Machine Learning course
advanced track

Lecture 4: Self-attention & Transformer

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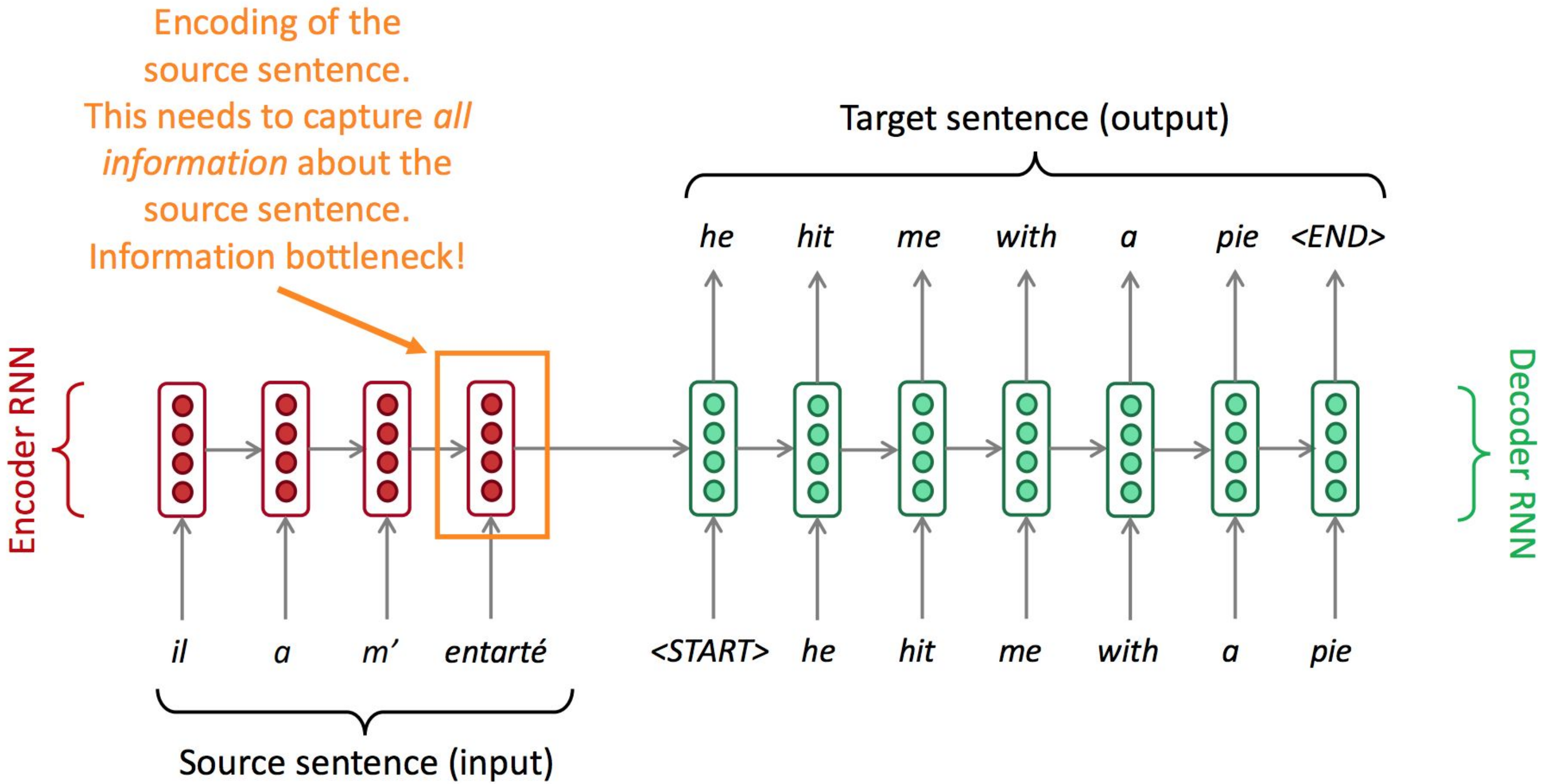
Outline

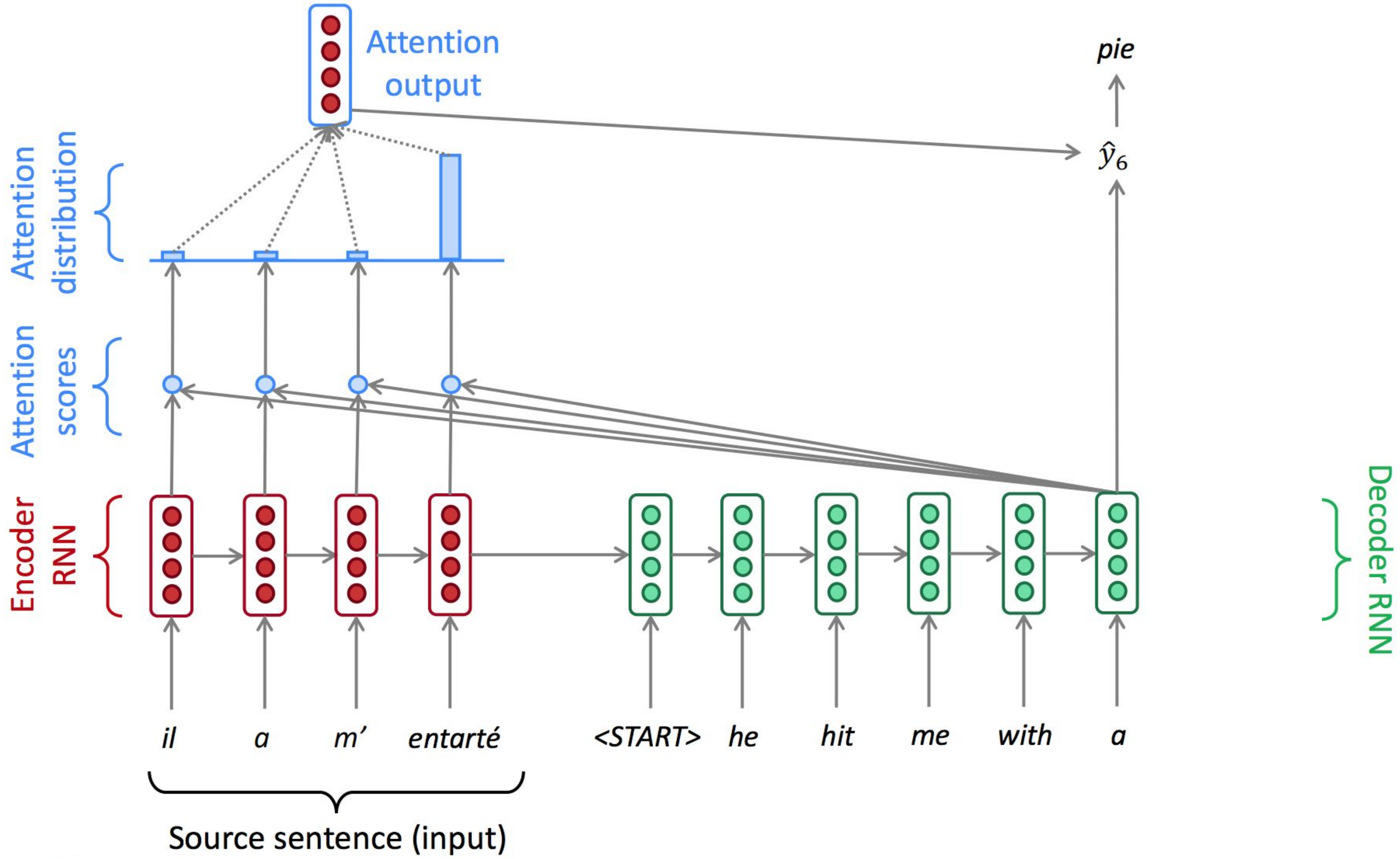
1. recap: Attention in seq2seq
2. Transformer architecture
3. Self-Attention
4. Positional encoding
5. Layer normalization
6. Q & A

Based on: http://web.stanford.edu/class/cs224n/slides/cs224n-2019-lecture08-nmt.pdf
https://jalammar.github.io/illustrated-transformer/

recap: Attention in seq2seq



recap: Attention in seq2seq



recap: Attention in seq2seq

We have encoder hidden states $h_1, \ldots, h_N \in \mathbb{R}^h$

On timestep *t*, we have decoder hidden state $s_t \in \mathbb{R}^h$

We get the attention scores $\boldsymbol{e}^t$ for this step:

$$\boldsymbol{e}^t = [\boldsymbol{s}_t^T \boldsymbol{h}_1, \ldots, \boldsymbol{s}_t^T \boldsymbol{h}_N] \in \mathbb{R}^N$$

We take softmax to get the attention distribution α^t for this step (this is a probability distribution and sums to 1)

$$\alpha^t = \mathrm{softmax}(\boldsymbol{e}^t) \in \mathbb{R}^N$$

We use α^t to take a weighted sum of the encoder hidden states to get the attention output $\boldsymbol{a}_t$

$$\boldsymbol{a}_t = \sum_{i=1}^{N} \alpha_i^t \boldsymbol{h}_i \in \mathbb{R}^h$$

Finally we concatenate the attention output $\boldsymbol{a}_t$ with the decoder hidden state s_t and proceed as in the non-attention seq2seq model

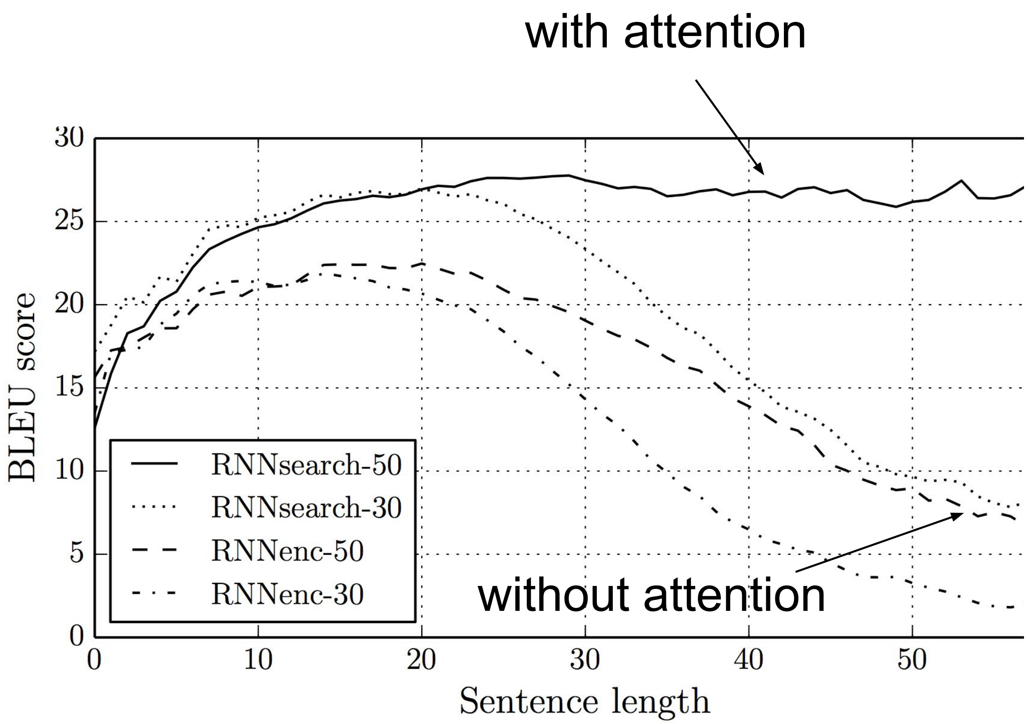
$$[\boldsymbol{a}_t; \boldsymbol{s}_t] \in \mathbb{R}^{2h}$$

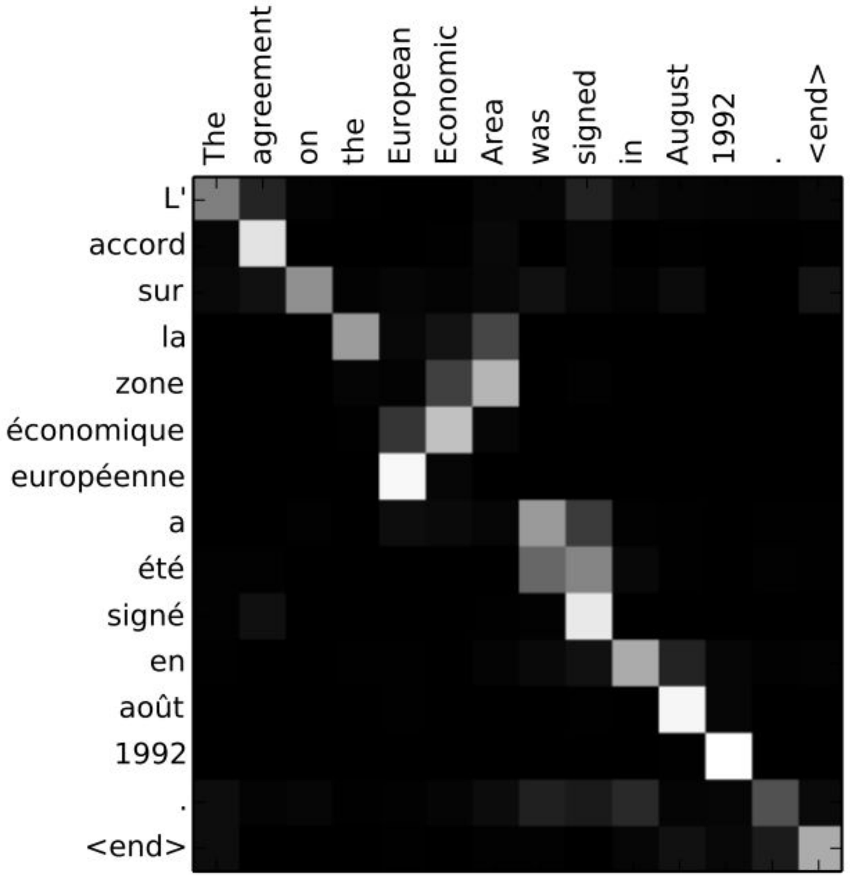
Attention variants

- Basic dot-product (the one discussed before): $\boldsymbol{e}_i = \boldsymbol{s}^T \boldsymbol{h}_i \in \mathbb{R}$
- Multiplicative attention: $\boldsymbol{e}_i = \boldsymbol{s}^T \boldsymbol{W} \boldsymbol{h}_i \in \mathbb{R}$
  - $\boldsymbol{W} \in \mathbb{R}^{d_2 \times d_1}$ - weight matrix
- Additive attention: $\boldsymbol{e}_i = \boldsymbol{v}^T \tanh(\boldsymbol{W}_1 \boldsymbol{h}_i + \boldsymbol{W}_2 \boldsymbol{s}) \in \mathbb{R}$
  - $\boldsymbol{W}_1 \in \mathbb{R}^{d_3 \times d_1}, \boldsymbol{W}_2 \in \mathbb{R}^{d_3 \times d_2}$ - weight matrices
  - $\boldsymbol{v} \in \mathbb{R}^{d_3}$ - weight vector

