Attention

CISC 7026: Introduction to Deep Learning

University of Macau

New laptop, bigger translation model, better captions?

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Final homework uploaded, due 12/18

All quiz 3 grades uploaded

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If you submitted a quiz but have no grade, come see me after class

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3 more lectures

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2. 11/25: Transformers

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3 more lectures

1. Today: Attention
2. 11/25: Transformers
3. 12/3: (Virtual) Introduction to reinforcement learning

Next term: CISC 7404 Special Topics in Artificial Intelligence (preliminary)

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Still designing course, but will focus on deep reinforcement learning

Agenda

1. GNN Review
2. VAE Review and Coding
3. Attention
4. Keys and Queries
5. Self Attention
6. Homework

Agenda

1. **GNN Review**
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GNN Review

Graph is a structure of nodes (vertices) and edges

GNN Review

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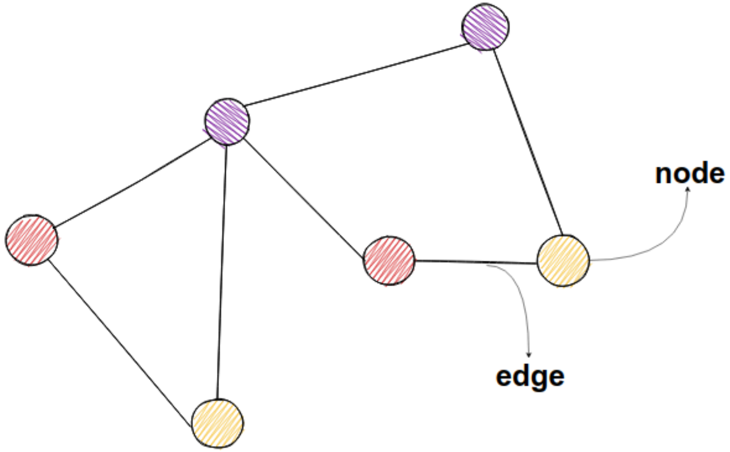

GNN Review

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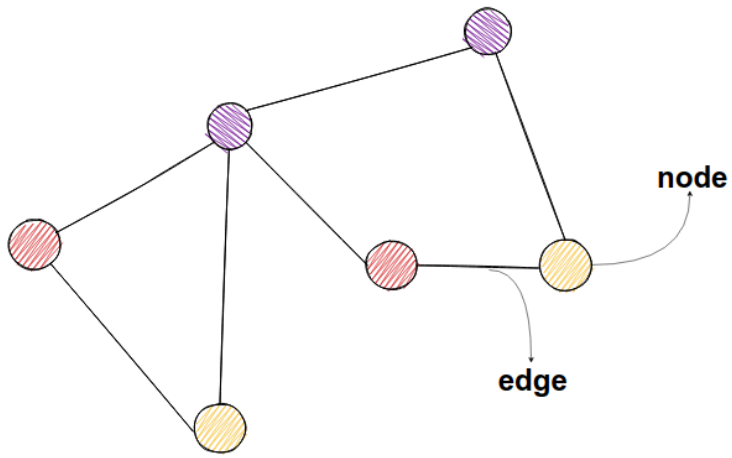

A **node** is a vector of information

GNN Review

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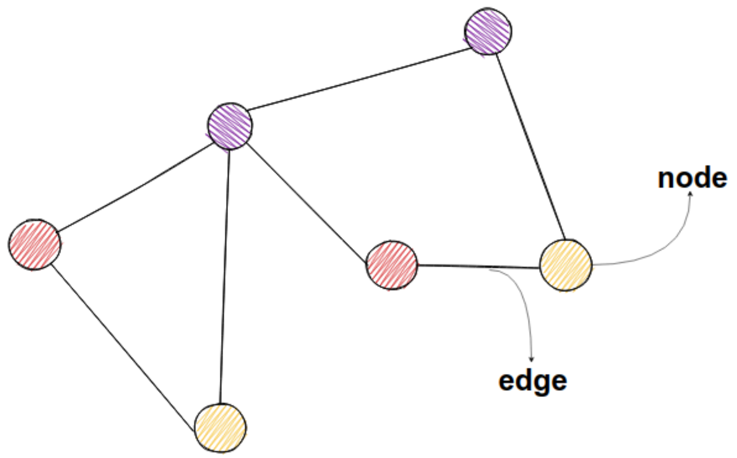

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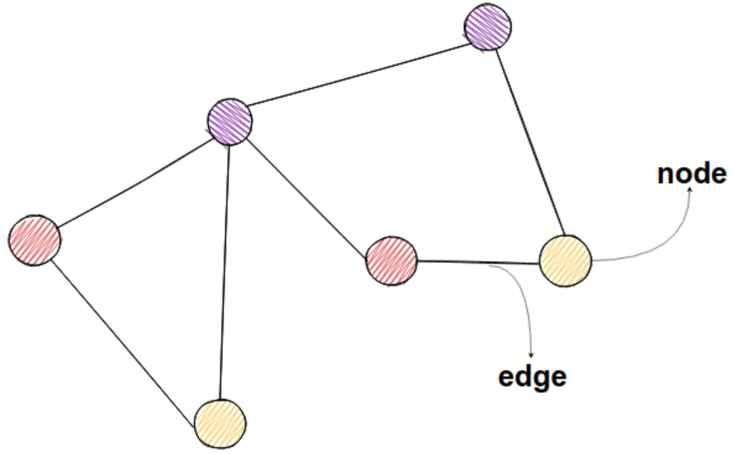

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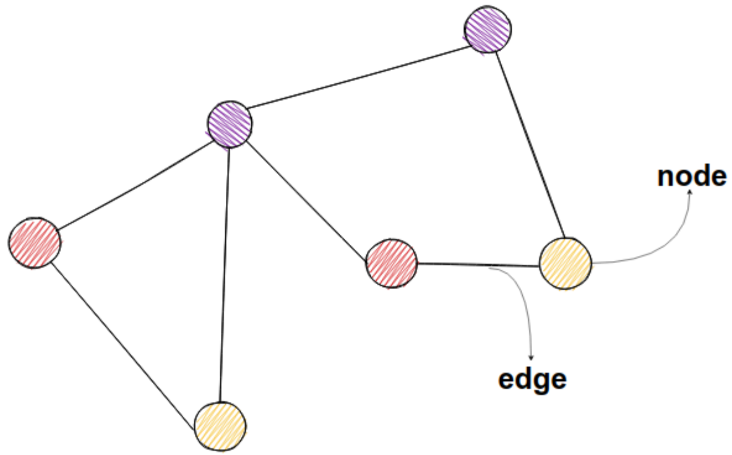

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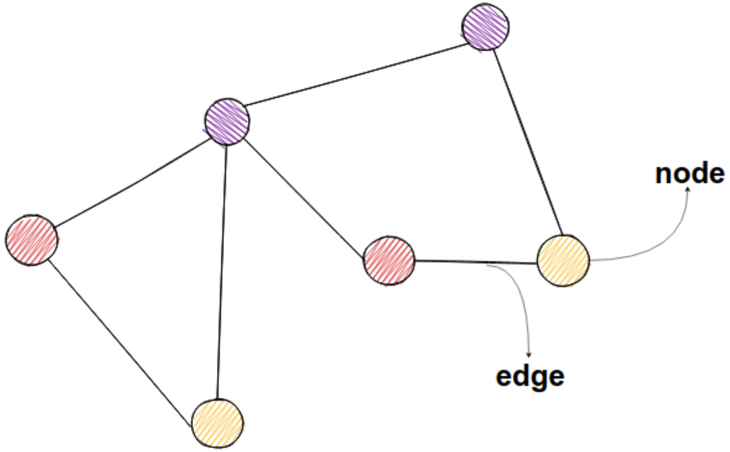

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If we connect nodes i and j with edge (i, j), then i and j are **neighbors**

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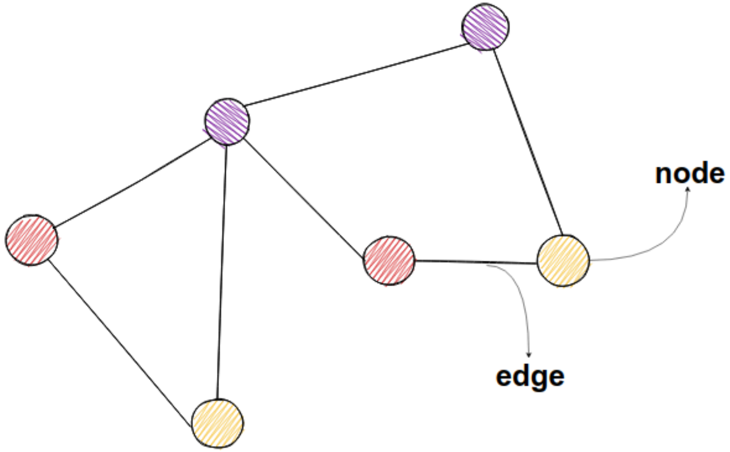

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The **neighborhood** $N(i)$ contains all neighbors of node i

GNN Review

Let us think of graphs as **signals**

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Question: Where did we see signals before?

