Attention and Transformers

CISC 7026: Introduction to Deep Learning

University of Macau

Agenda

1. GNN Review
2. VAE Review and Coding
3. Attention
4. Keys and Queries
5. Transformer
6. Positional Encoding
7. 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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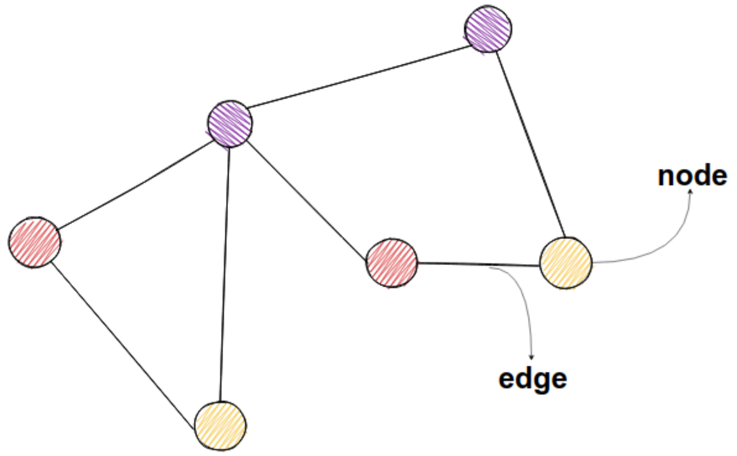

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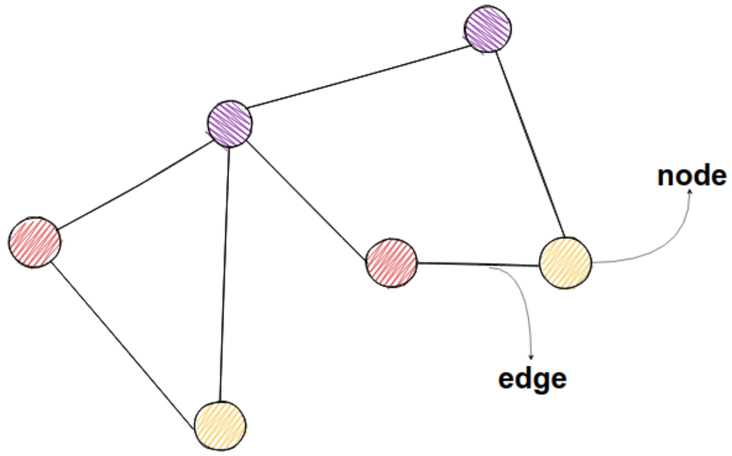

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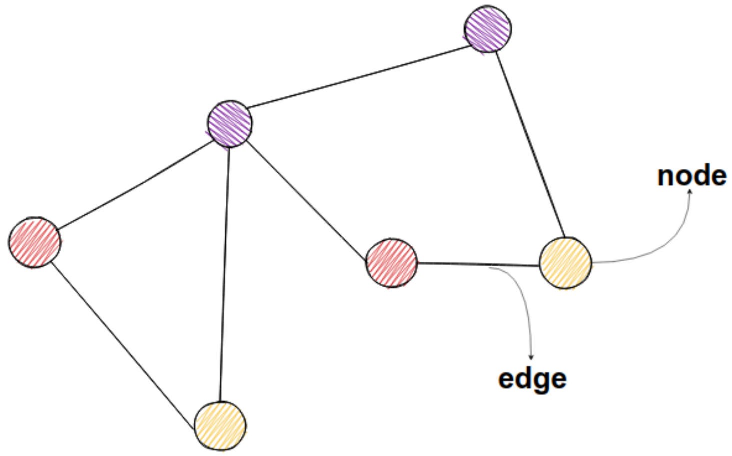

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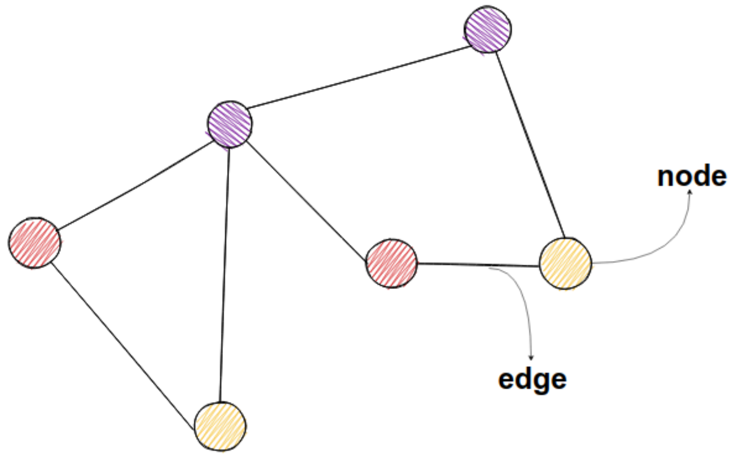
GNN Review



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

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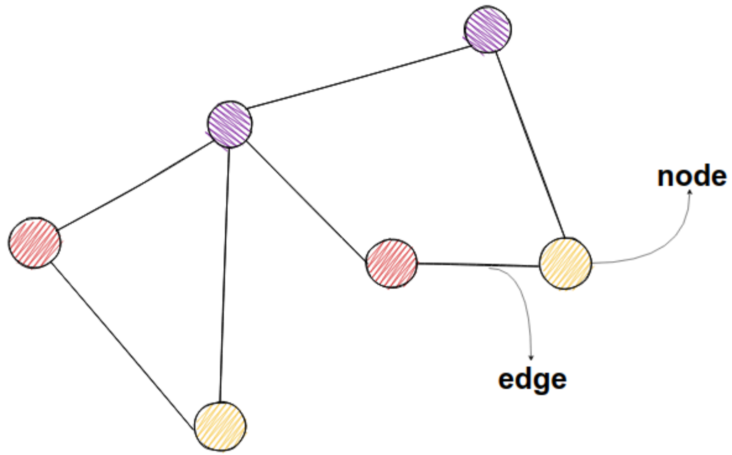

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The **neighborhood** $N(j)$ contains all neighbors of node j

GNN Review

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$$f(\boldsymbol{X}, \boldsymbol{E}, \boldsymbol{\theta})_j = \sigma\left(\boldsymbol{\theta}_1^\top \overline{\boldsymbol{x}}_j + \sum_{i \in N(j)} \boldsymbol{\theta}_2^\top \boldsymbol{x}_i\right)$$

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

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GNN Review

We can use pooling with graph convolutions too

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

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

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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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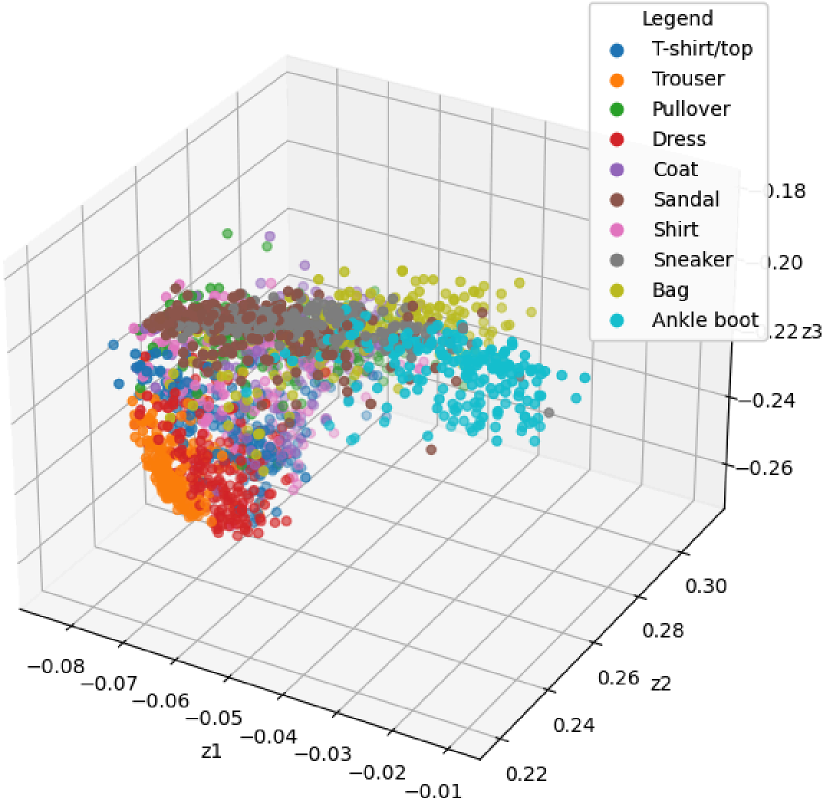
How does this work?

