Autoencoders and Generative Models

CISC 7026: Introduction to Deep Learning

University of Macau

Agenda

1. Review
2. Compression
3. Autoencoders
4. Applications
5. Variational Modeling
6. VAE Implementation
7. Coding

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Convolution works over inputs of any variables (time, space, etc)

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Recurrent neural networks only work with time

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Convolution makes use of locality and translation equivariance properties

Recurrent models do not assume locality or equivariance

Equivariance and locality make learning more efficient, but not all problems have this structure

Review

How do humans process temporal data?

Review

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Humans only perceive the present

Review

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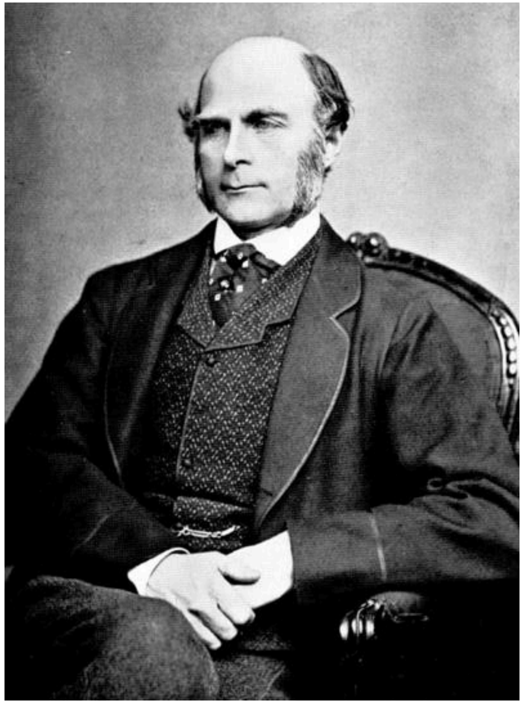
Humans only perceive the present

Humans process temporal data by storing and recalling memories

Review

Francis Galton (1822-1911)

photo composite memory



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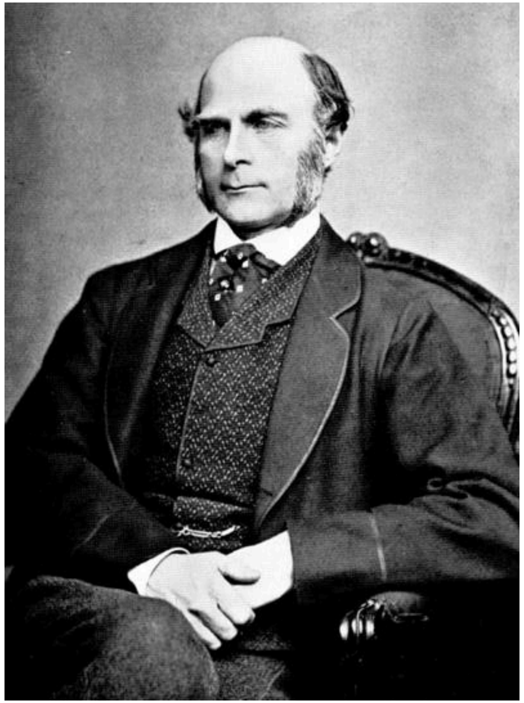
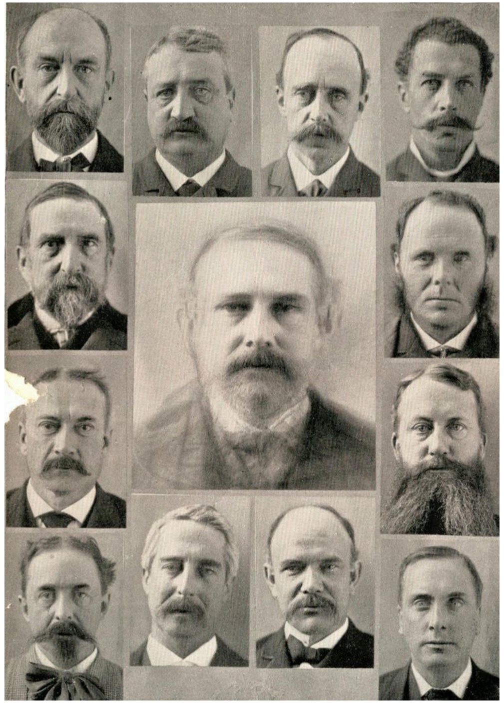


Composite photo of members of a party



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Task: Find a mathematical model of how our mind represents memories

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We repeat the same process for each new face

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We can rewrite f as a **recurrent function**

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Humans forget old information

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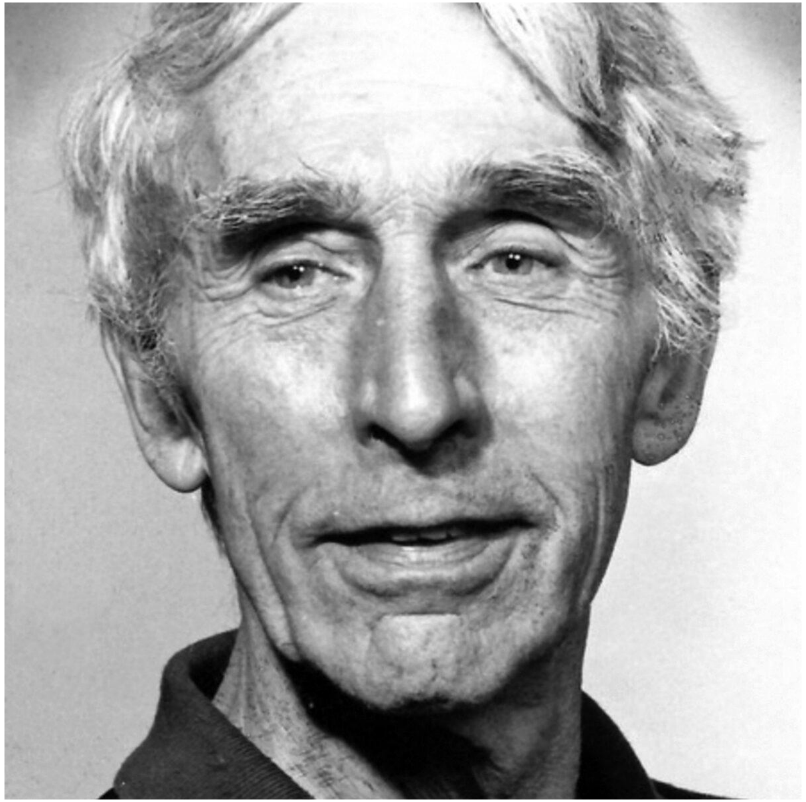
Murdock (1982)



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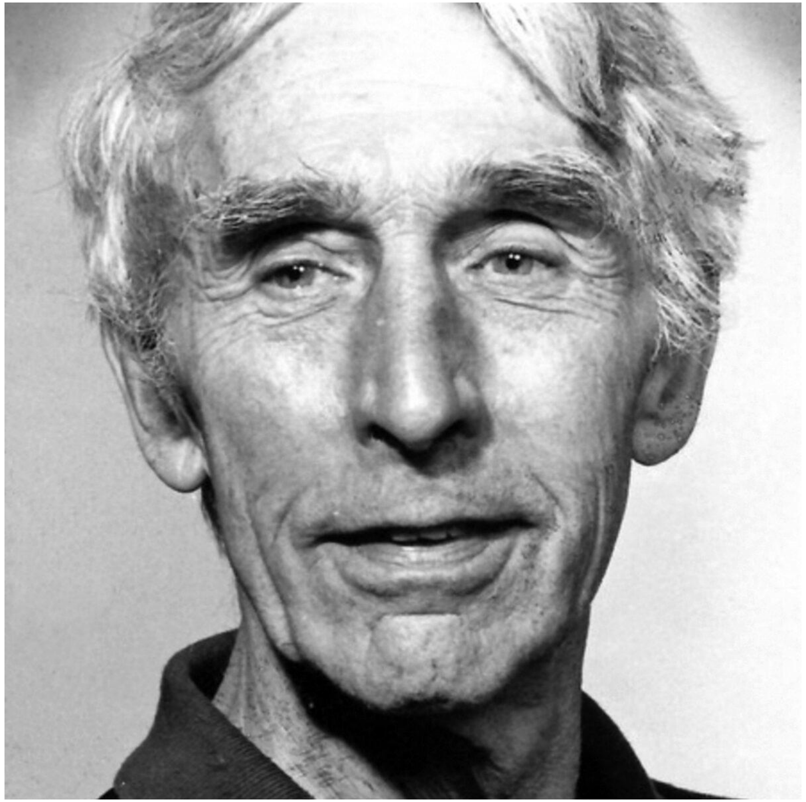

$$f(\boldsymbol{h}, \boldsymbol{x}, \boldsymbol{\theta}) = {\color{red}\gamma} \boldsymbol{h} + \boldsymbol{\theta}^\top \overline{\boldsymbol{x}}; \quad 0 < \gamma < 1$$

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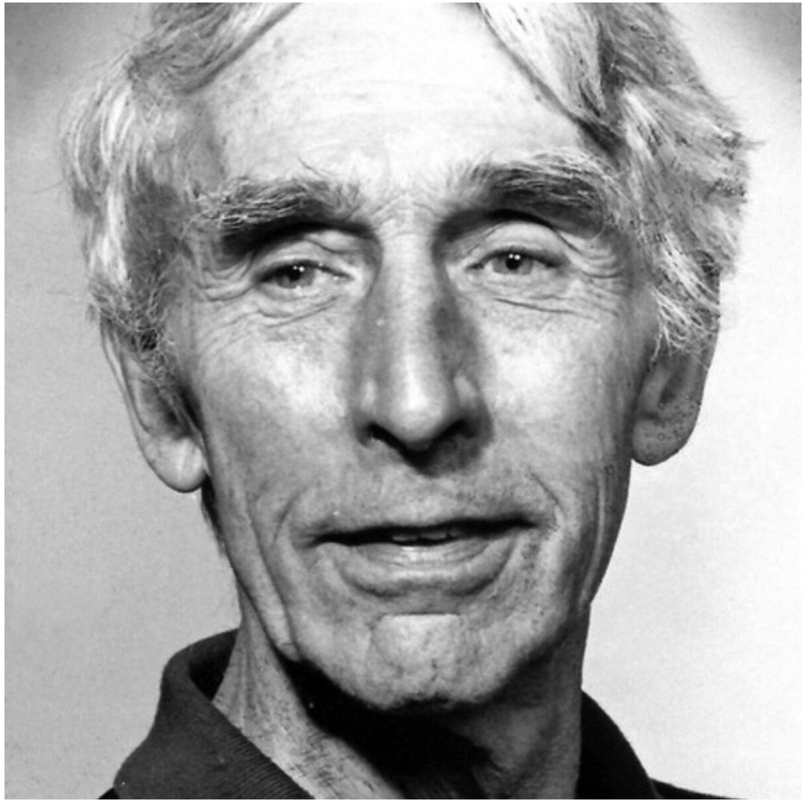

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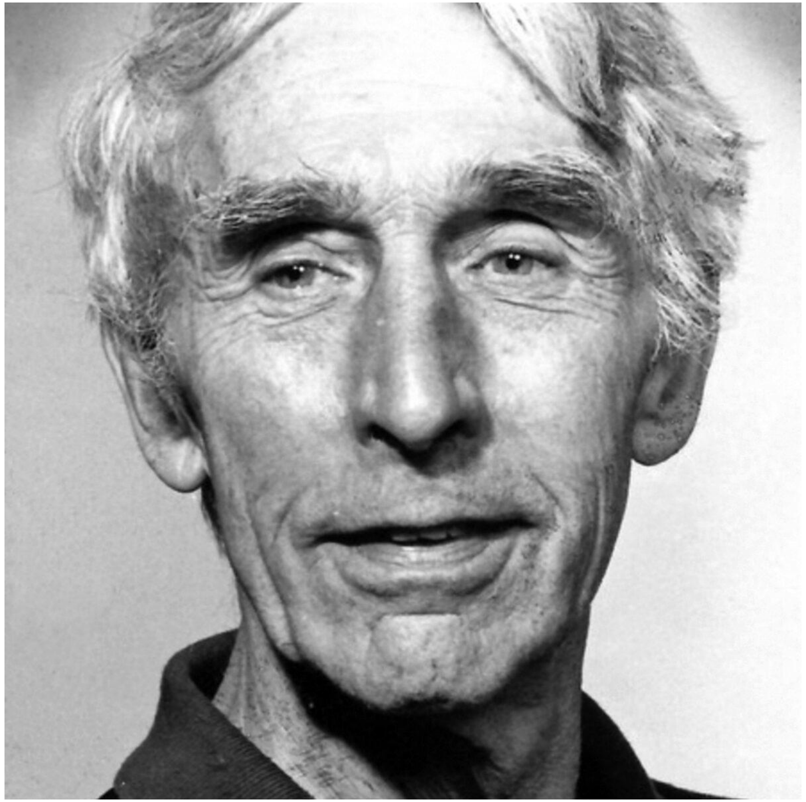

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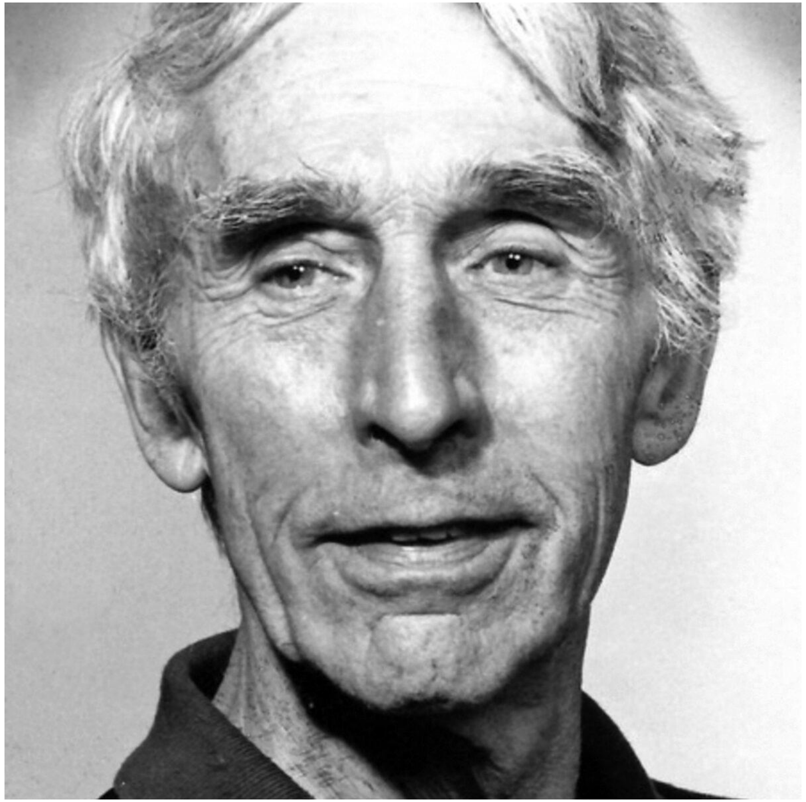

