

Advanced NLP -

Session 3: Attention & Transformers

Prof. Dr. Richard Sieg
TH Köln IWS - WS 25/26

Attention Is All You Need

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The Illustrated Transformer

by Jay Alammar

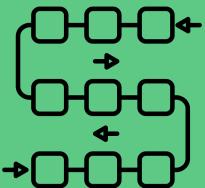
Agenda

01. Attention

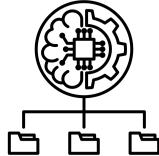
02. Transformer

03. Tutorial

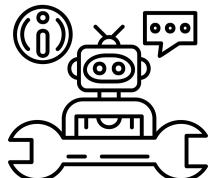
The 3 Ingredients of LLMs



Process long sequences and context



Efficient training on huge datasets



Follow (human) instructions

01.

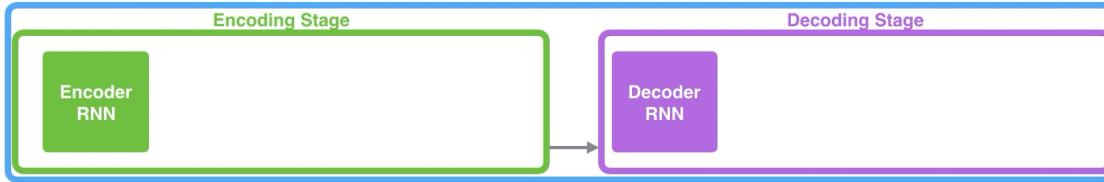
Attention

Recap: RNNs & LSTMs Issues

- The entire meaning of the source sentence is encapsulated in the last hidden state
- The decoder only uses this last hidden state but has not other interaction with the encoder
- Words are processed in sequential order and thus it is difficult to learn long-distance dependencies
- We have to compute the hidden states sequentially so we cannot parallelize and use GPUs for training and inference

Neural Machine Translation

SEQUENCE TO SEQUENCE MODEL



Je suis étudiant

Neural Machine Translation

SEQUENCE TO SEQUENCE MODEL WITH ATTENTION

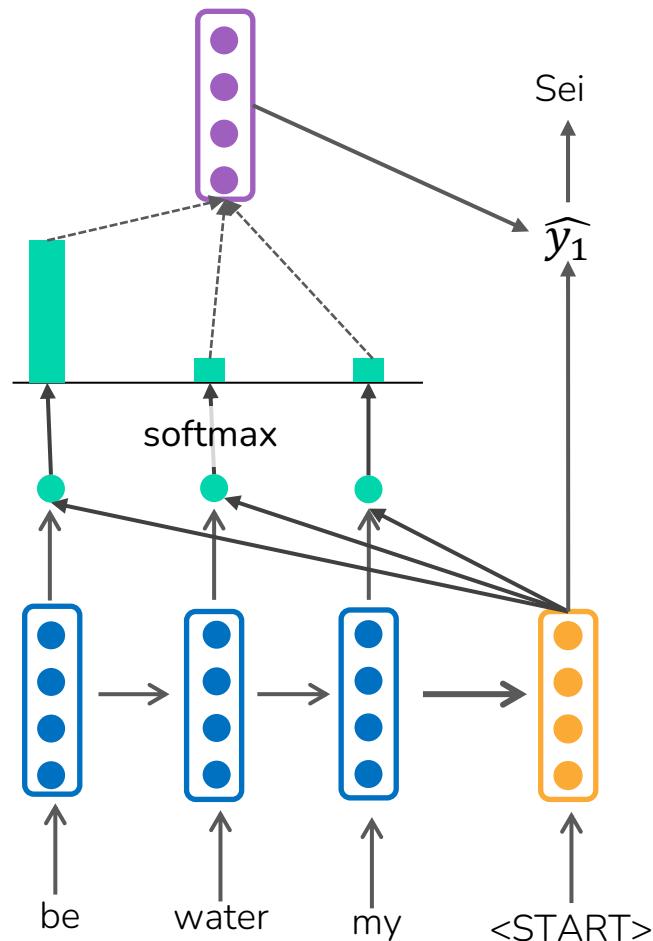


Je suis étudiant

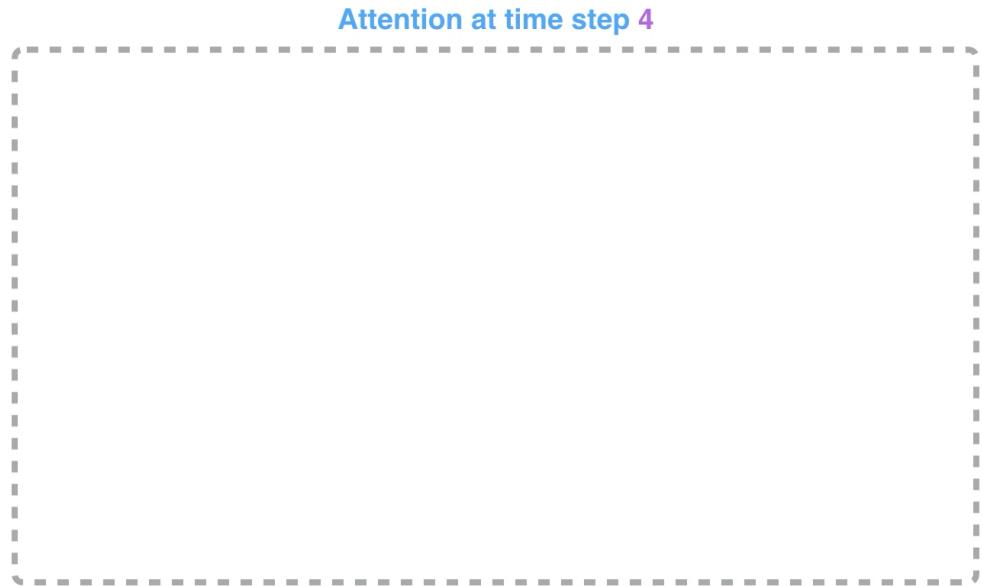
Attention Decoder
Bahdanau et al 2014
Luong et al 2015

