UNIVERSITY OF TECHNOLOGY
IN THE EUROPEAN CAPITAL OF CULTURE
CHEMNITZ

Neurocomputing

Transformers

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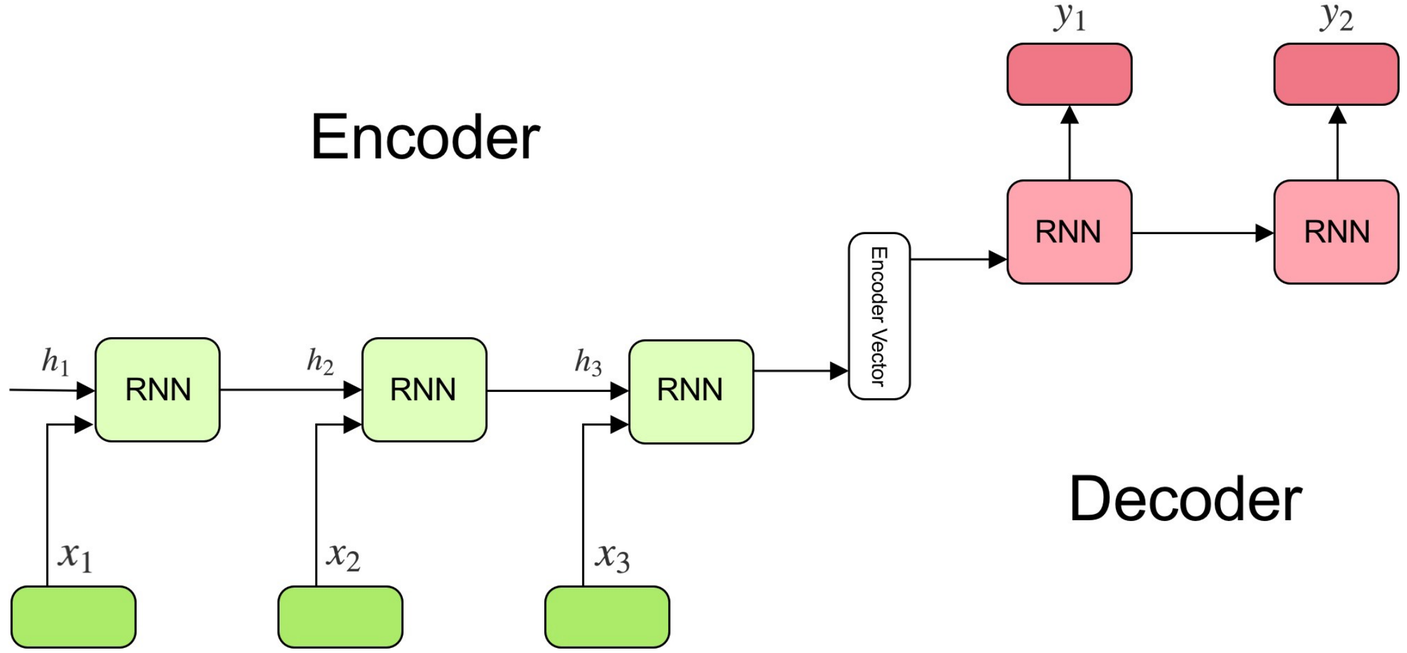
1 - Attentional recurrent networks

Many to Many: seq2seq

- The **state vector** obtained at the end of a sequence can be reused as an initial state for another LSTM.
- The goal of the **encoder** is to find a compressed representation of a sequence of inputs.
- The goal of the **decoder** is to generate a sequence from that representation.
- **Sequence-to-sequence** (seq2seq) models are recurrent autoencoders.



Sutskever, I., Vinyals, O., and Le, Q. V. (2014). Sequence to Sequence Learning with Neural Networks. arXiv:1409.3215

Attentional recurrent networks

- The problem with seq2seq is that it **compresses** the complete input sentence into a single state vector.

- For long sequences, the beginning of the sentence may not be present in the final state vector:
  - Truncated BPTT, vanishing gradients.
  - When predicting the last word, the beginning of the paragraph might not be necessary.
- Consequence: there is not enough information in the state vector to start translating.

Attentional recurrent networks

- A solution would be to concatenate the **state vectors** of all steps of the encoder and pass them to the decoder.

- **Problem 1:** it would make a lot of elements in the state vector of the decoder (which should be constant).
- **Problem 2:** the state vector of the decoder would depend on the length of the input sequence.

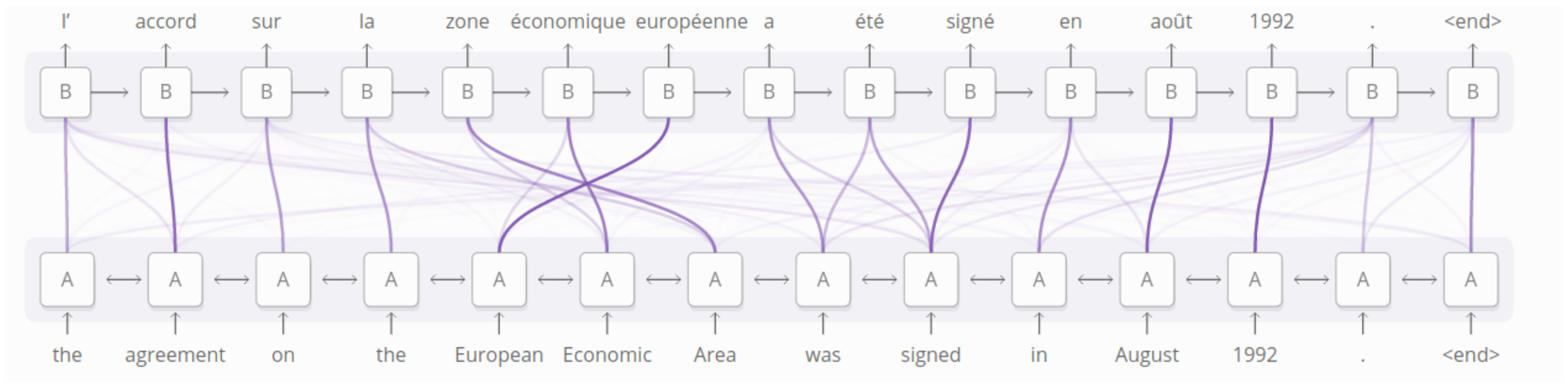
Attentional recurrent networks

- Attentional mechanisms let the decoder decide (by learning) which state vectors it needs to generate each word at each step.

- The **attentional context vector** of the decoder A_t^{decoder} at time t is a weighted average of all state vectors C_i^{encoder} of the encoder.

$$A_t^{\text{decoder}} = \sum_{i=0}^{T} a_i \, C_i^{\text{encoder}}$$

- The coefficients a_i are called the **attention scores** : how much attention is the decoder paying to each of the encoder's state vectors?



Attentional recurrent networks

- The attention scores a_i are computed as a **softmax** over the scores e_i (in order to sum to 1):

$$a_i = \frac{\exp e_i}{\sum_j \exp e_j} \Rightarrow A_t^{\text{decoder}} = \sum_{i=0}^{T} \frac{\exp e_i}{\sum_j \exp e_j} C_i^{\text{encoder}}$$

- The score e_i is computed using:
  - the previous output of the decoder $\mathbf{h}_{t-1}^{\text{decoder}}$.
  - the corresponding state vector C_i^{encoder} of the encoder at step i.
  - attentional weights W_a.

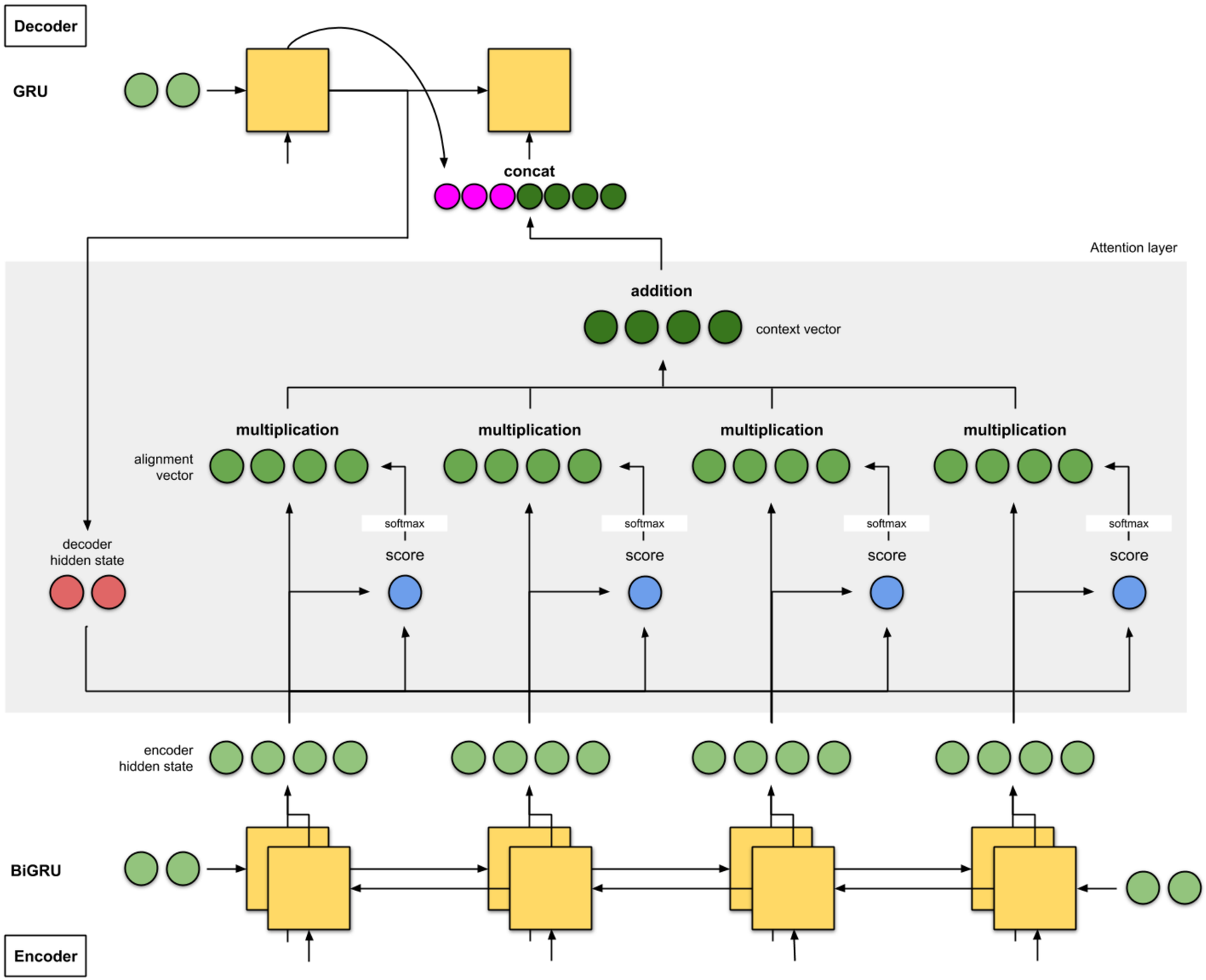
$$e_i = \tanh(W_a \, [\mathbf{h}_{t-1}^{\text{decoder}}; C_i^{\text{encoder}}])$$

- Everything is differentiable, these attentional weights can be learned with BPTT.

Attentional recurrent networks

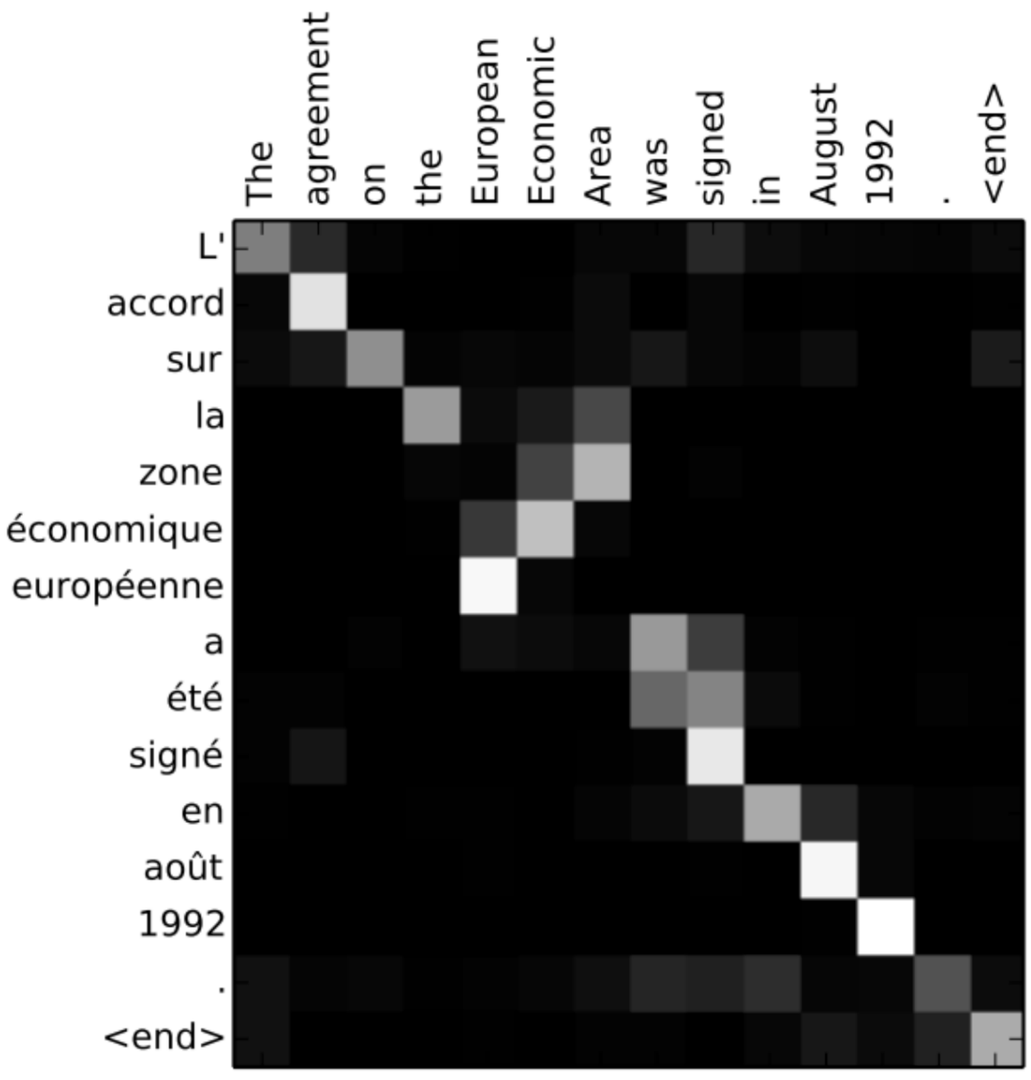
- The attentional context vector A_t^{decoder} is concatenated with the previous output $\mathbf{h}_{t-1}^{\text{decoder}}$ and used as the next input $\mathbf{x}_t^{\text{decoder}}$ of the decoder:

$$\mathbf{x}_t^{\text{decoder}} = [\mathbf{h}_{t-1}^{\text{decoder}}; A_t^{\text{decoder}}]$$


Decoder
GRU
concat
Attention layer
addition
context vector
multiplication
multiplication
multiplication
multiplication
alignment vector
softmax
softmax
softmax
softmax
score
score
score
score
decoder hidden state
encoder hidden state
BiGRU
Encoder

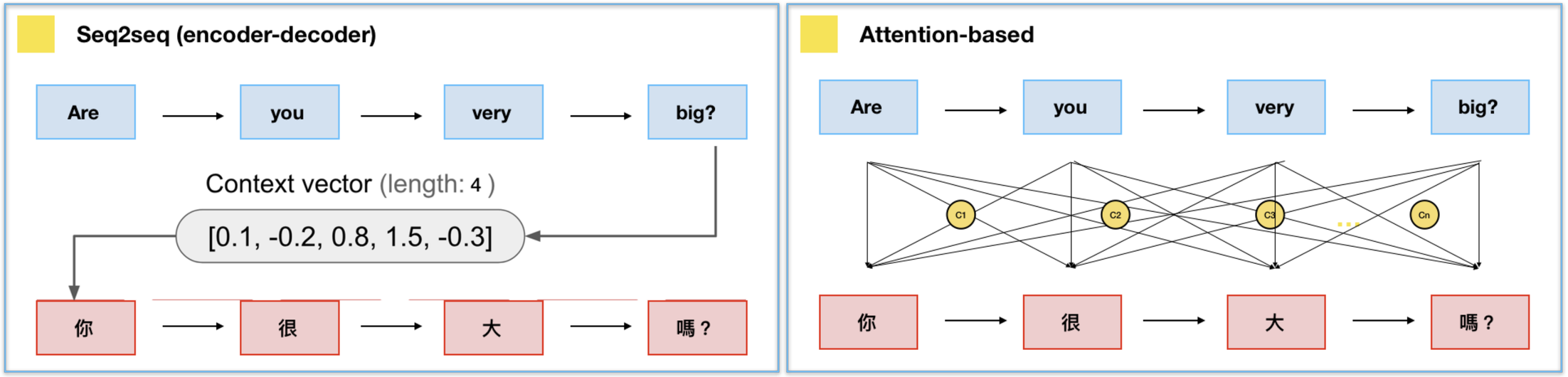
Attentional recurrent networks

- The attention scores or **alignment scores** a_i are useful to interpret what happened.
- They show which words in the original sentence are the most important to generate the next word.



Attentional recurrent networks

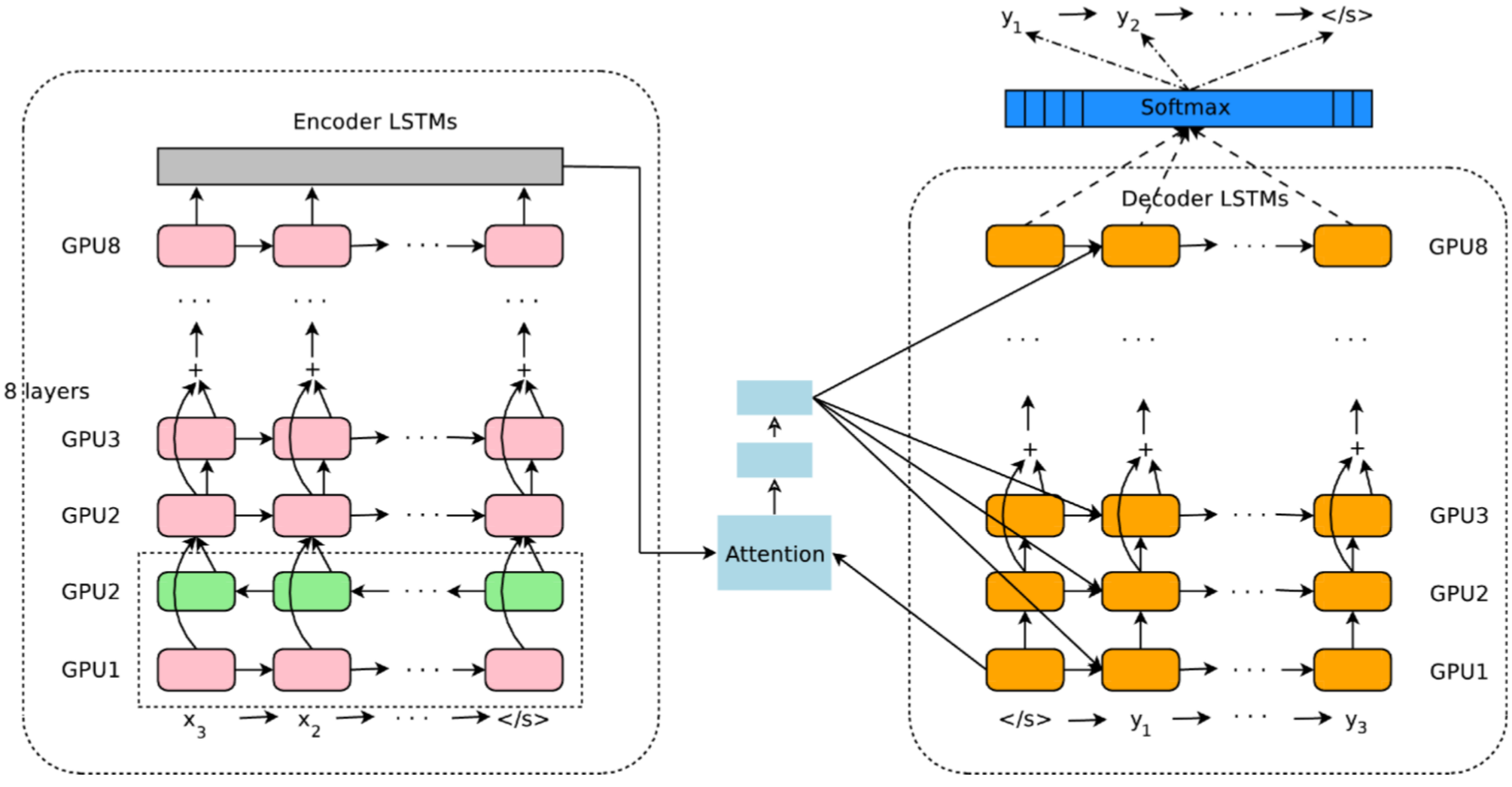
- **Attentional mechanisms** are now central to NLP.



- The whole **history** of encoder states is passed to the decoder, which learns to decide which part is the most important using **attention**.
- This solves the bottleneck of seq2seq architectures, at the cost of much more operations.
- They require to use fixed-length sequences (generally 50 words).

Google Neural Machine Translation (GNMT)

- Google Neural Machine Translation (GNMT) uses an attentional recurrent NN, with bidirectional GRUs, 8 recurrent layers on 8 GPUs for both the encoder and decoder.



