Attention in NNs: the advent of Transformers

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Outline

- Attention Mechanisms in Recurrent Networks
- Trasformers
  - Attention
  - Multiheaded attention
  - Attention in encoder-decoder networks
- BERT: Using attention for optimal encoding
- Applications to Language Processing
  - Fondational models
- Perspectives

Encoding and contexts

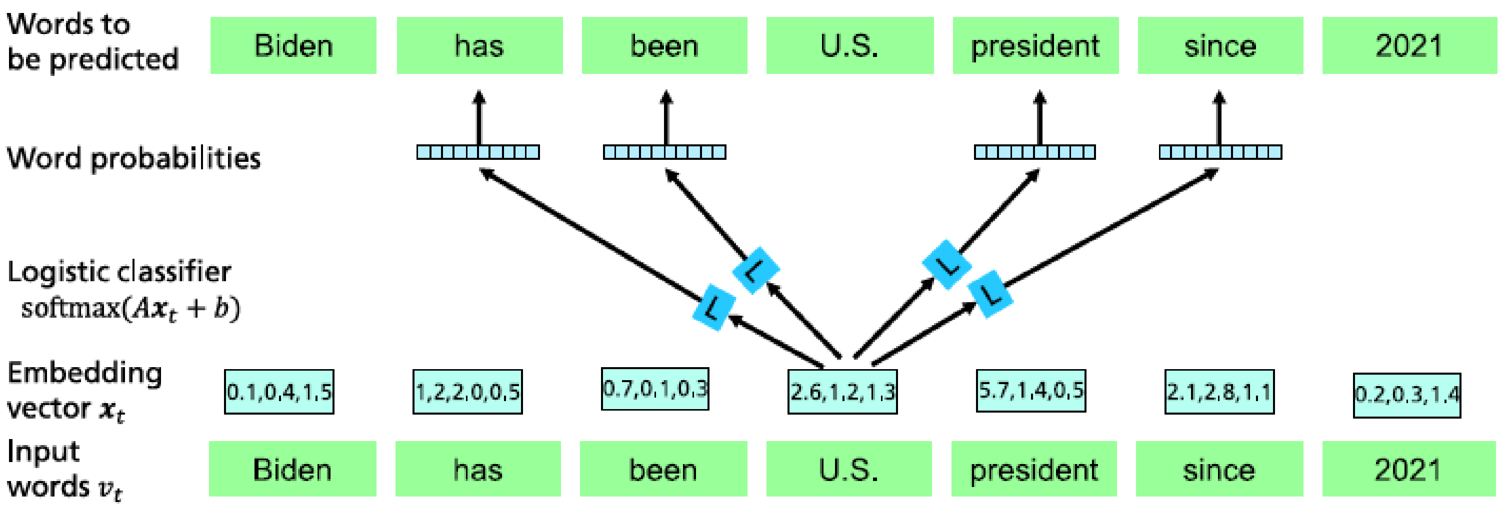


Fig. 1.2 Word2vec predicts the words in the neighborhood of a central word by logistic classifier *L*. The input to *L* is the embedding of the central word. By training with a large set of documents, the parameters of *L* as well as the embeddings are learned [54, p. 2].

- from Gerhard Paaß and Sven Giesselbach, *Foundation Models for Natural Language Processing: Pre-trained Language Models Integrating Media*, Springer-Verlag, 2023, URL: https://link.springer.com/book/9783031231896

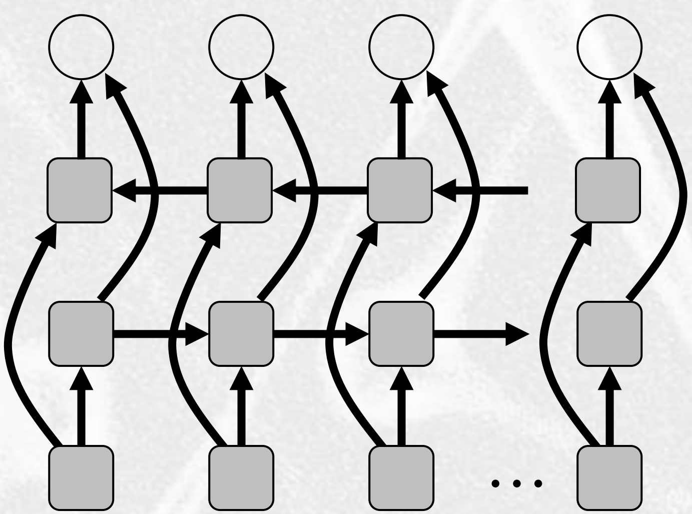
Other RNN architectures

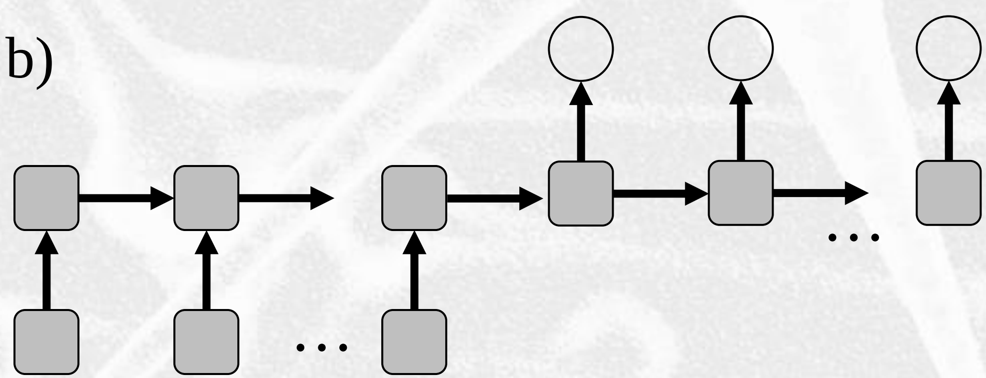
a) Recurrent networks can be made bidirectional, propagating information in both directions

- They have been used for a wide variety of applications, including protein secondary structure prediction and handwriting recognition

b) An "encoder-decoder" network creates a fixed-length vector representation for variable-length inputs, the encoding can be used to generate a variable-length sequence as the output

- Particularly useful for machine translation





Training different Types of RNNs

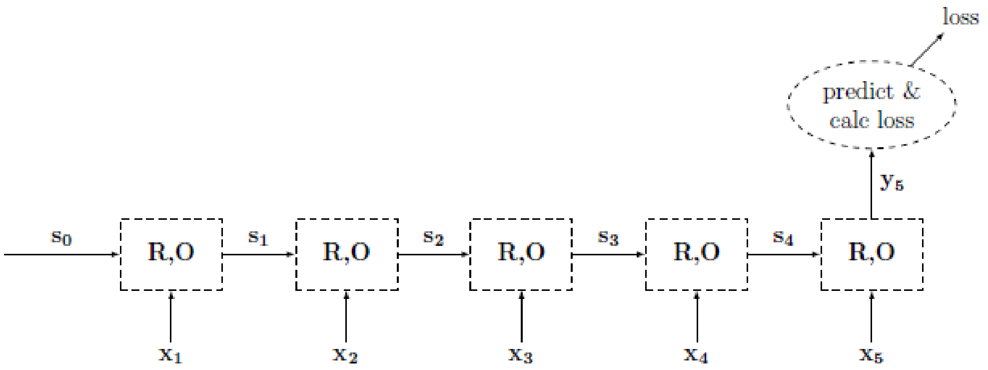


Figure 7: Acceptor RNN Training Graph.

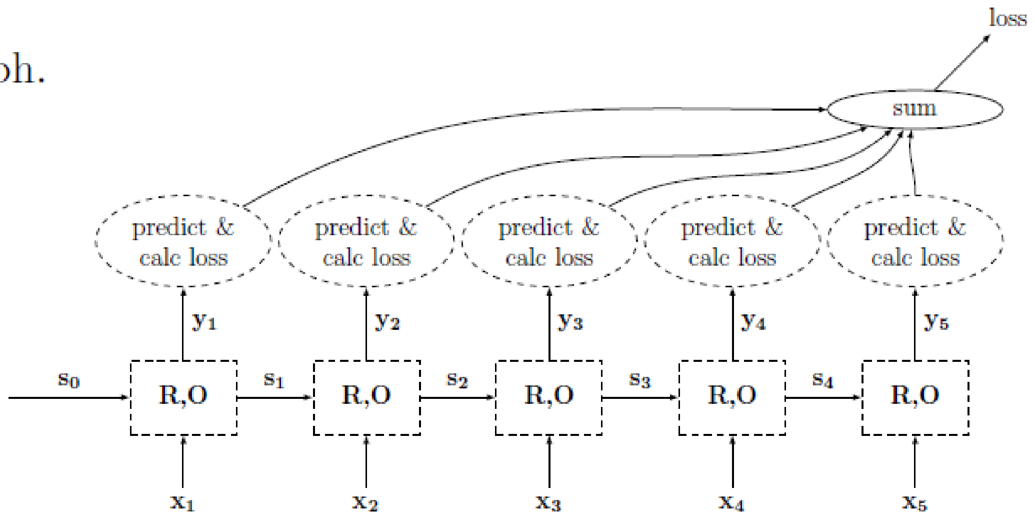


Figure 8: Transducer RNN Training Graph.

Training different Types of RNNs

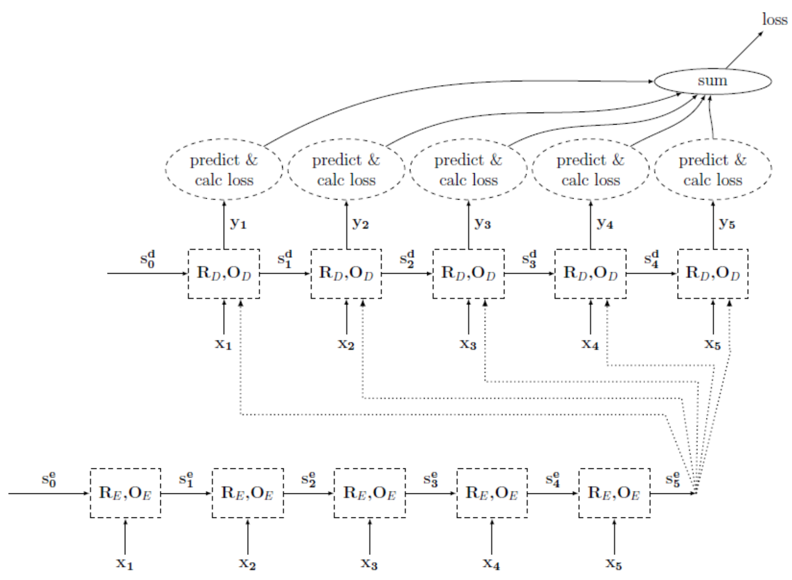


Figure 9: Encoder-Decoder RNN Training Graph.

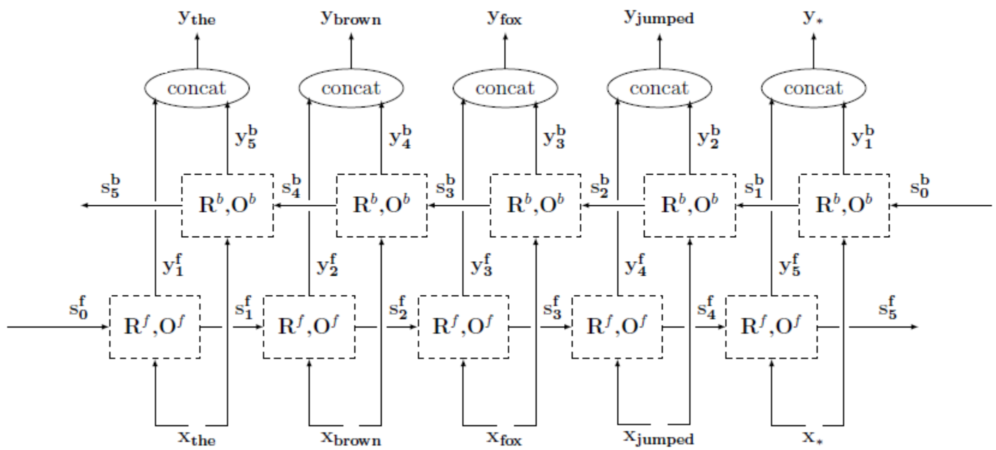
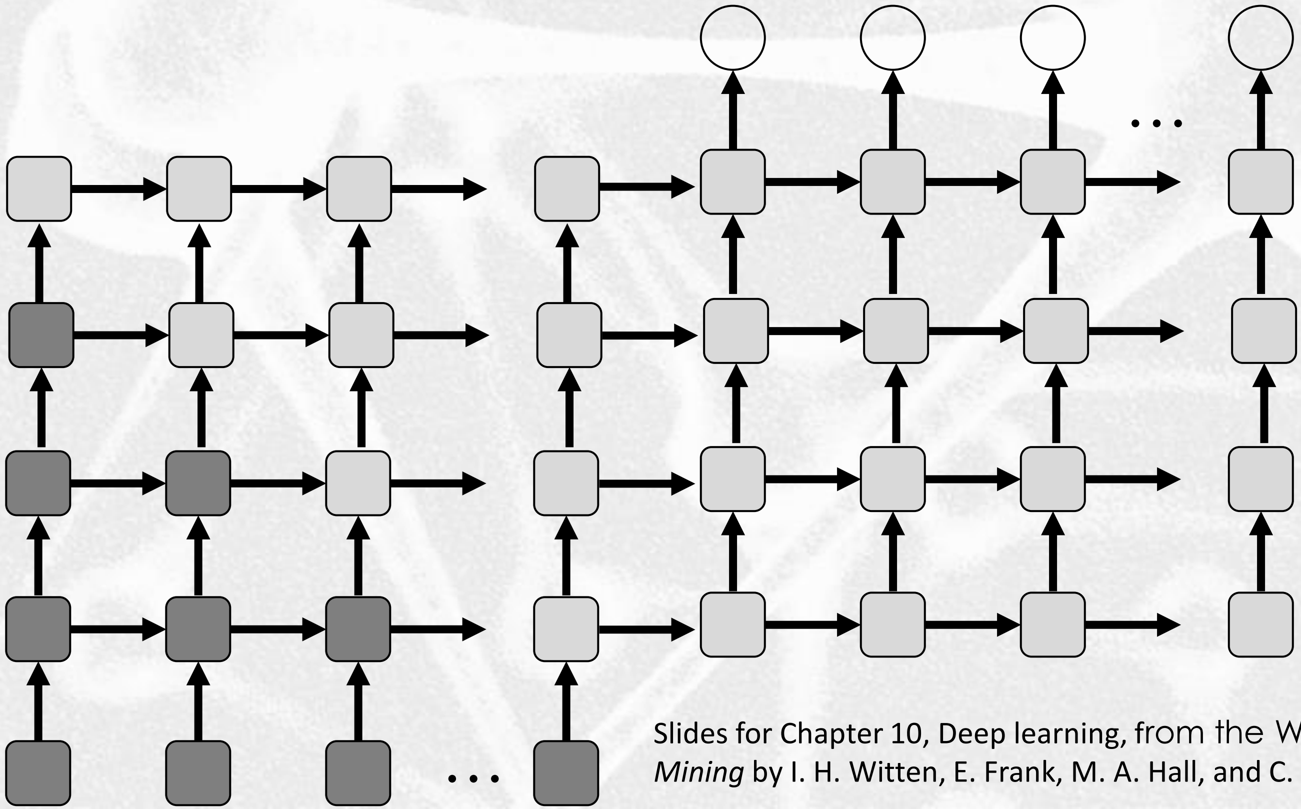


Figure 11: biRNN over the sentence "the brown fox jumped ."

Encoder-decoder deep architectures

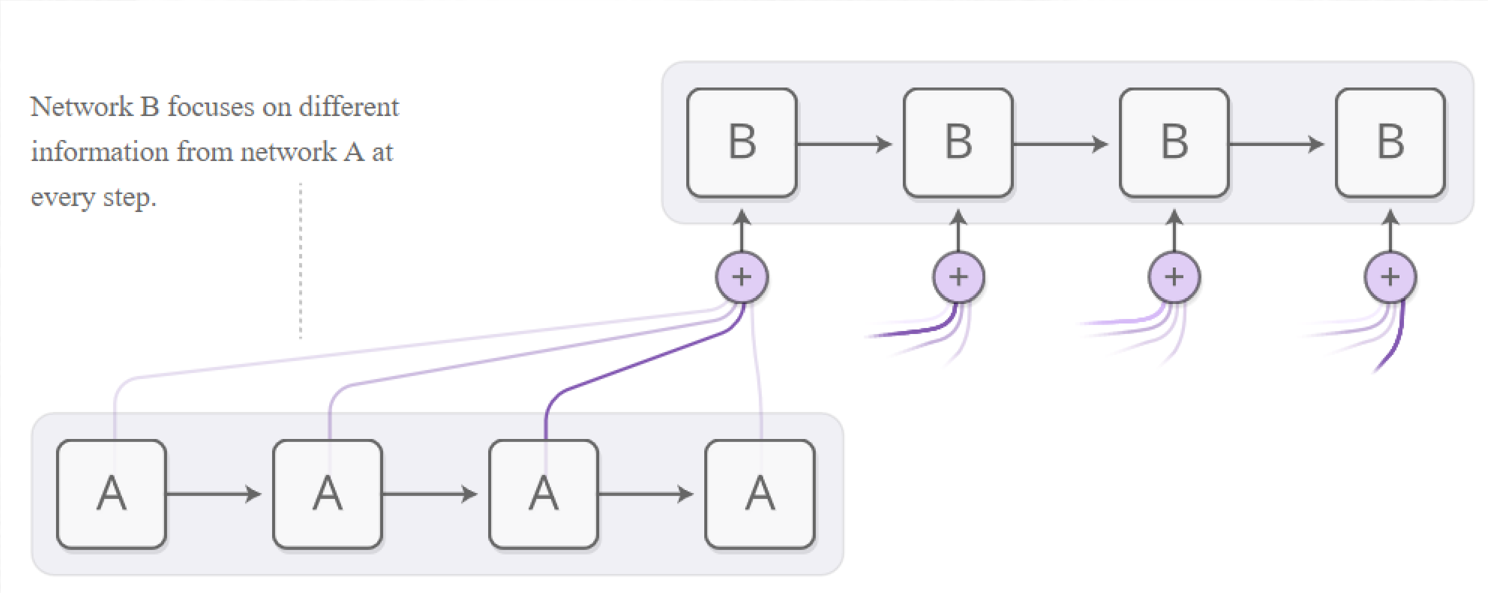
- Given enough data, a deep encoder-decoder architecture (see below) can yield results that compete with hand-engineered translation systems.

- The connectivity structure means that partial computations in the model can flow through the graph in a wave (darker nodes in fig.)



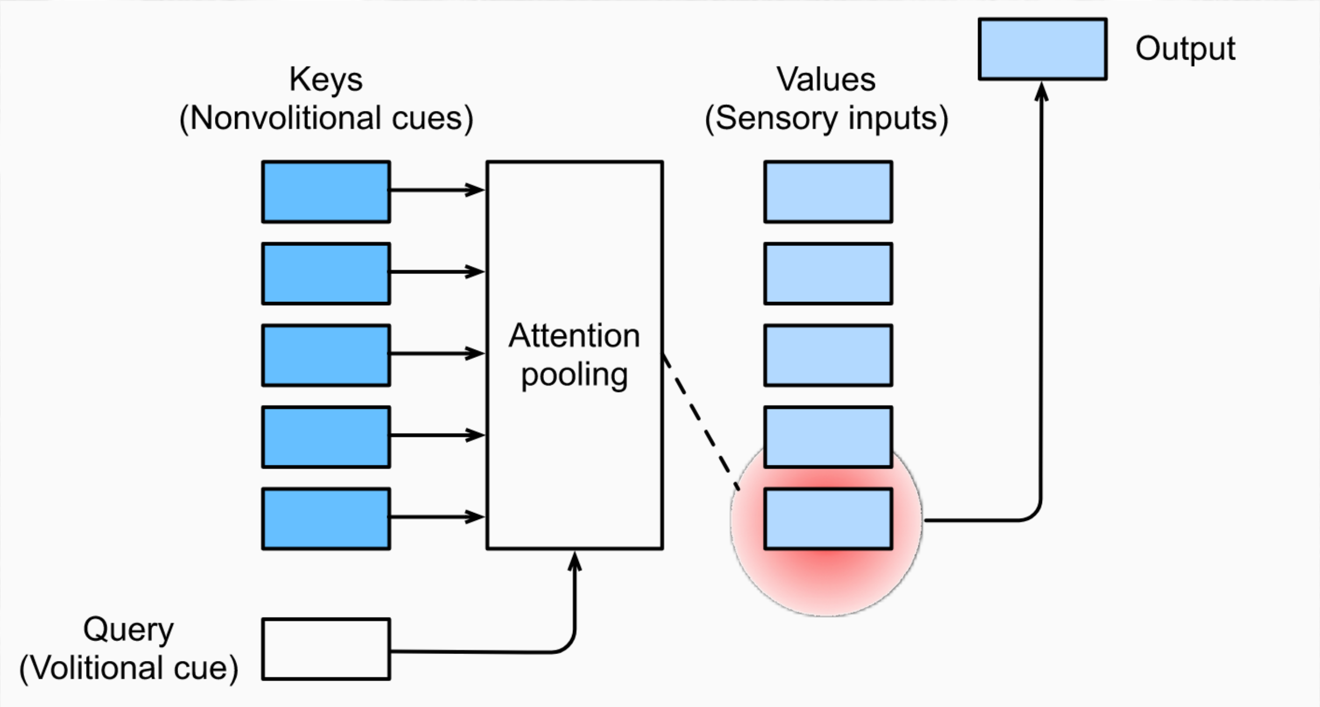
Attention-based RNNs

- A NN (e.g. B) is used to attend the outcome of a second network A, e.g. (Vaswani et al., 2017)

