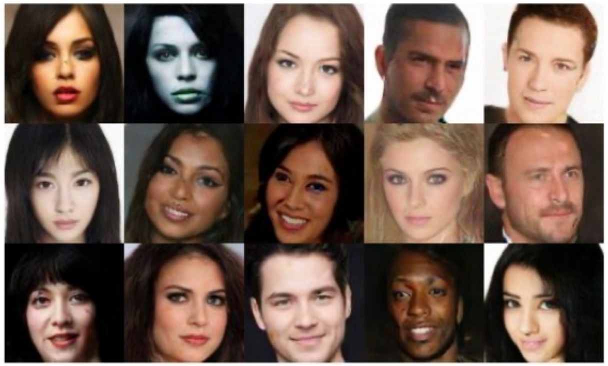
Given training data, generate new samples from same distribution



Formulate as density estimation problems:

- **Explicit density estimation**: explicitly define and solve for $p_{model}(x)$
- **Implicit density estimation**: learn model that can sample from $p_{model}(x)$ **without explicitly defining it.**

Why Generative Models


- Realistic samples for artwork, super-resolution, colorization, etc.
- Learn useful features for downstream tasks such as classification.
- Getting insights from high-dimensional data (physics, medical imaging, etc.)
- Modeling physical world for simulation and planning (robotics and reinforcement learning applications)
- Many more ...

Deep Generative models

- **Tractable density: PixelRNN/CNN**
- **Approximate density: Variational Autoencoder (VAE)**
- **Implicit density: Generative Adversarial Networks (GAN) and Diffusion Models**

Fully visible belief network (FVBN)

Explicit density model

$$p(x) = p(x_1, x_2, \ldots, x_n)$$

Likelihood of image x

Joint likelihood of each pixel in the image

Fully visible belief network (FVBN)

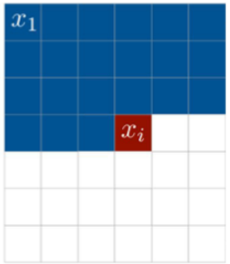
Explicit density model

Use chain rule to decompose likelihood of an image x into product of 1-d distributions:

$$p(x) = \prod_{i=1}^{n} p(x_i | x_1, ..., x_{i-1})$$

Likelihood of image x

Probability of i'th pixel value given all previous pixels



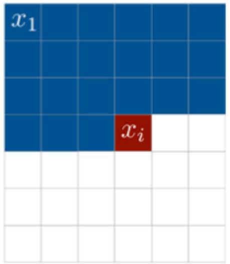
Then maximize likelihood of training data

Fully visible belief network (FVBN)

Explicit density model

Use chain rule to decompose likelihood of an image x into product of 1-d distributions:

$$p(x) = \prod_{i=1}^{n} p(x_i | x_1, ..., x_{i-1})$$



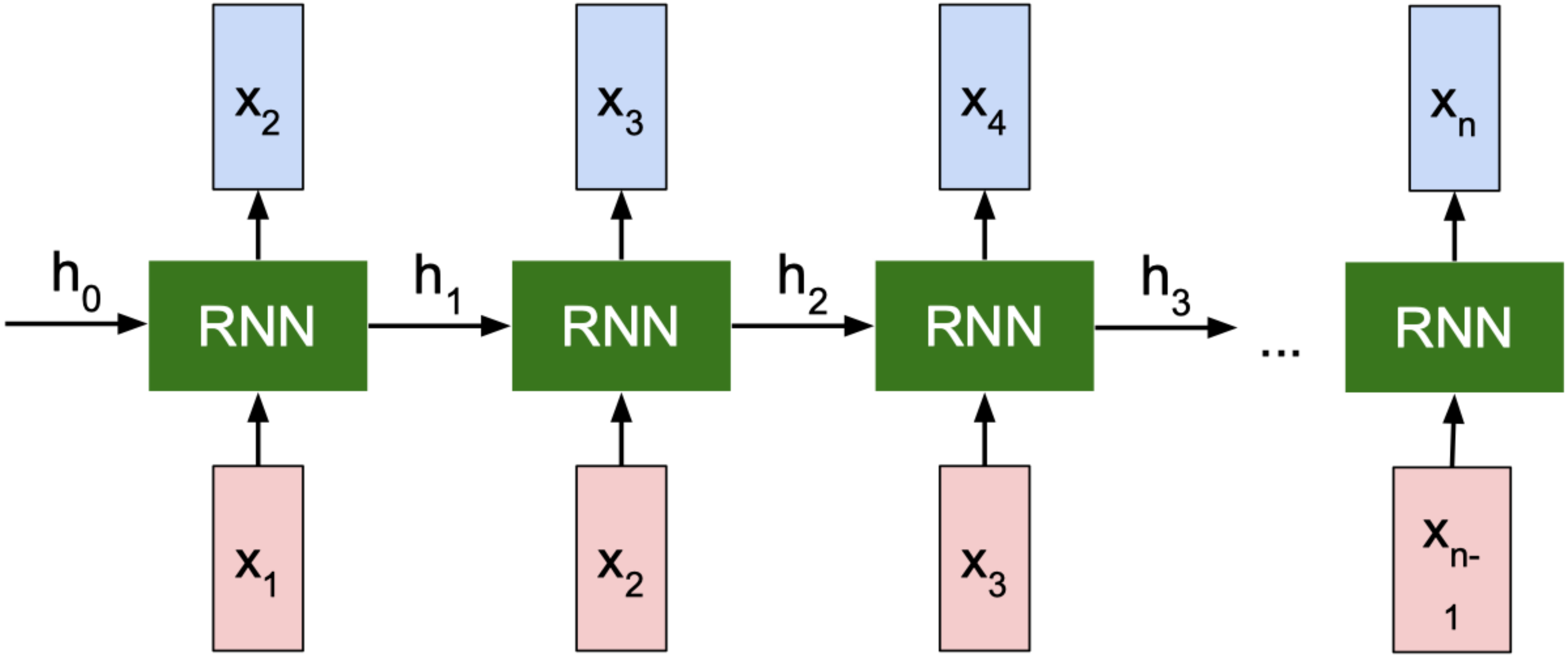
Likelihood of image x

Probability of i'th pixel value given all previous pixels

Complex distribution over pixel values => Express using a neural network!

Then maximize likelihood of training data

RNN

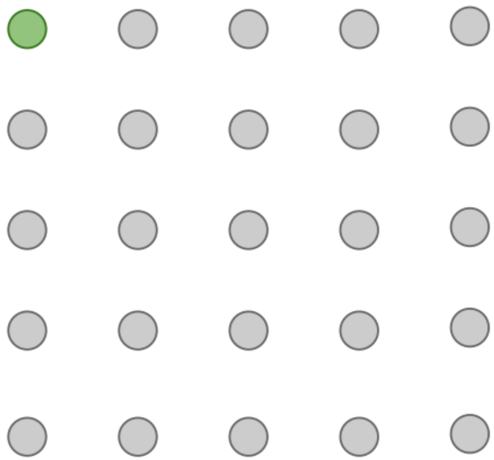


$$p(x_i|x_1, ..., x_{i-1})$$

PixelRNN

Generate image pixels starting from corner

Dependency on previous pixels modeled using an RNN (LSTM)



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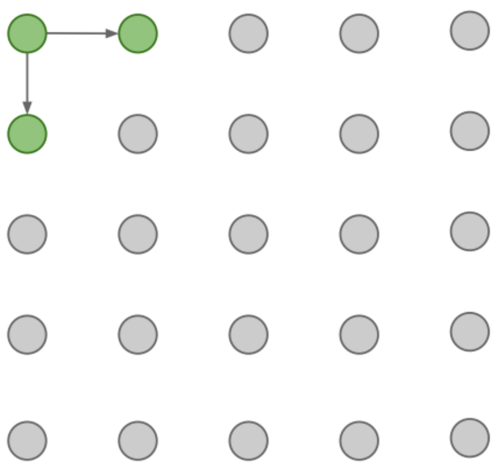

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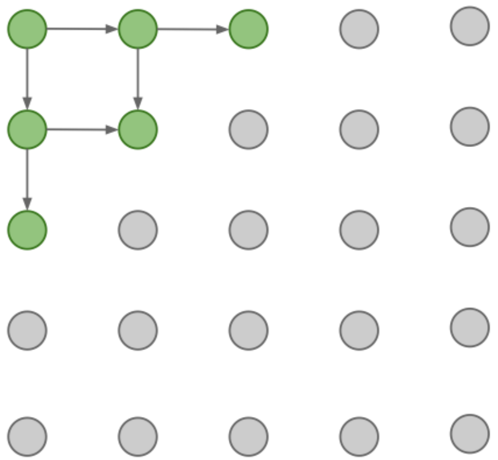
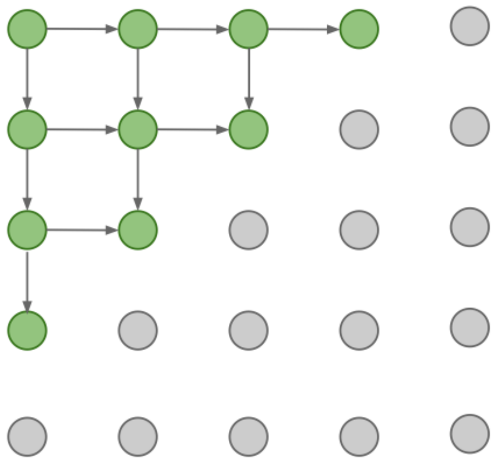


PixelRNN

Generate image pixels starting from corner

Dependency on previous pixels modeled using an RNN (LSTM)

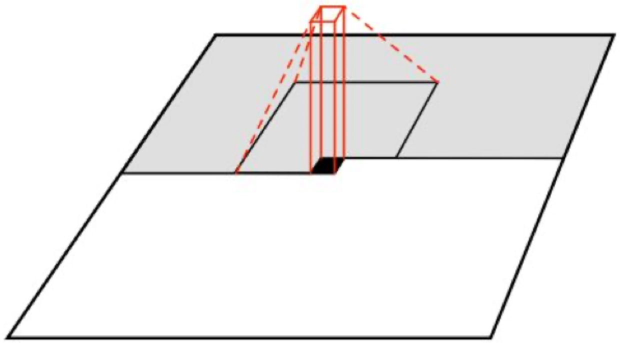
Drawback: sequential generation is slow in both training and inference!



