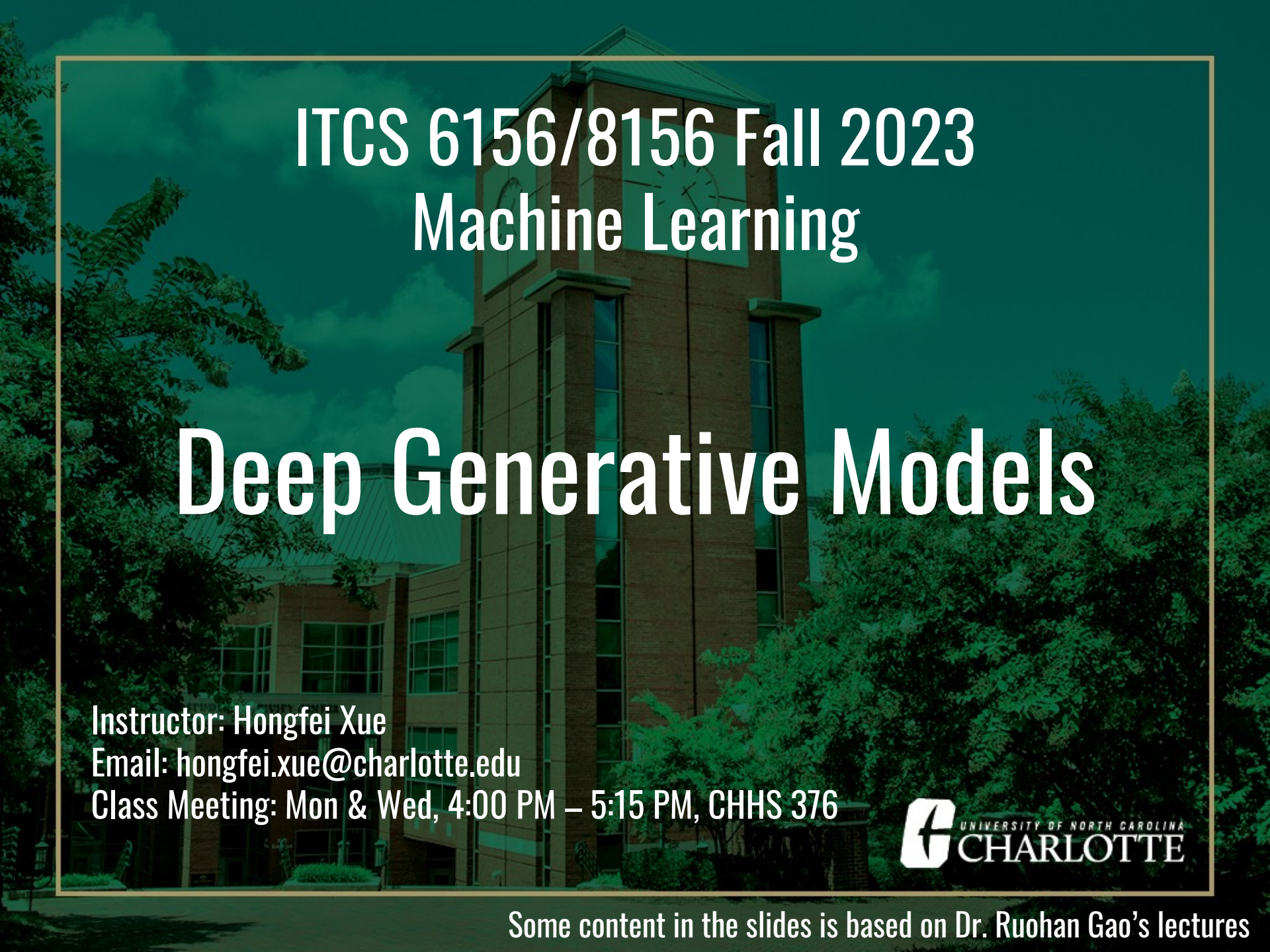

ITCS 6156/8156 Fall 2023
Machine Learning

Deep Generative Models

Instructor: Hongfei Xue
Email: hongfei.xue@charlotte.edu
Class Meeting: Mon & Wed, 4:00 PM – 5:15 PM, CHHS 376

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

Supervised Learning

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A cat sitting on a suitcase on the floor

Image captioning

Supervised vs Unsupervised Learning

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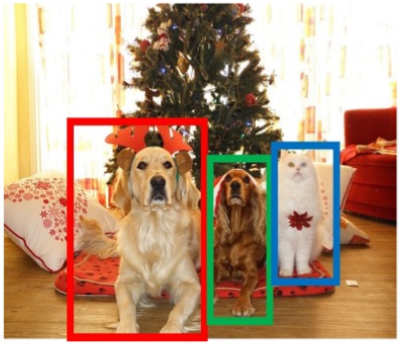

DOG, **DOG**, **CAT**

Object Detection

Supervised vs Unsupervised Learning

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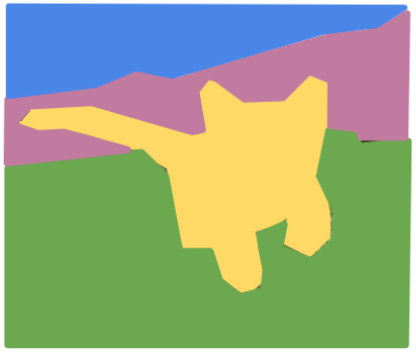


GRASS, CAT,
TREE, SKY

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.

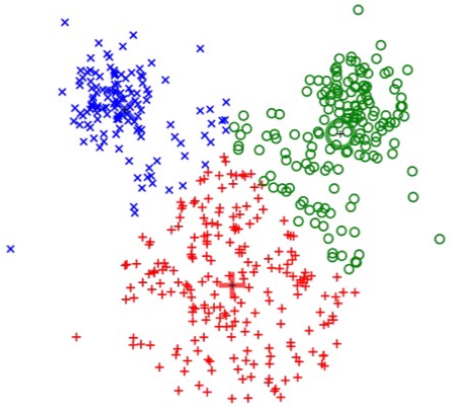
Supervised vs Unsupervised Learning

Unsupervised Learning

Data: x
Just data, no labels!

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

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



K-means clustering

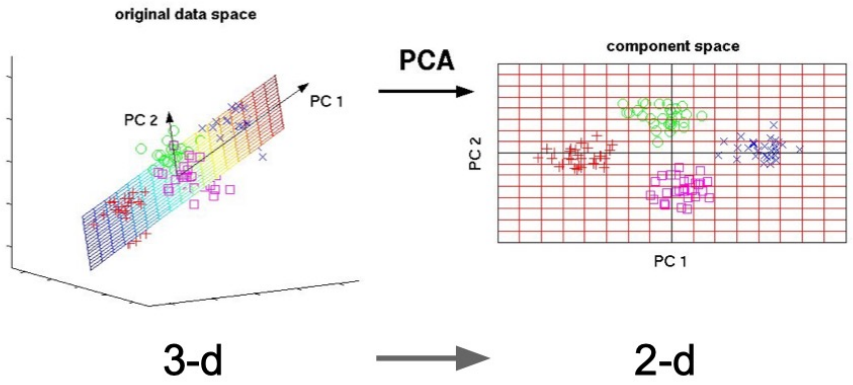
Supervised vs Unsupervised Learning

Unsupervised Learning

Data: x
Just data, no labels!

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

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



Principal Component Analysis
(Dimensionality reduction)

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, density estimation, etc.

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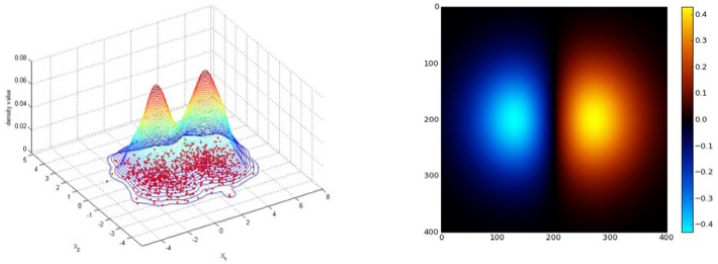
1-d density estimation



2-d density estimation

Modeling p(x)

2-d density images left and right are CC0 public domain

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.

Unsupervised Learning

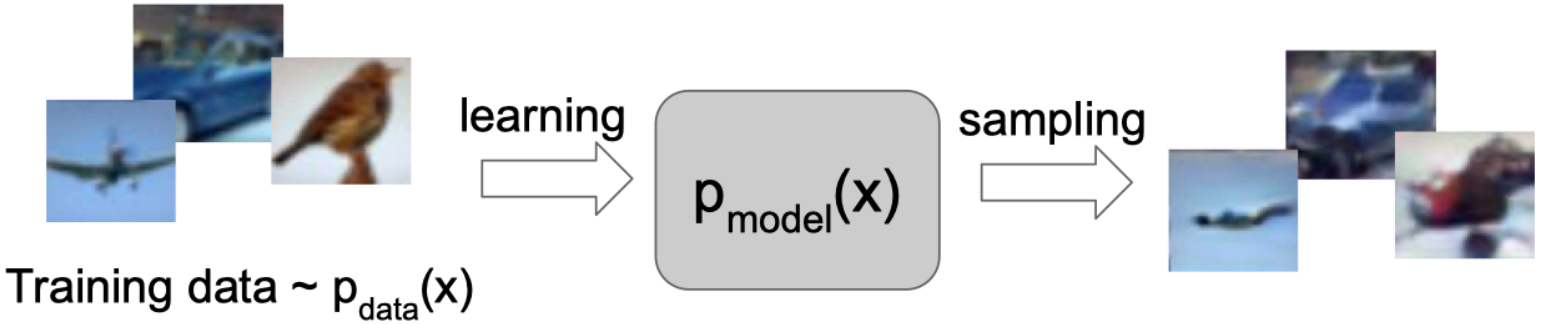
Data: x
Just data, no labels!

