Transformers and Large Language Models

COMP 4630 | Winter 2025

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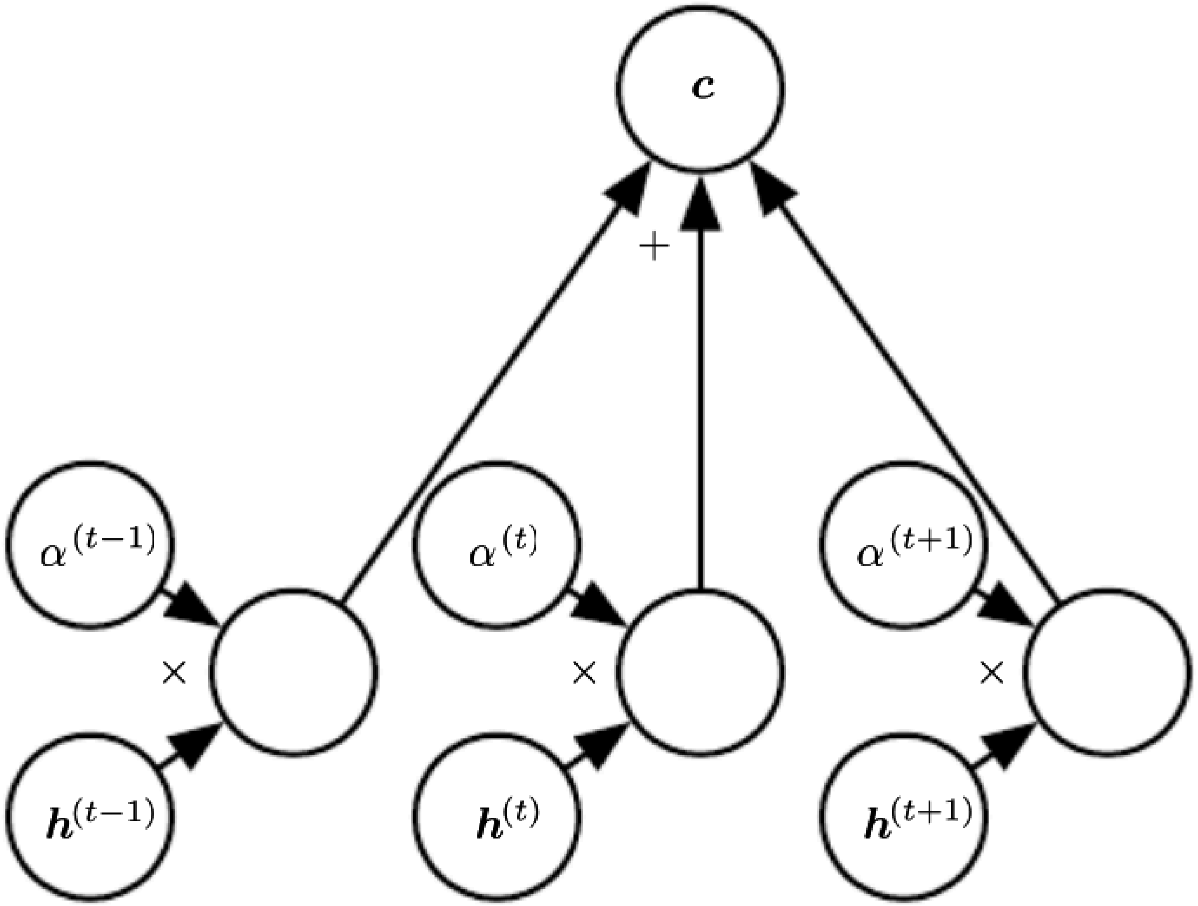
Overview

- Attention mechanisms
- Transformers and large language models
    - Multi-head attention, positional encoding, and magic
    - BERT, GPT, Llama, etc.
- References and suggested readings:
    - Scikit-learn book: Chapter 16
    - d2l.ai: Chapter 11

Attention Overview

- Basically a weighted average of the encoder states, called the **context**
- Weights α usually come from a softmax layer
- ❓ what does the use of softmax tell us about the weights?



