
Deep Learning 과정

# Self-Attention and Transformer

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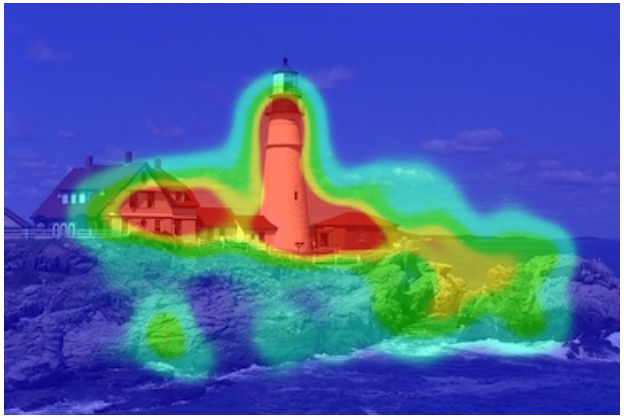
# Outline

- Attention
- Self-attention
- Transformer

# Attention Mechanism

Attention mechanisms in neural Networks

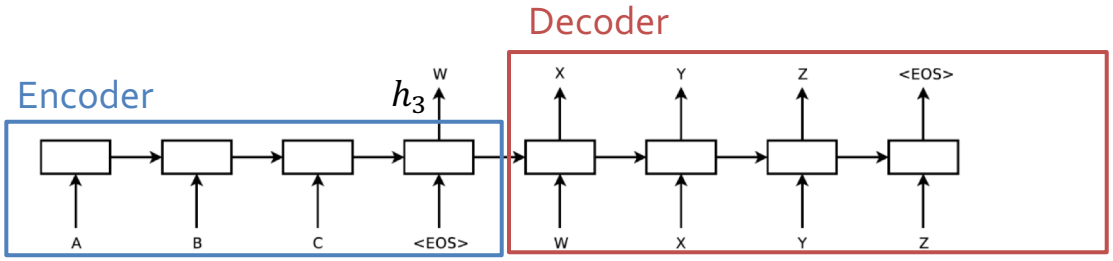
- Loosely based on the visual attention mechanism in humans
- Focus on a certain region of an image with high resolution while perceiving the surrounding image in low resolution
- Adjust the focal point over time



# Attention Mechanism

First successfully applied in neural machine translation

- In previous seq2seq model, the decoder generates a translation solely based on the last hidden state ($h_3$) from the encoder
- Could be unreasonable that (1) a single vector encodes all information about a potentially very long sentence and (2) the decoder produces a good translation based on only that
- What if the input sentence consists of 50 words?
- Multiple (practical) hacks: (i) reverse the input sentence, or (ii) feed the input sentence twice….



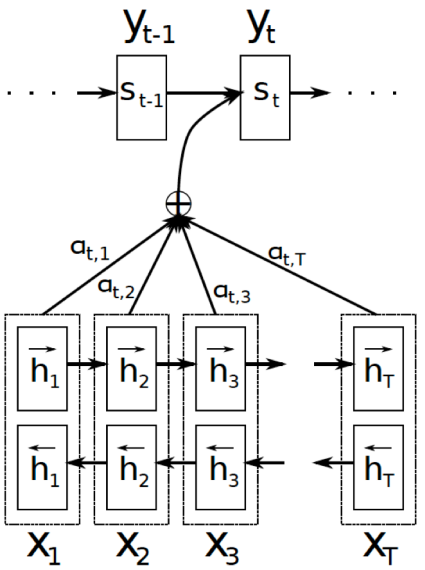
# Attention Mechanism

Solution: attention mechanisms!

- The decoder **attends** to different parts of the source sentence at each step of the output generation

Encoder: a bi-directional RNN

- $x_i/y_t$: a word of source/translated sentence
- Forward RNN reads the sentence, and calculates forward hidden states $(\overrightarrow{h_i}, \ldots, \overrightarrow{h_T})$
- The embedding of each word $x_j$ is obtained by the concatenation $h_i = [\overrightarrow{h_i}^T, \overleftarrow{h_i}^T]$






Bahdanau et al. Neural Machine Translation by Jointly Learning to Align and Translate. ICLR 2015

# Attention Mechanism

## Solution: attention mechanisms!

- The decoder **attends** to different parts of the source sentence at each step of the output generation