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

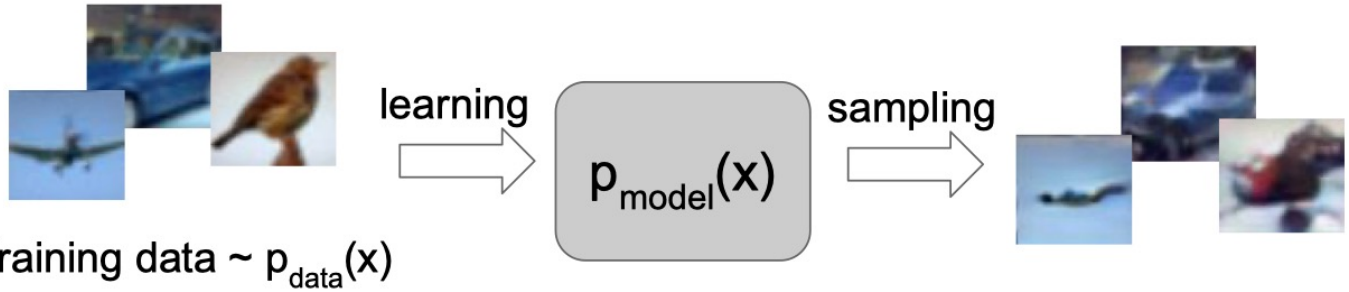


Objectives:

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

Generative Modeling

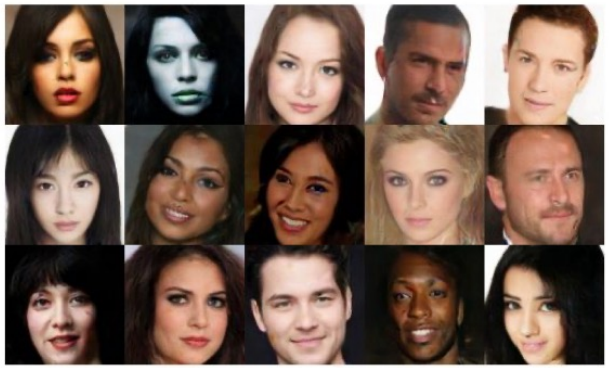
Given training data, generate new samples from same distribution



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)**

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)

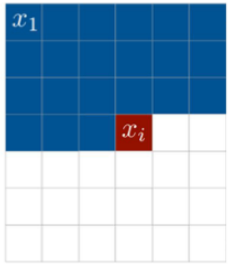
Explicit density model

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

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

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)

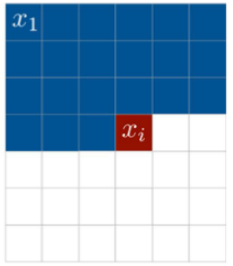
Explicit density model

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

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

Likelihood of image x

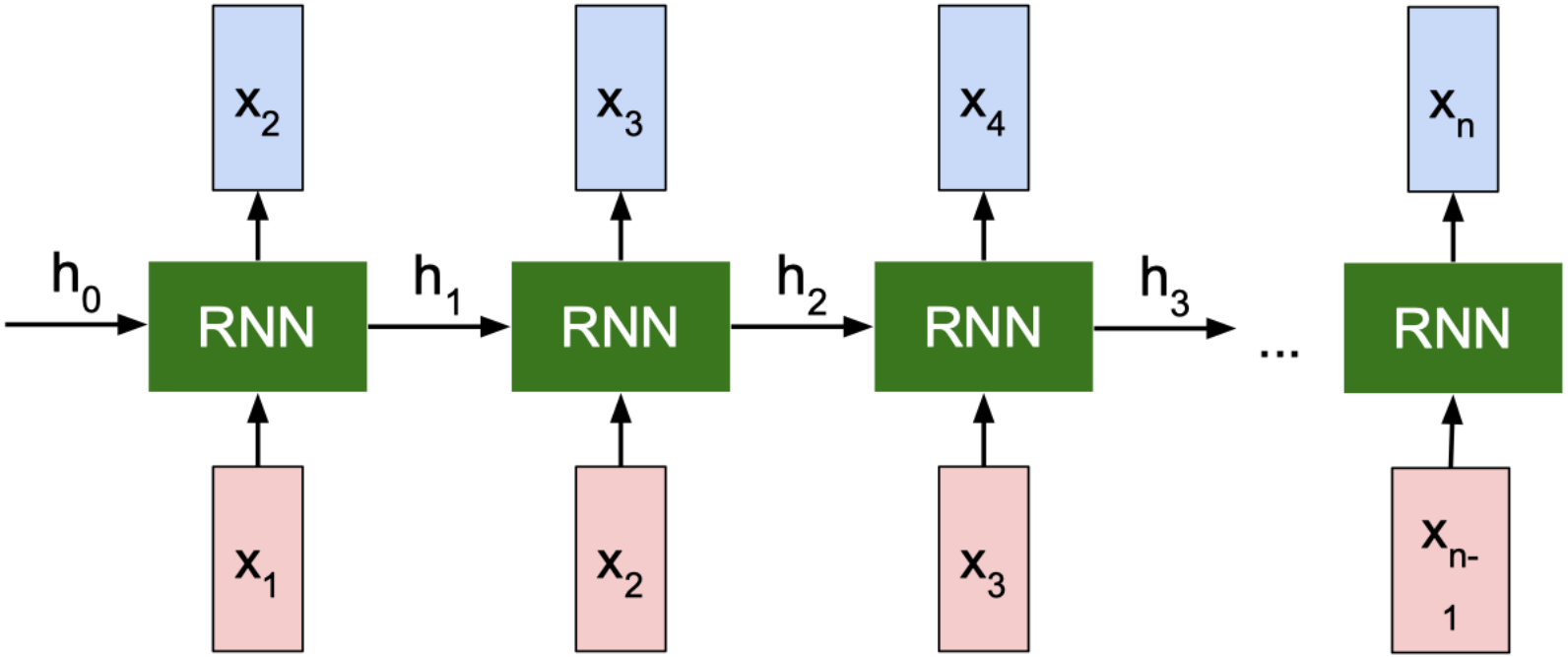
Probability of i'th pixel value given all previous pixels



Then maximize likelihood of training data

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

RNN

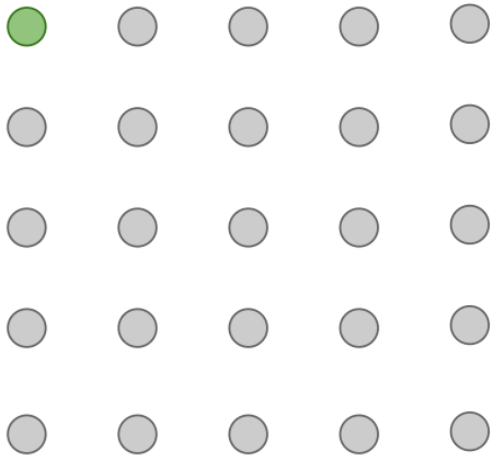


$$p(x_i|x_1, \ldots, x_{i-1})$$

PixelRNN

Generate image pixels starting from corner

Dependency on previous pixels modeled using an RNN (LSTM)



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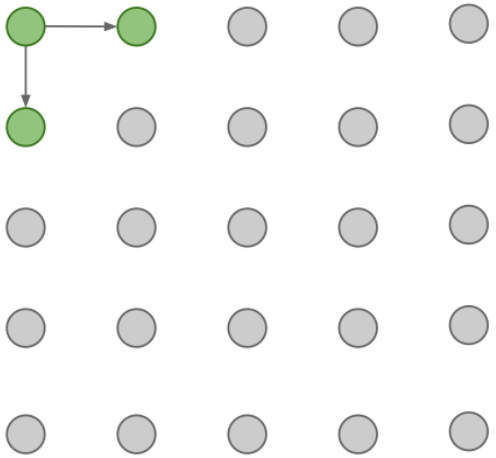

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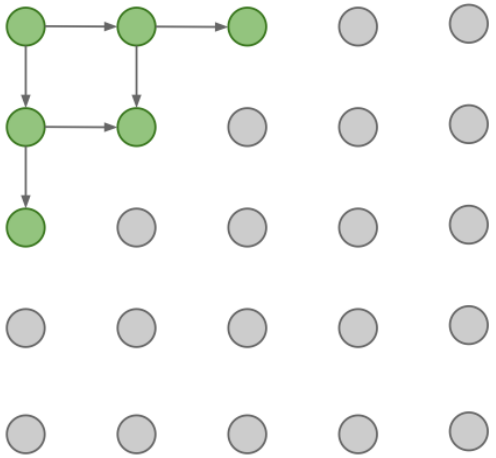

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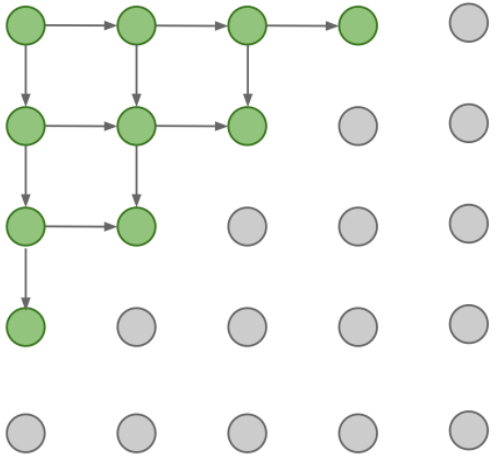
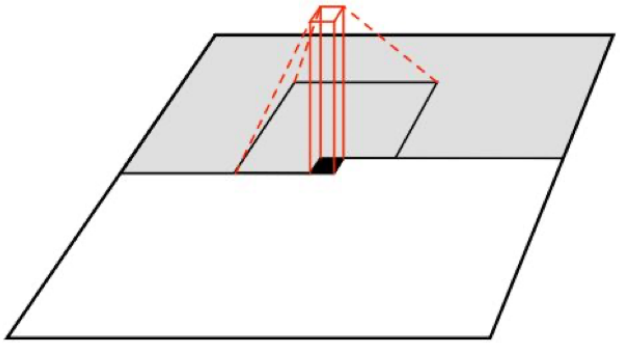


Drawback: sequential generation is slow in both training and inference!

PixelCNN

Still generate image pixels starting from corner

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



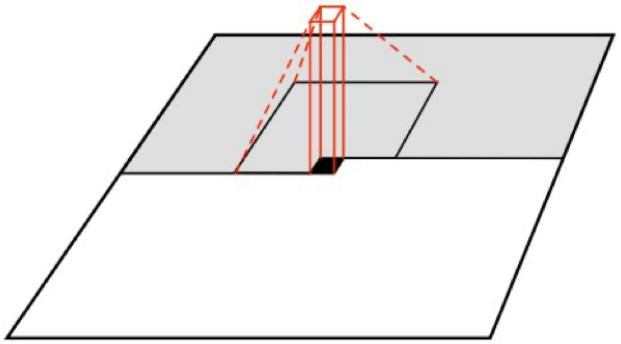
PixelCNN

Still generate image pixels starting from corner

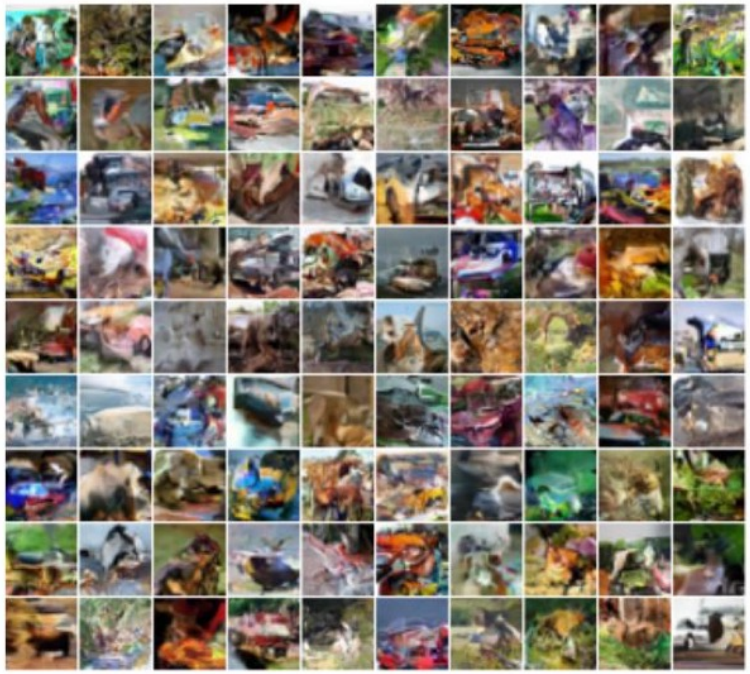
Dependency on previous pixels now modeled using a CNN over context region (masked convolution)

