

CS5242 : Neural Networks and Deep Learning

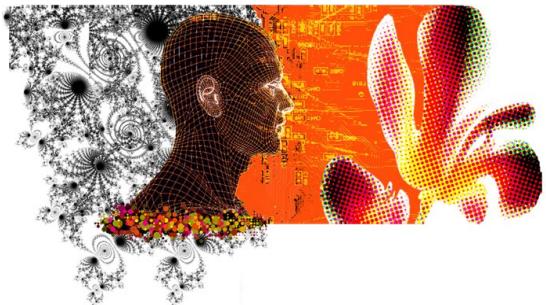
Lecture 7 : Attention Neural Networks

Semester 2 2024/25

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Outline

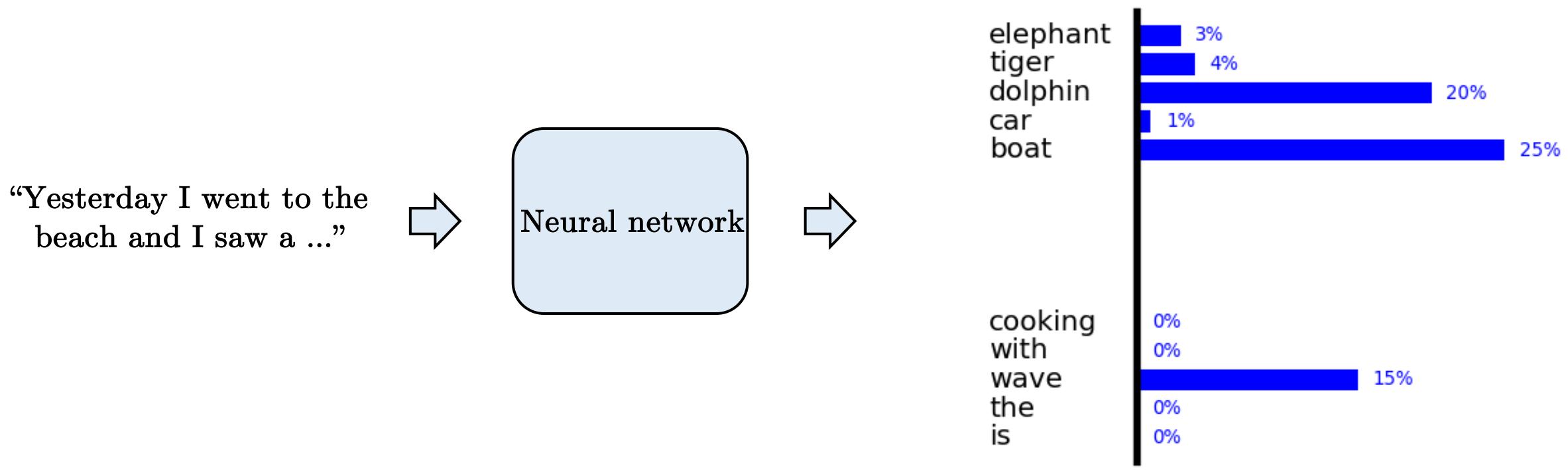
- Language Models
- Memory Networks
- Transformers
- Language Model Transformers
- Sequence-To-Sequence Transformers
- Transfer Learning
- Conclusion

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Language models

- Language model predicts the next word given a context window.
- Most fundamental problem in NLP.



Input:

Sequence of words

Output:

Probability distribution over
the dictionary/vocabulary

Recurrent neural networks

- Data structure
 - Input is an ordered sequence.
 - Input length and output length can be variable.
- RNNs are designed for sequences.
 - They learn a representation of sequence independently of its length.
 - Recurrence formula summarizes the sequence with a vector h :
- Weight sharing across time (translation invariance)
- They learn to keep or ignore information in the sequence for the downstream task.
 - Gating mechanism to forget/remember the past or the new input :

$$\sigma \odot h$$

Recurrent neural networks

- Performance
 - Significant **progress in NLP** but not a breakthrough.
 - Dominant in NLP for Machine Translation (MT), Q&A, summarization up to 2018.
- Limitation
 - RNNs **cannot learn long-term dependencies** (no more than 50 steps).
 - Hard to train because they are **non-linear dynamical systems**
 - Any small perturbation can amplify or vanish.
 - **Slow to train** because of their sequential nature (due to recurrence mechanism).
 - Important limitation when training on large-scale datasets.

Outline

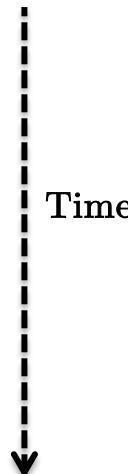
- Language Models
- **Memory Networks**
- Transformers
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Memory networks

- How do these models work?
- Let us consider a simple example from the bAbI dataset (Meta 2015).
- This dataset is used to evaluate simple reasoning property of models.
- Example :
 - Joe went to the kitchen
 - Joe picked up milk
 - Joe went to the bathroom
 - Joe put down the milk
 - Joe went to the bedroom
 - Question : Where is the milk?
 - Answer : ---

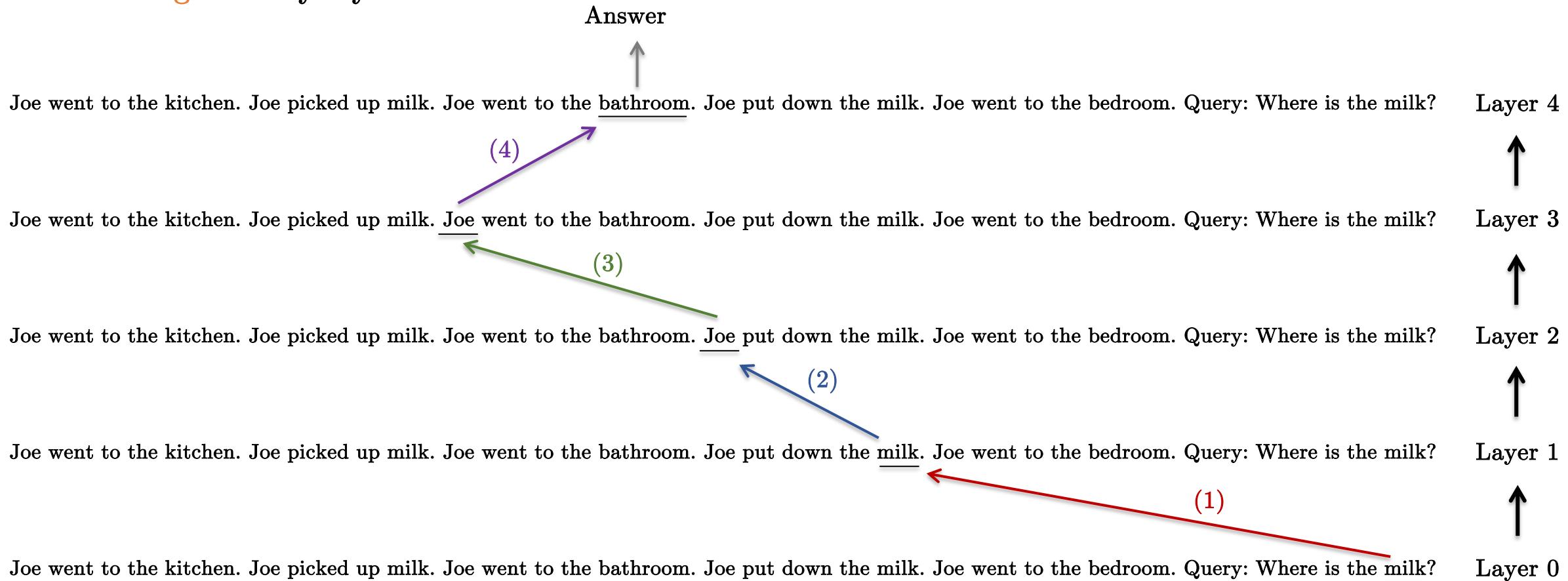
Memory networks

- Memory networks (Weston-Chopra-Bordes, Meta 2015) are designed to response to the questions with **multi-step** word matching :
 - Joe went to the kitchen
 - Joe picked up milk
 - Joe went to the bathroom
 - (3) 
 - (4) 
 - Joe put down the milk
 - (2) 
 - (1) 
 - Joe went to the bedroom
 - Question : Where is the milk?
 - Answer : bathroom
- This matching process is also called **multi-hop attention**.
- Multi-hop attention is a mechanism that performs **multi-step reasoning**.

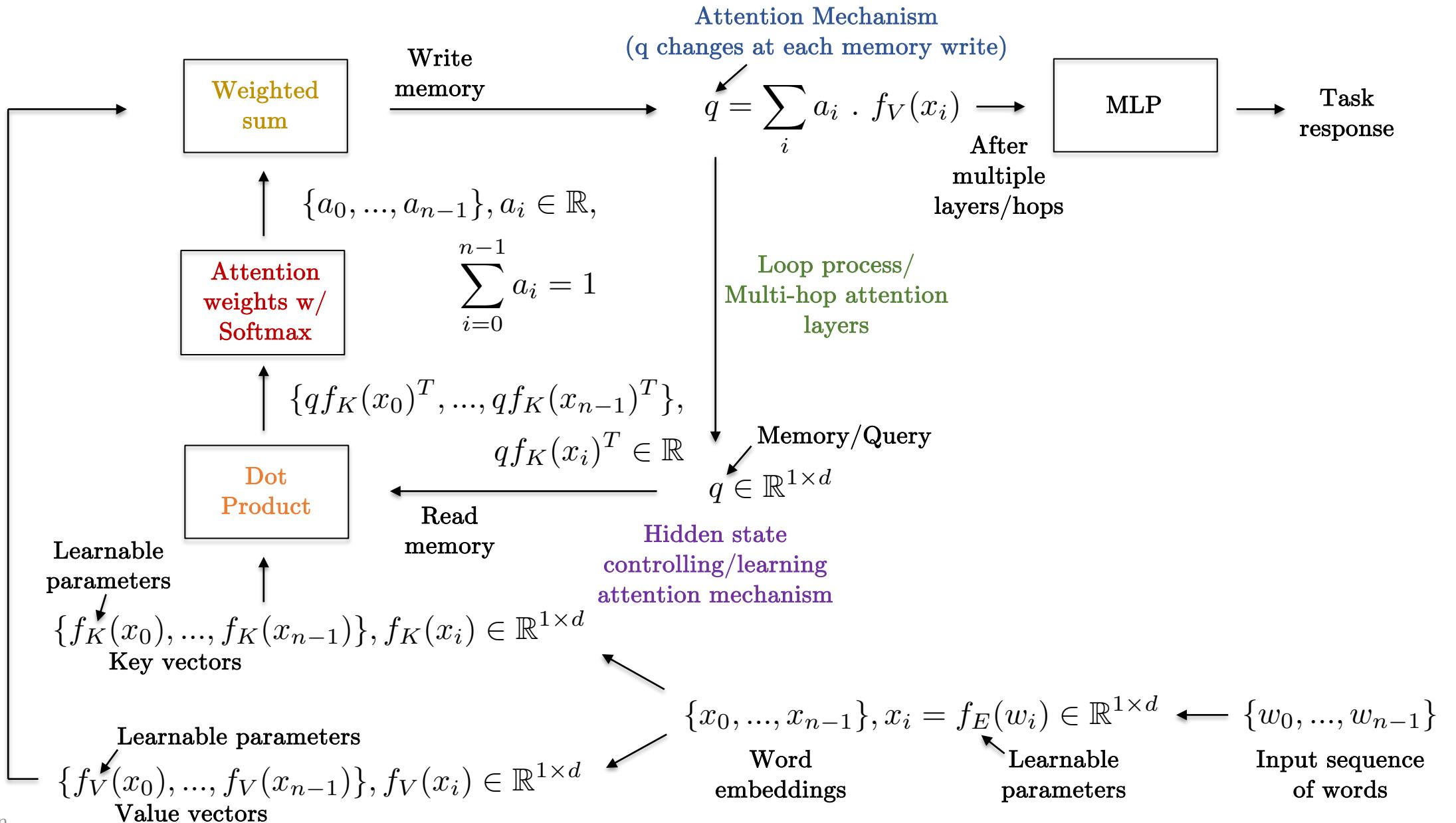


Multi-hop attention steps

- **Unrolling memory layers :**



Implementation



Formalization

- Input sequence of words : $\{w_0, \dots, w_{n-1}\}, w_i \in \{0, \dots, V - 1\}$

- Continuous representation/
word embedding : $\{x_0, \dots, x_{n-1}\}, x_i = f_E(w_i) \in \mathbb{R}^d$

- Hidden features :

$$\text{Key} = \begin{bmatrix} f_K(x_0) \\ \vdots \\ f_K(x_{n-1}) \end{bmatrix} \in \mathbb{R}^{n \times d} \quad q \in \mathbb{R}^{1 \times d} \quad \text{Query} \quad V = \begin{bmatrix} f_V(x_0) \\ \vdots \\ f_V(x_{n-1}) \end{bmatrix} \in \mathbb{R}^{n \times d} \quad \text{Value}$$

- Repeat K times :
 $a \leftarrow \text{Softmax}(qK^T) \in \mathbb{R}^{1 \times n}$
 $q \leftarrow aV = \text{Softmax}(qK^T)V \in \mathbb{R}^{1 \times d}$

- Output : $s = \text{MLP}(q) \in \mathbb{R}^V$

Properties

- This model is seen as **differentiable** memory computers, i.e. memory operations read and write can be differentiable and thus be used with backpropagation.
- This network can update its memory by stacking **multiple-hop attention layers** to perform **multi-step reasoning**.
- This model is based on the principle that **intelligence** requires an adaptive long-term memory, unlike RNNs which is limited to short-term memory.
- This technique is a **precursor** of Transformers.

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Limitations of memory networks

- Memory networks were promising, but not ground-breaking.
- Transformers designed the first efficient version of attention networks !
- Transformer improvements over memory networks :
 - Multiple queries (one per word)
 - Multi-head attention mechanism (more learning capacity)
 - Residual blocks (better backpropagation)

Self-attention mechanism

- Input set (continuous representation) :

$$\{x_0, \dots, x_{n-1}\}, \quad X = \begin{bmatrix} x_0 \\ \vdots \\ x_{n-1} \end{bmatrix} \in \mathbb{R}^{n \times d}$$

- Initiate hidden state :

$$H = X \in \mathbb{R}^{n \times d}$$

- Repeat K layers :

$$H \leftarrow \text{Softmax}(QK^T)V \in \mathbb{R}^{n \times d}$$

Self-attention layer

Differentiable dictionary
Dict is a standard structure in CS
Dict=(Key,Value)

Query the dictionary
for a key and its value.

$K = HW^K \in \mathbb{R}^{n \times d}, W^K \in \mathbb{R}^{d \times d}$

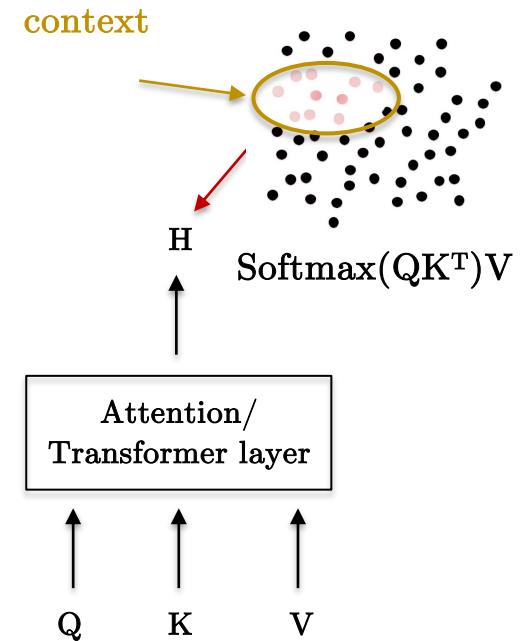
$V = HW^V \in \mathbb{R}^{n \times d}, W^V \in \mathbb{R}^{d \times d}$

$Q = HW^Q \in \mathbb{R}^{n \times d}, W^Q \in \mathbb{R}^{d \times d}$

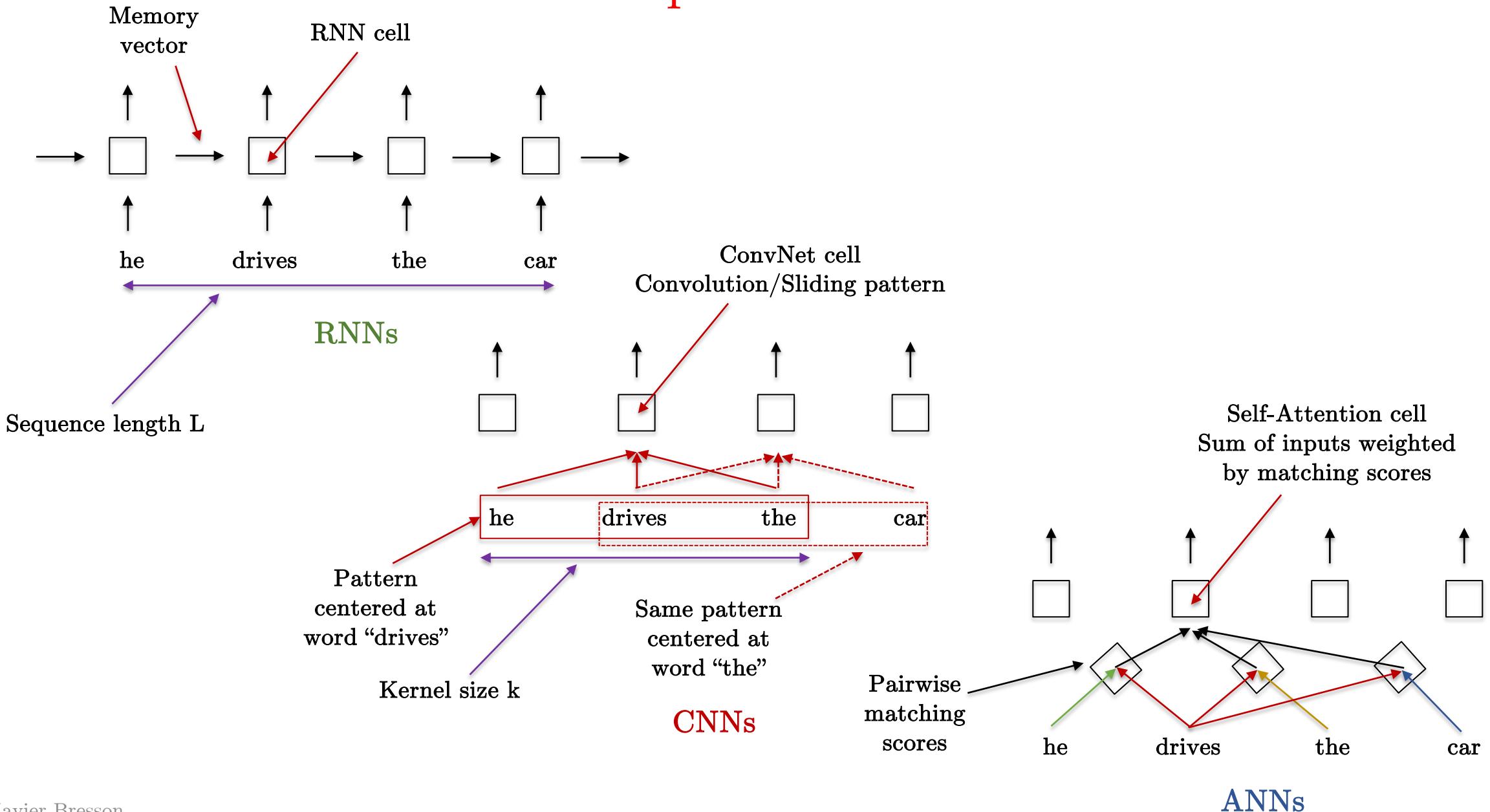
Learnable parameters

Context-to-word representation

- From **fixed word representation** to **context-to-word representation** :
$$H \leftarrow \text{Softmax}(QK^T)V \in \mathbb{R}^{n \times d}$$
- The new data representation is a sum of all input data weighted by the **pairwise matching** (or attention) scores.
- The subset of data with non-zero attention scores forms the **context**.
- The attention mechanism allows to **dynamically change** the word representation according to its context.
- Context-to-word is a powerful idea in NLP because a word may have different meanings, that can only be clarified in a particular context :
 - The vase **broke**. The news **broke**. Sandy **broke** the world record. Sandy **broke** the law. We **broke** even. The burglar **broke** into the house. Etc.



Computational cost



Computational cost

- RNN layer : $O(L \cdot d^2)$
- ConvNet layer : $O(L \cdot d^2 \cdot k)$
- Transformer layer : $O(L^2 \cdot d)$

Seems bad !

with L : sequence length, d : hidden feature size, k : kernel size

- Attention networks have actually less parameters to learn as long as $L \leq d$!