## Decoder by soft-attention

- The context vector $c_t$ with weight $\alpha_{it}$

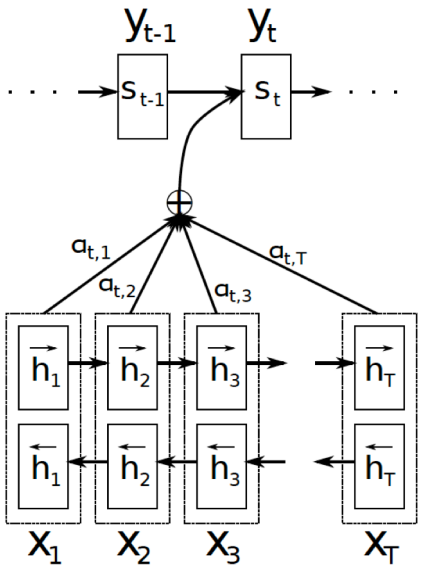
$$c_t = \sum_{i=1}^{T} \alpha_{ti}\, h_i$$

can consider all input $i$ according to its importance

$$\alpha_{ti} = \frac{\exp(e_{ti})}{\sum_{k=1}^{T} \exp(e_{tk})}$$

how much each input $i$ contributes to output $t$

$$e_{ti} = v^T \tanh(W s_{t-1} + V h_i)$$



# Attention Mechanism

## Solution: attention mechanisms!

- The decoder **attends** to different parts of the source sentence at each step of the output generation

## Decoder by soft-attention

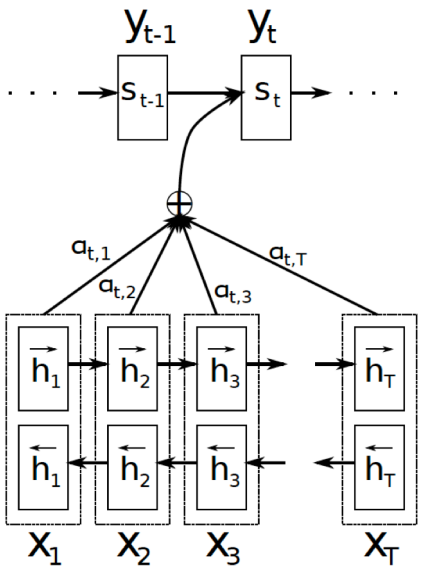
- The language model equation is

$$P(y_t|y_t, \dots, y_{t-1}, \boldsymbol{x}) = g(y_{t-1}, s_t, c_t)$$

where $g$ is a nonlinear (multi-layered) function for probability output (e.g. hidden layers + softmax)

$s_t$ is an RNN hidden state at time $t$

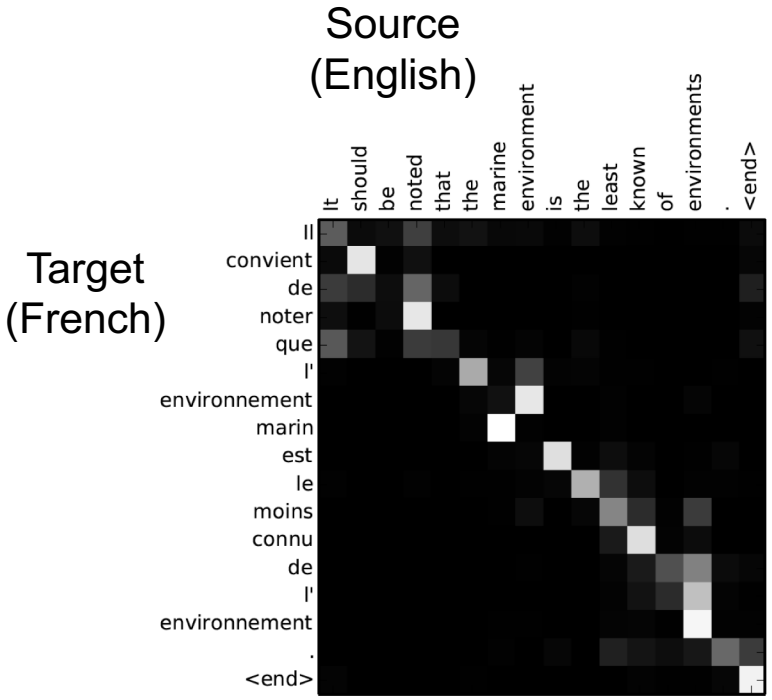
$$s_t = f(s_{t-1}, y_{t-1}, c_t)$$



# Attention Mechanism

Visualizing the attention weight matrix $\alpha$

- The decoder **attends** to different parts of the source sentence at each step of the output generation




