Attention and Transformers

CISC 7026: Introduction to Deep Learning

University of Macau

Agenda

1. GNN Review
2. VAE Review and Coding
3. Attention
4. Positional Encoding
5. Transformers
6. Coding

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1. **GNN Review**
2. VAE Review and Coding
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GNN Review

Graph is a structure of nodes (vertices) and edges

$$G = (\boldsymbol{X}, \boldsymbol{E}) \qquad \boldsymbol{X} \in \mathbb{R}^{T \times d_x} \qquad \boldsymbol{E} \in \mathcal{P}(\mathbb{Z}_T \times \mathbb{Z}_T)$$

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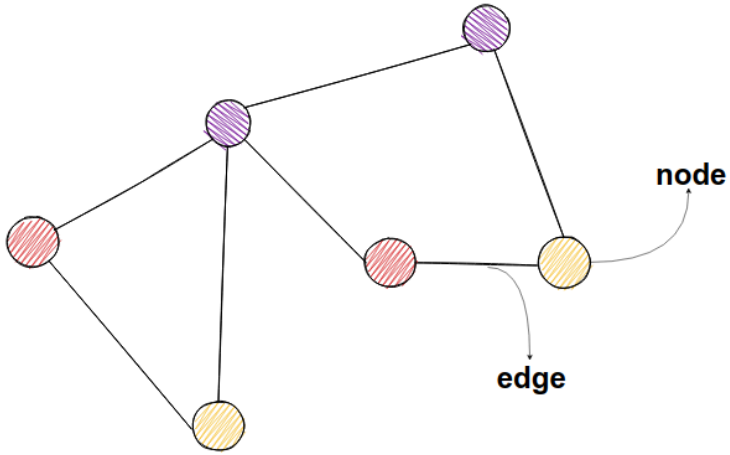

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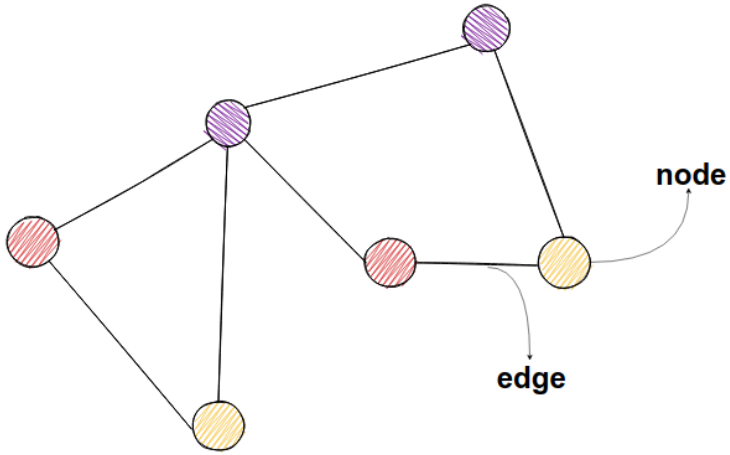

A **node** is a vector of information

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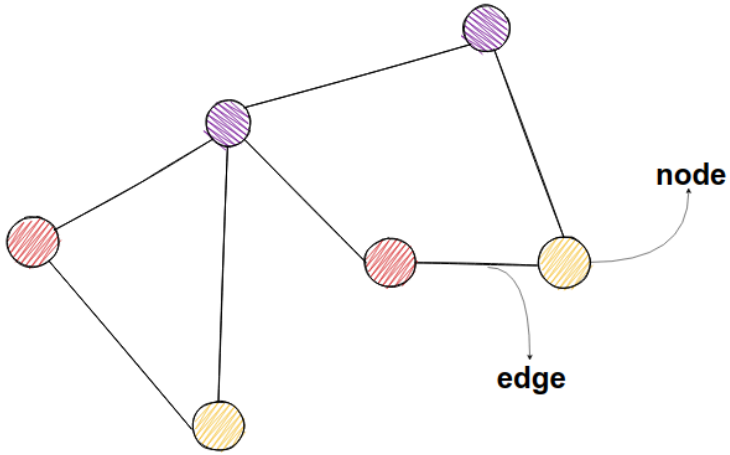

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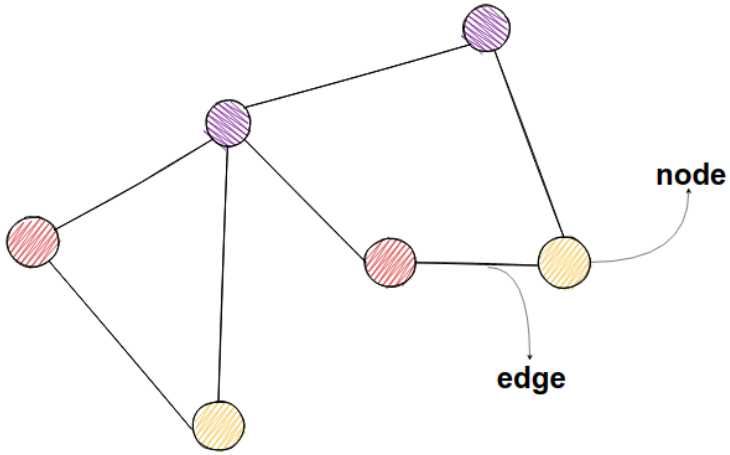
GNN Review



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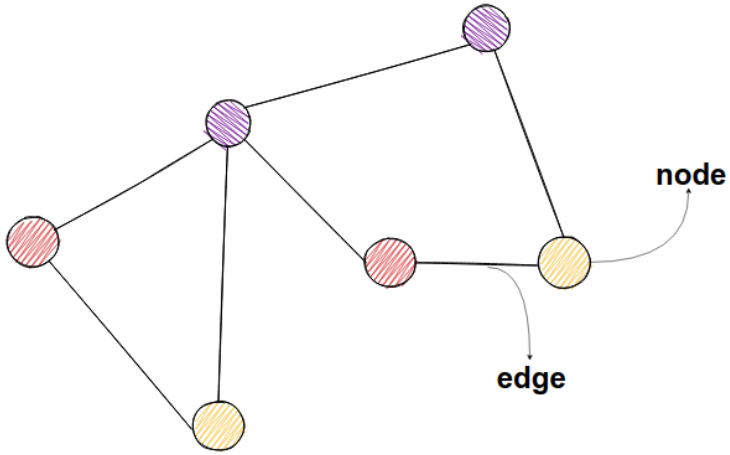

A **node** is a vector of information

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If we connect nodes i and j with edge (i, j), then i and j are **neighbors**

The **neighborhood** $N(j)$ contains all neighbors of node j

GNN Review

Prof. Li introduced the **graph convolution layer**

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This is just one node, we use this graph layer for all nodes in the graph

GNN Review

Graph convolution over all nodes in the graph

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$$f(\boldsymbol{X}, \boldsymbol{E}, \boldsymbol{\theta}) = \begin{bmatrix} f(\boldsymbol{X}, \boldsymbol{E}, \boldsymbol{\theta})_1 \\ f(\boldsymbol{X}, \boldsymbol{E}, \boldsymbol{\theta})_2 \\ \vdots \\ f(\boldsymbol{X}, \boldsymbol{E}, \boldsymbol{\theta})_T \end{bmatrix} = \begin{bmatrix} \sigma\left(\boldsymbol{\theta}_1^\top \overline{\boldsymbol{x}}_1 + \sum_{i \in N(1)} \boldsymbol{\theta}_2^\top \boldsymbol{x}_i\right) \\ \sigma\left(\boldsymbol{\theta}_1^\top \overline{\boldsymbol{x}}_2 + \sum_{i \in N(2)} \boldsymbol{\theta}_2^\top \boldsymbol{x}_i\right) \\ \vdots \\ \sigma\left(\boldsymbol{\theta}_1^\top \overline{\boldsymbol{x}}_T + \sum_{i \in N(T)} \boldsymbol{\theta}_2^\top \boldsymbol{x}_i\right) \end{bmatrix}$$

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Graph convolution over all nodes in the graph

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How does this compare to regular convolution (images, sound, etc)?

GNN Review

Standard convolution

$$\begin{bmatrix} \sigma\left(\boldsymbol{\theta}_1^\top \overline{\boldsymbol{x}}_1 + \sum_{i=1}^{k} \boldsymbol{\theta}_2^\top \boldsymbol{x}_i\right) \\ \sigma\left(\boldsymbol{\theta}_1^\top \overline{\boldsymbol{x}}_2 + \sum_{i=2}^{k+1} \boldsymbol{\theta}_2^\top \boldsymbol{x}_i\right) \\ \vdots \\ \sigma\left(\boldsymbol{\theta}_1^\top \overline{\boldsymbol{x}}_T + \sum_{i=T-k}^{T} \boldsymbol{\theta}_2^\top \boldsymbol{x}_i\right) \end{bmatrix}$$

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Question: What is the output size of standard convolution?

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Answer: $T - k - 1 \times d_h$

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GNN Review

We can use pooling with graph convolutions too

$$\text{SumPool}\left(\begin{bmatrix} \sigma\left(\boldsymbol{\theta}_1^\top \overline{\boldsymbol{x}}_1 + \sum_{i \in N(1)} \boldsymbol{\theta}_2^\top \boldsymbol{x}_i\right) \\ \sigma\left(\boldsymbol{\theta}_1^\top \overline{\boldsymbol{x}}_2 + \sum_{i \in N(2)} \boldsymbol{\theta}_2^\top \boldsymbol{x}_i\right) \\ \vdots \\ \sigma\left(\boldsymbol{\theta}_1^\top \overline{\boldsymbol{x}}_T + \sum_{i \in N(T)} \boldsymbol{\theta}_2^\top \boldsymbol{x}_i\right) \end{bmatrix}\right) =$$

$$\sigma\left(\boldsymbol{\theta}_1^\top \overline{\boldsymbol{x}}_1 + \sum_{i \in N(1)} \boldsymbol{\theta}_2^\top \boldsymbol{x}_i\right) + \sigma\left(\boldsymbol{\theta}_1^\top \overline{\boldsymbol{x}}_2 + \sum_{i \in N(2)} \boldsymbol{\theta}_2^\top \boldsymbol{x}_i\right) + \ldots$$

GNN Review

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$$\text{SumPool}(f(\boldsymbol{X}, \boldsymbol{E}, \boldsymbol{\theta})) = \text{SumPool}\left(\begin{bmatrix} f(\boldsymbol{X}, \boldsymbol{E}, \boldsymbol{\theta})_1 \\ f(\boldsymbol{X}, \boldsymbol{E}, \boldsymbol{\theta})_2 \\ \vdots \\ f(\boldsymbol{X}, \boldsymbol{E}, \boldsymbol{\theta})_T \end{bmatrix}\right)$$

$$= \text{SumPool}\left(\begin{bmatrix} f(\boldsymbol{X}, \boldsymbol{E}, \boldsymbol{\theta})_2 \\ f(\boldsymbol{X}, \boldsymbol{E}, \boldsymbol{\theta})_T \\ \vdots \\ f(\boldsymbol{X}, \boldsymbol{E}, \boldsymbol{\theta})_1 \end{bmatrix}\right)$$