PixelCNN

Still generate image pixels starting from corner

Dependency on previous pixels now modeled using a CNN over context region (**masked convolution**)



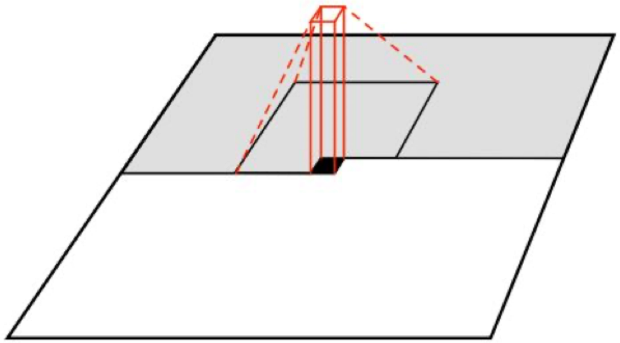
PixelCNN

Still generate image pixels starting from corner

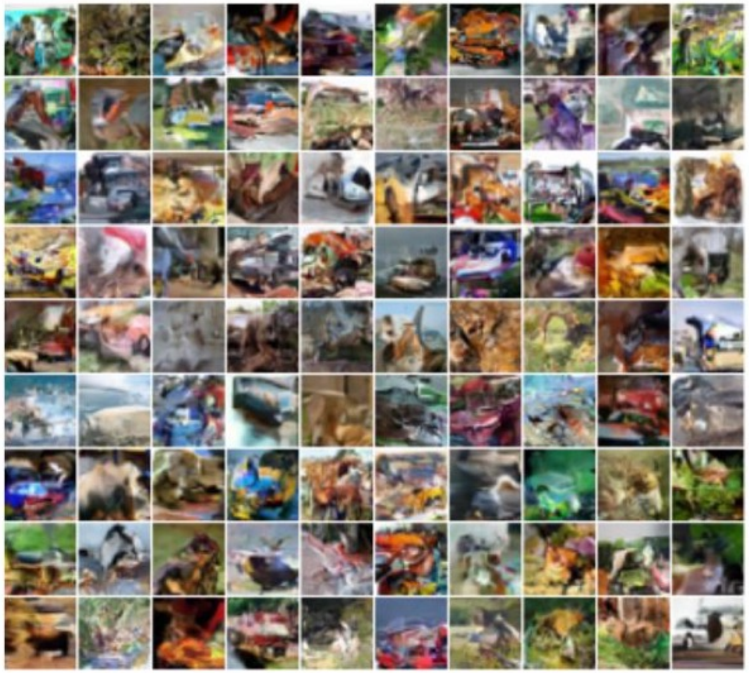
Dependency on previous pixels now modeled using a CNN over context region (masked convolution)

Training is faster than PixelRNN
(can parallelize convolutions since context region values known from training images)

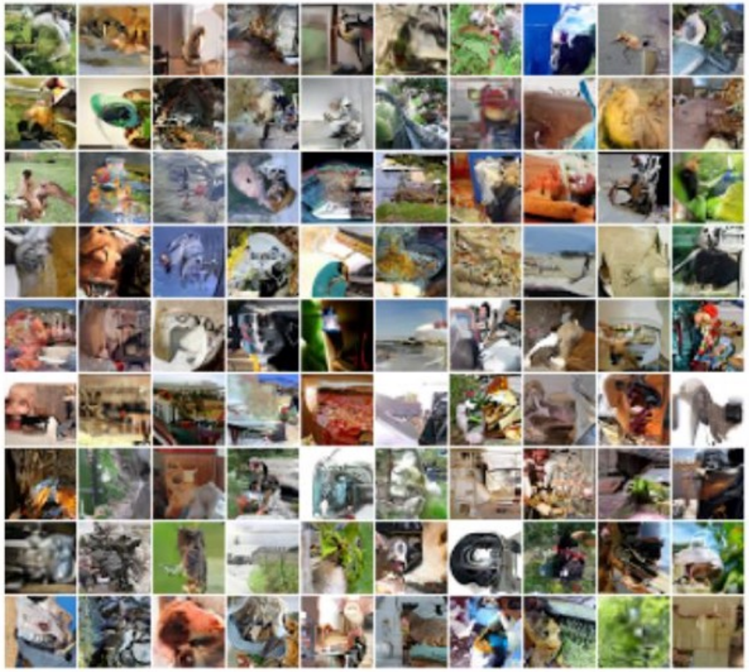
Generation is still slow:
For a 32x32 image, we need to do forward passes of the network 1024 times for a single image



Generation Samples



32x32 CIFAR-10



32x32 ImageNet

PixelRNN and PixelCNN

Pros:

- Can explicitly compute likelihood p(x)
- Easy to optimize
- Good samples

Con:

- Sequential generation => slow

Improving PixelCNN performance

- Gated convolutional layers
- Short-cut connections
- Discretized logistic loss
- Multi-scale
- Training tricks
- Etc…

See

- Van der Oord et al. NIPS 2016
- Salimans et al. 2017 (PixelCNN++)

Variational Autoencoders (VAE)

So far...

PixelRNN/CNNs define tractable density function, optimize likelihood of training data:

$$p_\theta(x) = \prod_{i=1}^{n} p_\theta(x_i | x_1, ..., x_{i-1})$$

Variational Autoencoders (VAEs) define intractable density function with latent **z**:

$$p_\theta(x) = \int p_\theta(z) p_\theta(x|z) dz$$

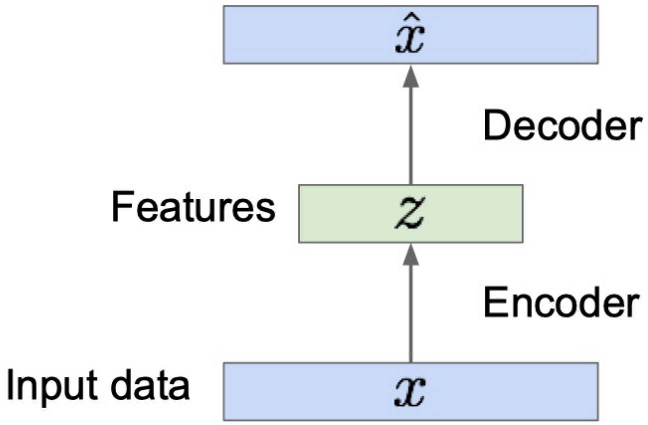
No dependencies among pixels, can generate all pixels at the same time!

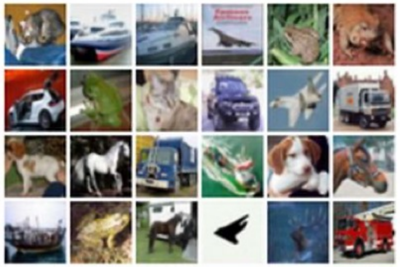
Cannot optimize directly, derive and optimize lower bound on likelihood instead

Why latent z?

Recap: Autoencoders

Unsupervised approach for learning a lower-dimensional feature representation from unlabeled training data



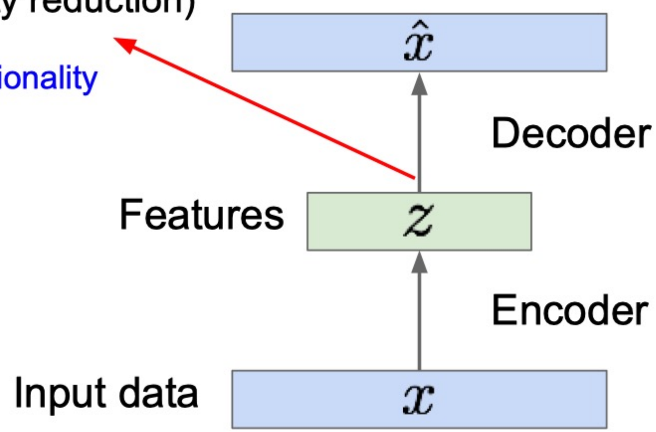


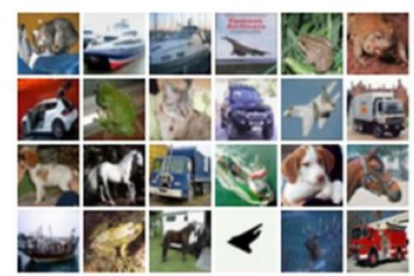
Recap: Autoencoders

Unsupervised approach for learning a lower-dimensional feature representation from unlabeled training data

z usually smaller than **x**
(dimensionality reduction)

Q: Why dimensionality reduction?





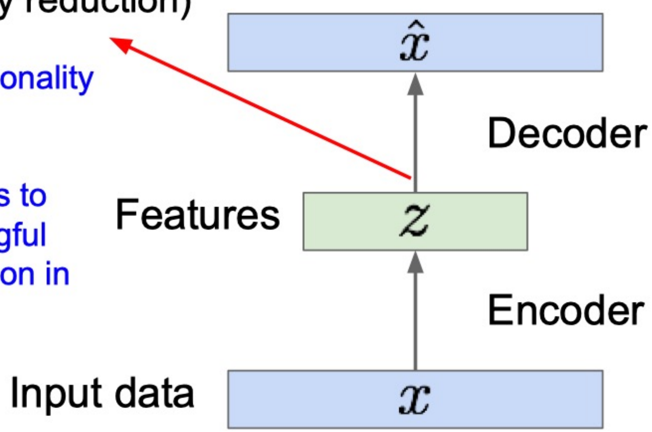
Recap: Autoencoders

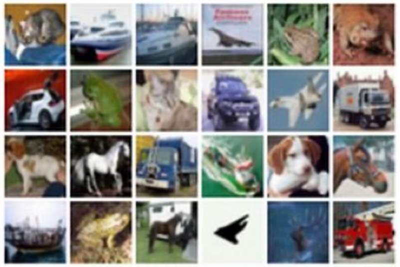
Unsupervised approach for learning a lower-dimensional feature representation from unlabeled training data

z usually smaller than **x** (dimensionality reduction)

Q: Why dimensionality reduction?

A: Want features to capture meaningful factors of variation in data

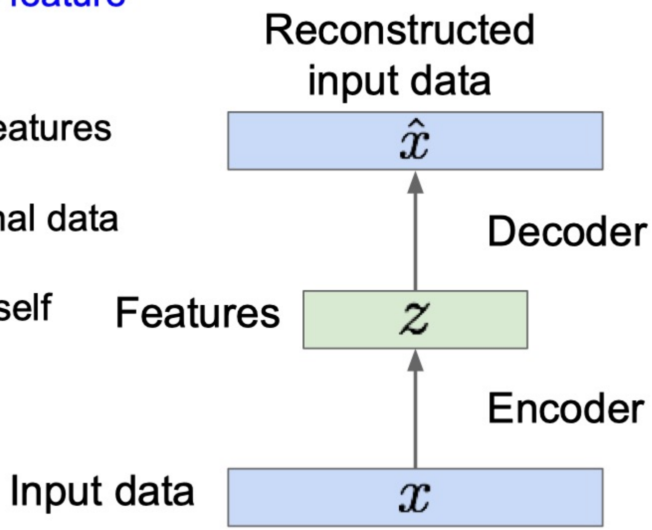


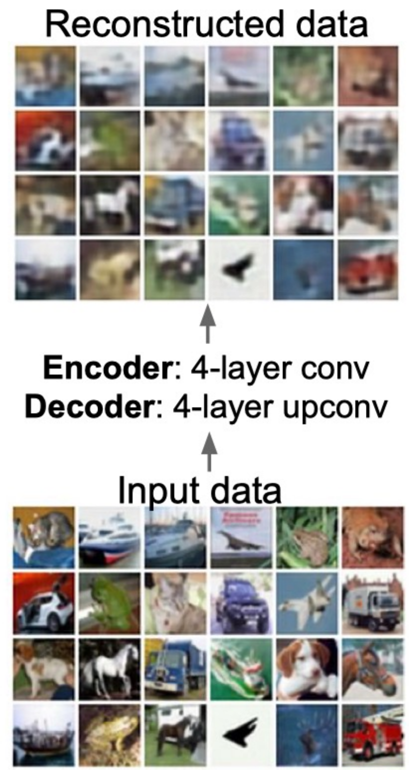


Recap: Autoencoders

How to learn this feature representation?

