Generative Models

Slides from Justin Johnson

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.

Classification

Cat

Slide from Justin Johnson

Supervised vs Unsupervised Learning

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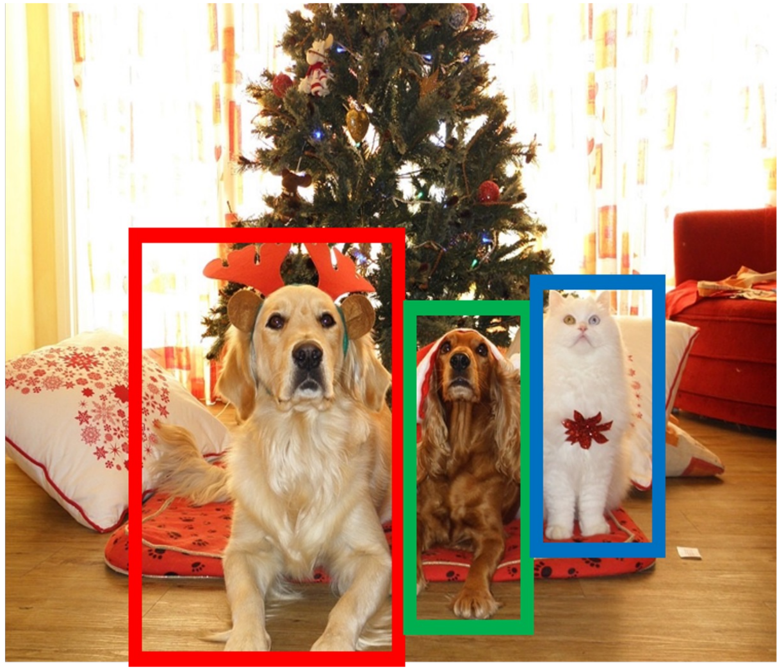
Object Detection



DOG, DOG, CAT

Slide from Justin Johnson

Supervised vs Unsupervised Learning

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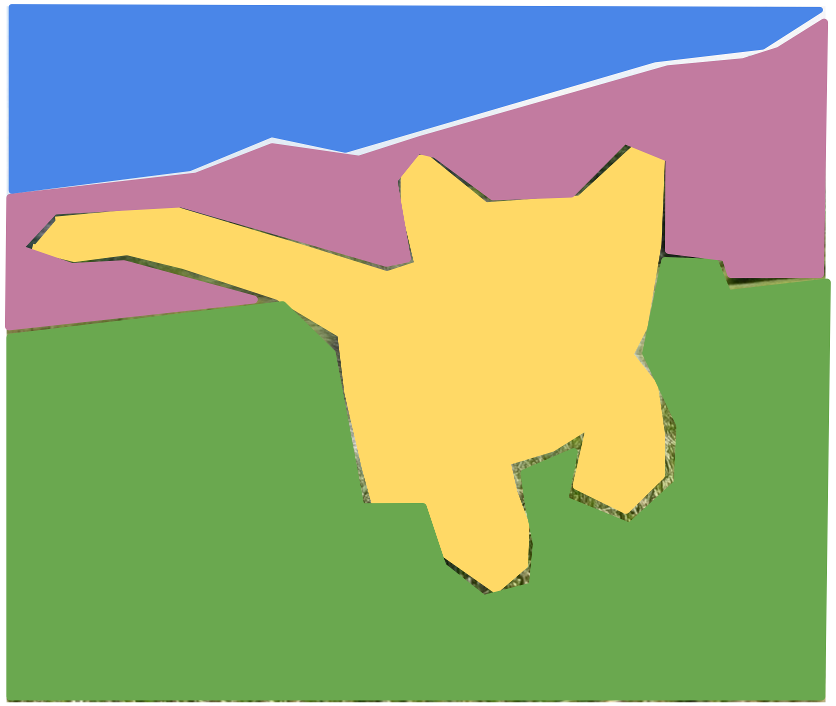
Semantic Segmentation



GRASS, CAT, TREE, SKY

Slide from Justin Johnson

Supervised vs Unsupervised Learning

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

Image captioning

A cat sitting on a suitcase on the floor

Slide from Justin Johnson

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

Unsupervised Learning

Data: x

Just data, no labels!

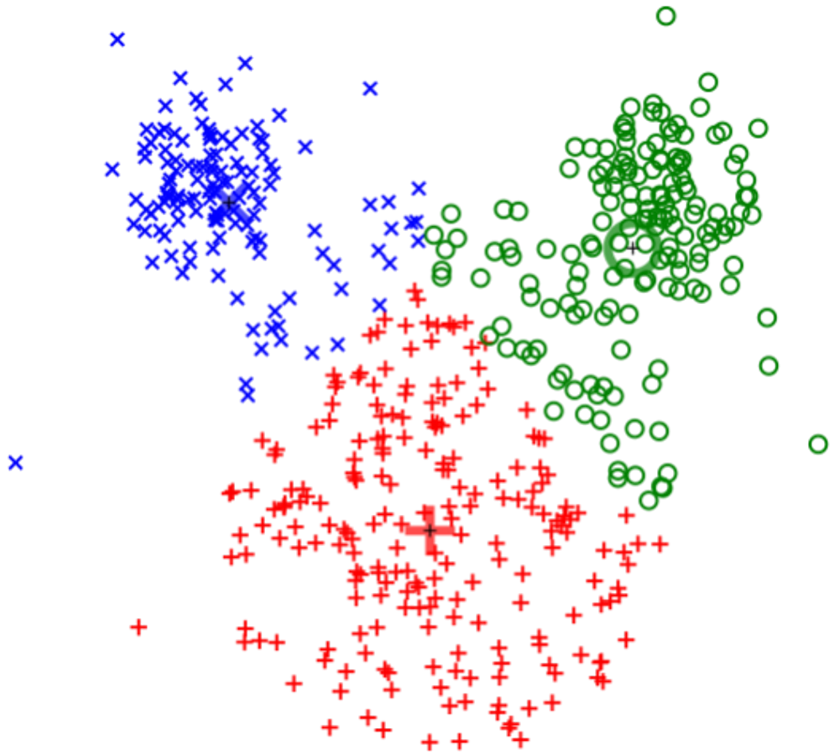
Goal: Learn some underlying hidden *structure* of the data

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

Slide from Justin Johnson

Supervised vs Unsupervised Learning

Clustering
(e.g. K-Means)



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

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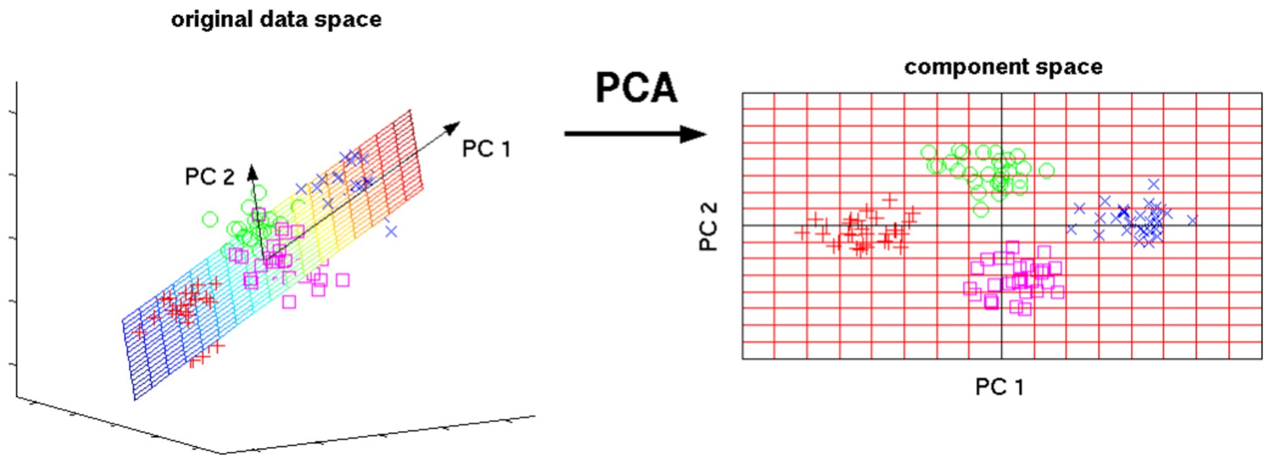
Supervised vs Unsupervised Learning

Dimensionality Reduction
(e.g. Principal Components Analysis)



3D → 2D

This image from Matthias Scholz is CC0 public domain

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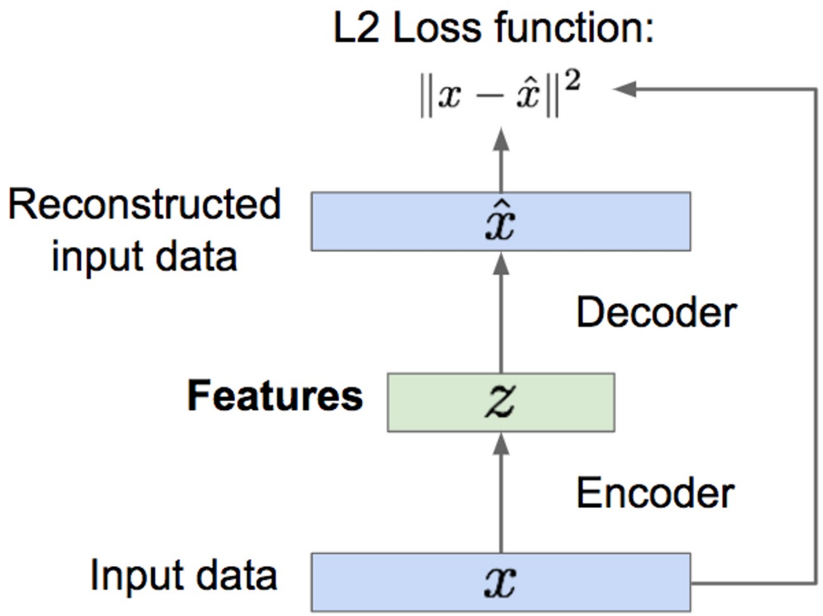
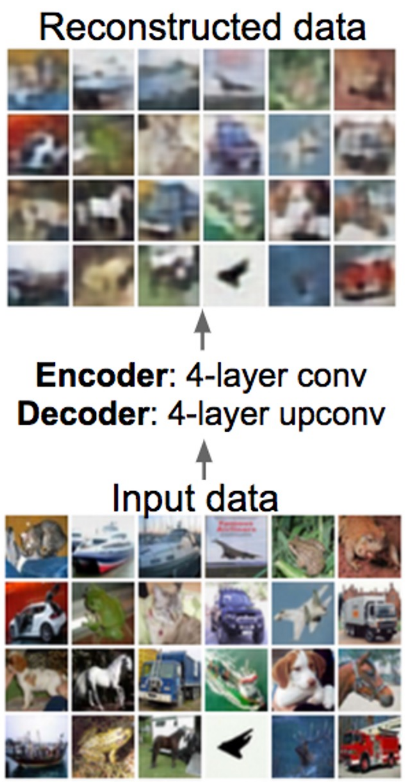
Supervised vs Unsupervised Learning

Feature Learning
(e.g. autoencoders)





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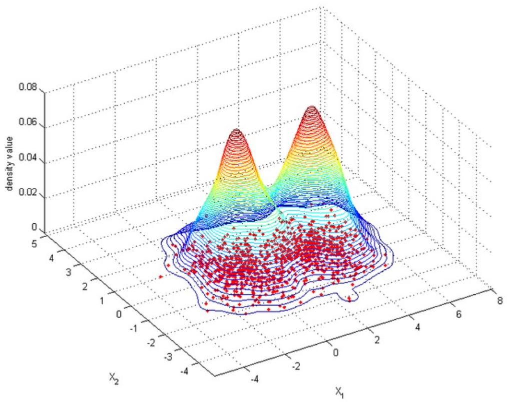
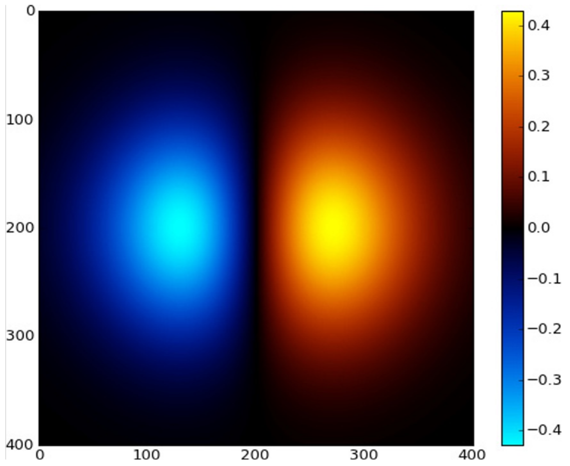
Supervised vs Unsupervised Learning

Learning the distribution
e.g. density estimation





Images left and right are CC0 public domain

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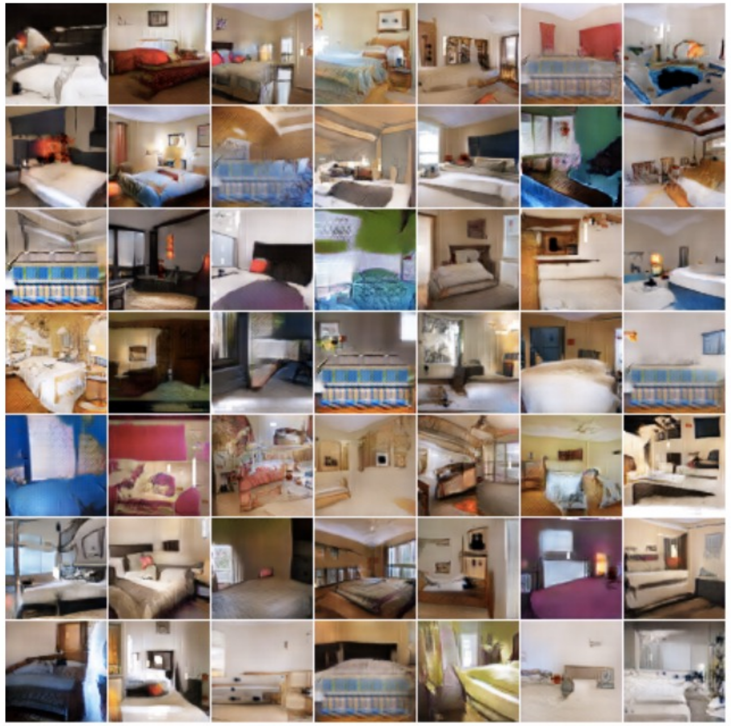
Examples: Clustering, dimensionality reduction, feature learning, density estimation, etc.

Slide from Justin Johnson

Supervised vs Unsupervised Learning

Learning the distribution
e.g. sampling from it



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Slide from Justin Johnson

Types of Generative Models

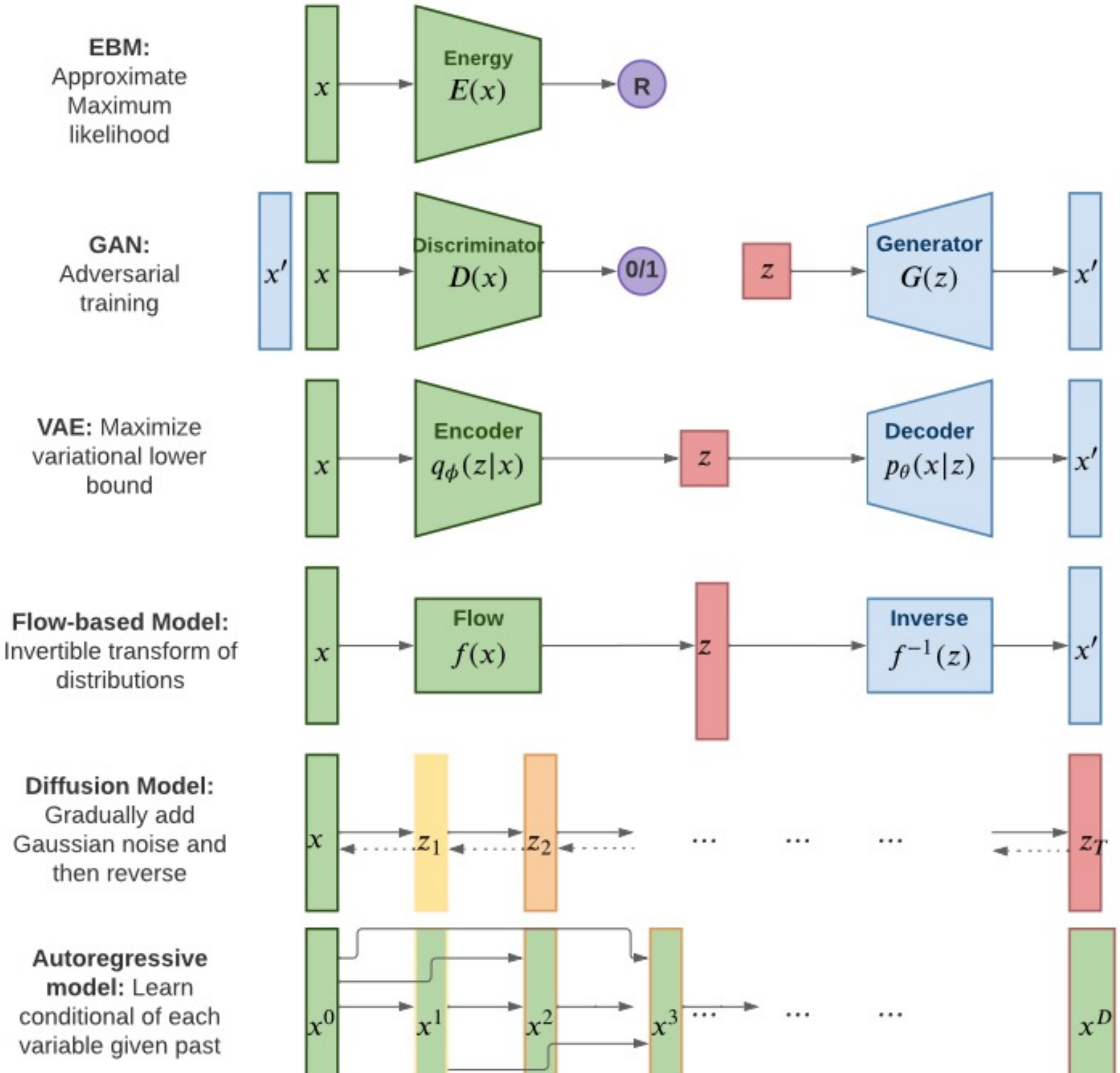
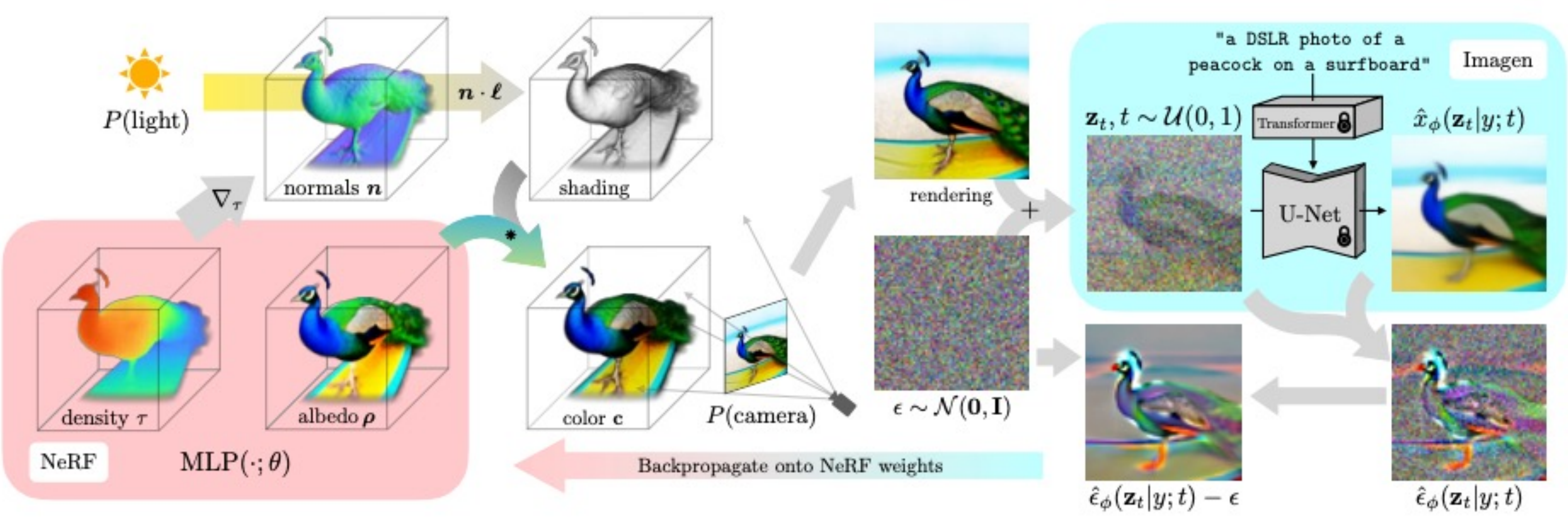


Figure from Probabilistic Machine Learning: Advanced Topics, adapted from https://lilianweng.github.io/posts/2021-07-11-diffusion-models/

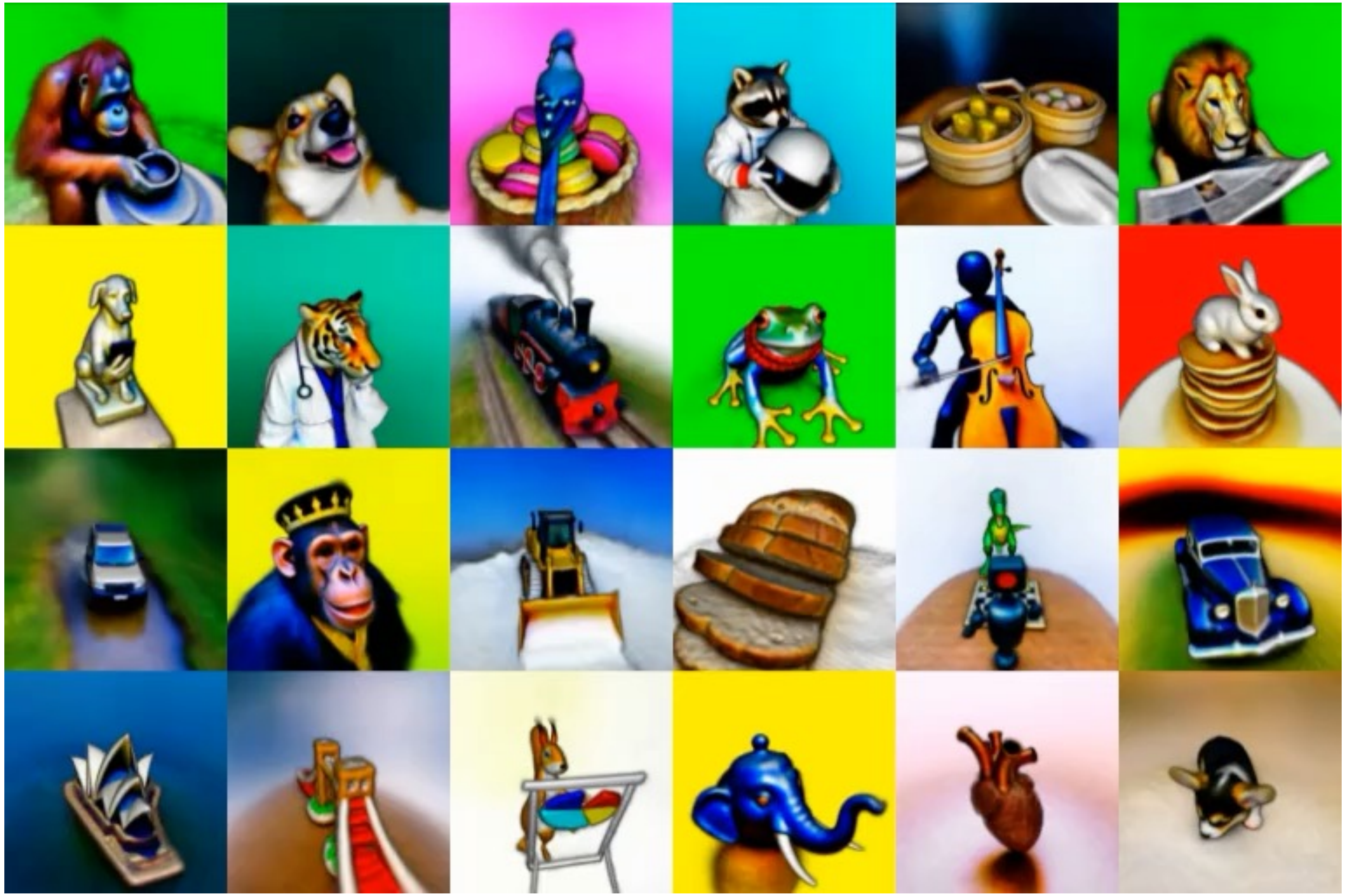
Application of Generative Models (Image in-painting)

Application of Generative Models (As a prior)



[Dream Fusion: Text-to-3D Using 2D Diffusion]

Application of Generative Models (As a prior)



[Dream Fusion: Text-to-3D Using 2D Diffusion]

Application of Generative Models (Image generation)

Text-to-Image Synthesis on LAION. 1.45B Model.