The model generates each output word by **attending** sequentially to different input state

# Cost of Attention

The size of attention weight matrix $\boldsymbol{\alpha}$ is quadratic

- e.g. if input/output sentence is 50 words long, then the size of $\boldsymbol{\alpha}$ is 50x50 = 2,500
- If we consider character-level tokenization, it could be prohibitively expensive

The previous attention mechanism is counter-intuitive

- For each output, we scan through all the input words (i.e. going back through all of our internal memory)
- Human instantaneously knows which parts of memory should be accessed
- Use reinforcement learning to predict an approximation location to focus to [Mnih 2014]

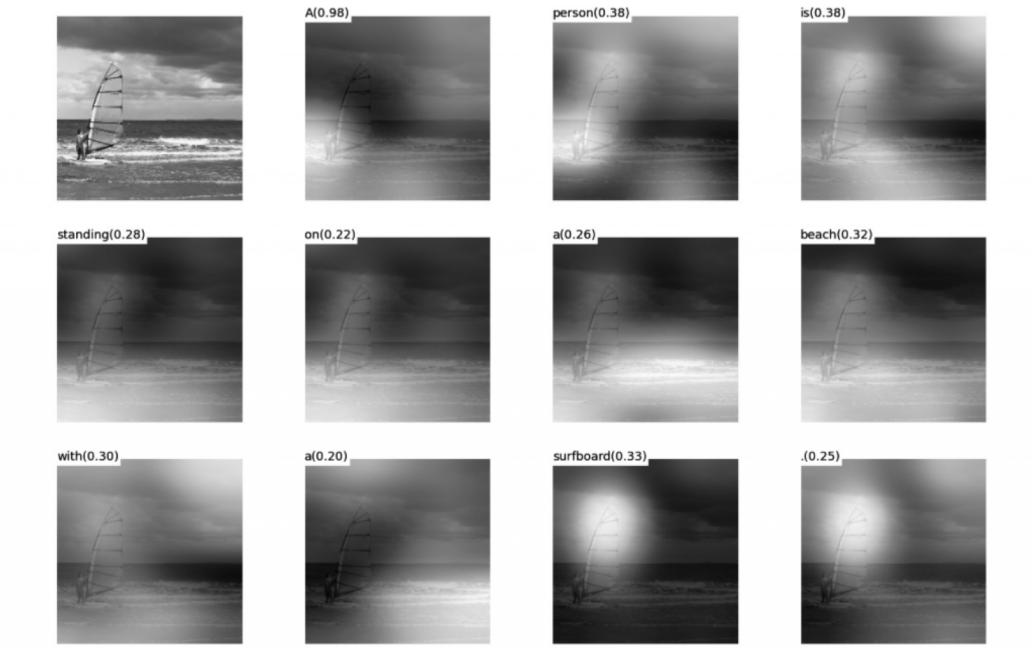


Mnih et al. Recurrent Models of Visual Attention. NIPS 2014

# Image Captioning with Visual Attention

Solution: attention mechanisms!

- The decoder attends to different parts of the source ~~sentence~~ image at each step of the output generation




(b) A person is standing on a beach with a surfboard.



Xu et al. Show, Attend and Tell: Neural Image Caption Generation with Visual Attention. ICML 2015