Train such that features can be used to reconstruct original data "Autoencoding" - encoding input itself

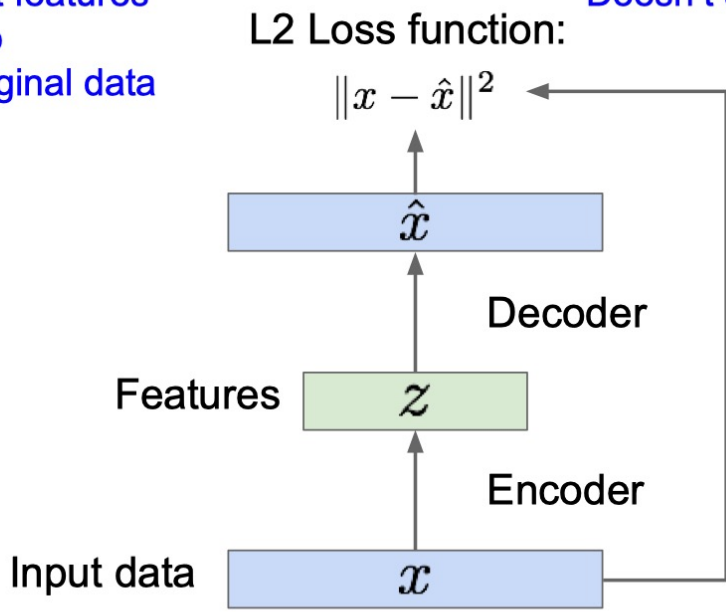


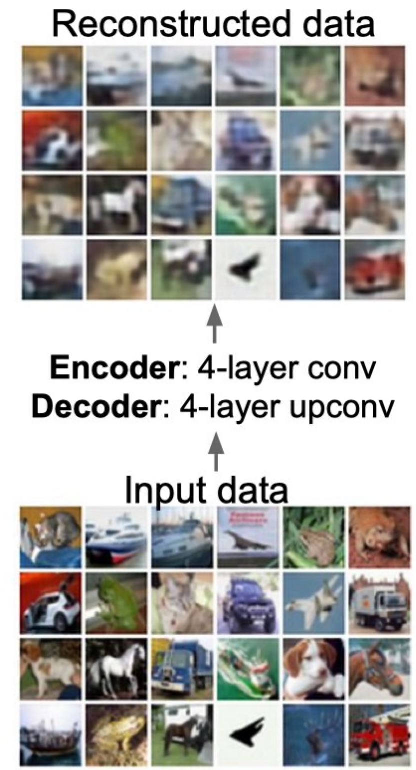


Recap: Autoencoders

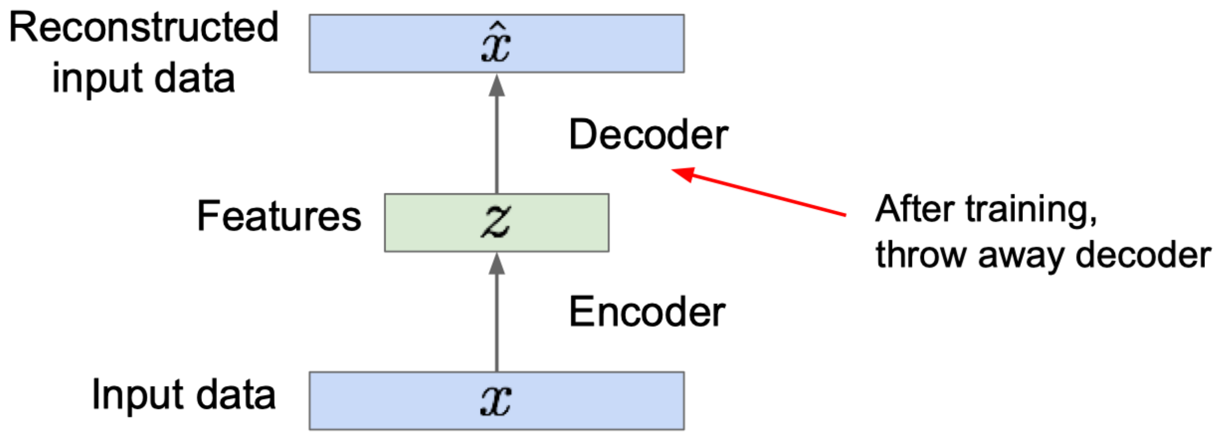
Train such that features can be used to reconstruct original data

Doesn't use labels!





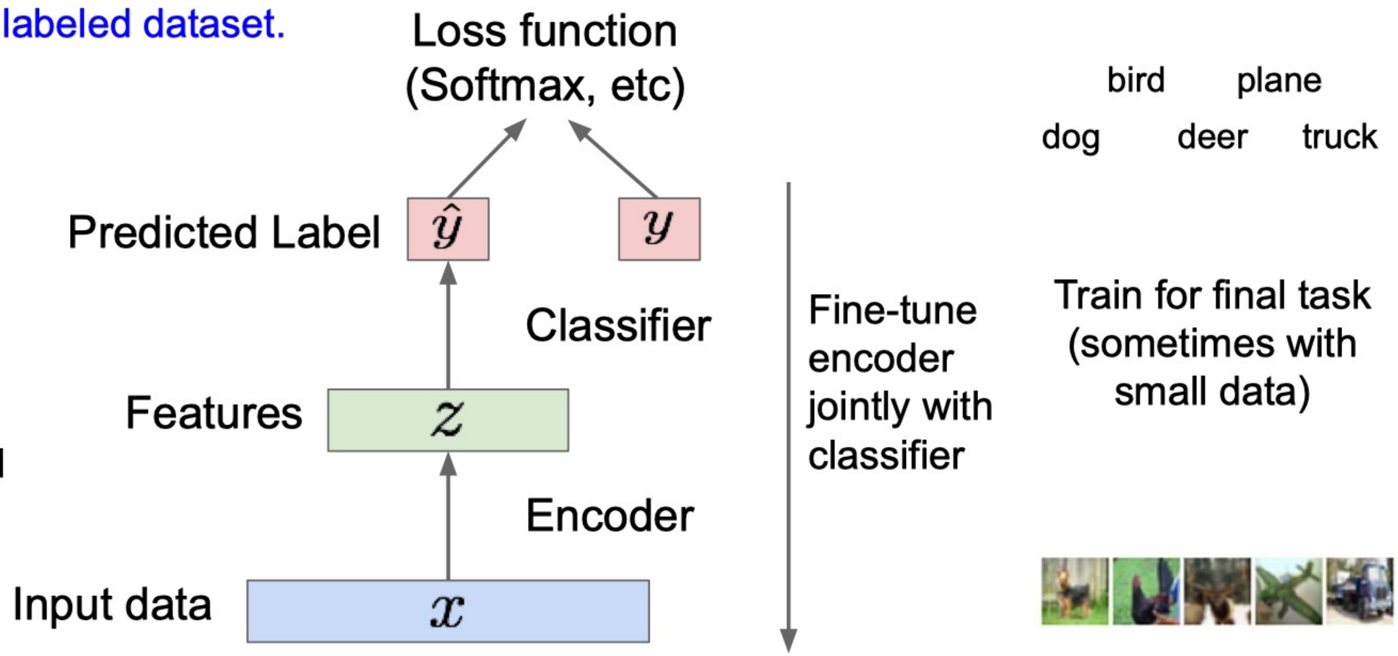
Recap: Autoencoders



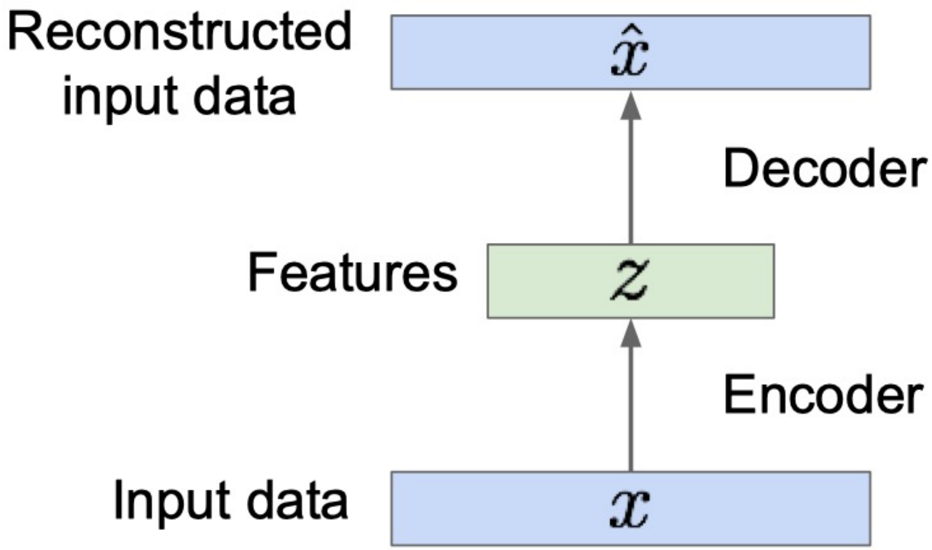
Recap: Autoencoders

Transfer from large, unlabeled dataset to small, labeled dataset.

Encoder can be used to initialize a **supervised** model



Recap: Autoencoders



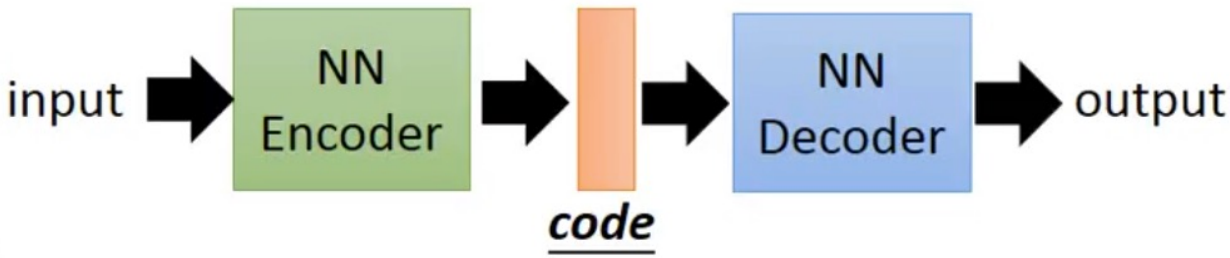
Autoencoders can reconstruct data, and can learn features to initialize a supervised model

Features capture factors of variation in training data.

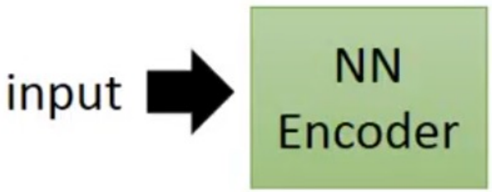
But we can't generate new images from an autoencoder because we don't know the space of z.

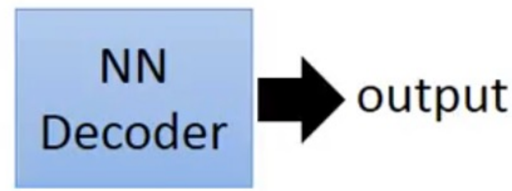
How do we make autoencoder a **generative model**?