'A street sign that reads "Latent Diffusion" '	*'A zombie in the style of Picasso'*	*'An image of an animal half mouse half octopus'*	*'An illustration of a slightly conscious neural network'*	*'A painting of a squirrel eating a burger'*	*'A watercolor painting of a chair that looks like an octopus'*	*'A shirt with the inscription: "I love generative models!" '*

Variational Autoencoders

Variational Autoencoders

PixelRNN / PixelCNN explicitly parameterizes density function with a neural network, so we can train to maximize likelihood of training data:

$$\mathrm{p}_W(x) = \prod_{t=1}^{T} p_W(x_t \mid x_1, \ldots, x_{t-1})$$

Variational Autoencoders (VAE) define an **intractable density** that we cannot explicitly compute or optimize

But we will be able to directly optimize a **lower bound** on the density

Slide from Justin Johnson

Variational Autoencoders

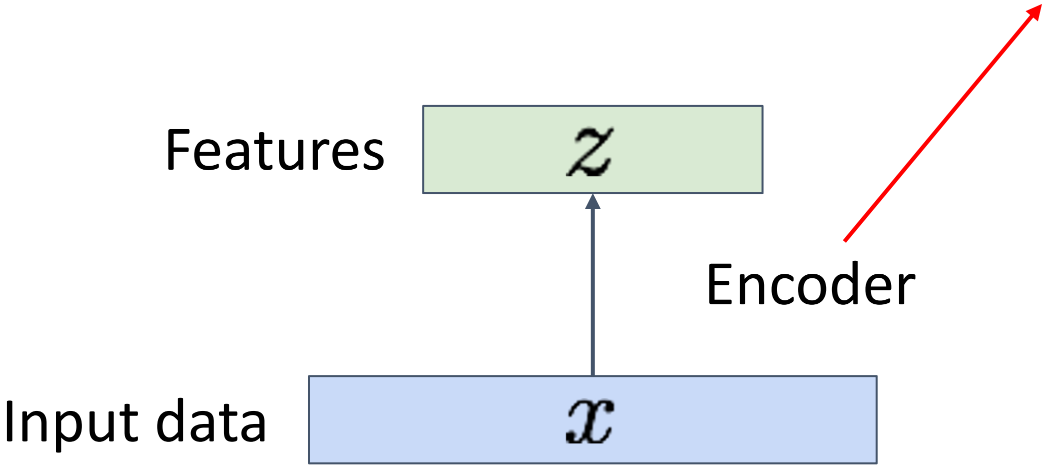
Slide from Justin Johnson

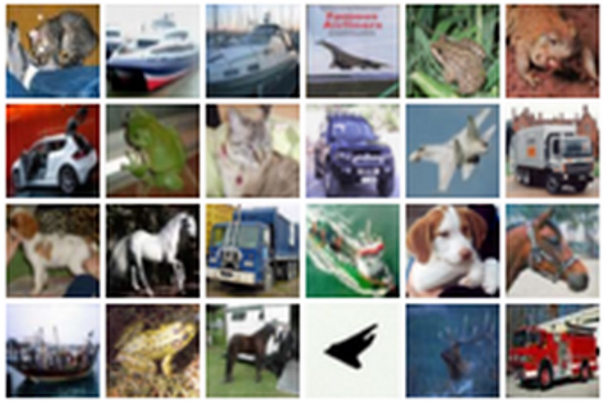
(Regular, non-variational) Autoencoders

Unsupervised method for learning feature vectors from raw data x, without any labels

Features should extract useful information (maybe object identities, properties, scene type, etc) that we can use for downstream tasks

Originally: Linear + nonlinearity (sigmoid)
Later: Deep, fully-connected
Later: ReLU CNN





Input Data

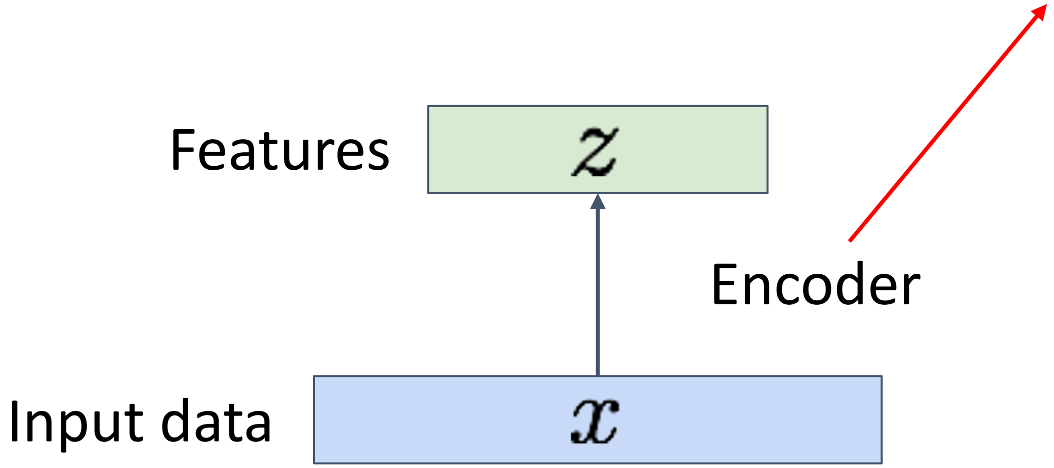
Slide from Justin Johnson

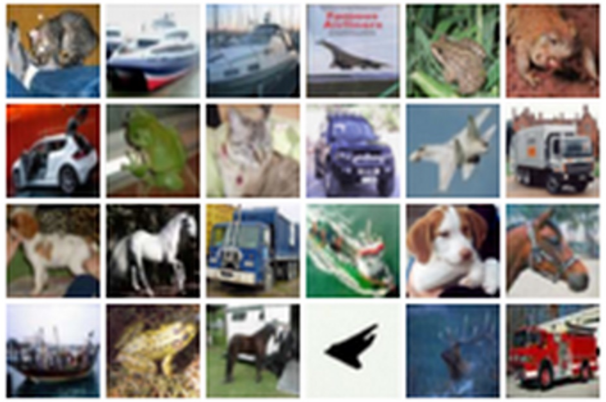
(Regular, non-variational) Autoencoders

Problem: How can we learn this feature transform from raw data?

Features should extract useful information (maybe object identities, properties, scene type, etc) that we can use for downstream tasks
But we can't observe features!

Originally: Linear + nonlinearity (sigmoid)
Later: Deep, fully-connected
Later: ReLU CNN





Input Data

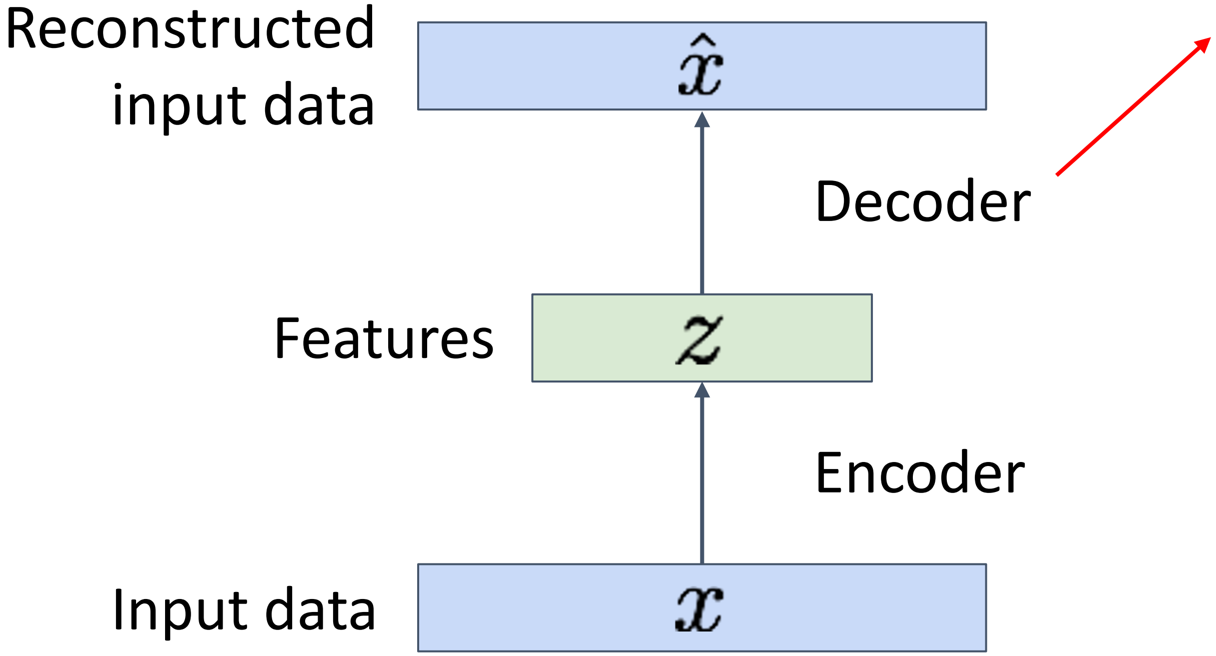
Slide from Justin Johnson

(Regular, non-variational) Autoencoders

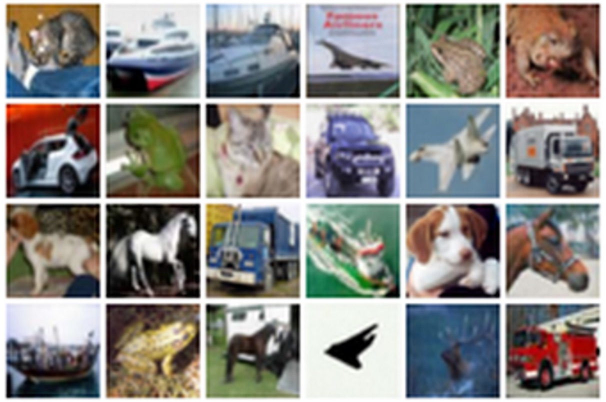
Problem: How can we learn this feature transform from raw data?

Idea: Use the features to reconstruct the input data with a **decoder**

"Autoencoding" = encoding itself



Originally: Linear + nonlinearity (sigmoid)
Later: Deep, fully-connected
Later: ReLU CNN (upconv)



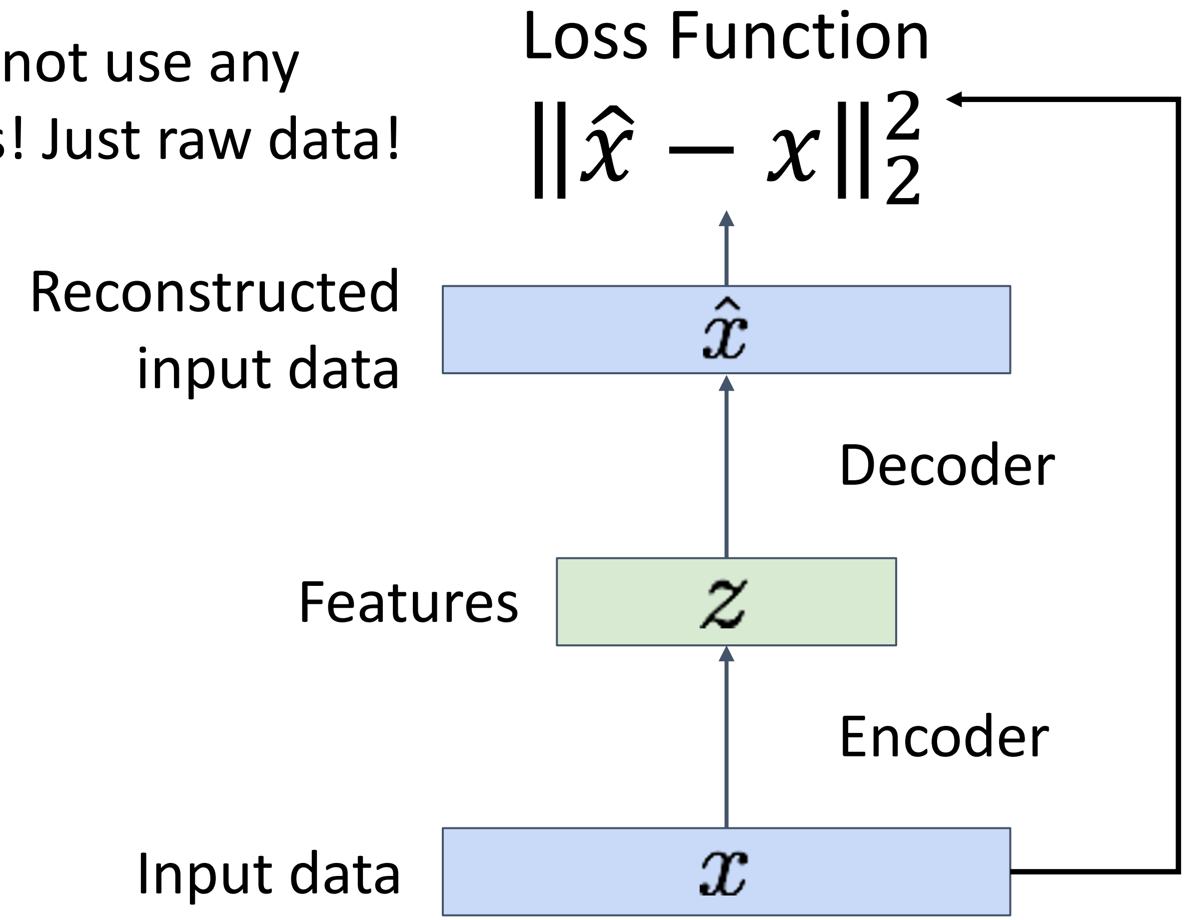
Input Data

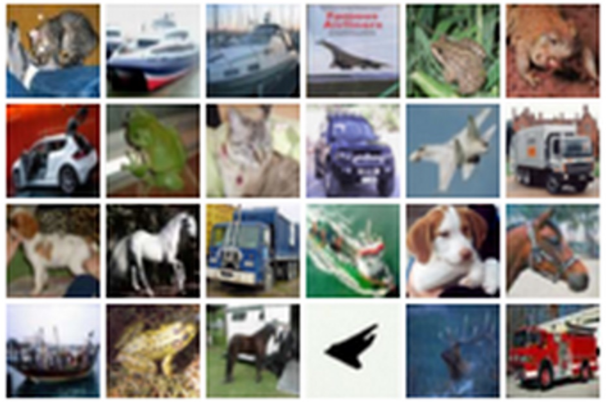
Slide from Justin Johnson

(Regular, non-variational) Autoencoders

Loss: L2 distance between input and reconstructed data.

Does not use any labels! Just raw data!





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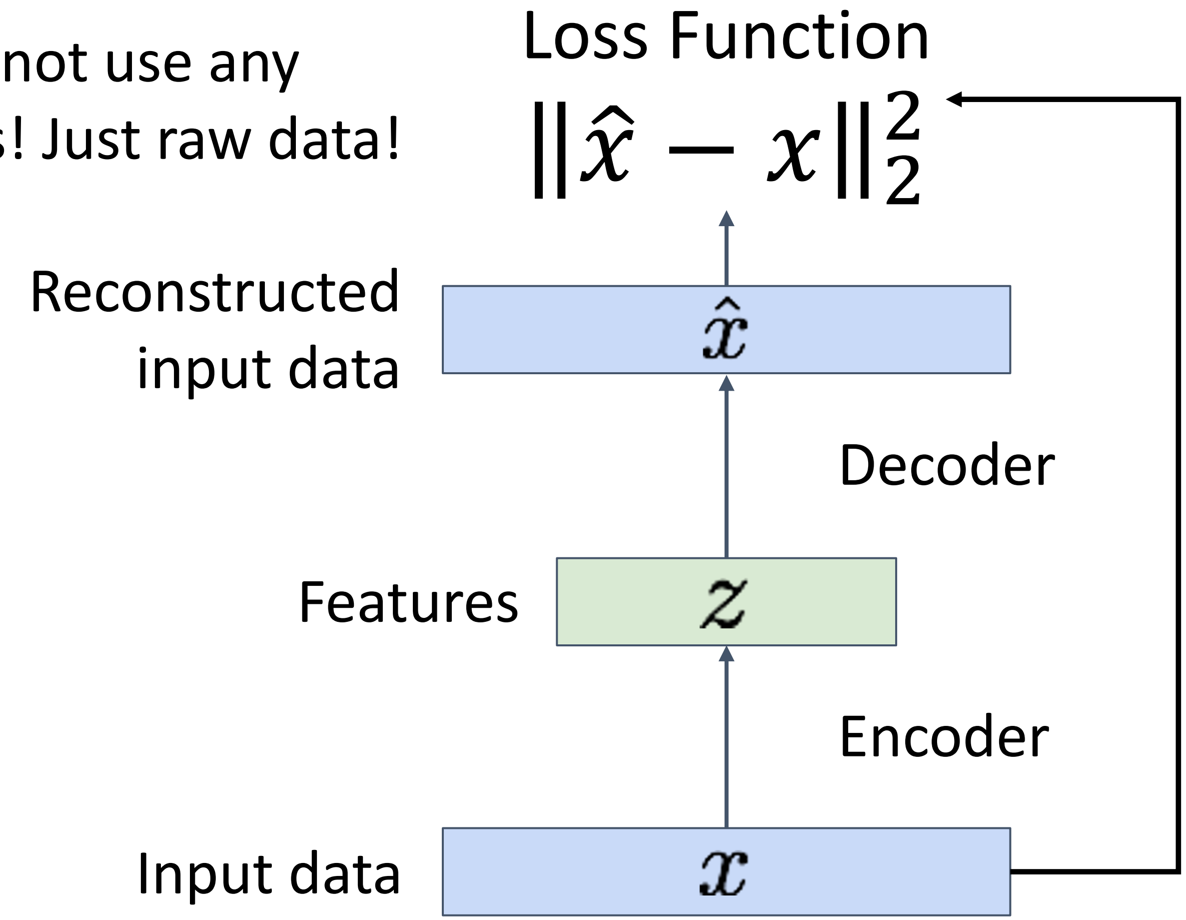

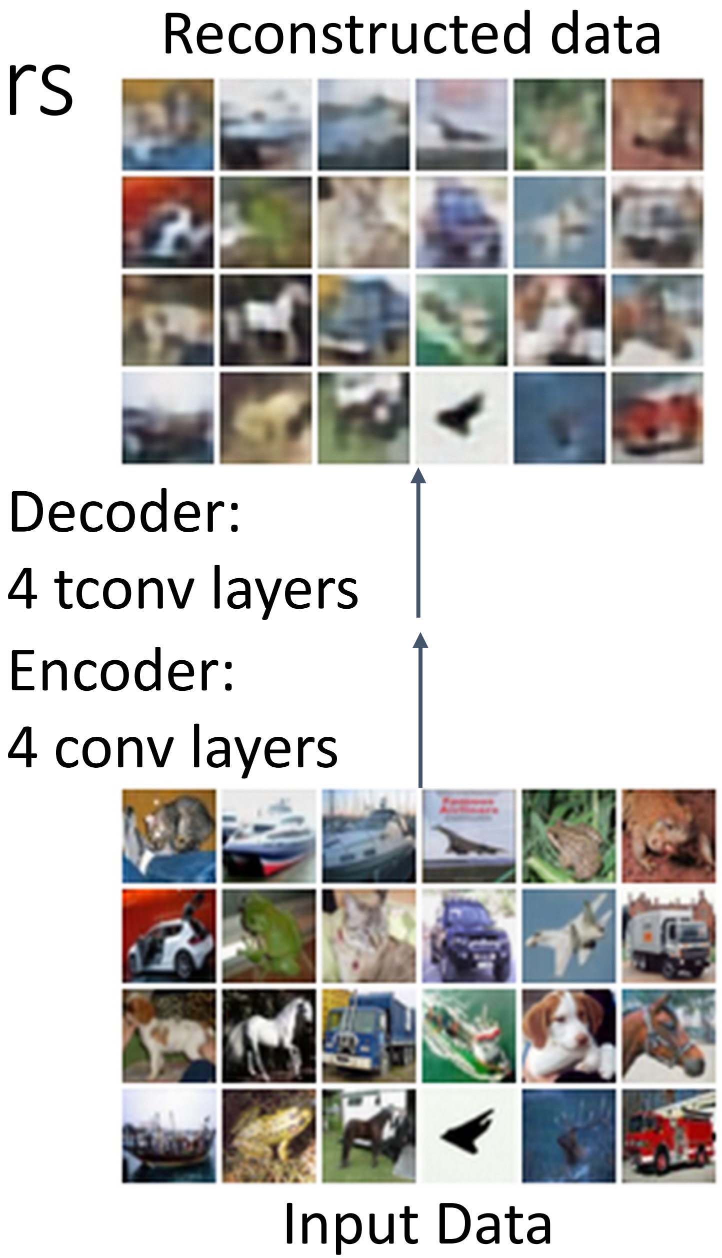

Slide from Justin Johnson

(Regular, non-variational) Autoencoders

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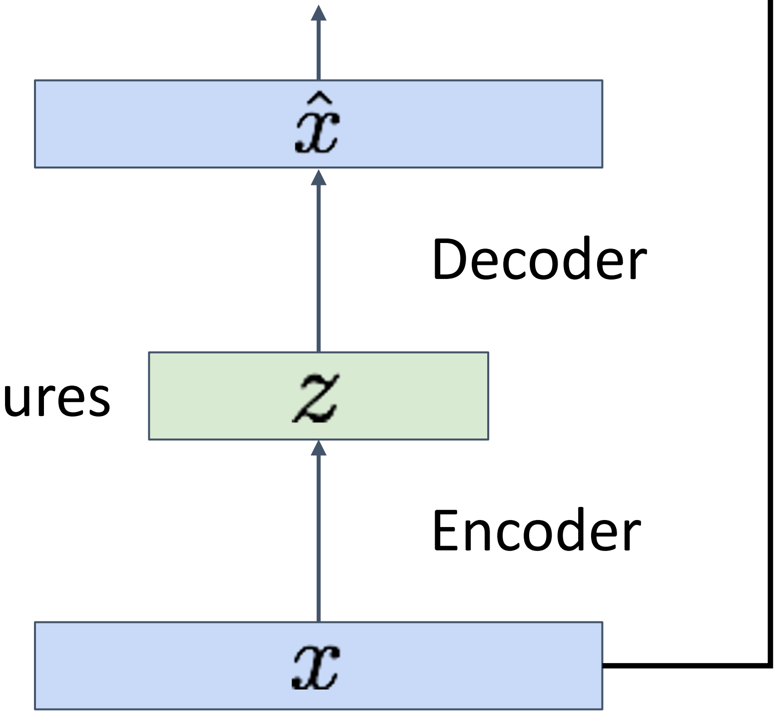
Does not use any labels! Just raw data!

