

Seq2seq, NMT, Transformer

Milan Straka

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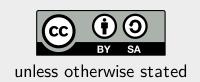








Charles University in Prague Faculty of Mathematics and Physics Institute of Formal and Applied Linguistics





Sequence-to-Sequence Architecture (Seq2seq)





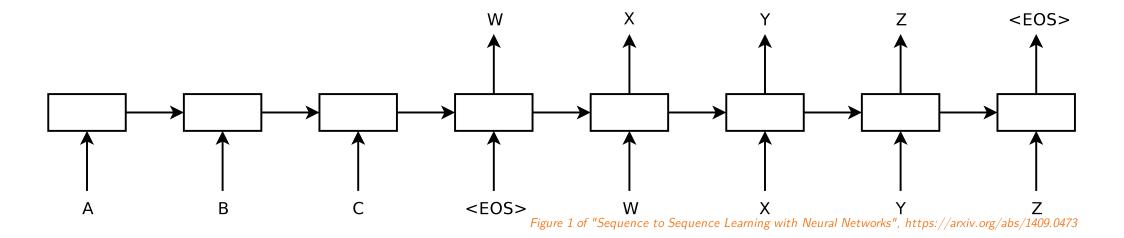
Sequence-to-Sequence is a name for an architecture allowing to produce an arbitrary output sequence y_1, \ldots, y_M from an input sequence x_1, \ldots, x_N .

Unlike span labeling/CTC, no assumptions are necessary and we condition each output sequence element on all input sequence elements and all already generated output sequence elements:

$$Pig(oldsymbol{y} \mid oldsymbol{X}ig) = \prod_{i=1}^M Pig(y_i \mid oldsymbol{x}_1, \dots, oldsymbol{x}_N, y_1, \dots, y_{i-1}ig).$$

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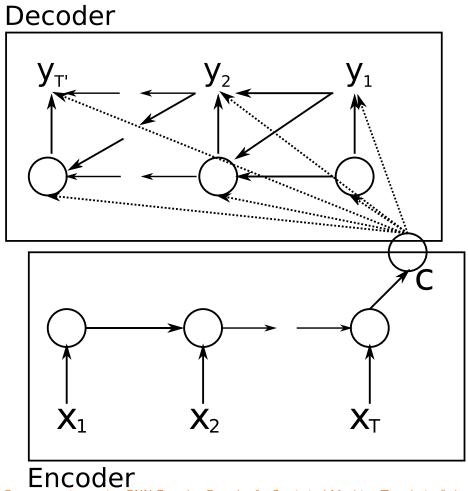


Figure 1 of "Learning Phrase Representations using RNN Encoder–Decoder for Statistical Machine Translation", https://arxiv.org/abs/1406.1078

NPFL138, Lecture 9

Seq2seq

Tying

Attention

SubWords

GNMT

Transformer

SelfAttention

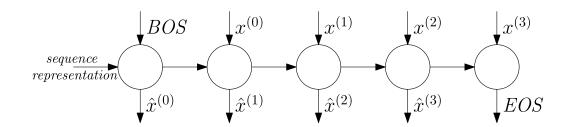
PosEmbed

Training



Training

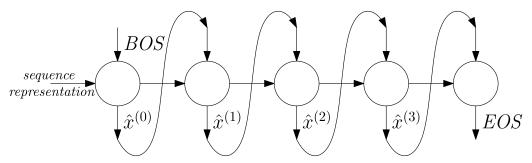
The so-called **teacher forcing** is used during training – the gold outputs are used as inputs during training.



Inference

During inference, the network processes its own predictions – such an approach is called **autoregressive decoding**.

Usually, the generated logits are processed by an rg max, the chosen word embedded and used as next input.





Word Embedding Tying

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Tying Word Embeddings



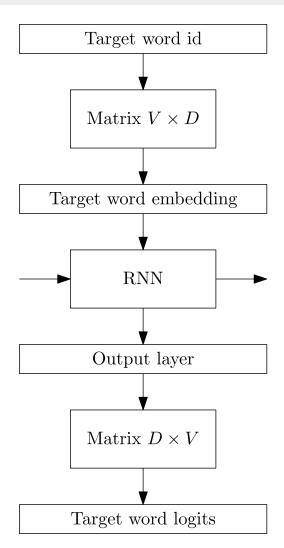
In the decoder, we both:

- ullet embed the previous prediction, using a matrix of size $\mathbb{R}^{V \times D}$, where V is the vocabulary size and D is the embedding size;
- classify the hidden state into current prediction, using a matrix of size $\mathbb{R}^{D imes V}$.

Both these matrices have similar meaning – they represent words in the embedding space (the first explicitly represents words by the embeddings, the second produces logits by computing weighted cosine similarity of the inputs and columns of the weight matrix).

Therefore, it makes sense to **tie** these matrices, i.e., to represent one of them as a transposition of the other.

• However, while the embedding matrix should usually have constant variance per dimension, the output layer should keep the variance of the RNN output; therefore, the output layer matrix is usually the embedding matrix divided by \sqrt{D} .



Training

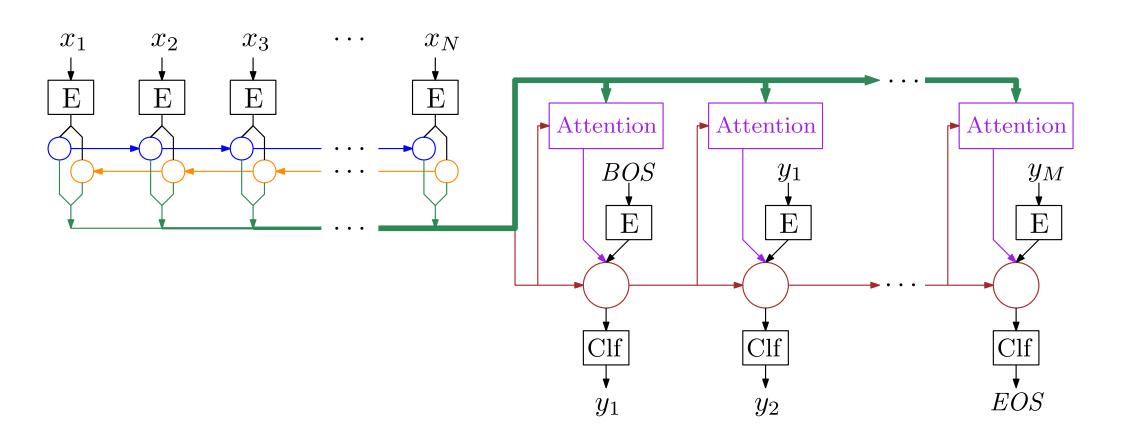


Attention

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Attention







Bahdanau (or Additive) Attention

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Bahdanau Attention



As another input during decoding, we add context vector c_i :

$$oldsymbol{s}_i = f(oldsymbol{s}_{i-1}, oldsymbol{y}_{i-1}, oldsymbol{c}_i).$$

We compute the context vector as a weighted combination of source sentence encoded outputs:

$$m{c}_i = \sum_j lpha_{ij} m{h}_j$$

The weights α_{ij} are softmax of e_{ij} over j,

$$oldsymbol{lpha}_i = \operatorname{softmax}(oldsymbol{e}_i),$$

with e_{ij} being

$$e_{ij} = oldsymbol{v}^ op anh(oldsymbol{V}oldsymbol{h}_j + oldsymbol{W}oldsymbol{s}_{i-1} + oldsymbol{b}).$$