Attention advantages

- "Free" word alignment
- Better results on long sequences

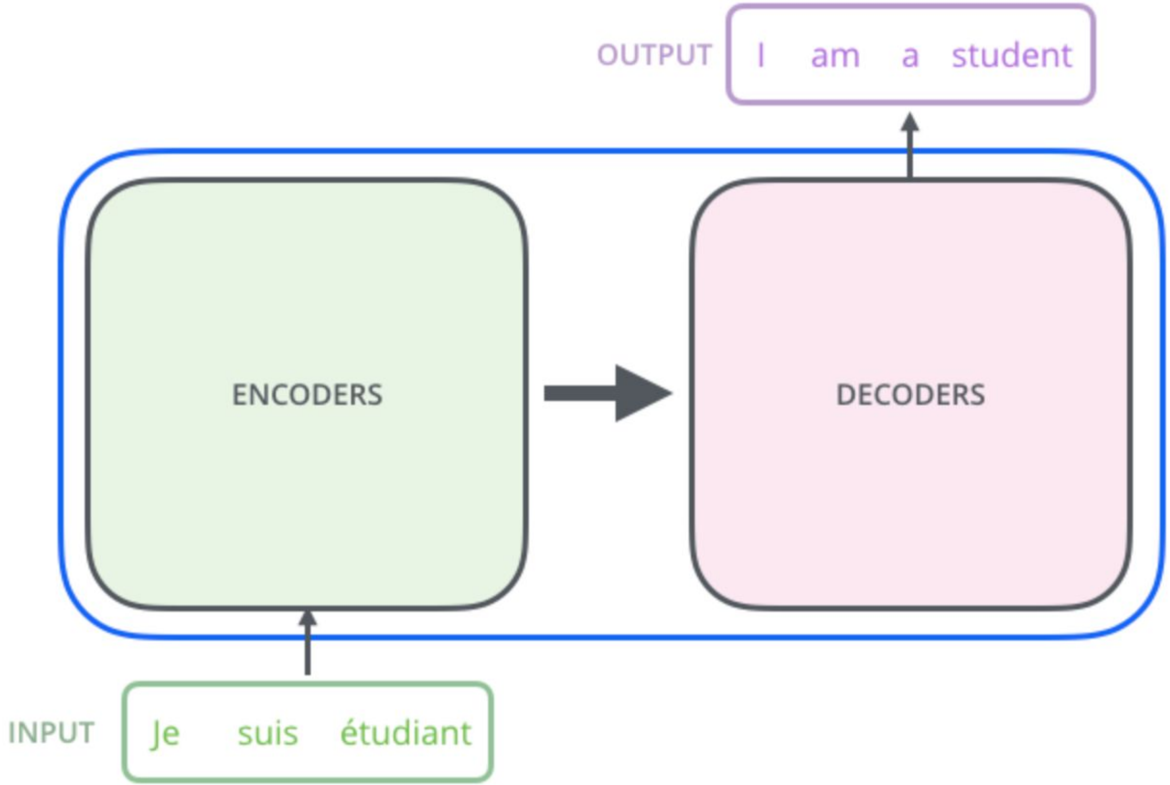




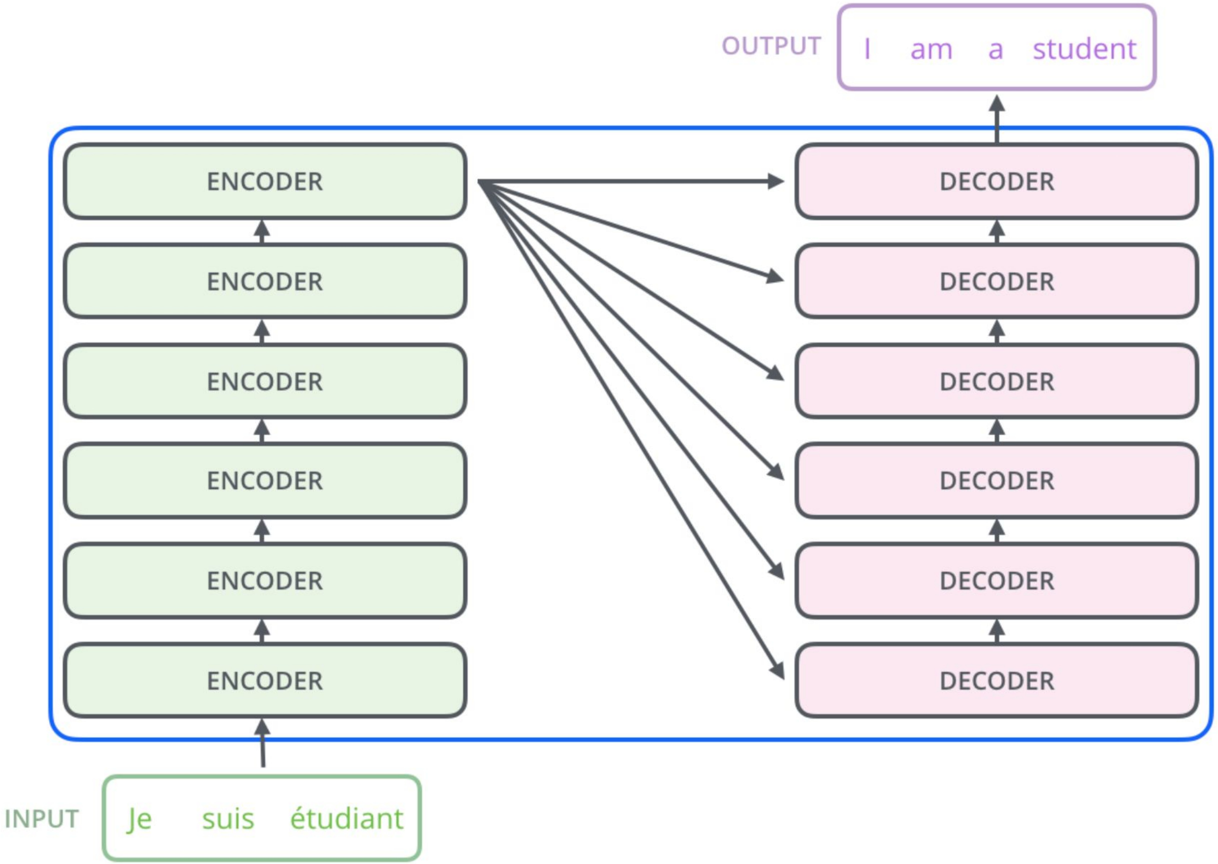
The Transformer

The Transformer

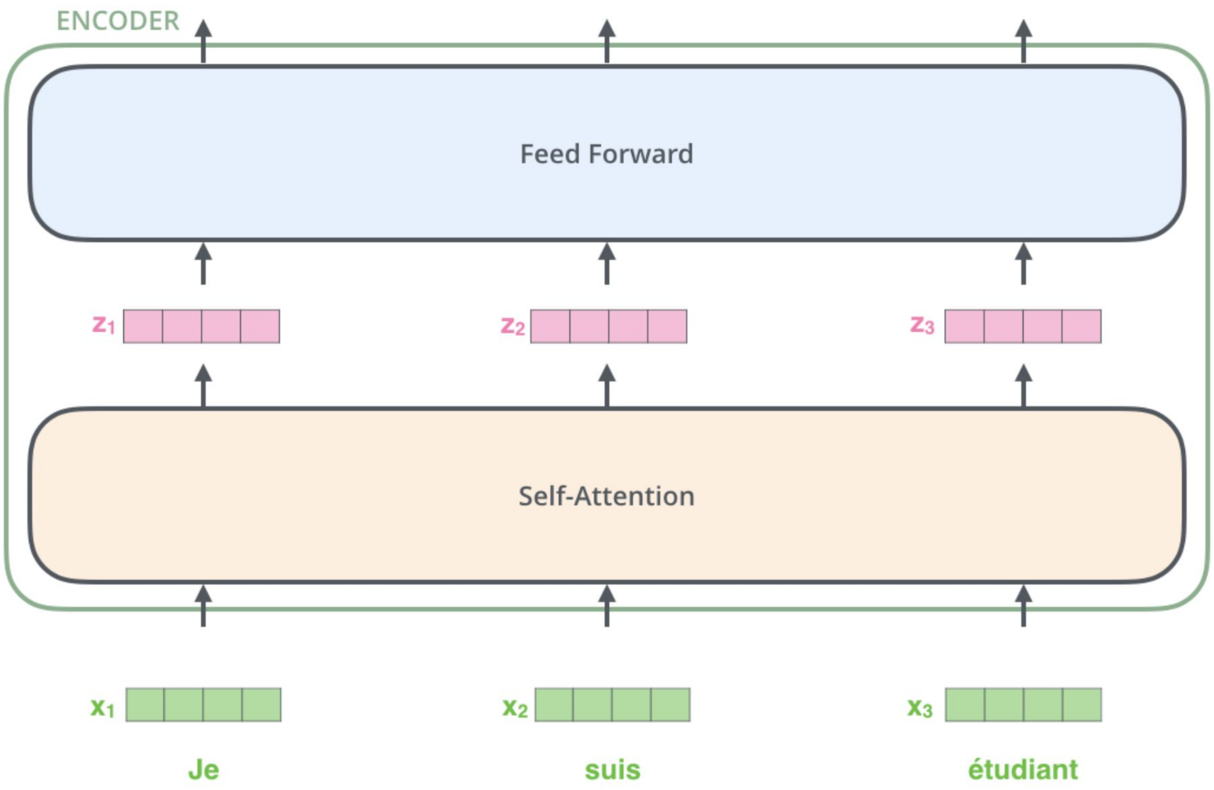
The Transformer



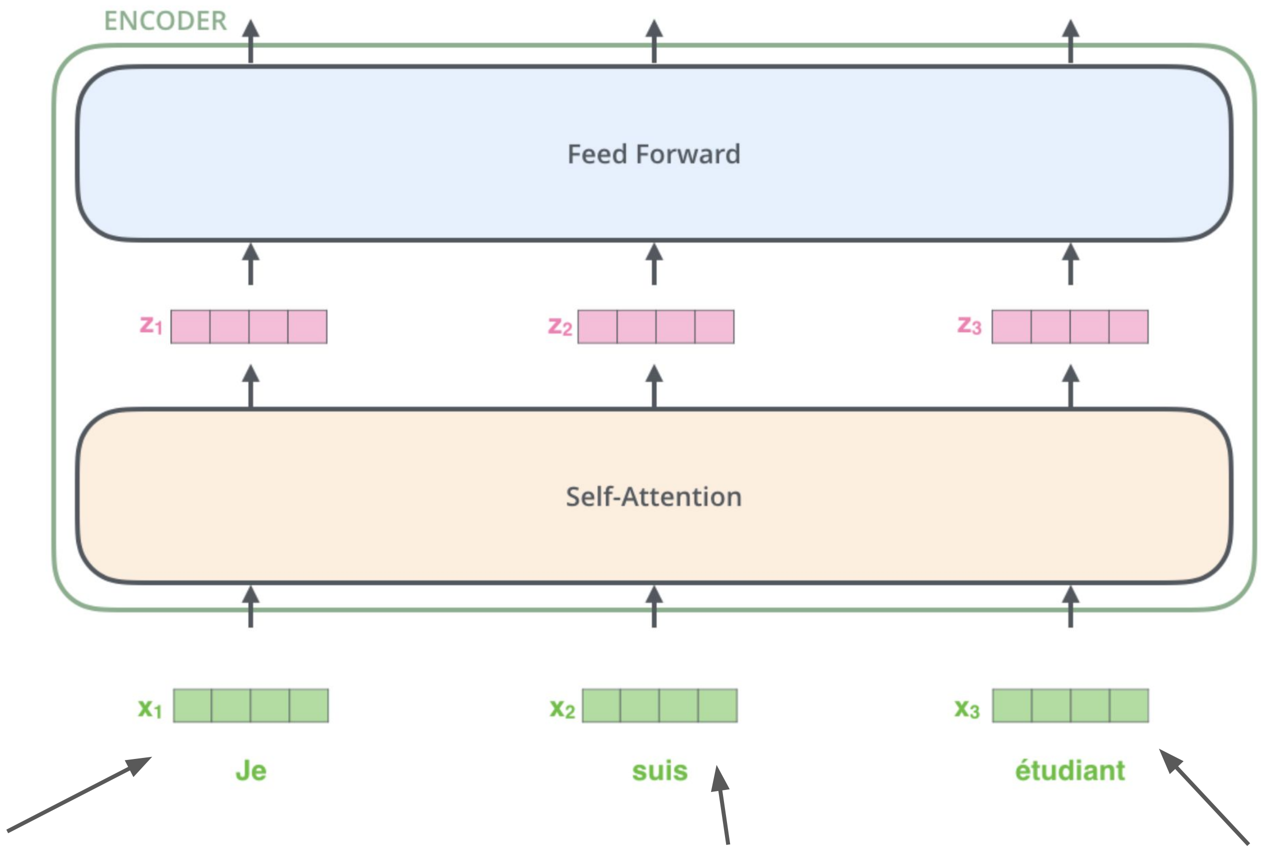
The Transformer



The Encoder Side



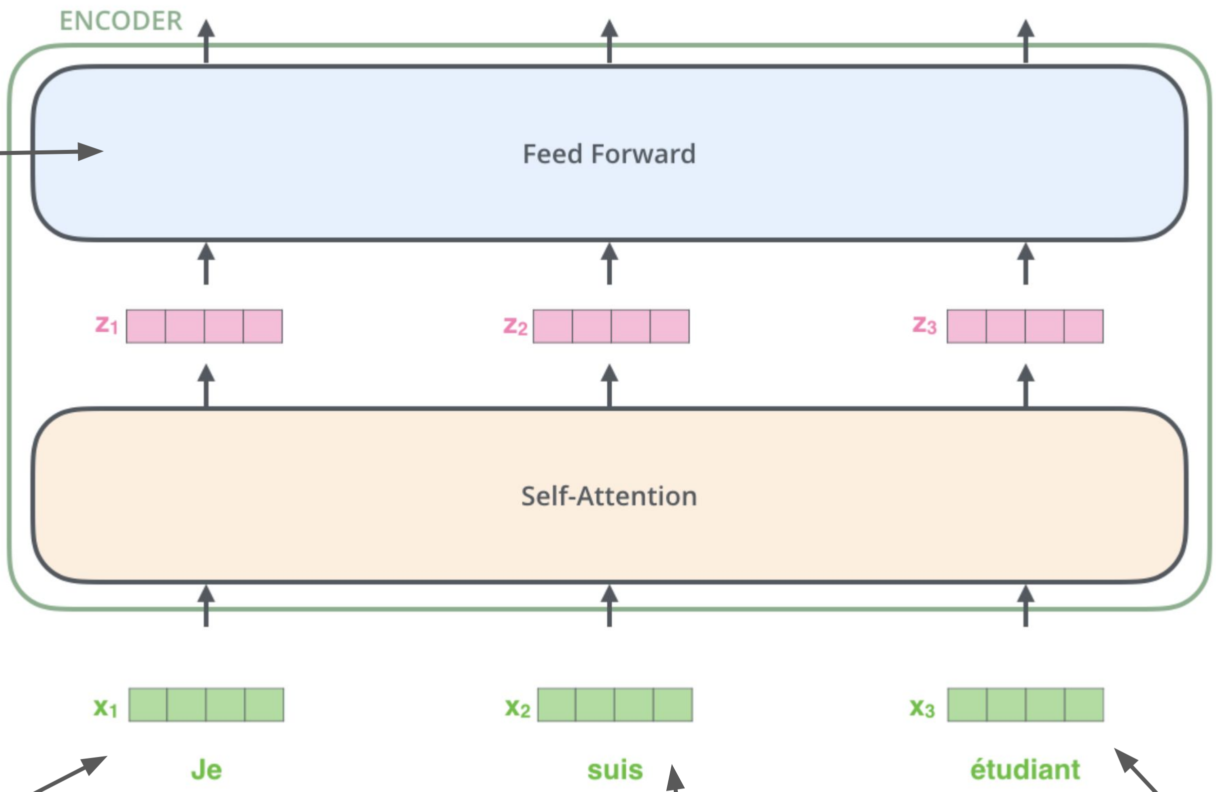
The Encoder Side



the word in each position flows through its own path in the encoder

The Encoder Side

Can be parallelized



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The Encoder Side

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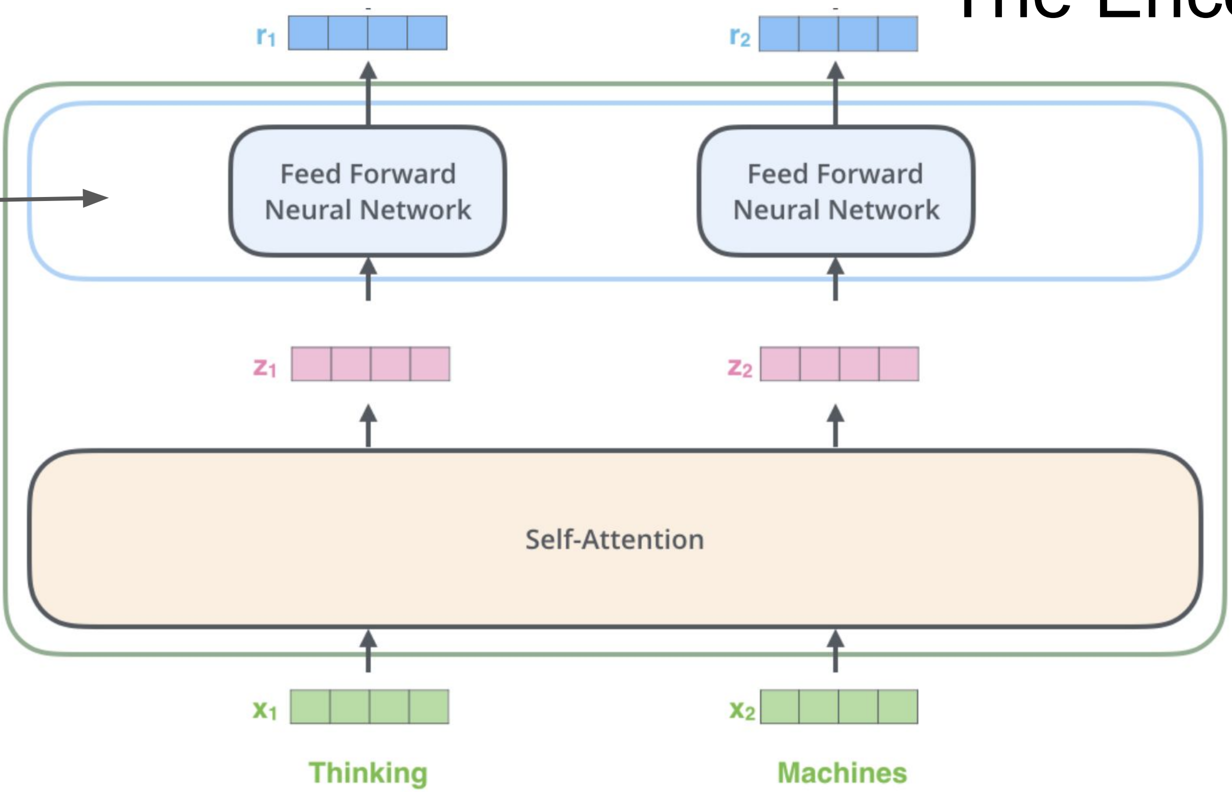

the word in each position flows through its own path in the encoder

The Transformer: quick overview

- Proposed in the paper “Attention is All You Need” (Ashish Vaswani et al.)
- No recurrent or convolutional neural networks -> just attention
- Beats seq2seq in machine translation task
  - 28.4 BLEU on the WMT 2014 English-to-German translation task
- Much faster
- Uses **self-attention** concept

Self-Attention

Self-Attention at a High Level

”`The animal didn't cross the street because it was too tired`”

- What does “it” in this sentence refer to?