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

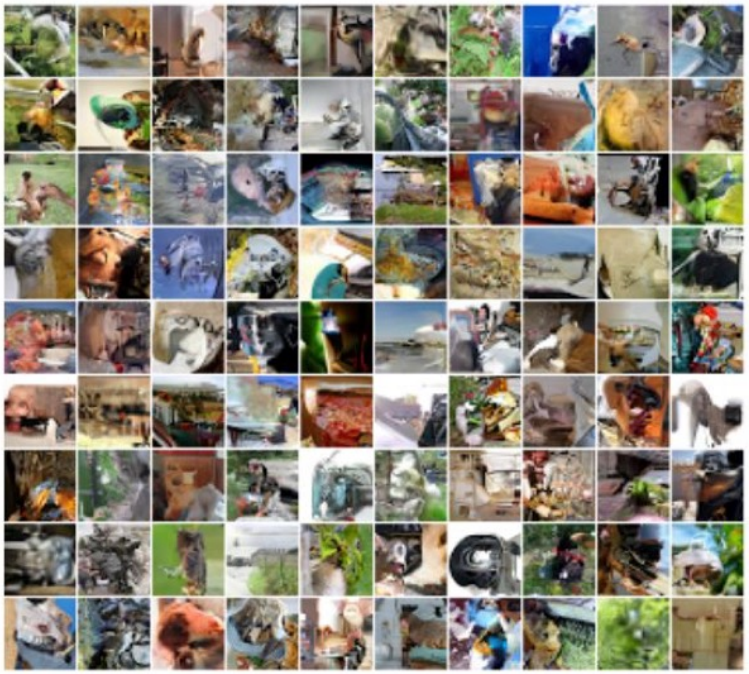
Generation is still slow:
For a 32x32 image, we need to do forward passes of the network 1024 times for a single image



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**:

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

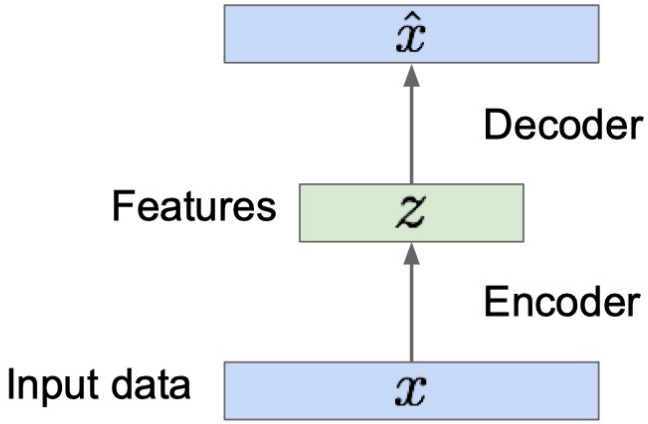
No dependencies among pixels, can generate all pixels at the same time!

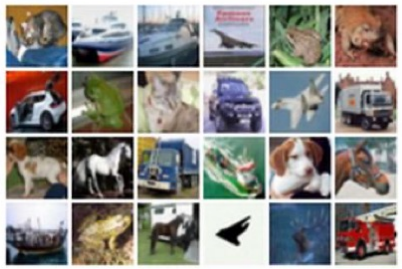
Cannot optimize directly, derive and optimize lower bound on likelihood instead

Why latent z?

Recap: Autoencoders

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



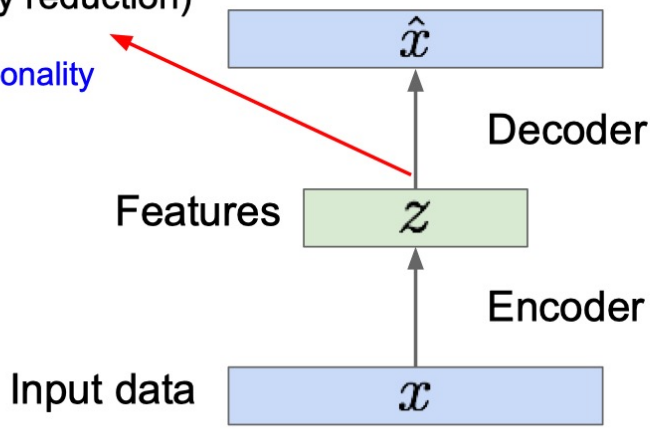


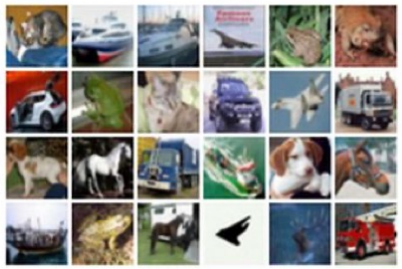
Recap: Autoencoders

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

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

Q: Why dimensionality reduction?





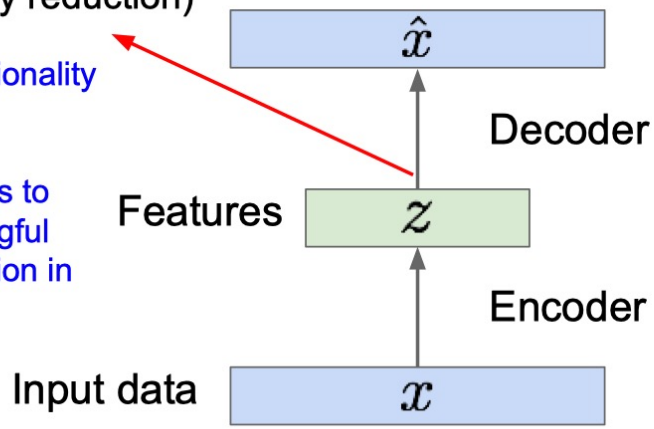
Recap: Autoencoders

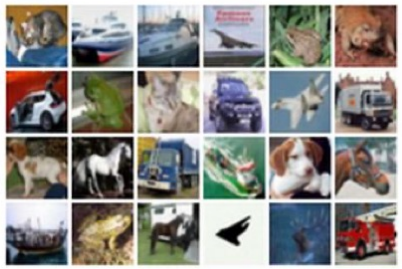
Unsupervised approach for learning a lower-dimensional feature representation from unlabeled training data

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

Q: Why dimensionality reduction?

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

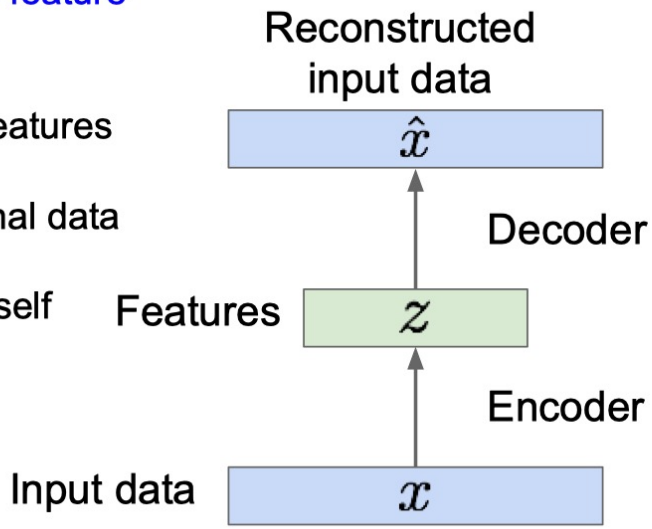


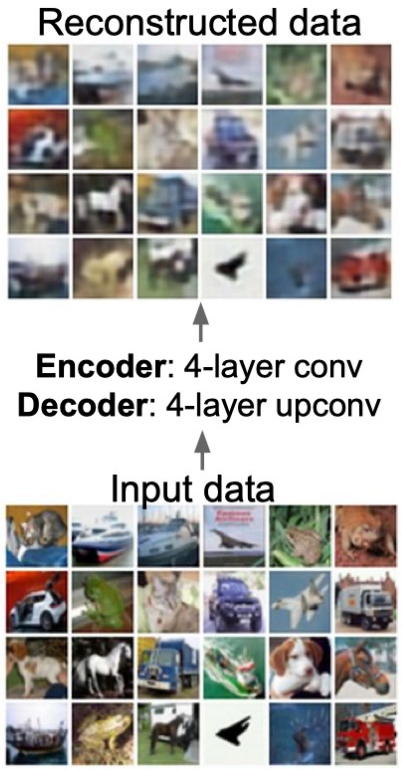


Recap: Autoencoders

How to learn this feature representation?