2 - Transformers

Attention Is All You Need

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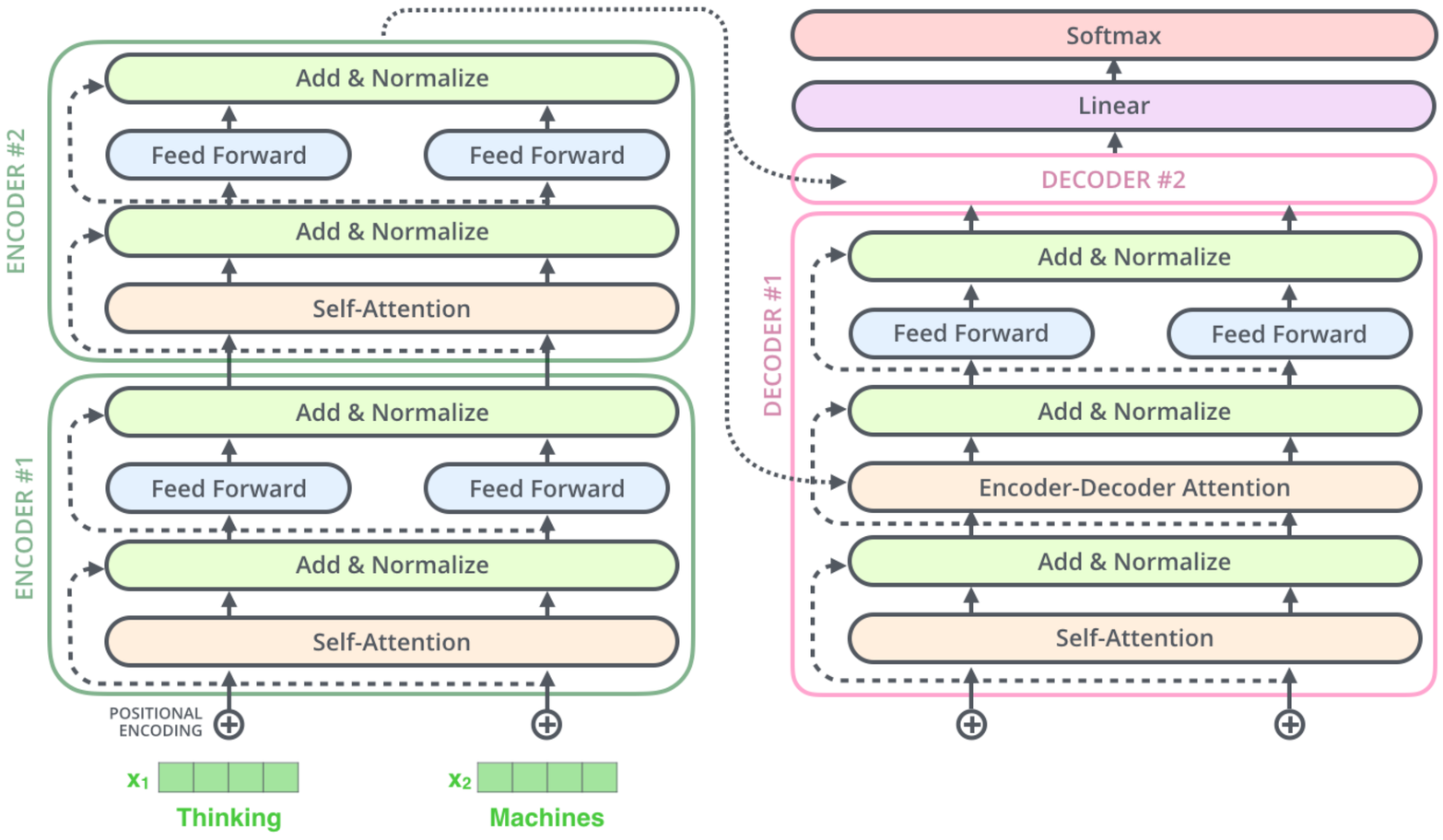
Transformer networks

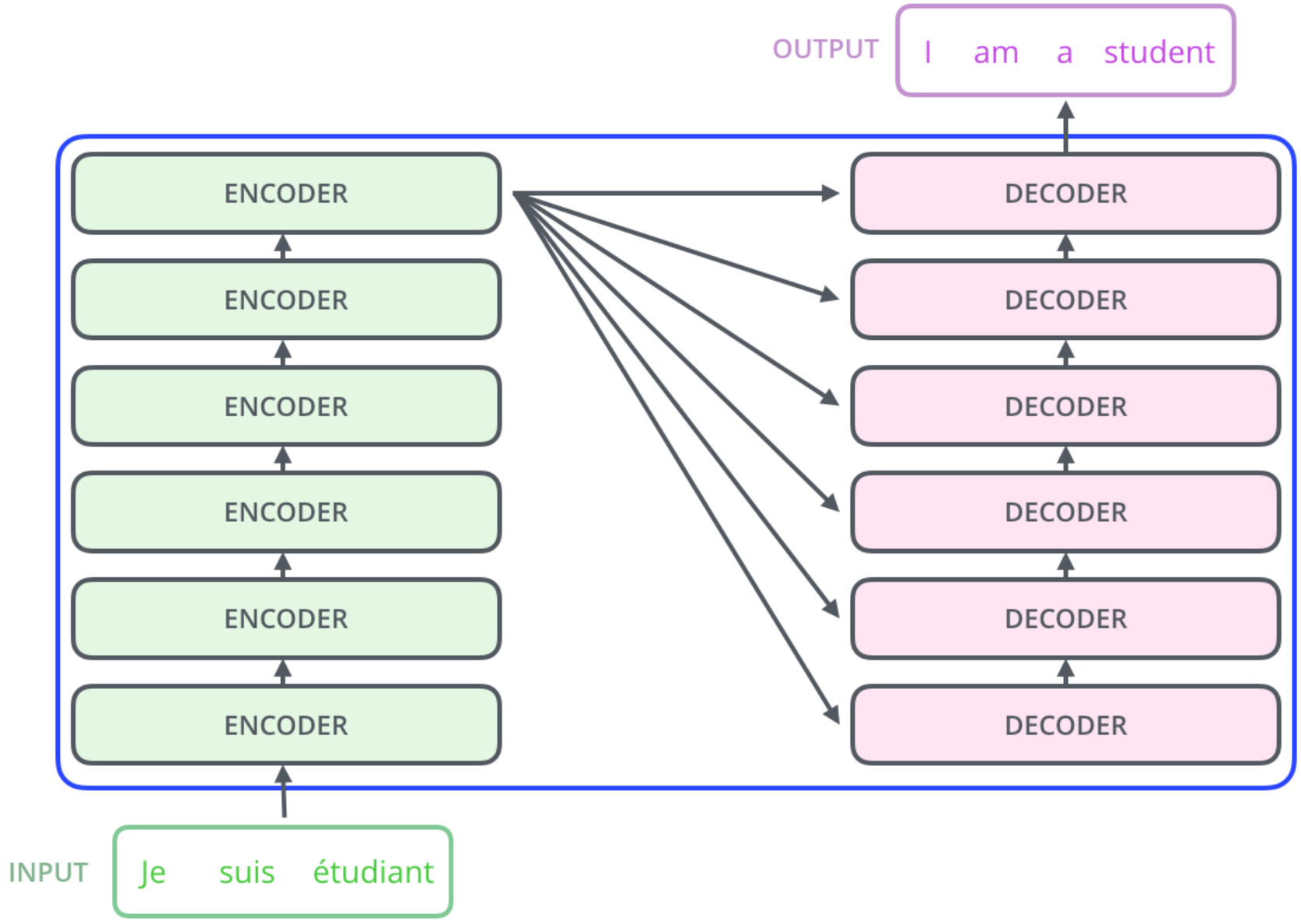
- Attentional mechanisms are so powerful that recurrent networks are not even needed anymore.
- **Transformer networks** use **self-attention** in a purely feedforward architecture and outperform recurrent architectures.
- Used in Google BERT and OpenAI GPT-3 for text understanding (e.g. search engine queries) and generation.



Source: http://jalammar.github.io/illustrated-transformer/

Transformer networks

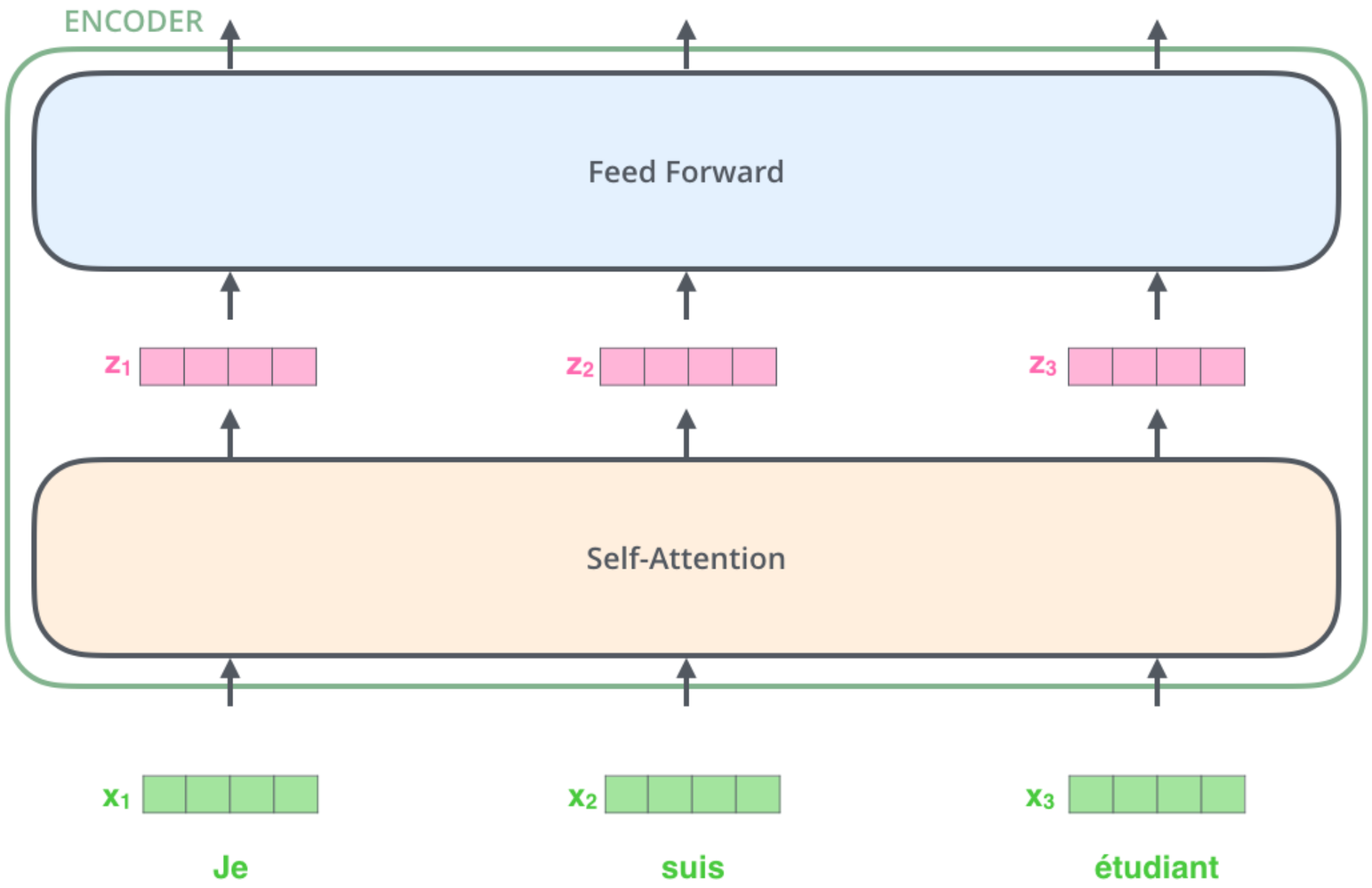
- Transformer networks use an **encoder-decoder** architecture, each with 6 stacked layers.



Source: http://jalammar.github.io/illustrated-transformer/

Encoder layer

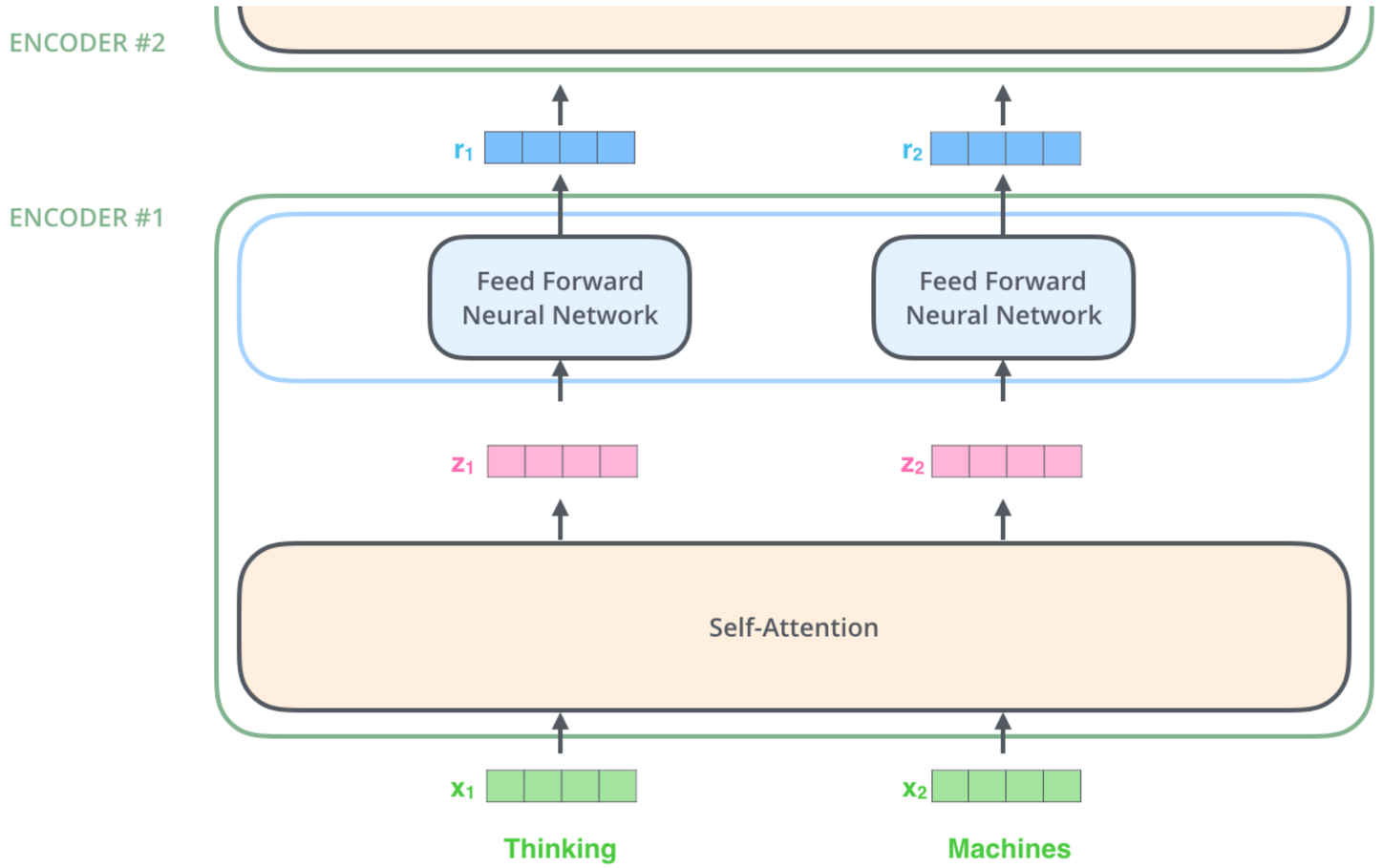
- Each layer of the encoder processes the n words of the input sentence **in parallel**.
- Word embeddings (as in word2vec) of dimension 512 are used as inputs (but learned end-to-end).



Source: http://jalammar.github.io/illustrated-transformer/

Encoder layer

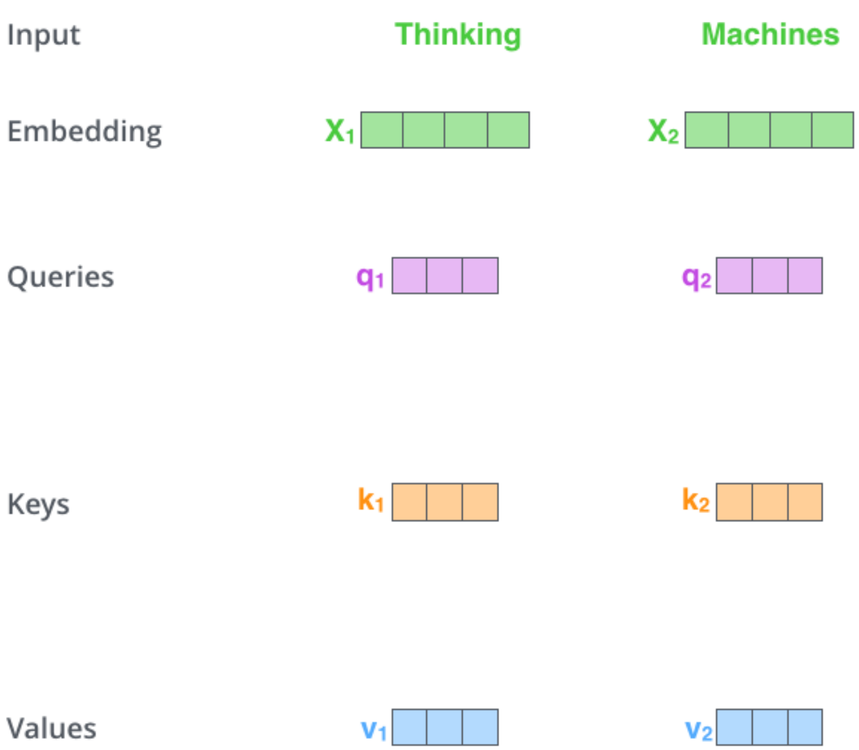
- Two operations are performed on each word embedding $\mathbf{x}_i$:
  - self-attention vector $\mathbf{z}_i$ depending on the other words.
  - a regular feedforward layer to obtain a new representation $\mathbf{r}_i$ (shared among all words).

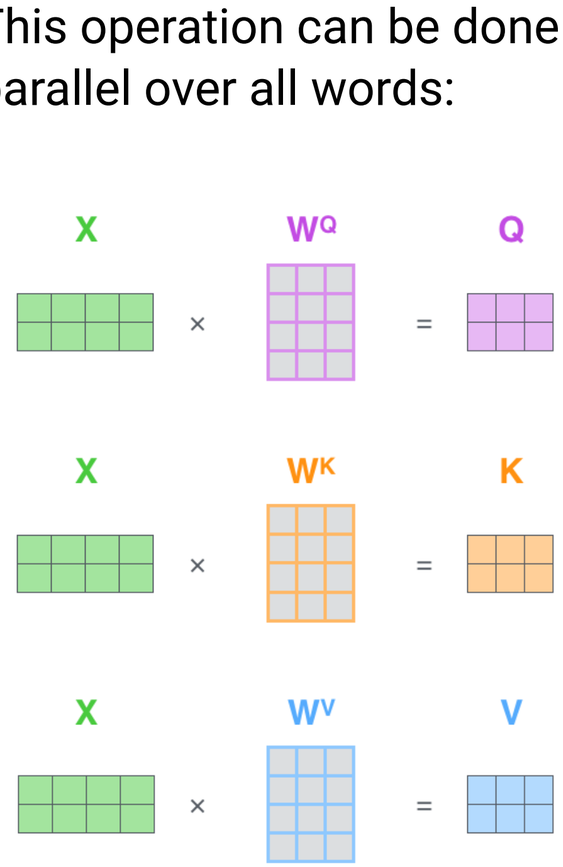


Source: http://jalammar.github.io/illustrated-transformer/

Self-attention

- The first step of self-attention is to compute for each word three vectors of length $d_k = 64$ from the embeddings $\mathbf{x}_i$ or previous representations $\mathbf{r}_i$ (d = 512).
  - The **query** $\mathbf{q}_i$ using W^Q.
  - The **key** $\mathbf{k}_i$ using W^K.
  - The **value** $\mathbf{v}_i$ using W^V.





- This operation can be done in parallel over all words:

Source: http://jalammar.github.io/illustrated-transformer/

Self-attention

- Why query / key / value? This a concept inspired from recommendation systems / databases.
- A Python dictionary is a set of key / value entries:

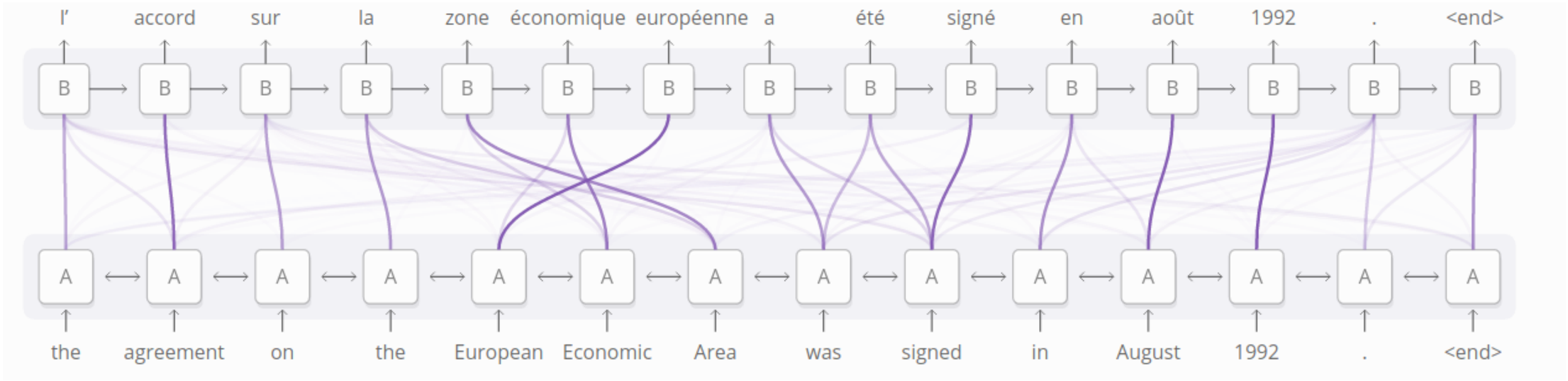
```
tel = {
    'jack': 4098,
    'sape': 4139
}
```

- The query would ask the dictionary to iterate over all entries and return the value associated to the key **equal or close to** the query.

```
tel['jacky'] # 4098
```

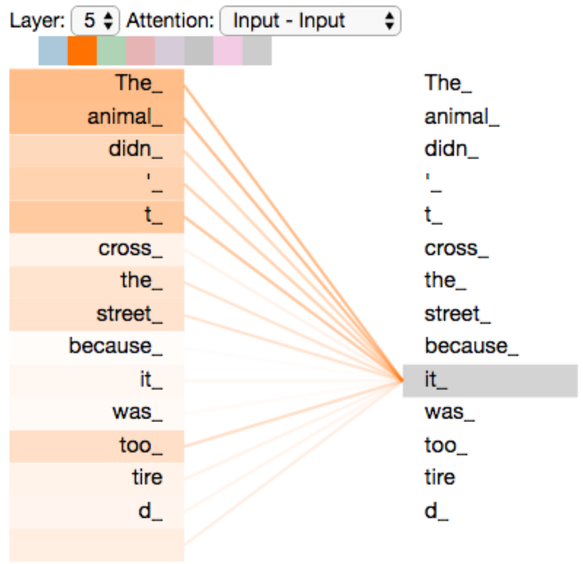
- This would be some sort of **fuzzy** dictionary.