Attention - Core Idea

- At each time step t in the decoder, we take the average of all encoder hidden states as an additional **context vector** combined with the hidden state
- Instead of just taking the normal average of all hidden states we take a **weighted average** depending on the current hidden state
- Weights are given by softmaxed **attention scores** so that they sum up to 1
- And these **attention scores** are learned by the neural network



1. The **Attention Decoder** receives **all** hidden states of the Encoder.
2. At each time step, we compute a score for each encoder hidden state (**attention**)
3. We multiply each hidden state with its **softmaxed** score
4. And add those vectors to get our new **context vector**
5. The context vector is then joined with the hidden state vector to generate the output distribution

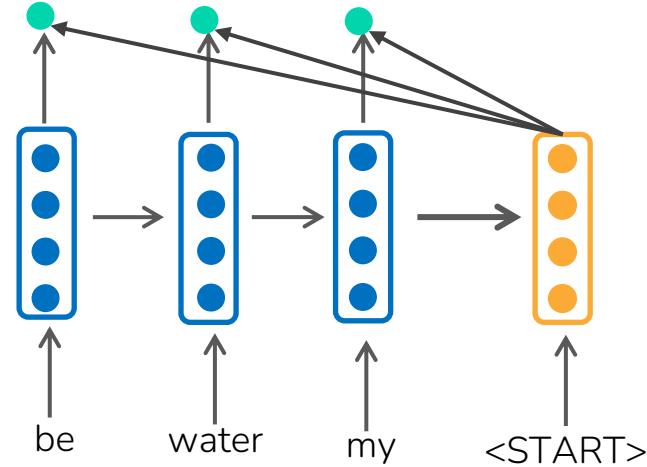


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Computing Attention Scores

- Easiest approach: Take the scalar/dot product between encoder and decoder hidden state $h_E \cdot h_D$
- More generally: Introduce a weight matrix: $h_E^T W h_d$
- Use a feed forward layer and project it to a scalar: $v^T \tanh(W_1 h_E + W_2 h_D)$



But still...

- The encoder and decoder work sequentially and we cannot parallelize computations
- The attention decoder now has all encoder hidden states but only the current decoder hidden state to work with
- Vanishing Gradients: Difficult to learn long-distance relationship

As it turns out:

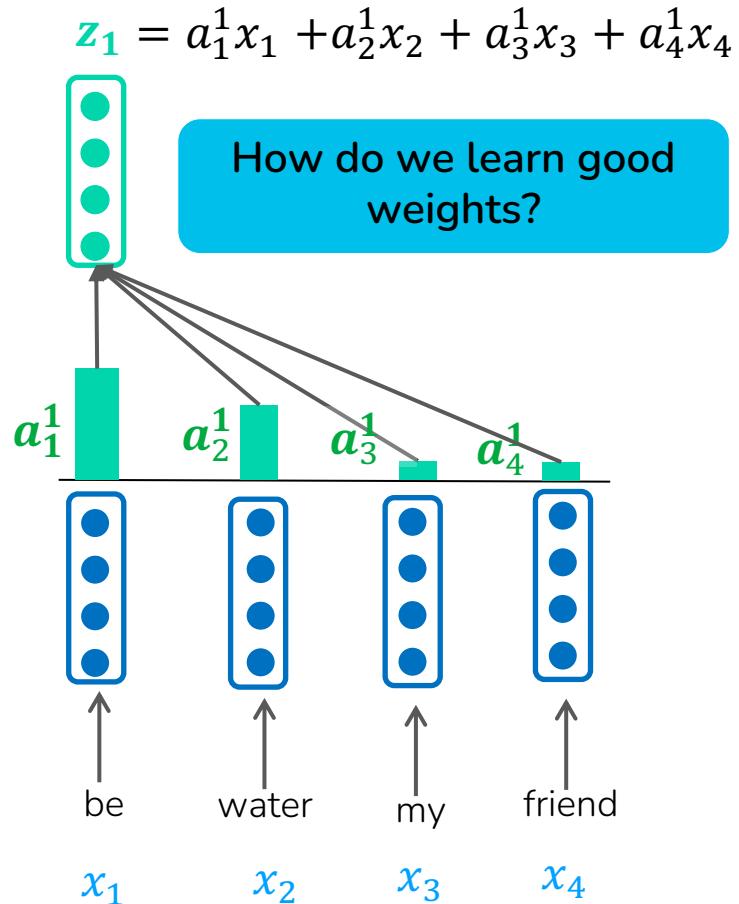
Attention Is All You Need

02.