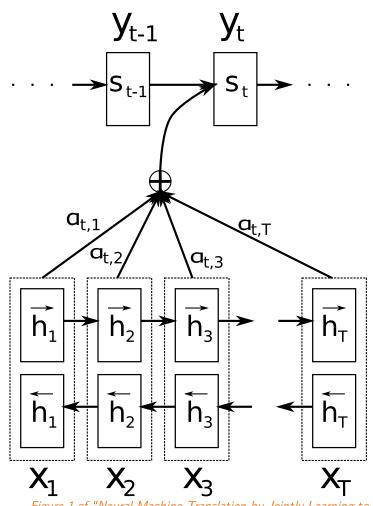
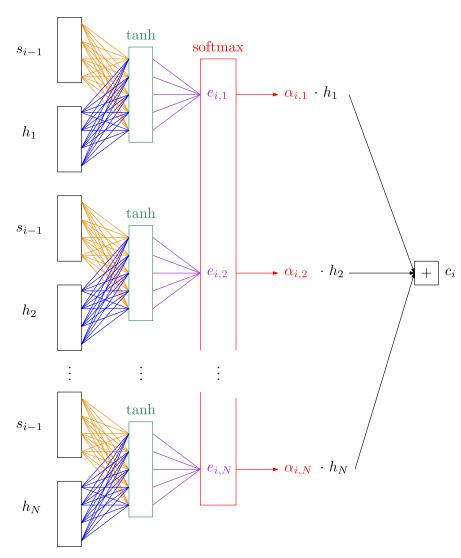


Figure 1 of "Neural Machine Translation by Jointly Learning to Align and Translate", https://arxiv.org/abs/1409.0473

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Bahdanau Attention Implementation

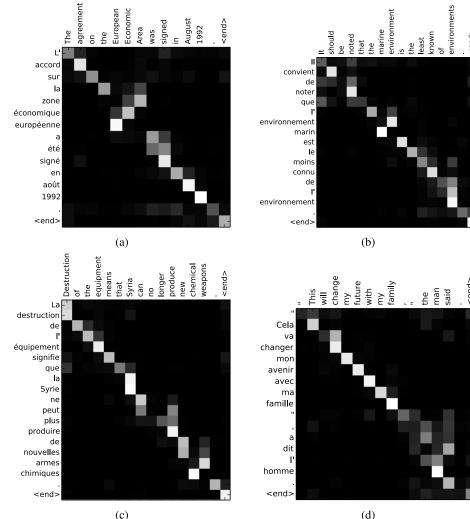






Trained Attention Visualization





(c) (d) Figure 3 of "Neural Machine Translation by Jointly Learning to Align and Translate", https://arxiv.org/abs/1409.0473



Luong (or Dot-Product) Attention

Luong Attention



In the described Bahdanau (additive) attention, we performed

$$e_{ij} = oldsymbol{v}^ op anh(oldsymbol{V}oldsymbol{h}_j + oldsymbol{W}oldsymbol{s}_{i-1} + oldsymbol{b}).$$

There are however other methods how Vh_j and Ws_{i-1} can be combined, most notably the Luong (or dot-product) attention, which uses just a dot product:

$$e_{ij} = ig(oldsymbol{V}oldsymbol{h}_jig)^Tig(oldsymbol{W}oldsymbol{s}_{i-1}ig).$$

The latter is easier to implement, but may sometimes be more difficult to train (scaling helps a bit, wait for the Transformer self-attention description); both approaches are used in quite a few papers.

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Subword Units (BPE, WordPieces)

Subword Units – BPE



Translate **subword units** instead of words. The subword units can be generated in several ways, the most commonly used are:

• **BPE**: Using the *byte pair encoding* algorithm. Start with individual characters plus a special end-of-word symbol •. Then, merge the most occurring symbol pair A, B by a new symbol AB, with the symbol pair never crossing word boundary (so that the end-of-word symbol cannot be inside a subword).

Considering text with words low, lowest, newer, wider, a possible sequence of merges:

$$egin{aligned} r & ullet & egin{aligned} r & ullet & eta & \ l & o &
ightarrow low \ lo & w &
ightarrow low \ e & r^ullet &
ightarrow er^ullet \end{aligned}$$

The BPE algorithm is executed on the training data, and it generates the resulting dictionary, merging rules, and training data encoded using this dictionary.

SubWords

Subword Units – BPE



- The end-of-word symbol was described to be at the end of a subword in the original paper.
- However, in existing implementations, we usually represent **beginning-of-word** symbol at the beginning of a subwords instead (usually a suitable encoded space).
- Furthermore, when considering multilingual models, there are in fact quite a lot of characters. Therefore, some tokenizers allow representing bytes of UTF-8 encoding.
 - Byte-level BPE or BBPE allows even subword splitting at arbitrary boundaries (inside a single UTF-8-encoded codepoint).
 - Sentence-piece model splits at Unicode codepoint boundaries, but can represent unknown characters using bytes of UTF-8 encoding.
- For example, a phrase "Přelétavý motýlek" can be tokenized as

```
# Using sentence-piece implementation of BPE:
['_Pře', 'lé', 'ta', 'vý', '_mot', 'ý', 'lek']
# Byte-level BPE, first trained on English data, the second on Czech data
['P', 'Å', 'Ļ', 'el', 'ét', 'av', 'Ã', '½', 'Ġmot', 'Ã', '½', 'le', 'k']
['PÅĻe', 'lét', 'avý', 'Ġmotý', 'lek']
```

Subword Units – WordPieces



• **WordPieces**: Given a text divided into subwords, we can compute unigram probability of every subword, and then get the likelihood of the text under a unigram language model by multiplying the probabilities of the subwords in the text.

When we have only a text and a subword dictionary, we divide the text in a greedy fashion, iteratively choosing the longest existing subword.

When constructing the subwords, we again start with individual characters (compared to BPE, we have a *start-of-word* character instead of an *end-of-word* character), and then repeatedly join such a pair of subwords that increases the unigram language model likelihood the most.

In the original implementation, the input data were once in a while "reparsed"
 (retokenized) in a greedy fashion with the up-to-date dictionary. However, the recent
 implementations do not seem to do it – but they retokenize the training data with the
 final dictionary, contrary to the BPE approach.

For both approaches, usually quite little subword units are used (32k-64k), often generated on the union of the two vocabularies of the source and target languages (the so-called *joint BPE* or *shared wordpieces*).

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BPE and WordPieces Comparison



Both the BPE and the WordPieces give very similar results; the biggest difference is that during the inference:

- for BPE, the sequence of merges must be performed in the same order as during the construction of the BPE (because we use the output of BPE as training data),
- for WordPieces, it is enough to find longest matches from the subword dictionary (because we reprocessed the training data with the final dictionary);
- note that the above difference is mostly artificial if we reparsed the training data in the BPE approach, we could also perform "greedy tokenization".

Of course, the two algorithms also differ in the way how they choose the pair of subwords to merge.

Both algorithms are implemented in quite a few libraries, most notably the sentencepiece library and the Hugging Face tokenizers package.