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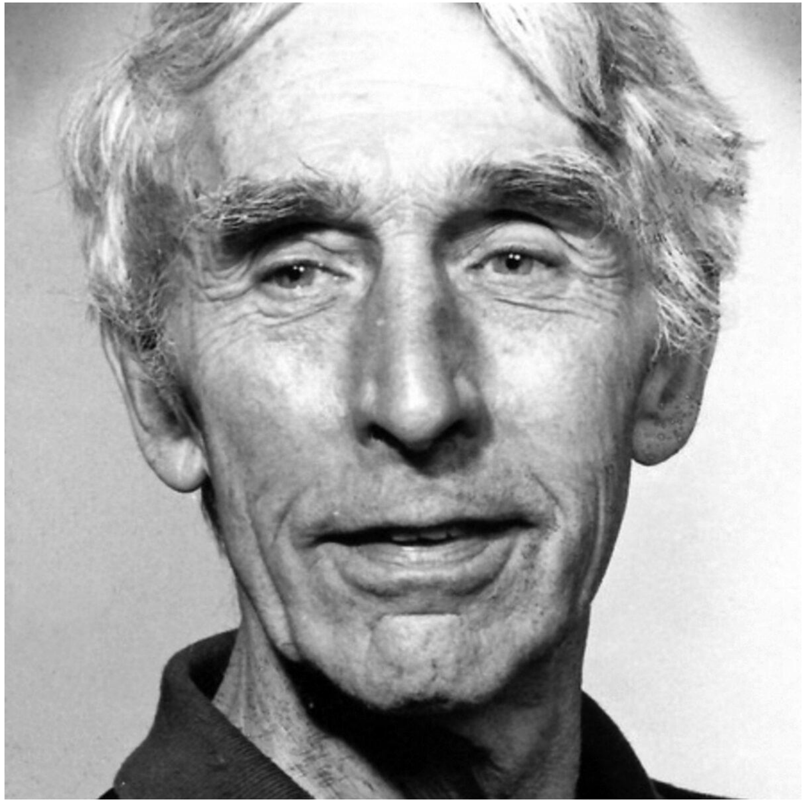

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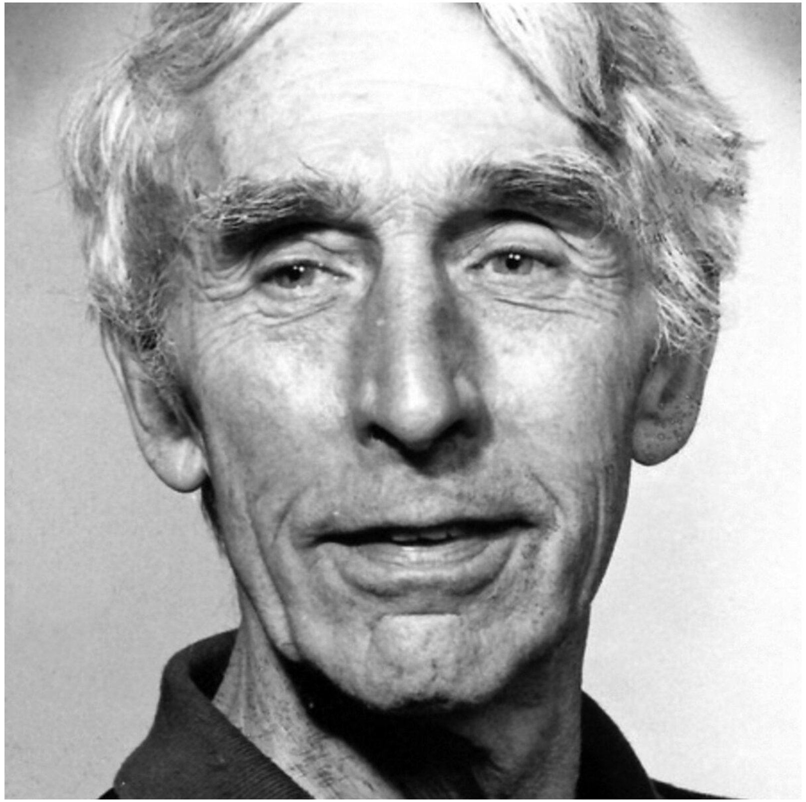

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$\boldsymbol{x}$: "What is your favorite ice cream flavor?"

$\boldsymbol{h}$: Everything you remember (hometown, birthday, etc)

g : Searches your memories for ice cream information, and responds "chocolate"

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Step 1: Perform scan to find recurrent states

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Step 2: Perform recall on recurrent states

$$\begin{bmatrix} \boldsymbol{y}_1 \\ \vdots \\ \boldsymbol{y}_T \end{bmatrix} = \begin{bmatrix} g(\boldsymbol{h}_1, \boldsymbol{x}_1, \boldsymbol{\theta}_g) \\ \vdots \\ g(\boldsymbol{h}_T, \boldsymbol{x}_T, \boldsymbol{\theta}_g) \end{bmatrix}$$

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The simplest recurrent neural network is the **Elman Network**

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Add forgetting

$$f(\boldsymbol{h}, \boldsymbol{x}, \boldsymbol{\theta}) = \sigma\left(\boldsymbol{\theta}_1^\top \boldsymbol{h} \odot f_{\text{forget}}(\boldsymbol{h}, \boldsymbol{x}, \boldsymbol{\theta}) + \boldsymbol{\theta}_2^\top \overline{\boldsymbol{x}}\right)$$

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When $f_{\text{forget}} < 1$, we forget some of our memories!

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Through gradient descent, neural network learns which memories to forget

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Minimal gated unit (MGU) is a modern RNN

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MGU defines two helper functions

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Minimal gated unit (MGU) is a modern RNN

MGU defines two helper functions

$$f_{\text{forget}}(\boldsymbol{h}, \boldsymbol{x}, \boldsymbol{\theta}) = \sigma(\boldsymbol{\theta}_1^\top \overline{\boldsymbol{x}} + \boldsymbol{\theta}_2^\top \boldsymbol{h})$$

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Left term forgets old, right term replaces forgotten memories

Review

Jax RNN https://colab.research.google.com/drive/147z7FNGyERV8oQ_4gZmxDVdeoNt0hKta#scrollTo=TUMonlJ1u8Va

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1. **Review**
2. Compression
3. Autoencoders
4. Applications
5. Variational Modeling
6. VAE Implementation
7. Coding

Agenda

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Question: What is missing?

Answer: Shrek lives in a swamp, Lord Farquaad, dragons, etc

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Let us examine a more principled form of video compression

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Shrek in 4k UHD:

$$X \in \mathbb{Z}_{255}^{3 \times 3840 \times 2160}, X^{90 \times 60 \times 24}$$

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Today, we use the H.264 video **encoder** to transform videos into a more compact representation

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We achieve a compression ratio of $3000 \text{ GB} \ / \ 60 \text{ GB} = 50$

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You CPU has a H.264 decoder built in to make this fast

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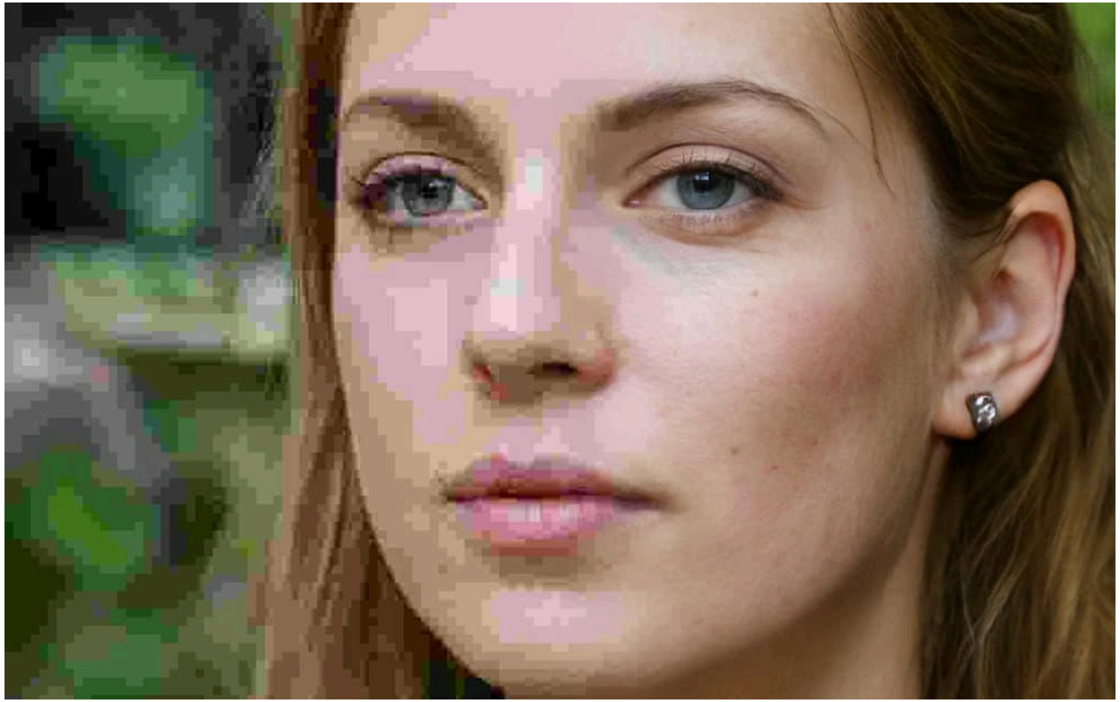

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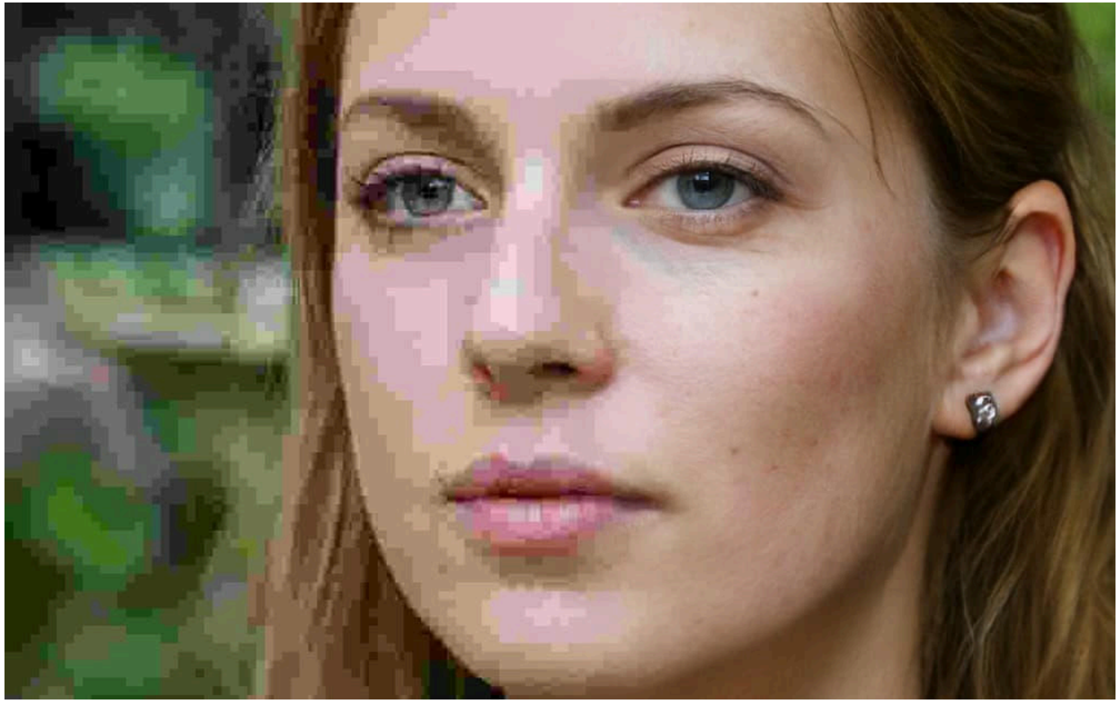

Question: Which is H.264?

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Encoders and decoders for images, videos, and music are functions

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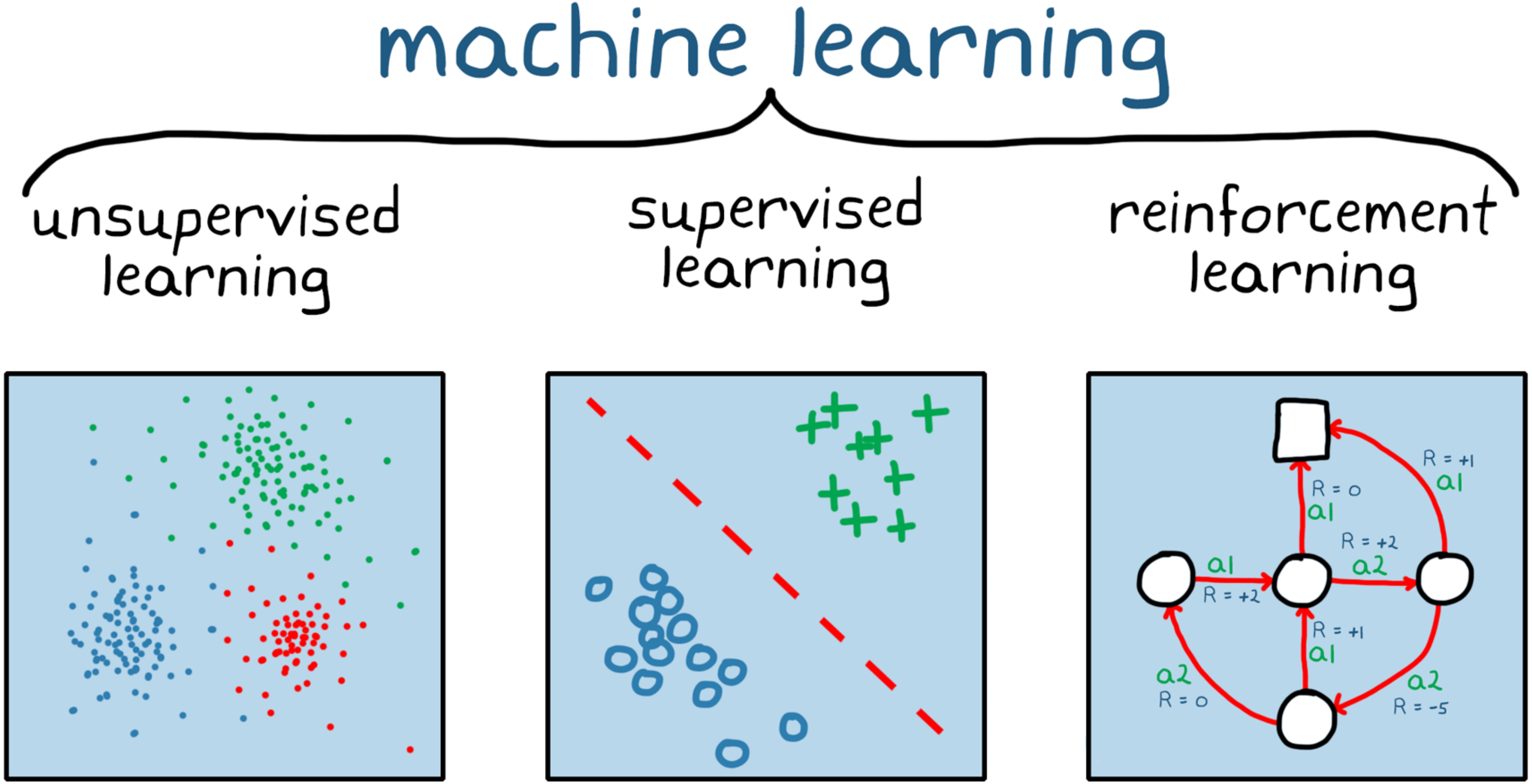
Training autoencoders is different than what we have seen before

Autoencoders



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The training algorithm may generate labels