- Example 1 : $L = 100, d = 1000, k = 3$

RNN: $O(10^8)$, ConvNet: $O(3 \cdot 10^8)$, Transformer: $O(10^7)$

- Example 2 : $L = 1000, d = 1000, k = 3$

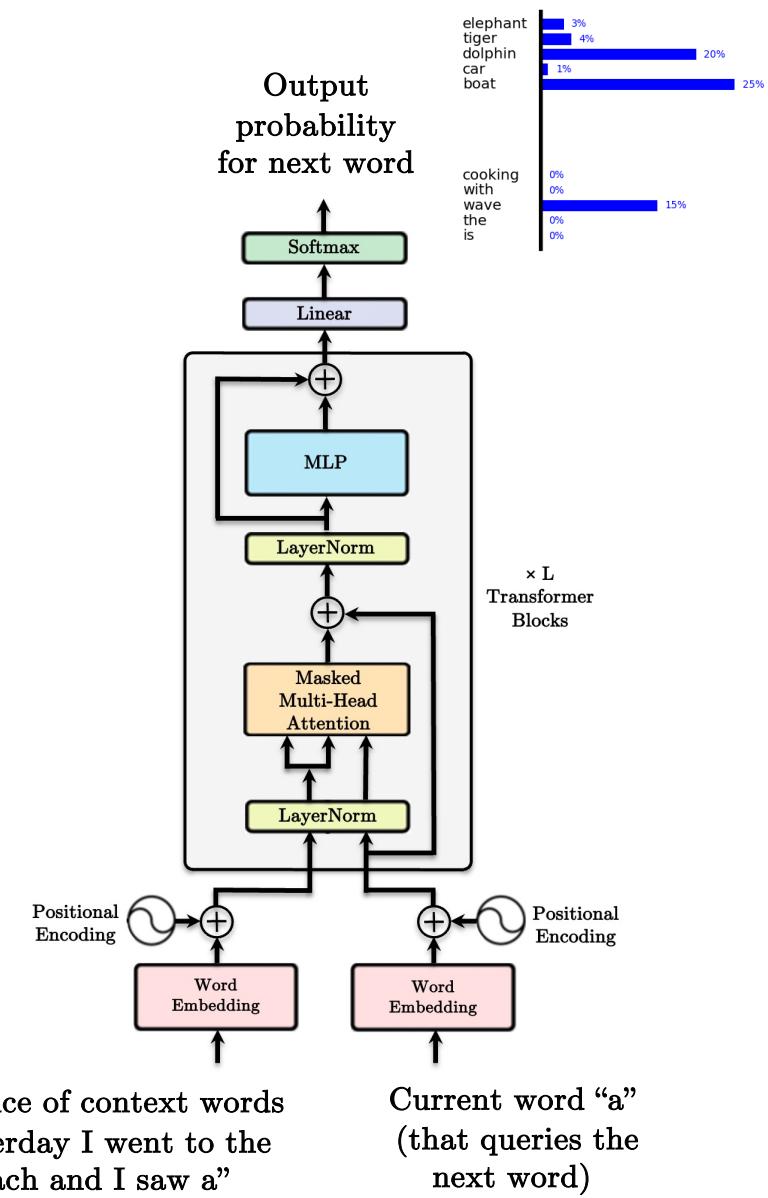
RNN: $O(10^9)$, ConvNet: $O(3 \cdot 10^9)$, Transformer: $O(10^9)$

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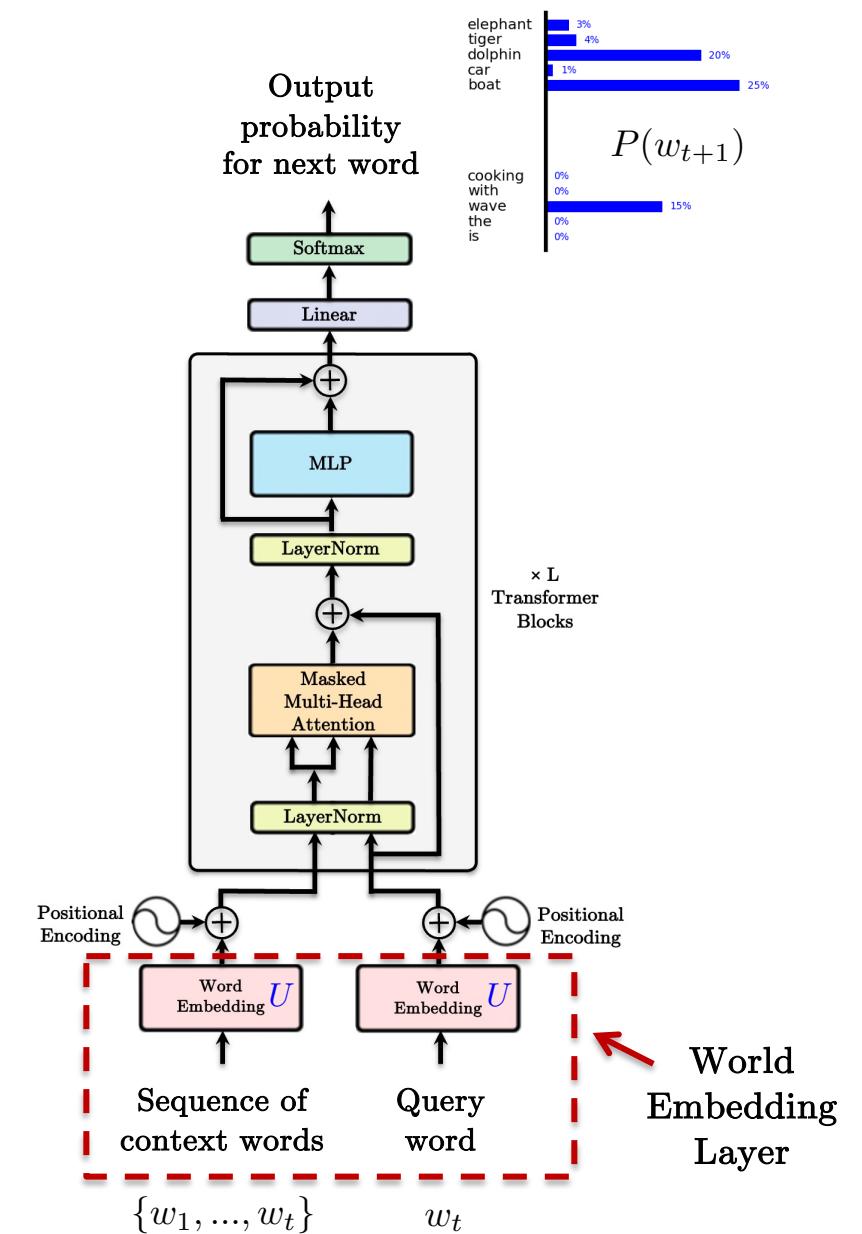
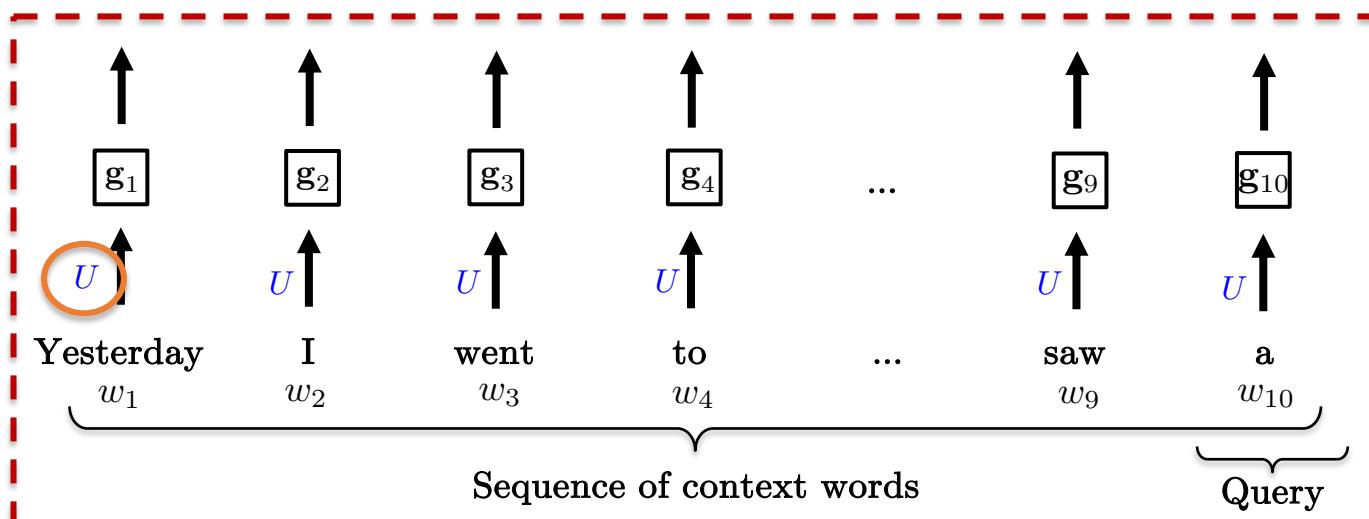
Language model transformers

- Given a sequence of words, predict the next word.
- This task to be successful requires a word representation that can be changed with different contexts.
- Transformers offer expressive word representation with its word-in-context property.
- A LM transformer is composed of three layers :
 - Word embedding layer
 - Attention layer
 - Classification layer



Word Embedding Layer

- Categorical variables (dictionary of 10,000 words) are
 - represented by one-hot vectors and then
 - embedded into a linear space.
- This is the same input embedding as in RNNs :
 - PyTorch `nn.Embedding()`



Multi-head attention

- Update equation for one MHA layer :

- PyTorch `nn.MultiheadAttention()`

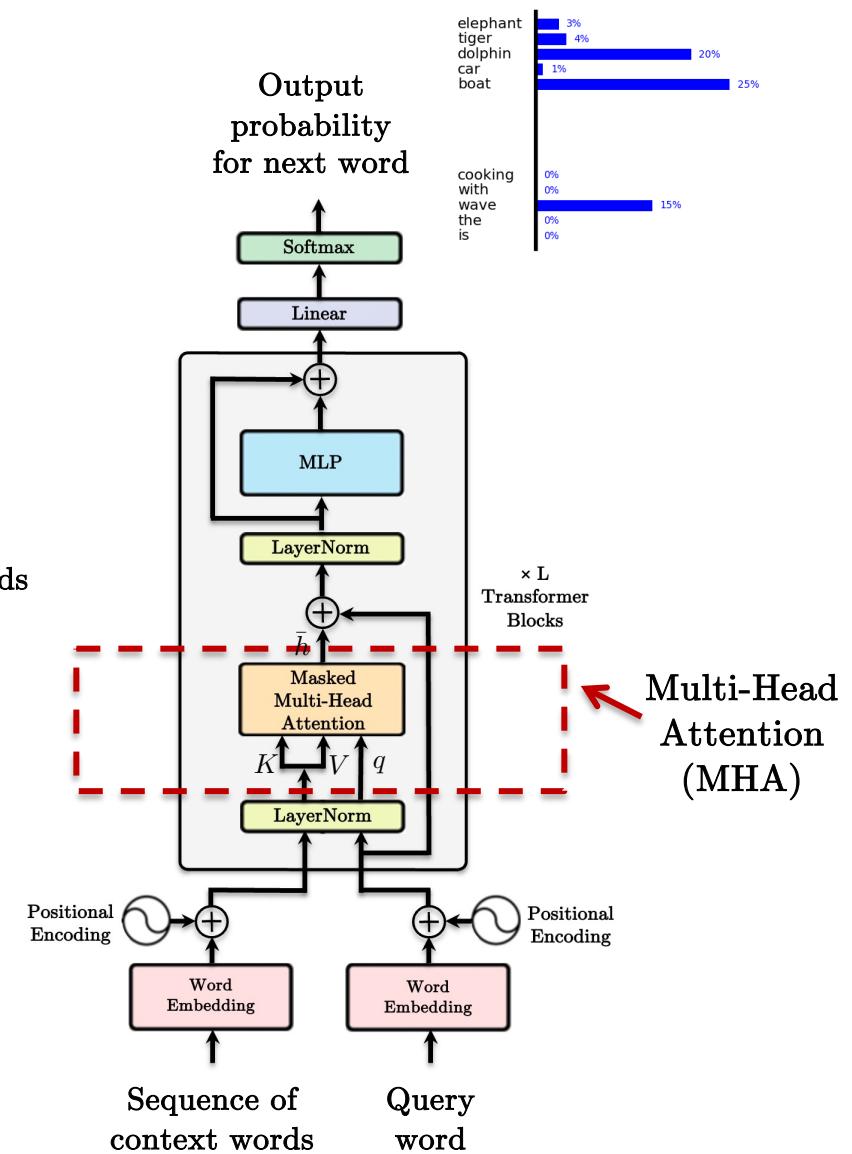
$$\begin{aligned}
 & \text{Query} \quad \text{Key} \quad \text{Value} \\
 & \bar{h} = \text{MHA}(q, K, V) \in \mathbb{R}^d, \quad q \in \mathbb{R}^d, \quad K \in \mathbb{R}^{L \times d}, \quad V \in \mathbb{R}^{L \times d} \\
 & = \left(\parallel_{h=1}^H \text{HA}_h(q, K, V) \right) W^O, \quad W^O \in \mathbb{R}^{d \times d} \\
 & \text{Concatenation operation with } q = g_t \in \mathbb{R}^d, \quad K = V = \{g_t, g_{t-1}, \dots, g_{t-(L-1)}\} \in \mathbb{R}^{L \times d} \\
 & \text{We consider sequence of L words}
 \end{aligned}$$

$$\text{HA}_h(q, K, V) = \text{Softmax}\left(\frac{q_h K_h^T}{\sqrt{d/H}}\right) V_h \in \mathbb{R}^{d/H}$$

$$\text{with } q_h = q W_h^q \in \mathbb{R}^{d/H}, \quad W_h^q \in \mathbb{R}^{d \times d/H}$$

$$K_h = K W_h^K \in \mathbb{R}^{n \times d/H}, \quad W_h^K \in \mathbb{R}^{d \times d/H}$$

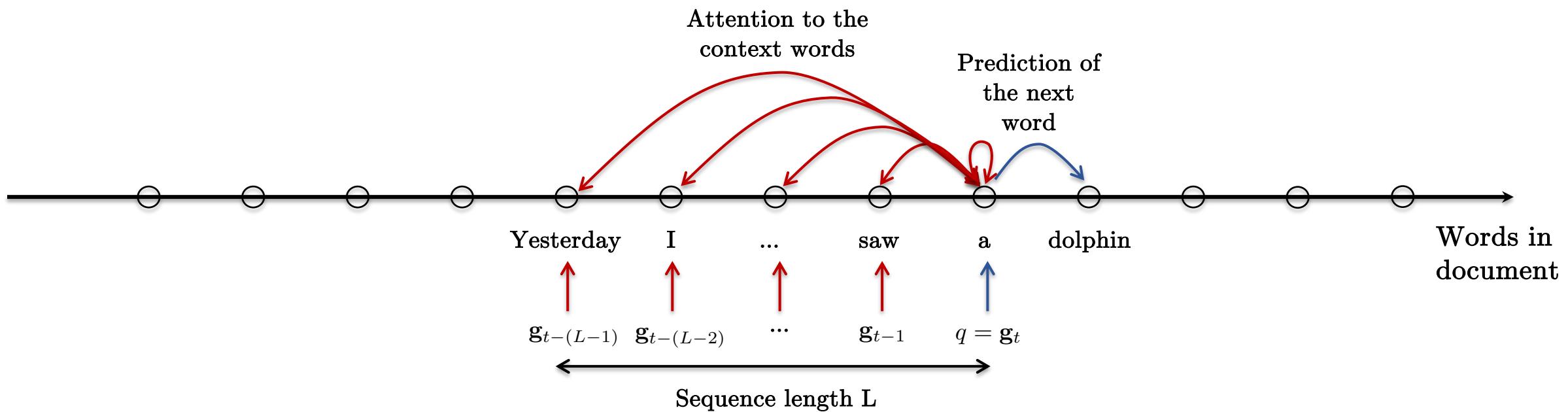
$$V_h = V W_h^V \in \mathbb{R}^{n \times d/H}, \quad W_h^V \in \mathbb{R}^{d \times d/H}$$



Head attention layer

- Equation of a single head attention layer :

$$\text{HA}(q, K, V) = \text{Softmax}\left(\frac{qK^T}{\sqrt{d}}\right)V \in \mathbb{R}^{1 \times d}, q \in \mathbb{R}^{1 \times d}, K \in \mathbb{R}^{L \times d}, V \in \mathbb{R}^{L \times d}$$



Transformer block

- Transformer or attention block layer (2017) :

$$\bar{h} = \text{LN}(q + \text{MHA}(q, K, V)) \in \mathbb{R}^d$$

$$h = \text{LN}(\bar{h} + \text{MLP}(\bar{h})) \in \mathbb{R}^d$$

Layer normalization

z-scoring with learnable parameters

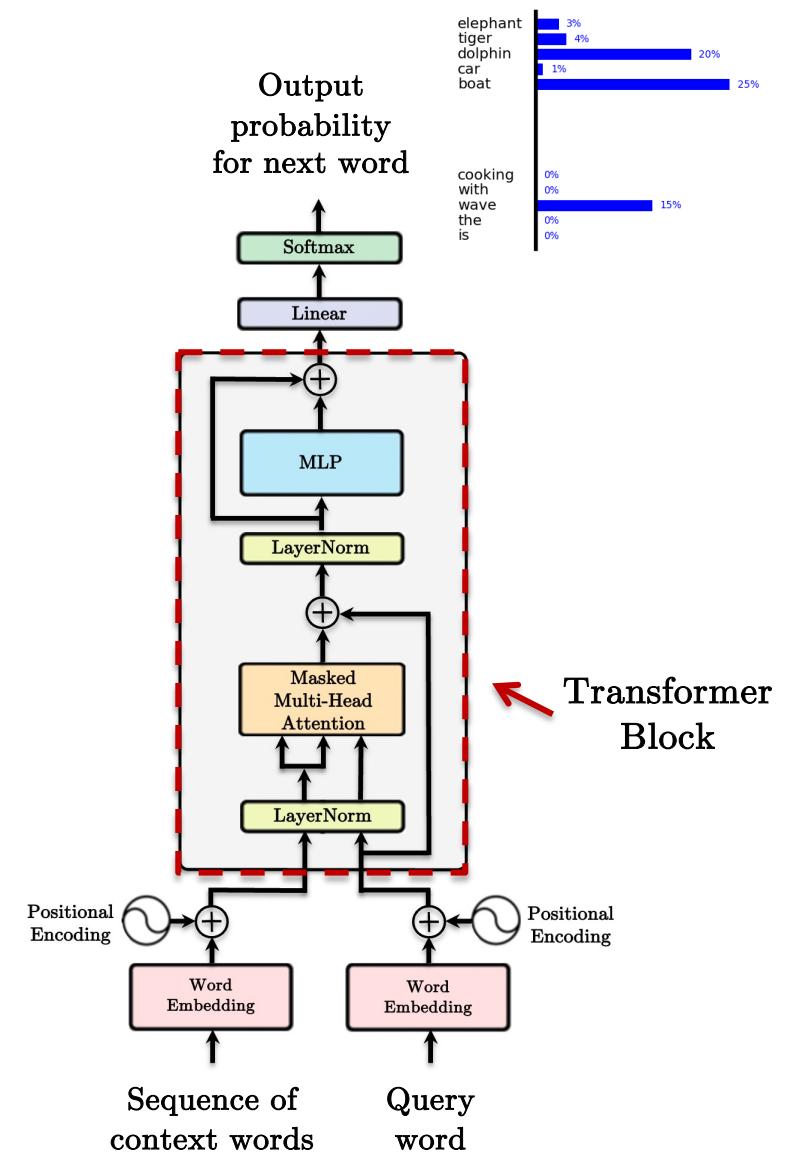
`nn.LayerNorm()`

Residual connection

- In 2019, LayerNorm (LN) was applied before non-linear operations :

$$\bar{h} = q + \text{MHA}(\text{LN}(q), \text{LN}(K), \text{LN}(V)) \in \mathbb{R}^d$$

$$h = \bar{h} + \text{MLP}(\text{LN}(\bar{h})) \in \mathbb{R}^d$$



LayerNorm and residual connection

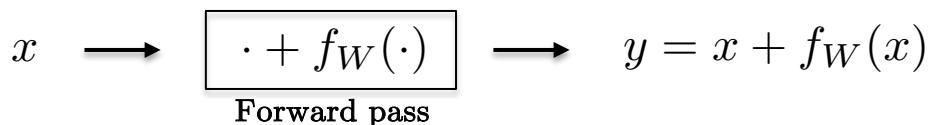
- Layer normalization :

$$\text{LN}(q) = a \odot \left(\frac{q - \mu}{\sigma} \right) + b \in \mathbb{R}^d$$

z-scoring

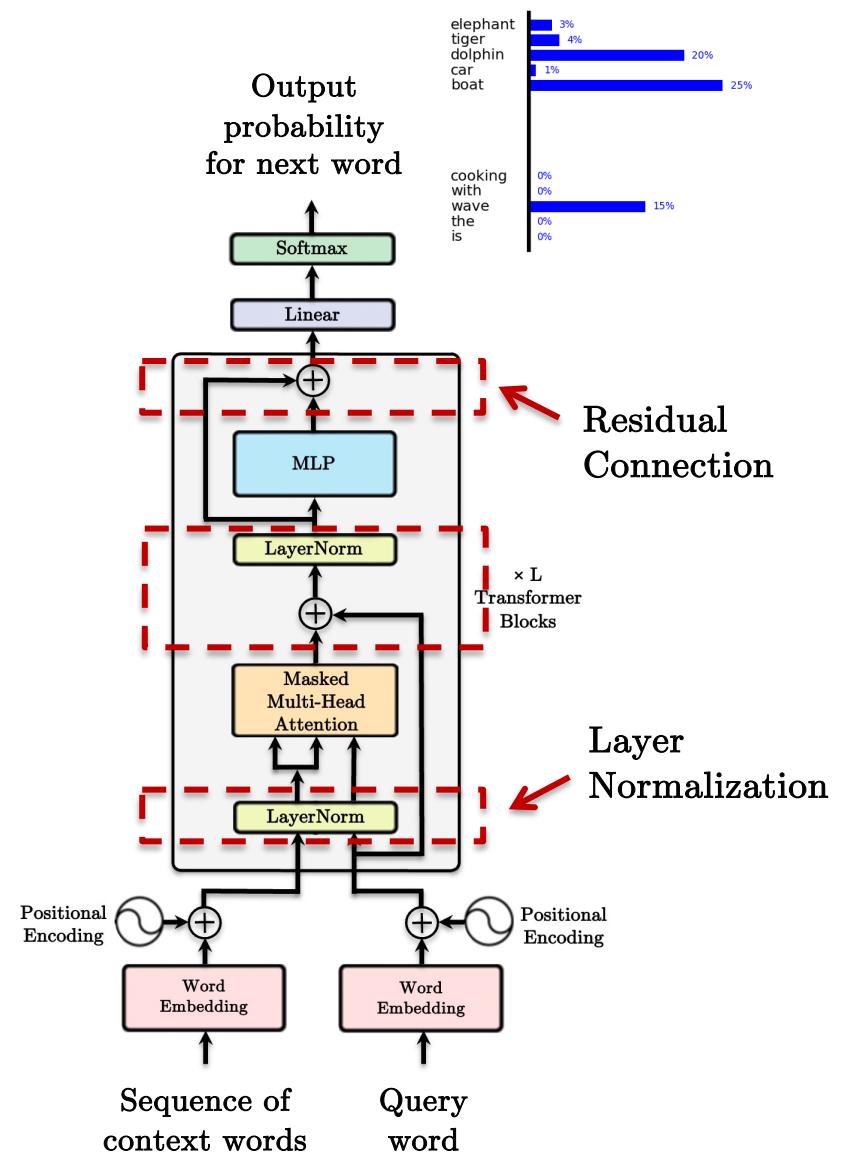
with $\mu = \text{Mean}(q) \in \mathbb{R}, \sigma = \text{Std}(q) \in \mathbb{R}, a, b \in \mathbb{R}^d$