Self-attention



- In attentional RNNs, the attention scores were used by each word generated by the decoder to decide which **input word** is relevant.
- If we apply the same idea to the **same sentence** (self-attention), the attention score tells how much words of the same sentence are related to each other (context).

  The animal didn't cross the street because it was too tired.
- The goal is to learn a representation for the word `it` that contains information about `the animal`, not `the street`.



Self-attention

- Each word $\mathbf{x}_i$ of the sentence generates its query $\mathbf{q}_i$, key $\mathbf{k}_i$ and value $\mathbf{v}_i$.

- For all other words $\mathbf{x}_j$, we compute the **match** between the query $\mathbf{q}_i$ and the keys $\mathbf{k}_j$ with a dot product:

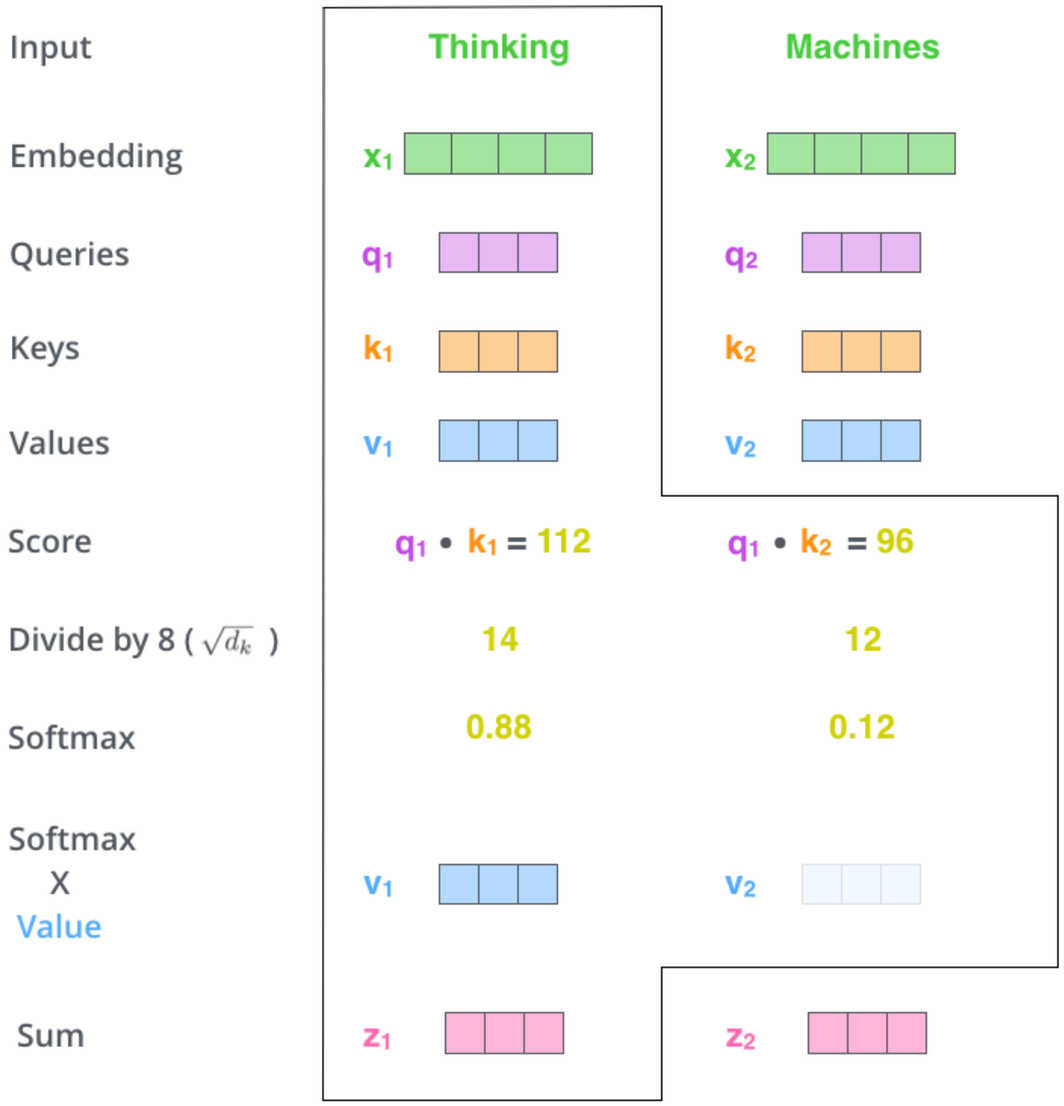
$$e_{i,j} = \mathbf{q}_i^T \mathbf{k}_j$$

- We normalize the scores by dividing by $\sqrt{d_k} = 8$ and apply a softmax:

$$a_{i,j} = \text{softmax}(\frac{\mathbf{q}_i^T \mathbf{k}_j}{\sqrt{d_k}})$$

- The new representation $\mathbf{z}_i$ of the word $\mathbf{x}_i$ is a weighted sum of the values of all other words, weighted by the attention score:

$$\mathbf{z}_i = \sum_j a_{i,j} \mathbf{v}_j$$



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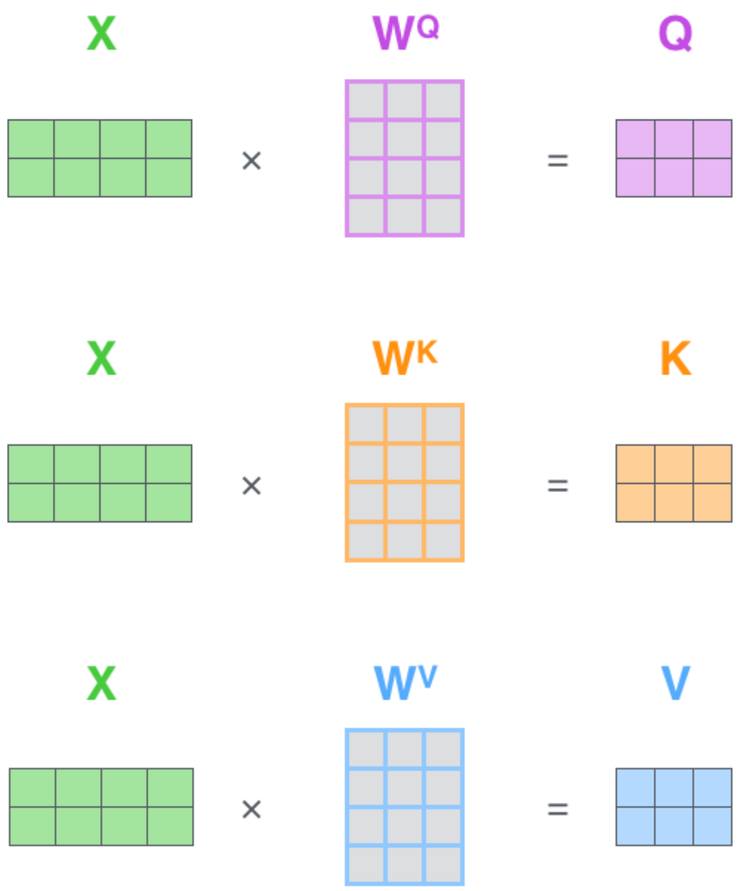
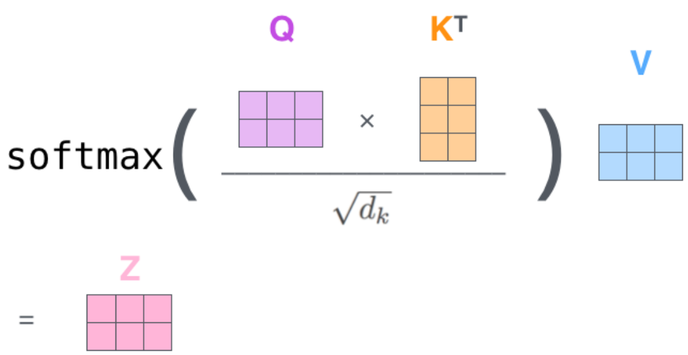
Self-attention



- If we concatenate the word embeddings into a $n \times d$ matrix X, self-attention only implies matrix multiplications and a row-based softmax:

$$\begin{cases} Q = X \times W^Q \\ K = X \times W^K \\ V = X \times W^V \\ Z = \text{softmax}(\frac{Q \times K^T}{\sqrt{d_k}}) \times V \end{cases}$$

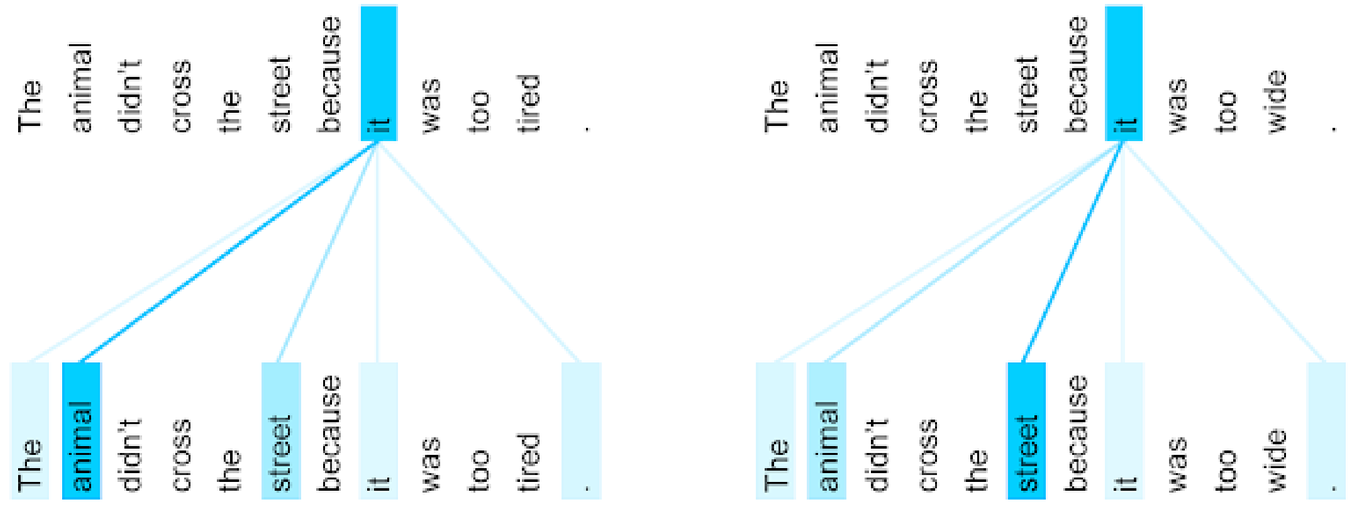


Source: http://jalammar.github.io/illustrated-transformer/

- Note 1: everything is differentiable, backpropagation will work.
- Note 2: the weight matrices do not depend on the length n of the sentence.

Multi-headed self-attention

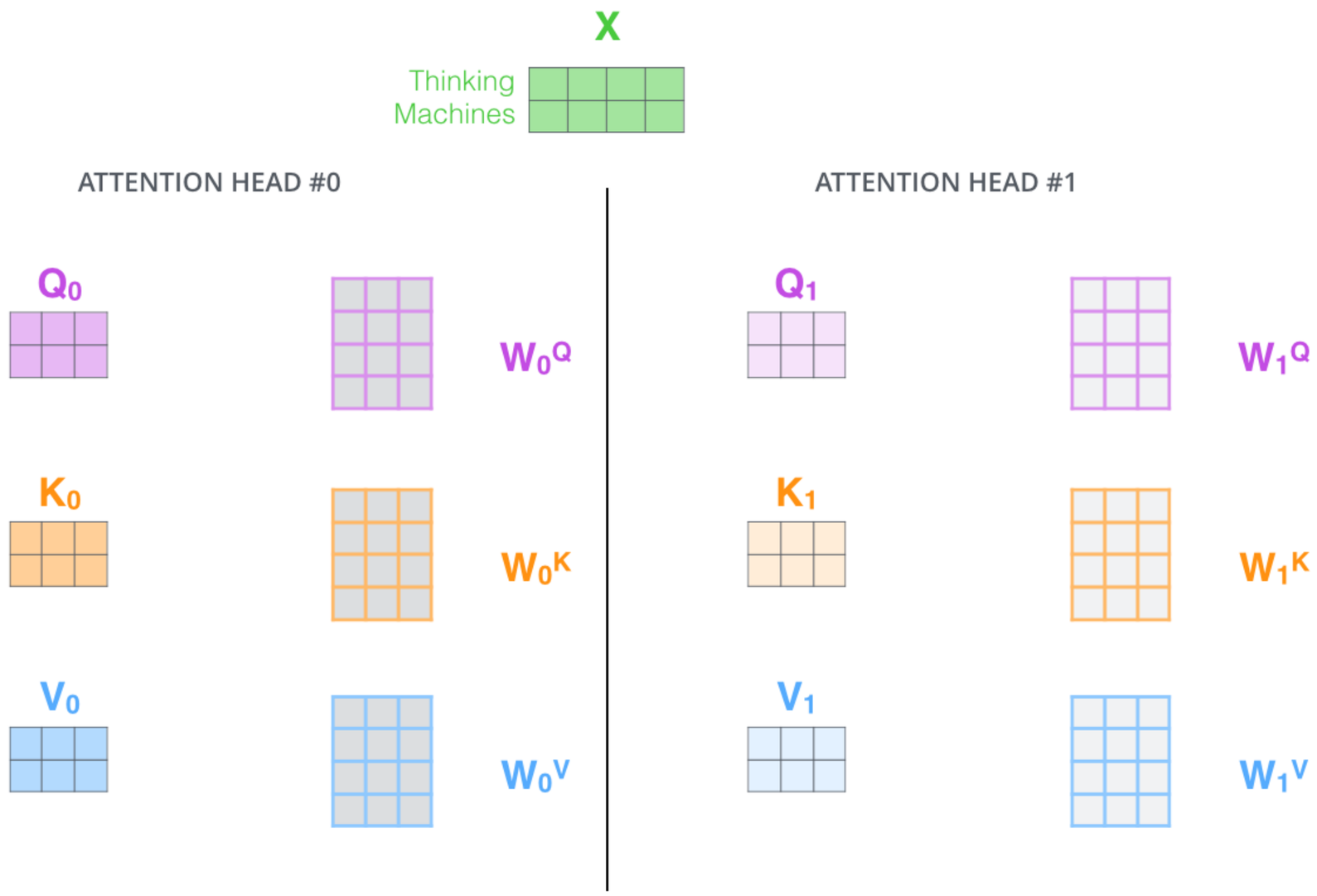
- In the sentence *The animal didn't cross the street because it was too tired.*, the new representation for the word `it` will hopefully contain features of the word `animal` after training.
- But what if the sentence was *The animal didn't cross the street because it was too* ***wide***.? The representation of `it` should be linked to `street` in that context.
- This is not possible with a single set of matrices W^Q, W^K and W^V, as they would average every possible context and end up being useless.



Source: https://ai.googleblog.com/2017/08/transformer-novel-neural-network.html

Multi-headed self-attention

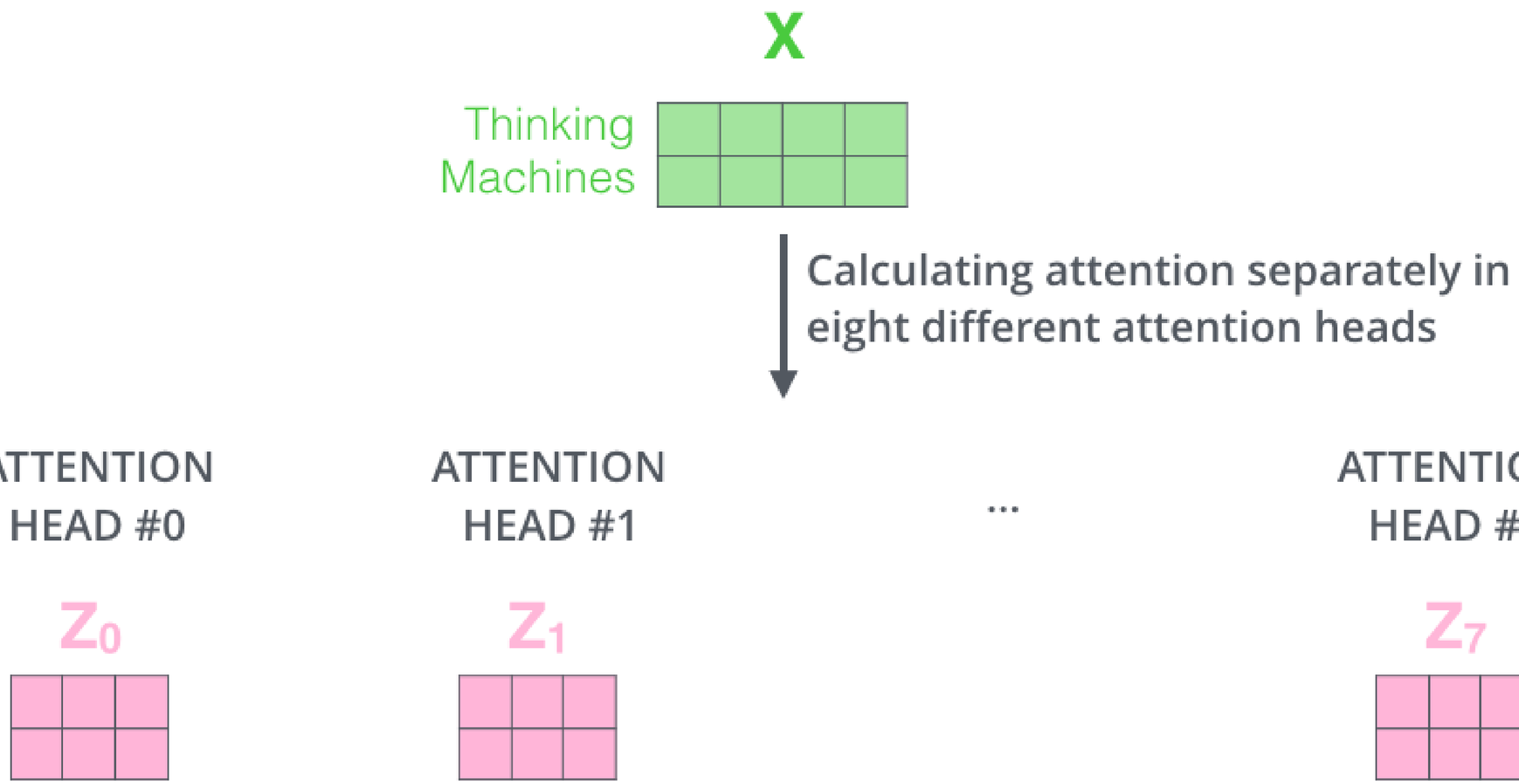
- The solution is to use **multiple attention heads** ($h = 8$) with their own matrices W_k^Q, W_k^K and W_k^V.