Variational Autoencoders

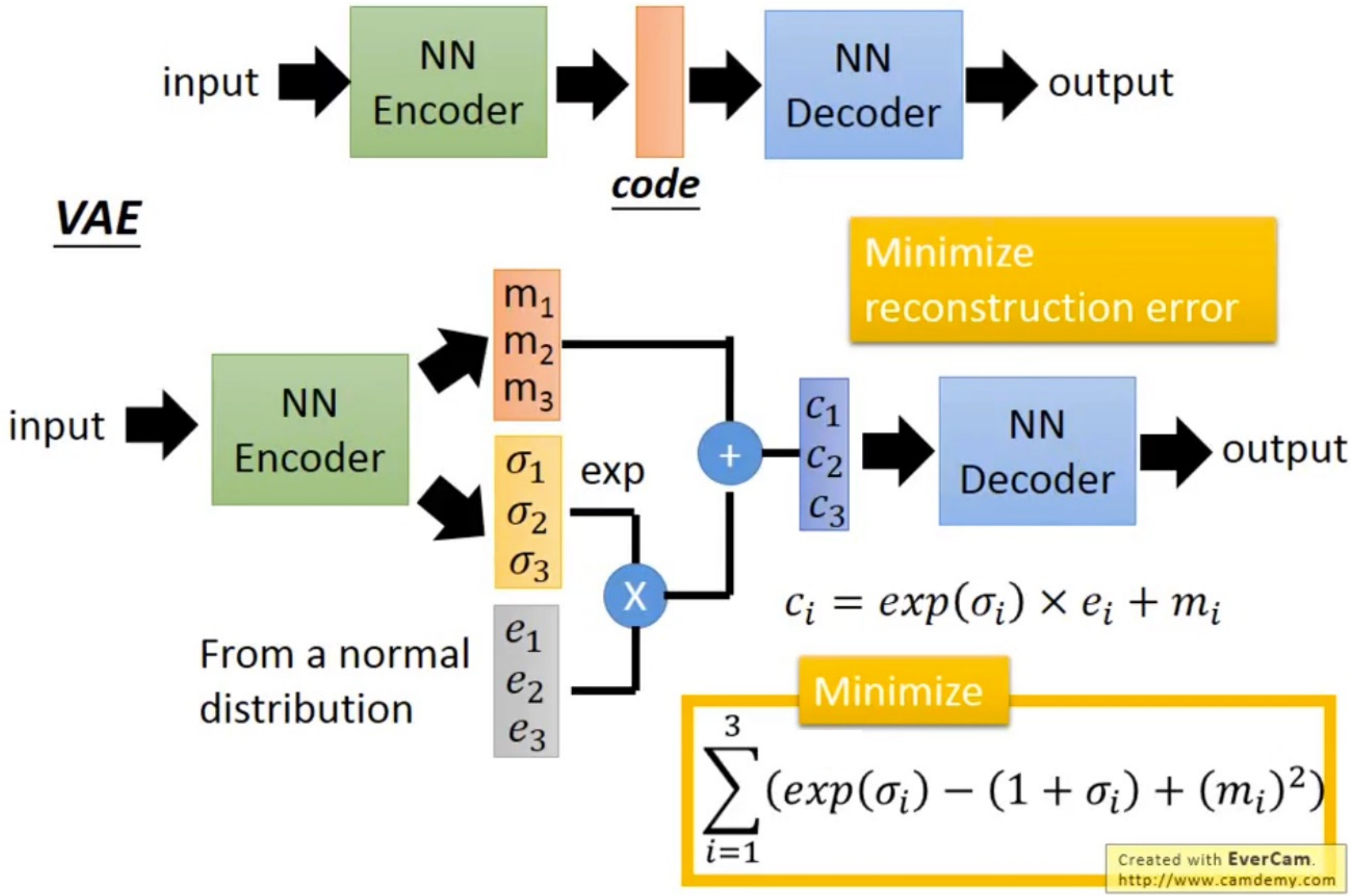


VAE



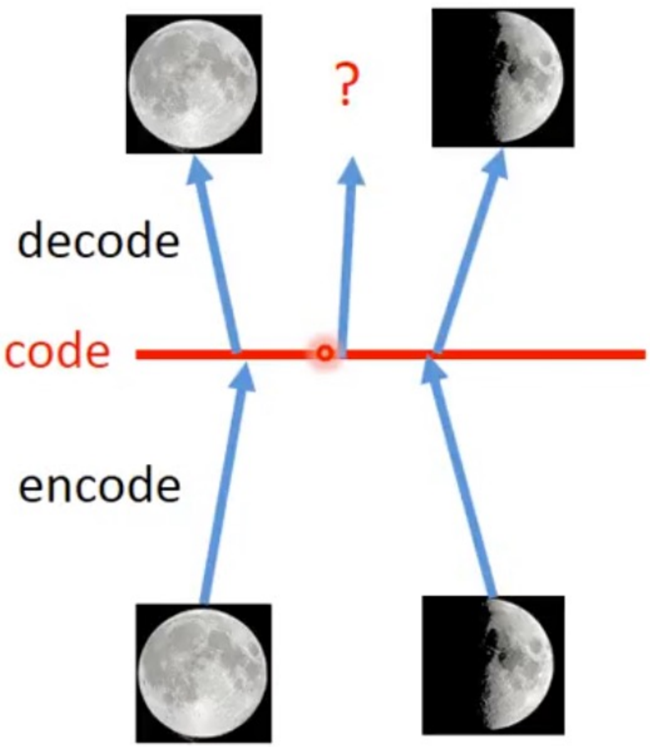


Variational Autoencoders



Why VAE?

Intuitive Reason



Variational Autoencoders

Why VAE?

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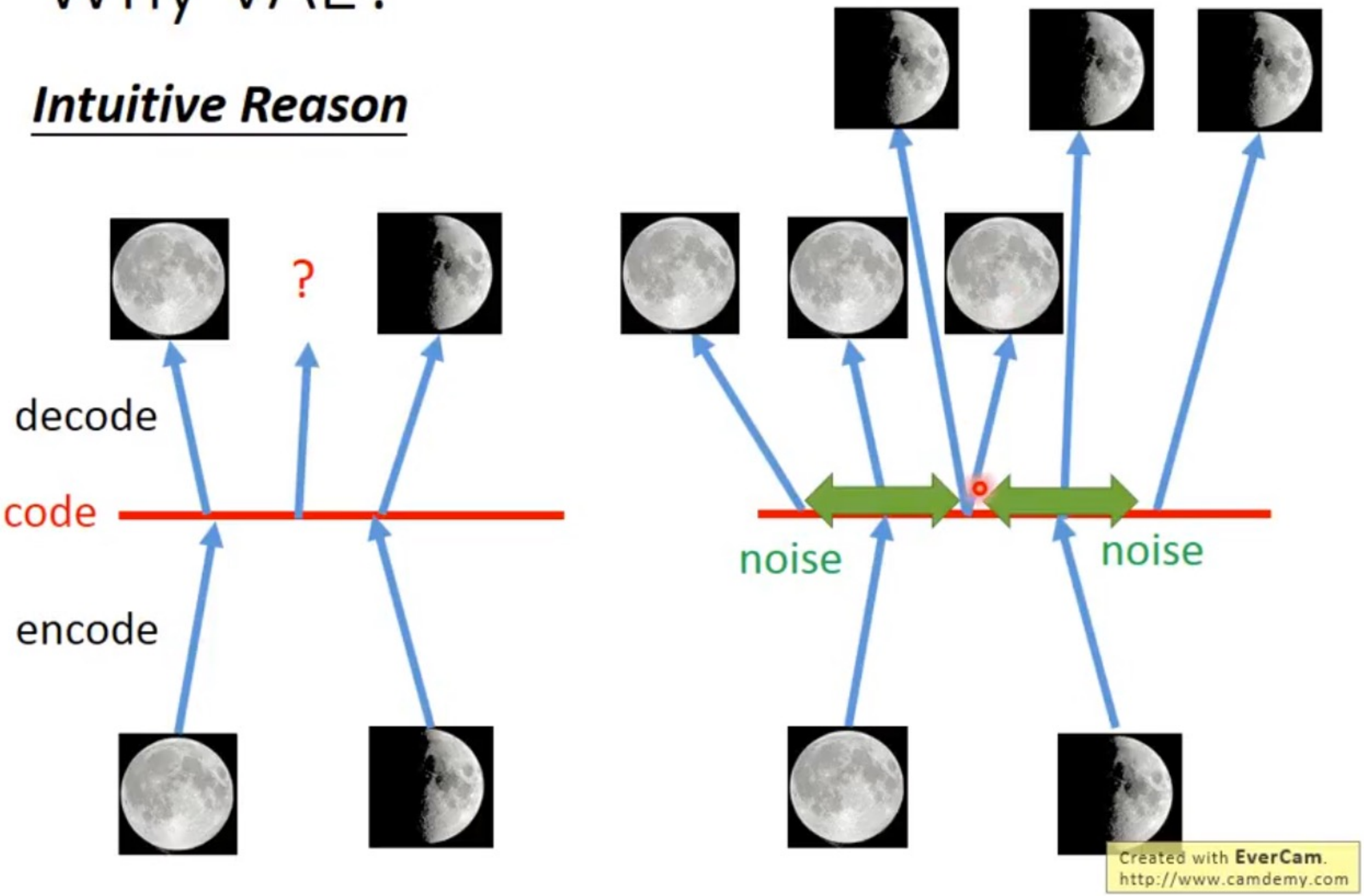
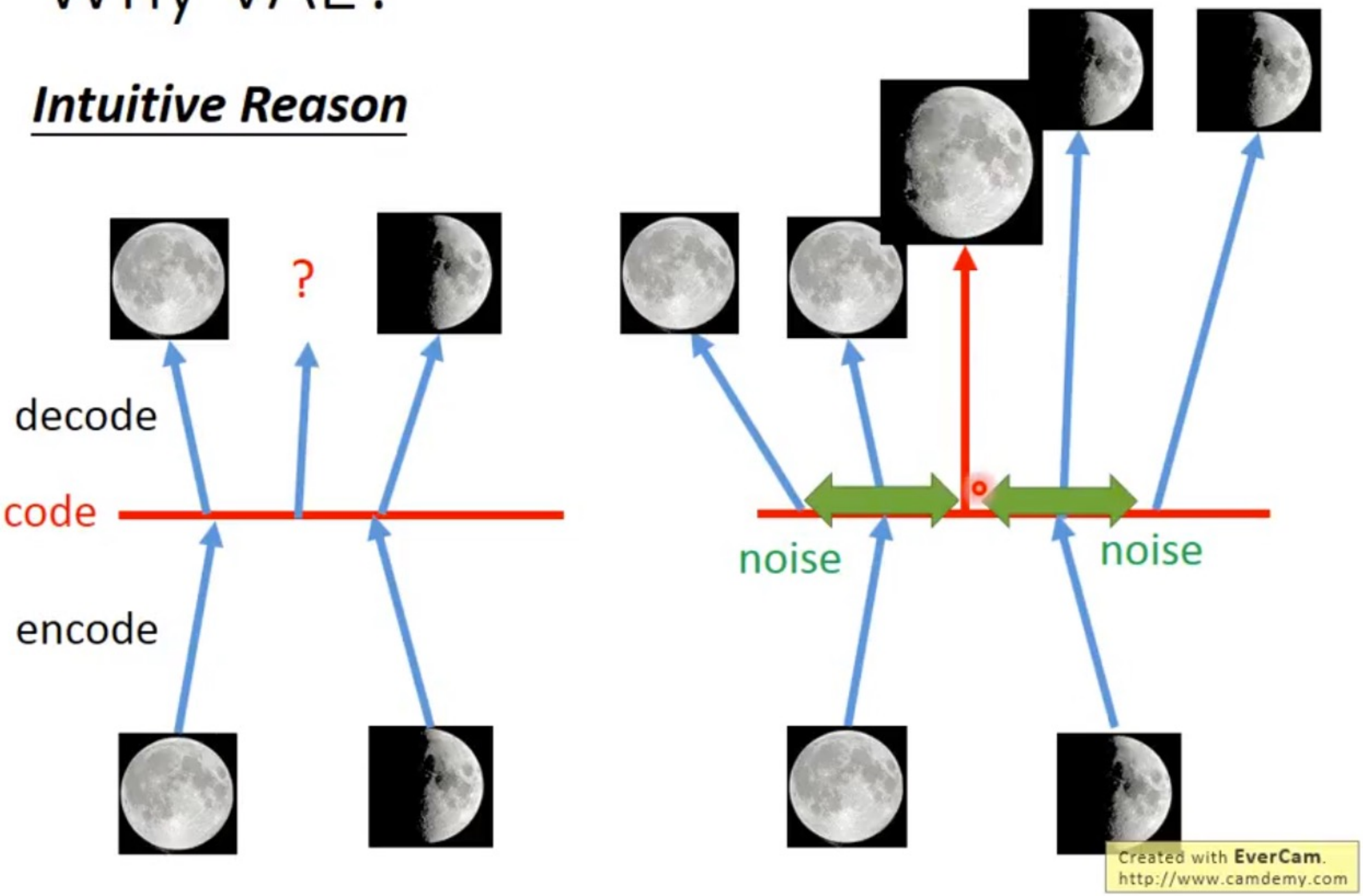


Variational Autoencoders

Why VAE?