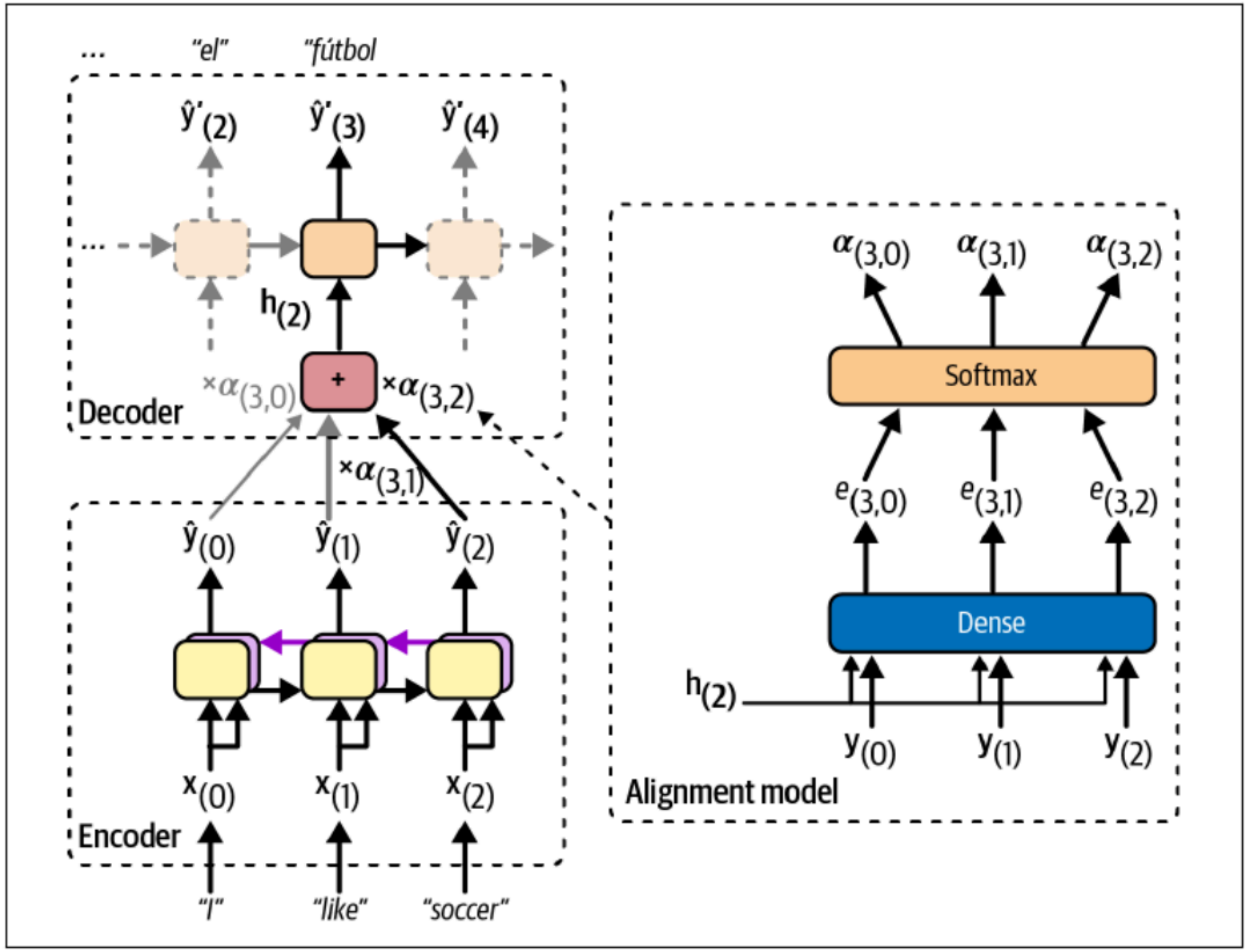


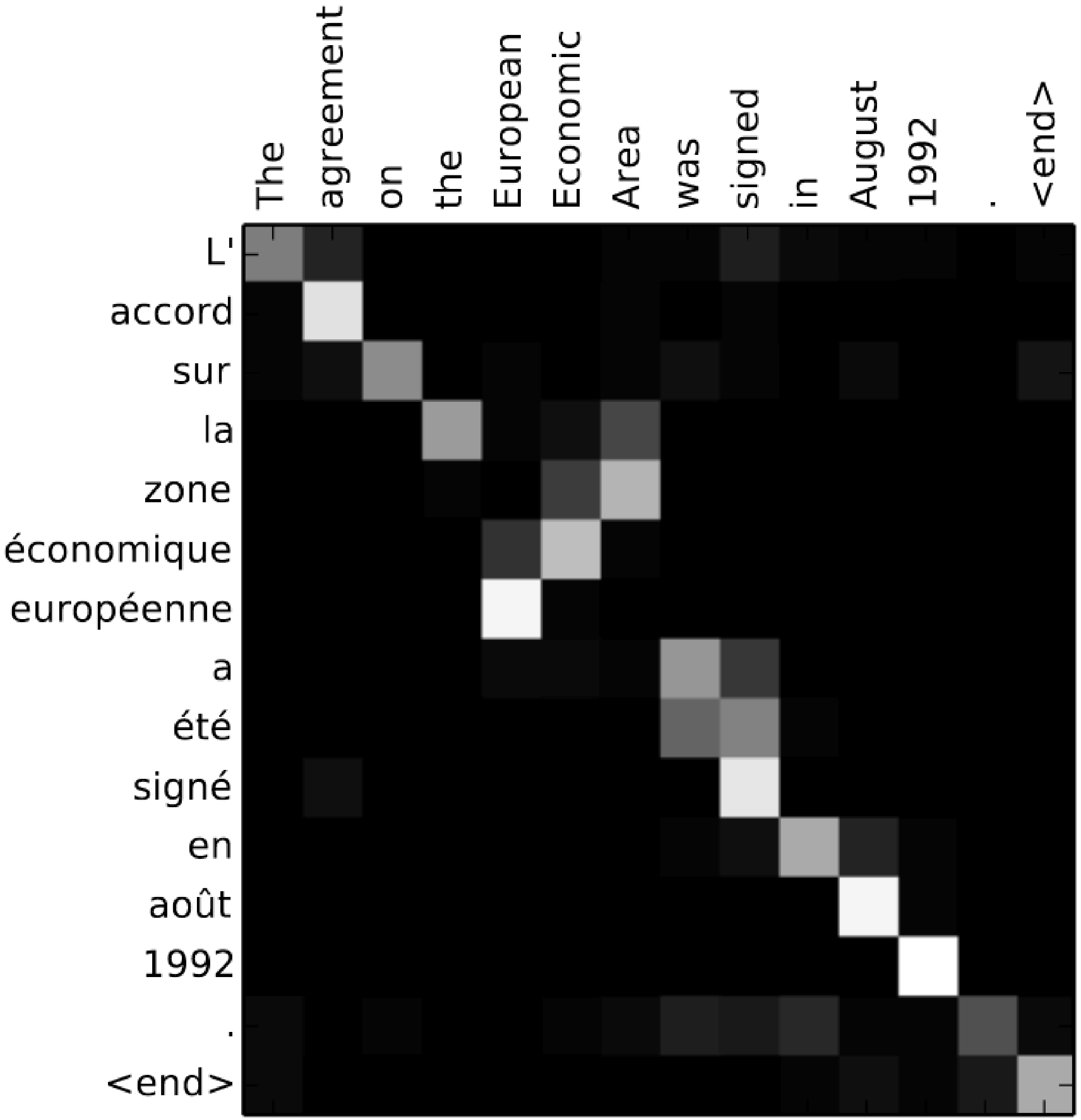
Figure 16-7. Neural machine translation using an encoder–decoder network with an attention model

Encoder-Decoder with Attention

- The **alignment model** is used to calculate attention weights
- The context vector changes at each time step!

Attention Example

- Attention weights can be visualized as a heatmap
- ❓ What can you infer from this heatmap?



The math version

The context vector $\mathbf{c}_t$ at each step t is computed from the alignment weights as:

$$\mathbf{c}_t = \sum_{i=1}^{n} \alpha_{ti} \mathbf{y}_i$$

where $\mathbf{y}_i$ is the encoder output at step i and α_{ti} is computed as:

$$\alpha_{ti} = \frac{\exp(e_{ti})}{\sum_{k=1}^{n} \exp(e_{tk})},$$

where e_{ti} is the **alignment score** or **energy** between the decoder hidden state at step t and the encoder output at step i.

Different kinds of attention

- The original Bahdanau attention (2014) model:

$$e_{ij} = \mathbf{v}_a^T \tanh(\mathbf{W}_a \mathbf{h}_{i-1} + \mathbf{U}_a \mathbf{y}_j)$$

  where $\mathbf{v}_a$, $\mathbf{W}_a$, and $\mathbf{U}_a$ are learned parameters

- Luong attention (2015), where the encoder outputs are **multiplied** by the decoder hidden state (dot product) at the **current step**

$$e_{ti} = \mathbf{h}_t^T \mathbf{y}_i$$

- ❓ What might be a benefit of dot-product attention?

