

Deep Learning

15 Self-Attention & Transformers - I

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Motivation

① Why does one need to think beyond LSTMs?

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- ② Sequential processing doesn't allow parallelization
 - Path length = $\mathcal{O}(n)$
 - RNNs need $\mathcal{O}(n)$ steps to process a sentence of length n

Motivation

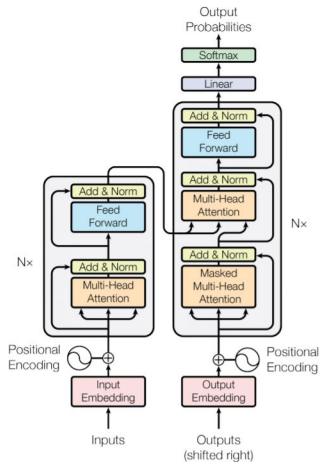
- ① (Despite the LSTM/GRU) RNNs need attention to deal with long-range dependencies

Motivation

- ① (Despite the LSTM/GRU) RNNs need attention to deal with long-range dependencies
- ② Since attention enables access to any state, do we need RNNs?

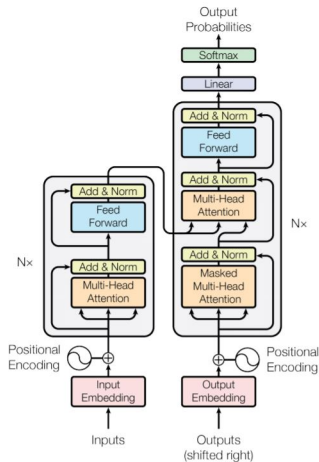
Transformers

- 1 Introduced by Vaswani et al.
NeurIPS 2017



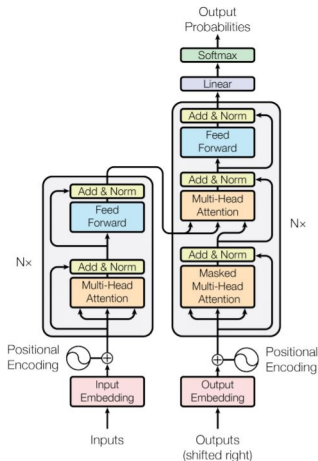
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- 2 Sequence to sequence modeling without RNNs



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- 2 Sequence to sequence modeling without RNNs
- 3 Transformer model is built on self-attention (no recurrence or convolutions)



Transformers

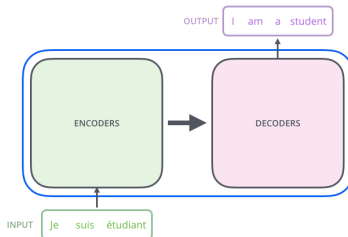


Credits: Jay Alammar

Transformers

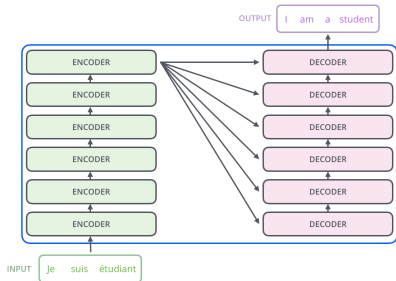


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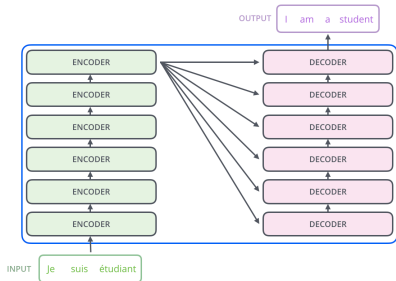
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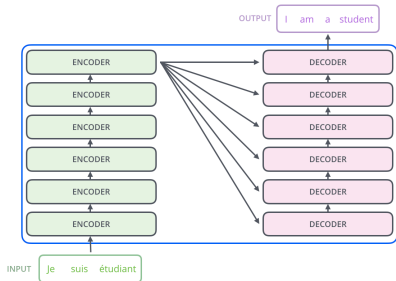
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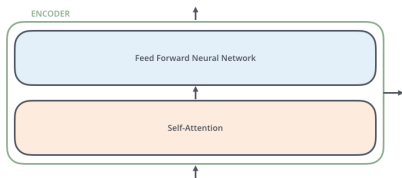
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- ① The Encoding module has a stack of encoders
- ② Same structure different parameters



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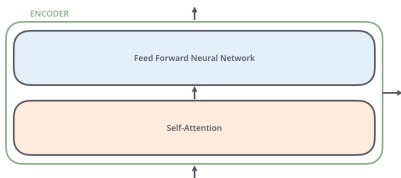
- ① The Encoding module has a stack of encoders
- ② Same structure different parameters
- ③ Similarly, the decoding module