- Residual/skip connection :



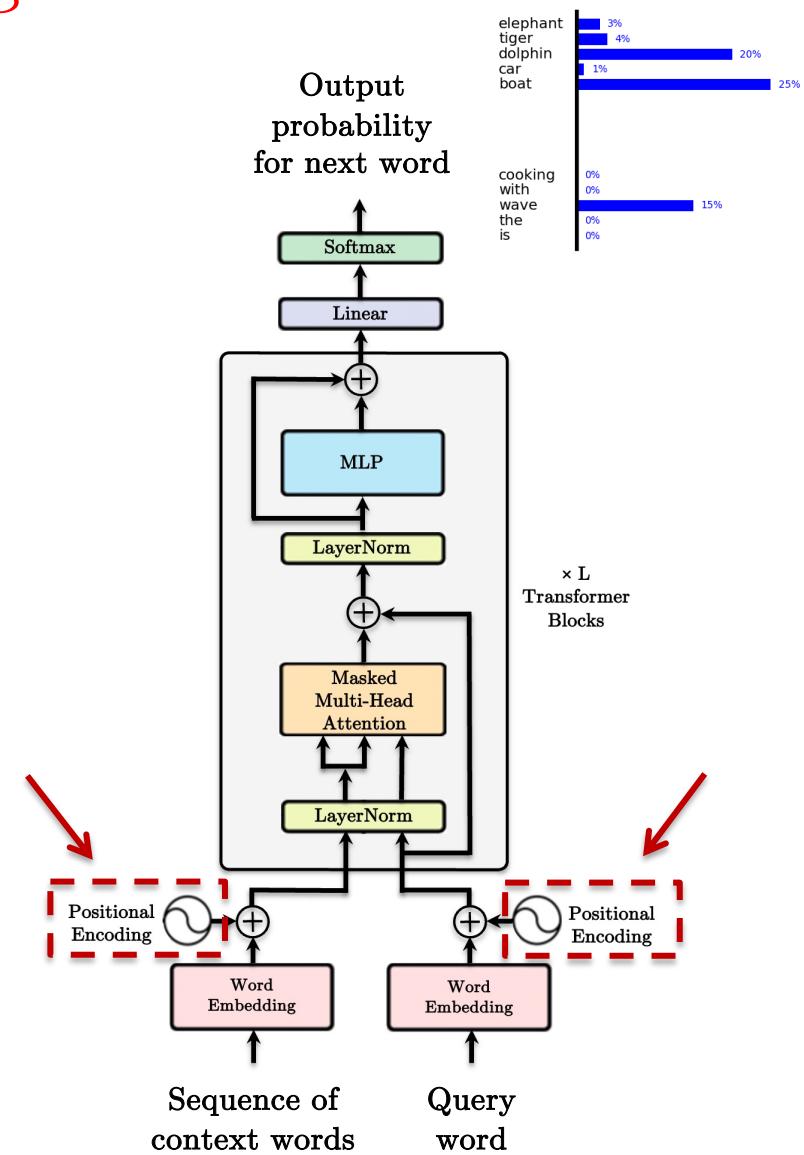
$$\begin{aligned} \frac{\partial L}{\partial x} &= \frac{\partial L}{\partial y} \frac{\partial y}{\partial x} \leftarrow \boxed{\cdot + f_W(\cdot)} \leftarrow \frac{\partial L}{\partial y} \\ &= \frac{\partial L}{\partial y} (\text{Id} + \nabla_x f_w) \\ &= \frac{\partial L}{\partial y} + \frac{\partial L}{\partial y} \nabla_x f_w \end{aligned}$$

No vanishing gradient
for residual connection



Positional encoding

- Transformers are designed to process **sets of vectors** but items in a set are **not** ordered.
- This is an **issue** for NLP tasks.
 - An **additional ordering feature** is required to inject causal ordering in the attention mechanism.
- Two classes of Positional Encoding (PE) :
 - Learnable vs non-learnable PE
- **Learnable PE** :
 - Embedding of discrete ordering index $0, 1, 2, 3, \dots, L-1$, with L is the sequence length.
 - Two issues :
 - Requires to know the maximum L value among all training sequences.
 - Some test sequences may have lengths not present in the train set.



Positional encoding

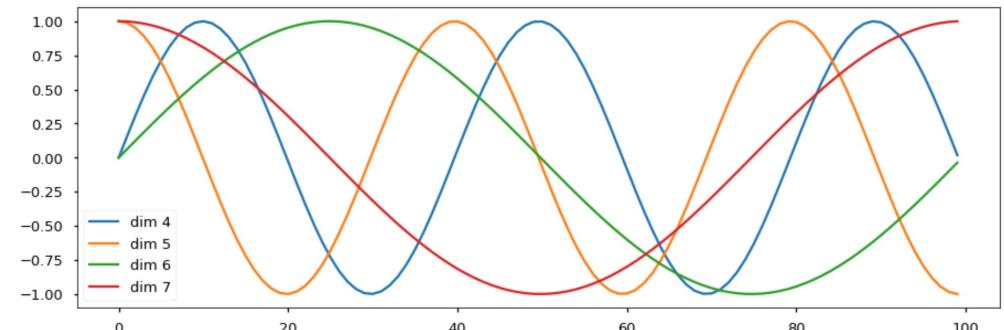
- Non-learnable PE :
 - Continuous ordering with `sin` and `cos` functions.
 - Advantages :
 - No training necessary
 - No need to know the maximum length in the train set.
 - Test sequences may have lengths not present in the train set.

$\text{PE}_t \in \mathbb{R}^d$ is defined as

$$\text{PE}_{t,i} = \begin{cases} \sin(2\pi f_i t) & \text{if } i \text{ is even,} \\ \cos(2\pi f_i t) & \text{if } i \text{ is odd,} \end{cases} \quad \text{with } f_i = \frac{10,000^{\frac{d}{12i}}}{2\pi}.$$

with $\|\text{PE}_t - \text{PE}_{t'}\|_2 \propto \text{Dist}(t, t') = |t - t'| \in \mathbb{R}_+$

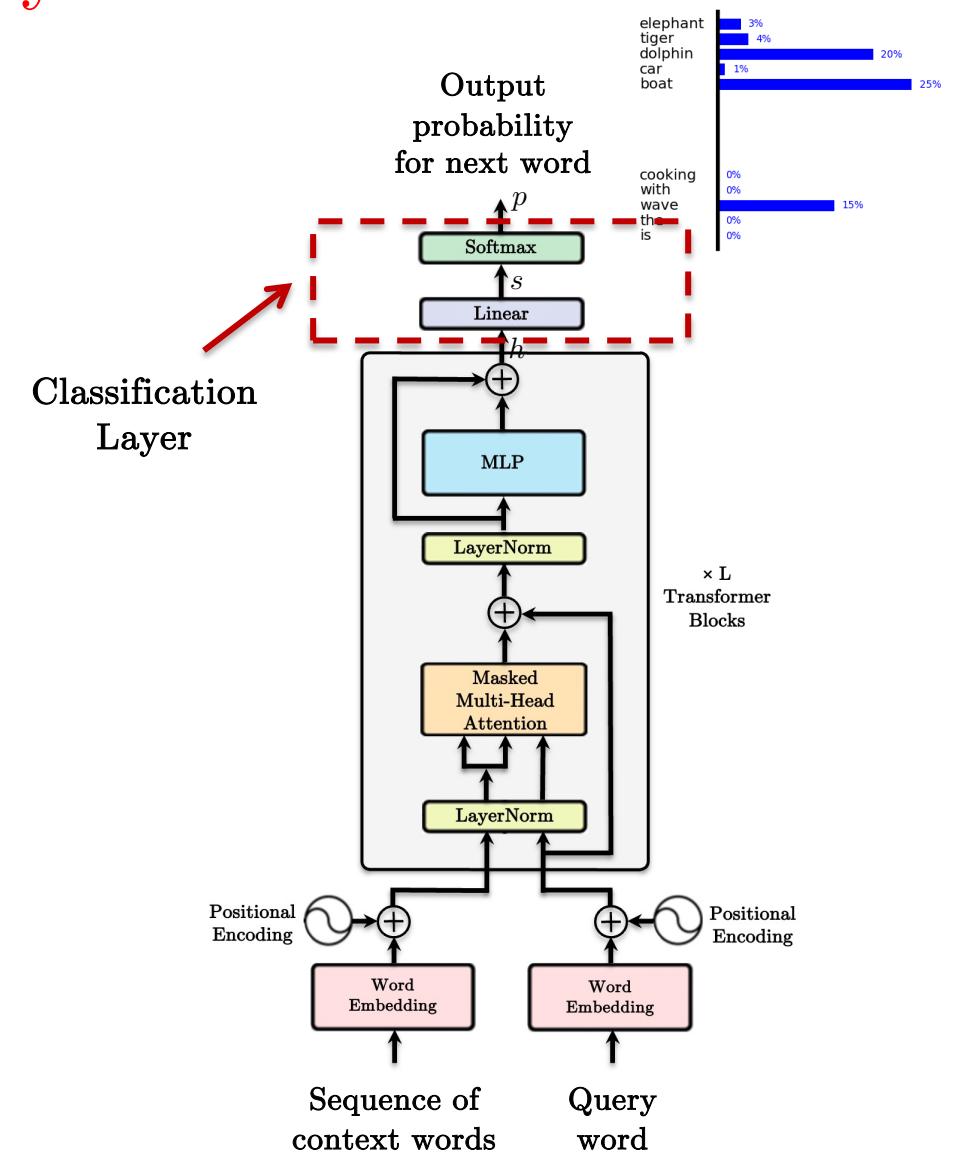
because these PEs are the eigenvectors of the line.



Classification layer

- The last layer is a standard linear layer to compute the scores of the next word in the sequence, followed by a Softmax function to produce the probability vector.

Linear layer
 $s = LL(h) \in \mathbb{R}^V$
 $p = \text{Softmax}(s) \in \mathbb{R}^V$



Efficient training

- It is possible to train **in parallel** the prediction of the next words in a sequence.
- For this, we need to hide the future words with a **masked attention matrix**.
- Here is the **process** :
 - Step 1 : Compute the attention matrix.
 - Step 2 : Mask next word to predict.
 - Step 3 : Softmax calculation.
 - Step 4 : Calculate weighted linear combination.

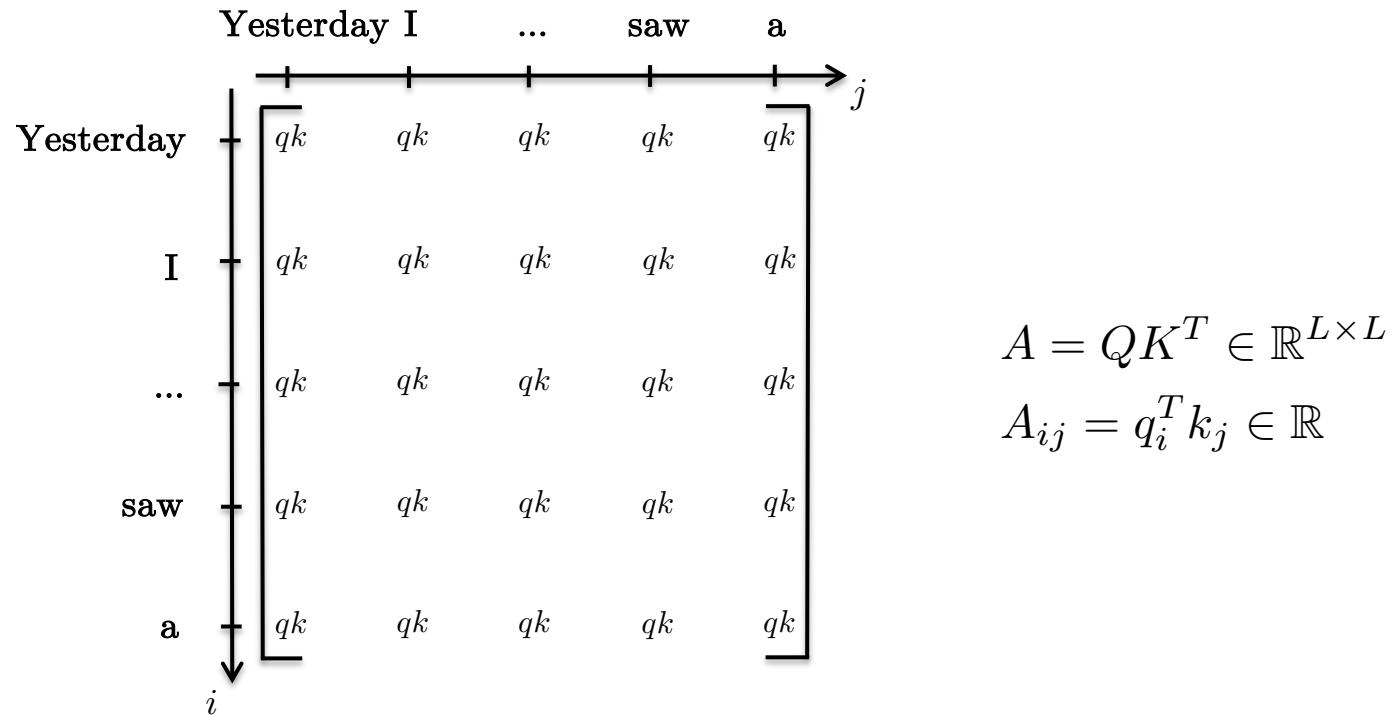
$$\text{Mask-HA}(Q, K, V) = \text{Softmax}\left(\frac{QK^T}{\sqrt{d}} \odot \text{Mask}\right)V,$$

with $Q, K, V \in \mathbb{R}^{L \times d}$, $\text{Mask} \in \mathbb{R}^{L \times L}$,

$$\text{and } \text{Mask}_{ij} = \begin{cases} 1 & \text{if attention between } i \text{ and } j \\ -\infty & \text{if no attention} \end{cases}$$

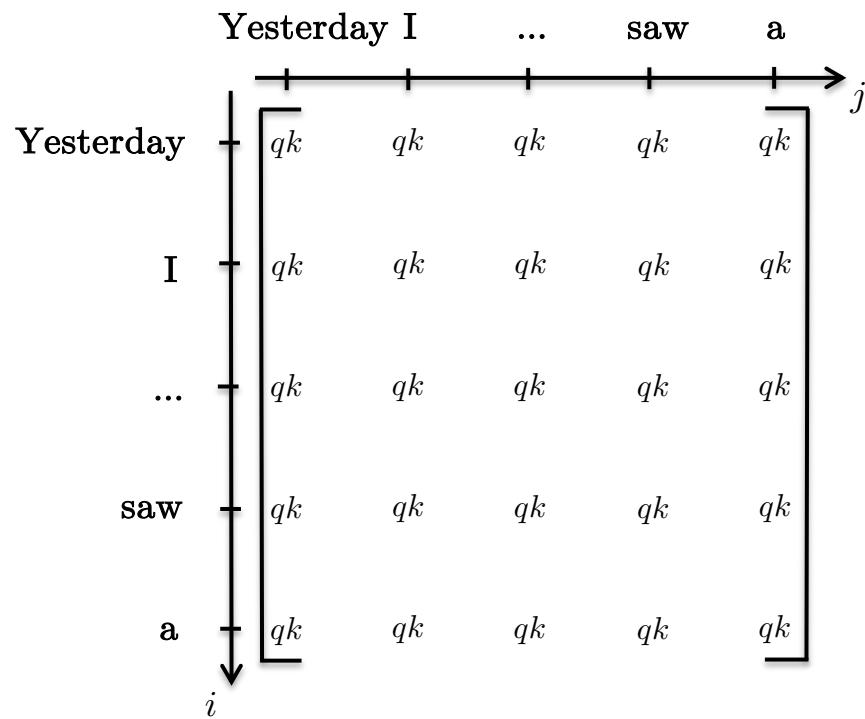
Attention matrix

- Step 1 : Compute the attention matrix A , i.e. A_{ij} is the dot product between word vector q_i and word vector k_j .
- Two similar vectors will receive a high value and inversely, two dissimilar ones a low value.



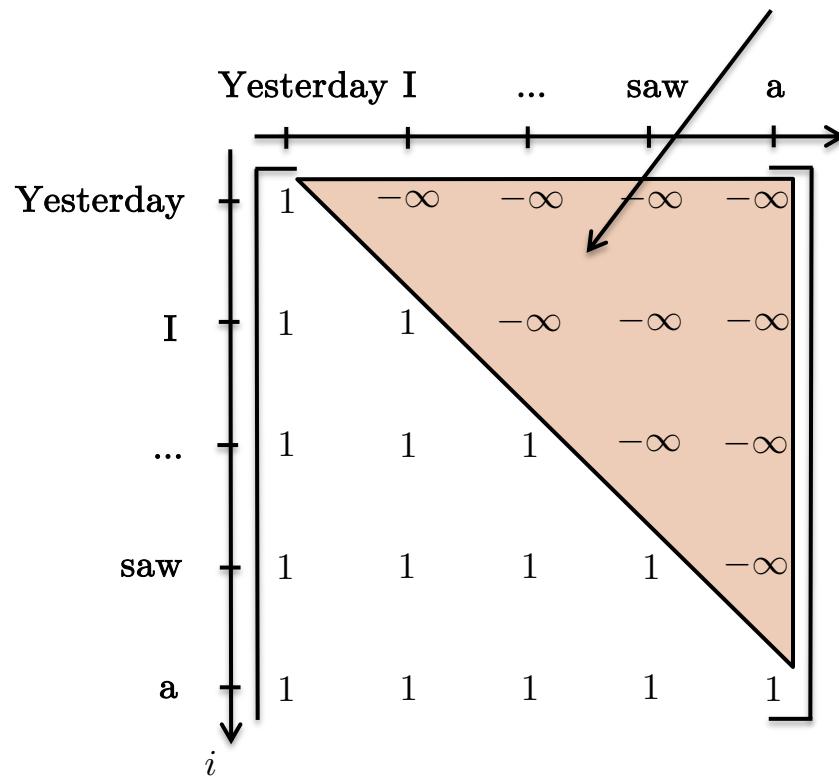
Masked attention

- Step 2 : Mask next word to predict



• Pointwise multiplication

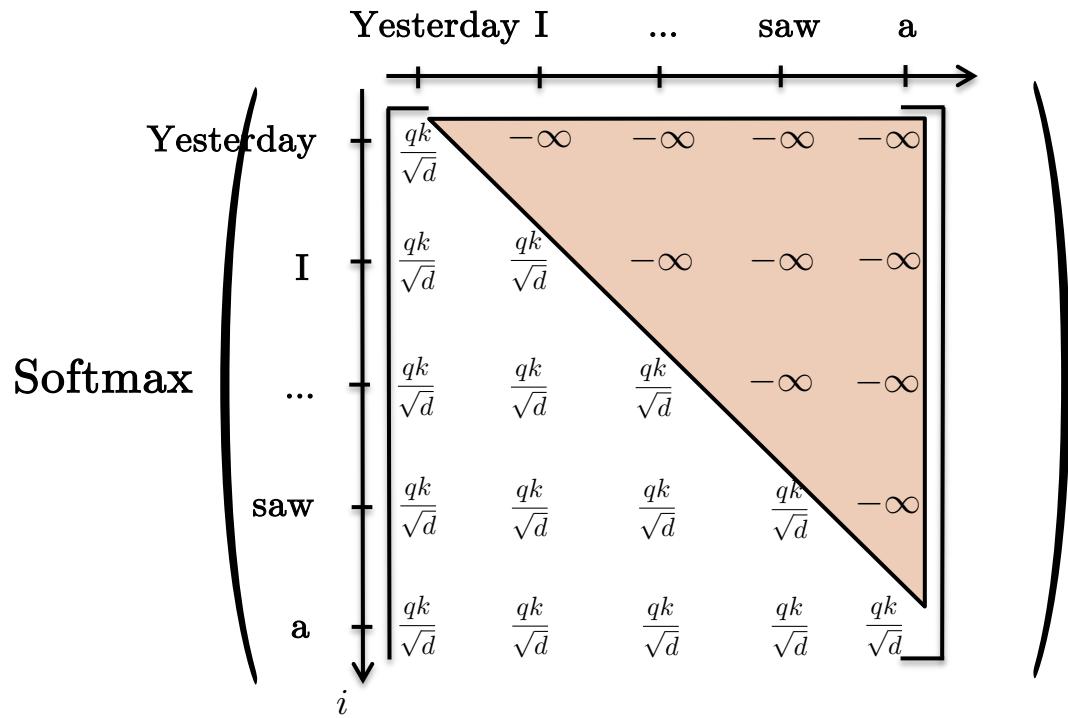
Hide these words during next word prediction