Self-Attention at a High Level

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- We want self-attention to associate “it” with “animal”

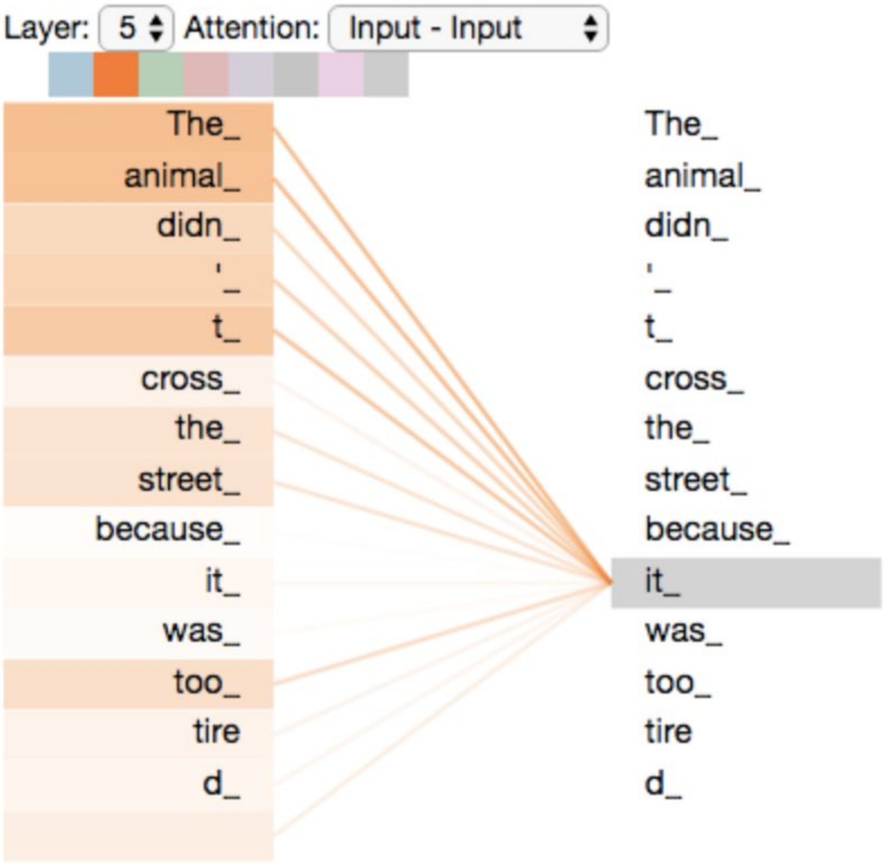
Self-Attention at a High Level

”`The animal didn't cross the street because it was too tired`”

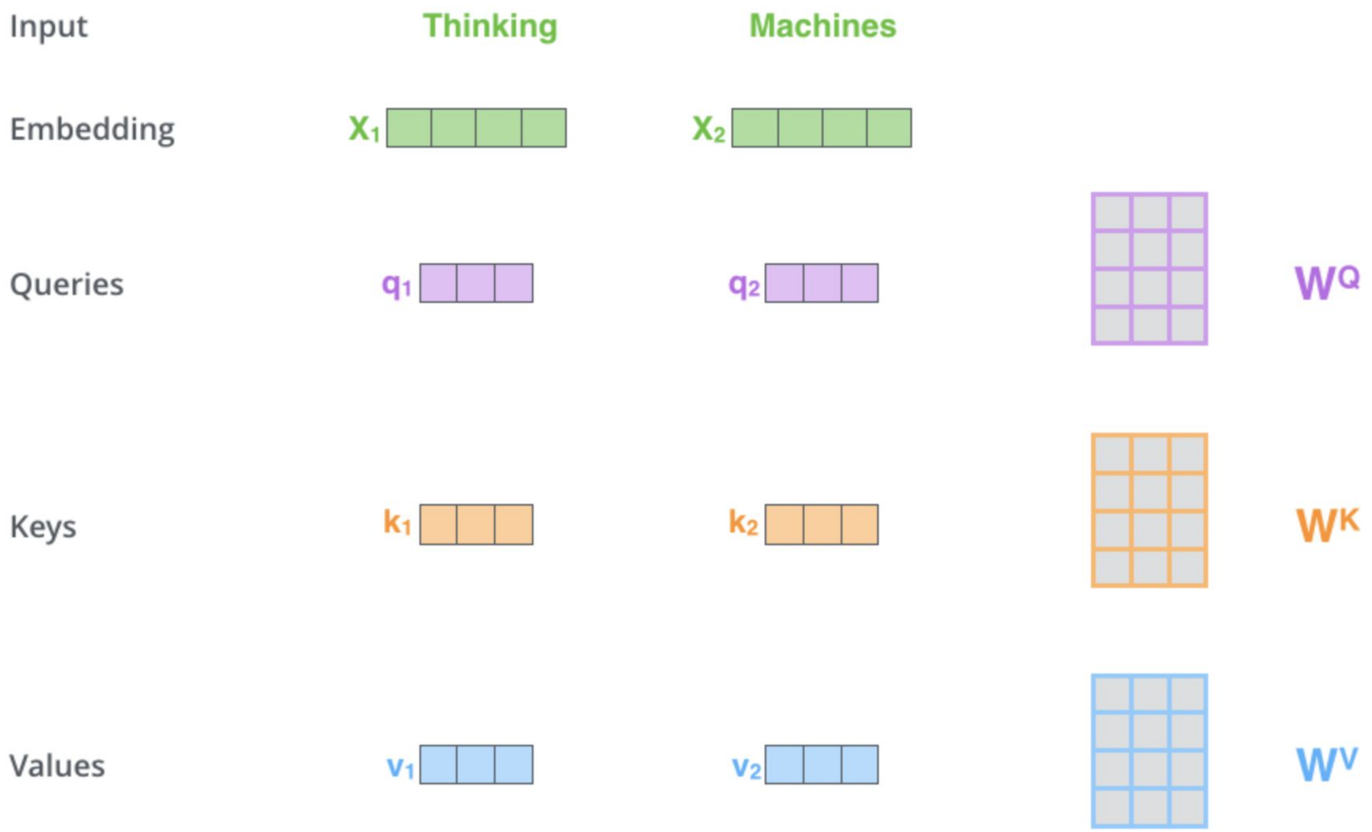
- What does “it” in this sentence refer to?
- We want self-attention to associate “it” with “animal”

- Self-attention is the method the Transformer uses to bake the “understanding” of other relevant words into the one we’re currently processing

Self-Attention at a High Level



Self-Attention: detailed explanation

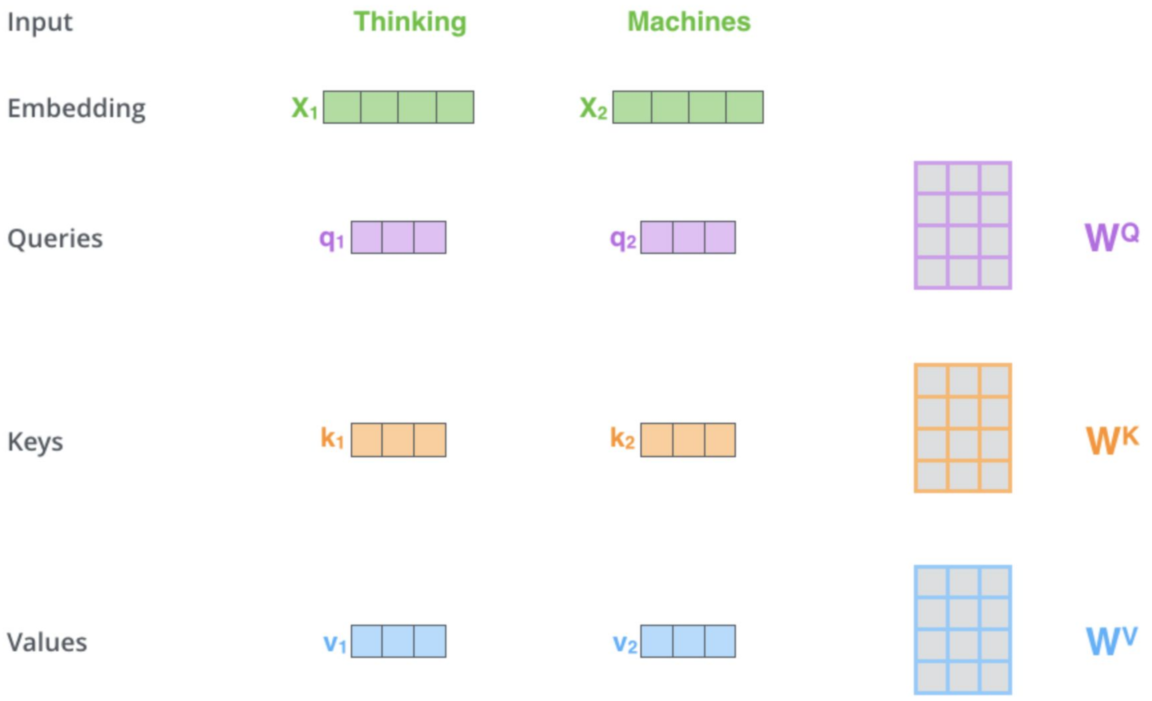


Self-Attention: detailed explanation

STEP 1:

create 3 vectors (Query, Key, Value)

from each of the encoder's input vectors



Self-Attention: detailed explanation

What are the “query”, “key”, and “value” vectors?

Self-Attention: detailed explanation

What are the “query”, “key”, and “value” vectors?

They’re abstractions that are useful for

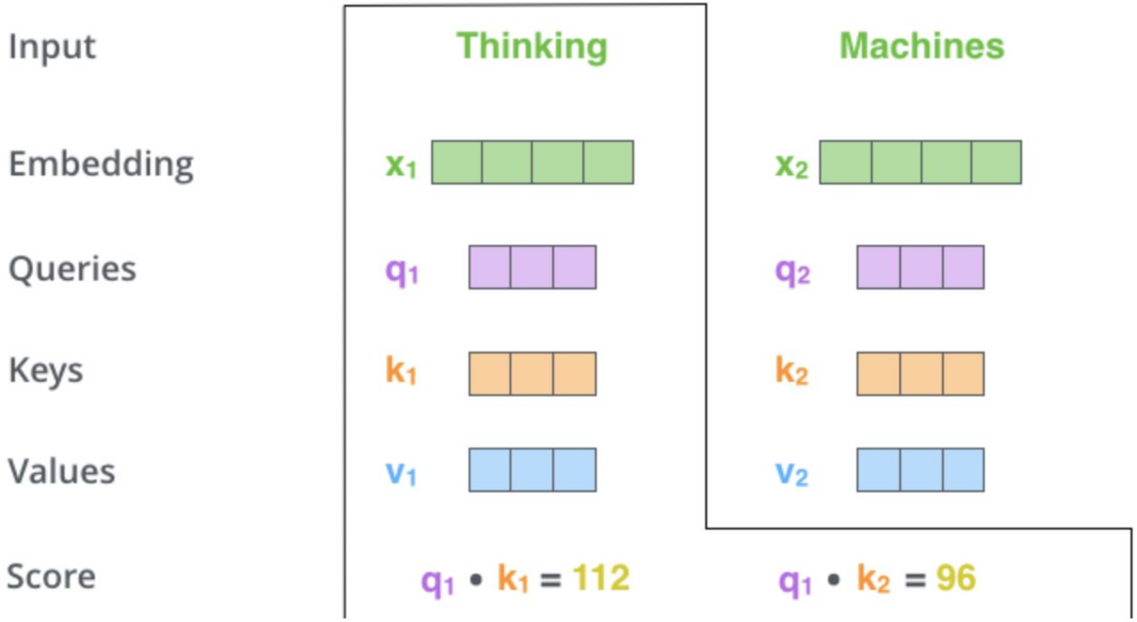
calculating and thinking about attention.

Self-Attention: detailed explanation

STEP 2:

calculate a score

(score each word of the input sentence against the current word)



Self-Attention: detailed explanation

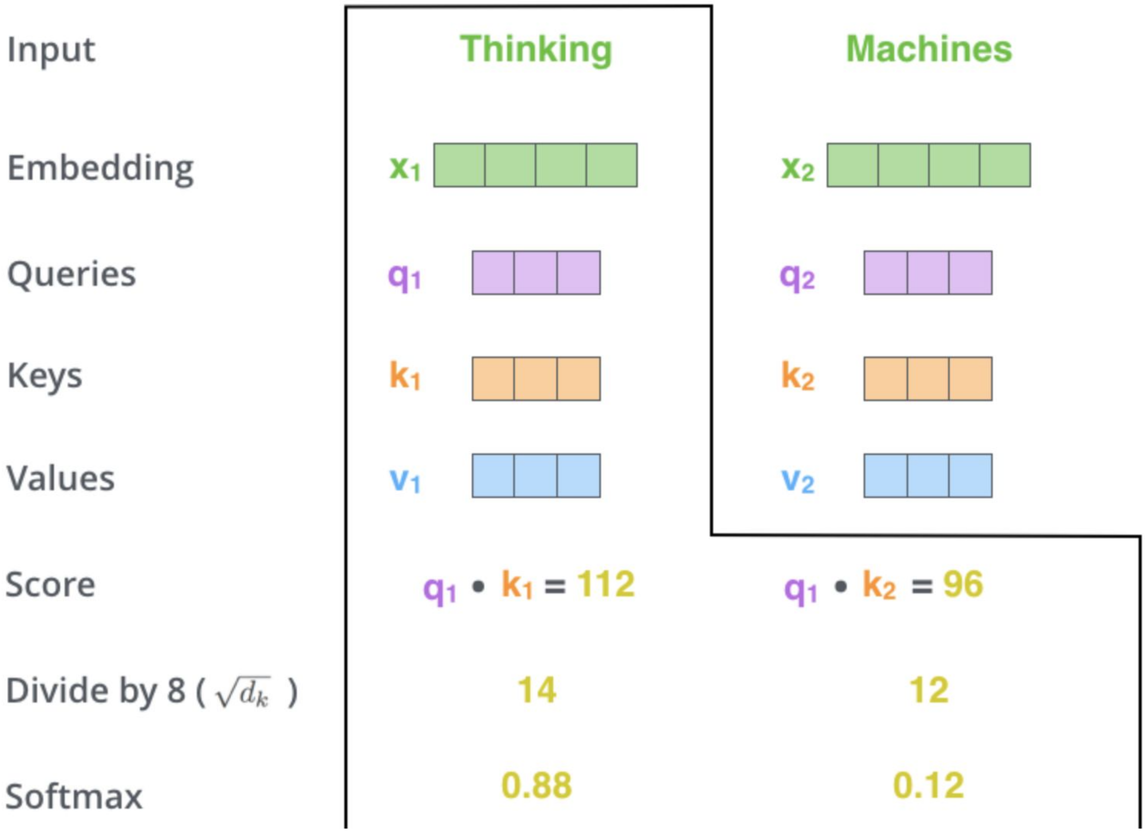
STEP 3:

divide the scores by 8

(the square root of the dimension of the key vectors)

STEP 4:

softmax



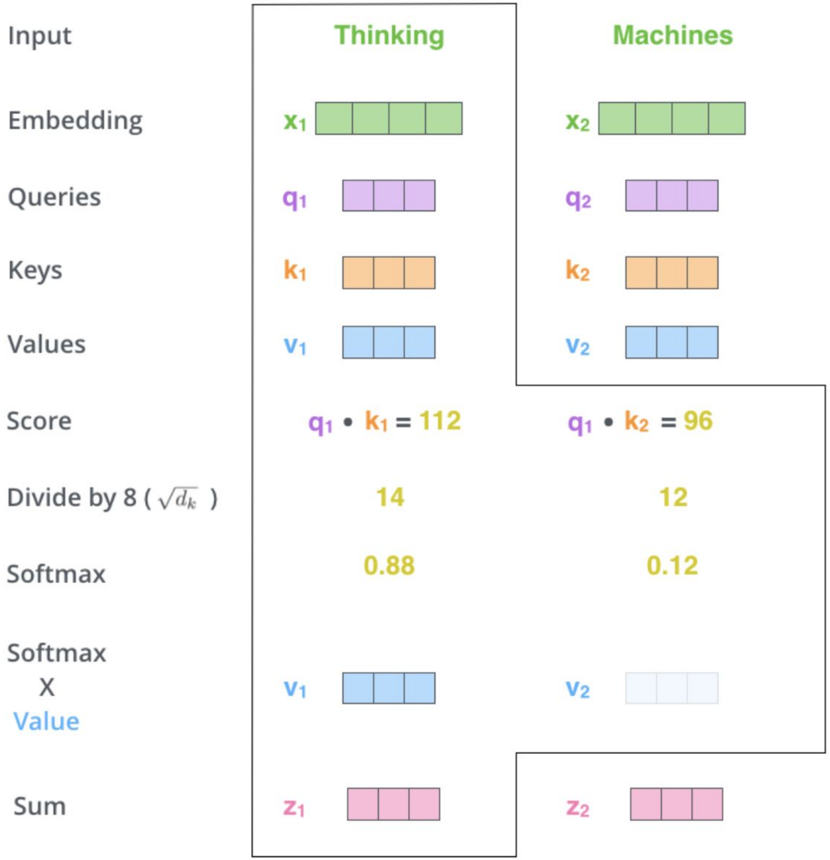
Self-Attention: detailed explanation

STEP 5:

