From Recurrent Neural Networks to Transformers

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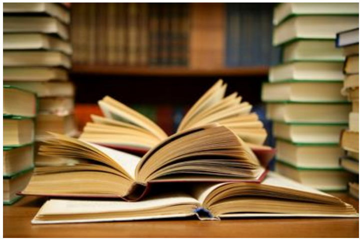
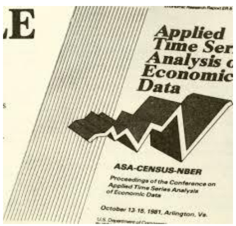
Dealing with sequential data

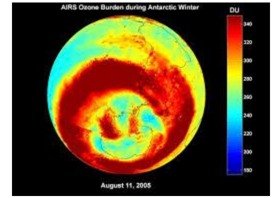


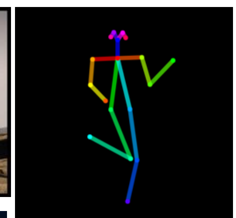


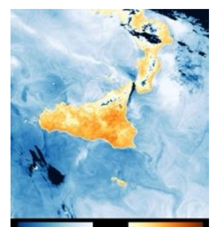
Text

Audio

IoT



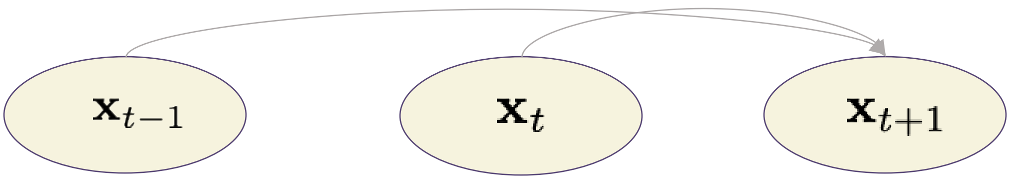




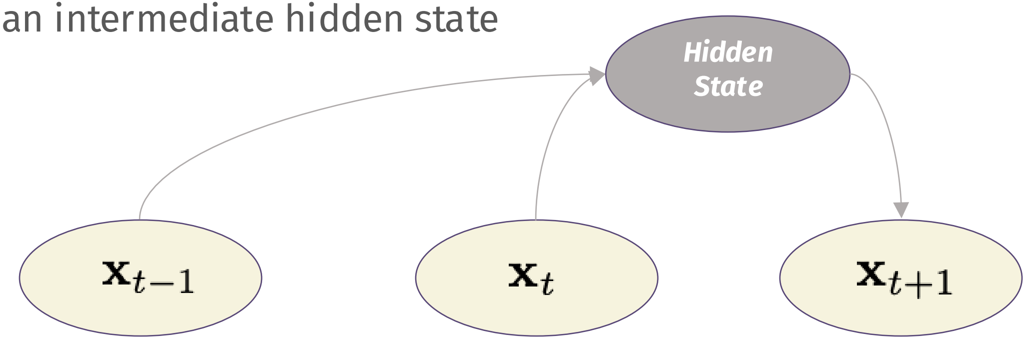
Sequences of
visual data

Dealing with sequences: a first summary

- Autoregressive models



- “Using” an intermediate hidden state



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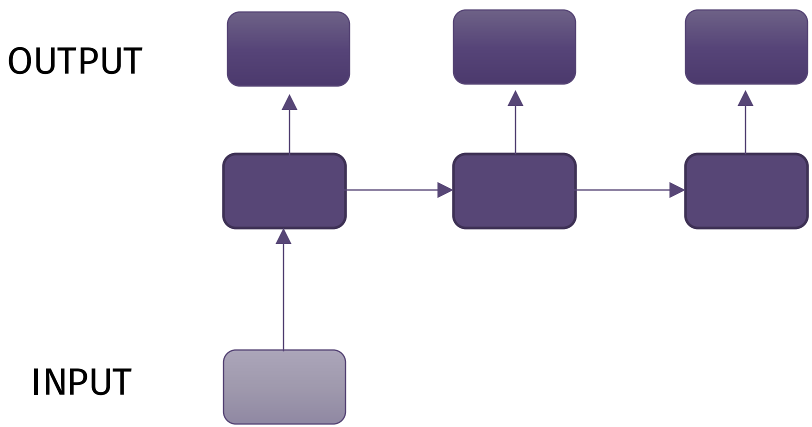
Different formulations of the problem

One-to-may: the input is in a standard format (not a sequence!), the output is a sequence

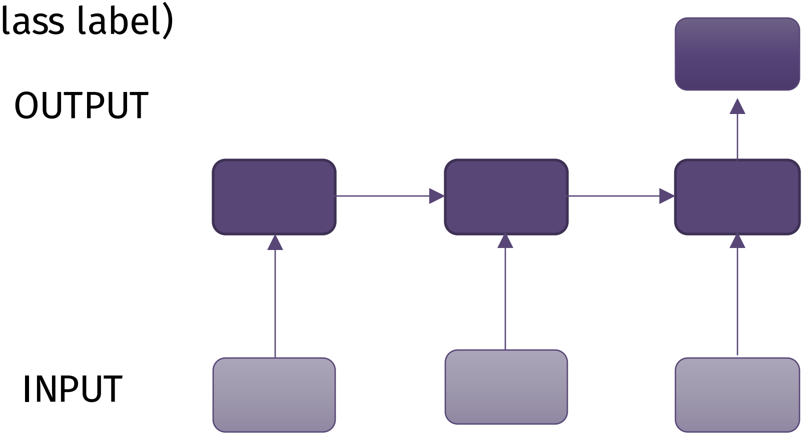
Example of applications: image captioning (input: image, output: text describing the image content)



Different formulations of the problem

Many-to-one: the input is a sequence, the output is a fixed-size vector (not a sequence!)

Example of applications: sentiment analysis (input: text, output: class label)



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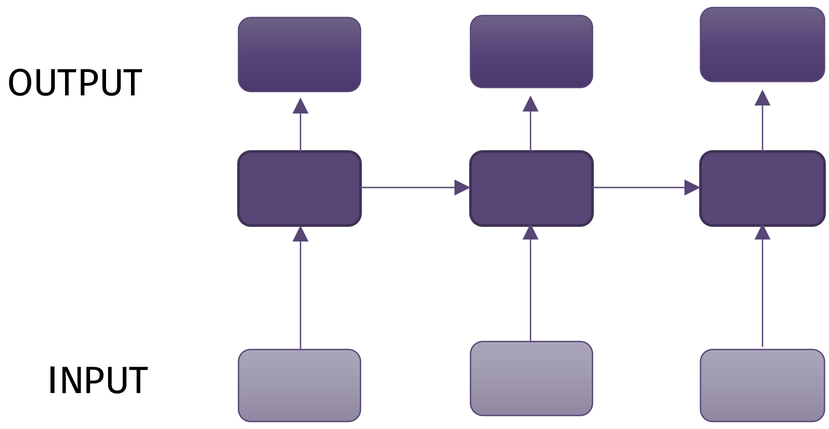
Different formulations of the problem

Direct Many-to-many: input and output are both sequences

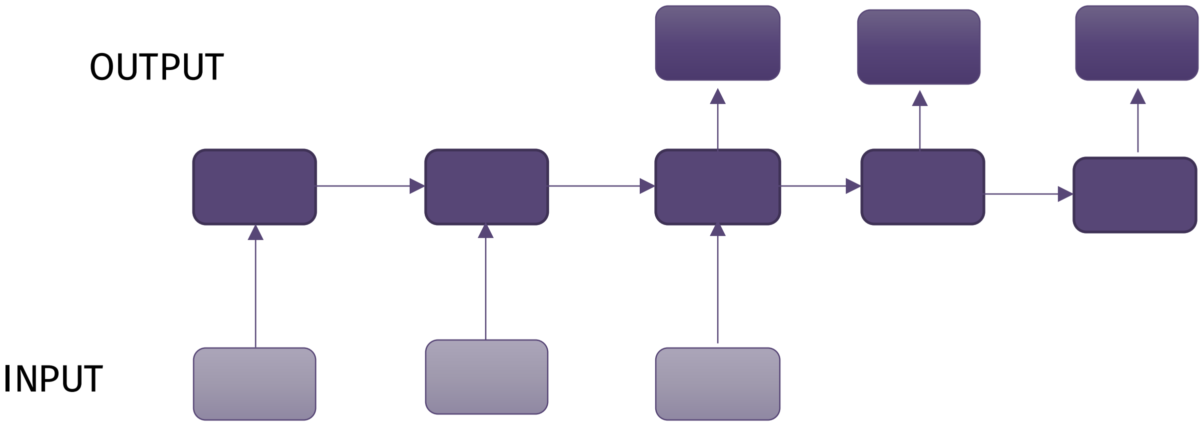
<u>Example of applications</u>: video captioning (input is a sequence of images, output is text)



Different formulations of the problem

Delayed Many-to-many: input and output are both sequences

Example of applications: language translation (input is a text, output is a text)



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Text data

- ML can not (directly) handle text data... we need a numerical descriptor
- Word embeddings can do the job

Vocabulary

my this I walk taking a the since am dog

Indexing

a → 0
am → 1
dog → 2
...
walk → N

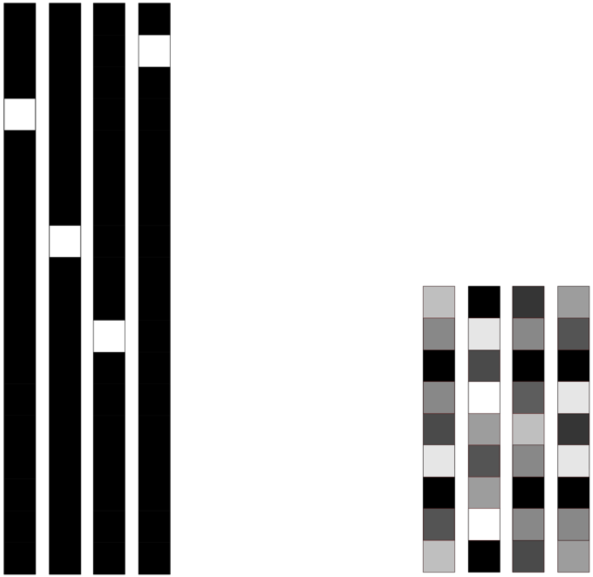
Embeddings

A = [1000...0]
Am = [0100...0]
dog = [0010...0]
Walk = [0000...1]

happy sad	*walk run*
dog cat	*day night*

No guarantee that words with similar meanings have descriptions close to each other in the embedding space...

One-hot encoding vs word embeddings



One-hot encoding:
- *Very sparse*
- *High dimensional*
- *Hard-coded*

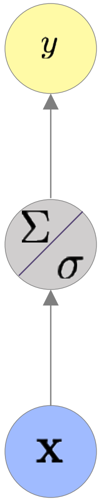
Word embeddings:
- *Dense*
- *Lower dimensional*
- *Learned from data*

Dealing with sequences: issues

- Handling sequences of **different lengths**
- Taking into account **short** and **long term** dependences
- Considering **order** between elements

Recurrent Neural Networks

Modelling sequences



Standard
one-to-one
vanilla
network

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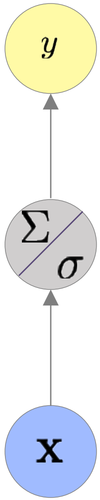
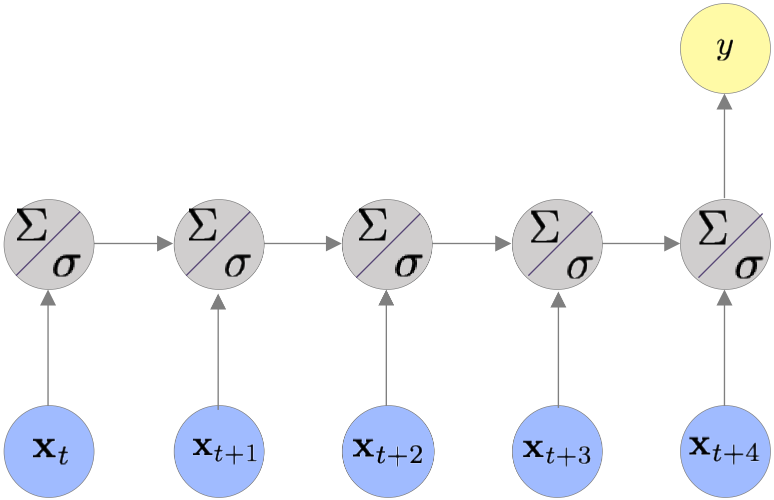


Standard one-to-one vanilla network



Adding recurrence over time

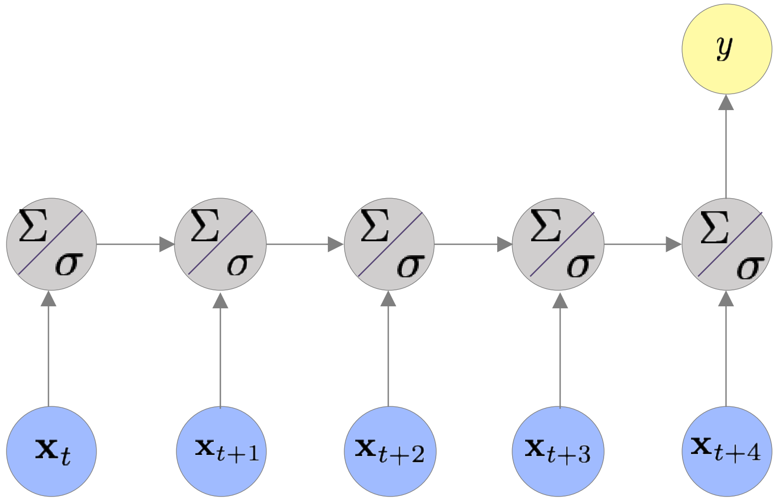
Recurrent Neural Networks (1986)

- Recurrence adds memory to the NN

- It also provides a way to model causal relationships between observations: the decision a recurrent net reached at time step t-1 affects the decision it will reach at time step t

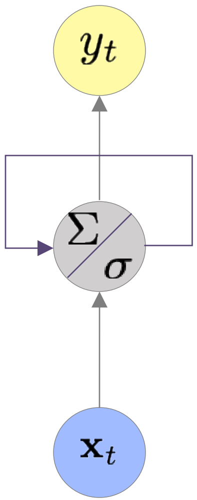
- RNNs have two sources of input: the present and the recent past, which are combined to determine how they respond to new data

Recurrent Neural Networks



Recurrent Neural Networks

The weight matrices are filters that determine ***how much importance to give to both the present input and the past hidden state***



$$\mathbf{x}_t \in \mathbb{R}^m$$

$$y_t \in \mathbb{R}$$

$$\mathbf{h}_t \in \mathbb{R}^p$$

$$\mathbf{h}_t = \sigma(W_h \mathbf{h}_{t-1} + W_x \mathbf{x}_t)$$

$$y_t = \sigma(W_y \mathbf{h}_t)$$

$$W_h \in \mathbb{R}^{p \times p} \qquad W_y \in \mathbb{R}^p$$

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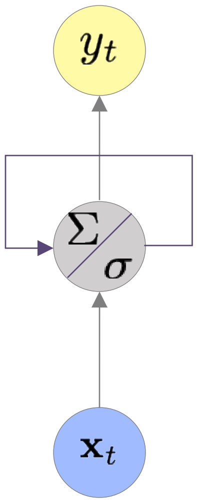

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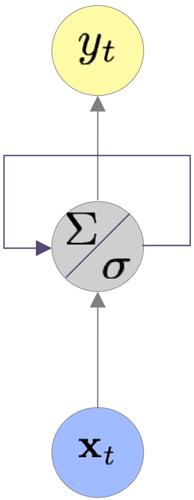

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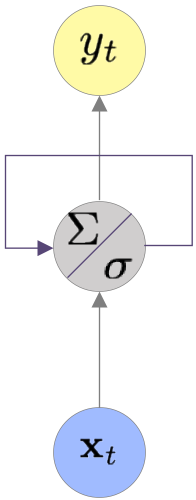

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IMPORTANT: weights do not depend on time → It's a parameter sharing

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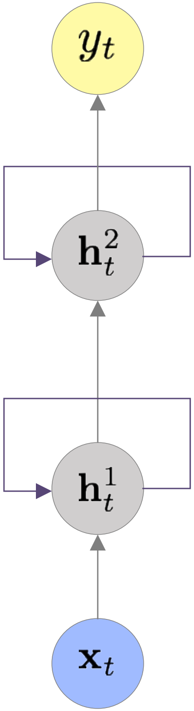
Recurrent Neural Networks