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VAE Review and Coding

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

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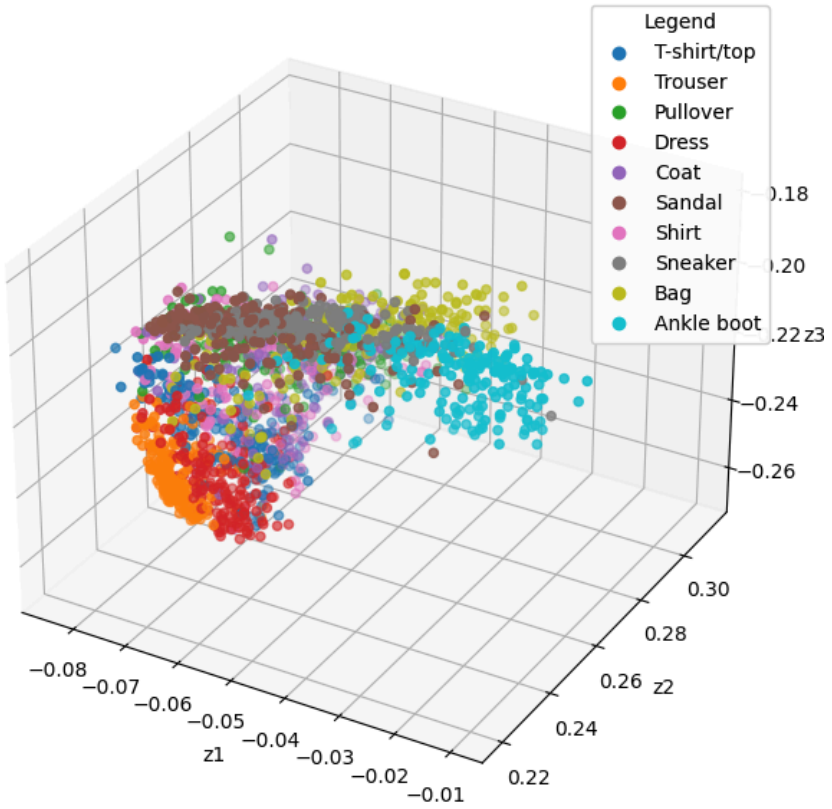
How does this work?

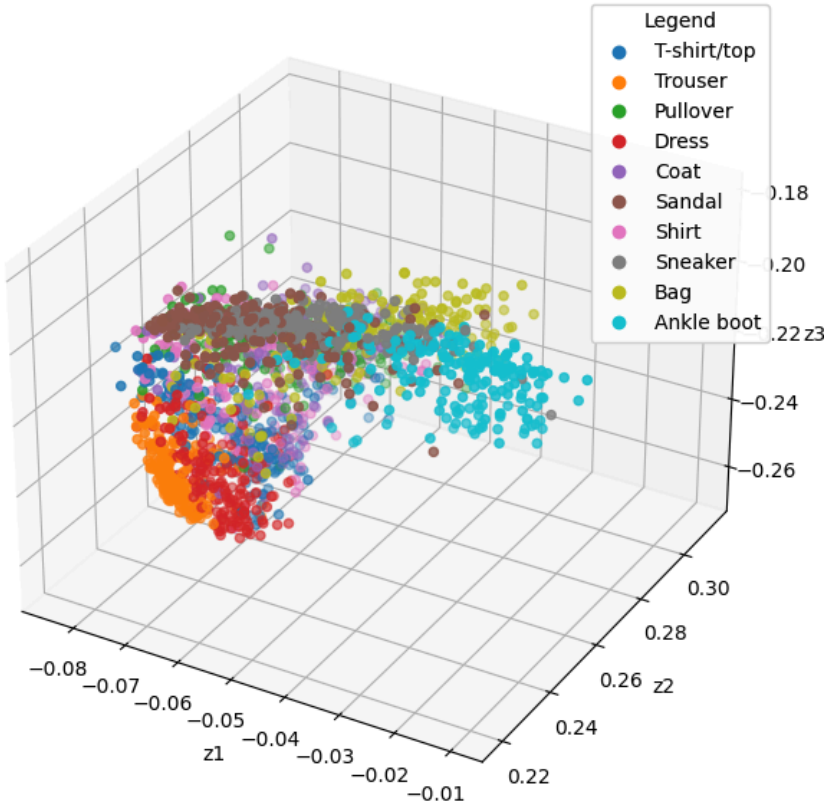
VAE Review and Coding

Latent space Z for autoencoder on the clothes dataset with $d_z = 3$



VAE Review and Coding

What happens if we decode a new point?



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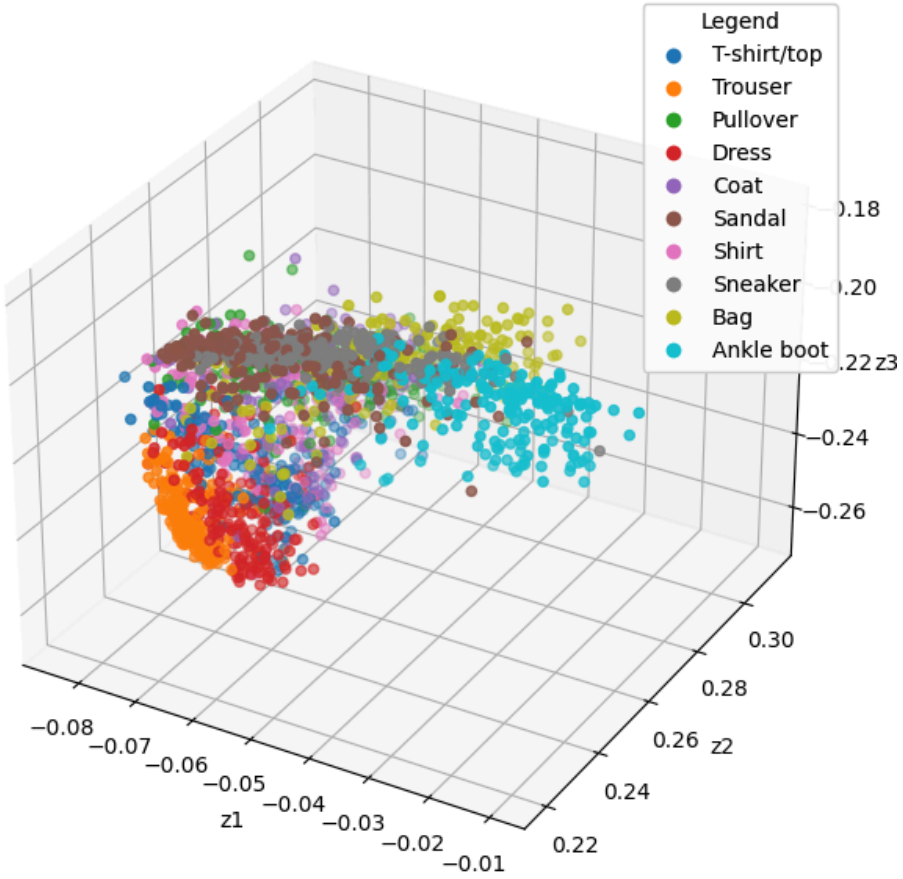
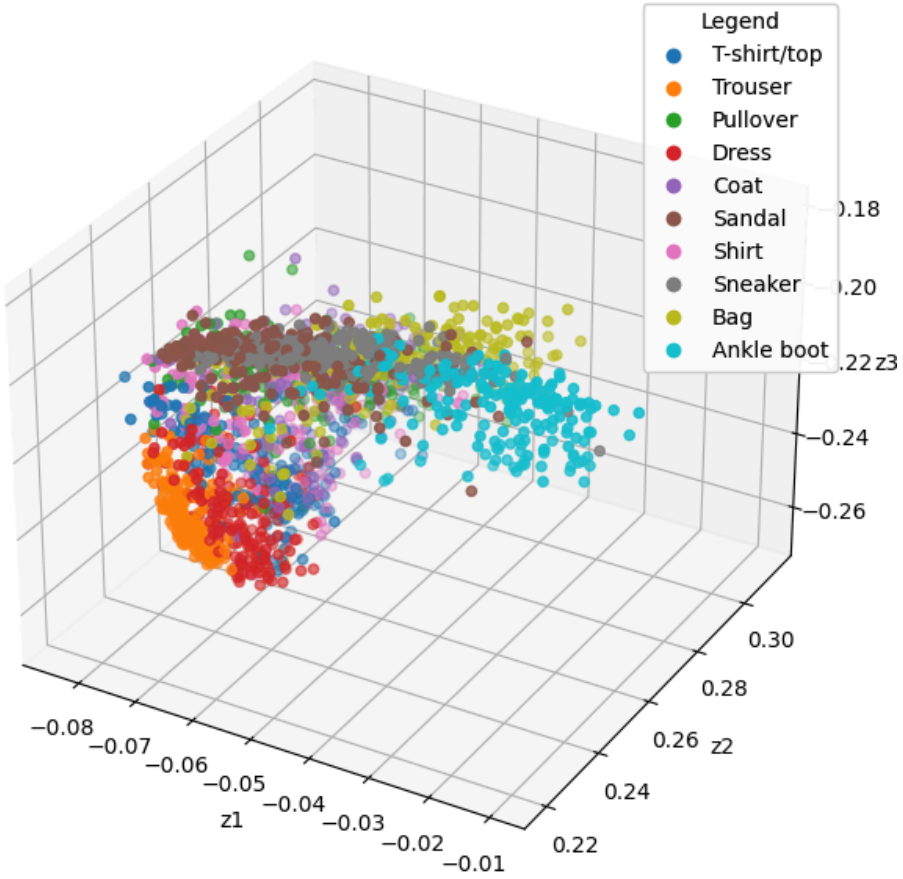


Autoencoder generative model:

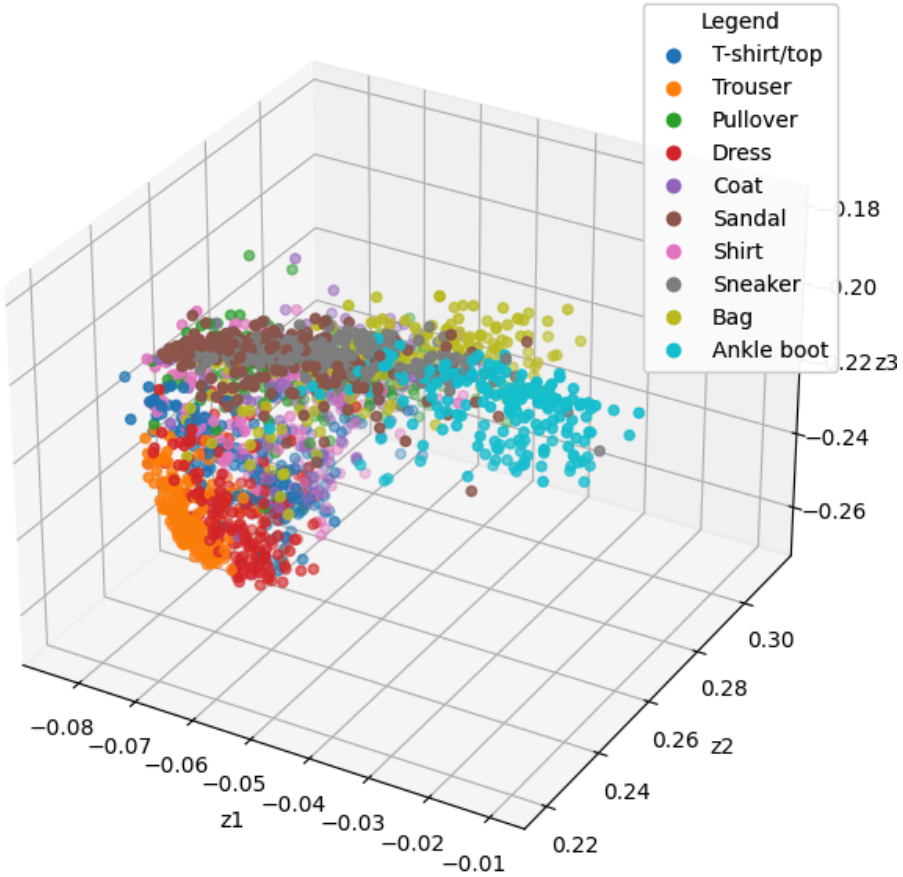
VAE Review and Coding



Autoencoder generative model:

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

VAE Review and Coding



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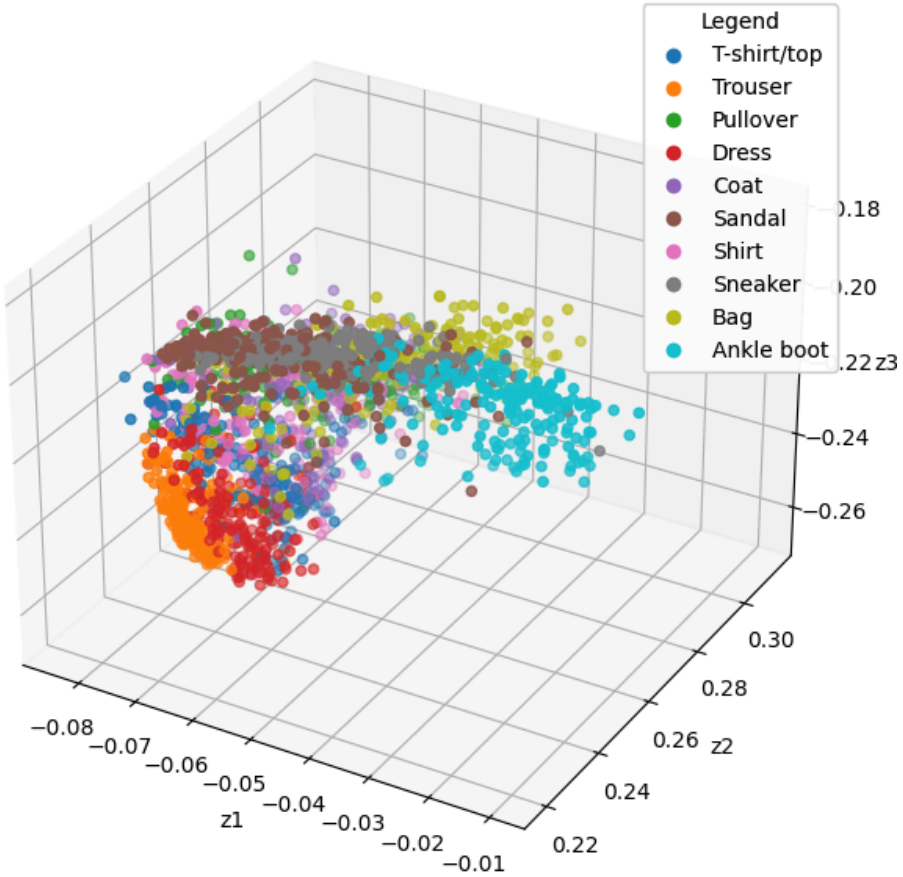
VAE Review and Coding



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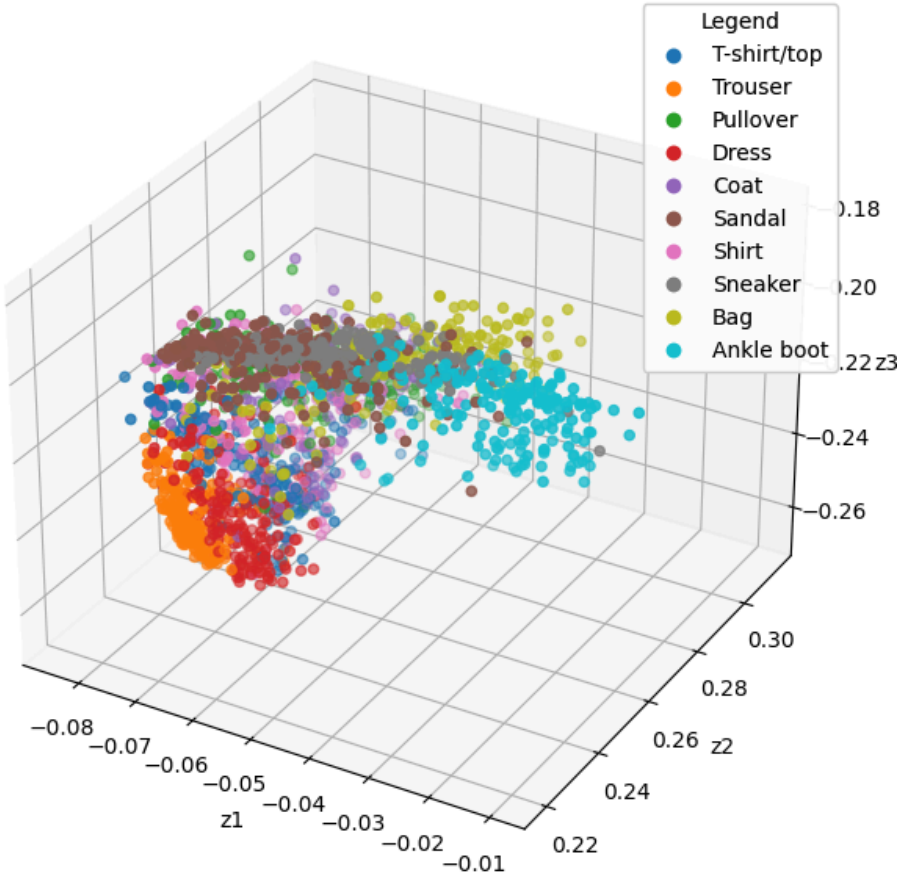

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Decode $\boldsymbol{z}_{\text{new}}$ into $\boldsymbol{x}_{\text{new}}$

VAE Review and Coding

VAE Review and Coding

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

VAE Review and Coding

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

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As d_z increases, points move further and further apart

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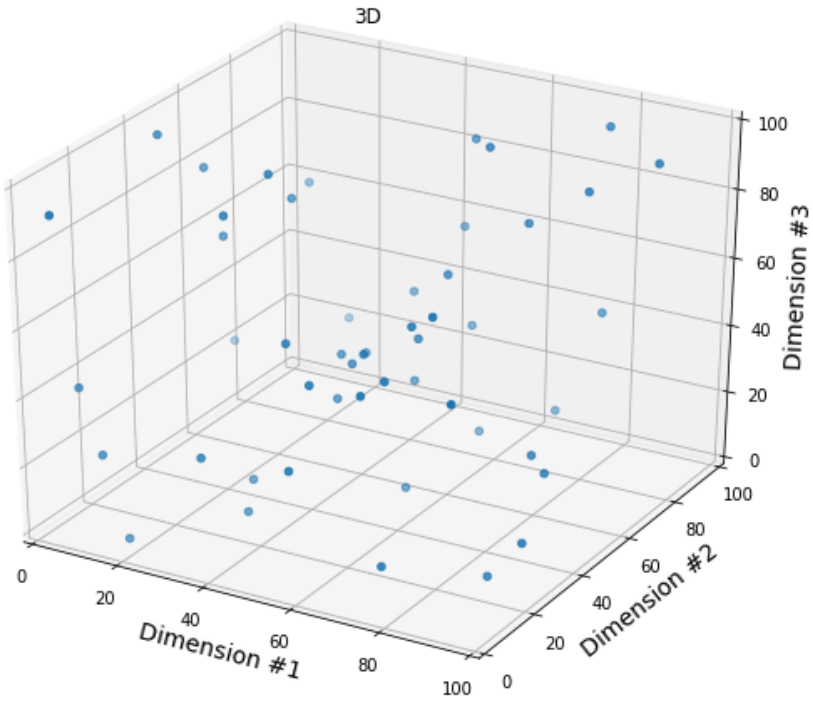

VAE Review and Coding

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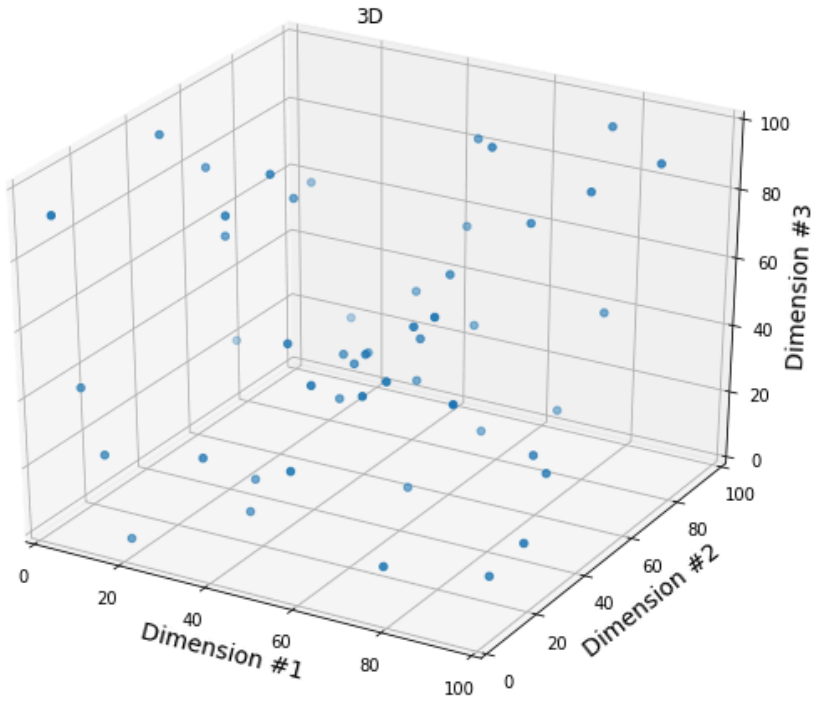

$f^{-1}(\boldsymbol{z} + \varepsilon)$ will produce either garbage, or $\boldsymbol{z}$

VAE Review and Coding

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VAE Review and Coding

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How?

VAE Review and Coding

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How?

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

VAE Review and Coding

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

How?