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$$\text{Node } i \quad \boldsymbol{x}(i) \in \mathbb{R}^{d_x}; \quad i \in 1, ..., T$$

GNN Review

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$$\text{Node } i \quad \boldsymbol{x}(i) \in \mathbb{R}^{d_x}; \quad i \in 1, ..., T$$

$$\text{Neighborhood of } i \quad \boldsymbol{N}(i) = \begin{bmatrix} i \\ j \\ k \\ \vdots \end{bmatrix}; \quad \boldsymbol{N}(i) \in \mathcal{P}(i); \quad i \in 1, ..., T$$

GNN Review

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

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Combine information from the neighbors of $\boldsymbol{x}(i)$

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Combine information from the neighbors of $\boldsymbol{x}(i)$

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

GNN Review

Apply graph convolution over all nodes in the graph

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$$f(\boldsymbol{x}, \boldsymbol{N}, \boldsymbol{\theta}) = \begin{bmatrix} f(\boldsymbol{x}, \boldsymbol{N}, \boldsymbol{\theta})(1) \\ f(\boldsymbol{x}, \boldsymbol{N}, \boldsymbol{\theta})(2) \\ \vdots \\ f(\boldsymbol{x}, \boldsymbol{N}, \boldsymbol{\theta})(T) \end{bmatrix} = \begin{bmatrix} \sigma\left(\sum_{j \in \boldsymbol{N}(1)} \boldsymbol{\theta}^\top \overline{\boldsymbol{x}}(j)\right) \\ \sigma\left(\sum_{j \in \boldsymbol{N}(2)} \boldsymbol{\theta}^\top \overline{\boldsymbol{x}}(j)\right) \\ \vdots \\ \sigma\left(\sum_{j \in \boldsymbol{N}(T)} \boldsymbol{\theta}^\top \overline{\boldsymbol{x}}(j)\right) \end{bmatrix}$$

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

GNN Review

Standard 1D convolution

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

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Question: What is the output size of standard convolution?

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Question: What is the output size of standard convolution?

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

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GNN Review

We can use pooling with graph convolutions too

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

$$\sigma\left(\sum_{j \in \boldsymbol{N}(1)} \boldsymbol{\theta}^\top \overline{\boldsymbol{x}}(j)\right) + \sigma\left(\sum_{j \in \boldsymbol{N}(2)} \boldsymbol{\theta}^\top \overline{\boldsymbol{x}}(j)\right) + \ldots + \sigma\left(\sum_{j \in \boldsymbol{N}(T)} \boldsymbol{\theta}^\top \overline{\boldsymbol{x}}(j)\right)$$

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VAE Review and Coding

We can use autoencoders as **generative models**

VAE Review and Coding

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A generative model learns the structure of data

VAE Review and Coding

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Using this structure, it generates **new** data

VAE Review and Coding

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VAE Review and Coding

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VAE Review and Coding

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VAE Review and Coding

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VAE Review and Coding

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If you like generative models, you should study Bayesian statistics

VAE Review and Coding

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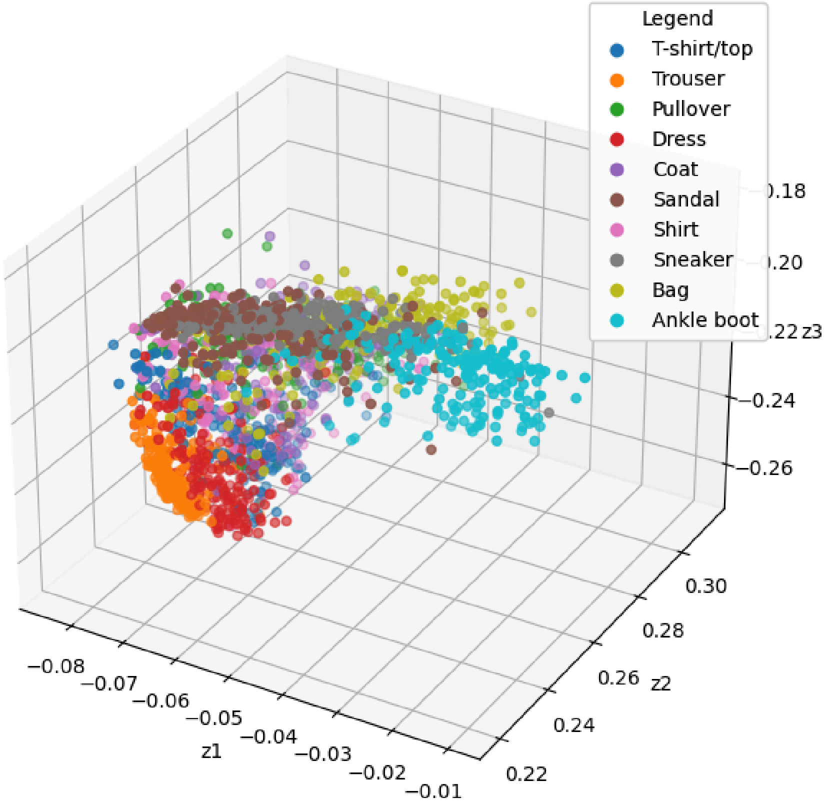
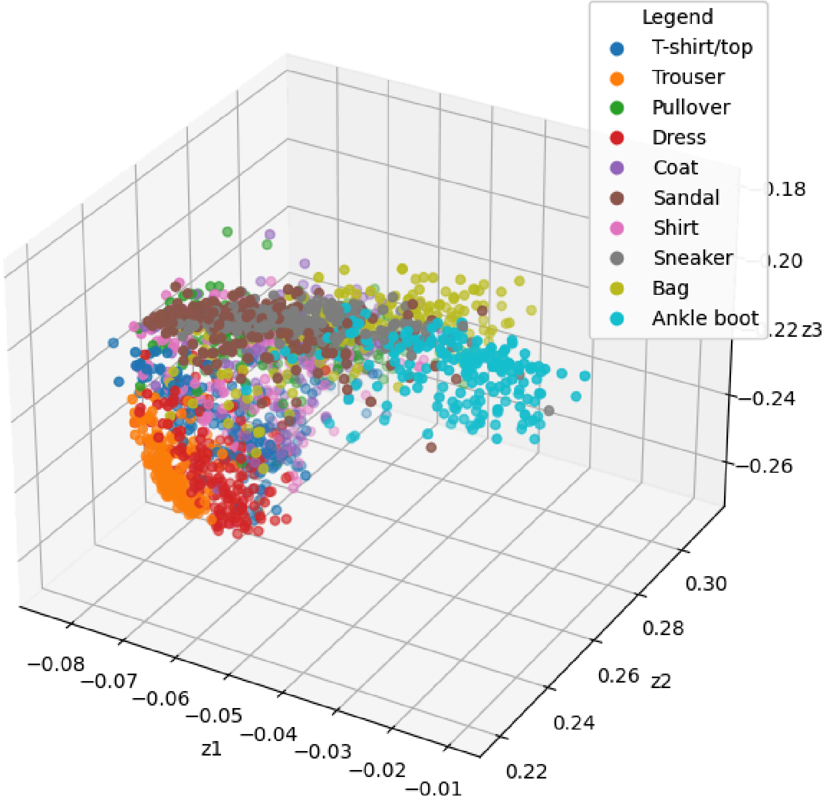
Back to the variational autoencoder