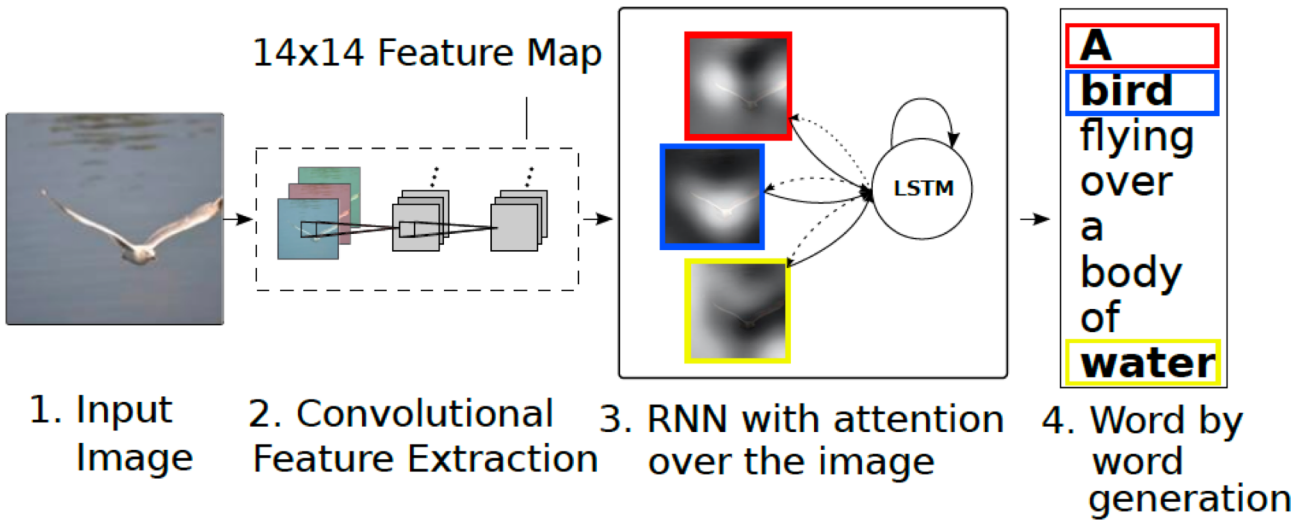
# Image Captioning with Visual Attention

Encoder: 14x14 CNN feature map

- Let the decoder to selectively focus on certain parts of an image

Decoder: LSTM layer

- Similar to the decoder of [Bahdanau et al. ICLR 2015]




Xu et al. Show, Attend and Tell: Neural Image Caption Generation with Visual Attention. ICML 2015

# Language Model Pretraining

Image:
H x W x 3

CNN

| | |
|---|---|
| a | b |
| c | d |

Grid of features
(Each D-dimensional)

Context vector $\boldsymbol{z}$
(D-dimensional)

From
RNN:

| | |
|---|---|
| $\alpha_a$ | $\alpha_b$ |
| $\alpha_c$ | $\alpha_d$ |

Distribution over
grid locations
$\alpha_a + \alpha_b + \alpha_c + \alpha_d = 1$

**Soft attention:**
Summarize ALL locations

$$z = \alpha_a a + \alpha_b b + \alpha_c c + \alpha_d d$$

Derivative $dz/d\alpha$ is nice!
Train with gradient descent

**Hard attention**:
(image cropping)
Sample ONE location
according to $\alpha, z$ = that vector

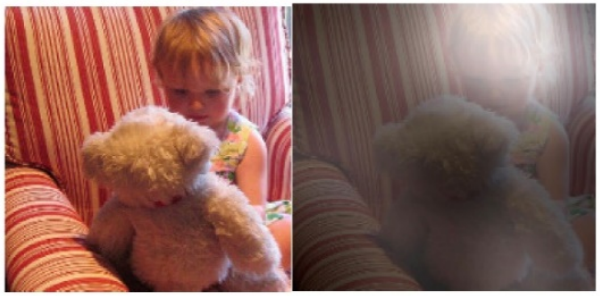
With argmax, $dz/d\alpha$ is zero
almost everywhere …
Can't use gradient descent;
need reinforcement learning

# Image Captioning with Visual Attention

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.



A little girl sitting on a bed with a teddy bear.

A group of people sitting on a boat in the water.

A giraffe standing in a forest with trees in the background.

# Video Captioning with Temporal Attention

Solution: attention mechanisms!

- The decoder attends to different parts of the source ~~sentence~~ frame at each step of the output generation

