

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

How do humans process temporal data?

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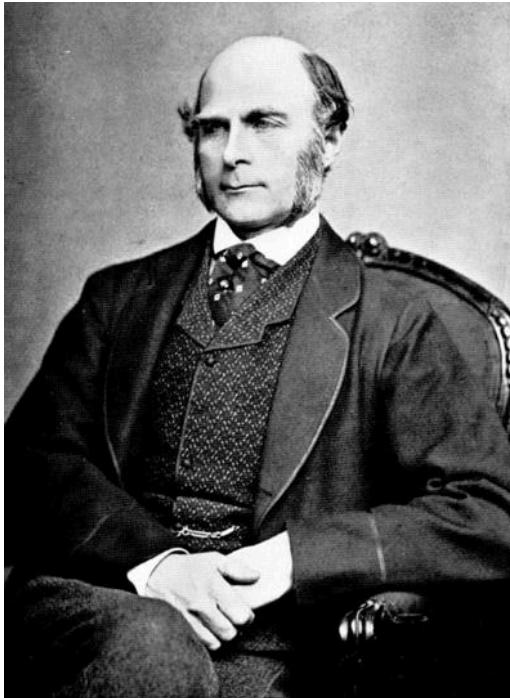
Humans only perceive the present

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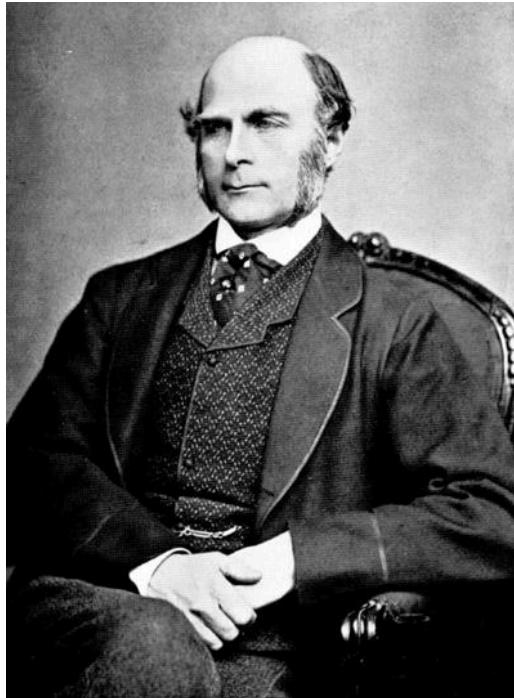
Humans process temporal data by storing and recalling memories

Francis Galton (1822-1911) photo composite memory

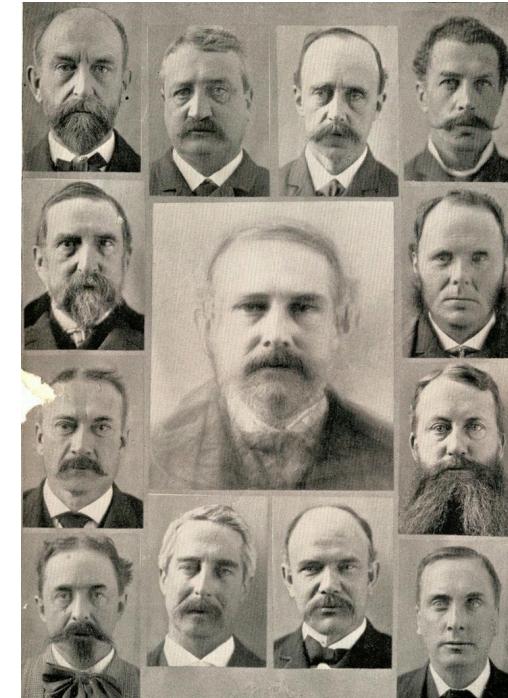


Review

Francis Galton (1822-1911)
photo composite memory



Composite photo of members of a
party



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

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

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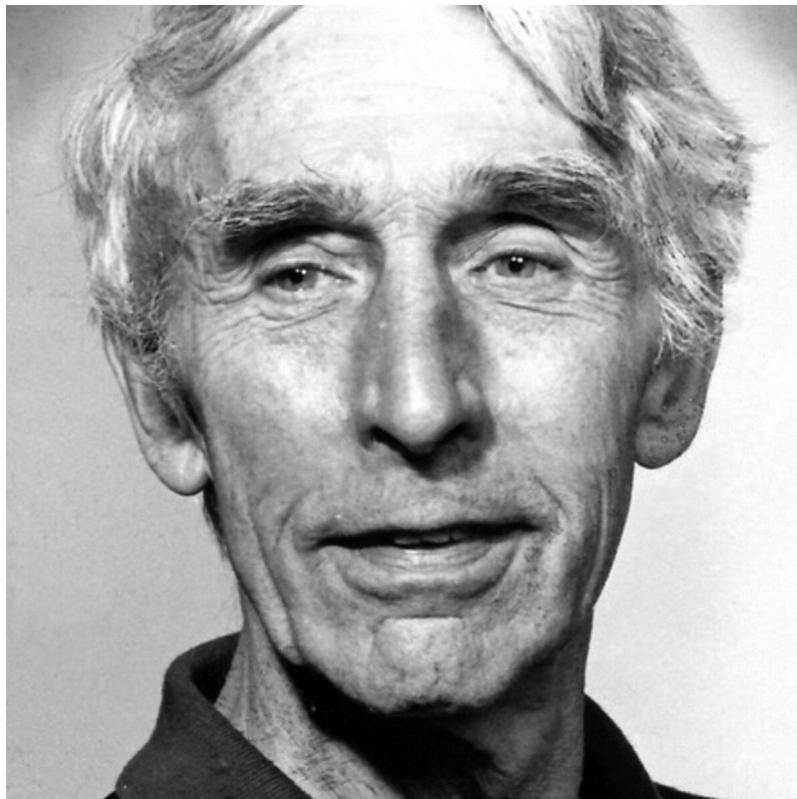
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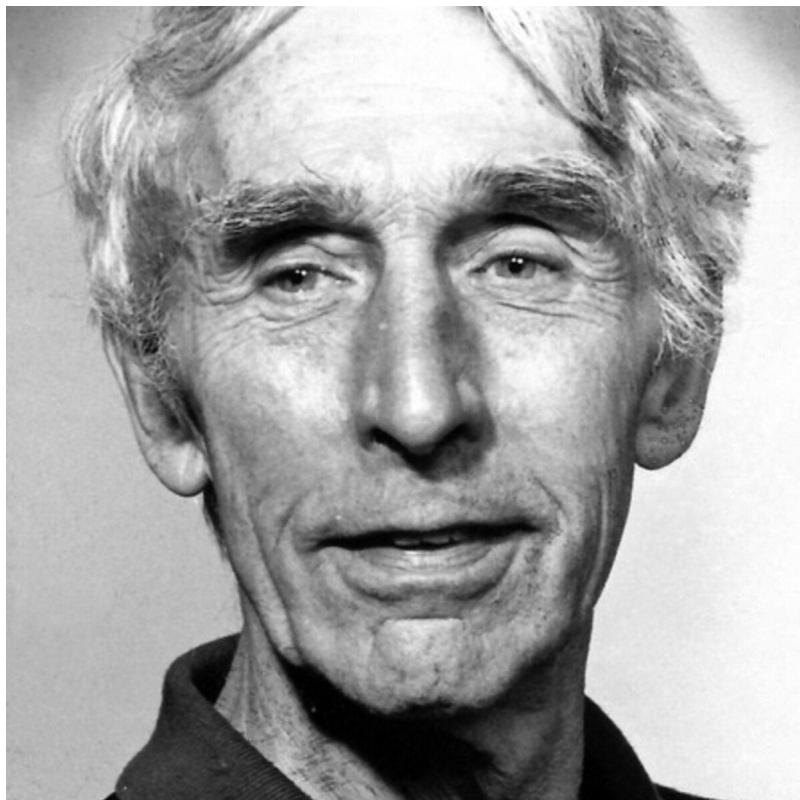
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Humans forget old information

Murdock (1982)

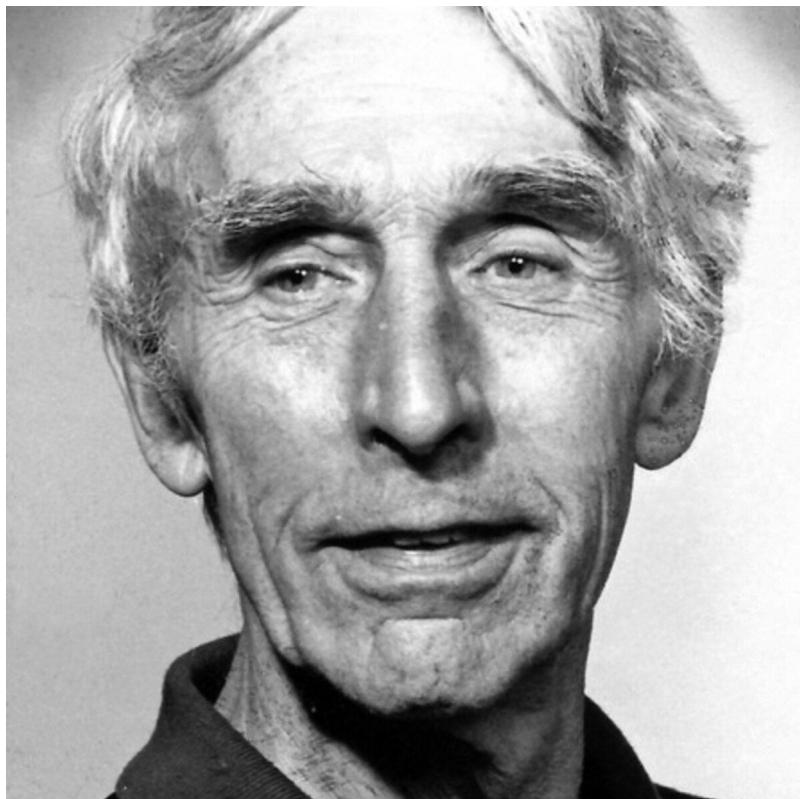


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$$f(\mathbf{h}, \mathbf{x}, \boldsymbol{\theta}) = \gamma \mathbf{h} + \boldsymbol{\theta}^\top \overline{\mathbf{x}}; \quad 0 < \gamma < 1$$

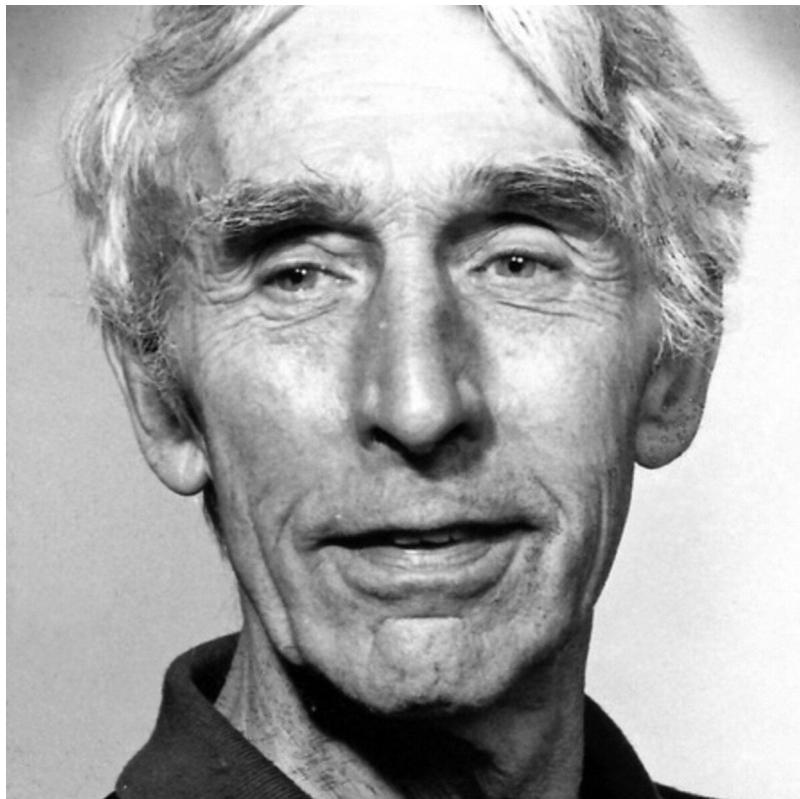
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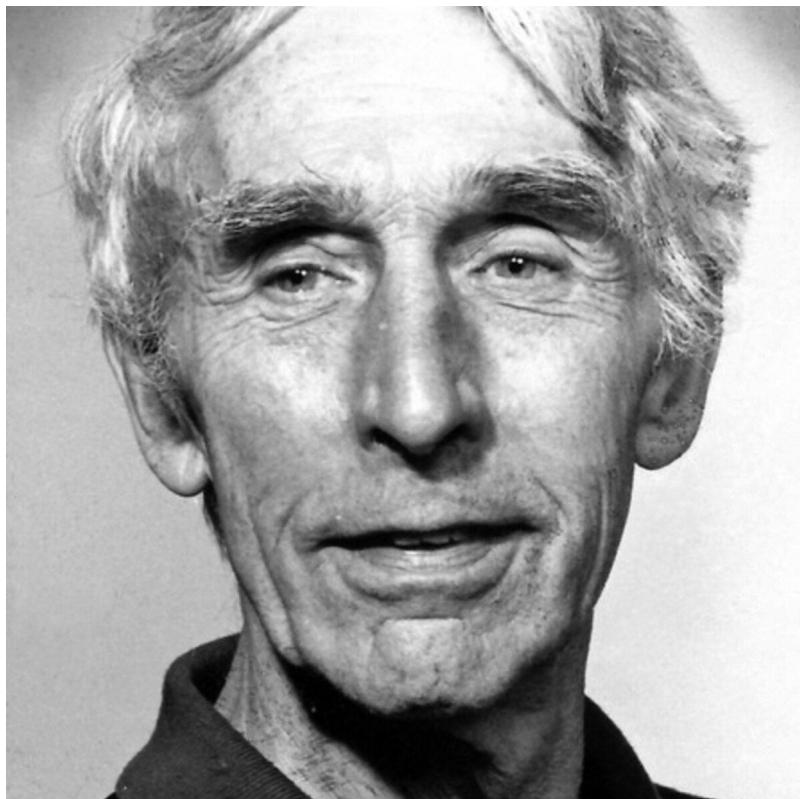