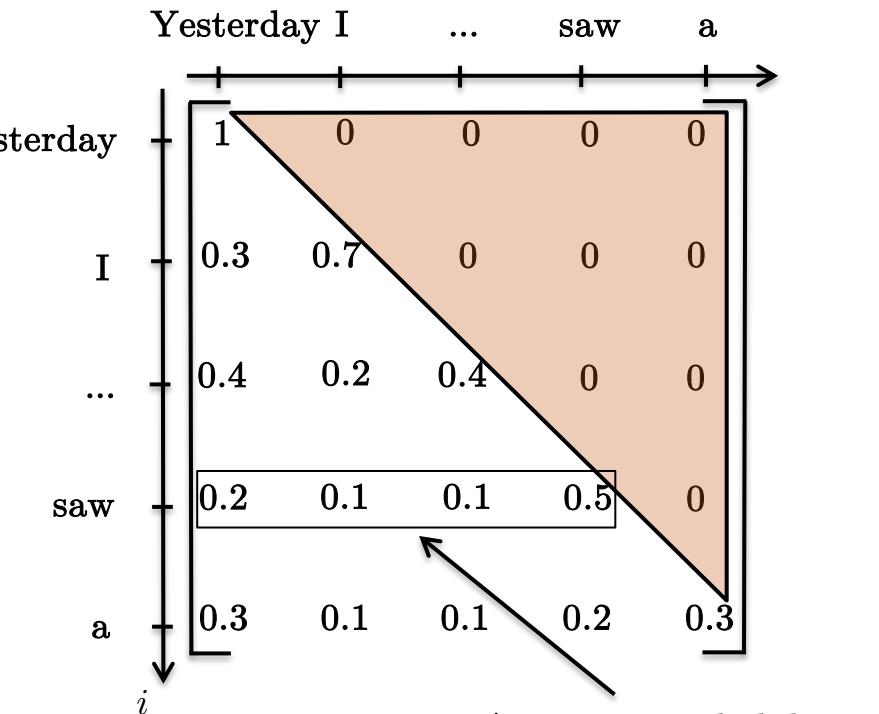
$$\text{Mask}_{ij} = \begin{cases} 1 & \text{if attention between } i \text{ and } j \\ -\infty & \text{if no attention} \end{cases}$$

Masked attention

- Step 3 : Softmax calculation



=



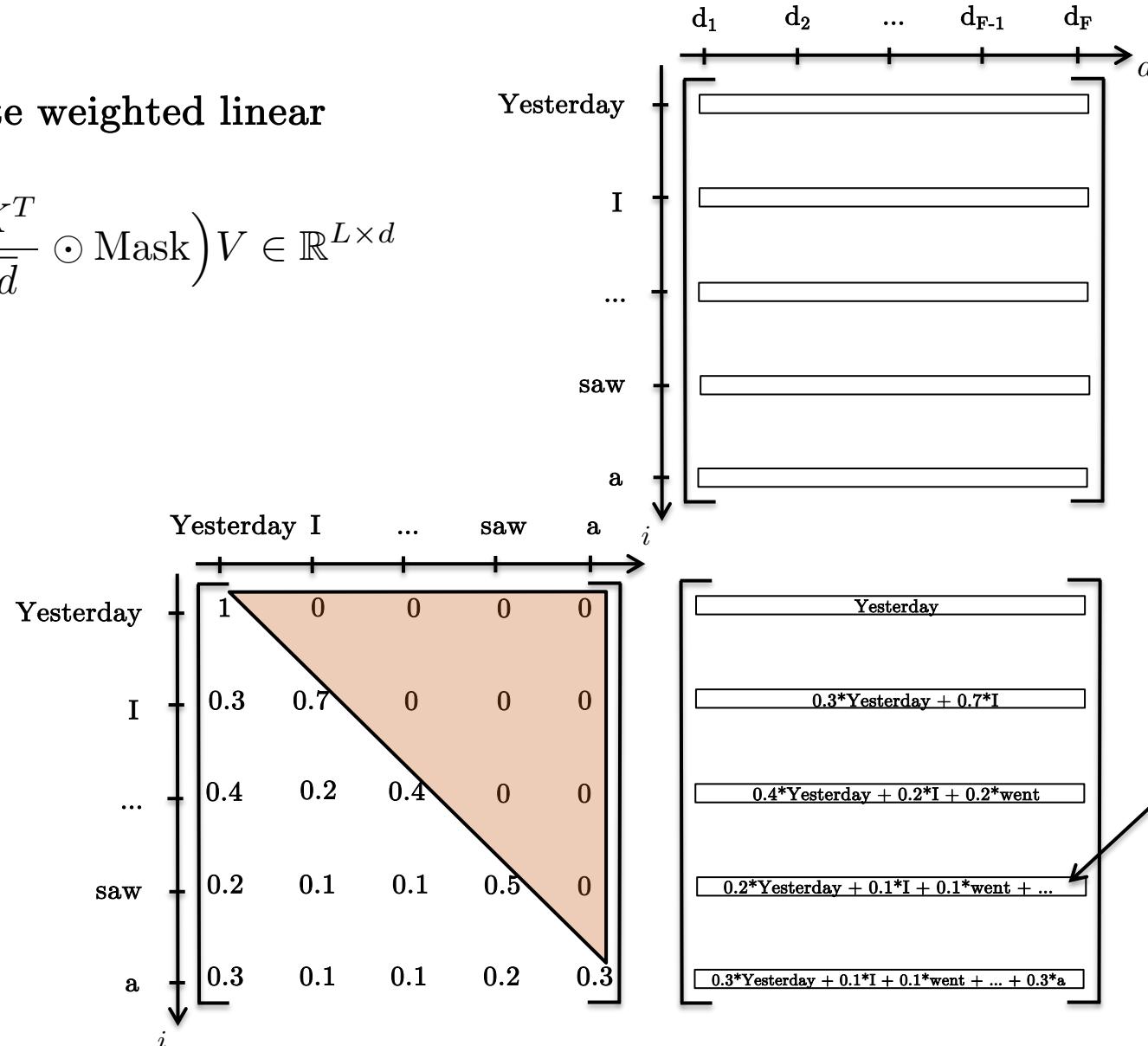
Attention probability
between "saw" and
"yesterday", "I", ... "saw".

$$\text{Softmax}_{\text{row}} \left(\frac{QK^T}{\sqrt{d}} \odot \text{Mask} \right) \in \mathbb{R}^{L \times L}$$

Updated word vectors

- Step 4 : Calculate weighted linear combination

$$\text{Softmax}_{\text{row}} \left(\frac{QK^T}{\sqrt{d}} \odot \text{Mask} \right) V \in \mathbb{R}^{L \times d}$$



Masked transformer blocks

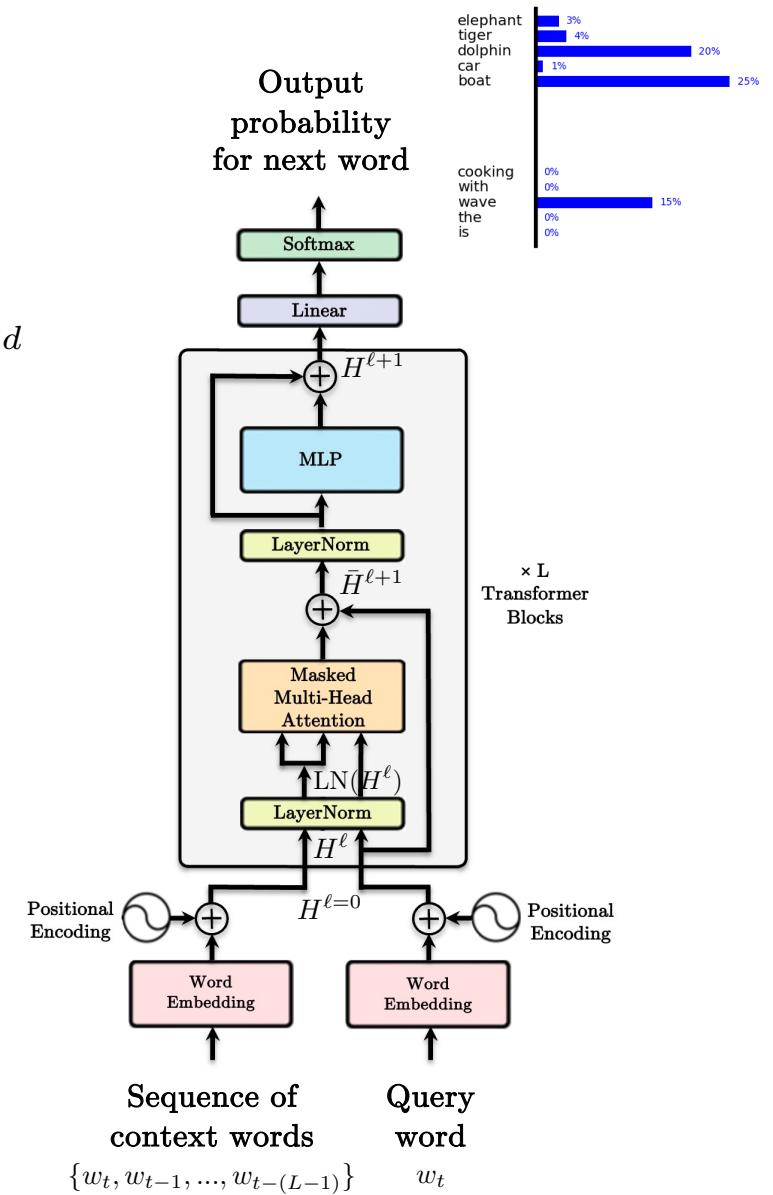
- Stack multiple masked transformer blocks :

For $\ell = 0, 1, 2, \dots, L - 1$

$$\bar{H}^{\ell+1} = H^\ell + \text{Mask-MHA}(\text{LN}(H^\ell), \text{LN}(H^\ell), \text{LN}(H^\ell)) \in \mathbb{R}^{L \times d}$$

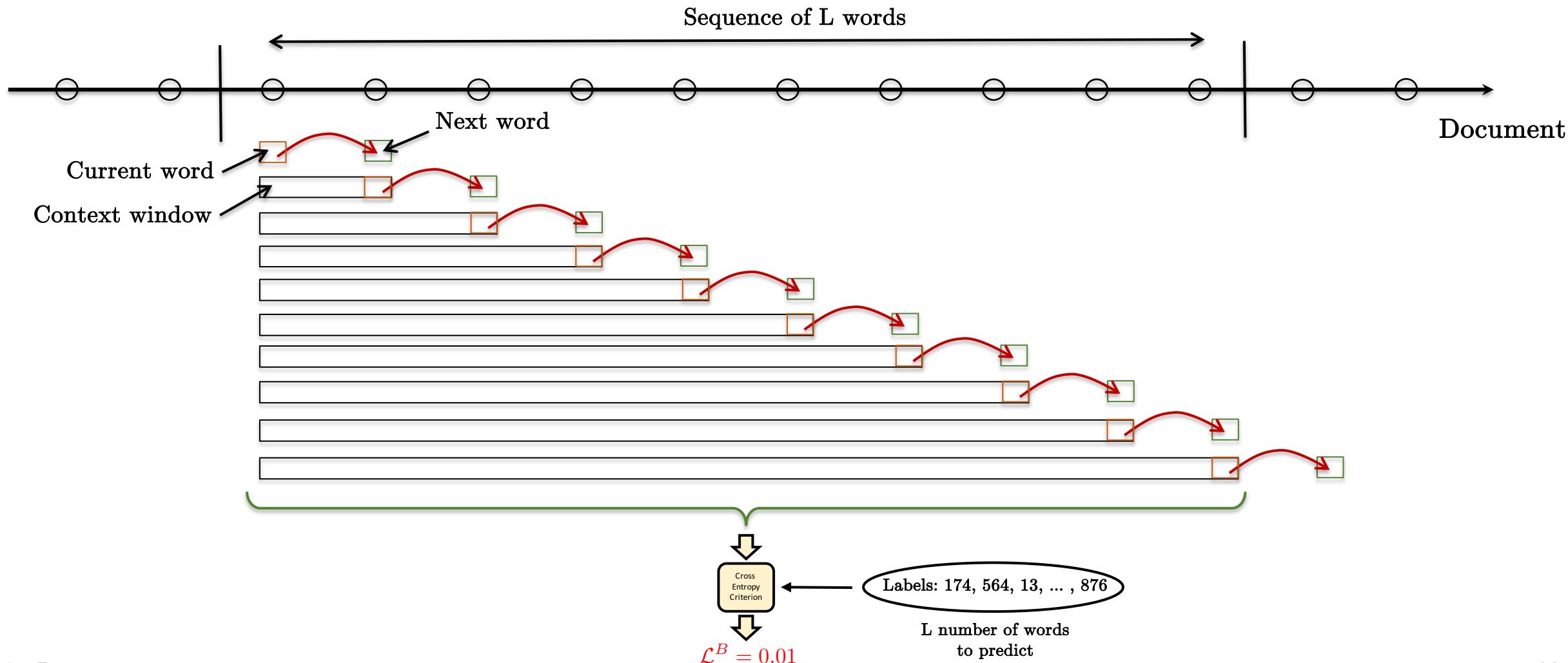
$$H^{\ell+1} = \bar{H}^{\ell+1} + \text{MLP}(\text{LN}(\bar{H}^{\ell+1})) \in \mathbb{R}^{L \times d}$$

with $H^{\ell=0} = \text{LL}(\{w_t, w_{t-1}, \dots, w_{t-(L-1)}\}) + \text{PE} \in \mathbb{R}^{L \times d}$



Training with mini-batch

- Training is done with a batch size of B sequences and batch length of L .



Generation

- The transformer network is trained in parallel (using the mask to hide the predicted words).
- After training, the mask is not required anymore (there are no future words to hide).
- And the sequence is generated auto-regressively, i.e. one word at a time.

Generate the next word w_{t+1} as follows:

Compute output of Transformer net:

for $\ell = 0, \dots, L - 1$

$$\bar{q}^{\ell+1} = q^\ell + \text{MHA}(\text{LN}(q^\ell), \text{LN}(K^\ell), \text{LN}(V^\ell)) \in \mathbb{R}^d$$

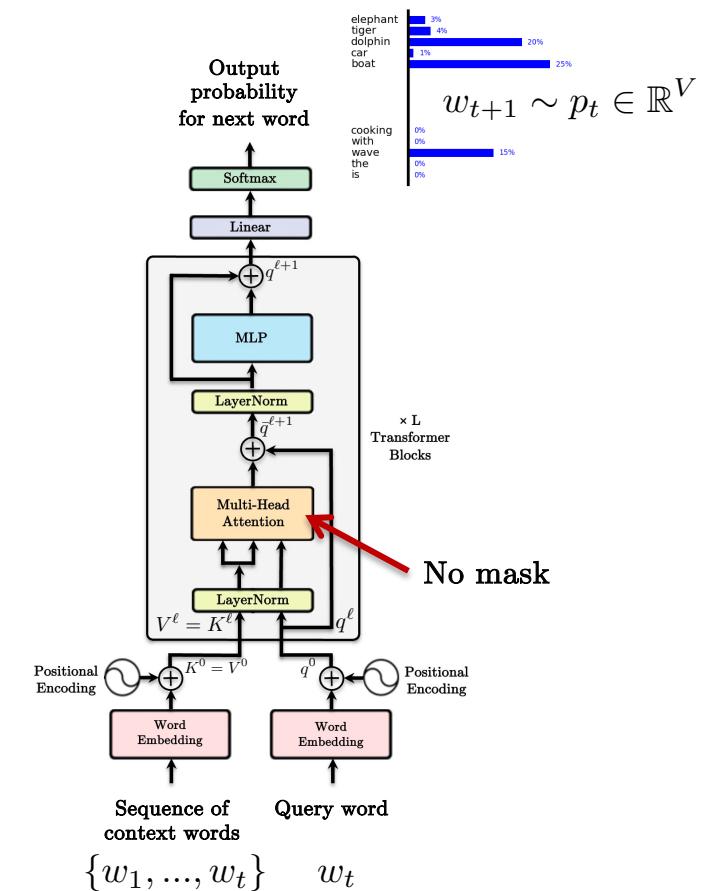
$$q^{\ell+1} = \bar{q}^{\ell+1} + \text{MLP}(\text{LN}(\bar{q}^{\ell+1})) \in \mathbb{R}^d$$

$$\text{with } q^{\ell=0} = \text{LL}(w_t) + \text{PE}_t \in \mathbb{R}^d$$

$$K^{\ell=0} = V^{\ell=0} = \text{LL}(\{w_1, \dots, w_t\}) + \text{PE} \in \mathbb{R}^{t \times d}$$

Get output probability $p_t = \text{Softmax}(\text{LL}(q^{\ell=L})) \in \mathbb{R}^V$

Sample next word probability $w_{t+1} \sim p_t$.



Lab 01

- PyTorch implementation of Language Model Transformers

jupyter transformer_language_modeling Last Checkpoint: 3 hours ago (autosaved)

File Edit View Insert Cell Kernel Widgets Help Trusted Python 3 (ipykernel) Logout

In [2]: # For Google Colaboratory
import sys
if 'google.colab' in sys.modules:
 # mount google drive
 from google.colab import drive
 drive.mount('/content/gdrive')
 # find automatically the path of the folder containing "file_name":
 file_name = 'transformer_language_modeling.ipynb'
 import subprocess
 path_to_file = subprocess.check_output('find . -type f -name \'' + str(file_name) + '\', shell=True).decode("utf-8")
 path_to_file = path_to_file.replace(file_name,'').replace('\n','')
 # if previous search failed or too long, comment the previous line and simply write down manually the path below:
 path_to_file = '/content/gdrive/My Drive/CS5242_notebooks/labs_lecture12/lab01_language_model/'
 print(path_to_file)
 # change current path to the folder containing "file_name"
 os.chdir(path_to_file)
 !pwd

Drive already mounted at /content/gdrive; to attempt to forcibly remount, call drive.mount("/content/gdrive", force_remount=True).
/content/gdrive/My Drive/CS5242_notebooks/labs_lecture12/lab01_language_model/
/content/gdrive/My Drive/CS5242_notebooks/labs_lecture12/lab01_language_model

In [3]: import torch
import torch.nn.functional as F
import torch.nn as nn
import math
import time
import utils

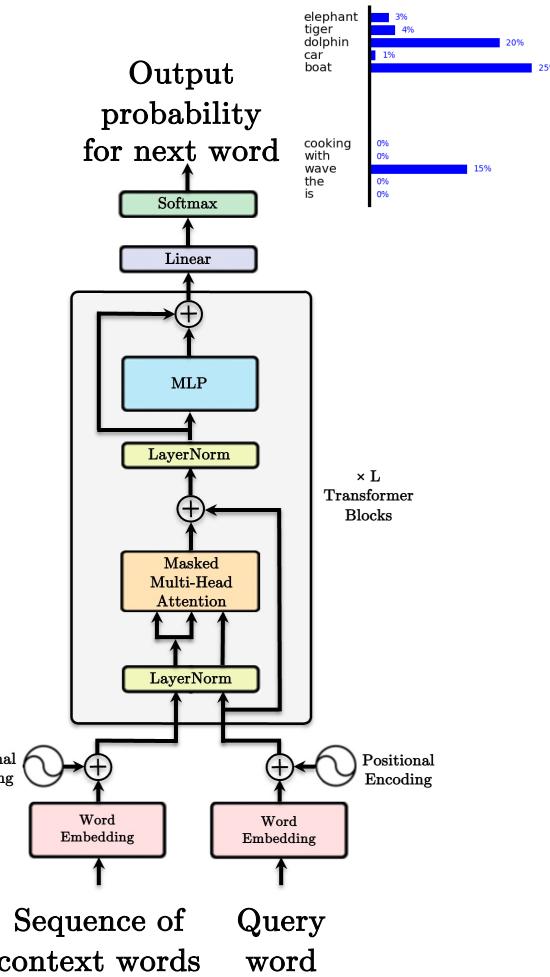
GPU

It is recommended to run this code on GPU:

- Time for 1 epoch on GPU: 48 sec w/ Google Colab Tesla P100-PCIE-16GB

In [4]: device= torch.device("cuda")
device= torch.device("cpu")
print(device)

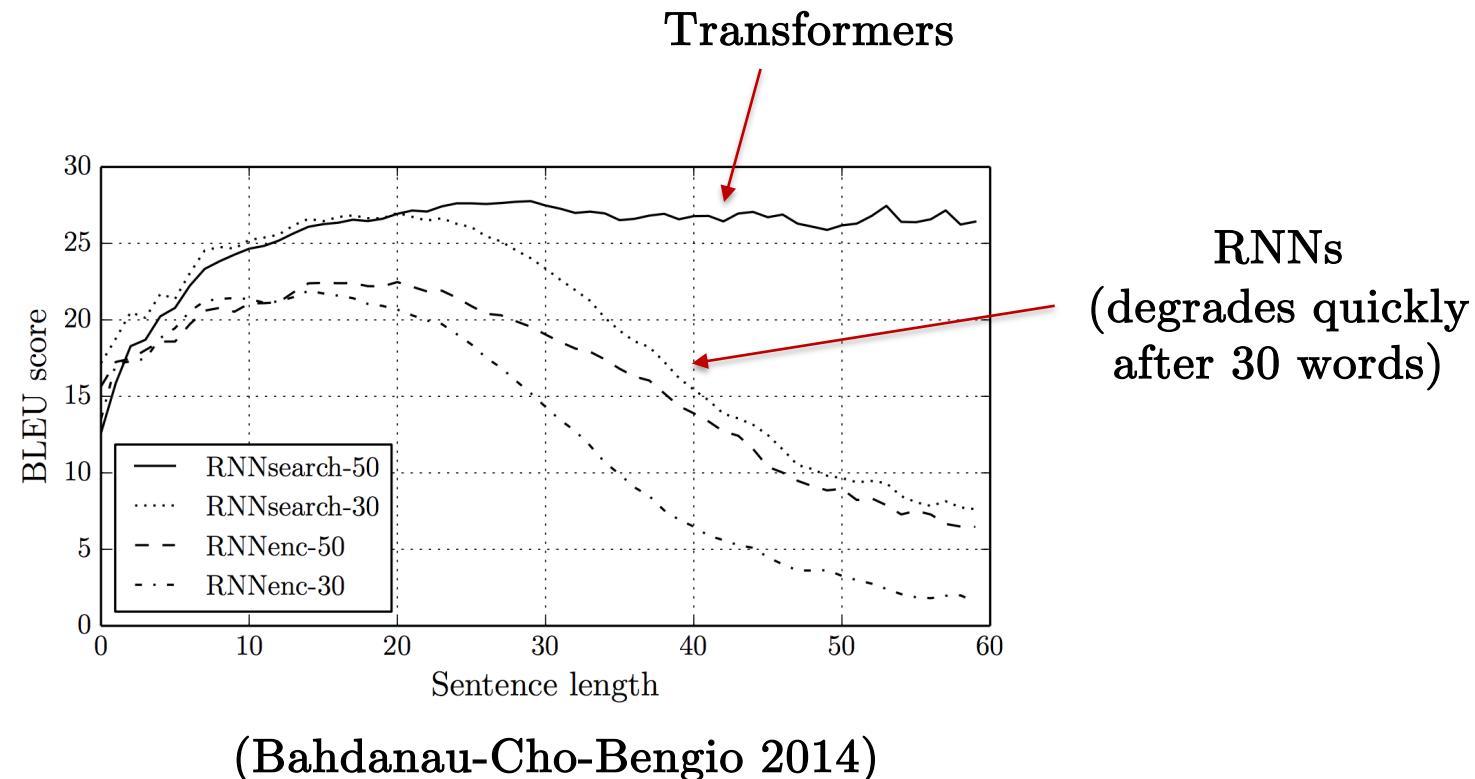
if torch.cuda.is_available():
 print('cuda available with GPU:',torch.cuda.get_device_name(0))



Lab 01

Attention mechanism

- It is a **breakthrough** idea in NLP !
- It is as **revolutionary** as CNNs in Computer Vision.