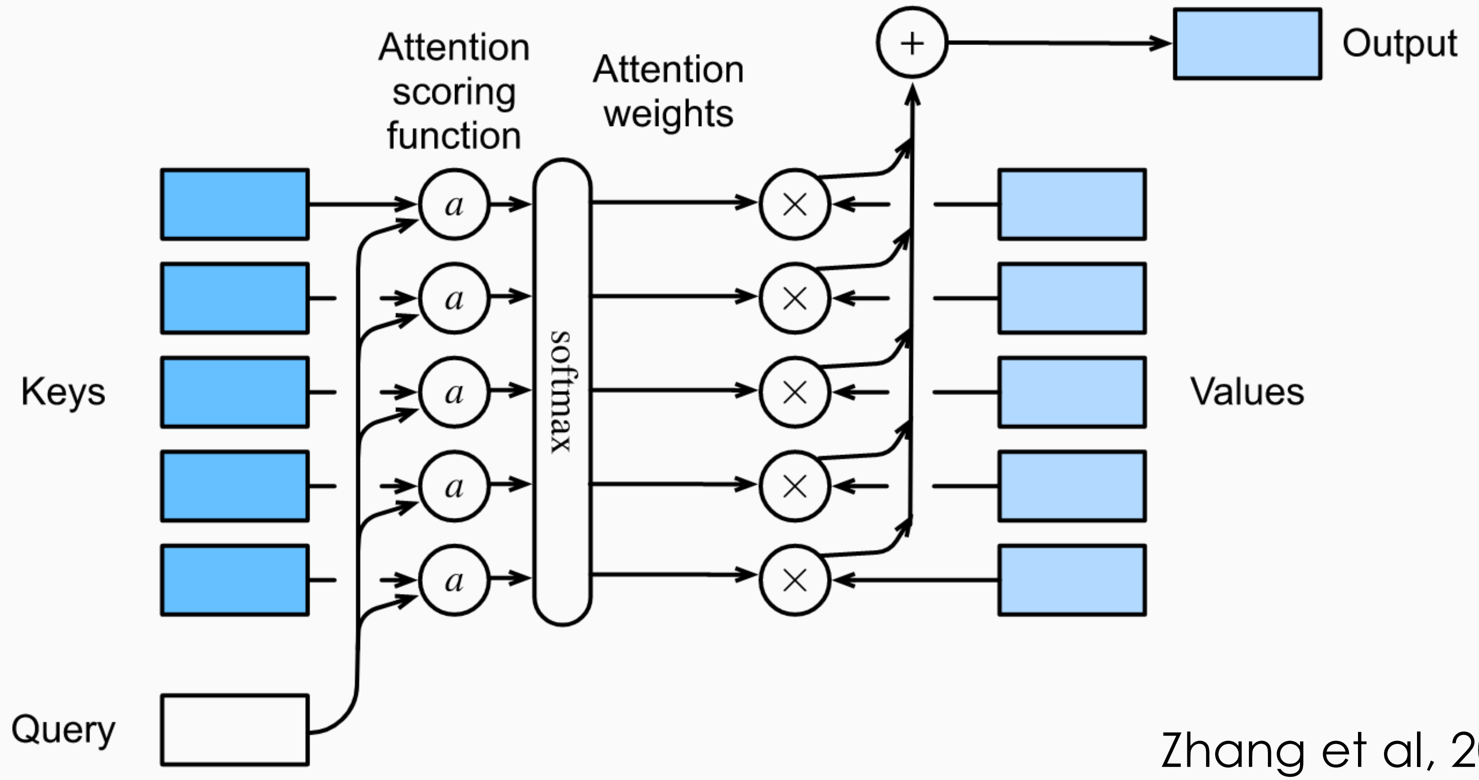


Attention: motivations

- From (*Dive into Deep Learning*, Zhang, Aston and Lipton, Zachary C. and Li, Mu and Smola, Alexander J., 2021).



Attention functions

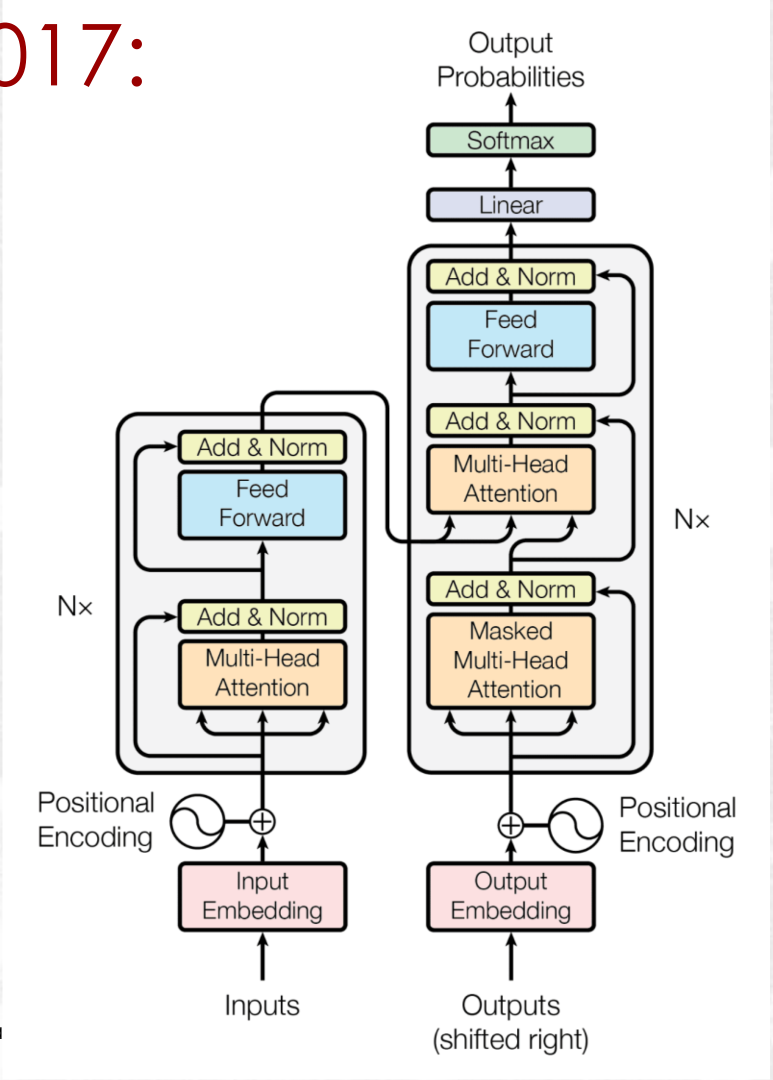


Zhang et al, 2021

Inside Attention

Going back in time to 2017: the Transformer

(Vaswani et al. 2017)



A Transformer: a neural architecture designed for **sequence-to-sequence tasks**.

- It takes a sequence of symbols as input and produces a sequence of symbols as output.

Before Transformers:

- Until 2017, these tasks were implemented using **Recurrent Neural Networks** (RNNs).
  - with limitations in handling long sequences.

Emergence of Attention:

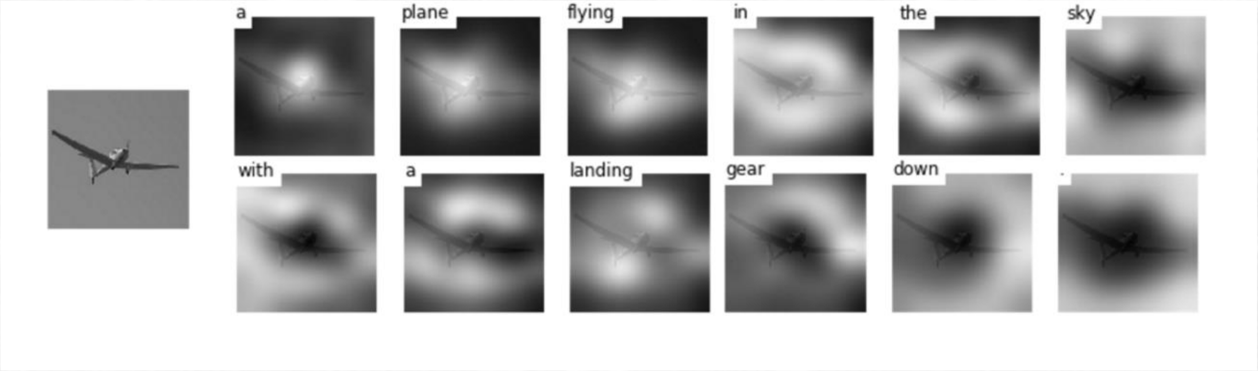
- Heavily used since 2015, allowed models to **focus on specific sections of a sequence** for better inference.

Ashish Vaswani, Noam Shazeer, Niki Parmar, Jakob Uszkoreit, Llion Jones, Aidan N. Gomez, Luka Polosukhin (2017). Attention Is All You Need. arXiv:1706.03762

The Importance of Attention in Neural Learning

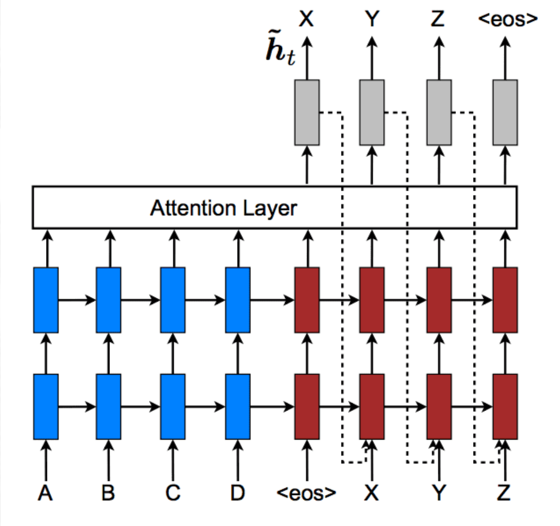
- **Revolution in Computer Vision**
  - It significantly improved **object detection** and **recognition in computer vision**.
  - It enables models to focus on relevant parts of an image, improving accuracy and efficiency.
  - **An interesting Survey:** `https://github.com/MenghaoGuo/Awesome-Vision-Attentions`

- **Breakthrough in tasks such as Image Captioning:**
  - Attention helps in **identifying key components** within images **to generate accurate and contextually relevant descriptions**.
  - **Seminal work:** (Xu et al, 2015) `https://arxiv.org/abs/1502.03044`

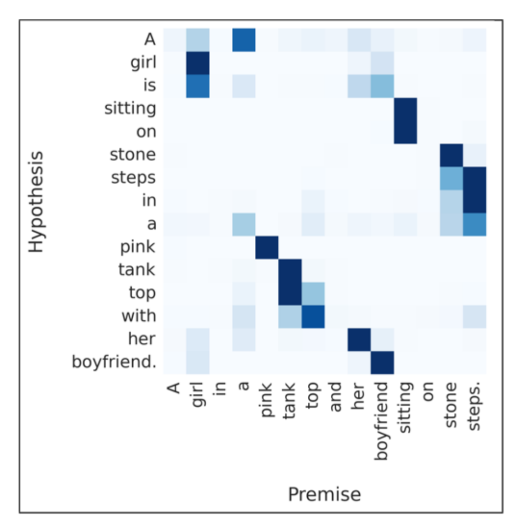


Enhancement in Recurrent Neural Networks

- For RNNs, **attention mechanisms** were used to address the **challenge of handling long sequences**.
- It allows RNNs to **focus on important parts** of the input sequence
  - improving performance in tasks like language translation and speech recognition.



(Luong et al, 2015)
Effective Approaches to Attention-based Neural Machine Translation
https://arxiv.org/abs/1508.04025

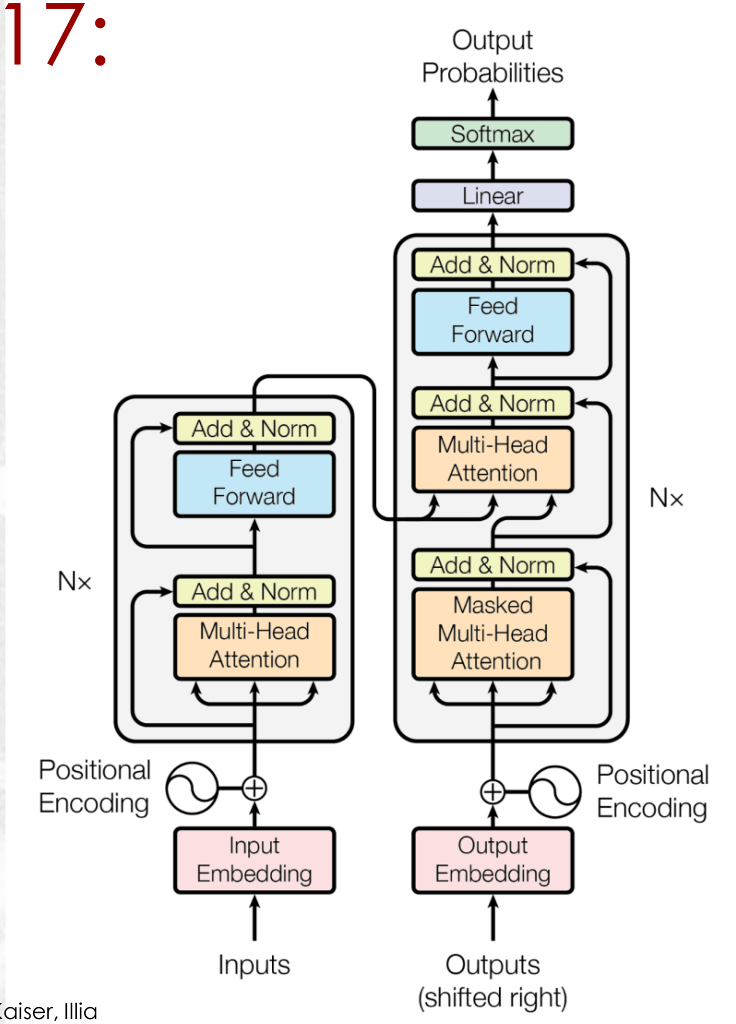


(Rocktäschel et, al., 2015)
Reasoning about Entailment with Neural Attention, 2015.
https://arxiv.org/abs/1508.04025

Going back in time to 2017: the Transformer

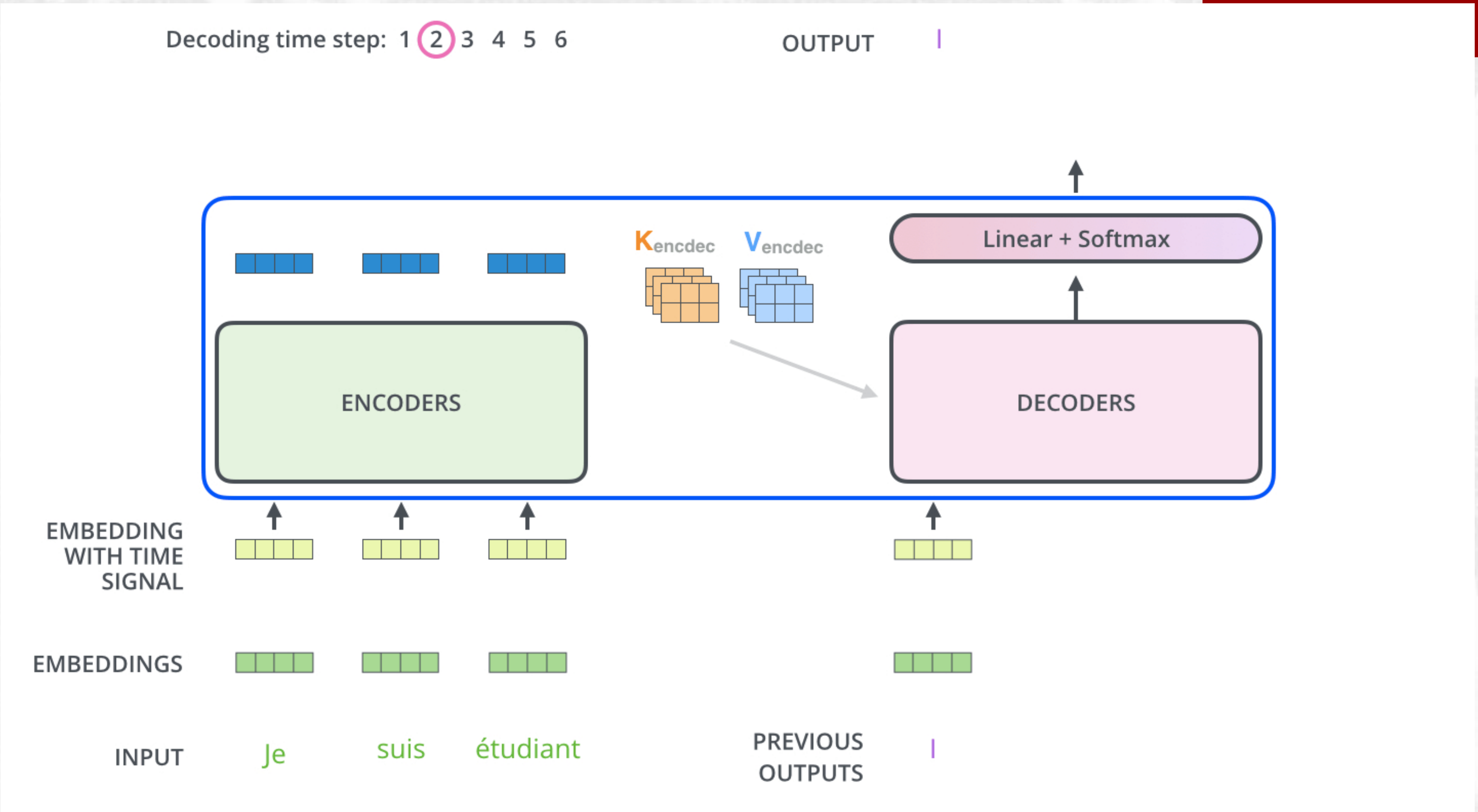
(Vaswani et al. 2017)

- **Attention in Transformers:**
  - In 2017, the **attention mechanism became an integral part** of this architecture.
  - a **significant evolution in seq2seq modeling**
- **Main advantages:**
  - Better with long range dependencies
  - Parallel processing (more scalable than RNNs)
  - State-of-the-art performances
- **Originally meant for Automatic machine translation:**
  - E.g., French to English



Ashish Vaswani, Noam Shazeer, Niki Parmar, Jakob Uszkoreit, Llion Jones, Aidan N. Gomez, Lukasz Kaiser, Illia Polosukhin (2017). Attention Is All You Need. arXiv:1706.03762

Seq2Seq: A transformer in action



Alammar, J (2018). The Illustrated Transformer [Blog post]. Retrieved from `https://jalammar.github.io/illustrated-transformer/`

Encoding/Decoding Architectures with Attention

- **Two components**
  - **Encoder:** Maps input sequence $X = (x_1, \dots, x_n)$ to continuous representations $Z = (z_1, \dots, z_n)$.
  - **Decoder:** Decoder uses Z to generate output sequence $Y = (y_1, \dots, y_m)$
- Encoder/Decoder process input vectors through **self-attention layer** and feed-forward network.
  - It enables to selectively **concentrate on pertinent parts of the input**
  - It improves **context awareness**
  - It allows to **consider positions** in the that also depends on the output

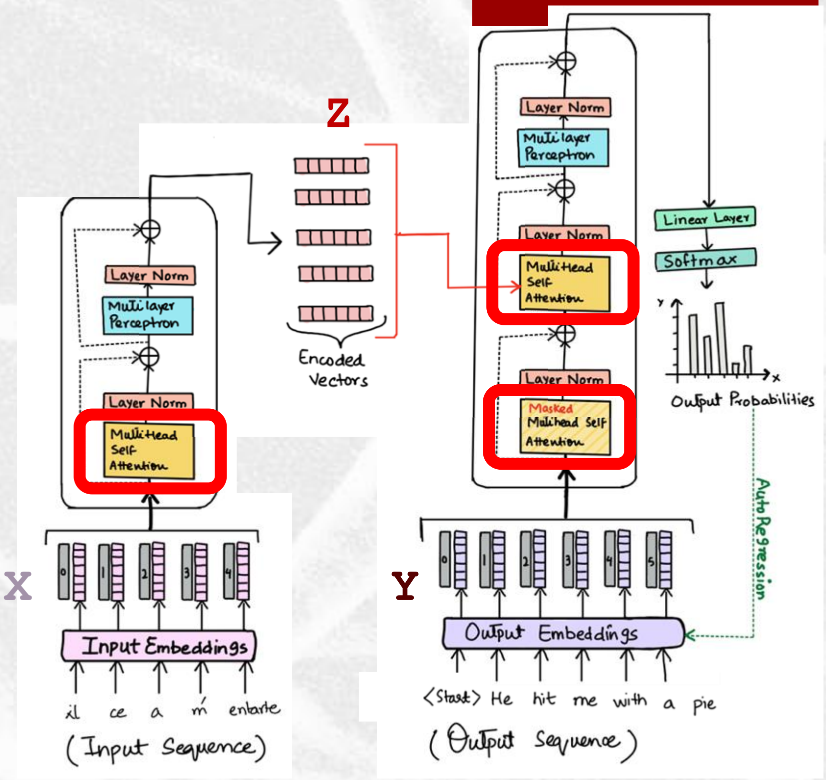
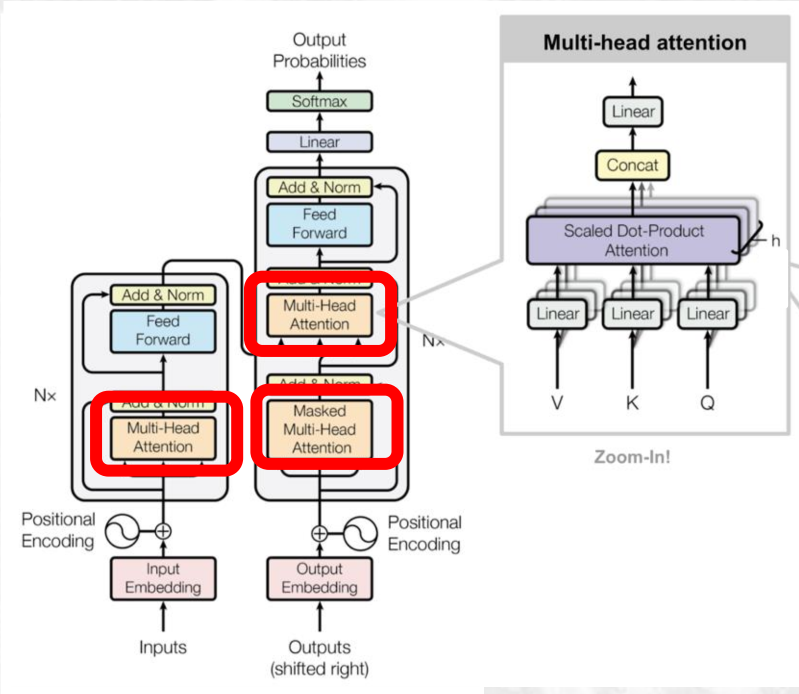


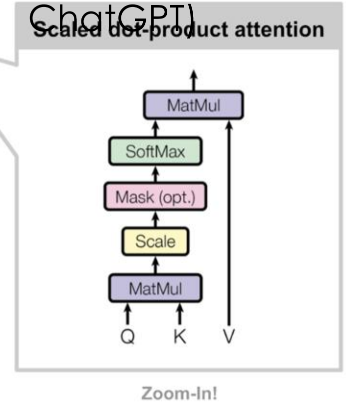
Image from https://medium.com/machine-intelligence-and-deep-learning-lab/transformer-the-self-attention-mechanism-d7d853c2c621

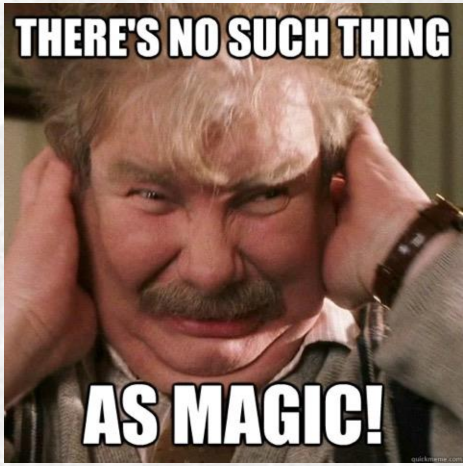
How does Self-attention work?