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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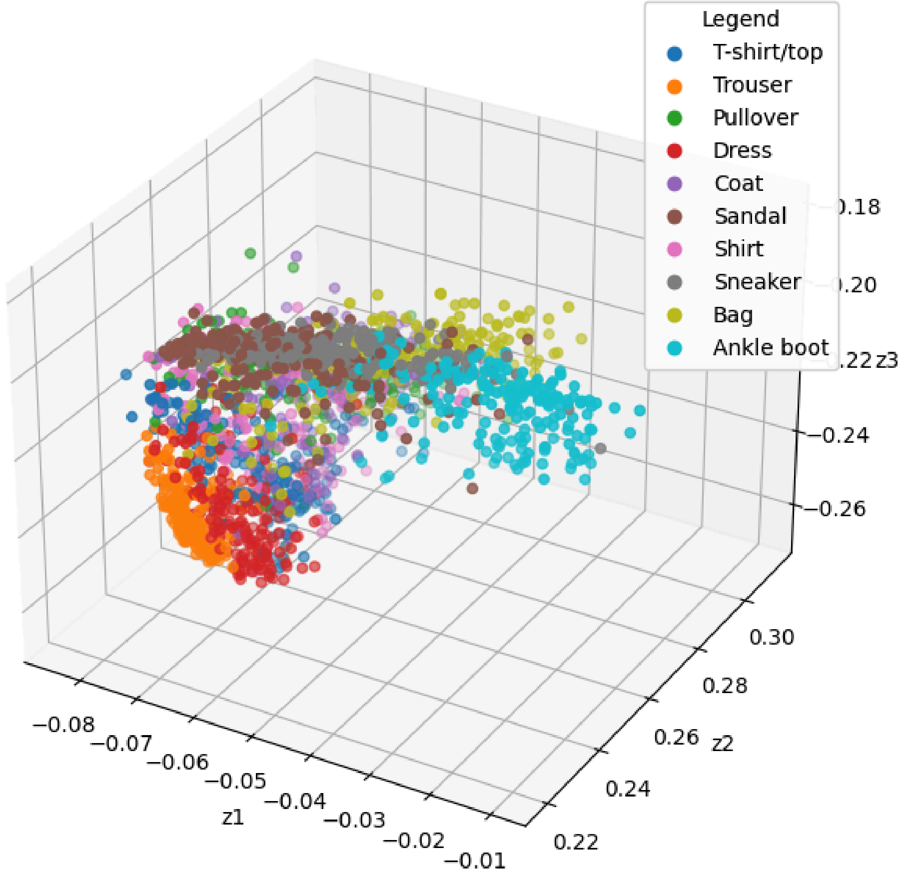
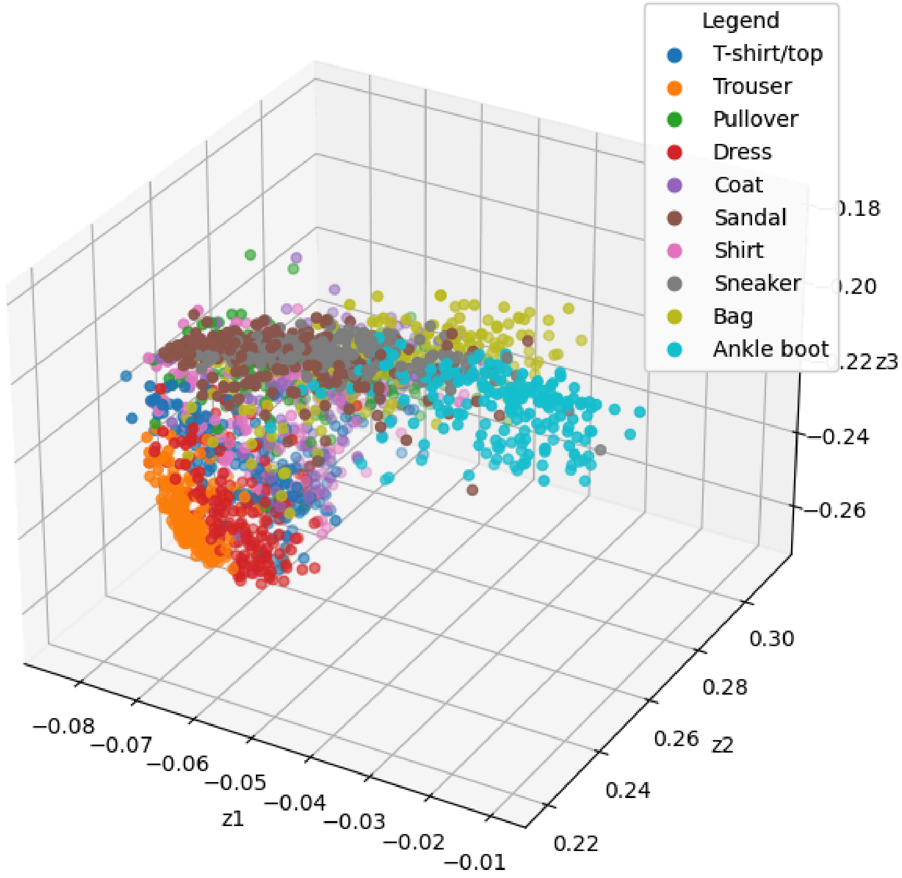


Autoencoder generative model:

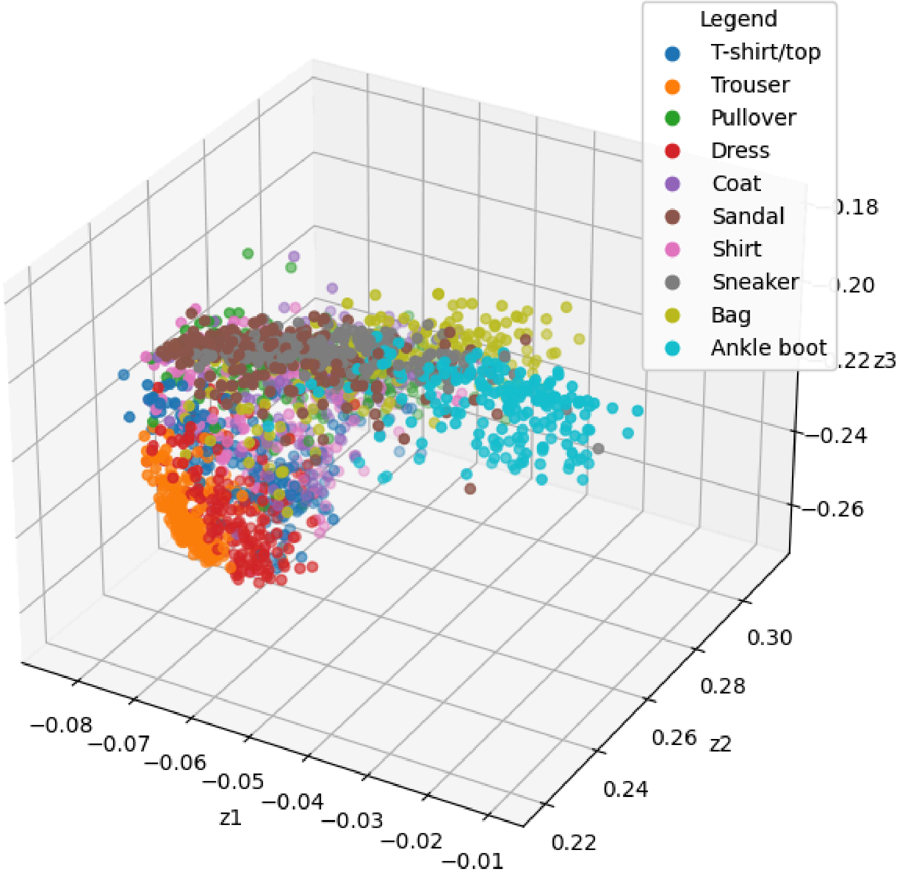
VAE Review and Coding



Autoencoder generative model:

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

VAE Review and Coding



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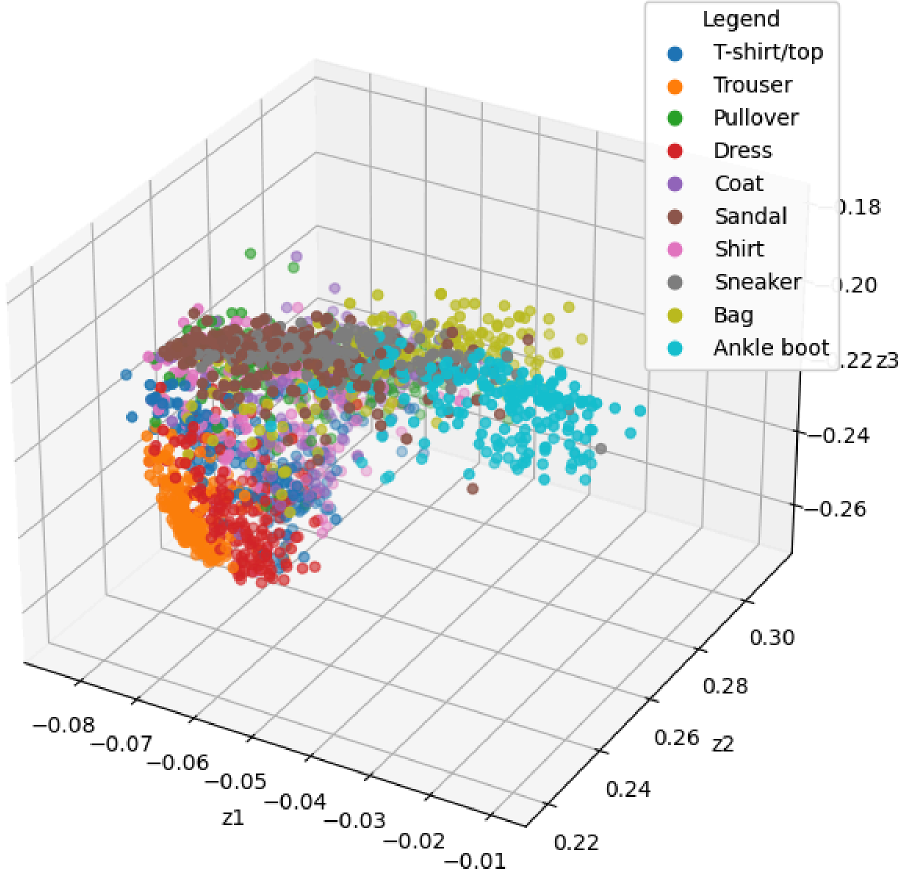
VAE Review and Coding