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Google Neural Machine Translation (GNMT)

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Google NMT



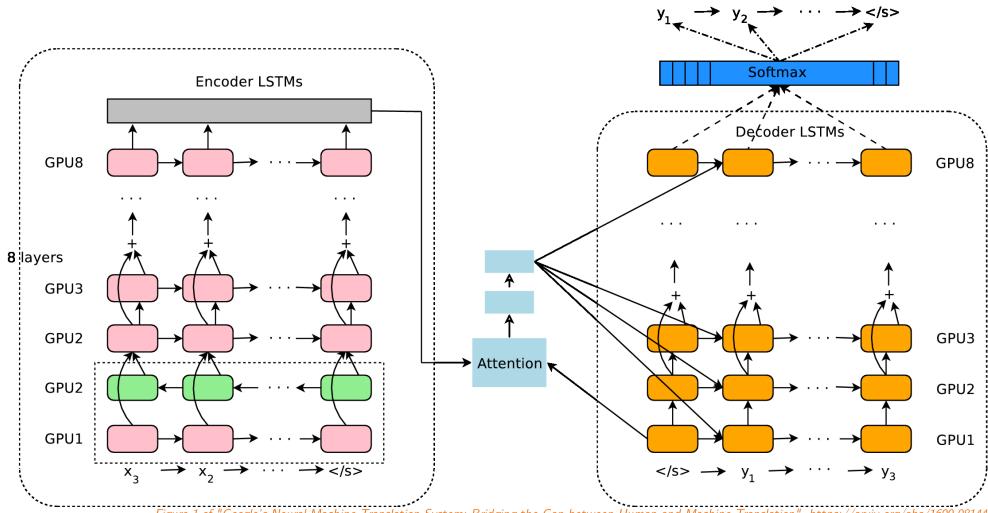
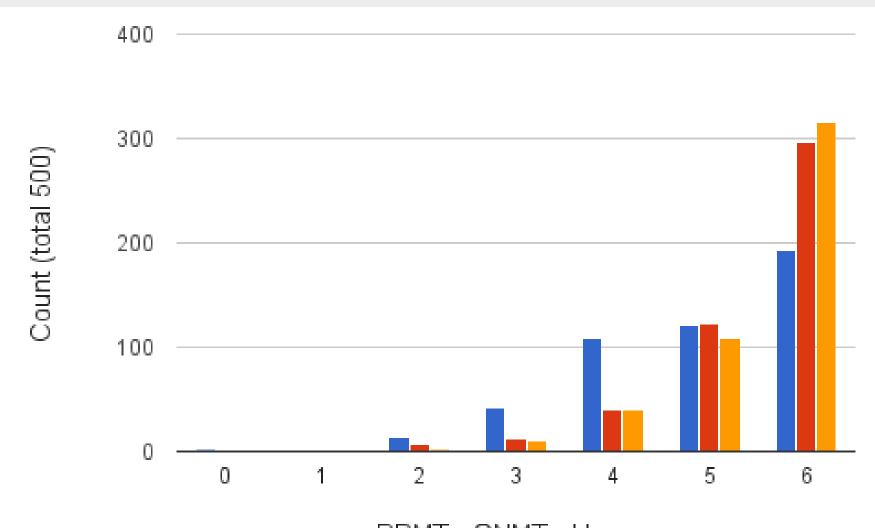


Figure 1 of "Google's Neural Machine Translation System: Bridging the Gap between Human and Machine Translation", https://arxiv.org/abs/1609.08144

Google NMT





PBMT - GNMT - Human
Figure 6 of "Google's Neural Machine Translation System: Bridging the Gap between Human and Machine Translation", https://arxiv.org/abs/1609.08144

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Beyond one Language Pair





Fig. 5. A selection of evaluation results, grouped by human rating.

Figure 5 of "Show and Tell: Lessons learned from the 2015 MSCOCO...", https://arxiv.org/abs/1609.06647

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Seg2seg

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Beyond one Language Pair



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What vegetable is the dog chewing on?

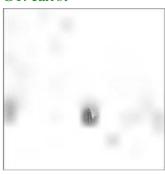
MCB: carrot

GT: carrot

What kind of dog is this?
MCB: husky
GT: husky

What kind of flooring does the room have? MCB: carpet GT: carpet









What color is the traffic light?
MCB: green

GT: green

Is this an urban area?
MCB: yes
GT: yes

Where are the buildings? MCB: in background GT: on left

Figure 6 of "Multimodal Compact Bilinear Pooling for VQA and Visual Grounding", https://arxiv.org/abs/1606.01847

Multilingual and Unsupervised Translation



Many attempts at multilingual translation.

- Individual encoders and decoders, shared attention.
- Shared encoders and decoders.

Surprisingly, even unsupervised translation can be performed. By unsupervised we understand settings where we have access to large monolingual corpora, but no parallel data.

In 2019, the best unsupervised systems were on par with the best 2014 supervised systems.

		WMT-14			
		fr-en	en-fr	de-en	en-de
Unsupervised	Proposed system detok. SacreBLEU*	33.5 33.2	36.2 33.6	27.0 26.4	22.5 21.2
Supervised	WMT best* Vaswani et al. (2017) Edunov et al. (2018)	35.0	35.8 41.0 45.6	29.0 - -	20.6 [†] 28.4 35.0

Table 3: Results of the proposed method in comparison to different supervised systems (BLEU).

Table 3 of "An Effective Approach to Unsupervised Machine Translation", https://arxiv.org/abs/1902.01313

Nowadays, language models like ChatGPT can be also considered unsupervised machine translation, and then achieve superior performance without explicit parallel data.

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Tying



The Transformer Architecture

Attention is All You Need



For some sequence processing tasks, *sequential* processing (as performed by recurrent neural networks) of its elements might be too restrictive.

Instead, we may want to be able to combine sequence elements independently on their distance.

Such processing is allowed in the **Transformer** architecture, originally proposed for neural machine translation in 2017 in *Attention is All You Need* paper.

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SubWords



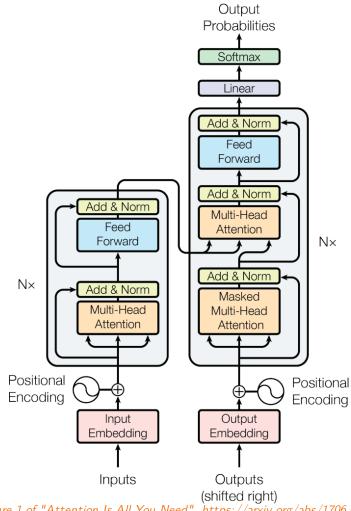
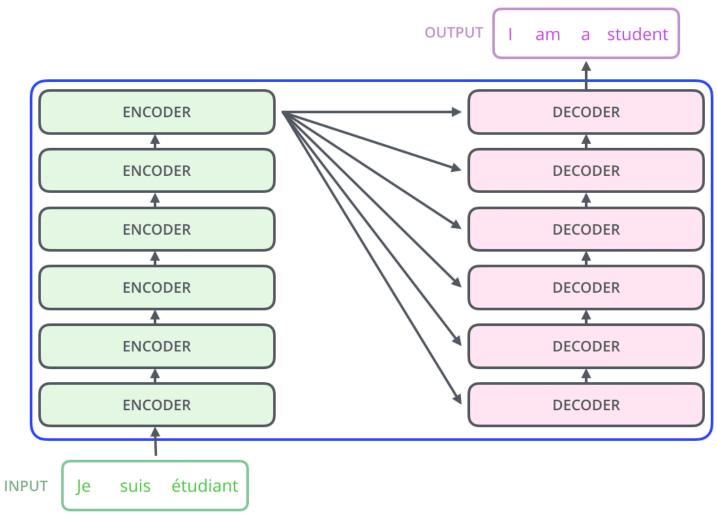


