Transformers

CISC 7026 - Introduction to Deep Learning

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Review

Review

Last time, we derived various forms of **attention**

We started with composite memory

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$$f(\boldsymbol{x}, \boldsymbol{\theta}) = \sum_{i=1}^{T} \boldsymbol{\theta}^\top \overline{\boldsymbol{x}}_i$$

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

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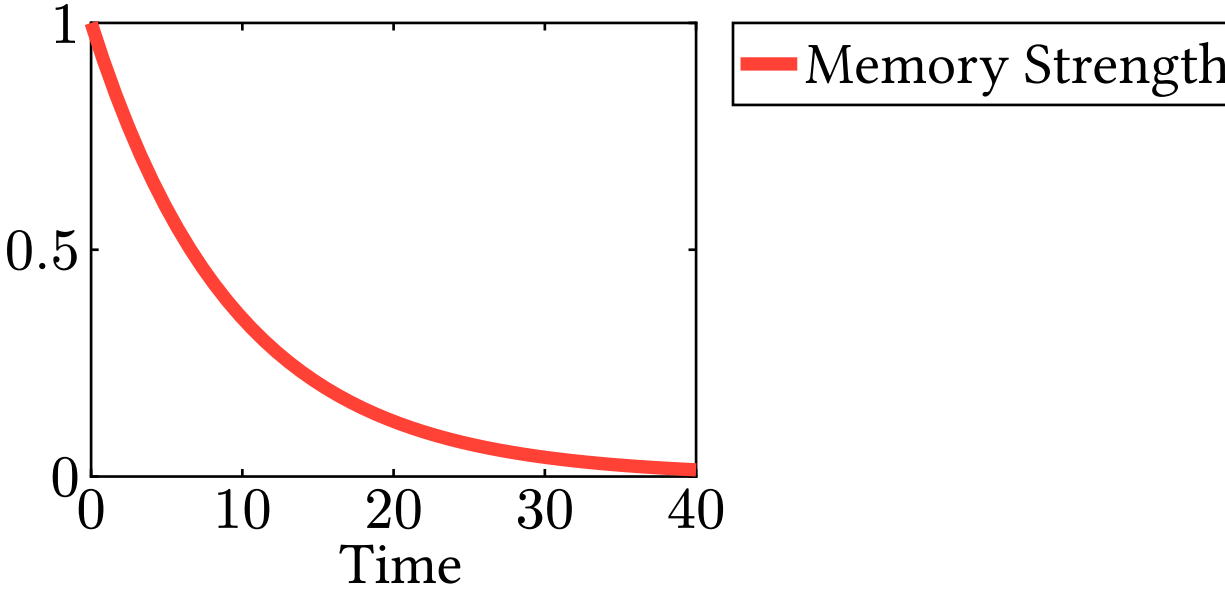

Review

We went to a party and the forgetting seemed ok

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10 PM

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10 PM 11 PM

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

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But we encountered problems when Taylor Swift arrived at the party

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But we encountered problems when Taylor Swift arrived at the party

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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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With our current model, we forget Taylor Swift!

Our model of human memory is incomplete

Review

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Last time we studied attention

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Overview of transformer application and domains

Going Deeper

Going Deeper

We previously reviewed training tricks

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We previously reviewed training tricks

- Deeper networks

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- Parameter initialization

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- Weight decay

Going Deeper

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- Deeper networks
- Parameter initialization
- Stochastic gradient descent
- Adaptive optimization
- Weight decay

These methods empirically improve performance, but we do not always understand why

Going Deeper

Modern transformers can be very deep

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For this reason, they use two new training tricks to enable very deep models

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Let us introduce these tricks

We will start with the **residual connection**

Going Deeper

Remember that a two-layer MLP is a universal function approximator

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$$\mid f(\boldsymbol{x}, \boldsymbol{\theta}) - g(\boldsymbol{x}) \mid < \varepsilon$$

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For certain problems, we need deeper networks

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Making the network too deep can hurt performance

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The theory is that the input information is **lost** somewhere in the network

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Making the network too deep can hurt performance

The theory is that the input information is **lost** somewhere in the network

$$\boldsymbol{y} = f_k(...f_2(f_1(\boldsymbol{x}, \boldsymbol{\theta}_1), \boldsymbol{\theta_2}), ..., \boldsymbol{\theta}_k)$$

Going Deeper

$$\boldsymbol{y} = f_k(...f_2(f_1(\boldsymbol{x}, \boldsymbol{\theta}_1), \boldsymbol{\theta_2}), ..., \boldsymbol{\theta}_k)$$

Claim: If the input information is present throughout the network, then we should be able to learn the identity function $f(x) = x$

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Question: We have seen a similar model, what was it?