Attention is all you need

- Some Googlers wanted to ditch RNNs
- If they can eliminate the sequential nature of the model, they can **parallelize** training on their massive GPU (TPU) clusters
- Problem: context matters!
- ❓ How can we preserve order, but also parallelize training?

Image from Merriam-Webster's Instagram Account

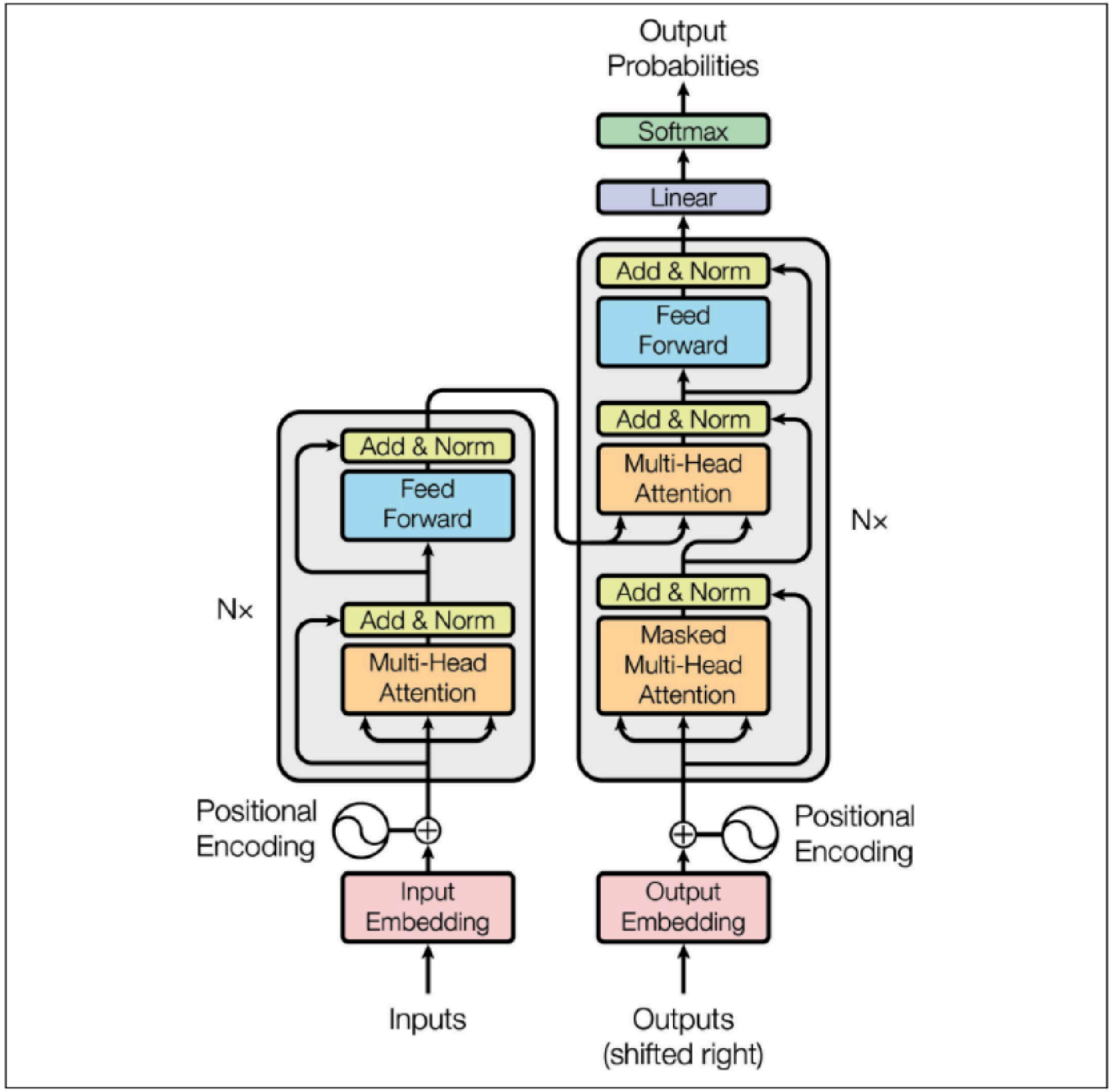


Figure 16-8. The original 2017 transformer architecture[22]