Transformers

Self-Attention

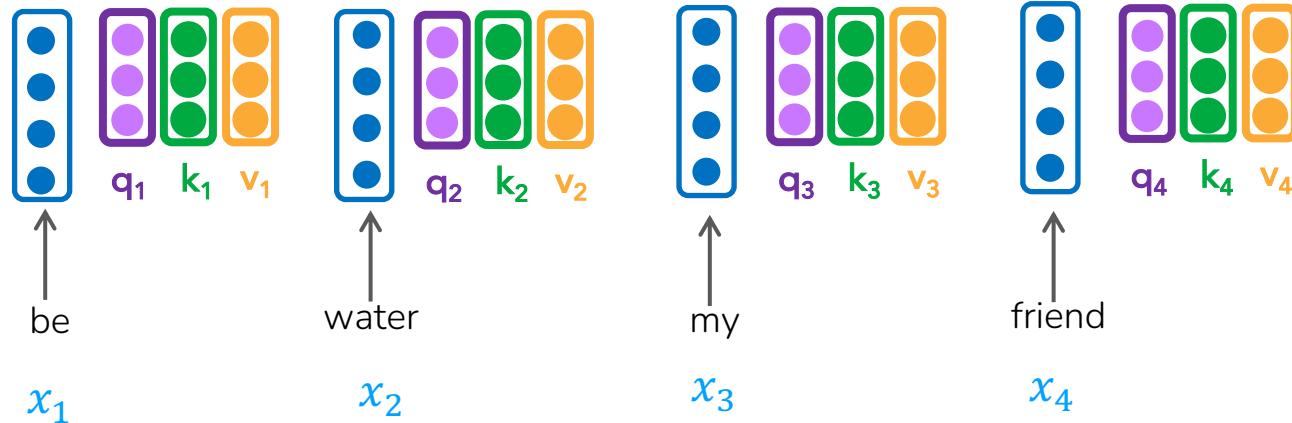
- Main idea: “Translate” a sequence into itself and calculate attention scores between the tokens of the sequence
- How much do the other (or previous) tokens in the sequence influence a token?
- This **self-attention** score yields a powerful representation of each token that encapsulates the whole context in a **context vector**
- And: All computations can be performed in parallel



Self-Attention

Divide by $\sqrt{\dim(k_i)}$ = 8 for more stability

$$\begin{array}{ll} s_4 = q_1 \cdot k_4 = 8 & a_4 = \sigma(s_4/8) = 0 \\ s_3 = q_1 \cdot k_3 = 16 & a_3 = \sigma(s_3/8) = .01 \\ s_2 = q_1 \cdot k_2 = 96 & a_2 = \sigma(s_2/8) = .12 \\ s_1 = q_1 \cdot k_1 = 112 & a_1 = \sigma(s_1/8) = .87 \end{array}$$



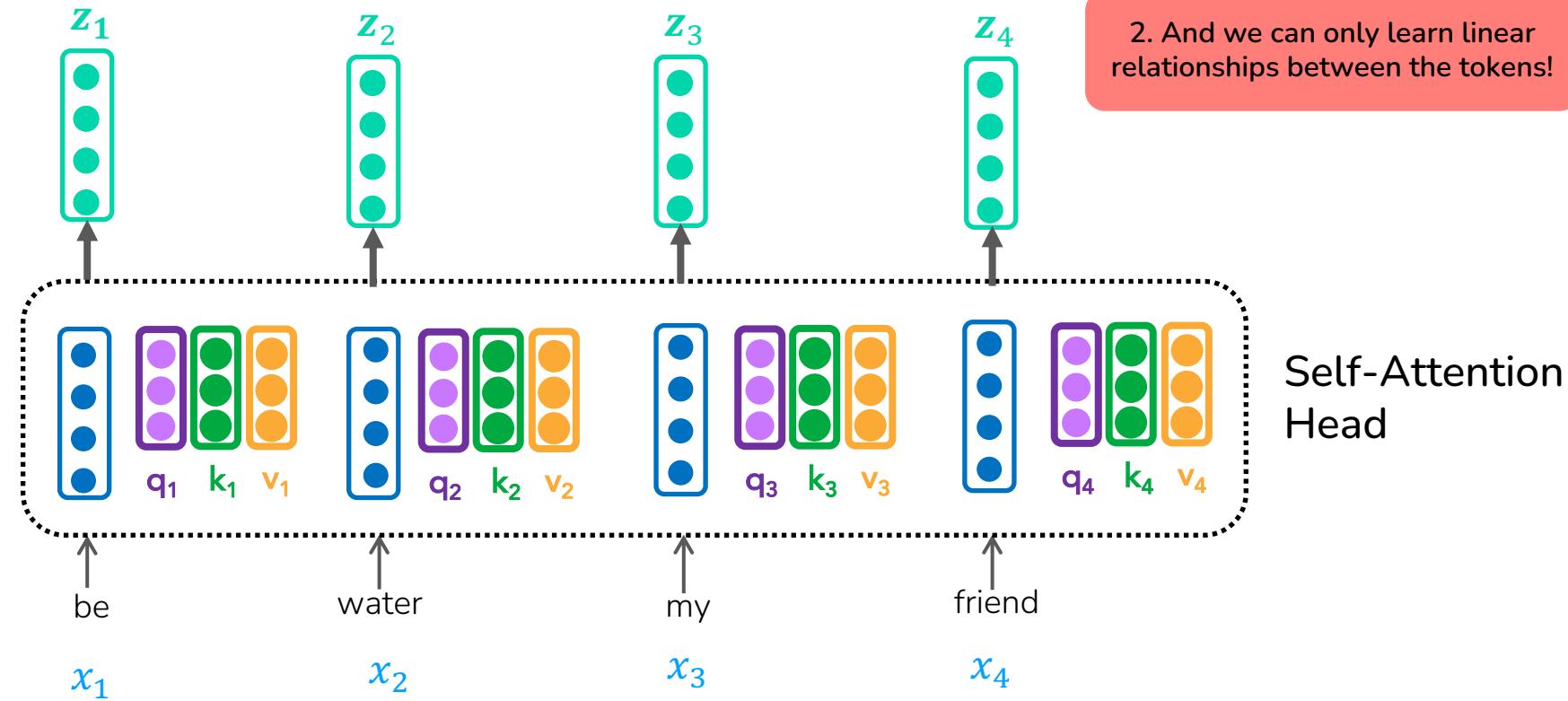
We need three weight matrices

$W_q, q_i = W_q x_i$	Queries
$W_k, k_i = W_k x_i$	Keys
$W_v, v_i = W_v x_i$	Values