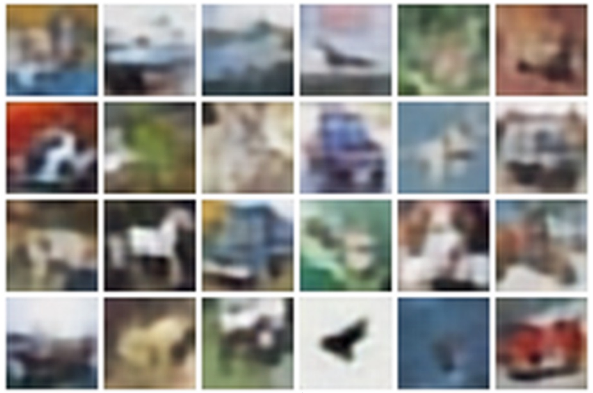
Loss Function

$$\|\hat{x} - x\|_2^2$$



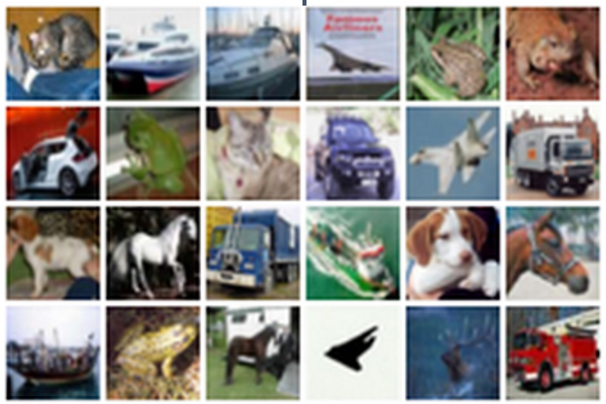
Features need to be **lower dimensional** than the data

Reconstructed data



Decoder:
4 tconv layers

Encoder:
4 conv layers

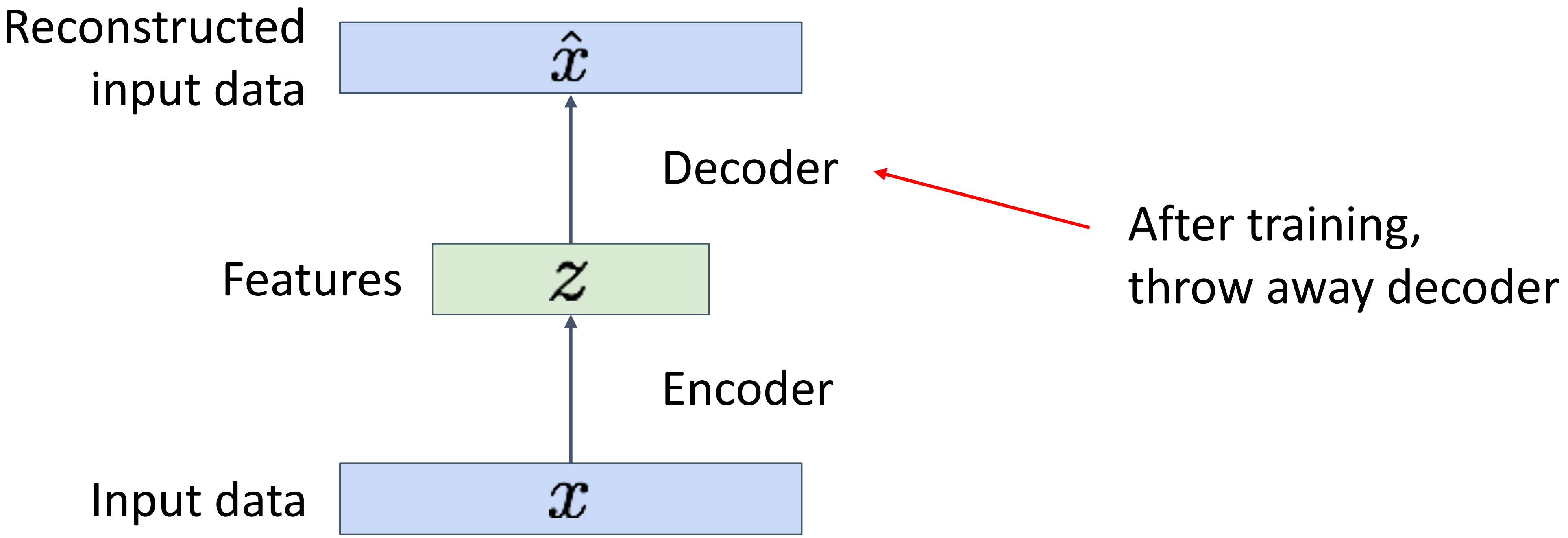


Input Data

Slide from Justin Johnson

(Regular, non-variational) Autoencoders

After training, **throw away decoder** and use encoder for a downstream task



Slide from Justin Johnson

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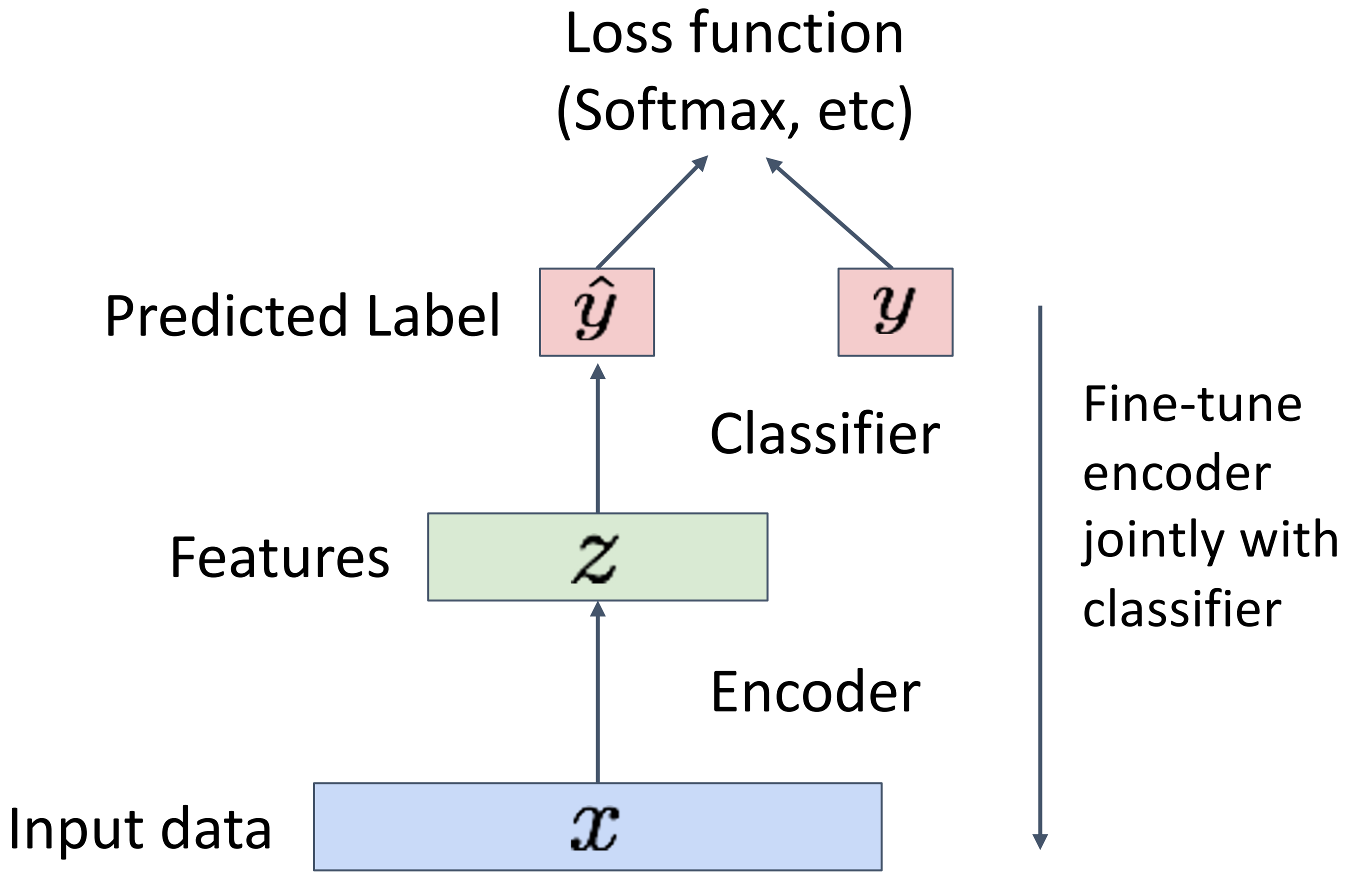

Encoder can be used to initialize a **supervised** model

Train for final task (sometimes with small data)

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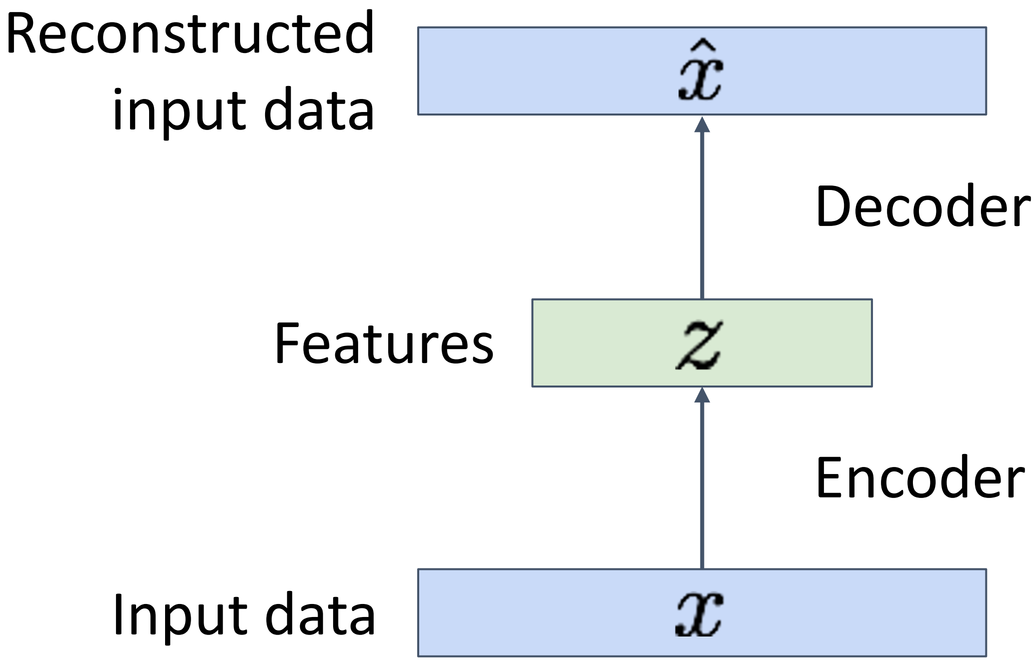
(Regular, non-variational) Autoencoders

Autoencoders learn **latent features** for data without any labels!

Can use features to initialize a **supervised** model

Not probabilistic: No way to sample new data from learned model



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Variational Autoencoders

Kingma and Welling, Auto-Encoding Variational Beyes, ICLR 2014

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Variational Autoencoders

Probabilistic spin on autoencoders:

1. Learn latent features z from raw data
2. Sample from the model to generate new data

Slide from Justin Johnson

Variational Autoencoders

Probabilistic spin on autoencoders:

1. Learn latent features z from raw data
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Assume training data $\{x^{(i)}\}_{i=1}^{N}$ is generated from unobserved (latent) representation **z**

Intuition: x is an image, **z** is latent factors used to generate **x:** attributes, orientation, etc.

Slide from Justin Johnson

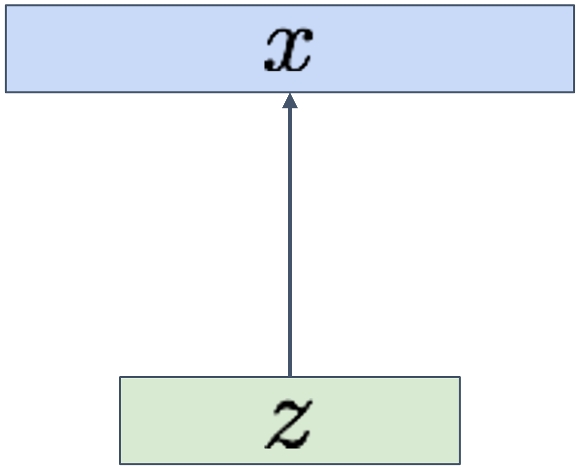
Variational Autoencoders

Probabilistic spin on autoencoders:
1. Learn latent features z from raw data
2. Sample from the model to generate new data

After training, sample new data like this:

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

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



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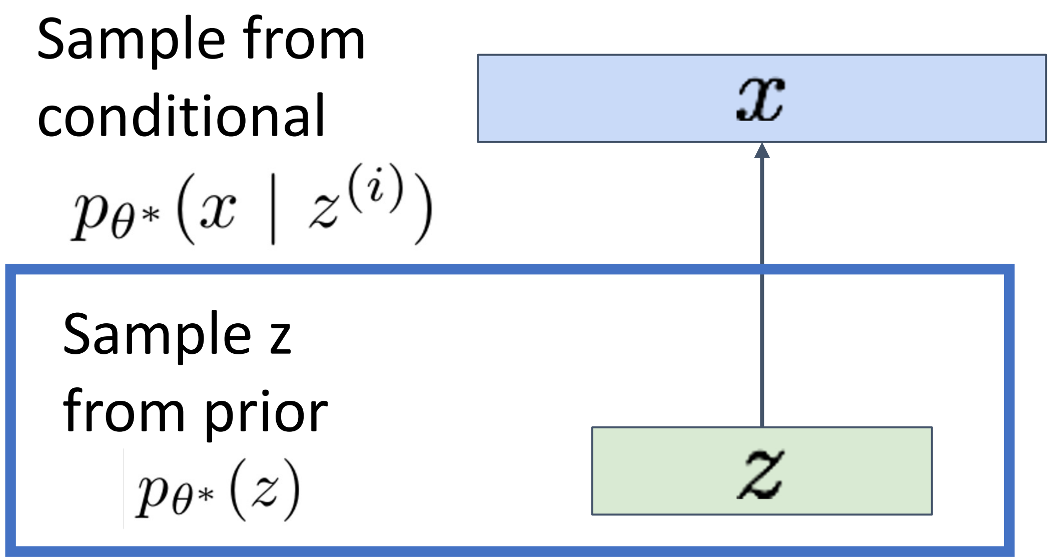

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Assume simple prior p(z), e.g. Gaussian

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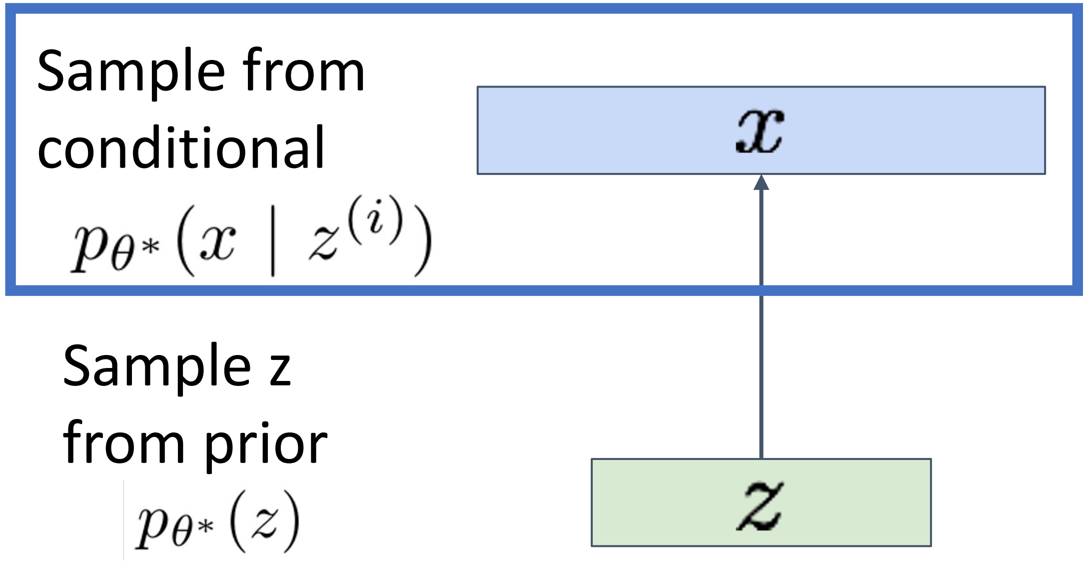

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Represent p(x|z) with a neural network (Similar to **decoder** from autencoder)

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Variational Autoencoders

Decoder must be **probabilistic**:
Decoder inputs z, outputs mean $\mu_{x|z}$ and (diagonal) covariance $\Sigma_{x|z}$

Sample x from Gaussian with mean $\mu_{x|z}$ and (diagonal) covariance $\Sigma_{x|z}$

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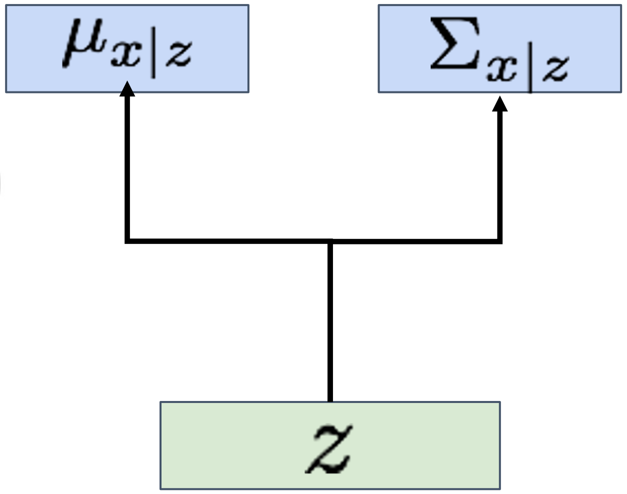

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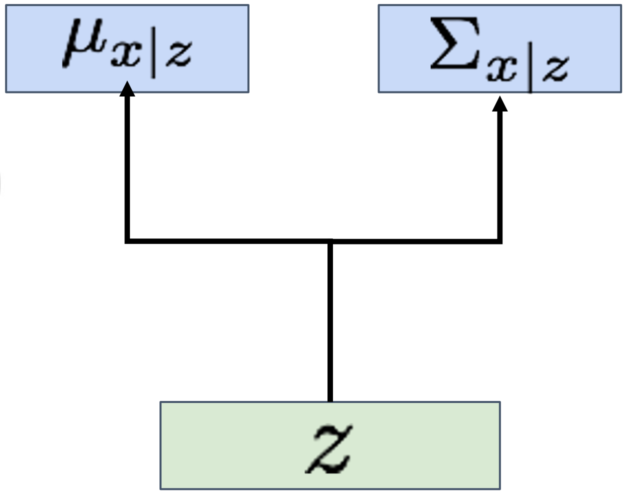

Assume training data $\{x^{(i)}\}_{i=1}^{N}$ is generated from unobserved (latent) representation **z**

How to train this model?

Basic idea: **maximize likelihood of data**

If we could observe the z for each x, then could train a *conditional generative model* p(x|z)

Slide from Justin Johnson

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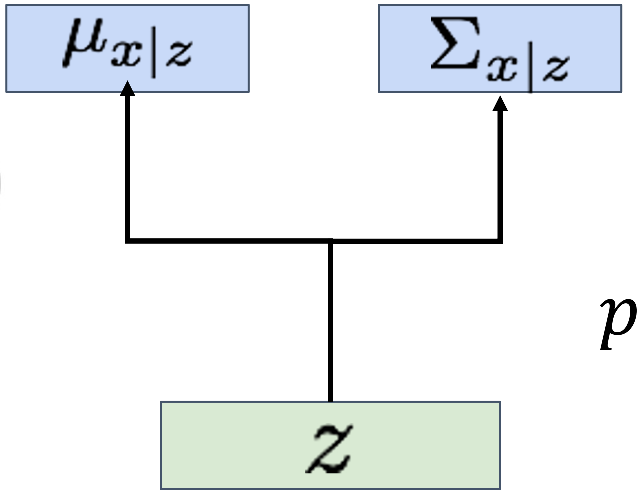

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How to train this model?

Basic idea: **maximize likelihood of data**

We don't observe z, so need to marginalize:

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

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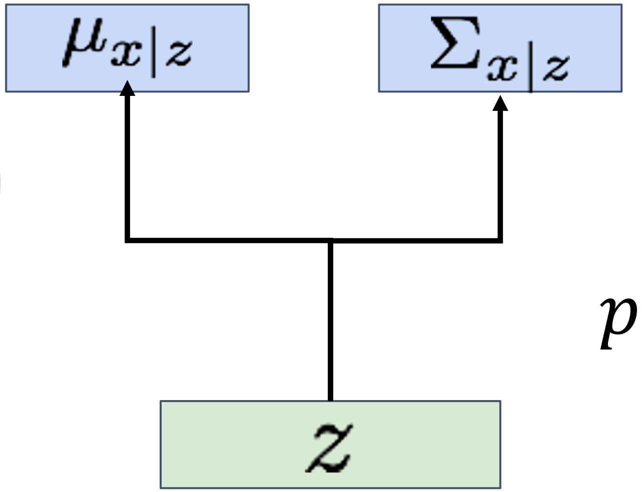

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Ok, can compute this with decoder network

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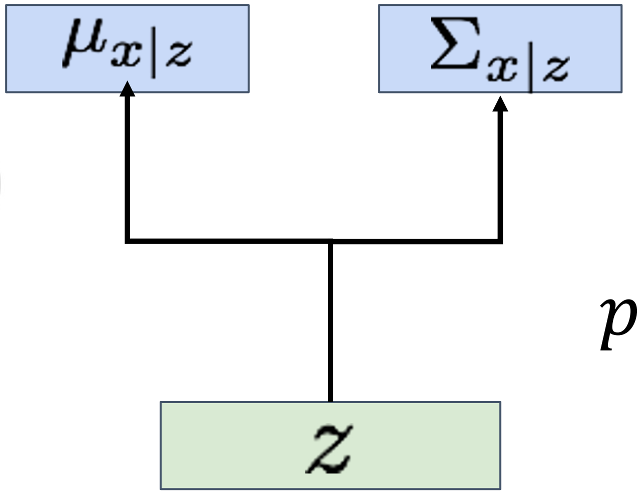

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Ok, we assumed Gaussian prior for z

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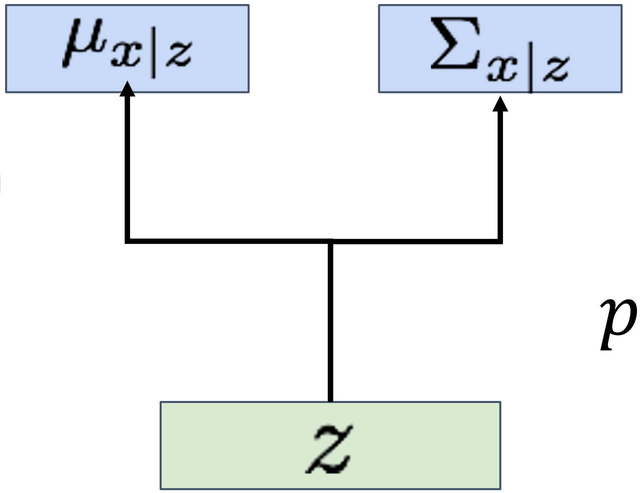

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$$p_\theta(x) = \int p_\theta(x,z)dz = \int p_\theta(x|z)p_\theta(z)dz$$

Problem: Impossible to integrate over all z!

Slide from Justin Johnson

Recall $p(x, z) = p(x \mid z)p(z) = p(z \mid x)p(x)$

Variational Autoencoders

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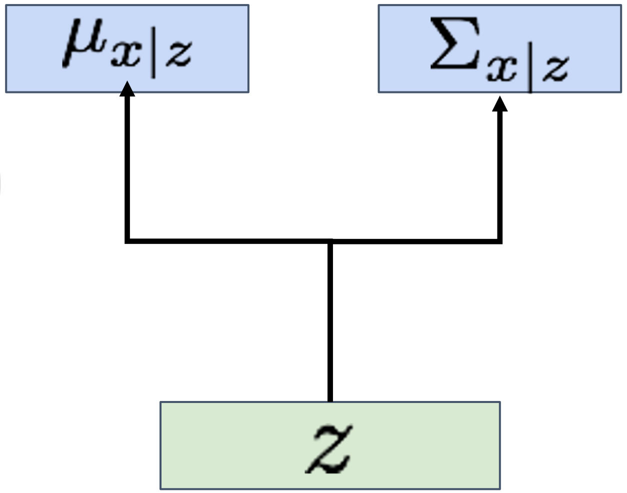


Assume training data $\{x^{(i)}\}_{i=1}^{N}$ is generated from unobserved (latent) representation **z**

How to train this model?