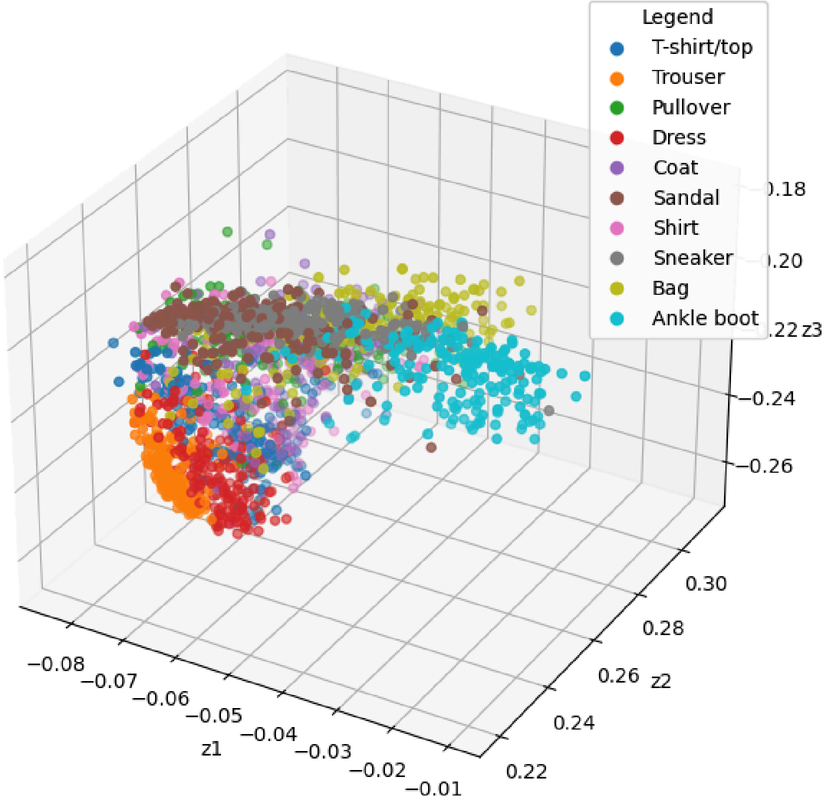
VAE Review and Coding

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

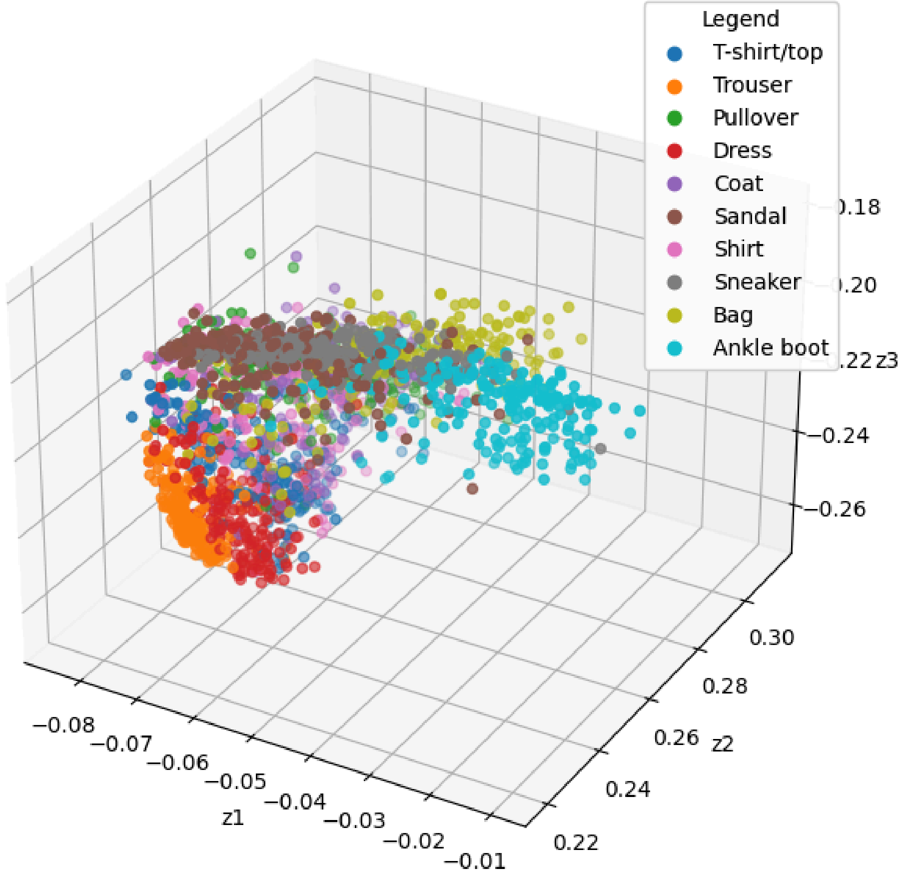


VAE Review and Coding

What happens if we decode a new point?

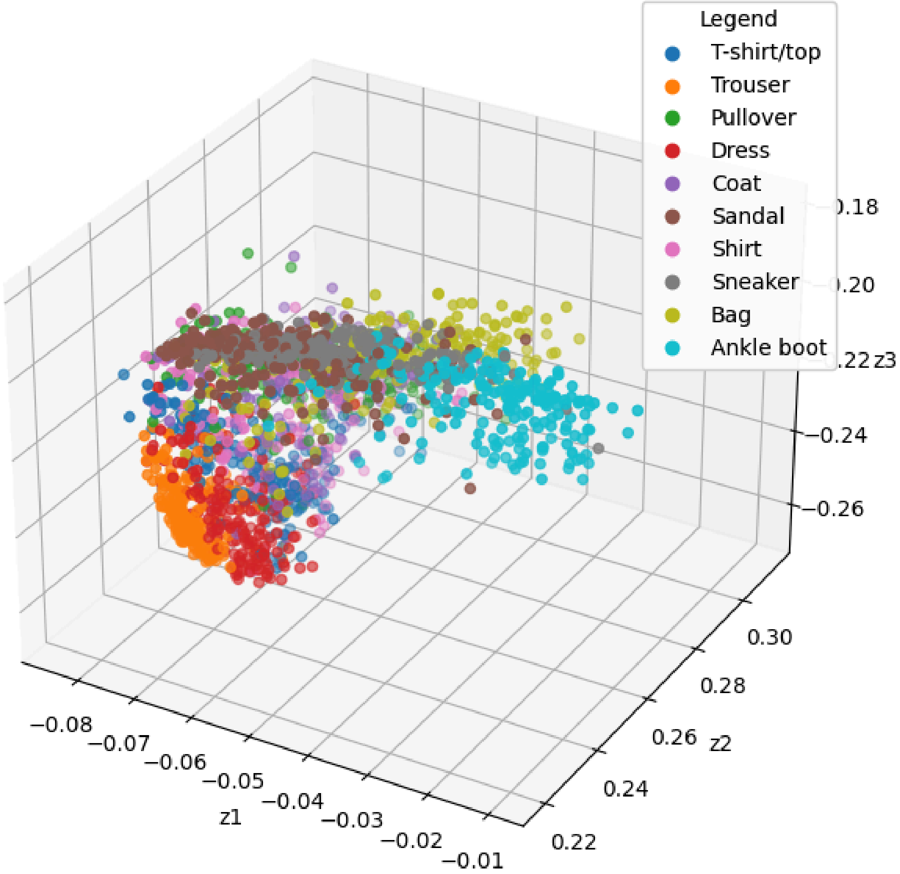


VAE Review and Coding



Autoencoder generative model:

VAE Review and Coding



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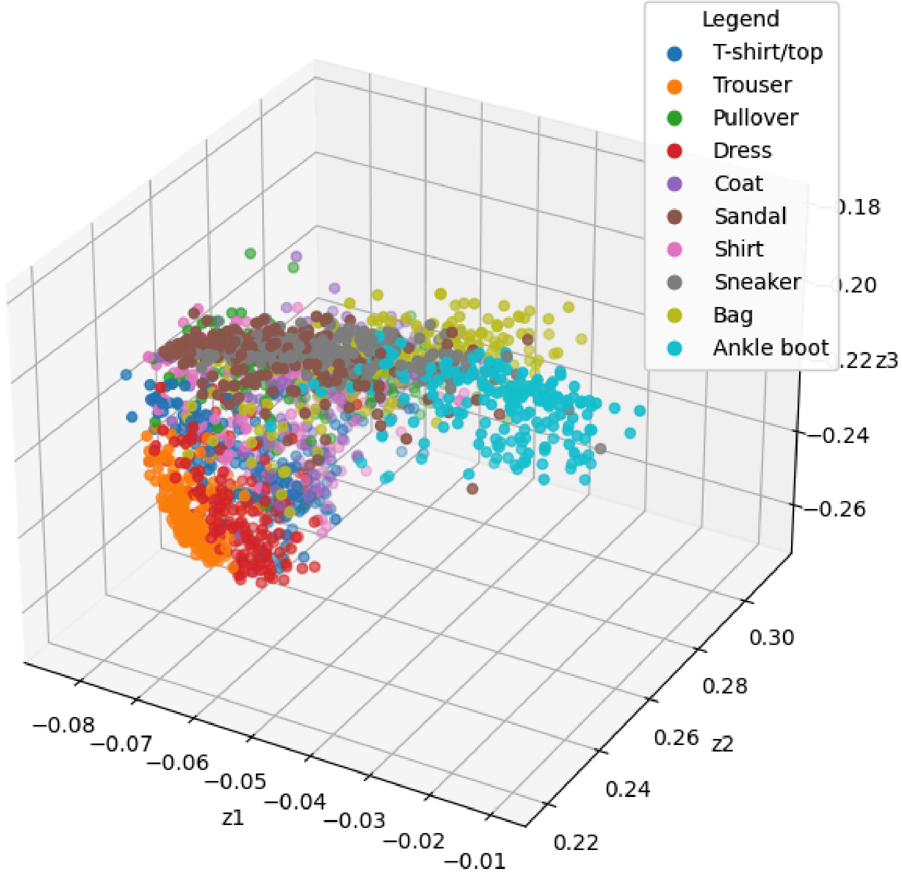
$$\text{Encode} \begin{bmatrix} \boldsymbol{x}_{[1]} \\ \vdots \\ \boldsymbol{x}_{[n]} \end{bmatrix} \text{ into } \begin{bmatrix} \boldsymbol{z}_{[1]} \\ \vdots \\ \boldsymbol{z}_{[n]} \end{bmatrix}$$