$$\begin{aligned} z_1 &= a_1 \cdot v_1 + a_2 \cdot v_2 + a_3 \cdot v_3 + a_4 \cdot v_4 \\ &= 0.87 \cdot v_1 + 0.12 \cdot v_2 + 0.01 \cdot v_3 + 0 \cdot v_4 \end{aligned}$$

$$\text{Attention}(Q, K, V) = \sigma(QK^T / \sqrt{d_k})V$$

Self-Attention

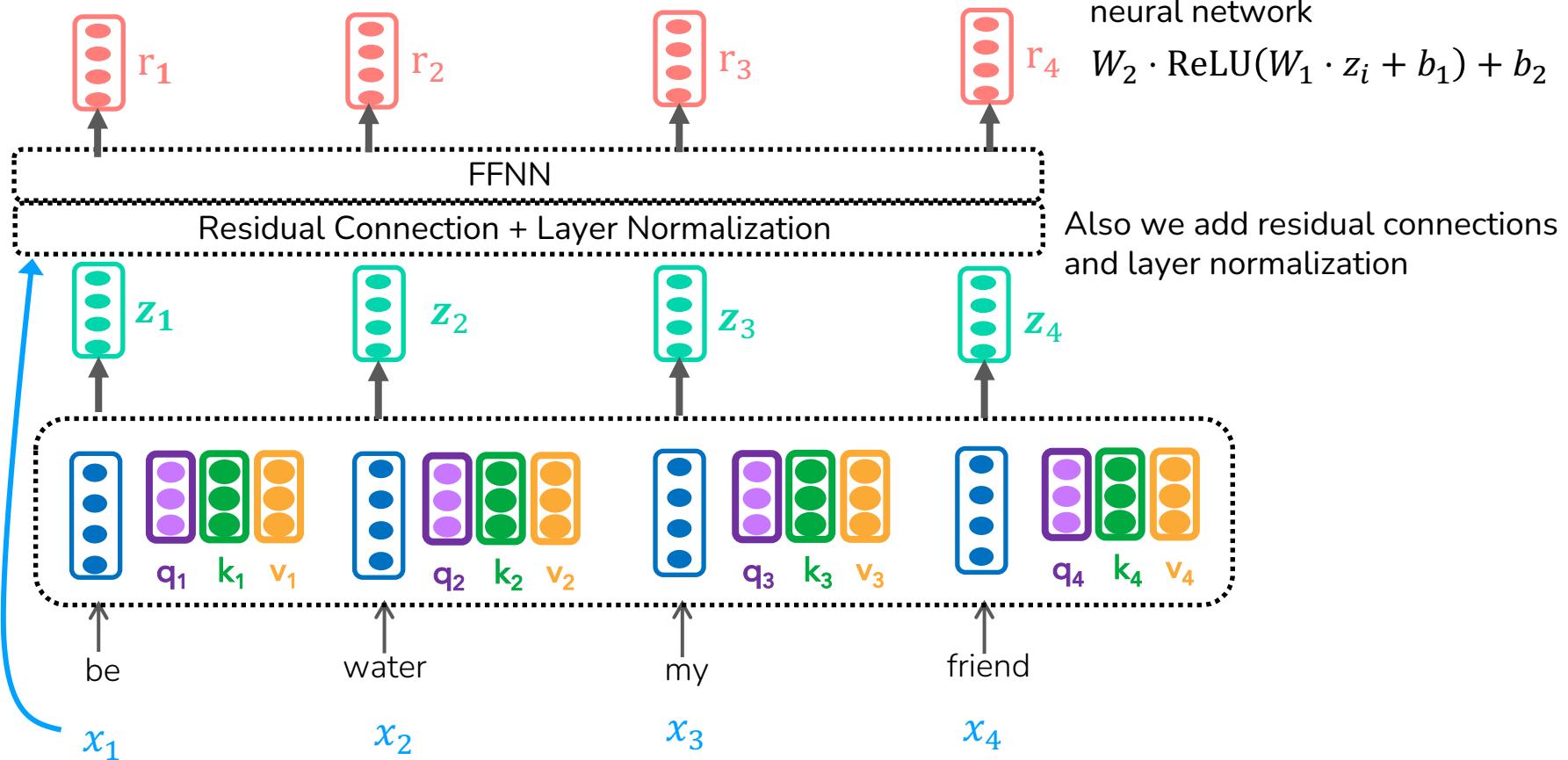


Fix: Sequence Order

- We do not have a concept for the position of a word (same as bag of words)
- **Solution:** Add position vectors to the embedding inputs $\tilde{x}_i = x_i + p_i$ where $p_i \in \mathbb{R}^d$ (**positional embedding**)
- These position vectors can be fixed or learned (out of scope of this lecture)
- Examples of fixed position vectors
- One-hot encodings $p_i = (0, \dots, 0, 1, 0, \dots, 0)$ (not useful in practice)
- **Sinusoidal** (original paper uses this)

$$p_i = (\sin(i/10000^{2 \cdot 1/d}), \cos(i/10000^{2 \cdot 1/d}), \dots, \sin(i/10000^{2 \cdot d/2/d}), \cos(i/10000^{2 \cdot d/2/d}))$$