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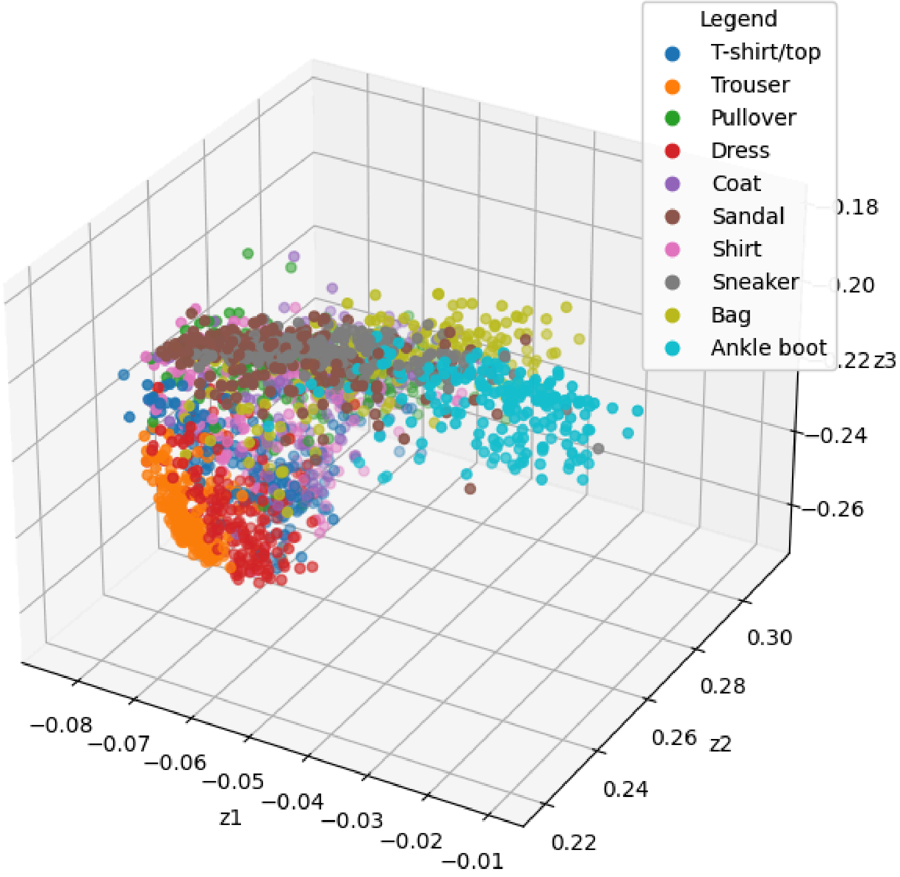
VAE Review and Coding



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

VAE Review and Coding

VAE Review and Coding

 

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

VAE Review and Coding

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

VAE Review and Coding

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As d_z increases, points move further and further apart

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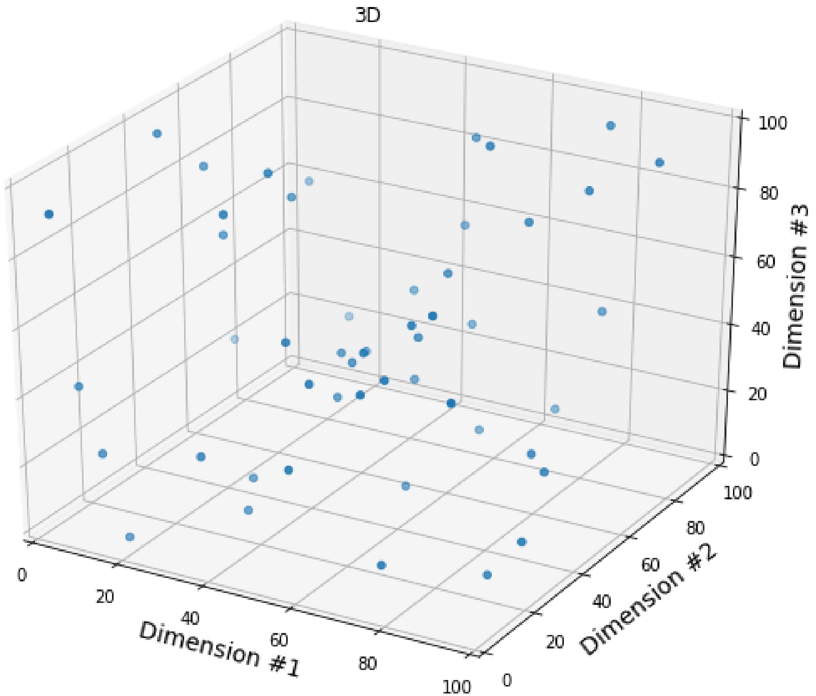

VAE Review and Coding

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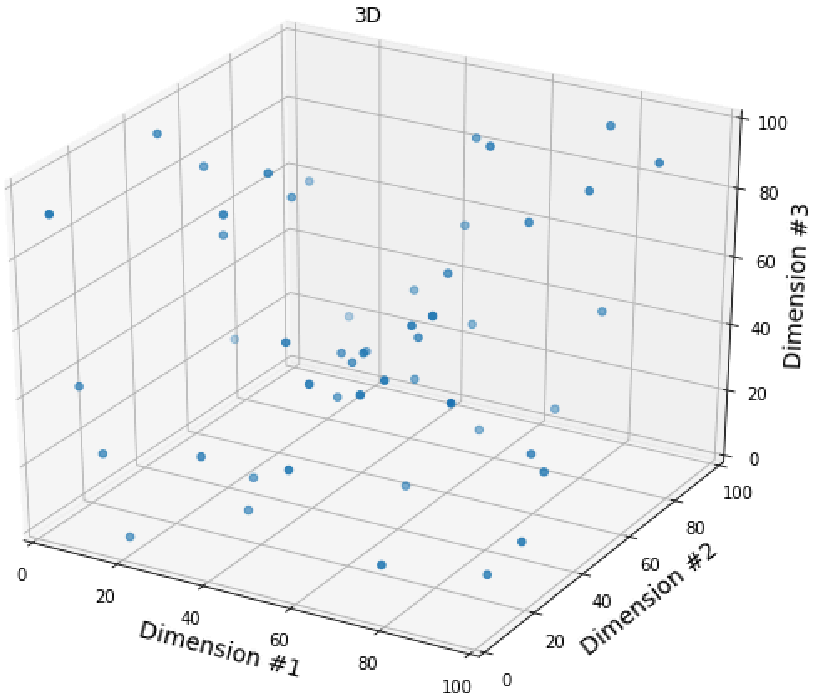

$f^{-1}(\boldsymbol{z} + \varepsilon)$ will produce either garbage, or $\boldsymbol{z}$

VAE Review and Coding

Variational autoencoders (VAEs) make $\boldsymbol{z}_{[1]}, ...\boldsymbol{z}_{[n]}$ normally distributed

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This keeps the point close together

VAE Review and Coding

Variational autoencoders (VAEs) make $\boldsymbol{z}_{[1]}, ...\boldsymbol{z}_{[n]}$ normally distributed

This keeps the point close together

We can sample new points $\boldsymbol{z}_{\text{new}} \sim N(\mathbf{0}, \mathbf{1})$

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

VAE Review and Coding

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

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

Given a prior distribution

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

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We want to approximate the dataset distribution

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

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We want to approximate the dataset distribution

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By approximating the marginal likelihood (from Bayes rule)

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

VAE Review and Coding

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

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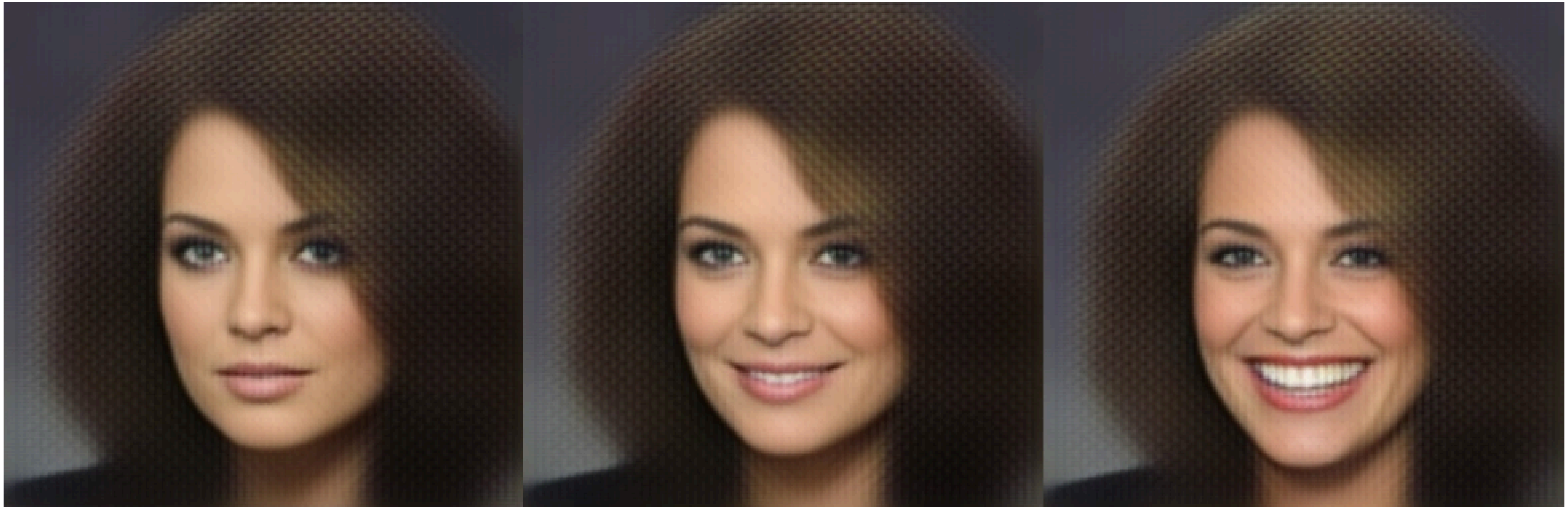
x :