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

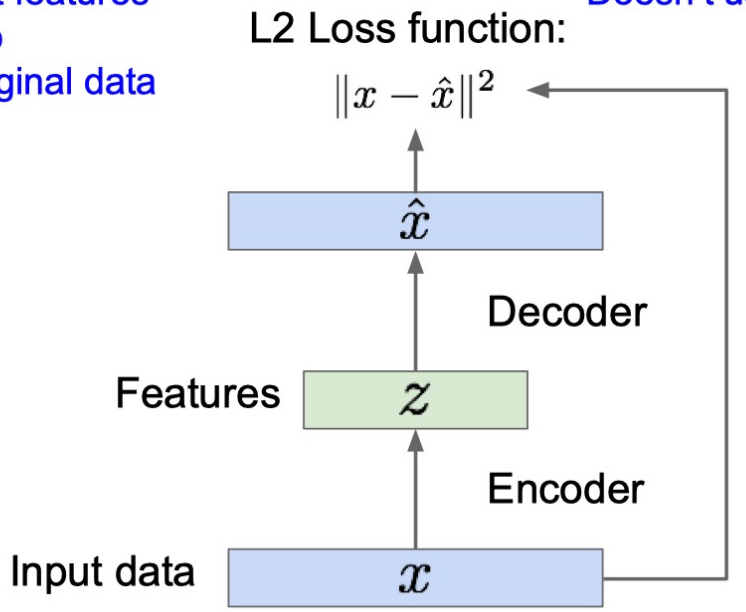


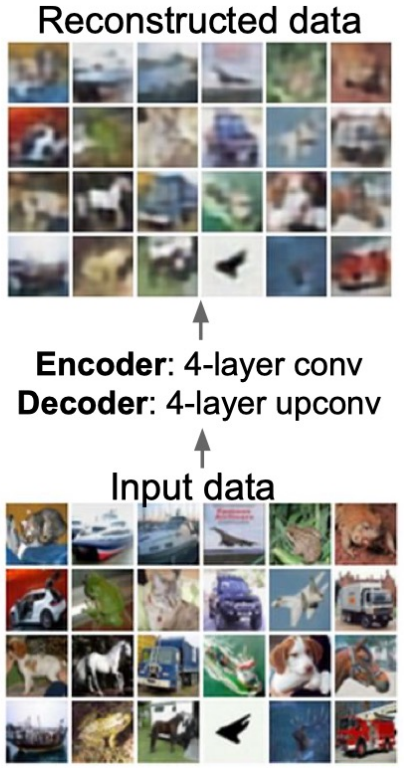


Recap: Autoencoders

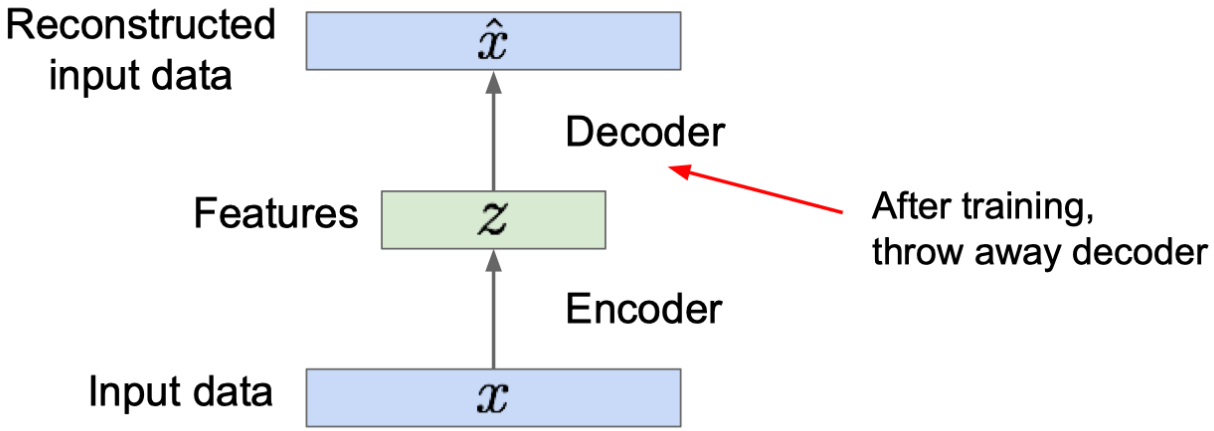
Train such that features can be used to reconstruct original data

Doesn't use labels!



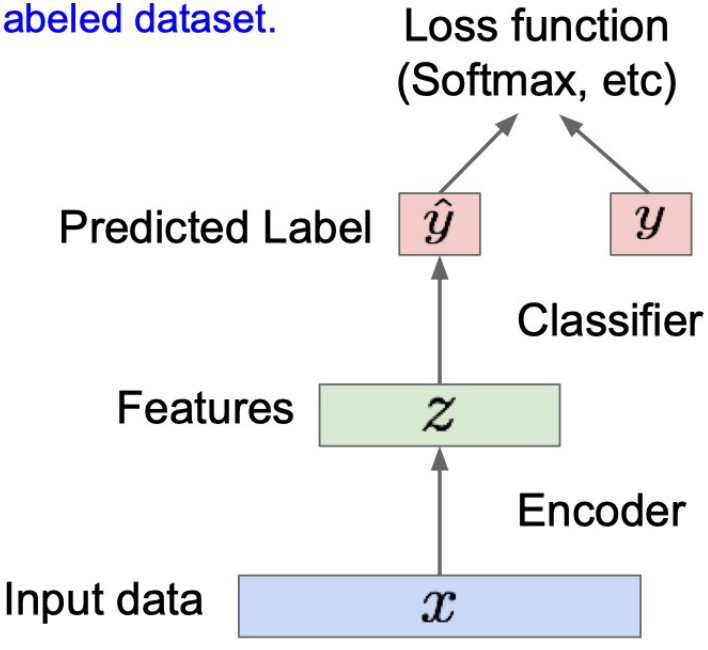


Recap: Autoencoders



Recap: Autoencoders

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



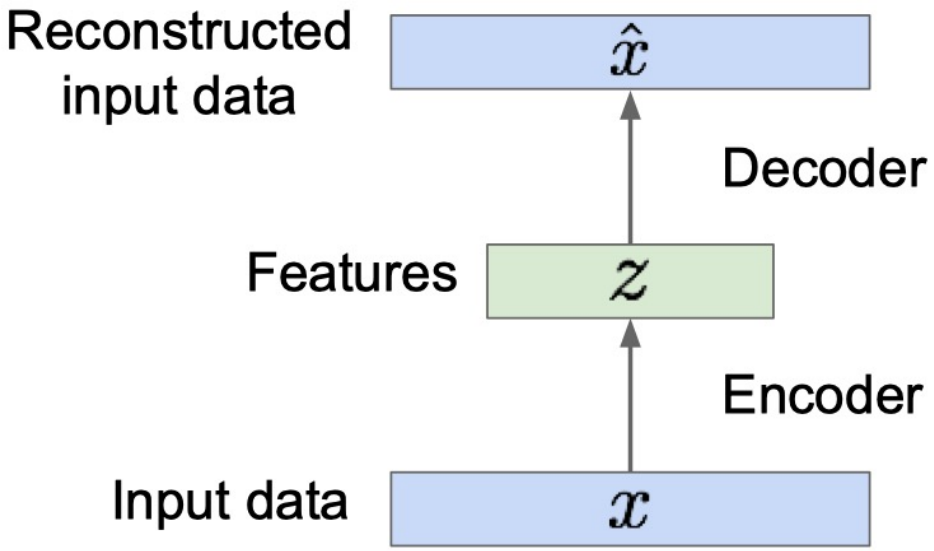
Encoder can be used to initialize a **supervised** model

Fine-tune encoder jointly with classifier

Train for final task (sometimes with small data)

bird plane
dog deer truck

Recap: Autoencoders



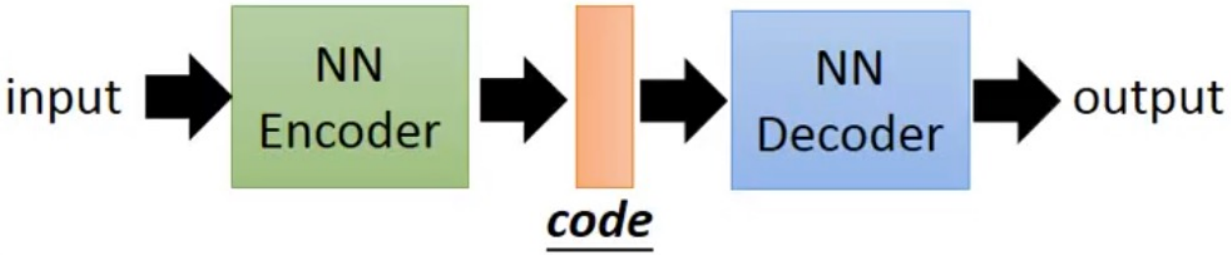
Autoencoders can reconstruct data, and can learn features to initialize a supervised model

Features capture factors of variation in training data.

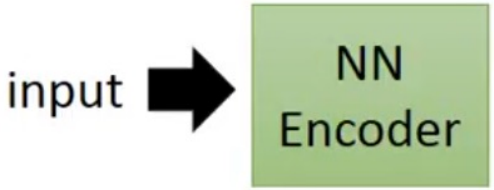
But we can't generate new images from an autoencoder because we don't know the space of z.

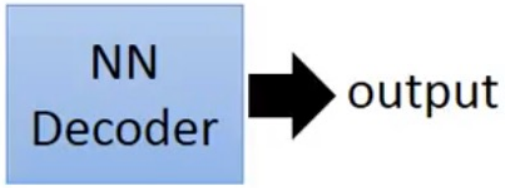
How do we make autoencoder a **generative model**?