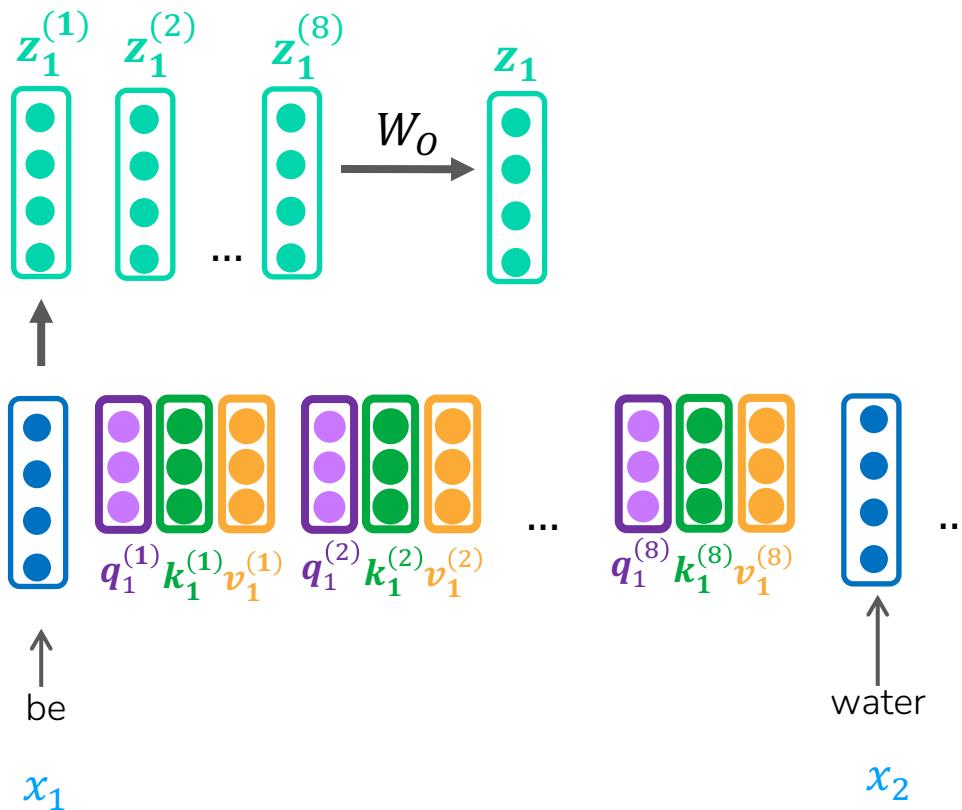
Fix: Non-Linearity



Let's stack things up!



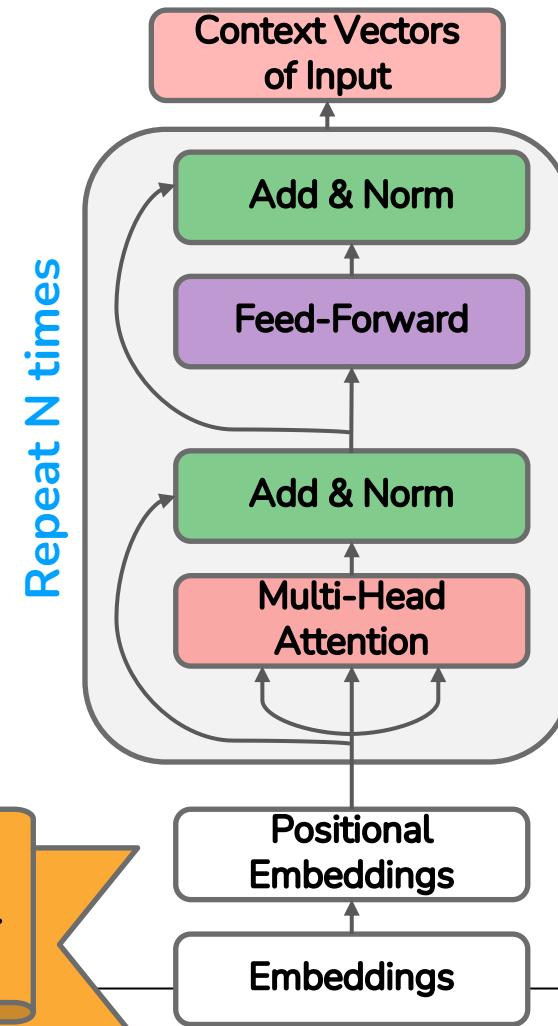
Multi-Head Attention



- We can use multiple weight matrices W_q, W_k, W_v in parallel
- This allows tokens to focus on different positions
- We call each set of these matrices an **attention head**
- The output z_i of each attention head is then concatenated $[z_1, \dots, z_h]$ and then projected back to the original dimension with a weight matrix W_o

Transformer Encoder

- Now we can stack multiple Transformer Blocks on top of each other.
- Each block has:
 - Multi-head attention
 - Residual connections and layer normalization
 - Feed-Forward Layer
 - Another layer of residual connections and normalization