It is not magic, it is not a human brain, it is **just matrix multiplication**



The core Component
(even many years later in ChatGPT)



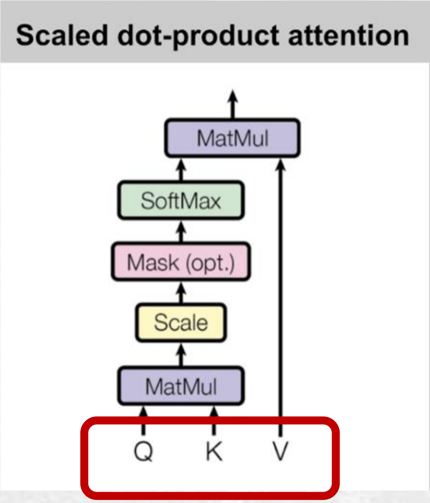


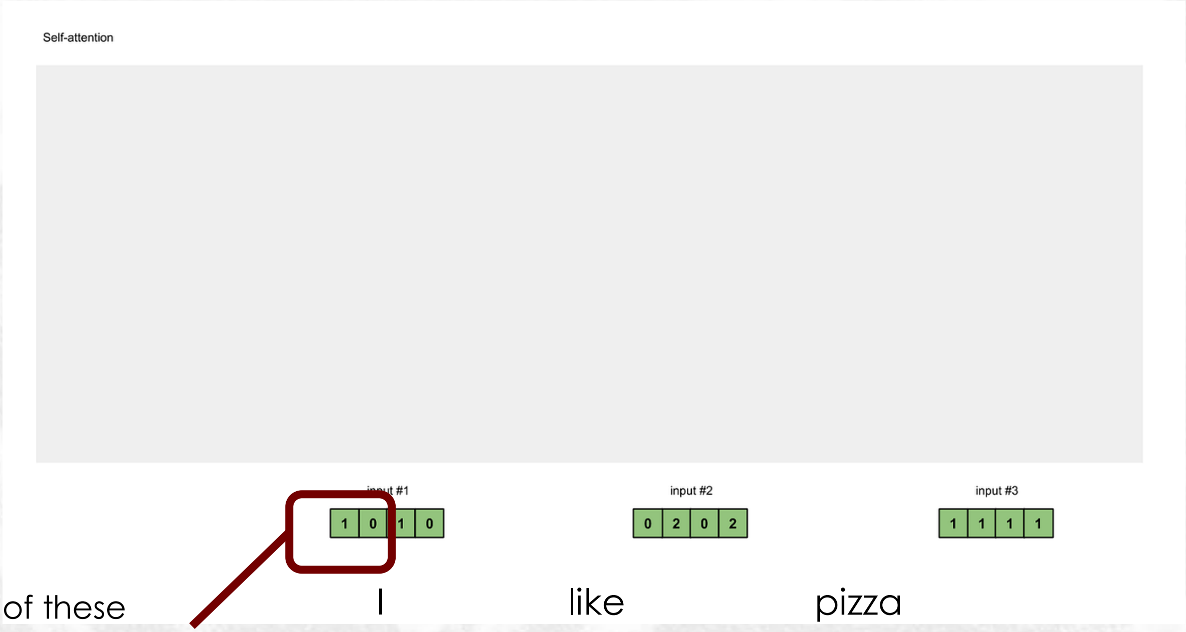
Many thanks to https://towardsdatascience.com/illustrated-self-attention-2d627e33b20a

«Attention in action»

Prepare inputs

Each word is associated to embeddings





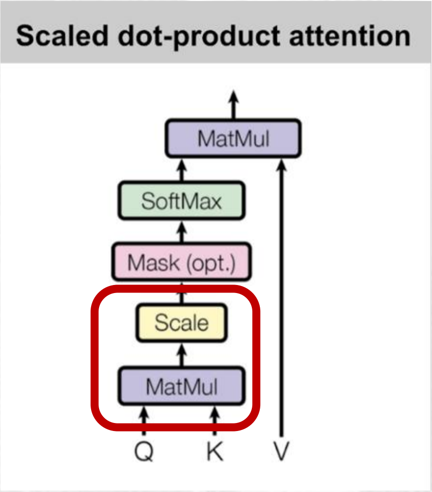
Positional Encoding: Part of these vector encodes the tokens' position

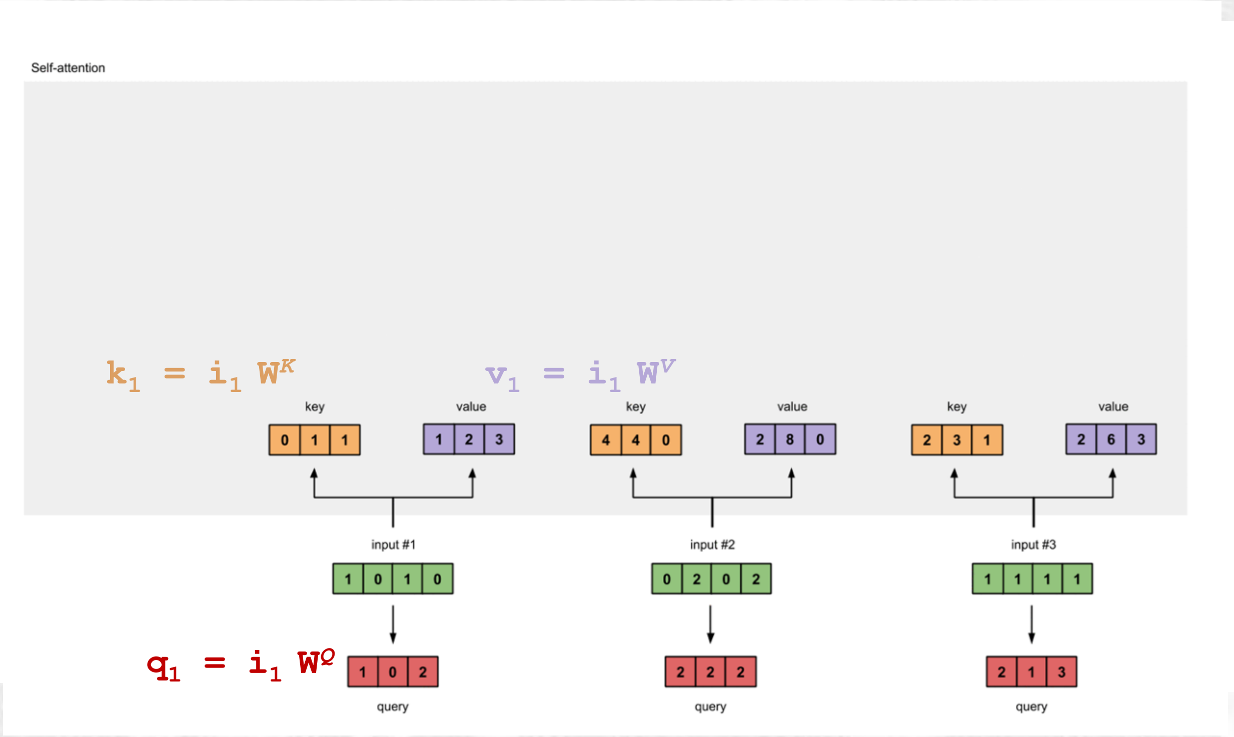
«Attention in action»

Compute Query, Key, and Value Vectors

For each word vector, calculate the Query, Key, and Value vectors by multiplying with respective weight matrices W^Q, W^K, W^V.

- $key_i = input_i\ W^K$
- $value_i = input_1\ W^V$
- $query_i = input_i\ W^Q$

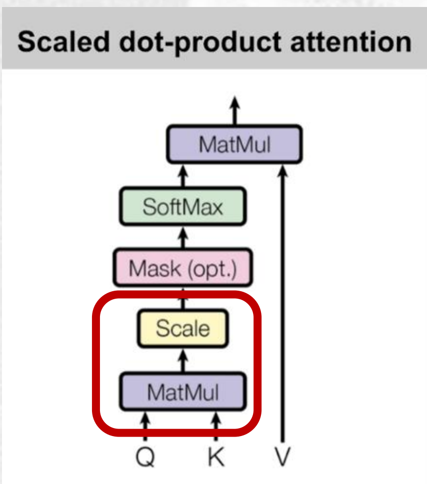


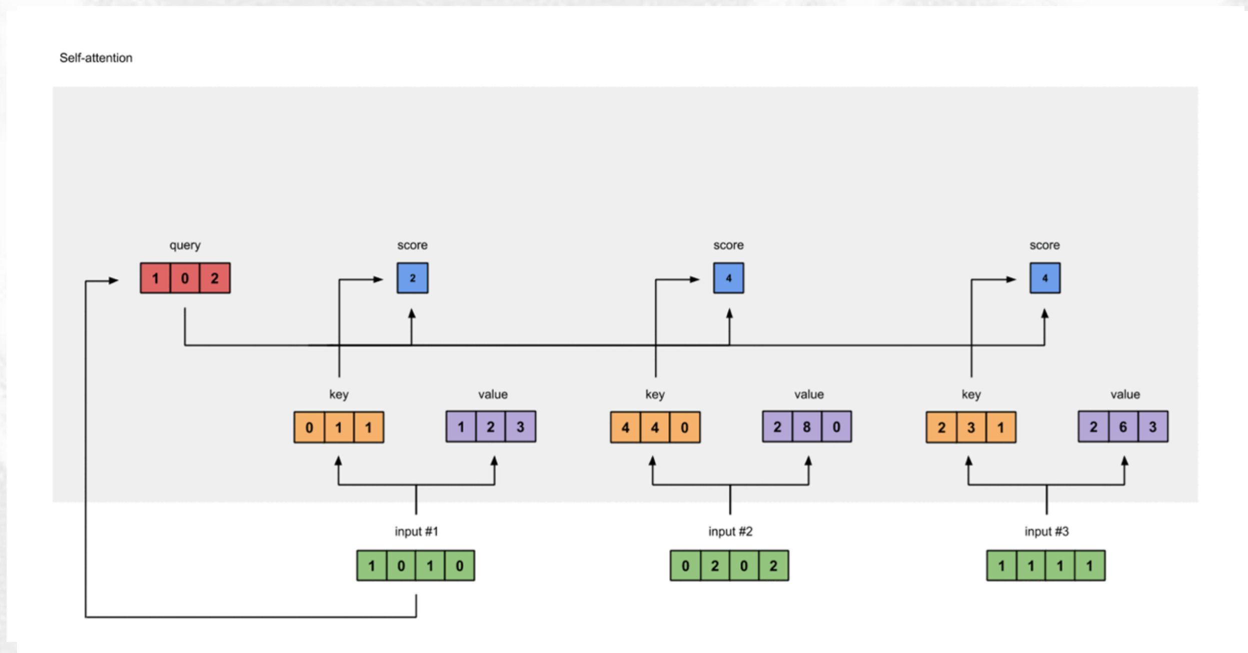


«Attention in action»

Calculate the Attention scores for $\texttt{input}_1$

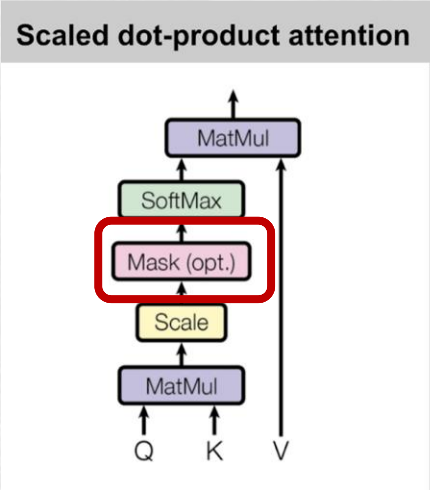
Attention scores are computed to «weight » the contribution of ALL words in the input sequence when representing $\texttt{input}_1$.

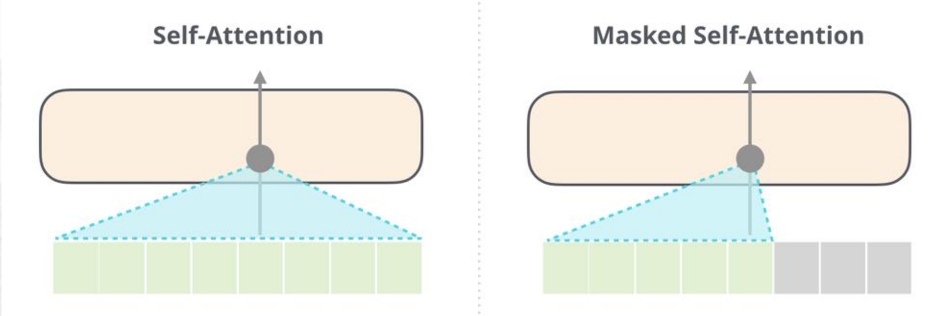




«Attention in action»
Role of Masked Attention

Use masked attention to handle sequences of different lengths

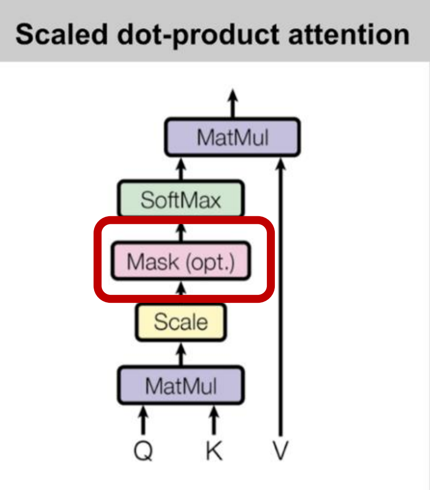


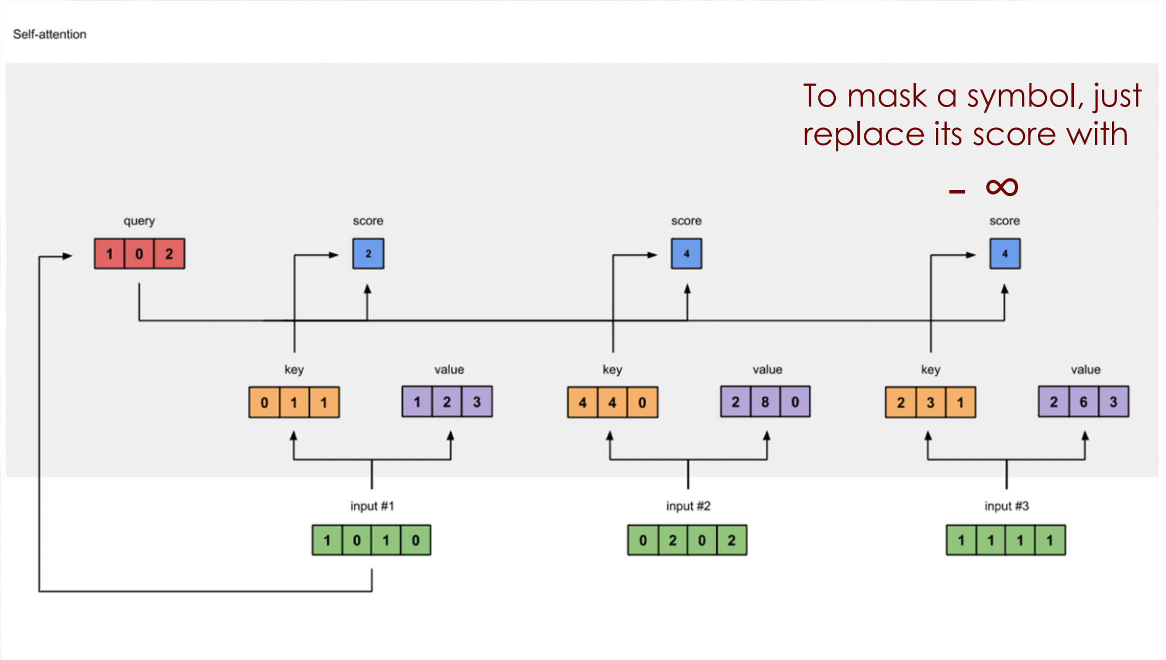


https://jalammar.github.io/illustrated-gpt2/

«Attention in action»
Role of Masked Attention (2)

Use masked attention to handle sequences of different lengths

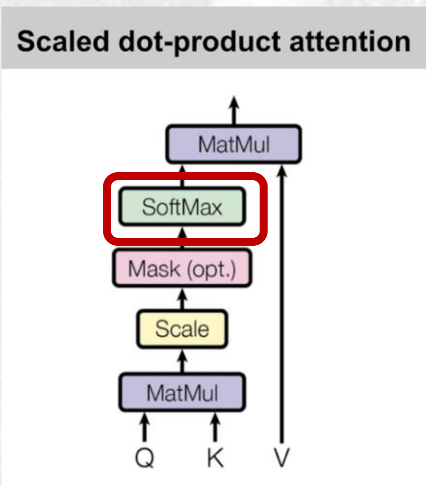


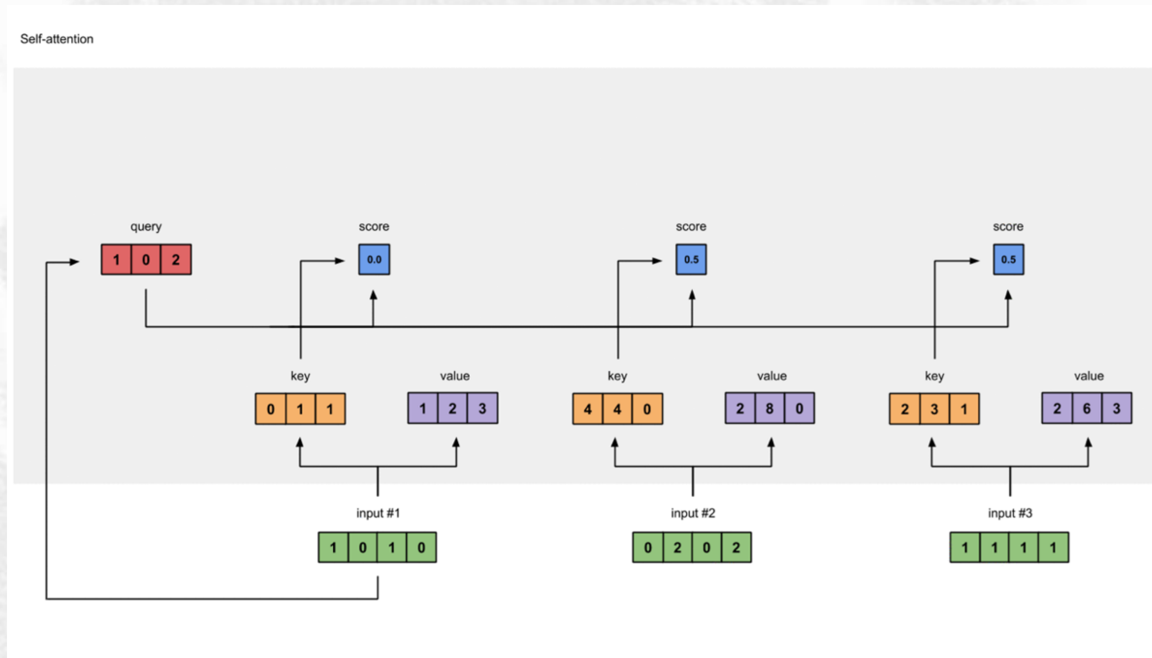


«Attention in action»
Calculate softmax

Softmax «simply» maps attention scores to a «probability» in [0, 1]

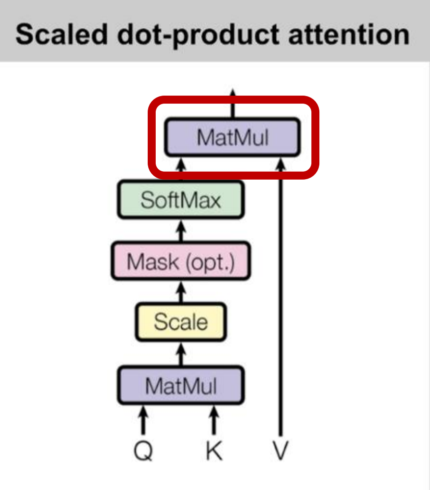
- The masked elements (i.e., with $-\infty$ gets a score near to 0)