Variational Autoencoders

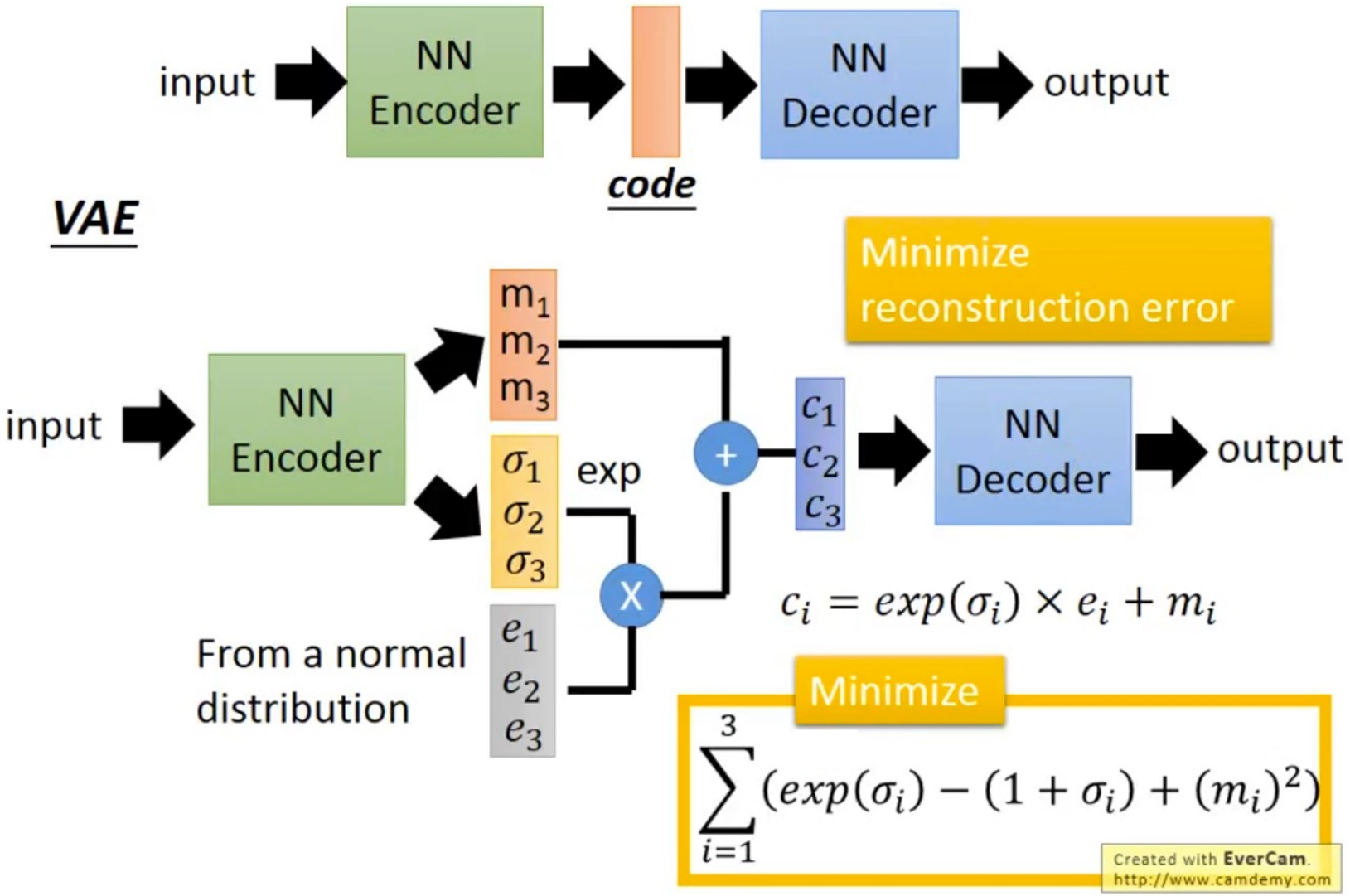


VAE





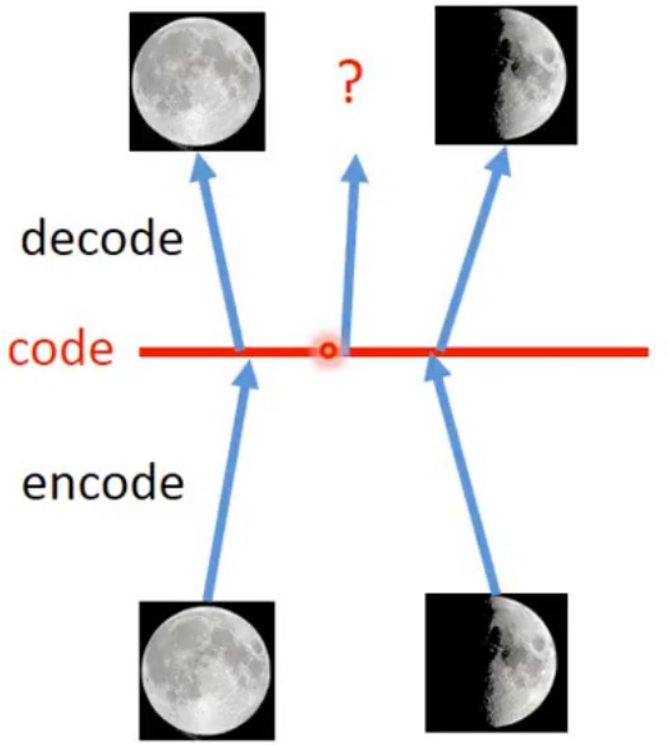
Variational Autoencoders



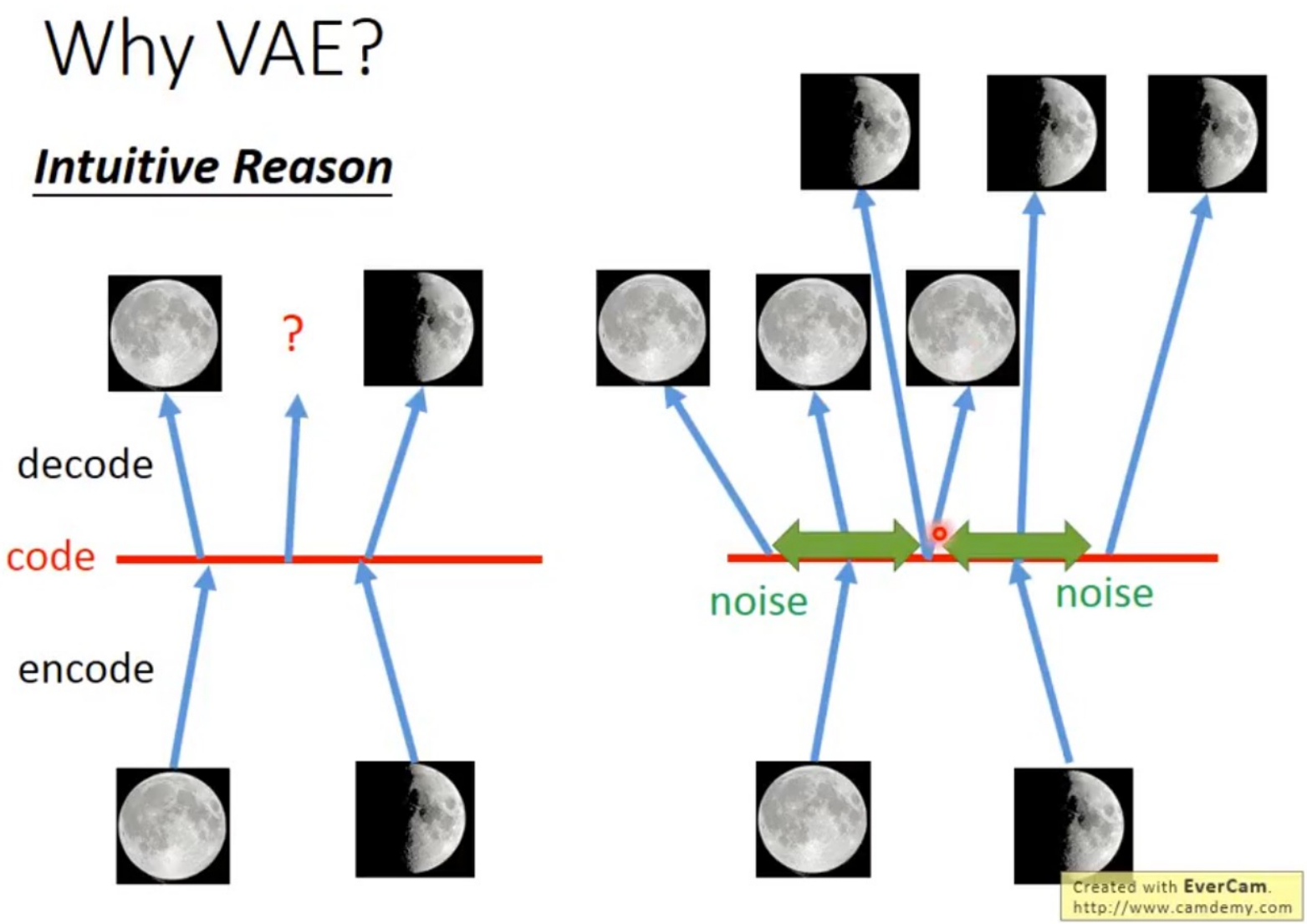
Variational Autoencoders

Why VAE?