We have built a
Transformer Encoder

Transformer Decoder

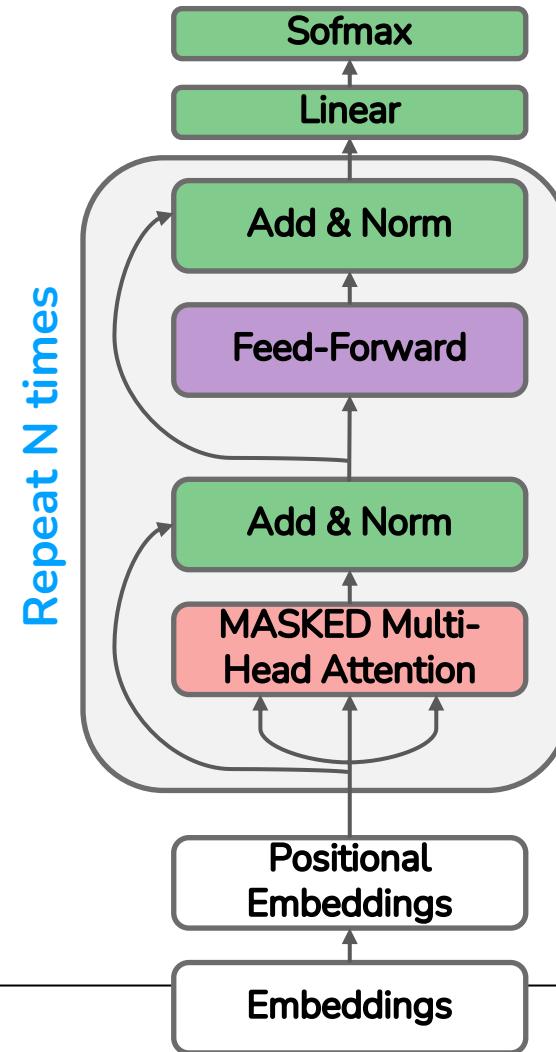
- The Decoder has to generate the output sequence
- So, during training we need to make sure that the Decoder can't look into the future
- Solution: Mask out the attention by setting the attention of future words to $-\infty$
- Our attention matrix becomes

$$e_{ij} = \begin{cases} q_i^T k_j, & j \leq i \\ -\infty, & j > i \end{cases}$$

		<Start>	be	water	my	friend
<START>		$-\infty$	$-\infty$	$-\infty$	$-\infty$	$-\infty$
be			$-\infty$	$-\infty$	$-\infty$	$-\infty$
water				$-\infty$	$-\infty$	$-\infty$
my						$-\infty$
friend						