Basic idea: **maximize likelihood of data**

Another idea: Try Bayes' Rule:

$$p_\theta(x) = \frac{p_\theta(x \mid z)p_\theta(z)}{p_\theta(z \mid x)}$$

Slide from Justin Johnson

Recall $p(x, z) = p(x \mid z)p(z) = p(z \mid x)p(x)$

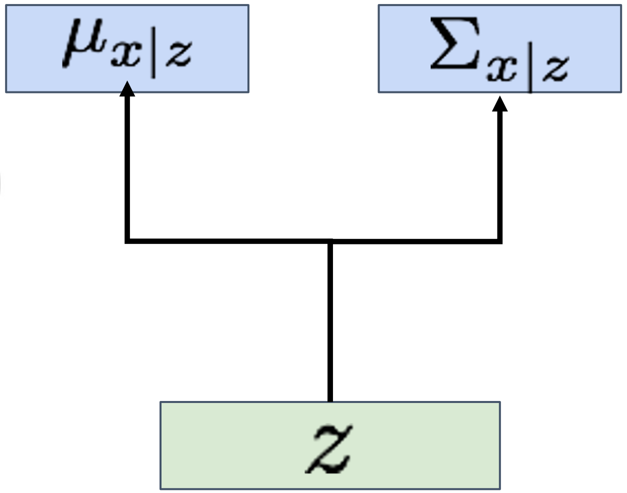
Variational Autoencoders

Decoder must be **probabilistic**:
Decoder inputs z, outputs mean $\mu_{x|z}$ and (diagonal) covariance $\Sigma_{x|z}$

Sample x from Gaussian with mean $\mu_{x|z}$ and (diagonal) covariance $\Sigma_{x|z}$

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

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



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Ok, compute with decoder network

Slide from Justin Johnson

Variational Autoencoders

Recall $p(x, z) = p(x \mid z)p(z) = p(z \mid x)p(x)$

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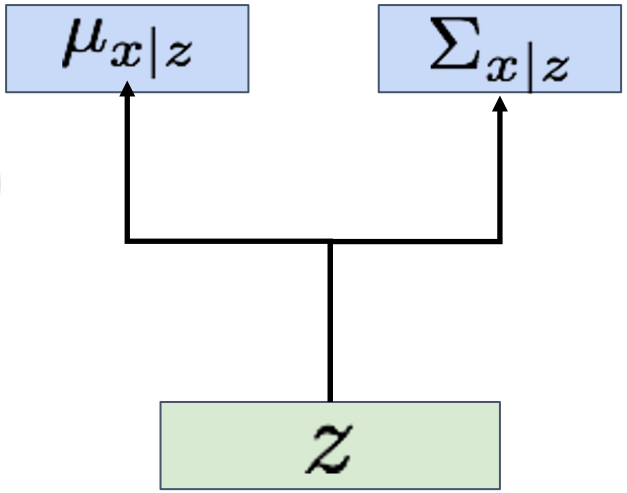

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Ok, we assumed Gaussian prior

Slide from Justin Johnson

Recall $p(x,z) = p(x \mid z)p(z) = p(z \mid x)p(x)$

Variational Autoencoders

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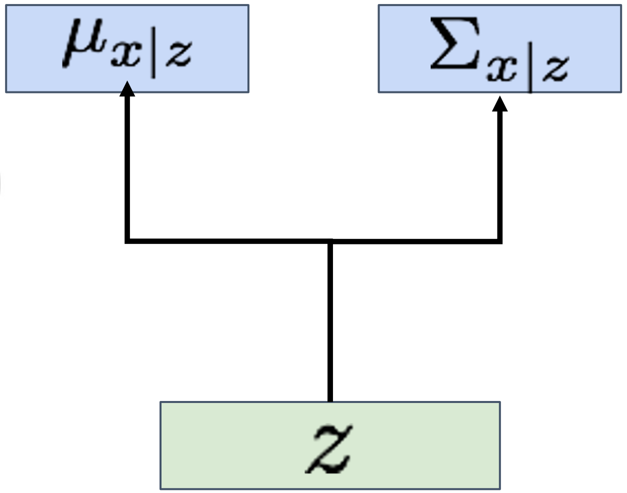

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Basic idea: **maximize likelihood of data**

Another idea: Try Bayes' Rule:

$$p_\theta(x) = \frac{p_\theta(x \mid z)p_\theta(z)}{p_\theta(z \mid x)}$$

Problem: No way to compute this!

Recall $p(x,z) = p(x \mid z)p(z) = p(z \mid x)p(x)$

Variational Autoencoders

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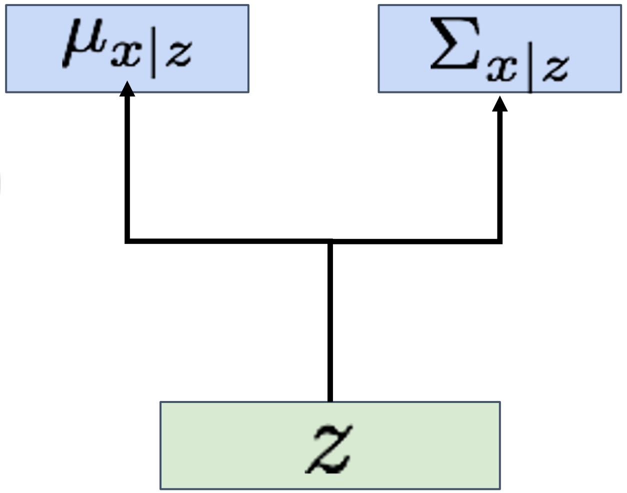

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Basic idea: **maximize likelihood of data**

Another idea: Try Bayes' Rule:

$$p_\theta(x) = \frac{p_\theta(x \mid z)p_\theta(z)}{p_\theta(z \mid x)}$$

Solution: Train another network **(encoder)** that learns $q_\phi(z \mid x) \approx p_\theta(z \mid x)$

Slide from Justin Johnson

Recall $p(x, z) = p(x \mid z)p(z) = p(z \mid x)p(x)$

Variational Autoencoders

Decoder must be **probabilistic**:
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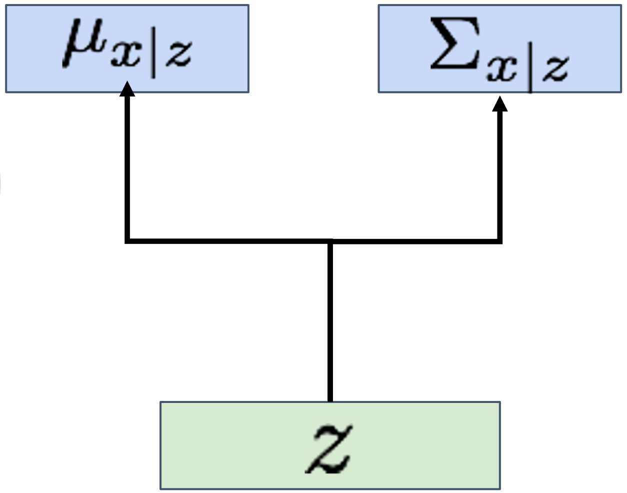


Assume training data $\{x^{(i)}\}_{i=1}^{N}$ is generated from unobserved (latent) representation **z**

How to train this model?

Basic idea: **maximize likelihood of data**

Another idea: Try Bayes' Rule:

$$p_\theta(x) = \frac{p_\theta(x \mid z)p_\theta(z)}{p_\theta(z \mid x)} \approx \frac{p_\theta(x \mid z)p_\theta(z)}{q_\phi(z \mid x)}$$

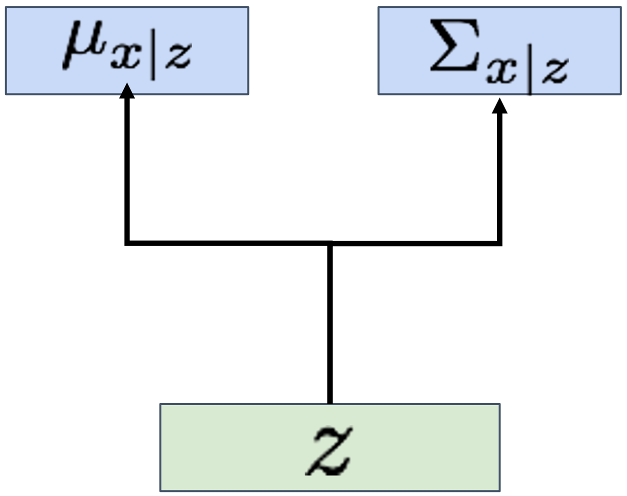
Use **encoder** to compute $q_\phi(z \mid x) \approx p_\theta(z \mid x)$

Slide from Justin Johnson

Variational Autoencoders

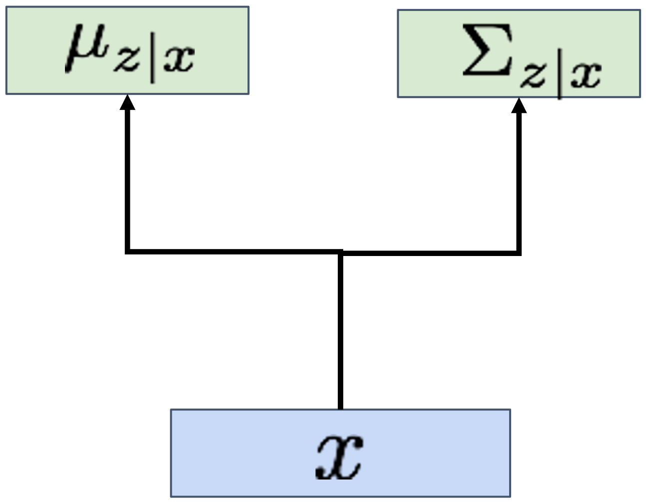
Decoder network inputs latent code z, gives distribution over data x

$$p_\theta(x \mid z) = N(\mu_{x|z}, \Sigma_{x|z})$$



Encoder network inputs data x, gives distribution over latent codes z

$$q_\phi(z \mid x) = N(\mu_{z|x}, \Sigma_{z|x})$$



If we can ensure that $q_\phi(z \mid x) \approx p_\theta(z \mid x)$,

then we can approximate

$$p_\theta(x) \approx \frac{p_\theta(x \mid z)p(z)}{q_\phi(z \mid x)}$$

Idea: Jointly train both encoder and decoder

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Variational Autoencoders

$$\log p_\theta(x) = \log \frac{p_\theta(x \mid z)p(z)}{p_\theta(z \mid x)}$$

Bayes' Rule

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Variational Autoencoders

$$\log p_\theta(x) = \log \frac{p_\theta(x \mid z)p(z)}{p_\theta(z \mid x)} = \log \frac{p_\theta(x|z)p(z)q_\phi(z|x)}{p_\theta(z|x)q_\phi(z|x)}$$

Multiply top and bottom by $q_\Phi(z|x)$

Slide from Justin Johnson

Variational Autoencoders

$$\log p_\theta(x) = \log \frac{p_\theta(x \mid z)p(z)}{p_\theta(z \mid x)} = \log \frac{p_\theta(x|z)p(z)q_\phi(z|x)}{p_\theta(z|x)q_\phi(z|x)}$$

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

Split up using rules for logarithms

Slide from Justin Johnson

Variational Autoencoders

$$\log p_\theta(x) = \log \frac{p_\theta(x \mid z)p(z)}{p_\theta(z \mid x)} = \log \frac{p_\theta(x|z)p(z)q_\phi(z|x)}{p_\theta(z|x)q_\phi(z|x)}$$

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Slide from Justin Johnson

Variational Autoencoders

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

$$\log p_\theta(x) = E_{z\sim q_\phi(z|x)}[\log p_\theta(x)]$$

We can wrap in an expectation since it doesn't depend on z

Slide from Justin Johnson

Variational Autoencoders

$$\log p_\theta(x) = \log \frac{p_\theta(x \mid z)p(z)}{p_\theta(z \mid x)} = \log \frac{p_\theta(x|z)p(z)q_\phi(z|x)}{p_\theta(z|x)q_\phi(z|x)}$$

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

$$\log p_\theta(x) = E_{z\sim q_\phi(z|x)}[\log p_\theta(x)]$$

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Slide from Justin Johnson

Variational Autoencoders

$$\log p_\theta(x) = \log \frac{p_\theta(x \mid z)p(z)}{p_\theta(z \mid x)} = \log \frac{p_\theta(x|z)p(z)q_\phi(z|x)}{p_\theta(z|x)q_\phi(z|x)}$$

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

$$= E_{z\sim q_\phi(z|x)}[\log p_\theta(x|z)] - D_{KL}\left(q_\phi(z|x), p(z)\right) + D_{KL}(q_\phi(z|x), p_\theta(z|x))$$

Data reconstruction

Slide from Justin Johnson

Variational Autoencoders

$$\log p_\theta(x) = \log \frac{p_\theta(x \mid z)p(z)}{p_\theta(z \mid x)} = \log \frac{p_\theta(x|z)p(z)q_\phi(z|x)}{p_\theta(z|x)q_\phi(z|x)}$$

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

$$= E_{z\sim q_\phi(z|x)}[\log p_\theta(x|z)] - D_{KL}\left(q_\phi(z|x), p(z)\right) + D_{KL}(q_\phi(z|x), p_\theta(z|x))$$

KL divergence between prior, and samples from the encoder network

Slide from Justin Johnson

Variational Autoencoders

$$\log p_\theta(x) = \log \frac{p_\theta(x \mid z)p(z)}{p_\theta(z \mid x)} = \log \frac{p_\theta(x|z)p(z)q_\phi(z|x)}{p_\theta(z|x)q_\phi(z|x)}$$

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

$$= E_{z\sim q_\phi(z|x)}[\log p_\theta(x|z)] - D_{KL}\left(q_\phi(z|x), p(z)\right) + D_{KL}(q_\phi(z|x), p_\theta(z|x))$$

KL divergence between encoder and posterior of decoder

Slide from Justin Johnson

Variational Autoencoders

$$\log p_\theta(x) = \log \frac{p_\theta(x \mid z)p(z)}{p_\theta(z \mid x)} = \log \frac{p_\theta(x|z)p(z)q_\phi(z|x)}{p_\theta(z|x)q_\phi(z|x)}$$

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

$$= E_{z\sim q_\phi(z|x)}[\log p_\theta(x|z)] - D_{KL}\left(q_\phi(z|x), p(z)\right) + D_{KL}(q_\phi(z|x), p_\theta(z|x))$$

KL is >= 0, so dropping this term gives a **lower bound** on the data likelihood:

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Variational Autoencoders

$$\log p_\theta(x) = \log \frac{p_\theta(x \mid z)p(z)}{p_\theta(z \mid x)} = \log \frac{p_\theta(x|z)p(z)q_\phi(z|x)}{p_\theta(z|x)q_\phi(z|x)}$$

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

$$= E_{z\sim q_\phi(z|x)}[\log p_\theta(x|z)] - D_{KL}\left(q_\phi(z|x), p(z)\right) + D_{KL}(q_\phi(z|x), p_\theta(z|x))$$

$$\log p_\theta(x) \geq E_{z\sim q_\phi(z|x)}[\log p_\theta(x|z)] - D_{KL}\left(q_\phi(z|x), p(z)\right)$$

Slide from Justin Johnson

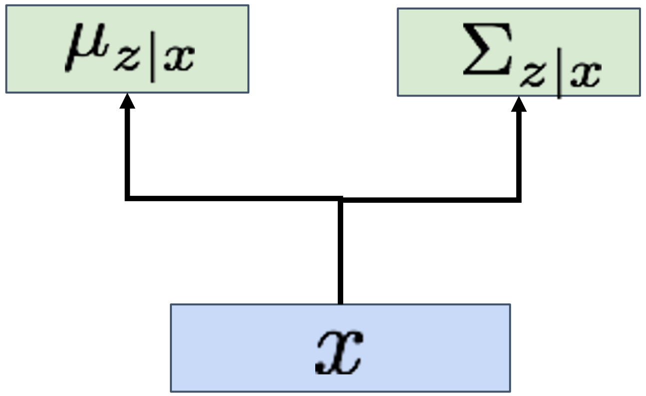
Variational Autoencoders

Jointly train **encoder** q and **decoder** p to maximize
the **variational lower bound** on the data likelihood
Also called **Evidence Lower Bound** (**ELBo**)

$$\log p_\theta(x) \geq E_{z\sim q_\phi(z|x)}[\log p_\theta(x|z)] - D_{KL}\left(q_\phi(z|x), p(z)\right)$$

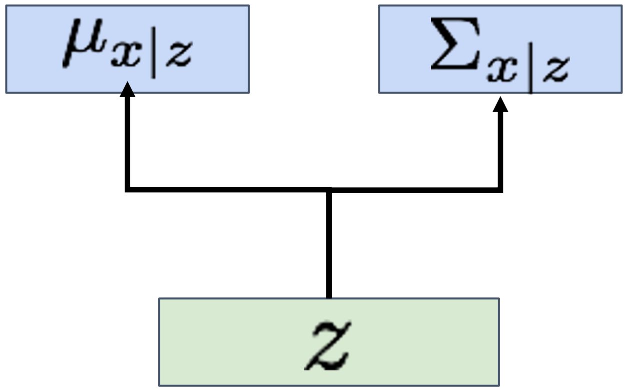
Encoder Network

$$q_\phi(z \mid x) = N(\mu_{z|x}, \Sigma_{z|x})$$



Decoder Network

$$p_\theta(x \mid z) = N(\mu_{x|z}, \Sigma_{x|z})$$



Slide from Justin Johnson

Example: Fully-Connected VAE

x: 28x28 image, flattened to 784-dim vector

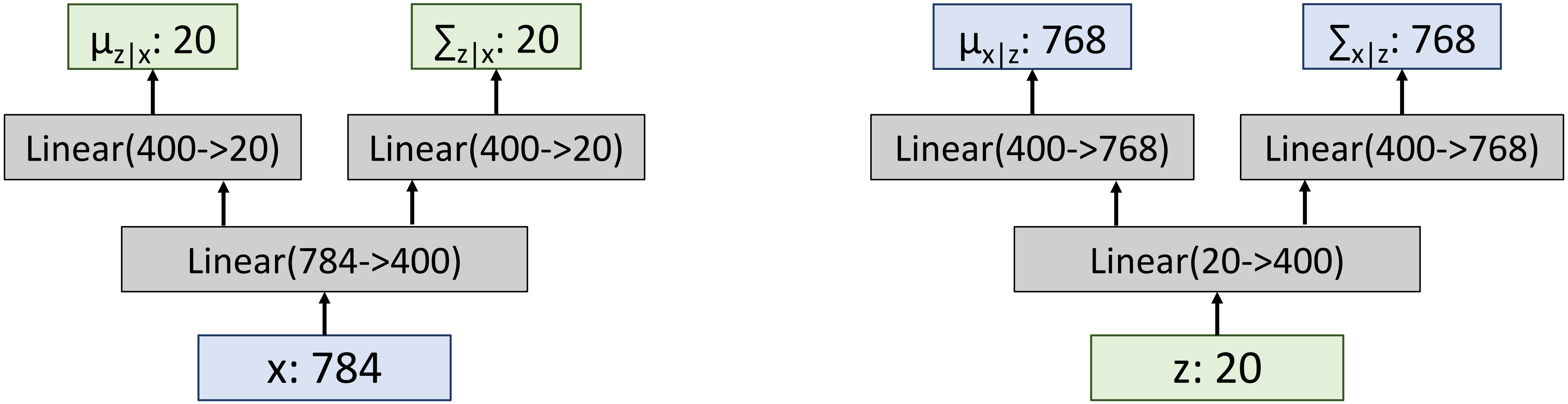
z: 20-dim vector

Encoder Network

$$q_\phi(z \mid x) = N(\mu_{z|x}, \Sigma_{z|x})$$

Decoder Network

$$p_\theta(x \mid z) = N(\mu_{x|z}, \Sigma_{x|z})$$



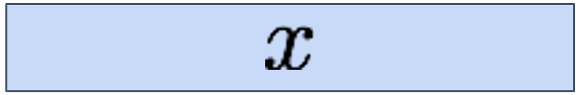
Slide from Justin Johnson

Variational Autoencoders

Train by maximizing the
variational lower bound

$$E_{z \sim q_\phi(z|x)}[\log p_\theta(x|z)] - D_{KL}\left(q_\phi(z|x), p(z)\right)$$

Input Data



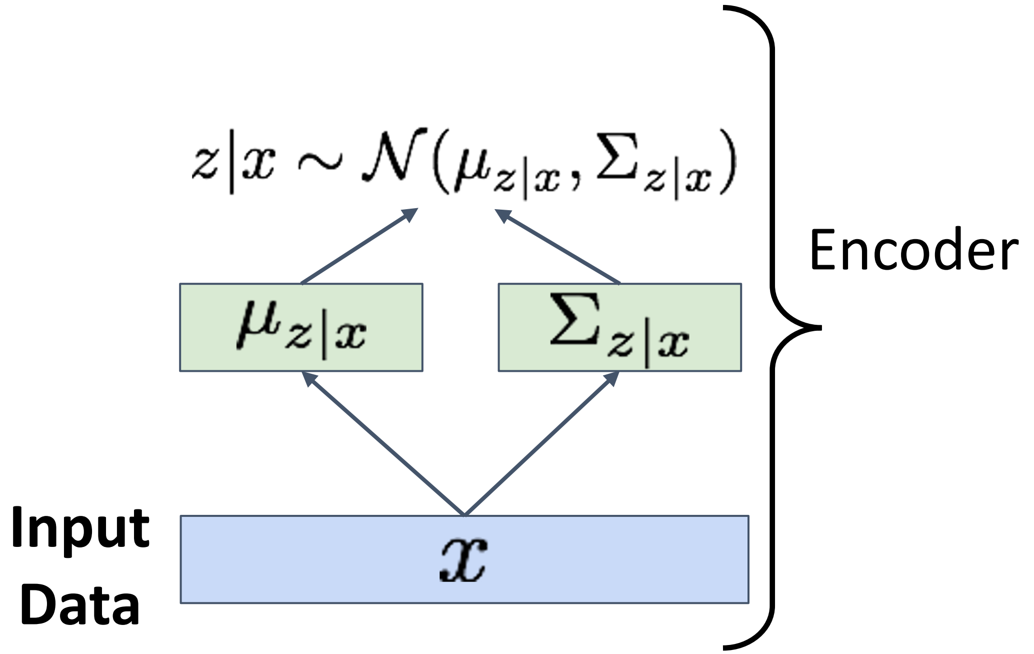
Slide from Justin Johnson

Variational Autoencoders

Train by maximizing the
variational lower bound

$$E_{z \sim q_\phi(z|x)}[\log p_\theta(x|z)] - D_{KL}\left(q_\phi(z|x), p(z)\right)$$

1. Run input data through **encoder** to get a distribution over latent codes



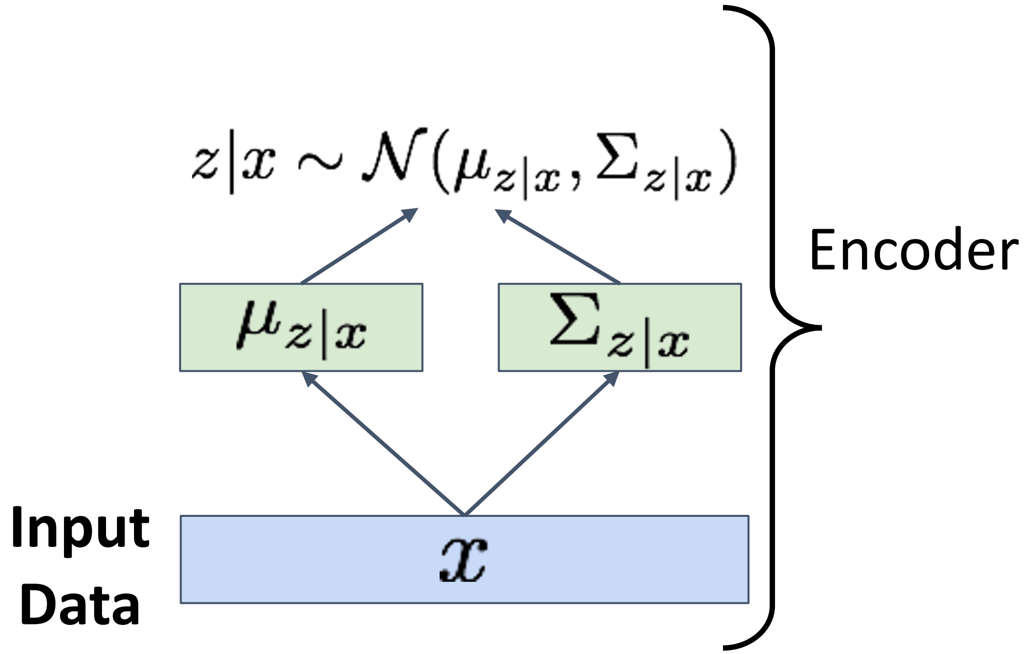
Slide from Justin Johnson

Variational Autoencoders

Train by maximizing the
variational lower bound

$$E_{z\sim q_\phi(z|x)}[\log p_\theta(x|z)] - \boxed{D_{KL}\left(q_\phi(z|x), p(z)\right)}$$