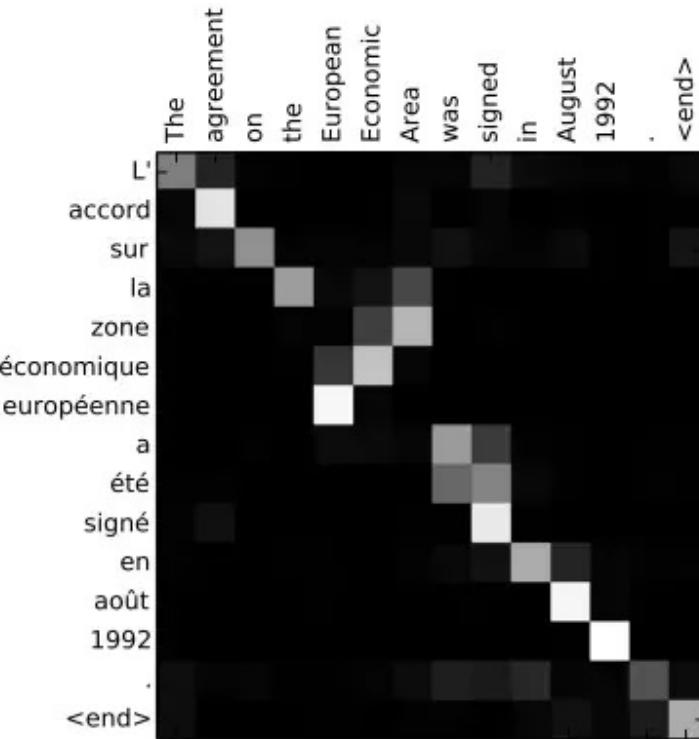


Why attention nets are better?

- Why casting the LM task as a soft alignment/attention problem is a great idea ?
- With RNNs, the very long sequence requires to be memorized and represented by a single vector.
- RNN architectures with a single memory vector cannot simply deal with long sequences (limit of non-linear dynamic systems).
- We ask too much to memorize everything with one vector!
- With attention, we distribute the memorization load over each pair of words.
- Each word in the target sequence only needs to find its match with the word (or a few words) in the source target.
- It solves the limitation of long-term dependencies in RNNs (a word in the target sequence communicates with all words in the source sequence).
- The matching is made easy by transforming the words with hidden representations.
- Attention is a key mathematical structure for NLP and several other domains.
- SOTA for all NLP tasks since 2019.

Attention interpretation

- The attention score matrix provides the matching between words in a sequence :



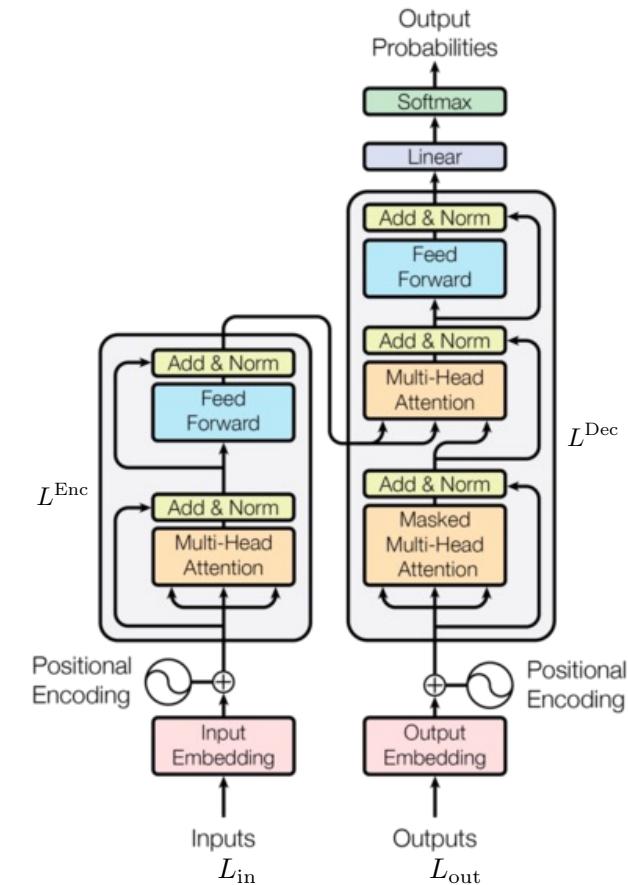
$$\text{Softmax}_{\text{row}}\left(\frac{QK^T}{\sqrt{d}}\right) \in \mathbb{R}^{L \times L}$$

Outline

- Language Models
- Memory Networks
- Transformers
- Language Model Transformers
- **Sequence-To-Sequence Transformers**
- Transfer Learning
- Conclusion

Seq2Seq Transformers

- Given a sequence of words, convert it into a different sequence.
- Basic tasks in NLP
 - Translation
 - Question & Answer
 - Summarization
- A Seq2Seq Transformer is composed of
 - Word embedding layer
 - Self-attention encoding layer
 - Self-attention decoding layer
 - Cross-attention layer
 - Classification layer



Input(EN): He drives the car

Output(FR): Il conduit la voiture

Seq2Seq Transformer Architecture
(Vaswani-et-al Google Brain 2017)

Self-attention encoder

- Encode the complete input sequence with a self-attention layer :

$$\bar{H} = \text{MHA}(H) \in \mathbb{R}^{L_{\text{in}} \times d}, H \in \mathbb{R}^{L_{\text{in}} \times d}$$

$$= \left(\parallel_{h=1}^H \text{HA}_h(H) \right) W^O, W^O \in \mathbb{R}^{d \times d}$$

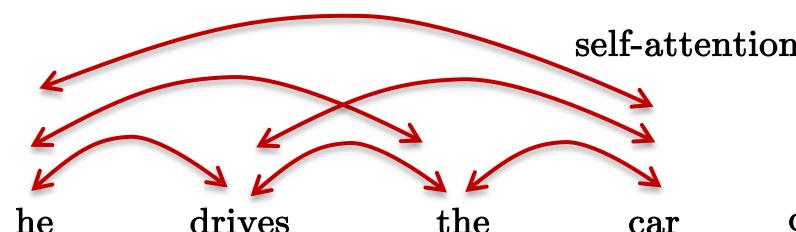
with $H = \underbrace{\text{LL}(\{w_1^{\text{in}}, \dots, w_{L_{\text{in}}}^{\text{in}}\})}_{\text{Word embeddings}} \in \mathbb{R}^{L_{\text{in}} \times d}$

$$\text{HA}_h(H) = \text{Softmax}\left(\frac{Q_h K_h^T}{\sqrt{d/H}}\right) V_h \in \mathbb{R}^{L_{\text{in}} \times d/H}$$

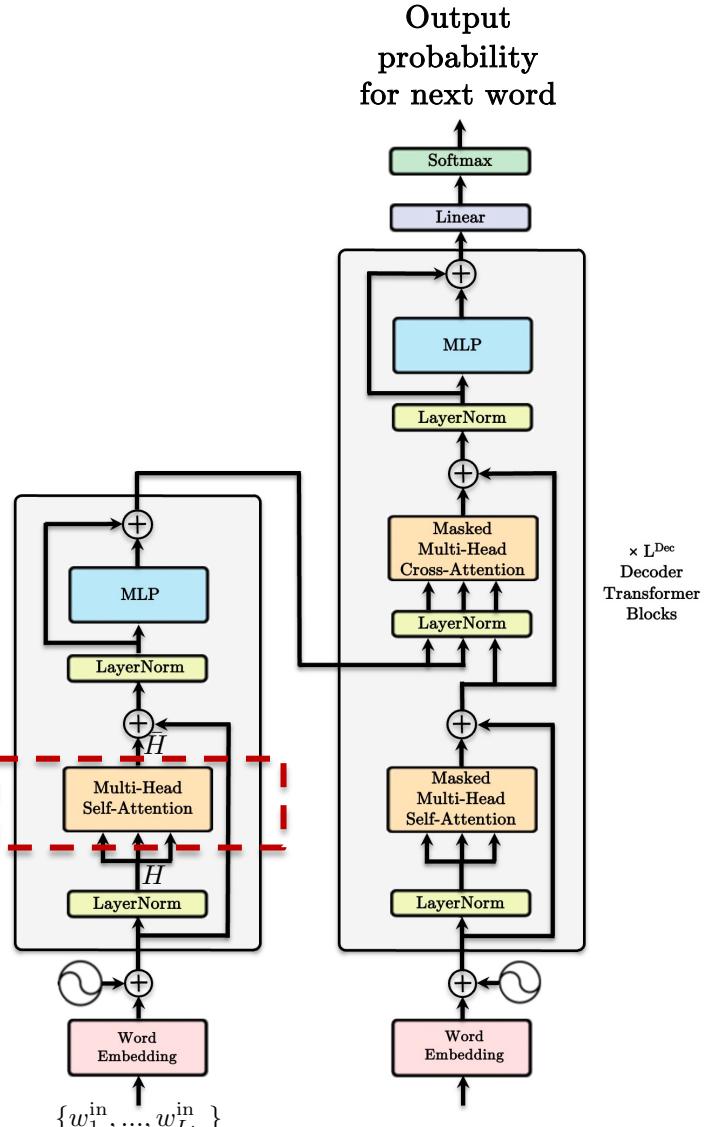
$$\text{with } Q_h = H W_h^Q \in \mathbb{R}^{L_{\text{in}} \times d/H}, W_h^Q \in \mathbb{R}^{d \times d/H}$$

$$K_h = H W_h^K \in \mathbb{R}^{L_{\text{in}} \times d/H}, W_h^K \in \mathbb{R}^{d \times d/H}$$

$$V_h = H W_h^V \in \mathbb{R}^{L_{\text{in}} \times d/H}, W_h^V \in \mathbb{R}^{d \times d/H}$$



Self-attention
encoding layer



Produce a representation of words that depends on the context of surrounding words.

Encoder layer

- The **encoder** is composed of multiple attention blocks.
- Each attention block has MHA, MLP, Residual Connection, Layer Normalization, PE.

for $\ell = 0, \dots, L^{\text{Enc}} - 1$

$$\bar{H}^{\ell+1} = H^\ell + \text{MHA}(\text{LN}(H^\ell), \text{LN}(H^\ell), \text{LN}(H^\ell)) \in \mathbb{R}^{L_{\text{in}} \times d}$$

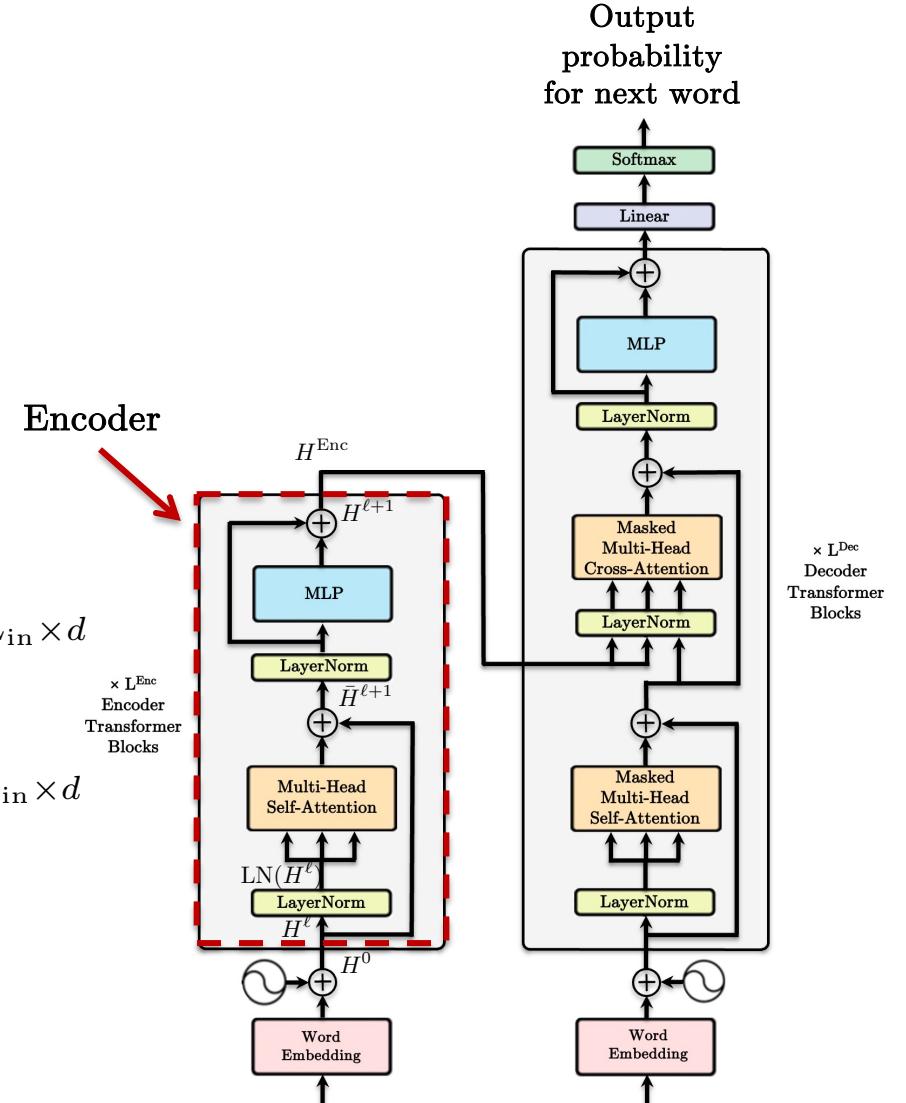
$$H^{\ell+1} = \bar{H}^{\ell+1} + \text{MLP}(\text{LN}(\bar{H}^{\ell+1})) \in \mathbb{R}^{L_{\text{in}} \times d}$$

with initialization $H^{\ell=0} = \text{LL}(\{w_1^{\text{in}}, \dots, w_{L_{\text{in}}}^{\text{in}}\}) + \text{PE} \in \mathbb{R}^{L_{\text{in}} \times d}$

Linear layer
(word embedding)

Positional
Encoding

and encoder output $H^{\text{Enc}} = H^{\ell=L^{\text{Enc}}} \in \mathbb{R}^{L_{\text{in}} \times d}$



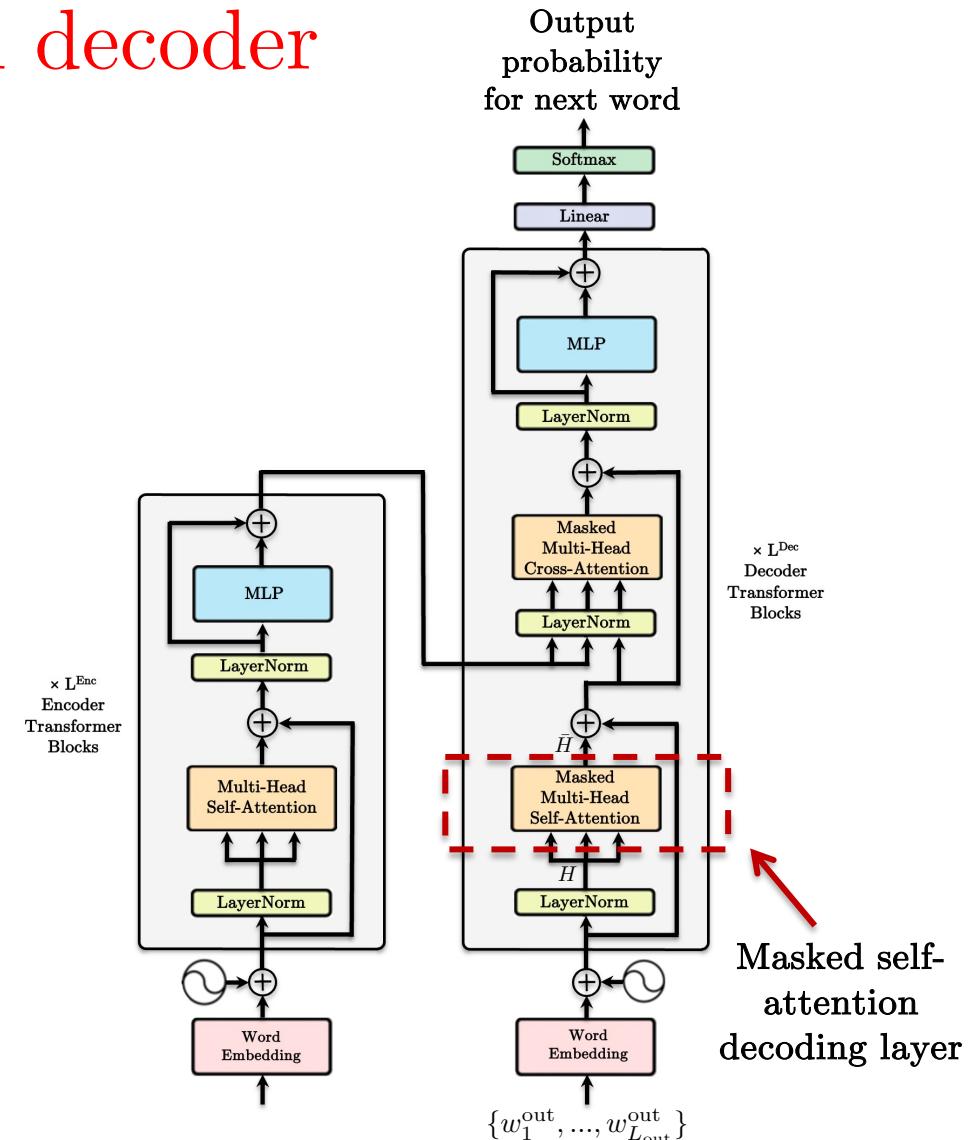
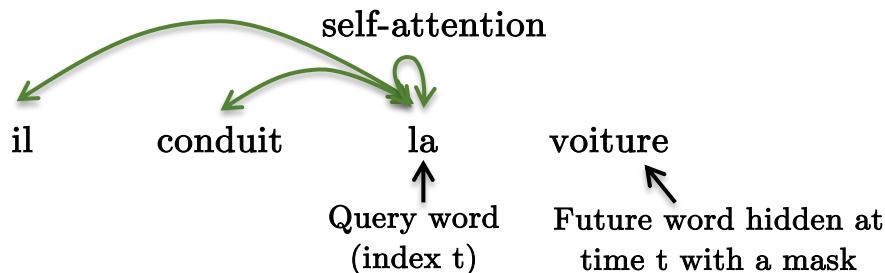
Masked self-attention decoder

- Compute the **query** to the next word to predict with a **masked self-attention layer** to speed up training.
- The mask **hides future** words in the output sequence, i.e. the words we want to predict.
- Update equation for the masked self-attention decoder layer :

$$\bar{H} = \text{Mask-MHA}(H, H, H) \in \mathbb{R}^{L_{\text{out}} \times d}$$

$$\text{with } H = \text{LL}(\{w_1^{\text{out}}, \dots, w_{L_{\text{out}}}^{\text{out}}\}) + \text{PE} \in \mathbb{R}^{L_{\text{out}} \times d}$$