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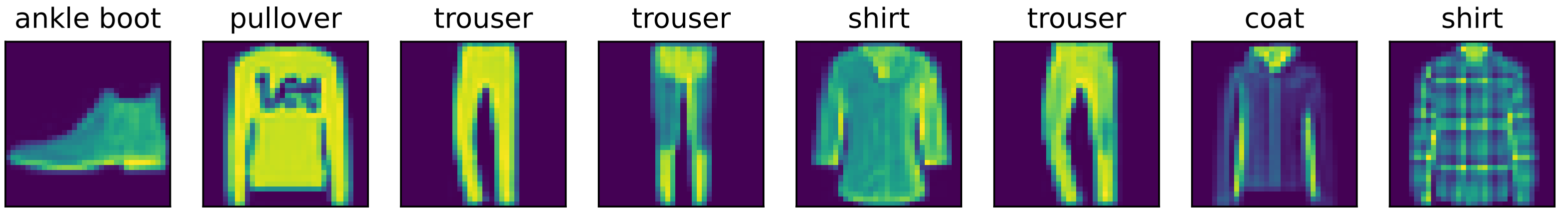

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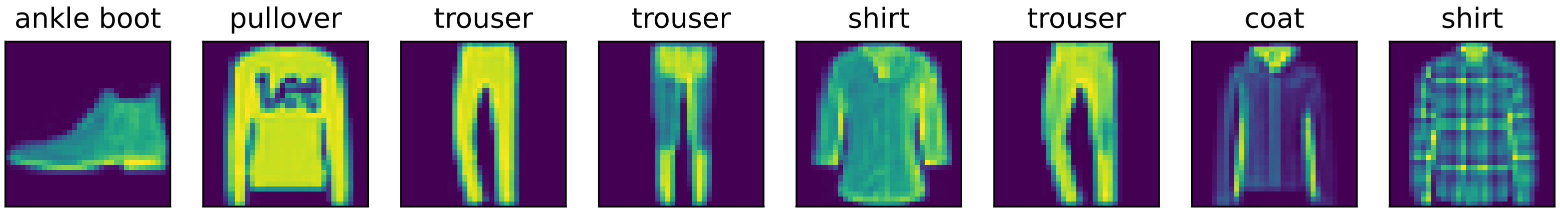

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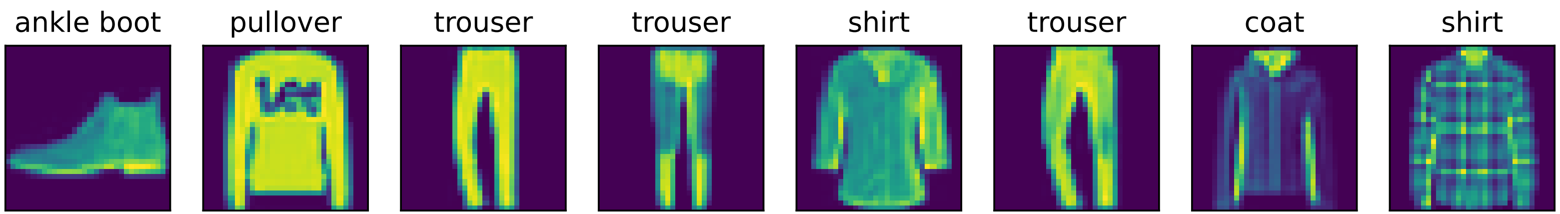

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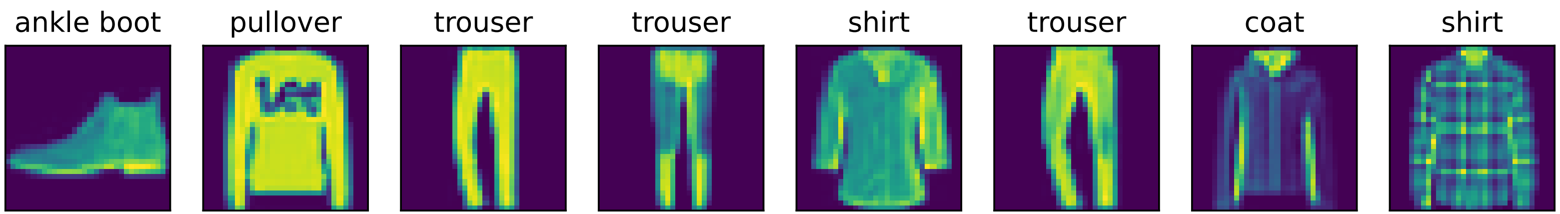

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Look for another solution

Autoencoders

Let us try another way

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Forces the networks to compress and reconstruct $\boldsymbol{x}$

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We call this the **reconstruction loss**

Autoencoders

$$\mathcal{L}(\boldsymbol{x}, \boldsymbol{\theta}) = \sum_{j=1}^{d_x} \left(x_j - f^{-1}(f(\boldsymbol{x}, \boldsymbol{\theta}_e), \boldsymbol{\theta}_d)_j \right)^2$$

Define over the entire dataset

$$\mathcal{L}(\boldsymbol{X}, \boldsymbol{\theta}) = \sum_{i=1}^{n} \sum_{j=1}^{d_x} \left(x_{[i],j} - f^{-1}\left(f\left(\boldsymbol{x}_{[i]}, \boldsymbol{\theta}_e\right), \boldsymbol{\theta}_d\right)_j \right)^2$$

We call this the **reconstruction loss**

It is an unsupervised loss because we only provide $\boldsymbol{X}$ and not $\boldsymbol{Y}$!

Autoencoders

First coding exercise

https://colab.research.google.com/drive/1UyR_W6NDIujaJXYlHZh6O3NfaCAMscpH#scrollTo=nmyQ8aE2pSbb

https://www.youtube.com/watch?v=UZDiGooFs54

Agenda

1. Review
2. Compression
3. **Autoencoders**
4. Applications
5. Variational Modeling
6. VAE Implementation
7. Coding

Agenda

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Applications

We can use autoencoders for more than compression

Applications

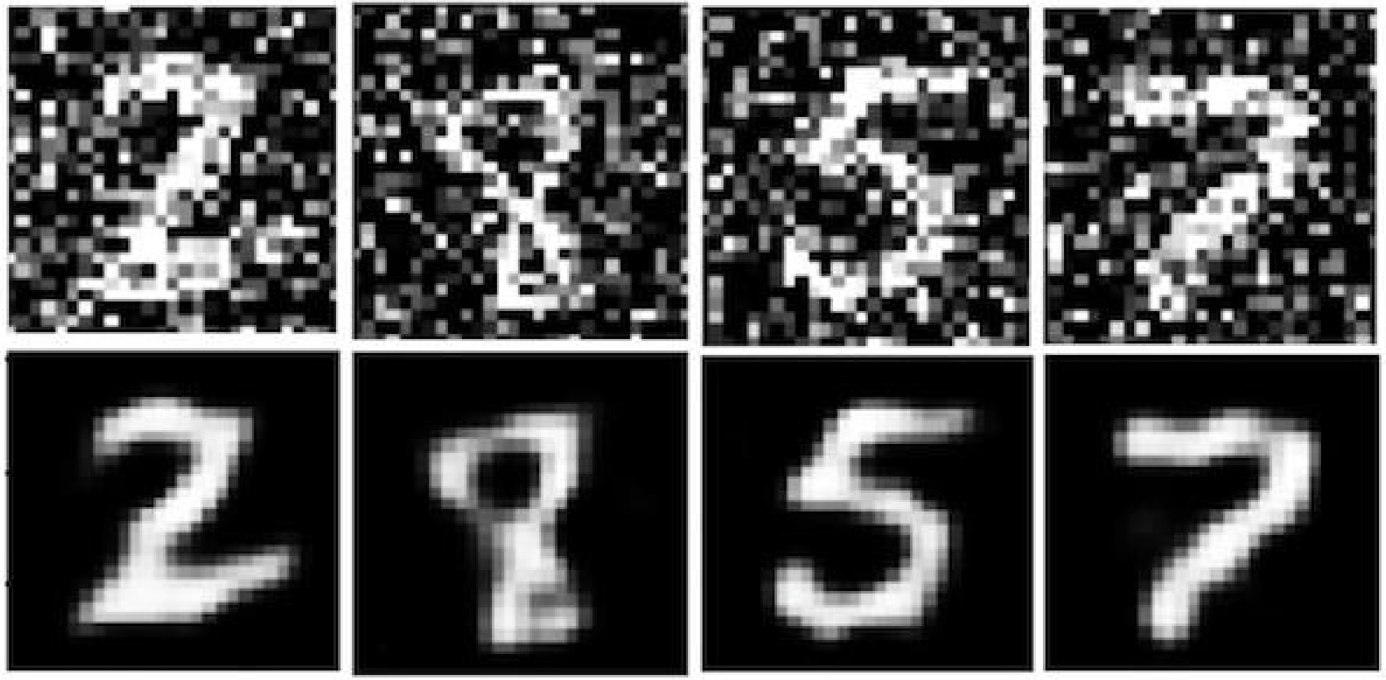
We can use autoencoders for more than compression

We can make **denoising autoencoders** that remove noise

Applications

We can use autoencoders for more than compression

We can make **denoising autoencoders** that remove noise



Applications

Generate some noise $\qquad \varepsilon \sim \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$

Applications

Generate some noise $\varepsilon \sim \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$

Add noise to the image $\boldsymbol{x} + \varepsilon$

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Original loss $\mathcal{L}(\boldsymbol{X}, \boldsymbol{\theta}) = \sum_{i=1}^{n} \sum_{j=1}^{d_x} \left(x_{[i],j} - f^{-1}\left(f\left(\boldsymbol{x}_{[i]}, \boldsymbol{\theta}_e \right), \boldsymbol{\theta}_d \right)_j \right)^2$

Applications

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Denoising loss $\qquad \mathcal{L}(\boldsymbol{X}, \boldsymbol{\theta}) = \sum_{i=1}^{n} \sum_{j=1}^{d_x} \left(x_{[i],j} - f^{-1}\left(f\left(\boldsymbol{x}_{[i]} + \boldsymbol{\varepsilon}, \boldsymbol{\theta}_e\right), \boldsymbol{\theta}_d\right)_j \right)^2$

Applications

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Autoencoder will learn to remove noise when reconstructing image

Applications

We can add camera blur too

Applications

We can add camera blur too

Applications

$$\mathrm{blur}(\boldsymbol{x} + \boldsymbol{\varepsilon})$$

Applications

$$\text{blur}(\boldsymbol{x} + \boldsymbol{\varepsilon})$$

Denoising deblur loss

$$\mathcal{L}(\boldsymbol{X}, \boldsymbol{\theta}) = \sum_{i=1}^{n} \sum_{j=1}^{d_x} \left(x_{[i],j} - f^{-1}\left(f\left(\text{blur}\left(\boldsymbol{x}_{[i]} + \boldsymbol{\varepsilon}\right), \boldsymbol{\theta}_e\right), \boldsymbol{\theta}_d\right)_j \right)^2$$

Applications

Now we can "enhance" images like in crime tv shows

Applications

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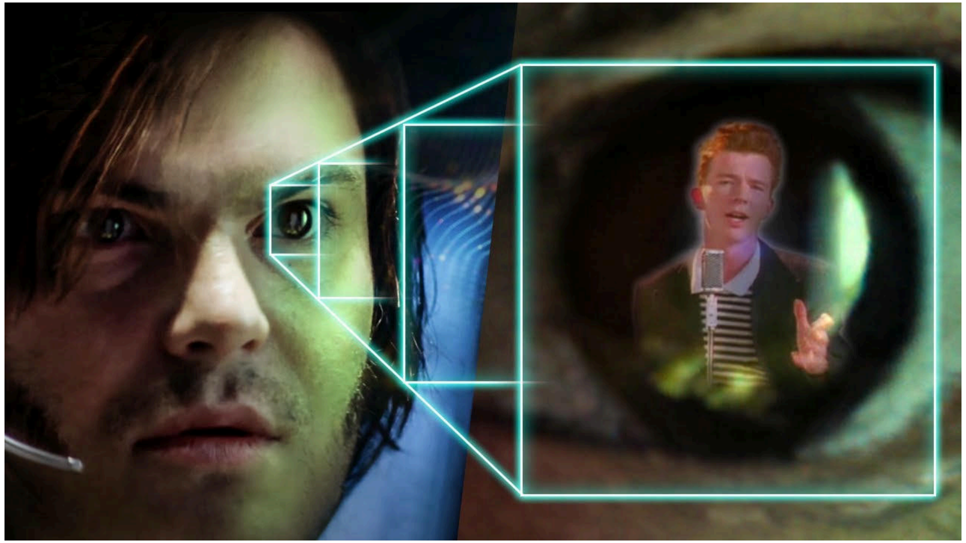
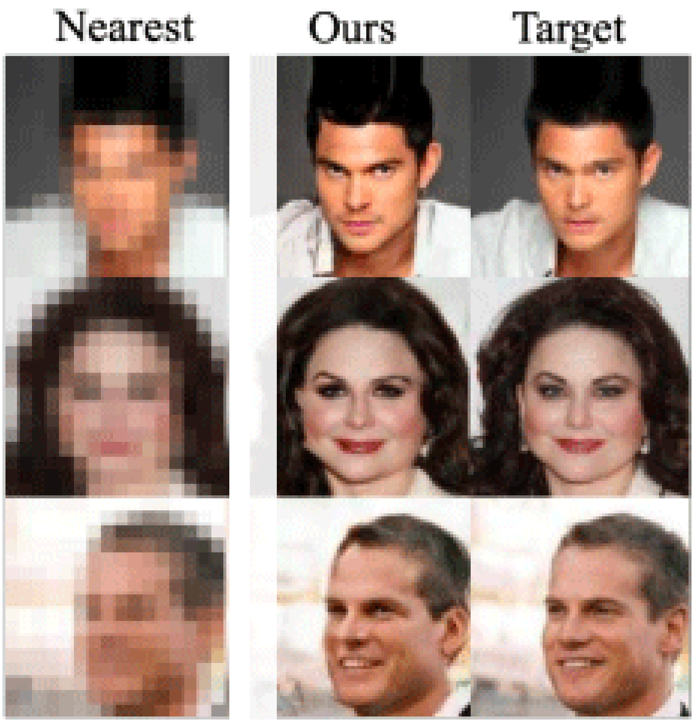


Applications

We can deblur faces from security cameras



Applications

We can even hide parts of the image

Applications

We can even hide parts of the image

A **masked autoencoder** will reconstruct the missing data

Applications

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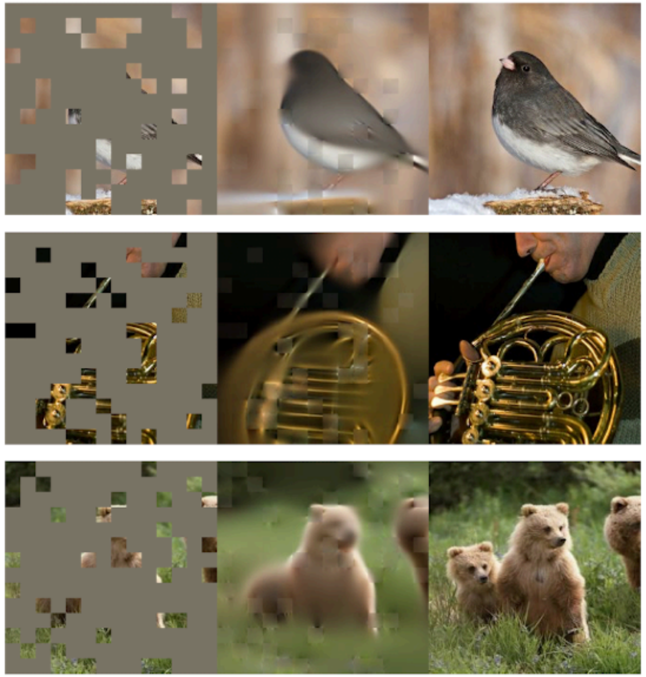
A **masked autoencoder** will reconstruct the missing data