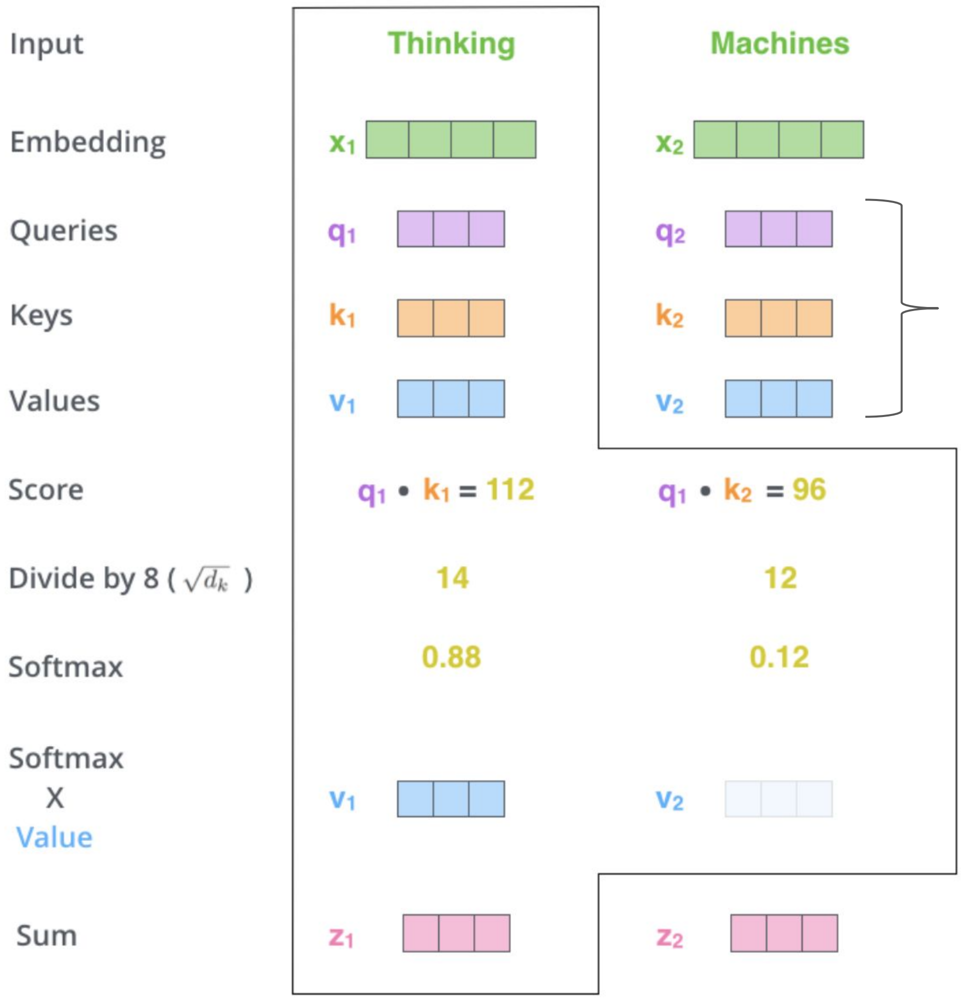
multiply each value vector by the softmax score

STEP 6:

sum up the weighted value vectors



Self-Attention



STEP 1: create Query, Key, Value

STEP 2: calculate scores

STEP 3: divide by $\sqrt{d_k}$

STEP 4: softmax

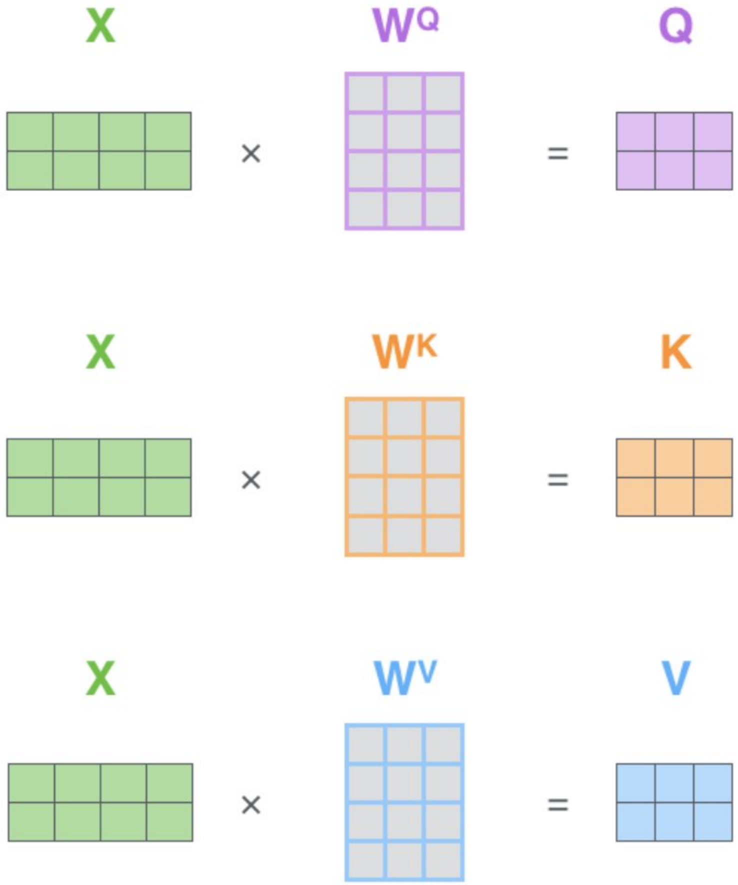
STEP 5: multiply each value vector by the softmax score

STEP 6: sum up the weighted value vectors

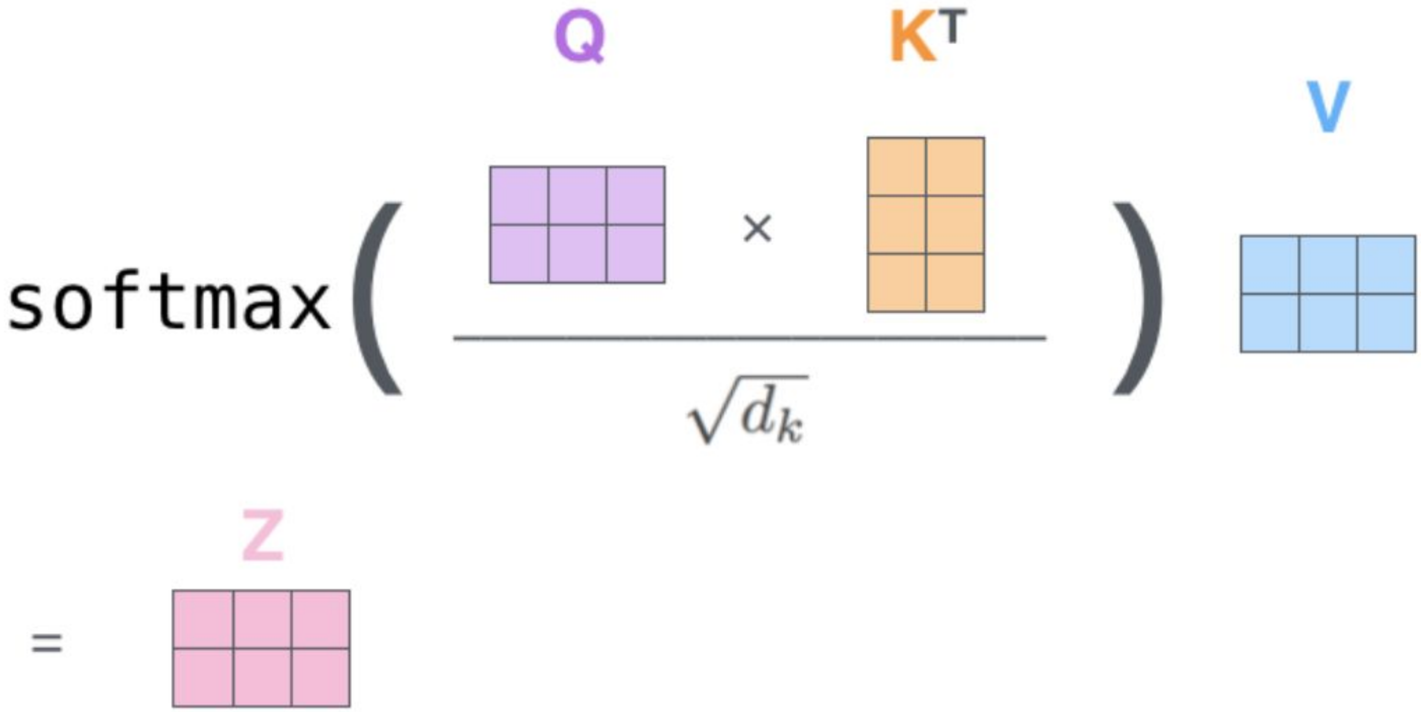
Self-Attention: Matrix Calculation

Pack embeddings into matrix **X**

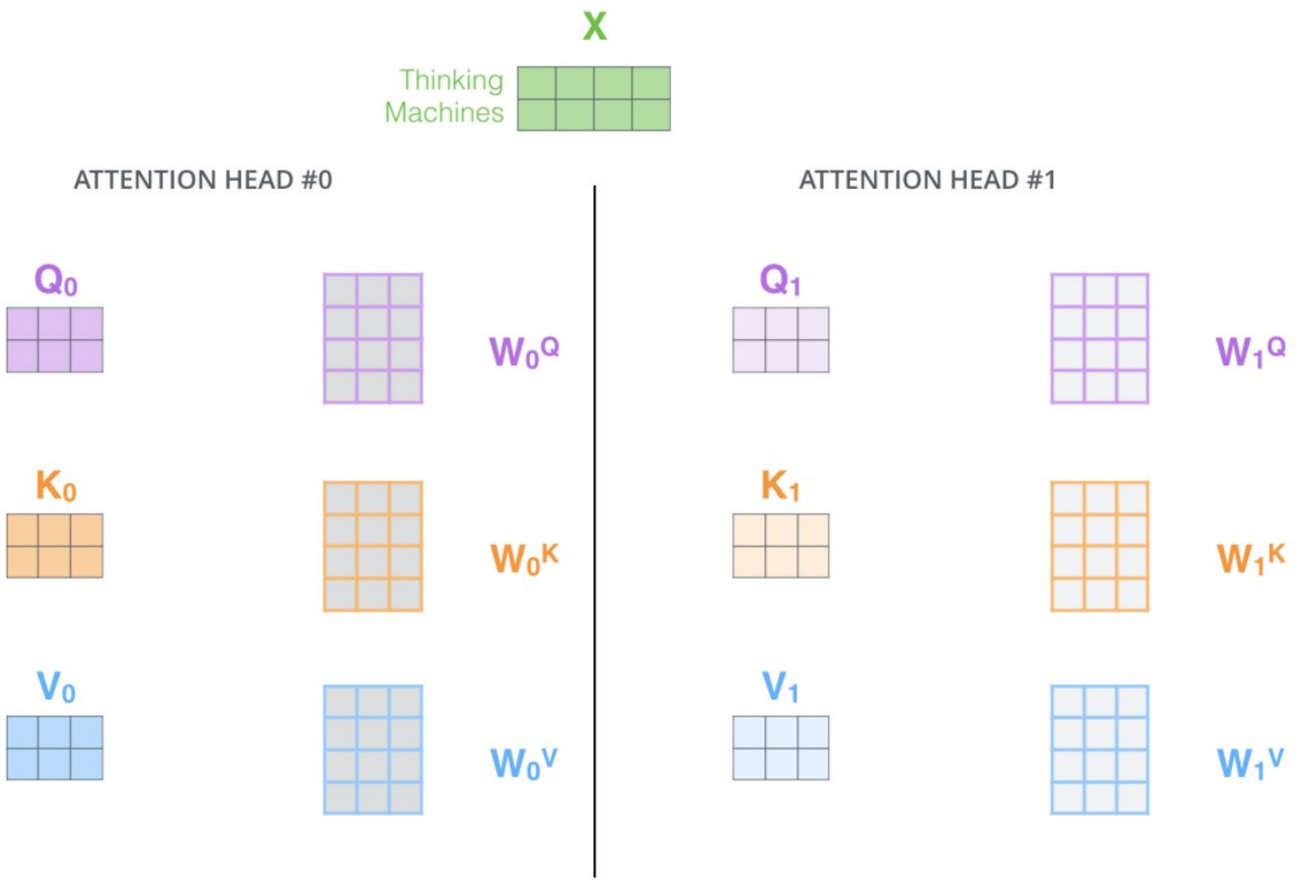
Multiply **X** by weight matrices we've trained (**Wk, Wq, Wv**)