Source: http://jalammar.github.io/illustrated-transformer/

Multi-headed self-attention

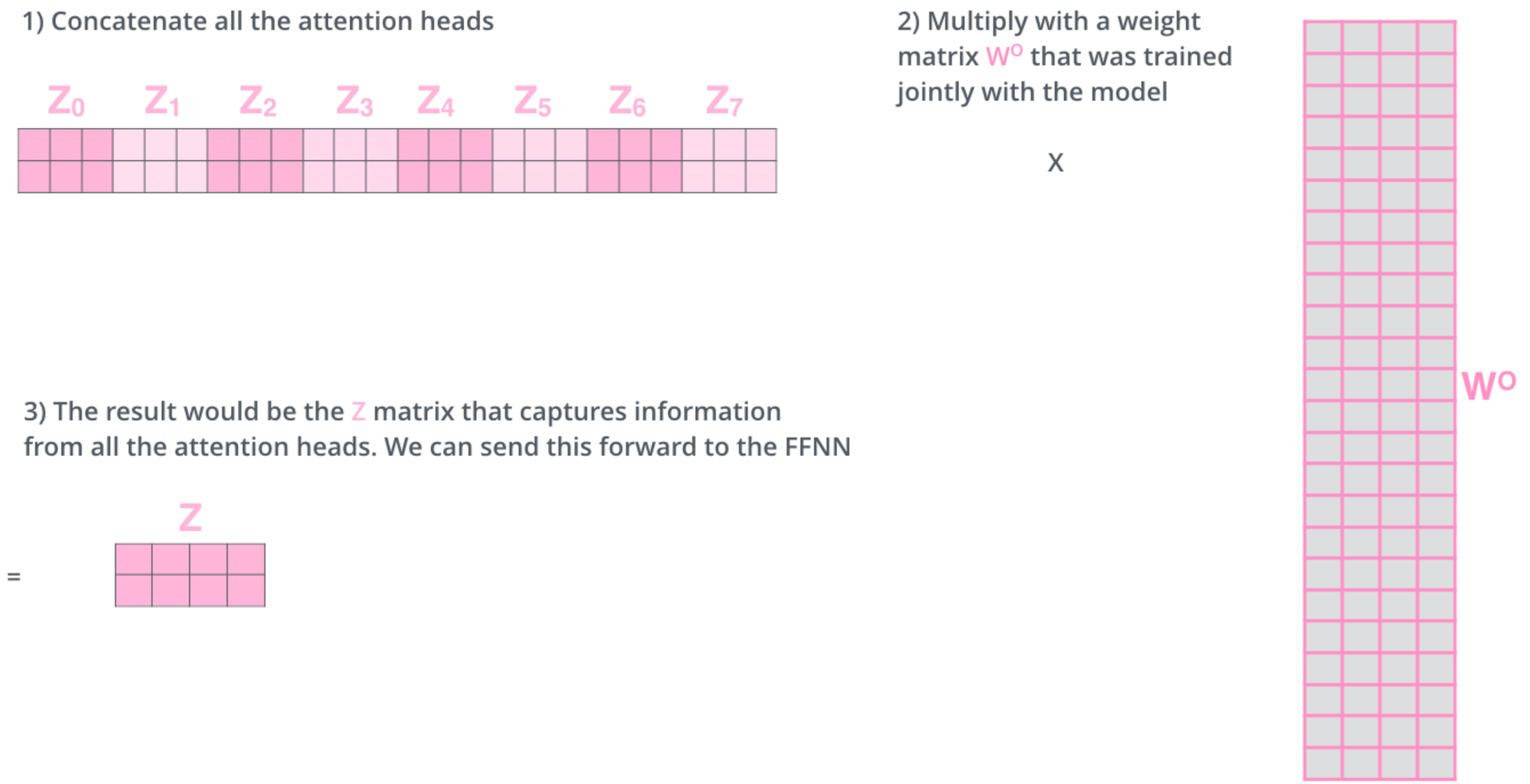
- Each **attention head** will output a vector $\mathbf{z}_i$ of size $d_k = 64$ for each word.
- How do we combine them?



Source: http://jalammar.github.io/illustrated-transformer/

Multi-headed self-attention

- The proposed solution is based on **ensemble learning** (stacking):
  - let another matrix W^O decide which attention head to trust…
  - 8×64 rows, 512 columns.



Source: http://jalammar.github.io/illustrated-transformer/

Multi-headed self-attention

1) This is our input sentence*

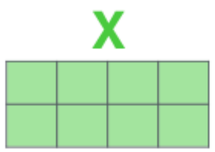
2) We embed each word*

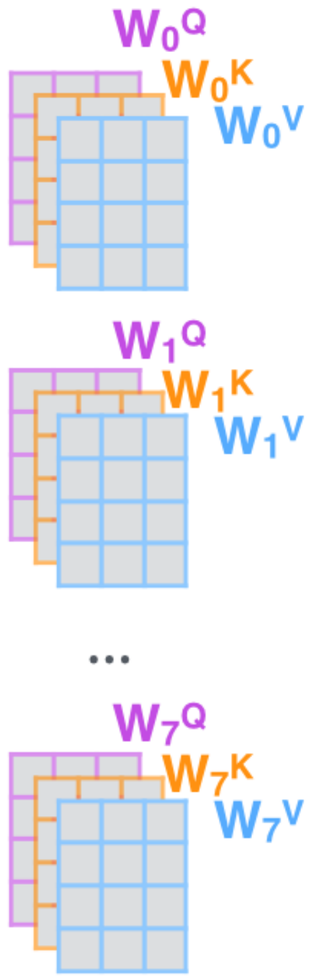
3) Split into 8 heads. We multiply X or R with weight matrices

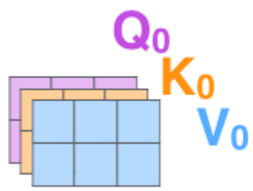
4) Calculate attention using the resulting Q/K/V matrices

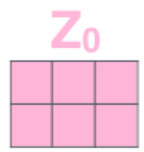
5) Concatenate the resulting Z matrices, then multiply with weight matrix W^O to produce the output of the layer

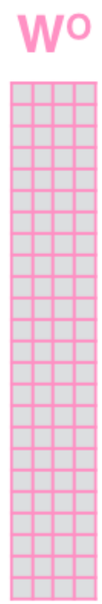
Thinking
Machines

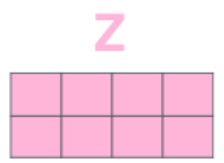


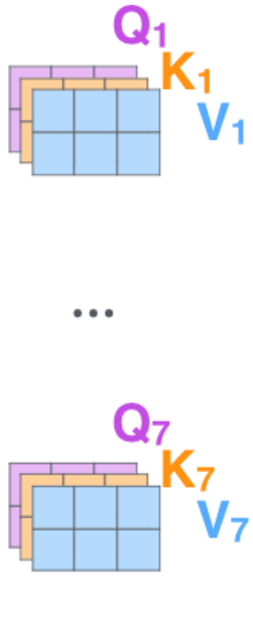










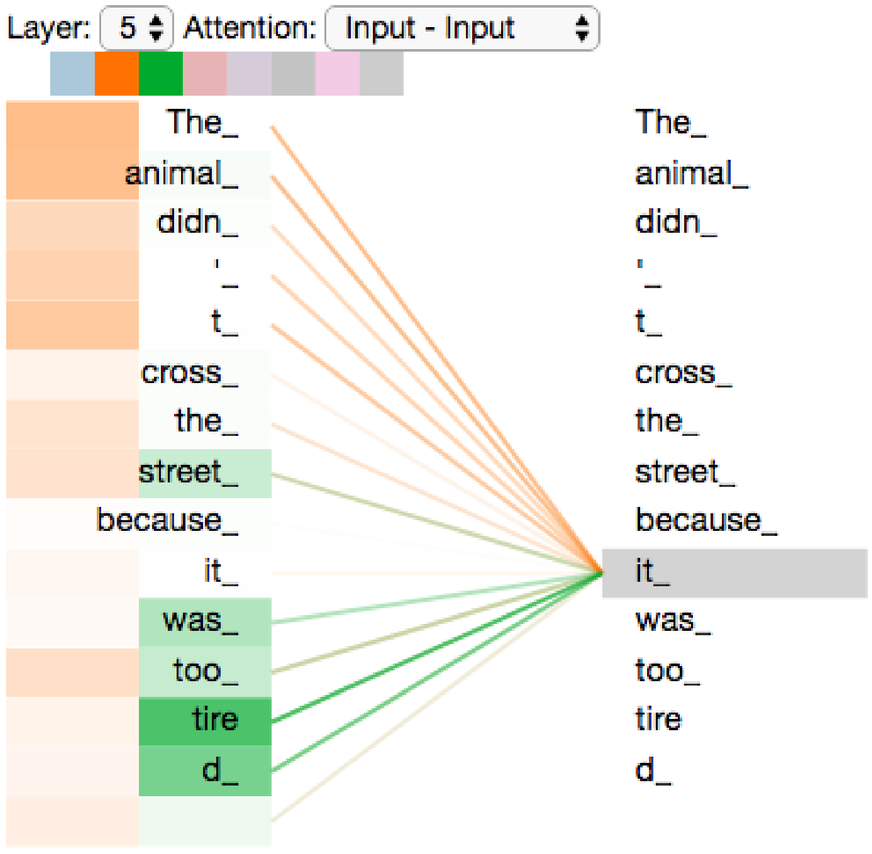


* In all encoders other than #0, we don't need embedding. We start directly with the output of the encoder right below this one

Source: http://jalammar.github.io/illustrated-transformer/

Multi-headed self-attention

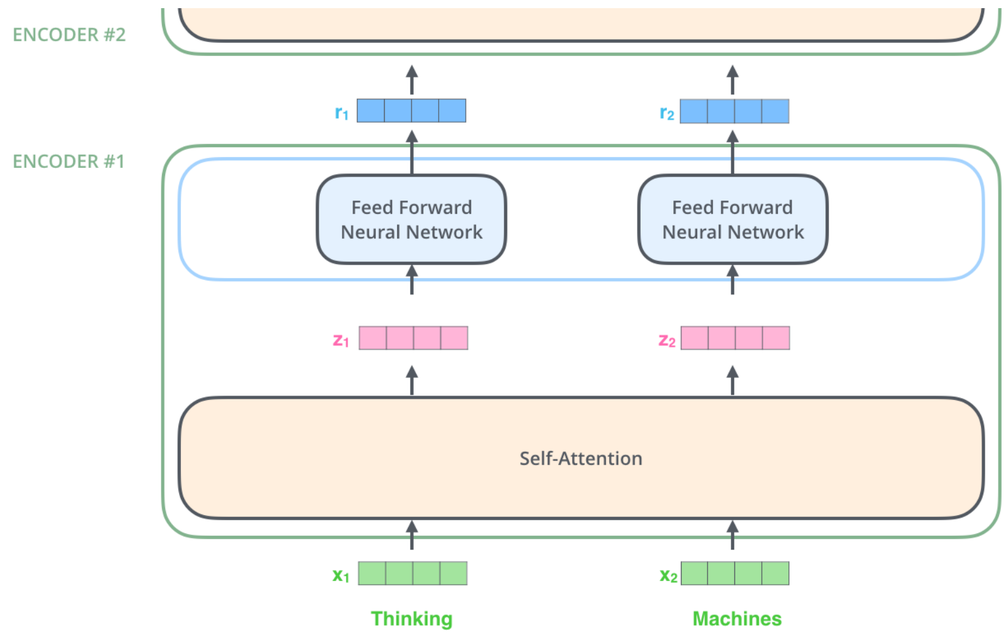
- Each attention head learns a different context:
  - `it` refers to `animal`.
  - `it` refers to `street`.
  - etc.
- The original transformer paper in 2017 used 8 attention heads.
- OpenAI's GPT-3 uses 96 attention heads…



Source: http://jalammar.github.io/illustrated-transformer/

Encoder layer

- Multi-headed self-attention produces a vector $\mathbf{z}_i$ for each word of the sentence.
- A regular feedforward MLP transforms it into a new representation $\mathbf{r}_i$.
  - one input layer with 512 neurons.
  - one hidden layer with 2048 neurons and a ReLU activation function.
  - one output layer with 512 neurons.
- The same NN is applied on all words, it does not depend on the length n of the sentence.



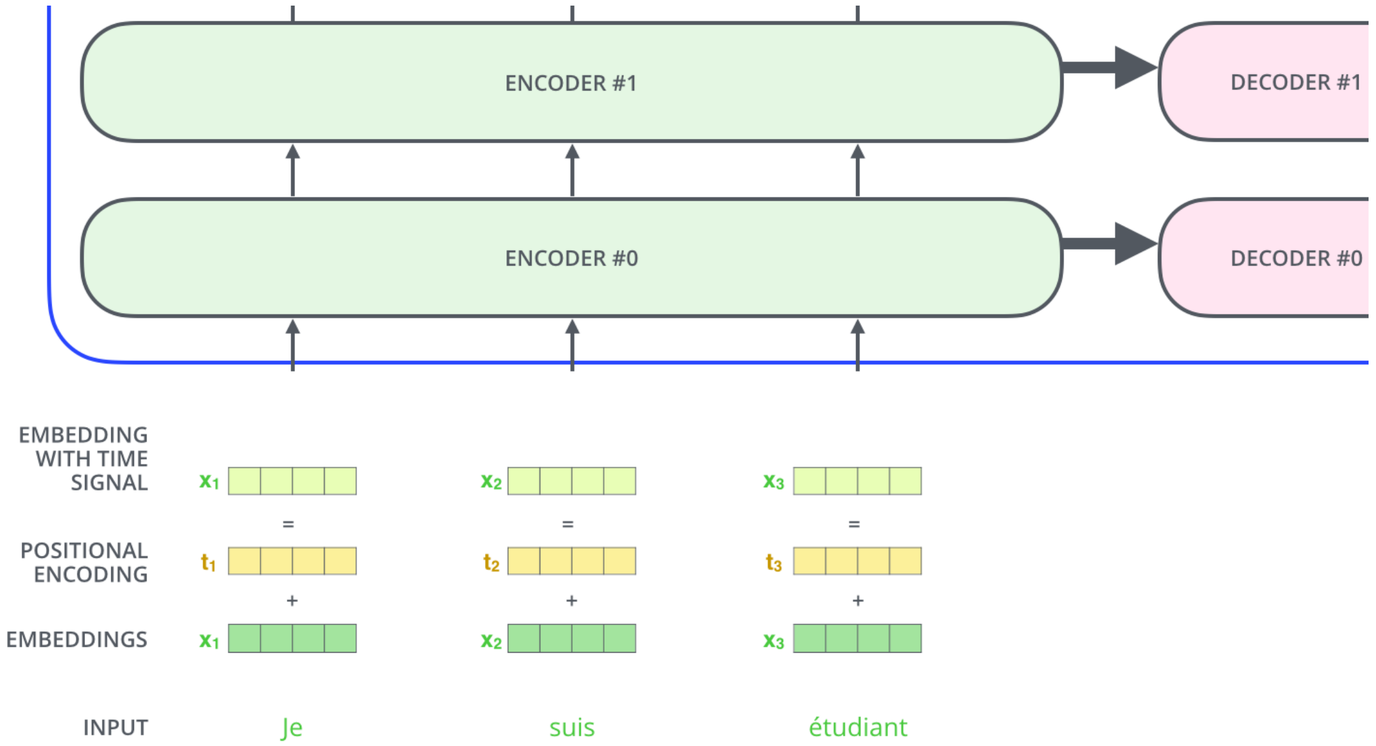
Source: http://jalammar.github.io/illustrated-transformer/

Positional encoding

- As each word is processed in parallel, the order of the words in the sentence is lost.

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

- We need to explicitly provide that information in the **input** using positional encoding.
- A simple method would be to append an index $i = 1, 2, \ldots, n$ to the word embeddings, but it is not very robust.



Source: http://jalammar.github.io/illustrated-transformer/

Positional encoding

- If the elements of the 512-d embeddings are numbers between 0 and 1, concatenating an integer between 1 and n will unbalance the dimensions.
- Normalizing that integer between 0 and 1 requires to know n in advance, this introduces a maximal sentence length…
- How about we append the binary code of that integer?

$0:$	0 0 0 0	$8:$	1 0 0 0
$1:$	0 0 0 1	$9:$	1 0 0 1
$2:$	0 0 1 0	$10:$	1 0 1 0
$3:$	0 0 1 1	$11:$	1 0 1 1
$4:$	0 1 0 0	$12:$	1 1 0 0
$5:$	0 1 0 1	$13:$	1 1 0 1
$6:$	0 1 1 0	$14:$	1 1 1 0
$7:$	0 1 1 1	$15:$	1 1 1 1

Source: https://kazemnejad.com/blog/transformer_architecture_positional_encoding/

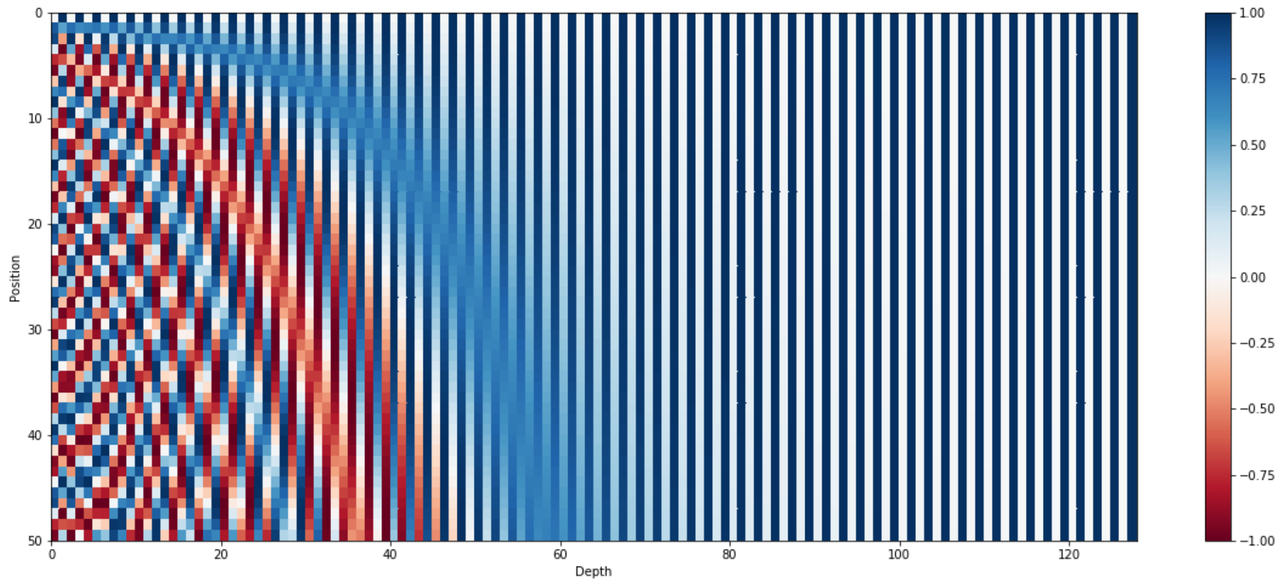
- Sounds good, we have numbers between 0 and 1, and we just need to use enough bits to encode very long sentences.
- However, representing a binary value (0 or 1) with a 64 bits floating number is a waste of computational resources.

Positional encoding

- We can notice that the bits of the integers oscillate at various frequencies:
  - the lower bit oscillates every number.
  - the bit before oscillates every two numbers.
  - etc.

0 :	0	0	0	0	8 :	1	0	0	0
1 :	0	0	0	1	9 :	1	0	0	1
2 :	0	0	1	0	10 :	1	0	1	0
3 :	0	0	1	1	11 :	1	0	1	1
4 :	0	1	0	0	12 :	1	1	0	0
5 :	0	1	0	1	13 :	1	1	0	1
6 :	0	1	1	0	14 :	1	1	1	0
7 :	0	1	1	1	15 :	1	1	1	1

- We could also represent the position of a word using sine and cosine functions at different frequencies (Fourier basis).
- We create a vector, where each element oscillates at increasing frequencies.
- The “code” for each position in the sentence is unique.

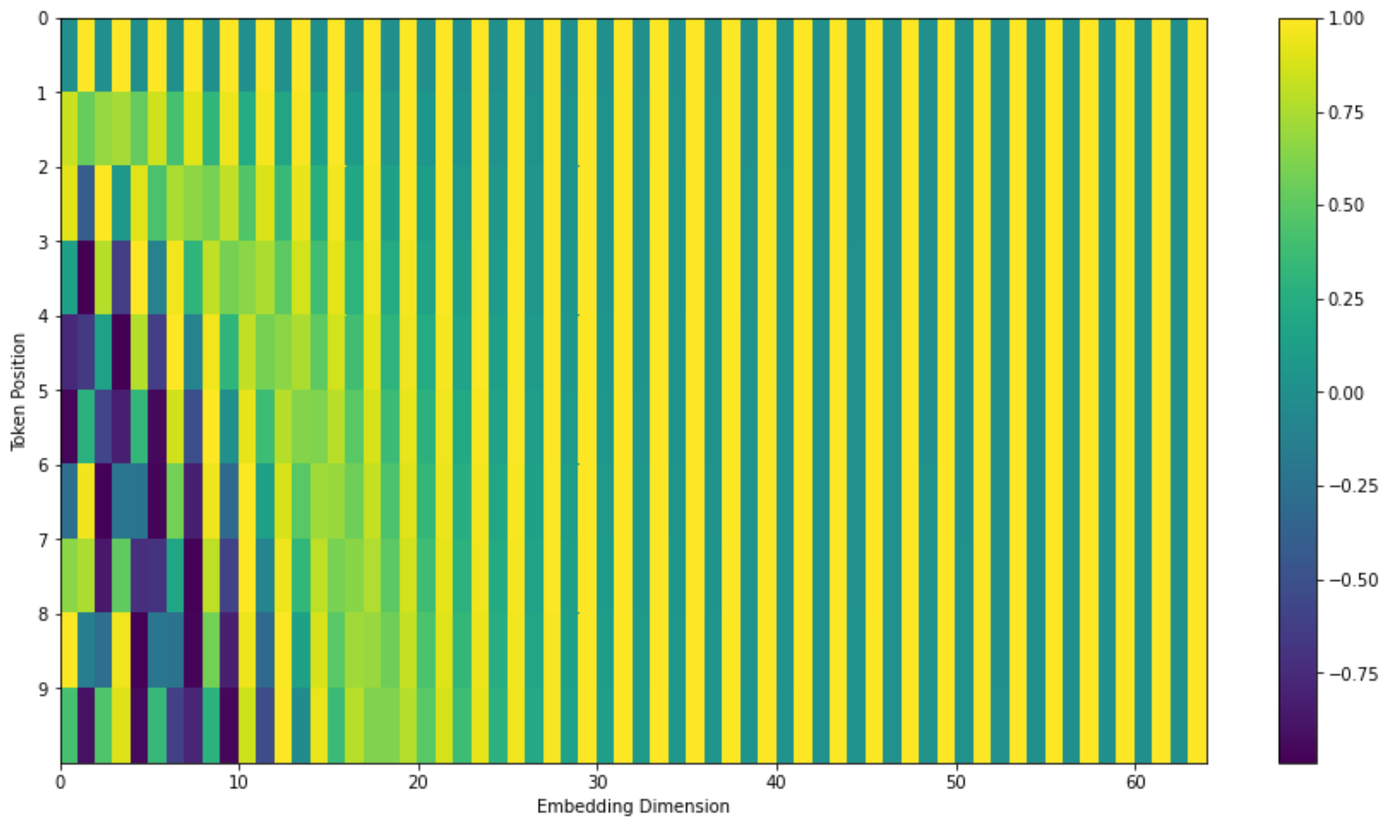


Source: https://kazemnejad.com/blog/transformer_architecture_positional_encoding/