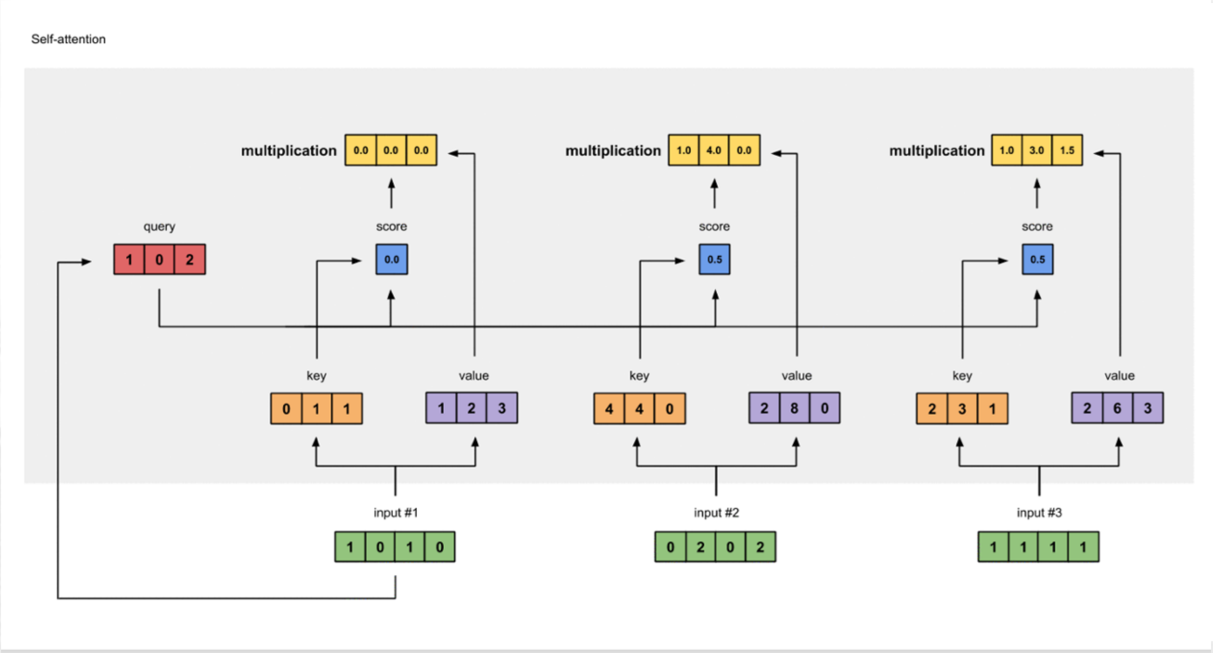




«Attention in action»
Multiply scores with values

Each $\texttt{input}_n$ (through each $\texttt{value}_n$) is weighted based of its importance in representing $\texttt{input}_1$

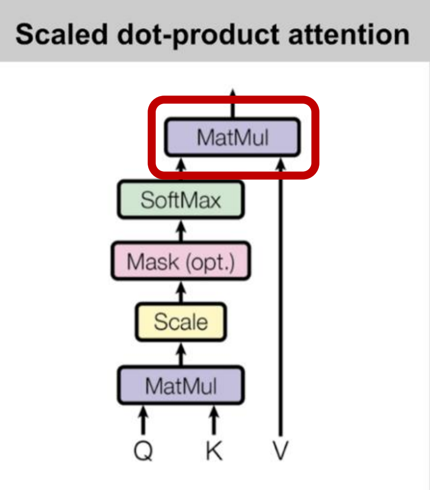


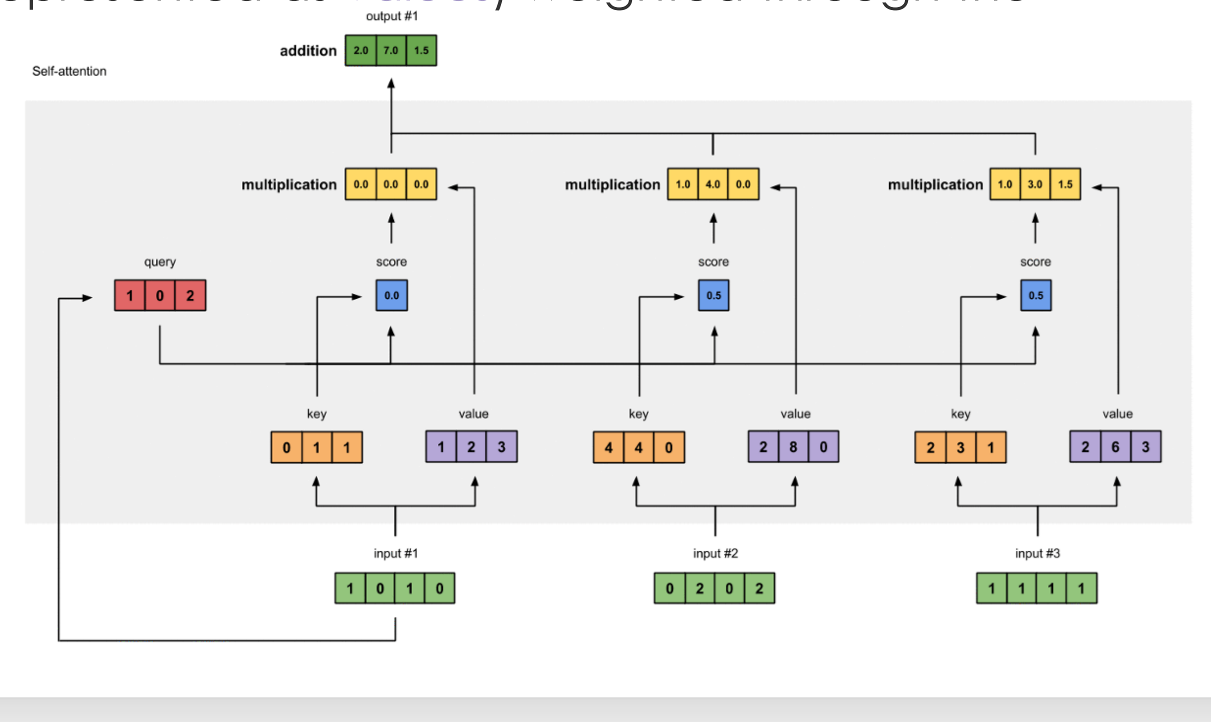


«Attention in action»

Complete the linear combination

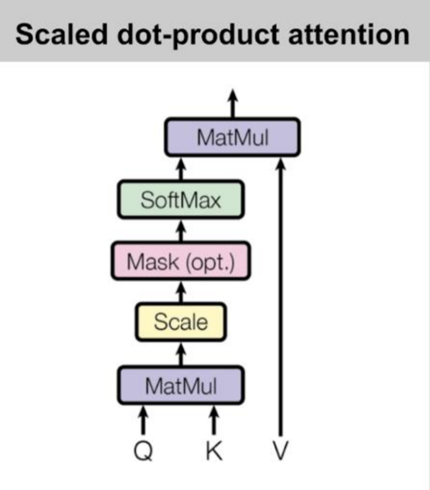
Sum weighted values to get $\texttt{output}_1$ that is the linear combination of all input elements (represented as values) weighted through the attention scores

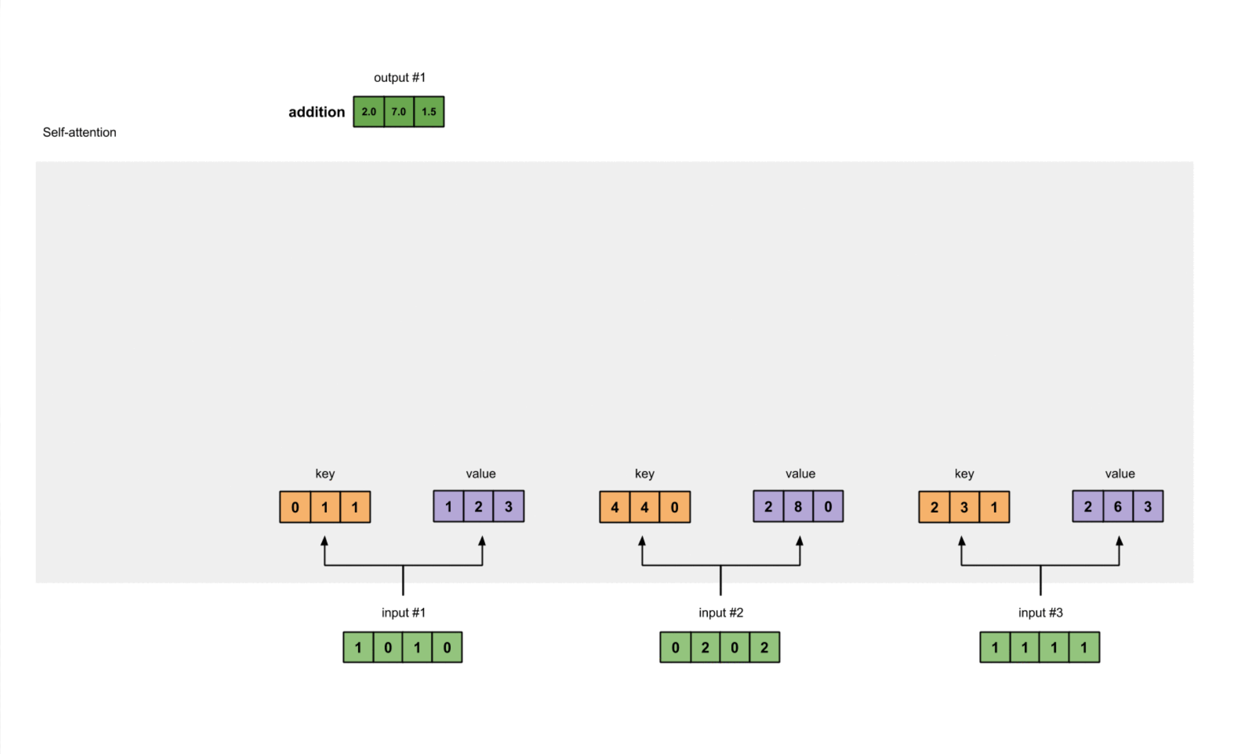




«Attention in action»

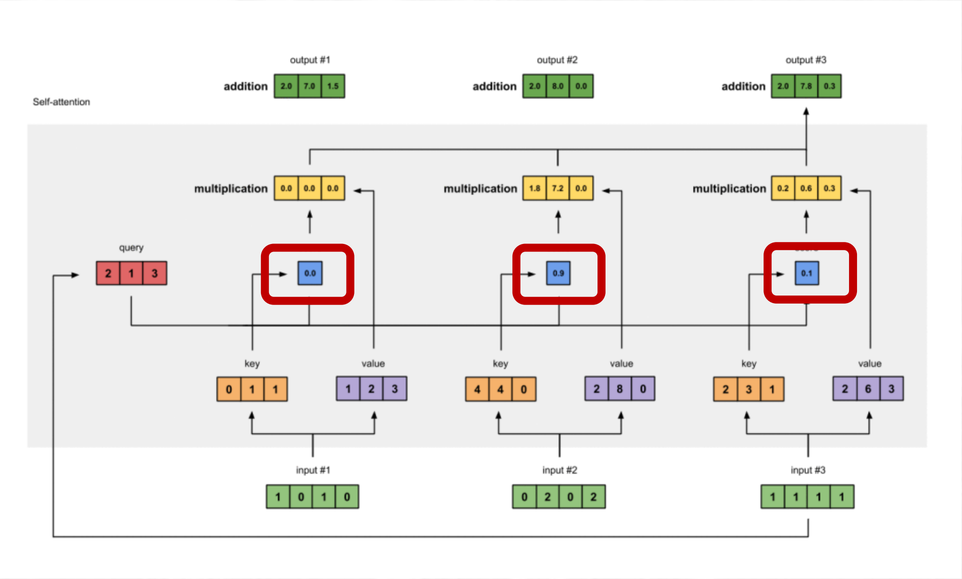
Repeat for `input`$_2$ and `input`$_3$



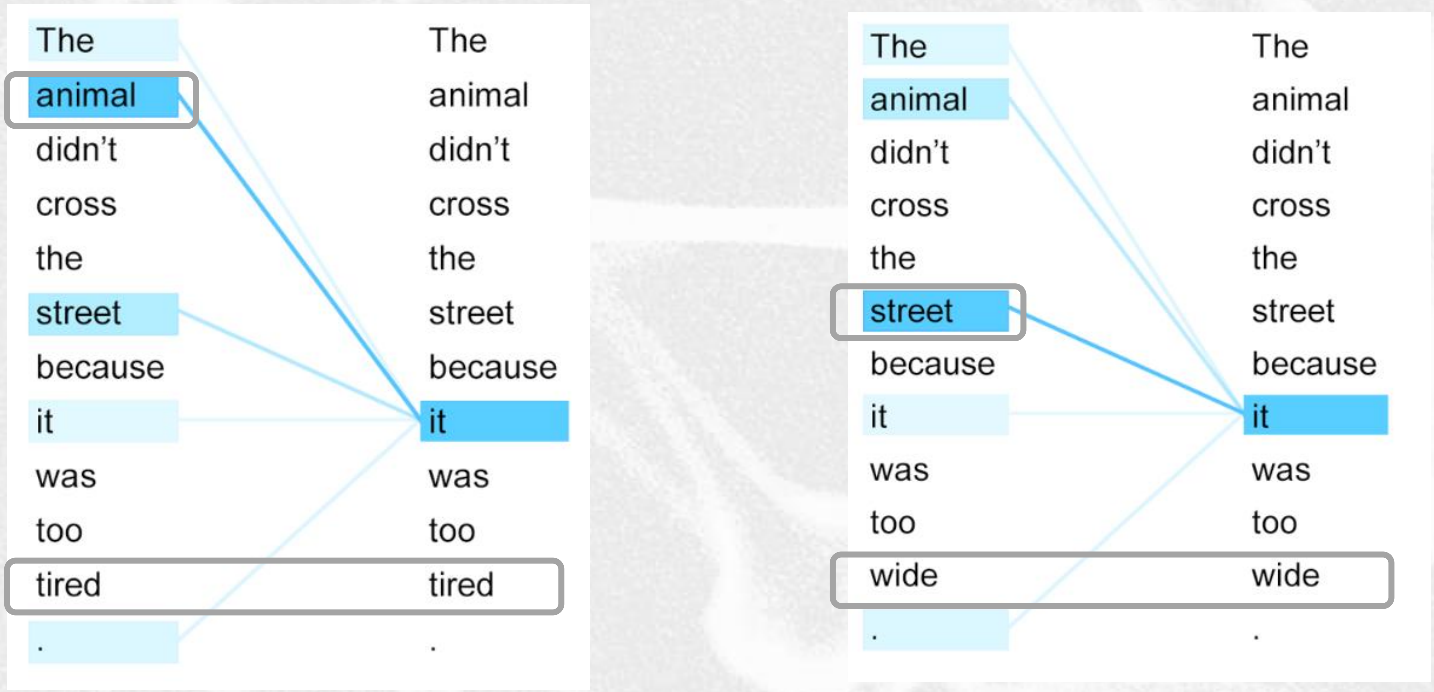


So… what is self-attention?

- It is not just a number, but a «probability distribution» for each symbol in input
  - And it allows weighting how **all words** are combined to generate the (hidden) representation of each word

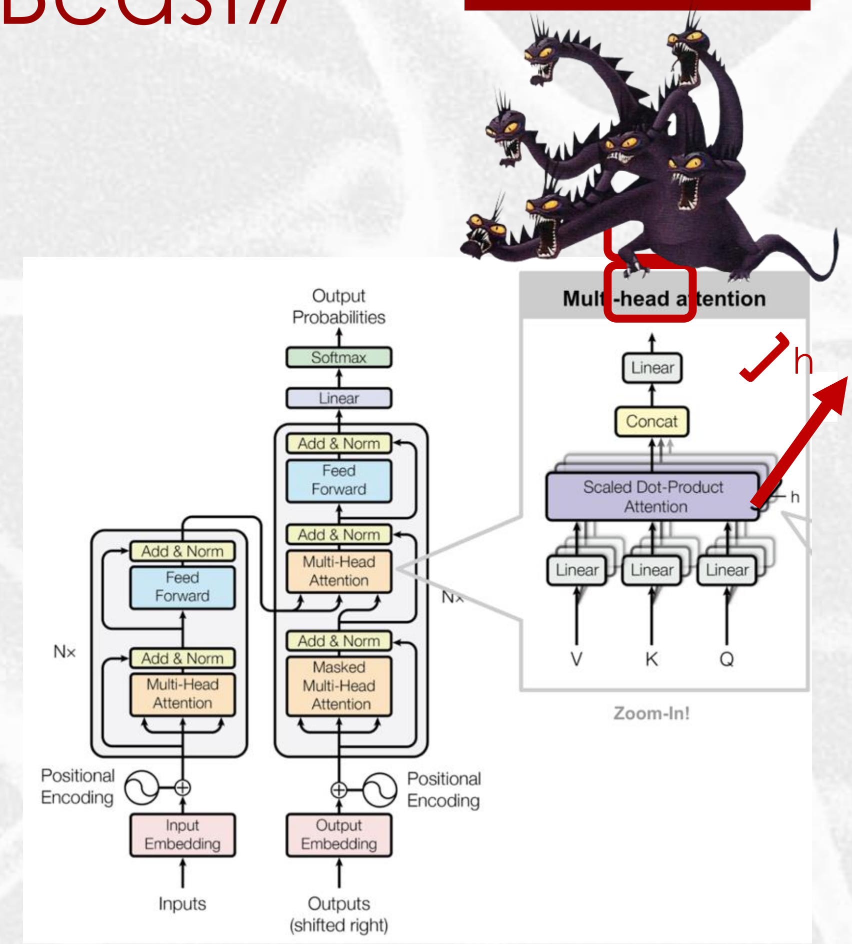


Self-Attention

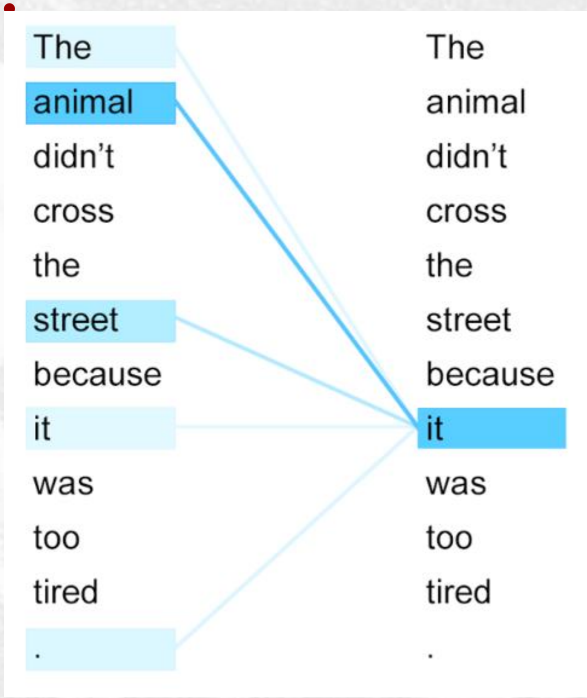


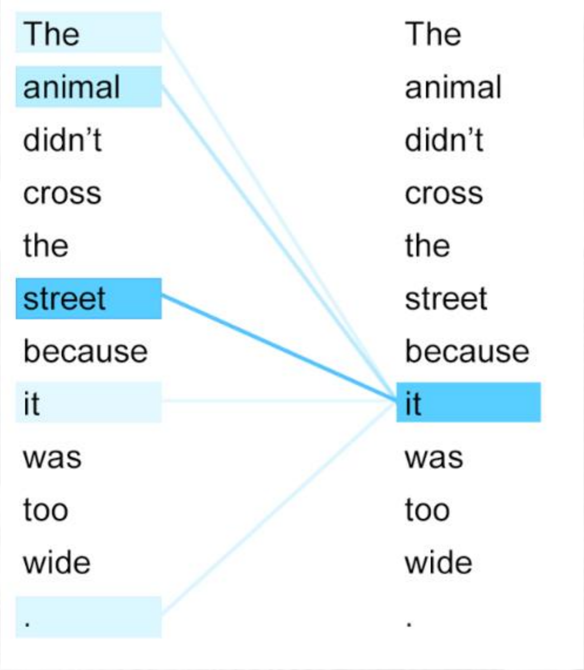
The Multi-Headed «Beast»

- Humans can attend to many things simultaneously.
- Can we extend attention to achieve the same?
- **Idea**: apply **Redundancy**, i.e., Scaled Dot-Product Attention **multiple times**
  - For each input, just generate h output
    - using h different different $(\mathbf{W}^Q, \mathbf{W}^K, \mathbf{W}^V)$)
  - Concatenate the h output vectors of each input
  - Use a linear layer to “restore” the initial dimensionality
    - **But combining all multiple evidences**