VAE Review and Coding



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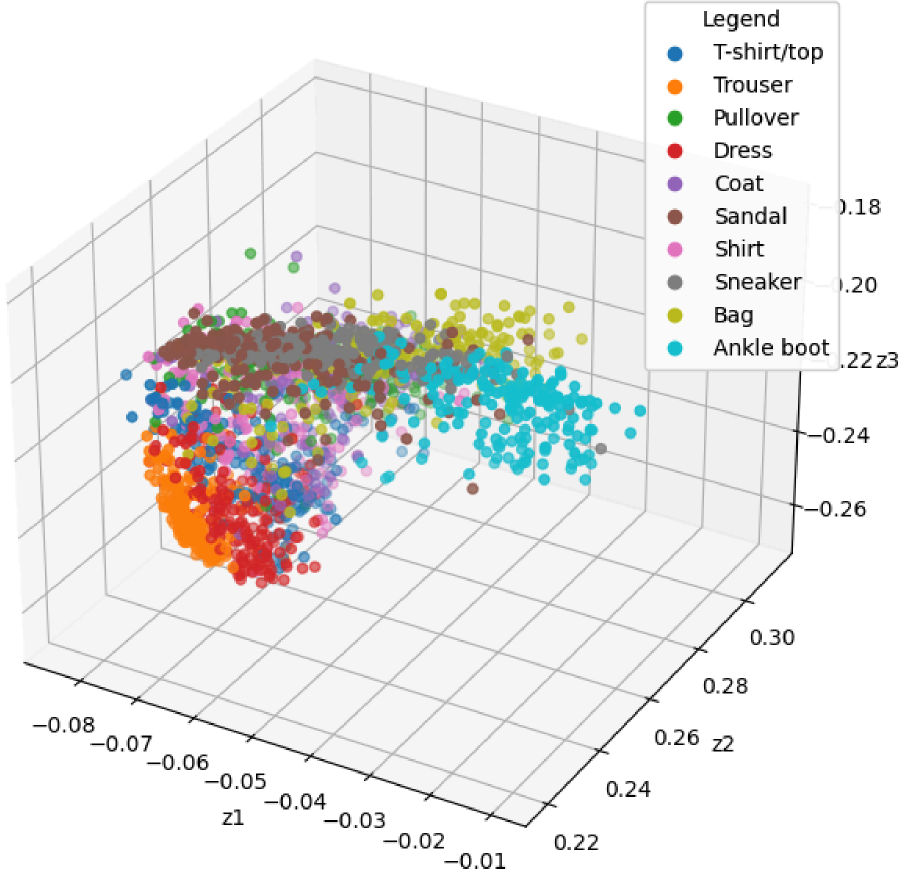
VAE Review and Coding



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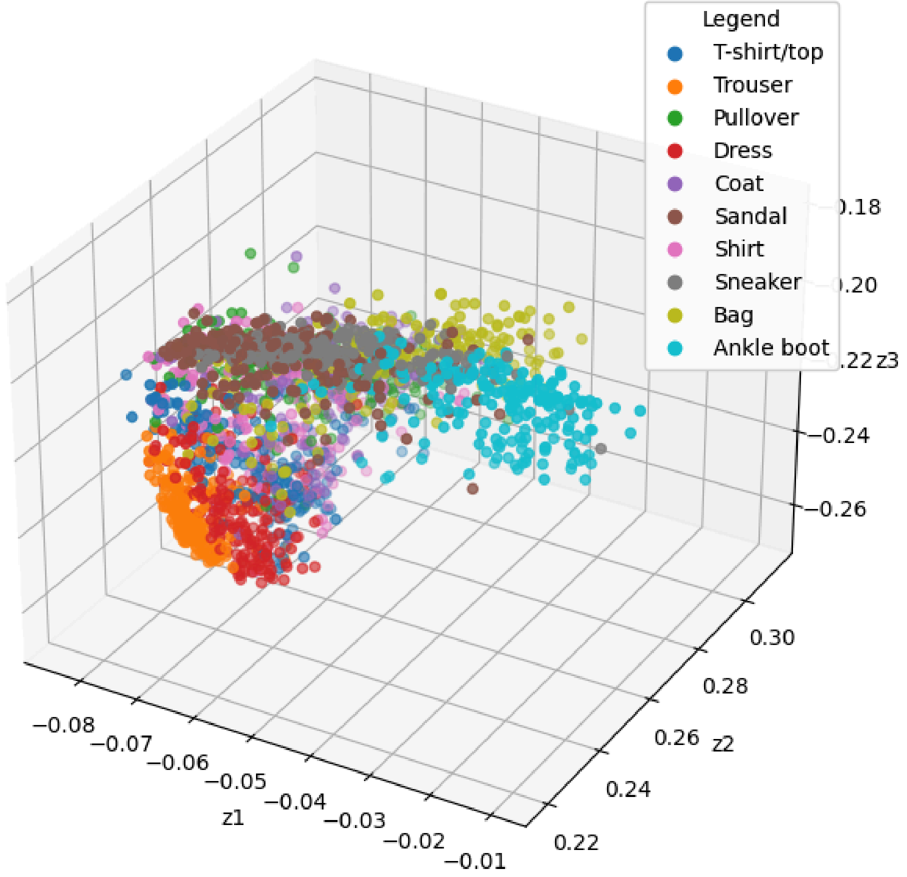

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Decode $\boldsymbol{z}_{\text{new}}$ into $\boldsymbol{x}_{\text{new}}$

VAE Review and Coding

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

VAE Review and Coding

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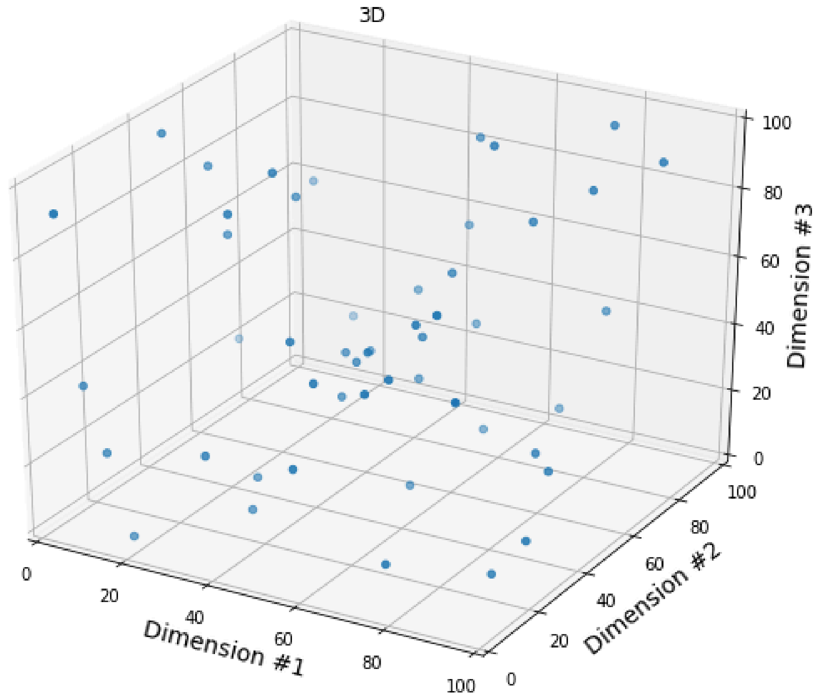

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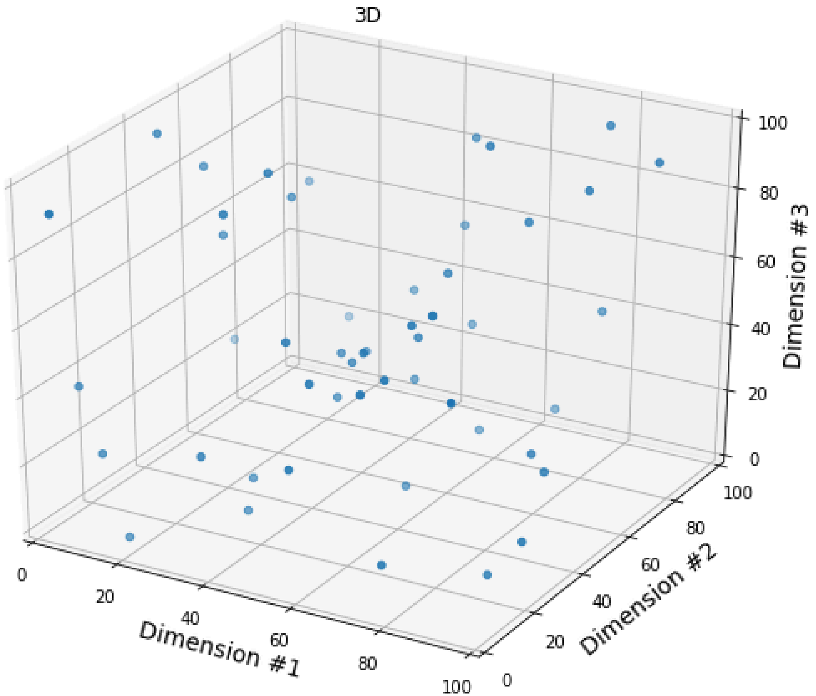

$f^{-1}(\boldsymbol{z} + \varepsilon)$ will produce either garbage, or $\boldsymbol{z}$

VAE Review and Coding

Variational autoencoders (VAEs) do three things:

VAE Review and Coding

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1. Make it easy to sample random z

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

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How?