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

VAE Review and Coding

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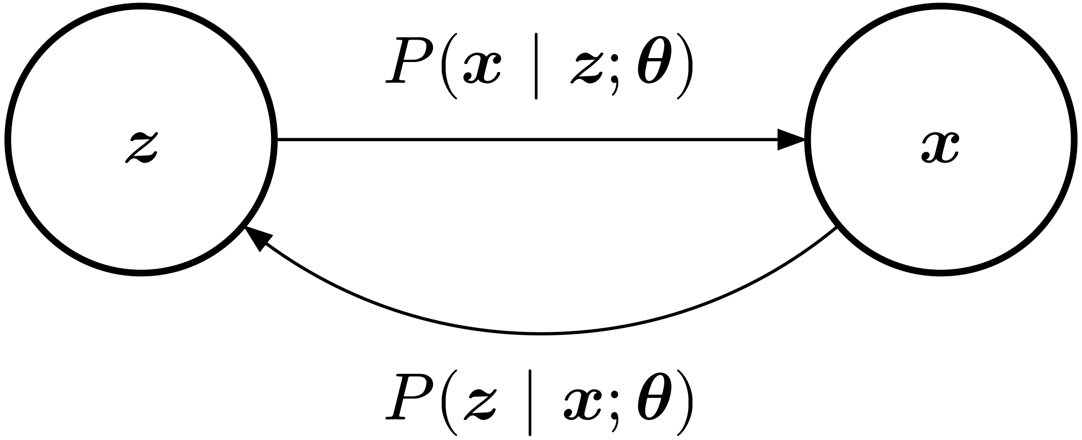

Decoder	Encoder
$P(\boldsymbol{x} \mid \boldsymbol{z}; \boldsymbol{\theta})$	$P(\boldsymbol{z} \mid \boldsymbol{x}; \boldsymbol{\theta})$
Generate new $\boldsymbol{x}$	Learn meaningful $\boldsymbol{z}$

VAE Review and Coding

How do we implement encoder 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(log_sigma))
```

VAE Review and Coding

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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 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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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)
```