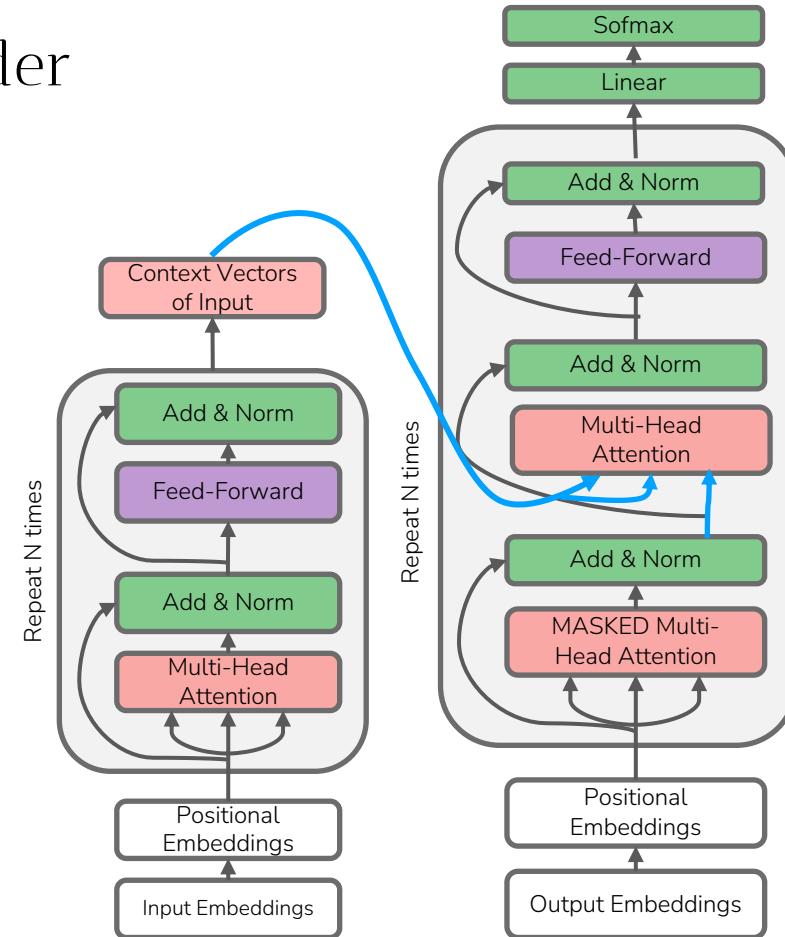
Transformer Decoder

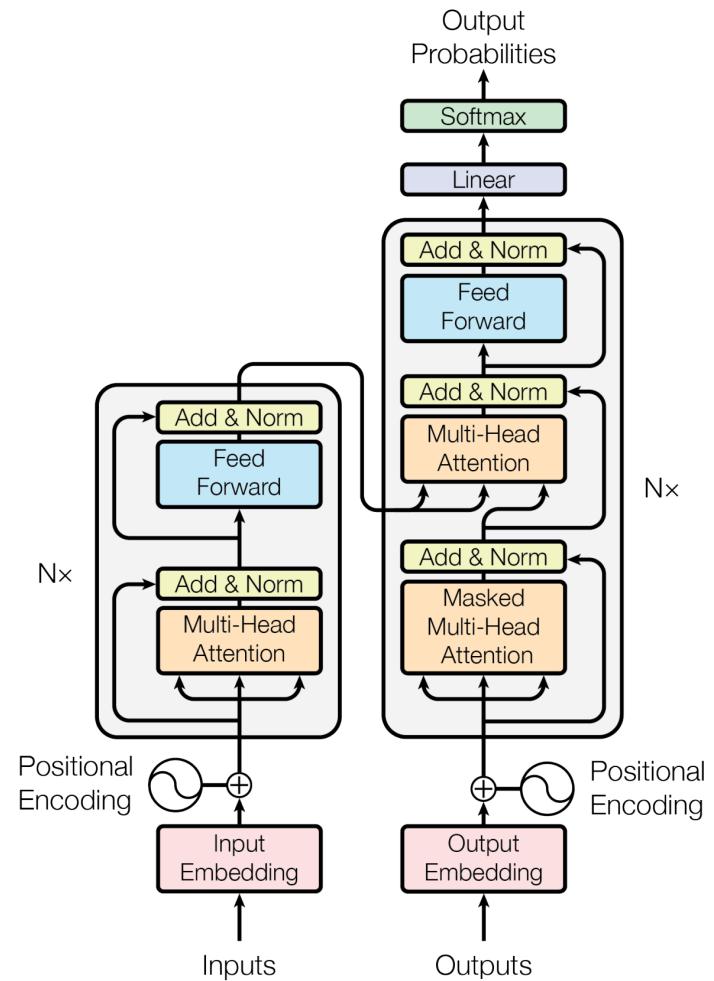
- The Transformer Decoder Block is the same as the Encoder just with Masked Multi-Head Attention
- So, the Decoder performs as an **auto-regressive** Language Model 🎉
- In the end, we add a Linear and a Softmax Layer to get the next word probabilities



The Transformer Encoder-Decoder

- For seq2seq tasks like Machine Translation, we can couple the Encoder and Decoder
- For this we add another Multi-Head Attention Block to the Decoder that receives the output vectors z_1, \dots, z_n from the Encoder (**Cross-Attention**)
- In this block, the keys and values are computed using the Encoder output vectors and the queries are computed using the Decoder input vectors h_1, \dots, h_n
- $k_i = W_k z_i, v_i = W_v z_i, q_i = W_q h_i$





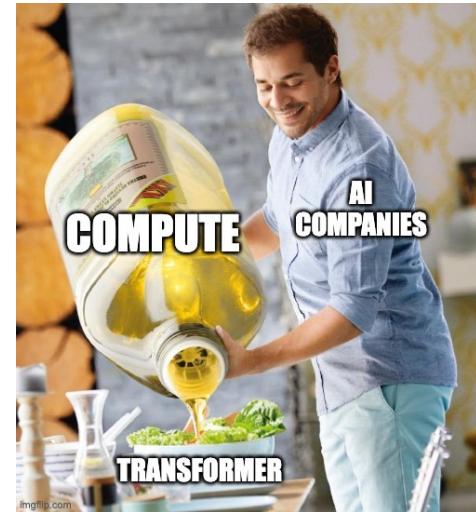
The Success of the Transformer

Model	BLEU		Training Cost (FLOPs)	
	EN-DE	EN-FR	EN-DE	EN-FR
ByteNet [18]	23.75			
Deep-Att + PosUnk [39]		39.2		$1.0 \cdot 10^{20}$
GNMT + RL [38]	24.6	39.92	$2.3 \cdot 10^{19}$	$1.4 \cdot 10^{20}$
ConvS2S [9]	25.16	40.46	$9.6 \cdot 10^{18}$	$1.5 \cdot 10^{20}$
MoE [32]	26.03	40.56	$2.0 \cdot 10^{19}$	$1.2 \cdot 10^{20}$
Deep-Att + PosUnk Ensemble [39]		40.4		$8.0 \cdot 10^{20}$
GNMT + RL Ensemble [38]	26.30	41.16	$1.8 \cdot 10^{20}$	$1.1 \cdot 10^{21}$
ConvS2S Ensemble [9]	26.36	41.29	$7.7 \cdot 10^{19}$	$1.2 \cdot 10^{21}$
Transformer (base model)	27.3	38.1	$3.3 \cdot 10^{18}$	
Transformer (big)	28.4	41.8	$2.3 \cdot 10^{19}$	

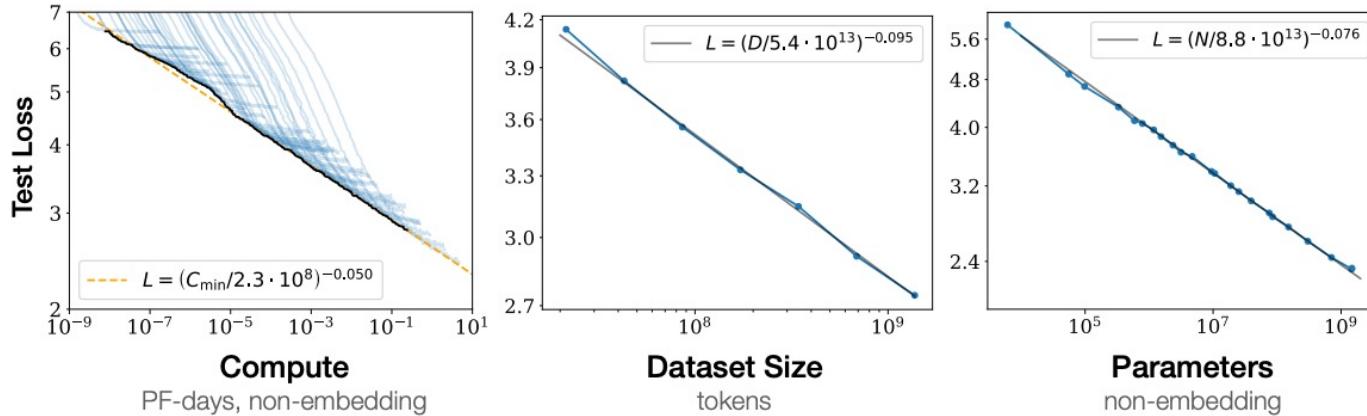
	Base	Big
Layers in Encoder & Decoder	6	6
#Heads	8	16
Model Dimension	512	1024
Feed-Forward Dimension	2048	4096