Intuitive Reason

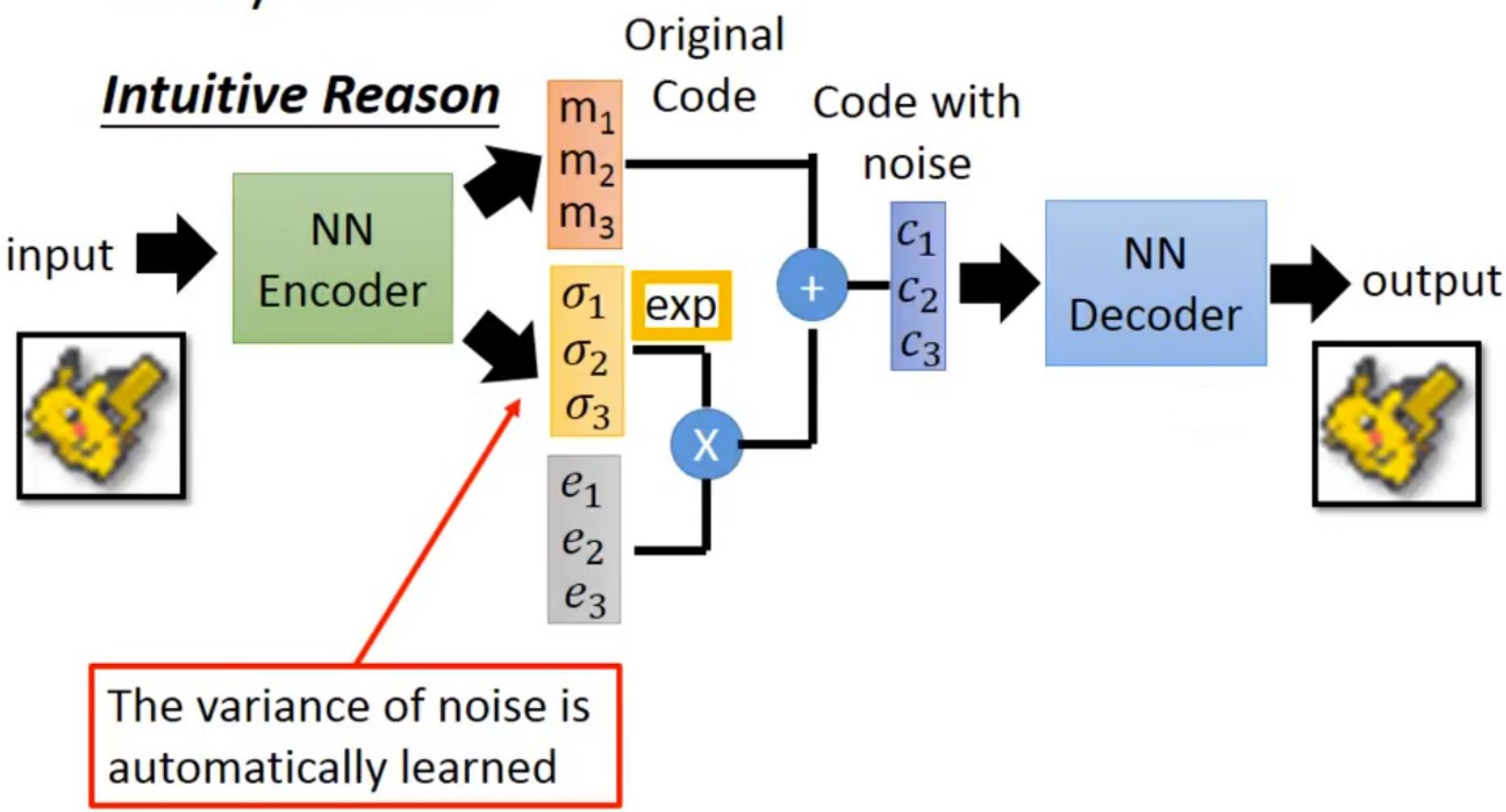


Variational Autoencoders: Simple Explanation

What will happen if we only minimize reconstruction error?

Why VAE?

Intuitive Reason



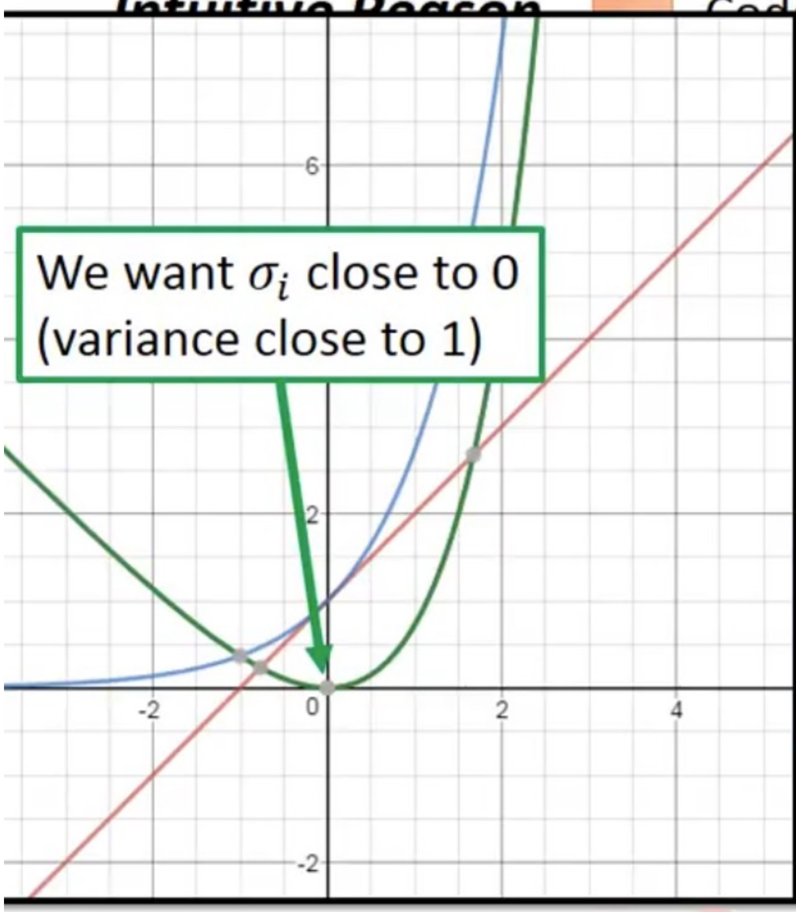
Variational Autoencoders: Simple Explanation

Why VAE?

What will happen if we only minimize reconstruction error?

Original

Code with noisy



c_1 c_2 c_3 → NN Decoder → output

Minimize

$$\sum_{i=1}^{3}\left(\underline{exp(\sigma_i)} - \underline{(1+\sigma_i)} + \underline{(m_i)^2}\right)$$

L2 regularization

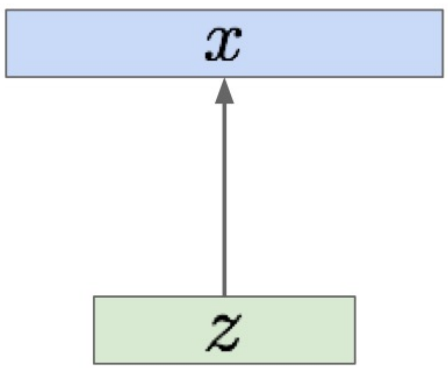
VAE: Probabilistic Perspective

Probabilistic spin on autoencoders - will let us sample from the model to generate data!

Assume training data $\{x^{(i)}\}_{i=1}^{N}$ is generated from the distribution of unobserved (latent) representation **z**

Intuition (remember from autoencoders!): **x** is an image, **z** is latent factors used to generate **x**: attributes, orientation, etc.

Sample from true conditional
$p_{\theta^*}(x \mid z^{(i)})$



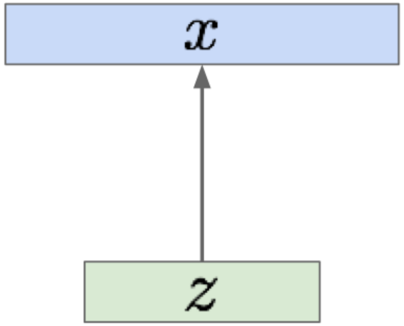
Sample from true prior
$z^{(i)} \sim p_{\theta^*}(z)$

VAE: A Probabilistic Perspective

We want to estimate the true parameters θ^* of this generative model given training data x.

Sample from true conditional

$p_{\theta^*}(x \mid z^{(i)})$



Sample from true prior

$z^{(i)} \sim p_{\theta^*}(z)$

How should we represent this model?

VAE: A Probabilistic Perspective

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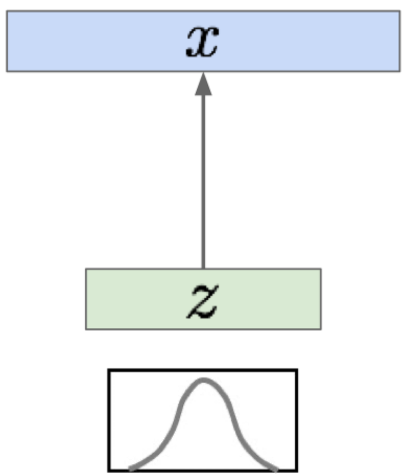


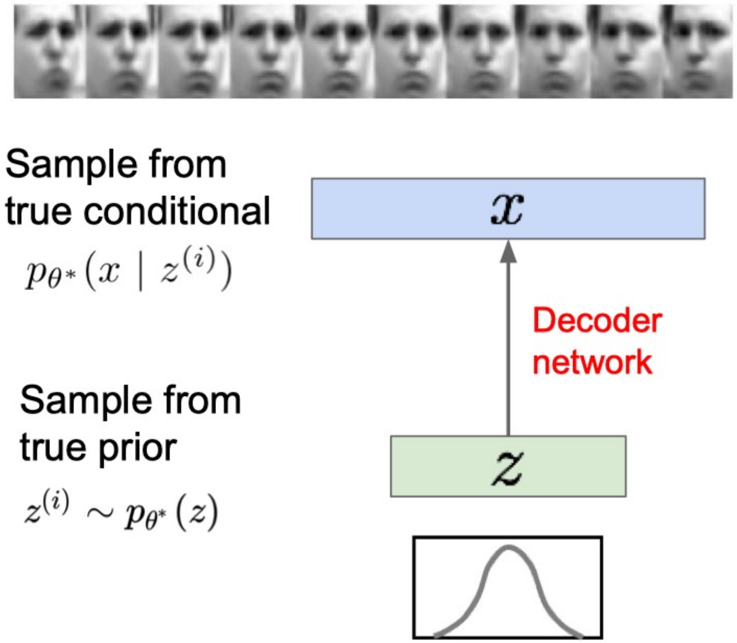
Sample from true prior

$z^{(i)} \sim p_{\theta^*}(z)$

How should we represent this model?