1. Run input data through **encoder** to get a distribution over latent codes
2. **Encoder output should match the prior p(z)!**



Slide from Justin Johnson

Variational Autoencoders

Train by maximizing the **variational lower bound**

$$E_{z\sim q_\phi(z|x)}[\log p_\theta(x|z)] - D_{KL}\left(q_\phi(z|x), p(z)\right)$$

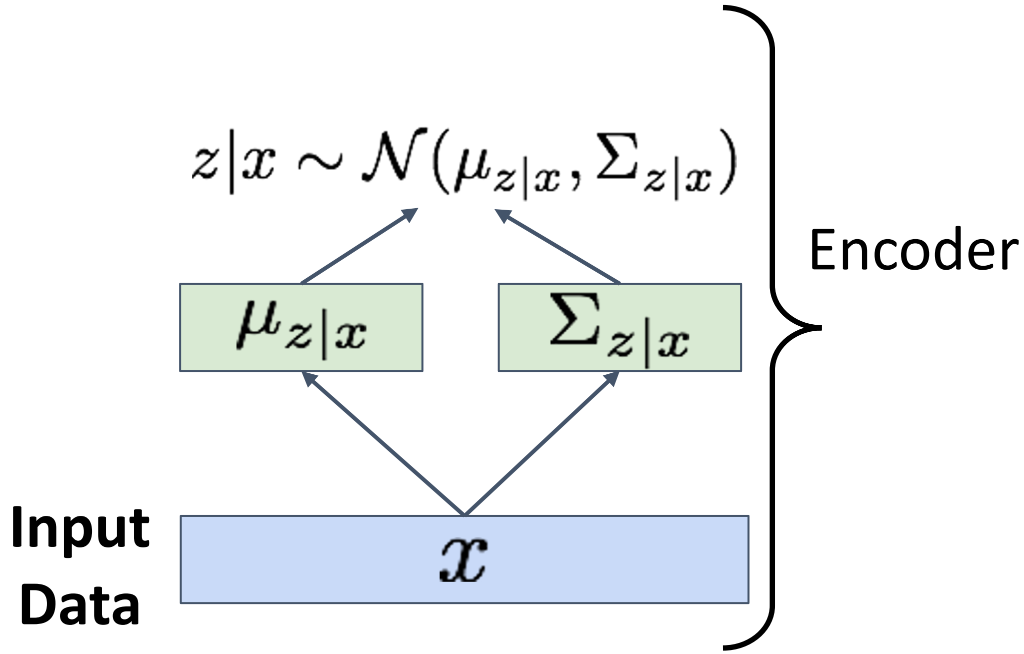
1. Run input data through **encoder** to get a distribution over latent codes
2. **Encoder output should match the prior p(z)!**

$$-D_{KL}\left(q_\phi(z|x), p(z)\right) = \int_Z q_\phi(z|x) \log \frac{p(z)}{q_\phi(z|x)} dz$$

$$= \int_Z N\left(z; \mu_{z|x}, \Sigma_{z|x}\right) \log \frac{N(z; 0, I)}{N\left(z; \mu_{z|x}, \Sigma_{z|x}\right)} dz$$

$$= \frac{1}{2}\sum_{j=1}^{J}\left(1 + \log\left(\left(\Sigma_{z|x}\right)_j^2\right) - \left(\mu_{z|x}\right)_j^2 - \left(\Sigma_{z|x}\right)_j^2\right)$$

Closed form solution when q_ϕ is diagonal Gaussian and p is unit Gaussian!
(Assume z has dimension J)



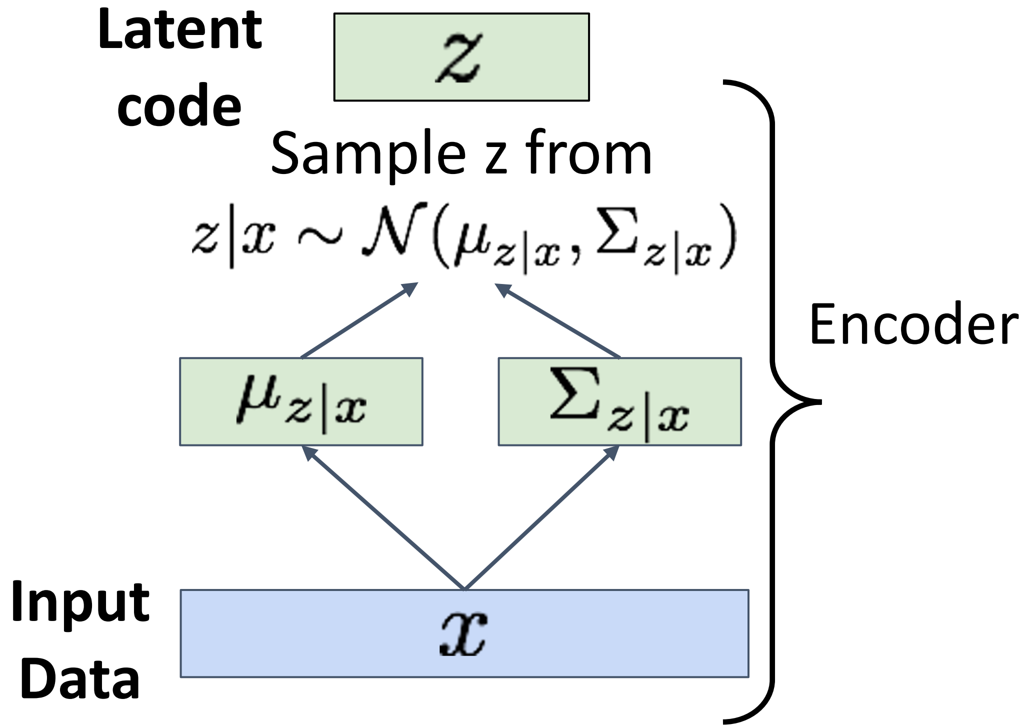
Slide from Justin Johnson

Variational Autoencoders

Train by maximizing the
variational lower bound

$$E_{z \sim q_\phi(z|x)}[\log p_\theta(x|z)] - \boxed{D_{KL}\left(q_\phi(z|x), p(z)\right)}$$

1. Run input data through **encoder** to get a distribution over latent codes
2. **Encoder output should match the prior p(z)!**
3. Sample code z from encoder output



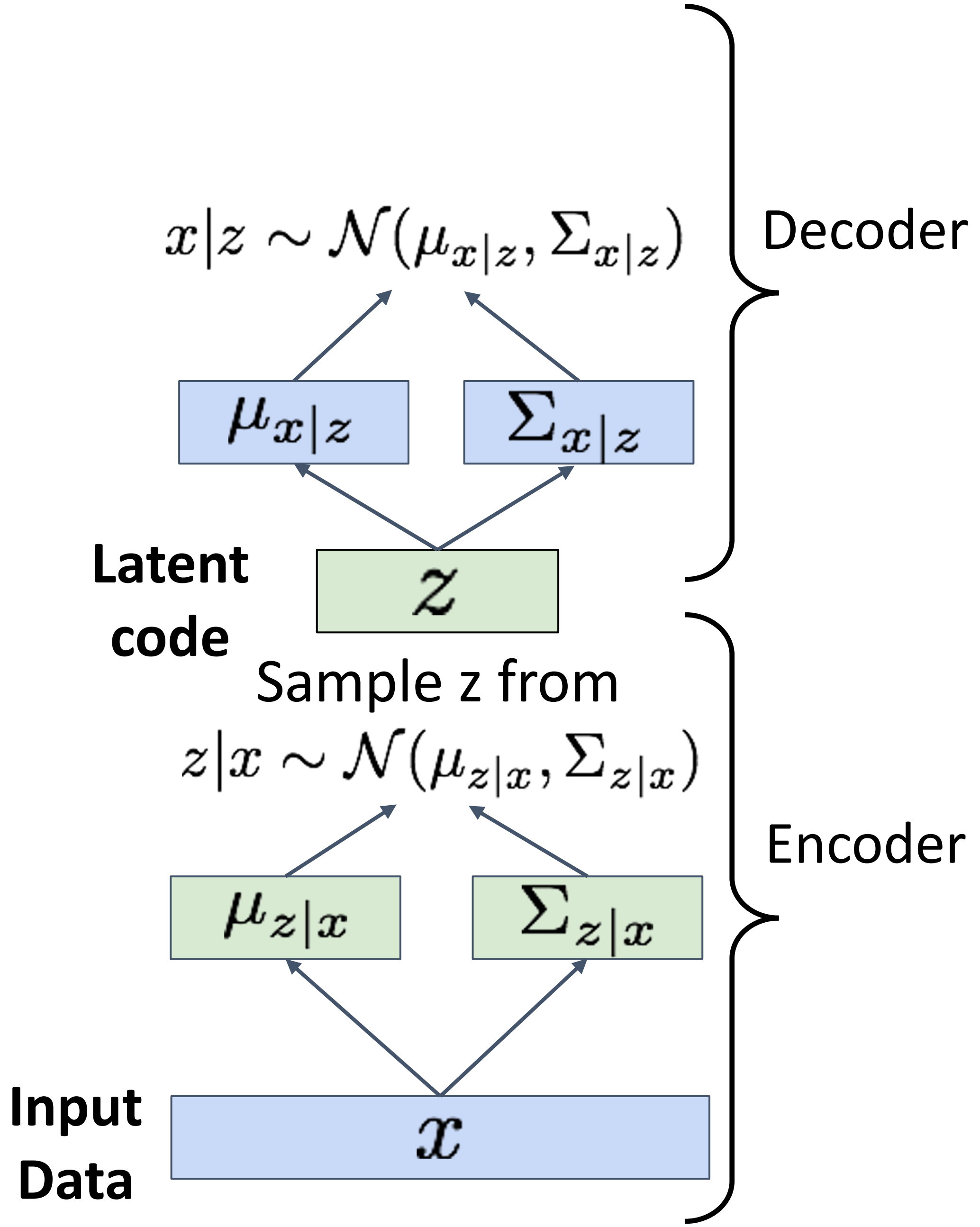
Slide from Justin Johnson

Variational Autoencoders

Train by maximizing the **variational lower bound**

$$E_{z \sim q_\phi(z|x)}[\log p_\theta(x|z)] - D_{KL}\left(q_\phi(z|x), p(z)\right)$$

1. Run input data through **encoder** to get a distribution over latent codes
2. **Encoder output should match the prior p(z)!**
3. Sample code z from encoder output
4. Run sampled code through **decoder** to get a distribution over data samples



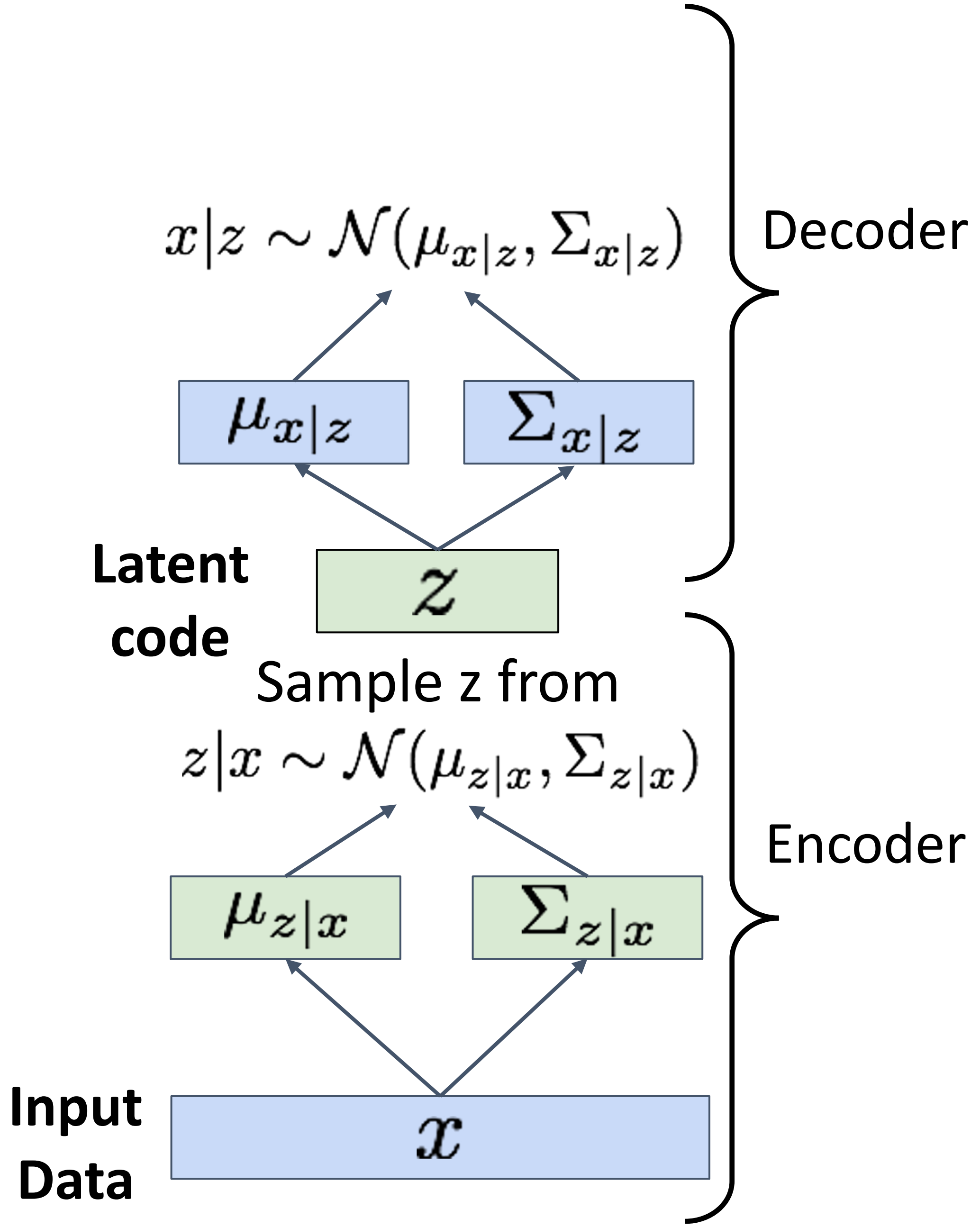
Slide from Justin Johnson

Variational Autoencoders

Train by maximizing the **variational lower bound**

$$E_{z \sim q_\phi(z|x)}[\log p_\theta(x|z)] - D_{KL}\left(q_\phi(z|x), p(z)\right)$$

1. Run input data through **encoder** to get a distribution over latent codes
2. **Encoder output should match the prior p(z)!**
3. Sample code z from encoder output
4. Run sampled code through **decoder** to get a distribution over data samples
5. **Original input data should be likely under the distribution output from (4)!**



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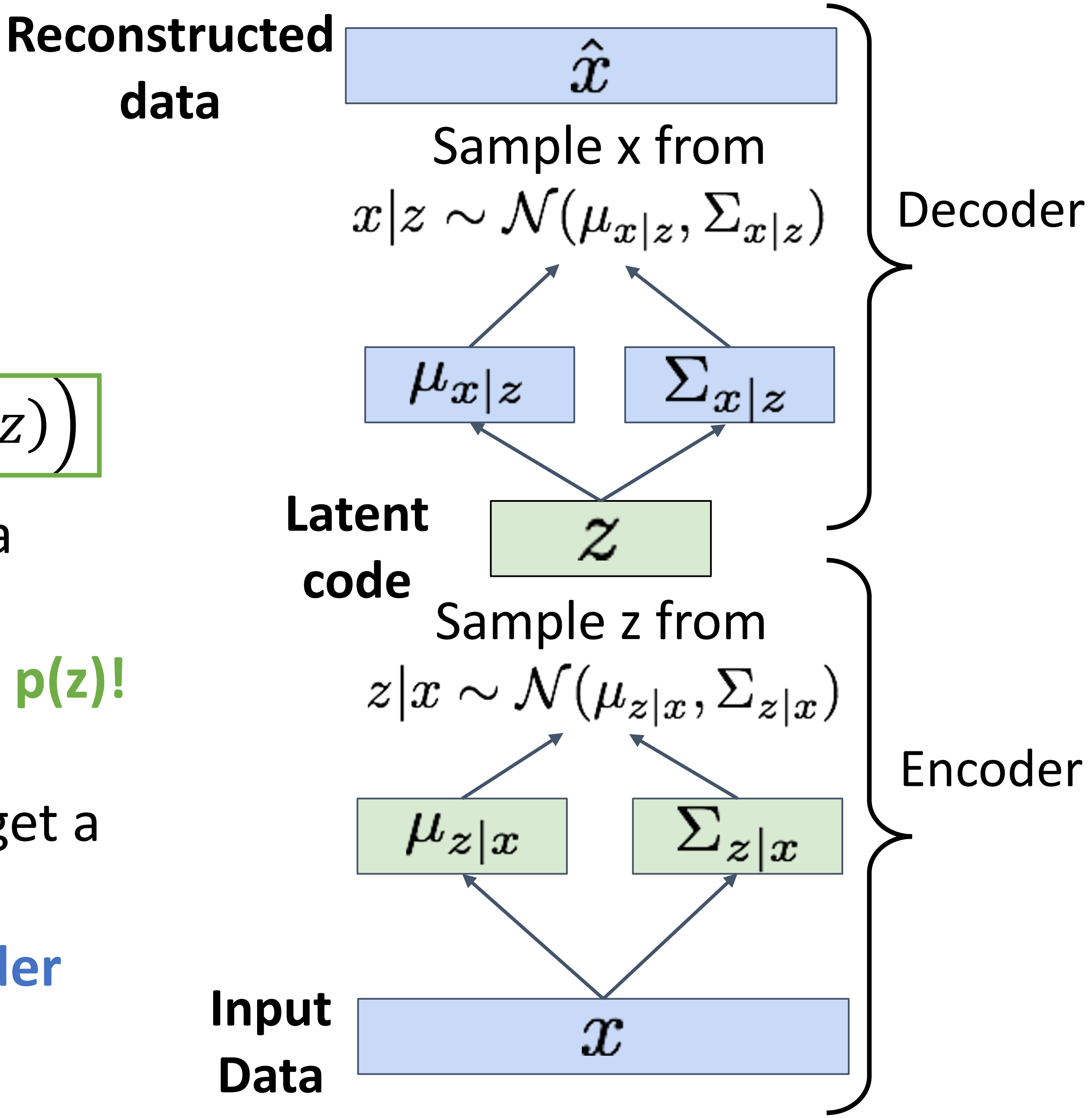
Variational Autoencoders

Train by maximizing the **variational lower bound**

$$E_{z\sim q_\phi(z|x)}[\log p_\theta(x|z)] - D_{KL}\left(q_\phi(z|x), p(z)\right)$$

1. Run input data through **encoder** to get a distribution over latent codes
2. **Encoder output should match the prior p(z)!**
3. Sample code z from encoder output
4. Run sampled code through **decoder** to get a distribution over data samples
5. **Original input data should be likely under the distribution output from (4)!**
6. Can sample a reconstruction from (4)



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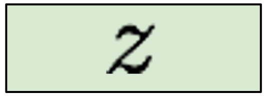
Variational Autoencoders: Generating Data

After training we can generate new data!

1. Sample z from prior p(z)

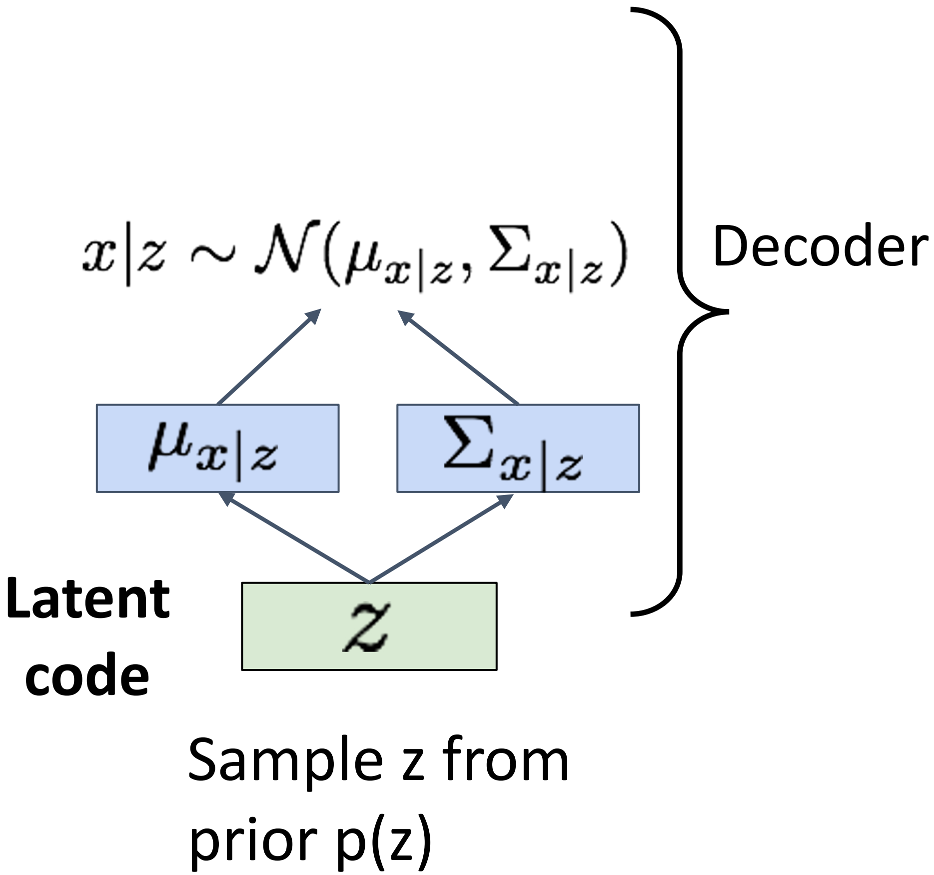


Slide from Justin Johnson

Variational Autoencoders: Generating Data

After training we can generate new data!