Positional encoding

- In practice, a 512-d vector is created using sine and cosine functions.

$$\begin{cases} t(\text{pos}, 2i) = \sin(\frac{\text{pos}}{10000^{2i/512}}) \\ t(\text{pos}, 2i+1) = \cos(\frac{\text{pos}}{10000^{2i/512}}) \end{cases}$$

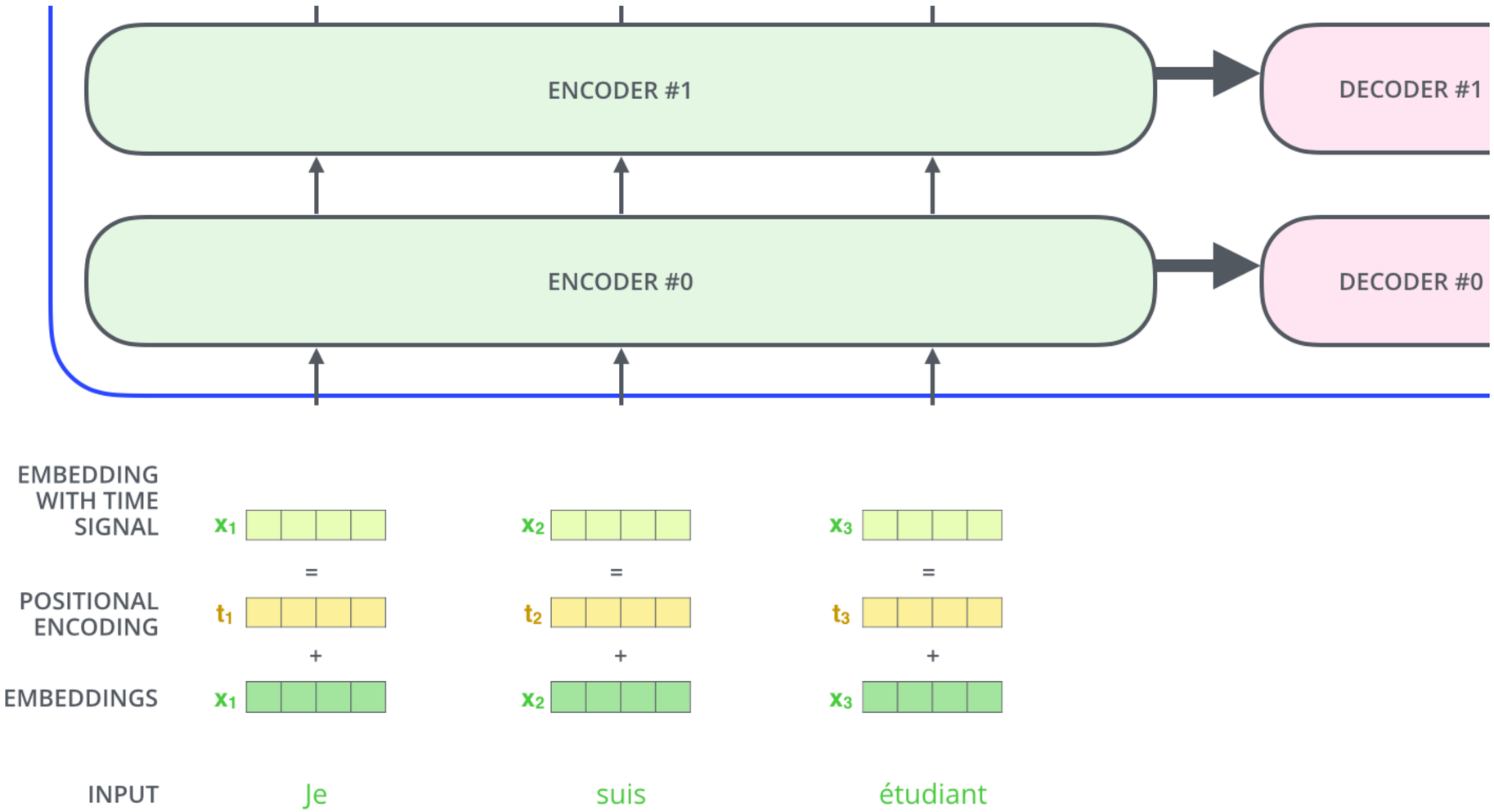


Source: http://jalammar.github.io/illustrated-transformer/

Positional encoding

- The positional encoding vector is **added** element-wise to the embedding, not concatenated!

$$\mathbf{x}_i = \mathbf{x}_i^{\text{embed}} + \mathbf{t}_i$$



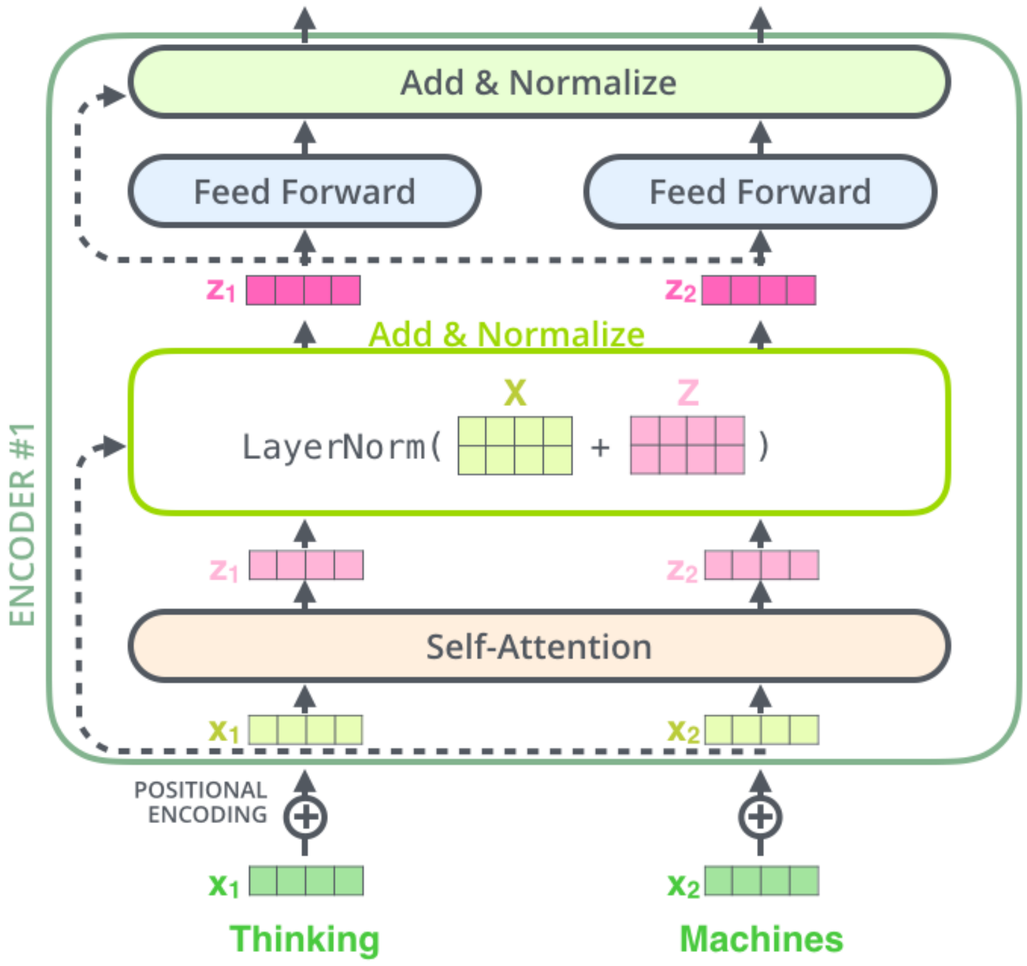
Source: http://jalammar.github.io/illustrated-transformer/

Encoder layer

- Last tricks of the encoder layers:
  - skip connections (residual layer)
  - layer normalization
- The input X is added to the output of the multi-headed self-attention and normalized (zero mean, unit variance).
- **Layer normalization** (Ba et al., 2016) is an alternative to batch normalization, where the mean and variance are computed over single vectors, not over a minibatch:

$$\mathbf{z} \leftarrow \frac{\mathbf{z} - \mu}{\sigma}$$

with $\mu = \frac{1}{d}\sum_{i=1}^{d} z_i$ and $\sigma = \frac{1}{d}\sum_{i=1}^{d}(z_i - \mu)^2$.

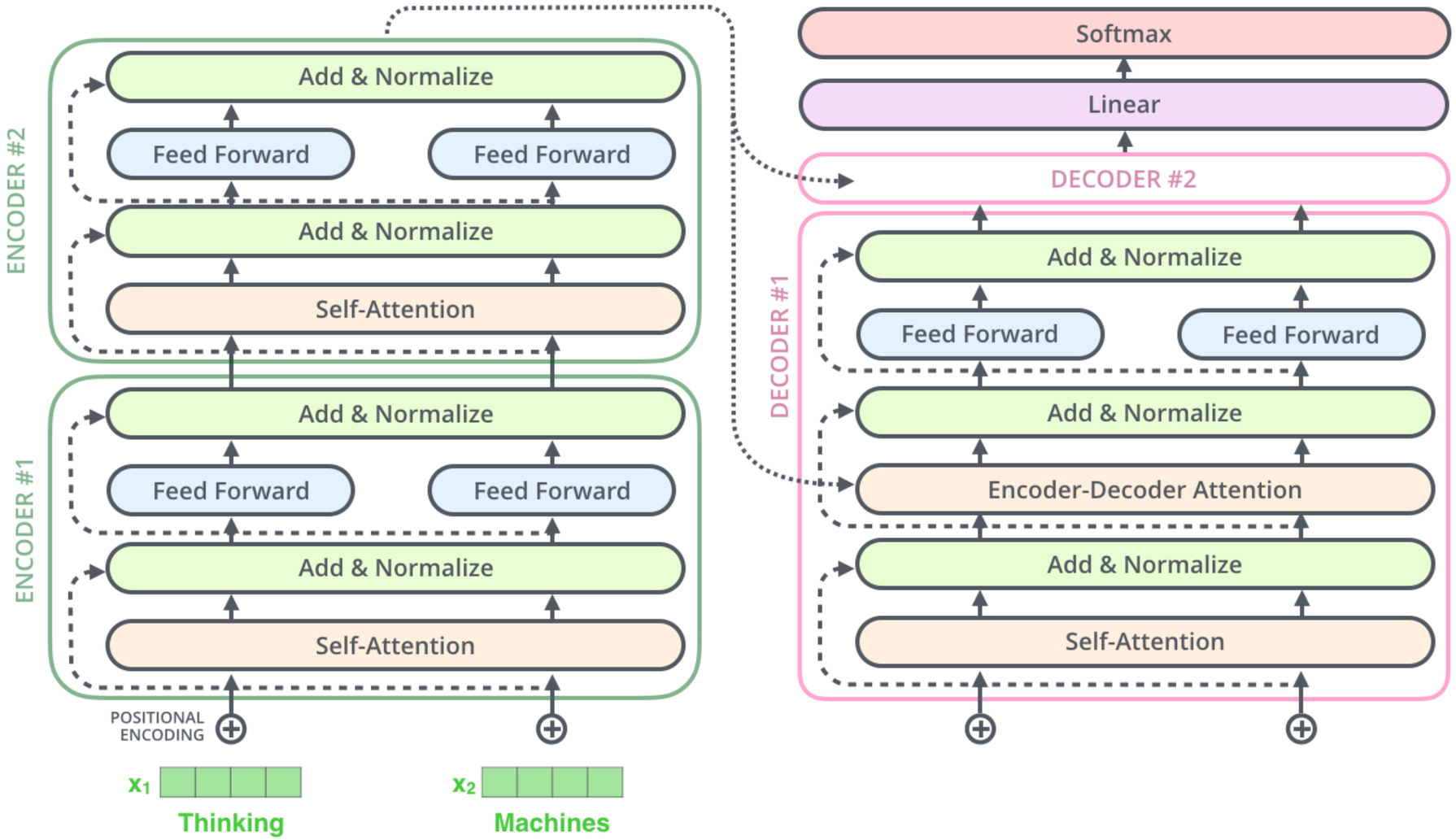


Source: http://jalammar.github.io/illustrated-transformer/

- The feedforward network also uses a skip connection and layer normalization.

Encoder

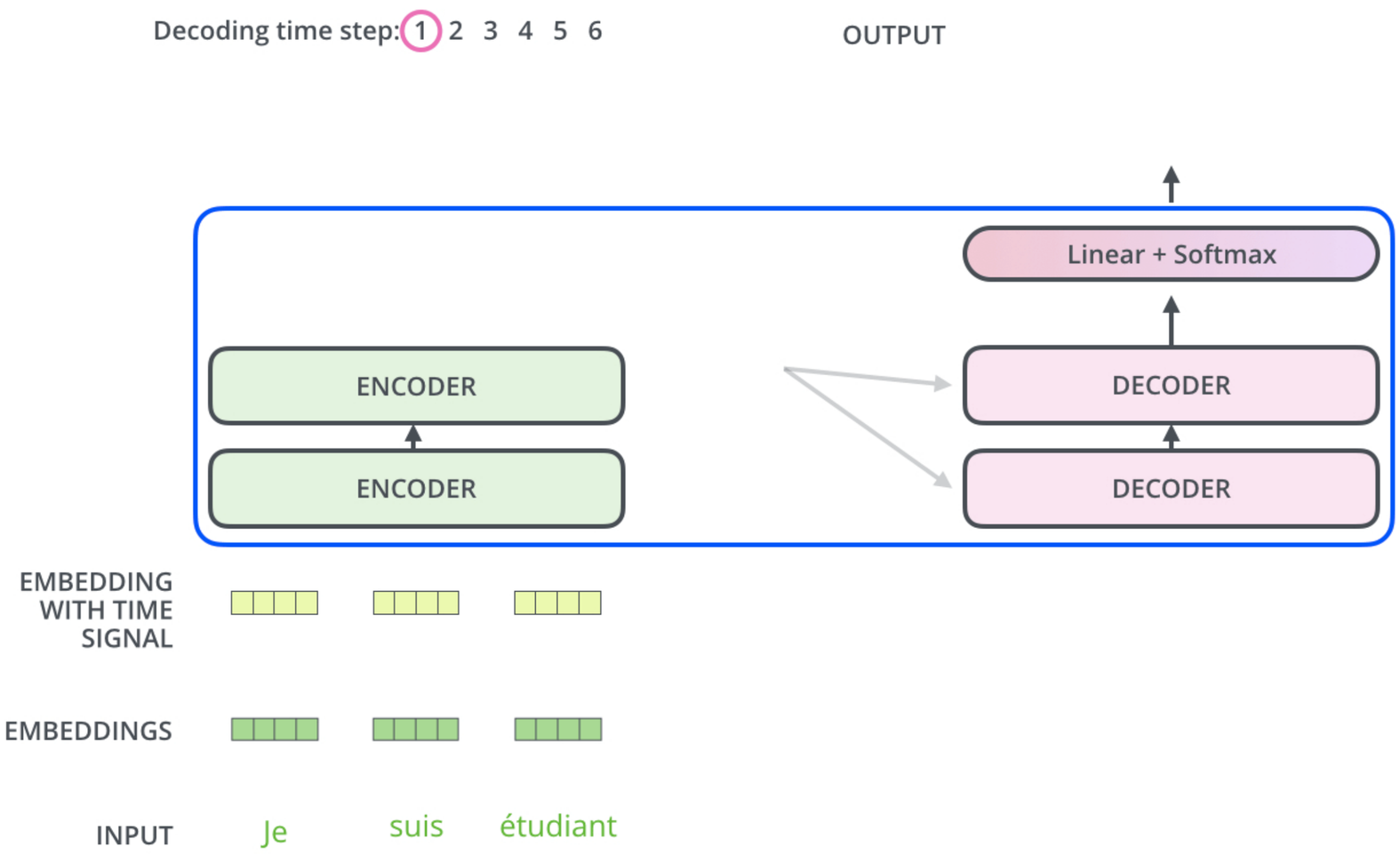
- We can now stack 6 (or more, 96 in GPT-3) of these encoder layers and use the final representation of each word as an input to the decoder.



Source: http://jalammar.github.io/illustrated-transformer/

Decoder

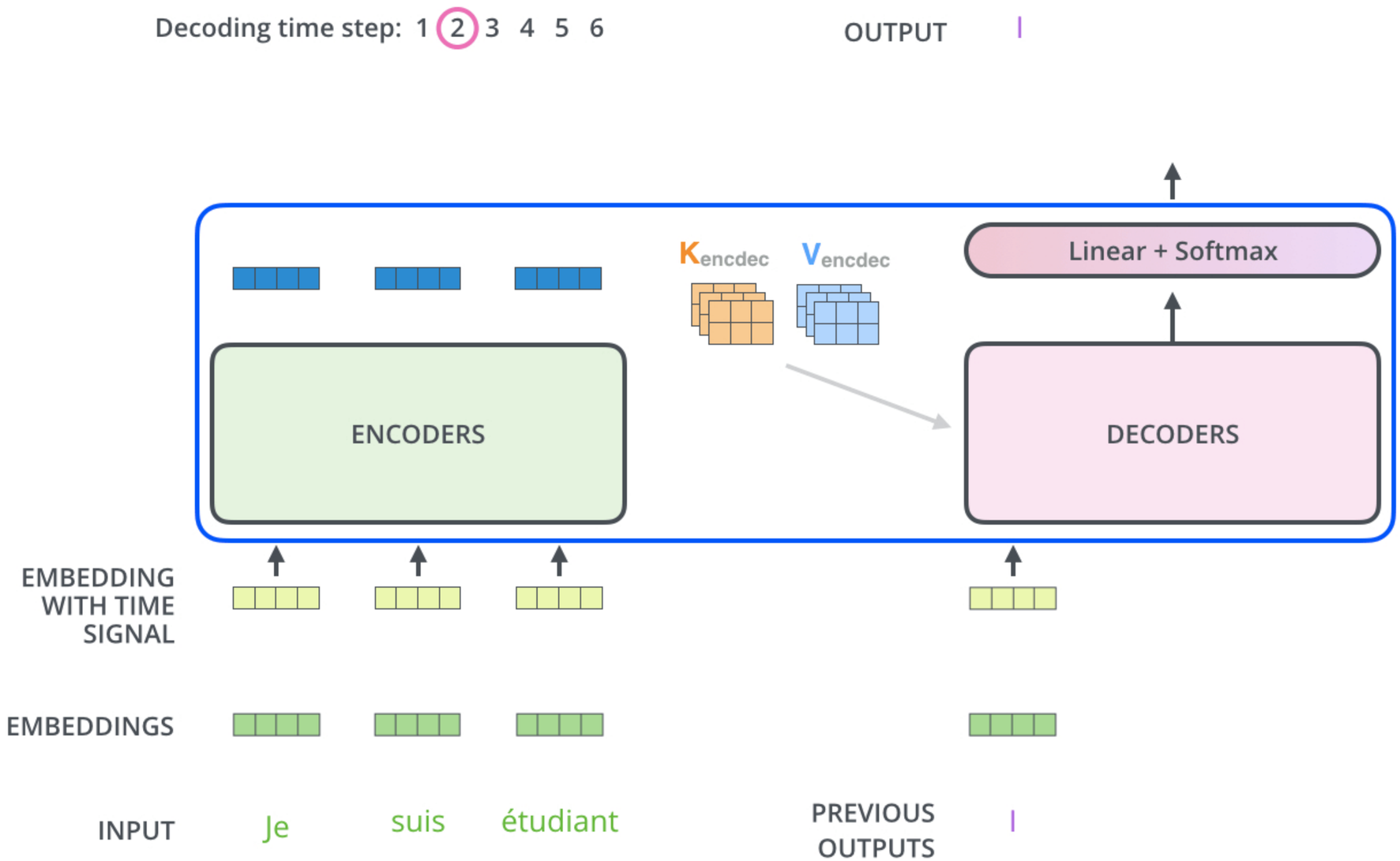
- In the first step of decoding, the final representations of the encoder are used as query and value vectors of the decoder to produce the first word.
- The input to the decoder is a “start of sentence” symbol.