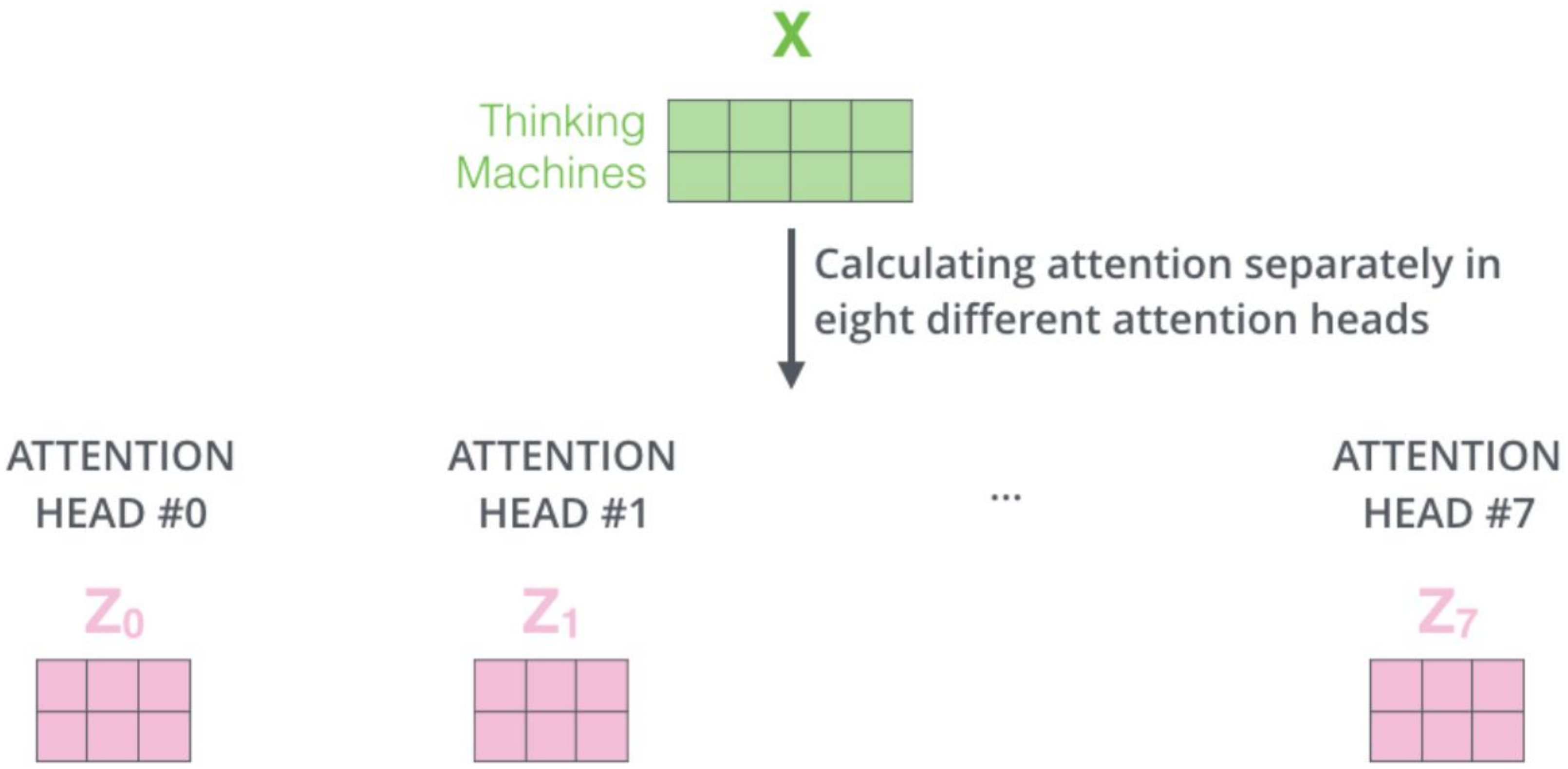
Self-Attention: Matrix Calculation



Multi-Head Attention



Multi-Head Attention



Multi-Head Attention

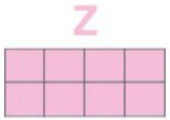
1) Concatenate all the attention heads

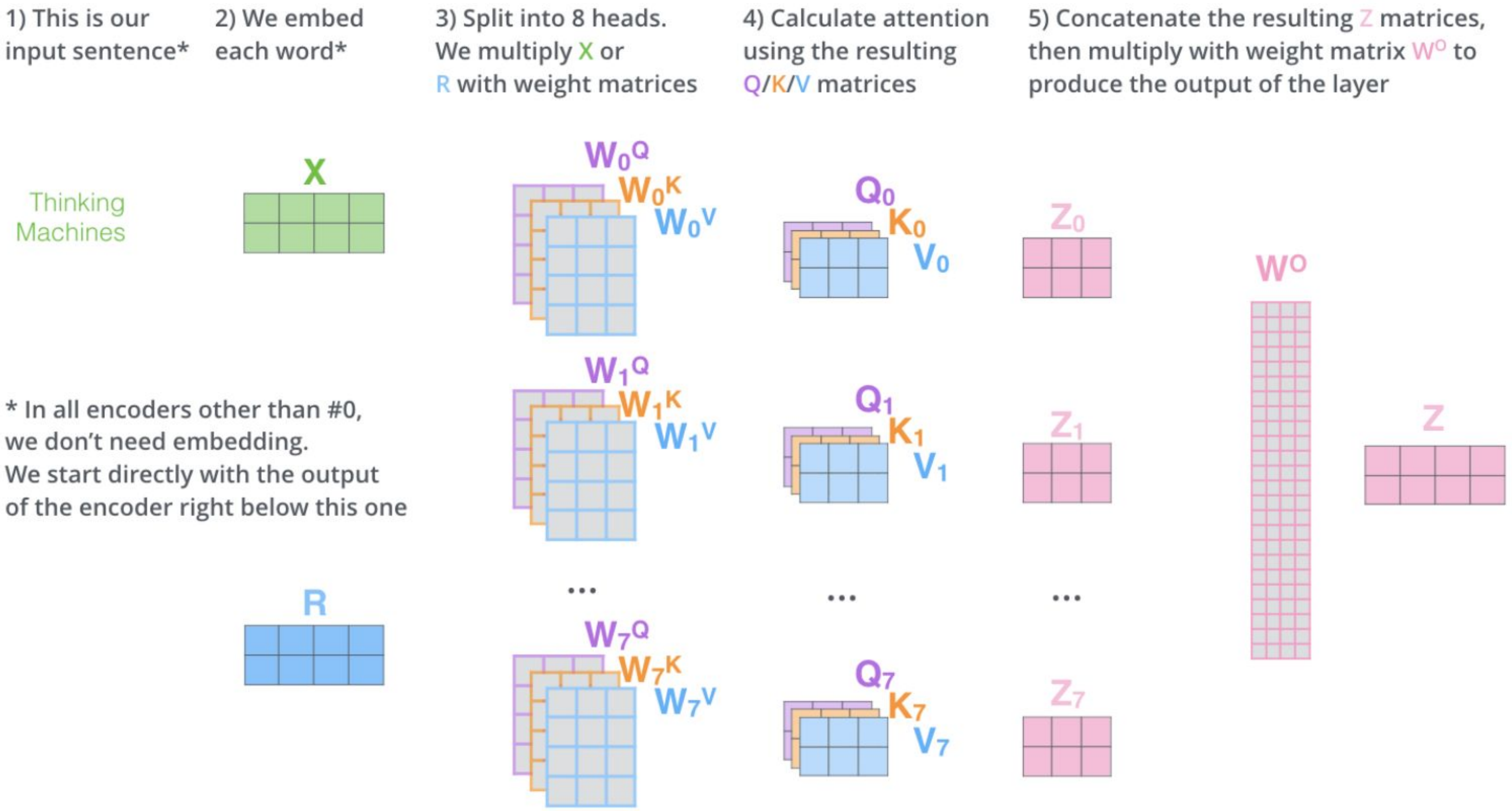
2) Multiply with a weight matrix W^O that was trained jointly with the model

X

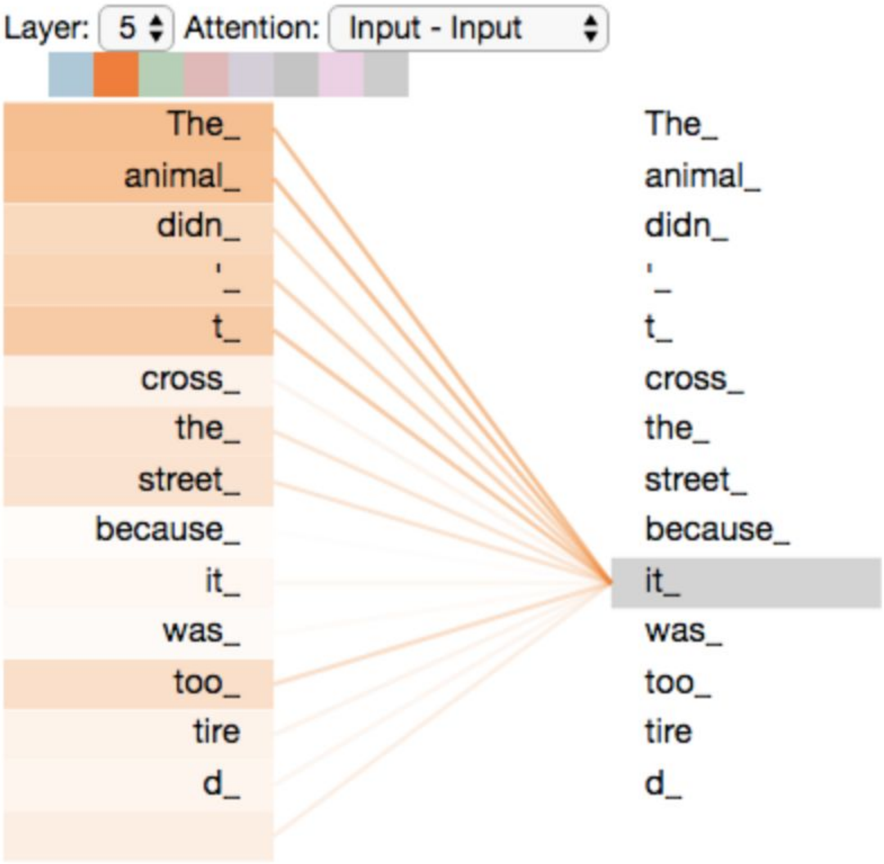
3) The result would be the Z matrix that captures information from all the attention heads. We can send this forward to the FFNN

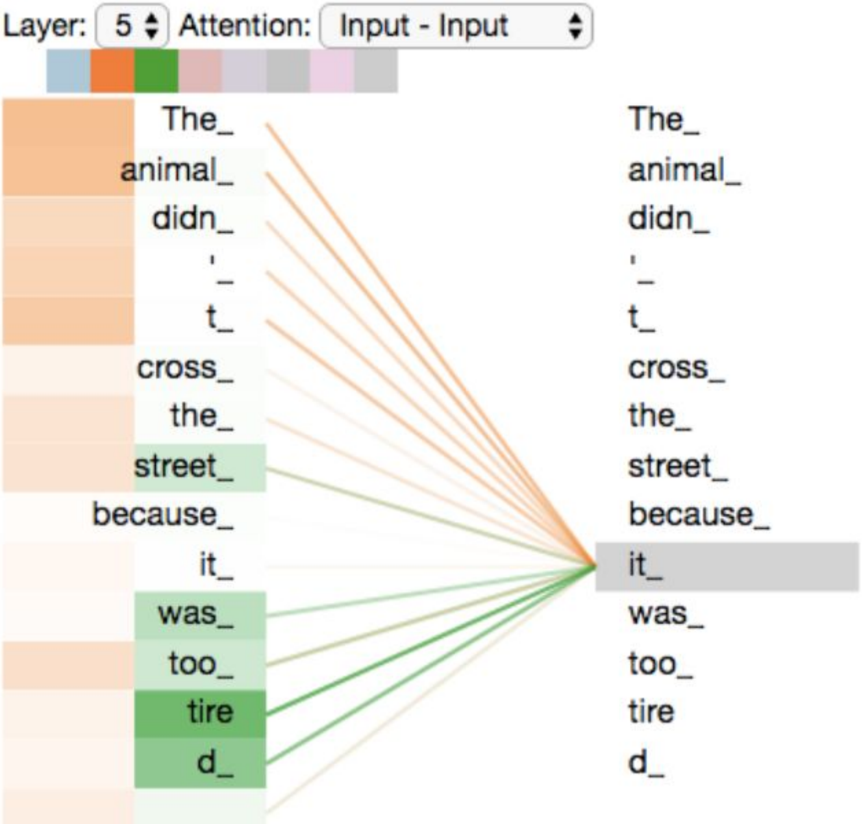
=



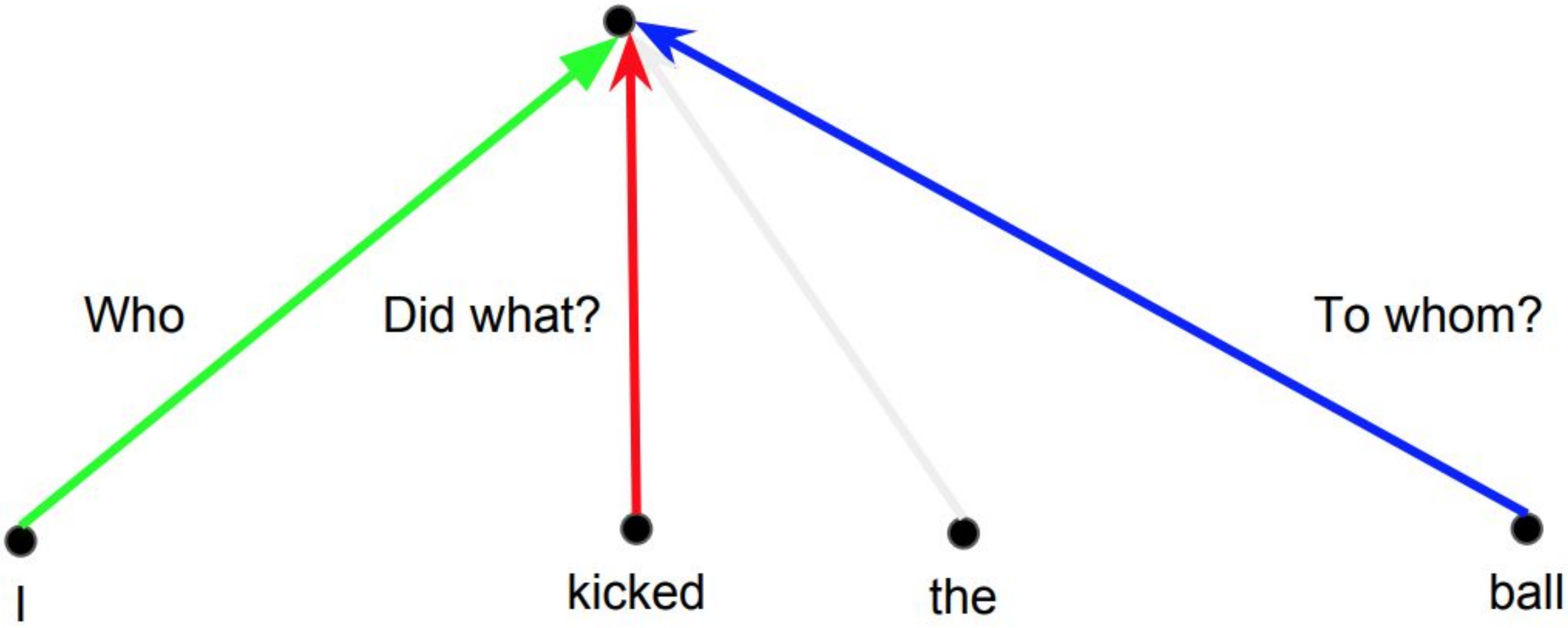

1) This is our input sentence*
2) We embed each word*
3) Split into 8 heads. We multiply X or R with weight matrices
4) Calculate attention using the resulting Q/K/V matrices
5) Concatenate the resulting Z matrices, then multiply with weight matrix W^O to produce the output of the layer
Thinking Machines
X
R
* In all encoders other than #0, we don't need embedding. We start directly with the output of the encoder right below this one
W_0^Q
W_0^K
W_0^V
W_1^Q
W_1^K
W_1^V
W_7^Q
W_7^K
W_7^V
Q_0
K_0
V_0
Q_1
K_1
V_1
Q_7
K_7
V_7
Z_0
Z_1
Z_7
W^O
Z
...

Multi-Head Attention

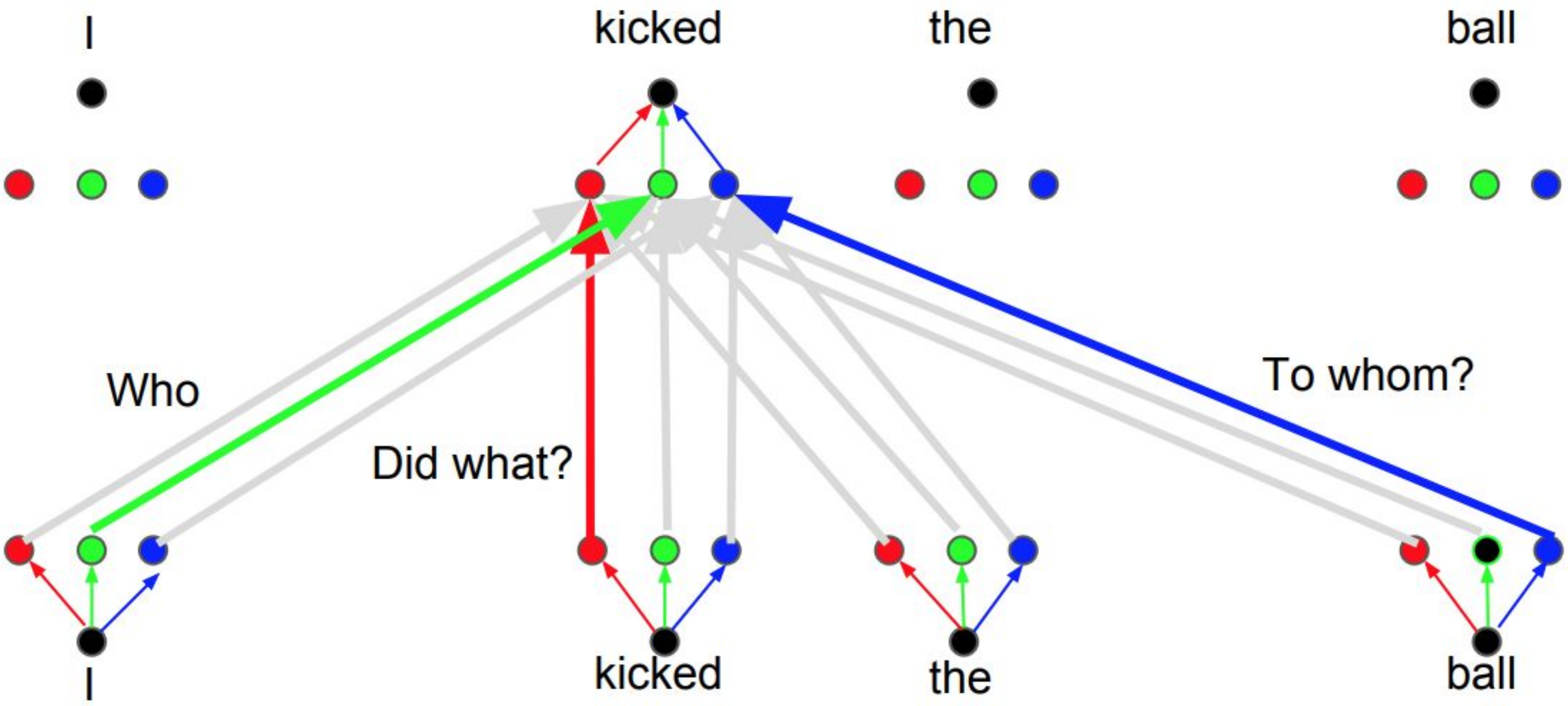




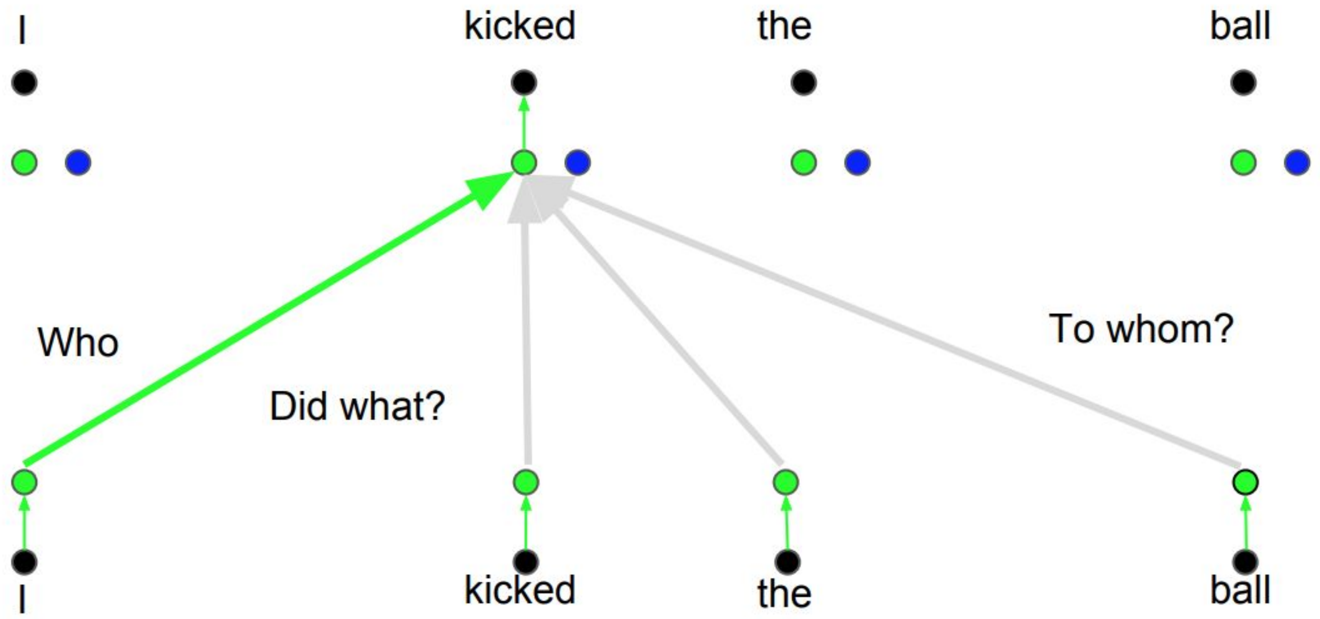
Why Multi-Head Attention?