VAE Review and Coding

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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, beta, 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 + beta * kl
```

VAE Review and Coding

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

https://colab.research.google.com/drive/1fwbkU46kvRWoisgIIZ2CFcynMReJsDUA

Show my results

https://openai.com/index/glow/

Agenda

1. GNN Review
2. **VAE Review and Coding**
3. Attention
4. Keys and Queries
5. Self Attention
6. Homework

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People use them for almost every task (even if they shouldn’t!)

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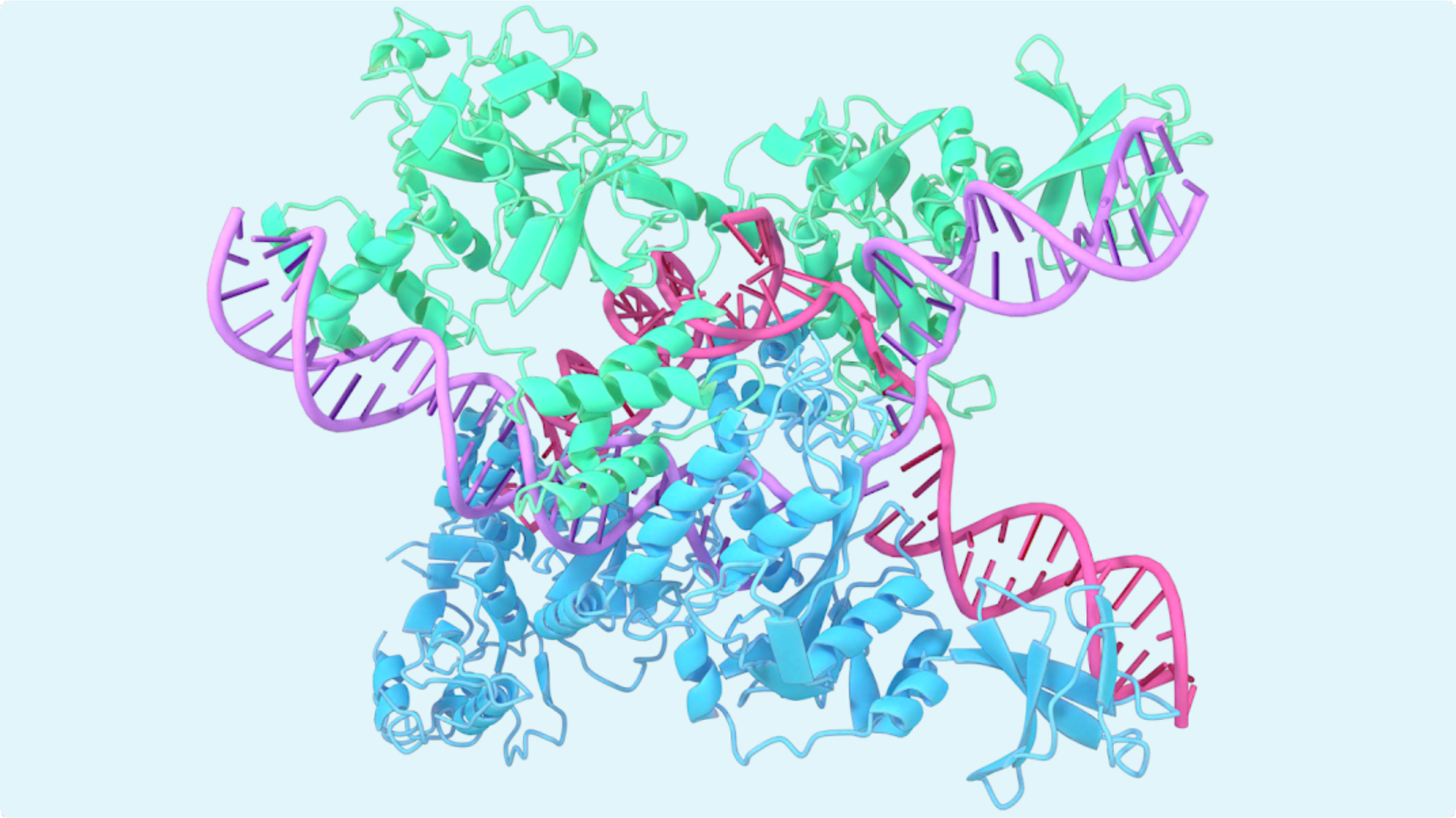
Let’s review some projects based on attention

Attention

AlphaFold (Nobel prize)

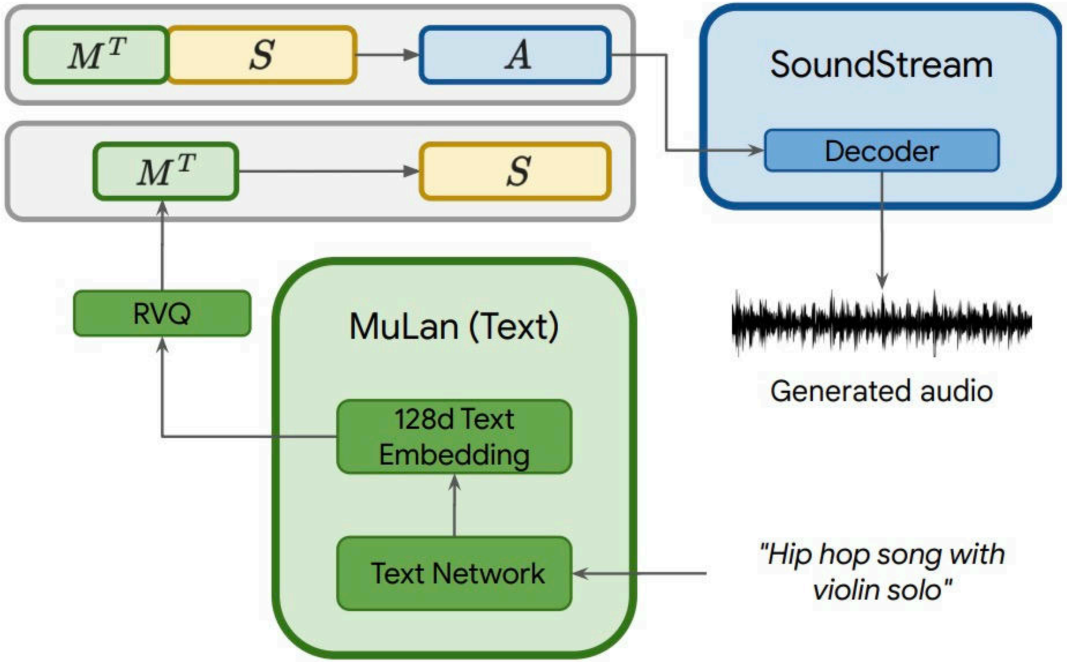


Attention

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

Attention

MusicTransformer, MuLan

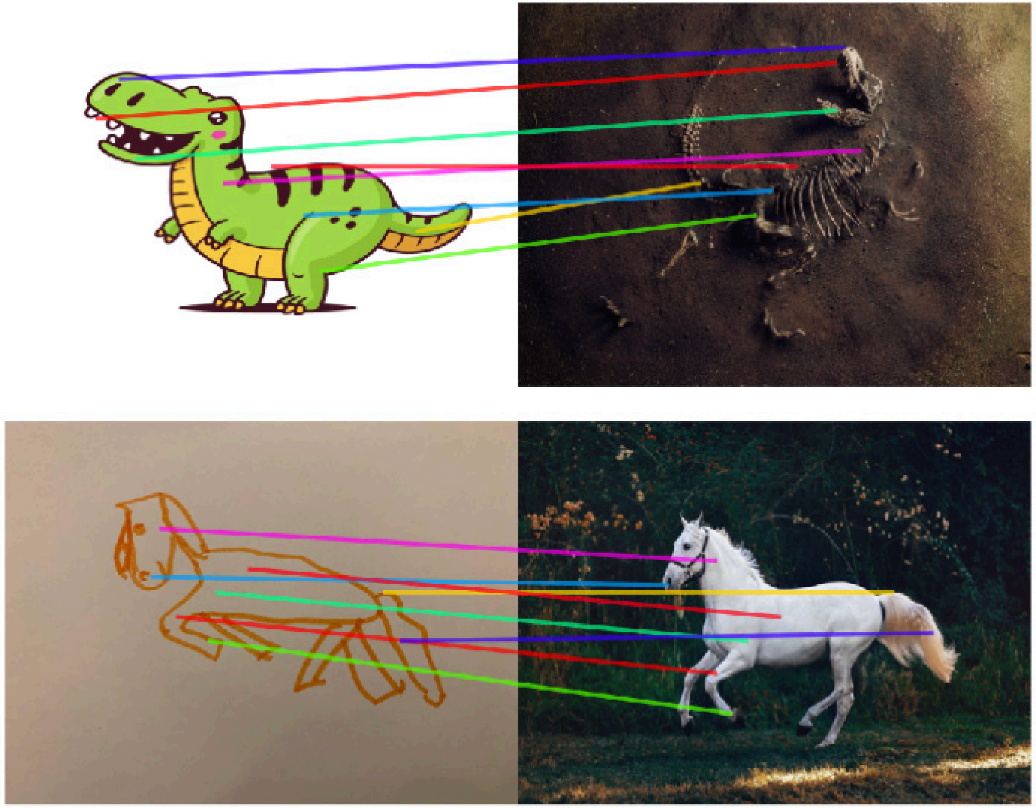


Attention

Google Translate, Baidu Translate, Apple Translate

Attention

ViT, DinoV2



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All these models are **transformers**

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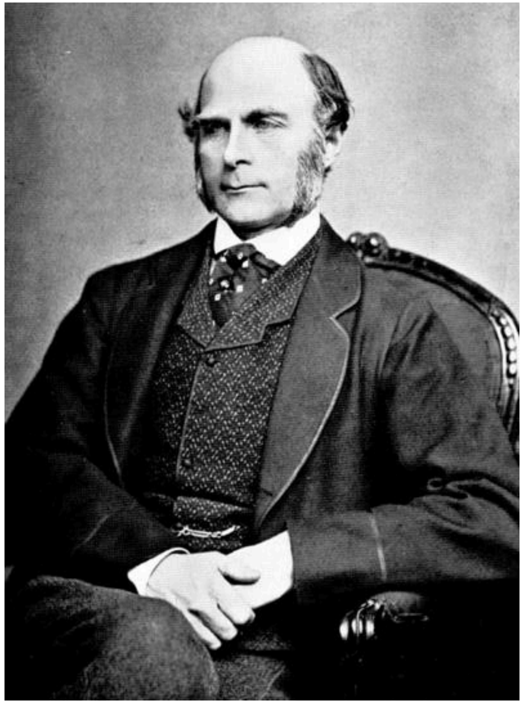
We can derive attention from composite memory

Attention

Francis Galton (1822-1911)
photo composite memory



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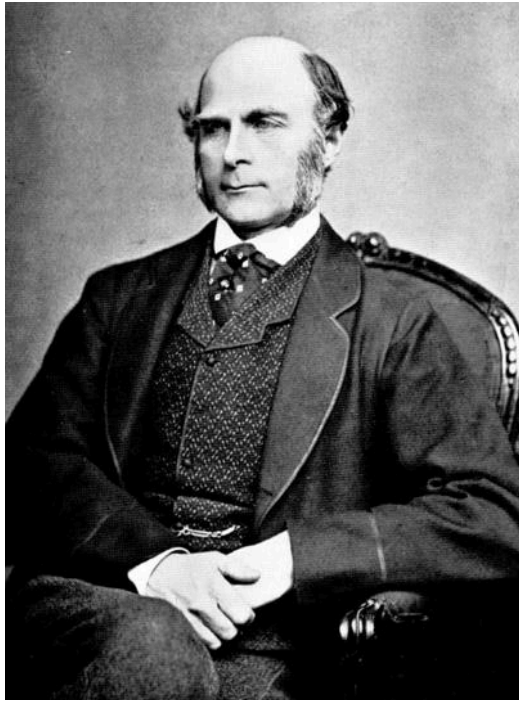
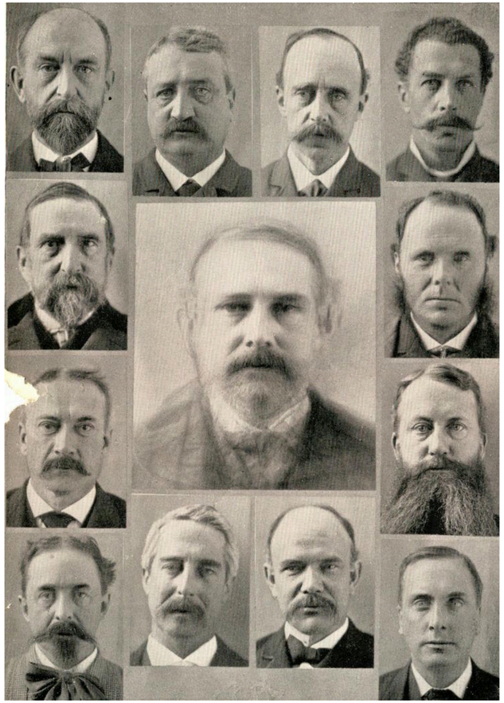


Composite photo of members of a party



Attention

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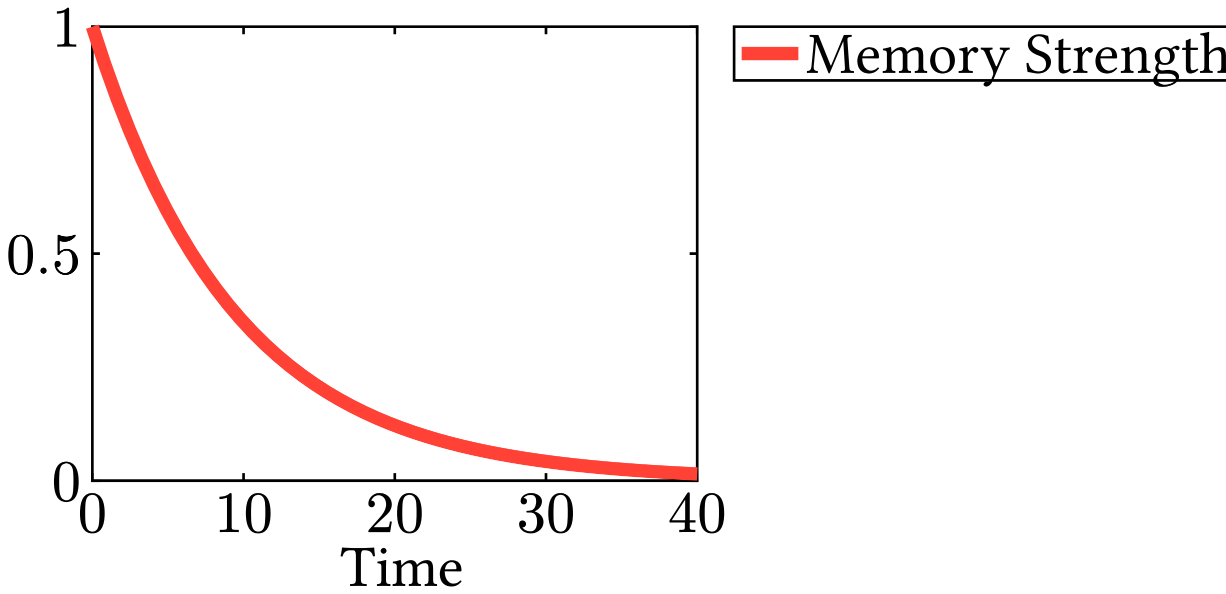

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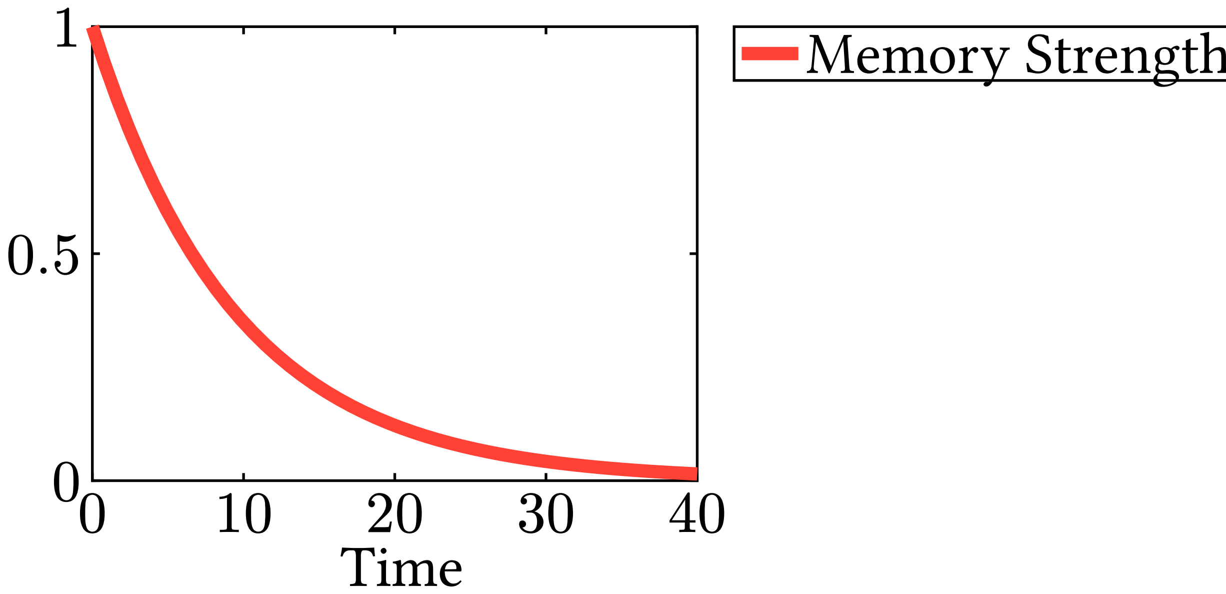

Question: Does this accurately model what **you** remember?

Attention

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10 PM 11 PM

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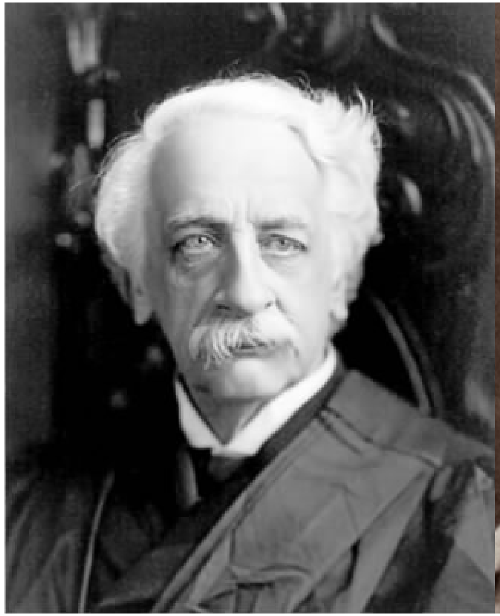
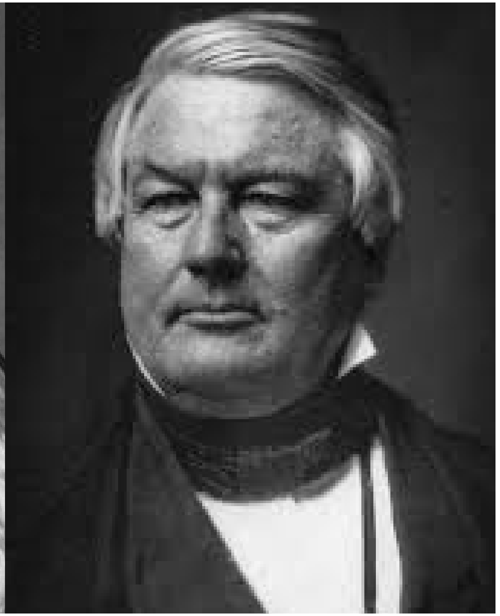


10 PM

11 PM

12 AM



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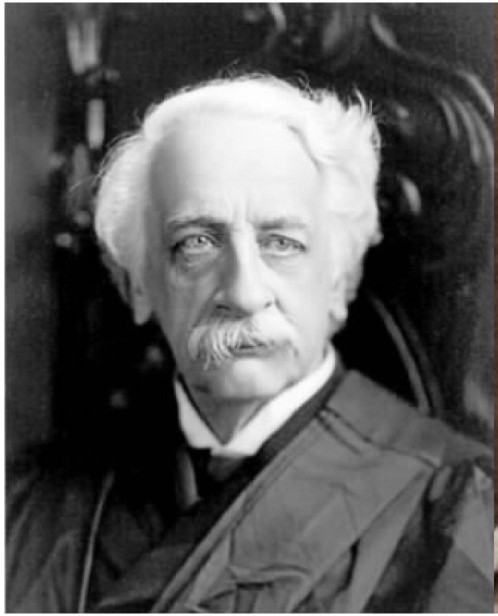


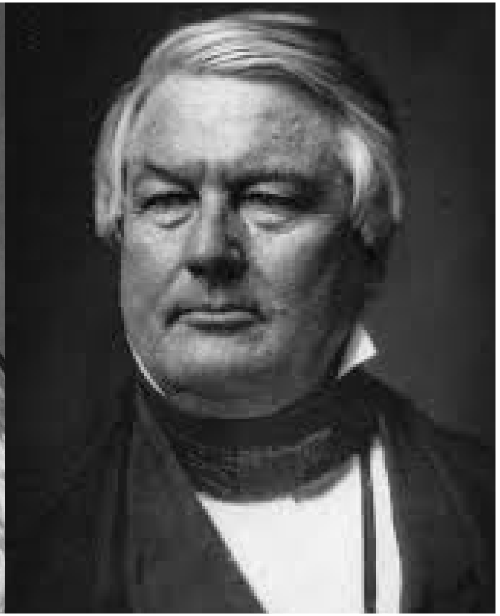

10 PM 11 PM 12 AM 1 AM

Attention

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Attention

Any questions before moving on?

Attention

Consider another party, with one more guest

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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

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We will forget meeting her!

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We will forget meeting her!

Question: Would you forget meeting Taylor Swift?

Attention

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Important memories persist longer than unimportant memories

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Important memories persist longer than unimportant memories

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

What does human memory actually look like?

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

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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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$$f_{\text{forget}}(\boldsymbol{x}, \boldsymbol{\theta}) = \sigma\left(\boldsymbol{\theta}_\lambda^\top \overline{\boldsymbol{x}}\right)$$

$$f(\boldsymbol{h}, \boldsymbol{x}, \boldsymbol{\theta}) = f_{\text{forget}}(\boldsymbol{x}, \boldsymbol{\theta}) \odot \boldsymbol{h} + \boldsymbol{\theta}_x^\top \overline{\boldsymbol{x}}$$

Attention

First, write our forgetting function with slightly different notation

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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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Only pay attention to important inputs

Attention

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

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Attention

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

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

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Question: What do the images look like now?

Attention

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

Question: What do the images look like now?

Attention

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!

Attention

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

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Question: How can we ensure that the attention sums to one?