Source: http://jalammar.github.io/illustrated-transformer/

Decoder

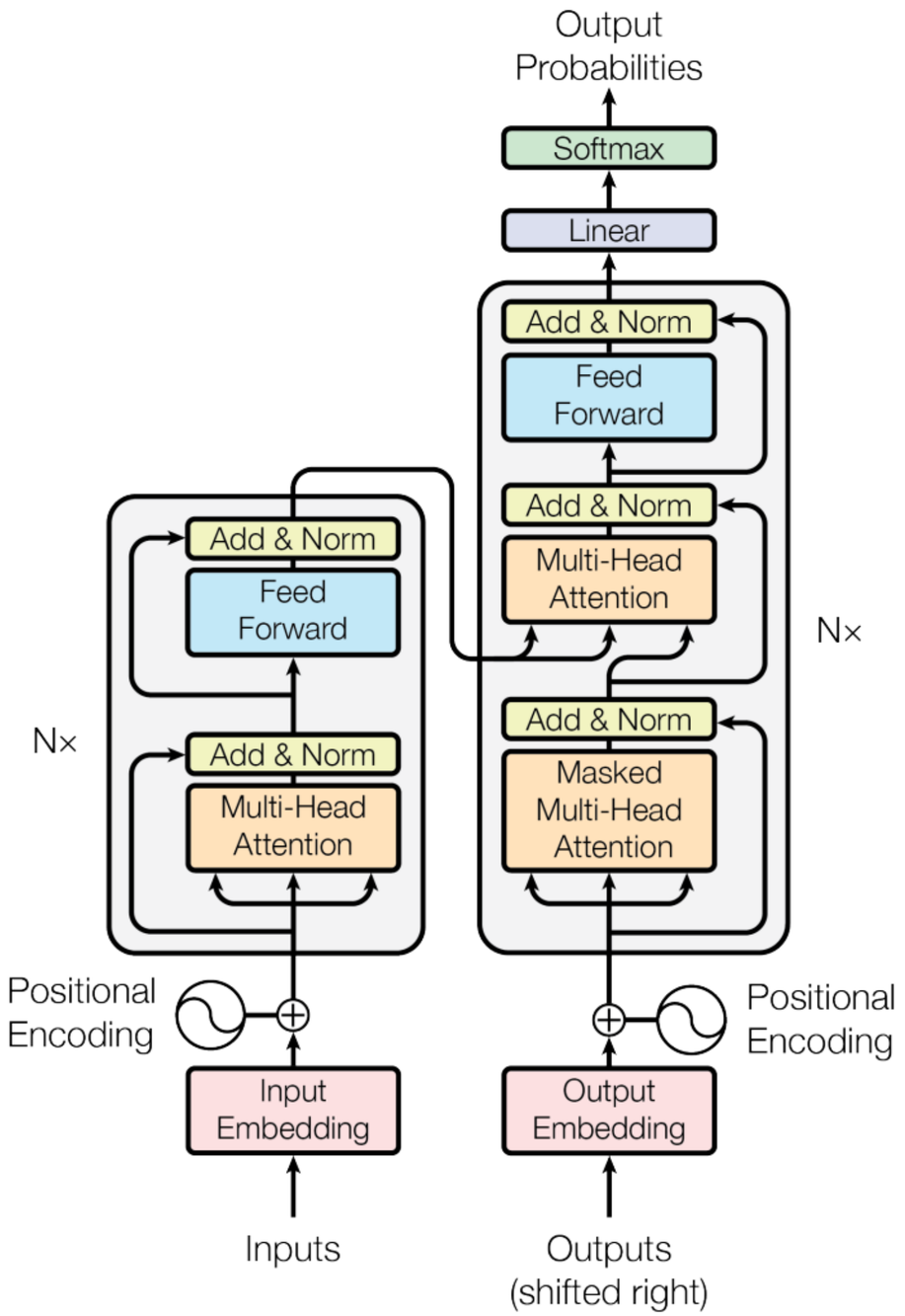
- The decoder is **autoregressive**: it outputs words one at a time, using the previously generated words as an input.



Source: http://jalammar.github.io/illustrated-transformer/

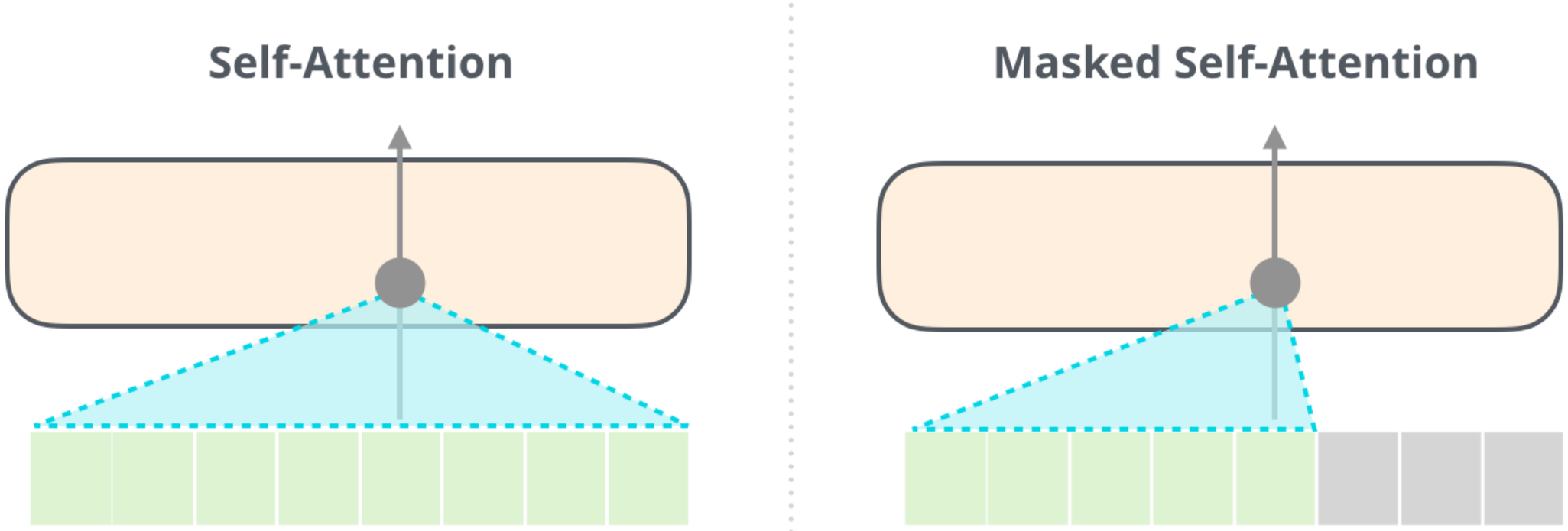
Decoder layer

- Each decoder layer has two multi-head attention sub-layers:
  - A self-attention sub-layer with query/key/values coming from the generated sentence.
  - An **encoder-decoder** attention sub-layer, with the query coming from the generated sentence and the key/value from the encoder.
- The encoder-decoder attention is the regular attentional mechanism used in seq2seq architectures.
- Apart from this additional sub-layer, the same residual connection and layer normalization mechanisms are used.



Masked self-attention

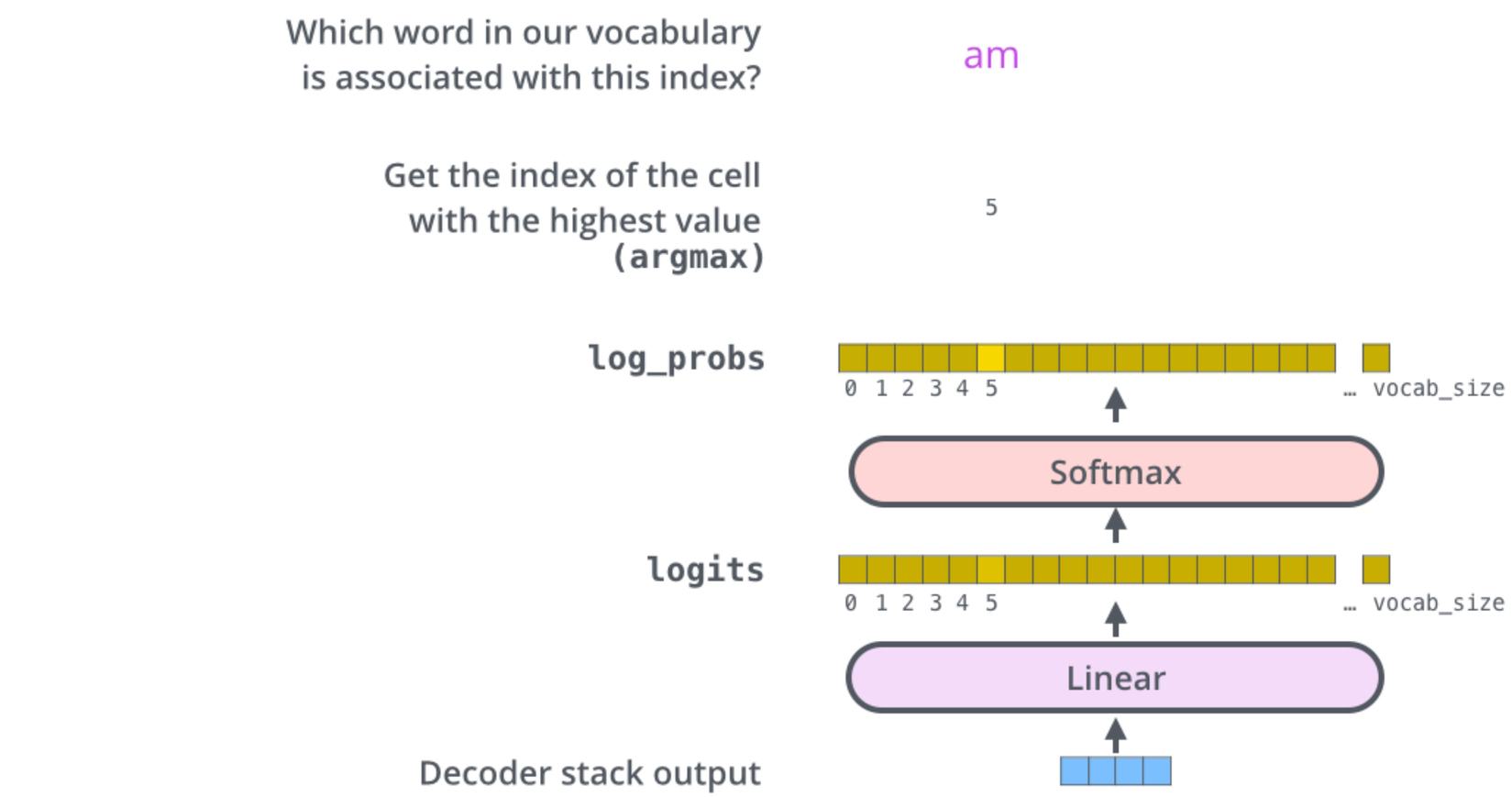
- When the sentence has been fully generated (up to the `<eos>` symbol), **masked self-attention** has to applied in order for a word in the middle of the sentence to not “see” the solution in the input when learning.
- As usual, learning occurs on minibatches of sentences, not on single words.



Source: https://jalammar.github.io/illustrated-gpt2/

Output

- The output of the decoder is a simple softmax classification layer, predicting the one-hot encoding of the word using a vocabulary (`vocab_size=25000`).



Source: http://jalammar.github.io/illustrated-transformer/

Training procedure

- The transformer is trained on the WMT datasets:
  - English-French: 36M sentences, 32000 unique words.
  - English-German: 4.5M sentences, 37000 unique words.
- Cross-entropy loss, Adam optimizer with scheduling, dropout. Training took 3.5 days on 8 P100 GPUs.
- The sentences can have different lengths, as the decoder is autoregressive.
- The transformer network beat the state-of-the-art performance in translation with less computations and without any RNN.

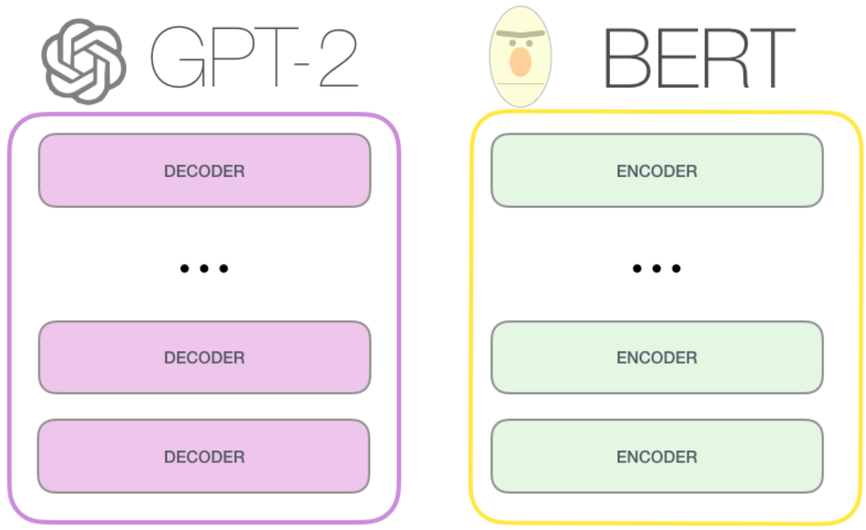
Table 2: The Transformer achieves better BLEU scores than previous state-of-the-art models on the English-to-German and English-to-French newstest2014 tests at a fraction of the training cost.

Model	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**	$2.3 \cdot 10^{19}$	

3 - Self-supervised transformers

Transformer-based language models

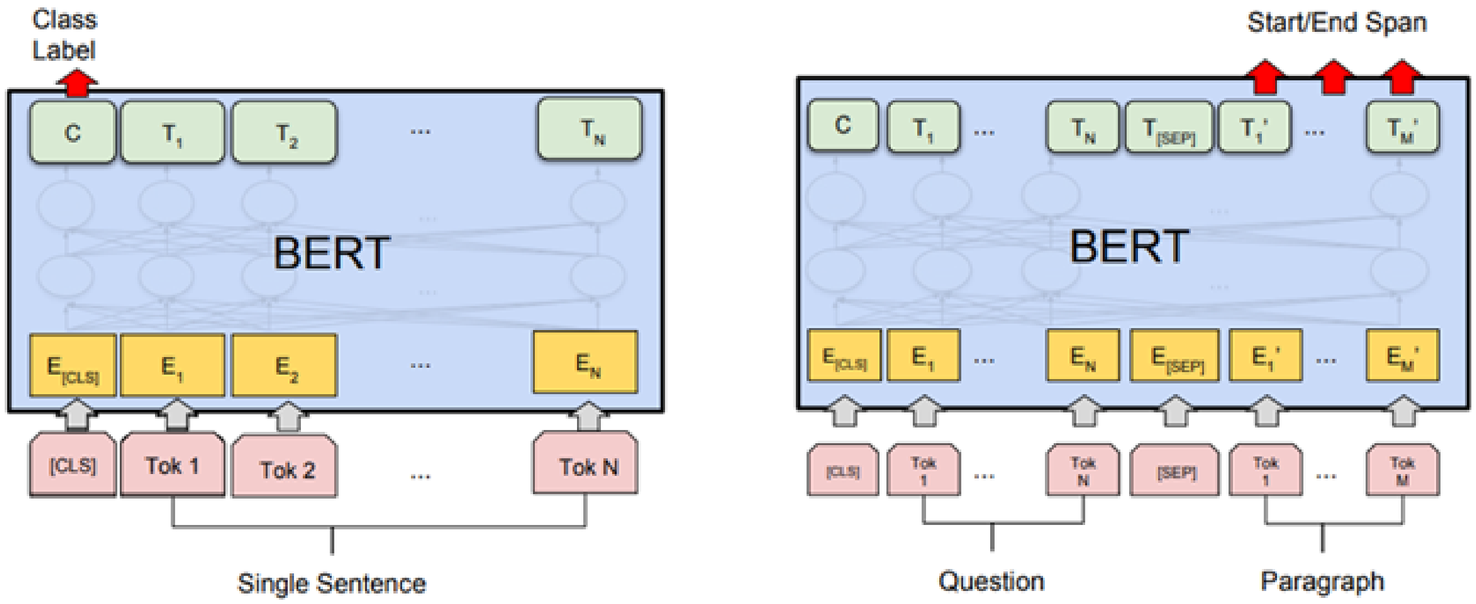
- The Transformer is considered as the **AlexNet** moment of natural language processing (NLP).
- However, it is limited to supervised learning of sentence-based translation.
- Two families of architectures have been developed from that idea to perform all NLP tasks using **unsupervised pretraining** or **self-supervised training**:
  - BERT (Bidirectional Encoder Representations from Transformers) from Google.
  - GPT (Generative Pre-trained Transformer) from OpenAI https://openai.com/blog/better-language-models/.



Source: https://jalammar.github.io/illustrated-gpt2/

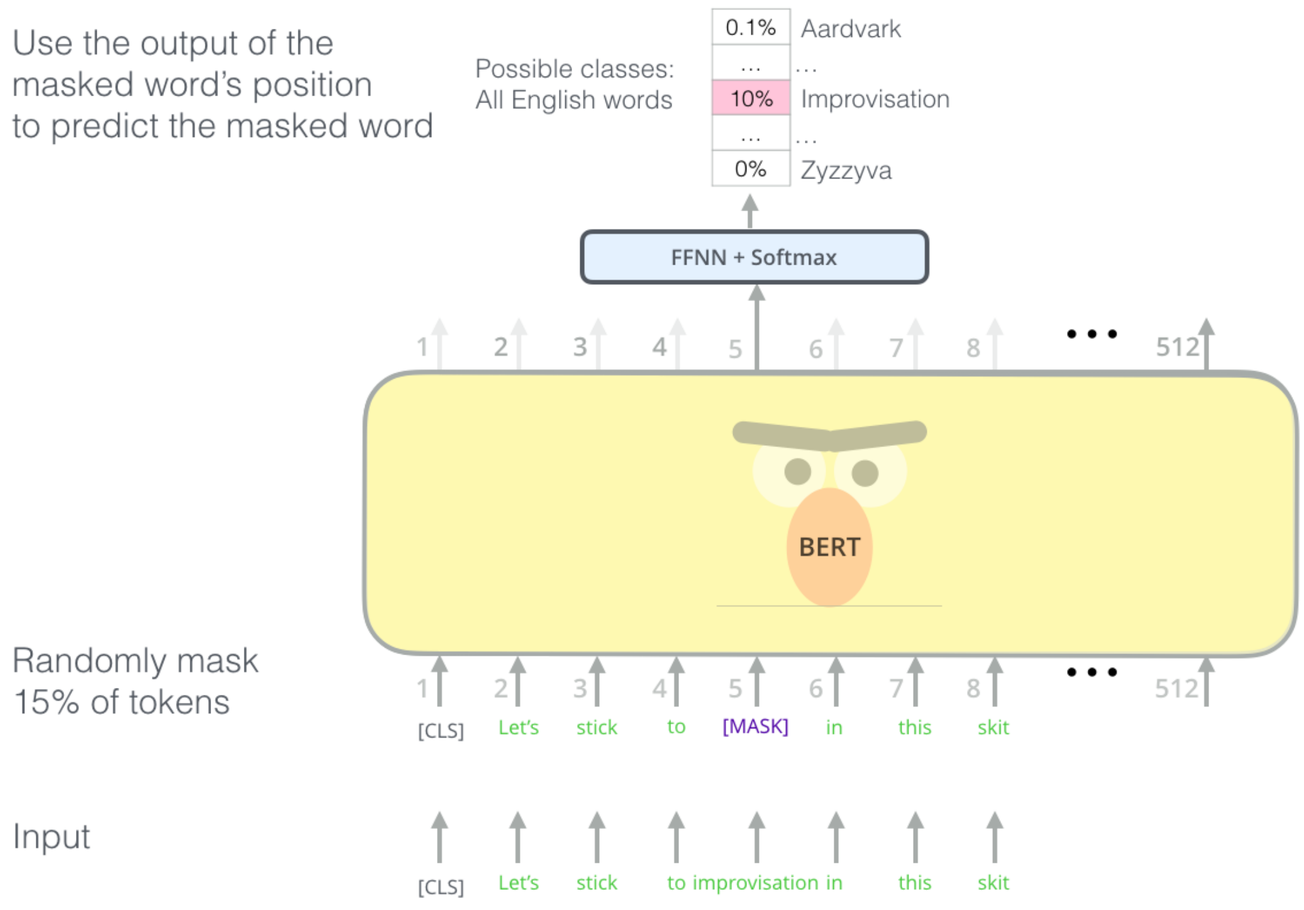
BERT - Bidirectional Encoder Representations from Transformers

- BERT only uses the encoder of the transformer (12 layers, 12 attention heads, $d = 768$).
- BERT is pretrained on two different unsupervised tasks before being fine-tuned on supervised tasks.



BERT - Bidirectional Encoder Representations from Transformers

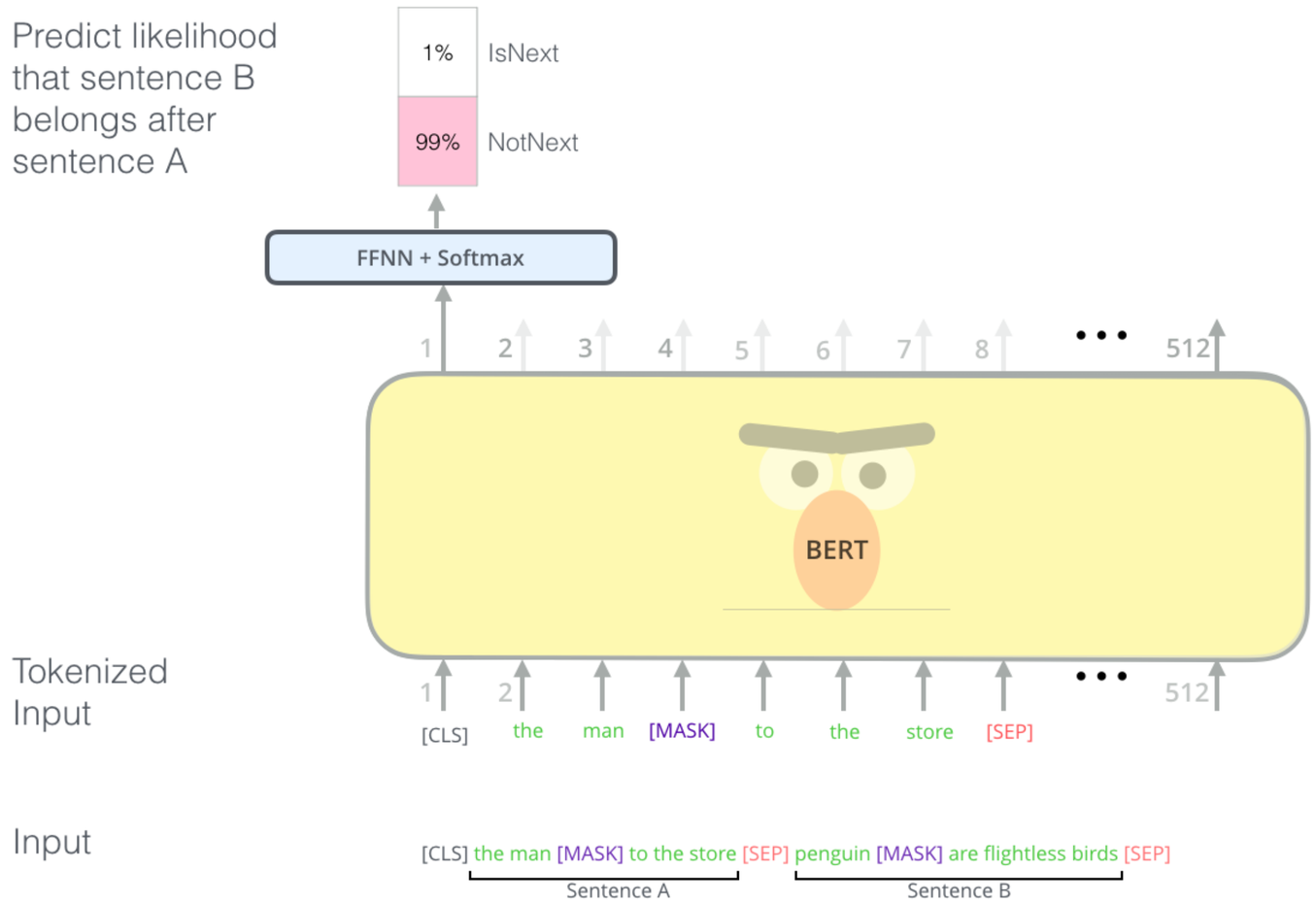
- **Task 1:** Masked language model. Sentences from BooksCorpus and Wikipedia (3.3G words) are presented to BERT during pre-training, with 15% of the words masked.
- The goal is to predict the masked words from the final representations using a shallow FNN.