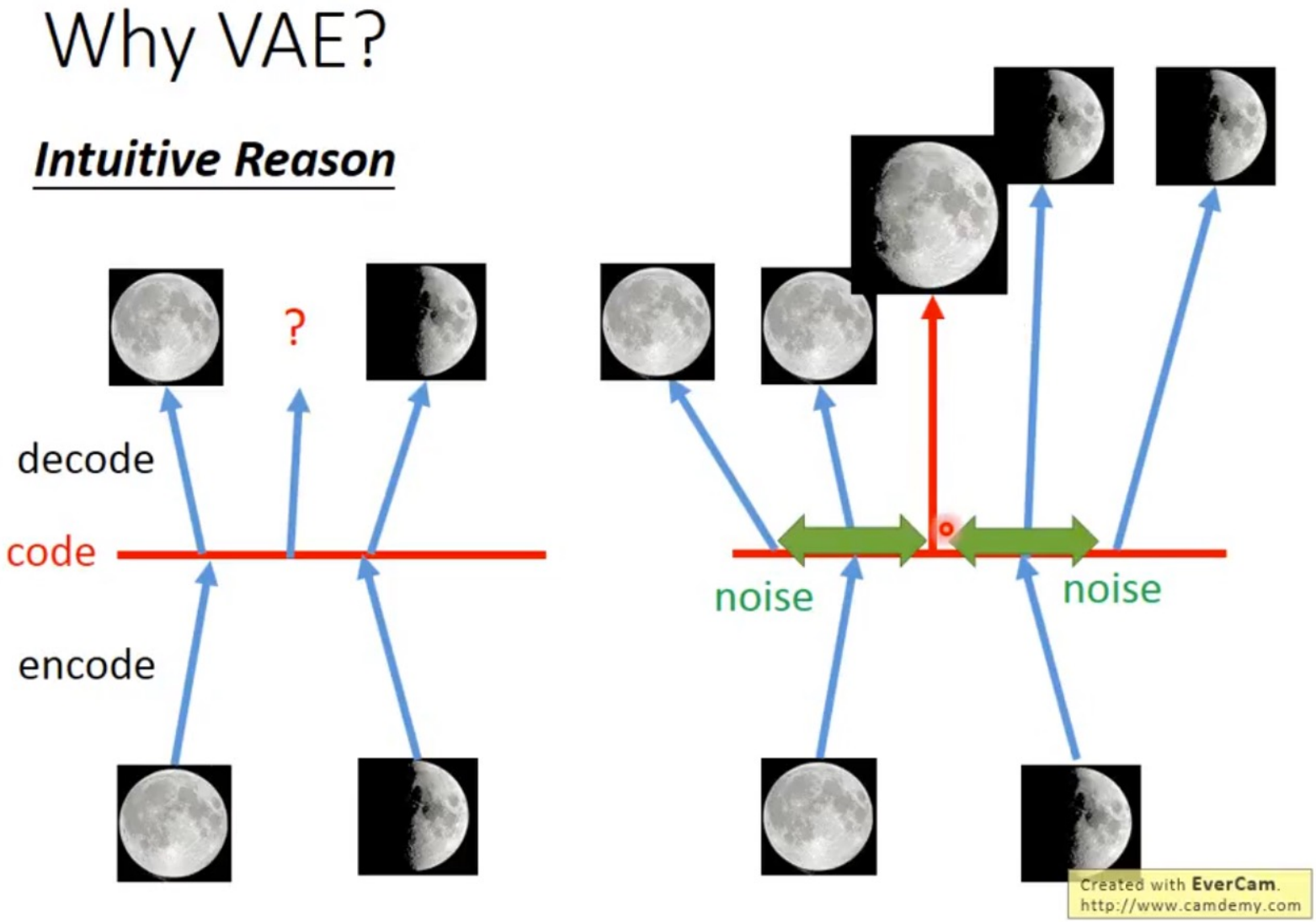
Intuitive Reason



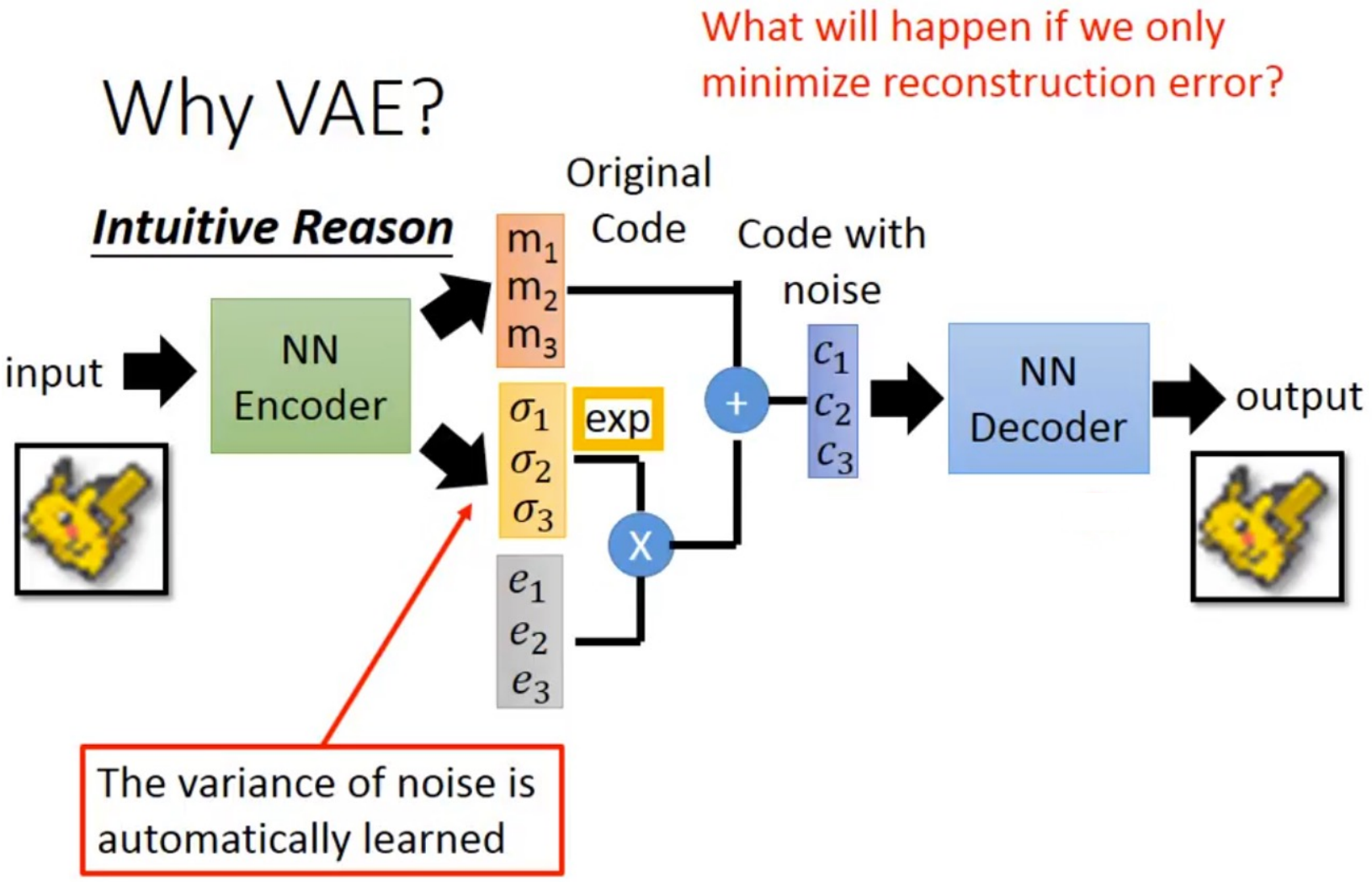
Variational Autoencoders



Variational Autoencoders



Variational Autoencoders: Simple Explanation



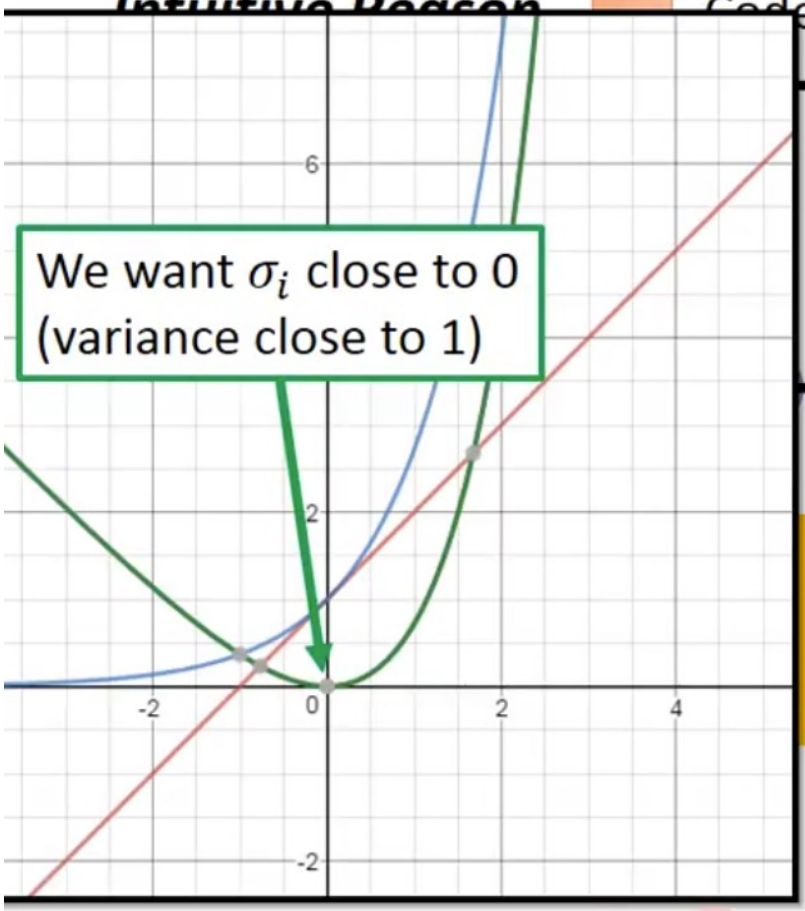
Variational Autoencoders: Simple Explanation

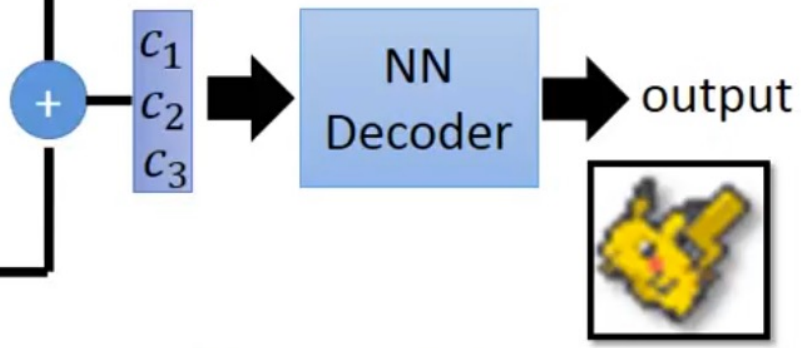
Why VAE?

What will happen if we only minimize reconstruction error?

Original

Code with noisy





Minimize

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

L2 regularization

VAE: Probabilistic Perspective

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

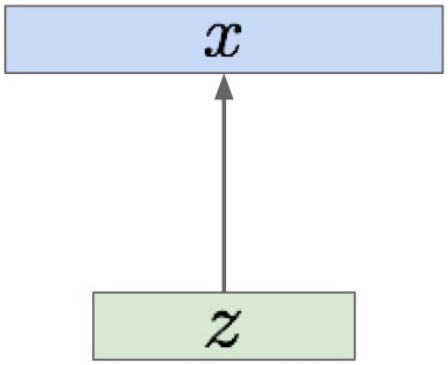
Assume training data $\{x^{(i)}\}_{i=1}^{N}$ is generated from the distribution of unobserved (latent) representation **z**

Sample from true conditional

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

Sample from true prior

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



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

VAE: A Probabilistic Perspective

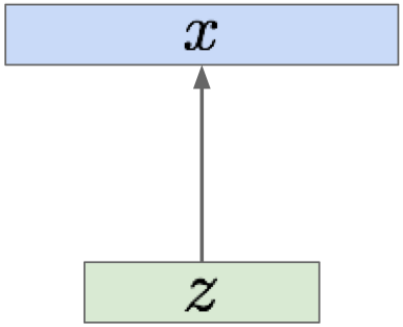
We want to estimate the true parameters θ^* of this generative model given training data x.

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

Sample from true conditional

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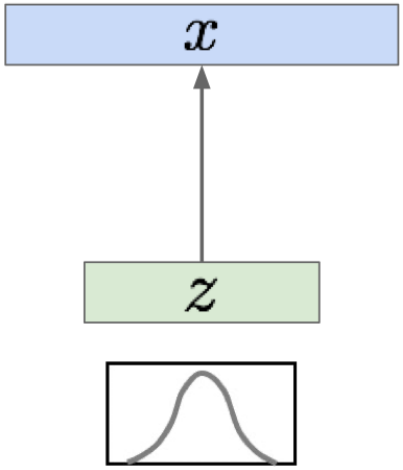

We want to estimate the true parameters θ^* of this generative model given training data x.

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.

VAE: A Probabilistic Perspective

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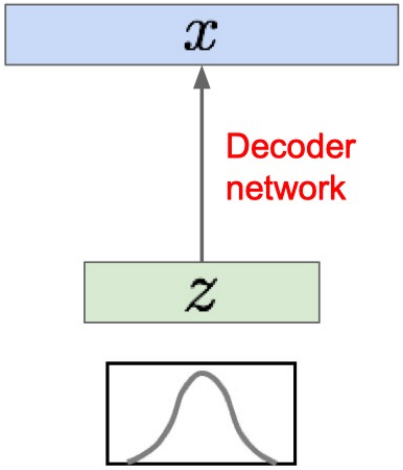

We want to estimate the true parameters θ^* of this generative model given training data x.

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?

Sample from true conditional

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

Sample from true prior

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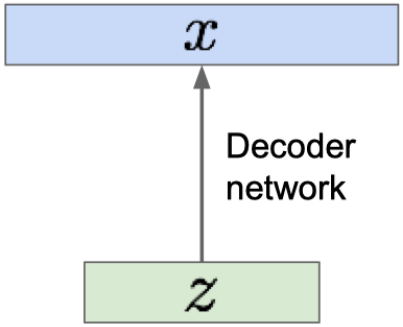

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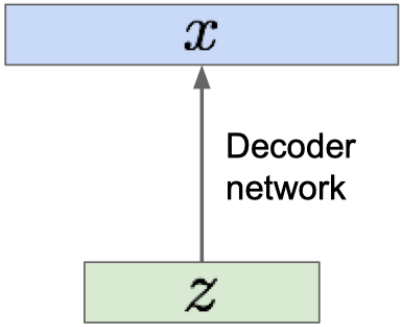


We want to estimate the true parameters θ^* of this generative model given training data x.