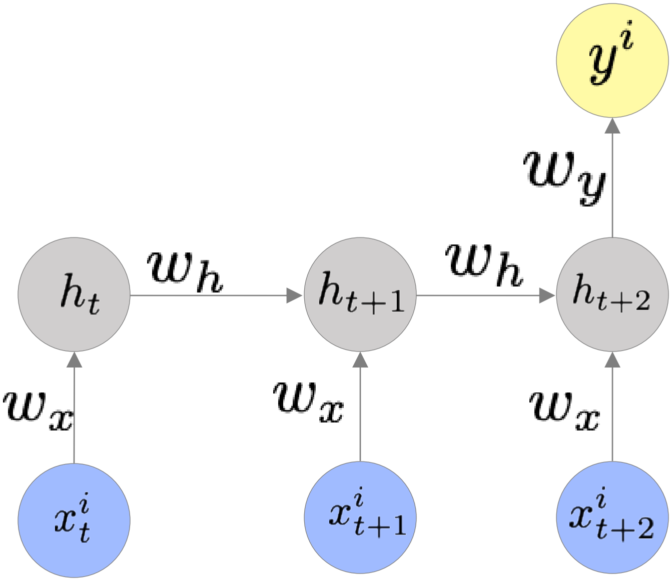
Having multiple hidden layers



$$\mathbf{h}_t^2 = \sigma(W_h^2 \mathbf{h}_{t-1}^2 + W_{12} \mathbf{h}_t^1)$$

$$\mathbf{h}_t^1 = \sigma(W_h^1 \mathbf{h}_{t-1}^1 + W_x \mathbf{x}_t)$$

Backpropagation: an example



$$\hat{y}^i = f_\sigma(w_y h_{t+2})$$

Let's assume everything (input, output, state, weights) is one-dimensional

$$h_{t+2} = f_\sigma(w_h h_{t+1} + w_x x_{t+2}^i)$$

$$h_{t+1} = f_\sigma(w_h h_t + w_x x_{t+1}^i)$$

$$h_t = f_\sigma(w_h h_{t-1} + w_x x_t^i)$$

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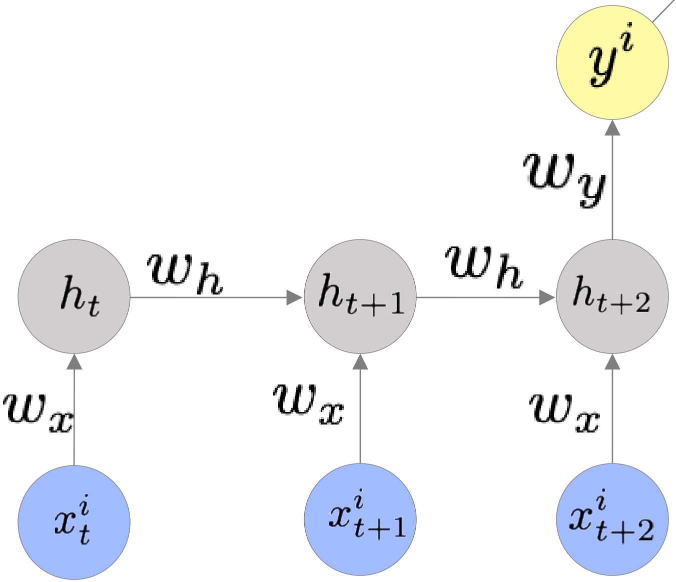
Backpropagation: an example

$$\boxed{J(S;\mathbf{w}) = \frac{1}{n}\sum_{i=1}^{n}(y^i - \hat{y}^i)^2}$$



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Let's consider the cost related to a single sample

$$J^i(\mathbf{w}) = (y^i - \hat{y}^i)^2$$

Backpropagation: an example

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$$J^i(\mathbf{w}) = (y^i - \hat{y}^i)^2$$

We want to estimate the partial derivative with respect a specific weight in the network

$$\frac{\partial J^i(\mathbf{w})}{\partial w_x}$$

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Backpropagation: an example

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Backpropagation: an example

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$$\frac{\partial J^i(\mathbf{w})}{\partial w_x} = \frac{\partial J^i(\mathbf{w})}{\partial \hat{y}^i}\frac{\partial \hat{y}^i}{\partial h_{t+2}}\sum_{k=t}^{t+2}\left(\frac{\partial h_{t+2}}{\partial h_k}\frac{\partial h_k}{\partial w_x}\right)$$

Backpropagation: an example

$$\frac{\partial J^i(\mathbf{w})}{\partial w_x} = \frac{\partial J^i(\mathbf{w})}{\partial \hat{y}^i} \frac{\partial \hat{y}^i}{\partial h_{t+2}} \sum_{k=t}^{t+2} (\frac{\partial h_{t+2}}{\partial h_k} \frac{\partial h_k}{\partial w_x})$$

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$$\frac{\partial h_{t+2}}{\partial h_k} = \prod_{j=k+1}^{t+2} \frac{\partial h_j}{\partial h_{j-1}}$$

Backpropagation: an example

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$$\frac{\partial h_{t+2}}{\partial h_k} = \prod_{j=k+1}^{t+2} \frac{\partial h_j}{\partial h_{j-1}}$$

- How to incorporate the contributions from all samples in the training set?
- What if multiple hidden layers are present?
- What if the output is a sequence?

Gradients-related issues for long-term dependences

- The computation of the loss gradient as successive multiplication leads to instability of the gradient and may take very long training times

- Many values < 1 lead to **vanishing** gradient problems

- Many values > 1 lead to **exploding** gradient problems

Exploding gradient

- Many values > 1 lead to **exploding** gradient problems: the update with SGD is done with very large steps, leading to bad results

- A possible solution is gradient clipping: if the gradient is greater than some threshold, scale it down before applying SGD update

- You make a step in the same direction but with a smaller step

Vanishing gradient

- Many values < 1 lead to **vanishing** gradient problems: gradient signal far over time is lost because it's much smaller than gradient signal from closer times

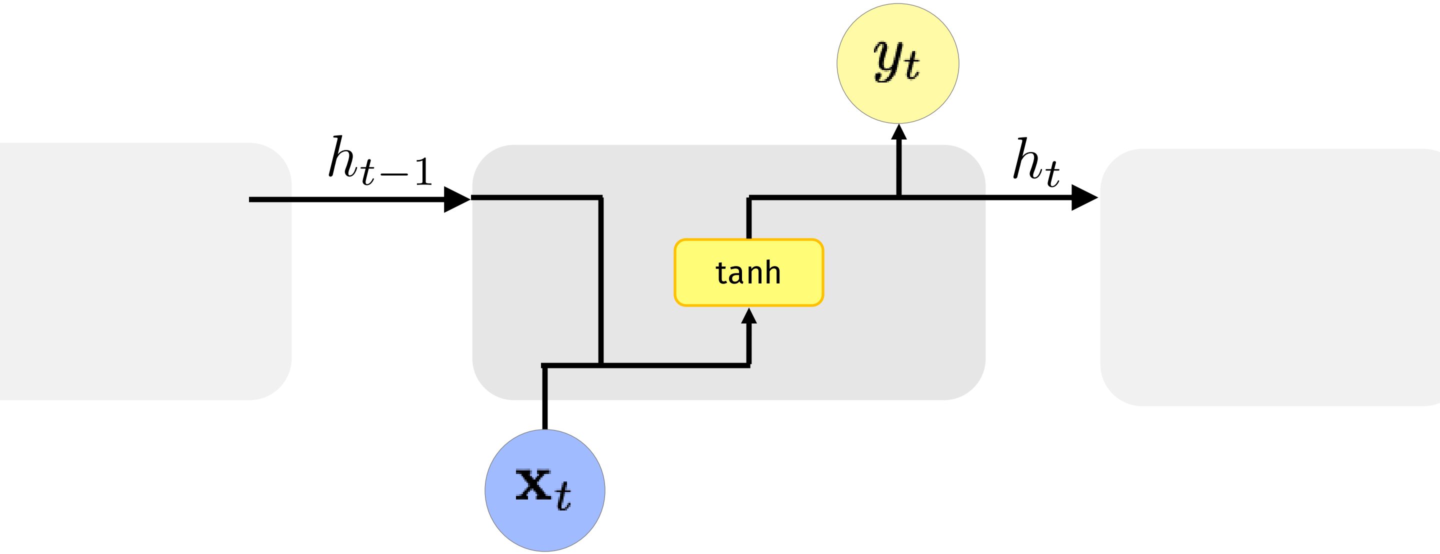
- Model weights are updated only with respect to near effects, not long-term effects

- A possible solution to learn long-term dependences in the data is to use **gated cells**

Long-Short Term Memory

RNNs cells

In standard RNNs, the cells contain a simple computation and their state is constantly re-written



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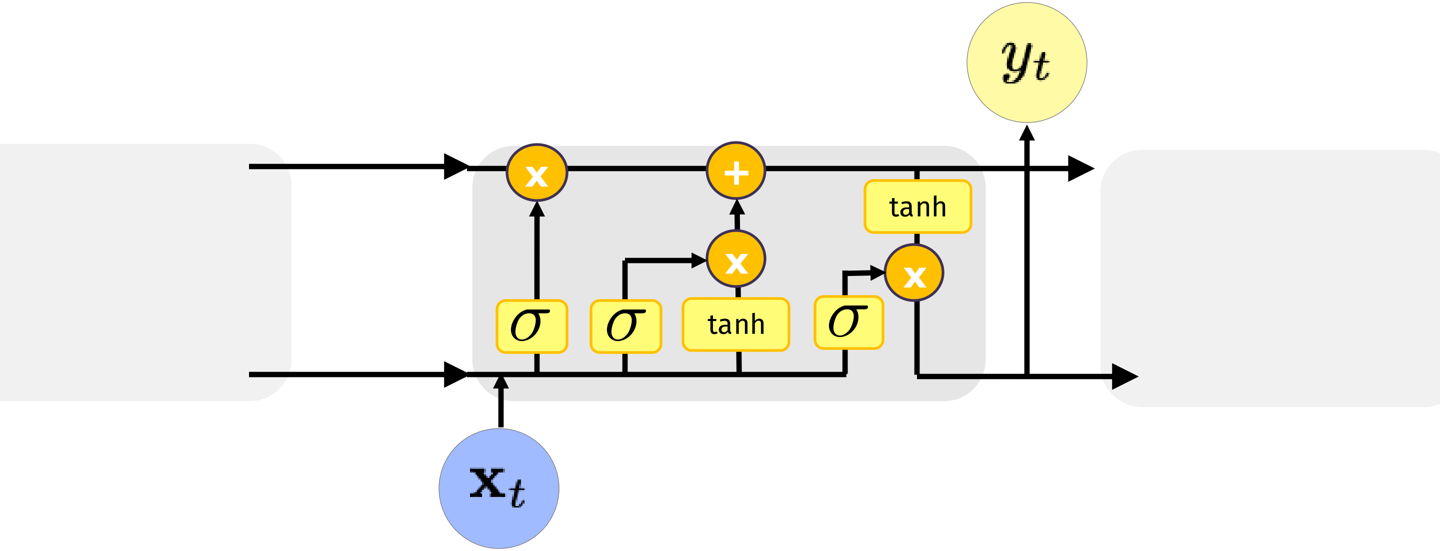
Gated cells

Gated cells contain computational blocks that control information flow



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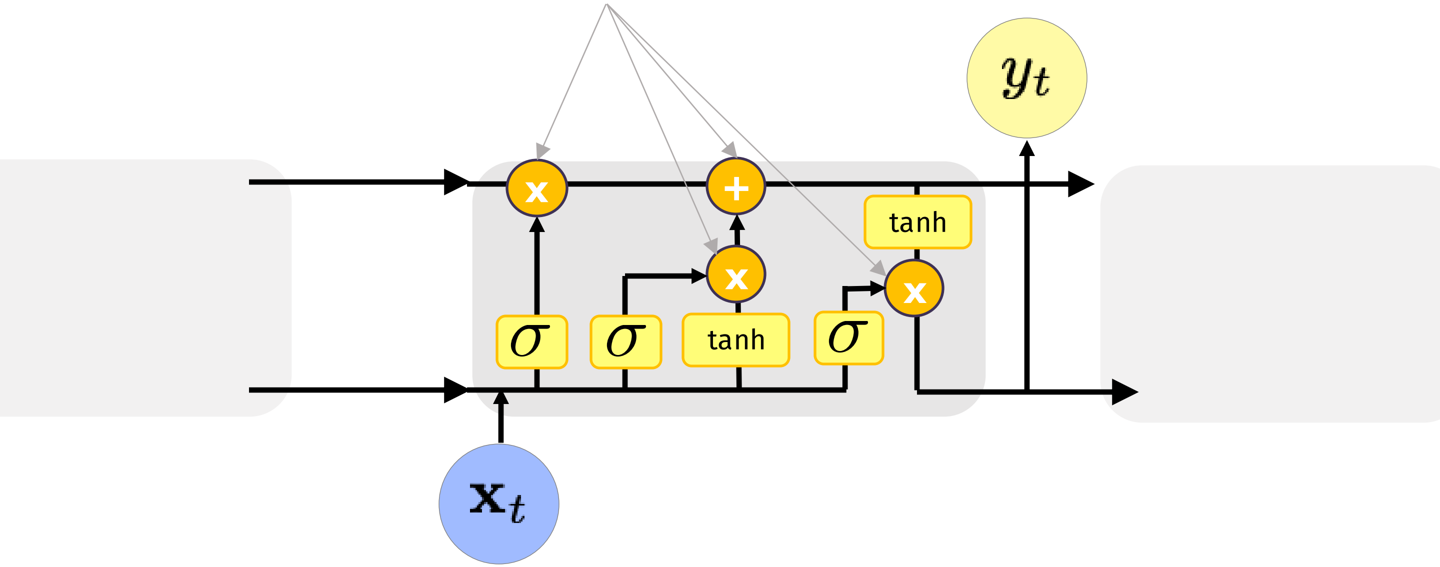


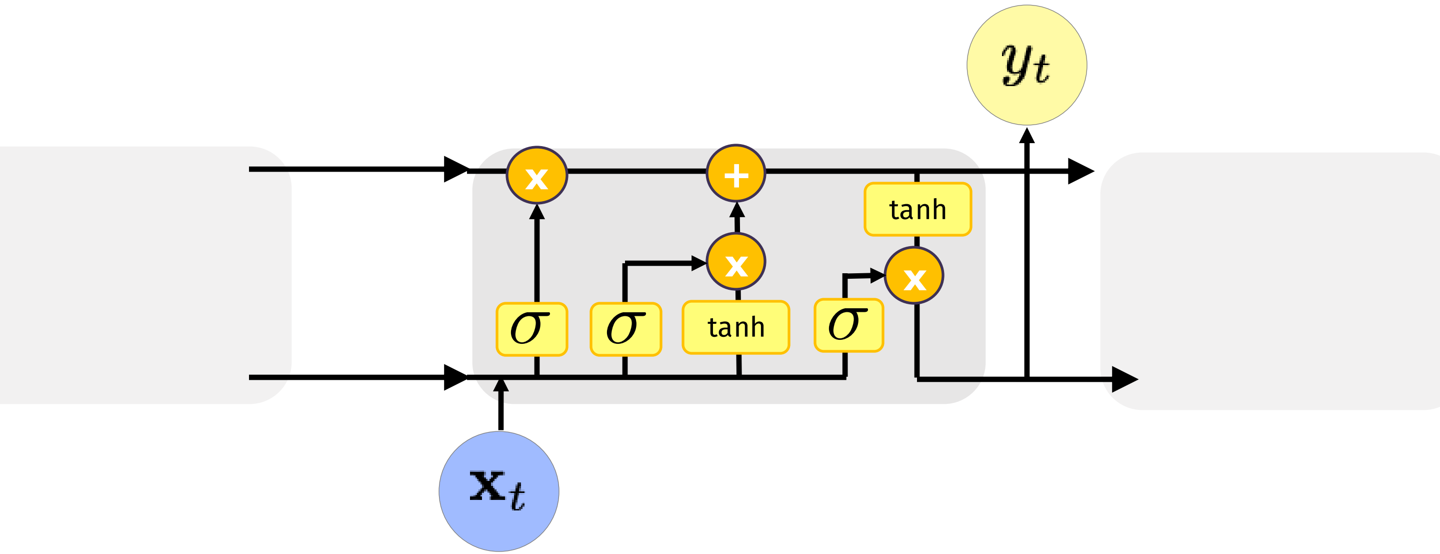
Long-short term memory (LSTM, 1997)

- They consider **connection weights that may change at each time step**
- Information is accumulated over a long duration
- Once the information has been used, it may be useful for the layer to forget the old state or keep the information
- The LSTM learns how to decide when to do that (this is in fact the role of gated units)

LSTM cell

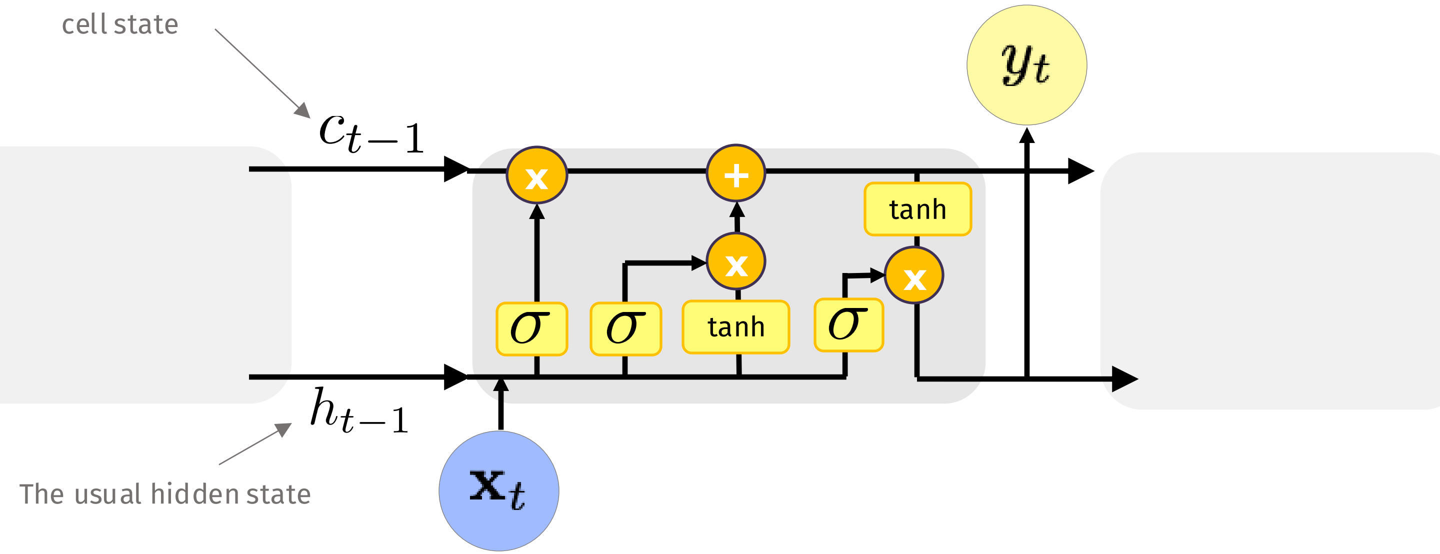
- It includes two states: a **hidden state** and a **cell state**, both vectors of length n
- The cell stores long-term information. The LSTM can **erase**, **write** and **read** information from the cell
- The selection of which information is erased/written/read is controlled by three corresponding **gates**, vectors again of length n
- Each element of the gates can be open (1), closed (0), or somewhere in-between
- The gates are dynamic: their value is computed based on the current context