Source: https://jalammar.github.io/illustrated-bert/

BERT - Bidirectional Encoder Representations from Transformers

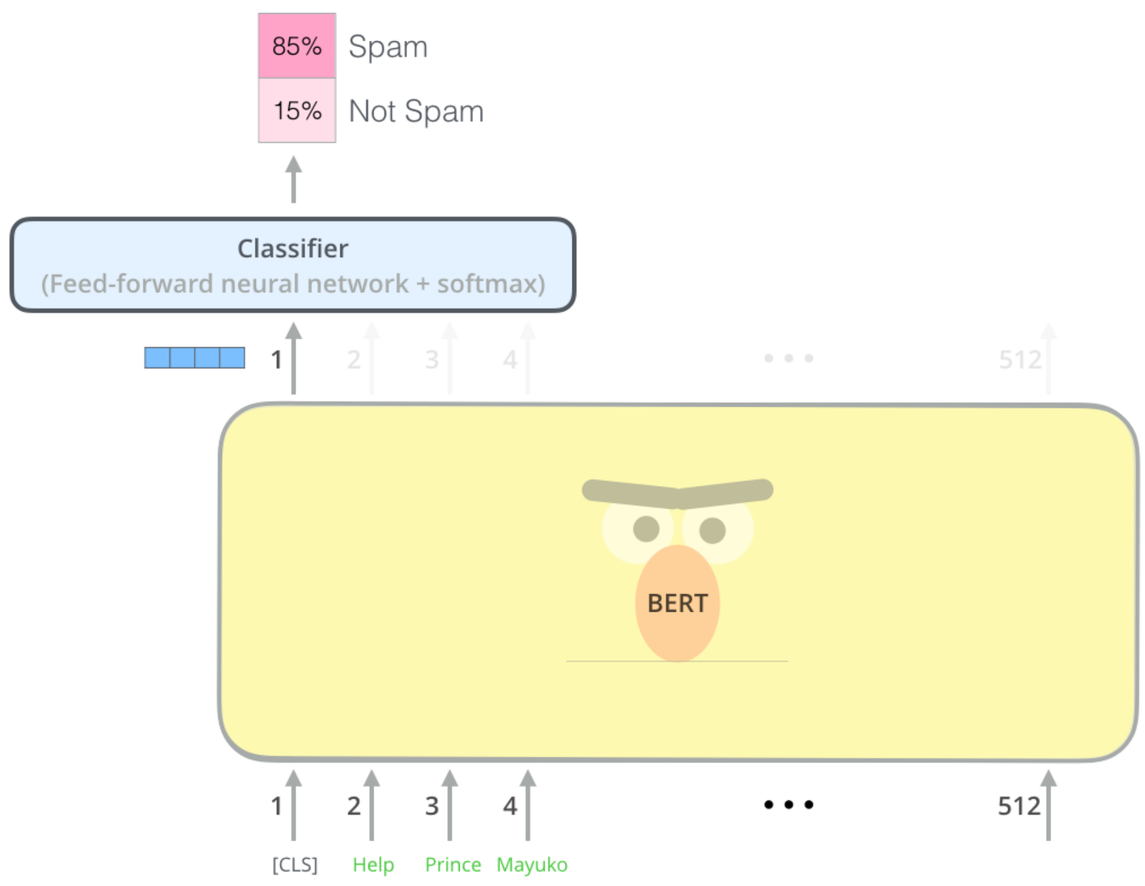
- **Task 2:** Next sentence prediction. Two sentences are presented to BERT.
- The goal is to predict from the first representation whether the second sentence should follow the first.



Source: https://jalammar.github.io/illustrated-bert/

BERT - Bidirectional Encoder Representations from Transformers

- Once BERT is pretrained, one can use **transfer learning** with or without fine-tuning from the high-level representations to perform:
  - sentiment analysis / spam detection
  - question answering

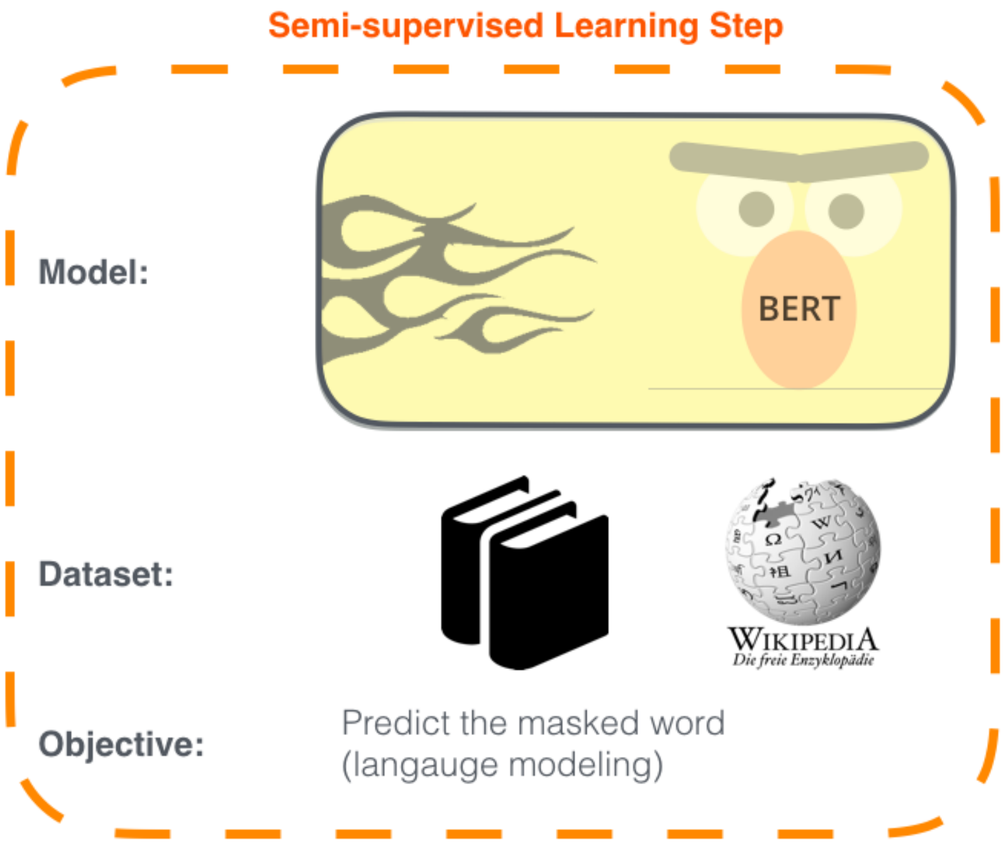


Source: https://jalammar.github.io/illustrated-bert/

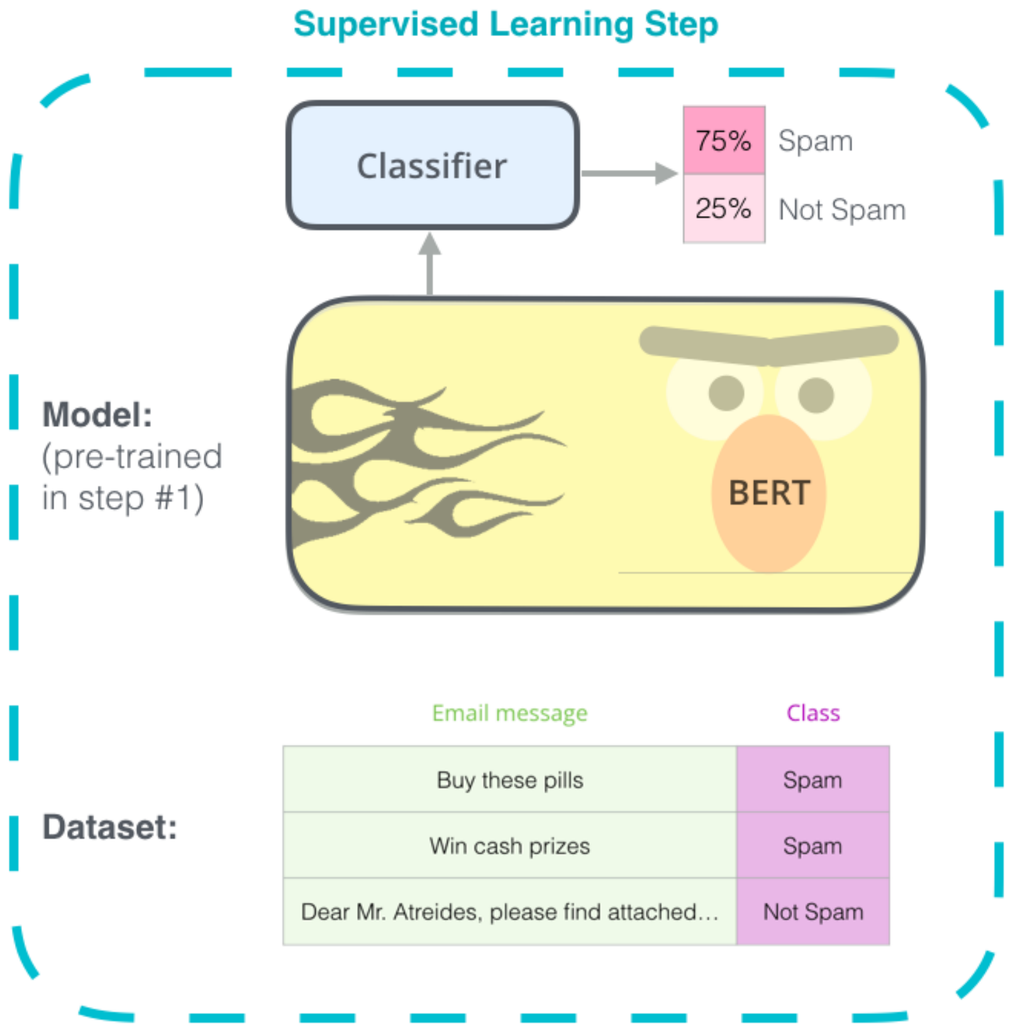
BERT - Bidirectional Encoder Representations from Transformers

1 - Semi-supervised training on large amounts of text (books, wikipedia..etc).

The model is trained on a certain task that enables it to grasp patterns in language. By the end of the training process, BERT has language-processing abilities capable of empowering many models we later need to build and train in a supervised way.



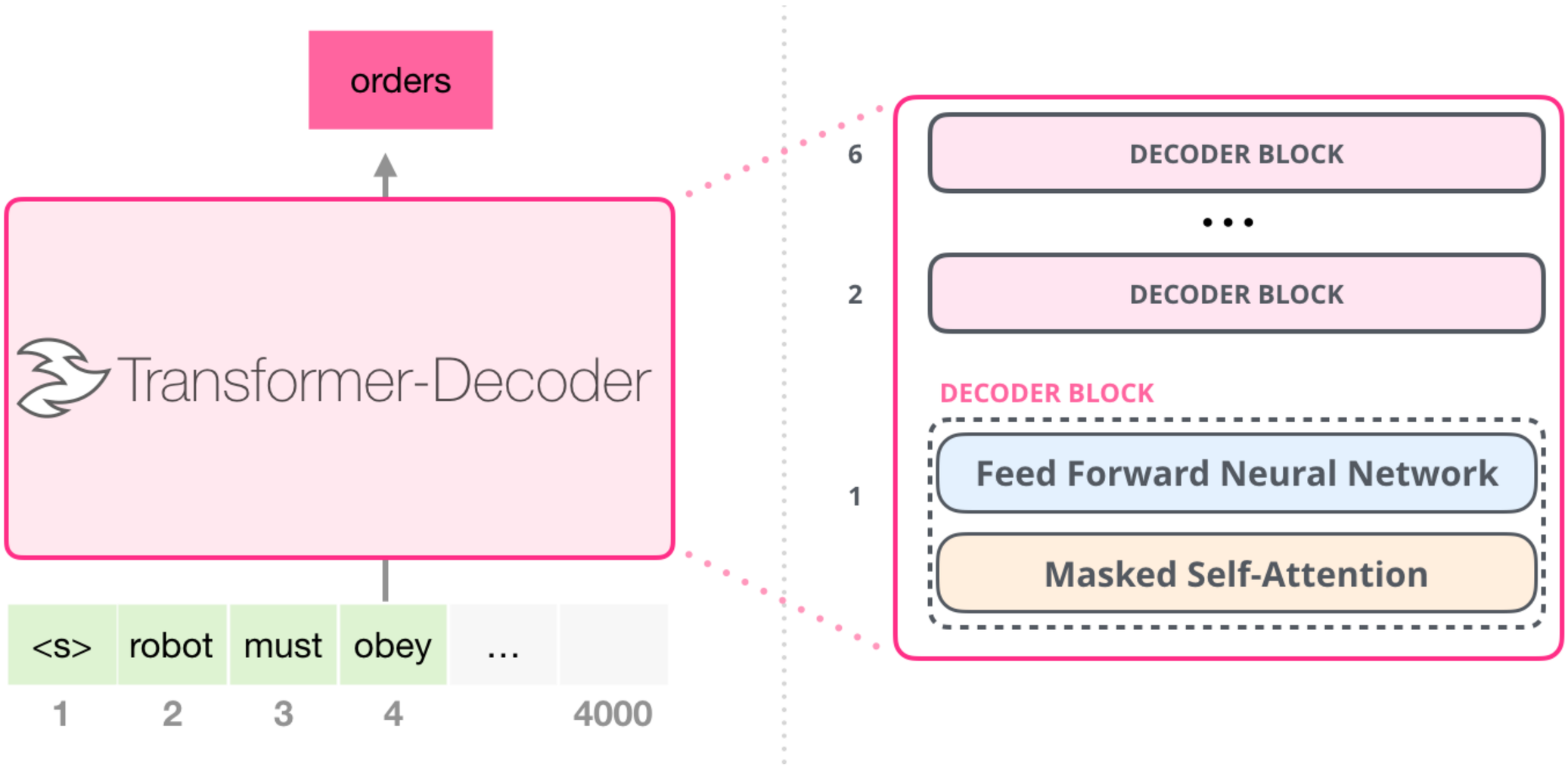
2 - Supervised training on a specific task with a labeled dataset.



Source: https://jalammar.github.io/illustrated-bert/

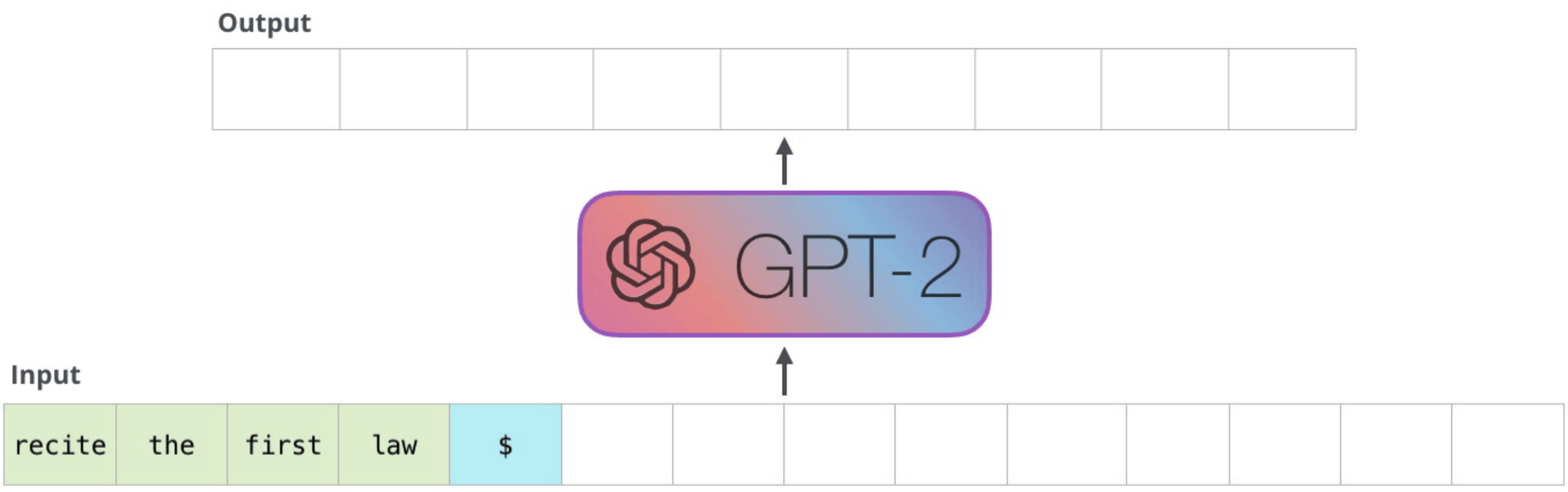
GPT - Generative Pre-trained Transformer

- As the Transformer, GPT is an **autoregressive** language model learning to predict the next word using only the transformer's **decoder**.



Source: https://jalammar.github.io/illustrated-gpt2/

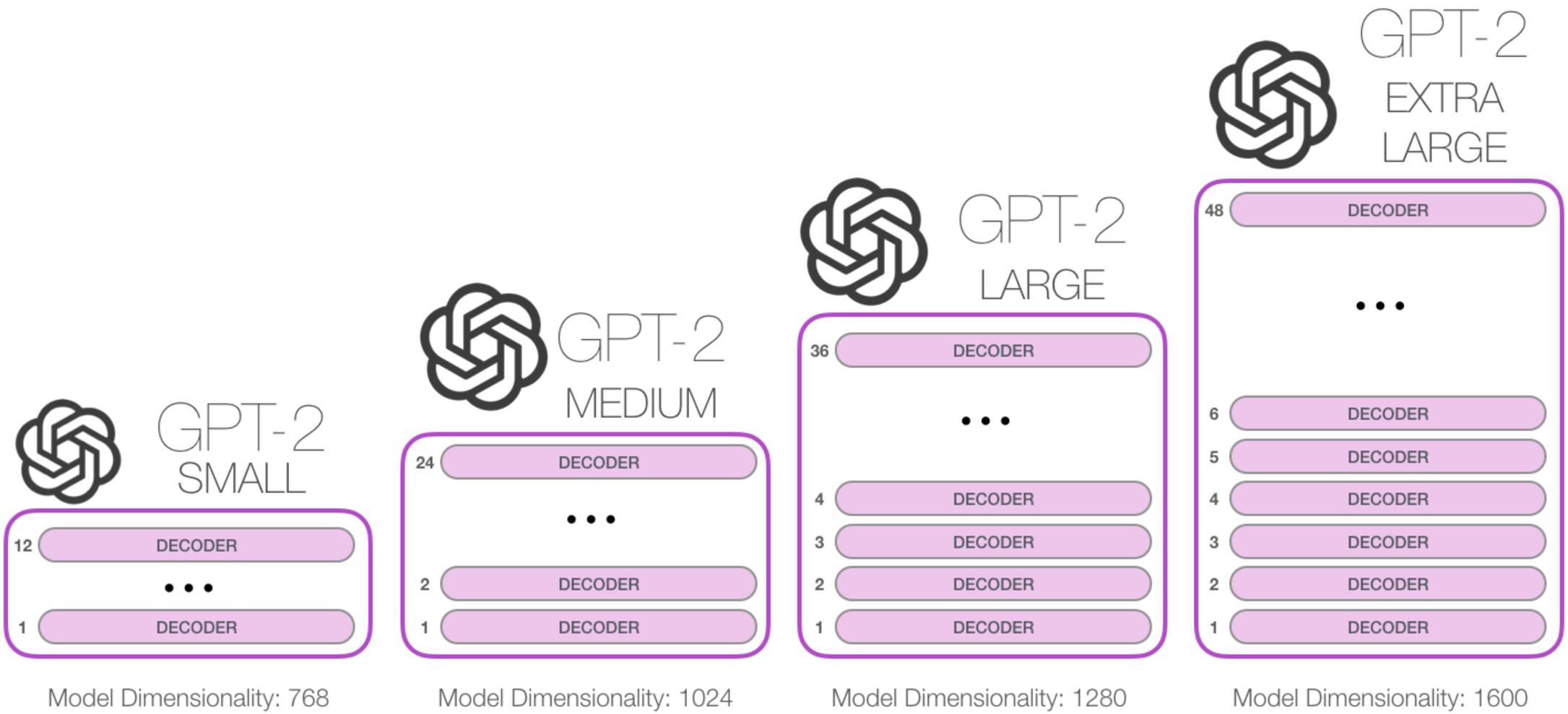
GPT - Generative Pre-trained Transformer