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

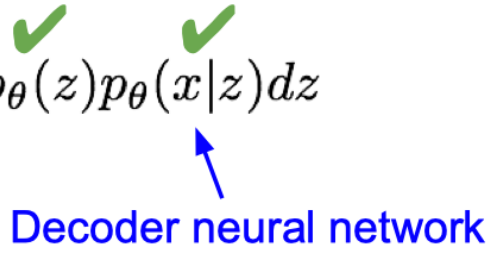
Data likelihood: $p_\theta(x) = \int p_\theta(z) p_\theta(x|z) dz$

✔

Simple Gaussian prior

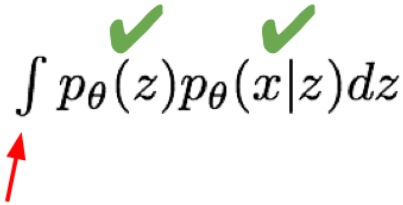
VAE: A Probabilistic Perspective

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



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

VAE: A Probabilistic Perspective

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

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Decoder: reconstruct the input data

Encoder: make approximate posterior distribution close to prior

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

VAE: A Probabilistic Perspective

Variational Autoencoders

Putting it all together: maximizing the likelihood lower bound

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

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

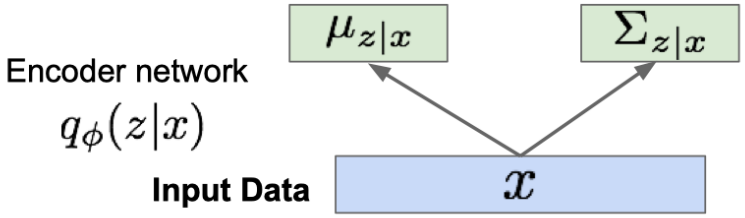
Input Data x

VAE: A Probabilistic Perspective

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

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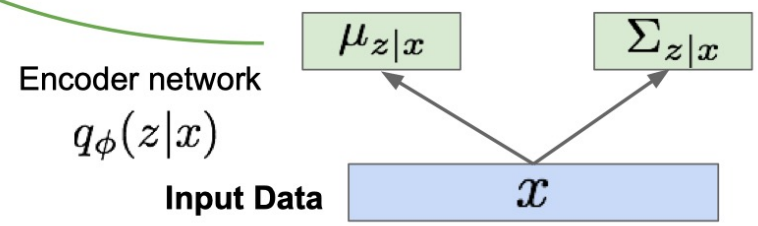
$$D_{KL}(\mathcal{N}(\mu_{z|x}, \Sigma_{z|x})||\mathcal{N}(0, I))$$

Have analytical solution

Make approximate posterior distribution close to prior



VAE: A Probabilistic Perspective

Variational Autoencoders

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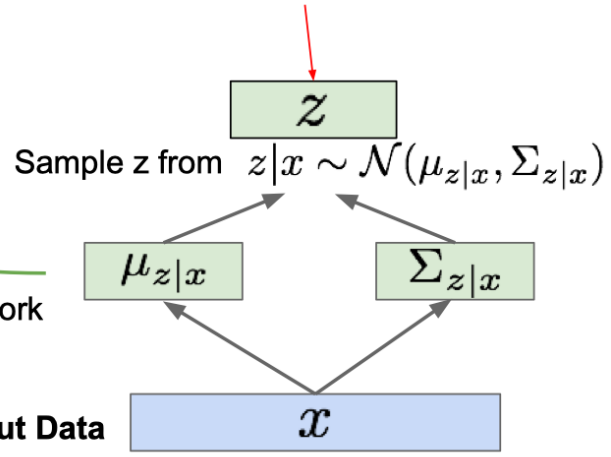
Make approximate posterior distribution close to prior

Not part of the computation graph!



VAE: A Probabilistic Perspective

Variational Autoencoders

Putting it all together: maximizing the likelihood lower bound

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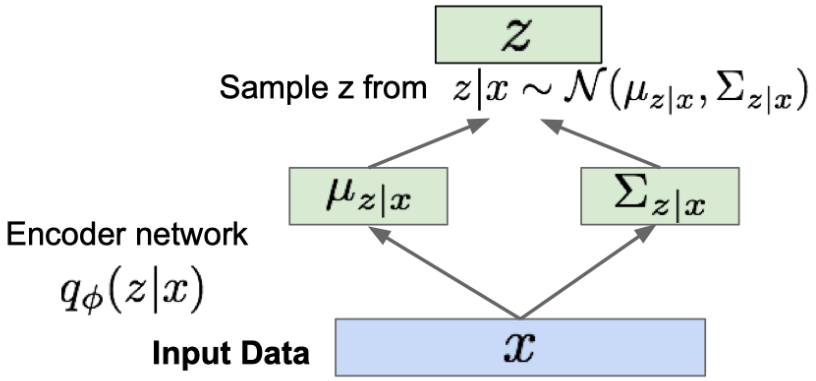
Reparameterization trick to make sampling differentiable:

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

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



VAE: A Probabilistic Perspective

Variational Autoencoders

Putting it all together: maximizing the likelihood lower bound

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

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

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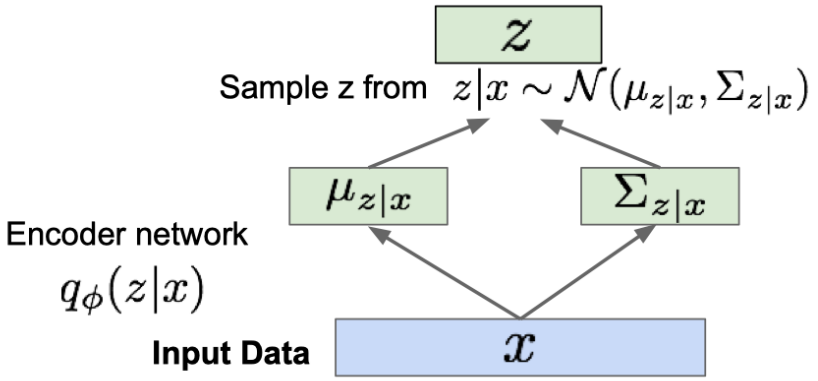
Input to the graph

Part of computation graph



VAE: A Probabilistic Perspective

Variational Autoencoders

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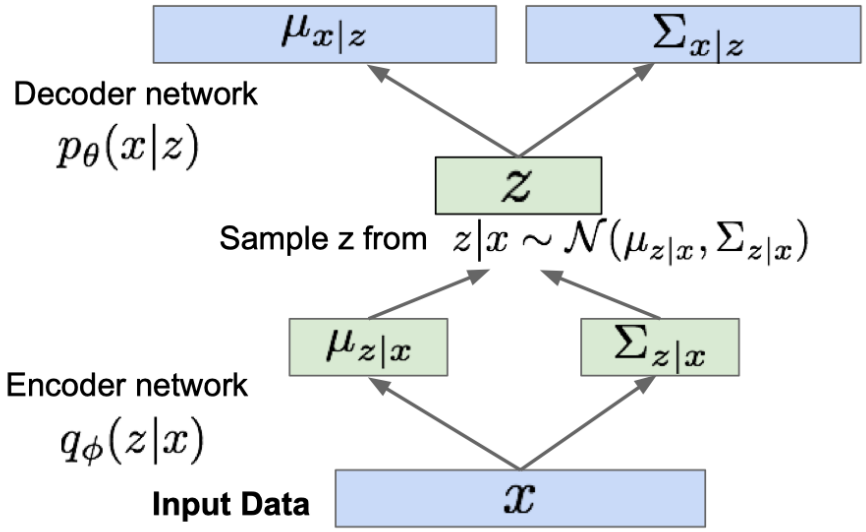


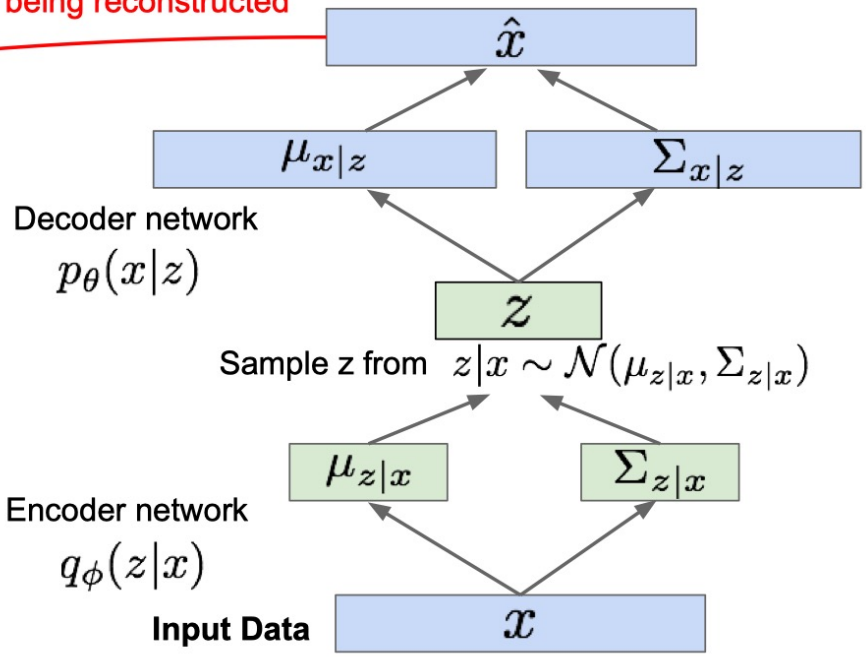
VAE: A Probabilistic Perspective

Variational Autoencoders

Putting it all together: maximizing the likelihood lower bound

Maximize likelihood of original input being reconstructed

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



VAE: A Probabilistic Perspective

Variational Autoencoders

Putting it all together: maximizing the likelihood lower bound

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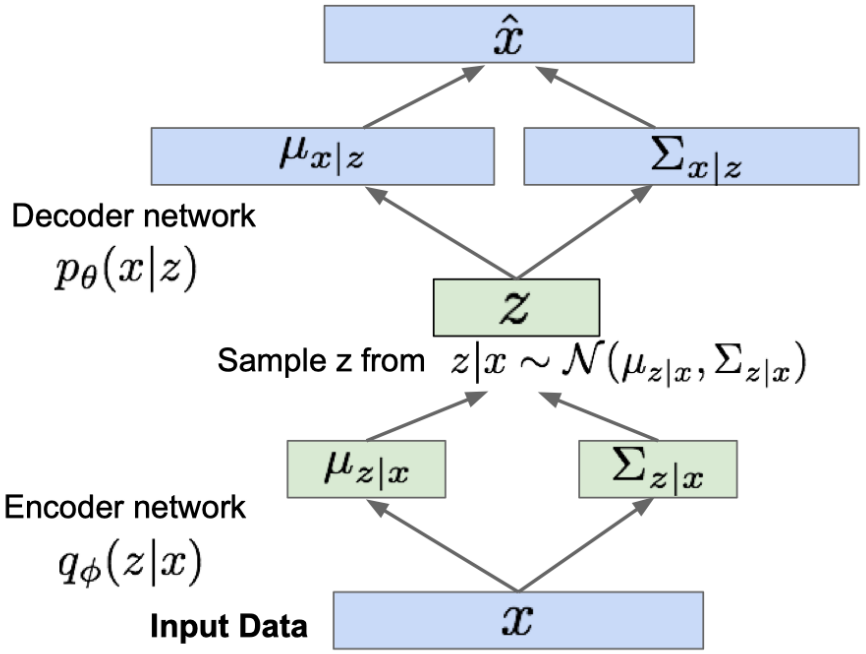
For every minibatch of input data: compute this forward pass, and then backprop!