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Question: How can we ensure that the attention sums to one?

Answer: Softmax!

Attention

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

Attention

Let us rewrite attention using softmax

Attention

Let us rewrite attention using softmax

The attention we pay to person i is

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

Attention

Attention

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

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

Attention

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

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

Attention

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

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

Attention

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

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

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

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

Attention

Attention

$$0.70 \cdot \boldsymbol{\theta}^\top \overline{\boldsymbol{x}}_1$$

Attention

$0.70 \cdot \boldsymbol{\theta}^\top \overline{\boldsymbol{x}}_1 \quad 0.04 \cdot \boldsymbol{\theta}^\top \overline{\boldsymbol{x}}_2$

Attention

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Attention

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

Attention

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

Attention

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

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

Attention

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

Attention

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Compute attention for all inputs at once

Attention

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

Attention

This is a simple form of attention

Attention

This is a simple form of attention

Next, we will investigate the attention used in transformers

Agenda

1. GNN Review
2. VAE Review and Coding
3. **Attention**
4. Keys and Queries
5. Self Attention
6. Homework

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Keys and Queries

The modern form of attention behaves like a database

Keys and Queries

The modern form of attention behaves like a database

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

Keys and Queries

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

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Keys and Queries

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

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Query: Which person will help me on my exam?

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Lawyer


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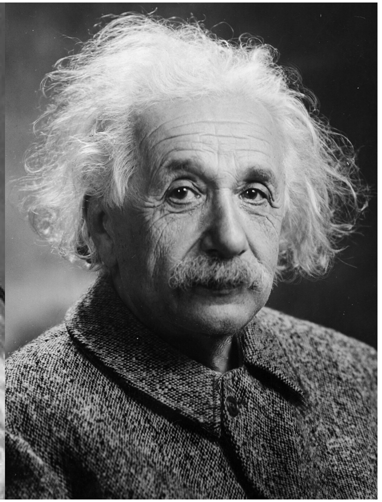
Chef


Scientist

Keys and Queries

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Query: Which person will help me on my exam?

Musician | Lawyer | Shopkeeper | Chef | Scientist

Keys and Queries

Query: I want to have fun

Keys and Queries

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Keys and Queries

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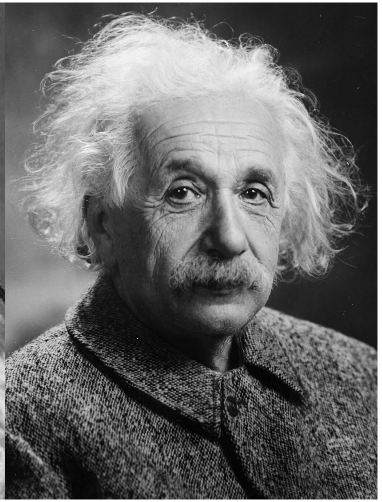

Scientist

Keys and Queries

Query: I want to have fun

Musician Lawyer Shopkeeper Chef Scientist

Keys and Queries

Query: I want to have fun

Musician   Lawyer   Shopkeeper   Chef   Scientist

How do we represent keys and queries mathematically?

Keys and Queries

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

Keys and Queries

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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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To determine if a key and query match, we will take the dot product

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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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Large dot product $\Rightarrow$ match! Small dot product $\Rightarrow$ no match.

Keys and Queries

Example:

Keys and Queries

Example:

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

Keys and Queries

Example:

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

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

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Example:

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Large attention!

Keys and Queries

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$$\boldsymbol{q}^\top \boldsymbol{k}_i = \left(\boldsymbol{\theta}_Q^\top \text{ Mathematician}\right)^\top \left(\boldsymbol{\theta}_K^\top\right.$$  $$\left.\right) = -50$$