Source: https://jalammar.github.io/illustrated-gpt2/

GPT - Generative Pre-trained Transformer

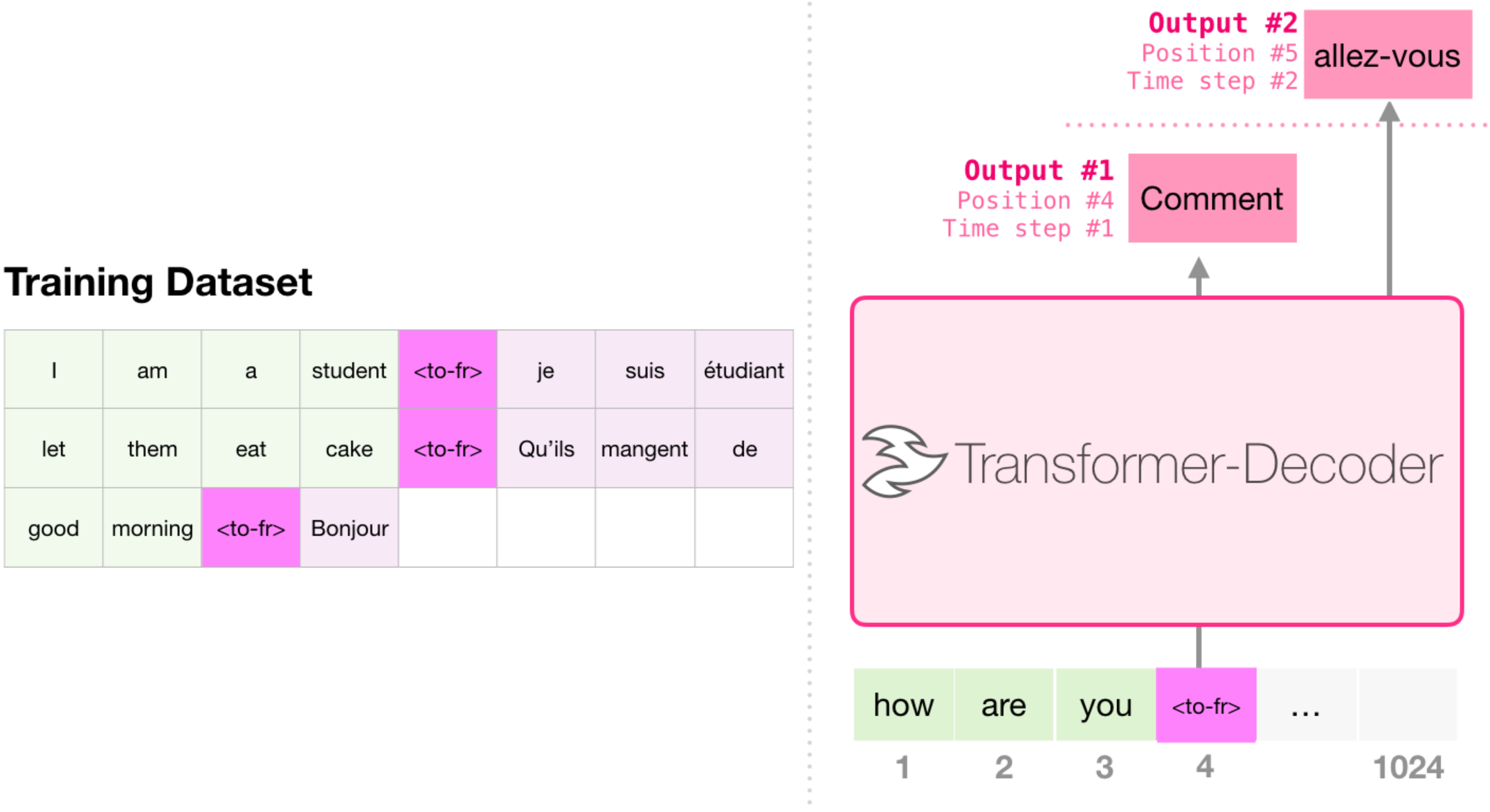
- GPT-2 comes in various sizes, with increasing performance.
- GPT-3 is even bigger, with 175 **billion** parameters and a much larger training corpus.



Source: https://jalammar.github.io/illustrated-gpt2/

GPT - Generative Pre-trained Transformer

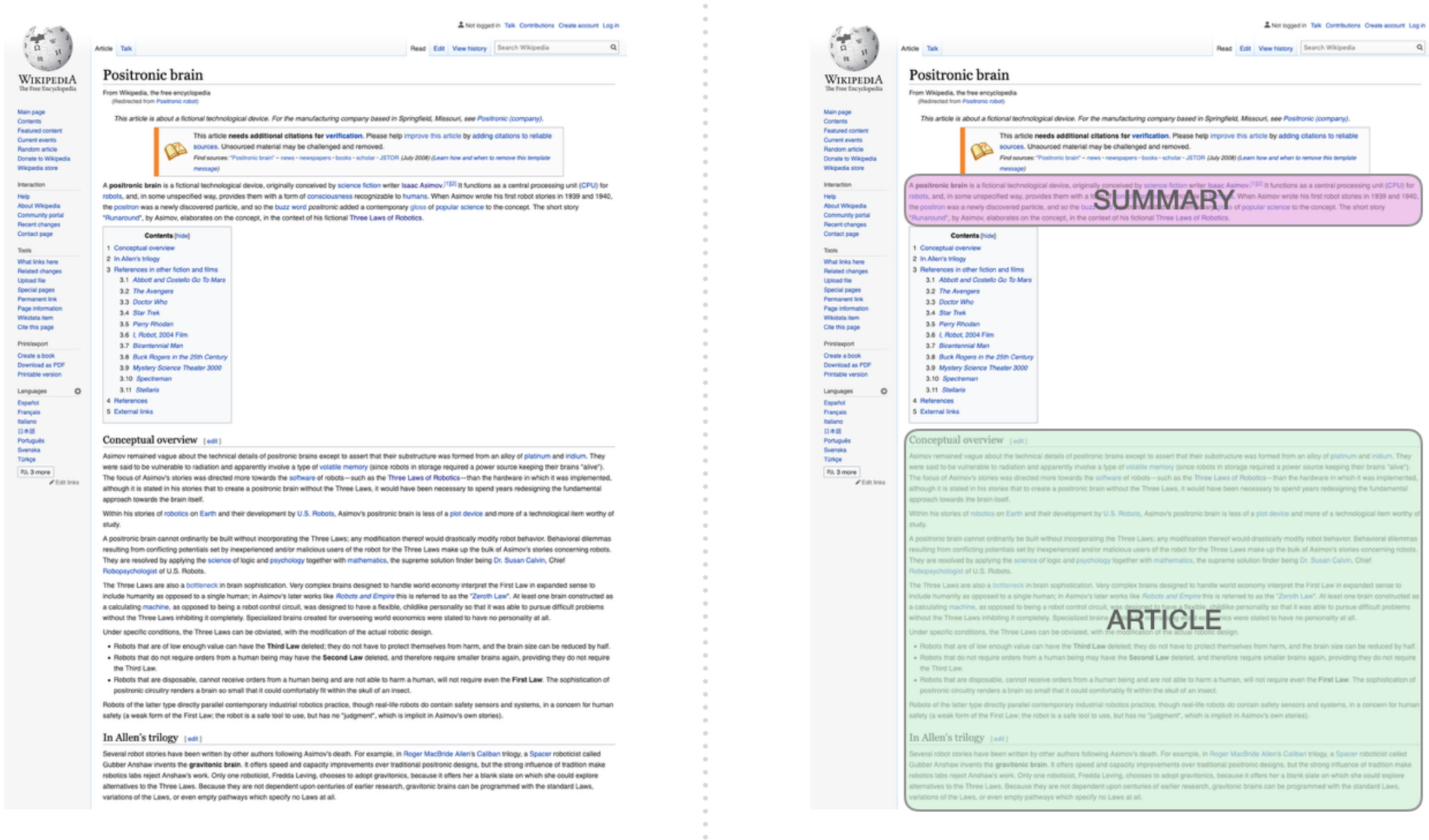
- GPT can be fine-tuned (transfer learning) to perform **machine translation**.



Source: https://jalammar.github.io/illustrated-gpt2/

GPT - Generative Pre-trained Transformer

- GPT can be fine-tuned to summarize Wikipedia articles.



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GPT - Generative Pre-trained Transformer

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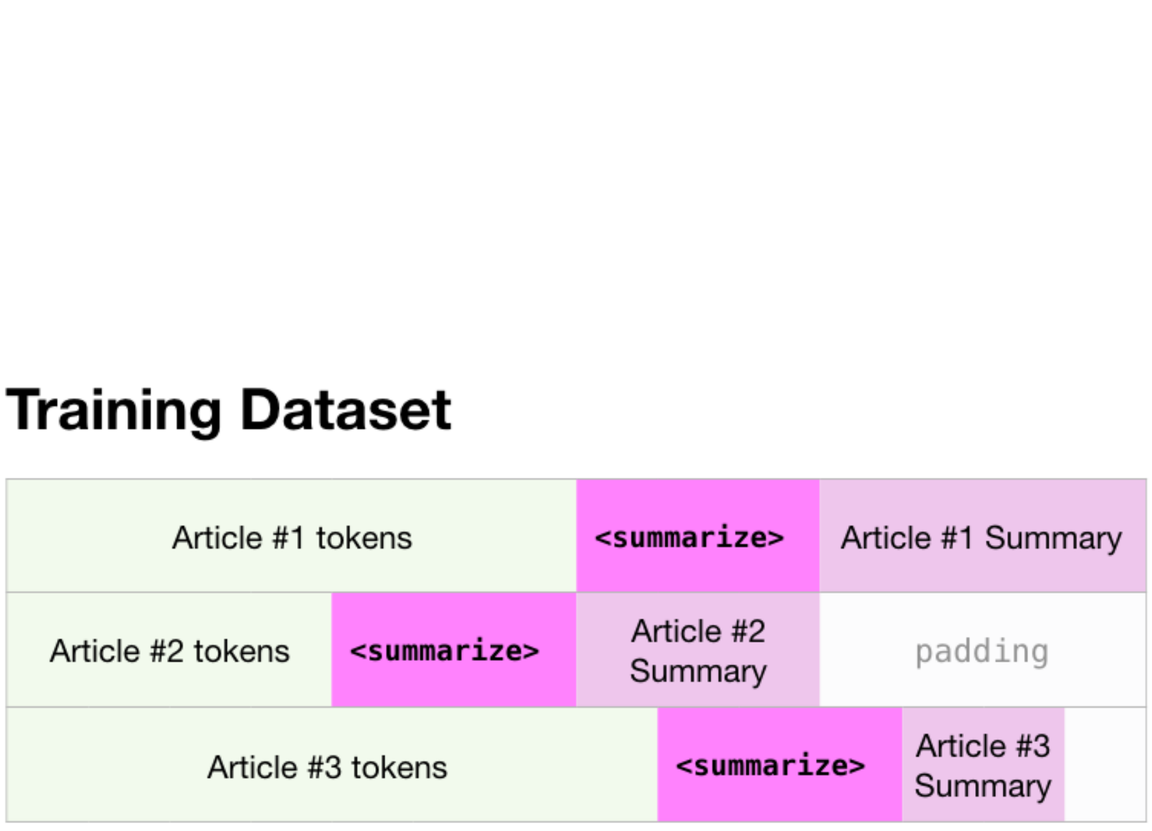
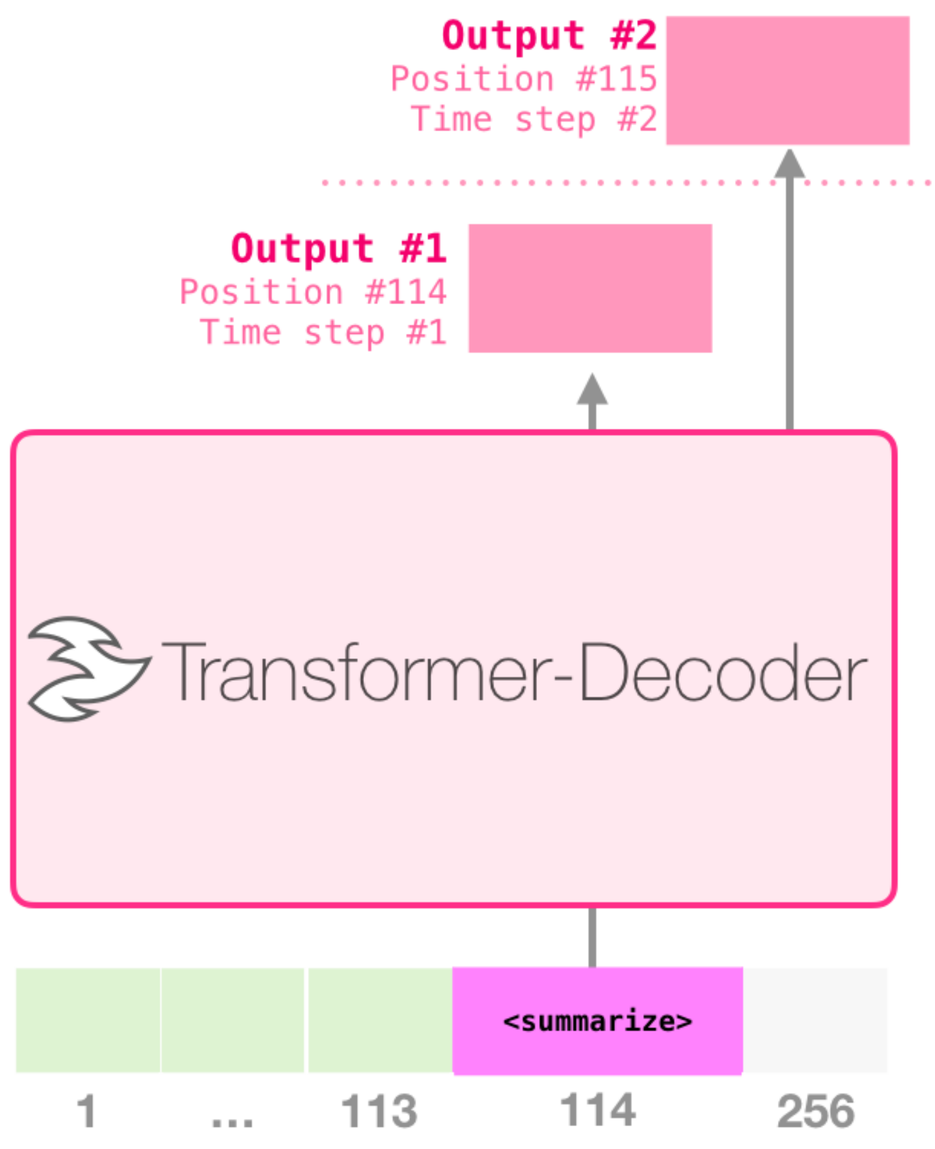




Source: https://jalammar.github.io/illustrated-gpt2/

Try transformers at https://huggingface.co/

```
pip install transformers
```

Write With Transformer `distil-gpt2`

Shuffle initial text Trigger autocomplete or `tab` Select suggestion `↑` `↓` and `enter` Cancel suggestion `esc`

Save & Publish

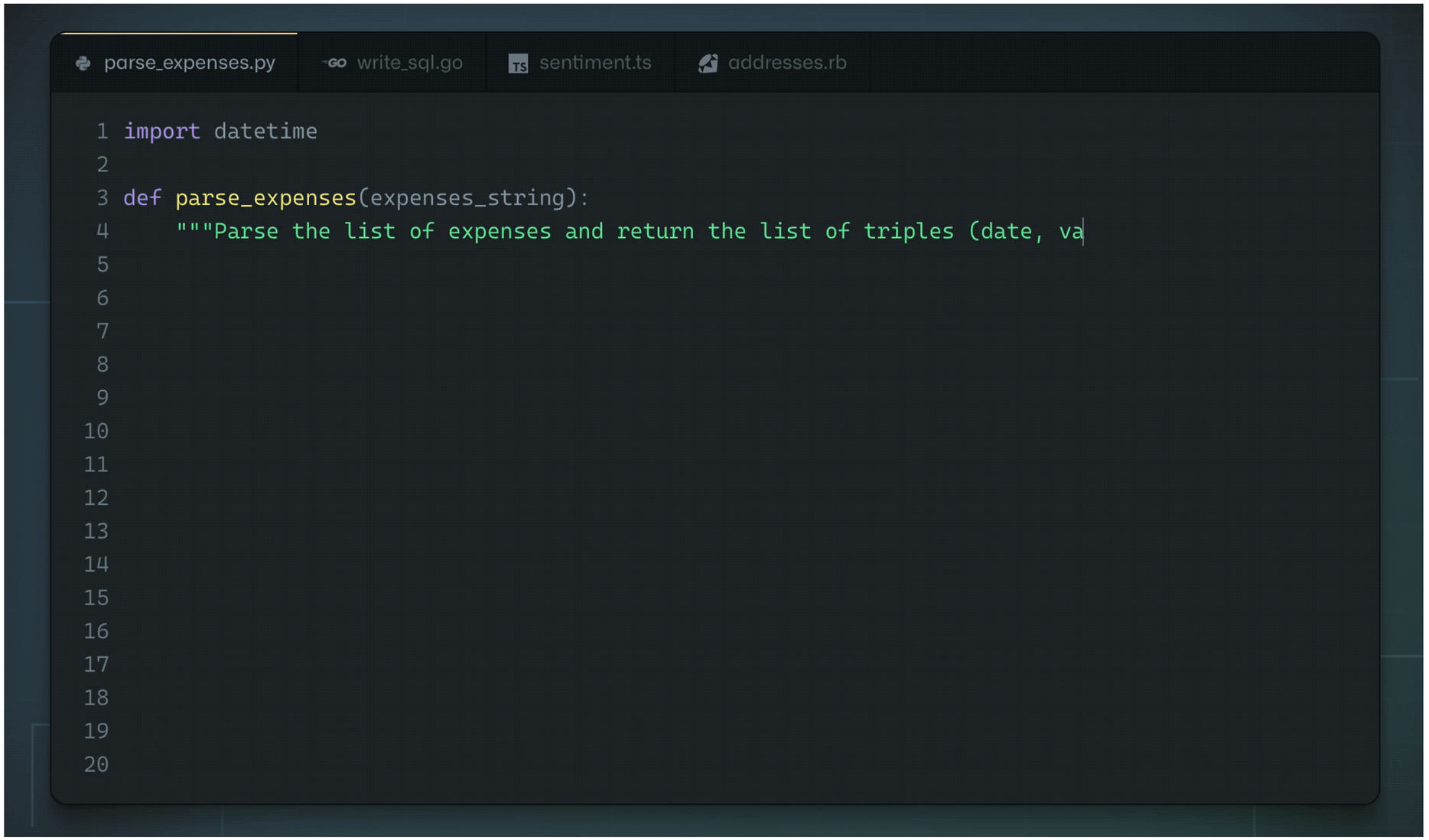
Neurocomputing is

- the leading topic of the next century.
- now more popular than a year ago, wit…
- a new field of study that explores the w…

Github copilot

- Github and OpenAI trained a GPT-3-like architecture on the available open source code.
- Copilot is able to “autocomplete” the code based on a simple comment/docstring.

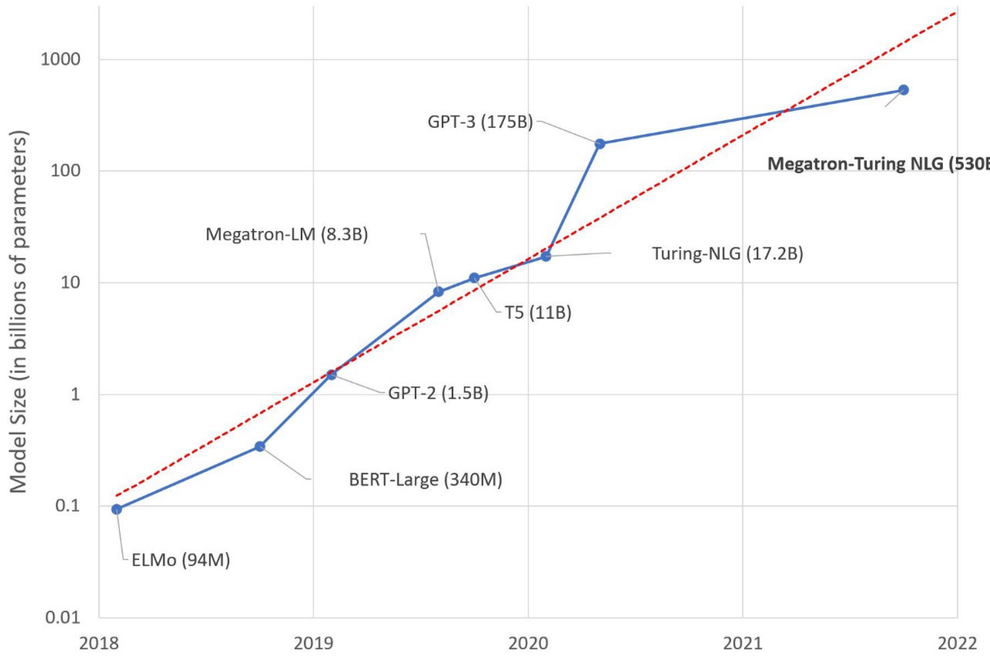
https://copilot.github.com/



ChatGPT

Transformers and NLP

- All NLP tasks (translation, sentence classification, text generation) are now done using **Large Language Models** (LLM), **self-supervisedly** pre-trained on huge corpuses.
- BERT can be used for feature extraction, while GPT is more generative.
- Transformer architectures seem to **scale**: more parameters = better performance. Is there a limit?



Source: https://julsimon.medium.com/large-language-models-a-new-moores-law-66623de5631b

- The price to pay is that these models are very expensive to train (training one instance of GPT-3 costs 12M$) and to use (GPT-3 is only accessible with an API).
- Many attempts have been made to reduce the size of these models while keeping a satisfying performance.
  - DistilBERT, RoBERTa, BART, T5, XLNet…
- See https://medium.com/mlearning-ai/recent-language-models-9fcf1b5f17f5

References

- Various great blog posts by Jay Alammar to understand attentional networks, transformers, etc:

https://jalammar.github.io/visualizing-neural-machine-translation-mechanics-of-seq2seq-models-with-attention/

http://jalammar.github.io/illustrated-transformer/

https://jalammar.github.io/illustrated-bert/

https://jalammar.github.io/illustrated-gpt2/

- Application of transformers outside NLP:

https://medium.com/swlh/transformers-are-not-only-for-nlp-cd837c9f175