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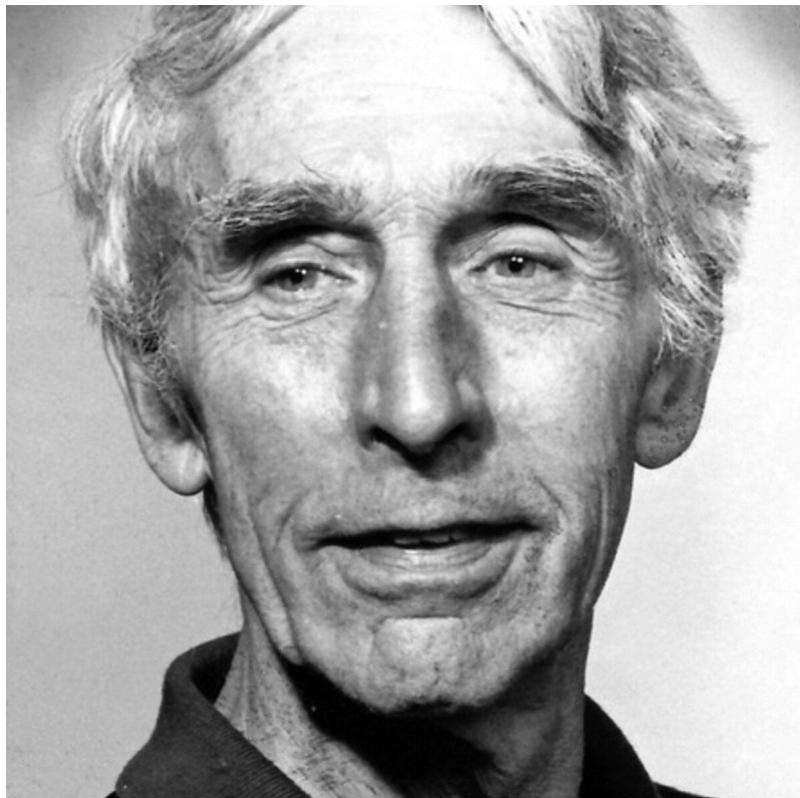
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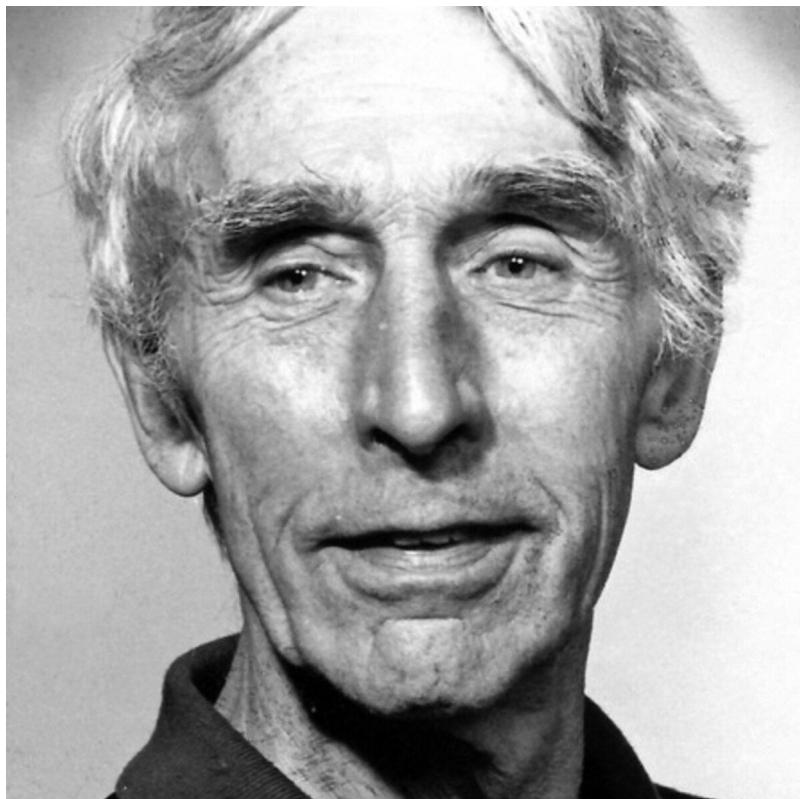
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$$h_T = \gamma^3 h_{T-3} + \gamma^2 \theta^\top \bar{x}_{T-2} + \gamma \theta^\top \bar{x}_{T-1} + \theta^\top \bar{x}_T$$

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h : Everything you remember (hometown, birthday, etc)

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

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$$\begin{bmatrix} \mathbf{y}_1 \\ \vdots \\ \mathbf{y}_T \end{bmatrix} = \begin{bmatrix} g(\mathbf{h}_1, \mathbf{x}_1, \theta_g) \\ \vdots \\ g(\mathbf{h}_T, \mathbf{x}_T, \theta_g) \end{bmatrix}$$

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Add forgetting

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Through gradient descent, neural network learns which memories to forget

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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=TUMonJ1u8Va

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Compression



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Question: What is missing?

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

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In compression, we reduce the size of data by removing information

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When you discuss films with friends, you summarize them

This is a form of **compression**

$$f \left(\begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix} \right) = \text{Green ogre and donkey save princess}$$

In compression, we reduce the size of data by removing information

Let us examine a more principled form of video compression

Compression

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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H.264 encoder selects 16×16 pixel blocks, estimates shift between frames, applies cosine transform, ...

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Question: What is the size of Z in GB?

Answer: 60 GB, original size was 3000 GB

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

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What happens on your computer when you watch Shrek?

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Download $z \in Z$ from the internet

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

Compression

Compression may be **lossy**

Compression

Compression may be **lossy** or **lossless**

Compression

Compression may be **lossy**

or **lossless**



Compression

Compression may be **lossy** or **lossless**



Question: Which is H.264?

Agenda

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

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

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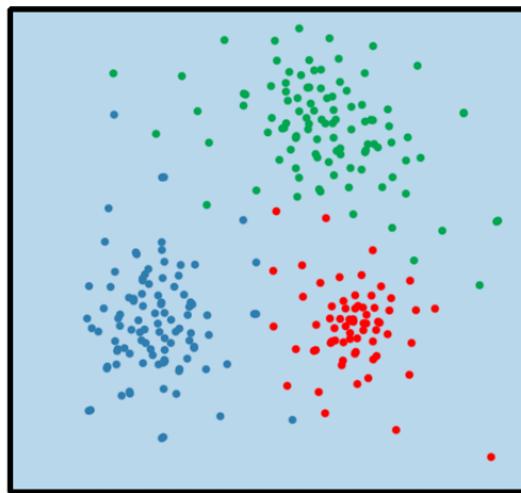
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Training autoencoders is different than what we have seen before

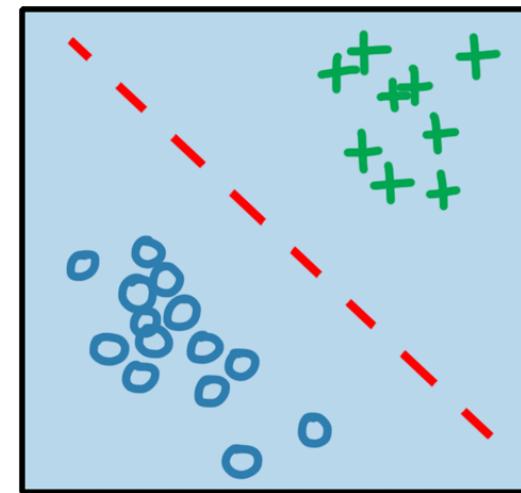
Autoencoders

machine learning

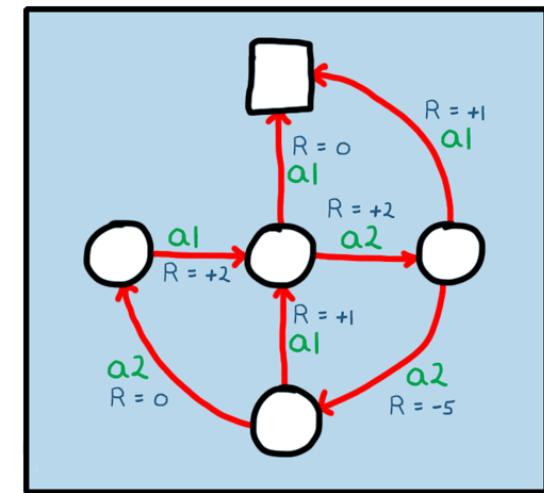
unsupervised
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supervised
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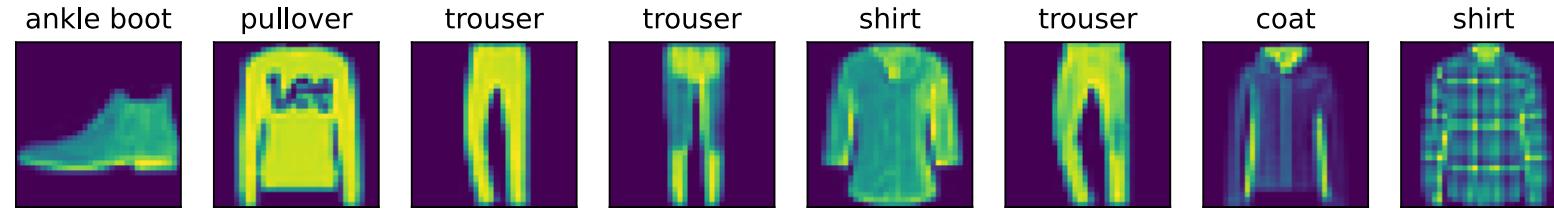
The training algorithm will learn **unsupervised** (only from \mathbf{X})

Autoencoders

Task: Compress images for your clothing website to save on costs

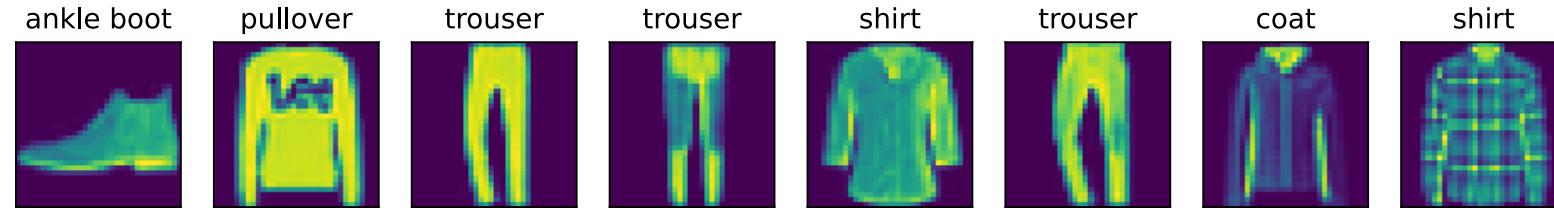
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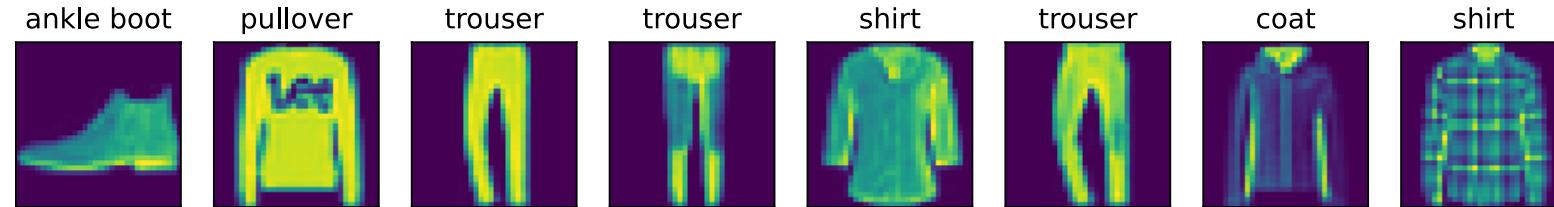