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

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

VAE Review and Coding

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

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

VAE Review and Coding

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 $\boldsymbol{z} \sim \mathcal{N}(0, 1)$

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

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

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

VAE Review and Coding

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

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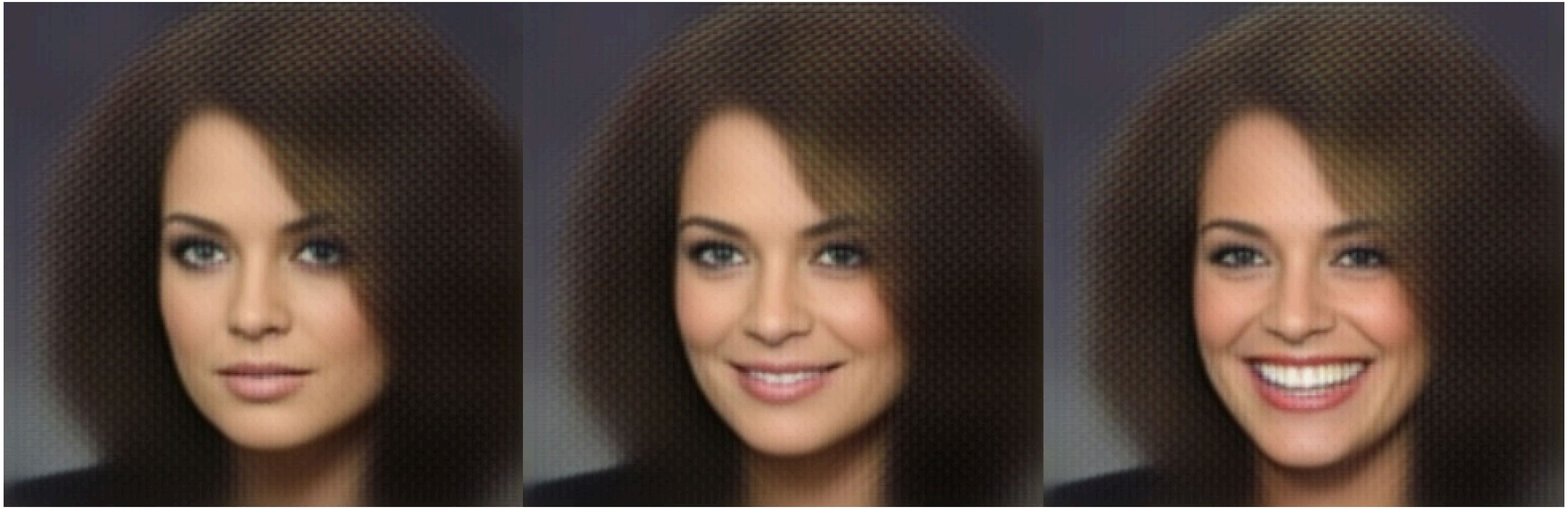
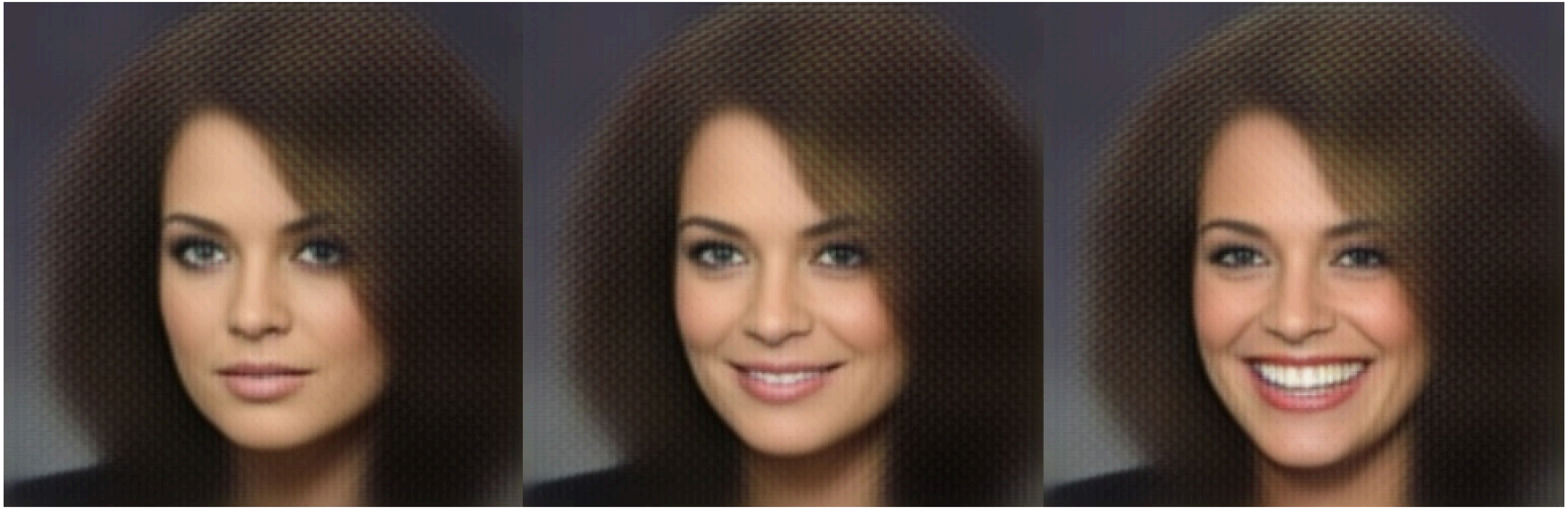
x : 

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

VAE Review and Coding



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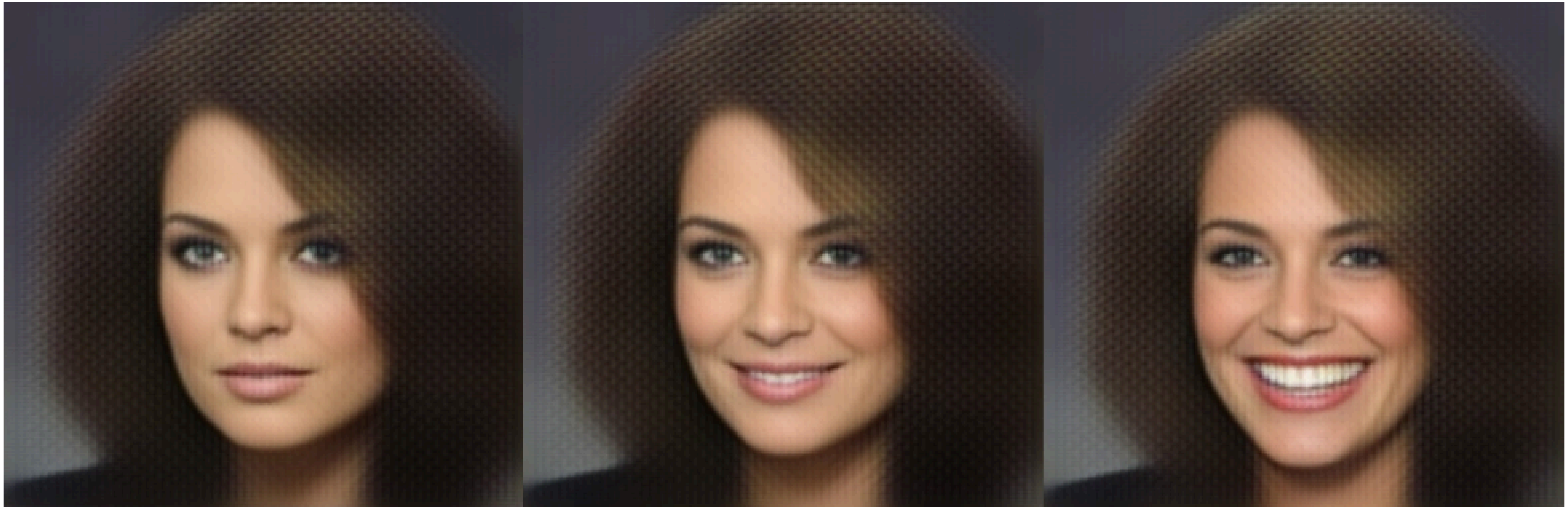
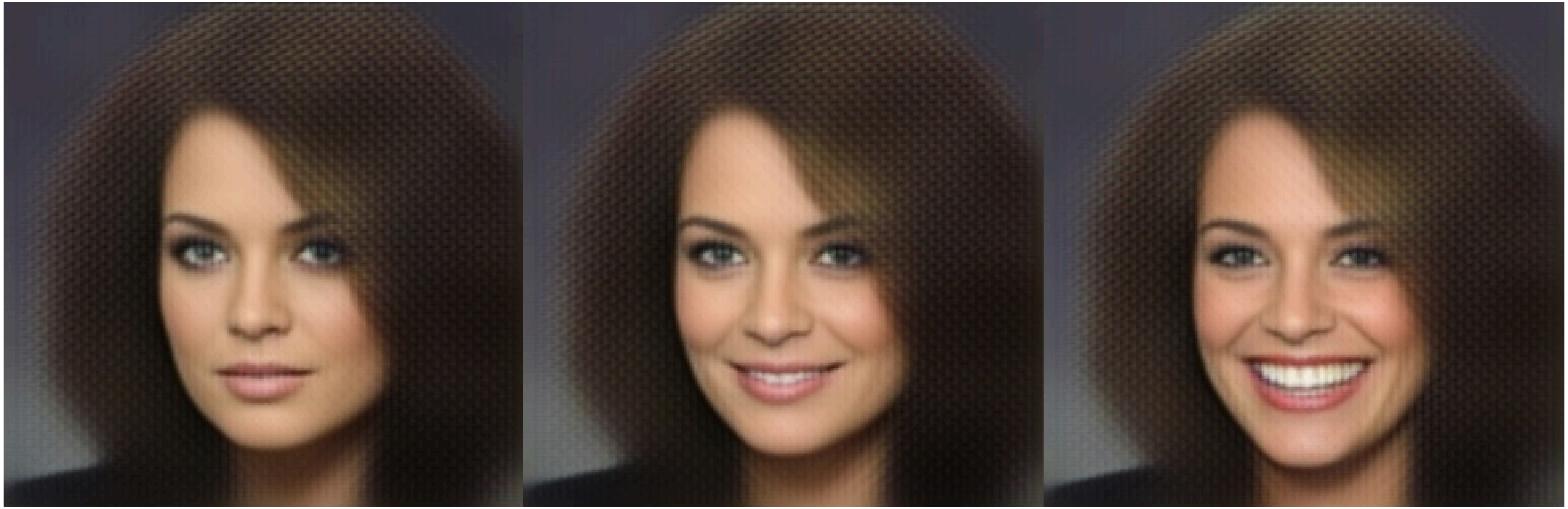