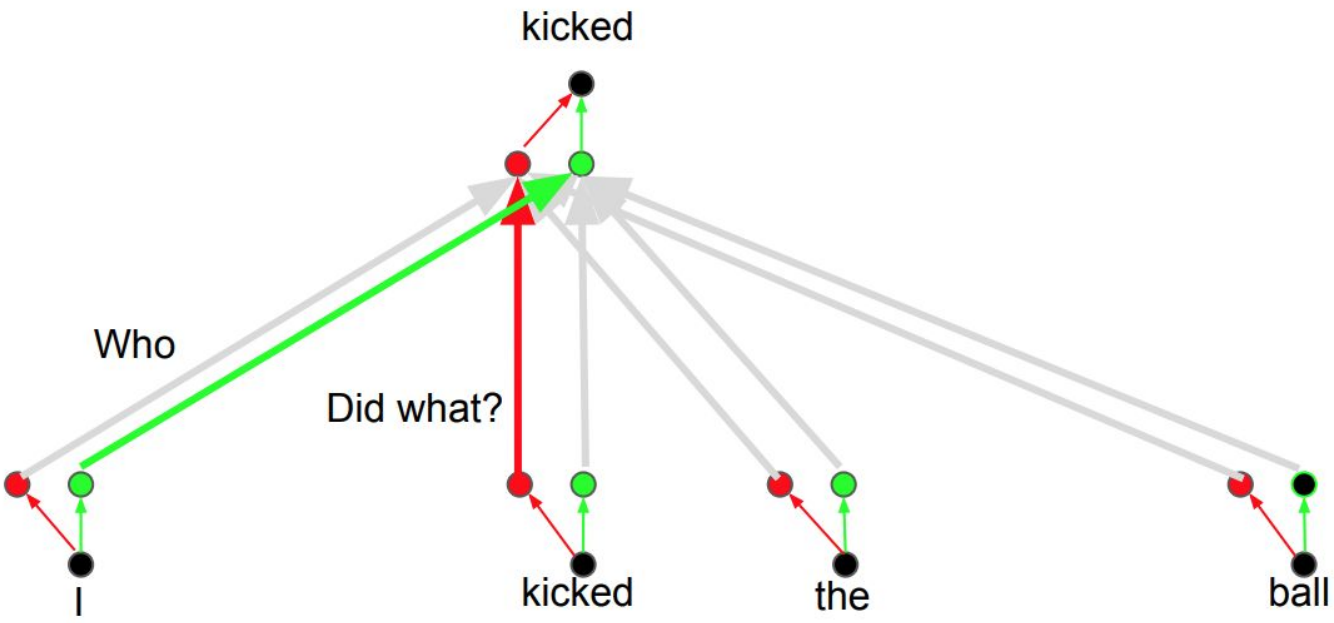
Why Multi-Head Attention?



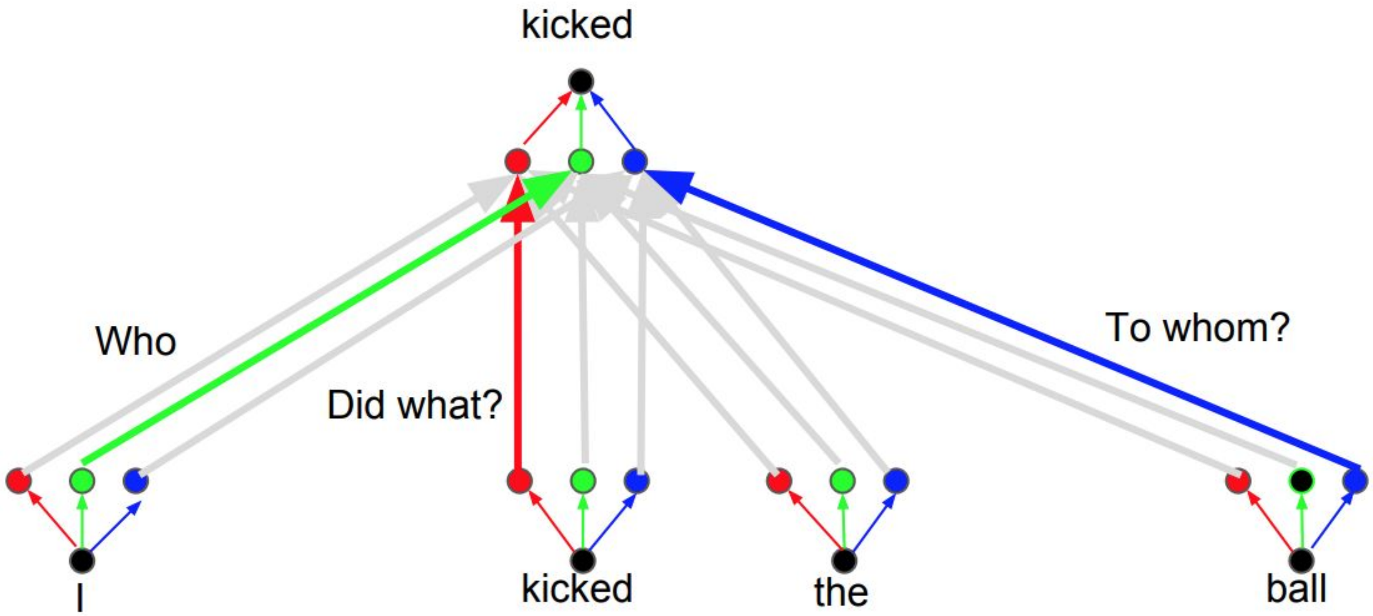
Attention head: Who



Attention head: Did What?

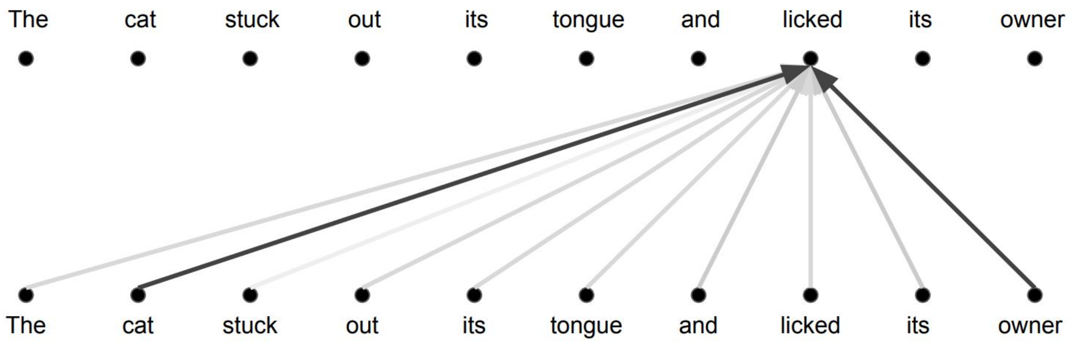


Attention head: To Whom?



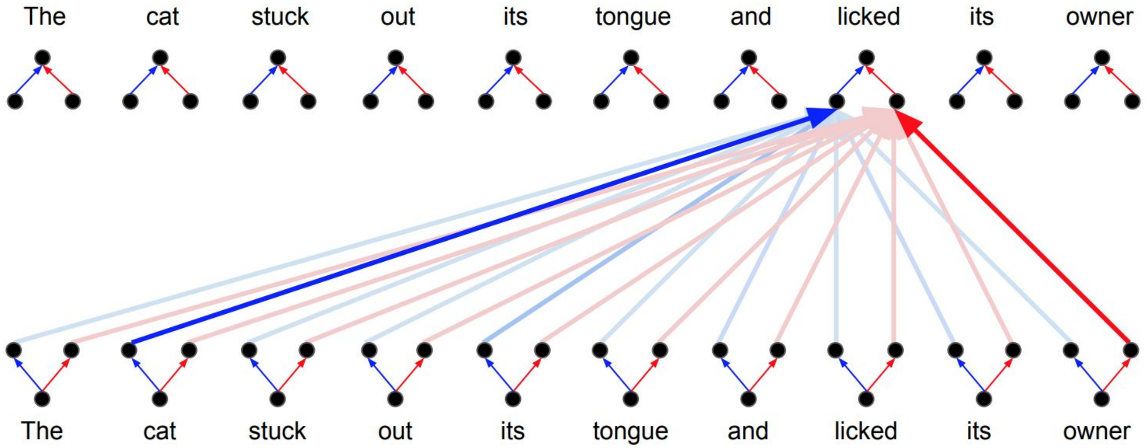
Attention vs. Multi-Head Attention

Attention: a weighted average



Multi-Head Attention:

parallel attention layers with different linear transformations on input and output.



Performance: WMT 2014 BLEU

	EN-DE	EN-FR
GNMT (orig)	24.6	39.9
ConvSeq2Seq	25.2	40.5
Transformer*	**28.4**	**41.8**

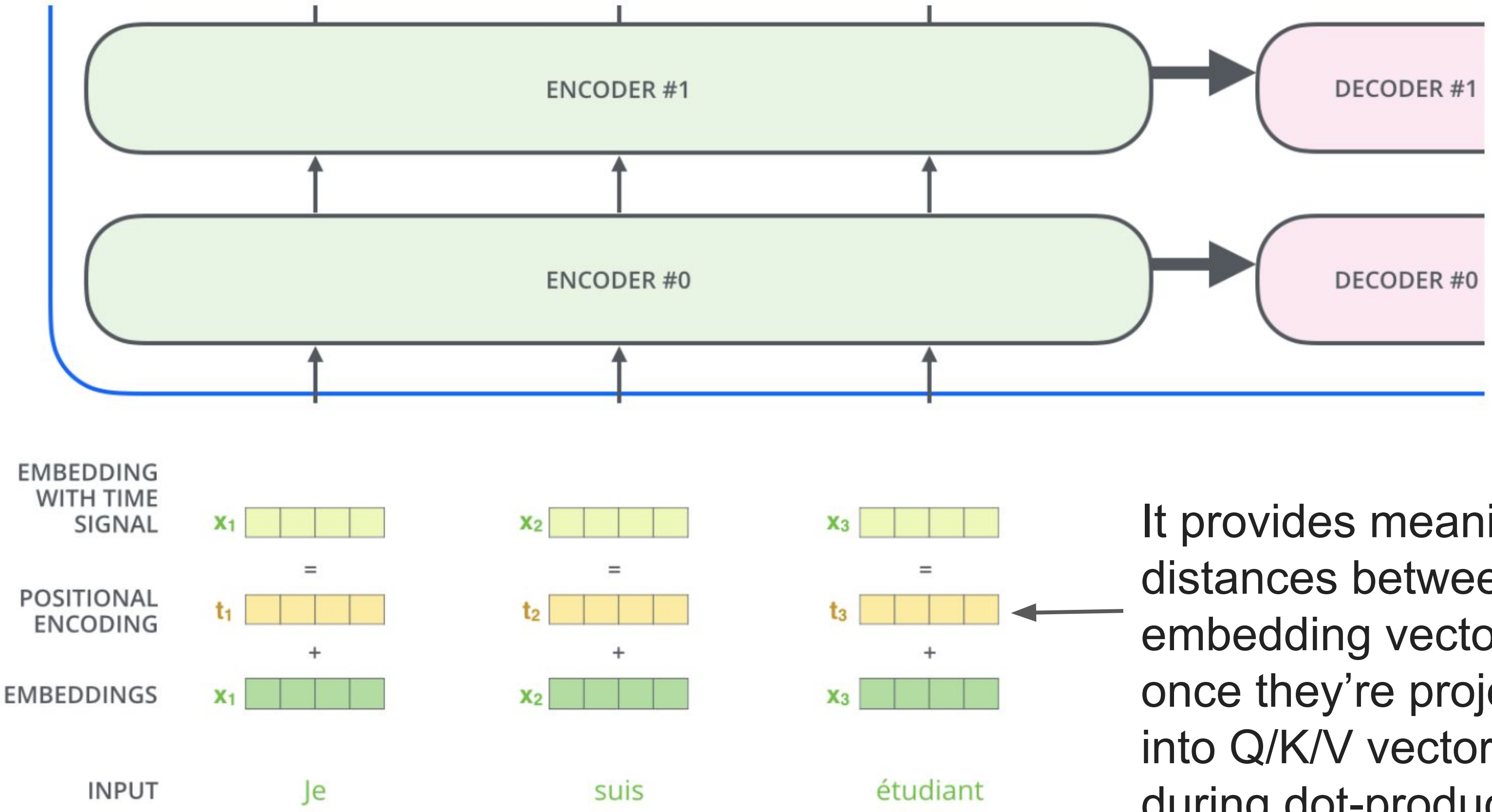
*Transformer models trained >3x faster than the others.

Research Challenges

- Constant ‘path length’ between any two positions.
- Unbounded memory.
- Trivial to parallelize (per layer).
- Models Self-Similarity.
- Relative attention provides expressive timing, equivariance, and extends naturally to graphs.

Positional Encoding

Positional Encoding



It provides meaningful distances between the embedding vectors once they're projected into Q/K/V vectors and during dot-product attention

Positional Encoding

$$PE_{(pos,\ 2i)} = sin(pos\,/\,10000^{2i\,/\,d_{\text{model}}})$$

$$PE_{(pos,\ 2i+1)} = cos(pos\,/\,10000^{2i\,/\,d_{\text{model}}})$$

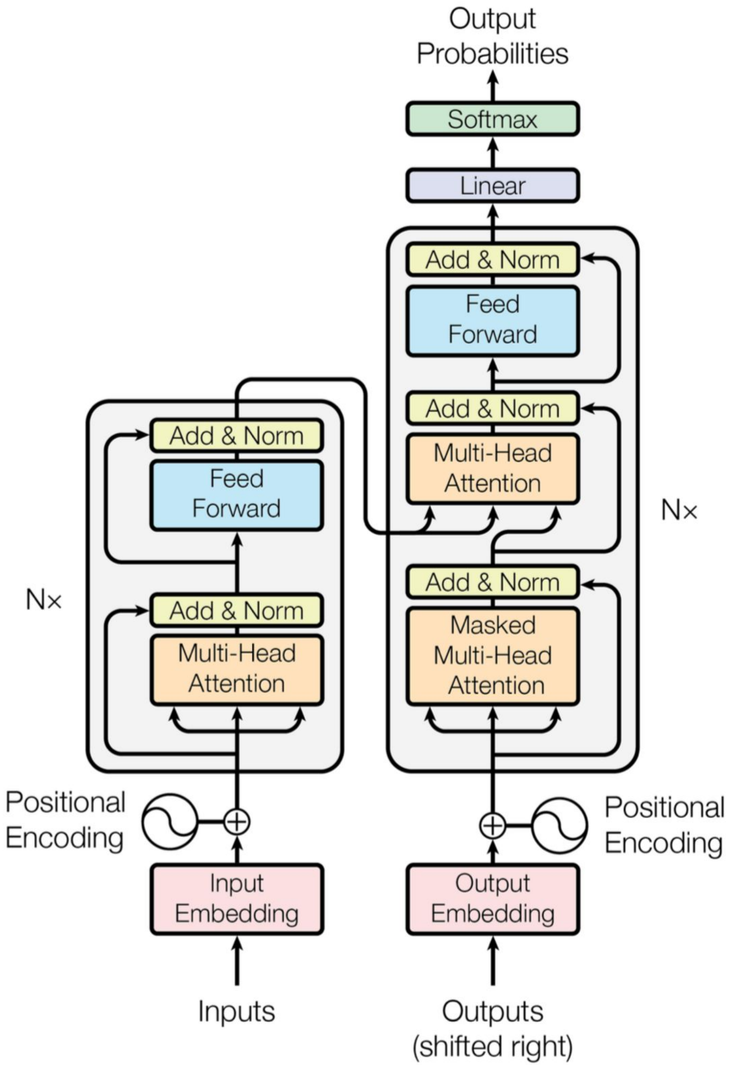
- *pos* is the position
- *i* is the dimension.