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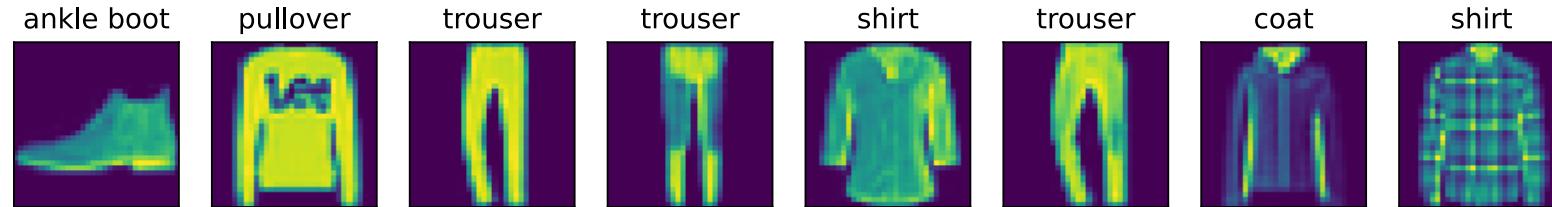
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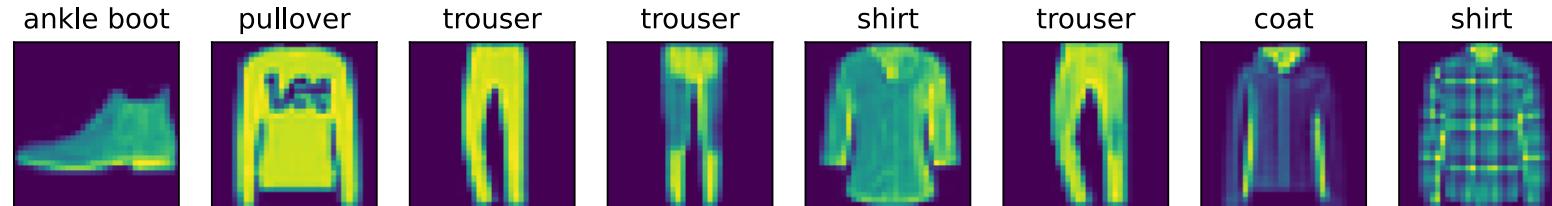
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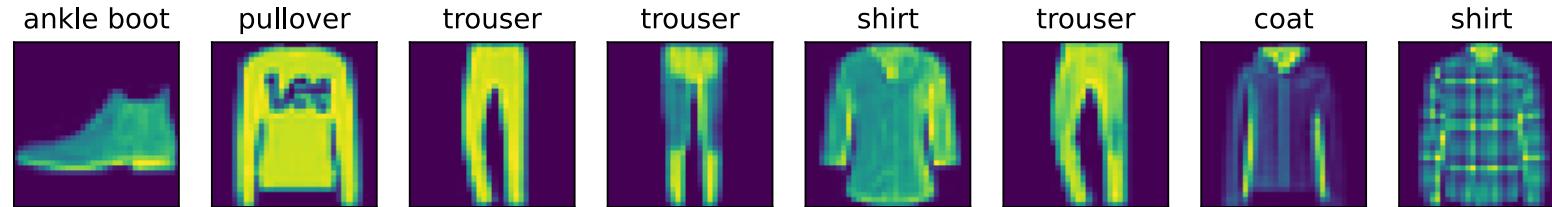
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Autoencoders

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How do we find θ ?

Autoencoders

Let us find f , then find the inverse f^{-1}

Autoencoders

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Start with a perceptron

Autoencoders

Let us find f , then find the inverse f^{-1}

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$$f(x, \theta) = \sigma(\theta^\top \bar{x}); \quad \theta \in \mathbb{R}^{d_x \times d_z}$$

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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}

Autoencoders

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We call this the **reconstruction loss**

It is an unsupervised loss because we only provide X and not Y !

Autoencoders

First coding exercise

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

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

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Applications

We can use autoencoders for more than compression

Applications

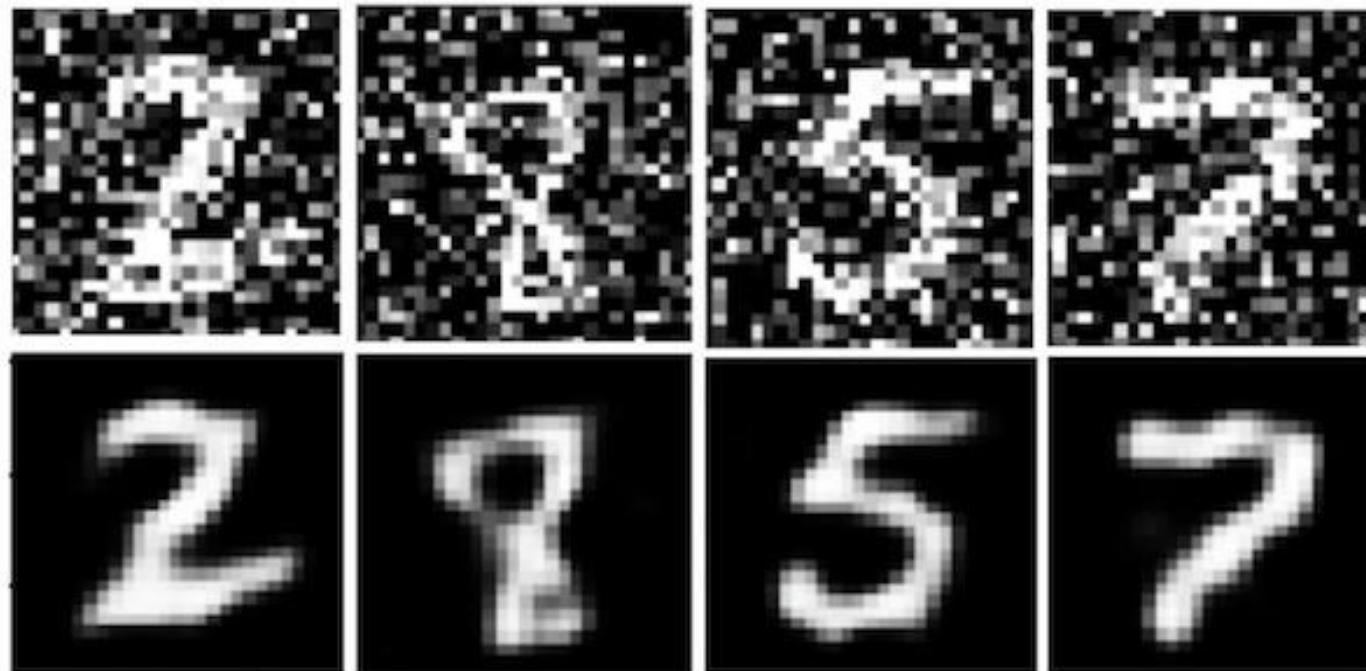
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Applications

Generate some noise

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

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Add noise to the image

$$x + \varepsilon$$

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

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

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$$x + \varepsilon$$

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

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

Autoencoder will learn to remove noise when reconstructing image

Applications

We can add camera blur too

Applications

We can add camera blur too



Applications

$$\text{blur}(x + \epsilon)$$

Applications

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

Denoising deblur loss

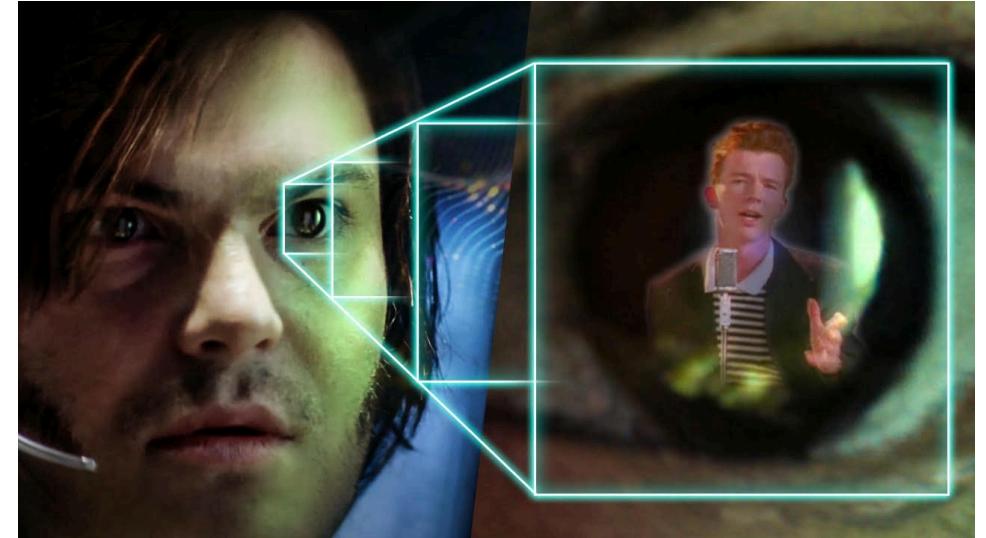
$$\mathcal{L}(\mathbf{X}, \boldsymbol{\theta}) = \sum_{i=1}^n \sum_{j=1}^{d_x} \left(x_{[i],j} - f^{-1} \left(f \left(\text{blur} \left(\mathbf{x}_{[i]} + \varepsilon \right), \boldsymbol{\theta}_e \right), \boldsymbol{\theta}_d \right)_j \right)^2$$