Applications

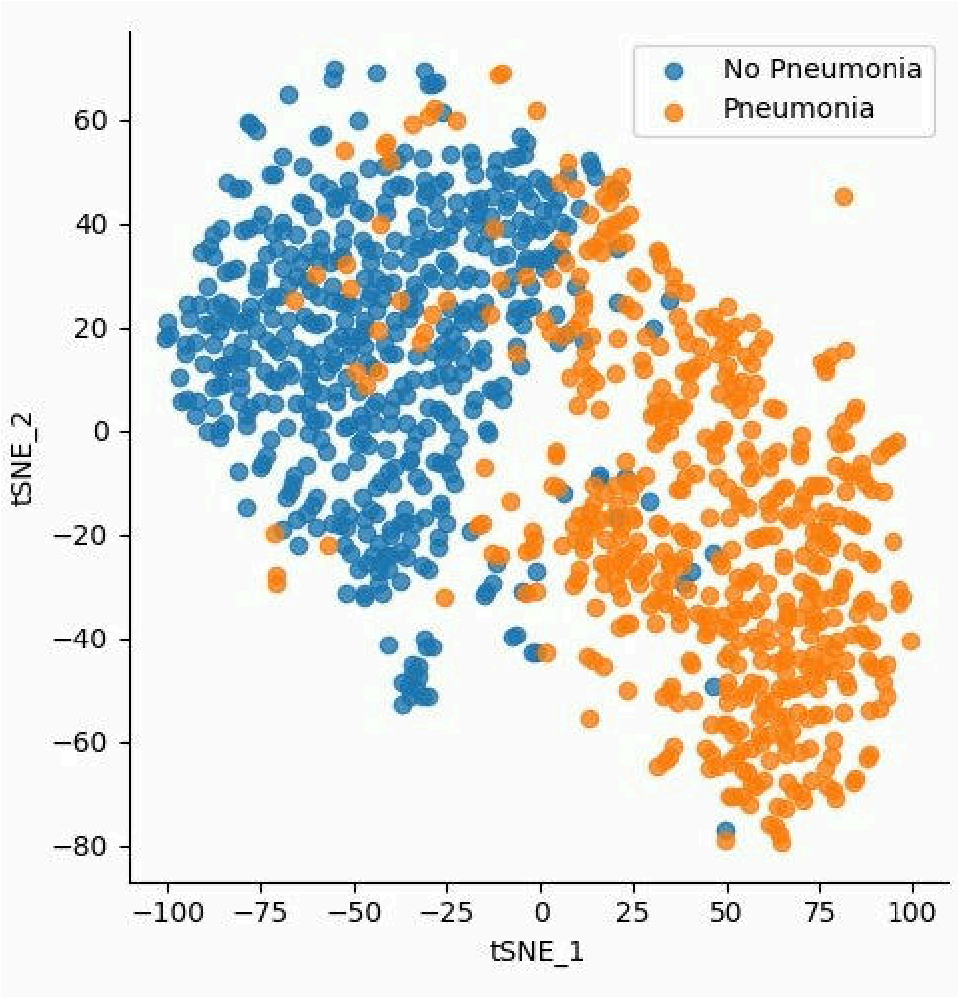
What is happening here? How can these models do this?

Applications

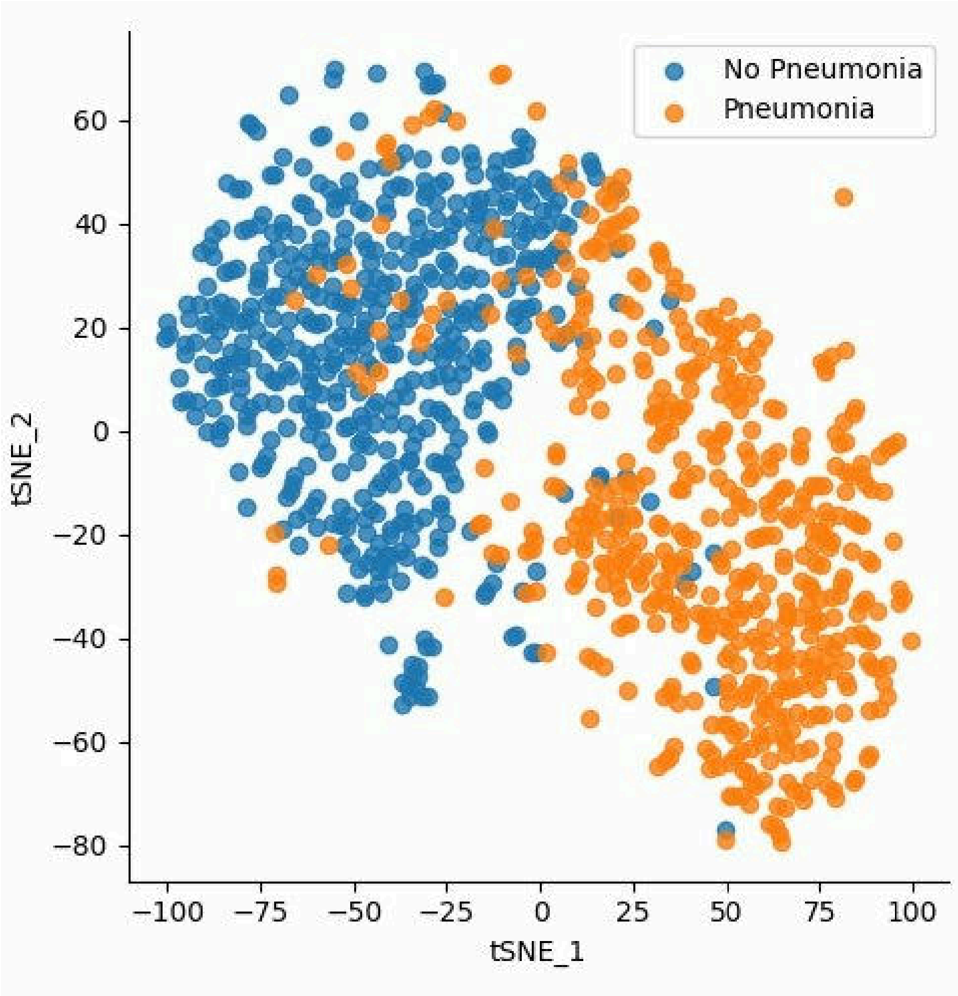
What is happening here? How can these models do this?

Autoencoders learn the structure of the dataset

Applications

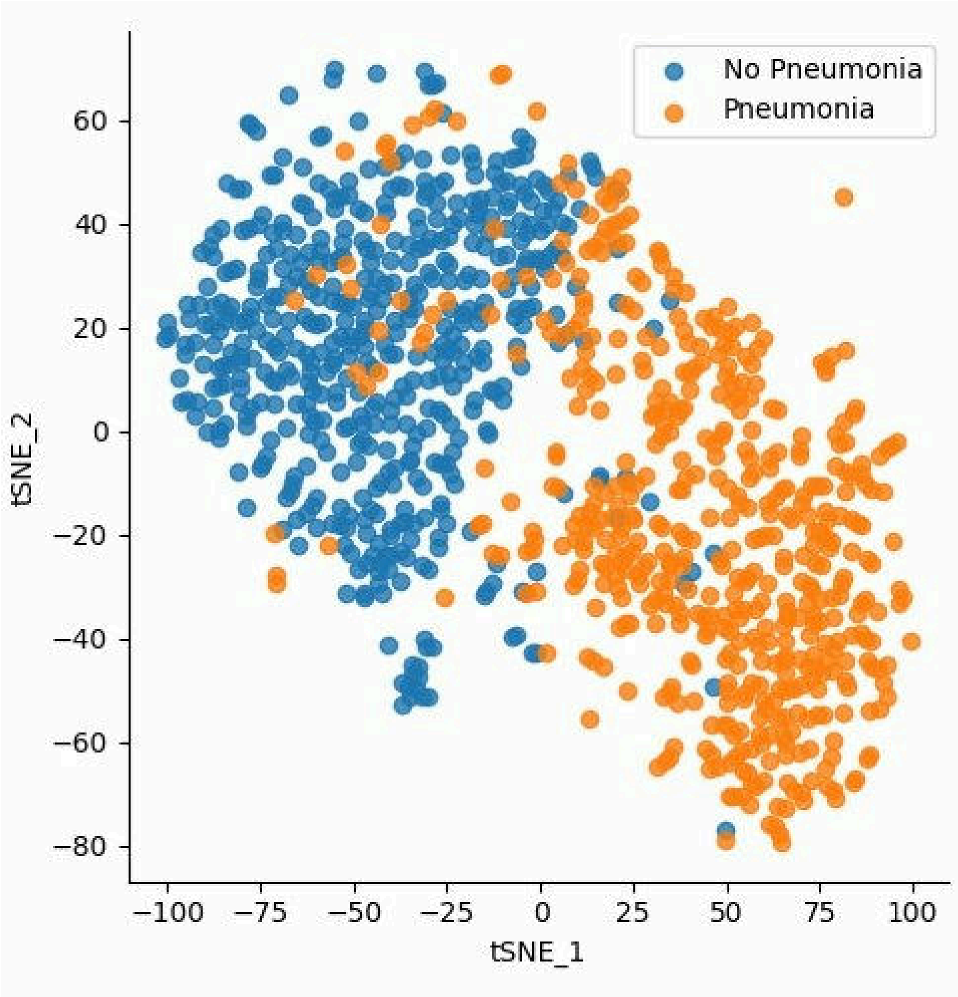


Applications



X : Pictures of human lungs

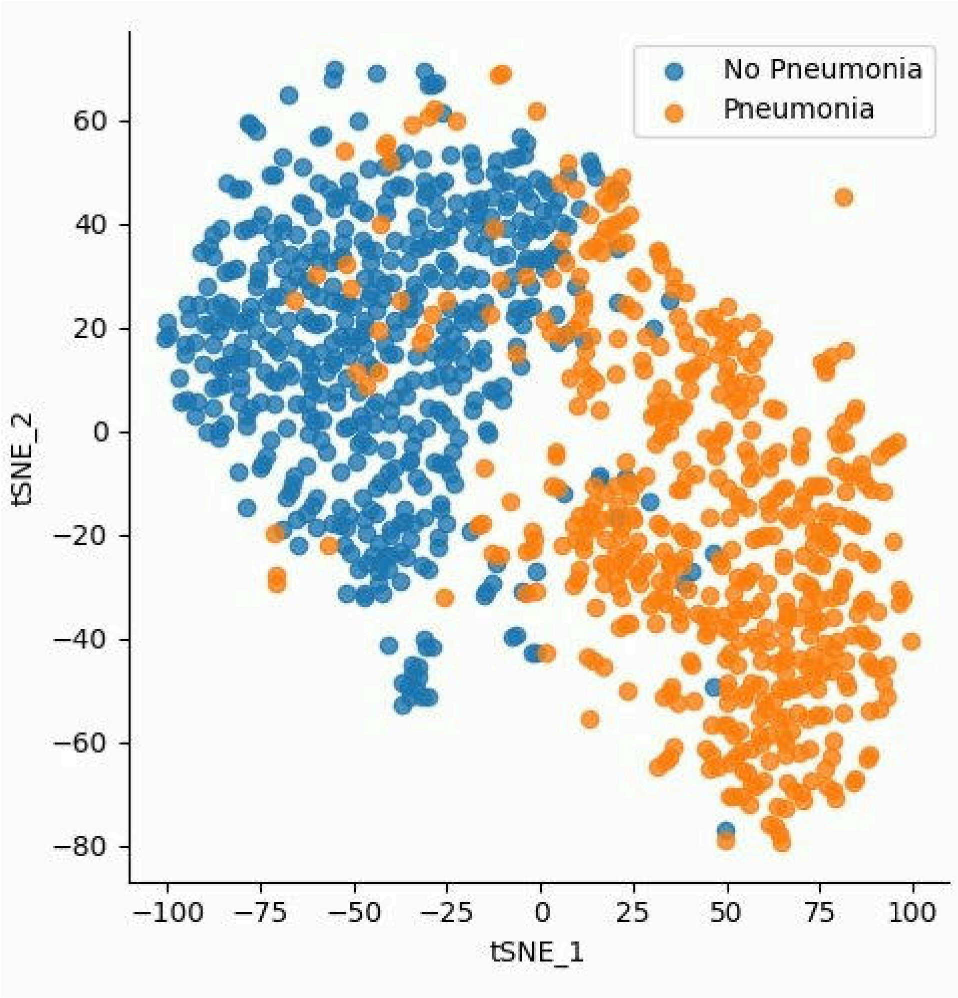
Applications



X : Pictures of human lungs

$Z \in \mathbb{R}^2$

Applications



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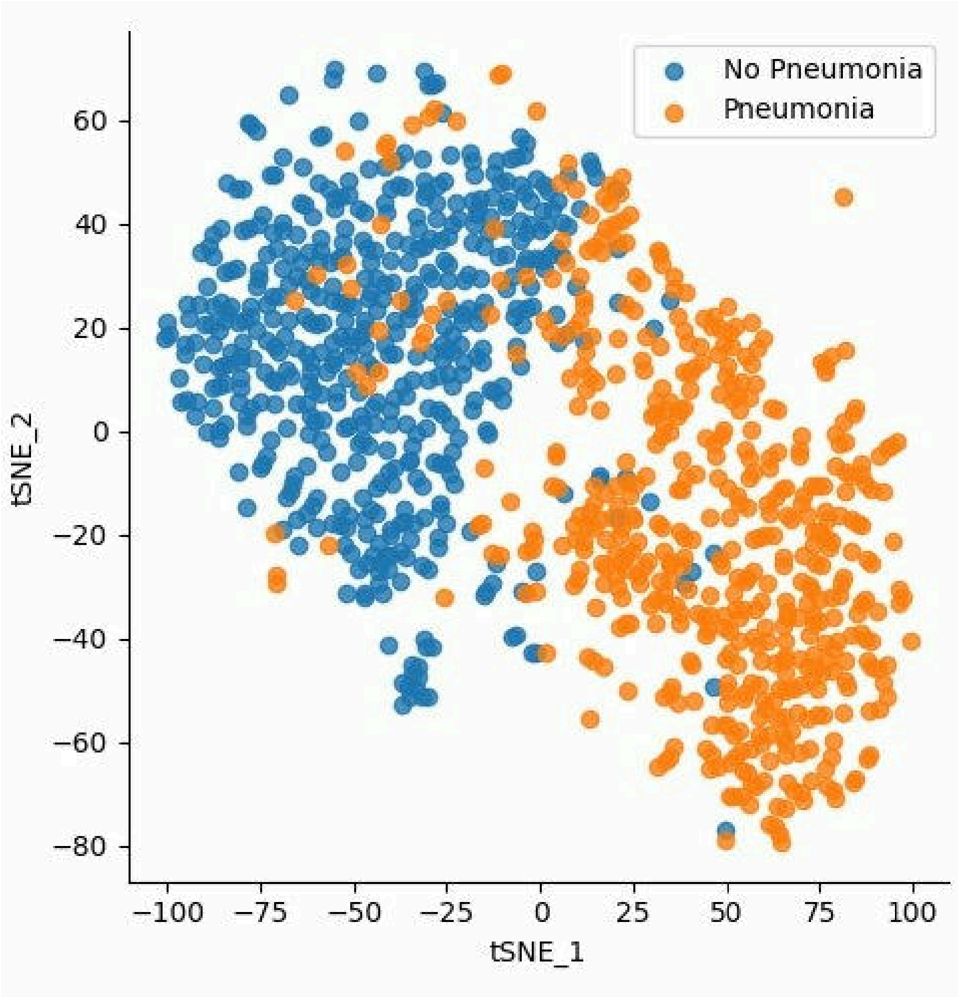
$Z \in \mathbb{R}^2$