Figure 1 of "Attention Is All You Need", https://arxiv.org/abs/1706.03762

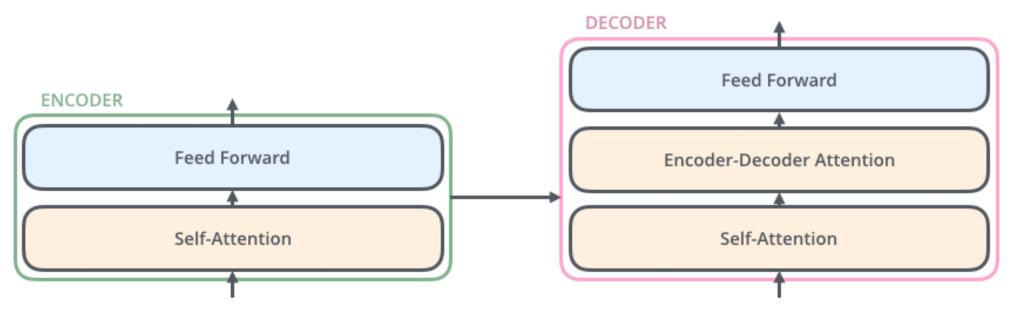




http://jalammar.github.io/images/t/The_transformer_encoder_decoder_stack.png

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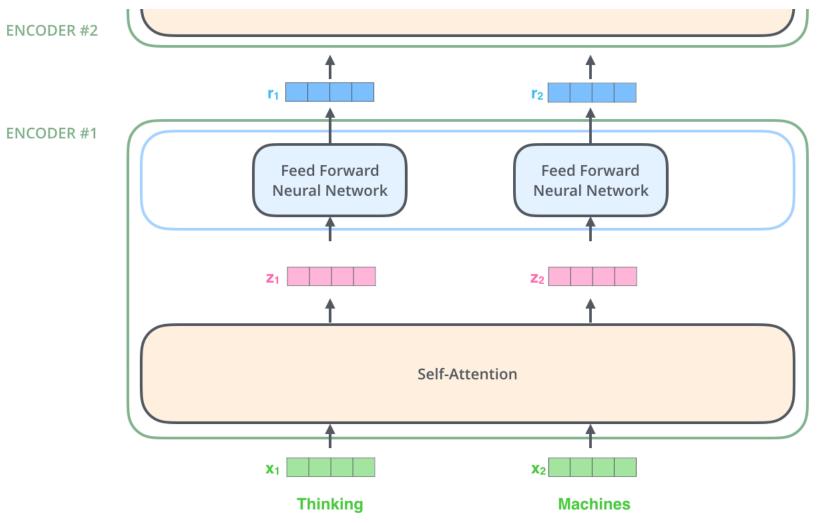


http://jalammar.github.io/images/t/Transformer_decoder.png

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http://jalammar.github.io/images/t/encoder_with_tensors_2.png

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Transformer – Self-Attention

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Transformer – Self-Attention



Assume that we have a sequence of n words represented using a matrix $m{X} \in \mathbb{R}^{n \times d}$.

The attention module for queries $Q \in \mathbb{R}^{n \times d_k}$, keys $K \in \mathbb{R}^{n \times d_k}$ and values $V \in \mathbb{R}^{n \times d_v}$ is defined as:

$$ext{Attention}(oldsymbol{Q}, oldsymbol{K}, oldsymbol{V}) = \operatorname{softmax}\left(rac{oldsymbol{Q}oldsymbol{K}^ op}{\sqrt{d_k}}
ight)oldsymbol{V}.$$

The queries, keys and values are computed from the input word representations $m{X}$ using a linear transformation as

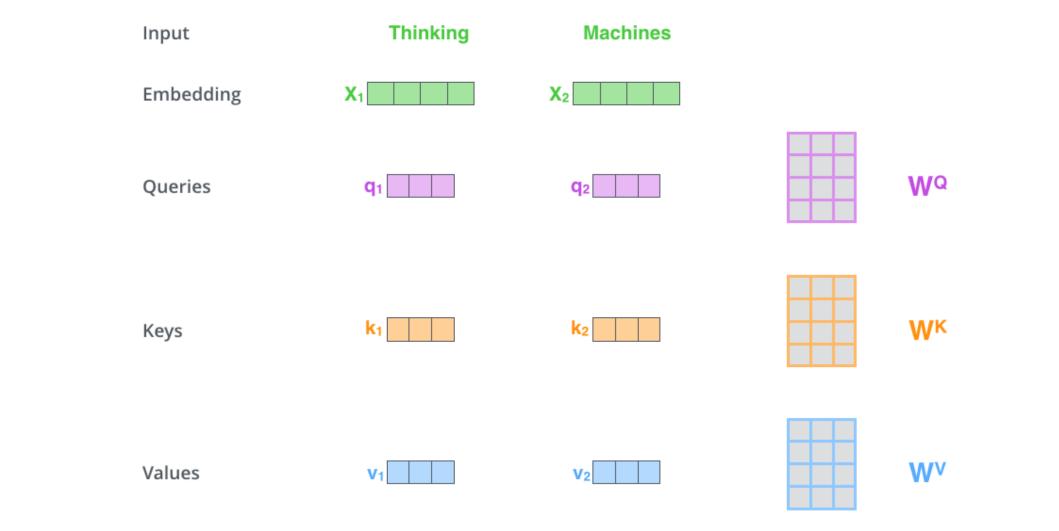
$$egin{aligned} oldsymbol{Q} &= oldsymbol{X} oldsymbol{W}^Q \ oldsymbol{K} &= oldsymbol{X} oldsymbol{W}^K \ oldsymbol{V} &= oldsymbol{X} oldsymbol{W}^V \end{aligned}$$

for trainable weight matrices $m{W}^Q, m{W}^K \in \mathbb{R}^{d imes d_k}$ and $m{W}^V \in \mathbb{R}^{d imes d_v}$.