Network can only see $\boldsymbol{x}$, it cannot directly observe $\boldsymbol{z}$

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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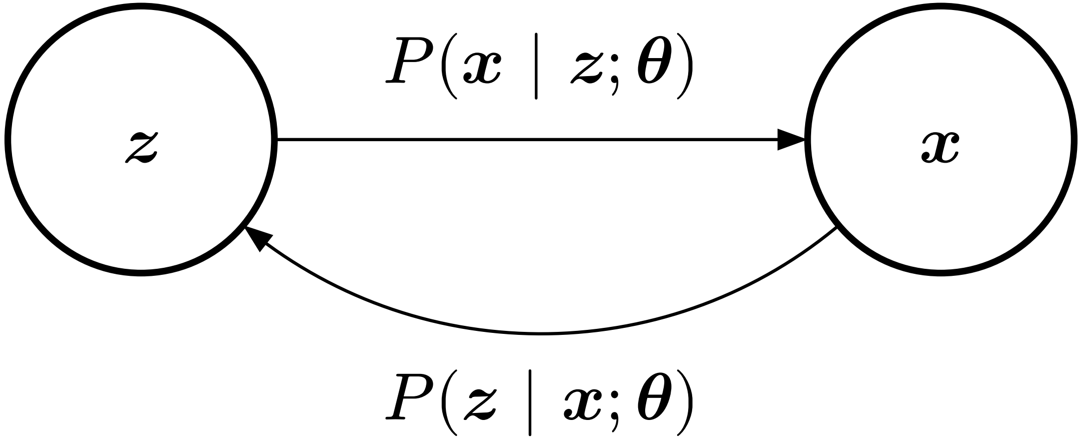

Decoder	Encoder
$P(\boldsymbol{x} \mid \boldsymbol{z}; \boldsymbol{\theta})$	$P(\boldsymbol{z} \mid \boldsymbol{x}; \boldsymbol{\theta})$

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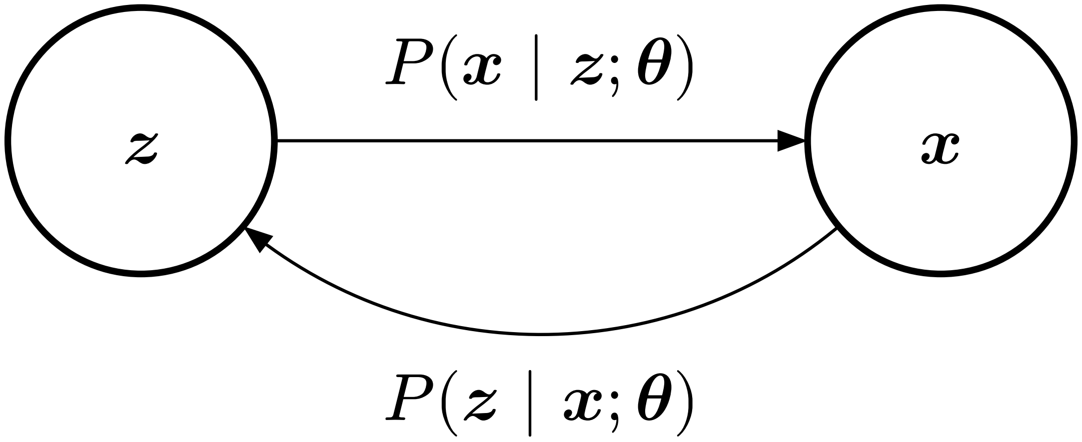

Decoder	Encoder
$P(\boldsymbol{x} \mid \boldsymbol{z}; \boldsymbol{\theta})$	$P(\boldsymbol{z} \mid \boldsymbol{x}; \boldsymbol{\theta})$

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

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

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We can use the same decoder as a standard autoencoder

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Encoder outputs a distribution ΔZ but decoder input is Z

Solution: Sample a vector $\boldsymbol{z}$ 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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$$\boldsymbol{z} = \boldsymbol{\mu} + \boldsymbol{\sigma} \odot \boldsymbol{\varepsilon}$$