1. Sample z from prior p(z)
2. Run sampled z through decoder to get distribution over data x

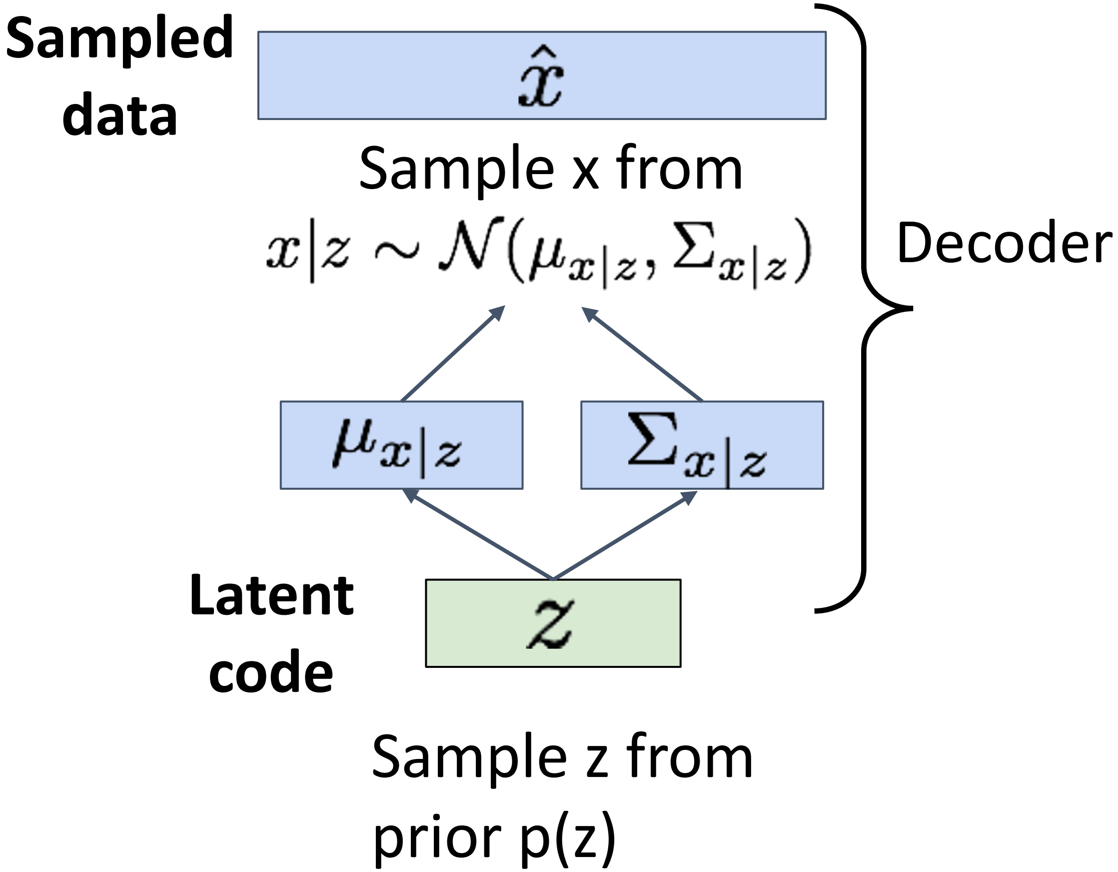


Slide from Justin Johnson

Variational Autoencoders: Generating Data

After training we can generate new data!

1. Sample z from prior p(z)
2. Run sampled z through decoder to get distribution over data x
3. Sample from distribution in (2) to generate data



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Variational Autoencoders: Generating Data

32x32 CIFAR-10

Labeled Faces in the Wild

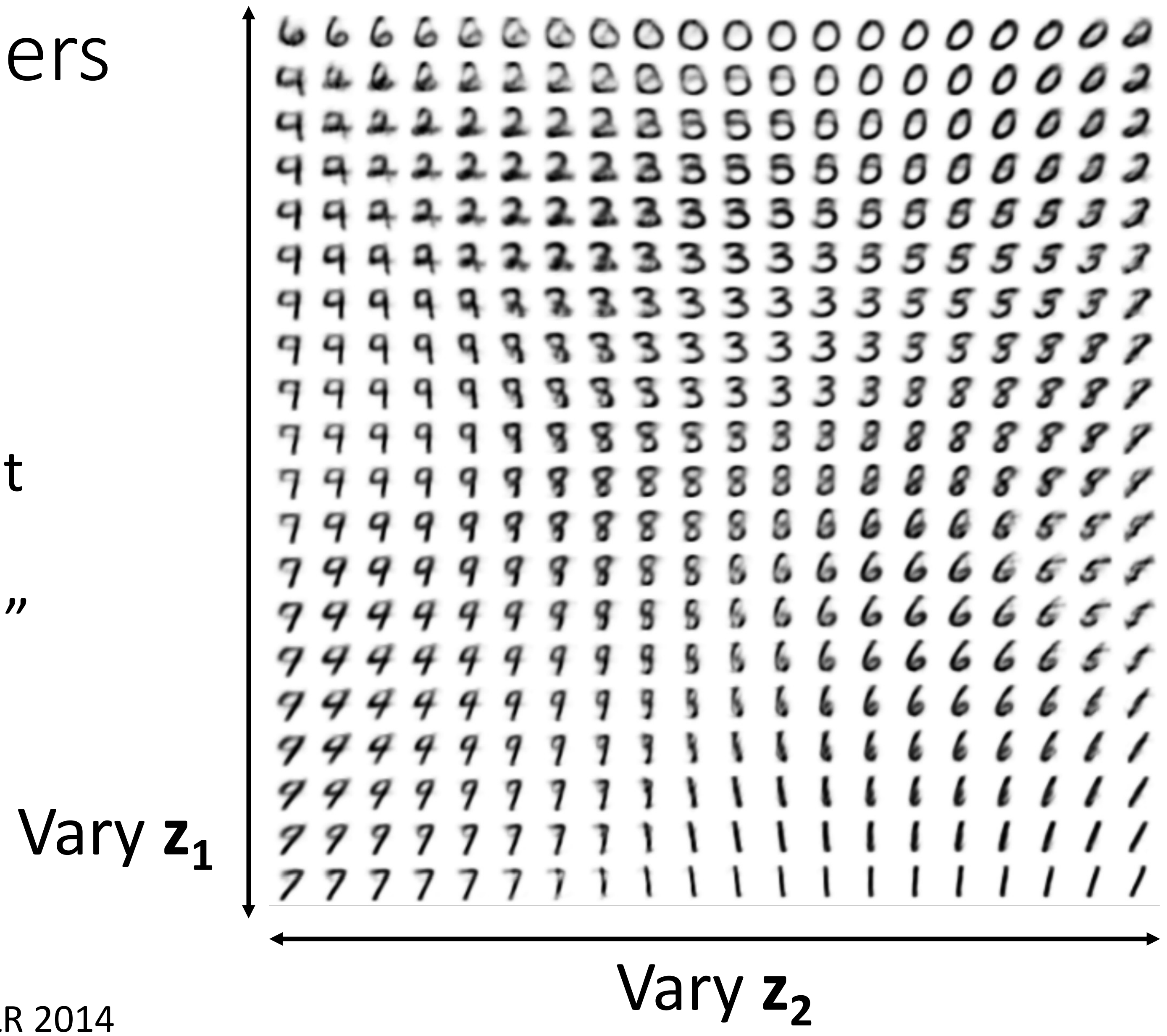
Figures from (L) Dirk Kingma et al. 2016; (R) Anders Larsen et al. 2017.

Slide from Justin Johnson

Variational Autoencoders

The diagonal prior on p(z) causes dimensions of z to be independent

"Disentangling factors of variation"



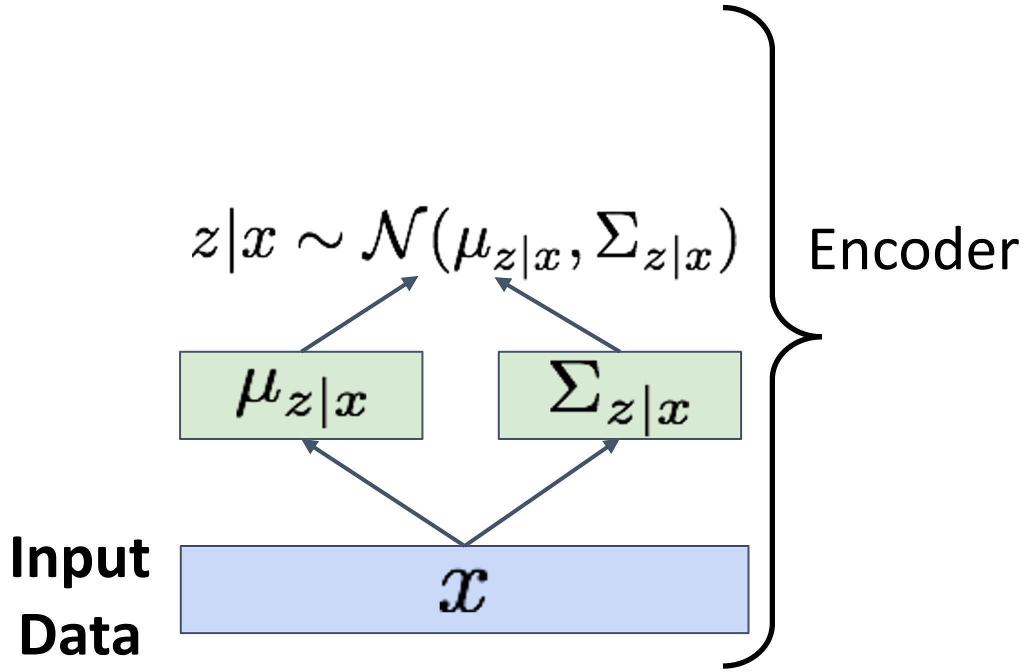
Kingma and Welling, Auto-Encoding Variational Beyes, ICLR 2014

Slide from Justin Johnson

Variational Autoencoders

After training we can **edit images**

1. Run input data through **encoder** to get a distribution over latent codes



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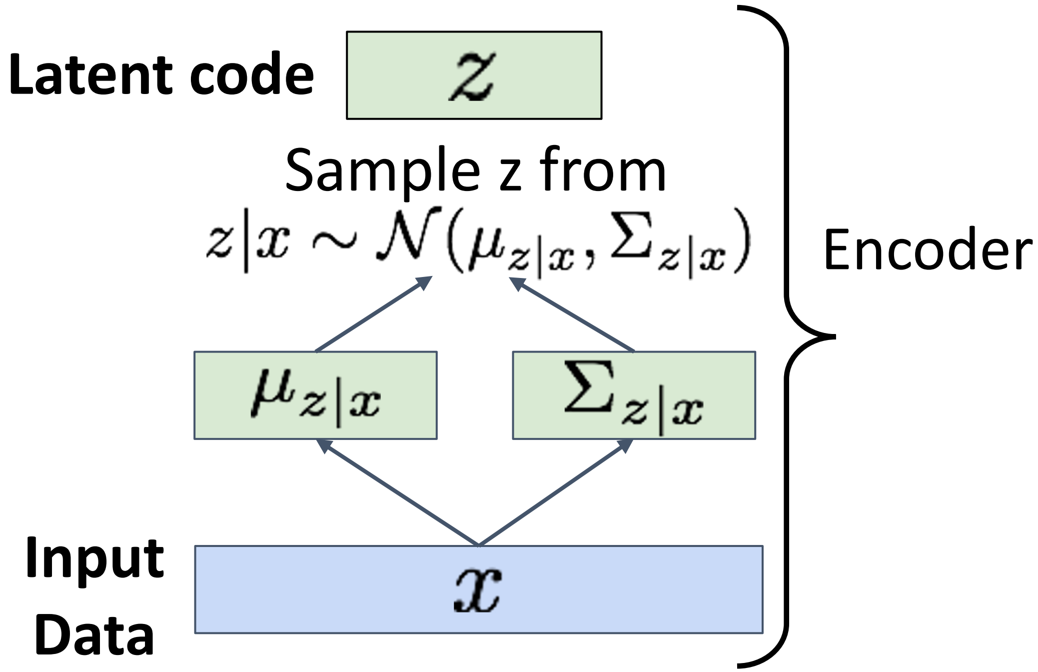
Variational Autoencoders

After training we can **edit images**

1. Run input data through **encoder** to get a distribution over latent codes
2. Sample code z from encoder output

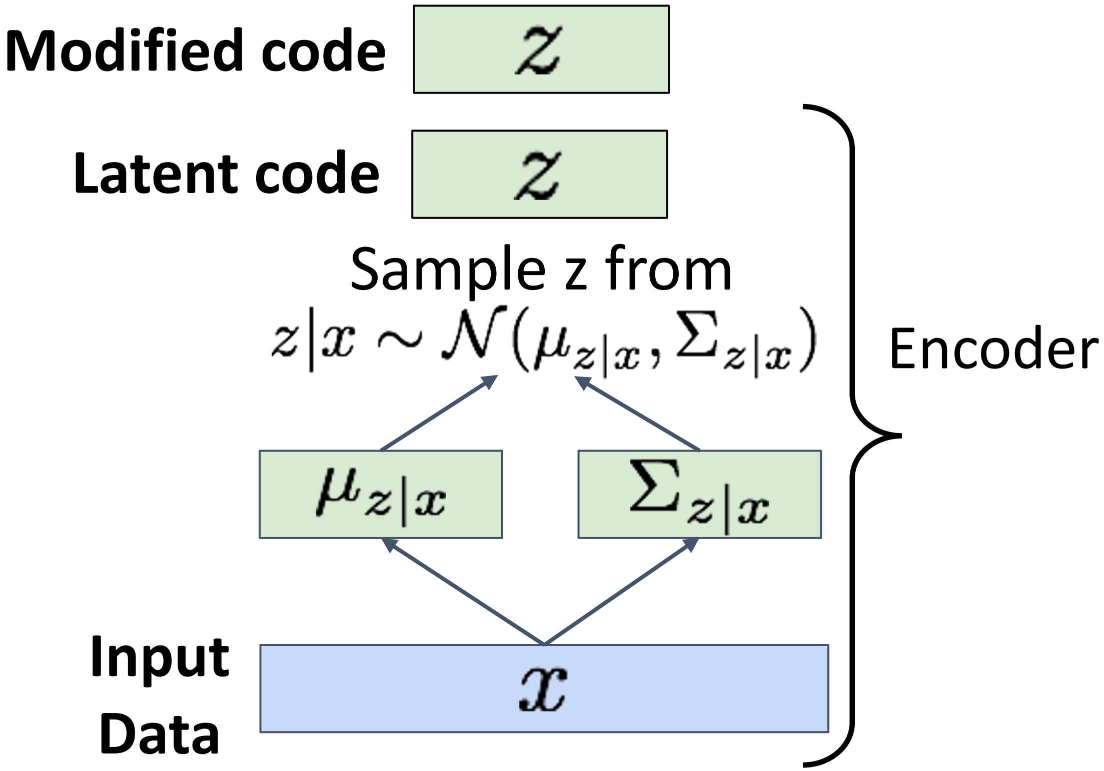


Slide from Justin Johnson

Variational Autoencoders

After training we can **edit images**

1. Run input data through **encoder** to get a distribution over latent codes
2. Sample code z from encoder output
3. Modify some dimensions of sampled code

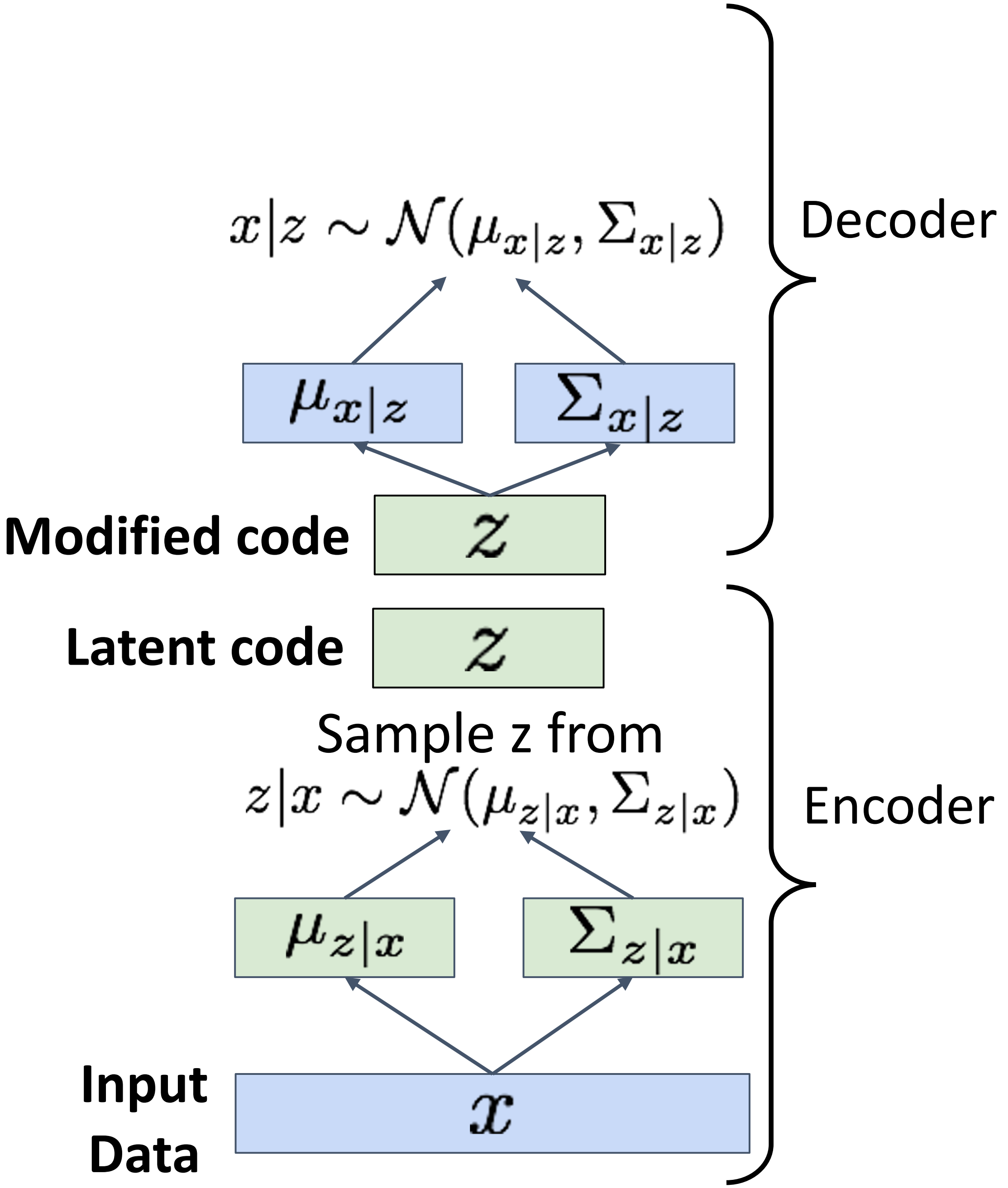


Slide from Justin Johnson

Variational Autoencoders

After training we can **edit images**

1. Run input data through **encoder** to get a distribution over latent codes
2. Sample code z from encoder output
3. Modify some dimensions of sampled code
4. Run modified z through **decoder** to get a distribution over data sample

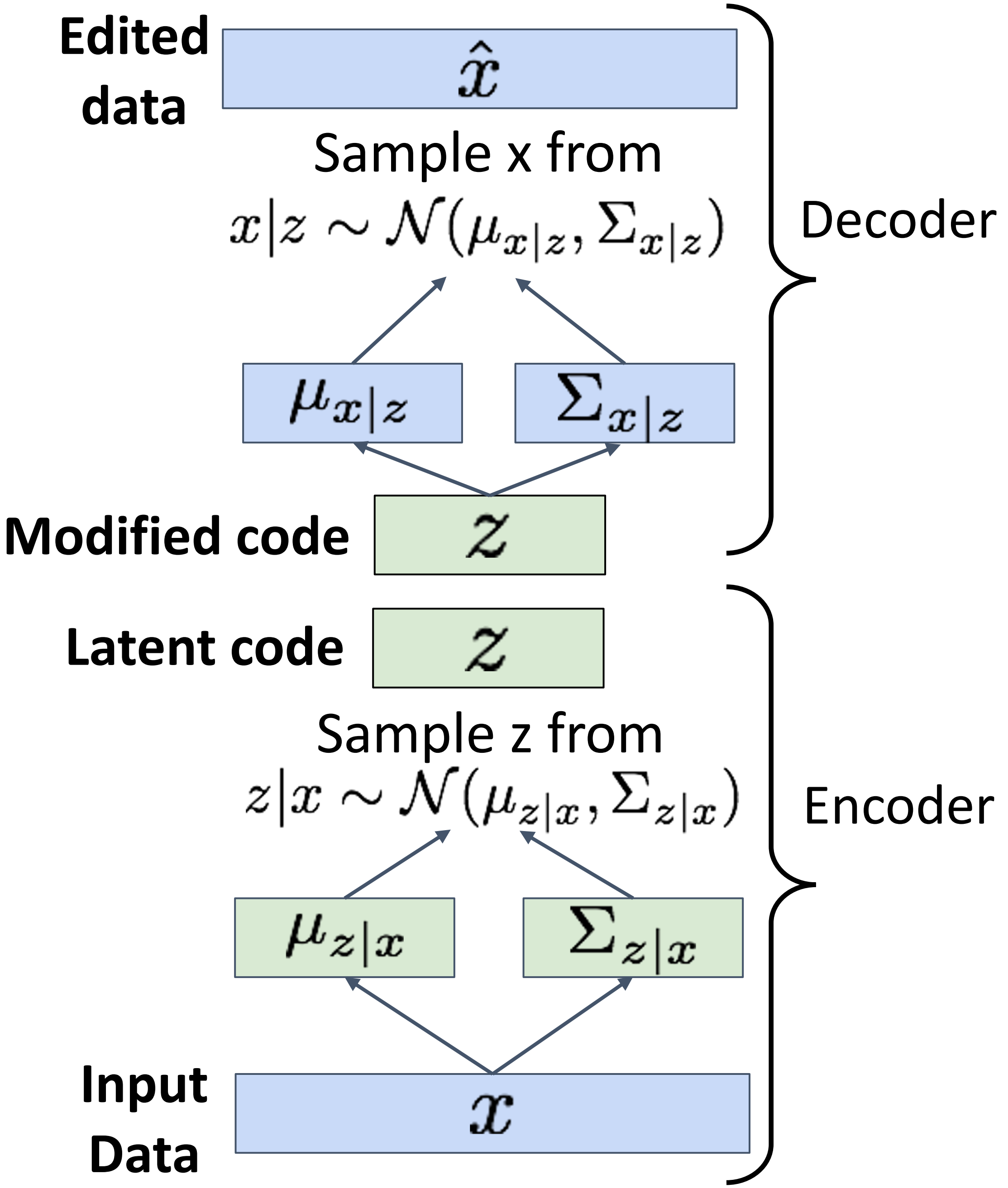


Slide from Justin Johnson

Variational Autoencoders

After training we can **edit images**

1. Run input data through **encoder** to get a distribution over latent codes
2. Sample code z from encoder output
3. Modify some dimensions of sampled code
4. Run modified z through **decoder** to get a distribution over data samples
5. Sample new data from (4)