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Question: We have seen a similar model, what was it?

Question: Do you agree or disagree with the claim?

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https://colab.research.google.com/drive/1qVIbQKpTuBYIa7FvC4IH-kJq-E0jmc0d#scrollTo=bg74S-AvbmJz

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Very deep networks struggle to learn the identity function

Going Deeper

$$\boldsymbol{x} = f_k(...f_2(f_1(\boldsymbol{x}, \boldsymbol{\theta}_1), \boldsymbol{\theta_2}), ..., \boldsymbol{\theta}_k)$$

Very deep networks struggle to learn the identity function

If the input information is available, then learning the identity function should be very easy!

Question: How can we prevent the input from getting lost?

Going Deeper

We can feed the input to each layer

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The first approach is called the **DenseNet** approach

Going Deeper

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\begin{aligned}
\boldsymbol{z}_1 &= f_1(\boldsymbol{x}, \boldsymbol{\theta}_1) \\
\boldsymbol{z}_2 &= f_2\left(\begin{bmatrix}\boldsymbol{x} \\ \boldsymbol{z}_1\end{bmatrix}, \boldsymbol{\theta}_2\right) \\
&\vdots \\
\boldsymbol{z}_k &= f_k\left(\begin{bmatrix}\boldsymbol{x} \\ \boldsymbol{z}_1 \\ \vdots \\ \boldsymbol{z}_{k-1}\end{bmatrix}, \boldsymbol{\theta}_k\right)
\end{aligned}
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Going Deeper

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Question: Any issues with the DenseNet approach?

Answer: Very deep networks require too many parameters!

Going Deeper

The next method is called the **ResNet** approach

$$
\begin{aligned}
\boldsymbol{z}_1 &= f_1(\boldsymbol{x}, \boldsymbol{\theta}_1) \\
\boldsymbol{z}_2 &= f_2(\boldsymbol{x}, \boldsymbol{\theta}_2) + \boldsymbol{x} \\
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For example, for an identity function we can easily learn

$$f(\boldsymbol{x}, \boldsymbol{\theta}) = 0; \quad f(\boldsymbol{x}, \boldsymbol{\theta}) + x = x$$

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This helps prevent information from getting lost in very deep networks

Going Deeper

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But we can still have very small or very large outputs from each layer

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$$f_1(\boldsymbol{x}, \boldsymbol{\theta}_1) = \sum_{i=1}^{d_x} \theta_{1,i} x_i$$

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$$f_1(\boldsymbol{x}, \boldsymbol{\theta}_1) = \sum_{i=1}^{d_x} \theta_{1,i} x_i$$

Question: If all $x_i = 1$, $\theta_{1,i} = 0.01$ and $d_x = 1000$, what is the output?

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What if we add another layer with the same d_x and θ?

$$f_2(\boldsymbol{z}, \boldsymbol{\theta}_2) = \sum_{i=1}^{1000} 0.01 \cdot 10 = 100$$

Going Deeper

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What if we add another layer with the same d_x and θ?

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Question: What is the problem?

Going Deeper

Let us look at the gradient

Going Deeper

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$$\nabla_{\boldsymbol{\theta}_1} f_2(f_1(\boldsymbol{x}, \boldsymbol{\theta}_1), \boldsymbol{\theta}_2) =$$

Going Deeper

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$$\nabla_{\boldsymbol{\theta}_1} f_2(f_1(\boldsymbol{x}, \boldsymbol{\theta}_1), \boldsymbol{\theta}_2) = \nabla_{\boldsymbol{\theta}_1}[f_2](f_1(\boldsymbol{x}, \boldsymbol{\theta}_1)) \cdot \nabla_{\boldsymbol{\theta}_1}[f_1](\boldsymbol{x}, \boldsymbol{\theta}_1)$$

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$$\approx 100 \cdot 10$$

Can cause exploding or vanishing gradient

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Can cause exploding or vanishing gradient

Deeper network $\Rightarrow$ worse exploding/vanishing issues

Question: What can we do?

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Let us look at the gradient

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First, layer normalization **centers** the output of the layer

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First, layer normalization **centers** the output of the layer

$$\mu = d_y \sum_{i=1}^{d_y} f(\boldsymbol{x}, \boldsymbol{\theta})_i$$

$$f(\boldsymbol{x}, \boldsymbol{\theta}) - \mu$$

Question: What does this do?

Going Deeper

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Question: What does this do?

Answer: Makes output have zero mean (both positive and negative values)

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Question: What does this do?