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

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

VAE Review and Coding

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

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

VAE Review and Coding

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

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

VAE Review and Coding

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

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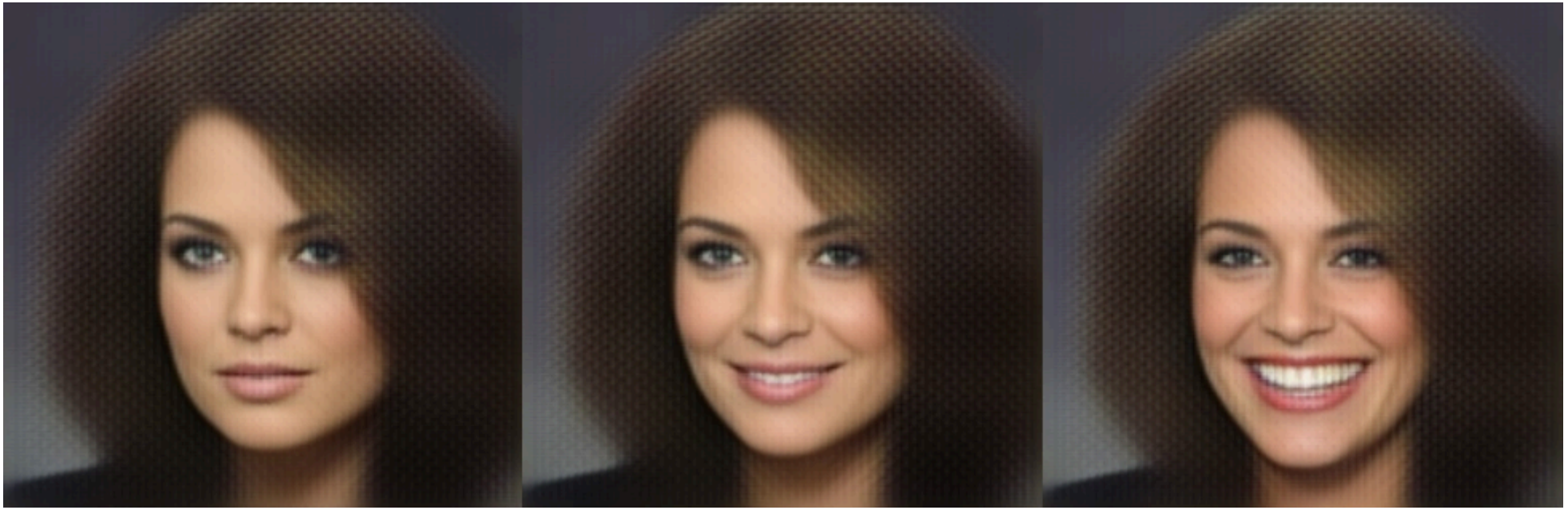
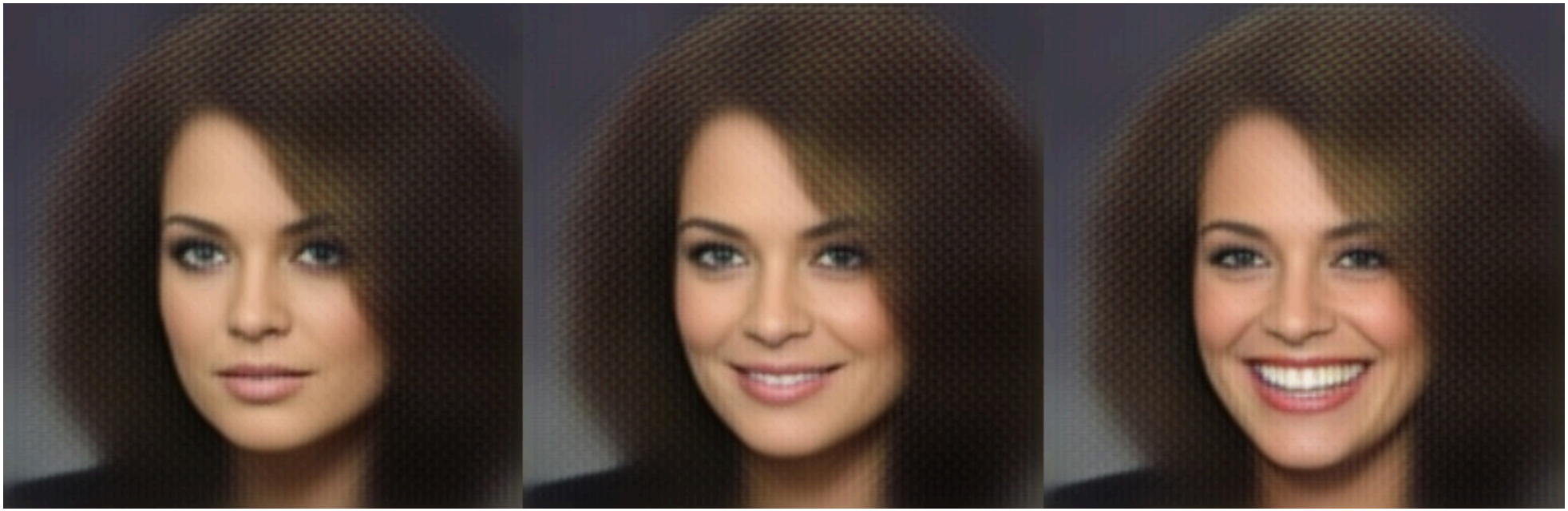
x :

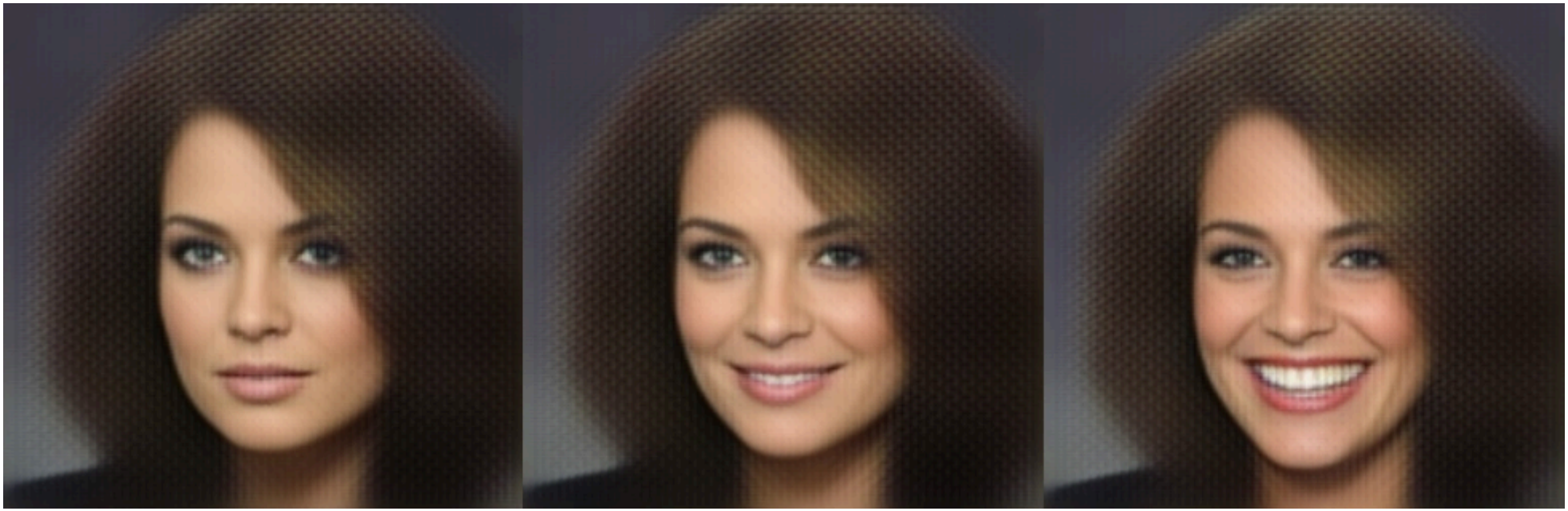


z : [woman brown hair (frown | smile)]

VAE Review and Coding

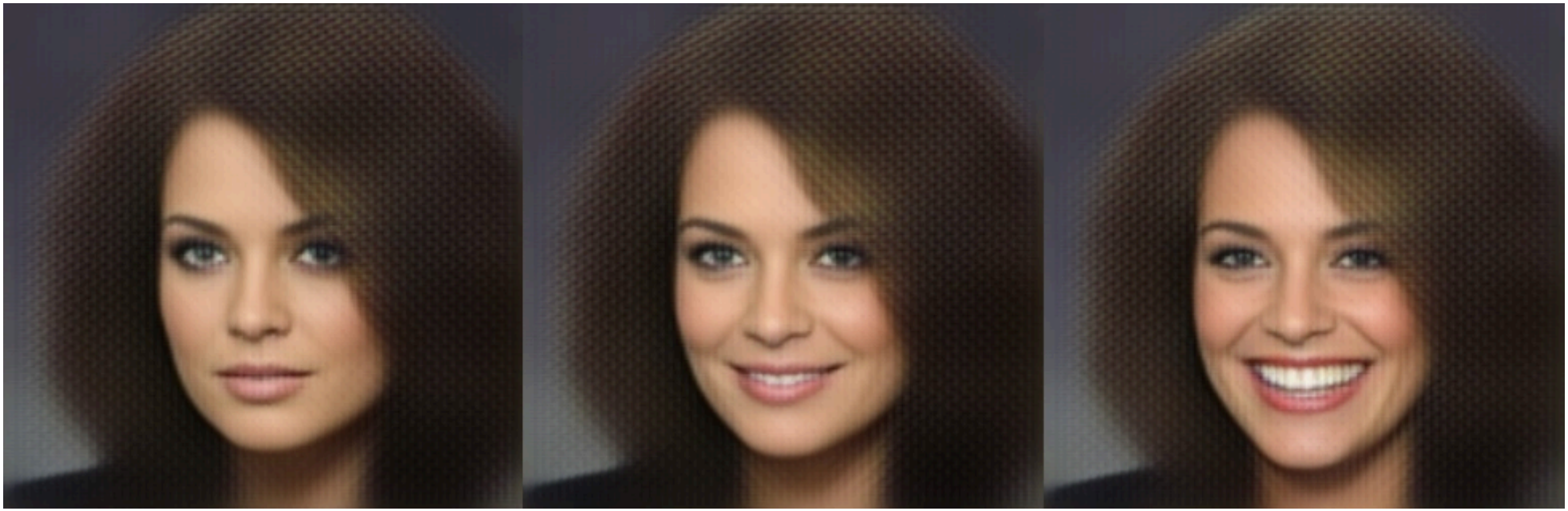


VAE Review and Coding



Network can only see x, it cannot directly observe z

VAE Review and Coding



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

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

VAE Review and Coding

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

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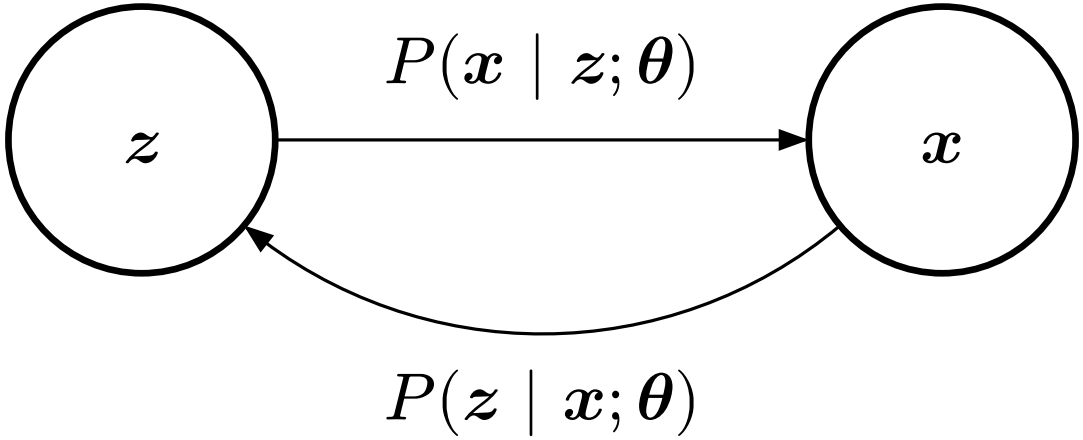