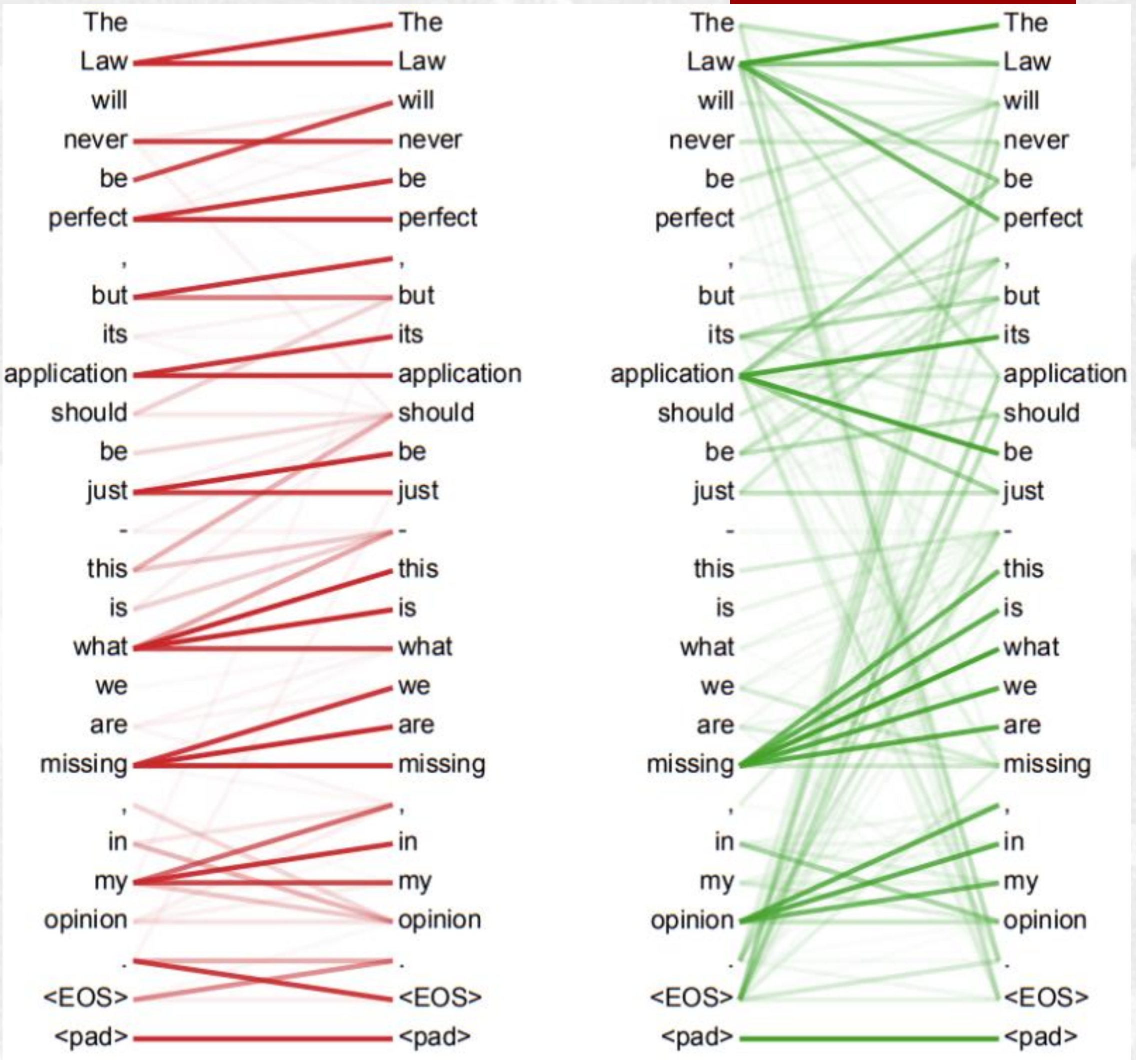


From «simple» attention…



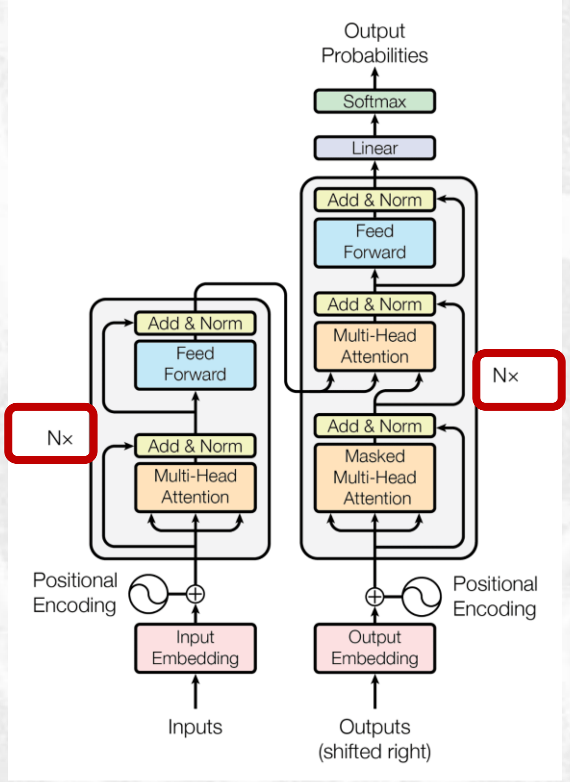


... to Multi-head Attention

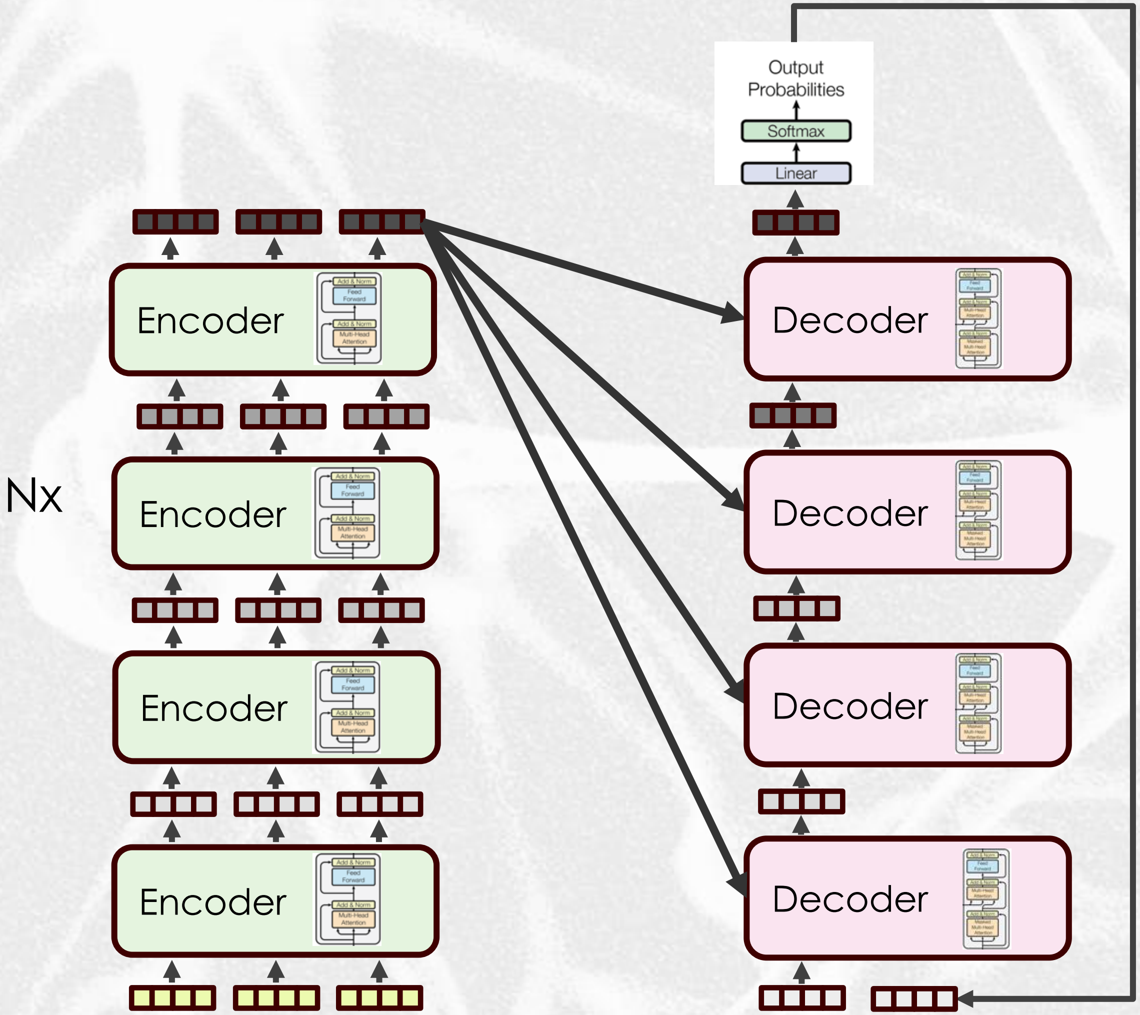


Where is the «Deep Learning»?

Encoders and decoders are repeated N times



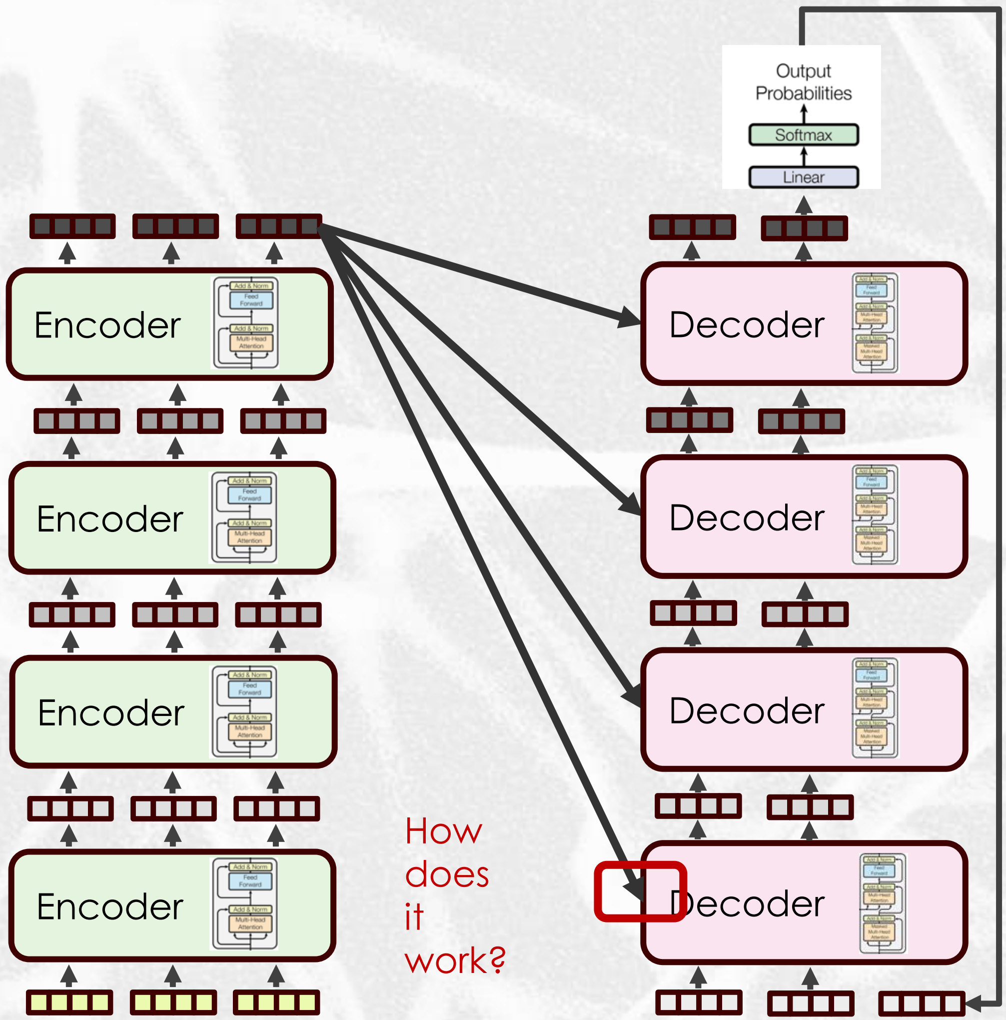
Again: the Transformer in Action



Generated hidden representations for each symbol initially rely on the first token, called `<start>`.

These representations are influenced by all hidden representations from the encoder.

Again: the Transformer in Action



After the generation begins…

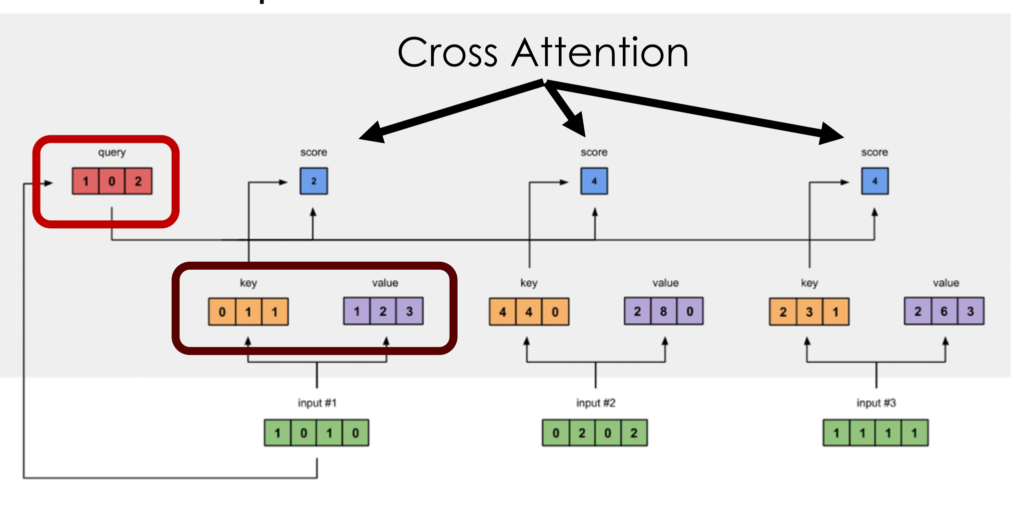
the **decoder's hidden representations simultaneously depend on all input tokens** attended to in the encoder…

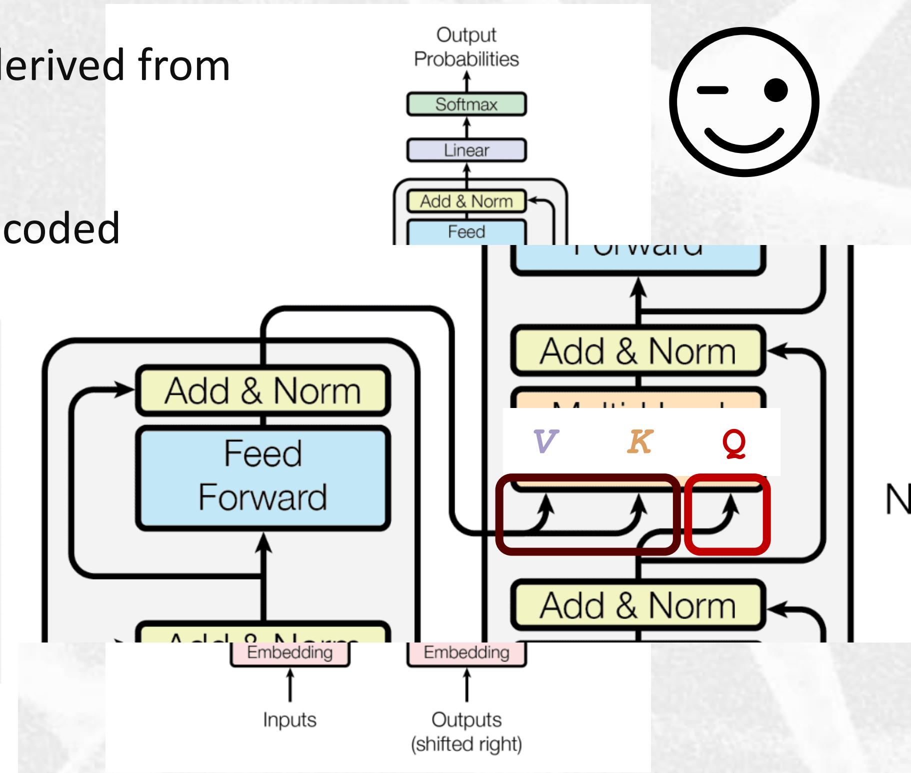
but **on the decoder's own previously generated hidden representations up to that point**.

How to combine Encoders and Decoders?

- In the decoder, key and value vector are derived from the input.
- The query, in contrast, depends on the decoded sequence.

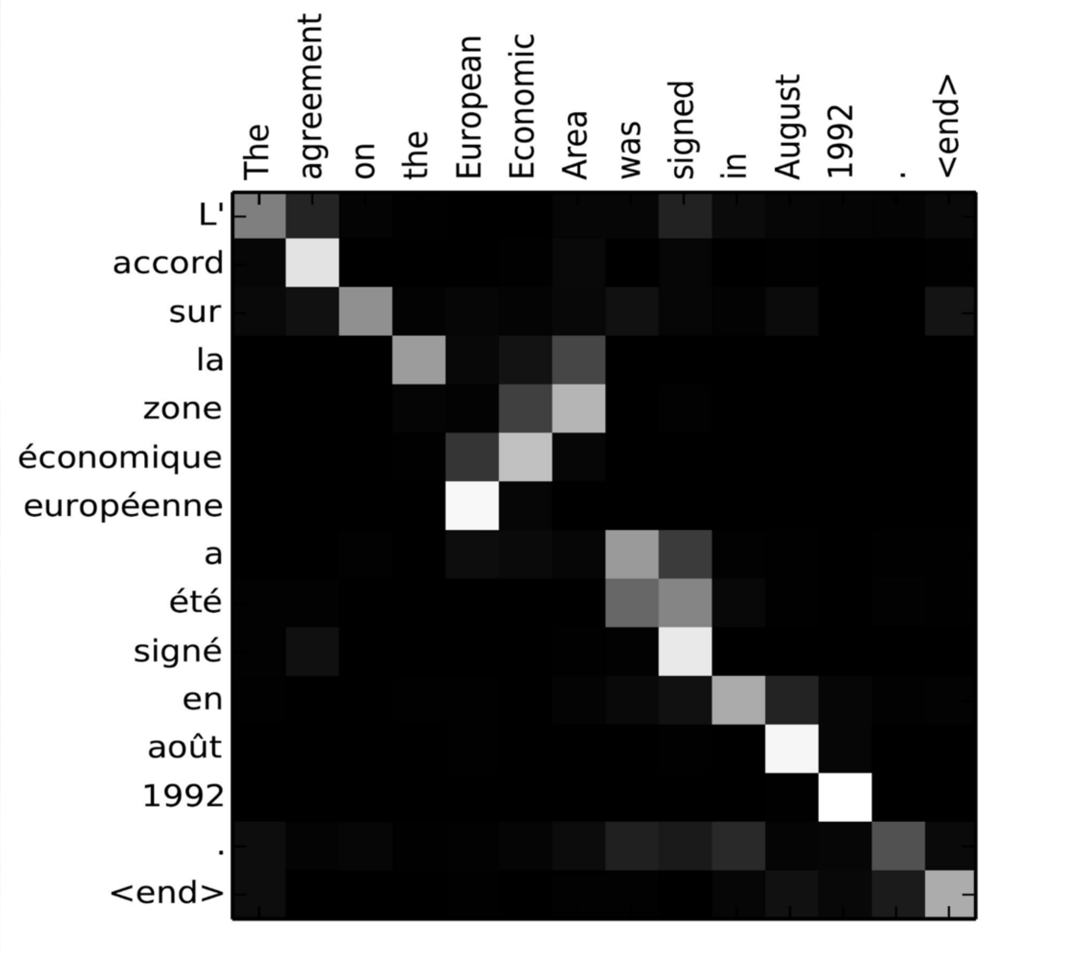
Self-attention





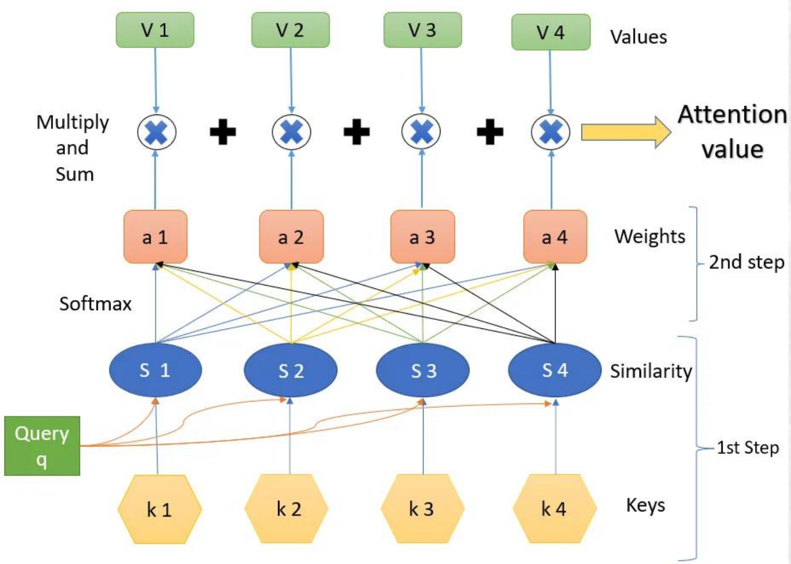
Cross-Attention

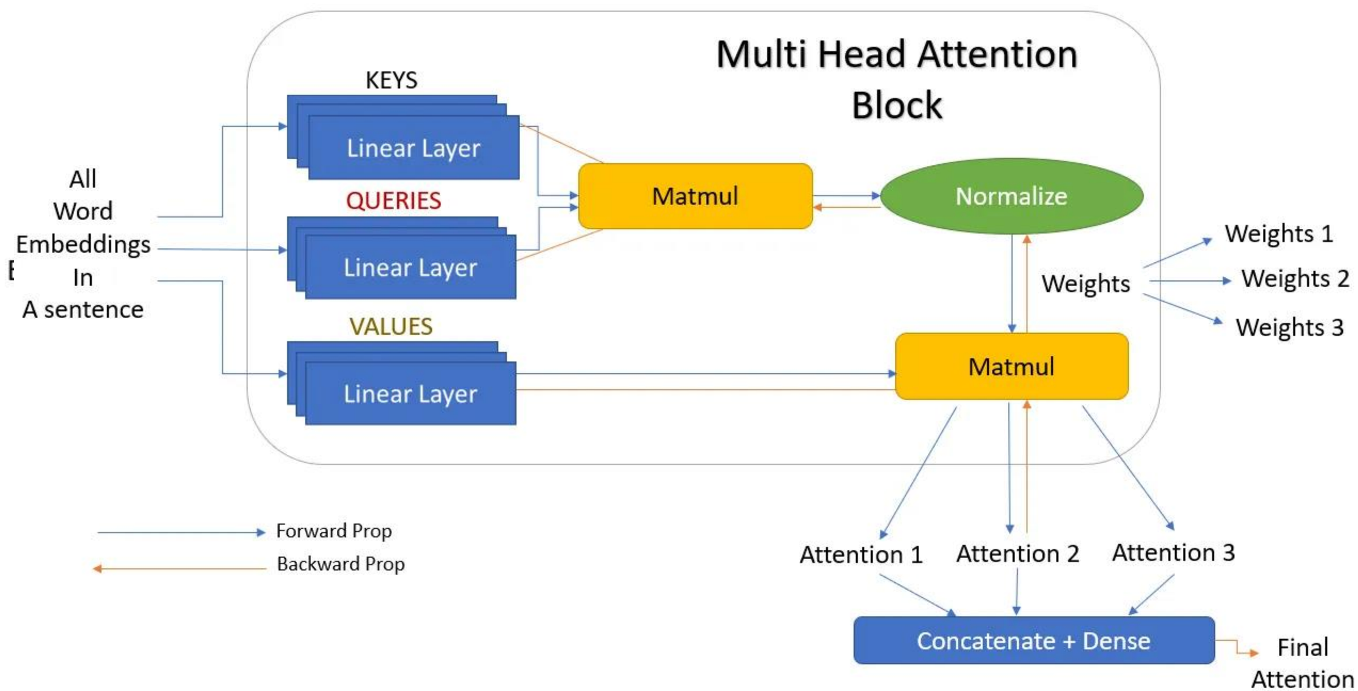
- Attention scores between input and output words
- White equals higher score
- The diagonal is highly correlated
- The scores reveal the grammatical difference for adjectives for the two languages (*zone économique européenne*)