LSTM cell: phases of the work



LSTM cell: phases of the work

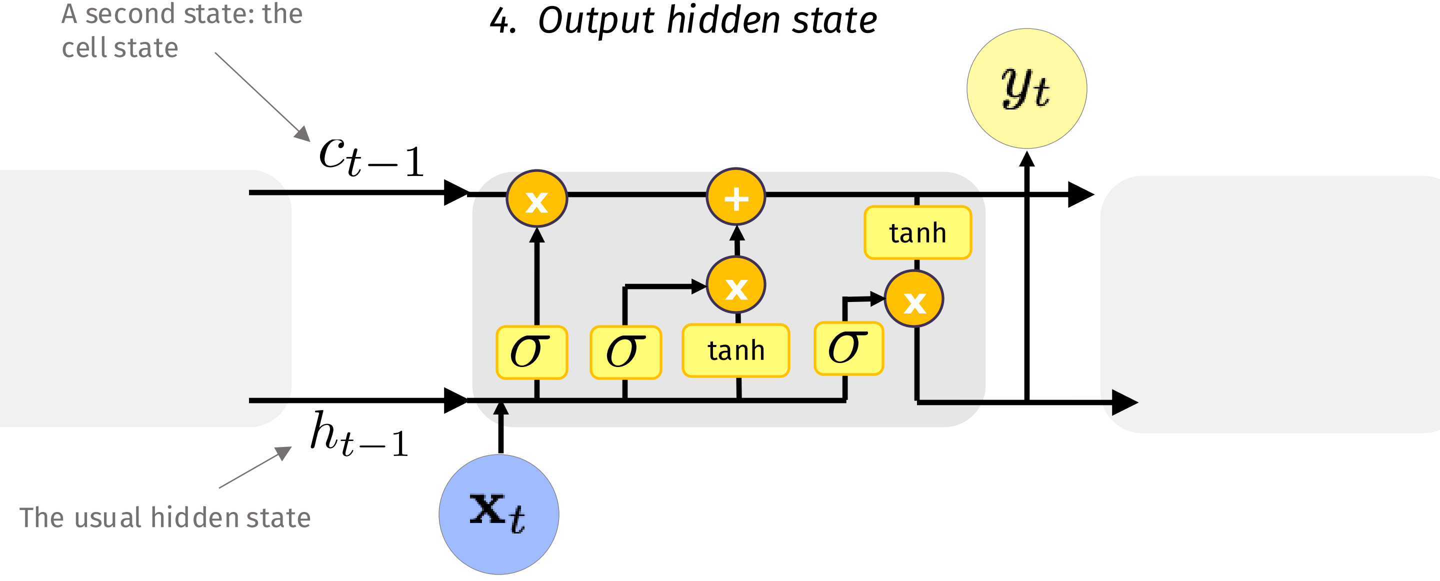
A second state: the
cell state



The usual hidden state

LSTM cell: phases of the work

1. *Forget*
2. *Store input*
3. *Update cell state*
4. *Output hidden state*



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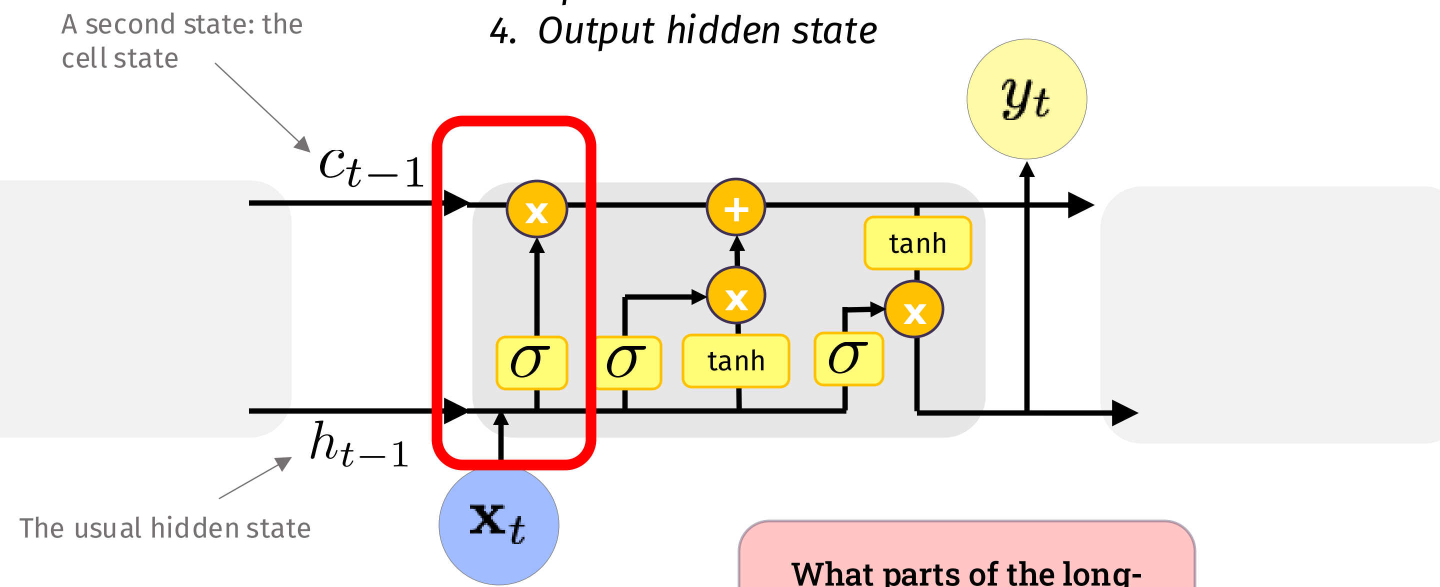

What parts of the long-term memory can now be forgotten?

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LSTM cell: phases of the work

1. *Forget*
2. ***Store input***
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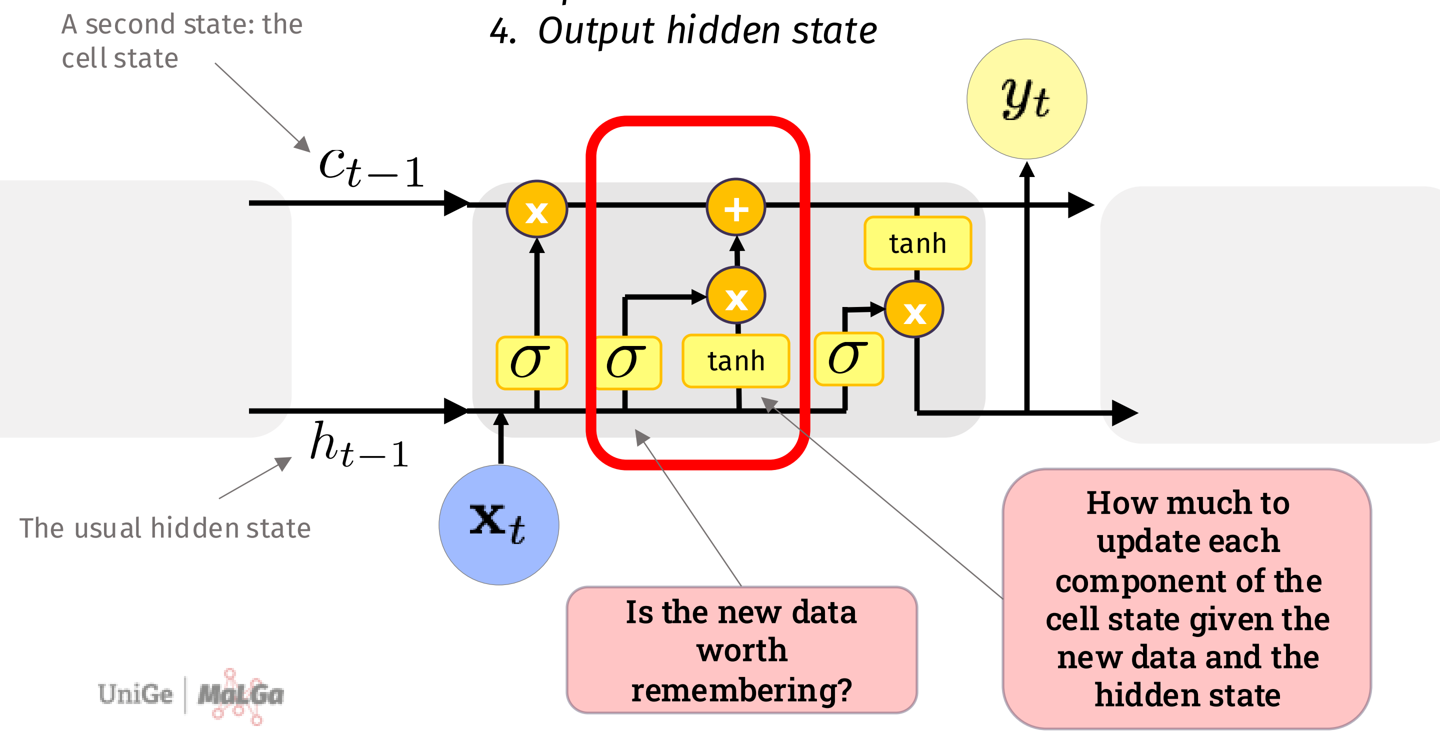

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1. *Forget*
2. *Store input*
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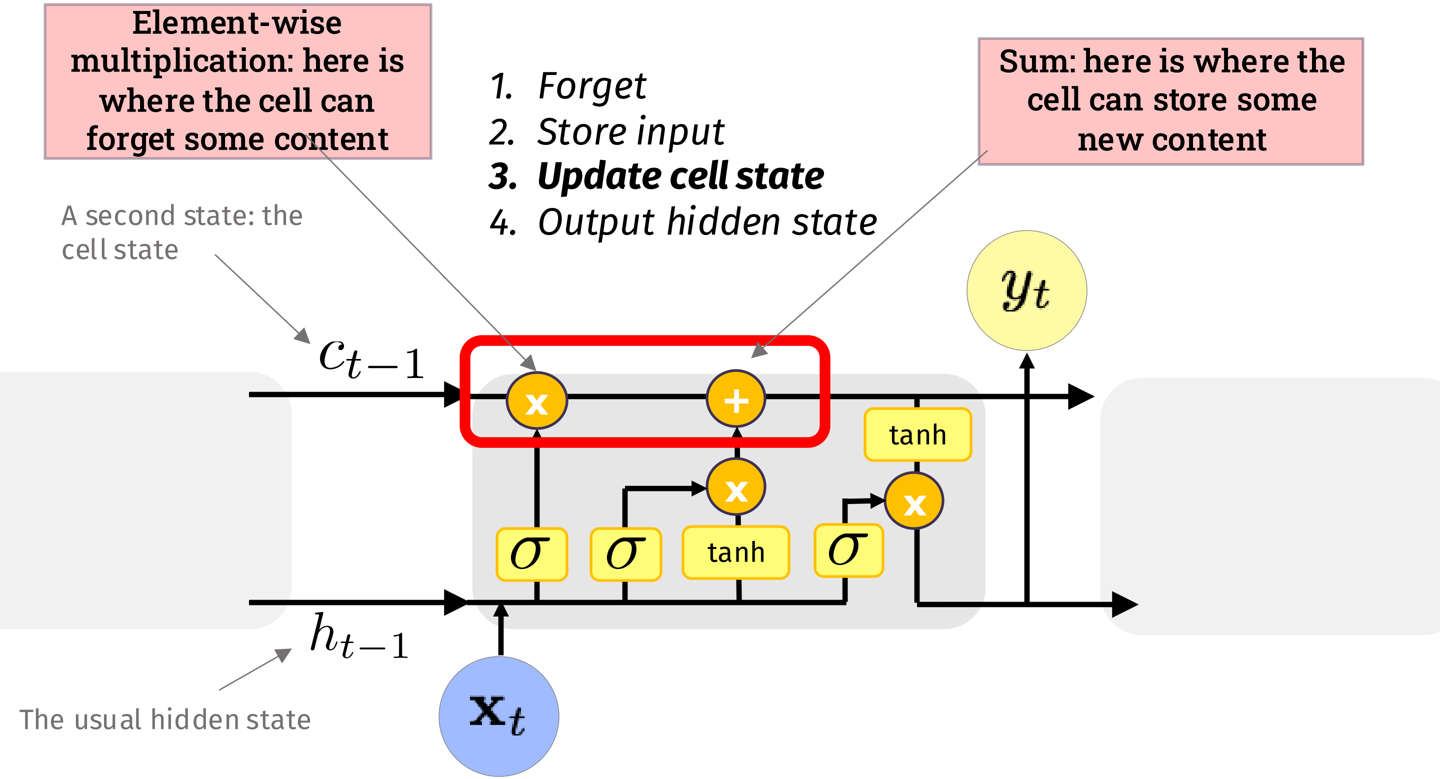
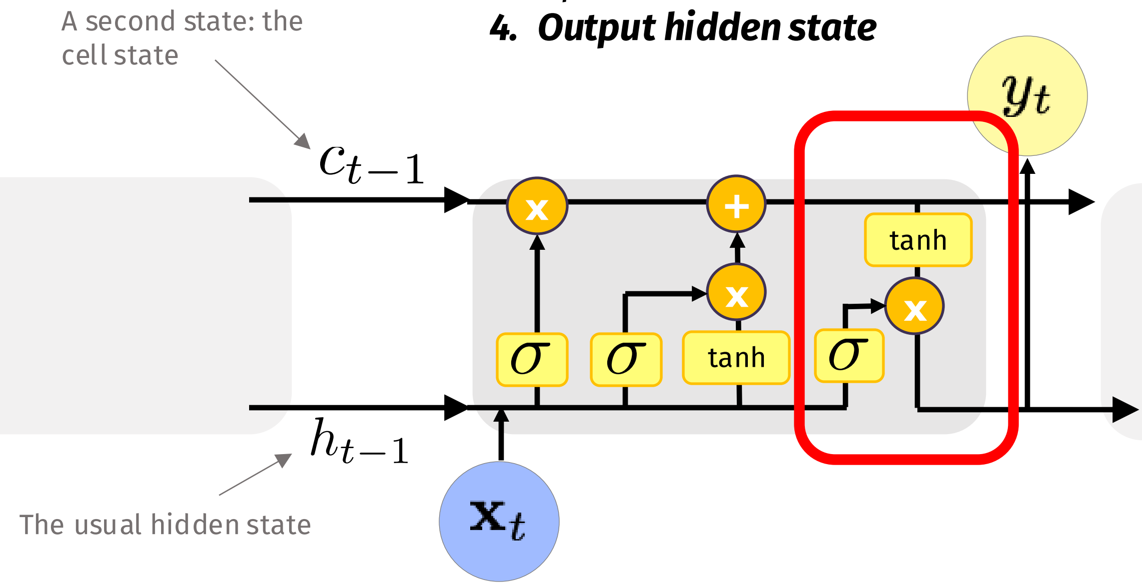
4. *Output hidden state*



The cell state values are selectively updated

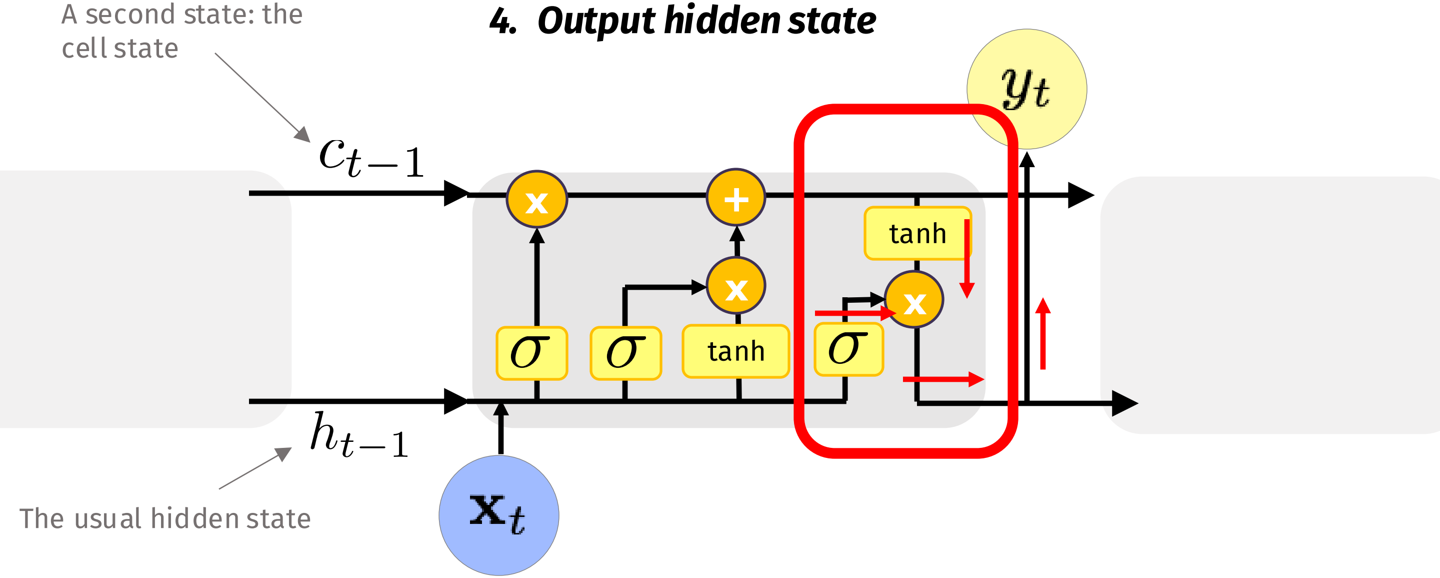
LSTM cell: phases of the work

1. *Forget*
2. *Store input*
3. *Update cell state*
4. ***Output hidden state***



LSTM cell: phases of the work

1. *Forget*
2. *Store input*
3. *Update cell state*
4. ***Output hidden state***



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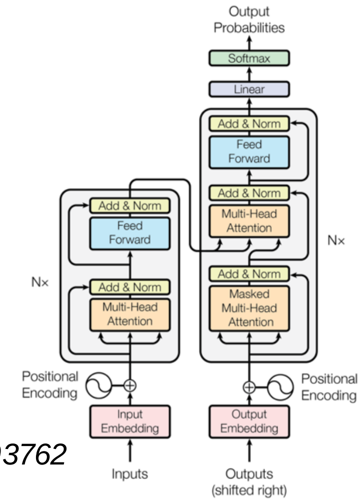
Variations on the theme and recent advances

GRU (Gated Recurrent Unit)

- It includes only the hidden state
- It also has two gates:
    - Update gate: it decides what information to keep and what to throw away
    - Reset gate: it decides how much past information to forget