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$$\mu = d_y \sum_{i=1}^{d_y} f(\boldsymbol{x}, \boldsymbol{\theta})_i \qquad\qquad f(\boldsymbol{x}, \boldsymbol{\theta}) - \mu$$

Then, layer normalization **rescales** the outputs

$$\sigma = \frac{\sqrt{\sum_{i=1}^{d_y} f(\boldsymbol{x}, \boldsymbol{\theta}_i - \mu)^2}}{d_y}$$

$$\mathrm{LN}(f(\boldsymbol{x}, \boldsymbol{\theta})) = \frac{f(\boldsymbol{x}, \boldsymbol{\theta}) - \mu}{\sigma}$$

Now, the output of the layer is normally distributed

Going Deeper

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- 99.7% of outputs $\in [-3, 3]$

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Going Deeper

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- 99.99% of outputs $\in [-4, 4]$
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This helps prevent vanishing and exploding gradients

Going Deeper

Now, let's combine residual connections and layer norm and try our very deep network again

TODO COLAB

Transformers

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Now we have everything we need to implement a transformer

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- Attention

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A deep neural network consists of many layers

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A deep neural network consists of many layers

A transformer consists of many **transformer blocks**

Transformers

```
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):
        x = self.norm1(self.attn(x) + x)
        x = self.norm2(self.mlp(x) + x)
        return x
```