Decoder

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Encoder

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VAE Review and Coding

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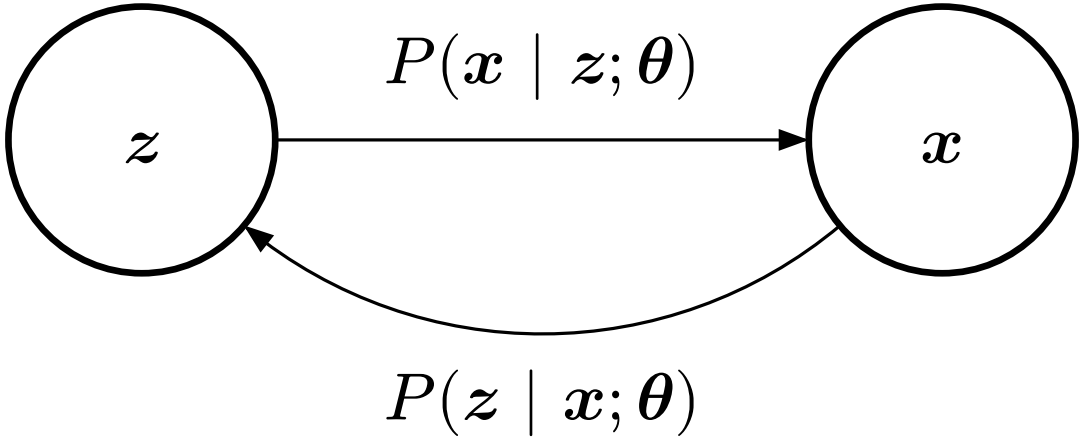

Decoder

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

Encoder

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

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

VAE Review and Coding

How do we implement f (i.e., $P(\boldsymbol{z} \mid \boldsymbol{x}; \boldsymbol{\theta})$)?

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

VAE Review and Coding

```
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 Review and Coding

We covered the encoder

$$f : X \times \Theta \mapsto \Delta Z$$

We can use the same decoder as a standard autoencoder

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Solution: Sample a vector z from the distribution ΔZ

VAE Review and Coding

Put it all together

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Step 1: Encode the input to a normal distribution

$$\boldsymbol{\mu}, \boldsymbol{\sigma} = f(\boldsymbol{x}, \boldsymbol{\theta}_e)$$

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VAE Review and Coding

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Step 3: Decode the sample

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

VAE Review and Coding

```
# Create normal distribution from input
mu, sigma = model.f(x)

# Randomly sample a z vector from our distribution
epsilon = jax.random.normal(key, x.shape[0])
z = mu + sigma * epsilon

# Decode/reconstruct z back into x
pred_x = model.f_inverse(z)
```

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VAE Review and Coding

From the KL divergence, we derived the **ELBO** loss for the VAE

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

$$\underbrace{\beta \left(\sum_{i=1}^{n} \sum_{j=1}^{d_z} \mu_{[i],j}^2 + \sigma_{[i],j}^2 - \log\left(\sigma_{[i],j}^2 \right) - 1 \right)}_{\text{Make } \boldsymbol{z} \text{ normally distributed}}$$

VAE Review and Coding