VAE: Generating Data

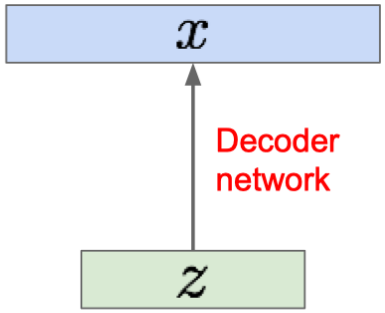
Our assumption about data generation process

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

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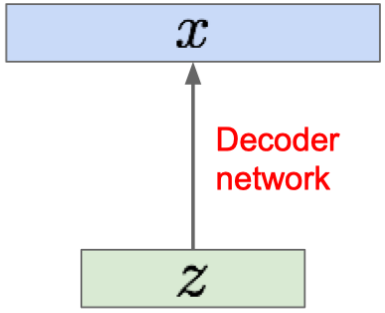
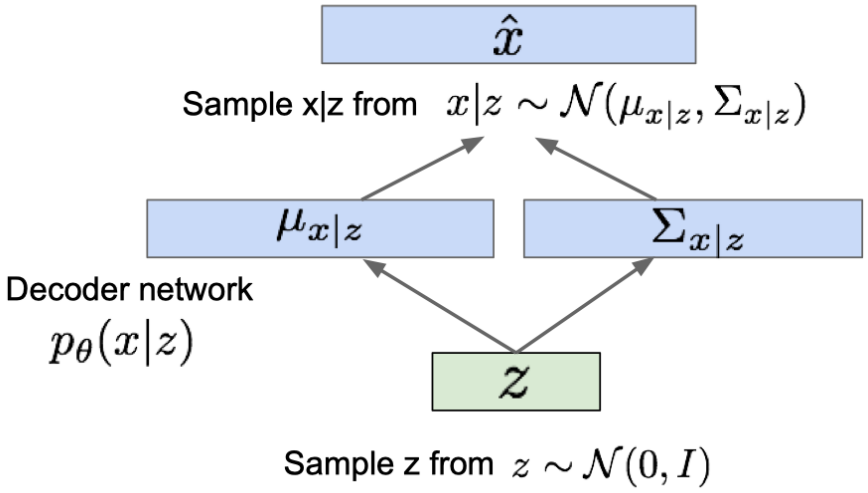


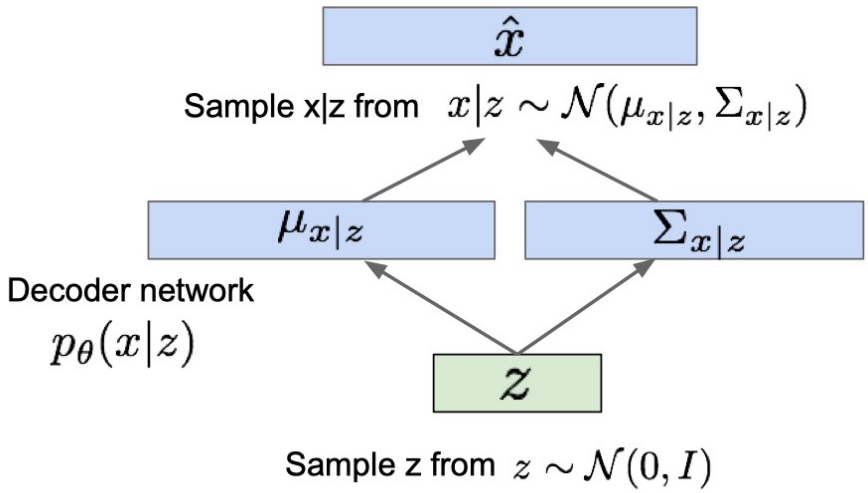
Now given a trained VAE: use decoder network & sample z from prior!

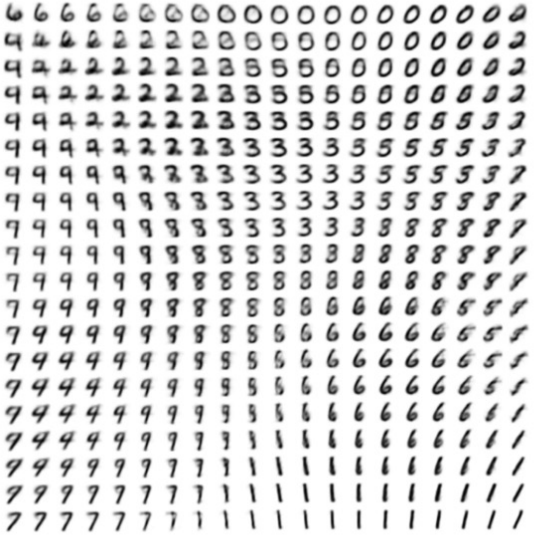


Kingma and Welling, "Auto-Encoding Variational Bayes", ICLR 2014

VAE: Generating Data

Use decoder network. Now sample z from prior!

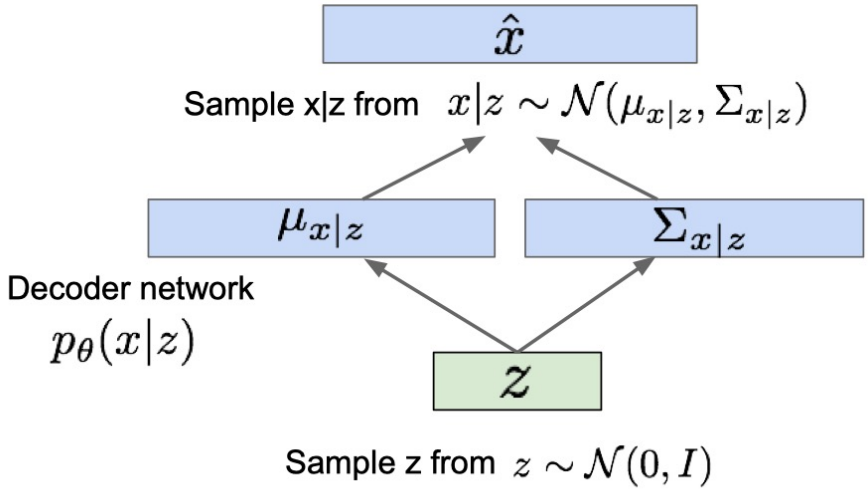




Kingma and Welling, "Auto-Encoding Variational Bayes", ICLR 2014

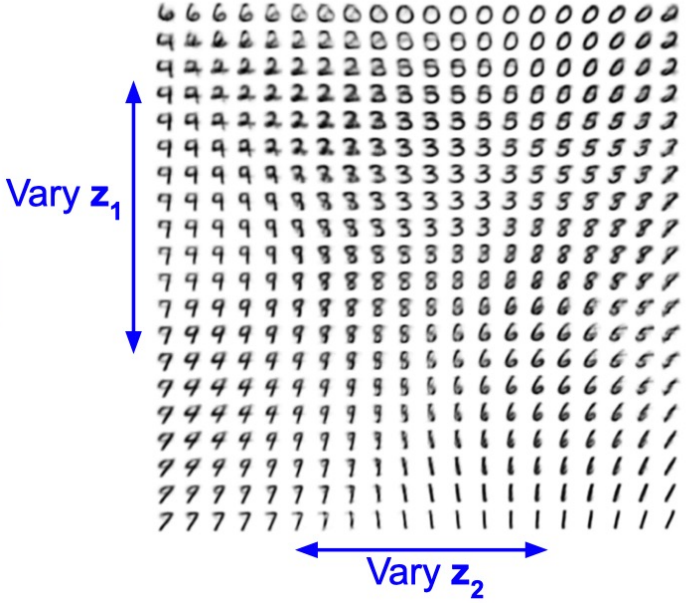
VAE: Generating Data

Use decoder network. Now sample z from prior!



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

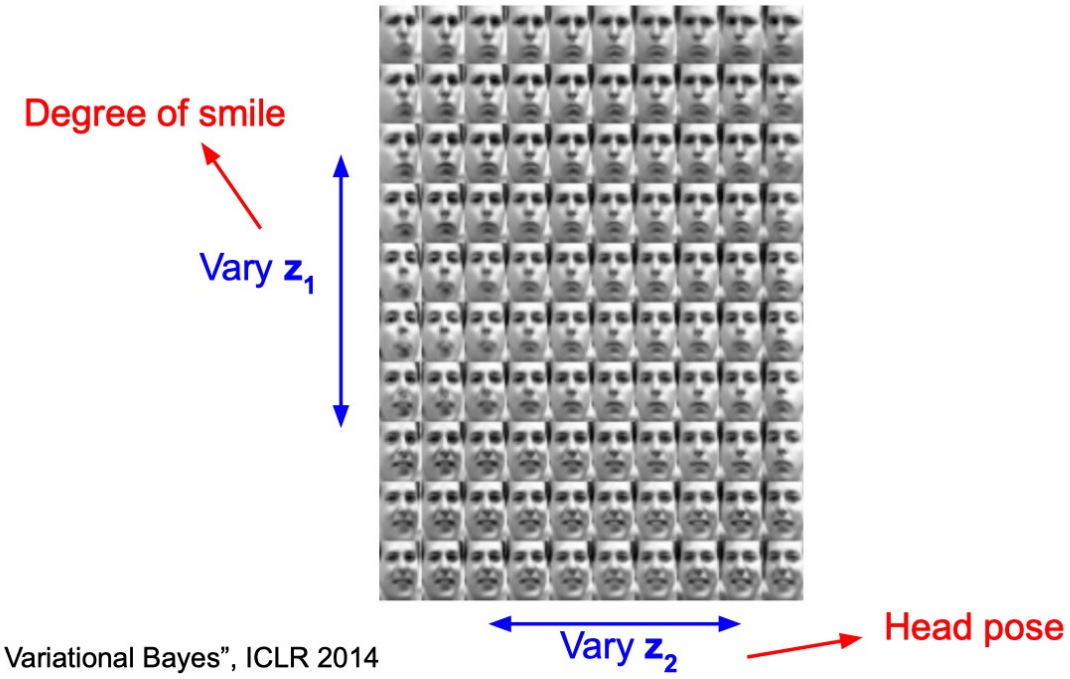
Data manifold for 2-d **z**



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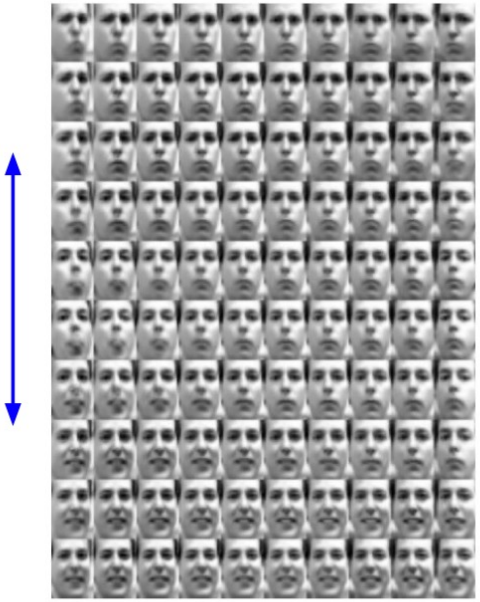
Also good feature representation that can be computed using $q_\phi(z|x)$!



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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