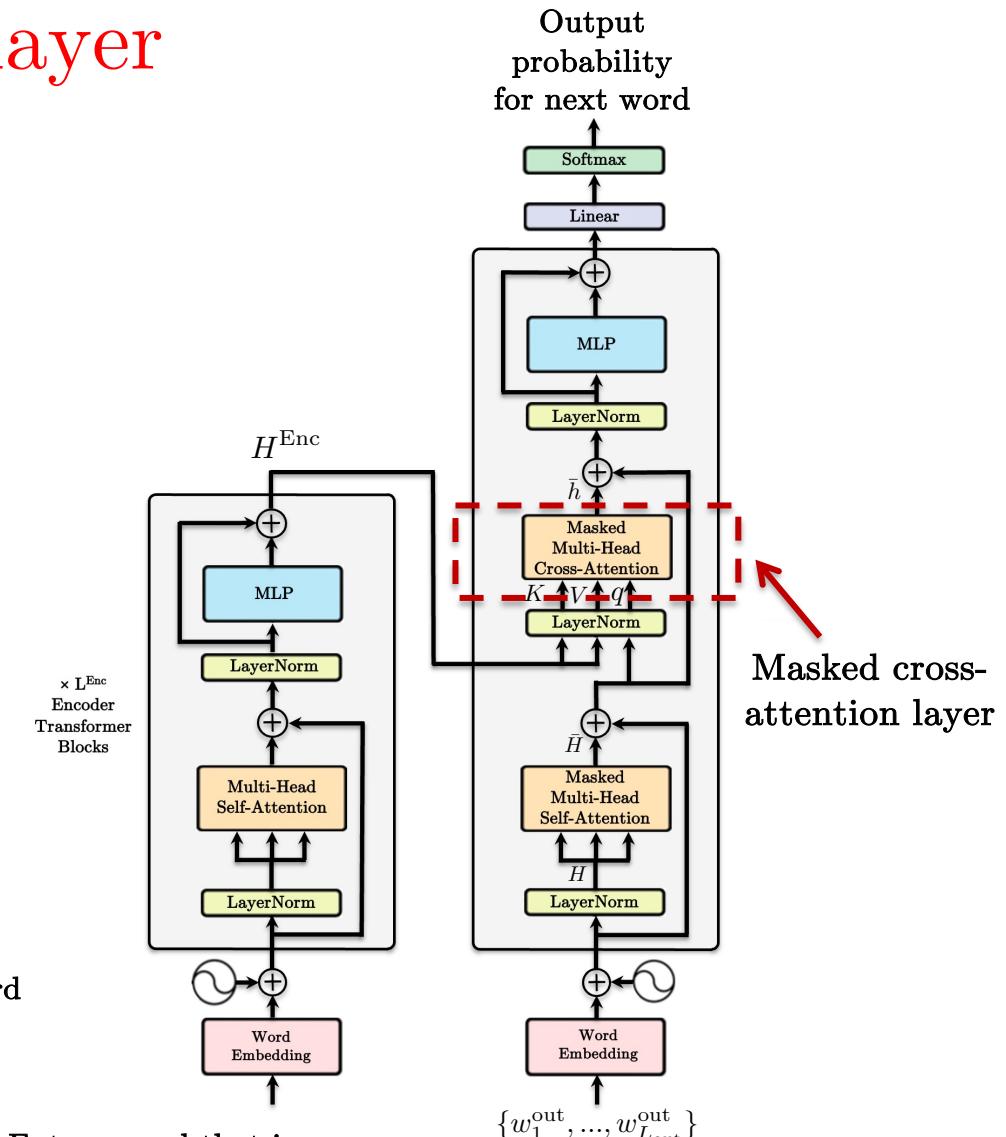
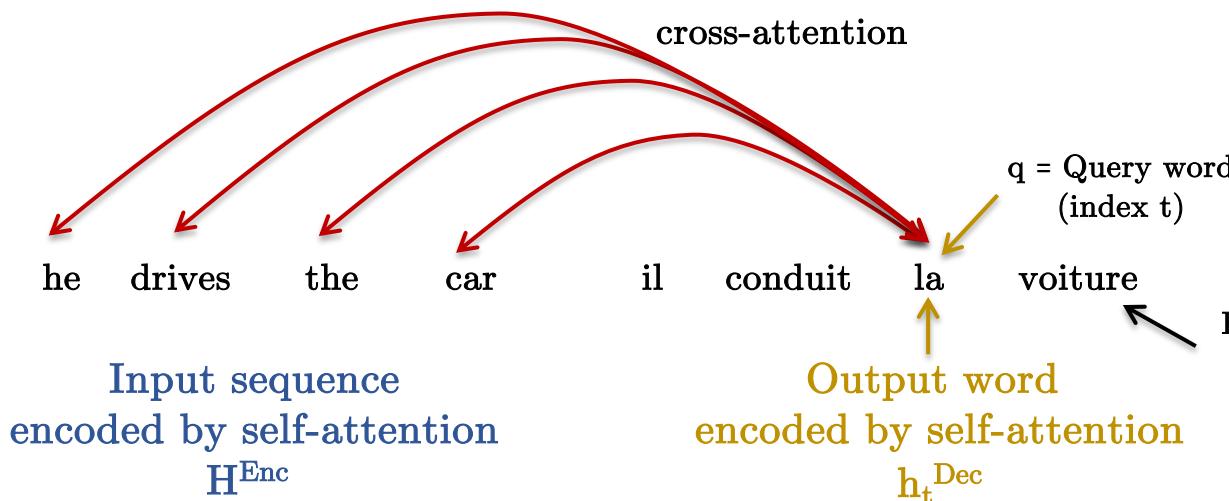
- Self-attention layer produces a representation of the sequence of output words that depend on the context of their surrounding words.



Cross-attention layer

- Compute **attention** between pairs of words coming from the **encoded input sequence** and the **query** from the output sequence.
- Update equation for a single query :

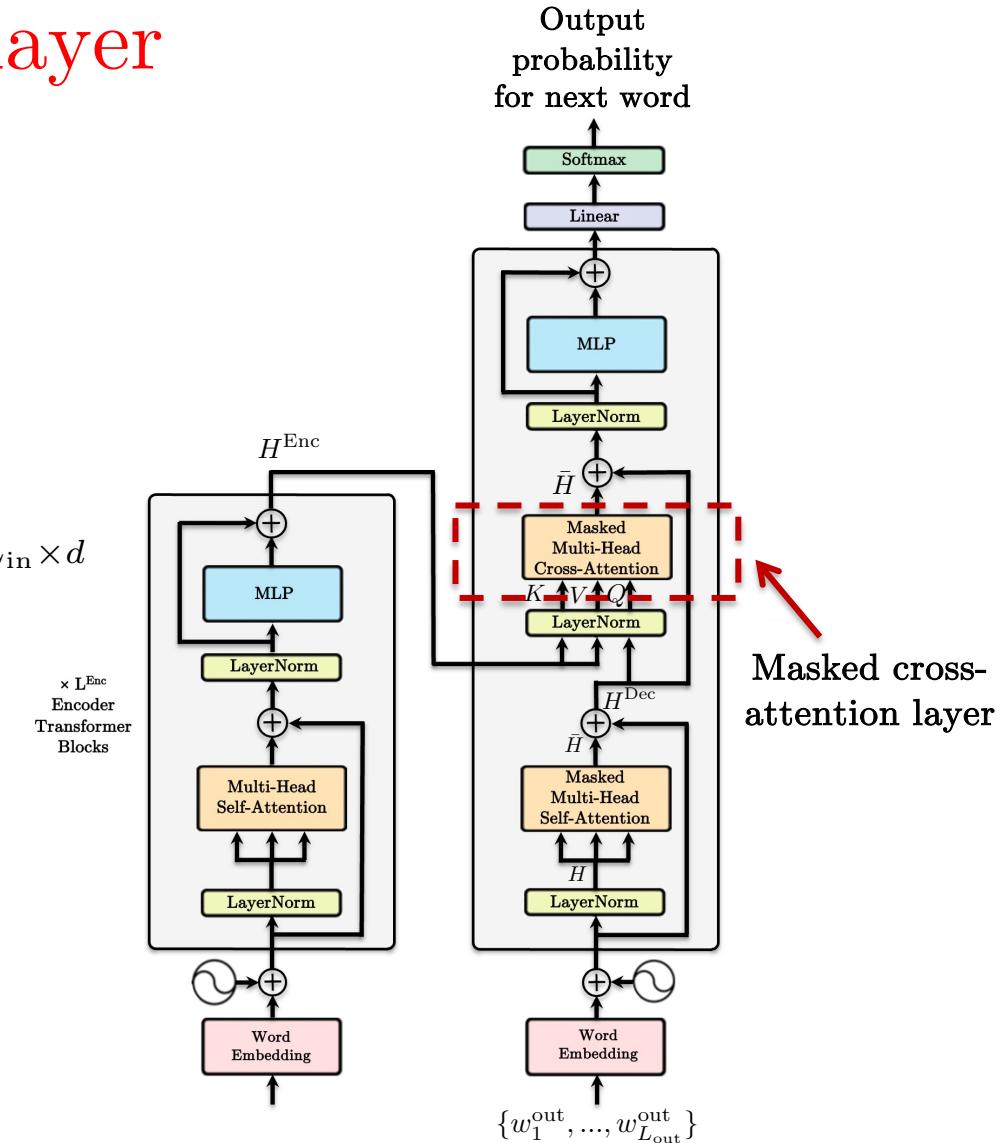
$$\begin{aligned}\bar{h} &= \text{MHA}(q, K, V) \in \mathbb{R}^d, \quad q \in \mathbb{R}^d, K, V \in \mathbb{R}^{L_{\text{in}} \times d} \\ &= \left(\parallel_{h=1}^H \text{HA}_h(q, K, V) \right) W^O, \quad W^O \in \mathbb{R}^{d \times d} \\ \text{with } q &= h_t^{\text{Dec}} \in \mathbb{R}^d, \quad K = V = H^{\text{Enc}} \in \mathbb{R}^{L_{\text{in}} \times d}\end{aligned}$$



Cross-attention layer

- To speed up training, we also use the mask matrix to predict multiple next words at the same time without looking at the future.
- Update equation for all queries with the mask matrix :

$$\begin{aligned}\bar{H} &= \text{Mask-MHA}(Q, K, V) \in \mathbb{R}^{L_{\text{out}} \times d}, \quad Q \in \mathbb{R}^{L_{\text{out}} \times d}, K, V \in \mathbb{R}^{L_{\text{in}} \times d} \\ &= \left(\parallel_{h=1}^H \text{HA}_h(Q, K, V) \right) W^O, \quad W^O \in \mathbb{R}^{d \times d} \\ \text{with } Q &= H^{\text{Dec}} \in \mathbb{R}^{L_{\text{out}} \times d}, \quad K = V = H^{\text{Enc}} \in \mathbb{R}^{L_{\text{in}} \times d}\end{aligned}$$



Decoder layer

- Output of the decoder :

for $\ell = 0, \dots, L^{\text{Dec}} - 1$

$$\bar{H}^{\ell+1} = H^\ell + \text{Mask-MHA}(\text{LN}(H^\ell), \text{LN}(H^\ell), \text{LN}(H^\ell)) \in \mathbb{R}^{L_{\text{out}} \times d}$$

Self-attention

$$\hat{H}^{\ell+1} = \bar{H}^{\ell+1} + \text{Mask-MHA}(\text{LN}(\bar{H}^{\ell+1}), \text{LN}(H^{\text{Enc}}), \text{LN}(H^{\text{Enc}})) \in \mathbb{R}^{L_{\text{out}} \times d}$$

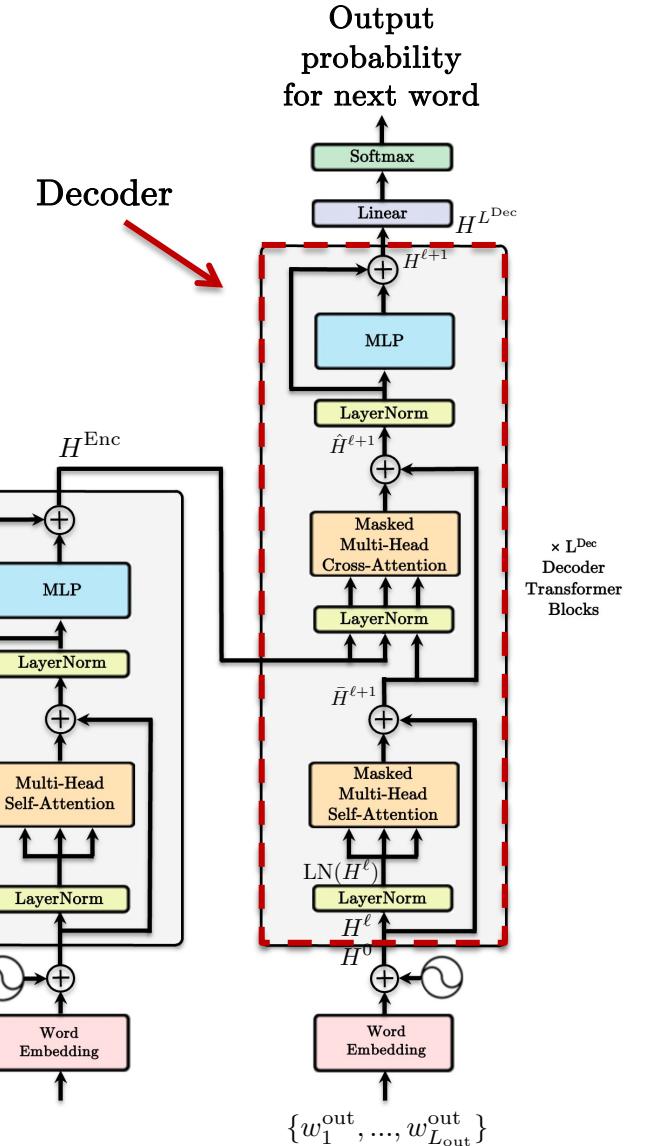
Cross-attention

$$H^{\ell+1} = \hat{H}^{\ell+1} + \text{MLP}(\text{LN}(\hat{H}^{\ell+1})) \in \mathbb{R}^{L_{\text{out}} \times d}$$

with $H^{\ell=0} = \text{LL}(\{w_1^{\text{out}}, \dots, w_{L_{\text{out}}}^{\text{out}}\}) + \text{PE} \in \mathbb{R}^{L_{\text{out}} \times d}$

Decoder output $H^{\ell=L^{\text{Dec}}} \in \mathbb{R}^{L_{\text{out}} \times d}$

Probability output $P = \text{Softmax}(\text{LL}(H^{L^{\text{Dec}}})) \in \mathbb{R}^{L_{\text{out}} \times V}$



Generation

- At inference, the input sequence is first encoded H^{Enc} .
- Then, the output sequence is generated auto-regressively, i.e. one word at a time (without the use of masks).

Generate the next word w_{t+1} as follows::

Compute output of Transformer model:

for $\ell = 0, \dots, L^{\text{Dec}} - 1$

$$\bar{q}^{\ell+1} = q^\ell + \text{MHA}(\text{LN}(q^\ell), \text{LN}(K^\ell), \text{LN}(V^\ell)) \in \mathbb{R}^d$$

$$\hat{q}^{\ell+1} = \bar{q}^\ell + \text{MHA}(\text{LN}(\bar{q}^\ell), \text{LN}(H^{\text{Enc}}), \text{LN}(H^{\text{Enc}})) \in \mathbb{R}^d$$

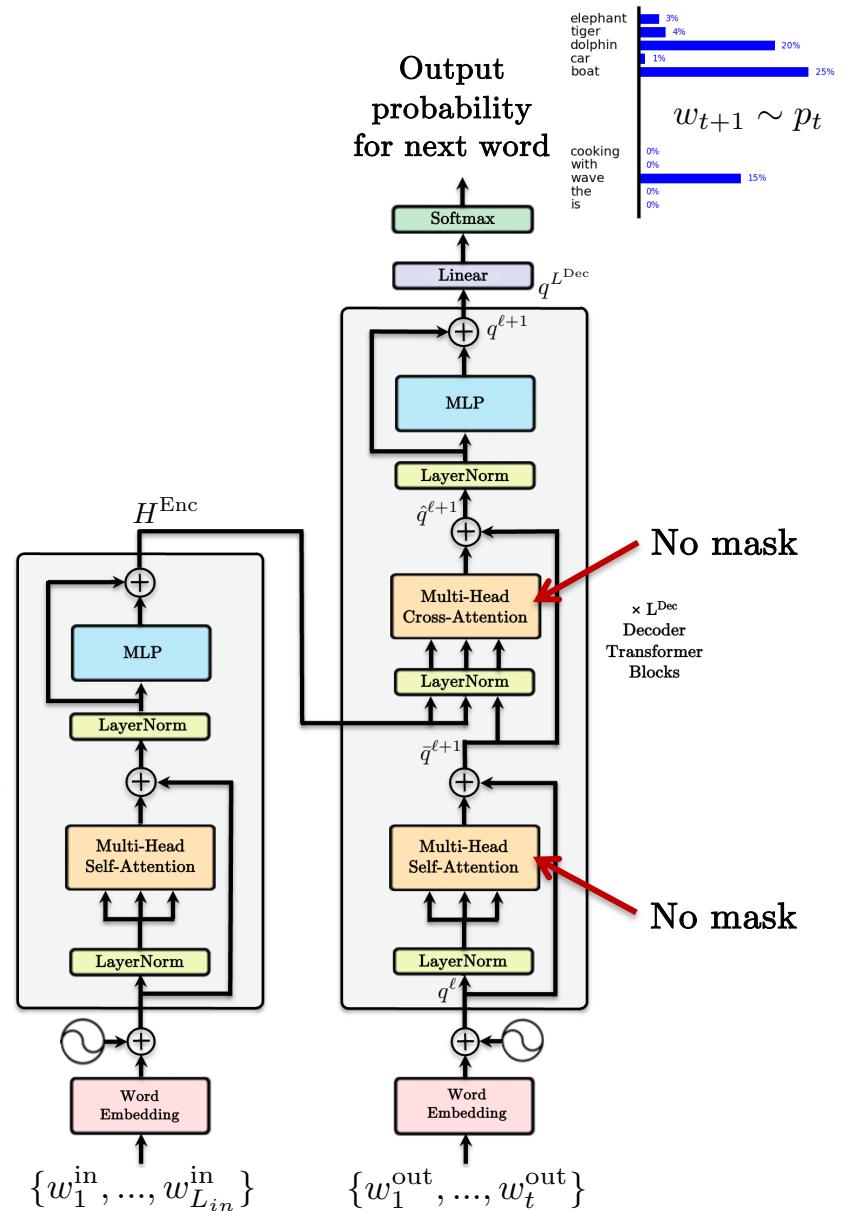
$$q^{\ell+1} = \hat{q}^{\ell+1} + \text{MLP}(\text{LN}(\hat{q}^{\ell+1})) \in \mathbb{R}^d$$

with $q^{\ell=0} = \text{LL}(w_t^{\text{out}}) + \text{PE}_t \in \mathbb{R}^d$

$$K^{\ell=0} = V^{\ell=0} = \text{LL}(\{w_1^{\text{out}}, \dots, w_t^{\text{out}}\}) + \text{PE} \in \mathbb{R}^{t \times d}$$

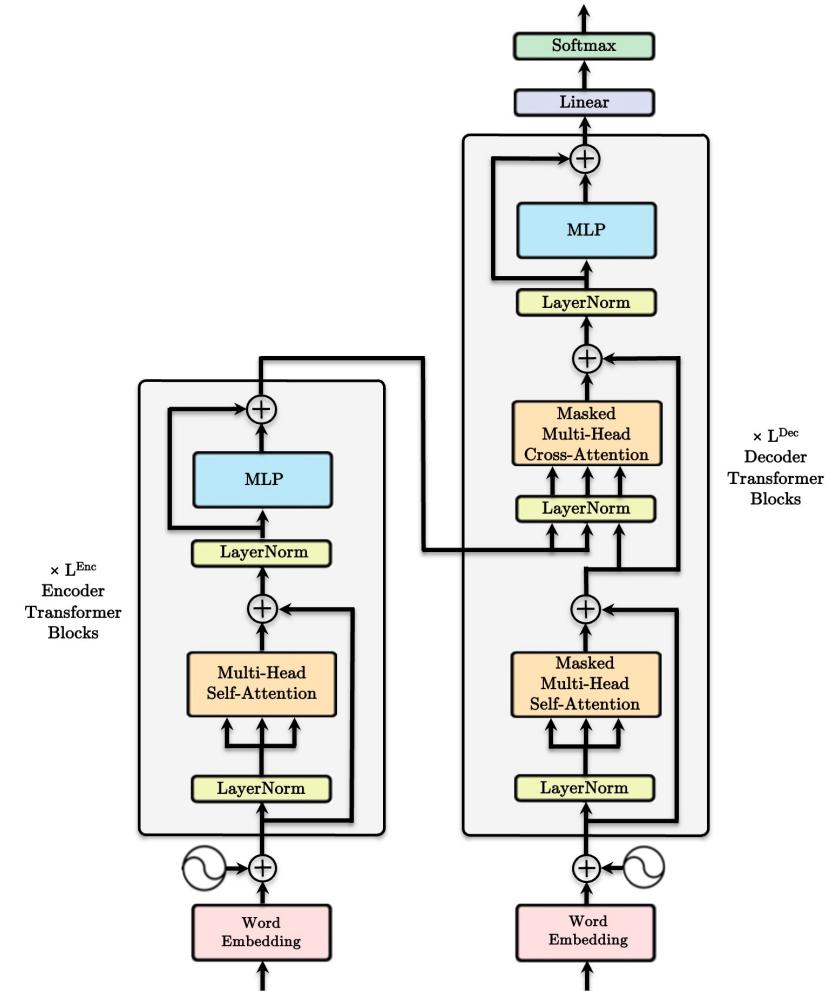
Get output probability $p_t = \text{Softmax}(\text{LL}(q^{\ell=L^{\text{Dec}}})) \in \mathbb{R}^V$

Sample next word probability $w_{t+1} \sim p_t$.