Applications

Now we can “enhance” images like in crime tv shows

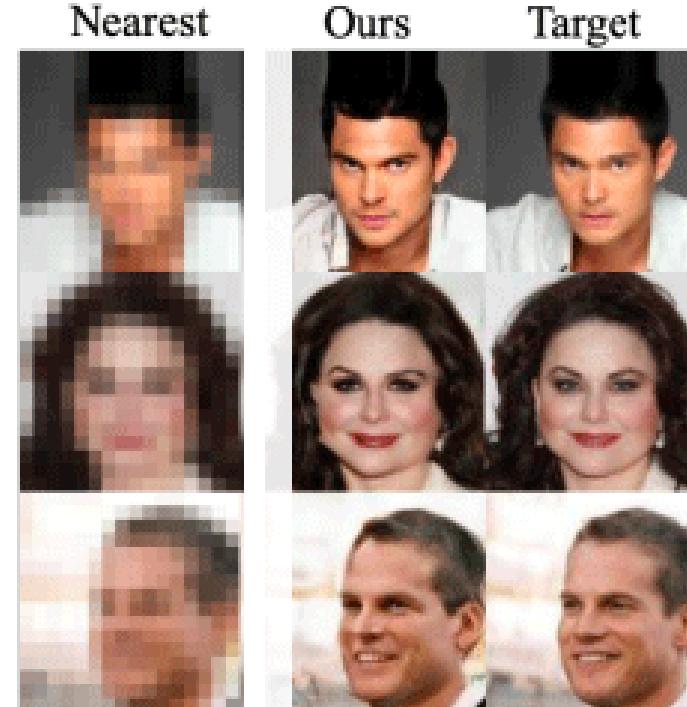
Applications

Now we can “enhance” images like in crime tv shows



Applications

We can deblur faces from security cameras



Applications

We can even hide parts of the image

Applications

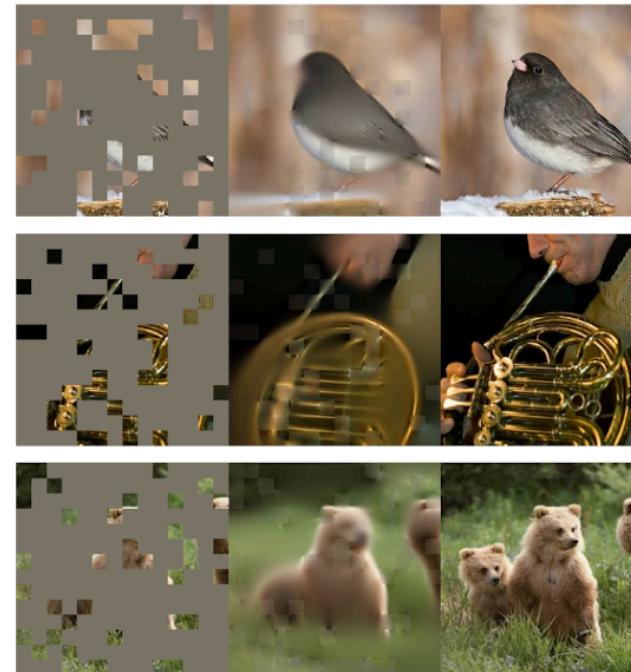
We can even hide parts of the image

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

Applications

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Applications

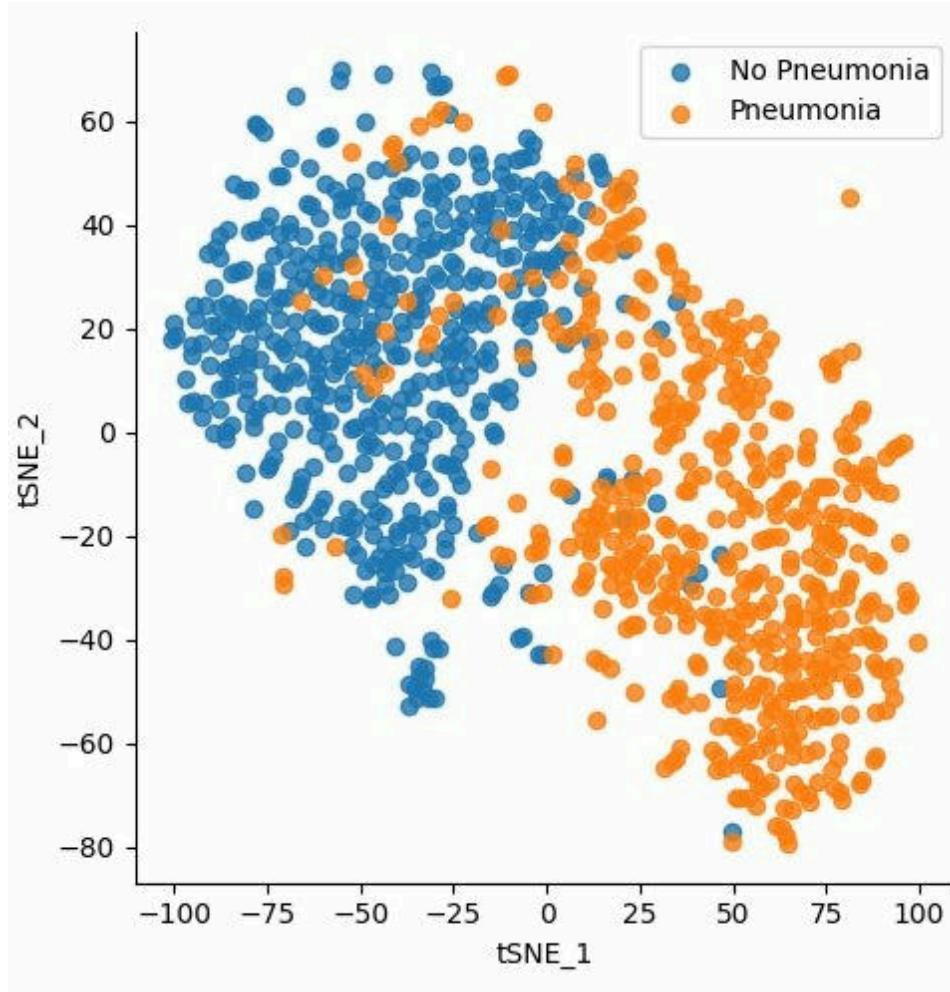
What is happening here? How can these models do this?

Applications

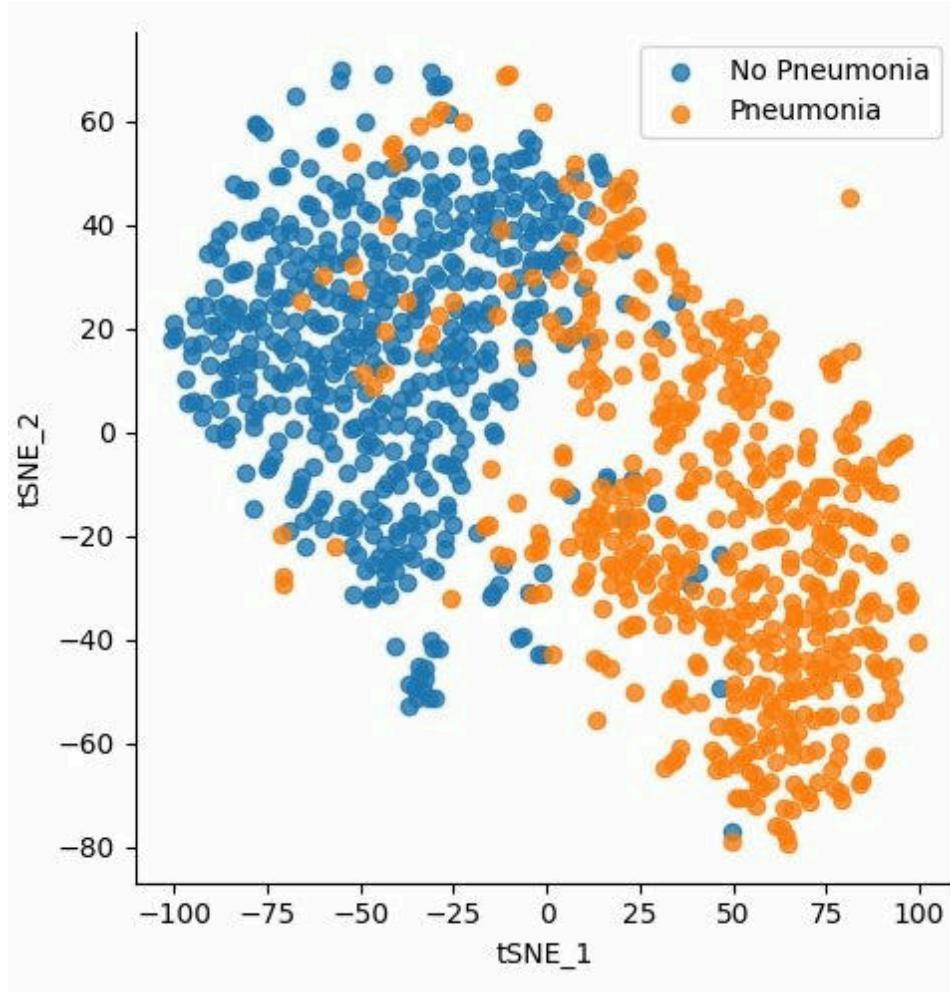
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Autoencoders learn the structure of the dataset

Applications

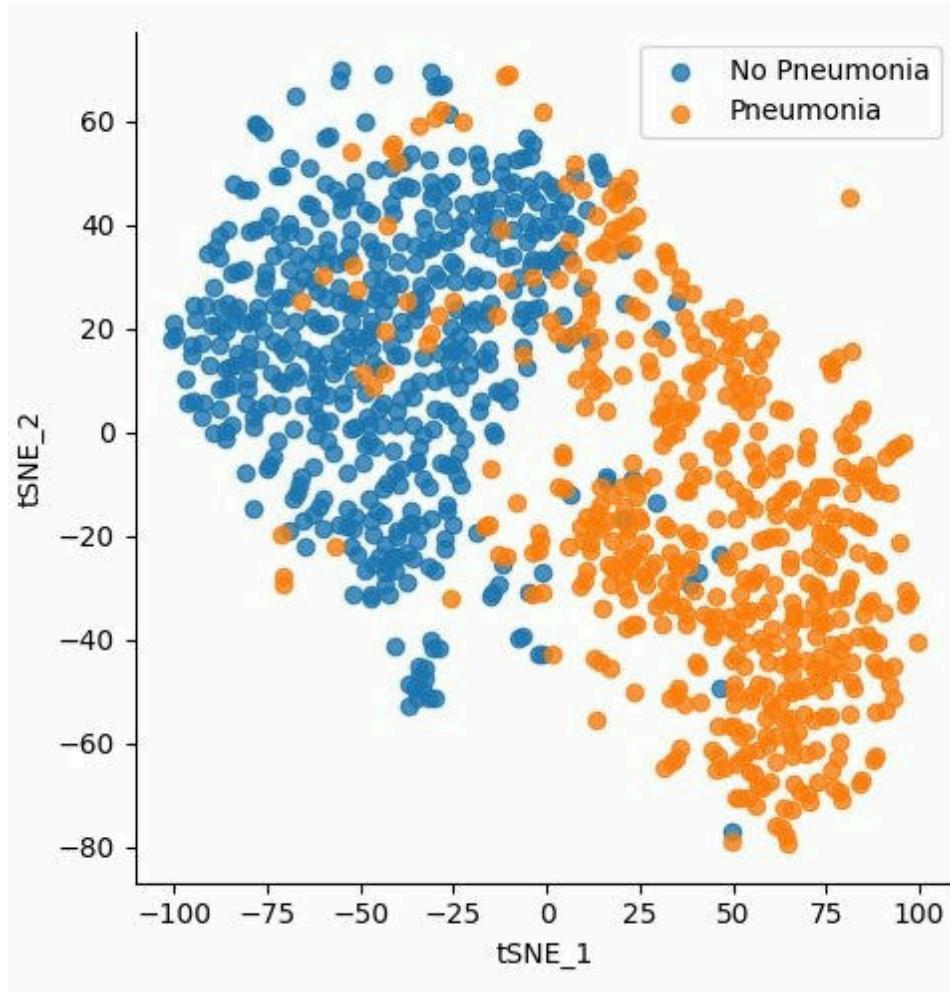


Applications



X : Pictures of human lungs

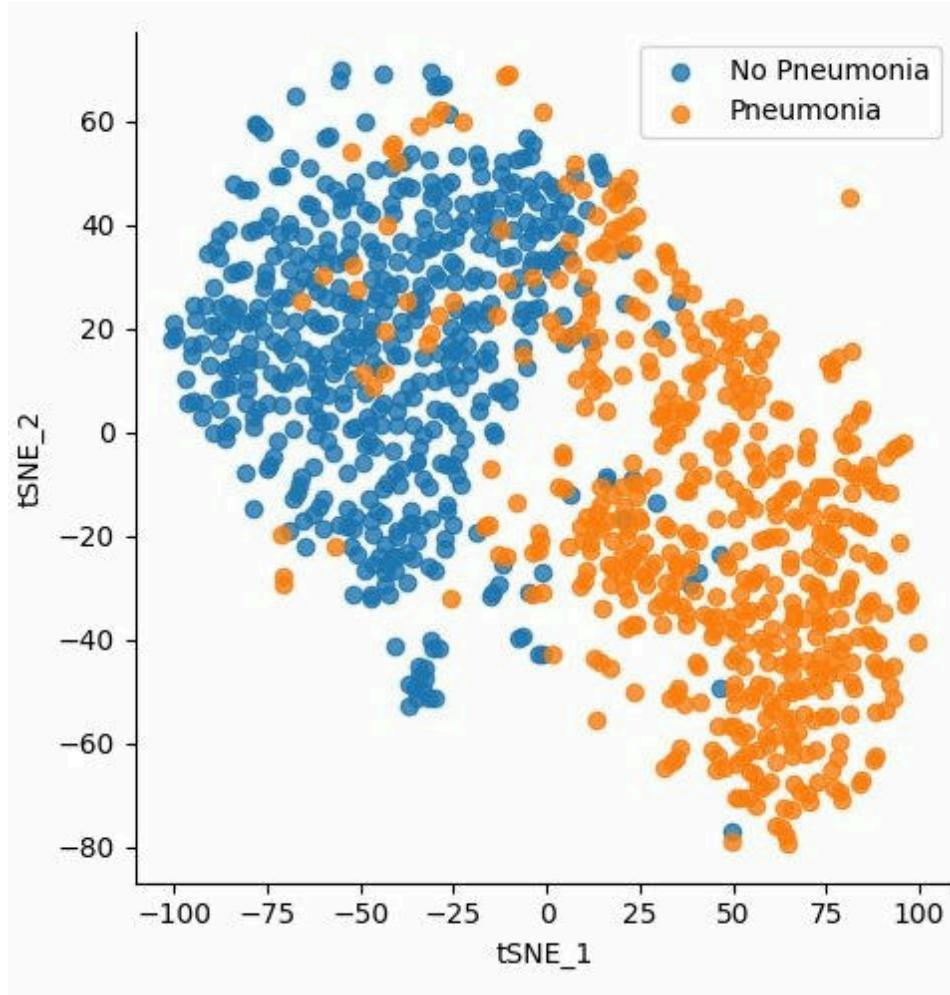
Applications



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

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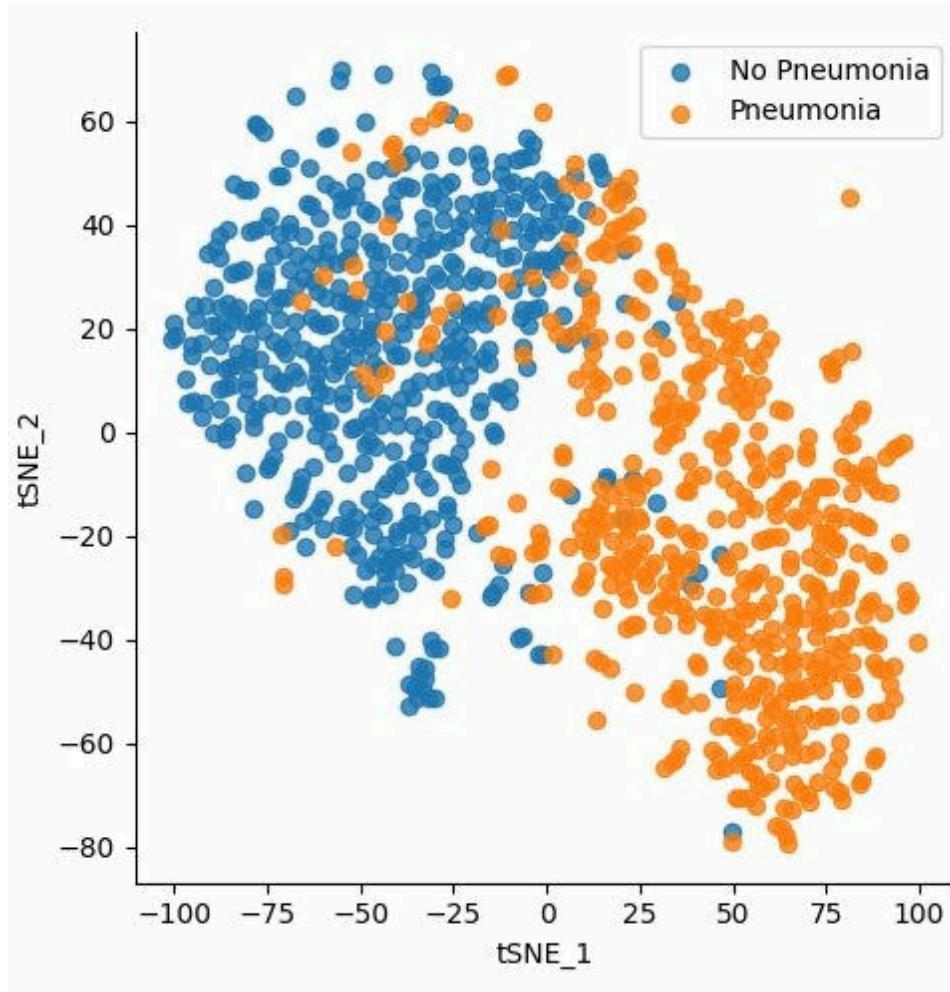