Learns the structure of lungs from images

Applications



X : Pictures of human lungs

$Z \in \mathbb{R}^2$

Learns the structure of lungs from images

Differentiates sick and healthy lungs without being told

Applications

If the dataset is lung images, the model learns the structure of lungs

Applications

If the dataset is lung images, the model learns the structure of lungs

If the dataset is pictures from our world, then the autoencoders learn the structure of the world

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Nobody tells them what a dog or cat is

Applications

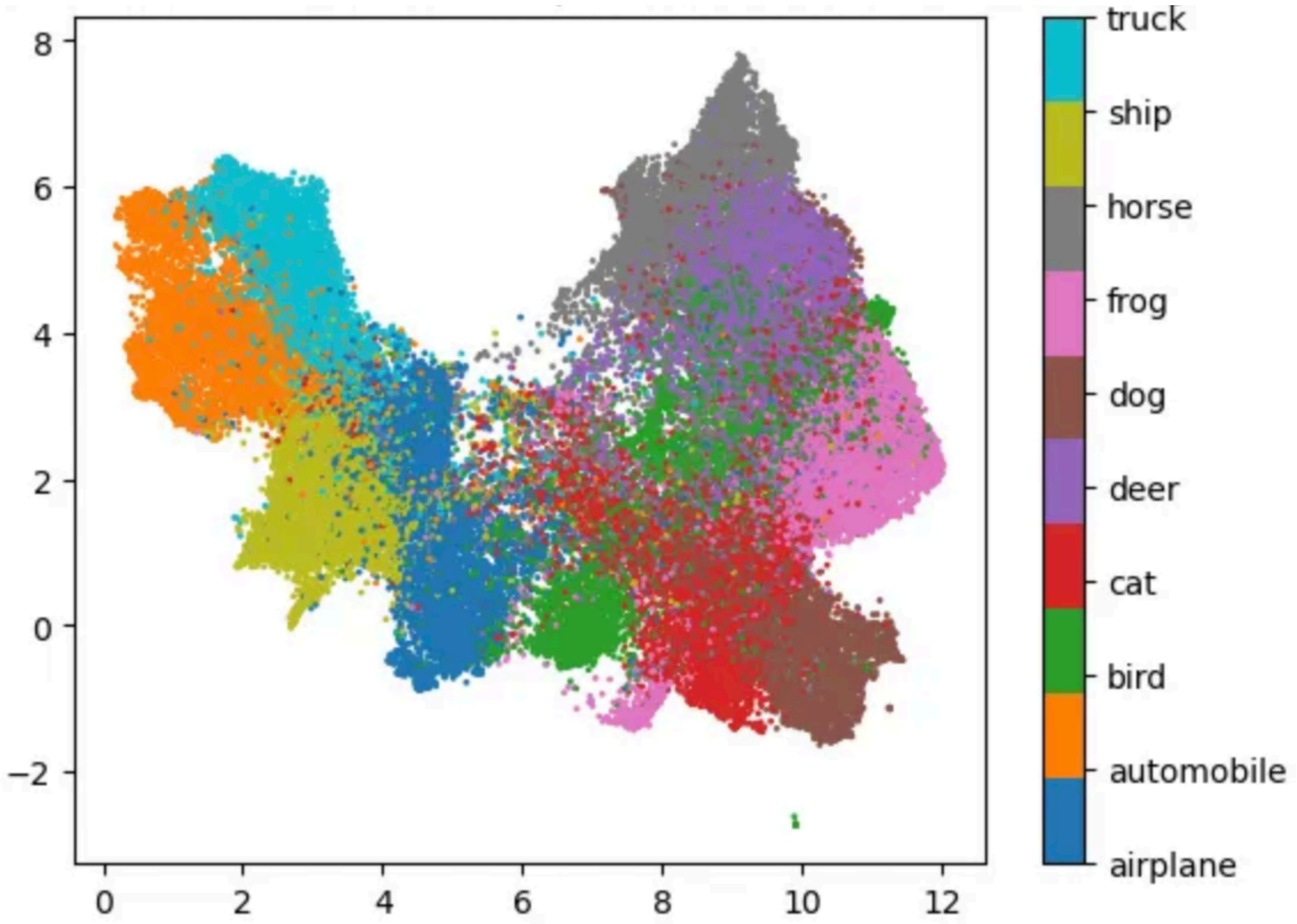
If the dataset is lung images, the model learns the structure of lungs

If the dataset is pictures from our world, then the autoencoders learn the structure of the world

Nobody tells them what a dog or cat is

They learn that on their own

Applications



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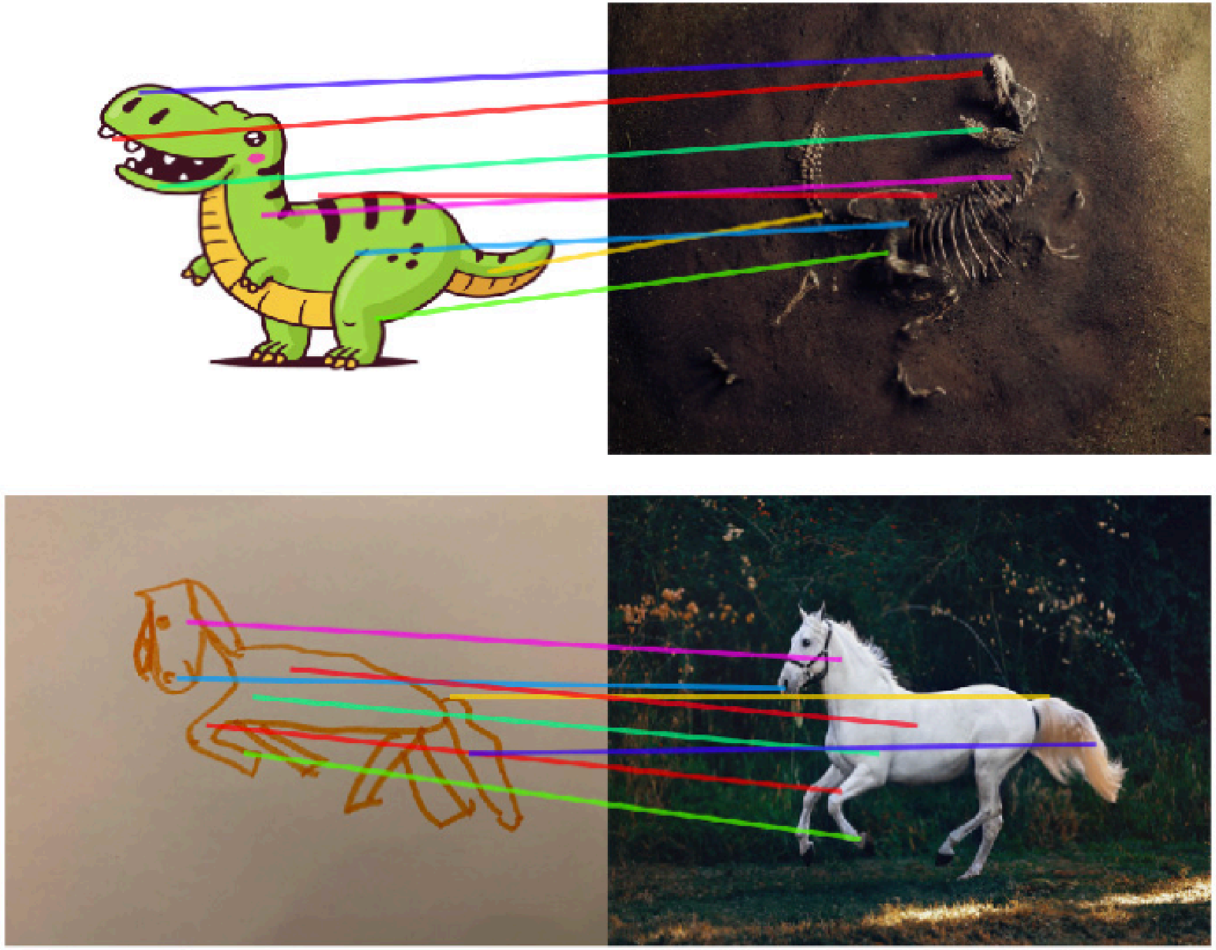

Applications

Some say “neural networks do not understand”, they just learn patterns

Applications

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Humans are also pattern recognition machines

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Applications

Some say "neural networks do not understand", they just learn patterns

Humans are also pattern recognition machines

These networks can understand our world

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Variational Modeling

Variational Modeling

These pictures were created by a **variational** autoencoder

Variational Modeling

 

These pictures were created by a **variational** autoencoder

But these people do not exist!

Variational Modeling

Autoencoders are useful for compression and denoising

Variational Modeling

Autoencoders are useful for compression and denoising

But we can also use them as **generative models**

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- Train on book dataset, write a **new** book

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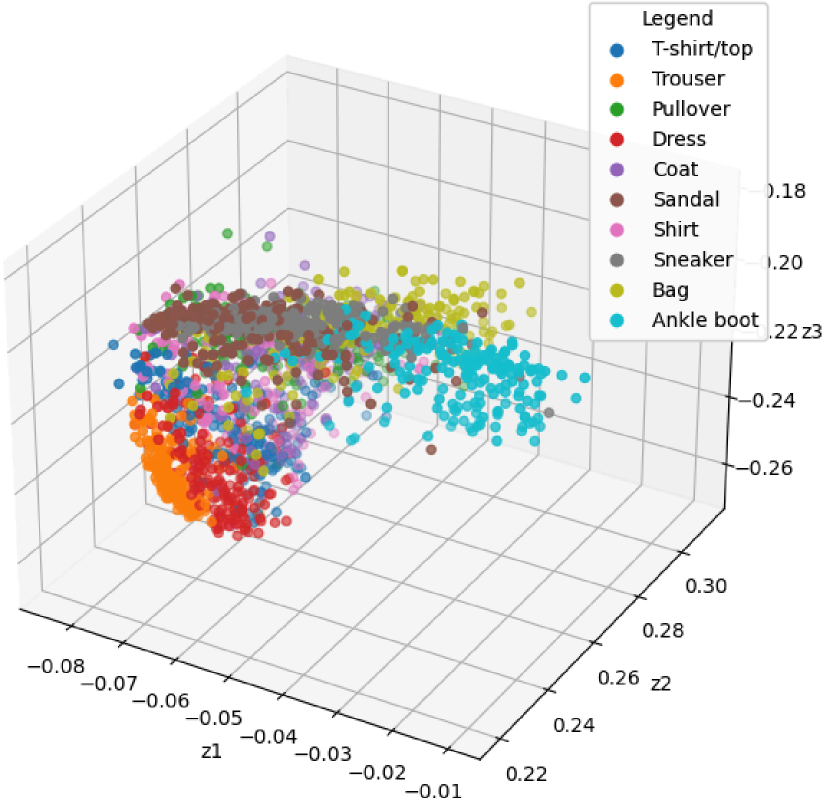
How does this work?

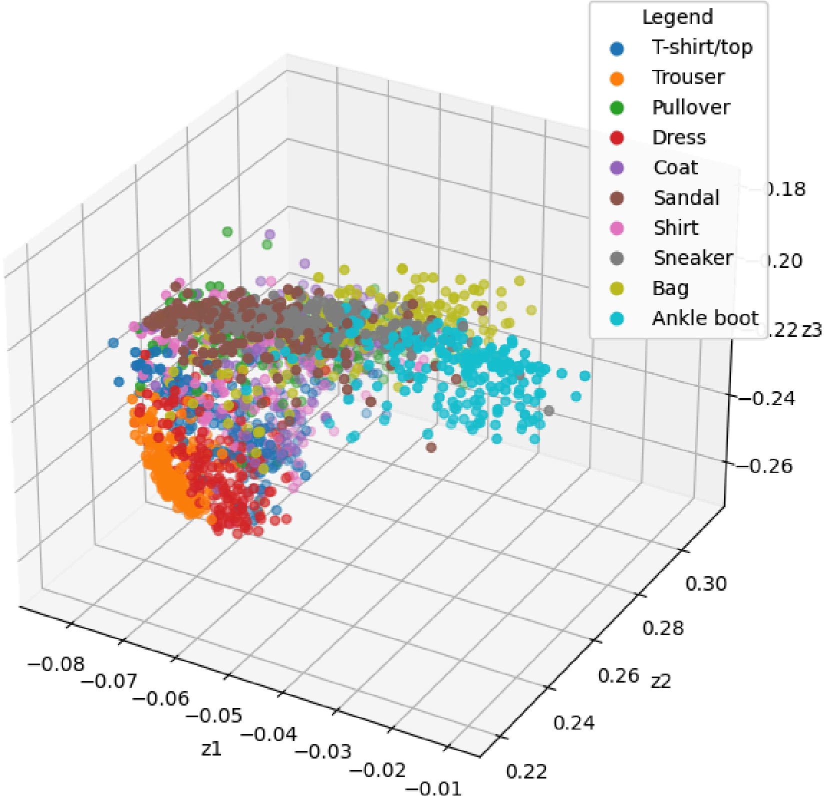
Variational Modeling

Latent space Z after training on the clothes dataset with $d_z = 3$

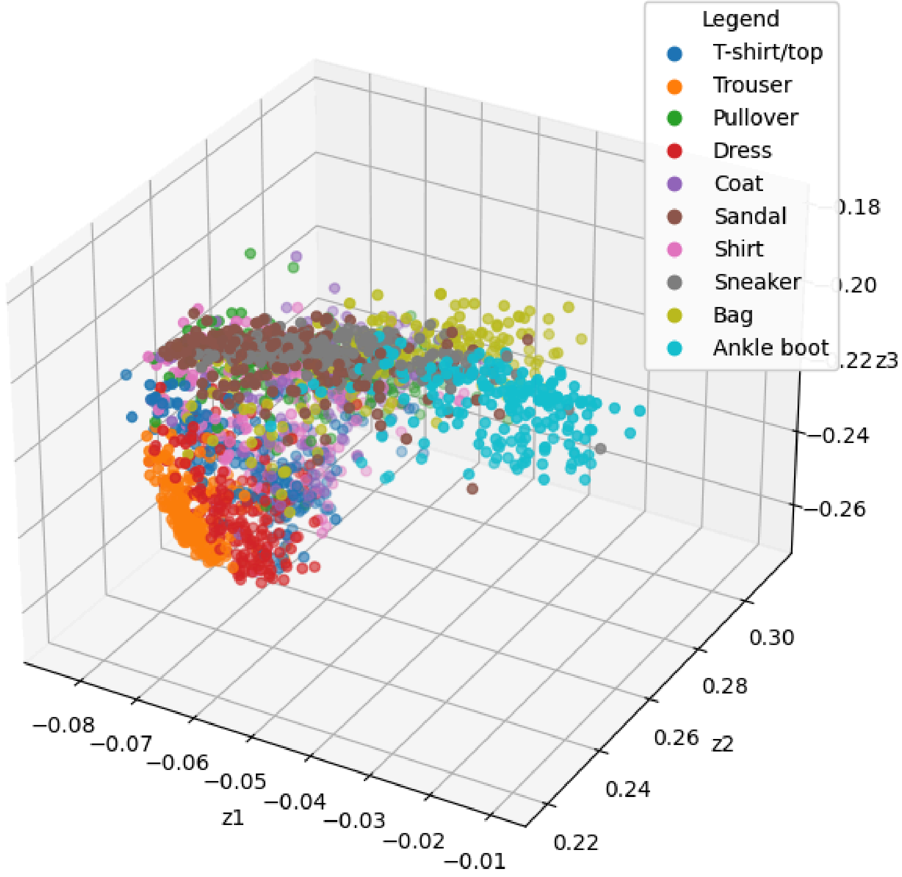


Variational Modeling

What happens if we decode a new point?