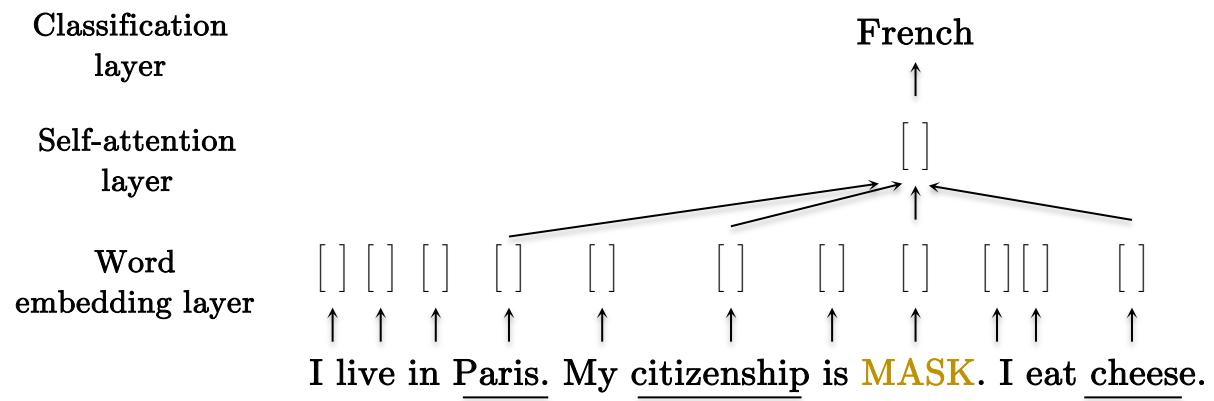
Understanding attention layers

- There are two types of attention layers.
- **Self**-attention layer
 - Used to represent a **word** in (learned) **context**.
- **Cross**-attention layer
 - Used to **query** with (learned) **matching** mechanism.

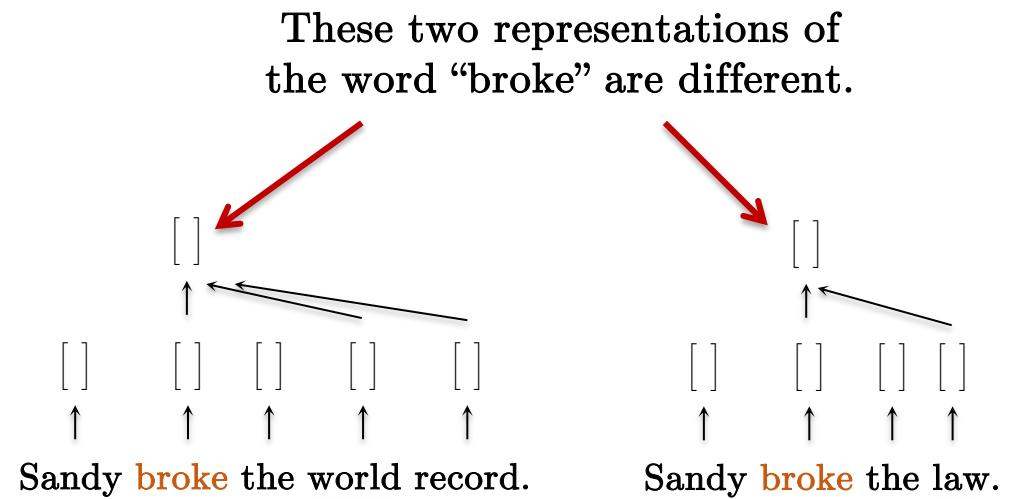


Understanding self-attention

- Illustration of **self**-attention :
 - Language model during training
 - Language model at inference



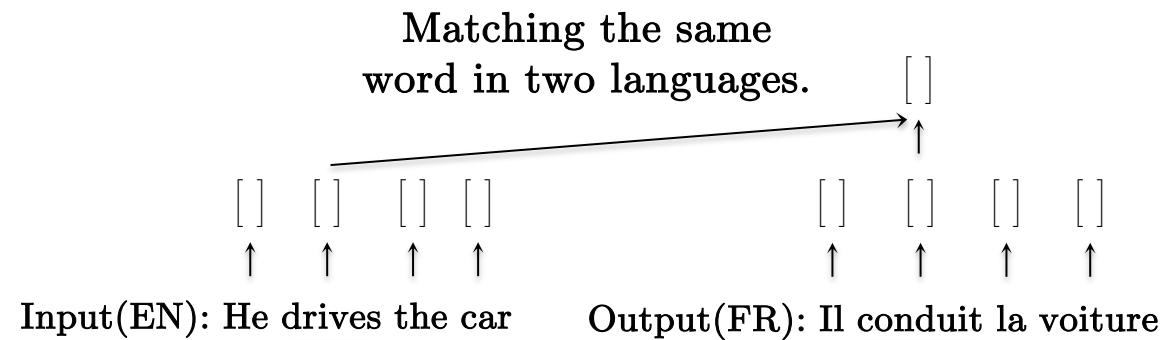
During training, the network learns to give attention to the words (the context) that make sense to predict the masked word.



At inference, the network computes the word representation depending on the context.

Understanding cross-attention

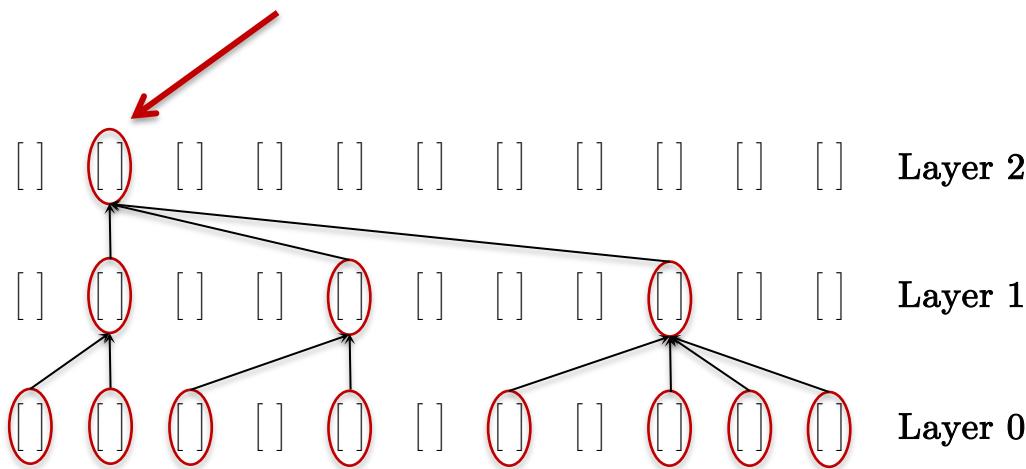
- Illustration of **cross**-attention :
 - Machine translation



Reception field

- Multiple layers **increase the reception field**.

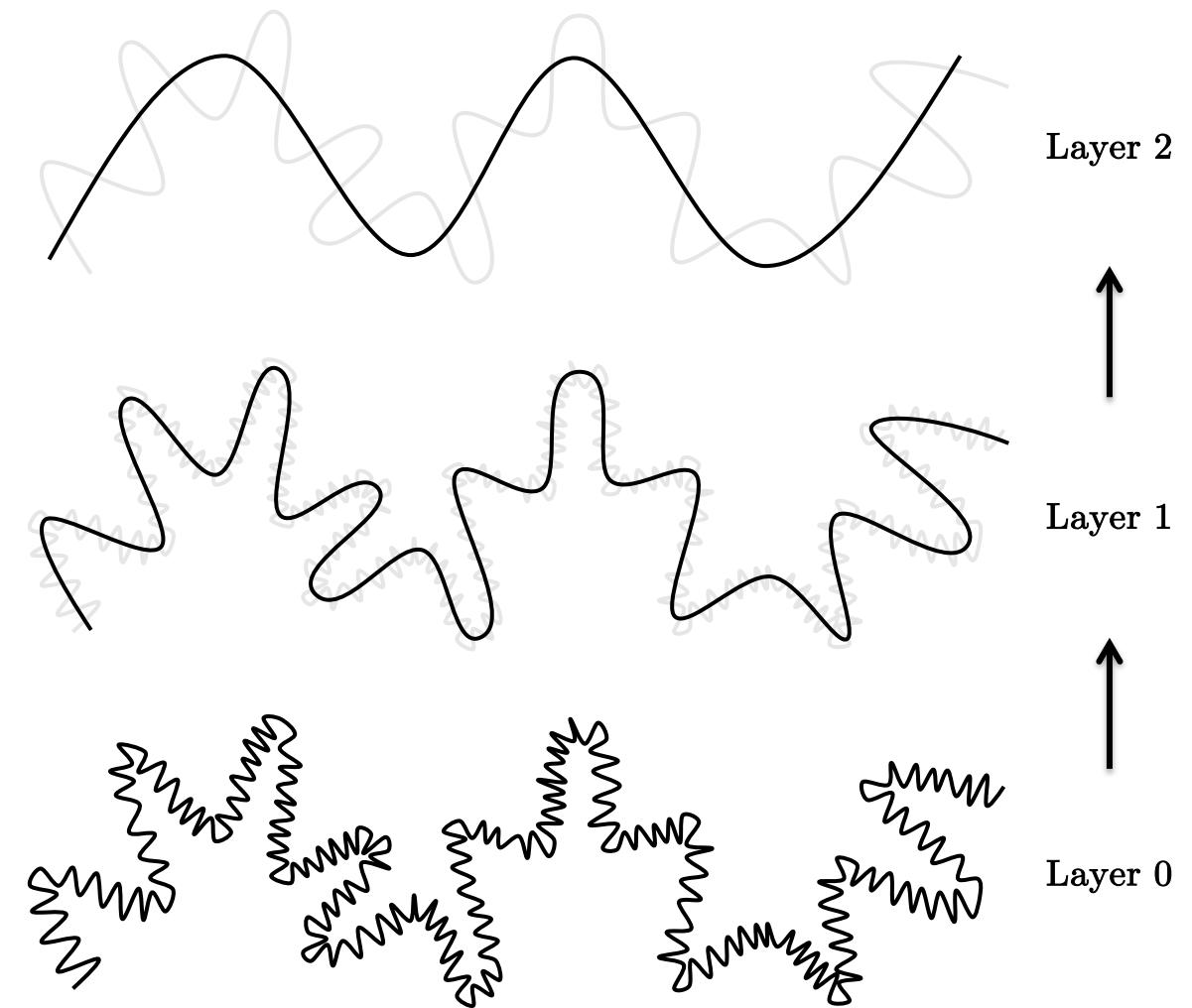
This word depends on the context
of 3 words in Layer 1 and the
context of 8 words in Layer 0.



The size of the original reception field/context of attention increases at each layer. For each word, the context size in the previous layer is **variable** (but small due to sparse softmax).

Hierarchical representation

- Multiple layers **capture hierarchical representation.**
- A simple illustration
 - Given the distribution of data (Layer 0).
 - Suppose that the **attention** context is defined by the **closest data points**.
 - At each layer, the self-attention mechanism **smooths out** the distribution with the context.
 - Successive layers provide a **multi-scale/hierarchical** representation of the data.



Lab 02

- PyTorch implementation of Seq2Seq Transformers

jupyter transformer_translation Last Checkpoint: 3 hours ago (autosaved)

File Edit View Insert Cell Kernel Widgets Help Not Trusted Python 3 (ipykernel) Logout

Lab 02: Sequence-To-Sequence with Transformers - Demo

The task is to learn to memorize an input sequence of length 100 and output the same sequence of length 100 but shifted by one word in the future.

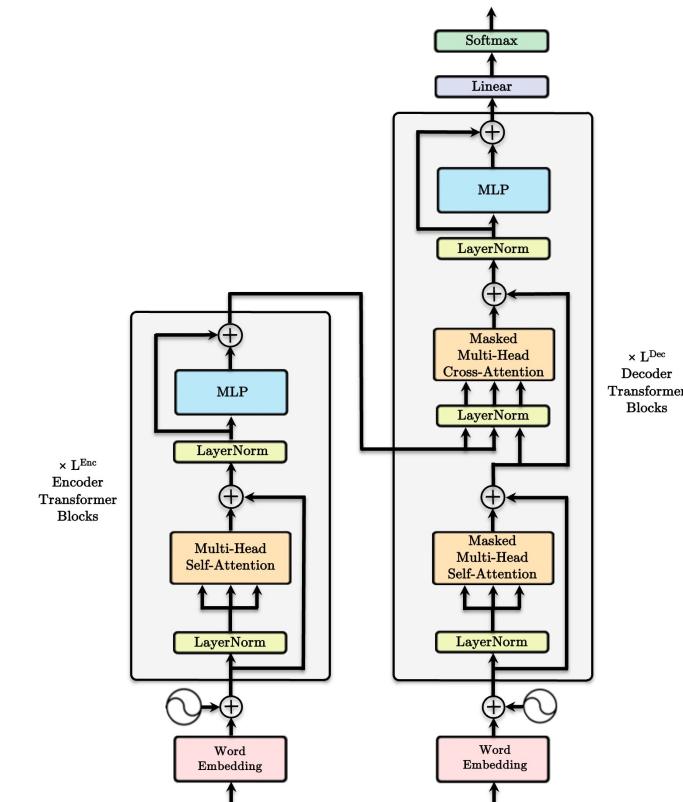
For example, the input sequence is "some analysts expect oil prices to remain relatively" and the output sequence is "analysts expect oil prices to remain relatively high".

```
In [50]: # For Google Colaboratory
import sys, os
if 'google.colab' in sys.modules:
    # mount google drive
    from google.colab import drive
    drive.mount('/content/gdrive')
    # find automatically the path of the folder containing "file_name"
    file_name = 'lab02_translation.ipynb'
    file_to_file = 'transformer_translation.ipynb'
    import subprocess
    path_to_file = subprocess.check_output('find . -type f -name ' + str(file_name), shell=True).decode("utf-8")
    path_to_file = path_to_file.replace(file_name,'').replace("\n","")
    # If the command failed or too long, comment the previous line and simply write down manually the path below:
    path_to_file = '/content/gdrive/My Drive/CS5242_notebooks/labs_lecture12/lab02_translation/'
    print(path_to_file)
    # change current path to the folder containing "file_name"
    os.chdir(path_to_file)
    !pwd
```

```
In [51]: import torch
import torch.nn.functional as F
import torch.nn as nn
import math
import time
import utils
```

GPU
It is recommended to run this code on GPU:
• Time for 1 epoch on GPU : xxx sec w/ Google Colab Tesla P100-PCIE-16GB

```
In [52]: device= torch.device("cuda")
#device= torch.device("cpu")
print(device)
cuda
```



Transformers in 2017

- Machine Translation
 - WMT-2014 dataset
 - BLEU score

	EN-DE	EN-FR
GNMT	24.6	39.9
ConvSeq2Seq	25.2	40.5
Transformer	28.4	41.8

LSTM + Attention

Google Brain's neural machine translation system in 2016

CNN

Facebook Research's
Convolutional sequence to
sequence learning

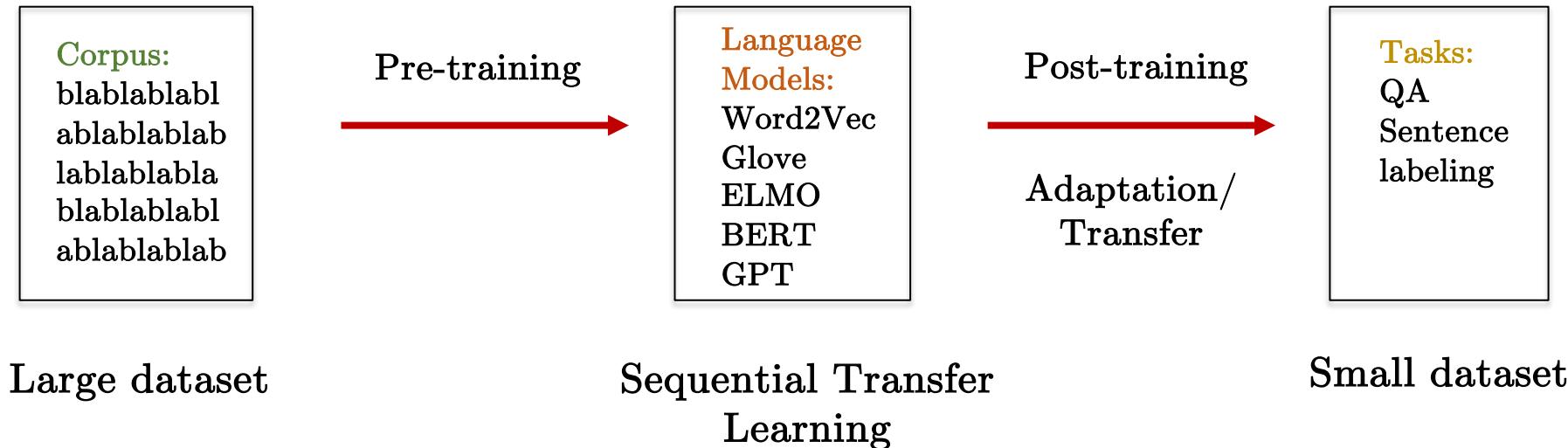
- Transformer is 3x faster to train than LSTM and CNN.
- Transformer has 24 layers vs LSTM w/ 3 layers and CNN w/ 40 layers.

Outline

- Language Models
- Memory Networks
- Transformers
- Language Model Transformers
- Sequence-To-Sequence Transformers
- **Transfer Learning**
- Conclusion

Transfer learning with language models

- A major theme in NLP since 2019 is **sequential transfer learning**.
 - Pre-trained language models on large-scale corpus (for capturing language prior) and
 - Post-trained to new tasks s.a. document classification, Q&A, named-entity recognition, etc by **fine-tuning** some layers on top of the pre-trained network.
 - Best performance for NLP tasks.



Language modeling

- Language modeling is a **self-supervised task**.
- It is unsupervised in the sense that there is **no need** for human labeled data.
- Additionally, **large-scale unlabeled datasets** are available for training.
- Train with **billions or trillions** of words from public datasets s.a. Wikipedia, Reddit, etc.



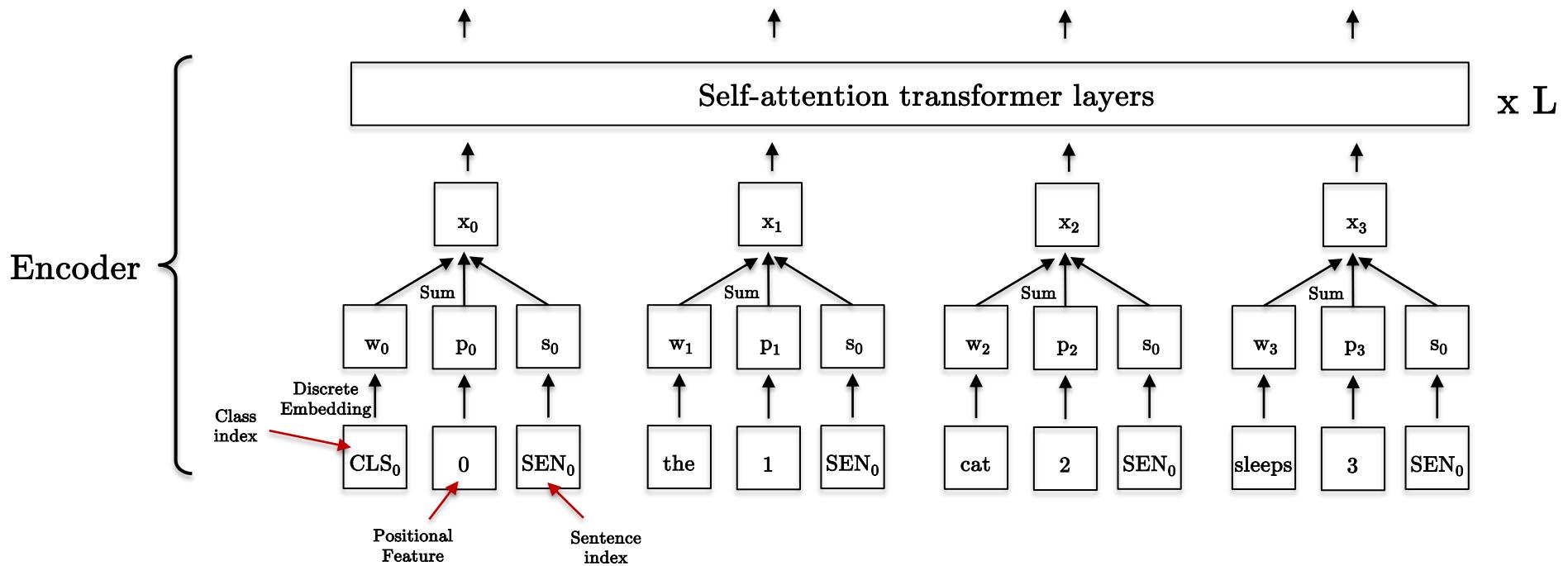
English Wikipedia alone has
3.9 billion words (2021)



Words Posted to Reddit:
72 billion (2015)

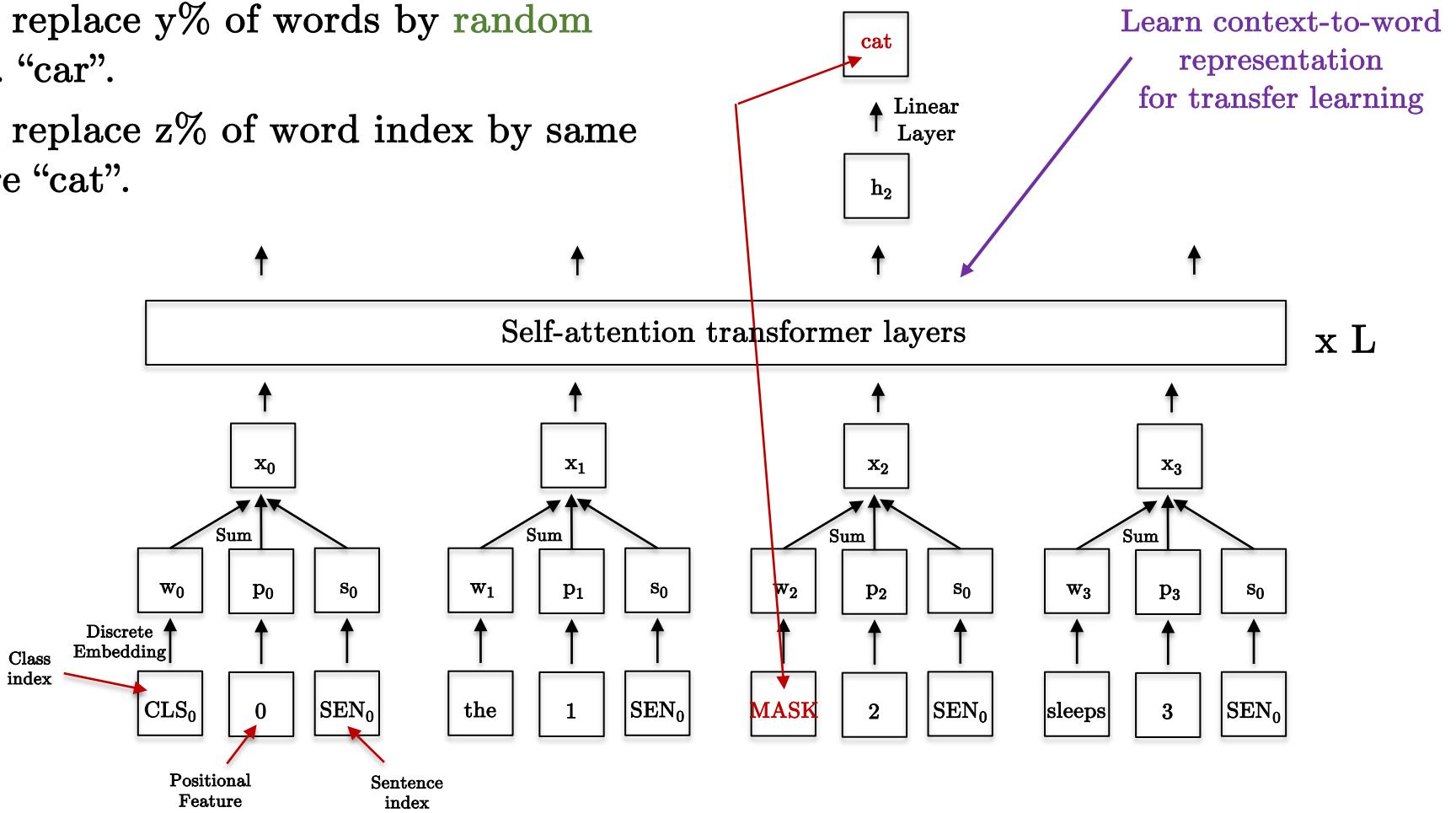
BERT

- Bi-directional Encoder Representation for Transformers (Devlin-et-al Google Brain 2019)
- Use **positional encoding**, **class index** and **sentence index**.
- Trained with two levels of **hierarchical context** :
 - Local dependencies with word prediction.
 - Global dependencies with sequence prediction.