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Learns the structure of lungs from images

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

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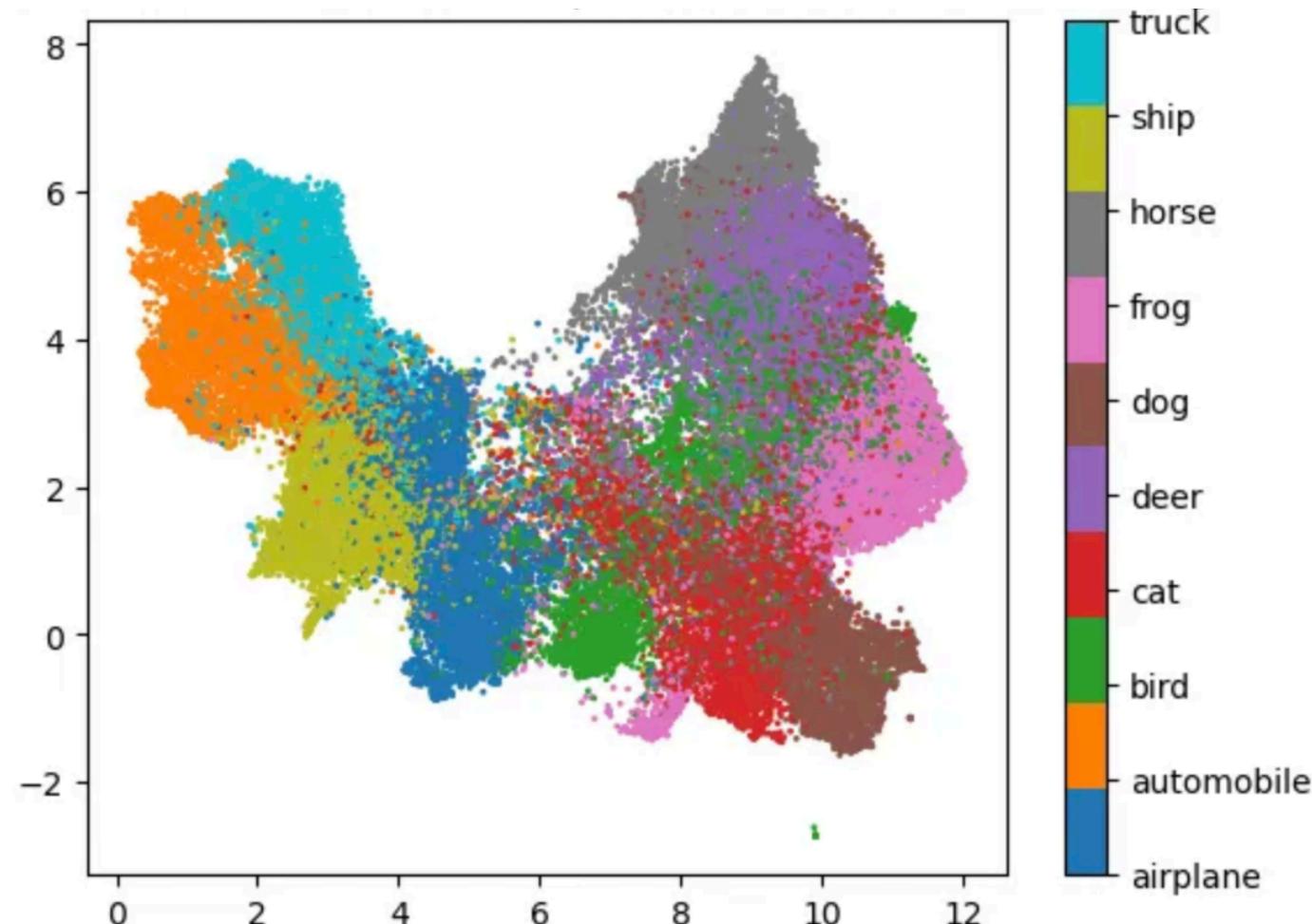
If the dataset is lung images, the model learns the structure of lungs

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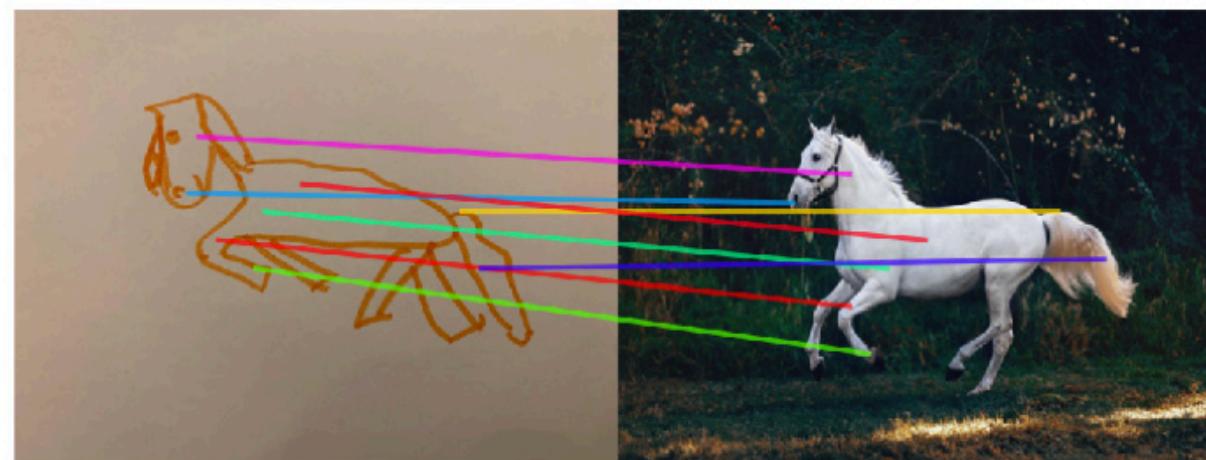
Nobody tells them what a dog or cat is

They learn that on their own

Applications



Applications



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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These networks can understand our world

Agenda

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

Agenda

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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**

Variational Modeling

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Variational Modeling

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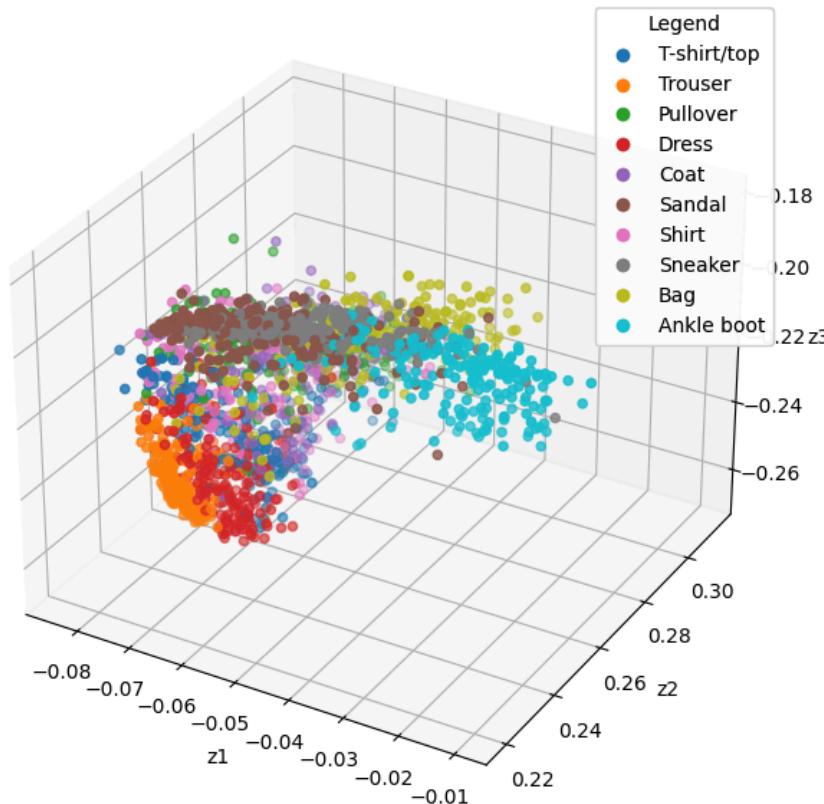
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How does this work?

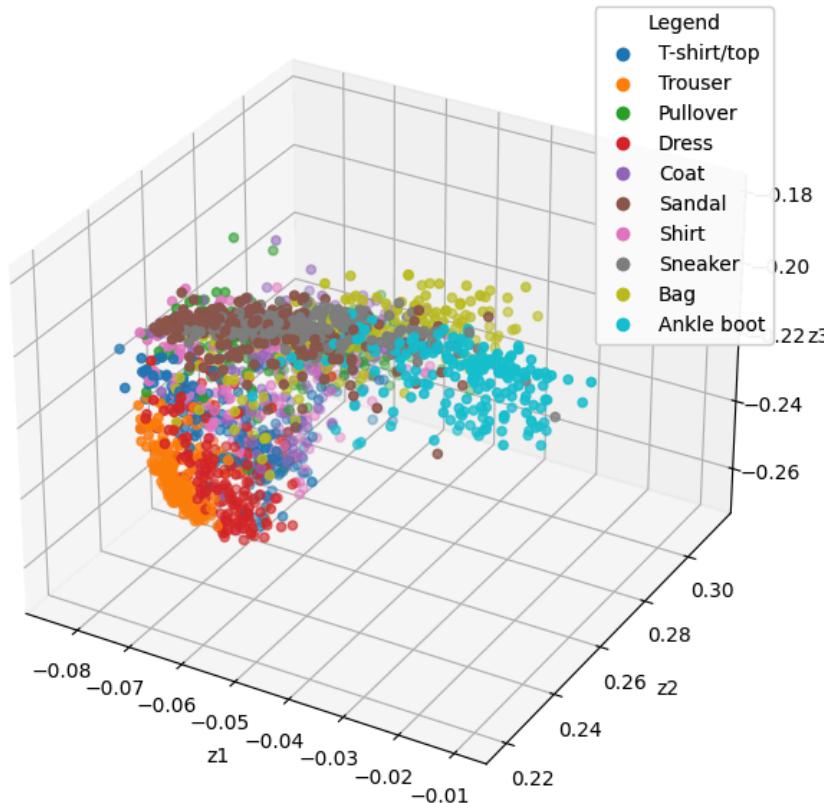
Variational Modeling

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

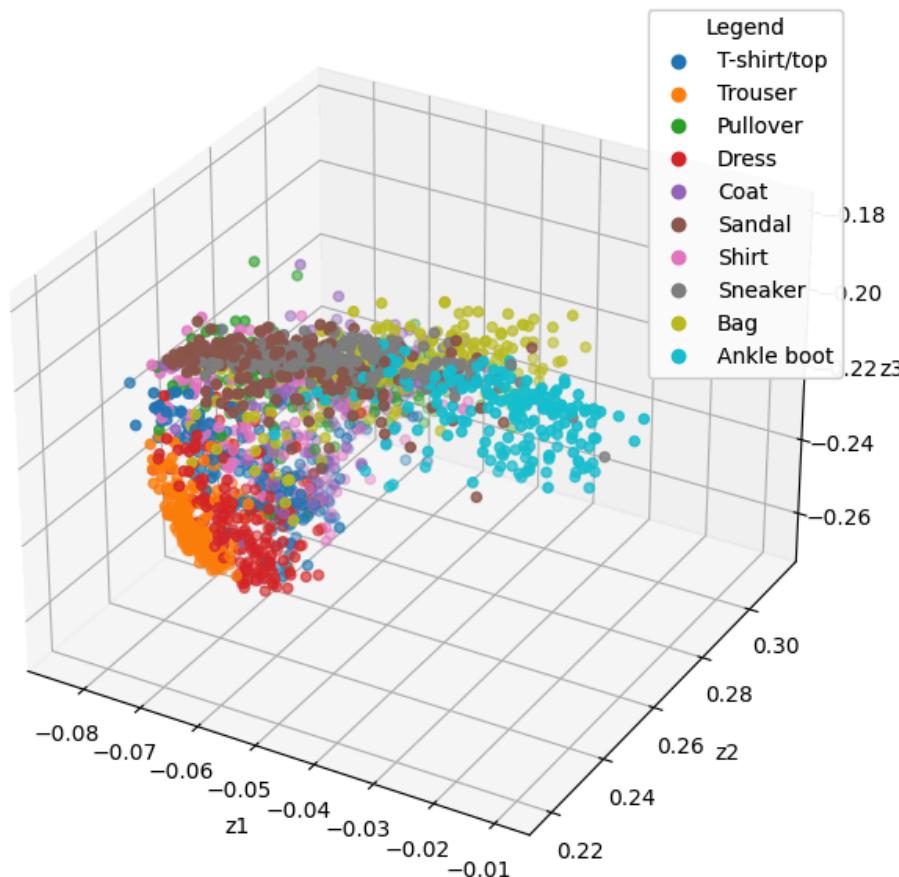


Variational Modeling

What happens if we decode a new point?