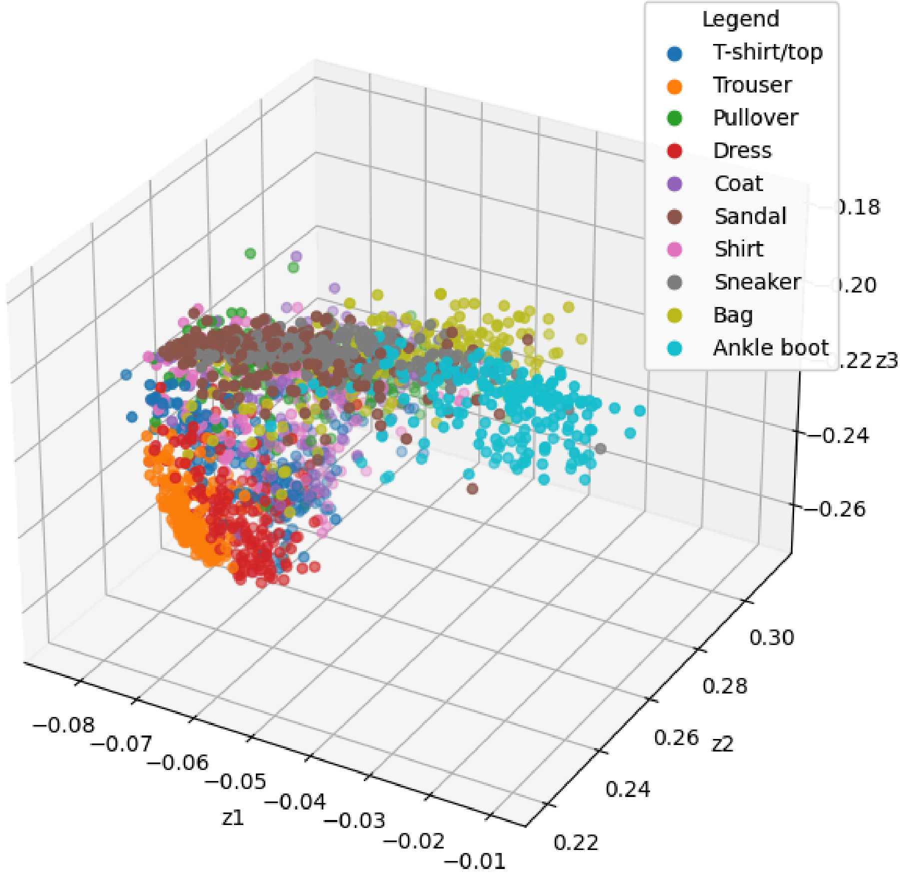


Variational Modeling



Autoencoder generative model:

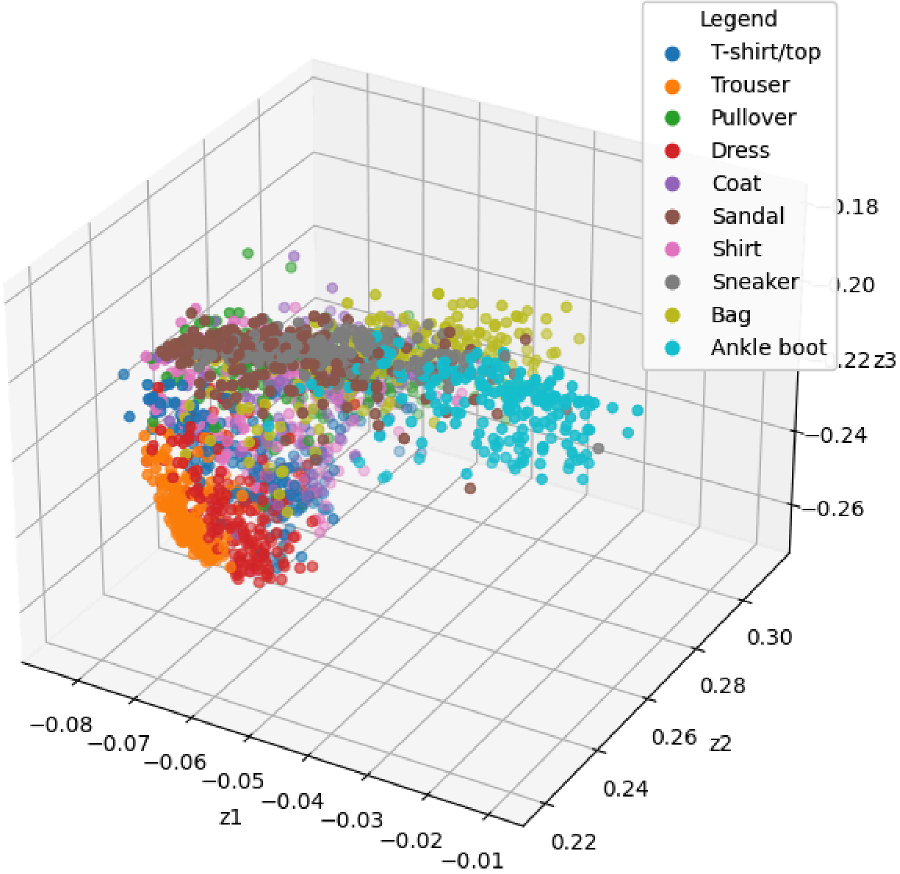
Variational Modeling



Autoencoder generative model:

$$\text{Encode} \begin{bmatrix} \boldsymbol{x}_{[1]} \\ \vdots \\ \boldsymbol{x}_{[n]} \end{bmatrix} \text{ into } \begin{bmatrix} \boldsymbol{z}_{[1]} \\ \vdots \\ \boldsymbol{z}_{[n]} \end{bmatrix}$$

Variational Modeling



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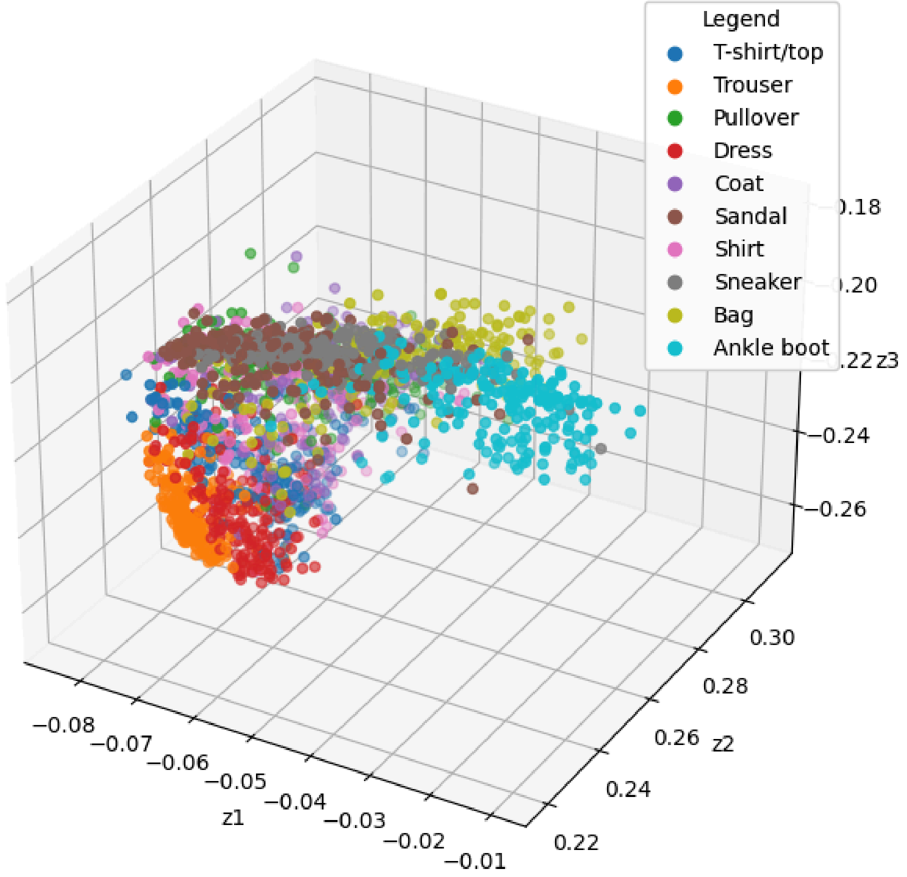
Pick a point $\boldsymbol{z}_{[k]}$

Variational Modeling



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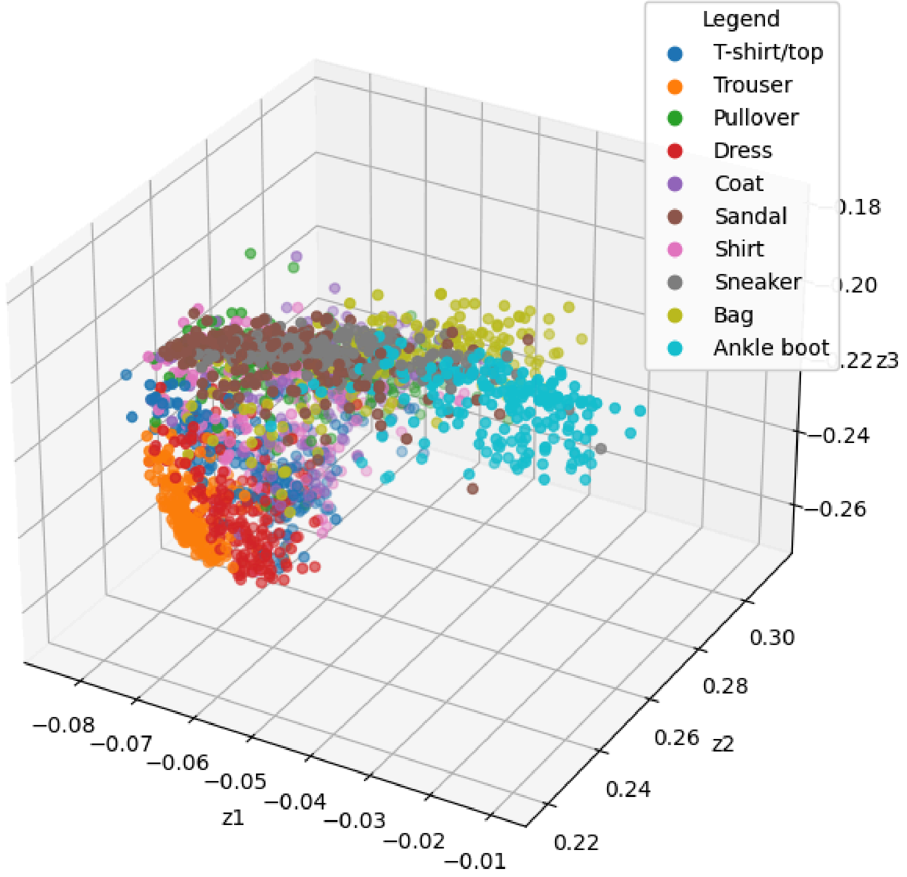
Variational Modeling



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Decode $\boldsymbol{z}_{\text{new}}$ into $\boldsymbol{x}_{\text{new}}$

Variational Modeling

Variational Modeling

$$f^{-1}(\boldsymbol{z}_k + \varepsilon, \boldsymbol{\theta}_d)$$

But there is a problem, the **curse of dimensionality**

Variational Modeling

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As d_z increases, points move further and further apart

Variational Modeling

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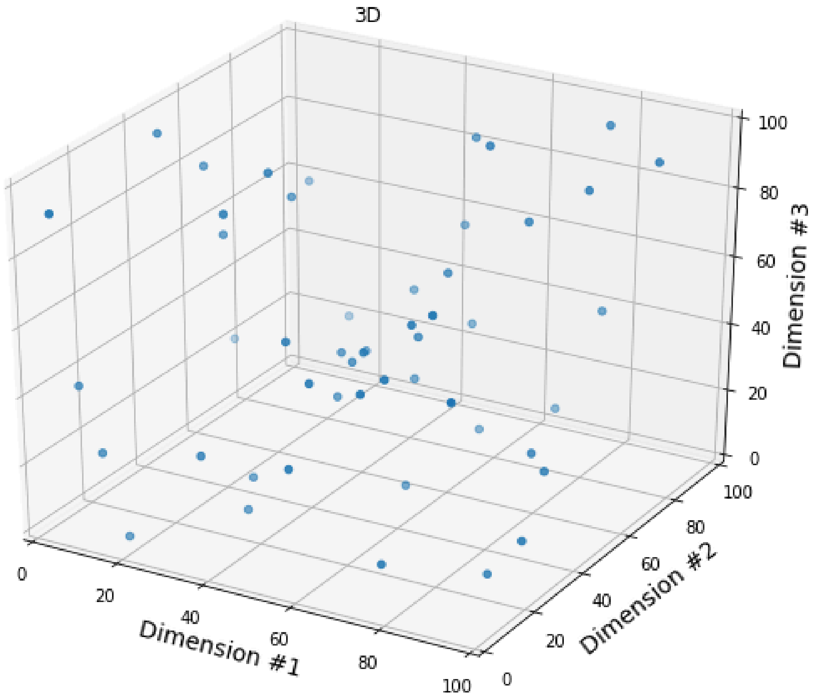

Variational Modeling

But there is a problem, the **curse of dimensionality**

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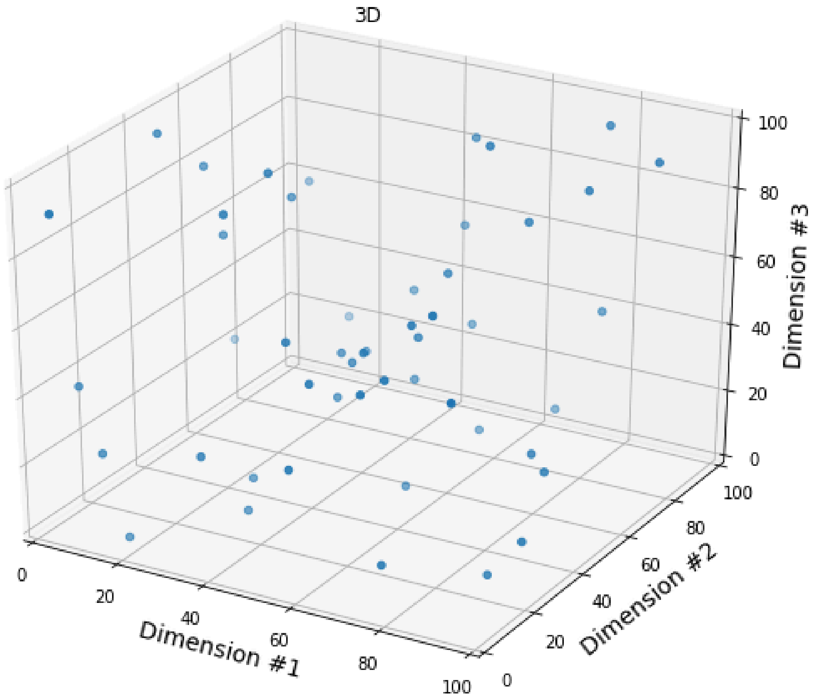

$f^{-1}(\boldsymbol{z} + \varepsilon)$ will produce either garbage, or $\boldsymbol{z}$

Variational Modeling

Question: What can we do?