Transformers

- Still encoder-decoder and sequence-to-sequence
- N encoder/decoder layers
- New stuff:
  - Multi-head attention
  - Positional encoding
  - Skip (residual) connections and layer normalization

Multi-head attention

- Each input is linearly projected h times with different learned projections
- The projections are aligned with independent attention mechanisms
- Outputs are concatenated and linearly projected back to the original dimension
- Concept: each layer can learn different relationships between tokens

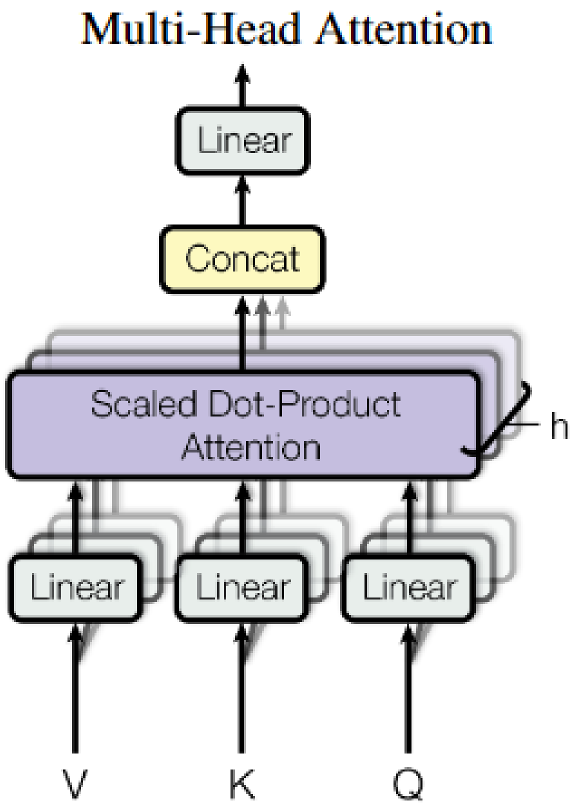


Figure from Attention is All you Need

What are V, K, and Q?

- Attention is described as **querying** a set of **key-value** pairs
- Kind of like a fuzzy dictionary lookup

$$\text{Attention}(\mathbf{Q}, \mathbf{K}, \mathbf{V}) = \text{softmax}\left(\frac{\mathbf{Q}\mathbf{K}^T}{\sqrt{d_k}}\right)\mathbf{V}$$

- $\mathbf{Q}$ is an $n_{queries} \times d_{keys}$ matrix, where d_{keys} is the dimension of the keys
- $\mathbf{K}$ is an $n_{keys} \times d_{keys}$ matrix
- $\mathbf{V}$ is an $n_{keys} \times d_{values}$ matrix
- The $\mathbf{QK^T}$ product is $n_{queries} \times n_{keys}$, representing the **alignment score** between queries and keys (dot product attention)

The various (multi) attention heads

- Encoder **self-attention** (query, key, value are all from the same sequence)
  - Learns relationships between input tokens (e.g. English words)
- Decoder **masked self-attention**:
  - Like the encoder, but only looks at previously generated tokens
  - Prevents the decoder from "cheating" by looking at future tokens
- Decoder **cross-attention**:
  - Decodes the output sequence by "attending" to the input sequence
  - Queries come from the previous decoder layer, keys and values come from the encoder (like prior work)
- ❓ What does stacking these modules N times do?