Each dimension of the positional encoding corresponds to a sinusoid.
The wavelengths form a geometric progression from 2pi to 2pi * 10 000

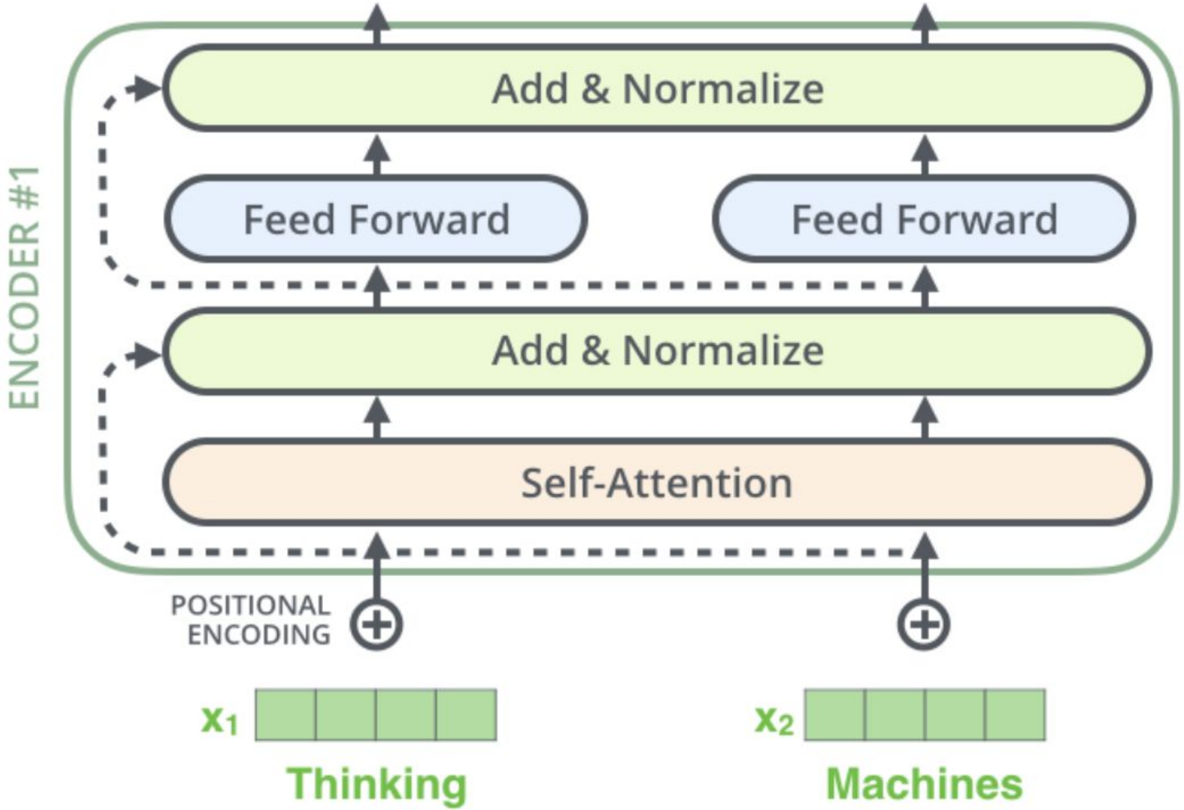
Positional Encoding

Layer Normalization

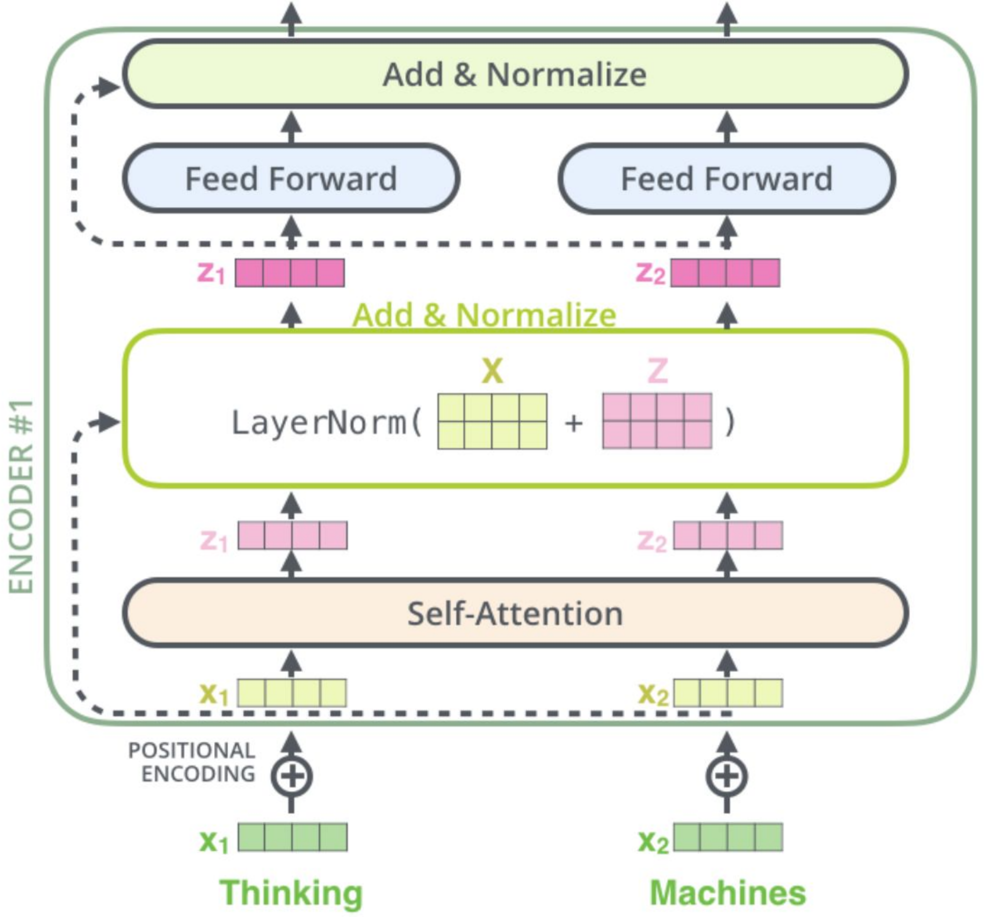
The Transformer: recap



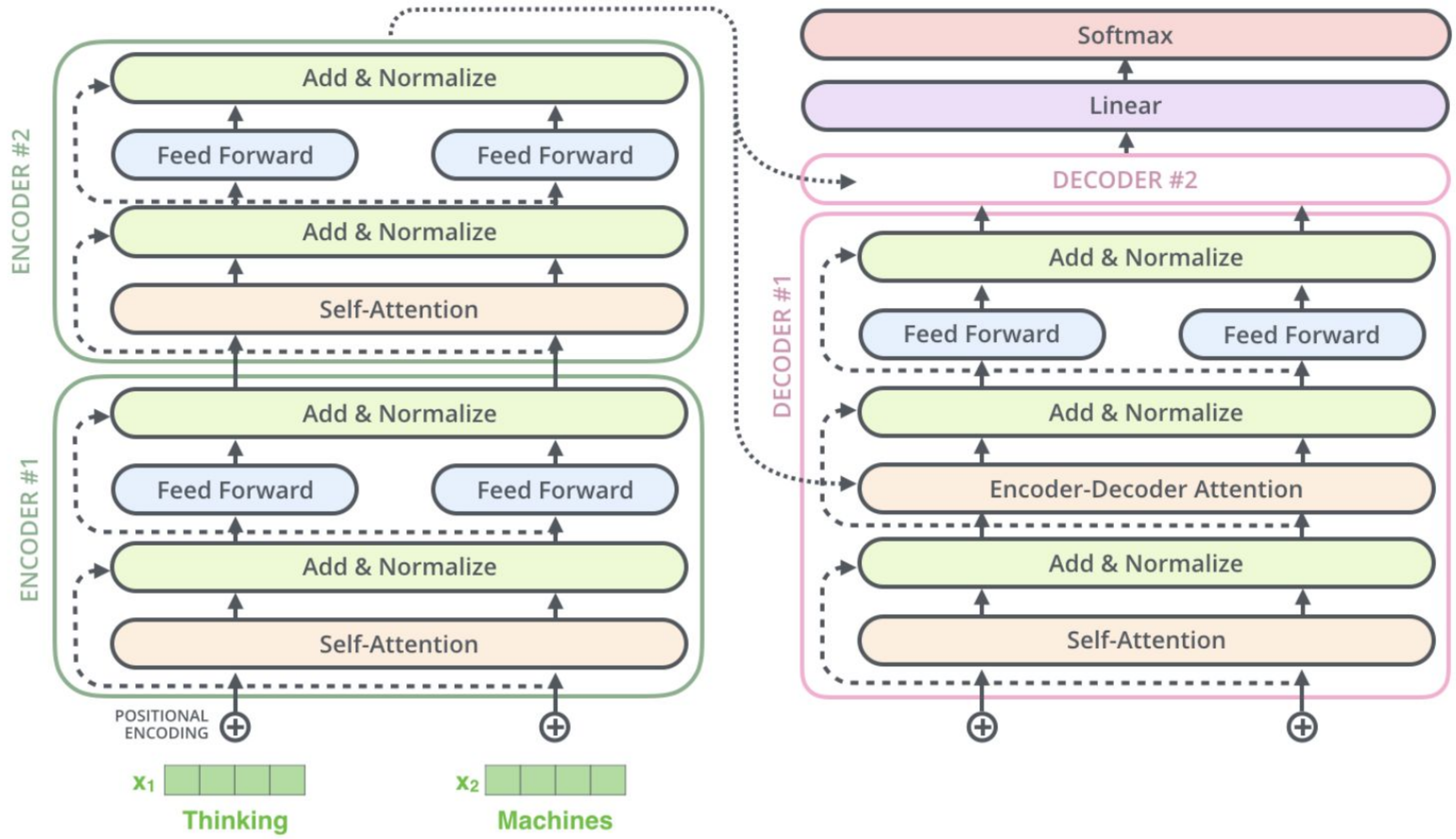
Layer Normalization



Layer Normalization

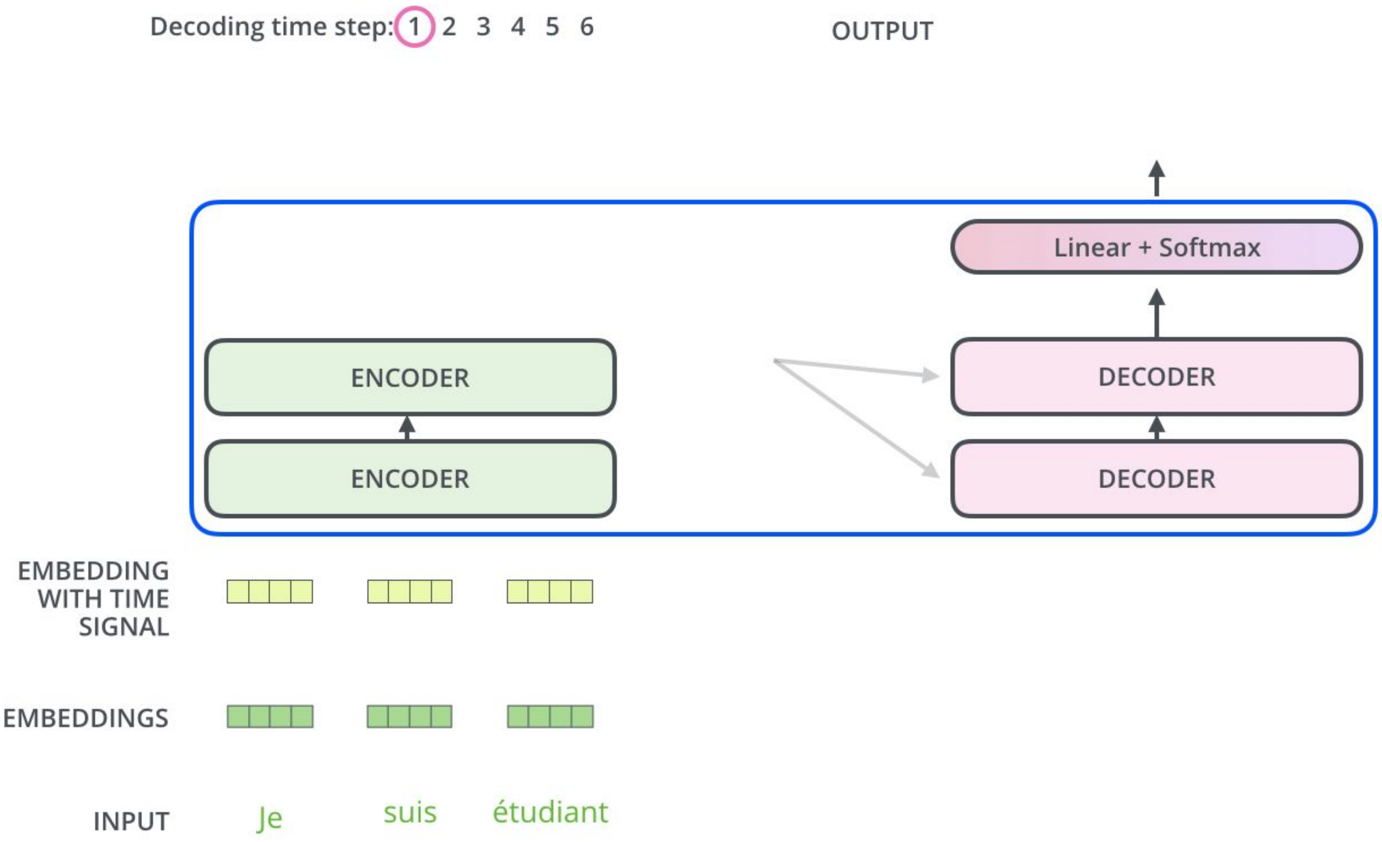


Layer Normalization



The Decoder

The Decoder Side



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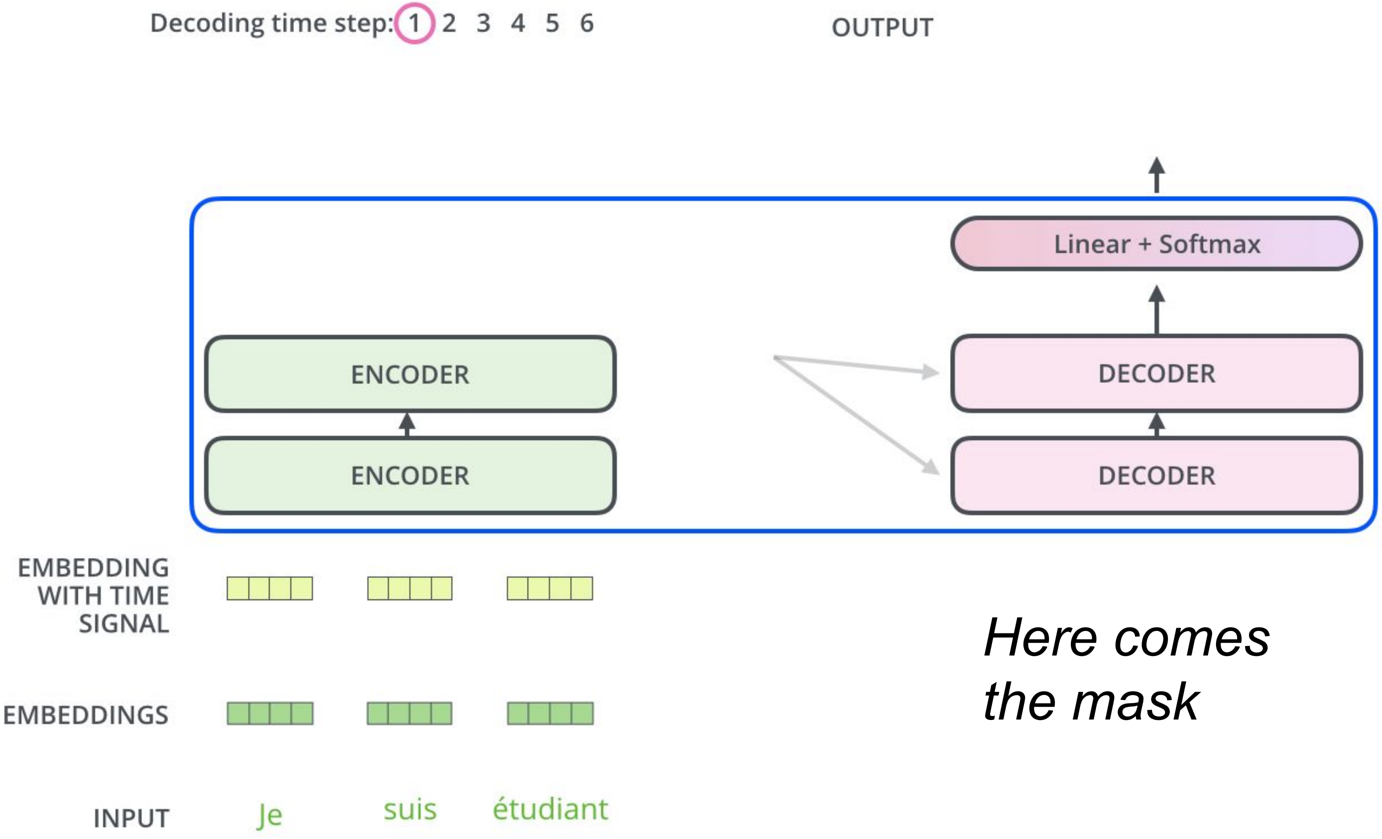