- 1 Encoder first has a self-attention layer

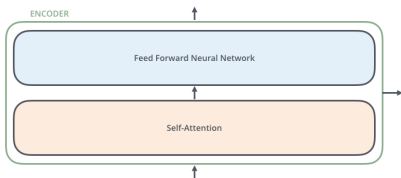
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Transformers



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- ① Encoder first has a self-attention layer
- ② Looks at the other words while encoding a specific word
- ③ Next a (same) feed-forward NN is applied at all positions

Attention vs Self-attention

- ① Encoder-Decoder Attention looks

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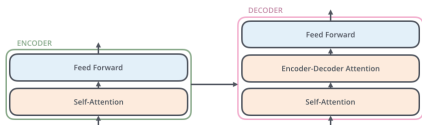
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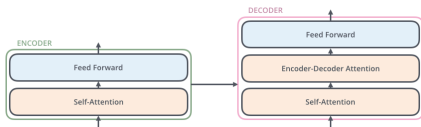
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Credits: Jay Alammar

- 1 Decoder has both the layers (self-attention and shared feed-forward)



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- 1 Decoder has both the layers (self-attention and shared feed-forward)
- 2 But, in the middle it has an **encoder-decoder attention layer**

Why the name 'Transformer'?

- ① Transforms a set of vectors in some representation space into a corresponding set of vectors (same dimensionality) in some new space

Why the name 'Transformer'?

- ① Transforms a set of vectors in some representation space into a corresponding set of vectors (same dimensionality) in some new space
- ② **Goal:** new space will have a **richer internal representation** that is better suited to solve the downstream task

Transformers-Encoding

- ① Start with turning each word into a vector at the bottom-most encoder

x_1 
Je

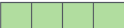
x_2 
suis

x_3 
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Transformers-Encoding

- ① Start with turning each word into a vector at the bottom-most encoder
- ② Others receive a list of vectors from the encoder immediately below

x_1 
Je

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Credits: Jay Alammar

Self-attention in Encoder vs. Decoder



- ① Who is doing: all source tokens

Self-attention in Encoder vs. Decoder



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- ② What are they doing (**repeat**)
 - look at each other
 - update representations

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Self-attention in Encoder vs. Decoder



- | | |
|---|--|
| ① Who is doing: all source tokens | ① Decoder |
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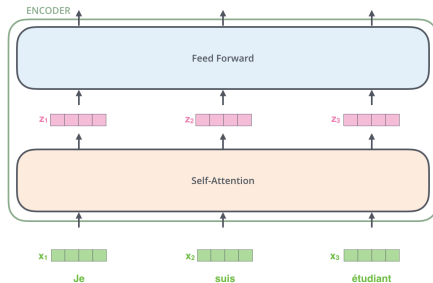
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 - look at each other
 - update representations
- ① Decoder
- ② Who is doing: target token at each time step
- ③ What are they doing (**repeat**)
 - looks at previous target tokens (self-attention)
 - looks at source representations (encoder-decoder attention)
 - update representation

Transformers-Encoding

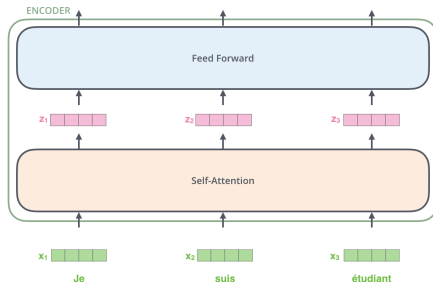
- ① Each word flows through the two layers of the encoder through its own path



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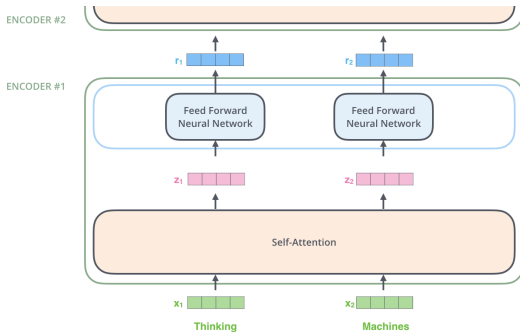
Transformers-Encoding

- ① Each word flows through the two layers of the encoder through its own path
- ② Self-attention layer has dependencies among them. However, the path length is $\mathcal{O}(1)$



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Transformers-Encoding



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Self-Attention

- ① The animal didn't cross the street because it was too tired
- ② The animal didn't cross the street because it was too wide