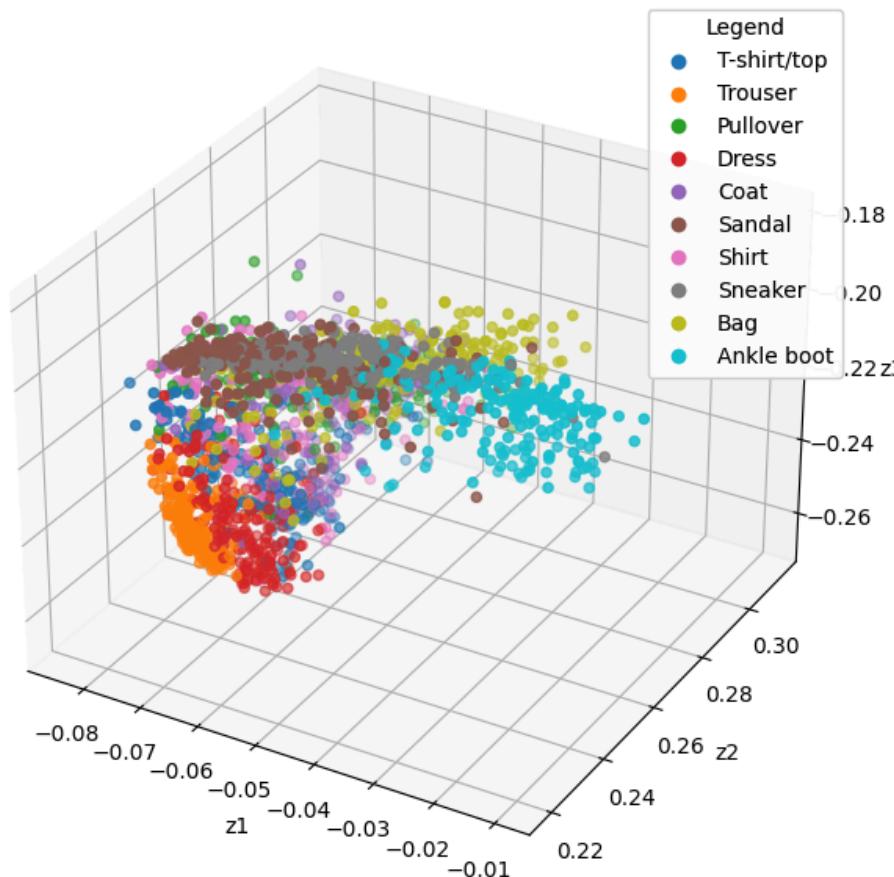


Variational Modeling



Autoencoder generative model:

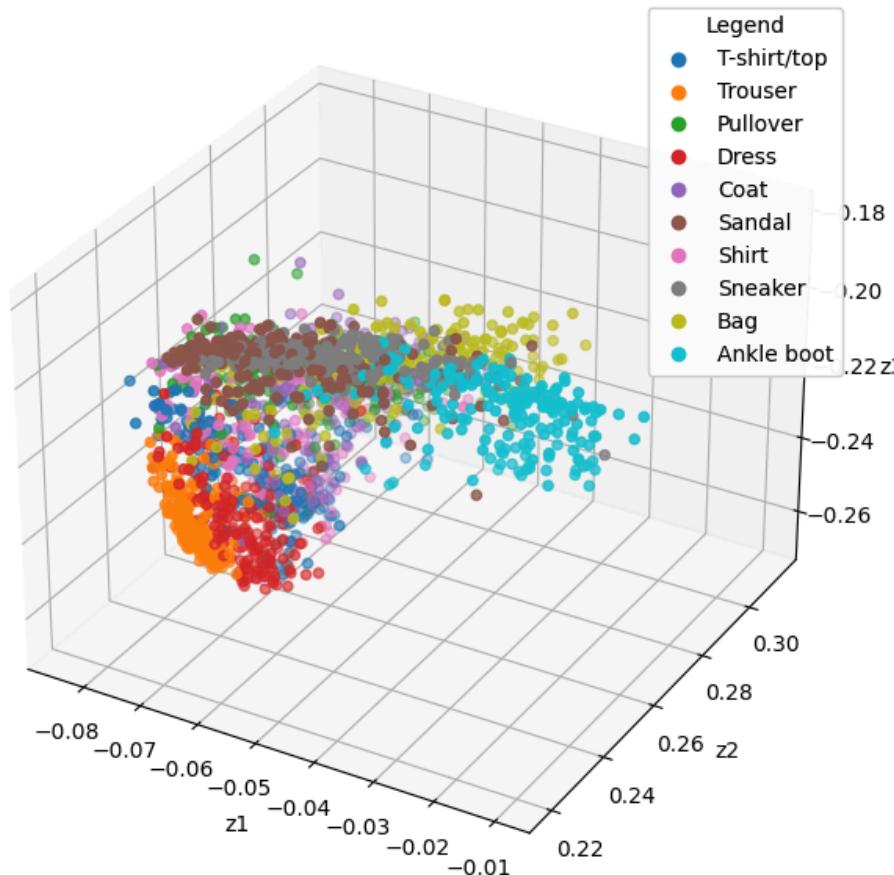
Variational Modeling



Autoencoder generative model:

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

Variational Modeling

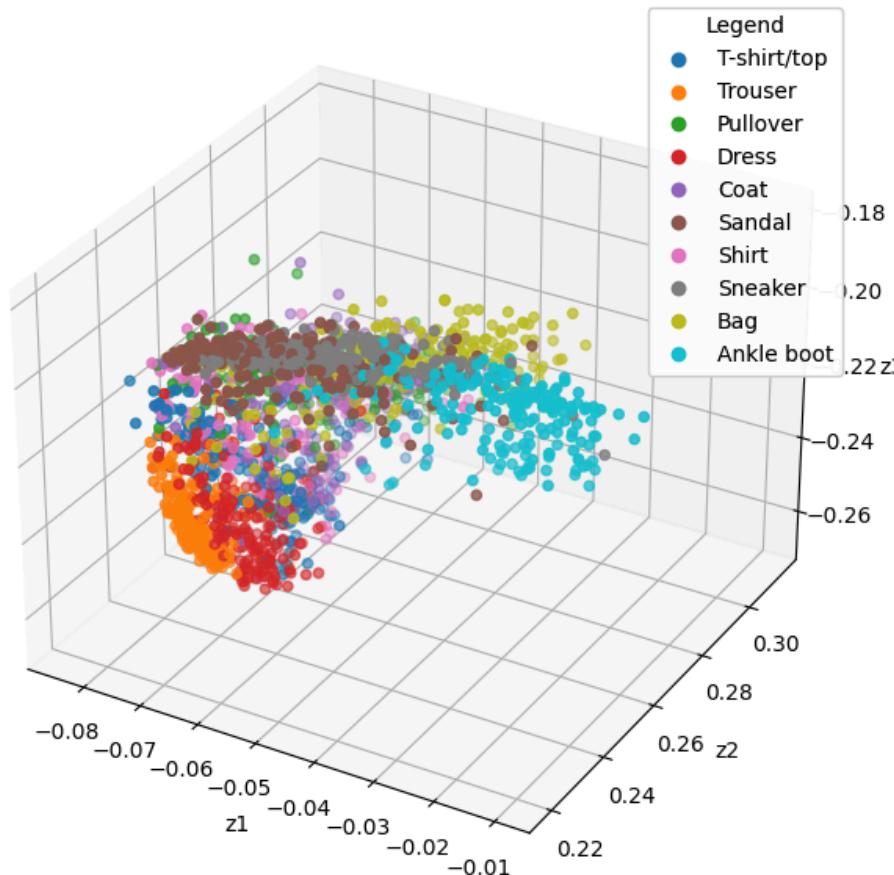


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Variational Modeling



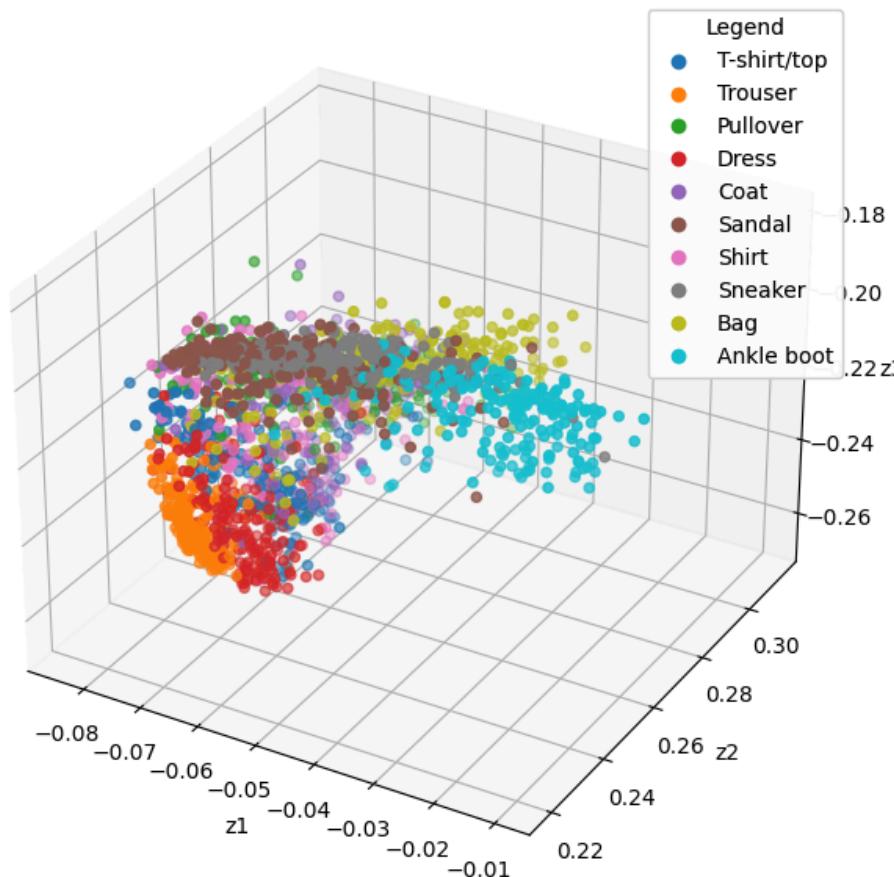
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Variational Modeling



Variational Modeling



$$f^{-1}(z_k + \epsilon, \theta_d)$$

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

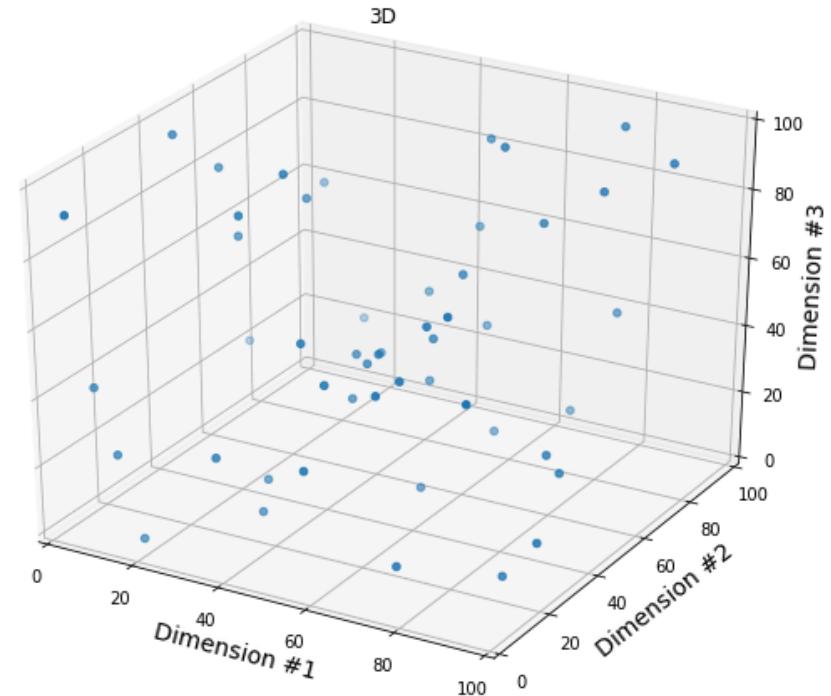
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As d_z increases, points move
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Variational Modeling