```
def L(model, x, m, n, key):
  mu, sigma = model.f(x) # Encode input into distribution
  # Sample from distribution
  z = mu + sigma * jax.random.normal(key, x.shape[0])
  # Reconstruct input
  pred_x = model.f_inverse(z)
  # Compute reconstruction and kl loss terms
  recon = jnp.sum((x - pred_x) ** 2)
  kl = jnp.sum(mu ** 2 + sigma ** 2 - jnp.log(sigma ** 2) -
1)
  # Loss function contains reconstruction and kl terms
  return m / n * recon + kl
```

VAE Review and Coding

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

Agenda

1. GNN Review
2. **VAE Review and Coding**
3. Attention
4. Positional Encoding
5. Transformers
6. Coding

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Attention

Today, we will investigate attention and transformers

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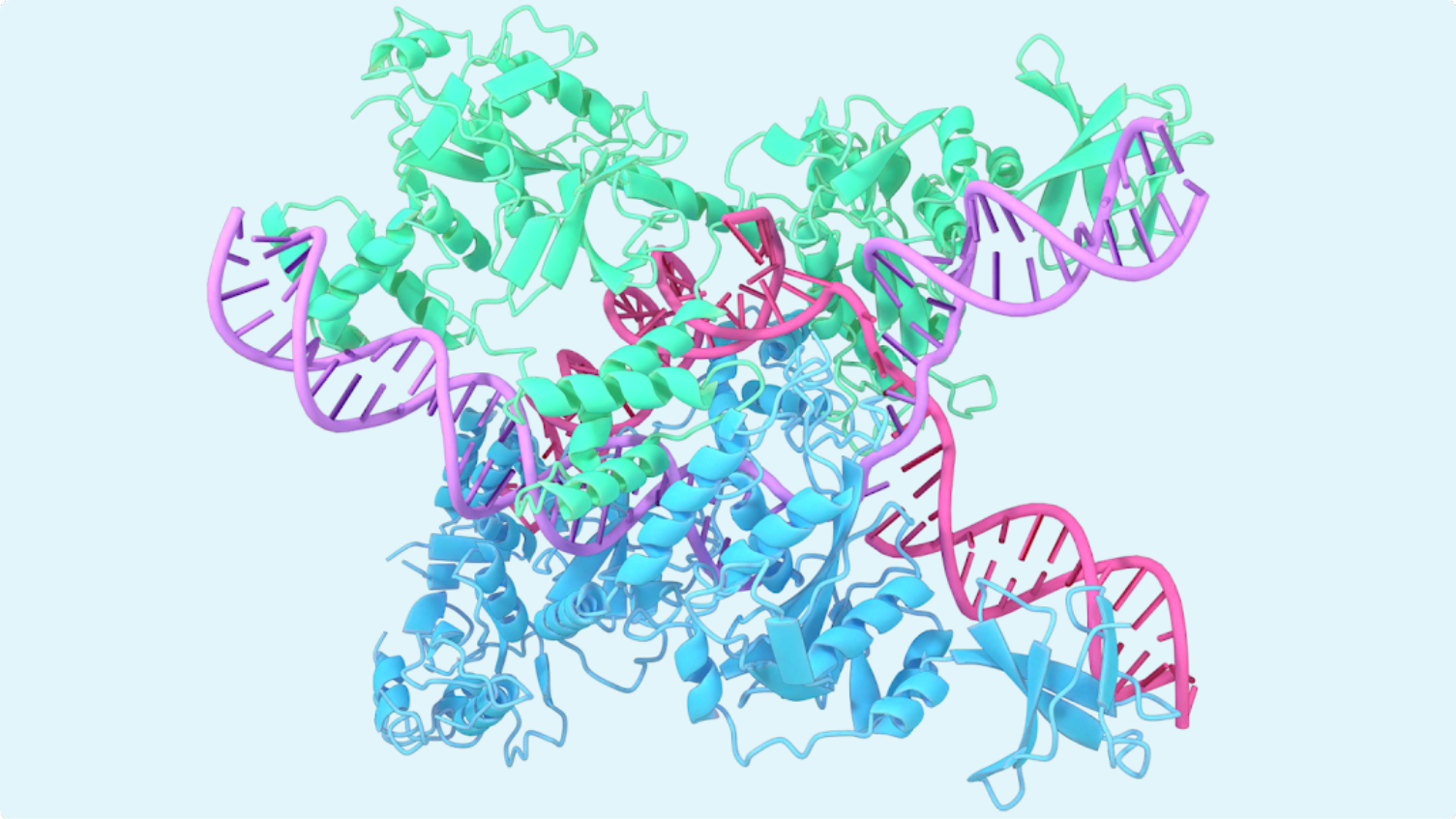
Let’s review some products based on attention

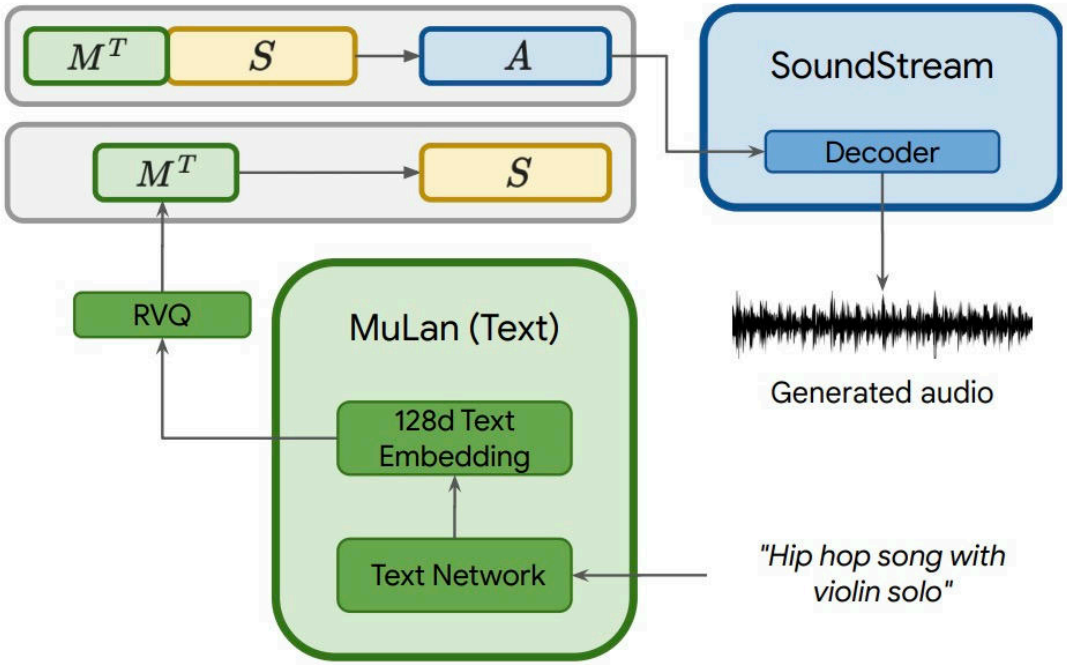
AlphaFold (Nobel prize)



Attention

ChatGPT, Qwen, LLaMA, Mistral, Doubou, Ernie chatbots

MusicTransformer, MuLan

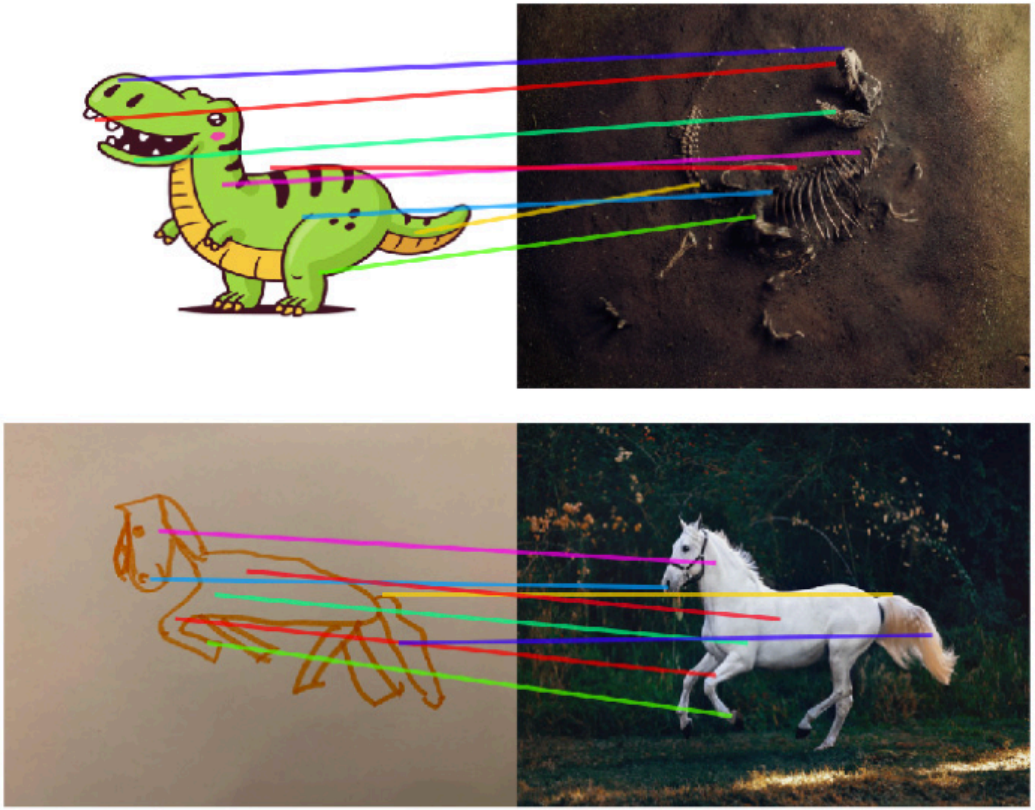


Attention

Google Translate, Baidu Translate, Apple Translate

Attention

ViT, DinoV2



Attention

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At the core of each transformer is **attention**

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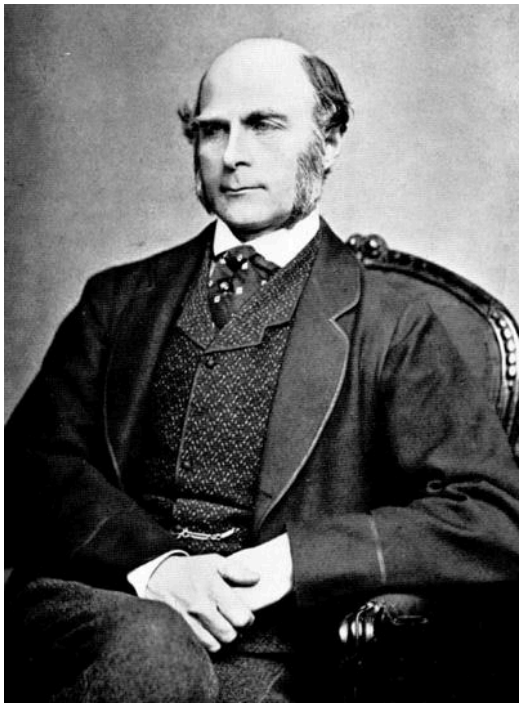
We can derive attention from composite memory

Attention

Francis Galton (1822-1911)
photo composite memory



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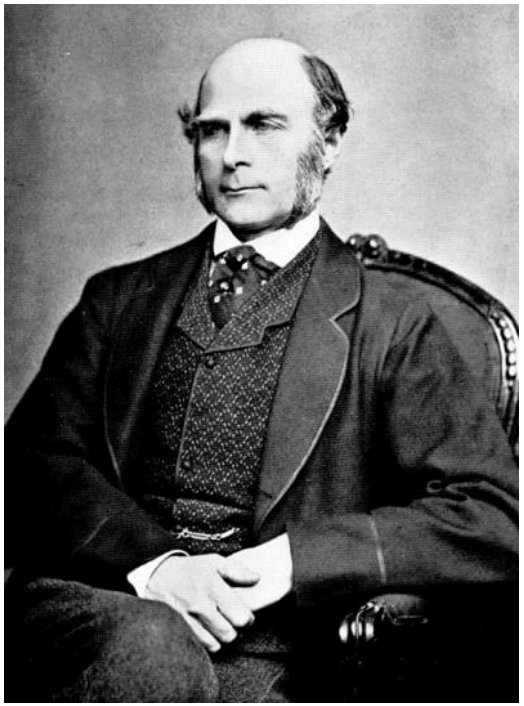

Composite photo of members of a party

Attention

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

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Attention

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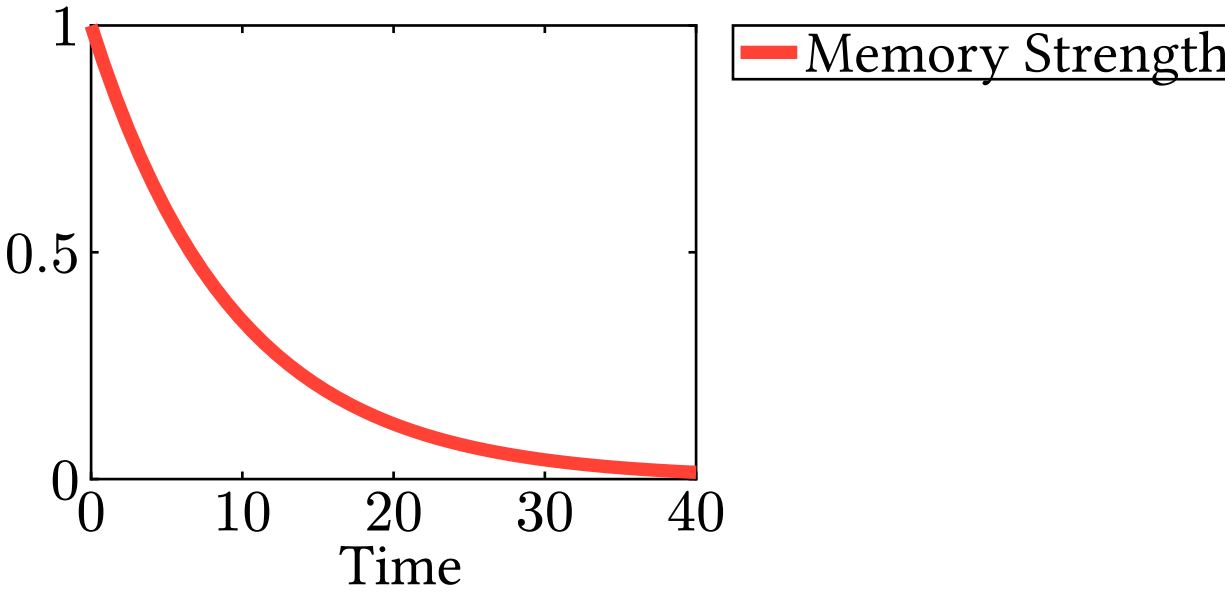

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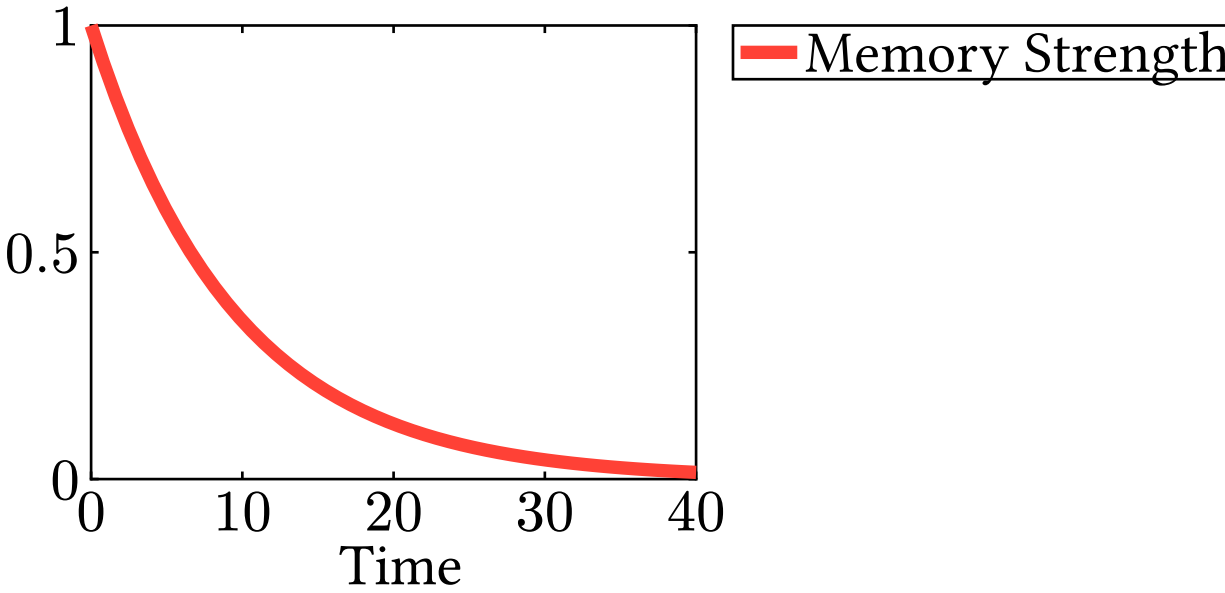

Question: Does this accurately model what you remember?

Attention

You go to a party and meet these people in order

Attention

According to forgetting, the memories should fade with time

$$\gamma^3 \boldsymbol{\theta}^\top \overline{\boldsymbol{x}}_1$$

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Attention

Consider the following case

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Attention

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$$\gamma^4 \boldsymbol{\theta}^\top \overline{\boldsymbol{x}}_1 \quad \gamma^3 \boldsymbol{\theta}^\top \overline{\boldsymbol{x}}_2 \quad \gamma^2 \boldsymbol{\theta}^\top \overline{\boldsymbol{x}}_3 \quad \gamma^1 \boldsymbol{\theta}^\top \overline{\boldsymbol{x}}_4 \quad \gamma^0 \boldsymbol{\theta}^\top \overline{\boldsymbol{x}}_5$$

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Question: What will happen to Taylor Swift?

Attention

$\gamma^4 \boldsymbol{\theta}^\top \overline{\boldsymbol{x}}_1$ $\gamma^3 \boldsymbol{\theta}^\top \overline{\boldsymbol{x}}_2$ $\gamma^2 \boldsymbol{\theta}^\top \overline{\boldsymbol{x}}_3$ $\gamma^1 \boldsymbol{\theta}^\top \overline{\boldsymbol{x}}_4$ $\gamma^0 \boldsymbol{\theta}^\top \overline{\boldsymbol{x}}_5$

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We will forget meeting her!

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Would you forget Taylor Swift at a party?

Attention

Our model of memory is incomplete

Attention

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Memories are not created equal, some are more important than others

My memory might actually be

$$1.0 \cdot \boldsymbol{\theta}^\top \overline{\boldsymbol{x}}_1 \qquad 0.1 \cdot \boldsymbol{\theta}^\top \overline{\boldsymbol{x}}_2 \qquad 0.1 \cdot \boldsymbol{\theta}^\top \overline{\boldsymbol{x}}_3 \qquad 0.5 \cdot \boldsymbol{\theta}^\top \overline{\boldsymbol{x}}_4 \qquad 0.1 \cdot \boldsymbol{\theta}^\top \overline{\boldsymbol{x}}_5$$

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Question: How can we achieve this forgetting?

Attention

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Let us do something similar

However, we will write it slightly differently (without recurrence)

Attention

First, write our forgetting function

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This is one form of **attention**

We only pay attention to specific inputs

Attention

We can use this simple form of attention to pay attention to Taylor Swift

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$$\lambda(\boldsymbol{x}_1, \boldsymbol{\theta}_\lambda) \quad \lambda(\boldsymbol{x}_2, \boldsymbol{\theta}_\lambda) \quad \lambda(\boldsymbol{x}_3, \boldsymbol{\theta}_\lambda) \quad \lambda(\boldsymbol{x}_4, \boldsymbol{\theta}_\lambda) \quad \lambda(\boldsymbol{x}_5, \boldsymbol{\theta}_\lambda)$$

$$\cdot \boldsymbol{\theta}^\top \overline{\boldsymbol{x}}_1 \quad \cdot \boldsymbol{\theta}^\top \overline{\boldsymbol{x}}_2 \quad \cdot \boldsymbol{\theta}^\top \overline{\boldsymbol{x}}_3 \quad \cdot \boldsymbol{\theta}^\top \overline{\boldsymbol{x}}_4 \quad \cdot \boldsymbol{\theta}^\top \overline{\boldsymbol{x}}_5$$

Attention

$$\lambda(\boldsymbol{x}_1, \boldsymbol{\theta}_\lambda) \cdot \boldsymbol{\theta}^\top \overline{\boldsymbol{x}}_1 \qquad \lambda(\boldsymbol{x}_2, \boldsymbol{\theta}_\lambda) \cdot \boldsymbol{\theta}^\top \overline{\boldsymbol{x}}_2 \qquad \lambda(\boldsymbol{x}_3, \boldsymbol{\theta}_\lambda) \cdot \boldsymbol{\theta}^\top \overline{\boldsymbol{x}}_3 \qquad \lambda(\boldsymbol{x}_4, \boldsymbol{\theta}_\lambda) \cdot \boldsymbol{\theta}^\top \overline{\boldsymbol{x}}_4 \qquad \lambda(\boldsymbol{x}_5, \boldsymbol{\theta}_\lambda) \cdot \boldsymbol{\theta}^\top \overline{\boldsymbol{x}}_5$$

Question: What do the images look like now?

Attention

$$\lambda(\boldsymbol{x}_1, \boldsymbol{\theta}_\lambda) \cdot \boldsymbol{\theta}^\top \overline{\boldsymbol{x}}_1 \quad \lambda(\boldsymbol{x}_2, \boldsymbol{\theta}_\lambda) \cdot \boldsymbol{\theta}^\top \overline{\boldsymbol{x}}_2 \quad \lambda(\boldsymbol{x}_3, \boldsymbol{\theta}_\lambda) \cdot \boldsymbol{\theta}^\top \overline{\boldsymbol{x}}_3 \quad \lambda(\boldsymbol{x}_4, \boldsymbol{\theta}_\lambda) \cdot \boldsymbol{\theta}^\top \overline{\boldsymbol{x}}_4 \quad \lambda(\boldsymbol{x}_5, \boldsymbol{\theta}_\lambda) \cdot \boldsymbol{\theta}^\top \overline{\boldsymbol{x}}_5$$

Question: What do the images look like now?

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This form of attention will learn to pay attention to everyone!