Choose prior p(z) to be simple, e.g. Gaussian. Reasonable for latent attributes, e.g. pose, how much smile.

VAE: A Probabilistic Perspective



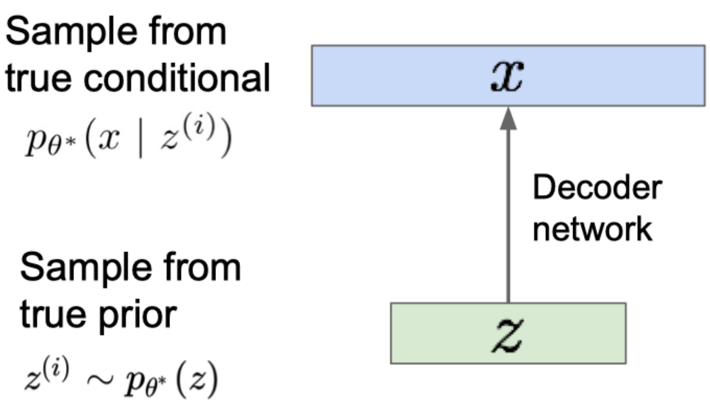
We want to estimate the true parameters θ^* of this generative model given training data x.

How should we represent this model?

Choose prior p(z) to be simple, e.g. Gaussian. Reasonable for latent attributes, e.g. pose, how much smile.

Conditional p(x|z) is complex (generates image) => represent with neural network

VAE: A Probabilistic Perspective



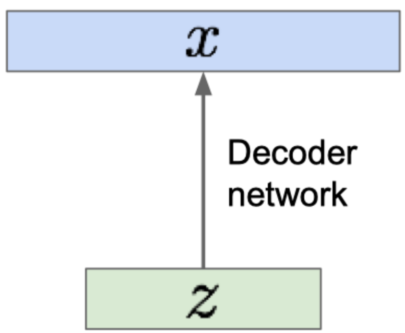
We want to estimate the true parameters θ^* of this generative model given training data x.

How to train the model?

VAE: A Probabilistic Perspective

Sample from
true conditional
$p_{\theta^*}(x \mid z^{(i)})$

Sample from
true prior
$z^{(i)} \sim p_{\theta^*}(z)$



We want to estimate the true parameters θ^*
of this generative model given training data x.

How to train the model?

Learn model parameters to maximize likeliho
of training data

$$p_\theta(x) = \int p_\theta(z) p_\theta(x|z) dz$$

Q: What is the problem with this?

Intractable!

VAE: A Probabilistic Perspective

Data likelihood: $p_\theta(x) = \int p_\theta(z) p_\theta(x|z) dz$

Simple Gaussian prior

VAE: A Probabilistic Perspective

Data likelihood: $p_\theta(x) = \int p_\theta(z) p_\theta(x|z) dz$

Decoder neural network

VAE: A Probabilistic Perspective

Data likelihood: $p_\theta(x) = \int p_\theta(z) p_\theta(x|z) dz$

Intractable to compute p(x|z) for every z!

VAE: A Probabilistic Perspective

Data likelihood: $p_\theta(x) = \int p_\theta(z) p_\theta(x|z) dz$

Posterior density: $p_\theta(z|x) = p_\theta(x|z) p_\theta(z) / p_\theta(x)$

Intractable data likelihood

VAE: A Probabilistic Perspective

Data likelihood: $p_\theta(x) = \int p_\theta(z) p_\theta(x|z) dz$

Posterior density also intractable: $p_\theta(z|x) = p_\theta(x|z) p_\theta(z) / p_\theta(x)$

Solution: In addition to modeling $p_\theta(x|z)$, learn $q_\phi(z|x)$ that approximates the true posterior $p_\theta(z|x)$.

Will see that the approximate posterior allows us to derive a lower bound on the data likelihood that is tractable, which we can optimize.

Variational inference is to approximate the unknown posterior distribution from only the observed data x

VAE: A Probabilistic Perspective

$$\log p_\theta(x^{(i)}) = \mathbf{E}_{z\sim q_\phi(z|x^{(i)})}\left[\log p_\theta(x^{(i)})\right] \quad (p_\theta(x^{(i)}) \text{ Does not depend on } z)$$

$$= \mathbf{E}_z\left[\log \frac{p_\theta(x^{(i)} \mid z)p_\theta(z)}{p_\theta(z \mid x^{(i)})}\right] \quad \text{(Bayes' Rule)}$$

$$= \mathbf{E}_z\left[\log \frac{p_\theta(x^{(i)} \mid z)p_\theta(z)}{p_\theta(z \mid x^{(i)})} \frac{q_\phi(z \mid x^{(i)})}{q_\phi(z \mid x^{(i)})}\right] \quad \text{(Multiply by constant)}$$

$$= \mathbf{E}_z\left[\log p_\theta(x^{(i)} \mid z)\right] - \mathbf{E}_z\left[\log \frac{q_\phi(z \mid x^{(i)})}{p_\theta(z)}\right] + \mathbf{E}_z\left[\log \frac{q_\phi(z \mid x^{(i)})}{p_\theta(z \mid x^{(i)})}\right] \quad \text{(Logarithms)}$$

$$= \mathbf{E}_z\left[\log p_\theta(x^{(i)} \mid z)\right] - D_{KL}(q_\phi(z \mid x^{(i)}) \,||\, p_\theta(z)) + D_{KL}(q_\phi(z \mid x^{(i)}) \,||\, p_\theta(z \mid x^{(i)}))$$

We want to maximize the data likelihood

Decoder network gives $p_\theta(x|z)$, can compute estimate of this term through sampling.

This KL term (between Gaussians for encoder and z prior) has nice closed-form solution!

$p_\theta(z|x)$ intractable (saw earlier), can't compute this KL term :(But we know KL divergence always >= 0.

VAE: A Probabilistic Perspective

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$$= \mathbf{E}_z\left[\log \frac{p_\theta(x^{(i)} \mid z)p_\theta(z)}{p_\theta(z \mid x^{(i)})}\right] \quad \text{(Bayes' Rule)}$$

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$$= \boxed{\underbrace{\mathbf{E}_z\left[\log p_\theta(x^{(i)} \mid z)\right] - D_{KL}(q_\phi(z \mid x^{(i)}) \,||\, p_\theta(z))}_{\mathcal{L}(x^{(i)},\theta,\phi)}} + \underbrace{D_{KL}(q_\phi(z \mid x^{(i)}) \,||\, p_\theta(z \mid x^{(i)}))}_{\boxed{\geq 0}}$$

Tractable lower bound which we can take gradient of and optimize! ($p_\theta(x|z)$ differentiable, KL term differentiable)

VAE: A Probabilistic Perspective

Decoder: reconstruct the input data

Encoder: make approximate posterior distribution close to prior

$$
\begin{aligned}
\log p_\theta(x^{(i)}) &= \mathbf{E}_{z\sim q_\phi(z|x^{(i)})}\left[\log p_\theta(x^{(i)})\right] \qquad (p_\theta(x^{(i)}) \text{ Does not depend on } z) \\
&= \mathbf{E}_z\left[\log \frac{p_\theta(x^{(i)} \mid z)p_\theta(z)}{p_\theta(z \mid x^{(i)})}\right] \qquad (\text{Bayes' Rule}) \\
&= \mathbf{E}_z\left[\log \frac{p_\theta(x^{(i)} \mid z)p_\theta(z)}{p_\theta(z \mid x^{(i)})}\frac{q_\phi(z \mid x^{(i)})}{q_\phi(z \mid x^{(i)})}\right] \qquad (\text{Multiply by constant}) \\
&= \mathbf{E}_z\left[\log p_\theta(x^{(i)} \mid z)\right] - \mathbf{E}_z\left[\log \frac{q_\phi(z \mid x^{(i)})}{p_\theta(z)}\right] + \mathbf{E}_z\left[\log \frac{q_\phi(z \mid x^{(i)})}{p_\theta(z \mid x^{(i)})}\right] \qquad (\text{Logarithms}) \\
&= \boxed{\underbrace{\mathbf{E}_z\left[\log p_\theta(x^{(i)} \mid z)\right] - D_{KL}(q_\phi(z \mid x^{(i)}) \,||\, p_\theta(z))}_{\mathcal{L}(x^{(i)},\theta,\phi)}} + \underbrace{D_{KL}(q_\phi(z \mid x^{(i)}) \,||\, p_\theta(z \mid x^{(i)}))}_{\boxed{\geq 0}}
\end{aligned}
$$

Tractable lower bound which we can take gradient of and optimize! ($p_\theta(x|z)$ differentiable, KL term differentiable)

Variational Autoencoders

Putting it all together: maximizing the likelihood lower bound

$$\underbrace{\mathbf{E}_z\left[\log p_\theta(x^{(i)} \mid z)\right] - D_{KL}(q_\phi(z \mid x^{(i)}) \,||\, p_\theta(z))}_{\mathcal{L}(x^{(i)}, \theta, \phi)}$$

VAE: A Probabilistic Perspective

Variational Autoencoders

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Let’s look at computing the KL divergence between the estimated posterior and the prior given some data

Input Data x

Variational Autoencoders

Putting it all together: maximizing the likelihood lower bound

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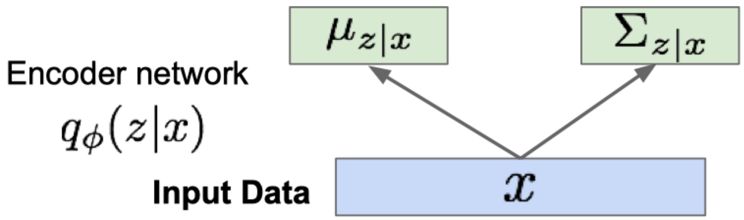