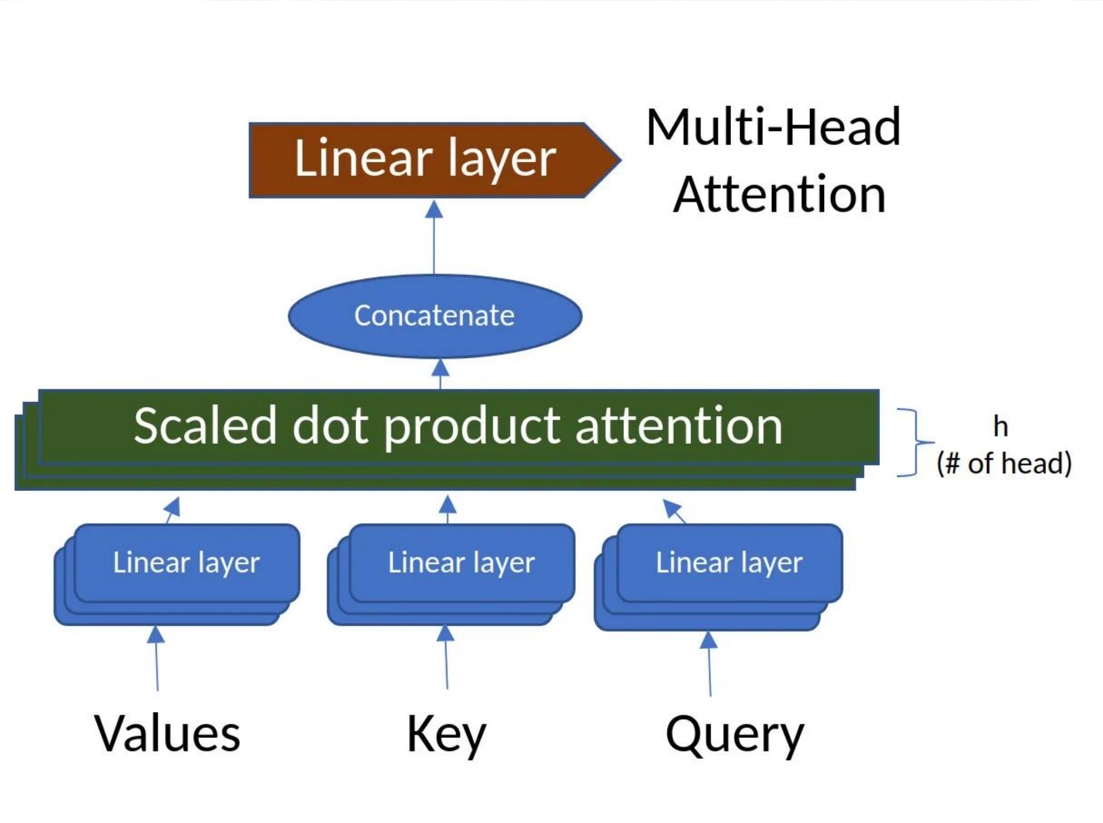


Advantages of Attention

- **Targeted Focus in Decoding:**
  - The decoder, with attention, can **strategically concentrate on relevant segments** of the source text
  - leading to more coherent and **contextually accurate** translations.
- **Addressing Vanishing Gradient Problem:** The mechanism offers a solution to the vanishing gradients issue
  - creating shortcuts between distant states in the sequence, facilitating smoother gradient flow during backpropagation.
- **Enhancing Model Interpretability:** we gain insights into what the model focuses on at each step


V 1
V 2
V 3
V 4
Values
Multiply and Sum
Attention value
a 1
a 2
a 3
a 4
Weights
2nd step
Softmax
S 1
S 2
S 3
S 4
Similarity
Query q
1st Step
k 1
k 2
k 3
k 4
Keys


Multi Head Attention Block
KEYS
Linear Layer
QUERIES
Linear Layer
VALUES
Linear Layer
All Word Embeddings In A sentence
Matmul
Normalize
Weights
Weights 1
Weights 2
Weights 3
Matmul
Attention 1
Attention 2
Attention 3
Concatenate + Dense
Final Attention
Forward Prop
Backward Prop


Linear layer
Multi-Head
Attention
Concatenate
Scaled dot product attention
h
(# of head)
Linear layer
Linear layer
Linear layer
Values
Key
Query

Attention functions: examples (1)

- In general, when queries and keys are vectors of different lengths, we can use additive attention as the scoring function. Given a query $\mathbf{q} \in \mathbb{R}^q$ and a key $\mathbf{k} \in \mathbb{R}^k$, the *additive attention* scoring function

$$a(\mathbf{q}, \mathbf{k}) = \mathbf{w}_v^\top \tanh(\mathbf{W}_q\mathbf{q} + \mathbf{W}_k\mathbf{k}) \in \mathbb{R},$$

- where learnable parameters $\mathbf{W}_q \in \mathbb{R}^{h\times q}$, $\mathbf{W}_k \in \mathbb{R}^{h\times k}$ and $\mathbf{w}_v \in \mathbb{R}^h$.
- In a learnable setting, the query and the key are concatenated and fed into an MLP with a single hidden layer whose number of hidden units is *h*, a hyperparameter. By using as the activation function and disabling bias terms, we implement additive attention in the following

Attention functions: scaled dot-product (2)

- When *q* and *k* are *d*-dimensional vectors whose independent dimensions have mean=0 and variance=1, their dot product has mean = 0 and a variance = *d*. To ensure that the variance of the dot product still remains one regardless of vector length, the *scaled dot-product attention* scoring function is adopted $a(\mathbf{q}, \mathbf{k}) = \mathbf{q}^\top \mathbf{k}/\sqrt{d}$
- It divides the dot product by $\sqrt{d}$. In practice, we often think in minibatches for efficiency, such as computing attention for *n* queries and *m* key-value pairs, where queries and keys are of length *d* and values are of length v. The scaled dot-product attention of queries $\mathbf{Q} \in \mathbb{R}^{n\times d}$, keys $\mathbf{K} \in \mathbb{R}^{m\times d}$, and values $\mathbf{V} \in \mathbb{R}^{m\times v}$ is

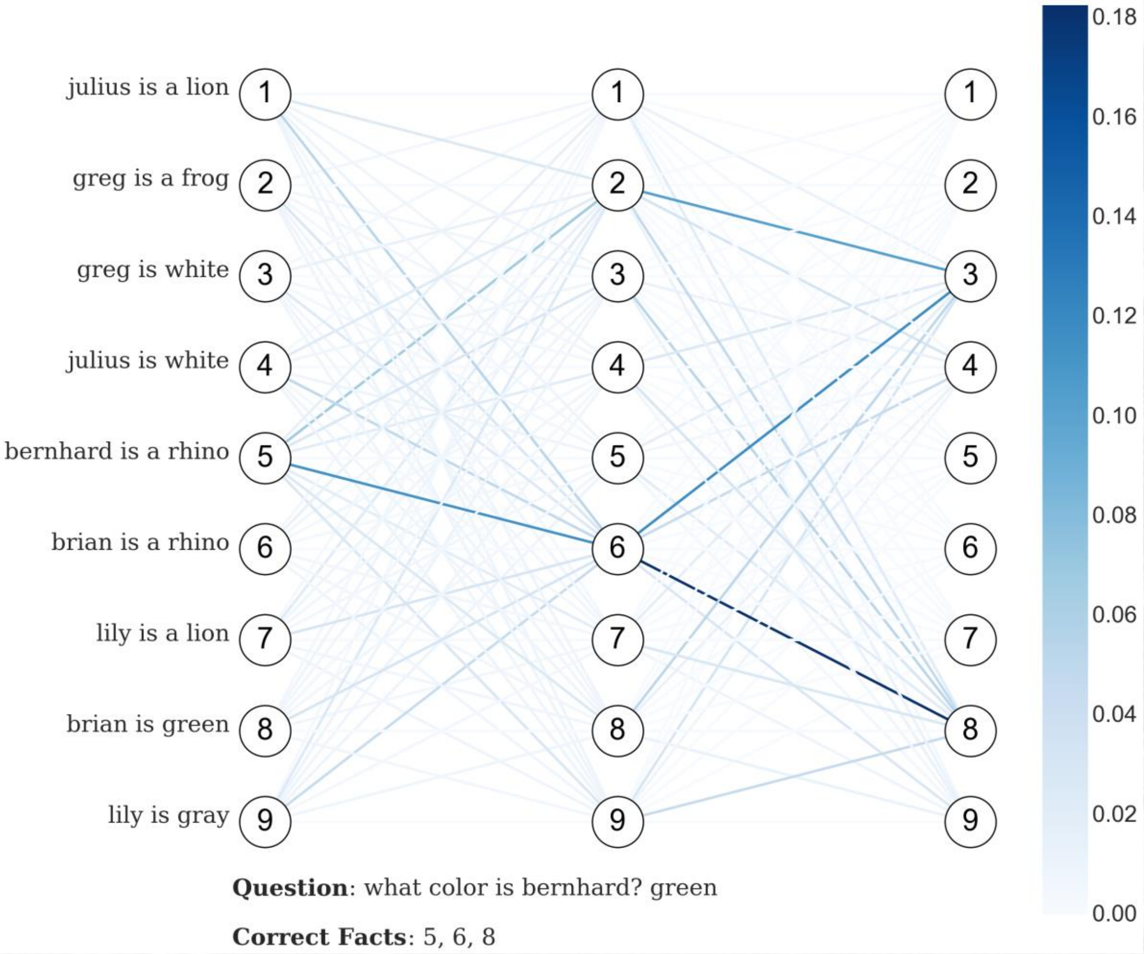
$$\mathrm{softmax}\left(\frac{\mathbf{Q}\mathbf{K}^\top}{\sqrt{d}}\right)\mathbf{V} \in \mathbb{R}^{n\times v}.$$

Attention & enconding

- IN a decoding process (e.g. machine translation) there are **three** kinds of dependencies for neural architectures
- Dependencies can establish between
- (1) the ***input and output*** tokens
- (2) the ***input tokens themselves***
- (3) the ***output tokens themselves***
- Examples:
  - MT
  - QA where the query the answer paragraph is the input and the matched answer is the output

Visualization of the attention distribution in QA

- Supporting fact sequences for an example question
- On the right the attentions over facts for individual sequences
  - Each sequence is mapped into a Markov process



From RNNs to Transformers

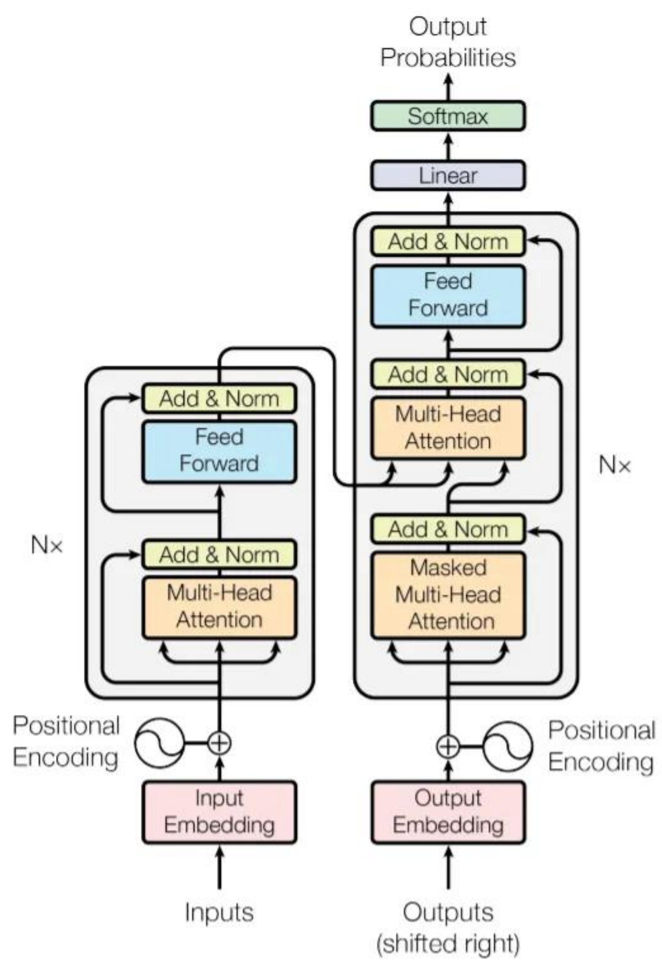
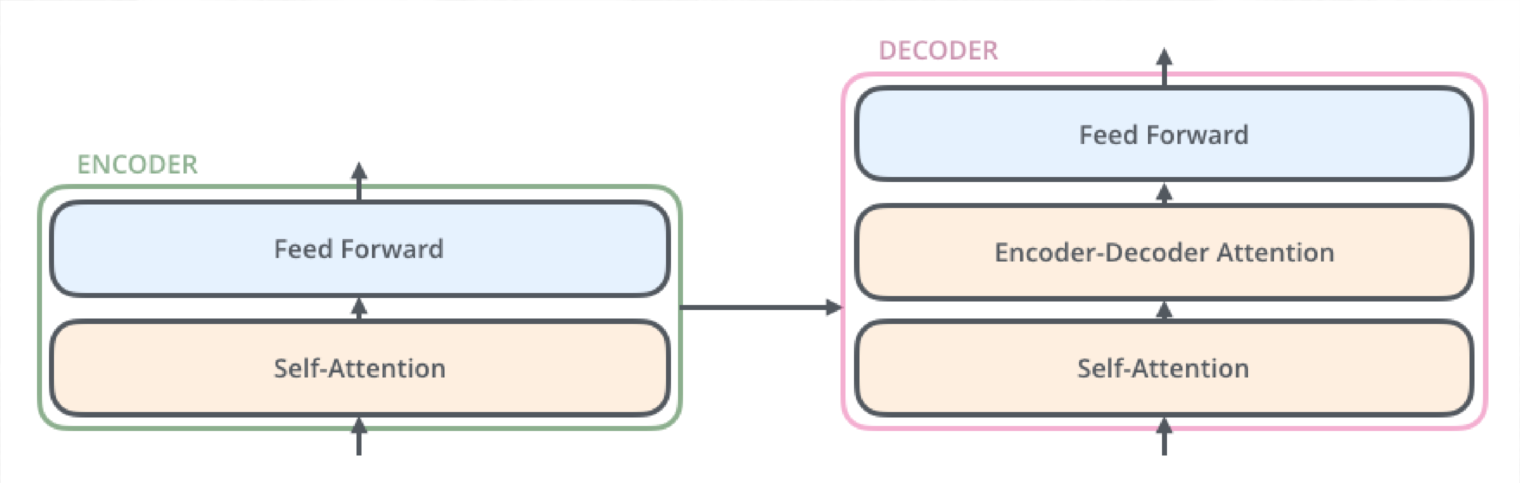


Figure 1: The Transformer - model architecture.

The Transformer was only the beginning

A transformer is made of two components

- Encoder
- Decoder



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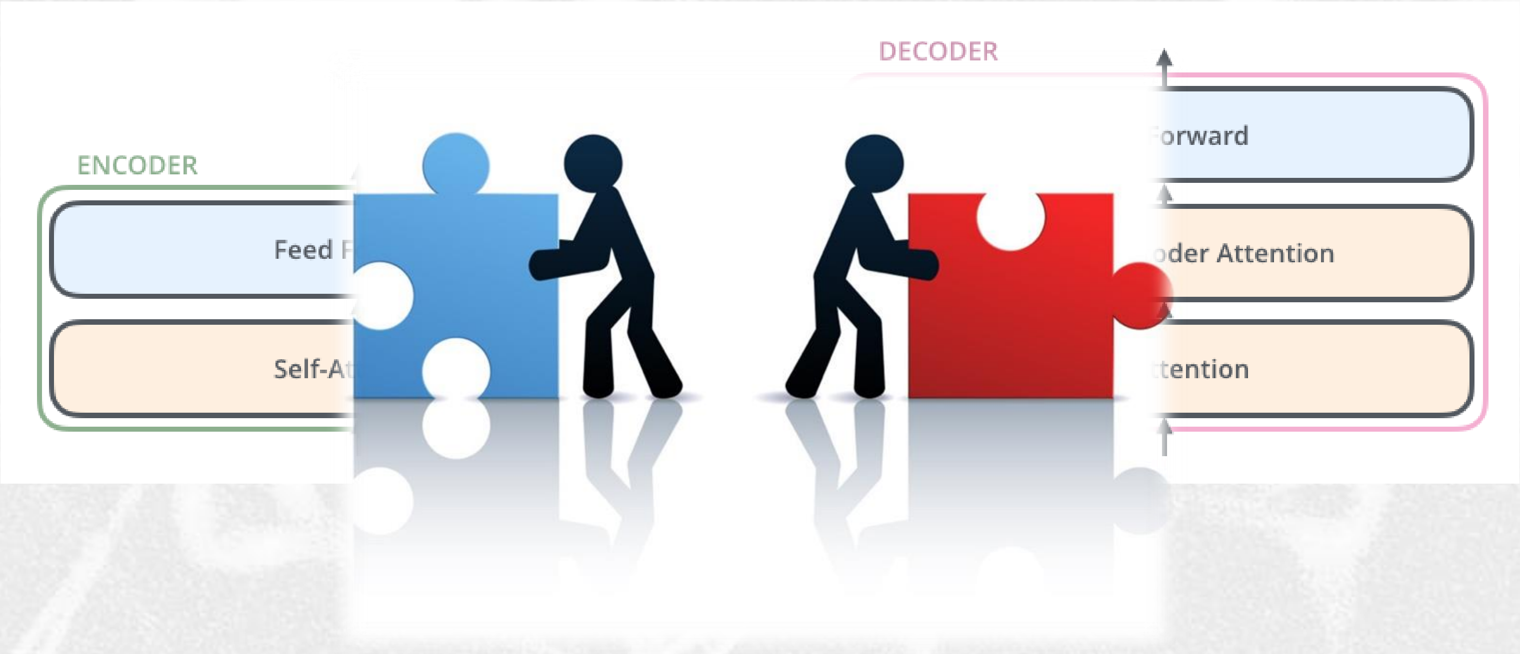
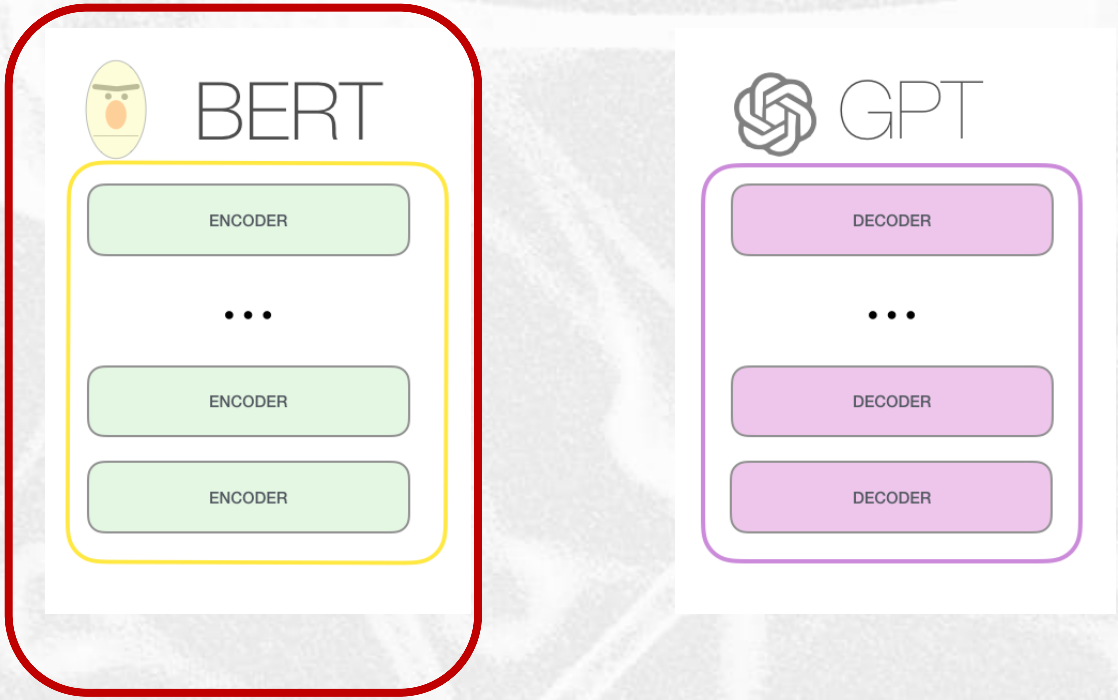


The transformer was only the beginning

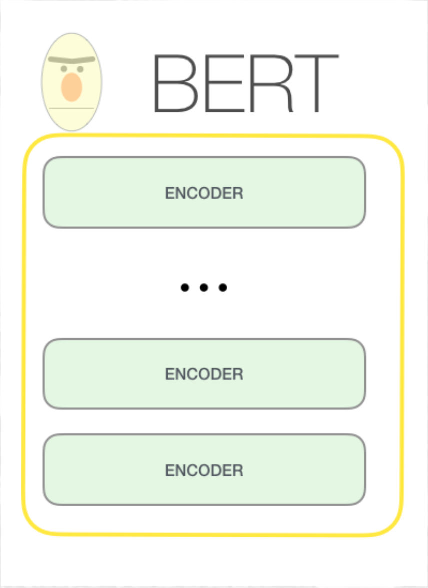
- This separation led to two «classes» of methods
  - **«Encoder-only» models**: the most famous one is BERT
  - **«Decoder–only» models:** the most famous one is GPT



BERT (Devlin et al, 2018)

Bidirectional Encoder Representations from Transformers

- Only the encoder is used
- Designed to generate **contextual meaningful representation** of input words
  - Representations are **context sensitive,** thanks to self-attention
  - Understand the context of a word in a sentence from **both left and right sides** (bidirectionally).
- Representations are embeddings
  - not suitable for text generation
  - … but for many other tasks



Images from `https://jalammar.github.io/illustrated-bert/`

Devlin, J., Chang, M. W., Lee, K., & Toutanova, K. (2018). Bert: Pre-training of deep bidirectional transformers for language understanding. arXiv:1810.04805.