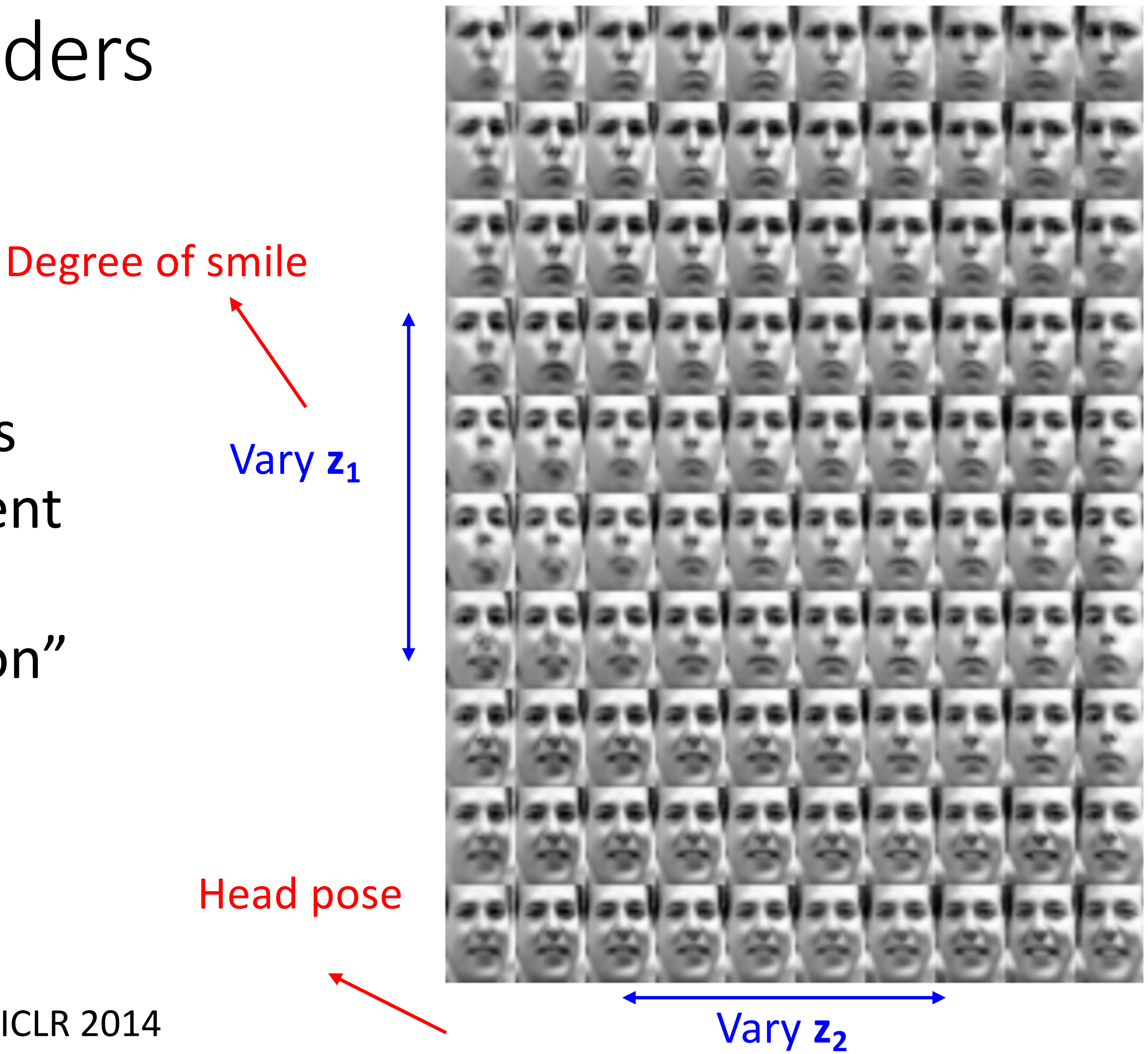


Slide from Justin Johnson

Variational Autoencoders

The diagonal prior on p(z) causes dimensions of z to be independent

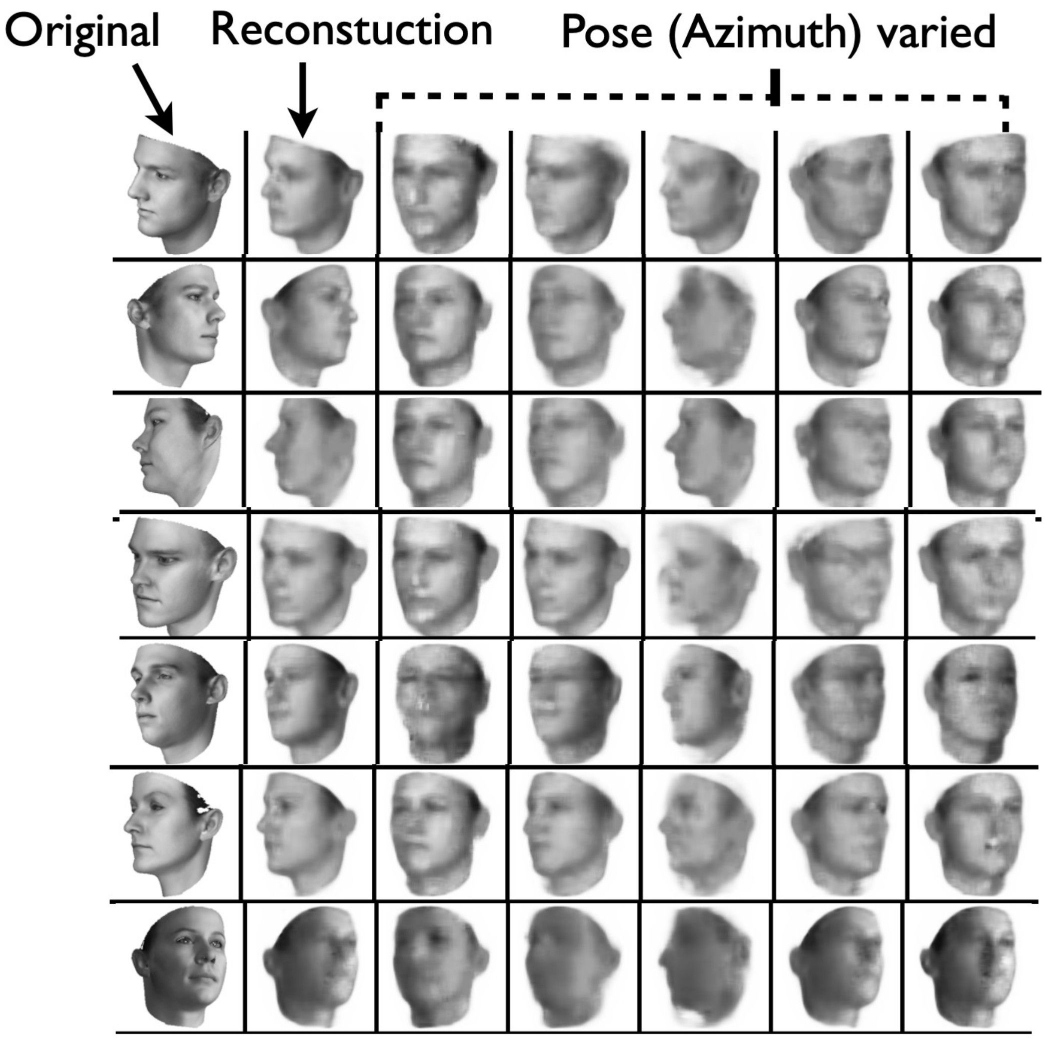
"Disentangling factors of variation"

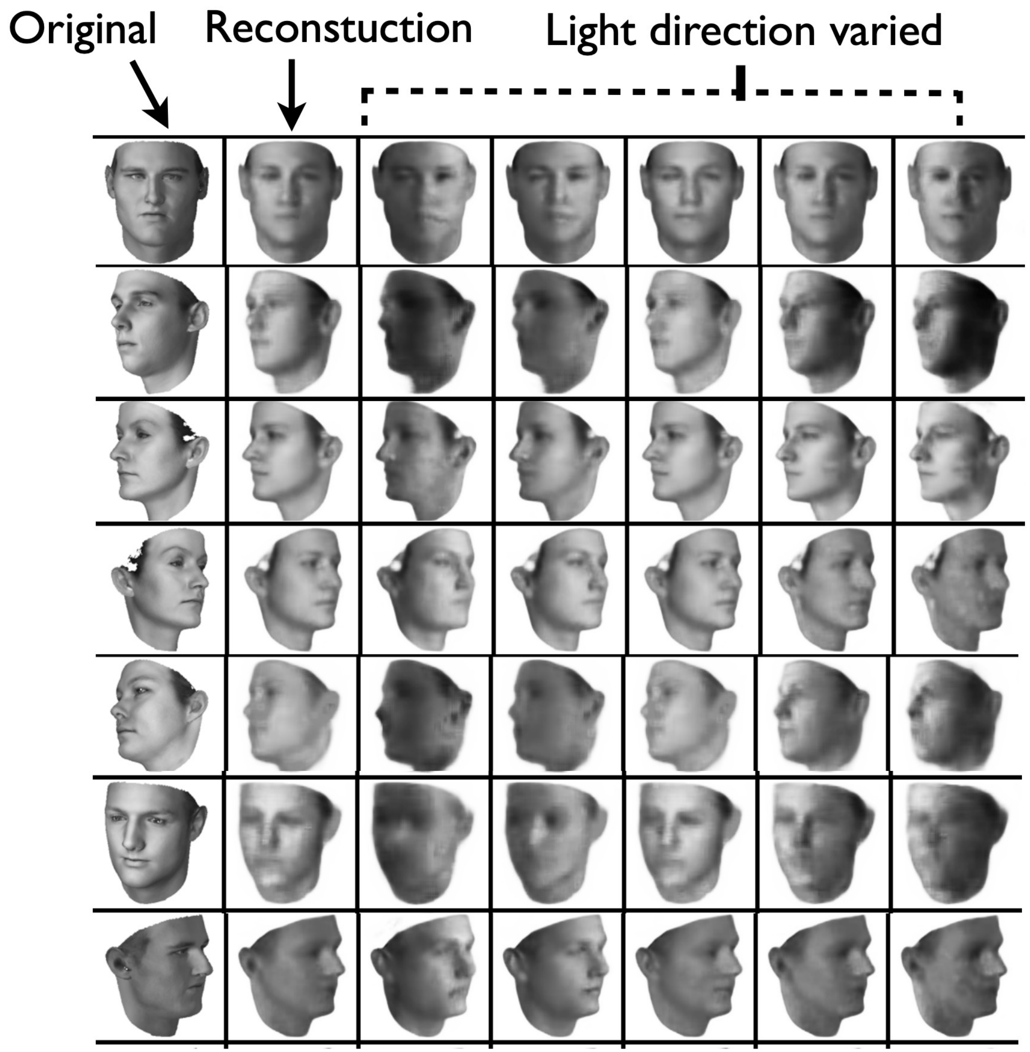


Kingma and Welling, Auto-Encoding Variational Beyes, ICLR 2014

Slide from Justin Johnson

Variational Autoencoders: Image Editing



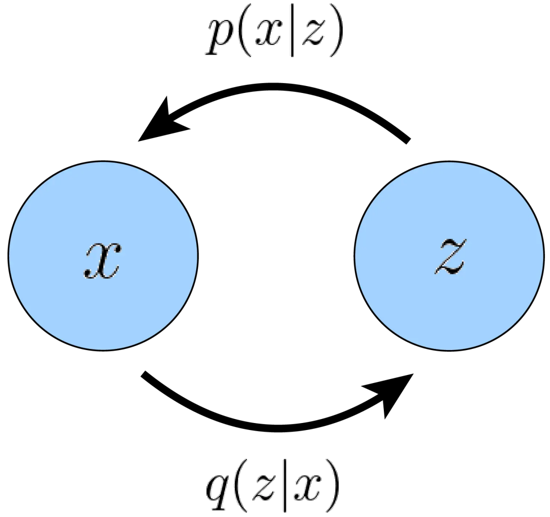


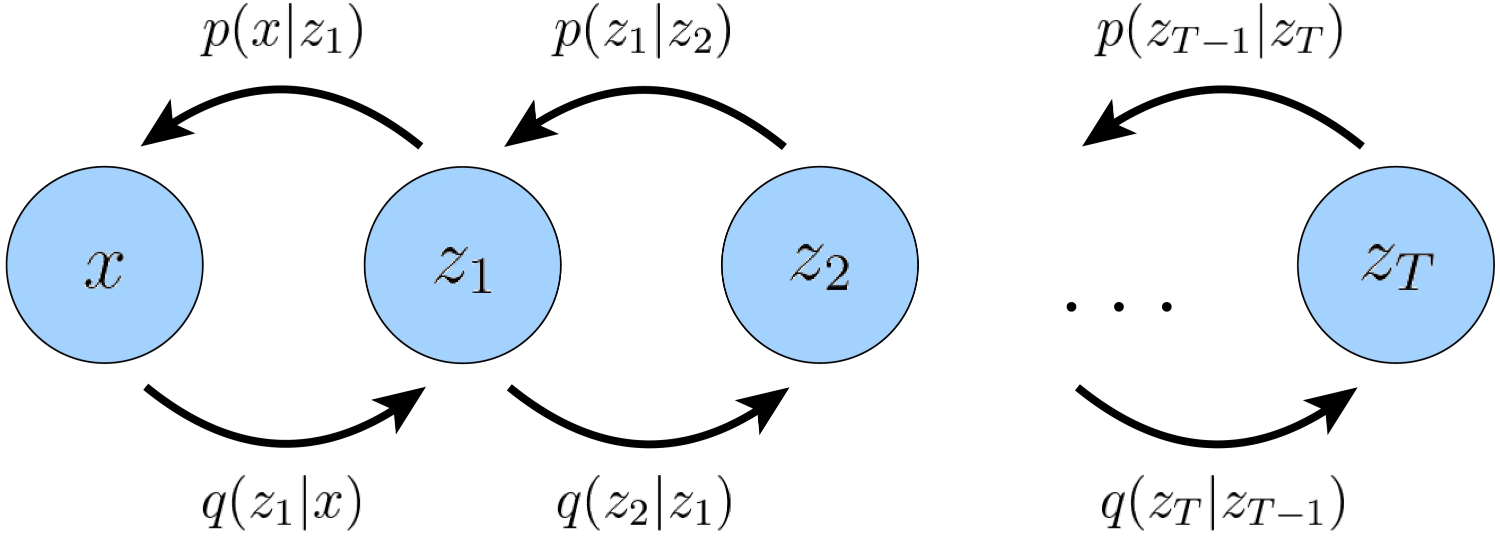
Kulkarni et al, "Deep Convolutional Inverse Graphics Networks", NeurIPS 2014

Slide from Justin Johnson

Diffusion Models

(Markovian) Hierarchical Variational Autoencoders





$$p(\boldsymbol{x}, \boldsymbol{z}_{1:T}) = p(\boldsymbol{z}_T) p_{\boldsymbol{\theta}}(\boldsymbol{x}|\boldsymbol{z}_1) \prod_{t=2}^{T} p_{\boldsymbol{\theta}}(\boldsymbol{z}_{t-1}|\boldsymbol{z}_t)$$

$$q_{\boldsymbol{\phi}}(\boldsymbol{z}_{1:T}|\boldsymbol{x}) = q_{\boldsymbol{\phi}}(\boldsymbol{z}_1|\boldsymbol{x}) \prod_{t=2}^{T} q_{\boldsymbol{\phi}}(\boldsymbol{z}_t|\boldsymbol{z}_{t-1})$$

Diffusion Models

A Markovian Hierarchical Variational Autoencoder with three key restrictions

1. The latent dimension is exactly equal to the data dimension

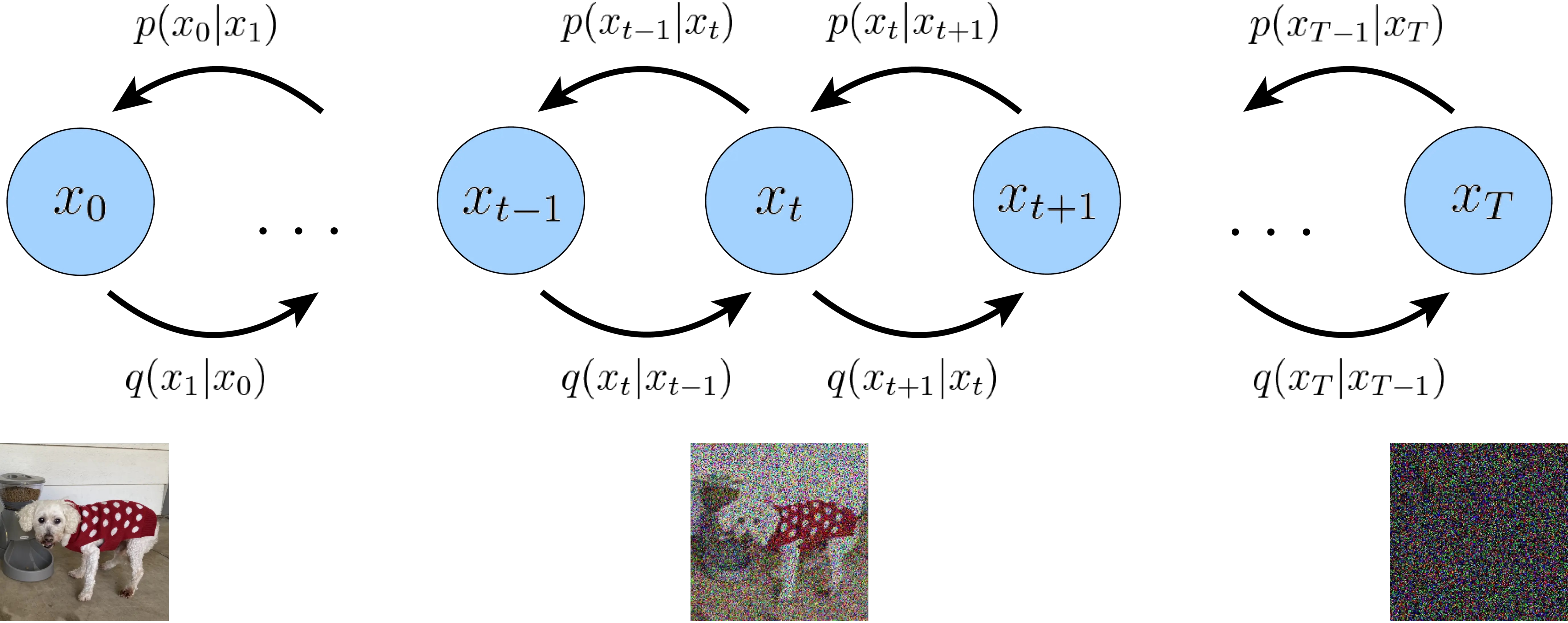
2. The structure of the latent encoder at each timestep is not learned; it is pre-defined as a linear Gaussian model. In other words, it is a Gaussian distribution centered around the output of the previous timestep

3. The Gaussian parameters of the latent encoders vary over time in such a way that the distribution of the latent at final timestep T is a standard Gaussian

Diffusion Models

$$q(\boldsymbol{x}_t|\boldsymbol{x}_{t-1}) = \mathcal{N}(\boldsymbol{x}_t; \sqrt{\alpha_t}\boldsymbol{x}_{t-1}, (1-\alpha_t)\mathbf{I})$$

$$p(\boldsymbol{x}_T) = \mathcal{N}(\boldsymbol{x}_T; \mathbf{0}, \mathbf{I})$$



ELBO for Diffusion Models

$$
\begin{aligned}
\log p(\boldsymbol{x}) &\geq \mathbb{E}_{q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)}\left[\log \frac{p(\boldsymbol{x}_{0:T})}{q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)}\right] \\
&= \mathbb{E}_{q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)}\left[\log \frac{p(\boldsymbol{x}_T)\prod_{t=1}^{T} p_{\boldsymbol{\theta}}(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t)}{\prod_{t=1}^{T} q(\boldsymbol{x}_t|\boldsymbol{x}_{t-1})}\right] \\
&= \mathbb{E}_{q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)}\left[\log \frac{p(\boldsymbol{x}_T)p_{\boldsymbol{\theta}}(\boldsymbol{x}_0|\boldsymbol{x}_1)\prod_{t=2}^{T} p_{\boldsymbol{\theta}}(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t)}{q(\boldsymbol{x}_1|\boldsymbol{x}_0)\prod_{t=2}^{T} q(\boldsymbol{x}_t|\boldsymbol{x}_{t-1})}\right] \\
&= \mathbb{E}_{q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)}\left[\log \frac{p(\boldsymbol{x}_T)p_{\boldsymbol{\theta}}(\boldsymbol{x}_0|\boldsymbol{x}_1)\prod_{t=2}^{T} p_{\boldsymbol{\theta}}(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t)}{q(\boldsymbol{x}_1|\boldsymbol{x}_0)\prod_{t=2}^{T} q(\boldsymbol{x}_t|\boldsymbol{x}_{t-1},\boldsymbol{x}_0)}\right] \\
&= \mathbb{E}_{q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)}\left[\log \frac{p_{\boldsymbol{\theta}}(\boldsymbol{x}_T)p_{\boldsymbol{\theta}}(\boldsymbol{x}_0|\boldsymbol{x}_1)}{q(\boldsymbol{x}_1|\boldsymbol{x}_0)} + \log \prod_{t=2}^{T} \frac{p_{\boldsymbol{\theta}}(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t)}{q(\boldsymbol{x}_t|\boldsymbol{x}_{t-1},\boldsymbol{x}_0)}\right] \\
&= \mathbb{E}_{q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)}\left[\log \frac{p(\boldsymbol{x}_T)p_{\boldsymbol{\theta}}(\boldsymbol{x}_0|\boldsymbol{x}_1)}{q(\boldsymbol{x}_1|\boldsymbol{x}_0)} + \log \prod_{t=2}^{T} \frac{p_{\boldsymbol{\theta}}(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t)}{\frac{q(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t,\boldsymbol{x}_0)q(\boldsymbol{x}_t|\boldsymbol{x}_0)}{q(\boldsymbol{x}_{t-1}|\boldsymbol{x}_0)}}\right]
\end{aligned}
$$

ELBO for Diffusion Models

$$
\begin{aligned}
&= \mathbb{E}_{q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)}\left[\log \frac{p(\boldsymbol{x}_T)p_{\boldsymbol{\theta}}(\boldsymbol{x}_0|\boldsymbol{x}_1)}{q(\boldsymbol{x}_1|\boldsymbol{x}_0)} + \log \prod_{t=2}^{T} \frac{p_{\boldsymbol{\theta}}(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t)}{\frac{q(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t,\boldsymbol{x}_0)\cancel{q(\boldsymbol{x}_t|\boldsymbol{x}_0)}}{\cancel{q(\boldsymbol{x}_{t-1}|\boldsymbol{x}_0)}}}\right] \\
&= \mathbb{E}_{q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)}\left[\log \frac{p(\boldsymbol{x}_T)p_{\boldsymbol{\theta}}(\boldsymbol{x}_0|\boldsymbol{x}_1)}{\cancel{q(\boldsymbol{x}_1|\boldsymbol{x}_0)}} + \log \frac{\cancel{q(\boldsymbol{x}_1|\boldsymbol{x}_0)}}{q(\boldsymbol{x}_T|\boldsymbol{x}_0)} + \log \prod_{t=2}^{T} \frac{p_{\boldsymbol{\theta}}(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t)}{q(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t,\boldsymbol{x}_0)}\right] \\
&= \mathbb{E}_{q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)}\left[\log \frac{p(\boldsymbol{x}_T)p_{\boldsymbol{\theta}}(\boldsymbol{x}_0|\boldsymbol{x}_1)}{q(\boldsymbol{x}_T|\boldsymbol{x}_0)} + \sum_{t=2}^{T} \log \frac{p_{\boldsymbol{\theta}}(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t)}{q(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t,\boldsymbol{x}_0)}\right] \\
&= \mathbb{E}_{q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)}\left[\log p_{\boldsymbol{\theta}}(\boldsymbol{x}_0|\boldsymbol{x}_1)\right] + \mathbb{E}_{q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)}\left[\log \frac{p(\boldsymbol{x}_T)}{q(\boldsymbol{x}_T|\boldsymbol{x}_0)}\right] + \sum_{t=2}^{T} \mathbb{E}_{q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)}\left[\log \frac{p_{\boldsymbol{\theta}}(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t)}{q(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t,\boldsymbol{x}_0)}\right] \\
&= \mathbb{E}_{q(\boldsymbol{x}_1|\boldsymbol{x}_0)}\left[\log p_{\boldsymbol{\theta}}(\boldsymbol{x}_0|\boldsymbol{x}_1)\right] + \mathbb{E}_{q(\boldsymbol{x}_T|\boldsymbol{x}_0)}\left[\log \frac{p(\boldsymbol{x}_T)}{q(\boldsymbol{x}_T|\boldsymbol{x}_0)}\right] + \sum_{t=2}^{T} \mathbb{E}_{q(\boldsymbol{x}_t,\boldsymbol{x}_{t-1}|\boldsymbol{x}_0)}\left[\log \frac{p_{\boldsymbol{\theta}}(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t)}{q(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t,\boldsymbol{x}_0)}\right] \\
&= \underbrace{\mathbb{E}_{q(\boldsymbol{x}_1|\boldsymbol{x}_0)}\left[\log p_{\boldsymbol{\theta}}(\boldsymbol{x}_0|\boldsymbol{x}_1)\right]}_{\text{reconstruction term}} - \underbrace{D_{\mathrm{KL}}(q(\boldsymbol{x}_T|\boldsymbol{x}_0) \parallel p(\boldsymbol{x}_T))}_{\text{prior matching term}} - \sum_{t=2}^{T} \underbrace{\mathbb{E}_{q(\boldsymbol{x}_t|\boldsymbol{x}_0)}\left[D_{\mathrm{KL}}(q(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t,\boldsymbol{x}_0) \parallel p_{\boldsymbol{\theta}}(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t))\right]}_{\text{denoising matching term}}
\end{aligned}
$$