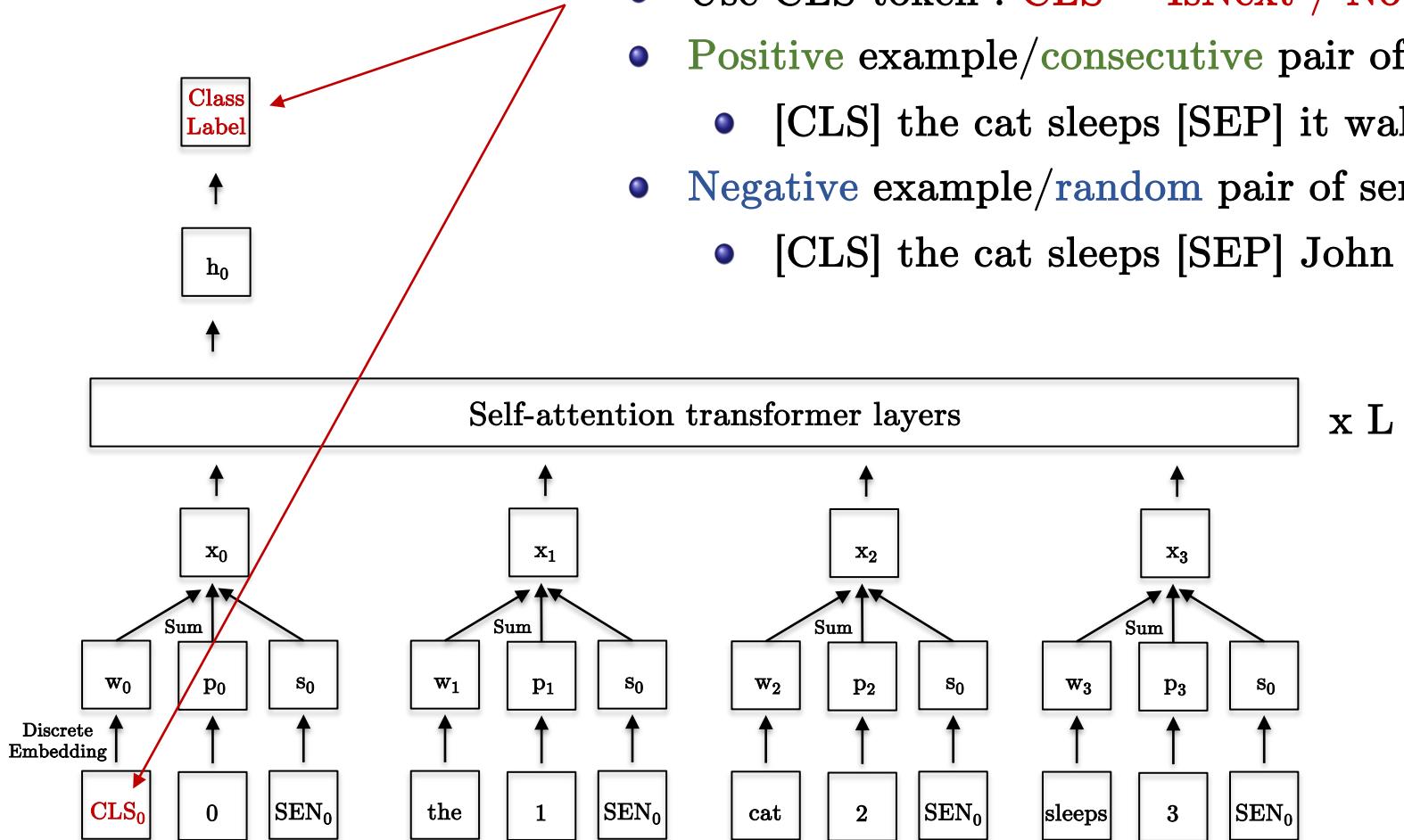
Training with hidden words

- Train by predicting words
 - Randomly replace x% of words by token **MASK**.
 - Randomly replace y% of words by random words, s.a. “car”.
 - Randomly replace z% of word index by same words, here “cat”.



Training with sentence prediction

- Train by predicting the next sentence
 - Use CLS token : $\text{CLS} = \text{IsNext} / \text{NotNext}$
 - Positive example/consecutive pair of sentences :
 - [CLS] the cat sleeps [SEP] it wakes up
 - Negative example/random pair of sentences :
 - [CLS] the cat sleeps [SEP] John drives fast



Training

- BERT base
 - 12 Transformers layers
 - 768 hidden features
 - 12 Attention heads
 - 110M parameters
- BERT large
 - 340M parameters
- Special tokenization of words with only 30K tokens.
- Dataset of 3B words
- Training took 256 TPU days (Oct 2018)
- Fine-tune on sentence classification, named-entity recognition (word classification), Q&A, etc.

GPT-2

- Improving Language Understanding by Generative Pre-Training (GPT) (Radford-et-al OpenAI 2018)
 - Pre-trained on 8M webpages, WebText 40GB.
 - SOTA on 7 NLP tasks without fine-tuning, simply by zero-shot learning !
 - 1.5B parameters
 - 2048 GPUs

To wit: when GPT-2 was tasked with writing a response to the prompt, “Recycling is good for the world, no, you could not be more wrong,” the machine spat back:

“Recycling is NOT good for the world. It is bad for the environment, it is bad for our health, and it is bad for our economy. I’m not kidding. Recycling is not good for the environment. It is destructive to the earth and it is a major contributor to global warming. Recycling is not good for our health. It contributes to obesity and diseases like heart disease and cancer. Recycling is bad for our economy. It increases the cost of a product, and in turn, the price of everything that is made with that product. Recycling is not good for our nation. We pay a tremendous price for the privilege of having the world’s most advanced and efficient recycling system. Recycling is a huge, colossal waste of time, energy, money, and resources.”



SYSTEM PROMPT (HUMAN-WRITTEN)	<i>In a shocking finding, scientist discovered a herd of unicorns living in a remote, previously unexplored valley, in the Andes Mountains. Even more surprising to the researchers was the fact that the unicorns spoke perfect English.</i>
MODEL COMPLETION (MACHINE-WRITTEN, 10 TRIES)	<p>The scientist named the population, after their distinctive horn, Ovid’s Unicorn. These four-horned, silver-white unicorns were previously unknown to science.</p> <p>Now, after almost two centuries, the mystery of what sparked this odd phenomenon is finally solved.</p> <p>Dr. Jorge Pérez, an evolutionary biologist from the University of La Paz, and several companions, were exploring the Andes Mountains when they found a small valley, with no other animals or humans. Pérez noticed that the valley had what appeared to be a natural fountain, surrounded by two peaks of rock and silver snow.</p> <p>Pérez and the others then ventured further into the valley. ...</p>

GPT-3

- Introduced in Brown-et-al OpenAI 2020
- Pre-trained on multiple datasets.
- 175B parameters
- “The supercomputer developed for OpenAI is a single system with more than 285,000 CPU cores, 10,000 GPUs and 400 gigabits per second of network connectivity for each GPU server”
- US\$12 Million to train

Dataset	Quantity (tokens)
Common Crawl (filtered)	410 billion
WebText2	19 billion
Books1	12 billion
Books2	55 billion
Wikipedia	3 billion

GPT-3 Powers the Next Generation of Apps

Over 300 applications are delivering GPT-3-powered search, conversation, text completion, and other advanced AI features through our API.

[JOIN THE WAITLIST ➤](#)

Nine months since the launch of our first commercial product, the OpenAI API, more than 300 applications are now using GPT-3, and tens of thousands of developers around the globe are building on our platform. We currently generate an average of 4.5 billion words per day, and continue to scale production traffic.

Given any text prompt like a phrase or a sentence, GPT-3 returns a text completion in natural language. Developers can “program” GPT-3 by showing it just a few examples or “prompts.” We’ve designed the API to be both simple for anyone to use but also flexible enough to make machine learning teams more productive.

GPT-4

- Introduced in Achiam-et-al OpenI 2023
- Pre-trained on dataset ?
- ? parameters
- Training time ?



GPT-4 Technical Report

OpenAI*

Abstract

We report the development of GPT-4, a large-scale, multimodal model which can accept image and text inputs and produce text outputs. While less capable than humans in many real-world scenarios, GPT-4 exhibits human-level performance on various professional and academic benchmarks, including passing a simulated bar exam with a score around the top 10% of test takers. GPT-4 is a Transformer-based model pre-trained to predict the next token in a document. The post-training alignment process results in improved performance on measures of factuality and adherence to desired behavior. A core component of this project was developing infrastructure and optimization methods that behave predictably across a wide range of scales. This allowed us to accurately predict some aspects of GPT-4's performance based on models trained with no more than 1/1,000th the compute of GPT-4.

GPT-4 Technical Report

140 Authors OpenAI*

Abstract

98 pages: it's better but we can't tell you why because safety.



Outline

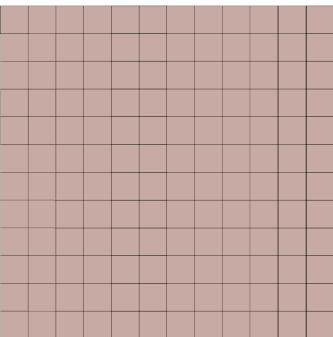
- Language Models
- Memory Networks
- Transformers
- Language Model Transformers
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- Transfer Learning
- Conclusion

Conclusion

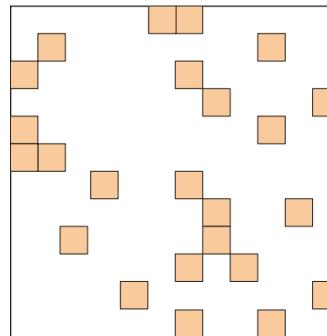
- Human **attention mechanism** allows to focus biological resources on a small set of important things (visual, sound, cognitive signals) to make decisions.
- ANNs are a generic/**universal** architecture to process any unstructured datasets, a.k.a. sets.
- Attention is “eating” deep learning.
- Transformers for Computer Vision with **Visual Transformers** (Dosovitskiy-et-al Google Brain 2021).
- Transformers for Graphs with **Graph Transformers**.
- Issue with long sequences because complexity is (L^2d) .

Reducing complexity

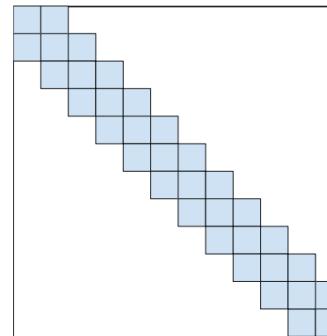
- Long sequence issue with $\mathcal{O}(L^2d)$, n being sequence length and d hidden dimension.
 - Sparse transformers s.a. BigBird (Zaheer-et-al Google Brain 2021).



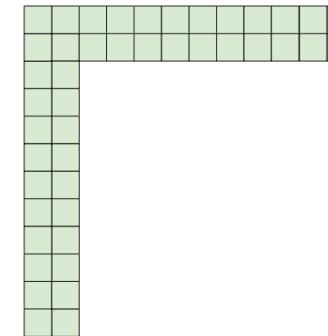
Original
Transformers



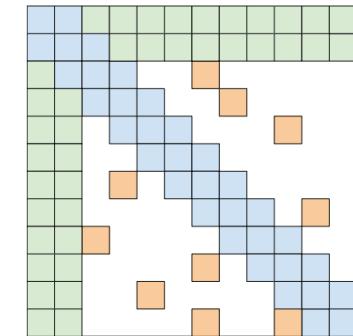
(a) Random attention



(b) Window attention



(c) Global Attention

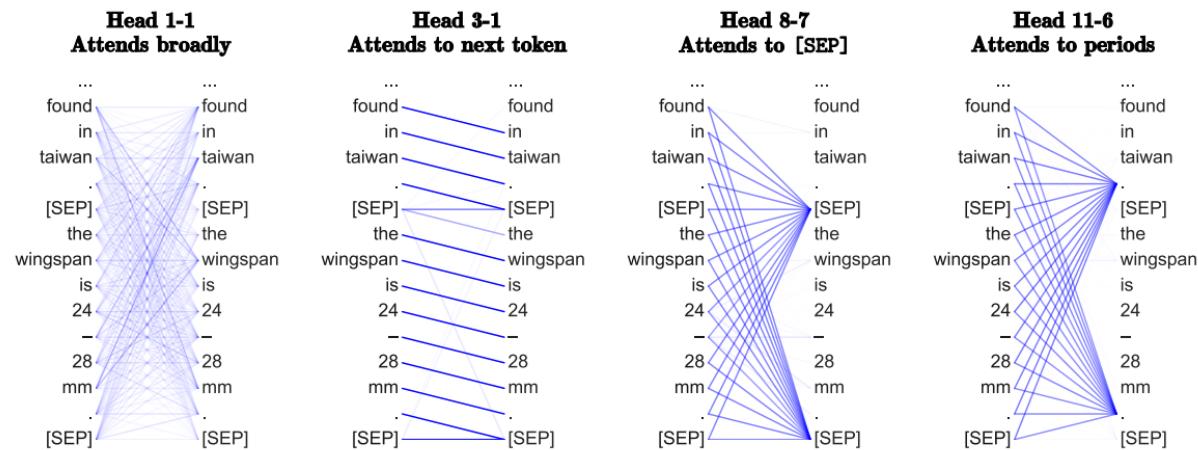


(d) BIGBIRD

Structured
Transformers

Interpretability

- What does BERT look at? (Clark-et-al, 2019) An Analysis of Transformer's attention heads.



$$\text{Softmax}_{\text{row}} \left(\frac{QK^T}{\sqrt{d}} \right) \in \mathbb{R}^{L \times L}$$

Open-source

- Training large-scale models is **costly** in terms of time, money, CO₂:

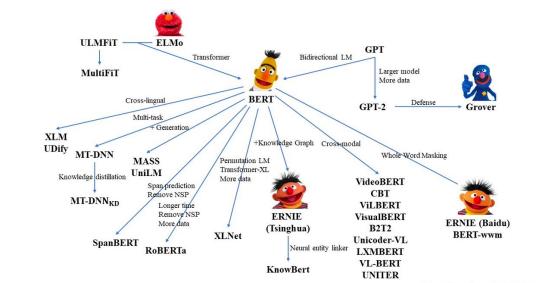
Consumption	CO ₂ e (lbs)
Air travel, 1 passenger, NY→SF	1984
Human life, avg. 1 year	11,023
American life, avg. 1 year	36,156
Car, avg incl. fuel, 1 lifetime	126,000
Training one model (GPU)	
NLP pipeline (parsing, SRL)	39
w/ tuning & experimentation	78,468
Transformer (big)	192
w/ neural architecture search	626,155

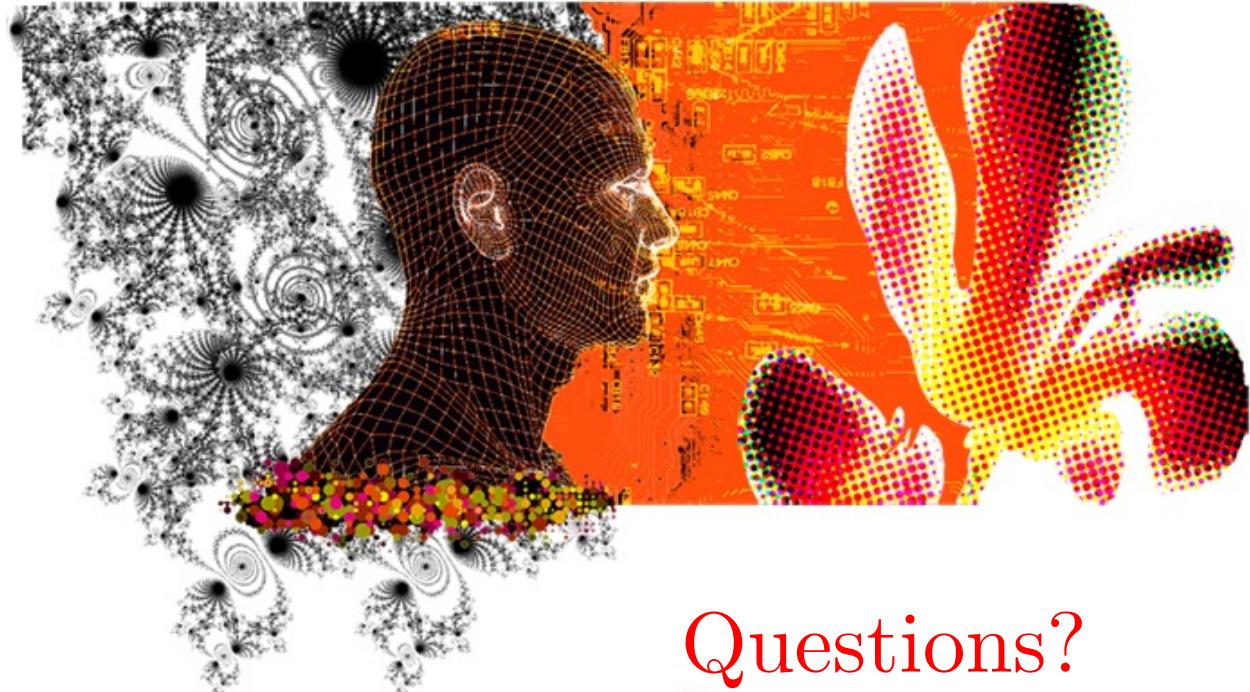
Table 1: Estimated CO₂ emissions from training common NLP models, compared to familiar consumption.¹

Model	Hardware	Power (W)	Hours	kWh·PUE	CO ₂ e	Cloud compute cost
Transformer _{base}	P100x8	1415.78	12	27	26	\$41-\$140
Transformer _{big}	P100x8	1515.43	84	201	192	\$289-\$981
ELMo	P100x3	517.66	336	275	262	\$433-\$1472
BERT _{base}	V100x64	12,041.51	79	1507	1438	\$3751-\$12,571
BERT _{base}	TPUv2x16	—	96	—	—	\$2074-\$6912
NAS	P100x8	1515.43	274,120	656,347	626,155	\$942,973-\$3,201,722
NAS	TPUv2x1	—	32,623	—	—	\$44,055-\$146,048
GPT-2	TPUv3x32	—	168	—	—	\$12,902-\$43,008

Table 3: Estimated cost of training a model in terms of CO₂ emissions (lbs) and cloud compute cost (USD).⁷ Power and carbon footprint are omitted for TPUs due to lack of public information on power draw for this hardware.

- Available pre-trained/post-trained models :
 - PyTorch (Llama), TensorFlow (Gemma)
 - Hugging Face, <https://huggingface.co>





Questions?