VAE: A Probabilistic Perspective

Variational Autoencoders

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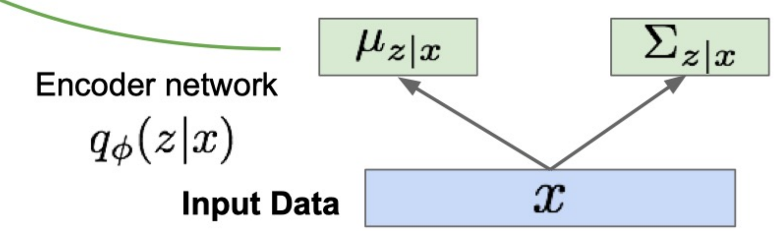
$$\underbrace{\mathbf{E}_z\left[\log p_\theta(x^{(i)} \mid z)\right] - \boxed{D_{KL}(q_\phi(z \mid x^{(i)}) \,||\, p_\theta(z))}}_{\mathcal{L}(x^{(i)}, \theta, \phi)}$$

$$D_{KL}(\mathcal{N}(\mu_{z|x}, \Sigma_{z|x}) || \mathcal{N}(0, I))$$

Have analytical solution

Make approximate posterior distribution close to prior



VAE: A Probabilistic Perspective

Variational Autoencoders

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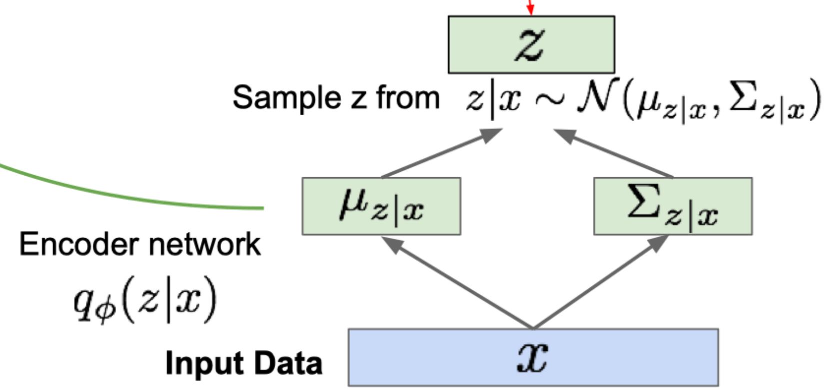
$$\underbrace{\boxed{\mathbf{E}_z\left[\log p_\theta(x^{(i)} \mid z)\right]} - D_{KL}(q_\phi(z \mid x^{(i)}) \,||\, p_\theta(z))}_{\mathcal{L}(x^{(i)}, \theta, \phi)}$$

Make approximate posterior distribution close to prior

Not part of the computation graph!



VAE: A Probabilistic Perspective

Variational Autoencoders

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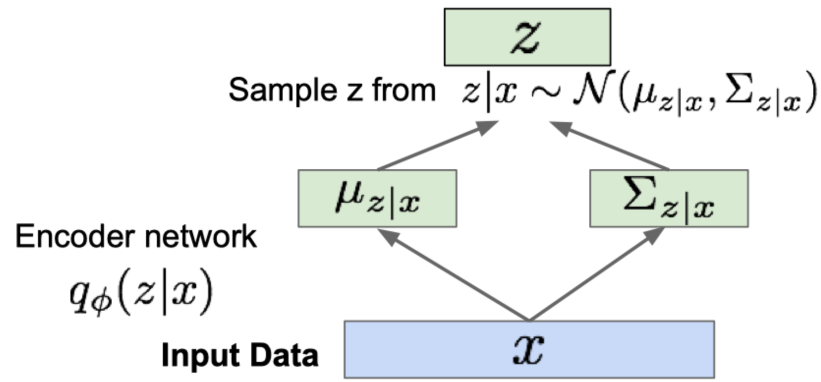
$$\underbrace{\boxed{\mathbf{E}_z\left[\log p_\theta(x^{(i)} \mid z)\right]} - D_{KL}(q_\phi(z \mid x^{(i)}) \,||\, p_\theta(z))}_{\mathcal{L}(x^{(i)}, \theta, \phi)}$$

Reparameterization trick to make sampling differentiable:

Sample $\epsilon \sim \mathcal{N}(0, I)$

$$z = \mu_{z|x} + \epsilon\sigma_{z|x}$$



VAE: A Probabilistic Perspective

Variational Autoencoders

Putting it all together: maximizing the likelihood lower bound

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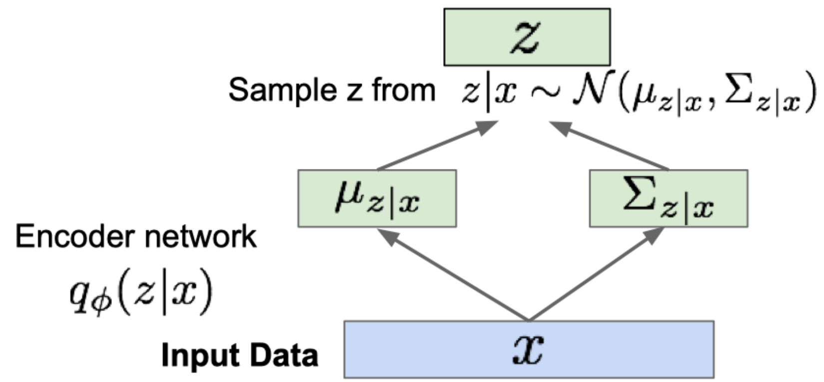
Reparameterization trick to make sampling differentiable:

Sample $\epsilon \sim \mathcal{N}(0, I)$

Input to the graph

$$z = \boxed{\mu_{z|x}} + \boxed{\epsilon}\boxed{\sigma_{z|x}}$$

Part of computation graph



VAE: A Probabilistic Perspective

Variational Autoencoders

Putting it all together: maximizing the likelihood lower bound

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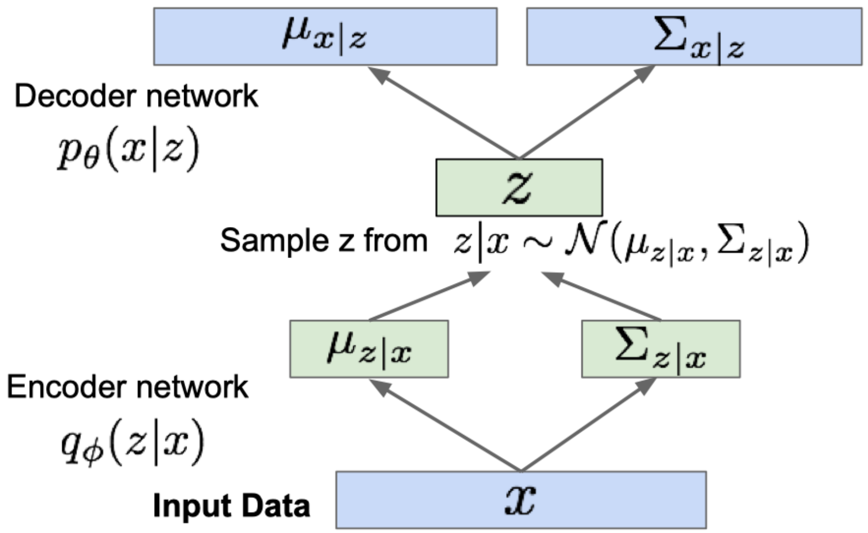


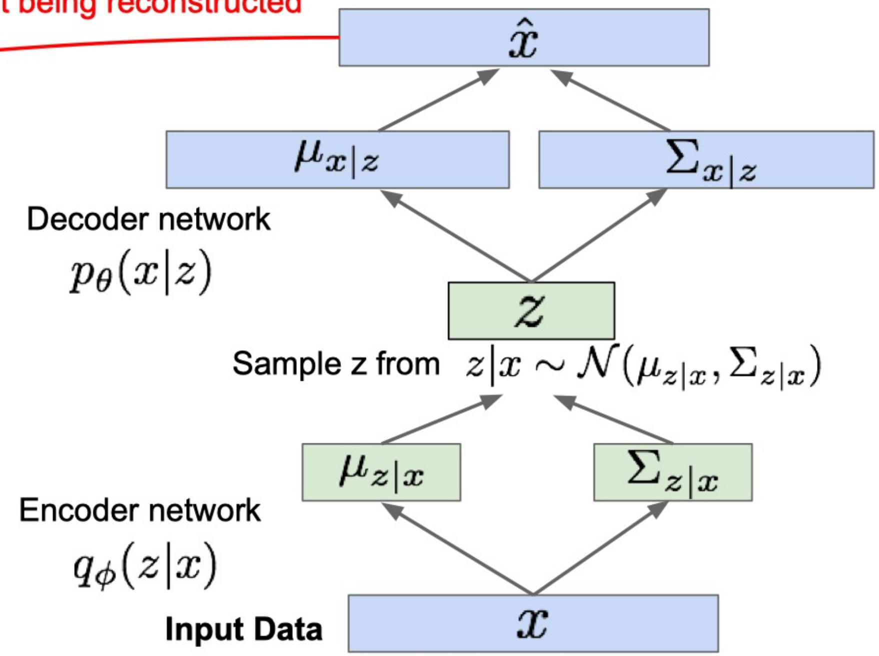
VAE: A Probabilistic Perspective

Variational Autoencoders

Maximize likelihood of original input being reconstructed

Putting it all together: maximizing the likelihood lower bound

$$\underbrace{\boxed{\mathbf{E}_z\left[\log p_\theta(x^{(i)} \mid z)\right]} - D_{KL}(q_\phi(z \mid x^{(i)}) \,||\, p_\theta(z))}_{\mathcal{L}(x^{(i)},\theta,\phi)}$$



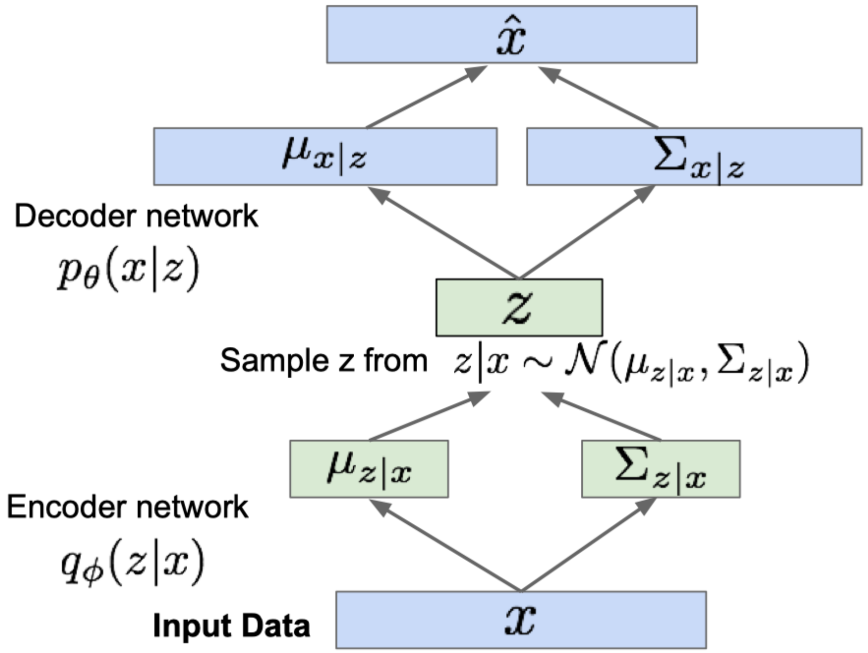
VAE: A Probabilistic Perspective

Variational Autoencoders

Putting it all together: maximizing the likelihood lower bound

$$\underbrace{\boxed{\mathbf{E}_z\left[\log p_\theta(x^{(i)} \mid z)\right] - D_{KL}(q_\phi(z \mid x^{(i)}) \,||\, p_\theta(z))}}_{\mathcal{L}(x^{(i)},\theta,\phi)}$$

For every minibatch of input data: compute this forward pass, and then backprop!