Transformers

- It includes an attention mechanism that decides at each step which other part of a certain sequence is important



https://arxiv.org/abs/1706.03762

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Self-attention and Transformers

Transformer (2017)

Originally proposed for language translation, they can be highly parallelized

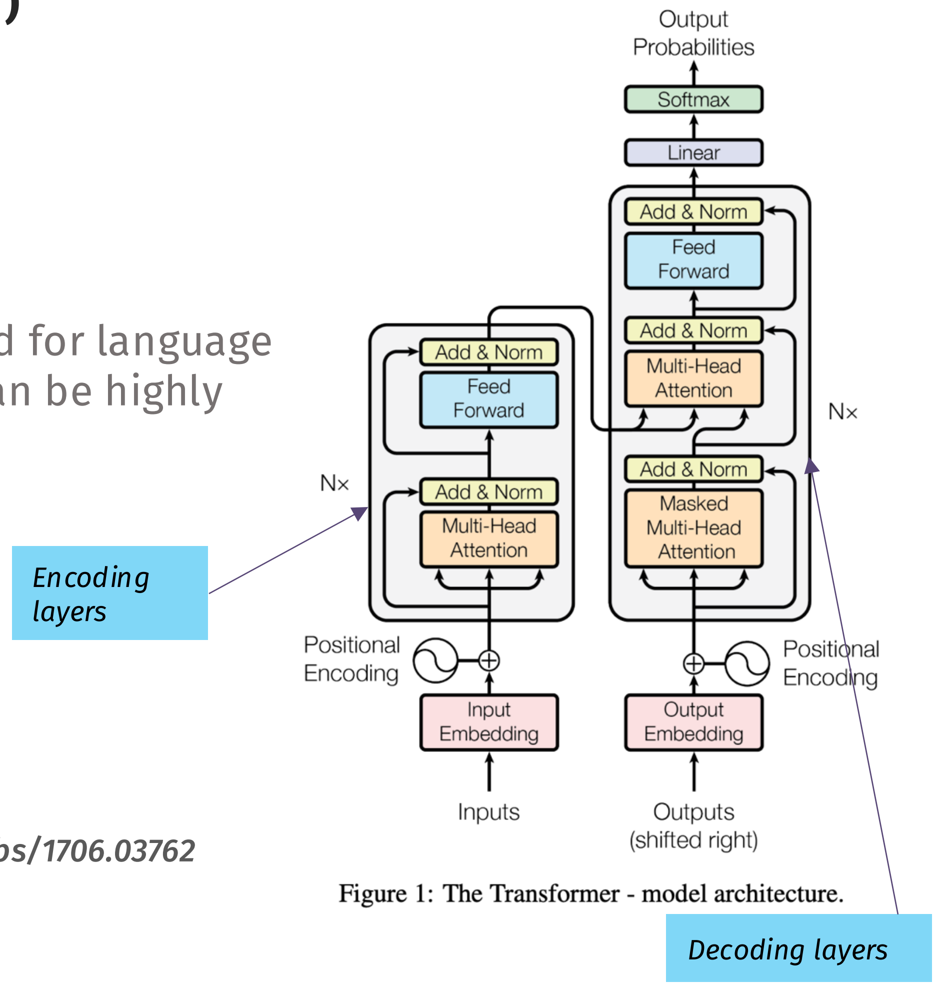

Figure 1: The Transformer - model architecture.

From https://arxiv.org/abs/1706.03762

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Transformer

- As other models for sequence transduction (e.g. language translation), they are based on an encoder-decoder structure

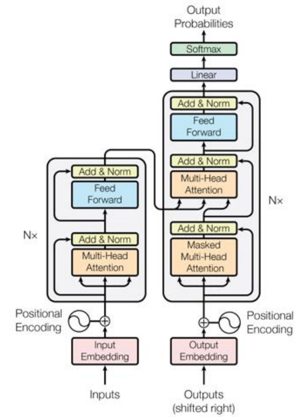


Figure 1: The Transformer - model architecture.

$$(x_1, \ldots, x_n)$$

Input sequence

ENCODING

$$\mathbf{z} = (z_1, \ldots, z_n)$$

Sequence of representations

DECODING

$$(y_1, \ldots, y_n)$$

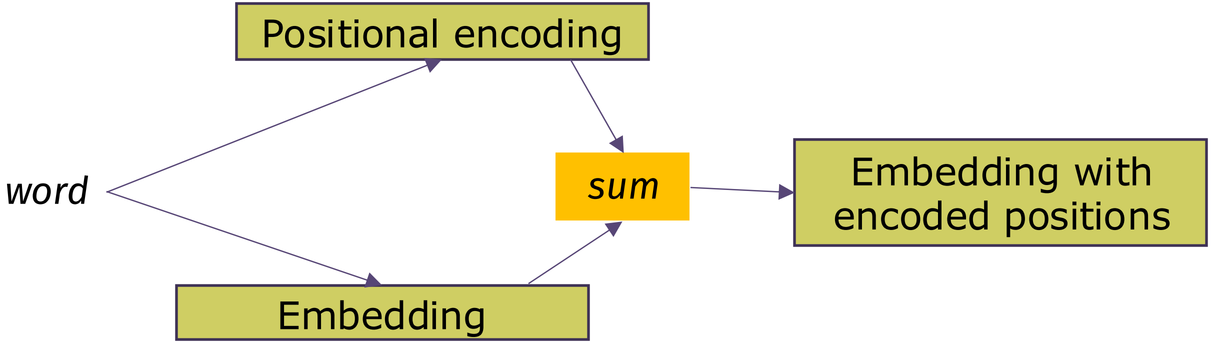
Output, generated one element at a time

[input] tokens

At each time step the model is auto-regressive, as the previously generated symbols are used as additional output in the decoder

What about the position of the words in the sequence?

- We need to «guide» the network to see the words in the correct order
- This is done by means of positional encoding



Transformer: main structure

A stack of N identical layers each one composed by multi-head self-attention and a fully connected net

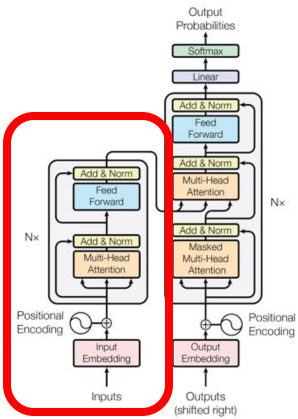
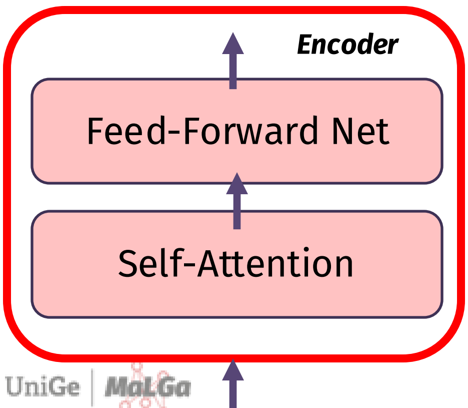


Figure 1: The Transformer - model architecture.



Transformer: main structure

A stack of N identical layers each one composed by multi-head self-attention and a fully connected net

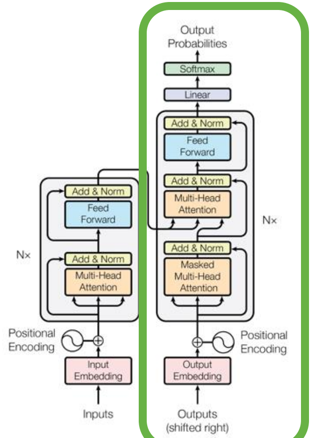
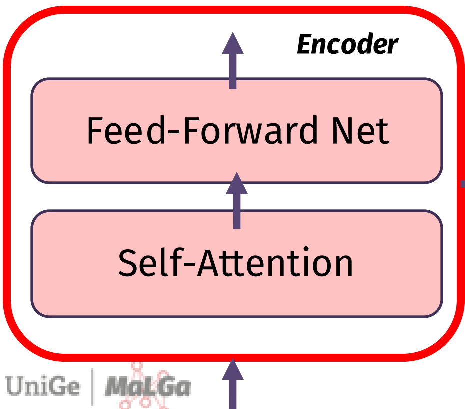
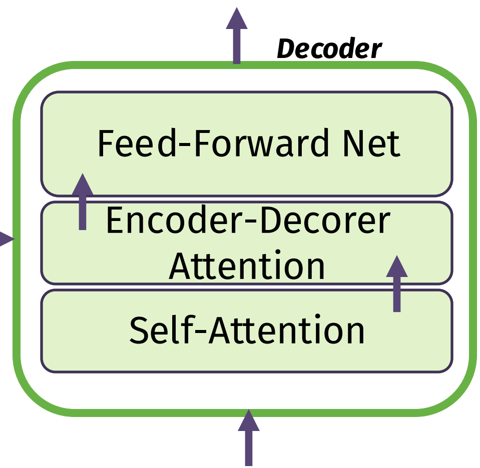


Figure 1: The Transformer - model architecture.

A stack of N identical layers each one composed by masked multi-head self-attention, multi-head self-attention, and a fully connected net





Transformer: main structure

A stack of N identical layers each one composed by multi-head self-attention and a fully connected net

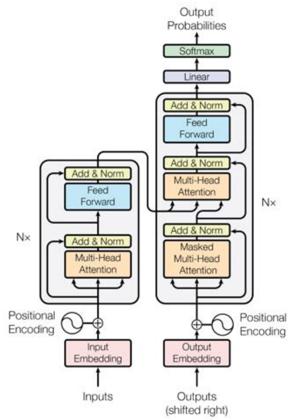


Figure 1: The Transformer - model architecture.

A stack of N identical layers each one composed by masked multi-head self-attention, multi-head self-attention, and a fully connected net

<u>RESIDUAL CONNECTION</u>: the output of each layer is

$$\sigma(x + f(x))$$

Where x is the input to the layer, while f(x) is the function implemented by the layer itself

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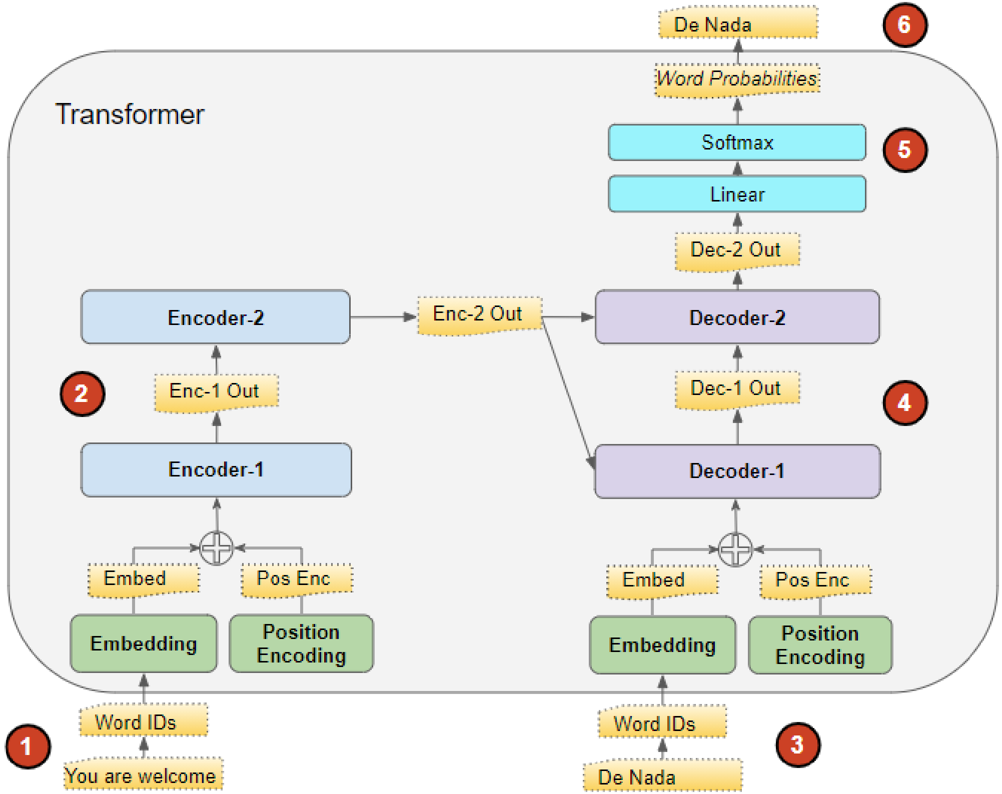
What is self-attention?

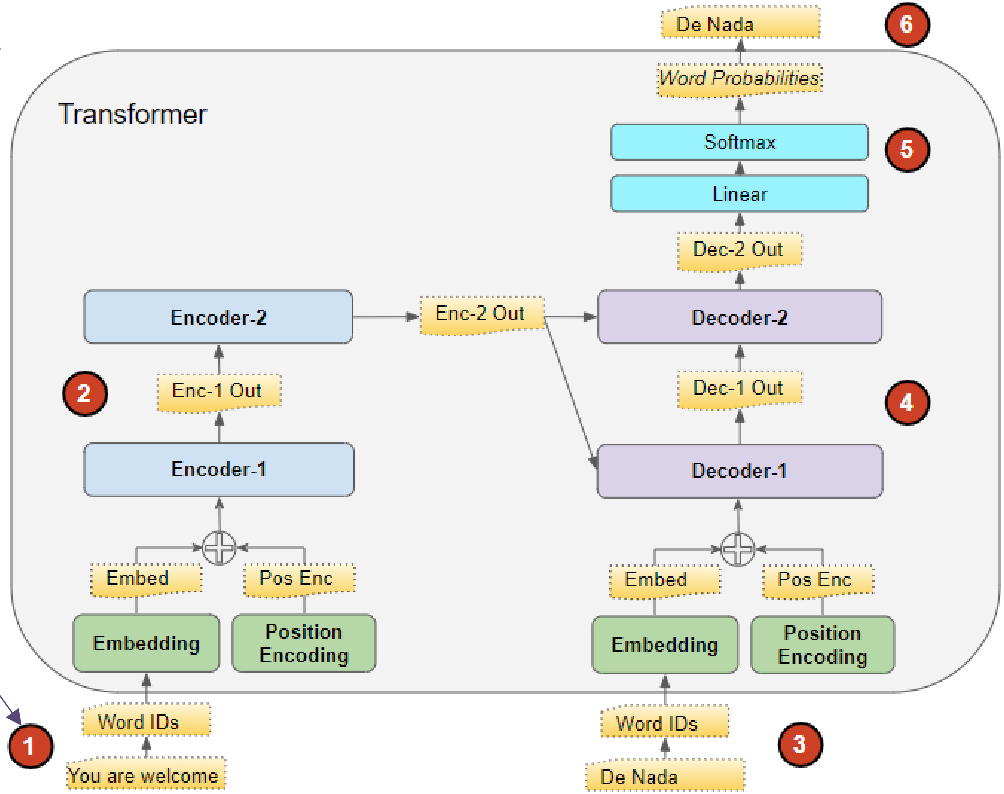
Example from https://towardsdatascience.com/transformers-explained-visually-part-1-overview-of-functionality-95a6dd460452

Training a Transformer



Example from https://towardsdatascience.com/transformers-explained-visually-part-1-overview-of-functionality-95a6dd460452

Training a Transformer

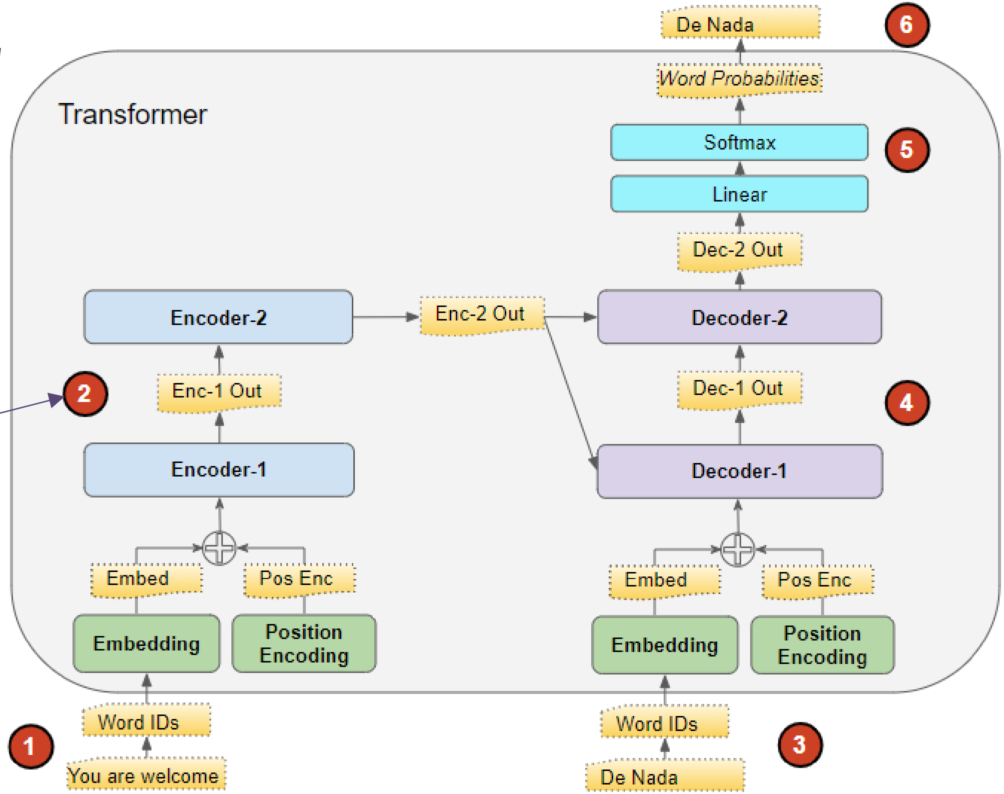


The input sequence is converted into embeddings+positional encoding

Example from https://towardsdatascience.com/transformers-explained-visually-part-1-overview-of-functionality-95a6dd460452