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Transformer – Self-Attention

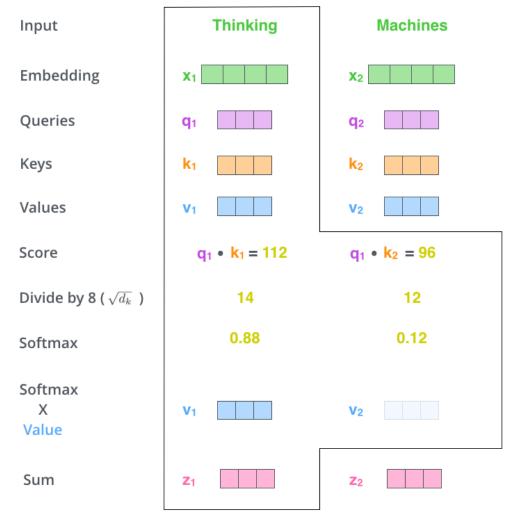




http://jalammar.github.io/images/t/transformer_self_attention_vectors.png

Transformer – Self-Attention



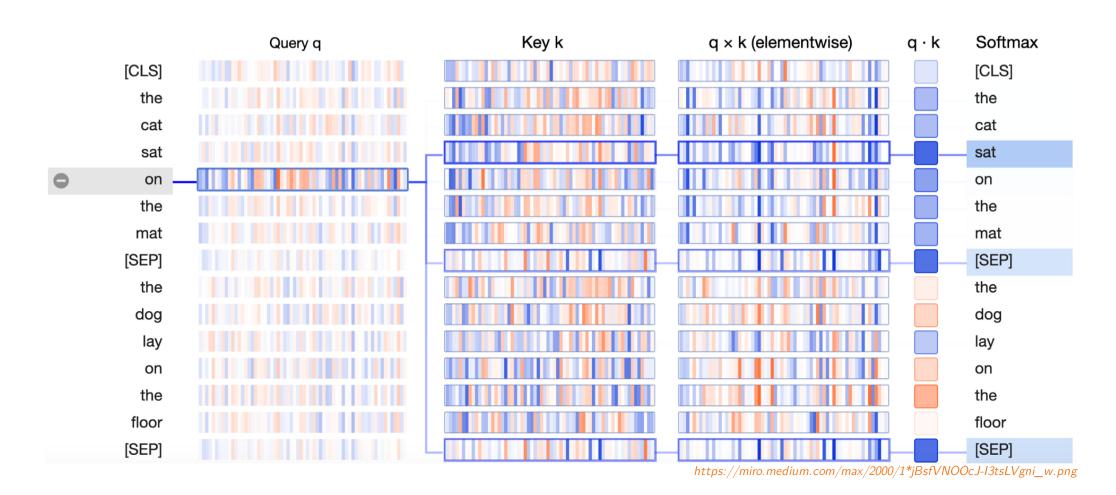


http://jalammar.github.io/images/t/self-attention-output.png

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Transformer – Self-Attention





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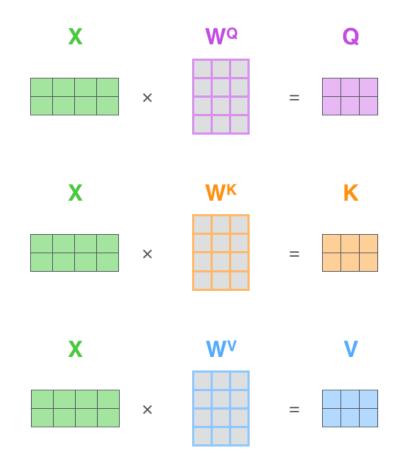
SelfAttention

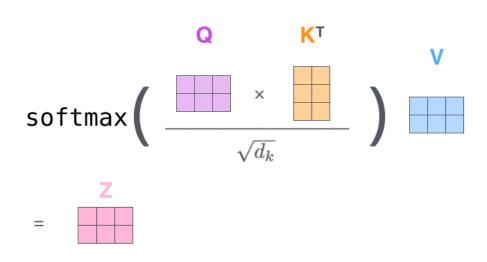
PosEmbed

Training 38/65

Transformer – Self-Attention







http://jalammar.github.io/images/t/self-attention-matrix-calculation-2.png

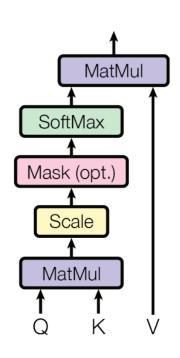
http://jalammar.github.io/images/t/self-attention-matrix-calculation.png

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Multihead attention is used in practice. Instead of using one huge attention, we split queries, keys and values to several groups (similar to how ResNeXt works), compute the attention in each of the groups separately, concatenate the results and multiply them by a matrix \boldsymbol{W}^O .

Scaled Dot-Product Attention



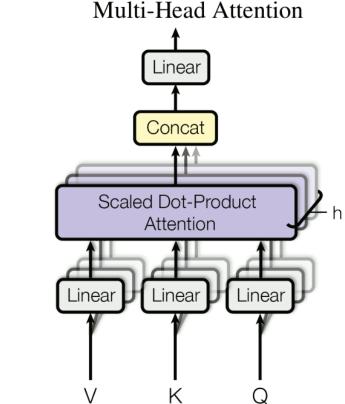
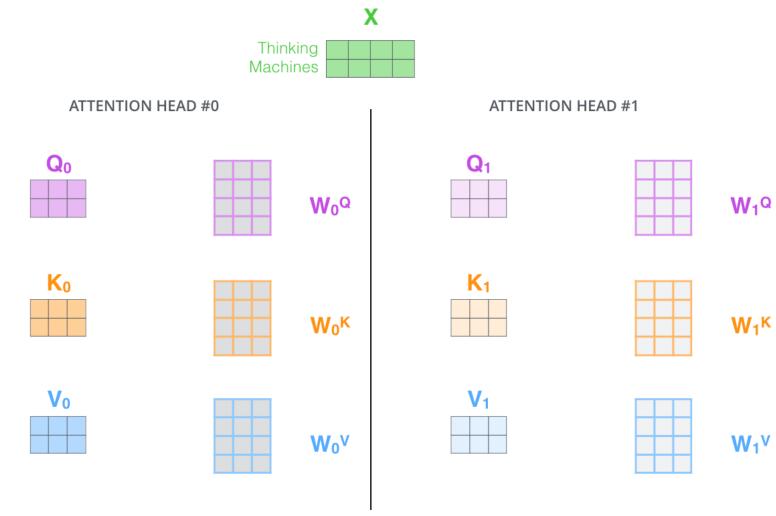


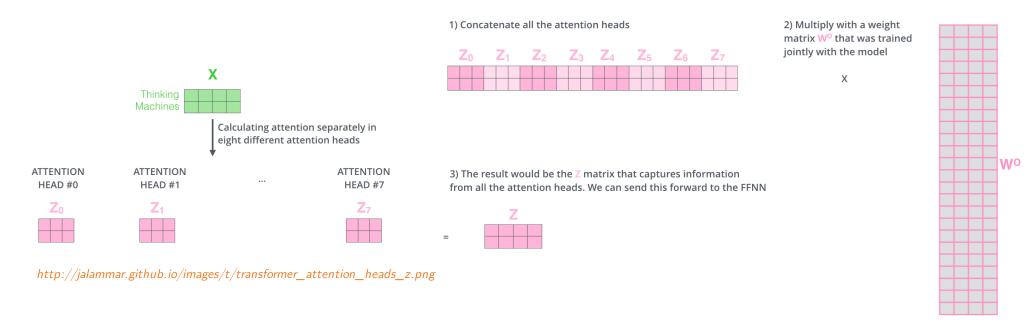
Figure 2 of "Attention Is All You Need", https://arxiv.org/abs/1706.03762





http://jalammar.github.io/images/t/transformer_attention_heads_qkv.png





http://jalammar.github.io/images/t/transformer_attention_heads_weight_matrix_o.png



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

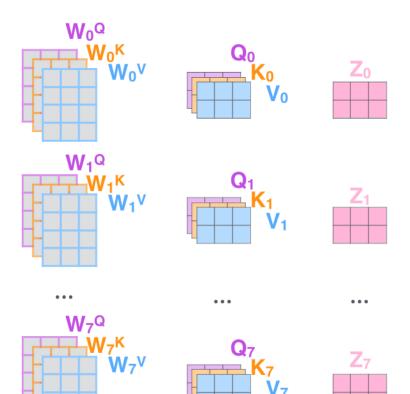
5) Concatenate the resulting Z matrices, then multiply with weight matrix W^o to produce the output of the layer