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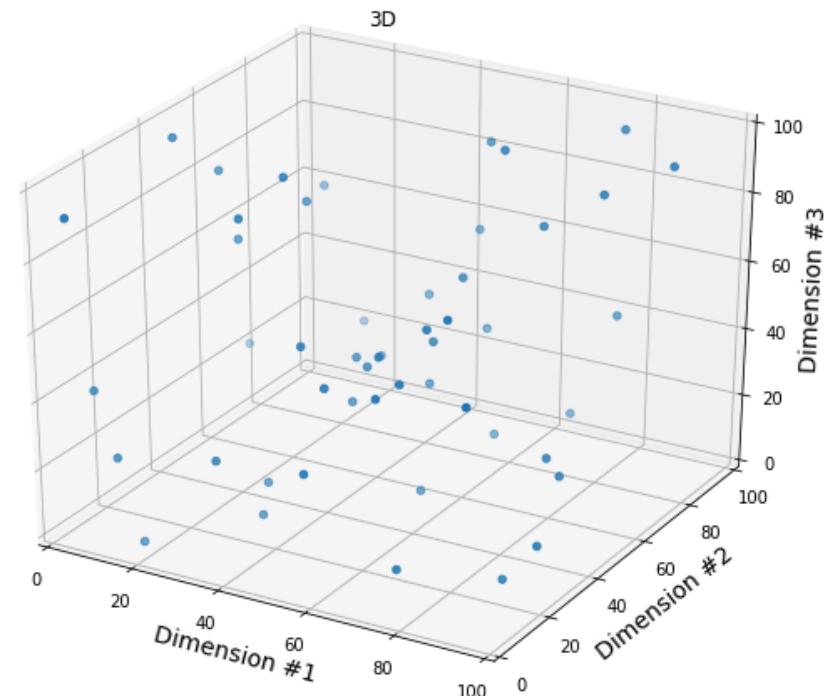
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Variational Modeling

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

Variational Modeling

Question: What can we do?

Variational Modeling

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Answer: Force the points to be close together!

Variational Modeling

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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)

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Variational Modeling

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How?

Variational Modeling

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Variational Modeling

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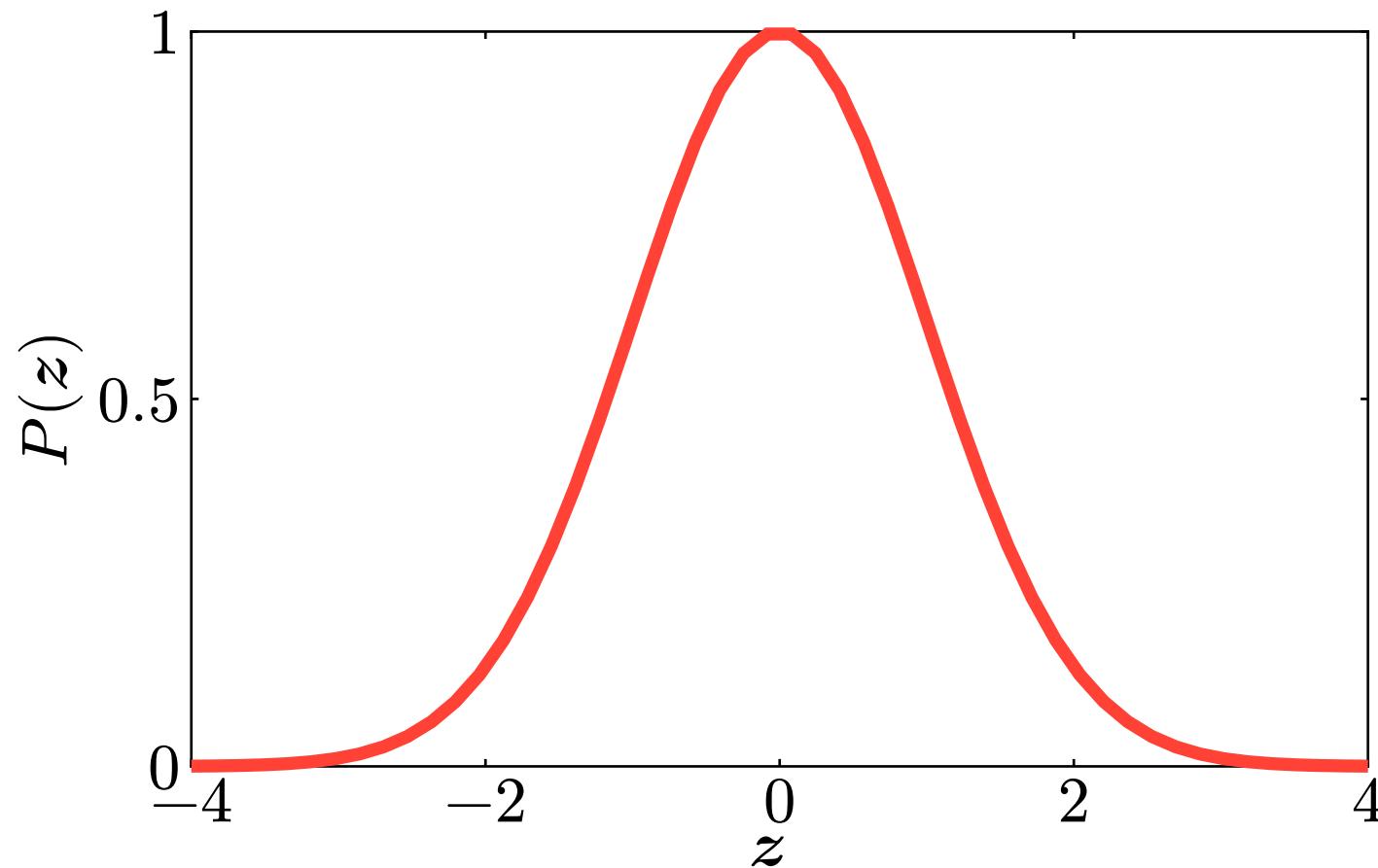
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How?

Make $z_{[1]}, \dots, z_{[n]}$ normally distributed

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

Variational Modeling



Variational Modeling

If $z_{[1]}, \dots, z_{[n]}$ are distributed following $\mathcal{N}(0, 1)$:

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Variational Modeling

If $z_{[1]}, \dots, z_{[n]}$ are distributed following $\mathcal{N}(0, 1)$:

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

Variational Modeling

So how do we ensure that $z_{[1]}, \dots, z_{[n]}$ are normally distributed?

Variational Modeling

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Variational Modeling

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

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

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Large $P(x; \theta)$



$P(x; \theta) \approx 0$



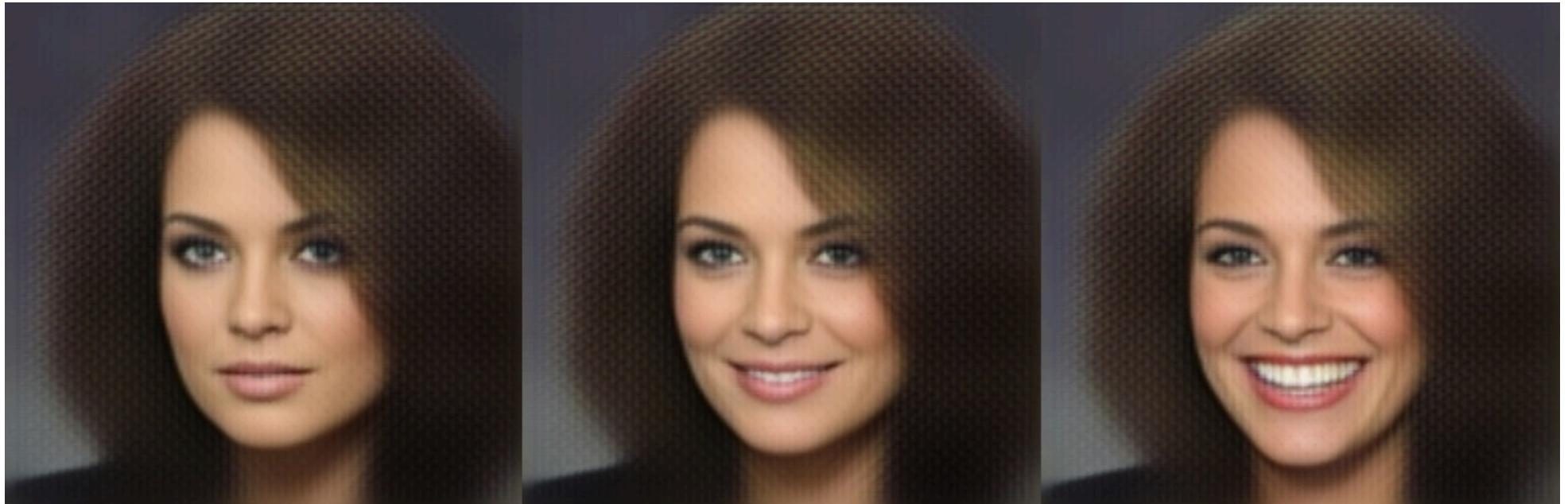
Variational Modeling

Key idea 2: There is some latent variable z which generates data x

Variational Modeling

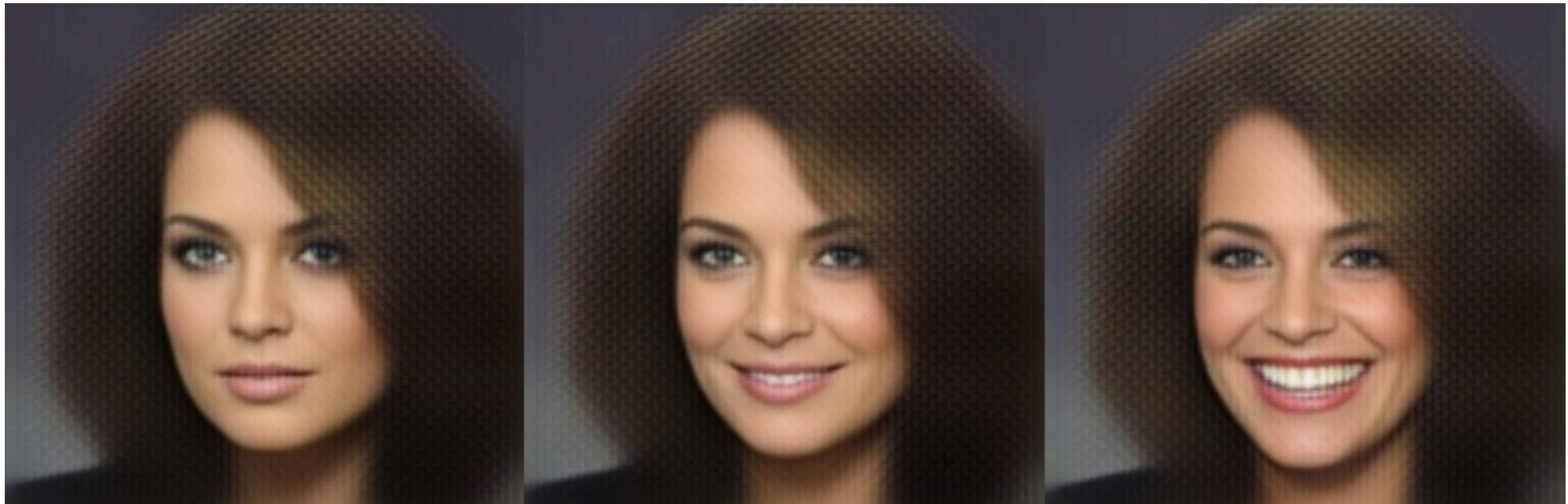
Key idea 2: There is some latent variable z which generates data x