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$$1.0 \cdot \boldsymbol{\theta}^\top \overline{\boldsymbol{x}}_1 \qquad 1.0 \cdot \boldsymbol{\theta}^\top \overline{\boldsymbol{x}}_2 \qquad 1.0 \cdot \boldsymbol{\theta}^\top \overline{\boldsymbol{x}}_3 \qquad 1.0 \cdot \boldsymbol{\theta}^\top \overline{\boldsymbol{x}}_4 \qquad 1.0 \cdot \boldsymbol{\theta}^\top \overline{\boldsymbol{x}}_5$$

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Not a good model of attention!

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We should normalize $\lambda(\boldsymbol{x}, \boldsymbol{\theta}_\lambda)$ to model a finite attention span

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For example, we can make

$$\sum_{i=1}^{T} \lambda(\boldsymbol{x}, \boldsymbol{\theta}_\lambda) = 1$$

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Question: Do we know of any functions with this property?

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This will limit the total amount of attenion that we have

Question: Do we know of any functions with this property?

Answer: Softmax!

Attention

The softmax function maps real numbers to the simplex (probabilities)

$$\text{softmax} : \mathbb{R}^k \mapsto \Delta^{k-1}$$

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$$\text{softmax} : \mathbb{R}^k \mapsto \Delta^{k-1}$$

$$\text{softmax}\left(\begin{bmatrix} x_1 \\ \vdots \\ x_k \end{bmatrix}\right) = \frac{\exp(\boldsymbol{x})}{\sum_{i=1}^{k} \exp(x_i)} = \begin{bmatrix} \frac{\exp(x_1)}{\exp(x_1)+\exp(x_2)+\ldots \exp(x_k)} \\ \frac{\exp(x_2)}{\exp(x_1)+e^{x_2}+\ldots \exp(x_k)} \\ \vdots \\ \frac{\exp(x_k)}{\exp(x_1)+\exp(x_2)+\ldots \exp(x_k)} \end{bmatrix}$$

Attention

Let us rewrite attention using softmax

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Let us rewrite attention using softmax

The attention we pay to person i is

$$\lambda\left(\begin{bmatrix}\boldsymbol{x}_1\\ \vdots \\ \boldsymbol{x}_T\end{bmatrix}, \boldsymbol{\theta}_\lambda\right)_i = \frac{\exp\left(\boldsymbol{\theta}_\lambda^\top \overline{\boldsymbol{x}}_i\right)}{\sum_{j=1}^{T} \exp\left(\boldsymbol{\theta}_\lambda^\top \overline{\boldsymbol{x}}_j\right)}$$

Attention

$$\lambda\left(\begin{bmatrix}\boldsymbol{x}_1\\ \vdots\\ \boldsymbol{x}_5\end{bmatrix}, \boldsymbol{\theta}_\lambda\right)_1 \lambda\left(\begin{bmatrix}\boldsymbol{x}_1\\ \vdots\\ \boldsymbol{x}_5\end{bmatrix}, \boldsymbol{\theta}_\lambda\right)_2 \lambda\left(\begin{bmatrix}\boldsymbol{x}_1\\ \vdots\\ \boldsymbol{x}_5\end{bmatrix}, \boldsymbol{\theta}_\lambda\right)_3 \lambda\left(\begin{bmatrix}\boldsymbol{x}_1\\ \vdots\\ \boldsymbol{x}_5\end{bmatrix}, \boldsymbol{\theta}_\lambda\right)_4 \lambda\left(\begin{bmatrix}\boldsymbol{x}_1\\ \vdots\\ \boldsymbol{x}_5\end{bmatrix}, \boldsymbol{\theta}_\lambda\right)_5$$

$$\cdot\, \boldsymbol{\theta}^\top \overline{\boldsymbol{x}}_1 \qquad \cdot\, \boldsymbol{\theta}^\top \overline{\boldsymbol{x}}_2 \qquad \cdot\, \boldsymbol{\theta}^\top \overline{\boldsymbol{x}}_3 \qquad \cdot\, \boldsymbol{\theta}^\top \overline{\boldsymbol{x}}_4 \qquad \cdot\, \boldsymbol{\theta}^\top \overline{\boldsymbol{x}}_5$$

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$$\lambda\left(\begin{bmatrix}\boldsymbol{x}_1\\ \vdots\\ \boldsymbol{x}_5\end{bmatrix}, \boldsymbol{\theta}_\lambda\right)_1 \lambda\left(\begin{bmatrix}\boldsymbol{x}_1\\ \vdots\\ \boldsymbol{x}_5\end{bmatrix}, \boldsymbol{\theta}_\lambda\right)_2 \lambda\left(\begin{bmatrix}\boldsymbol{x}_1\\ \vdots\\ \boldsymbol{x}_5\end{bmatrix}, \boldsymbol{\theta}_\lambda\right)_3 \lambda\left(\begin{bmatrix}\boldsymbol{x}_1\\ \vdots\\ \boldsymbol{x}_5\end{bmatrix}, \boldsymbol{\theta}_\lambda\right)_4 \lambda\left(\begin{bmatrix}\boldsymbol{x}_1\\ \vdots\\ \boldsymbol{x}_5\end{bmatrix}, \boldsymbol{\theta}_\lambda\right)_5$$

$$\cdot \boldsymbol{\theta}^\top \overline{\boldsymbol{x}}_1 \qquad \cdot \boldsymbol{\theta}^\top \overline{\boldsymbol{x}}_2 \qquad \cdot \boldsymbol{\theta}^\top \overline{\boldsymbol{x}}_3 \qquad \cdot \boldsymbol{\theta}^\top \overline{\boldsymbol{x}}_4 \qquad \cdot \boldsymbol{\theta}^\top \overline{\boldsymbol{x}}_5$$

Attention

$$0.70 \cdot \boldsymbol{\theta}^\top \overline{\boldsymbol{x}}_1 \quad 0.04 \cdot \boldsymbol{\theta}^\top \overline{\boldsymbol{x}}_2 \quad 0.03 \cdot \boldsymbol{\theta}^\top \overline{\boldsymbol{x}}_3 \quad 0.20 \cdot \boldsymbol{\theta}^\top \overline{\boldsymbol{x}}_4 \quad 0.03 \cdot \boldsymbol{\theta}^\top \overline{\boldsymbol{x}}_5$$

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$$0.70 + 0.04 + 0.03 + 0.20 + 0.03 = 1.0$$

Attention

$$\lambda\left(\begin{bmatrix}\boldsymbol{x}_1\\ \vdots \\ \boldsymbol{x}_T\end{bmatrix}, \boldsymbol{\theta}_\lambda\right)_i = \frac{\exp\left(\boldsymbol{\theta}_\lambda^\top \overline{\boldsymbol{x}}\right)}{\sum_{j=1}^{T} \exp\left(\boldsymbol{\theta}_\lambda^\top \overline{\boldsymbol{x}}_j\right)}$$

$$\lambda\left(\begin{bmatrix}\boldsymbol{x}_1\\ \vdots \\ \boldsymbol{x}_T\end{bmatrix}, \boldsymbol{\theta}_\lambda\right) = \begin{bmatrix}\frac{\exp\left(\boldsymbol{\theta}_\lambda^\top \overline{\boldsymbol{x}}_1\right)}{\sum_{j=1}^{T} \exp\left(\boldsymbol{\theta}_\lambda^\top \overline{\boldsymbol{x}}_j\right)}\\ \vdots \\ \frac{\exp\left(\boldsymbol{\theta}_\lambda^\top \overline{\boldsymbol{x}}_T\right)}{\sum_{j=1}^{T} \exp\left(\boldsymbol{\theta}_\lambda^\top \overline{\boldsymbol{x}}_j\right)}\end{bmatrix}$$

Keys and Queries

Attention

The modern form of attention behaves like a database

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We label each person at the party with a **key**

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The key describes the content of each $\boldsymbol{x}$

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Musician

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Musician Lawyer

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Musician Lawyer Shopkeeper

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Musician Lawyer Shopkeeper Chef Scientist

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The key describes the content of each $\boldsymbol{x}$

Musician Lawyer Shopkeeper Chef Scientist

Attention

Attention

Then we compute a **query** that corresponds to the key

Query: Which person will help me on my exam?

Attention

Then we compute a **query** that corresponds to the key

Query: Which person will help me on my exam?

Musician Lawyer Shopkeeper Chef Scientist

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Then we compute a **query** that corresponds to the key

Query: Which person will help me on my exam?

Musician Lawyer Shopkeeper Chef Scientist

Attention