Transformers

```
class Transformer(nn.Module):
    def __init__(self):
        self.block1 = TransformerBlock()
        self.block2 = TransformerBlock()
        self.block3 = TransformerBlock()

    def forward(self, x):
        x = self.block1(x)
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Question: What are the input/output shapes of the transformer?

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```

Question: What are the input/output shapes of the transformer?

Answer: $f : \mathbb{R}^{T \times d_x} \mapsto \mathbb{R}^{T \times d_h}$

Positional Encoding

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Our transformer maps T inputs to T outputs

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Our transformer maps T inputs to T outputs

- T words in a sentence

Positional Encoding

Our transformer maps T inputs to T outputs

- T words in a sentence
- T pixels in an image

Positional Encoding

Our transformer maps T inputs to T outputs

- T words in a sentence
- T pixels in an image
- T amino acids in a protein

Positional Encoding

Our transformer maps T inputs to T outputs

- T words in a sentence
- T pixels in an image
- T amino acids in a protein

Question: Does the order of the T inputs matter?

Positional Encoding

Our transformer maps T inputs to T outputs

- T words in a sentence
- T pixels in an image
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Question: Does the order of the T inputs matter?

Answer: In some tasks, yes! In others, no

Positional Encoding

Question: Detecting birds in an image of T pixels, does order matter?

Positional Encoding

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Positional Encoding

Question: T robots searching for an object. Does order matter?

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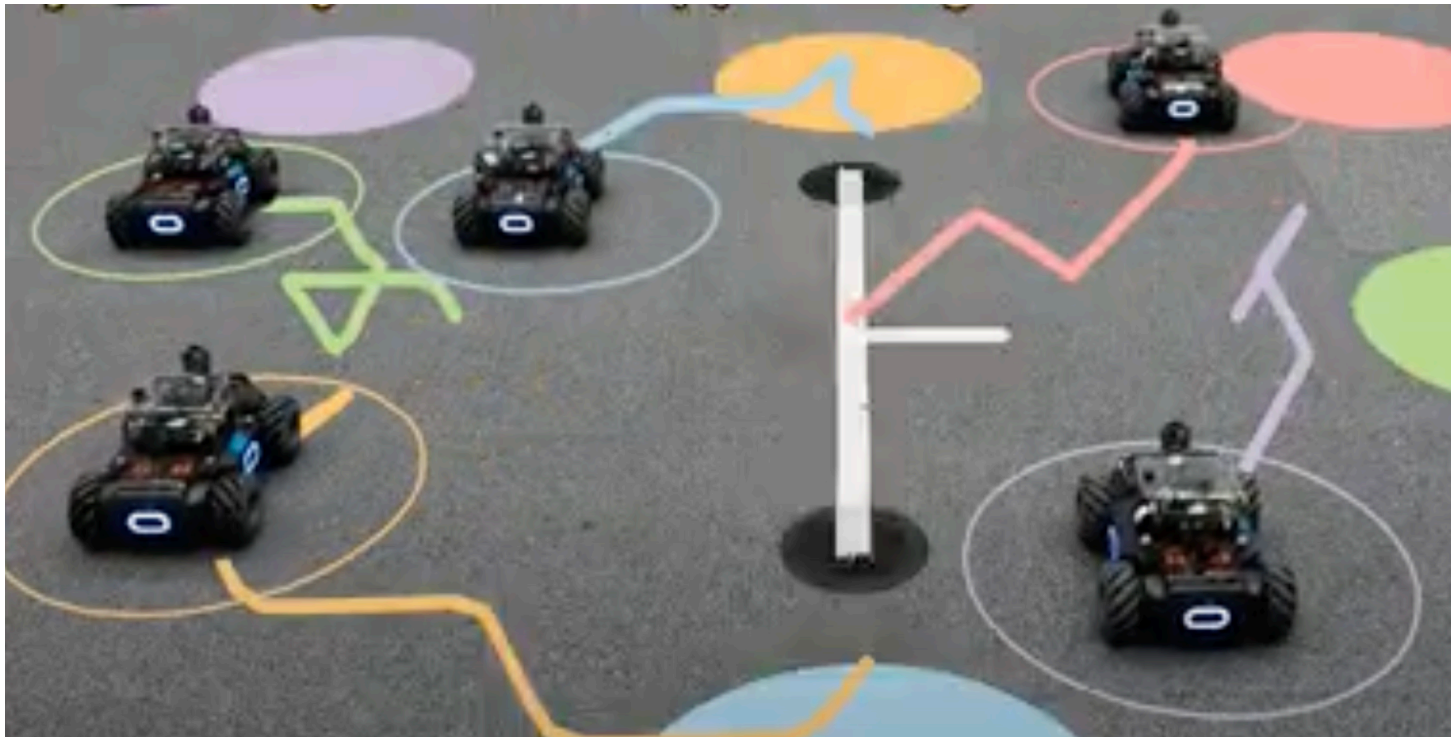

Positional Encoding

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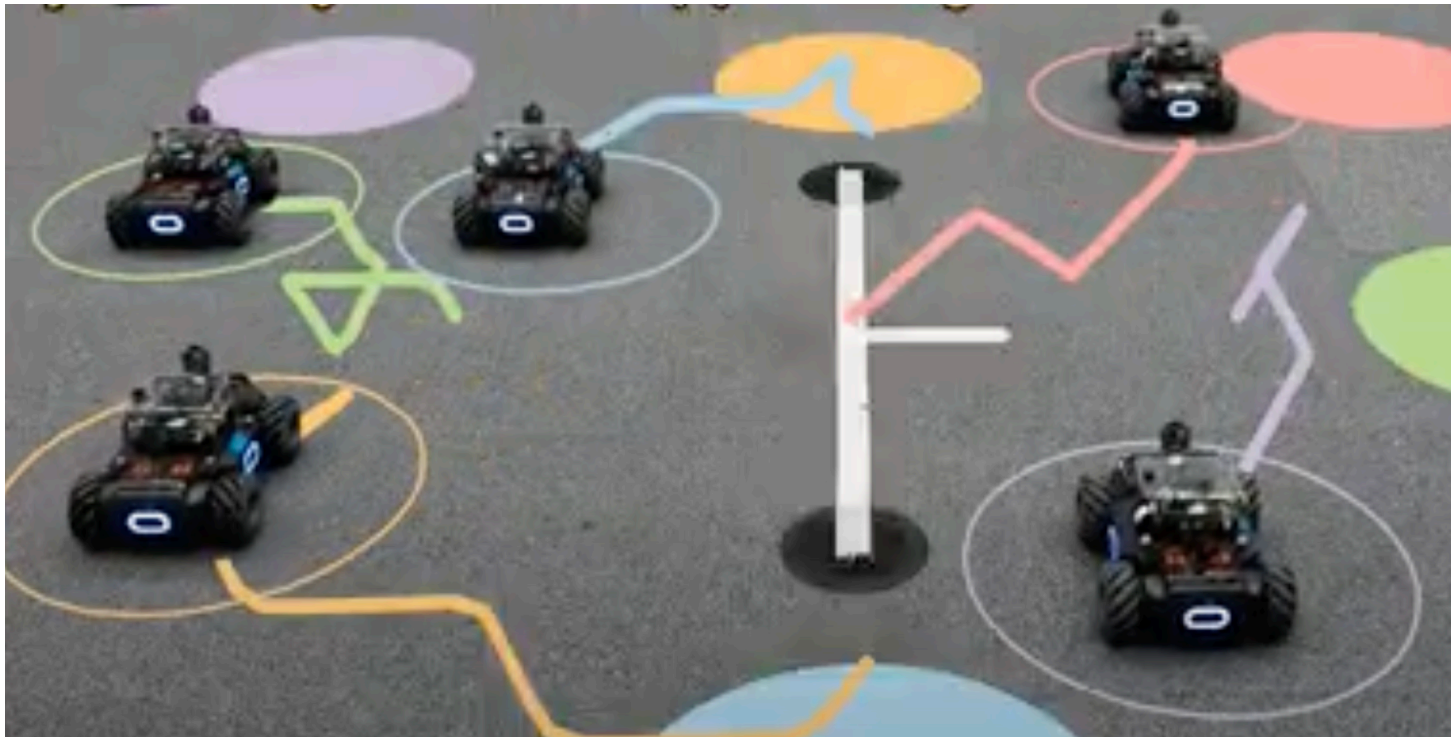

Answer: No!

Positional Encoding

Question: We translate a sentence containing T words. Does order matter?

$$\begin{bmatrix} \boldsymbol{x}_1 \\ \boldsymbol{x}_2 \\ \boldsymbol{x}_3 \\ \boldsymbol{x}_4 \\ \boldsymbol{x}_5 \end{bmatrix} = \begin{bmatrix} \text{The} \\ \text{dog} \\ \text{licks} \\ \text{the} \\ \text{owner} \end{bmatrix}$$

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Answer: Yes!

Positional Encoding

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Question: Does the transformer know the order of the T inputs?

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Define a **permutation matrix** $\boldsymbol{P} \in \{0,1\}^{T \times T}$ that reorders the inputs

Positional Encoding

For some tasks, we must know the order of the inputs

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Positional Encoding

Example 1:

$$P = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}; \quad a = \begin{bmatrix} 3 \\ 4 \\ 5 \end{bmatrix};$$