Training a Transformer

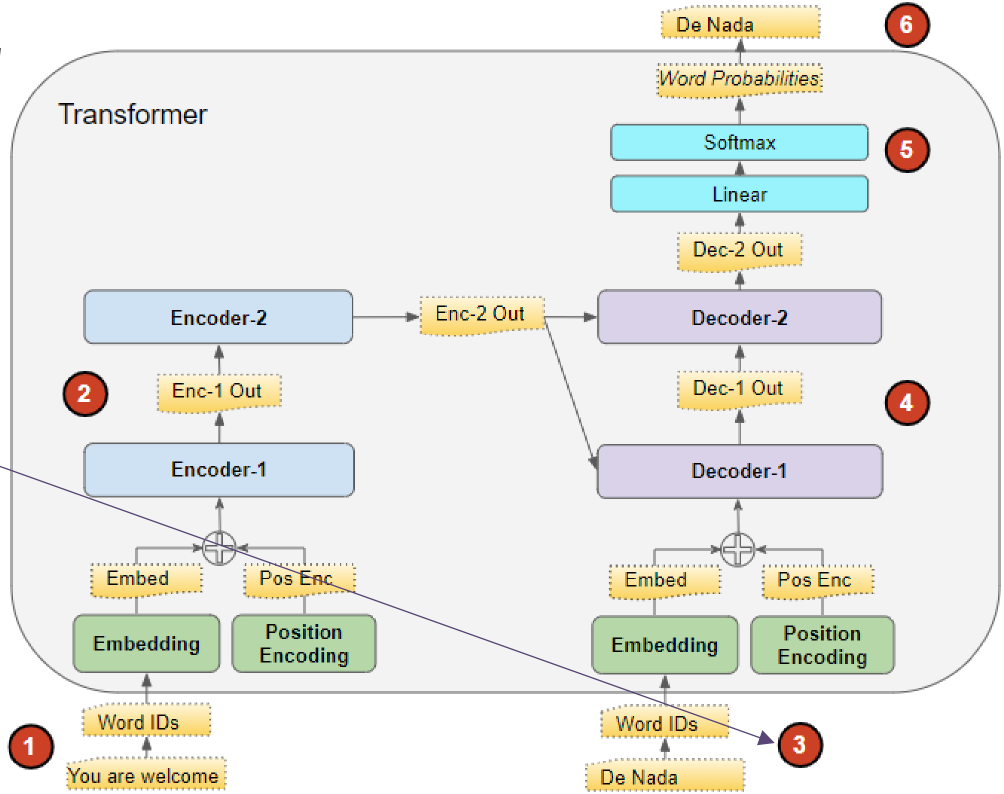
The encoders in the stack process the embeddings and produce an encoded representation



Example from https://towardsdatascience.com/transformers-explained-visually-part-1-overview-of-functionality-95a6dd460452

Training a Transformer

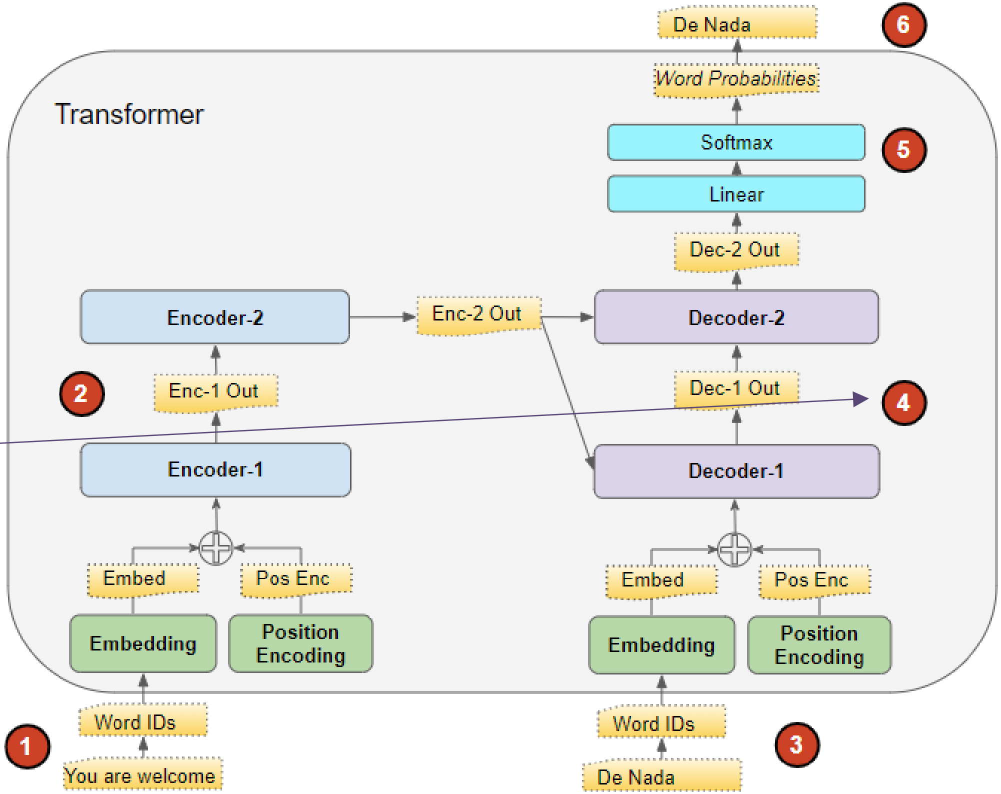
The target sequence is converted into embeddings+positional encoding



Example from https://towardsdatascience.com/transformers-explained-visually-part-1-overview-of-functionality-95a6dd460452

Training a Transformer

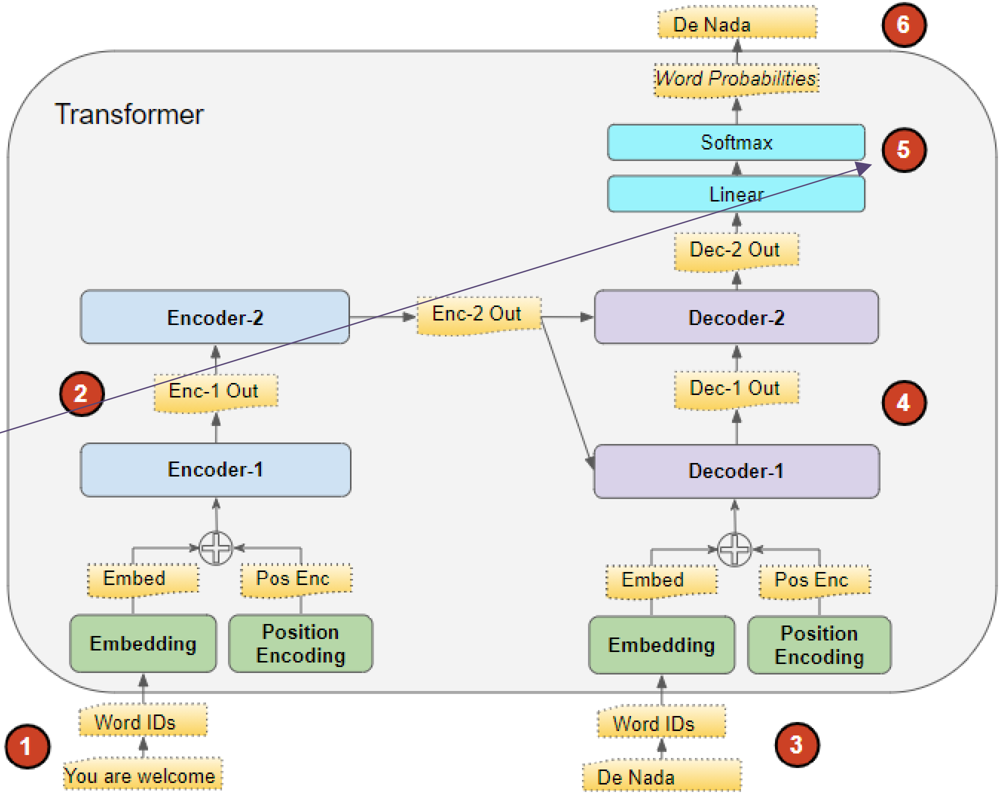
The decoders in the stack processes the embeddings + the encoded representation to produce a decoded representation of the target sequence.



Example from https://towardsdatascience.com/transformers-explained-visually-part-1-overview-of-functionality-95a6dd460452

Training a Transformer

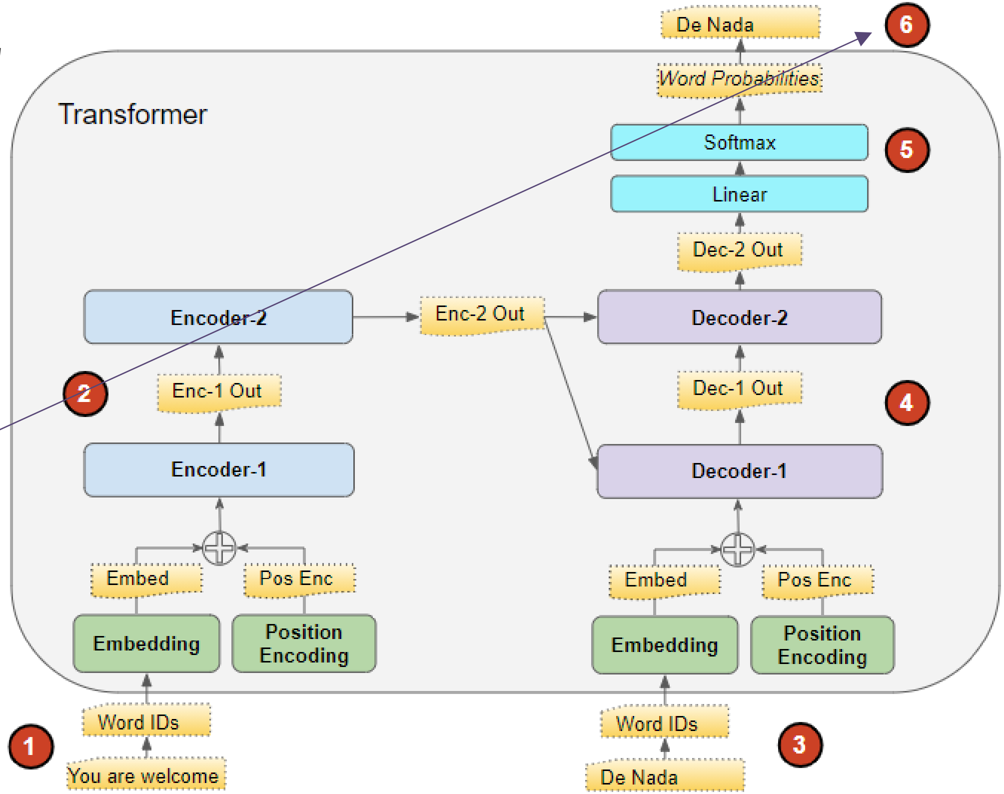
The output layer converts the decoded representations into word probabilities and produce the output



Example from https://towardsdatascience.com/transformers-explained-visually-part-1-overview-of-functionality-95a6dd460452

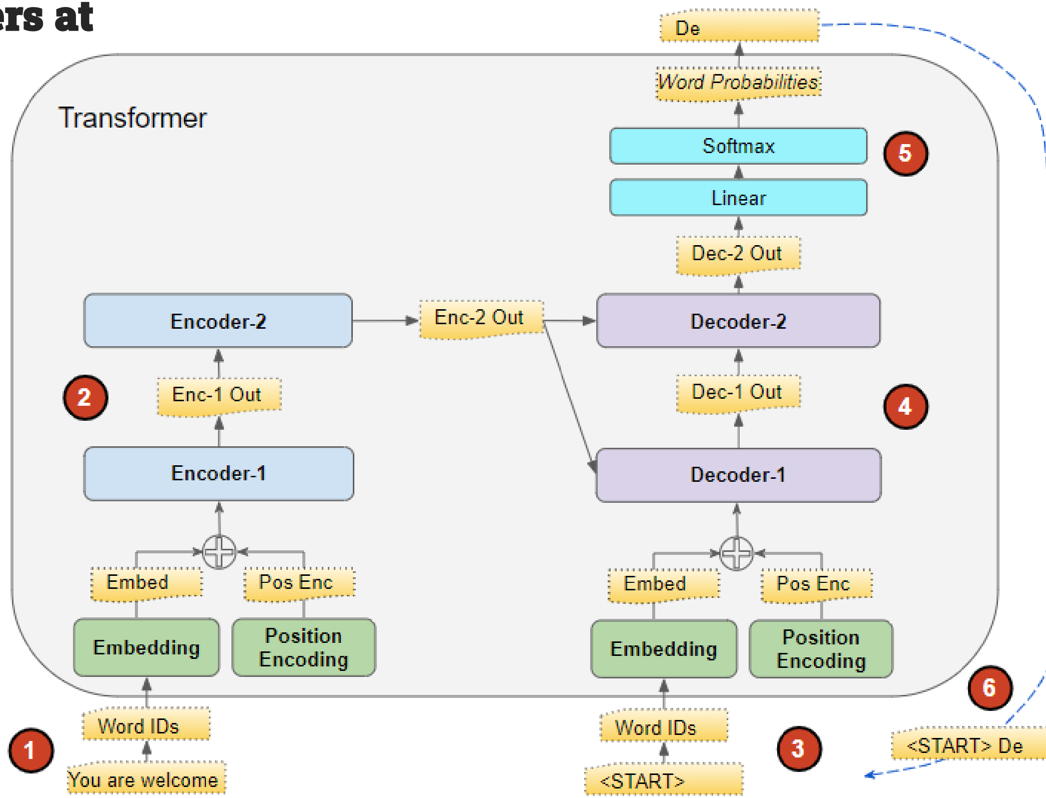
Training a Transformer

The loss function is computed for the back-propagation



Example from https://towardsdatascience.com/transformers-explained-visually-part-1-overview-of-functionality-95a6dd460452

Transformers at inference time



Example from https://towardsdatascience.com/transformers-explained-visually-part-1-overview-of-functionality-95a6dd460452

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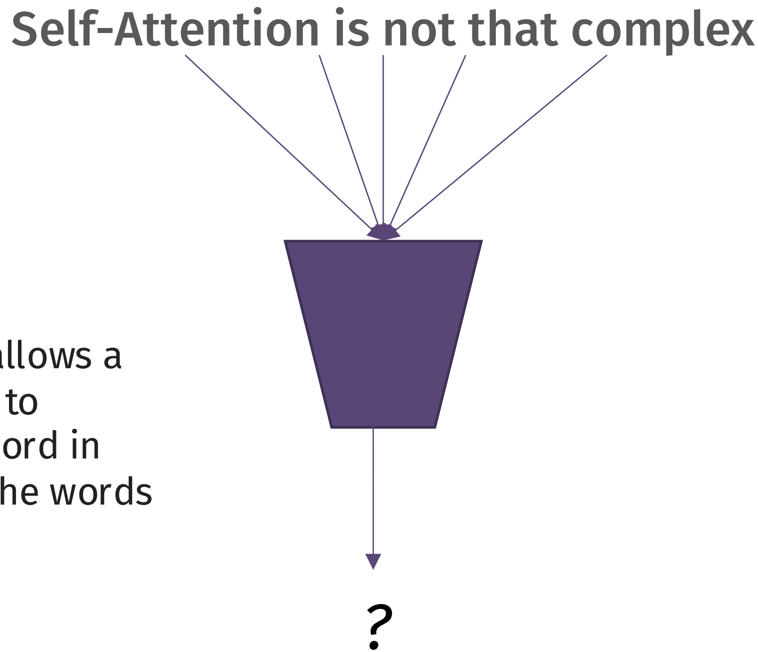
Understanding self-attention

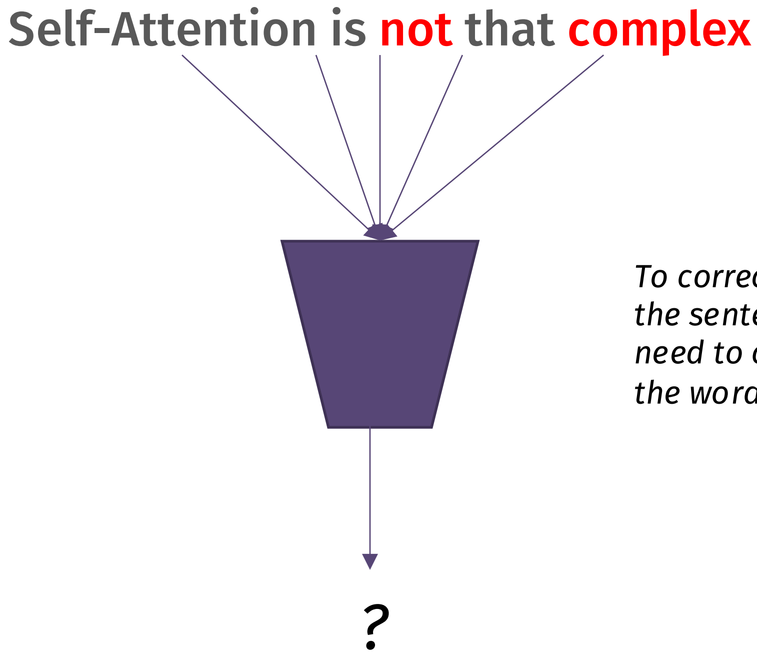
What is self-attention?



Self-attention allows a neural network to understand a word in the context of the words around it.

Inspired by https://twitter.com/MishaLaskin/status/1479246928454037508

What is self-attention?

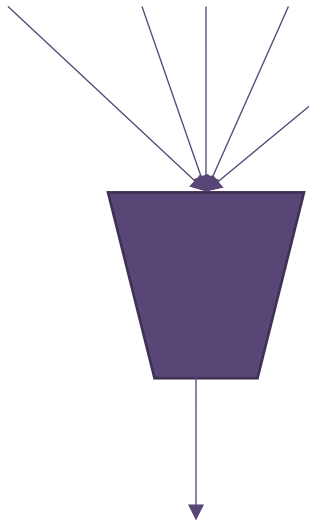


To correctly classify the sentence we need to consider all the words in it

Inspired by https://twitter.com/MishaLaskin/status/1479246928454037508

What is self-attention?

Self-Attention is **not** that **complex**



?