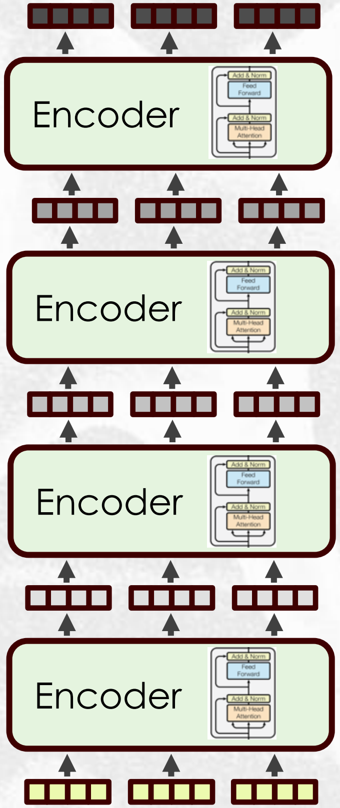
BERT (Devlin et al, 2018)

Why should it work?

- It is just a piece of the Transformer architecture seen a few slides ago.

The GREAT IDEA: Pre-Training the encoder

- Pre-trained on a large corpus of text and then fine-tuned for specific tasks like question answering, sentiment analysis, etc.



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Devlin, J., Chang, M. W., Lee, K., & Toutanova, K. (2018). Bert: Pre-training of deep bidirectional transformers for language understanding. arXiv:1810.04805.

No pre-training no party! The Revolution of Pre-Training in NLP

- **Simple idea:** train a (possibly large) model on a different task and re-use it on your task
  - circumventing the need for training from scratch
  - facilitating “quicker”, more effective deployment of the model
- **Precedent in Computer Vision**:
  - This strategy mirrors developments in computer vision
  - Architectures pre-trained on classification tasks using datasets like ImageNet
  - When applied on related task, these “starting point” achieve very good results
- **Addressing Overfitting in Large Models**:
  - With **increasing model sizes** and parameter counts, the **risk of overfitting grows**
  - Pre-training on vast datasets mitigates this by providing a broad learning base.

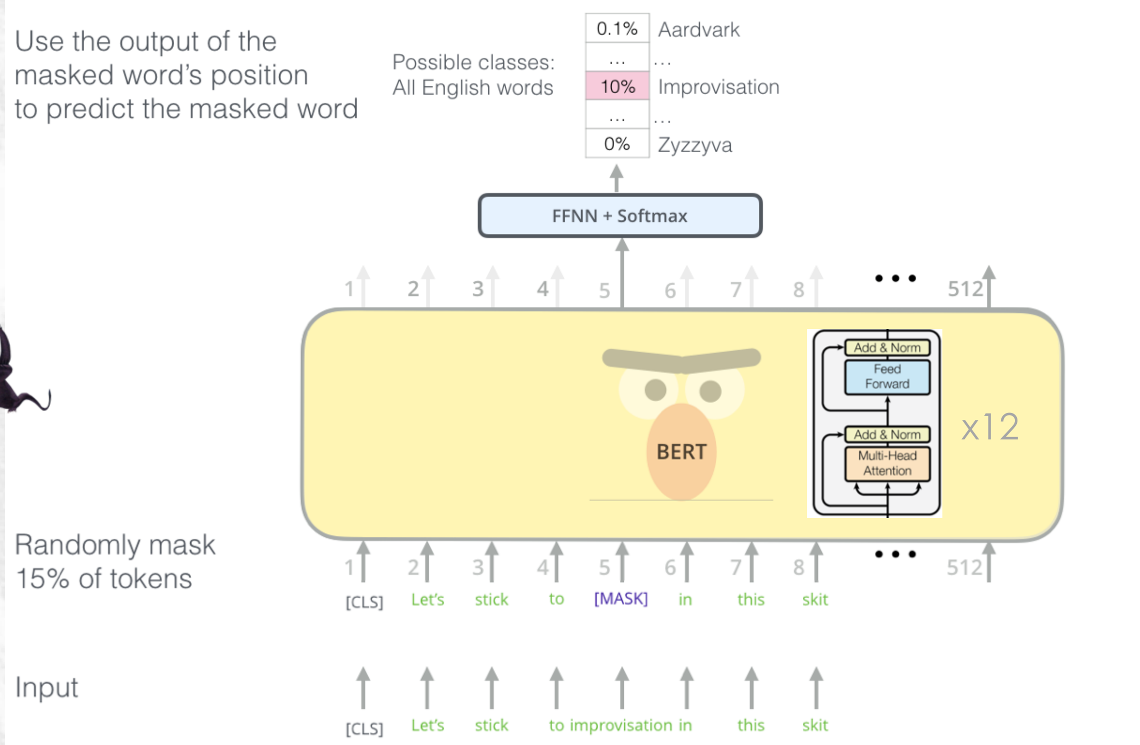
Towards Foundation Models

- **Emergence of Foundation Models in NLP**:
  - Large-scale models trained on linguistic tasks, forming a versatile base that can be fine-tuned for various specific applications.
- **Everybody worked on customizing Foundation Models:**
  - Leverage the extensive knowledge encapsulated in Foundation Models by fine-tuning them for particular NLP tasks.
- If you are interested in foundation models
  - [Zhou et al, 2023] A Comprehensive Survey on Pretrained Foundation Models: A History from BERT to ChatGPT
  - `https://arxiv.org/abs/2302.09419`

Pretraining BERT

- BERT takes a sequence of tokens as input
  - Utilizes **self-attention across layers** to **generate context-aware** representations of each token in the sequence.
  - In each layer, h=12 $\mathbf{W}^Q, \mathbf{W}^K, \mathbf{W}^V$ matrices

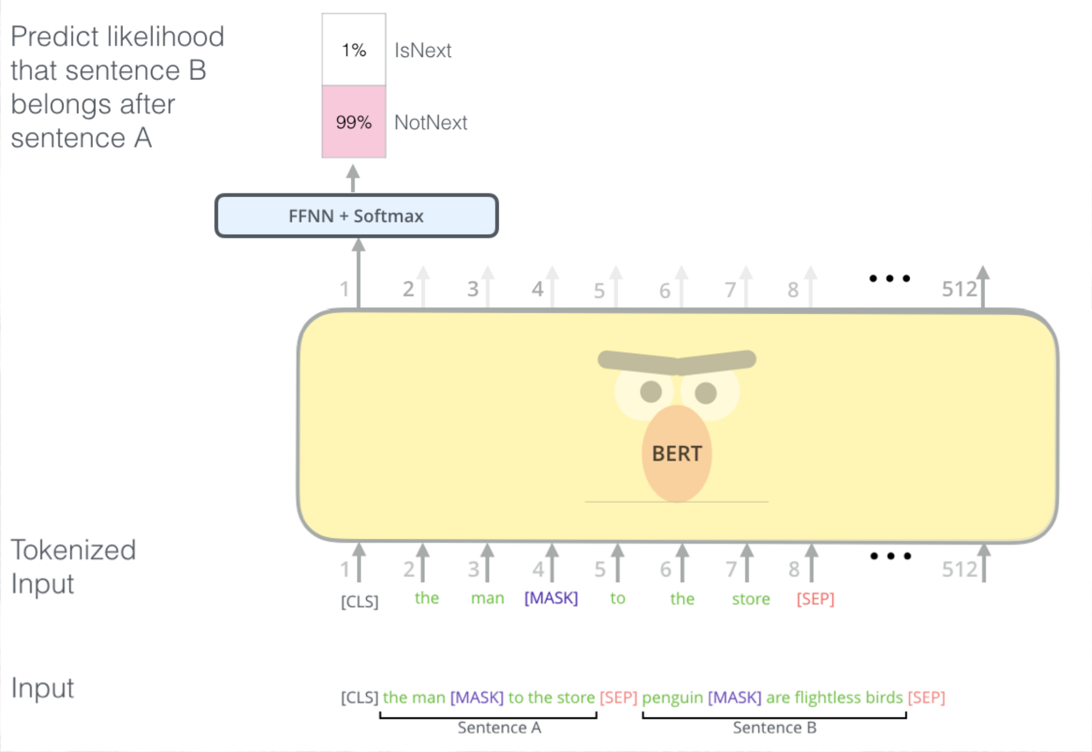
- **Pre-training tasks:**
  - **Masked-language modeling**



Pretraining BERT (2)

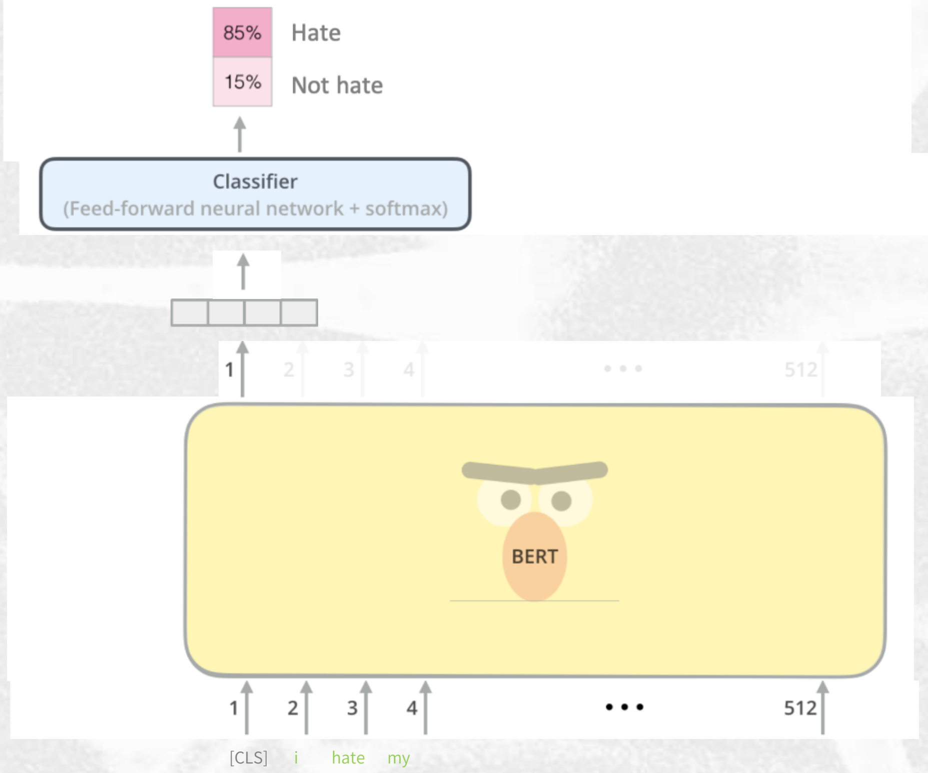
- BERT takes a sequence of tokens as input
  - Utilizes **self-attention across layers** to **generate context-aware** representations of each token in the sequence.
  - In each layer, h=12 $\mathbf{W}^Q, \mathbf{W}^K, \mathbf{W}^V$ matrices
- **Pre-training tasks:**
  - Masked-language modeling
  - **Next sentence prediction**

Pretrained using the Toronto BookCorpus (800M words) and English Wikipedia (2,500M words)



BERT and fine-tuning

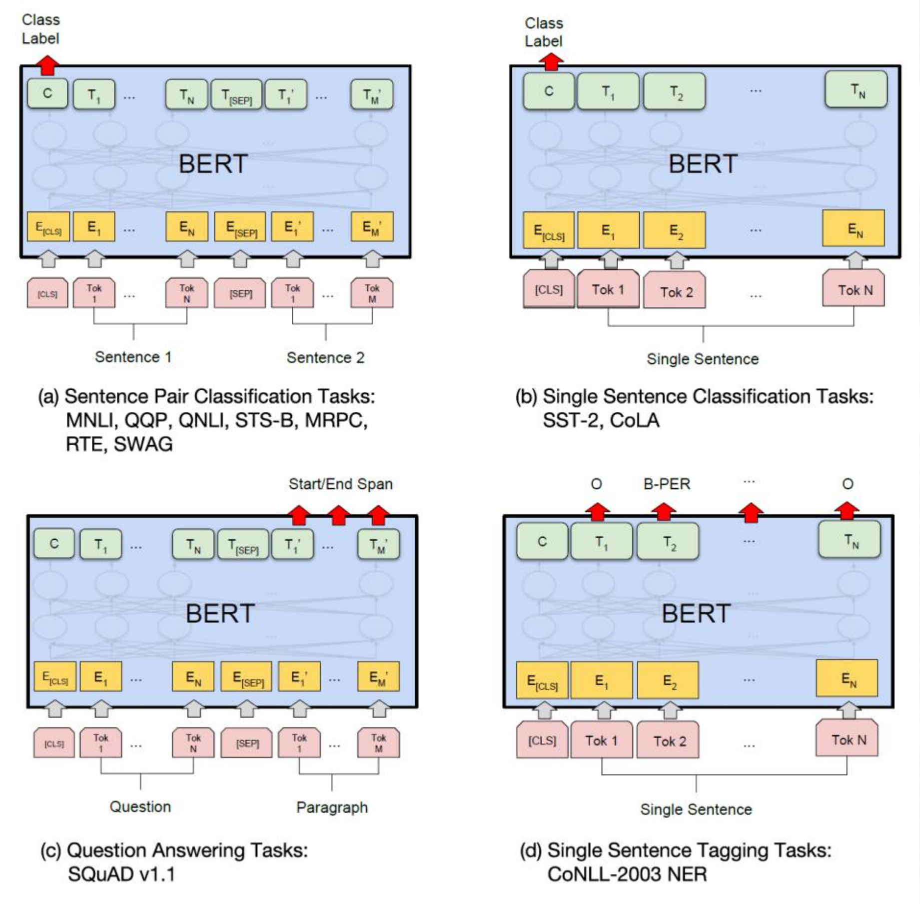
- Once pretrained, we can **apply it to new sentences**
- BERT will **produce encoded representations** for each input symbol
- And it can be used in **different classification tasks**, just adding a new (linear) classifier…
- … through fine-tuning of the entire architecture
- not trivial to forget what learned during the pre-training



Devlin, J., Chang, M. W., Lee, K., & Toutanova, K. (2018). Bert: Pre-training of deep bidirectional transformers for language understanding. arXiv:1810.04805.

BERT in action

- The final layer outputs hidden representations, which can be utilized with a simple linear classifier
- to address a broad spectrum of NLP tasks efficiently.



(a) Sentence Pair Classification Tasks: MNLI, QQP, QNLI, STS-B, MRPC, RTE, SWAG

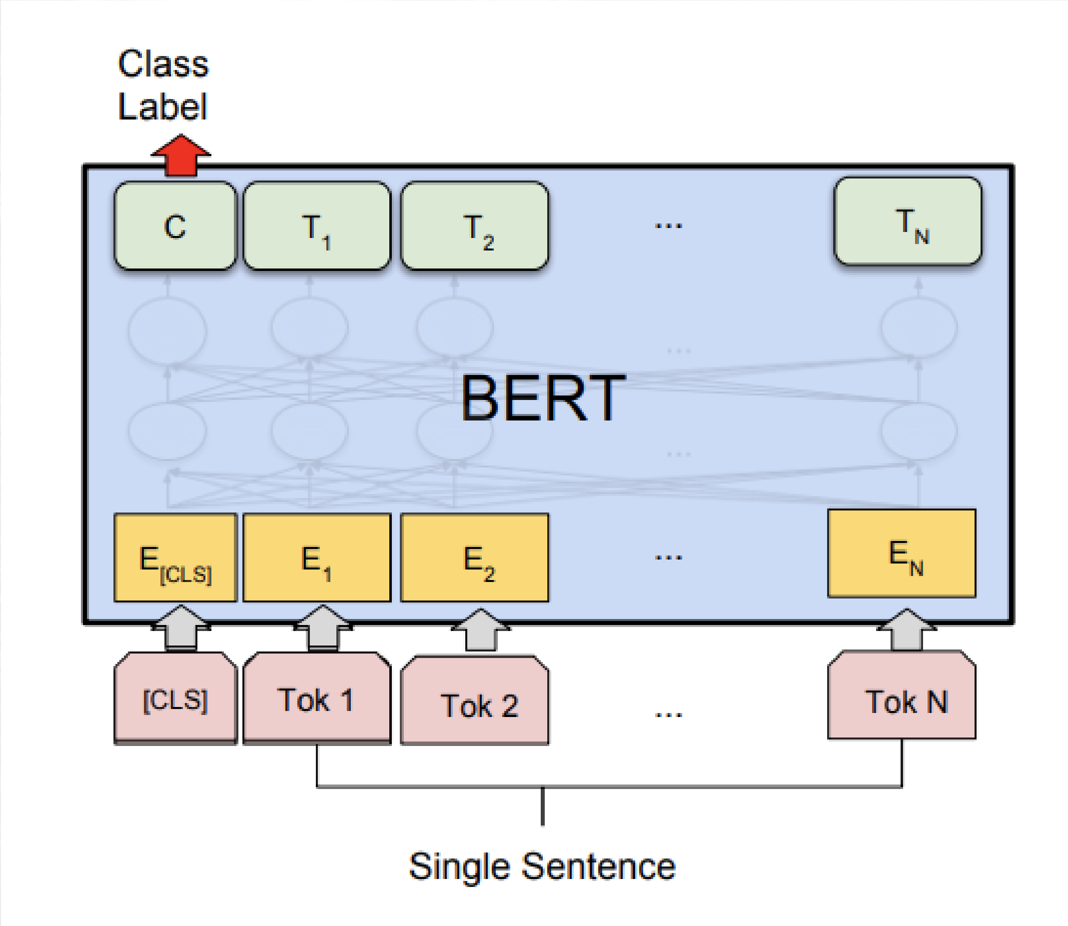
(b) Single Sentence Classification Tasks: SST-2, CoLA

(c) Question Answering Tasks: SQuAD v1.1

(d) Single Sentence Tagging Tasks: CoNLL-2003 NER

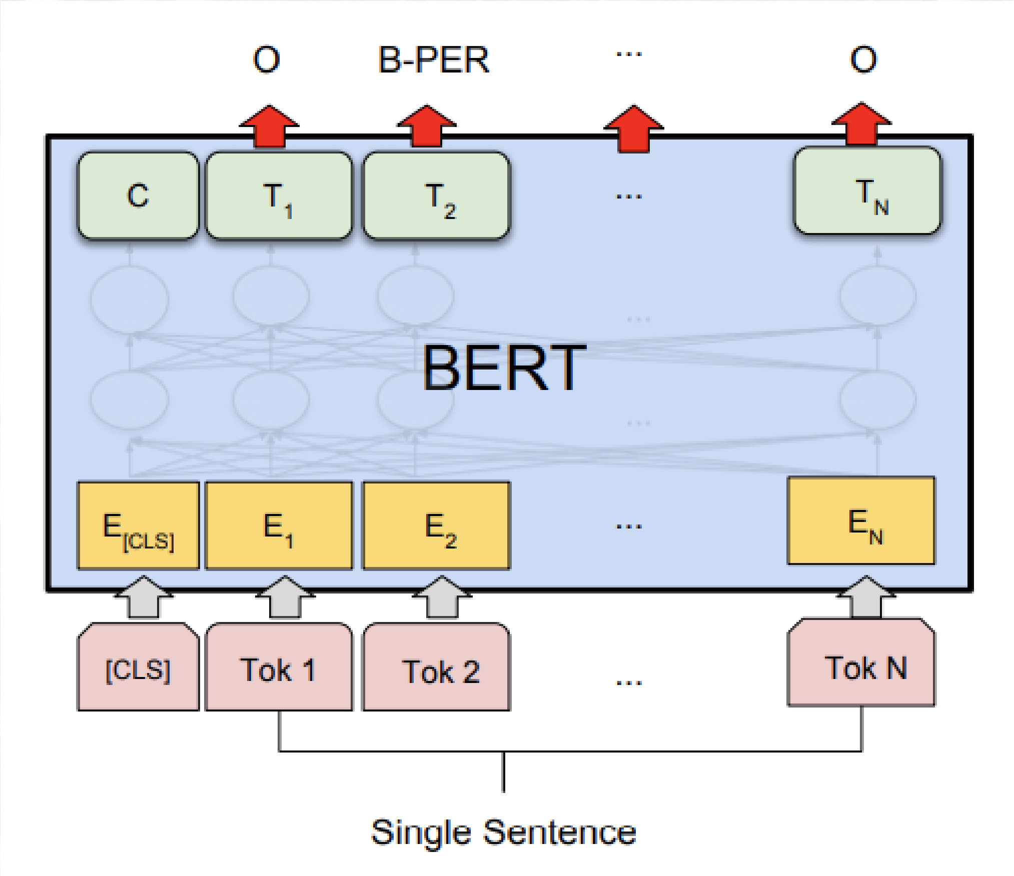
Devlin, J., Chang, M. W., Lee, K., & Toutanova, K. (2018). Bert: Pre-training of deep bidirectional transformers for language understanding. arXiv:1810.04805.