The Success of the Transformer

- As it turns out, the Transformer architecture is amazing for pre-training models on huge datasets (see next lecture)
- And the Encoder (BERT etc) or Decoder (GPT etc) themselves make great Language Models
- The rest is scaling (although attention has quadratic costs)

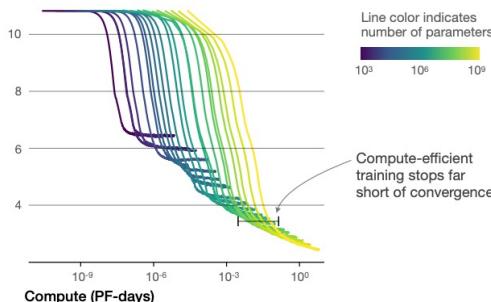
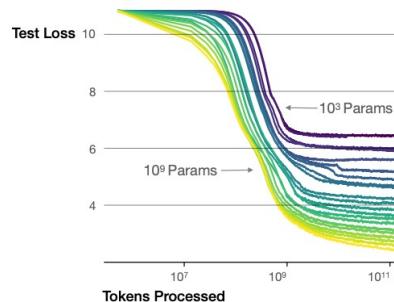


Scaling Transformer Models

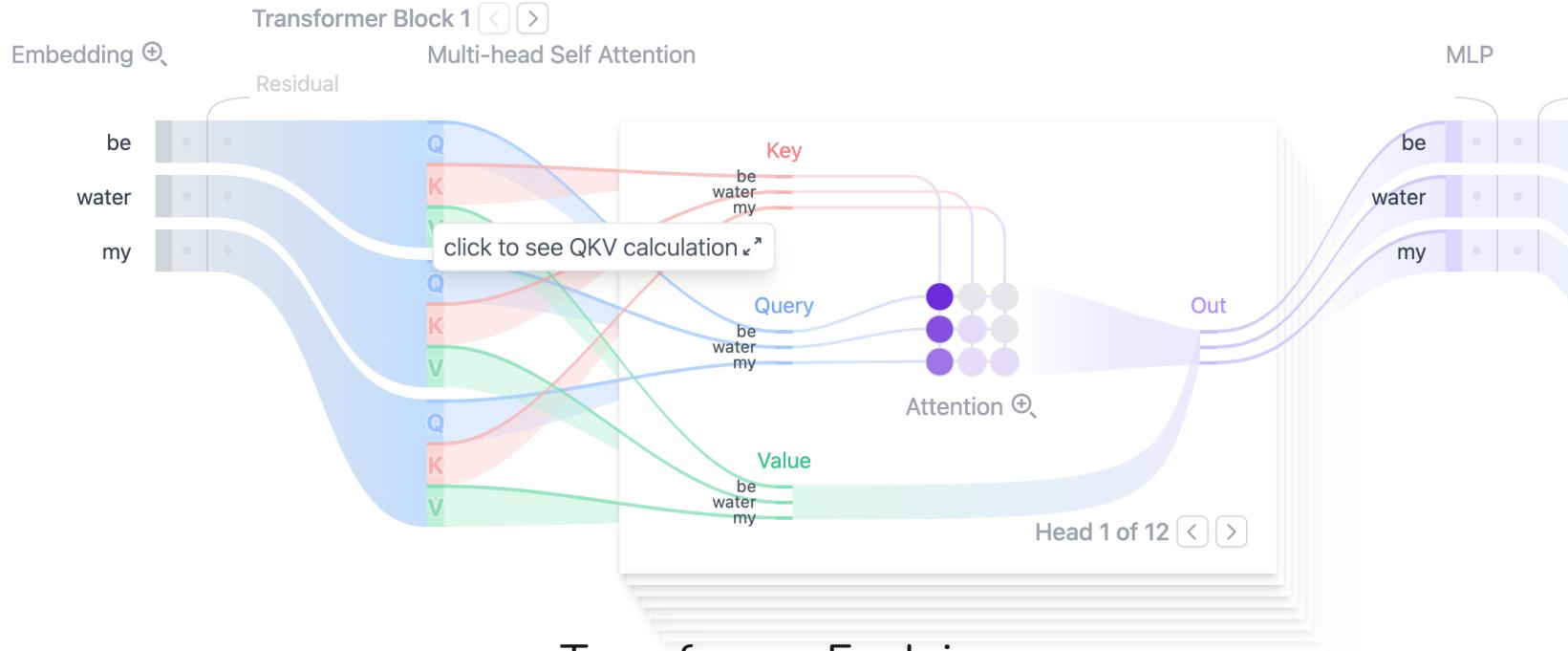


Larger models require **fewer samples** to reach the same performance

The optimal model size grows smoothly with the loss target and compute budget



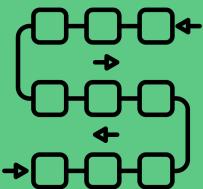
Folks do great visualizations of the transformer



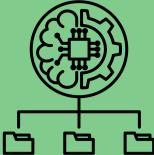
Transformer Explainer

Next lecture: BertViz in the tutorial session

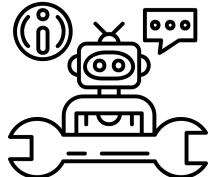
The 3 Ingredients of LLMs



Process long sequences and context



Efficient training on huge datasets



Follow (human) instructions

Tutorial