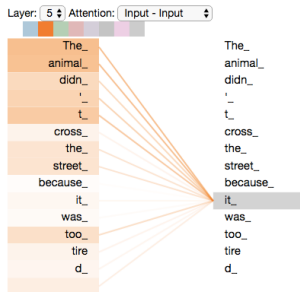
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- ③ What does 'it' refer to?
- ④ Easy for humans, but not so much for the traditional Seq2Seq models

Self-Attention

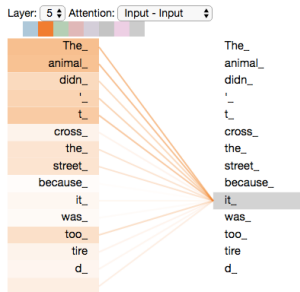
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Self-Attention

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- ② Unlike RNNs, we don't keep hidden states from previous positions here!



Credits: Jay Alammar

Attention weights

① Input tokens x_1, x_2, \dots, x_N

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Attention weights

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- ② Output tokens $\mathbf{y}_1, \mathbf{y}_2, \dots, \mathbf{y}_N$
- ③ $\mathbf{y}_n = \sum_{m=1}^N \mathbf{a}_{nm} \cdot \mathbf{x}_m$
- ④ $a_{mn} \geq 0$ and $\sum_{m=1}^N a_{mn} = 1$ Why?

How to compute the Attention weights?



- ① A simple way is to use the 'dot product' self-attention

How to compute the Attention weights?



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②
$$a_{nm} = \frac{\exp(\mathbf{x}_n^T \mathbf{x}_m)}{\sum_{m'=1}^N \exp(\mathbf{x}_n^T \mathbf{x}_{m'})}$$

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⑤ Each of the feature values in a token plays an equal role in determining the attention weights

Some terminology from Information Retrieval

- ① Consider a streaming platform and the problem of choosing which movie to watch

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- ⑤ The movie file itself is the **Value**

Self-Attention

$$\textcircled{1} \quad \mathbf{Q} = \mathbf{XW}^{(q)}$$

Self-Attention

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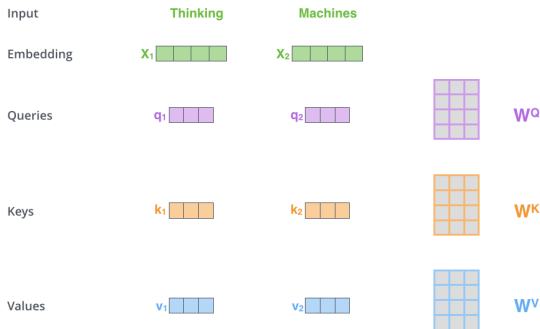
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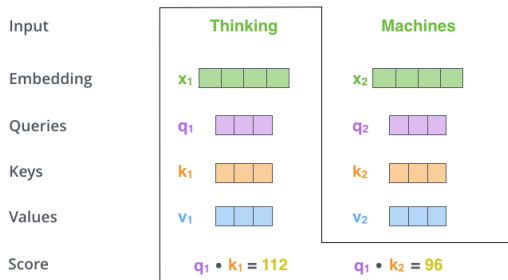
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Self-Attention



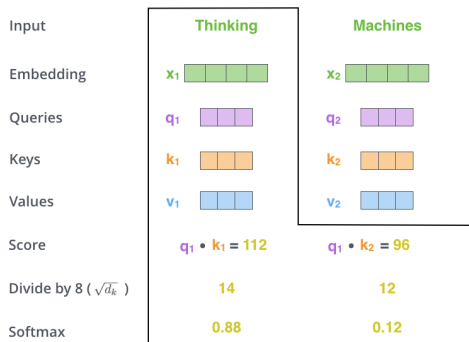
Credits: Jay Alammar

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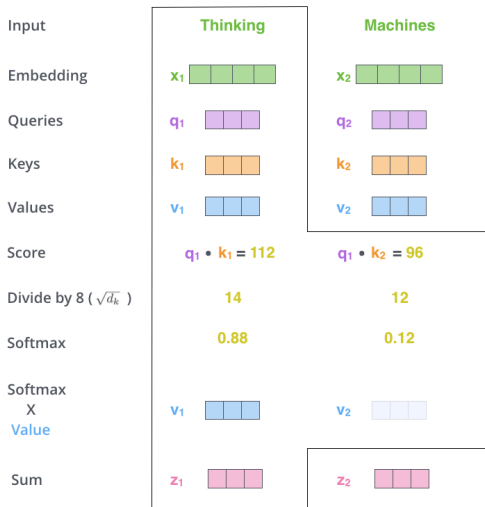
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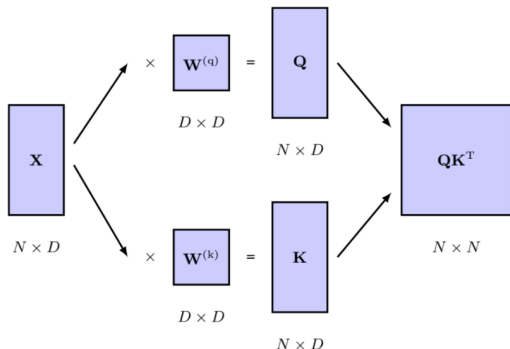
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Self-Attention