Step 3: Decode the sample

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

VAE Review and Coding

```python
# 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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$$\arg \min_{\boldsymbol{\theta}} \mathrm{KL}(P(\boldsymbol{x}), P(\boldsymbol{x}; \boldsymbol{\theta}))$$

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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. Keys and Queries
5. Transformer
6. Positional Encoding
7. Coding

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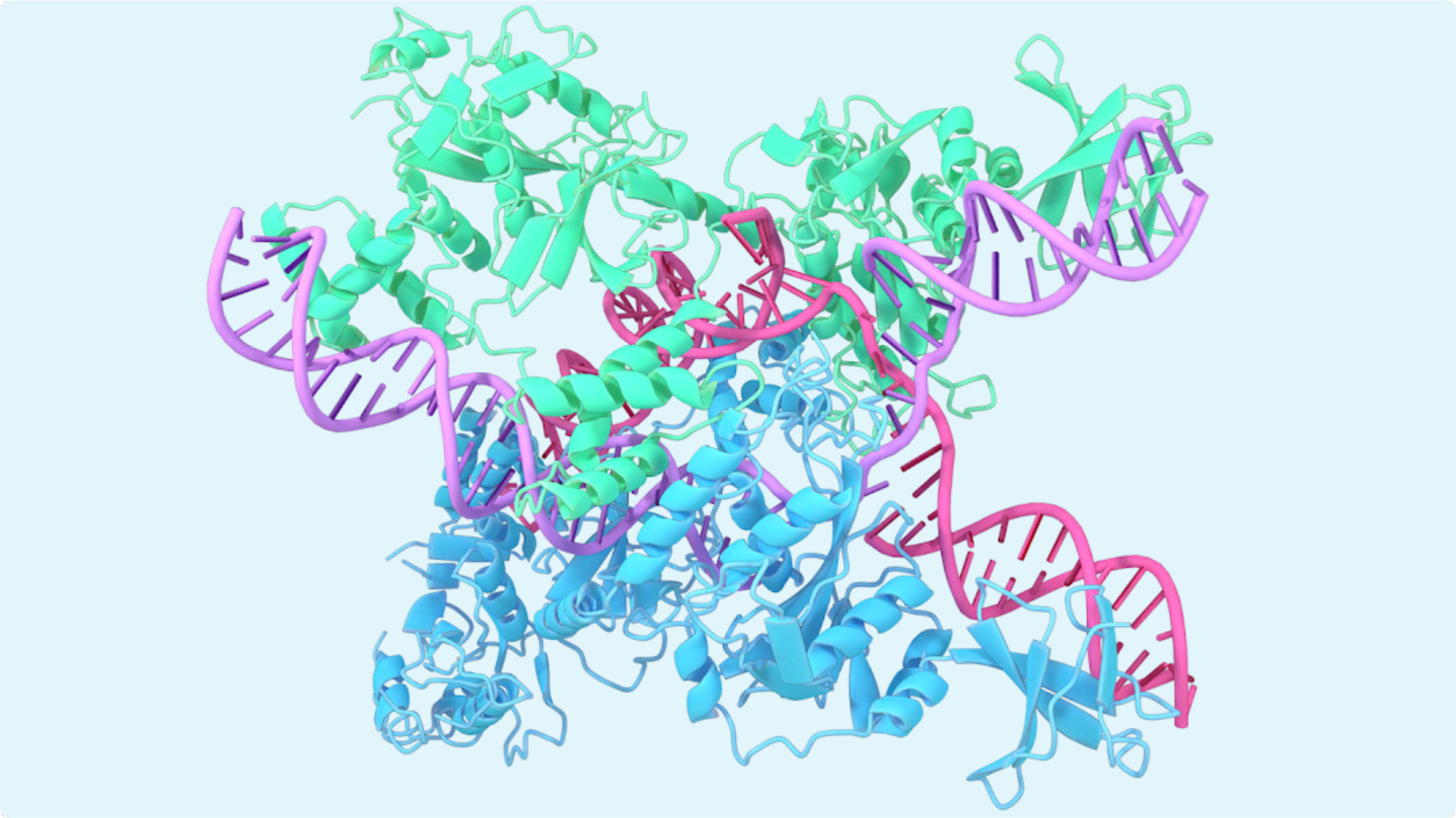
Let's review some products based on attention

Attention

AlphaFold (Nobel prize)

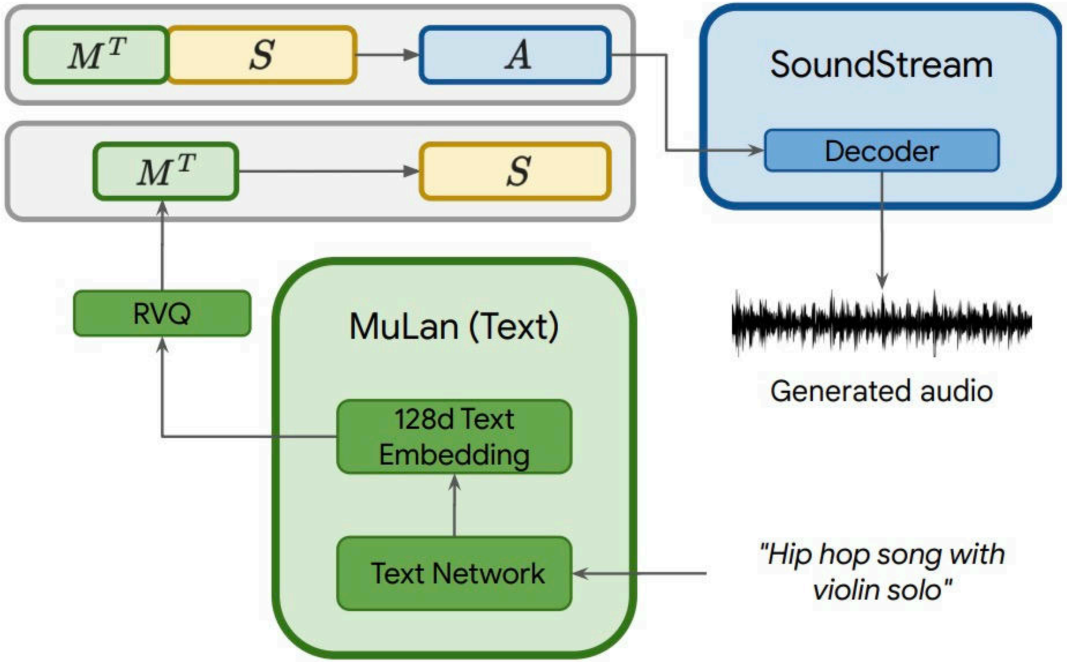


Attention

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

Attention

MusicTransformer, MuLan

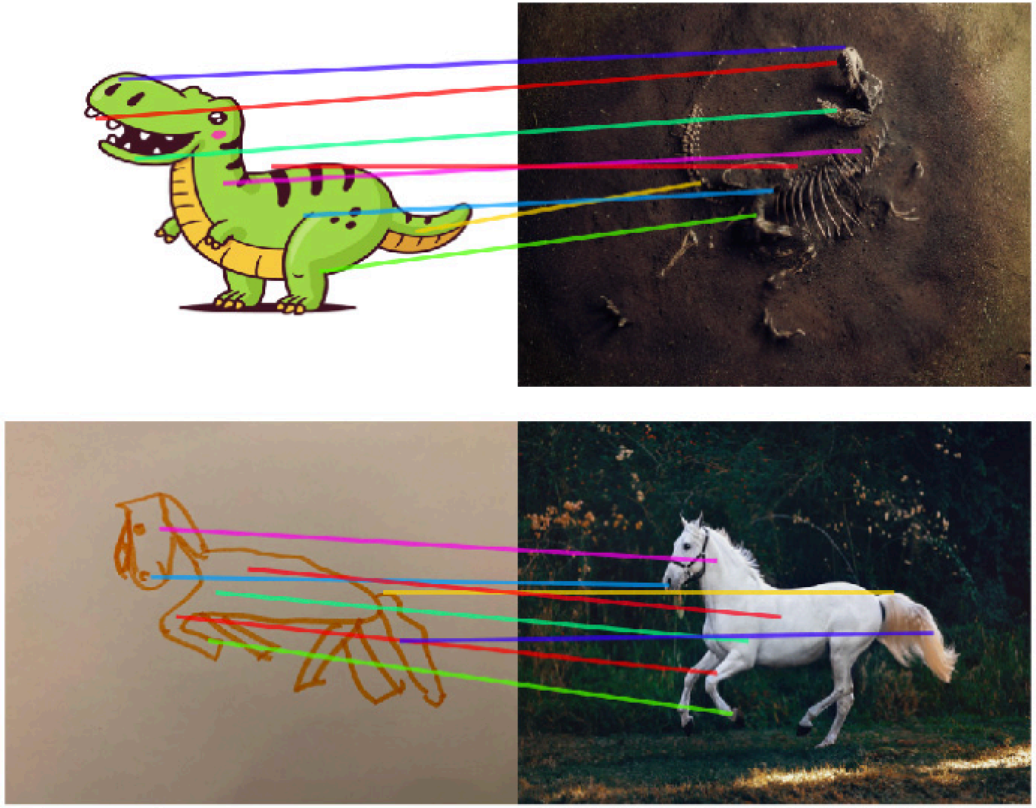


Attention

Google Translate, Baidu Translate, Apple Translate

Attention

ViT, DinoV2



Attention

All these models are **transformers**

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

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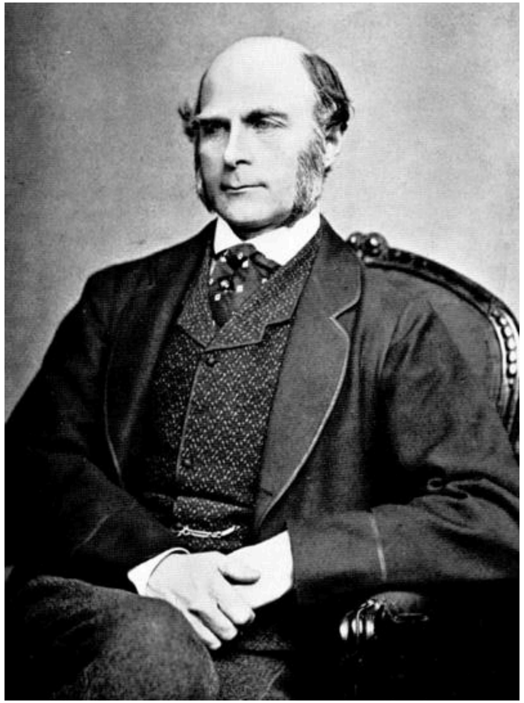
We can derive attention from composite memory

Attention

Francis Galton (1822-1911)
photo composite memory



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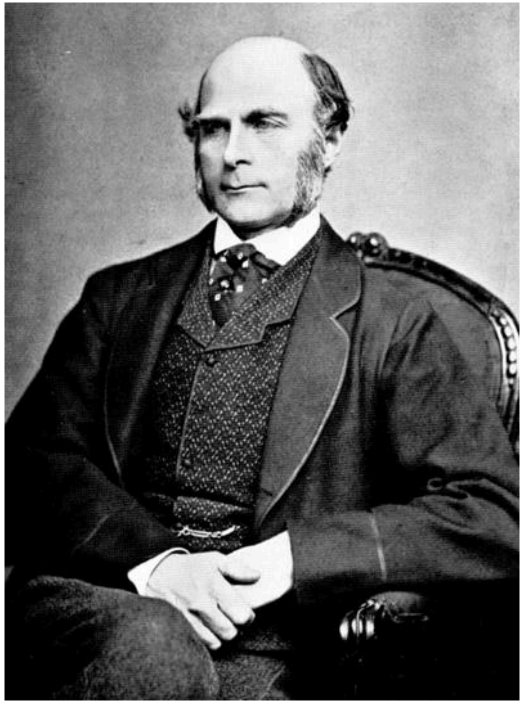
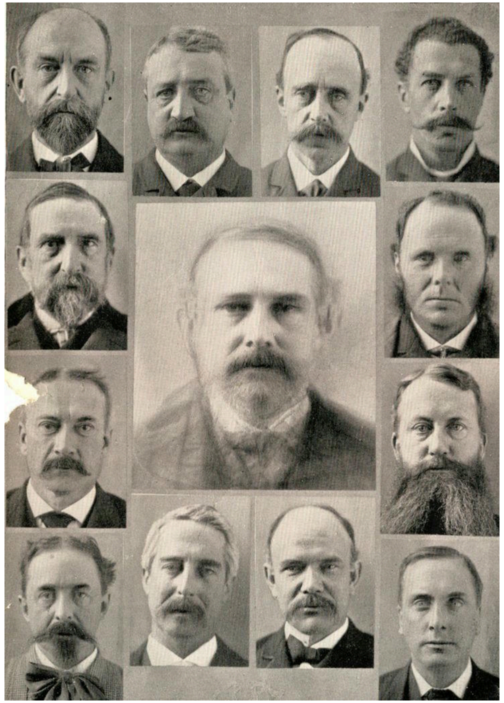


Composite photo of members of a party



Attention

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Limited space, cannot remember everything

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$$\sum_{i=1}^{T} \gamma^{T-i} \cdot \boldsymbol{\theta}^\top \overline{\boldsymbol{x}}_i$$

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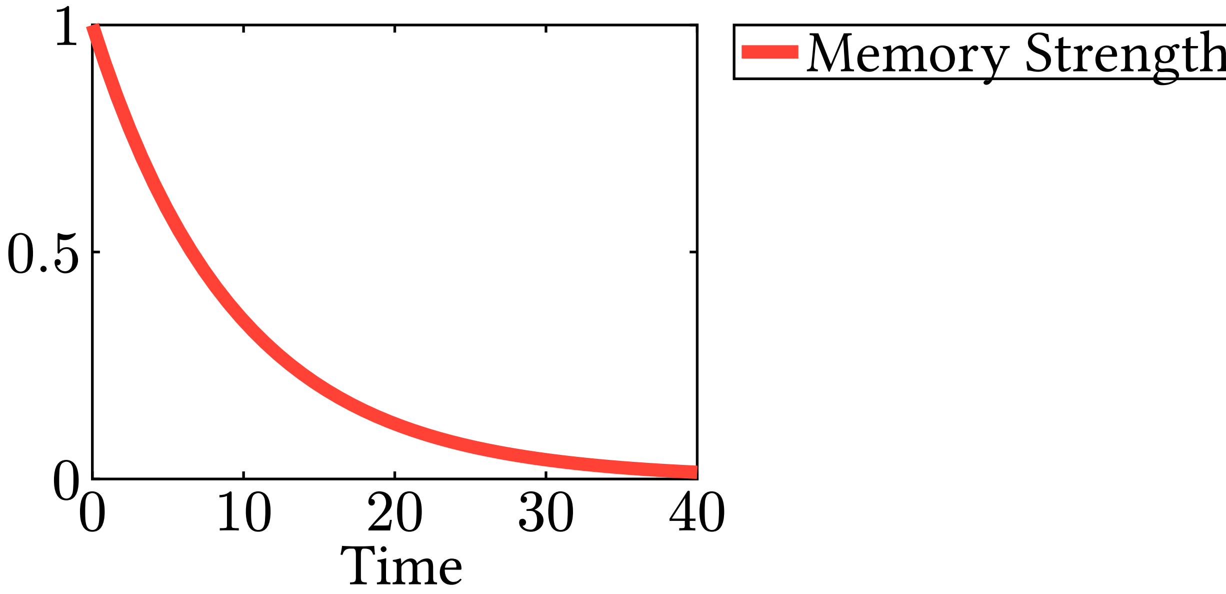

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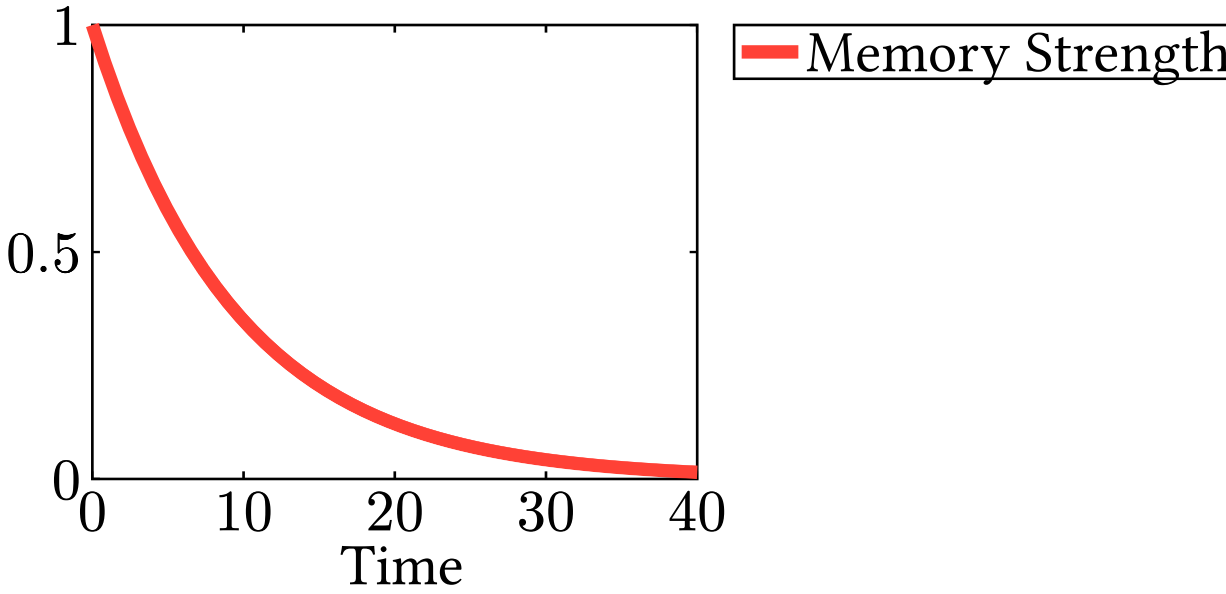
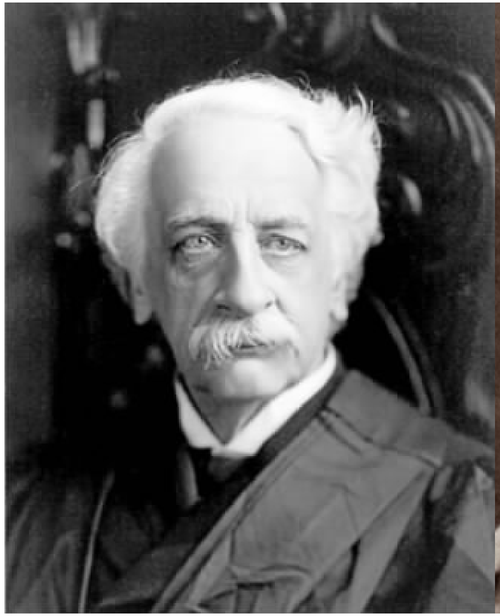
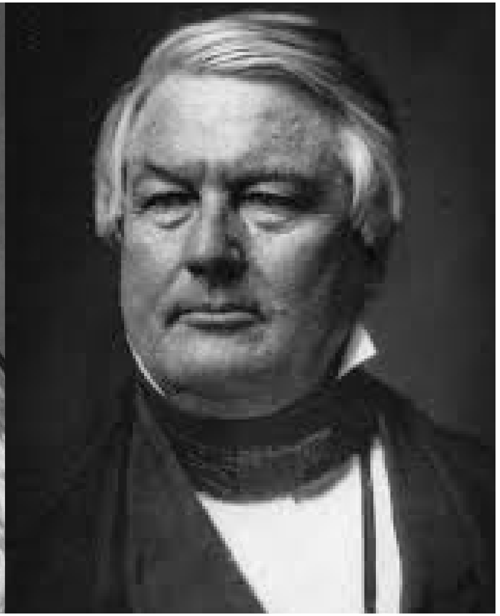


Question: Does this accurately model what you remember?

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 another party

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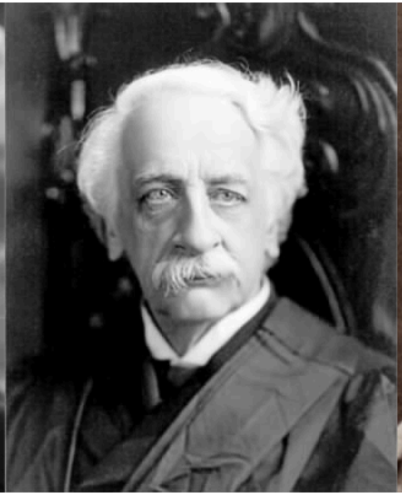


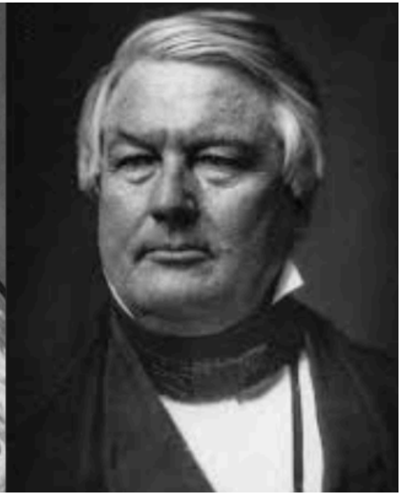

$\gamma^4 \boldsymbol{\theta}^\top \overline{\boldsymbol{x}}_1$ $\gamma^3 \boldsymbol{\theta}^\top \overline{\boldsymbol{x}}_2$ $\gamma^2 \boldsymbol{\theta}^\top \overline{\boldsymbol{x}}_3$ $\gamma^1 \boldsymbol{\theta}^\top \overline{\boldsymbol{x}}_4$ $\gamma^0 \boldsymbol{\theta}^\top \overline{\boldsymbol{x}}_5$

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Question: What will happen to Taylor Swift?

Attention

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

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We will forget meeting her!

Attention

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Question: Would you forget meeting Taylor Swift?

Attention

Our model of memory is incomplete

Attention

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

Attention

Our model of memory is incomplete

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

We will **pay more attention** to certain memories

My memory might actually be

$$1.0 \cdot \boldsymbol{\theta}^\top \overline{\boldsymbol{x}}_1$$

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Question: How can we achieve this forgetting?

Attention

In our composite model, forgetting is a function of time

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Question: Any forgetting mechanism that is not a function of time?

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Attention

First, write our forgetting function

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$$\lambda(\boldsymbol{x}, \boldsymbol{\theta}_\lambda) = \sigma\left(\boldsymbol{\theta}_\lambda^\top \overline{\boldsymbol{x}}\right); \quad \boldsymbol{\theta}_\lambda \in \mathbb{R}^{(d_x+1) \times 1}$$

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This is one form of **attention**

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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

Attention

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Attention

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

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

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Question: What do the images look like now?

Attention

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

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

Attention

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

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

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Not a good model of attention!

Attention

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

Attention

Let us rewrite attention using softmax

Attention

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

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

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

Attention

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

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

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

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Agenda

1. GNN Review
2. VAE Review and Coding
3. **Attention**
4. Keys and Queries
5. Transformer
6. Positional Encoding
7. Coding

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Keys and Queries

The modern form of attention behaves like a database

Keys and Queries

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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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Keys and Queries

We can search our keys using a **query**

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Query: Which person will help me on my exam?

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Keys and Queries

Query: I want to have fun

Keys and Queries

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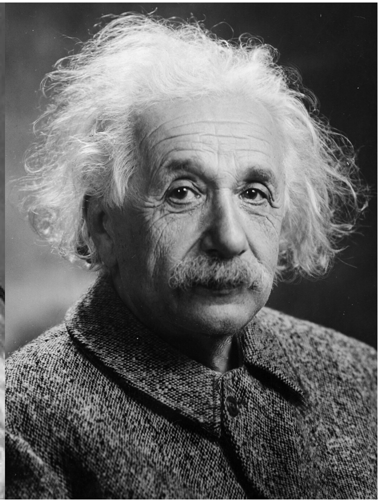

Scientist

Keys and Queries

Query: I want to have fun

Musician

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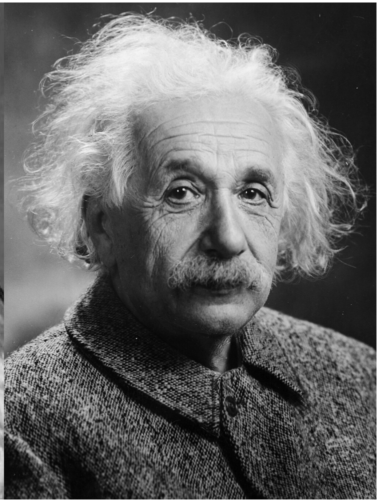