Variational Modeling

Question: What can we do?

Answer: Force the points to be close together!

Variational Modeling

Question: What can we do?

Answer: Force the points to be close together!

We will use a **variational autoencoder** (VAE)

Variational Modeling

VAE discovered by Diederik Kingma (also adam optimizer)

Variational Modeling

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Variational Modeling

Variational autoencoders (VAEs) do three things:

Variational Modeling

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1. Make it easy to sample random $\boldsymbol{z}$

Variational Modeling

Variational autoencoders (VAEs) do three things:

1. Make it easy to sample random $\boldsymbol{z}$
2. Keep all $\boldsymbol{z}_{[1]}, ...\boldsymbol{z}_{[n]}$ close together in a small region

Variational Modeling

Variational autoencoders (VAEs) do three things:

1. Make it easy to sample random $\boldsymbol{z}$
2. Keep all $\boldsymbol{z}_{[1]}, ...\boldsymbol{z}_{[n]}$ close together in a small region
3. Ensure that $\boldsymbol{z} + \boldsymbol{\varepsilon}$ is always meaningful

Variational Modeling

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How?

Variational Modeling

Variational autoencoders (VAEs) do three things:

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How?

Make $\boldsymbol{z}_{[1]}, ..., \boldsymbol{z}_{[n]}$ normally distributed

Variational Modeling

Variational autoencoders (VAEs) do three things:

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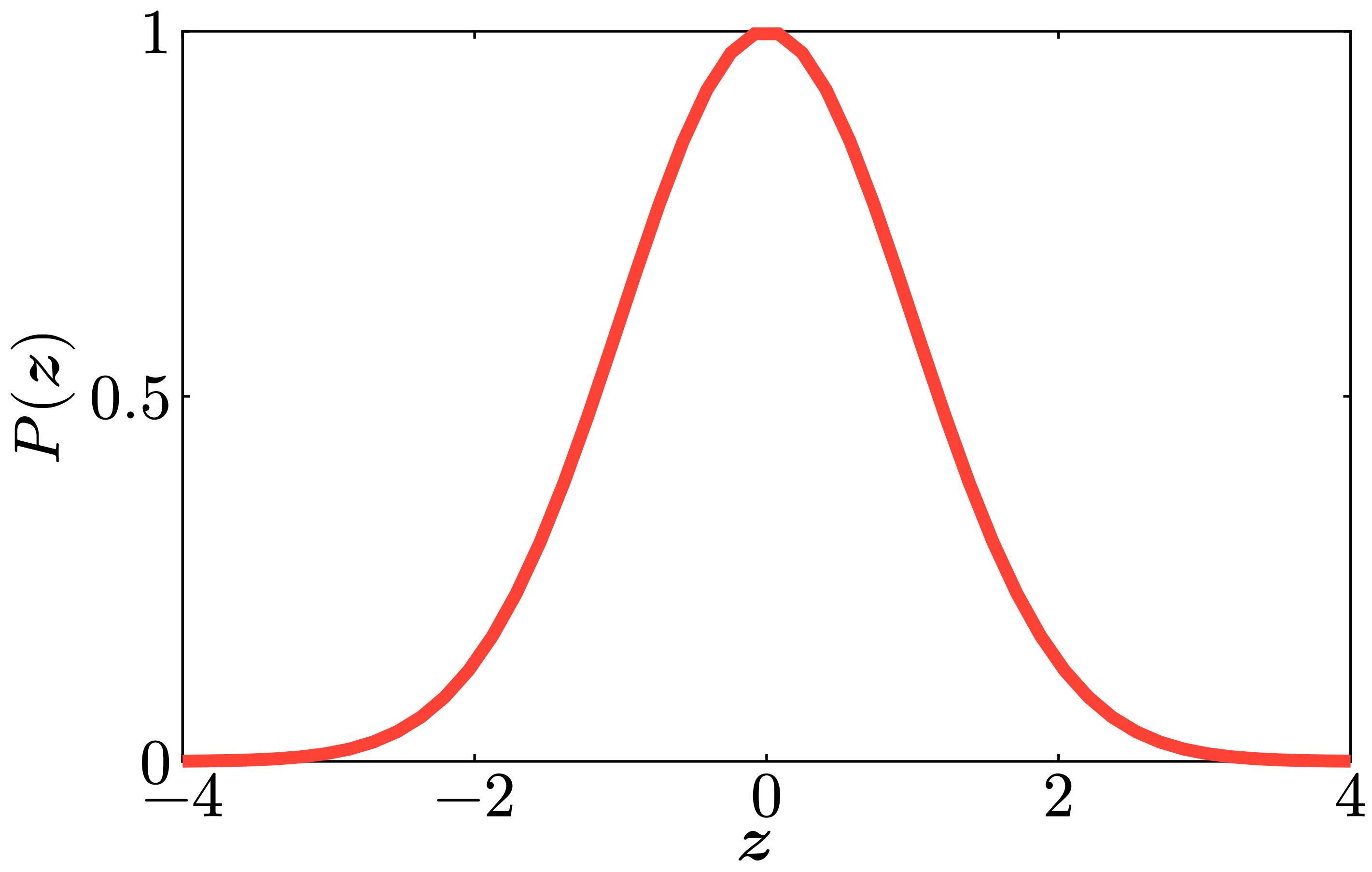
How?

Make $\boldsymbol{z}_{[1]}, ..., \boldsymbol{z}_{[n]}$ normally distributed

$$\boldsymbol{z} \sim \mathcal{N}(\mu, \sigma), \quad \mu = 0, \sigma = 1$$

Variational Modeling



Variational Modeling

If $\boldsymbol{z}_{[1]}, ..., \boldsymbol{z}_{[n]}$ are distributed following $\mathcal{N}(0, 1)$:

Variational Modeling

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1. 99.7% of $\boldsymbol{z}_{[1]}, ..., \boldsymbol{z}_{[n]}$ lie within $3\sigma = [-3, 3]$

Variational Modeling

If $\boldsymbol{z}_{[1]}, ..., \boldsymbol{z}_{[n]}$ are distributed following $\mathcal{N}(0, 1)$:

1. 99.7% of $\boldsymbol{z}_{[1]}, ..., \boldsymbol{z}_{[n]}$ lie within $3\sigma = [-3, 3]$
2. Make it easy to generate new $\boldsymbol{z}$, just sample $\boldsymbol{z} \sim \mathcal{N}(0, 1)$

Variational Modeling

So how do we ensure that $\boldsymbol{z}_{[1]}, ..., \boldsymbol{z}_{[n]}$ are normally distributed?

Variational Modeling

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We have to remember conditional probabilities

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$$P(\text{rain} \mid \text{cloud}) = \text{Probability of rain, given that it is cloudy}$$

Variational Modeling

So how do we ensure that $\boldsymbol{z}_{[1]}, ..., \boldsymbol{z}_{[n]}$ are normally distributed?

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$$P(\text{rain} \mid \text{cloud}) = \text{Probability of rain, given that it is cloudy}$$

Variational Modeling

Key idea 1: We want to model the distribution over the dataset X

$$P(\boldsymbol{x}; \boldsymbol{\theta}), \quad \boldsymbol{x} \sim \boldsymbol{X}$$

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We want to learn $\boldsymbol{\theta}$ that best models the distribution of possible faces

Variational Modeling

Key idea 1: We want to model the distribution over the dataset X

$$P(\boldsymbol{x}; \boldsymbol{\theta}), \quad \boldsymbol{x} \sim \boldsymbol{X}$$

We want to learn $\boldsymbol{\theta}$ that best models the distribution of possible faces

Large $P(\boldsymbol{x}; \boldsymbol{\theta})$

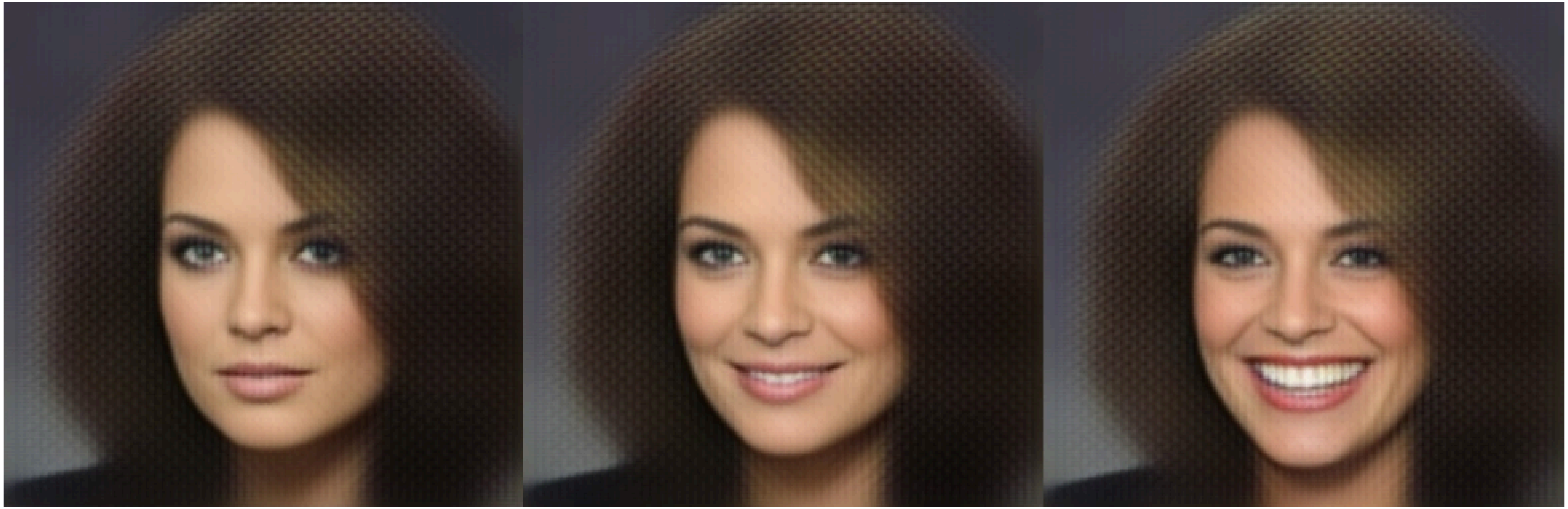
$P(\boldsymbol{x}; \boldsymbol{\theta}) \approx 0$

Variational Modeling

Key idea 2: There is some latent variable $\boldsymbol{z}$ which generates data $\boldsymbol{x}$

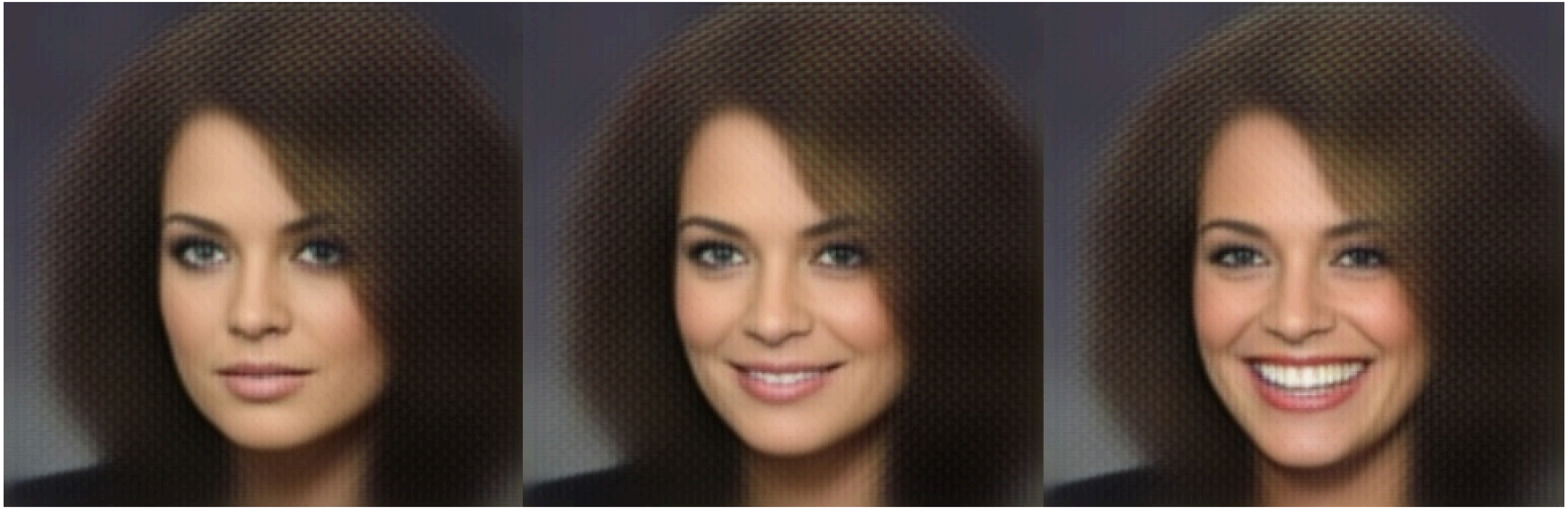
Variational Modeling

Key idea 2: There is some latent variable $\boldsymbol{z}$ which generates data $\boldsymbol{x}$