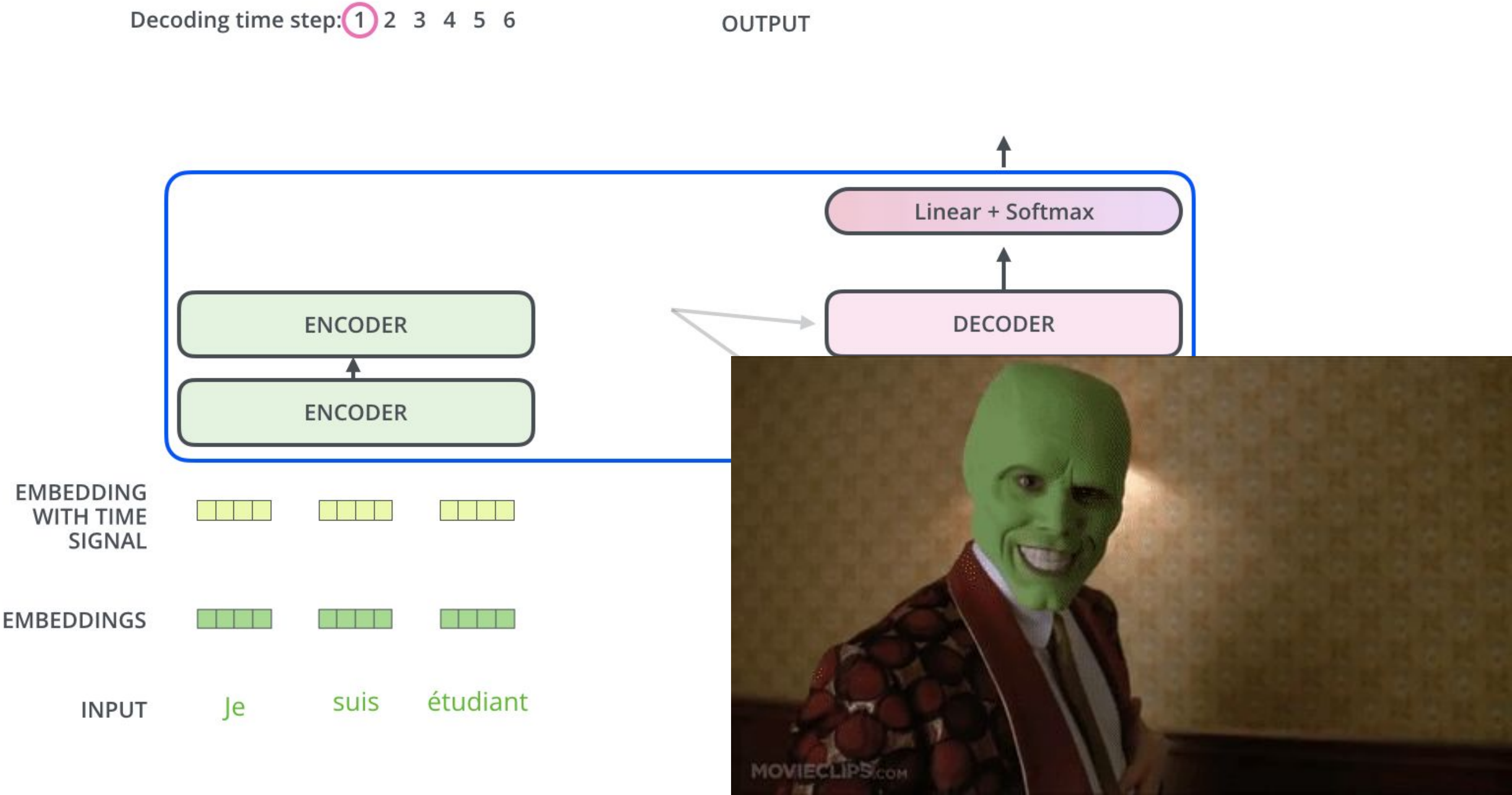
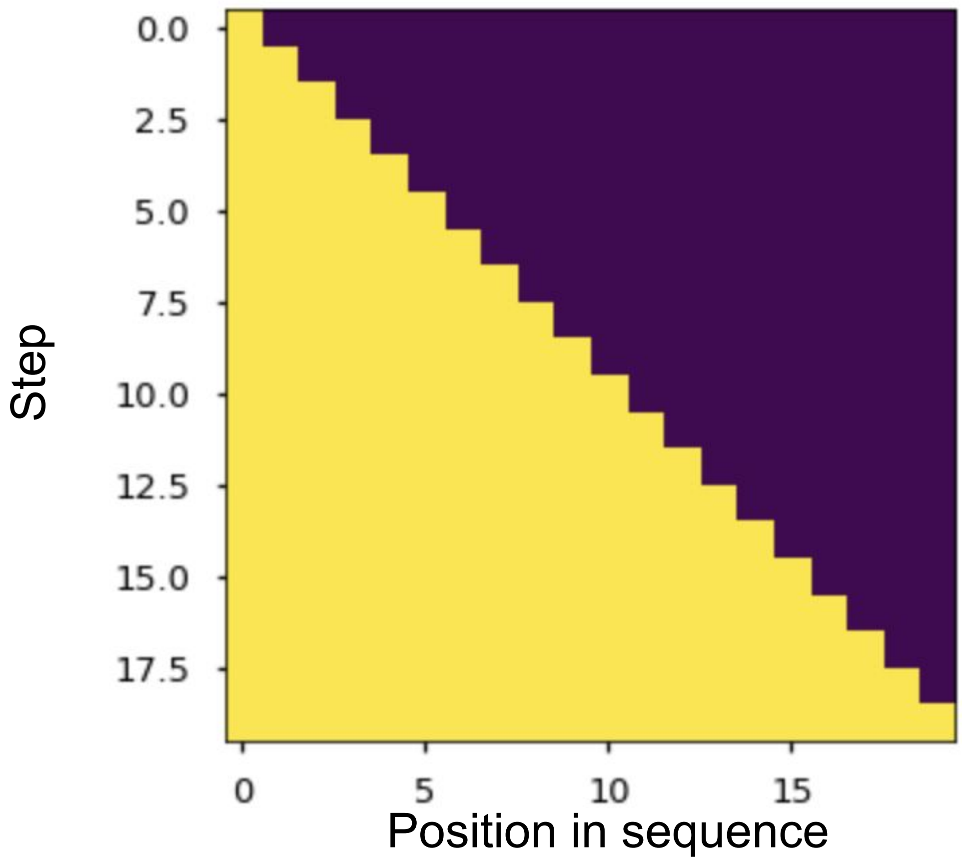


Here comes the mask

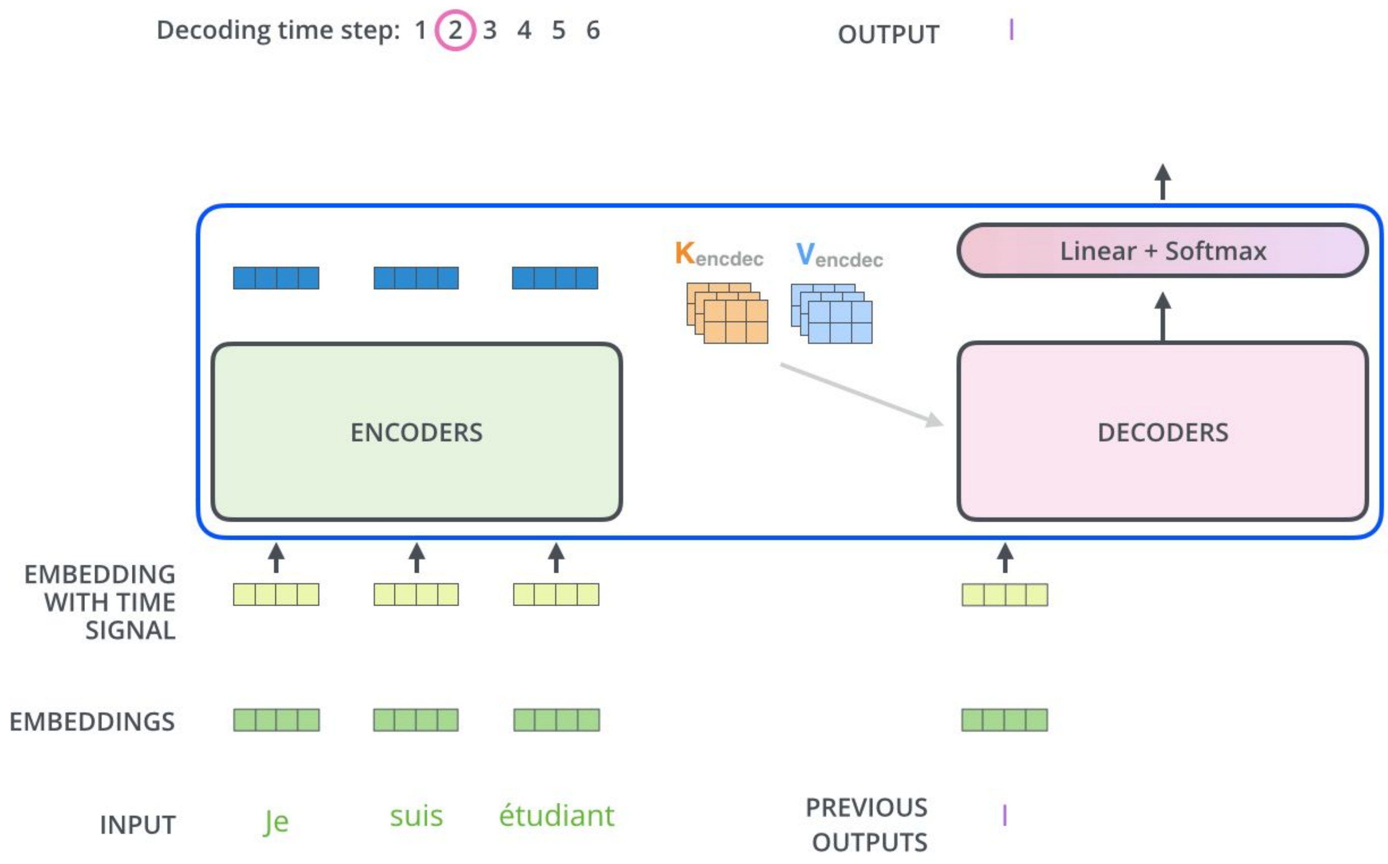
The Decoder Side



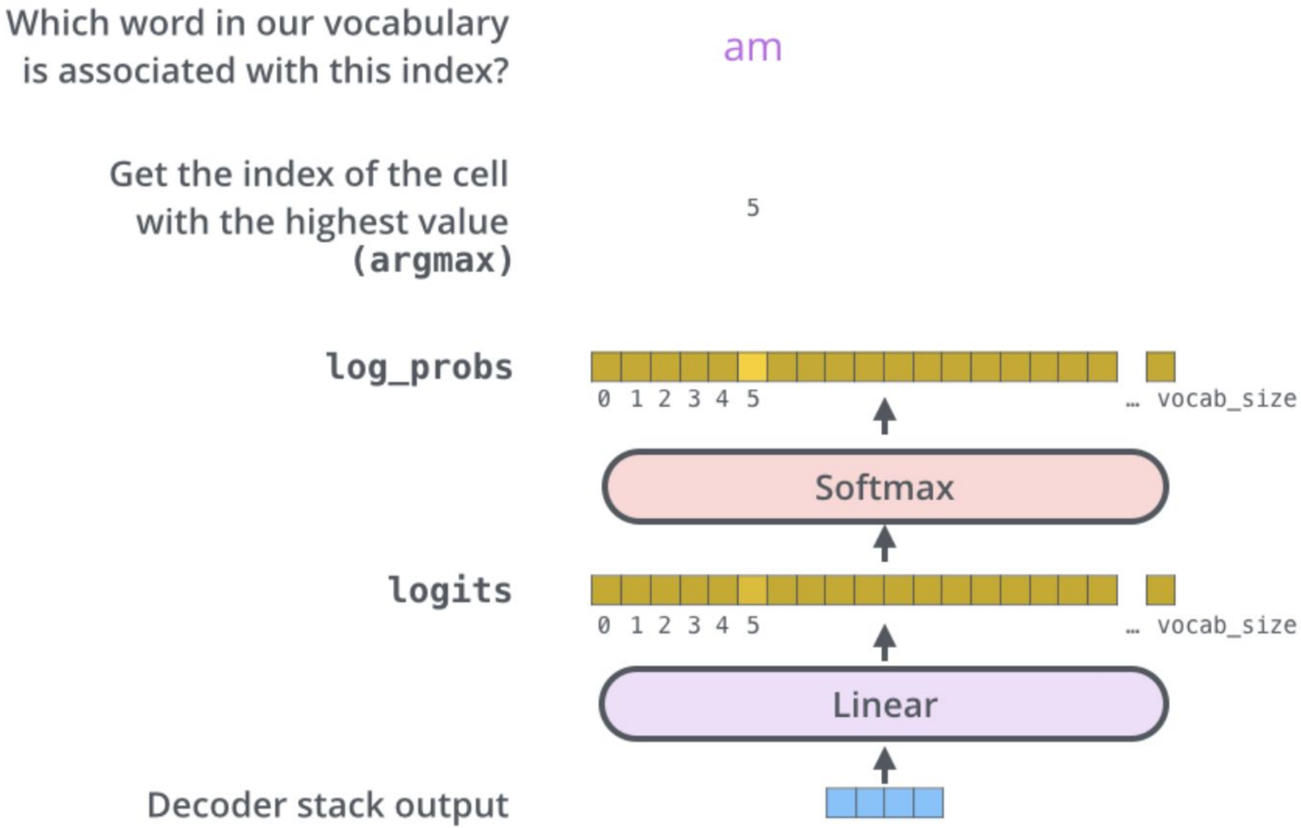
The masked decoder input



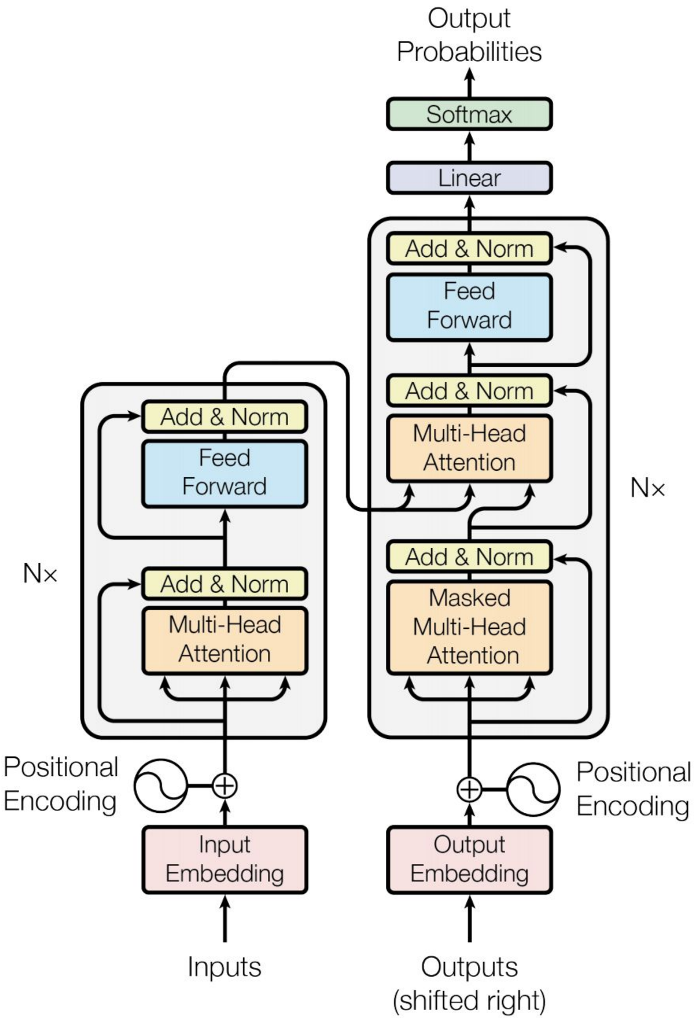
The Decoder Side



Final Linear and Softmax Layer



The Transformer



Outro and Q&A

- Transformer is novel and very powerful architecture
- It is worth it to understand how Self-Attention works
- Physical analogues can help you

- Further readings are available in the repo