Scientist

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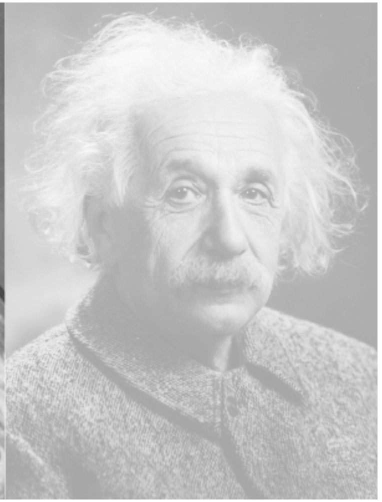
Musician Lawyer Shopkeeper Chef Scientist







How do we represent this mathematically?

Keys and Queries

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

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

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Create keys for all inputs

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Create keys for all inputs

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

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Example:

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

Keys and Queries

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

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

Keys and Queries

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$\boldsymbol{q}^\top \boldsymbol{k}_i = \left(\boldsymbol{\theta}_Q^\top \text{ Musician}\right)^\top \Big(\boldsymbol{\theta}_K^\top$  $\Big) = 100$

Keys and Queries

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Large attention!

Keys and Queries

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Keys and Queries

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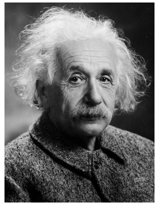
$$\left.\right) = -50$$

Small attention!

Keys and Queries

Example:

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

Keys and Queries

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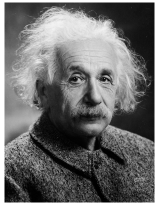
$$\boldsymbol{k}_i = \boldsymbol{\theta}_K^\top$$ 

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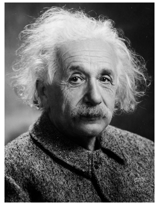
$$\boldsymbol{k}_i = \boldsymbol{\theta}_K^\top$$ 

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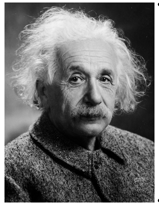
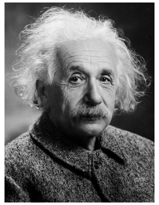
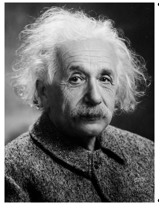
$$\boldsymbol{q}^\top \boldsymbol{k}_i = \left(\boldsymbol{\theta}_Q^\top \text{ Mathematician}\right)^\top \left(\boldsymbol{\theta}_K^\top \right.$$  $$\left. \right) = 90$$

Keys and Queries

Example:

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

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

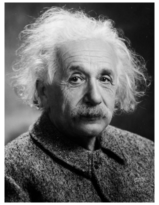
$\boldsymbol{q}^\top \boldsymbol{k}_i = (\boldsymbol{\theta}_Q^\top \text{ Mathematician})^\top (\boldsymbol{\theta}_K^\top$  $) = 90$

Large attention!

Keys and Queries

Example:

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



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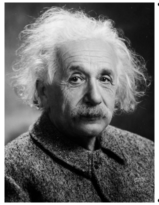
$$\boldsymbol{q}^\top \boldsymbol{k}_i = \left(\boldsymbol{\theta}_Q^\top \text{ Mathematician}\right)^\top \Bigg(\boldsymbol{\theta}_K^\top$$



$$\Bigg) = 90$$

Large attention!

Remember, there are multiple inputs to pay attention to

Keys and Queries

We compute attention for each input

Keys and Queries

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

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Question: Anything missing from before?

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Question: Anything missing from before?

Answer: Normalize attention to sum to one!

Keys and Queries

Normalize, only pay attention to important matches

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

Keys and Queries

Normalize, only pay attention to important matches

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We call this **dot-product attention**

Keys and Queries

Query: Which person will help me on my exam?

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$\boldsymbol{q}^\top \boldsymbol{k}_1$ $\boldsymbol{q}^\top \boldsymbol{k}_2$ $\boldsymbol{q}^\top \boldsymbol{k}_3$ $\boldsymbol{q}^\top \boldsymbol{k}_4$ $\boldsymbol{q}^\top \boldsymbol{k}_5$

Keys and Queries

Query: Which person will help me on my exam?

$\boldsymbol{q}^\top \boldsymbol{k}_1$	$\boldsymbol{q}^\top \boldsymbol{k}_2$	$\boldsymbol{q}^\top \boldsymbol{k}_3$	$\boldsymbol{q}^\top \boldsymbol{k}_4$	$\boldsymbol{q}^\top \boldsymbol{k}_5$
-1.71	0.60	-1.01	-0.61	2.73

softmax

Keys and Queries

Query: Which person will help me on my exam?

$\boldsymbol{q}^\top \boldsymbol{k}_1$	$\boldsymbol{q}^\top \boldsymbol{k}_2$	$\boldsymbol{q}^\top \boldsymbol{k}_3$	$\boldsymbol{q}^\top \boldsymbol{k}_4$	$\boldsymbol{q}^\top \boldsymbol{k}_5$
-1.71	0.60	-1.01	-0.61	2.73

$$\text{softmax}$$

0.01	0.10	0.02	0.03	0.84

Keys and Queries

Query: Which person will help me on my exam?

$\boldsymbol{q}^\top \boldsymbol{k}_1$	$\boldsymbol{q}^\top \boldsymbol{k}_2$	$\boldsymbol{q}^\top \boldsymbol{k}_3$	$\boldsymbol{q}^\top \boldsymbol{k}_4$	$\boldsymbol{q}^\top \boldsymbol{k}_5$
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Put dot product attention into our composite model

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In dot-product attention, we call $\boldsymbol{\theta}_V^\top \boldsymbol{x}_i$ the **value**

Keys and Queries

$$\boldsymbol{q}^\top \boldsymbol{k}_1 \quad \boldsymbol{q}^\top \boldsymbol{k}_2 \quad \boldsymbol{q}^\top \boldsymbol{k}_3 \quad \boldsymbol{q}^\top \boldsymbol{k}_4 \quad \boldsymbol{q}^\top \boldsymbol{k}_5$$

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

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Agenda

1. GNN Review
2. VAE Review and Coding
3. Attention
4. **Keys and Queries**
5. Transformer
6. Positional Encoding
7. Coding

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Transformer

Previously, we chose our own $\boldsymbol{x}_q = \text{Musician}$

Transformer

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We can also create queries from all the inputs

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

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We call this dot-product **self** attention

Transformer

Writing dot-product self attention in matrix form is easier

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This operation powers today's biggest models

Transformer

$$\boldsymbol{Q} \in \mathbb{R}^{T \times d_h} \quad \boldsymbol{K} \in \mathbb{R}^{T \times d_h} \quad \boldsymbol{V} \in \mathbb{R}^{T \times d_h}$$

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Transformer