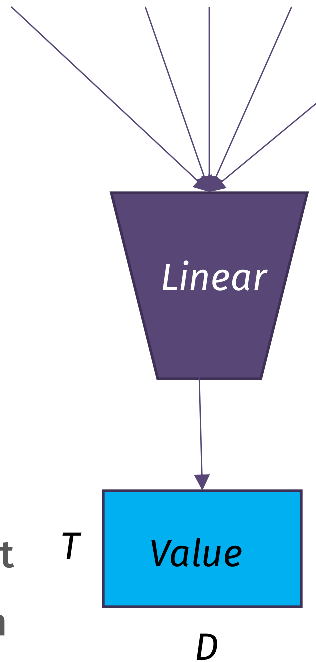
To correctly classify the sentence we need to consider all the words in it

NOT ONLY: we also need to understand the relations between them

Inspired by https://twitter.com/MishaLaskin/status/1479246928454037508

What is self-attention?

Self-Attention is **not** that **complex**



We encode each word (text) into a numerical embedding of size N

We pass the T words embeddings through a linear layer, obtaining the values, each one of size D

Value: the relevant content of a token

$$X \in \mathbb{R}^{T \times N}$$

$$W_V \in \mathbb{R}^{N \times D}$$

$$V = XW_V$$

Inspired by https://twitter.com/MishaLaskin/status/1479246928454037508

Combining values/words

	Self-Attention	is	not	that	complex
Self-Attention	1	1	1	1	1
is	1	1	1	1	1
not	1	1	1	1	1
that	1	1	1	1	1
complex	1	1	1	1	1

T x T

$$V = XW_V$$

T **Value** *D*

T **Attention** *D*

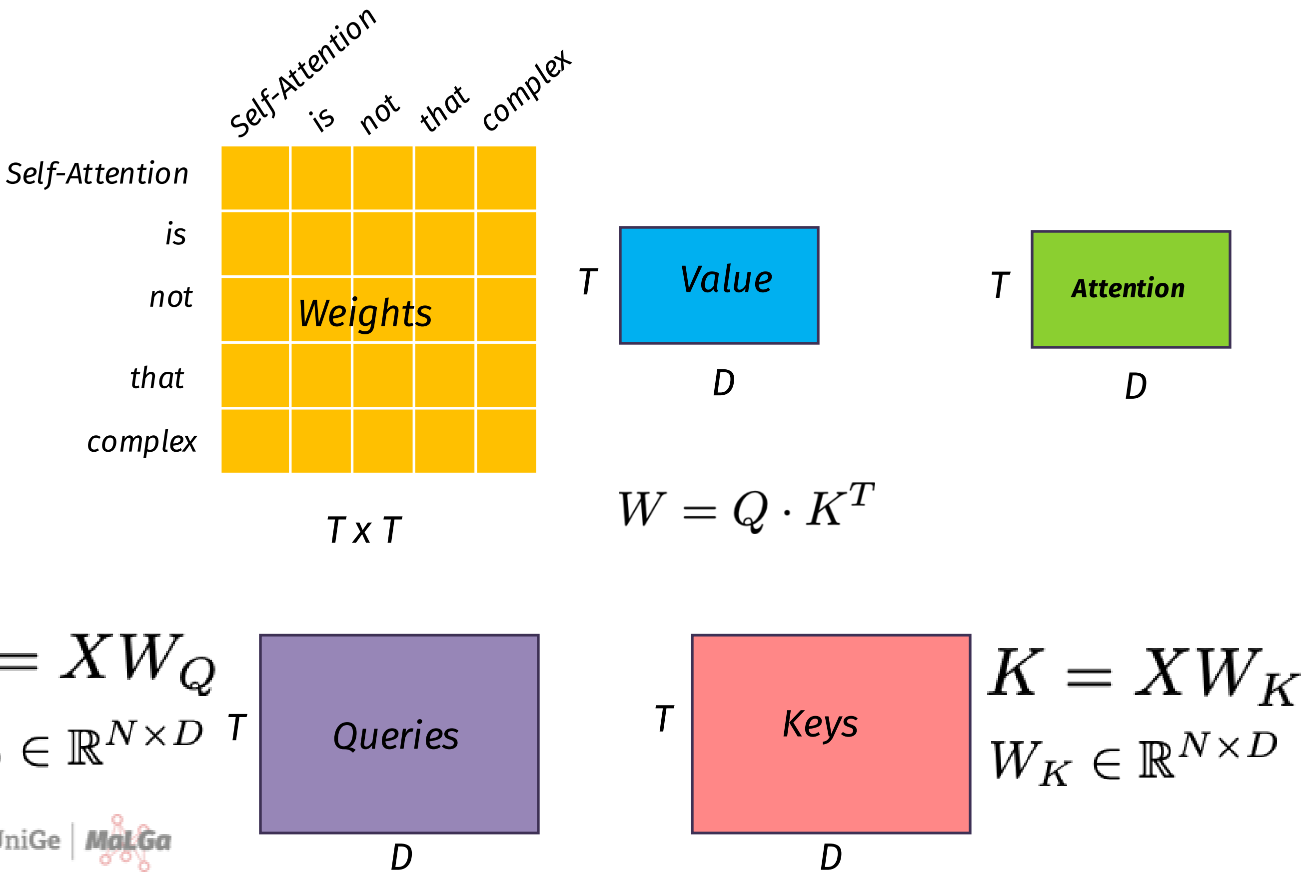
This is what we want to obtain

Here we would assume the same importance for all relationships... but we would like that, for instance, the relation between «not» and «complex» was more important than the one between «is» and «too»

Inspired by https://twitter.com/MishaLaskin/status/1479246928454037508

Learning the attention weights

Inspired by https://twitter.com/MishaLaskin/status/1479246928454037508



$$W = Q \cdot K^T$$

$$Q = XW_Q$$

$$W_Q \in \mathbb{R}^{N \times D}$$

$$K = XW_K$$

$$W_K \in \mathbb{R}^{N \times D}$$

Intuitions

- Each token's embedding x is transformed into three vectors: **Query (Q)**, **Key (K)**, and **Value (V)**
- A web search analogy:
  - **Query (Q)** is the search text you type in the search engine bar. This is the token for which you want to *find more information*
  - **Key (K)** is the title of each web page in the search result window. It represents the possible tokens the query can attend to
  - **Value (V)** is the actual content of the web pages shown.

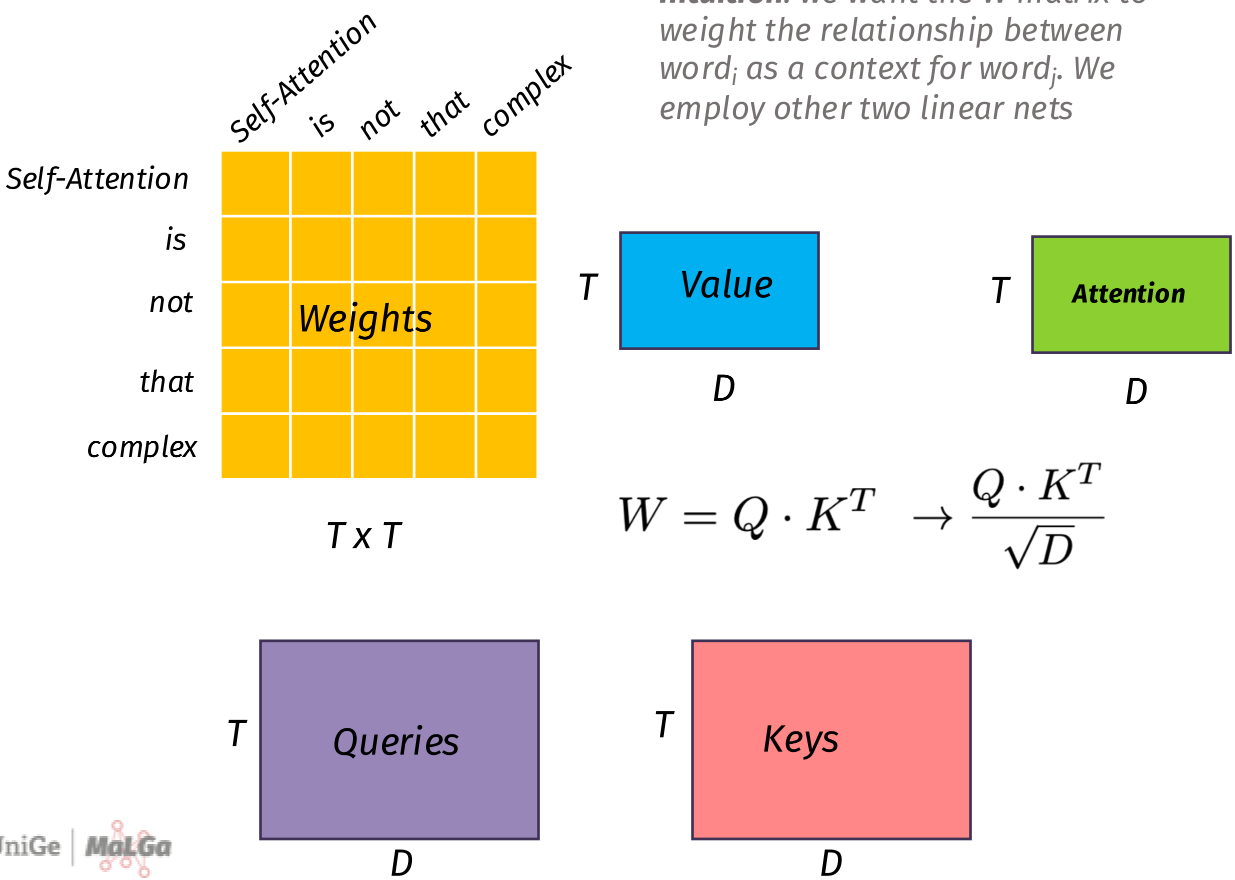
Once we matched the appropriate search term (Query) with the relevant results (Key), we want to get the content (Value) of the most relevant pages

From https://poloclub.github.io/transformer-explainer/

Learning the attention weights

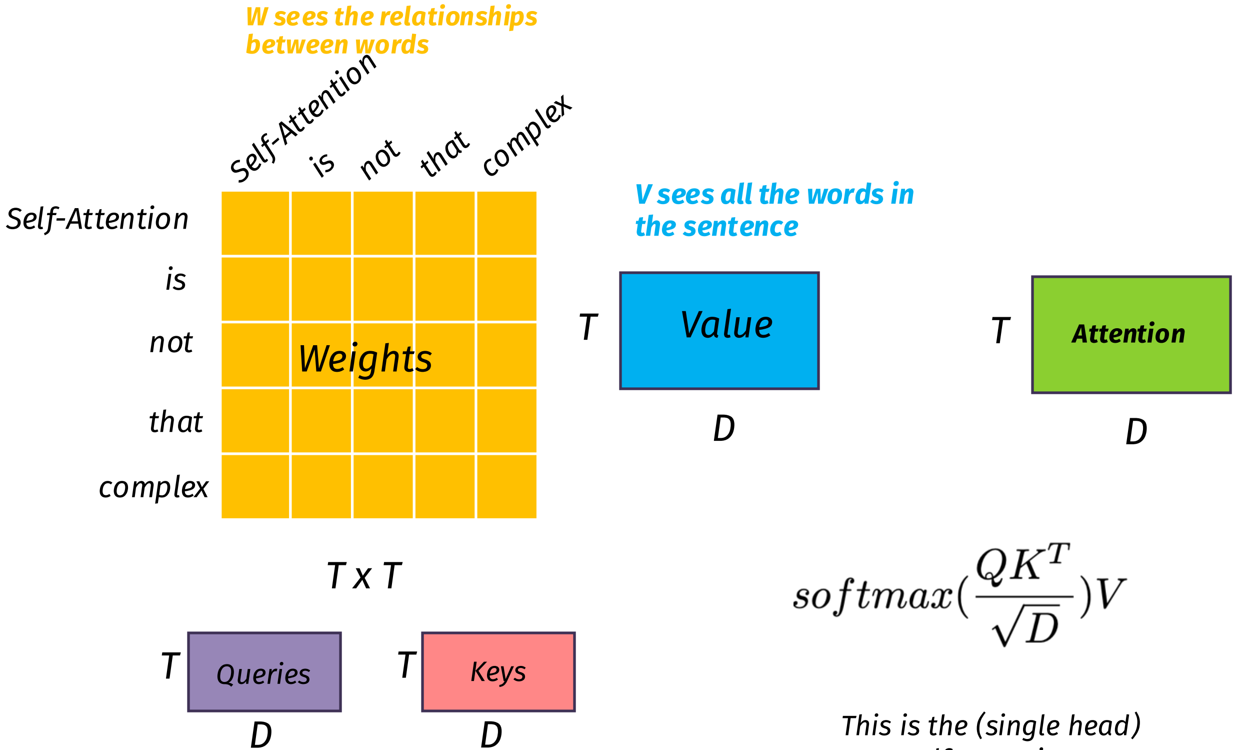
Inspired by https://twitter.com/MishaLaskin/status/1479246928454037508

Intuition: *we want the W matrix to weight the relationship between word$_i$ as a context for word$_j$. We employ other two linear nets*



$$W = Q \cdot K^T \quad \rightarrow \frac{Q \cdot K^T}{\sqrt{D}}$$

Single-head attention

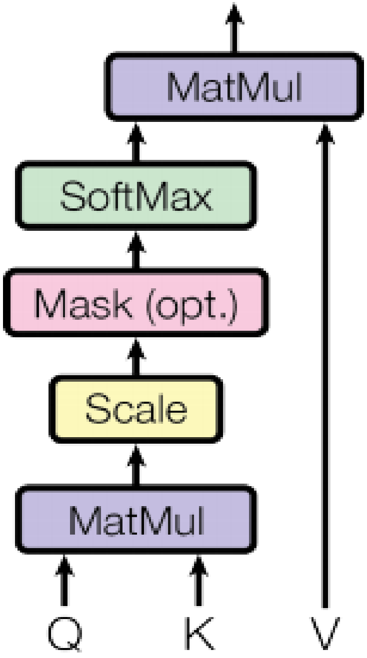


$$softmax(\frac{QK^T}{\sqrt{D}})V$$

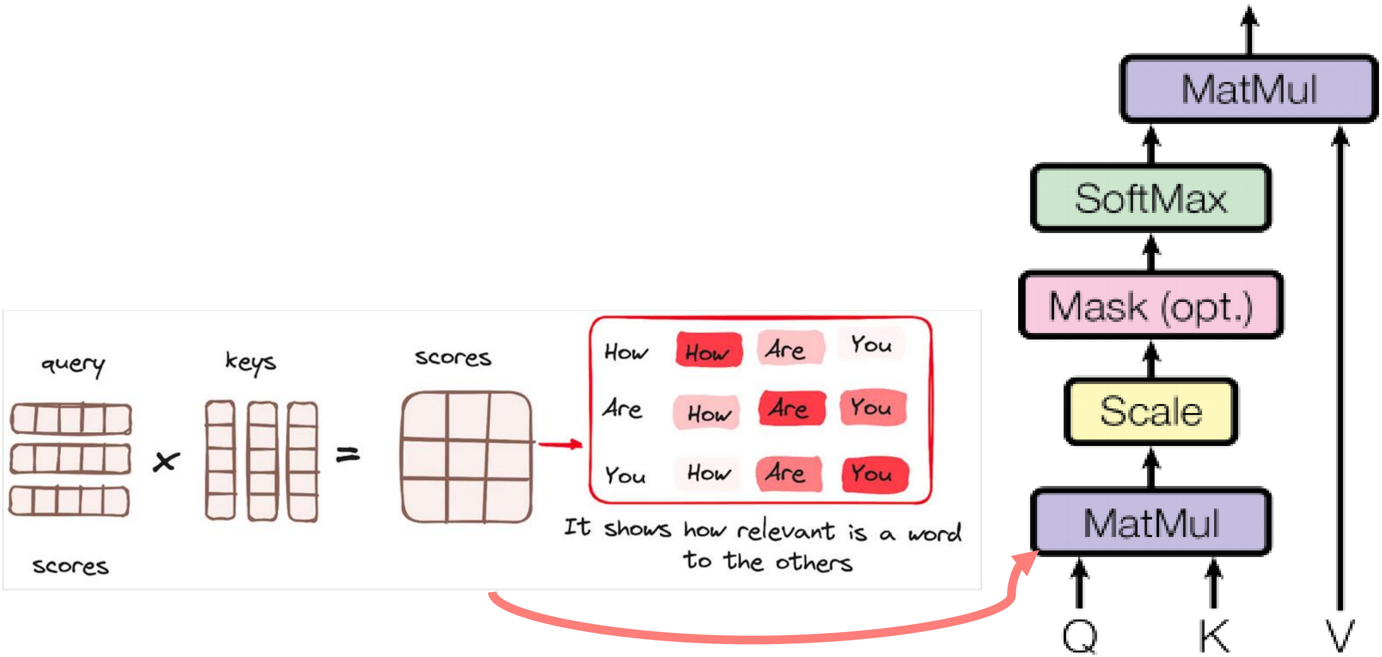
This is the (single head) self-attention

Inspired by https://twitter.com/MishaLaskin/status/1479246928454037508

Single-head attention
[Nothing but a Scaled Dot-Product]

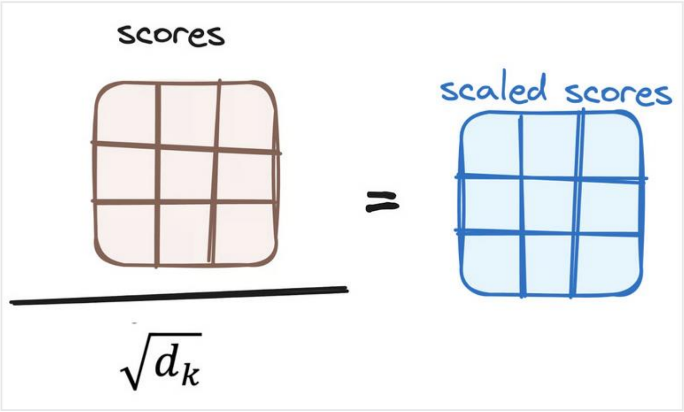


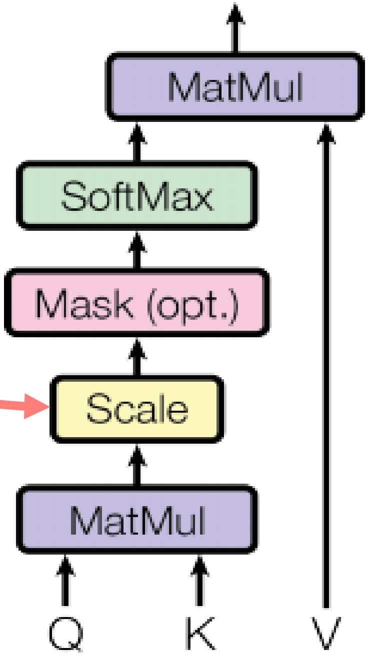
Single-head attention
[Nothing but a Scaled Dot-Product]