$x :$



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

Variational Modeling

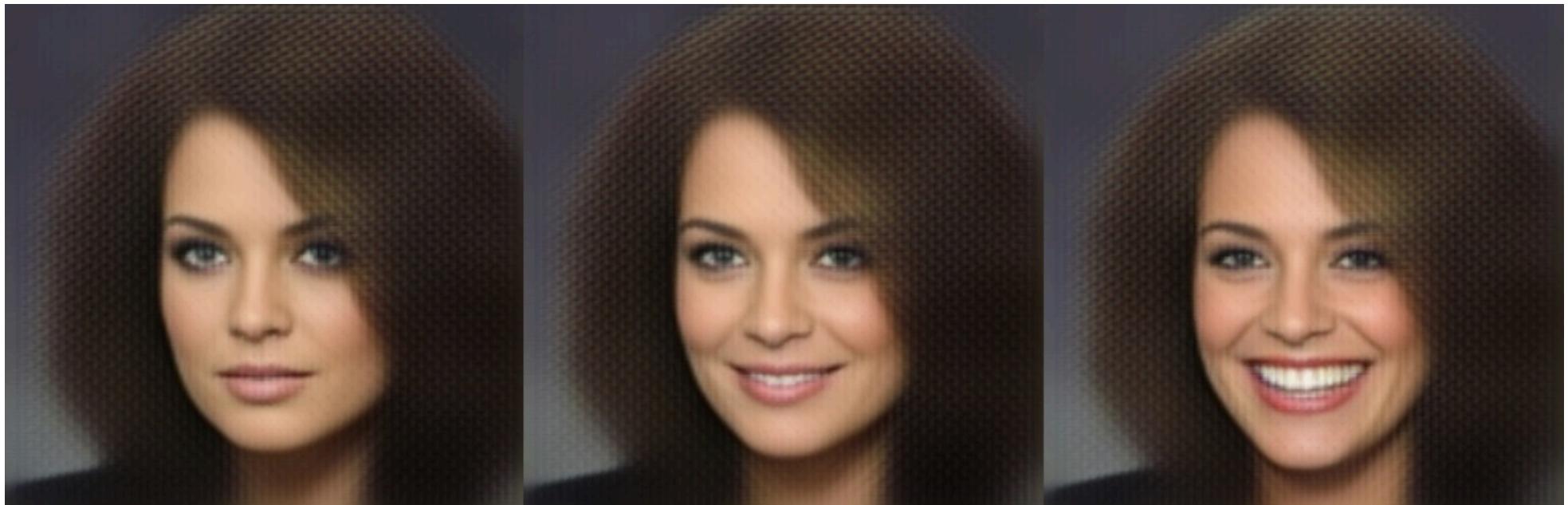


Variational Modeling



Network can only see x , it cannot directly observe z

Variational Modeling



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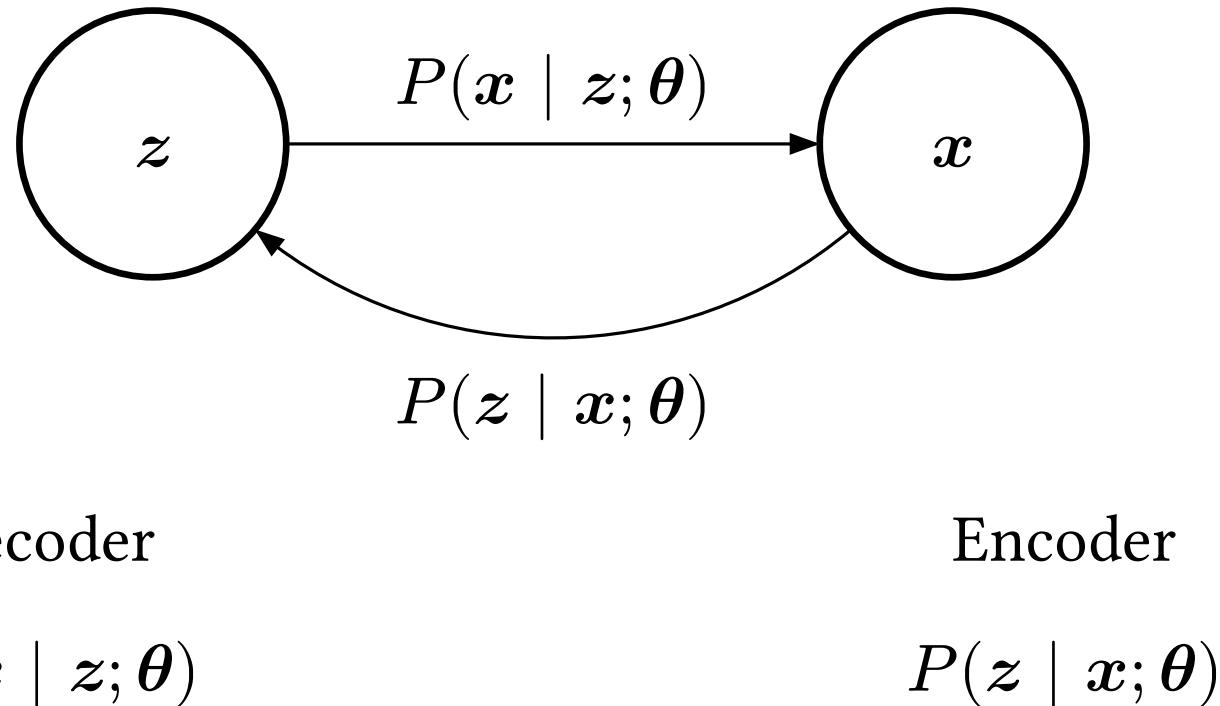
Given x , find the probability that the person is smiling $P(z \mid x; \theta)$

Variational Modeling

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

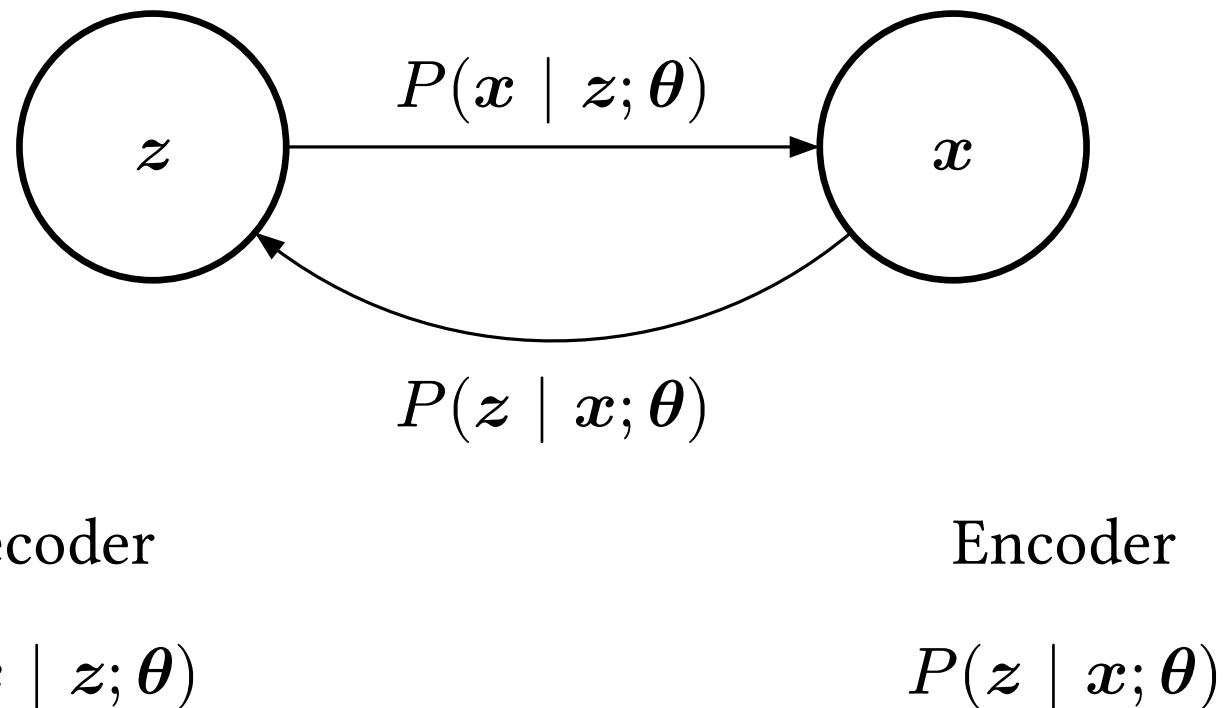
Variational Modeling

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Variational Modeling

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

Variational Modeling

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

Variational Modeling

$$P(z, x; \theta) = P(x | z; \theta) P(z; \theta)$$

We can choose any distribution for $P(z)$

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

We can randomly generate z , which we can decode into new x !

Variational Modeling

Now, all we must do is find θ that best explains the dataset distribution

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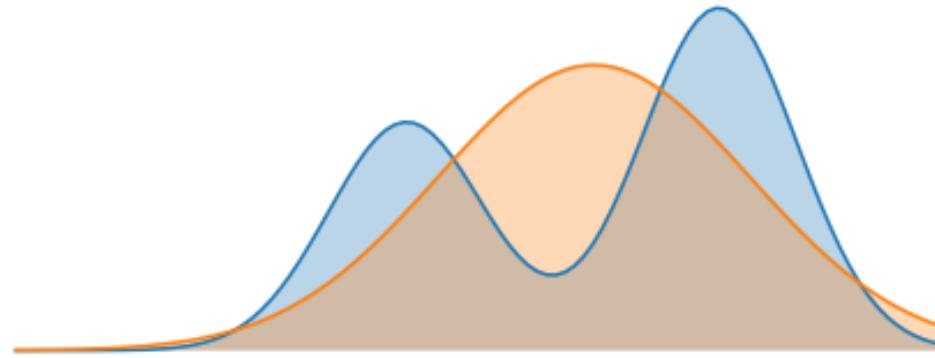
Question: How do we measure the distance between probability distributions?

Variational Modeling

Answer: KL divergence

Variational Modeling

Answer: KL divergence



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

Variational Modeling

Learn the parameters for our model

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$$\arg \min_{\theta} \text{KL}(P(x), P(x; \theta))$$

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

Variational Modeling

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Variational Modeling

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How is this ELBO helpful?

Decoder

$$P(x \mid z; \theta)$$

Encoder

$$P(z \mid x; \theta)$$

Prior

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

Variational Modeling

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Decoder	Encoder	Prior
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Now we know how to train our autoencoder!

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Our encoder should output d_z means and d_z standard deviations

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

VAE Implementation

```
core = nn.Sequential(...)  
mu_layer = nn.Linear(d_h, d_z)  
# Neural networks output real numbers  
# But sigma must be positive  
# Output log sigma, because e^(sigma) is always positive  
log_sigma_layer = nn.Linear(d_h, d_z)  
# Alternatively, one sigma for all data  
log_sigma = jnp.ones((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

VAE Implementation

We can sample from the distribution

$$\mu, \sigma = f(x, \theta_e)$$

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

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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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This trick only works with certain distributions

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Step 3: Decode the sample

$$x = f^{-1}(z, \theta_d)$$

VAE Implementation

One last thing, implement the loss function

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Decoder	Encoder	Prior
$P(x \mid z; \theta)$	$P(z \mid x; \theta)$	$P(z) = \mathcal{N}(0, 1)$

VAE Implementation

One last thing, implement the loss function

Decoder

$$P(x \mid z; \theta)$$

Encoder

$$P(z \mid x; \theta)$$

Prior

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

$$\mathcal{L}(x, \theta) = \arg \min_{\theta} \left[\underbrace{-\log P(x \mid z; \theta)}_{\text{Reconstruction error}} + \underbrace{\frac{1}{2} \text{KL}(P(z \mid x; \theta), P(z))}_{\text{Constrain latent}} \right]$$

VAE Implementation

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Start with the KL term first

VAE Implementation

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VAE Implementation

$$\mathcal{L}(\mathbf{x}, \boldsymbol{\theta}) = \arg \min_{\boldsymbol{\theta}} \left[-\log P(\mathbf{x} \mid \mathbf{z}; \boldsymbol{\theta}) + \frac{1}{2} \text{KL}(P(\mathbf{z} \mid \mathbf{x}; \boldsymbol{\theta}), P(\mathbf{z})) \right]$$

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

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

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$$= \sum_{j=1}^{d_z} \left(\mathbf{x}_j - f^{-1}(f(\mathbf{x}, \boldsymbol{\theta}_e), \boldsymbol{\theta}_d)_j \right)^2 - \left(\sum_{j=1}^{d_z} \mu_j^2 + \sigma_j^2 - \log(\sigma_j^2) - 1 \right)$$

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Finally, define over the entire dataset

$$\mathcal{L}(X, \theta) = \sum_{i=1}^n \sum_{j=1}^{d_z} \left(x_{[i],j} - f^{-1}(f(x_{[i]}, \theta_e), \theta_d)_j \right)^2 - \left(\sum_{i=1}^n \sum_{j=1}^{d_z} \mu_{[i],j}^2 + \sigma_{[i],j}^2 - \log(\sigma_{[i],j}^2) - 1 \right)$$

VAE Implementation

$$\begin{aligned}\mathcal{L}(\mathbf{X}, \boldsymbol{\theta}) = & \sum_{i=1}^n \sum_{j=1}^{d_z} \left(x_{[i],j} - f^{-1} \left(f \left(\mathbf{x}_{[i]}, \boldsymbol{\theta}_e \right), \boldsymbol{\theta}_d \right)_j \right)^2 - \\ & \left(\sum_{i=1}^n \sum_{j=1}^{d_z} \mu_{[i],j}^2 + \sigma_{[i],j}^2 - \log(\sigma_{[i],j}^2) - 1 \right)\end{aligned}$$

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

VAE Implementation

Another paper finds hyperparameter β also helps

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

VAE Implementation

```
def L(model, x, m, n, 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 ** 2) -
    1)

    return m / n * recon + kl
```

VAE Implementation

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

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

4 Nov - Compensatory rest day (holiday), no lecture

11 Nov - Quiz on autoencoders (not VAE) and Prof. Li on GNNs

18 Nov - Attention and transformers

25 Nov - Reinforcement learning

1 Dec - Foundation models (virtual, optional)