```
class Attention(nn.Module):
    def __init__(self):
        self.theta_K = nn.Linear(d_x, d_h, bias=False)
        self.theta_Q = nn.Linear(d_x, d_h, bias=False)
        self.theta_V = nn.Linear(d_x, d_h, bias=False)

    def forward(self, x):
        A = softmax(self.theta_Q(x) @ self.theta_K(x) / d_h)
        return A @ self.theta_V(x)
```

Transformer

Transformers

Transformer

If you understand attention, transformers are very simple

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Each transformer consists of many "transformer blocks"

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If you understand attention, transformers are very simple

Each transformer consists of many “transformer blocks”

A transformer block is attention and an MLP

Transformer

```python
class TransformerBlock(nn.Module):
    def __init__(self):
        self.attn = Attention()
        self.mlp = Sequential(
            Linear(d_h, d_h), LeakyReLU(), Linear(d_h, d_h))
        self.norm1 = nn.LayerNorm(d_h)
        self.norm2 = nn.LayerNorm(d_h)

    def forward(self, x):
        # Residual connection
        x = self.norm1(self.attn(x) + x)
        x = self.norm2(self.mlp(x) + x)
        return x
```

Transformer

```python
class Transformer(nn.Module):
    def __init__(self):
        self.block1 = TransformerBlock()
        self.block2 = TransformerBlock()
        ...

    def forward(self, x):
        x = self.block1(x)
        x = self.block2(x)
        ...
        return x
```

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Coding

Transformers are an operation on **sets**