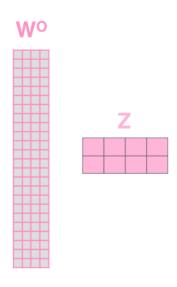
Thinking Machines



* In all encoders other than #0, we don't need embedding. We start directly with the output of the encoder right below this one



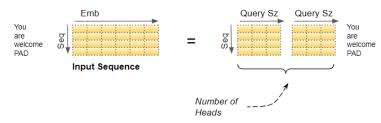




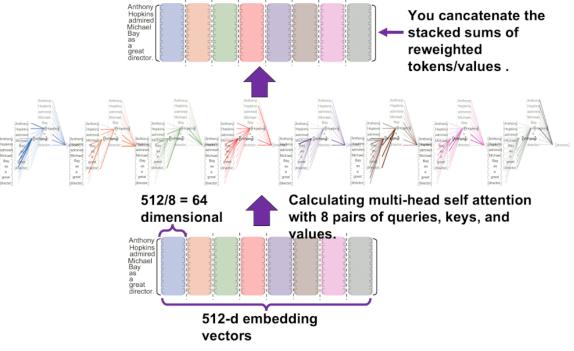
http://jalammar.github.io/images/t/transformer_multi-headed_self-attention-recap.png



When multihead attention is used, we first generate query/key/value vectors of the same dimension, and then split them into smaller pieces. Therefore, multihead attention does not increase complexity (much) and is analogous to ResNeXt/GroupNorm.



https://towardsdatascience.com/wp-content/uploads/2021/01/175EUBJLaqAMcDjgwWVh-_A.png



https://data-science-blog.com/wp-content/uploads/2022/01/mha_3-1030x608.png

Why Attention



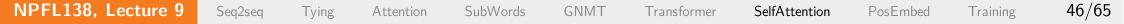
Table 1: Maximum path lengths, per-layer complexity and minimum number of sequential operations for different layer types. n is the sequence length, d is the representation dimension, k is the kernel size of convolutions and r the size of the neighborhood in restricted self-attention.

Layer Type	Complexity per Layer	Sequential Operations	Maximum Path Length
Self-Attention	$O(n^2 \cdot d)$	O(1)	O(1)
Recurrent	$O(n \cdot d^2)$	O(n)	O(n)
Convolutional	$O(\hat{k}\cdot n\cdot \hat{d}^2)$	O(1)	$O(log_k(n))$
Self-Attention (restricted)	$O(r \cdot n \cdot d)$	O(1)	O(n/r)

Table 1 of "Attention Is All You Need", https://arxiv.org/abs/1706.03762



Transformer – Feed Forward Networks



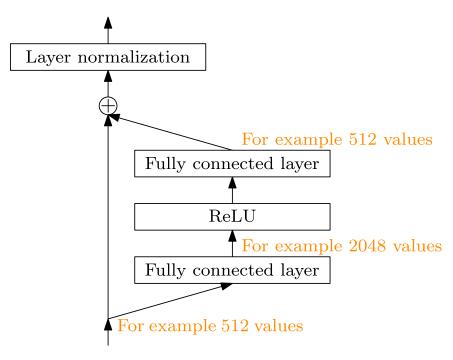
Transformer – Feed Forward Networks

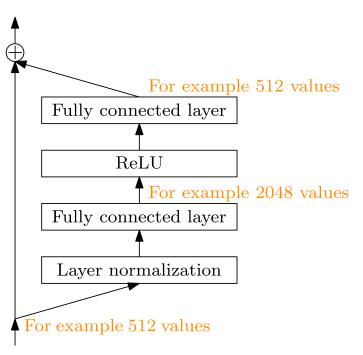


Feed Forward Networks

The self-attention is complemented with FFN layers, which is a fully connected ReLU layer with four times as many hidden units as inputs, followed by another fully connected layer without activation.

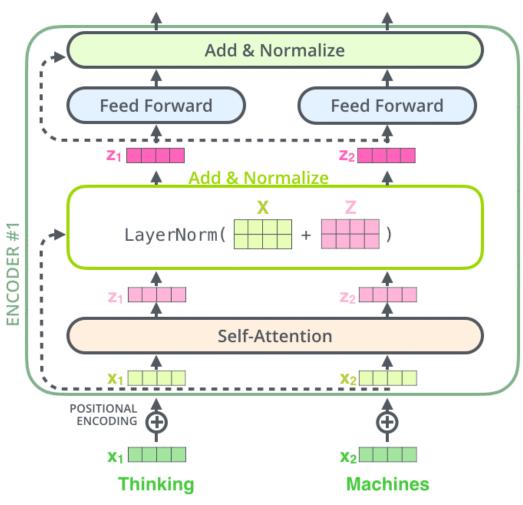
Original "Post-LN" configuration Improved "Pre-LN" configuration since 2020





Transformer – Post-LN Configuration including Residuals





http://jalammar.github.io/images/t/transformer_resideual_layer_norm_2.png

Transformer – Pre-LN Configuration

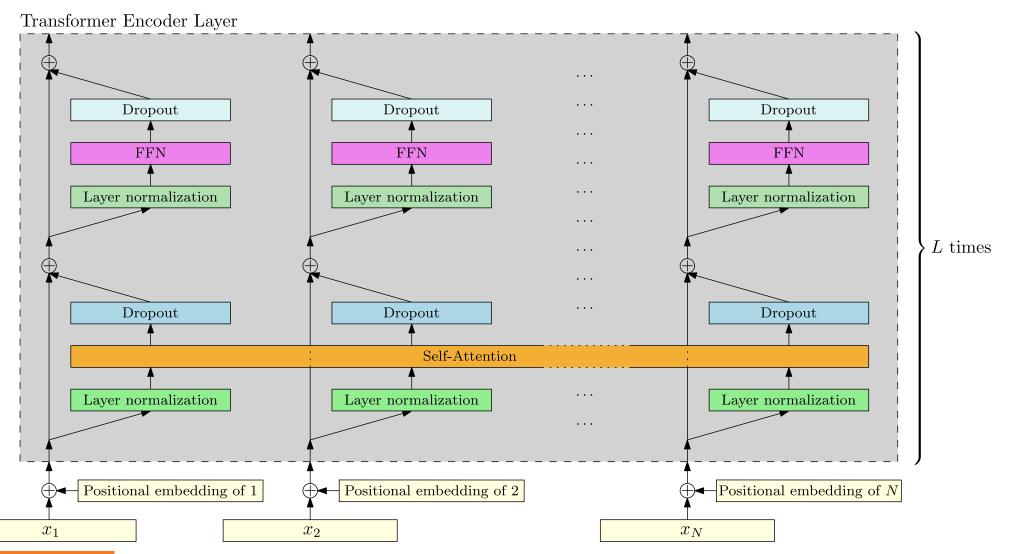
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Seq2seq