Drawings from https://www.datacamp.com/tutorial/how-transformers-work

Single-head attention
[Nothing but a Scaled Dot-Product]





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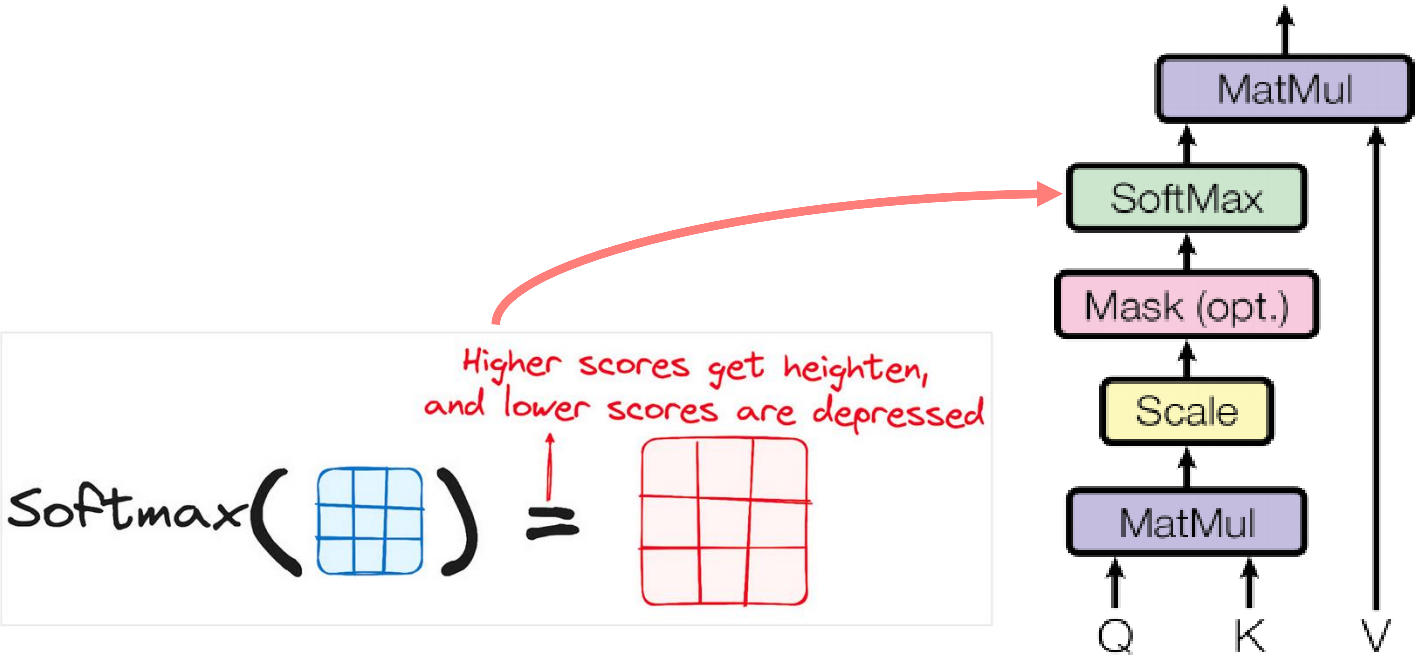

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Single-head attention
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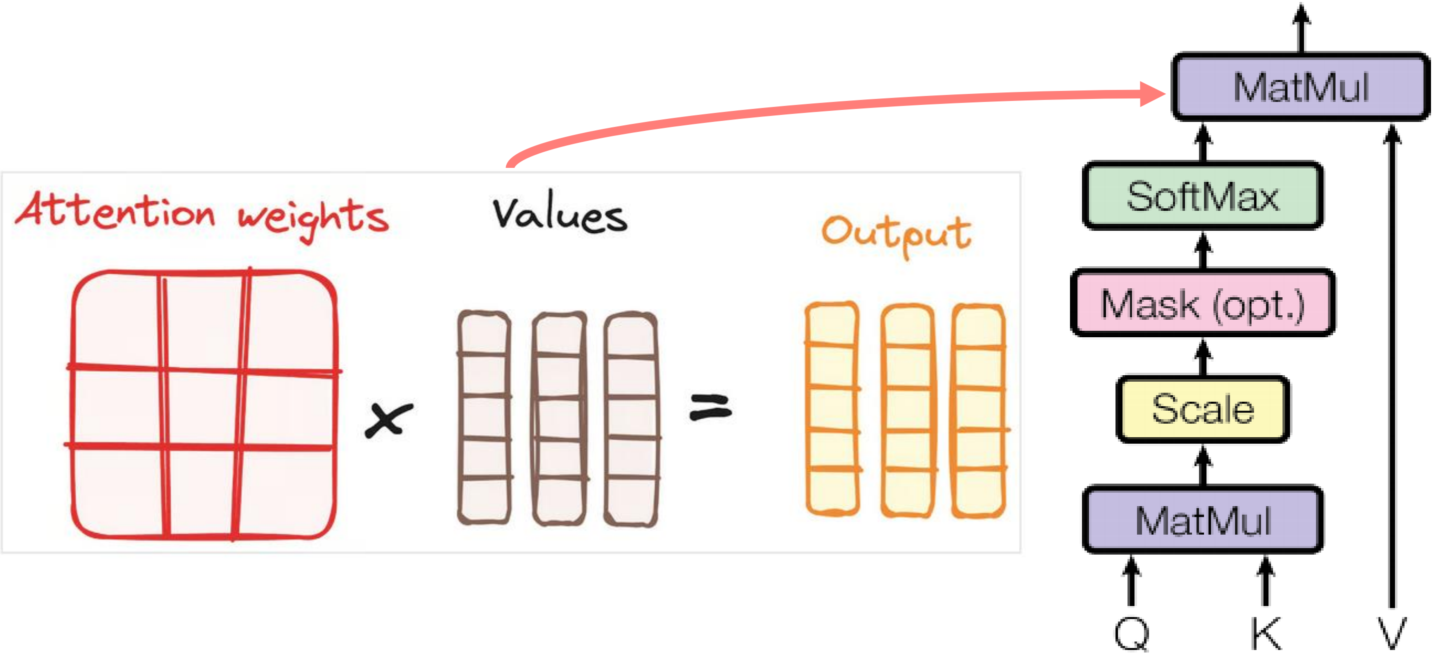


Drawings from https://www.datacamp.com/tutorial/how-transformers-work

Going back to the overall architecture

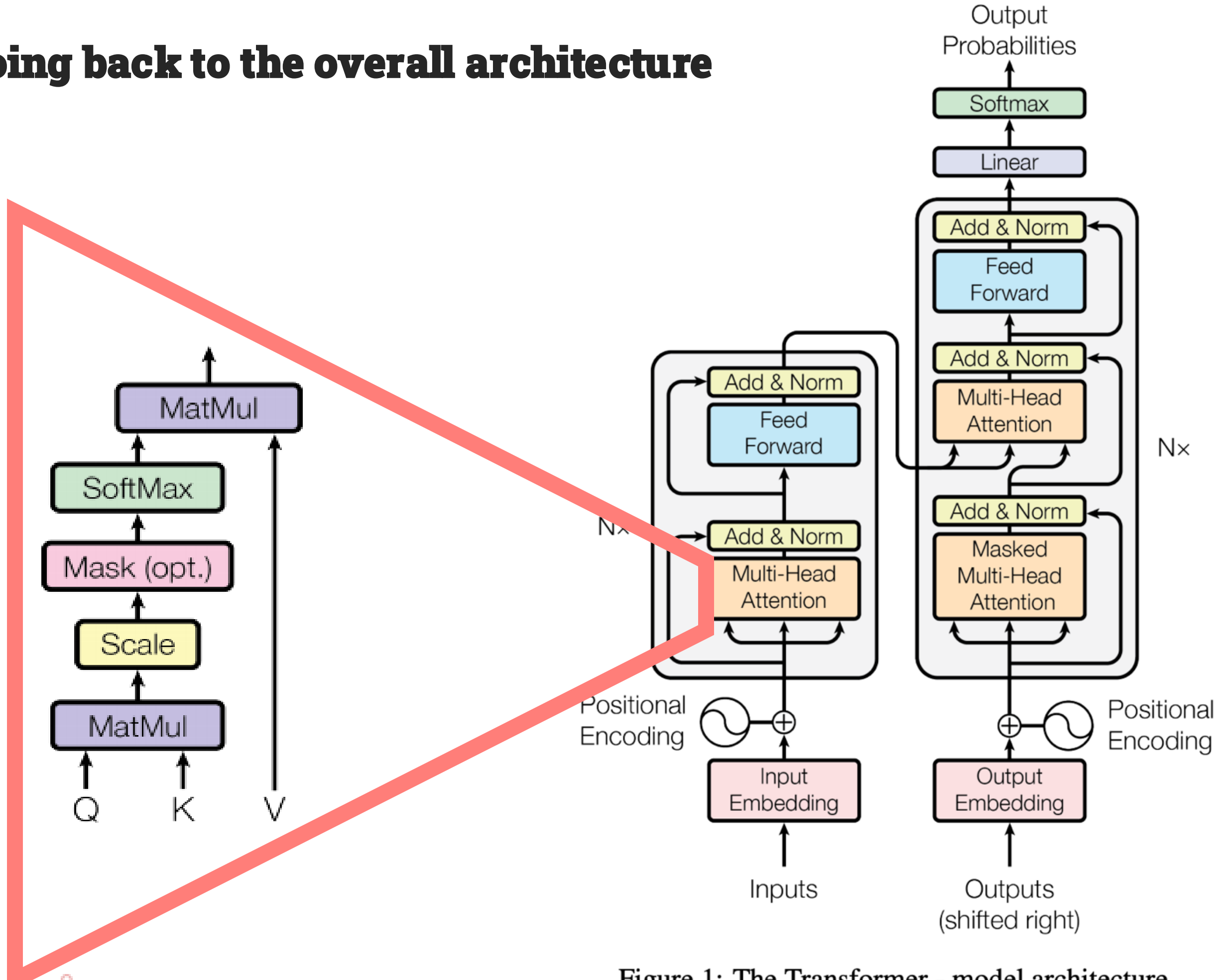
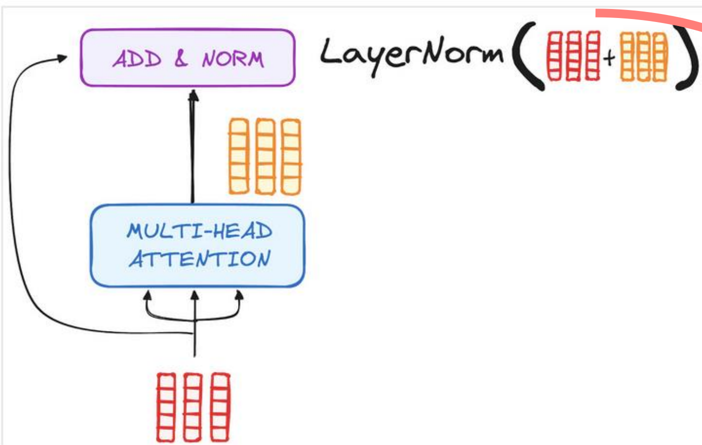


Figure 1: The Transformer - model architecture.

Going back to the overall architecture



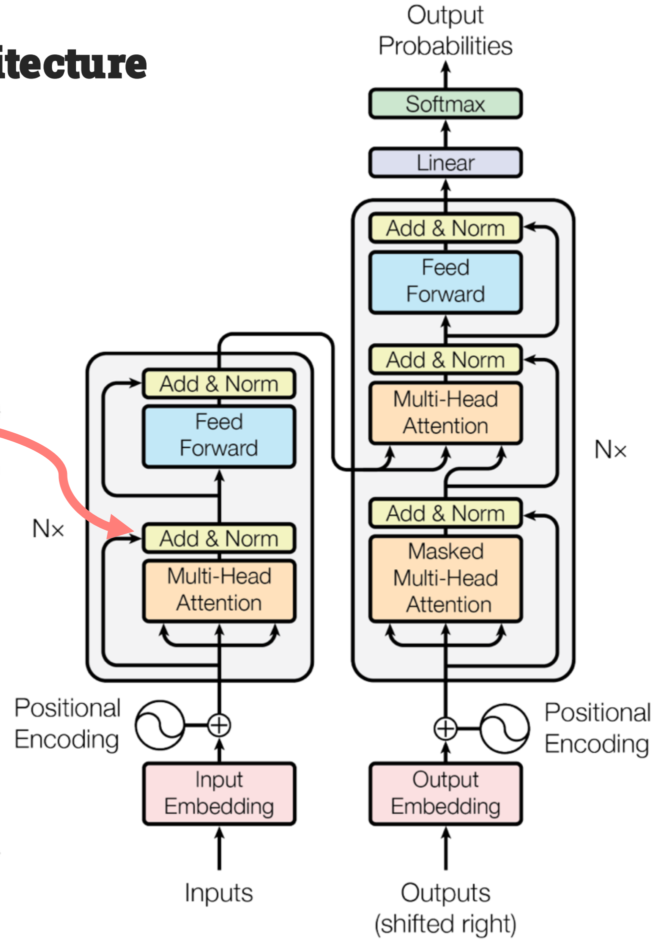
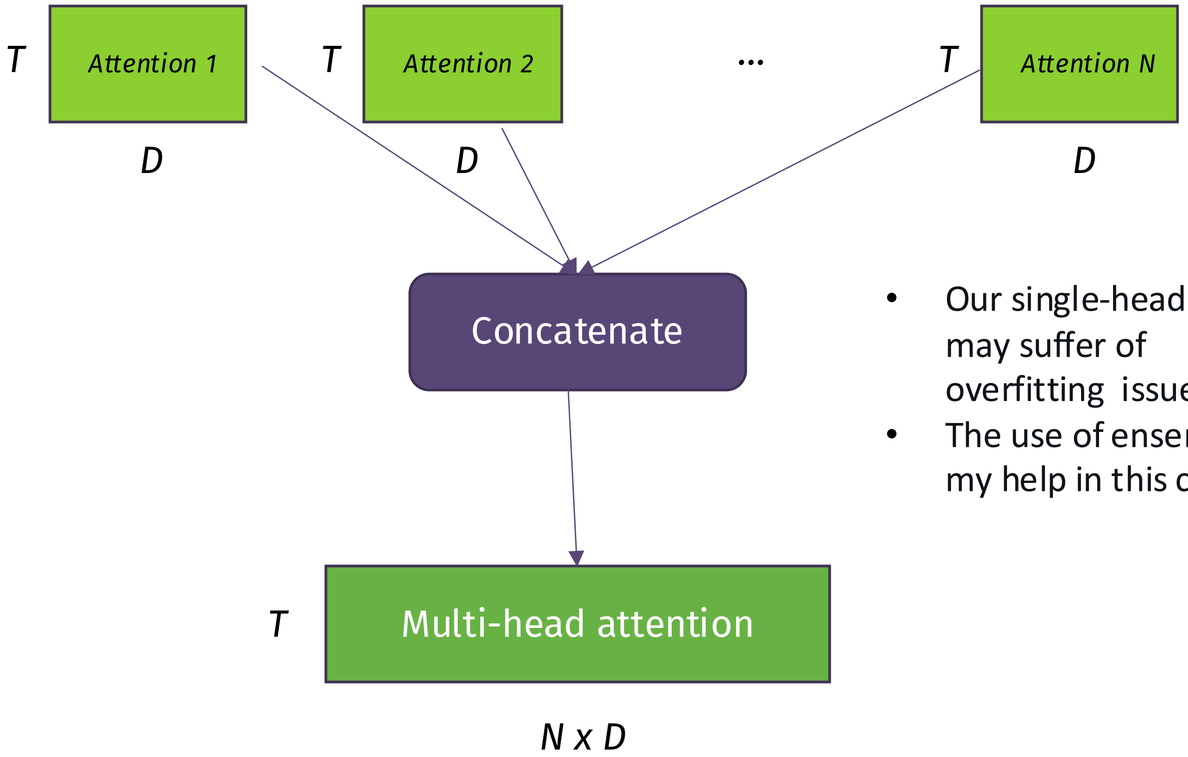


Figure 1: The Transformer - model architecture.