Positional encoding

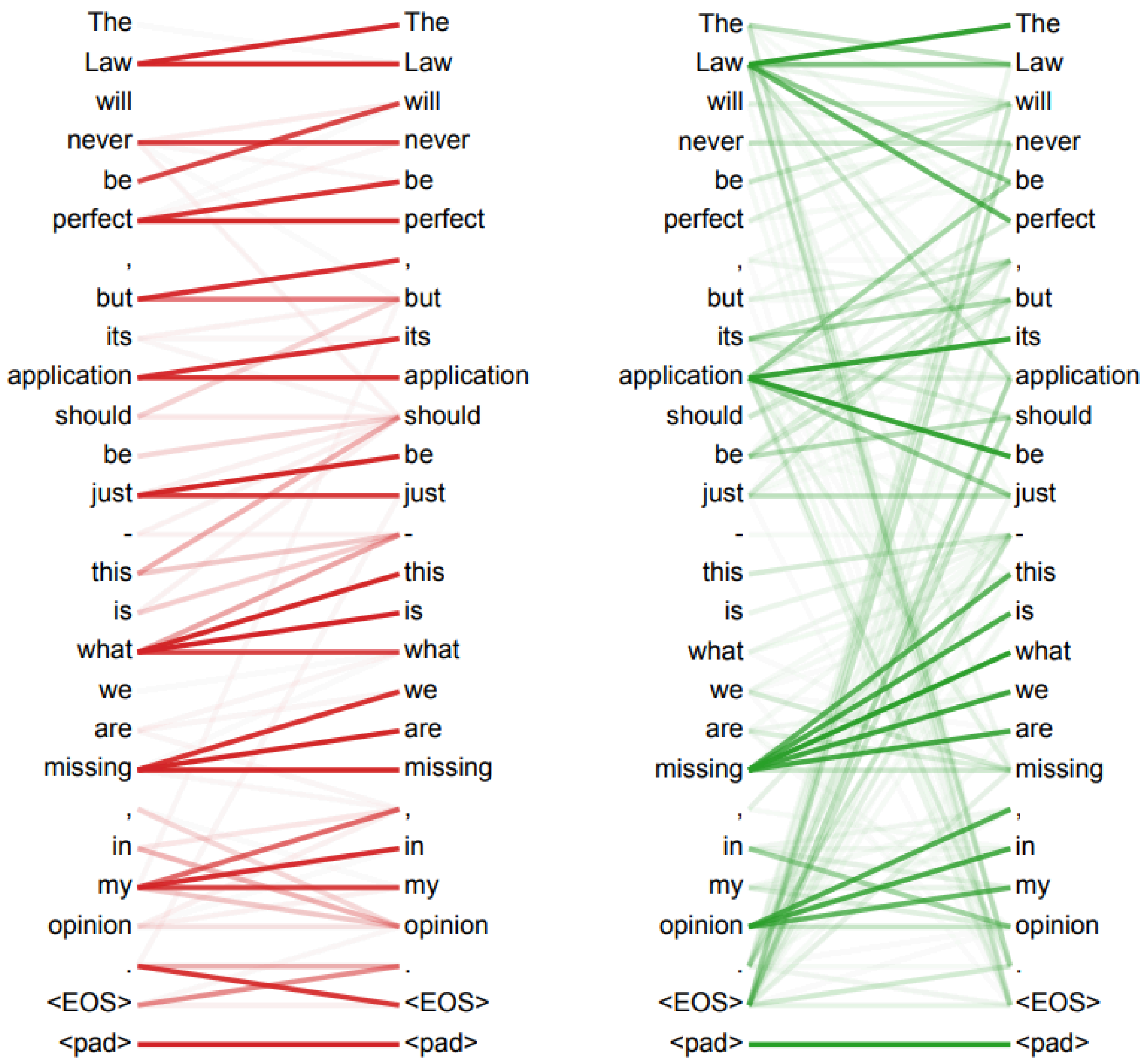
- By getting rid of RNNs, we're down to a bag of words
- **Positional encoding** re-introduces the concept of order
- Simple approach for word position p and dimension i:

$$\mathrm{PE}(p, 2i) = \sin\left(\frac{p}{10000^{2i/d}}\right)$$
$$\mathrm{PE}(p, 2i+1) = \cos\left(\frac{p}{10000^{2i/d}}\right)$$

- resulting vector is **added** to the input embeddings
- ❓ Why sinusoids? What other approaches might work?

Interpretability

- The arXiv version of the paper has some fun visualizations
- This is Figure 5, showing learned attention from two different heads of the encoder self-attention layer



A smattering of Large language models

- GPT (2018): Train to predict the next word on a lot of text, then **fine-tune**
  - Used only masked self-attention layers (the decoder part)
- BERT (2018): Bidirectional Encoder Representations from Transformers
  - Train to predict missing words in a sentence, then **fine-tune**
  - Used unmasked self-attention layers only (the encoder part)
- GPT-2 (2019): Bigger, better, and capable even without fine-tuning
- Llama (2023): Accessible and open source language model
- DeepSeek (2024): Significantly more efficient, but accused of being a distillation of OpenAI's models

Hugging Face

- Hugging Face provides a whole ecosystem for working with transformers
- Easiest way is with the `pipeline` interface for inference:

```
from transformers import pipeline
nlp = pipeline("sentiment-analysis") # for example
nlp("Cats are fickle creatures")
```

- Hugging Face models can be fine-tuned on your own data, but for that you'll need to use the `transformers` library

And now for something completely different: Reinforcement learning