BERT (Devlin et al. '18)



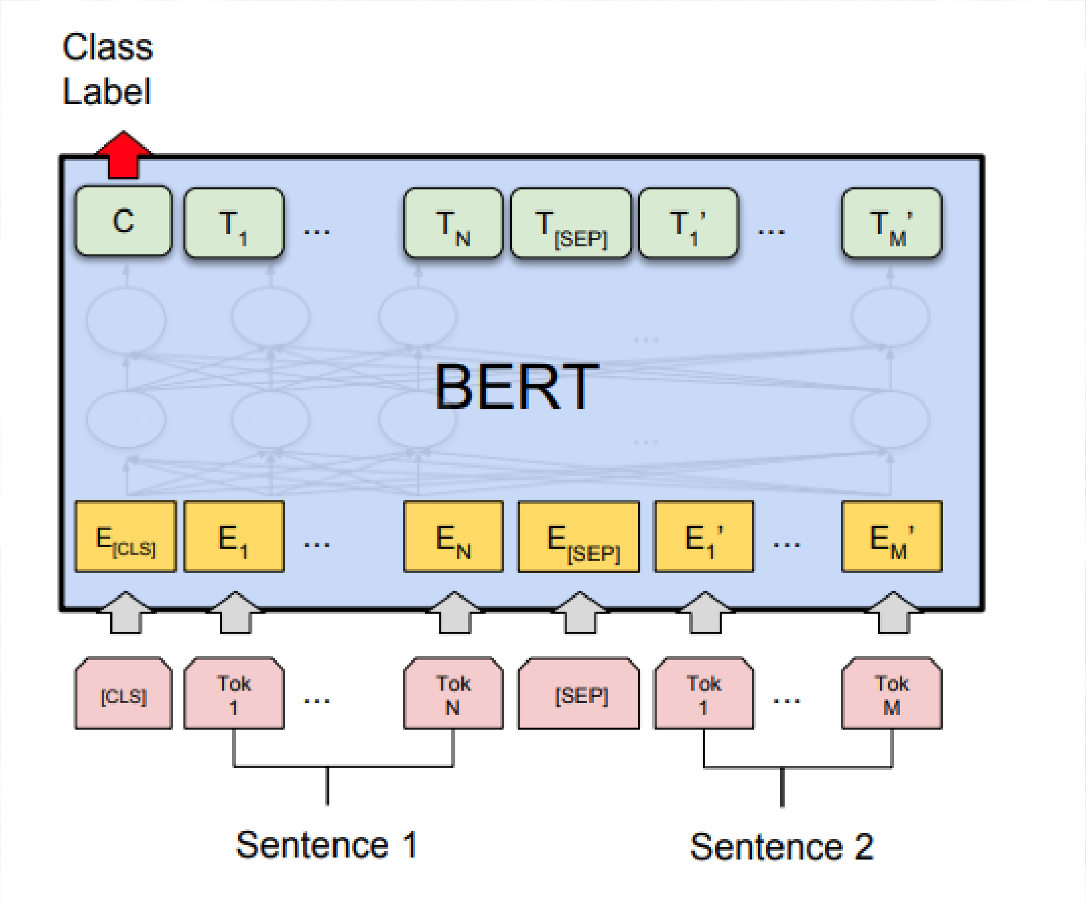
BERT for single sentence classification (Sentiment analysis, Intent Classification, etc.)

BERT (Devlin et al. '18)



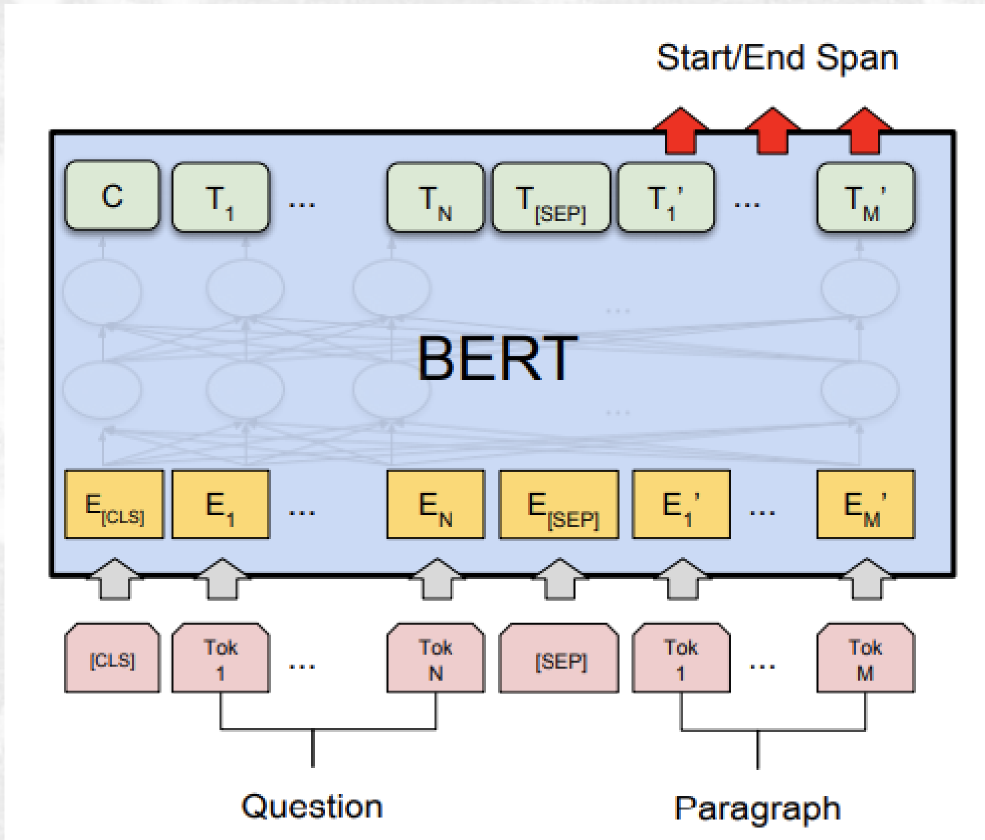
BERT for Sequence Tagging Tasks (e.g., POS tagging, Named Entity Recognition, etc.)

BERT (Devlin et al. '18)



BERT for sentence pairs classification (Paraphrase Identification, answer selection in QA, Recognizing Textual Entailment)

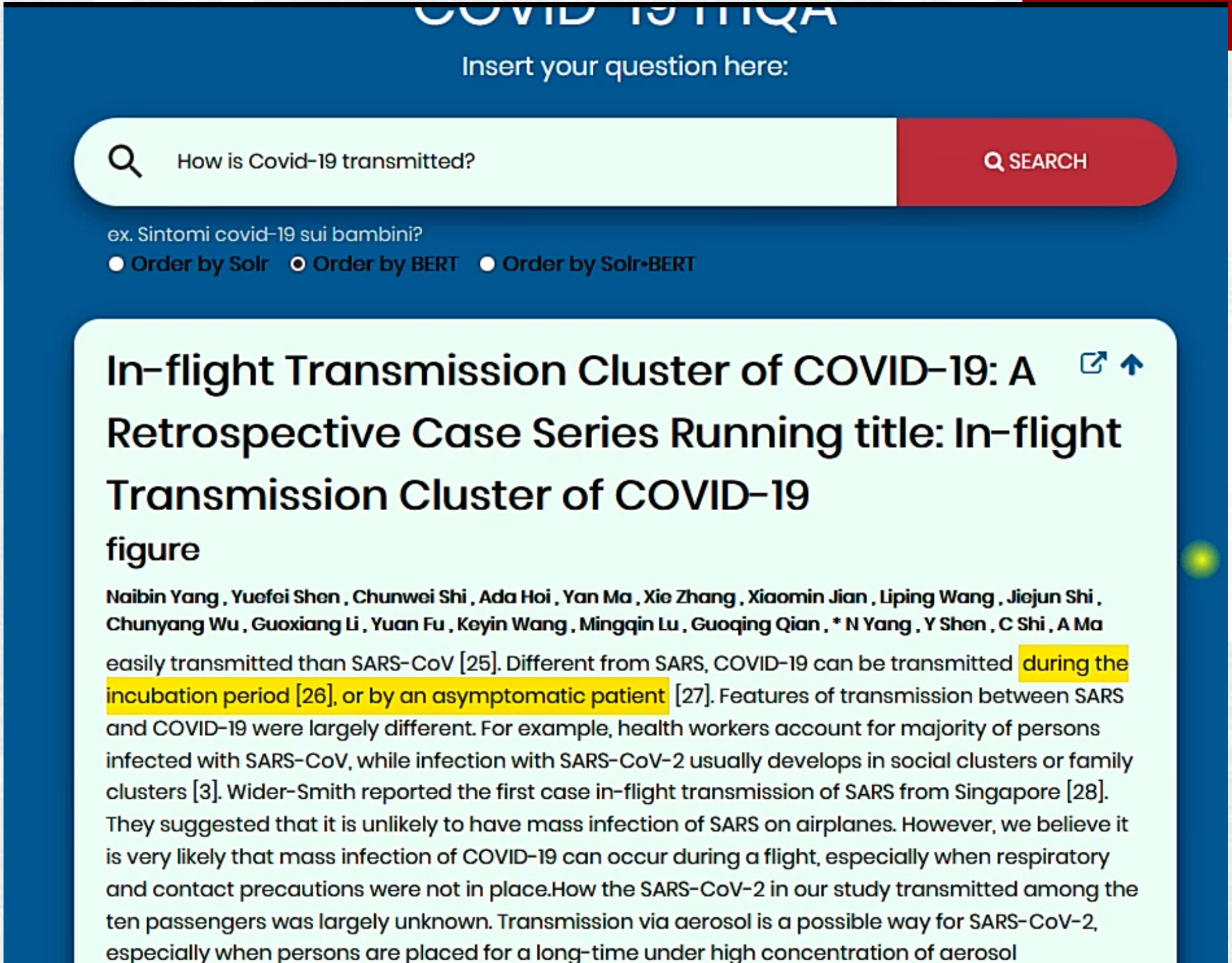
BERT (Devlin et al. '18)



BERT for Answer Span Selection in Question Answering

A QA example on SquAD

- Cross-lingual Question Answering

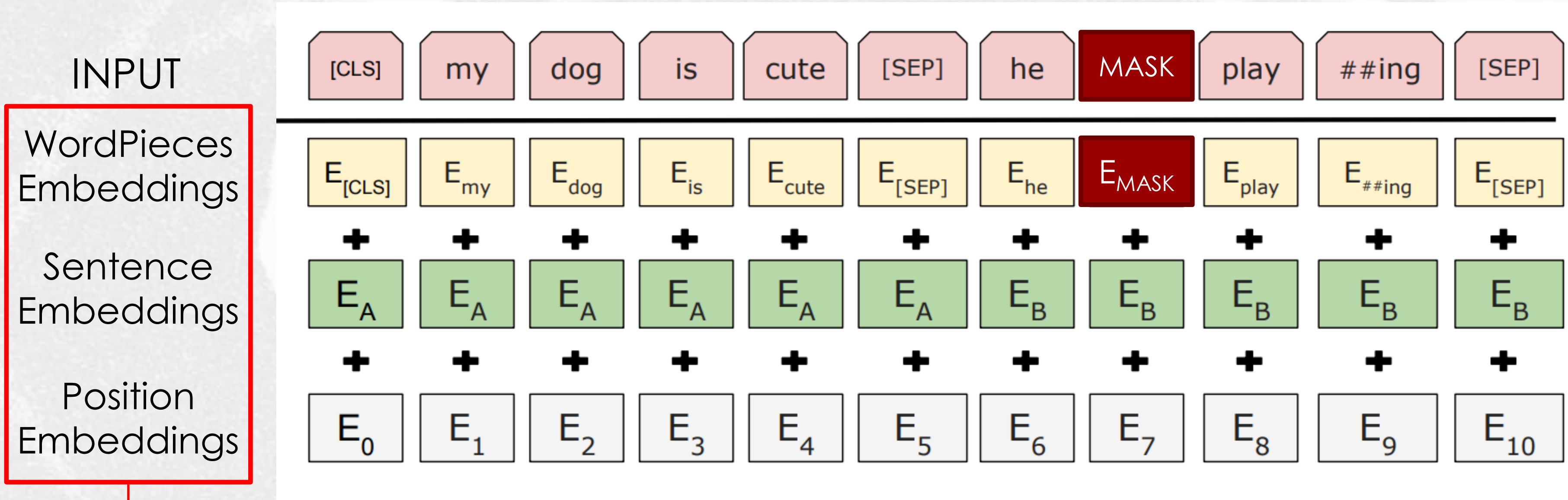


HUGGING FACE

BERT and «sons»

- A wide array of architectures, modeled and pre-trained, draw inspiration from BERT, featuring subtle but impactful variations.
- Selected **Notable Variants**:
  - **RoBERTa**: Streamlines BERT's pre-training approach and leverages an expanded dataset for training.
  - **ELECTRA**: Introduces a unique twist by replacing tokens with similar ones, then focusing on identifying these alterations.
  - **ALBERT**: Implements layer-wise parameter sharing to enhance efficiency.
  - **XLM**: Extends RoBERTa's capabilities across multiple languages.
- **Italian Contributions:**
  - Italy's own spin-offs include Alberto, UMBERTO, and Gilberto, each adding unique flavors to the BERT family.

BERT pretraining:
Input representations



All these embeddings are learned during the (pre)training process

In pre-training 15% of the input tokens are masked for the masked LM task

A complex application of LSTM (and recently Transformers): Image captioning

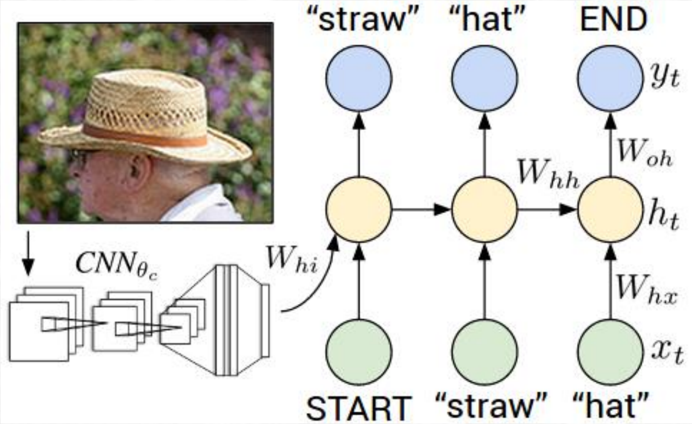
A woman is throwing a frisbee in a park.

A dog is standing on a hardwood floor.

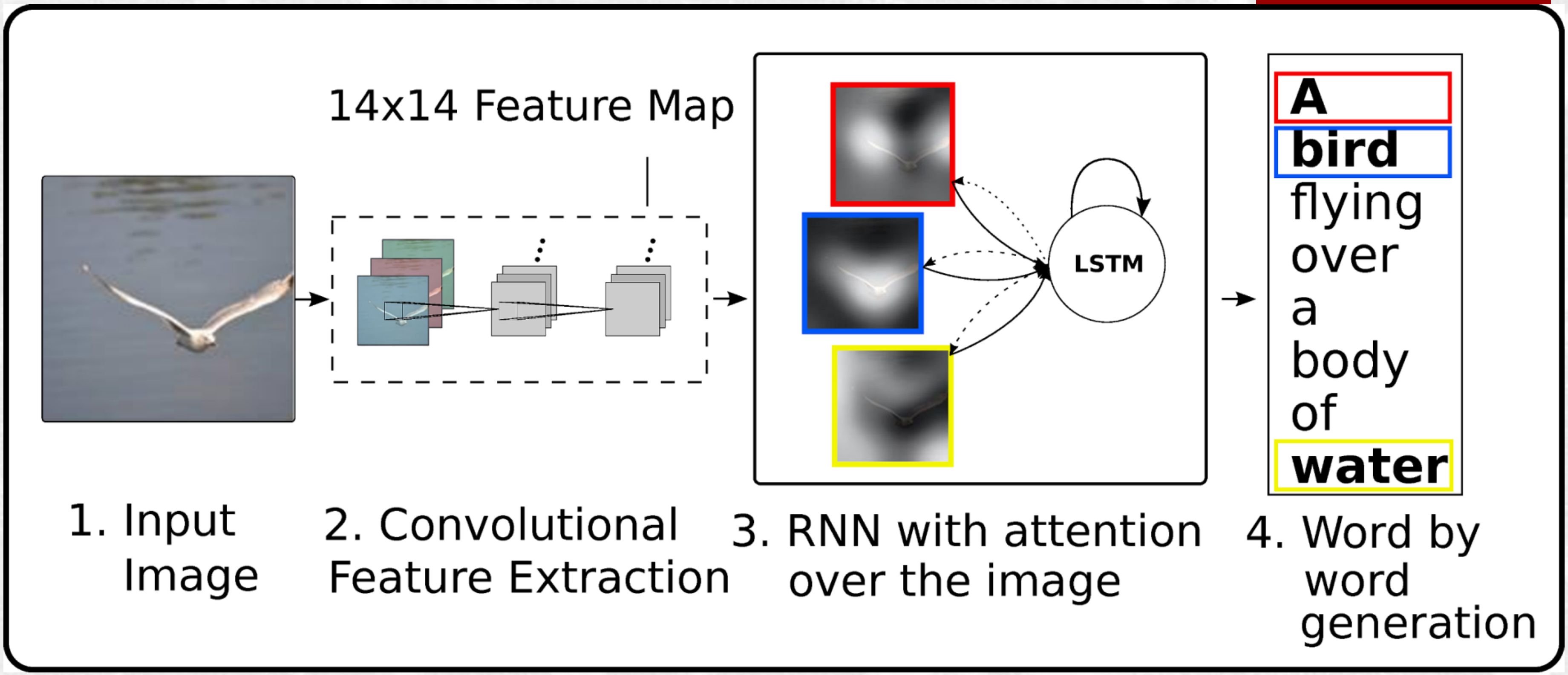
A stop sign is on a road with a mountain in the background.

Image Captioning

- Image to captions
  - Convolutional Neural Network to learn a representation of the image
  - (Bi-directional) Recurrent Neural Network to generate a caption describing the image
    - its input is the representation computed from the CNN
    - its output is a sequence of words, i.e. the caption



"baseball player is throwing ball in game."

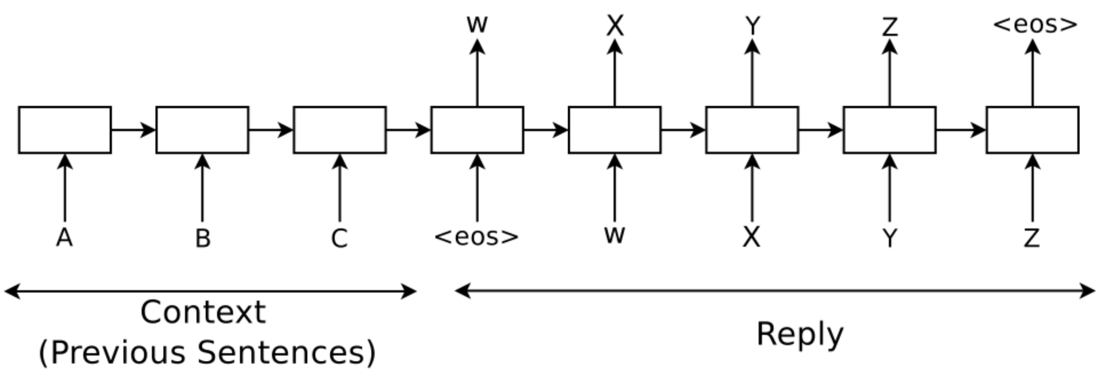

14x14 Feature Map
LSTM
A
bird
flying
over
a
body
of
water
1. Input Image
2. Convolutional Feature Extraction
3. RNN with attention over the image
4. Word by word generation

Attention: a dynamic rendering

Neural Conversation Model

- Learn to answer question in a conversation
- For example, an IT help desk
  - model the input sequence
  - produce a output sequence

Machine: *hi*
Human: *hello*
Machine: *could you please let me know what are the operating systems you are using ?*
Human: *i am using linux*
Machine: *ok it was in the ssl vpn on which you stated it was broken*
Machine: *please check if you are logged in to corp network*
Machine: *what is the error that you are running please*
Human: *i am seeing an error related to vpn*
Machine: *what is the error message that you are getting when connecting to vpn using network connect ?*
Human: *connection refused or something like that*



Transformers

- (Vaswani 2017), Attention is all you need, https://arxiv.org/abs/1706.03762
- (Devlin et al 2018), BERT: Pre-training of Deep Bidirectional Transformers for Language Understanding, https://arxiv.org/abs/1810.04805
- An interesting introduction to the attention mechanism:
  - **All you need to know about 'Attention' and 'Transformers' — In-depth Understanding — Part 1**, A. Sarkar, URL: https://towardsdatascience.com/all-you-need-to-know-about-attention-and-transformers-in-depth-understanding-part-1-552f0b41d021#4c16
- Other Task specific works:
  - Dzmitry Bahdanau, Kyunghyun Cho, and Yoshua Bengio. Neural machine translation by jointly learning to align and translate. CoRR, abs/1409.0473, 2014.
  - Effective Approaches to Attention-based Neural Machine Translation, Minh-Thang Luong Hieu Pham Christopher D. Manning, 2015, https://arxiv.org/abs/1508.04025v5
  - Yoon Kim, Carl Denton, Luong Hoang, and Alexander M. Rush. Structured attention networks. In International Conference on Learning Representations, 2017.