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PosEmbed

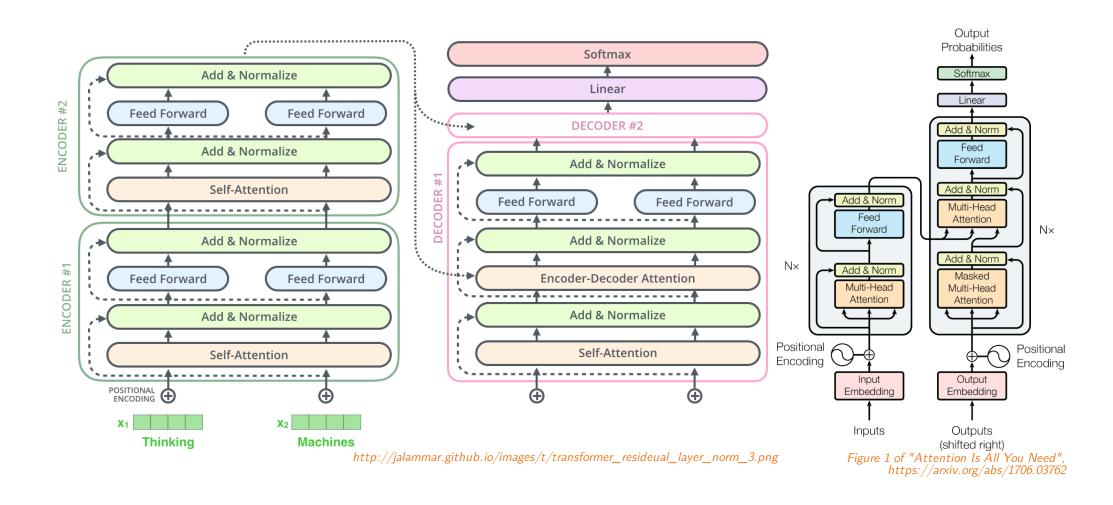
Training

SubWords

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Transformer – Decoder





Transformer – Decoder



Masked Self-Attention

During decoding, the self-attention must attend only to earlier positions in the output sequence.

This is achieved by **masking** future positions, i.e., zeroing their weights out, which is usually implemented by setting them to $-\infty$ before the softmax calculation.

Encoder-Decoder Attention

In the encoder-decoder attentions, the *queries* comes from the decoder, while the keys and the values originate from the encoder.

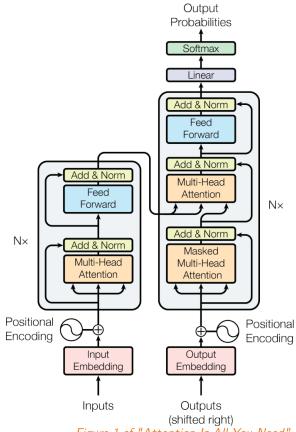
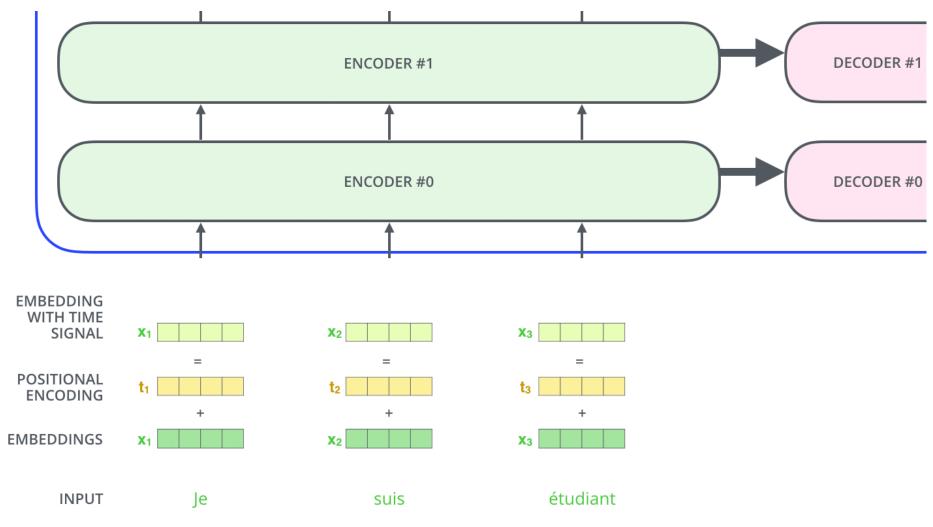


Figure 1 of "Attention Is All You Need", https://arxiv.org/abs/1706.03762







http://jalammar.github.io/images/t/transformer_positional_encoding_vectors.png



Positional Embeddings

We need to encode positional information (which was implicit in RNNs).

- Learned embeddings for every position.
- Sinusoids of different frequencies:

$$ext{PE}_{(pos,2i)} = \sin\left(pos/10000^{2i/d}
ight) \ ext{PE}_{(pos,2i+1)} = \cos\left(pos/10000^{2i/d}
ight)$$

This choice of functions should allow the model to attend to relative positions, since for any fixed k, PE_{pos+k} is a linear function of PE_{pos} , because

$$egin{aligned} ext{PE}_{(pos+k,2i)} &= \sin \left((pos+k)/10000^{2i/d}
ight) \ &= \sin \left(pos/10000^{2i/d}
ight) \cdot \cos \left(k/10000^{2i/d}
ight) + \cos \left(pos/10000^{2i/d}
ight) \cdot \sin \left(k/10000^{2i/d}
ight) \ &= of\!f\!set_{(k,2i)} \cdot ext{PE}_{(pos,2i)} + of\!f\!set_{(k,2i+1)} \cdot ext{PE}_{(pos,2i+1)}. \end{aligned}$$



Positional Embeddings

Sinusoids of different frequencies

In the original description of positional embeddings (the one used on the previous slide), the sines and cosines are interleaved, so for d=6, the positional embeddings would look like:

$$ext{PE}_{pos} = \left(\sin\left(rac{pos}{10000^0}
ight), \cos\left(rac{pos}{10000^0}
ight), \sin\left(rac{pos}{10000^{1/3}}
ight), \cos\left(rac{pos}{10000^{1/3}}
ight), \sin\left(rac{pos}{10000^{2/3}}
ight), \cos\left(rac{pos}{10000^{2/3}}
ight)
ight).$$

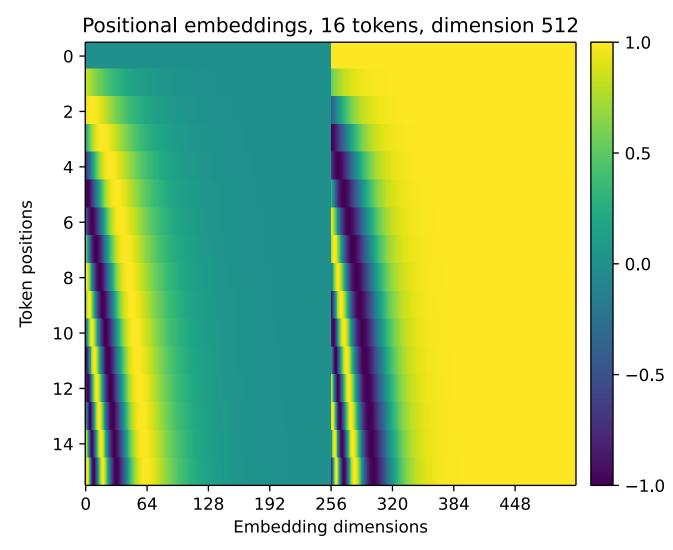
However, in practice, most implementations concatenate first all the sines and only then all the cosines:

$$\widehat{ ext{PE}}_{pos} = igg(\sinig(rac{pos}{10000^0}ig), \sinig(rac{pos}{10000^{1/3}}ig), \sinig(rac{pos}{10000^{2/3}}ig), \cosig(rac{pos}{10000^0}ig), \cosig(rac{pos}{10000^{1/3}}ig), \cosig(rac{pos}{10000^{2/3}}ig)ig).$$