VAE: Generating Data

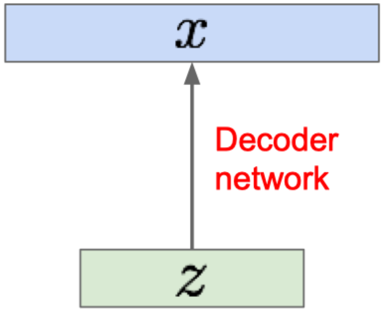
Our assumption about data generation process

Sample from true conditional

$p_{\theta^*}(x \mid z^{(i)})$

Sample from true prior

$z^{(i)} \sim p_{\theta^*}(z)$



Kingma and Welling, “Auto-Encoding Variational Bayes”, ICLR 2014

VAE: Generating Data

Our assumption about data generation process

Sample from true conditional

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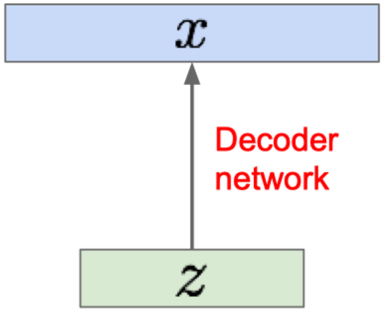
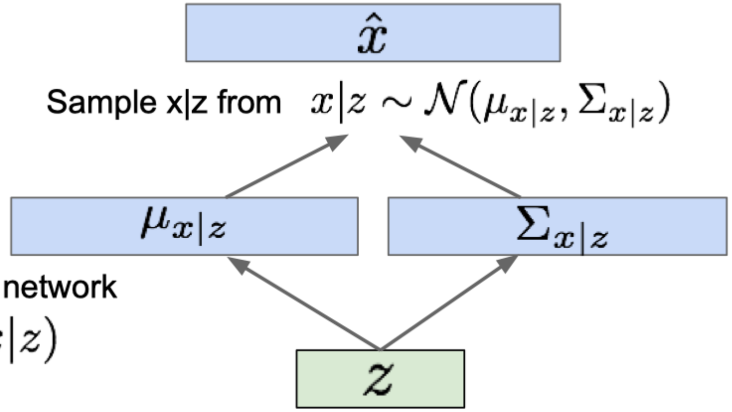


Sample from true prior

$z^{(i)} \sim p_{\theta^*}(z)$

Now given a trained VAE:
use decoder network & sample z from prior!



Sample x|z from $x|z \sim \mathcal{N}(\mu_{x|z}, \Sigma_{x|z})$

Decoder network

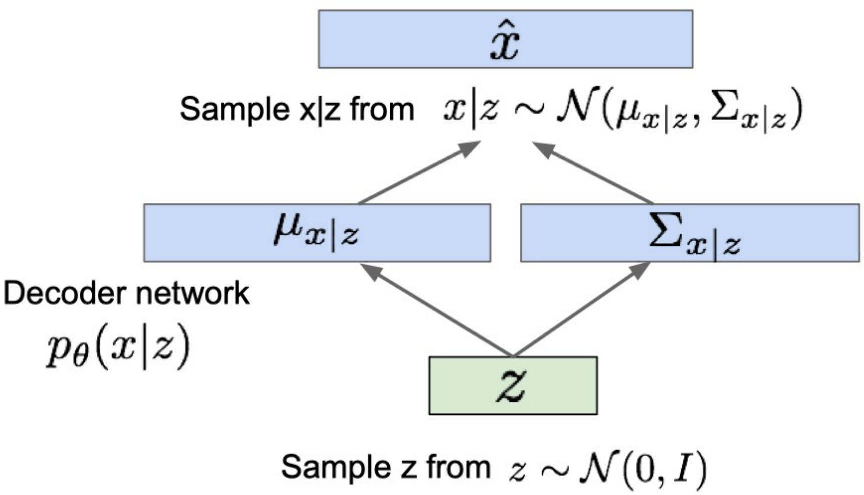
$p_\theta(x|z)$

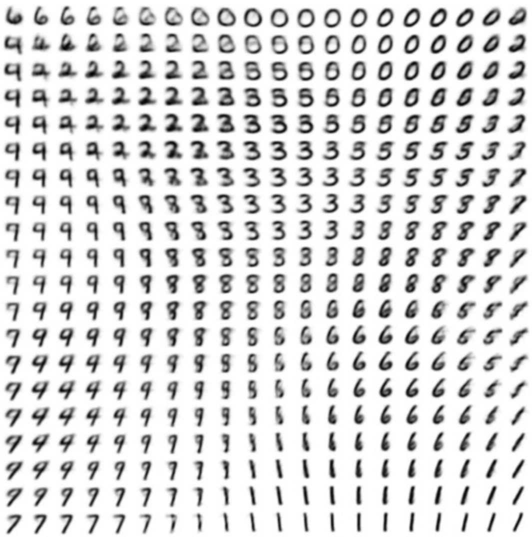
Sample z from $z \sim \mathcal{N}(0, I)$

Kingma and Welling, “Auto-Encoding Variational Bayes”, ICLR 2014

VAE: Generating Data

Use decoder network. Now sample z from prior!





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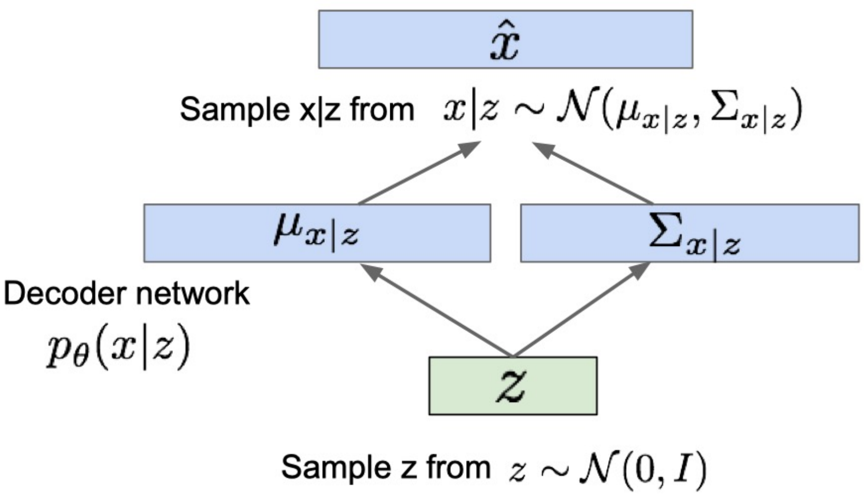
VAE: Generating Data

Use decoder network. Now sample z from prior!



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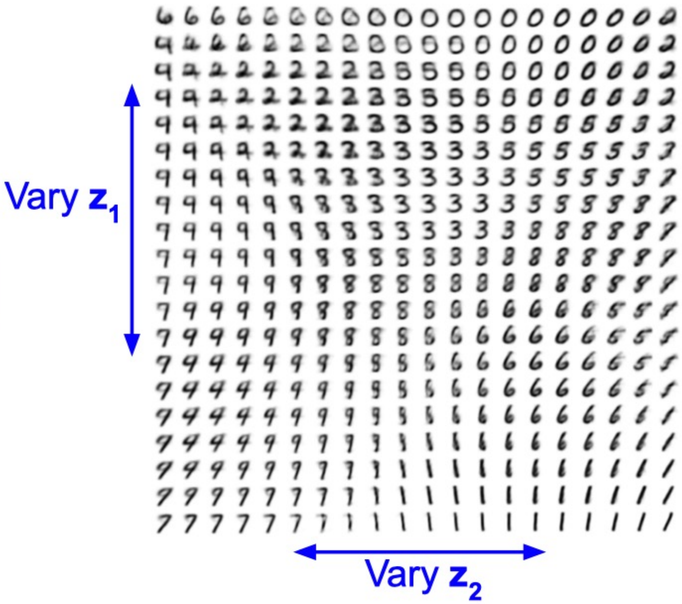
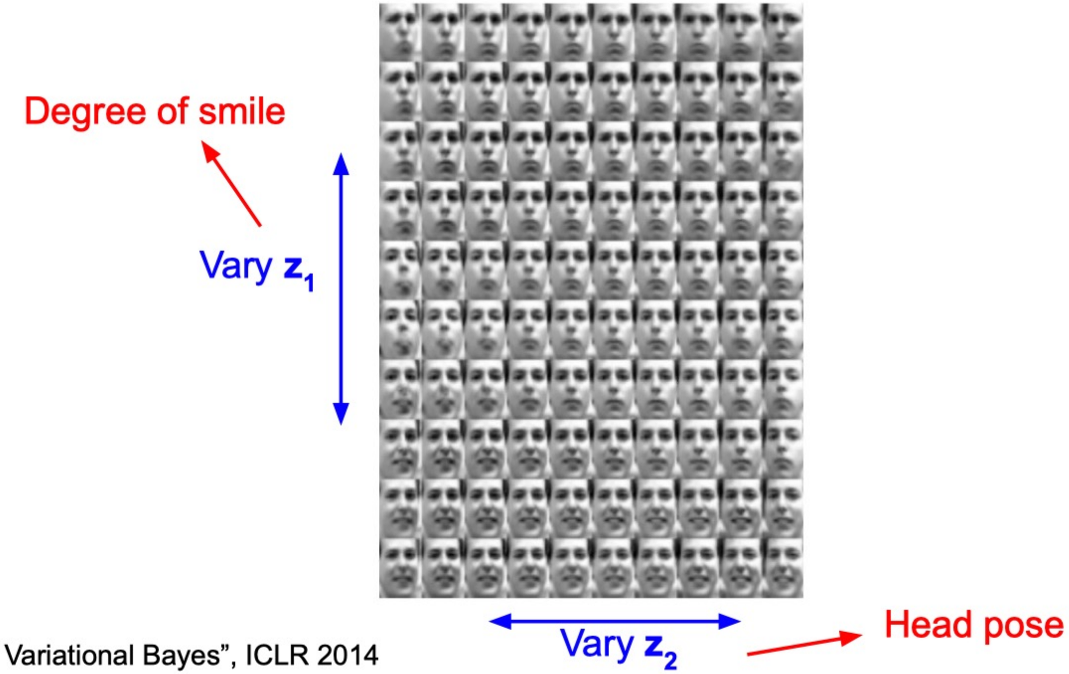
Data manifold for 2-d **z**



VAE: Generating Data

Diagonal prior on **z** => independent latent variables

Different dimensions of **z** encode interpretable factors of variation



Kingma and Welling, "Auto-Encoding Variational Bayes", ICLR 2014

VAE: Generating Data

Diagonal prior on **z** => independent latent variables

Different dimensions of **z** encode interpretable factors of variation

Also good feature representation that can be computed using $q_\phi(z|x)$!

Degree of smile

Vary $\mathbf{z}_1$

Vary $\mathbf{z}_2$

Head pose

Kingma and Welling, "Auto-Encoding Variational Bayes", ICLR 2014

VAE

Probabilistic spin to traditional autoencoders => allows generating data
Defines an intractable density => derive and optimize a (variational) lower bound

Pros:

- Principled approach to generative models
- Interpretable latent space.
- Allows inference of q(z|x), can be useful feature representation for other tasks

Cons:

- Maximizes lower bound of likelihood: okay, but not as good evaluation as PixelRNN/PixelCNN
- Samples blurrier and lower quality compared to state-of-the-art (GANs)

Active areas of research:

- More flexible approximations, e.g. richer approximate posterior instead of diagonal Gaussian, e.g., Gaussian Mixture Models (GMMs), Categorical Distributions.
- Learning disentangled representations.

Questions?

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