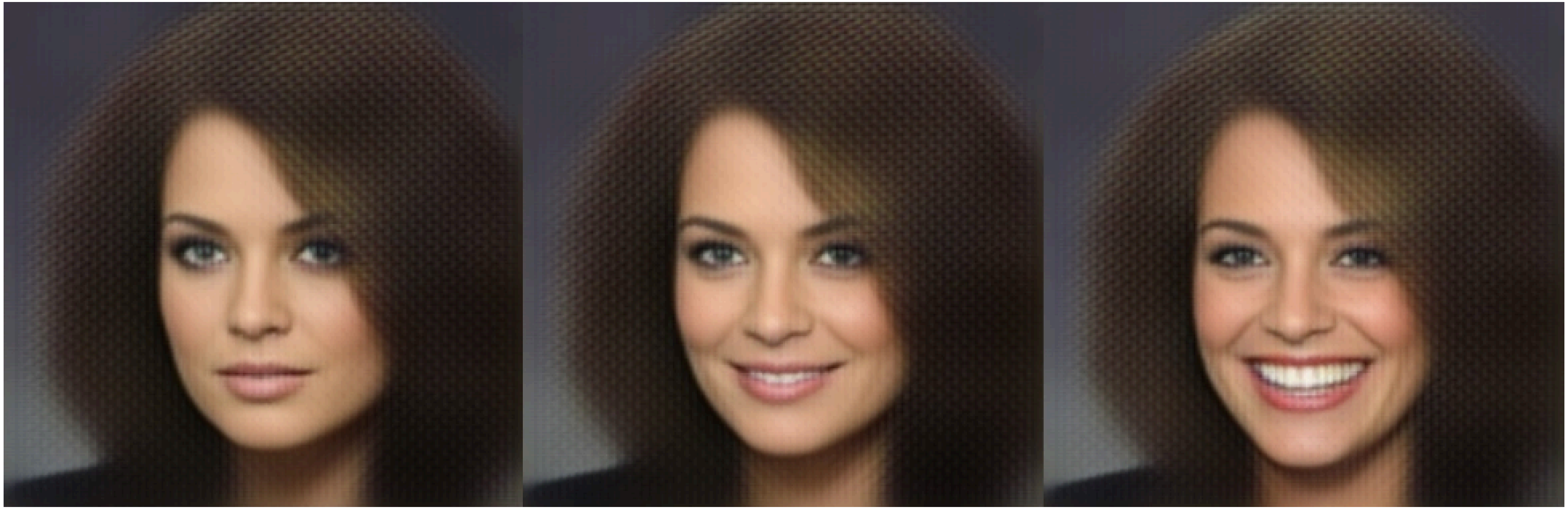
x : 

$$z : [\text{woman brown hair (frown} \mid \text{smile)}]$$

Variational Modeling

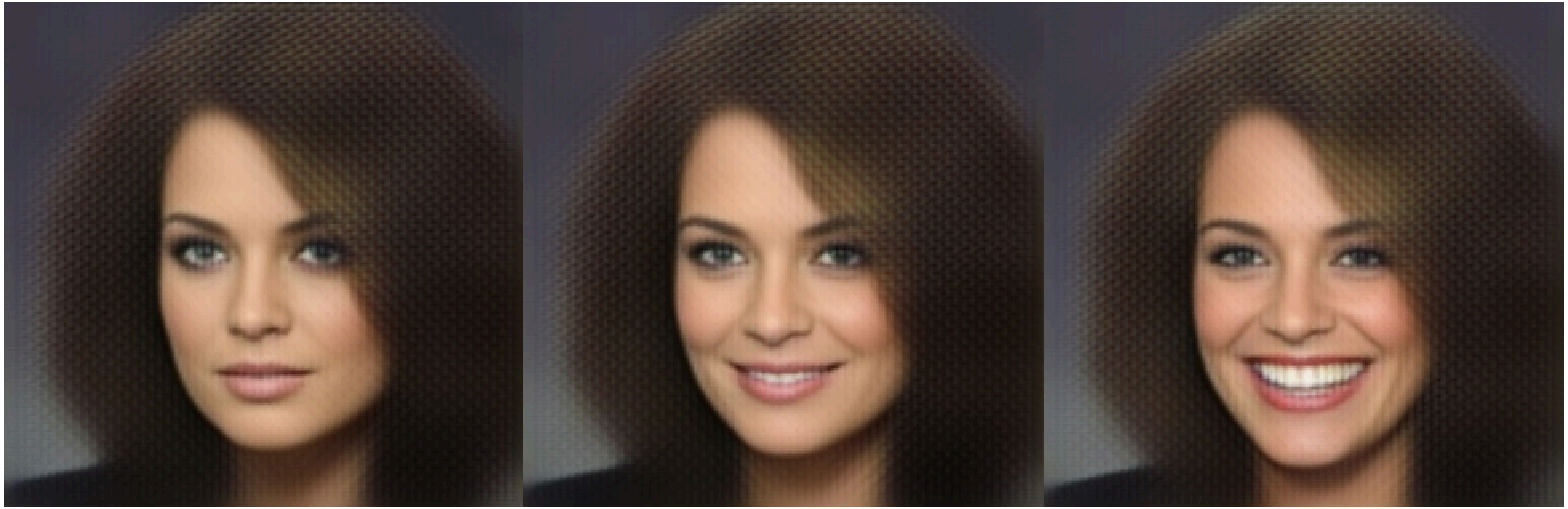


Variational Modeling



Network can only see $\boldsymbol{x}$, it cannot directly observe $\boldsymbol{z}$

Variational Modeling



Network can only see $\boldsymbol{x}$, it cannot directly observe $\boldsymbol{z}$

Given $\boldsymbol{x}$, find the probability that the person is smiling $P(\boldsymbol{z} \mid \boldsymbol{x}; \boldsymbol{\theta})$

Variational Modeling

We cast the autoencoding task as a **variational inference** problem

Variational Modeling

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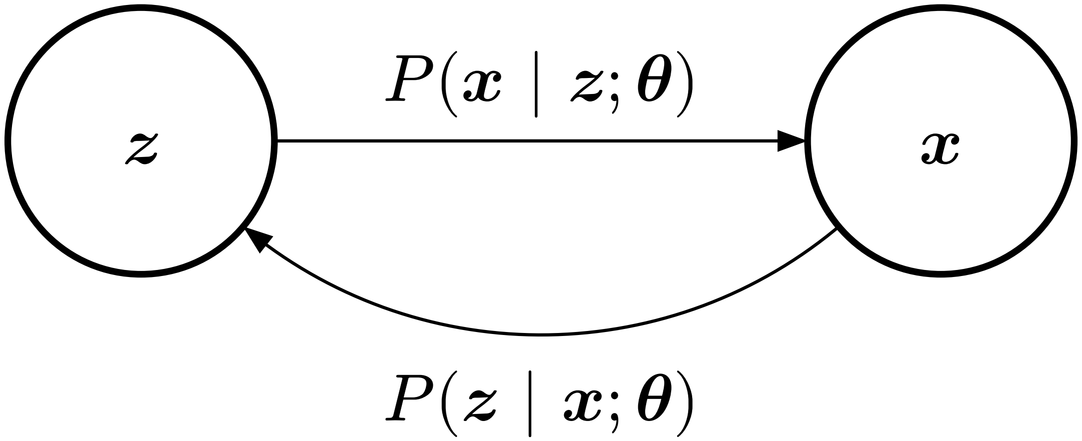


Decoder

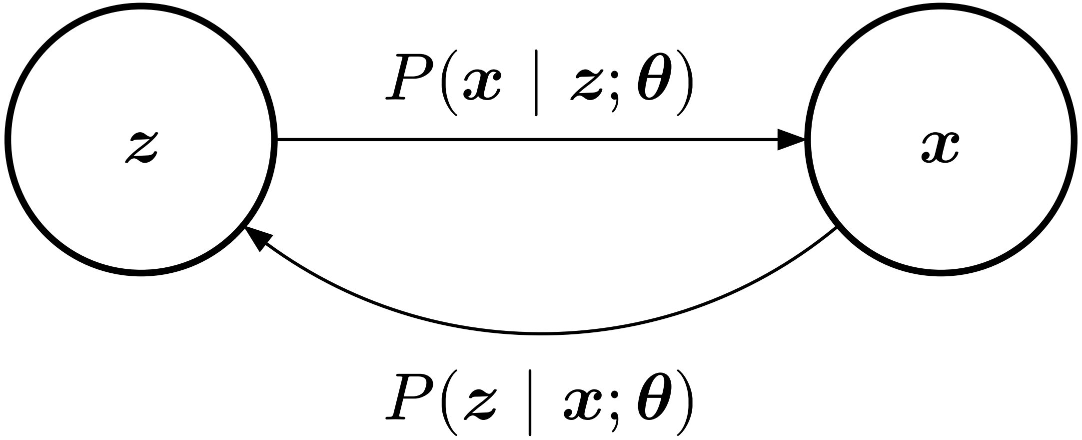
$$P(\boldsymbol{x} \mid \boldsymbol{z}; \boldsymbol{\theta})$$

Encoder

$$P(\boldsymbol{z} \mid \boldsymbol{x}; \boldsymbol{\theta})$$

Variational Modeling

We cast the autoencoding task as a **variational inference** problem



Decoder	Encoder
$P(\boldsymbol{x} \mid \boldsymbol{z}; \boldsymbol{\theta})$	$P(\boldsymbol{z} \mid \boldsymbol{x}; \boldsymbol{\theta})$

We want to learn both the encoder and decoder: $P(\boldsymbol{z}, \boldsymbol{x}; \boldsymbol{\theta})$

Variational Modeling

$$P(\boldsymbol{z}, \boldsymbol{x}; \boldsymbol{\theta}) = P(\boldsymbol{x} \mid \boldsymbol{z}; \boldsymbol{\theta}) \ P(\boldsymbol{z}; \boldsymbol{\theta})$$

Variational Modeling

$$P(\boldsymbol{z}, \boldsymbol{x}; \boldsymbol{\theta}) = P(\boldsymbol{x} \mid \boldsymbol{z}; \boldsymbol{\theta}) \ P(\boldsymbol{z}; \boldsymbol{\theta})$$

We can choose any distribution for $P(\boldsymbol{z})$

Variational Modeling

$$P(\boldsymbol{z}, \boldsymbol{x}; \boldsymbol{\theta}) = P(\boldsymbol{x} \mid \boldsymbol{z}; \boldsymbol{\theta}) \; P(\boldsymbol{z}; \boldsymbol{\theta})$$

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Variational Modeling

$$P(\boldsymbol{z}, \boldsymbol{x}; \boldsymbol{\theta}) = P(\boldsymbol{x} \mid \boldsymbol{z}; \boldsymbol{\theta}) \; P(\boldsymbol{z}; \boldsymbol{\theta})$$

We can choose any distribution for $P(\boldsymbol{z})$

$$P(\boldsymbol{z}) = \mathcal{N}(\mathbf{0}, \mathbf{1})$$

We can generate all possible $\boldsymbol{x}$ by sampling $\boldsymbol{z} \sim \mathcal{N}(\mathbf{0}, \mathbf{1})$

Variational Modeling

$$P(\boldsymbol{z}, \boldsymbol{x}; \boldsymbol{\theta}) = P(\boldsymbol{x} \mid \boldsymbol{z}; \boldsymbol{\theta}) \ P(\boldsymbol{z}; \boldsymbol{\theta})$$

We can choose any distribution for $P(\boldsymbol{z})$

$$P(\boldsymbol{z}) = \mathcal{N}(\mathbf{0}, \mathbf{1})$$

We can generate all possible $\boldsymbol{x}$ by sampling $\boldsymbol{z} \sim \mathcal{N}(\mathbf{0}, \mathbf{1})$

We can randomly generate $\boldsymbol{z}$, which we can decode into new $\boldsymbol{x}$!

Variational Modeling

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Question: How do we measure the distance between probability distributions?

Variational Modeling

Answer: KL divergence

Variational Modeling

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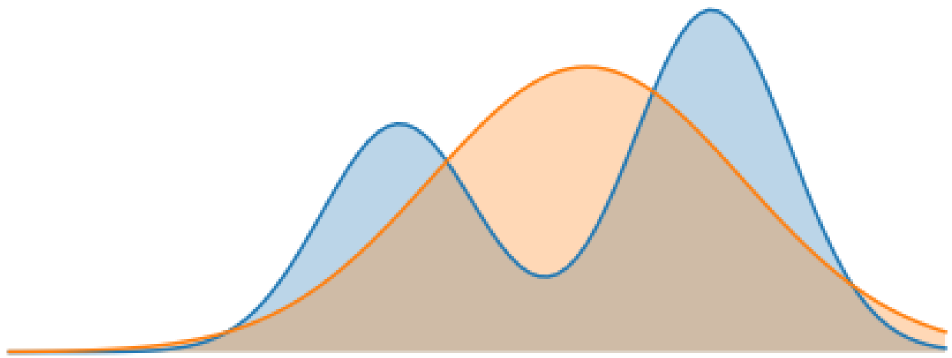

$$\mathrm{KL}(P, Q) = \sum_i P(i) \log \frac{P(i)}{Q(i)}$$

Variational Modeling

Learn the parameters for our model

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We call this the **Evidence Lower Bound Objective** (ELBO)

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Now we know how to train our autoencoder!

Agenda

1. Review
2. Compression
3. Autoencoders
4. Applications
5. **Variational Modeling**
6. VAE Implementation
7. Coding

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VAE Implementation

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$$f : X \times \Theta \mapsto \mathbb{R}^{d_z} \times \mathbb{R}_+^{d_z}$$

VAE Implementation

```
core = nn.Sequential(...)
mu_layer = nn.Linear(d_h, d_z)
# Neural networks output real numbers
# But sigma must be positive
# So we output log sigma, because e^(sigma) is always
positive
log_sigma_layer = nn.Linear(d_h, d_z)

tmp = core(x)
mu = mu_layer(tmp)
log_sigma = log_sigma_layer(tmp)
distribution = (mu, exp(sigma))
```

VAE Implementation

We covered the encoder

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We can use the same decoder as a standard autoencoder

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Answer: Encoder outputs a distribution ΔZ but decoder input is Z

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We can sample from the distribution

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Question: Why does this matter?

Answer: Must be differentiable for gradient descent

VAE Implementation

VAE paper proposes the **reparameterization trick**

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$$\boldsymbol{z} \sim \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\sigma})$$

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This trick only works with certain distributions

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Step 3: Decode the sample

$$\boldsymbol{x} = f^{-1}(\boldsymbol{z}, \boldsymbol{\theta}_d)$$

VAE Implementation

One last thing, implement the loss function

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Start with the KL term first

VAE Implementation

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$P(\boldsymbol{z})$ and $f(\boldsymbol{x}, \boldsymbol{\theta}_e)$ are Gaussian, we can simplify KL term

$$\mathcal{L}(\boldsymbol{x}, \boldsymbol{\theta}) = \underbrace{\log P(\boldsymbol{x} \mid \boldsymbol{z})}_{\text{Reconstruction error}} - \left(\sum_{j=1}^{d_z} \mu_j^2 + \sigma_j^2 - \log(\sigma^2) - 1 \right)$$

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Finally, define over the entire dataset

$$\mathcal{L}(\boldsymbol{X}, \boldsymbol{\theta}) = \sum_{i=1}^{n} \sum_{j=1}^{d_z} \left(x_{[i],j} - f^{-1}\left(f\left(\boldsymbol{x}_{[i]}, \boldsymbol{\theta}_e\right), \boldsymbol{\theta}_d\right)_j \right)^2 -$$

$$\left(\sum_{i=1}^{n} \sum_{j=1}^{d_z} \mu_{[i],j}^2 + \sigma_{[i],j}^2 - \log\left(\sigma_{[i],j}^2\right) - 1 \right)$$

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Scale of two terms can vary, we do not want one term to dominate

VAE Implementation

Paper suggests using minibatch size m and dataset size n

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$$\mathcal{L}(\boldsymbol{X}, \boldsymbol{\theta}) = \frac{m}{n} \sum_{i=1}^{n} \sum_{j=1}^{d_z} \left(x_{[i],j} - f^{-1}\left(f\left(\boldsymbol{x}_{[i]}, \boldsymbol{\theta}_e \right), \boldsymbol{\theta}_d \right)_j \right)^2 -$$

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$$\beta \left(\sum_{i=1}^{n} \sum_{j=1}^{d_z} \mu_{[i],j}^2 + \sigma_{[i],j}^2 - \log\left(\sigma_{[i],j}^2 \right) - 1 \right)$$

VAE Implementation

```
def L(model, x, m, n, beta, key):
  mu, sigma = model.f(x)
  epsilon = jax.random.normal(key, x.shape[0])
  z = mu + sigma * epsilon
  pred_x = model.f_inverse(z)

  recon = jnp.sum((x - pred_x) ** 2)
  kl = jnp.sum(mu ** 2 + sigma ** 2 - jnp.log(sigma) - 1)

  return m / n * recon + beta * kl
```

VAE Implementation

Coding VAE

https://colab.research.google.com/drive/1UyR_W6NDIujaJXYlHZh6O3NfaCAMscpH#scrollTo=nmyQ8aE2pSbb

https://www.youtube.com/watch?v=UZDiGooFs54