Query: I want to have fun

Attention

Query: I want to have fun

Musician	Lawyer	Shopkeeper	Chef	Scientist

Attention

Query: I want to have fun

Musician Lawyer Shopkeeper Chef Scientist

Attention

Query: I want to have fun

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How do we represent this mathematically?

Attention

For each input, we create a key $\boldsymbol{k}$

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$$\boldsymbol{k}_j = \boldsymbol{\theta}_K^\top \boldsymbol{x}_j, \quad \boldsymbol{k}_j \in \mathbb{R}^{d_h}$$

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Do this for all inputs

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$$\boldsymbol{k}_j = \boldsymbol{\theta}_K^\top \boldsymbol{x}_j, \quad \boldsymbol{k}_j \in \mathbb{R}^{d_h}$$

Do this for all inputs

$$\boldsymbol{K} = \begin{bmatrix} \boldsymbol{k}_1 \\ \boldsymbol{k}_2 \\ \vdots \\ \boldsymbol{k}_T \end{bmatrix} = \begin{bmatrix} \boldsymbol{\theta}_K^\top \boldsymbol{x}_1 \\ \boldsymbol{\theta}_K^\top \boldsymbol{x}_2 \\ \vdots \\ \boldsymbol{\theta}_K^\top \boldsymbol{x}_T \end{bmatrix}, \quad \boldsymbol{K} \in \mathbb{R}^{T \times d_h}$$

Attention

Now, create a query from some $\boldsymbol{x}_q$

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$$\boldsymbol{q} = \boldsymbol{\theta}_Q^\top \boldsymbol{x}_q, \quad \boldsymbol{q} \in \mathbb{R}^{d_h}$$

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We determine how well a key matches the query with the dot product

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$$\boldsymbol{q}^\top \boldsymbol{k}_i = \left(\boldsymbol{\theta}_Q^\top \boldsymbol{x}_q\right)^\top \left(\boldsymbol{\theta}_K^\top \boldsymbol{x}_i\right)$$

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Now, create a query from some $\boldsymbol{x}_q$

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$$\boldsymbol{q}^\top \boldsymbol{k}_i = \left(\boldsymbol{\theta}_Q^\top \boldsymbol{x}_q\right)^\top \left(\boldsymbol{\theta}_K^\top \boldsymbol{x}_i\right)$$

Question: What is the shape of $\boldsymbol{q}^\top \boldsymbol{k}_i$?

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Answer: $(1, d_h) \times (d_h, 1) = 1$, the output is a scalar

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Answer: $(1, d_h) \times (d_h, 1) = 1$, the output is a scalar

Example:

$$\boldsymbol{k}_i = \boldsymbol{\theta}_K^\top$$

Attention

Example:

$$\boldsymbol{k}_i = \boldsymbol{\theta}_K^\top$$ 

$$\boldsymbol{q} = \boldsymbol{\theta}_Q^\top \text{ Musician}$$

Attention

Example:

$$\boldsymbol{k}_i = \boldsymbol{\theta}_K^\top$$ 

$$\boldsymbol{q} = \boldsymbol{\theta}_Q^\top \text{ Musician}$$

$$\boldsymbol{q}^\top \boldsymbol{k}_i = \left(\boldsymbol{\theta}_Q^\top \text{ Musician}\right)^\top \left(\boldsymbol{\theta}_K^\top \right.$$  $$\left. \right) = 5.6$$

Attention

Example:

$$\boldsymbol{k}_i = \boldsymbol{\theta}_K^\top$$ 

$$\boldsymbol{q} = \boldsymbol{\theta}_Q^\top \text{ Musician}$$

$$\boldsymbol{q}^\top \boldsymbol{k}_i = \left(\boldsymbol{\theta}_Q^\top \text{ Musician}\right)^\top \left(\boldsymbol{\theta}_K^\top \right.$$  $$\left. \right) = 5.6$$

Large attention!

Attention

Example:

$$\boldsymbol{k}_i = \boldsymbol{\theta}_K^\top$$

Attention

Example:

$$\boldsymbol{k}_i = \boldsymbol{\theta}_K^\top$$ 

$$\boldsymbol{q} = \boldsymbol{\theta}_Q^\top \text{ Mathematician}$$

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$$\boldsymbol{q}^\top \boldsymbol{k}_i = \left(\boldsymbol{\theta}_Q^\top \text{ Mathematician}\right)^\top \left(\boldsymbol{\theta}_K^\top \right.$$  $$\left.\right) = -4.5$$

Attention

Example:

$$\boldsymbol{k}_i = \boldsymbol{\theta}_K^\top$$ 

$$\boldsymbol{q} = \boldsymbol{\theta}_Q^\top \text{ Mathematician}$$

$$\boldsymbol{q}^\top \boldsymbol{k}_i = \left(\boldsymbol{\theta}_Q^\top \text{ Mathematician}\right)^\top \left(\boldsymbol{\theta}_K^\top \right.$$  $$\left.\right) = -4.5$$

Small attention!

Attention

We compute the similarity between keys and queries using the dot product

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We compute the similarity between keys and queries using the dot product

$$\boldsymbol{q}^\top \boldsymbol{K} = \boldsymbol{q}^\top \begin{bmatrix} \boldsymbol{k}_1 \\ \boldsymbol{k}_2 \\ \vdots \\ \boldsymbol{k}_T \end{bmatrix} = \begin{bmatrix} \left(\boldsymbol{\theta}_Q^\top \boldsymbol{x}_q\right)^\top \left(\boldsymbol{\theta}_K^\top \boldsymbol{x}_1\right) \\ \left(\boldsymbol{\theta}_Q^\top \boldsymbol{x}_q\right)^\top \left(\boldsymbol{\theta}_K^\top \boldsymbol{x}_2\right) \\ \vdots \\ \left(\boldsymbol{\theta}_Q^\top \boldsymbol{x}_q\right)^\top \left(\boldsymbol{\theta}_K^\top \boldsymbol{x}_T\right) \end{bmatrix}$$

Attention

Another guest shows up to the party

Who do we pay attention to, Taylor Swift or Einstein?

It depends if you like music or science more

Attention

$$\lambda\left(\begin{bmatrix}\boldsymbol{x}_1\\ \vdots \\ \boldsymbol{x}_T\end{bmatrix}, \boldsymbol{\theta}_\lambda\right) = \frac{\exp\left(\boldsymbol{\theta}_\lambda^\top \overline{\boldsymbol{x}}\right)}{\sum_{j=1}^{k} \exp\left(\boldsymbol{\theta}_\lambda^\top \overline{\boldsymbol{x}}_j\right)}$$

Let us rewrite f as a single function

$$f_i\left(\begin{bmatrix}\boldsymbol{x}_1\\ \vdots \\ \boldsymbol{x}_T\end{bmatrix}, \boldsymbol{x}_i, \boldsymbol{\theta}\right) = \left(\frac{\exp\left(\boldsymbol{\theta}_\lambda^\top \overline{\boldsymbol{x}}_i\right)}{\sum_{j=1}^{T} \exp\left(\boldsymbol{\theta}_\lambda^\top \overline{\boldsymbol{x}}_j\right)}\right) \boldsymbol{\theta}^\top \overline{\boldsymbol{x}}_i$$

Parameters notation is a bit messy, let us clarify

Attention

$$f_i\left(\begin{bmatrix}\boldsymbol{x}_1\\ \vdots \\ \boldsymbol{x}_T\end{bmatrix}, \boldsymbol{x}_i, \boldsymbol{\theta}\right) = \left(\frac{\exp\left(\boldsymbol{\theta}_\lambda^\top \overline{\boldsymbol{x}}_i\right)}{\sum_{j=1}^{T}\exp\left(\boldsymbol{\theta}_\lambda^\top \overline{\boldsymbol{x}}_j\right)}\right)\boldsymbol{\theta}_V^\top \overline{\boldsymbol{x}}_i$$

Attention

$$f\left(\begin{bmatrix}\boldsymbol{x}_1\\ \vdots \\ \boldsymbol{x}_T\end{bmatrix}, \begin{bmatrix}\boldsymbol{x}_1\\ \vdots \\ \boldsymbol{x}_T\end{bmatrix}, \boldsymbol{\theta}\right) = \sum_{i=1}^{T}\left(\frac{\exp\left(\boldsymbol{\theta}_\lambda^\top \overline{\boldsymbol{x}}_i\right)}{\sum_{j=1}^{T}\exp\left(\boldsymbol{\theta}_\lambda^\top \overline{\boldsymbol{x}}_j\right)}\right)\boldsymbol{\theta}^\top \overline{\boldsymbol{x}}_i$$

Attention

TODO: Add query with science/einstein, music/taylor

TODO: Remove xbar because attention does not use bias?