Multi-head attention



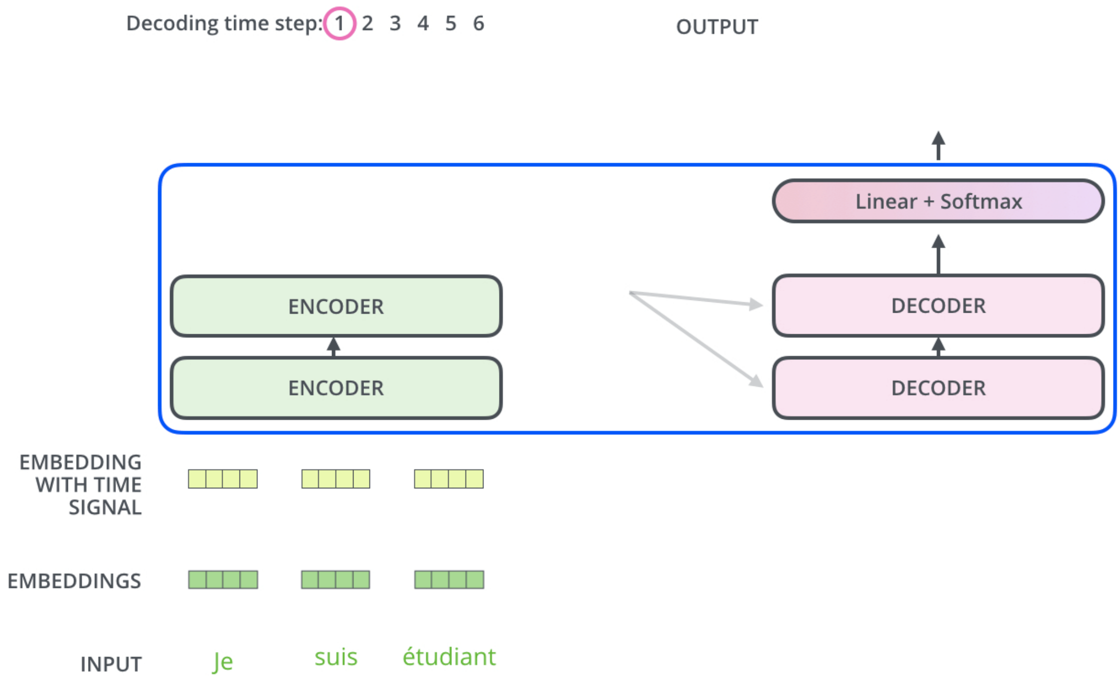
- Our single-head net may suffer of overfitting issues
- The use of ensembles my help in this case

Multi-head attention

When it will translate the word "it" the decoder will take into account the importance of "cat" and "hungry"

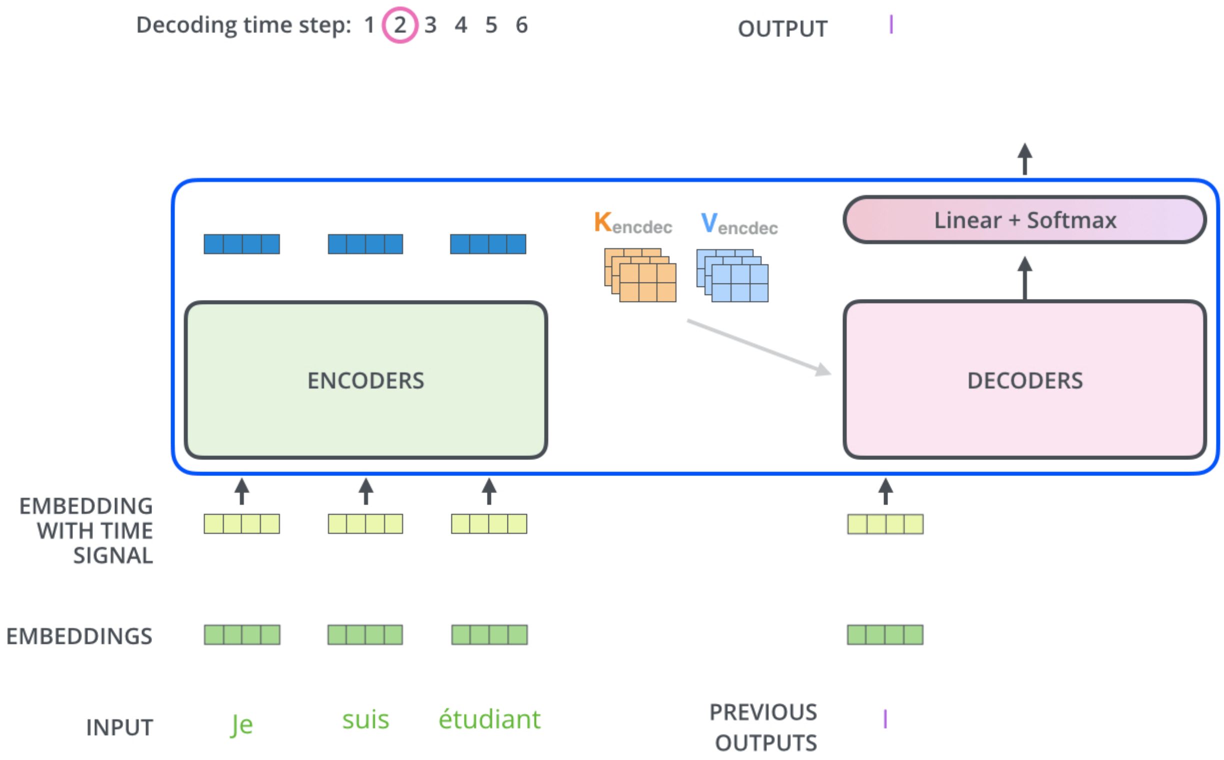
From https://towardsdatascience.com/transformers-explained-visually-part-1-overview-of-functionality-95a6dd460452/

The decoder side



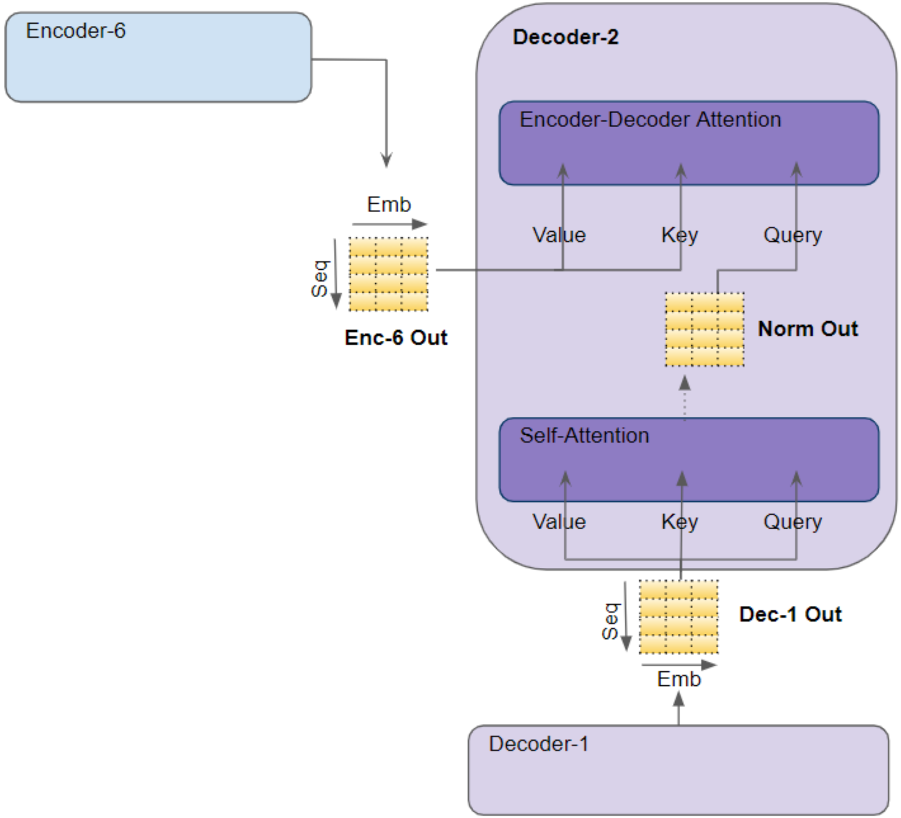
From http://jalammar.github.io/illustrated-transformer/

The decoder side



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

Encoder-Decoder attention

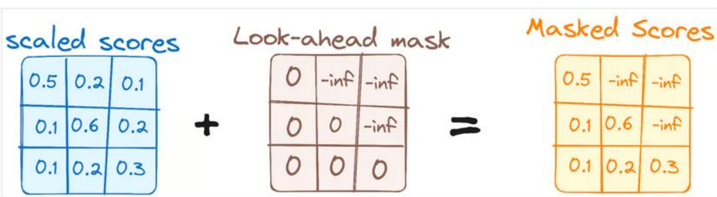


https://towardsdatascience.com/transformers-explained-visually-part-2-how-it-works-step-by-step-b49fa4a64f34/

Decoder behind the scenes

- In the decoder, the self-attention layer is only allowed to consider earlier positions in the output sequence (it can not “see” the future)

- This is achieved using masked attention: future positions are set to –inf before the softmax step



Drawings from https://www.datacamp.com/tutorial/how-transformers-work

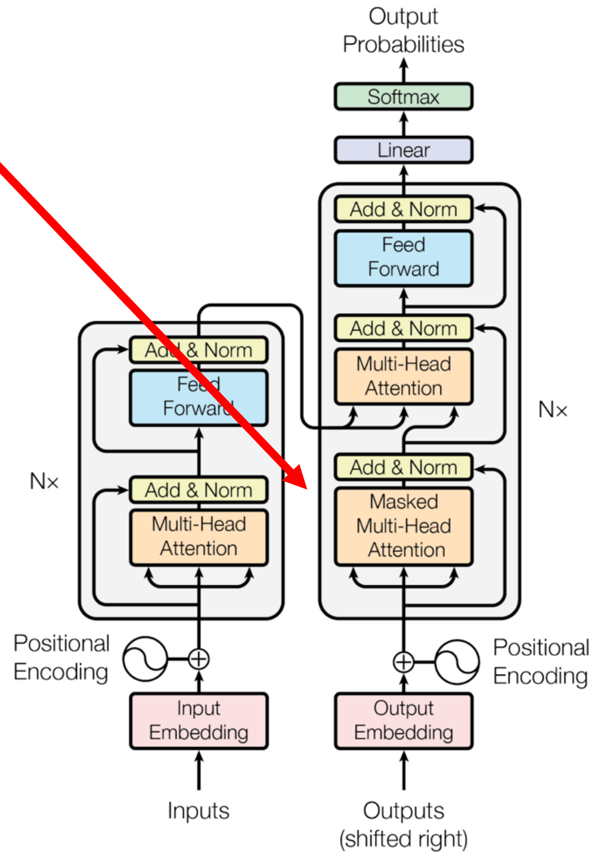
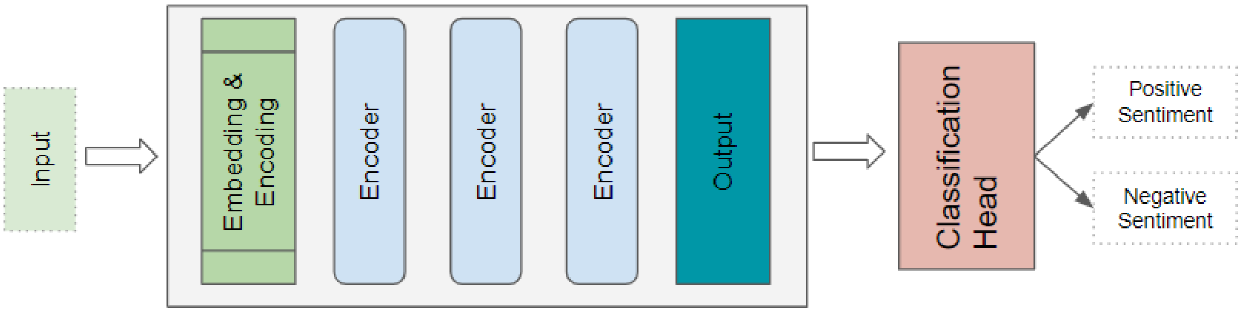


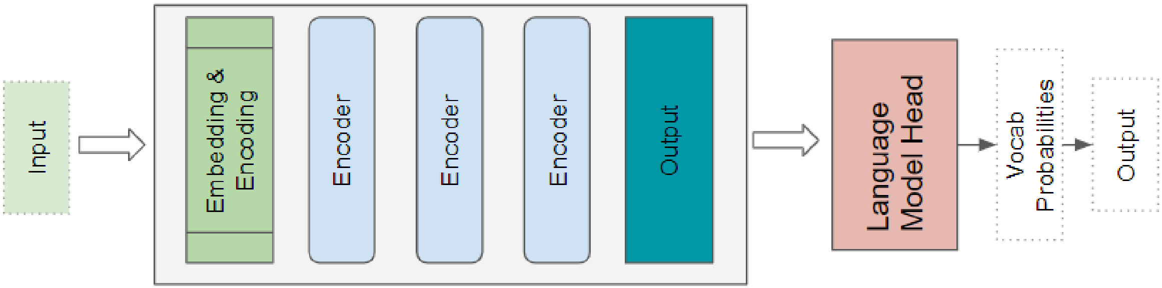
Figure 1: The Transformer - model architecture.

Encode to classify



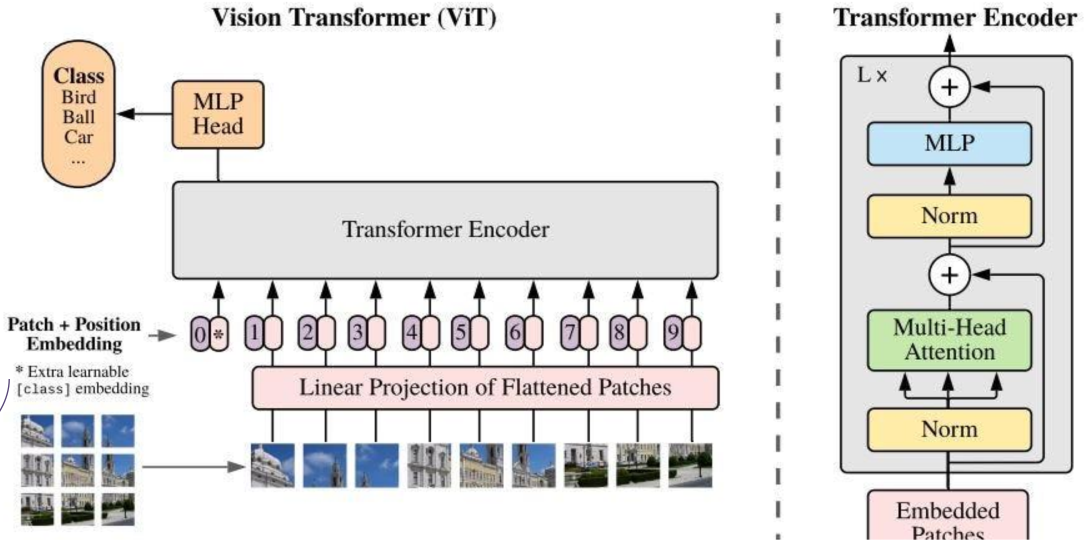
https://towardsdatascience.com/transformers-explained-visually-part-1-overview-of-functionality-95a6dd460452/

Encode to generate



https://towardsdatascience.com/transformers-explained-visually-part-1-overview-of-functionality-95a6dd460452/

Variants: vision transformers

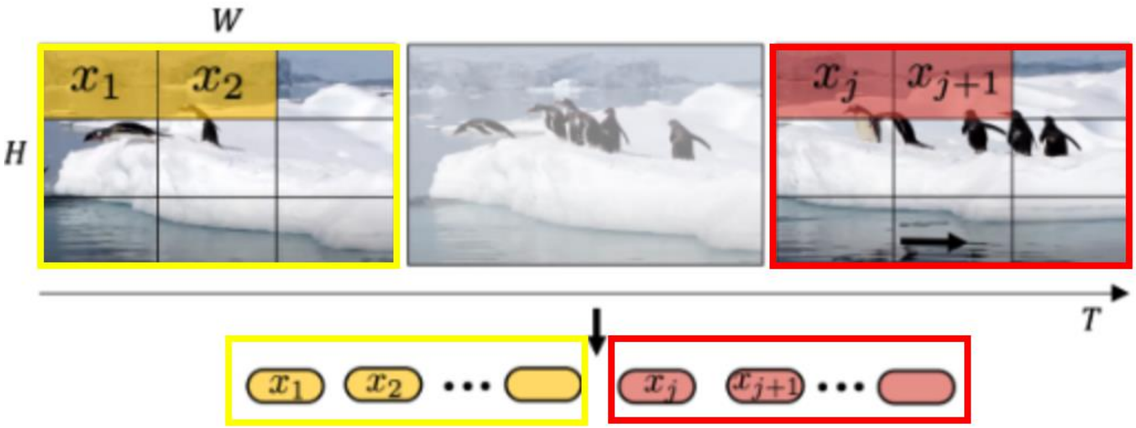


"Imagine you're reading a book, but instead of reading the entire book, you summarize it with a single sentence that captures the main theme. The "[class]" token is that sentence."

https://paperswithcode.com/paper/an-image-is-worth-16x16-words-transformers-1

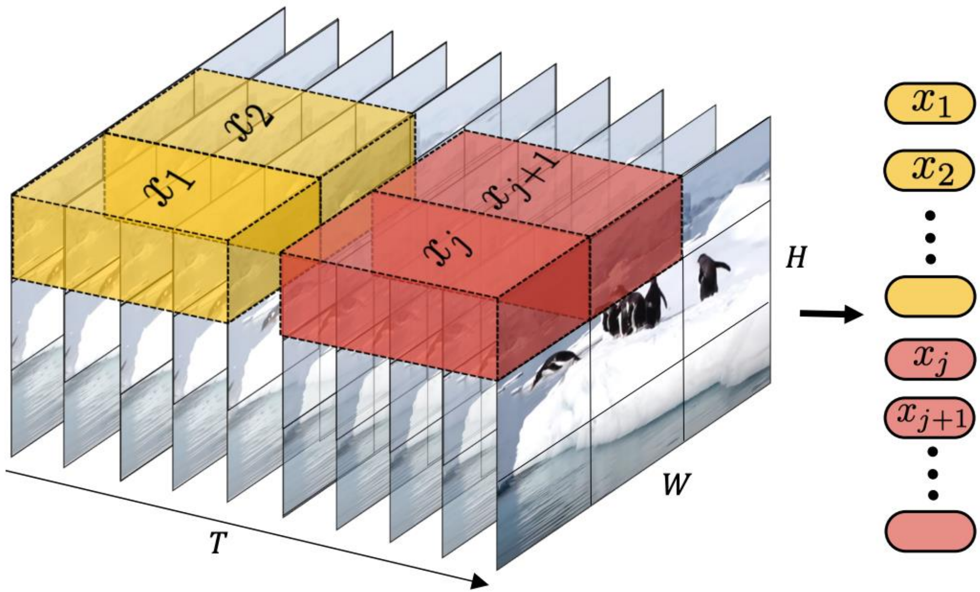
https://saadsohail5104.medium.com/understanding-the-role-of-the-class-token-in-vision-transformers-vit-d0f7750d7066

Variants: extensions to videos



https://medium.com/aiguys/vivit-video-vision-transformer-648a5fff68a4

Variants: extensions to videos



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Links

https://poloclub.github.io/transformer-explainer/

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https://towardsdatascience.com/transformers-explained-visually-part-2-how-it-works-step-by-step-b49fa4a64f34/

https://www.datacamp.com/tutorial/how-transformers-work

https://medium.com/aiguys/vivit-video-vision-transformer-648a5fff68a4

https://saadsohail5104.medium.com/understanding-the-role-of-the-class-token-in-vision-transformers-vit-d0f7750d7066

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