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

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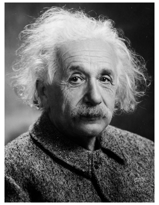
Small attention!

Keys and Queries

Example:

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

Keys and Queries

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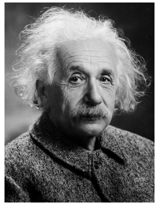
$$\boldsymbol{k}_i = \boldsymbol{\theta}_K^\top$$ 

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Keys and Queries

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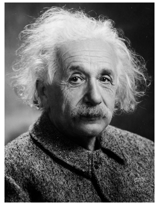
$\boldsymbol{k}_i = \boldsymbol{\theta}_K^\top$ 

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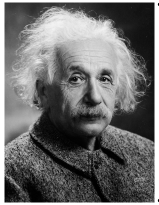
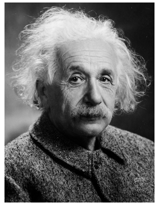
$\boldsymbol{q}^\top \boldsymbol{k}_i = \left(\boldsymbol{\theta}_Q^\top \text{ Mathematician}\right)^\top \Big(\boldsymbol{\theta}_K^\top$  $\Big) = 90$

Keys and Queries

Example:

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

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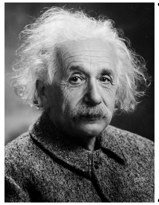
$\boldsymbol{q}^\top \boldsymbol{k}_i = \left(\boldsymbol{\theta}_Q^\top \text{ Mathematician}\right)^\top \left(\boldsymbol{\theta}_K^\top\right.$  $\left.\right) = 90$

Large attention!

Keys and Queries

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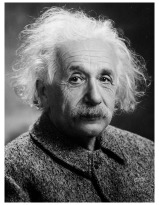
$$\boldsymbol{k}_i = \boldsymbol{\theta}_K^\top$$ 

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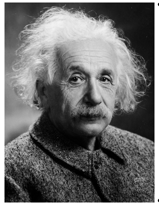
$$\boldsymbol{q}^\top \boldsymbol{k}_i = \left(\boldsymbol{\theta}_Q^\top \text{ Mathematician}\right)^\top \Bigg(\boldsymbol{\theta}_K^\top$$  $$\Bigg) = 90$$

Large attention!

Remember, there are multiple inputs to pay attention to

Keys and Queries

We compute a key for each input

$$\boldsymbol{K} = [\boldsymbol{k}_1 \ \ \boldsymbol{k}_2 \ \ \dots \ \ \boldsymbol{k}_T] = [\boldsymbol{\theta}_K^\top \boldsymbol{x}_1 \ \ \boldsymbol{\theta}_K^\top \boldsymbol{x}_2 \ \ \dots \ \ \boldsymbol{\theta}_K^\top \boldsymbol{x}_T], \quad \boldsymbol{K} \in \mathbb{R}^{d_h \times T}$$

Keys and Queries

We compute a key for each input

$$\boldsymbol{K} = [\boldsymbol{k}_1 \ \ \boldsymbol{k}_2 \ \ \ldots \ \ \boldsymbol{k}_T] = \left[\boldsymbol{\theta}_K^\top \boldsymbol{x}_1 \ \ \boldsymbol{\theta}_K^\top \boldsymbol{x}_2 \ \ \ldots \ \ \boldsymbol{\theta}_K^\top \boldsymbol{x}_T\right], \quad \boldsymbol{K} \in \mathbb{R}^{d_h \times T}$$

Keys and Queries

Then compute attention for each key

$$\boldsymbol{q}^\top \boldsymbol{K} = \boldsymbol{q}^\top [\boldsymbol{k}_1 \ \ \boldsymbol{k}_2 \ \ \dots \ \ \boldsymbol{k}_T] = [\boldsymbol{q}^\top \boldsymbol{k}_1 \ \ \boldsymbol{q}^\top \boldsymbol{k}_2 \ \ \dots \ \ \boldsymbol{q}^\top \boldsymbol{k}_T]$$

Keys and Queries

Then compute attention for each key

$$\boldsymbol{q}^\top \boldsymbol{K} = \boldsymbol{q}^\top [\boldsymbol{k}_1 \ \ \boldsymbol{k}_2 \ \ \ldots \ \ \boldsymbol{k}_T] = [\boldsymbol{q}^\top \boldsymbol{k}_1 \ \ \boldsymbol{q}^\top \boldsymbol{k}_2 \ \ \ldots \ \ \boldsymbol{q}^\top \boldsymbol{k}_T]$$

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Do not forget to normalize with softmax!

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

Agenda

1. GNN Review
2. VAE Review and Coding
3. Attention
4. **Keys and Queries**
5. Self Attention
6. Homework

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Self Attention

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

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

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This operation powers today's biggest models

Self Attention

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

$$\underbrace{\operatorname{attn}\left(\begin{bmatrix} \boldsymbol{x}_1 \\ \vdots \\ \boldsymbol{x}_T \end{bmatrix}, \boldsymbol{\theta} \right)}_{\mathbb{R}^{T \times d_h}} = \operatorname{softmax} \overbrace{\left(\frac{\boldsymbol{Q}\boldsymbol{K}^\top,}{\sqrt{d_h}} \right)}^{\mathbb{R}^{T \times T}} \underbrace{\boldsymbol{V}}_{\mathbb{R}^{T \times d_h}}$$

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Self Attention

```python
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).T / d_h, axis=1
        )
        return A @ self.theta_V(x)
```

Self Attention

Next lecture, we will create the transformer

Self Attention

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We will also discuss foundation models

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Homework

https://colab.research.google.com/drive/18VBb7sz0u8ul5vsFEJnQaepn0pQy4cUa?usp=sharing