ELBO for Diffusion Models

$$
\begin{aligned}
&= \mathbb{E}_{q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)}\left[\log \frac{p(\boldsymbol{x}_T)p_{\boldsymbol{\theta}}(\boldsymbol{x}_0|\boldsymbol{x}_1)}{q(\boldsymbol{x}_1|\boldsymbol{x}_0)} + \log \prod_{t=2}^{T} \frac{p_{\boldsymbol{\theta}}(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t)}{\frac{q(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t,\boldsymbol{x}_0)\cancel{q(\boldsymbol{x}_t|\boldsymbol{x}_0)}}{\cancel{q(\boldsymbol{x}_{t-1}|\boldsymbol{x}_0)}}}\right] \\
&= \mathbb{E}_{q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)}\left[\log \frac{p(\boldsymbol{x}_T)p_{\boldsymbol{\theta}}(\boldsymbol{x}_0|\boldsymbol{x}_1)}{\cancel{q(\boldsymbol{x}_1|\boldsymbol{x}_0)}} + \log \frac{\cancel{q(\boldsymbol{x}_1|\boldsymbol{x}_0)}}{q(\boldsymbol{x}_T|\boldsymbol{x}_0)} + \log \prod_{t=2}^{T} \frac{p_{\boldsymbol{\theta}}(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t)}{q(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t,\boldsymbol{x}_0)}\right] \\
&= \mathbb{E}_{q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)}\left[\log \frac{p(\boldsymbol{x}_T)p_{\boldsymbol{\theta}}(\boldsymbol{x}_0|\boldsymbol{x}_1)}{q(\boldsymbol{x}_T|\boldsymbol{x}_0)} + \sum_{t=2}^{T} \log \frac{p_{\boldsymbol{\theta}}(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t)}{q(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t,\boldsymbol{x}_0)}\right] \\
&= \mathbb{E}_{q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)}\left[\log p_{\boldsymbol{\theta}}(\boldsymbol{x}_0|\boldsymbol{x}_1)\right] + \mathbb{E}_{q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)}\left[\log \frac{p(\boldsymbol{x}_T)}{q(\boldsymbol{x}_T|\boldsymbol{x}_0)}\right] + \sum_{t=2}^{T} \mathbb{E}_{q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)}\left[\log \frac{p_{\boldsymbol{\theta}}(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t)}{q(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t,\boldsymbol{x}_0)}\right] \\
&= \mathbb{E}_{q(\boldsymbol{x}_1|\boldsymbol{x}_0)}\left[\log p_{\boldsymbol{\theta}}(\boldsymbol{x}_0|\boldsymbol{x}_1)\right] + \mathbb{E}_{q(\boldsymbol{x}_T|\boldsymbol{x}_0)}\left[\log \frac{p(\boldsymbol{x}_T)}{q(\boldsymbol{x}_T|\boldsymbol{x}_0)}\right] + \sum_{t=2}^{T} \mathbb{E}_{q(\boldsymbol{x}_t,\boldsymbol{x}_{t-1}|\boldsymbol{x}_0)}\left[\log \frac{p_{\boldsymbol{\theta}}(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t)}{q(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t,\boldsymbol{x}_0)}\right] \\
&= \underbrace{\mathbb{E}_{q(\boldsymbol{x}_1|\boldsymbol{x}_0)}\left[\log p_{\boldsymbol{\theta}}(\boldsymbol{x}_0|\boldsymbol{x}_1)\right]}_{\text{reconstruction term}} - \underbrace{D_{\mathrm{KL}}(q(\boldsymbol{x}_T|\boldsymbol{x}_0) \parallel p(\boldsymbol{x}_T))}_{\text{prior matching term}} - \sum_{t=2}^{T} \underbrace{\mathbb{E}_{q(\boldsymbol{x}_t|\boldsymbol{x}_0)}\left[D_{\mathrm{KL}}(q(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t,\boldsymbol{x}_0) \parallel p_{\boldsymbol{\theta}}(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t))\right]}_{\text{denoising matching term}}
\end{aligned}
$$

Computing the Denoising Matching Term

$$= \underbrace{\mathbb{E}_{q(\boldsymbol{x}_1|\boldsymbol{x}_0)}\left[\log p_{\boldsymbol{\theta}}(\boldsymbol{x}_0|\boldsymbol{x}_1)\right]}_{\text{reconstruction term}} - \underbrace{D_{\mathrm{KL}}(q(\boldsymbol{x}_T|\boldsymbol{x}_0) \parallel p(\boldsymbol{x}_T))}_{\text{prior matching term}} - \sum_{t=2}^{T} \underbrace{\mathbb{E}_{q(\boldsymbol{x}_t|\boldsymbol{x}_0)}\left[D_{\mathrm{KL}}(q(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t, \boldsymbol{x}_0) \parallel p_{\boldsymbol{\theta}}(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t))\right]}_{\text{denoising matching term}}$$

$$q(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t, \boldsymbol{x}_0) = \frac{q(\boldsymbol{x}_t|\boldsymbol{x}_{t-1}, \boldsymbol{x}_0)q(\boldsymbol{x}_{t-1}|\boldsymbol{x}_0)}{q(\boldsymbol{x}_t|\boldsymbol{x}_0)}$$

$$= \frac{\mathcal{N}(\boldsymbol{x}_t; \sqrt{\alpha_t}\boldsymbol{x}_{t-1}, (1-\alpha_t)\mathbf{I})\mathcal{N}(\boldsymbol{x}_{t-1}; \sqrt{\bar{\alpha}_{t-1}}\boldsymbol{x}_0, (1-\bar{\alpha}_{t-1})\mathbf{I})}{\mathcal{N}(\boldsymbol{x}_t; \sqrt{\bar{\alpha}_t}\boldsymbol{x}_0, (1-\bar{\alpha}_t)\mathbf{I})}$$

$$= \exp\left\{-\frac{1}{2}\left(\frac{1}{\frac{(1-\alpha_t)(1-\bar{\alpha}_{t-1})}{1-\bar{\alpha}_t}}\right)\left[\boldsymbol{x}_{t-1}^2 - 2\frac{\sqrt{\alpha_t}(1-\bar{\alpha}_{t-1})\boldsymbol{x}_t + \sqrt{\bar{\alpha}_{t-1}}(1-\alpha_t)\boldsymbol{x}_0}{1-\bar{\alpha}_t}\boldsymbol{x}_{t-1}\right]\right\}$$

$$\propto \mathcal{N}(\boldsymbol{x}_{t-1}; \underbrace{\frac{\sqrt{\alpha_t}(1-\bar{\alpha}_{t-1})\boldsymbol{x}_t + \sqrt{\bar{\alpha}_{t-1}}(1-\alpha_t)\boldsymbol{x}_0}{1-\bar{\alpha}_t}}_{\mu_q(\boldsymbol{x}_t, \boldsymbol{x}_0)}, \underbrace{\frac{(1-\alpha_t)(1-\bar{\alpha}_{t-1})}{1-\bar{\alpha}_t}\mathbf{I}}_{\boldsymbol{\Sigma}_q(t)})$$

Loss Function

$$= \underbrace{\mathbb{E}_{q(\boldsymbol{x}_1|\boldsymbol{x}_0)}\left[\log p_{\boldsymbol{\theta}}(\boldsymbol{x}_0|\boldsymbol{x}_1)\right]}_{\text{reconstruction term}} - \underbrace{D_{\mathrm{KL}}(q(\boldsymbol{x}_T|\boldsymbol{x}_0) \parallel p(\boldsymbol{x}_T))}_{\text{prior matching term}} - \sum_{t=2}^{T} \underbrace{\mathbb{E}_{q(\boldsymbol{x}_t|\boldsymbol{x}_0)}\left[D_{\mathrm{KL}}(q(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t, \boldsymbol{x}_0) \parallel p_{\boldsymbol{\theta}}(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t))\right]}_{\text{denoising matching term}}$$

$$q(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t, \boldsymbol{x}_0) \propto \mathcal{N}(\boldsymbol{x}_{t-1}; \underbrace{\frac{\sqrt{\alpha_t}(1-\bar{\alpha}_{t-1})\boldsymbol{x}_t + \sqrt{\bar{\alpha}_{t-1}}(1-\alpha_t)\boldsymbol{x}_0}{1-\bar{\alpha}_t}}_{\mu_q(\boldsymbol{x}_t, \boldsymbol{x}_0)}, \underbrace{\frac{(1-\alpha_t)(1-\bar{\alpha}_{t-1})}{1-\bar{\alpha}_t}\mathbf{I}}_{\boldsymbol{\Sigma}_q(t)})$$

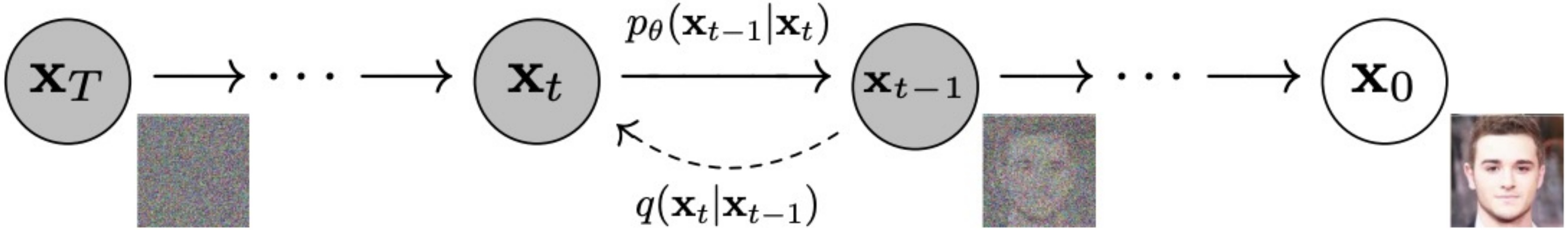
We will assume $p_\theta(x_{t-1}|x_t)$ can be approximated as a Gaussian.

$$D_{\mathrm{KL}}(\mathcal{N}(\boldsymbol{x}; \boldsymbol{\mu}_x, \boldsymbol{\Sigma}_x) \parallel \mathcal{N}(\boldsymbol{y}; \boldsymbol{\mu}_y, \boldsymbol{\Sigma}_y)) = \frac{1}{2}\left[\log\frac{|\boldsymbol{\Sigma}_y|}{|\boldsymbol{\Sigma}_x|} - d + \mathrm{tr}(\boldsymbol{\Sigma}_y^{-1}\boldsymbol{\Sigma}_x) + (\boldsymbol{\mu}_y - \boldsymbol{\mu}_x)^T\boldsymbol{\Sigma}_y^{-1}(\boldsymbol{\mu}_y - \boldsymbol{\mu}_x)\right]$$

$$\arg\min_{\boldsymbol{\theta}} D_{\mathrm{KL}}(q(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t, \boldsymbol{x}_0) \parallel p_{\boldsymbol{\theta}}(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t)) = \arg\min_{\boldsymbol{\theta}} \frac{1}{2\sigma_q^2(t)}\left[\left\|\boldsymbol{\mu}_{\boldsymbol{\theta}} - \boldsymbol{\mu}_q\right\|_2^2\right]$$

$$= \arg\min_{\boldsymbol{\theta}} \frac{1}{2\sigma_q^2(t)} \frac{\bar{\alpha}_{t-1}(1-\alpha_t)^2}{(1-\bar{\alpha}_t)^2}\left[\left\|\hat{\boldsymbol{x}}_{\boldsymbol{\theta}}(\boldsymbol{x}_t, t) - \boldsymbol{x}_0\right\|_2^2\right]$$

DDPMs: Basic idea



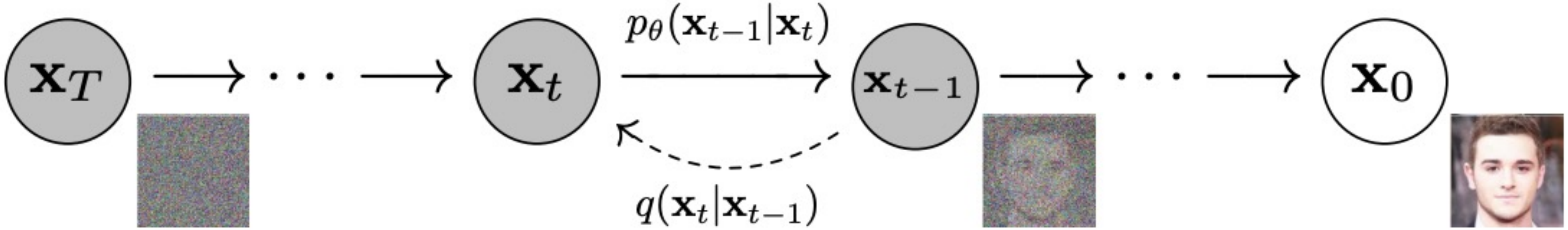
Unconditional CIFAR10 sample generation

J. Ho et al. [Denoising diffusion probabilistic models](). NeurIPS 2020

Blog introduction: https://lilianweng.github.io/posts/2021-07-11-diffusion-models/

CVPR 2022 tutorial

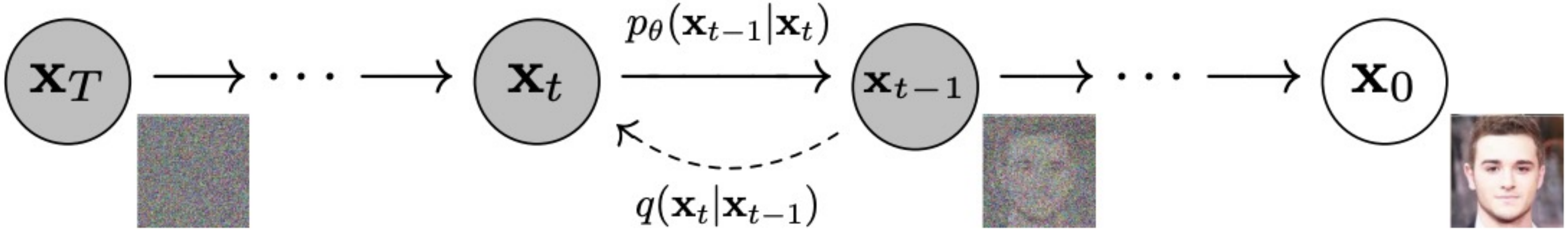
DDPMs: Basic idea



- *Forward process* q turns images into Gaussian noise
- *Reverse process* p turns noise into images
- Provided the increments of t are small enough, $p_\theta(x_{t-1}|x_t)$ is Gaussian and we can train a neural network to estimate the mean of x_{t-1} given x_t

J. Ho et al. Denoising diffusion probabilistic models. NeurIPS 2020

DDPMs: Basic idea



Algorithm 1 Training

1: **repeat**

2: $\mathbf{x}_0 \sim q(\mathbf{x}_0)$

3: $t \sim \text{Uniform}(\{1, \ldots, T\})$

4: $\boldsymbol{\epsilon} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$

5: Take gradient descent step on

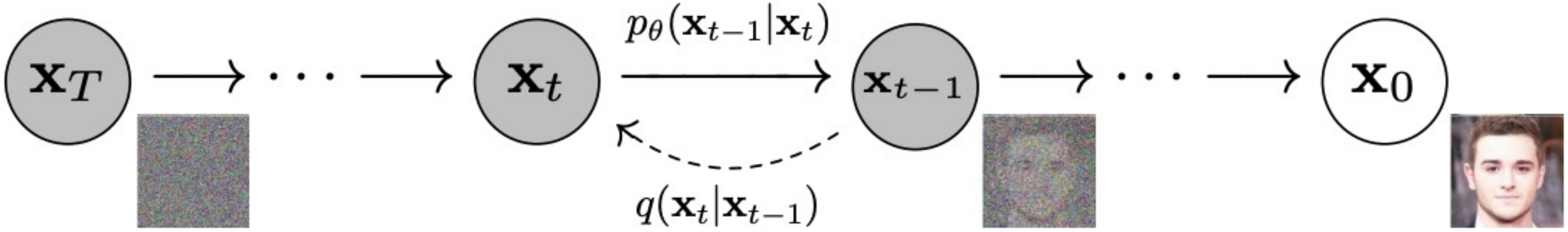
$$\nabla_\theta \left\| \boldsymbol{\epsilon} - \boldsymbol{\epsilon}_\theta(x_t , t) \right\|^2$$

6: **until** converged

- $\epsilon_\theta(x_t, t)$ is the predicted noise component of image x_t given noise level t
- Network parameters θ are updated to reduce L2 error between actual noise ϵ and predicted noise $\epsilon_\theta(x_t, t)$

J. Ho et al. Denoising diffusion probabilistic models. NeurIPS 2020

DDPMs: Basic idea



Algorithm 1 Training

repeat
  $\mathbf{x}_0 \sim q(\mathbf{x}_0)$
  $t \sim \mathrm{Uniform}(\{1, \ldots, T\})$
  $\boldsymbol{\epsilon} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
  Take gradient descent step on

$$\nabla_\theta \left\| \boldsymbol{\epsilon} - \boldsymbol{\epsilon}_\theta(\sqrt{\bar{\alpha}_t}\mathbf{x}_0 + \sqrt{1-\bar{\alpha}_t}\boldsymbol{\epsilon}, t) \right\|^2$$

until converged

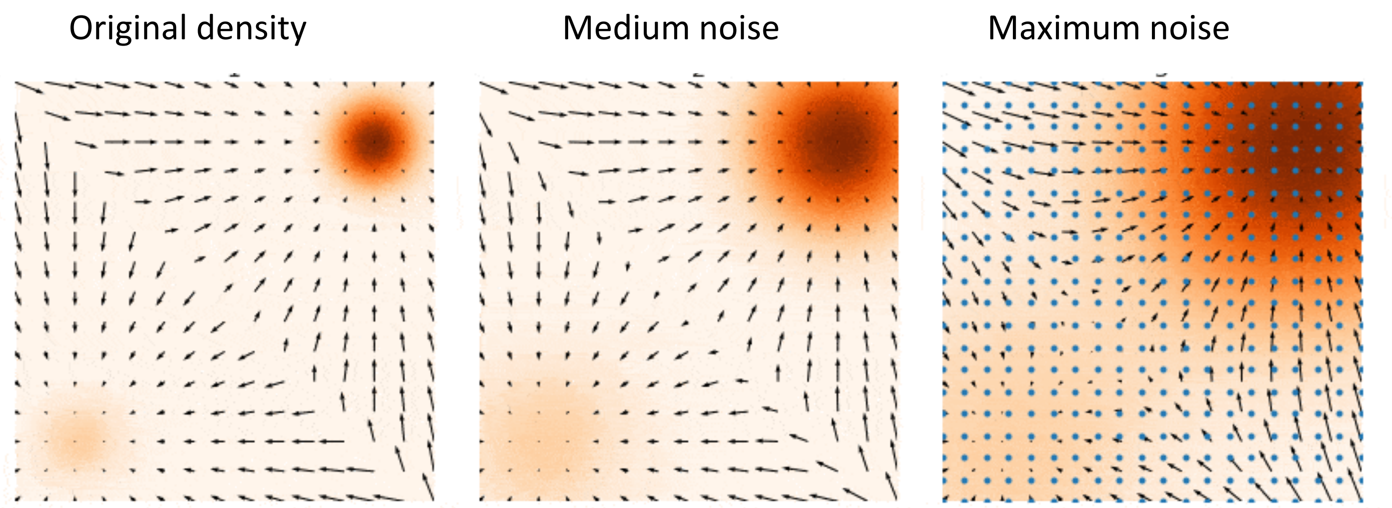
Algorithm 2 Sampling

$\mathbf{x}_T \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
for $t = T, \ldots, 1$ **do**
  $\mathbf{z} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$ if $t > 1$, else $\mathbf{z} = \mathbf{0}$
  $\mathbf{x}_{t-1} = \frac{1}{\sqrt{\alpha_t}}\left(\mathbf{x}_t - \frac{1-\alpha_t}{\sqrt{1-\bar{\alpha}_t}}\boldsymbol{\epsilon}_\theta(\mathbf{x}_t, t)\right) + \sigma_t \mathbf{z}$
end for
return $\mathbf{x}_0$

J. Ho et al. Denoising diffusion probabilistic models. NeurIPS 2020

Alternate viewpoint: Score-based generative modeling

- It can be shown that $\epsilon_\theta(x_t, t) \approx -\nabla_{x_t} \log q(x_t)$, where $\nabla_{x_t} \log q(x_t)$ is the *score function* of the (noisy) data distribution
- To sample from the original data density $q(x_0)$, we can use *annealed Langevin dynamics,* i.e., start by sampling from noise-perturbed versions of the data distribution and gradually reduce the amount of noise



Algorithm 1 Annealed Langevin dynamics.

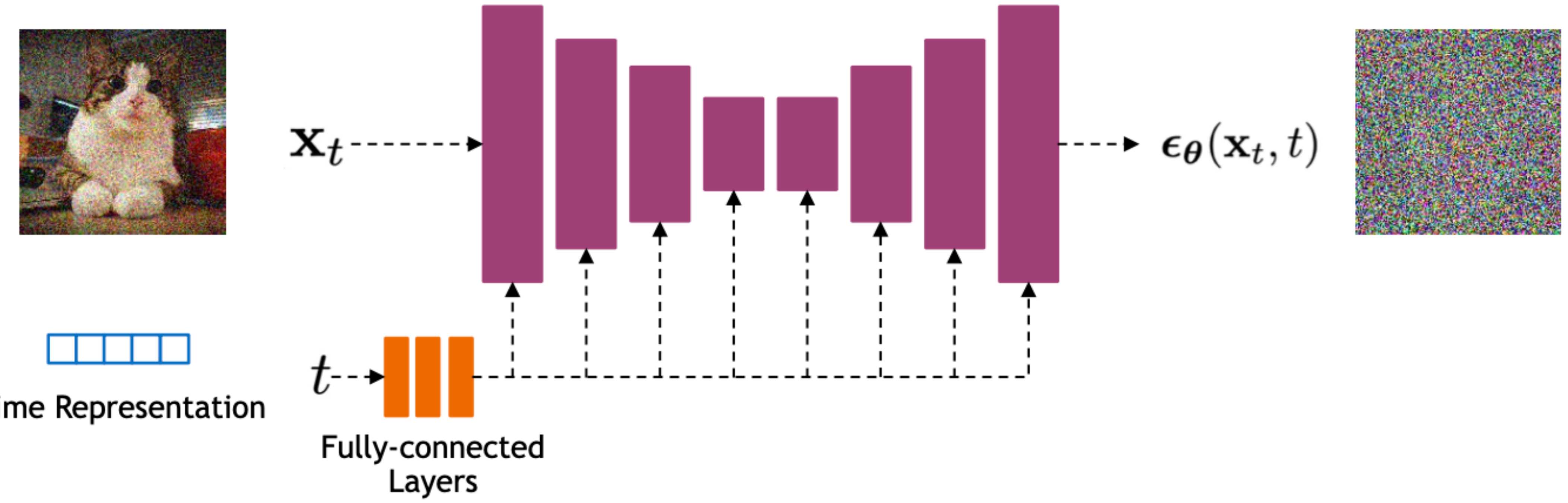
Require: $\{\sigma_i\}_{i=1}^{L}, \epsilon, T$.

Initialize $\tilde{\mathbf{x}}_0$
for $i \leftarrow 1$ to L **do**
  $\alpha_i \leftarrow \epsilon \cdot \sigma_i^2/\sigma_L^2$ ▷ α_i is the step size.
  for $t \leftarrow 1$ to T **do**
    Draw $\mathbf{z}_t \sim \mathcal{N}(0, I)$
    $\tilde{\mathbf{x}}_t \leftarrow \tilde{\mathbf{x}}_{t-1} + \frac{\alpha_i}{2}\mathbf{s}_\theta(\tilde{\mathbf{x}}_{t-1}, \sigma_i) + \sqrt{\alpha_i}\,\mathbf{z}_t$
  end for
  $\tilde{\mathbf{x}}_0 \leftarrow \tilde{\mathbf{x}}_T$
end for
return $\tilde{\mathbf{x}}_T$

Y. Song and S. Ermon. Generative Modeling by Estimating Gradients of the Data Distribution. NeurIPS 2019
https://yang-song.net/blog/2021/score/

DDPMs: Implementation

- U-Net architectures are typically used to represent $\epsilon_\theta(x_t, t)$
  - Bells and whistles: residual blocks, self-attention



- Time is encoded using sinusoidal positional embeddings or random Fourier features, fed into the U-Net using addition or adaptive normalization

Source: CVPR 2002 DM tutorial