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Positional Encoding

$$f\left(\boldsymbol{P}\begin{bmatrix}\boldsymbol{x}_1\\ \vdots \\ \boldsymbol{x}_n\end{bmatrix}\right) = \boldsymbol{P}f\left(\begin{bmatrix}\boldsymbol{x}_1\\ \vdots \\ \boldsymbol{x}_n\end{bmatrix}\right)$$

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Which is a transformer?

Positional Encoding

Recall dot product self attention

Positional Encoding

Recall dot product self attention

$$\boldsymbol{Q} = [\boldsymbol{q}_1 \;\; \boldsymbol{q}_2 \;\; \ldots \;\; \boldsymbol{q}_T] = \left[\boldsymbol{\theta}_Q^\top \boldsymbol{x}_1 \;\; \boldsymbol{\theta}_Q^\top \boldsymbol{x}_2 \;\; \ldots \;\; \boldsymbol{\theta}_Q^\top \boldsymbol{x}_T\right]$$

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$$\boldsymbol{V} = [\boldsymbol{v}_1 \;\; \boldsymbol{v}_2 \;\; \ldots \;\; \boldsymbol{v}_T] = \left[\boldsymbol{\theta}_V^\top \boldsymbol{x}_1 \;\; \boldsymbol{\theta}_V^\top \boldsymbol{x}_2 \;\; \ldots \;\; \boldsymbol{\theta}_V^\top \boldsymbol{x}_T\right]$$

Positional Encoding

Recall dot product self attention

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$$\text{attn}\left(\begin{bmatrix}\boldsymbol{x}_1 \\ \vdots \\ \boldsymbol{x}_T\end{bmatrix}, \boldsymbol{\theta}\right) = \text{softmax}\left(\frac{\boldsymbol{Q}\boldsymbol{K}^\top}{\sqrt{d_h}}\right)\boldsymbol{V}$$

Positional Encoding

$$\text{attn}\left(\boldsymbol{P}\begin{bmatrix}\boldsymbol{x}_1\\ \vdots \\ \boldsymbol{x}_T\end{bmatrix}, \boldsymbol{\theta}\right) = \text{softmax}\left(\frac{(\boldsymbol{PQ})(\boldsymbol{PK})^\top}{\sqrt{d_h}}\right)(\boldsymbol{PV})$$

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Question: What does this mean?

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Question: What does this mean?

Answer: Attention is equivariant, order **does not** matter

Positional Encoding

Transformer cannot determine order of inputs! **Equivariant** to ordering

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The following sentences are the same to a transformer

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This is a problem! For some tasks, we care about input order

Text Transformers

Image Transformers

Unsupervised Training

Unsupervised Training

Predict the future

World Models

World Models

What if transformers could interact with the world?

Course Evaluation

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Department instructed me to ask you for course feedback

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We take this feedback seriously

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Your feedback will impact future courses (and my job)

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Please scan the QR code and complete the survey

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https://isw.um.edu.mo/siaweb

Course Evaluation

Research data labeling and collection

If you participated, come up