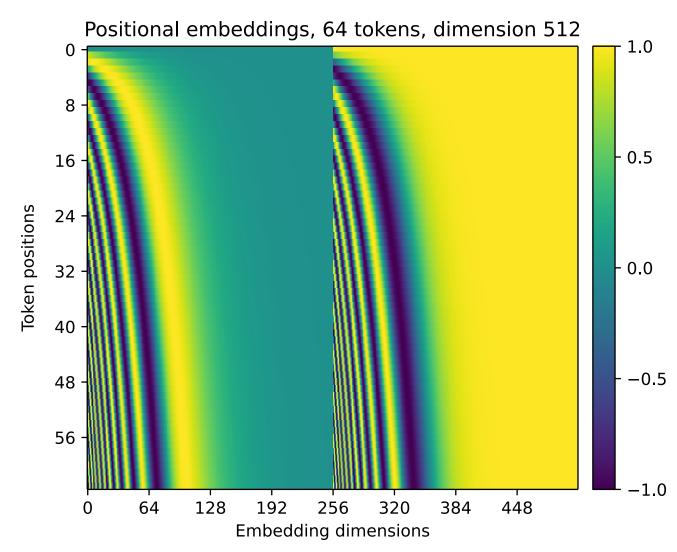
This is also how we visualize the positional embeddings on the following slides.

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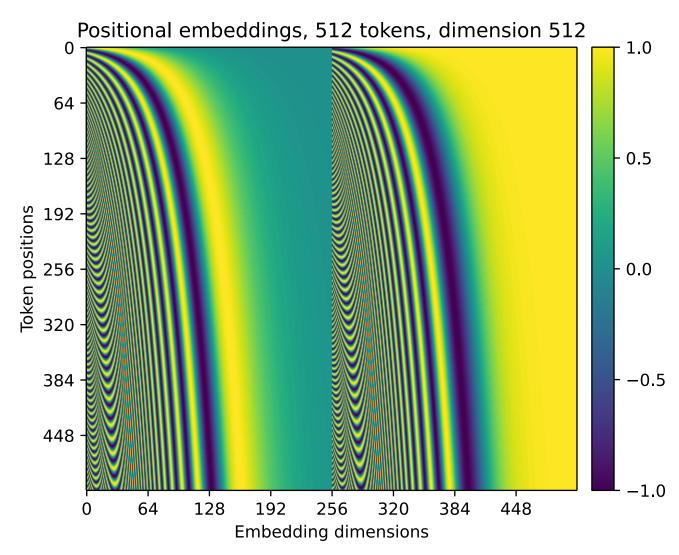
















Transformer – Training

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Transformer – Training



Regularization

The network is regularized by:

- dropout of input embeddings,
- dropout of each sub-layer, just before it is added to the residual connection (and then normalized),
- label smoothing.

Default dropout rate and also label smoothing weight is 0.1.

Parallel Execution

Because of the *masked attention*, training can be performed in parallel.

However, inference is still sequential.

Transformer – Training



Optimizer

Adam optimizer (with $\beta_2=0.98$, smaller than the default value of 0.999) is used during training, with the learning rate decreasing proportionally to inverse square root of the step number.

Warmup

Furthermore, during the first $warmup_steps$ updates, the learning rate is increased linearly from zero to its target value.

$$learning_rate = rac{1}{\sqrt{d_{\mathrm{model}}}} \min \left(rac{1}{\sqrt{step_num}}, rac{step_num}{warmup_steps} \cdot rac{1}{\sqrt{warmup_steps}}
ight).$$

In the original paper, 4000 warmup steps were proposed.

Note that the goal of warmup is mostly to prevent divergence early in training; the Pre-LN configuration usually trains well even without warmup.

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Transformers Results



Table 2: The Transformer achieves better BLEU scores than previous state-of-the-art models on the English-to-German and English-to-French newstest2014 tests at a fraction of the training cost.

Model	BL	EU	Training Co	Training Cost (FLOPs)			
Model	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	$2.0\cdot10^{19}$	$1.2\cdot 10^{20}$			
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 ·	10^{18}			
Transformer (big)	28.4	41.8	$2.3 \cdot$	10^{19}			

Table 2 of "Attention Is All You Need", https://arxiv.org/abs/1706.03762

Subwords were constructed using BPE with a shared vocabulary of about 37k tokens.

Transformers Ablations on En→De newtest2014 Dev



	N	d_{model}	$d_{ m ff}$	h	d_k	d_v	P_{drop}	ϵ_{ls}	train steps	PPL (dev)	BLEU (dev)	params ×10 ⁶
base	6	512	2048	8	64	64	0.1	0.1	100K	4.92	25.8	65
(A)				1	512	512				5.29	24.9	
				4	128	128				5.00	25.5	
				16	32	32				4.91	25.8	
				32	16	16				5.01	25.4	
(B)					16					5.16	25.1	58
					32					5.01	25.4	60
(C)	2									6.11	23.7	36
	4									5.19	25.3	50
	8									4.88	25.5	80
		256			32	32				5.75	24.5	28
		1024			128	128				4.66	26.0	168
			1024							5.12	25.4	53
			4096							4.75	26.2	90
(D)							0.0			5.77	24.6	
							0.2			4.95	25.5	
								0.0		4.67	25.3	
								0.2		5.47	25.7	
(E)	positional embedding instead of sinusoids							4.92	25.7			
big	6	1024	4096	16			0.3		300K	4.33	26.4	213

Table 4 of "Attention Is All You Need", https://arxiv.org/abs/1706.03762

The PPL is *perplexity per wordpiece*, where perplexity is $e^{H(P)}$, i.e., e^{loss} in our case.

Training

Decoder-Only Models



In seq2seq architecture, we have both an **encoder** and a **decoder**.

However, for text generation (chatbots, for example), a decoder-only model suffices.

- Examples include GPT-1 (2018), GPT-2 (2019), ChatGPT, Copilot, Llama, ...
- The decoder-only models are trained as language models, i.e., they estimate conditional probability of a word given its previous context (like Elmo).
- They consist purely of the decoder part of a Transformer (so they do not contain neither an encoder nor encoder-decoder attention; consequently, all their self-attentions are masked).
- On https://bbycroft.net/llm, you can find a 3D visualization and the description of the Transformer computation steps of several GPT models.

Summary



- **Seq2seq** is a general architecture of producing an output sequence from an input sequence.
- It is usually trained using **teacher forcing**, and use **autoregressive decoding**.
- Attention allows focusing on any part of a sequence in every time step.
- Transformer provides more powerful sequence-to-sequence architecture and also sequence element representation architecture compared to RNNs, but requires substantially more data.
 - When data are plentiful, best models for processing text, speech, and vision data utilize the Transformer architecture (together with convolutions in the vision domain).
- In seq2seq architecture, we have both an **encoder** and the **decoder**. However, text generation (i.e., in chatbots) is usually performed by **decoder-only** models.