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Self-Attention



Credits: The Bishop's book

Self-Attention

$$Y \quad N \times D_v = \text{Softmax} \left\{ QK^T \quad N \times N \right\} \times V \quad N \times D_v$$

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Scaled Self-Attention

- ① Gradients of the softmax become exponentially small for large input magnitudes

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- ③ If the elements of q and v vectors are independent $N(0, 1)$ distributed, the variance of the dot product $\rightarrow D_k$
- ④ Hence, normalize the product by the standard deviation
$$\mathbf{Y} = \text{Attention}(\mathbf{Q}, \mathbf{K}, \mathbf{V}) = \text{Softmax}\left[\frac{\mathbf{QK}^T}{\sqrt{D_k}}\right]\mathbf{V}$$

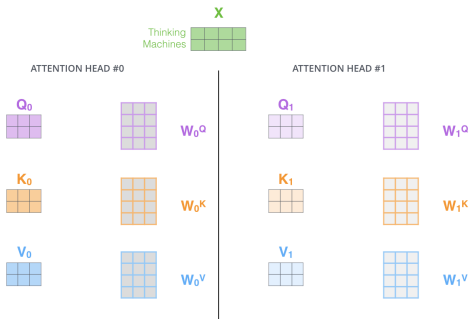
Multi-headed Self-Attention

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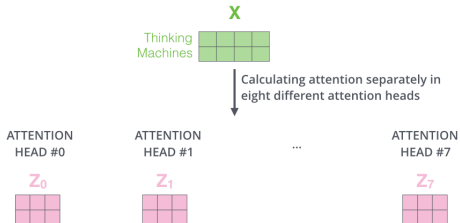
- ① There may be multiple patterns of attention that are relevant at the same time
- ② E.g., some patterns relevant to the 'tense' while others might be associated with the 'vocabulary.'

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Multi-headed Self-Attention

- ① Expands the model's ability to focus on different relevant positions in the i/p

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- ② Enables different 'representational subspace'

Multi-headed Self-Attention

1) Concatenate all the attention heads



2) Multiply with a weight matrix W^O that was trained jointly with the model

x

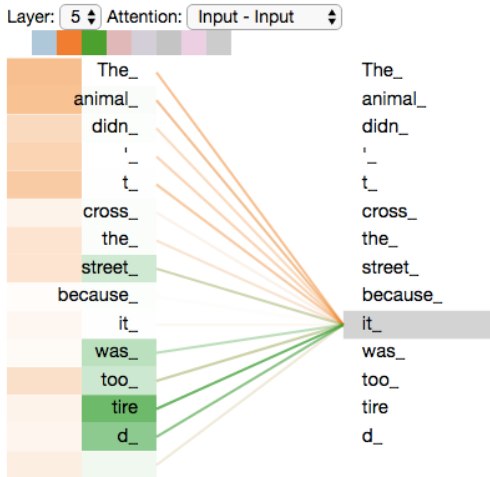


3) The result would be the Z matrix that captures information from all the attention heads. We can send this forward to the FFNN



Credits: Jay Alammar

Multi-headed Self-Attention



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Transformer Layers

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- ② → stack multiple self-attention layers
- ③ To improve the training efficiency, introduce residual connections (requires to maintain the dimensionality)
- ④ Followed by Layer normalization
 $\mathbf{Z} = \text{LayerNorm}[\mathbf{Y}(\mathbf{X}) + \mathbf{X}]$

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Transformer Layers

- ① Output vectors are constrained to lie in the subspace spanned by the i/p vectors
- ② Enhance the expressive capability/flexibility by post-processing using a nonlinear neural net (MLP)
- ③ This should not affect the transformer's ability to process variable length i/p
- ④ Same share net applies to all the o/p tokens (followed by residual connection and normalization)

$$\tilde{\mathbf{X}} = \mathbf{LayerNorm}[\mathbf{MLP}[\mathbf{Z}] + \mathbf{Z}]$$