Video captioning

- Given a short video clip, generate a descriptive sentence

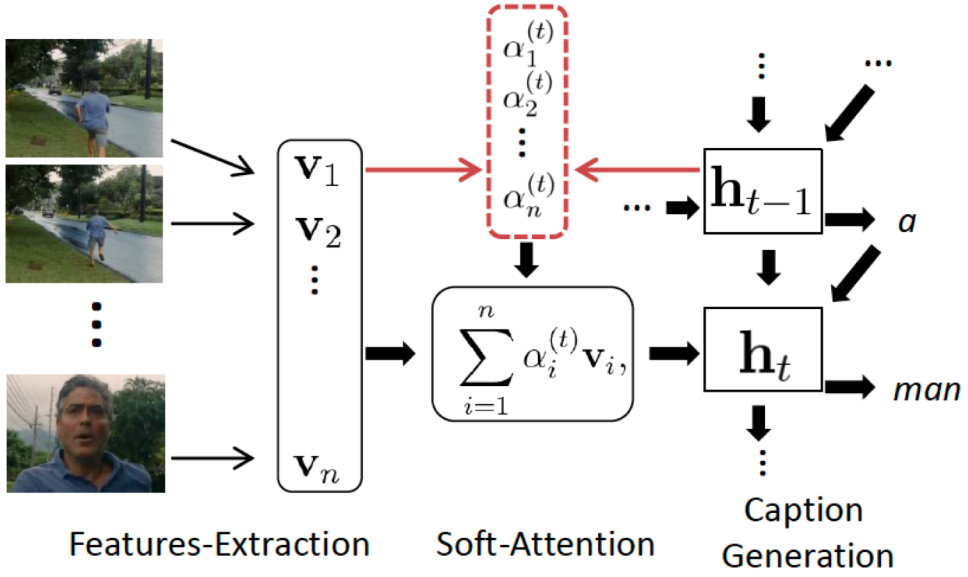

Yao et al. Describing Videos by Exploiting Temporal Structure. CVPR 2015

# Video Captioning with Temporal Attention

Encoder: 3D spatio-temporal CNN features for frames

Decoder: LSTM layer

- Similar to the decoder of [Bahdanau et al. ICLR 2015]
- $\boldsymbol{h}_t$ : hidden state at time $t$



# Video Captioning with Temporal Attention

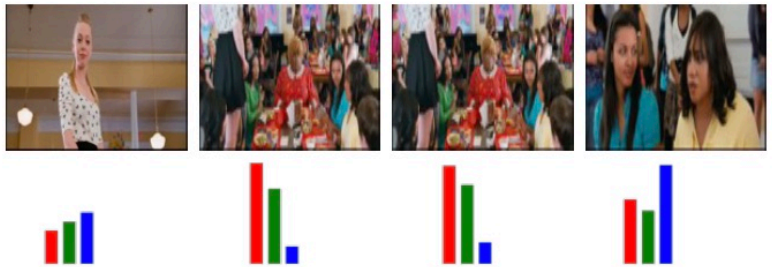
***+Local+Global:*** A **man** and a **woman** are **talking** on the **road**

***Ref:*** A man and a woman ride a motorcycle

***+Local+Global:*** **Someone** is **frying** a **fish** in a **pot**

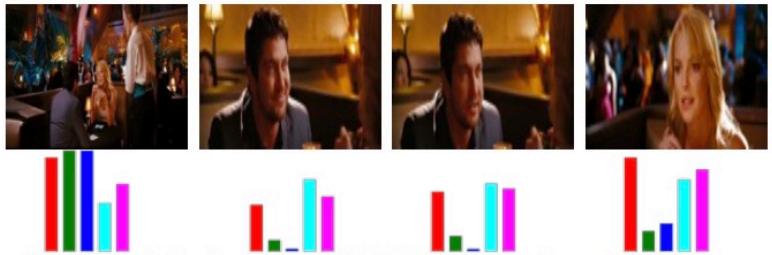
***+Local:*** Someone is frying something
***+Global:*** The person is cooking
***Basic:*** A man cooking its kitchen

***Ref:*** A woman is frying food



***+Local+Global:*** the **girl** **grins** at **him**

***Ref:*** SOMEONE and SOMEONE swap a look



***+Local+Global:*** as **SOMEONE** **sits** on the **table**, **SOMEONE** shifts his **gaze** to SOMEONE

***+Local:*** with a smile SOMEONE arrives
***+Global:*** SOMEONE sits at a table
***Basic:*** now, SOMEONE grins

***Ref:*** SOMEONE gaze at SOMEONE

# Memory Networks

Attention mechanisms

- The decoder attends to different parts of the source sentence/image/frame at each step of the output generation

Another interpretation: memory

- If we regard the source as the information in the memory, attention corresponds to selective memory access with weights

Memory networks = neural networks with external memory

- Prevents suffering from vanishing gradient problem



http://www.wildml.com/2016/01/attention-and-memory-in-deep-learning-and-nlp/

# End-to-End Memory Networks

Neural networks (RNN) + explicit storage + attention

Application: question answering

- (i) input: a set of sentences $\{x_i\}$, (ii) query $q$, and (iii) a single word answer
- Word/sentence order matters

```
Sam walks into the kitchen.
Sam picks up an apple.
Sam walks into the bedroom.
Sam drops the apple.
Q: Where is the apple?
A. Bedroom
```

```
Brian is a lion.
Julius is a lion.
Julius is white.
Bernhard is green.
Q: What color is Brian?
A. White
```

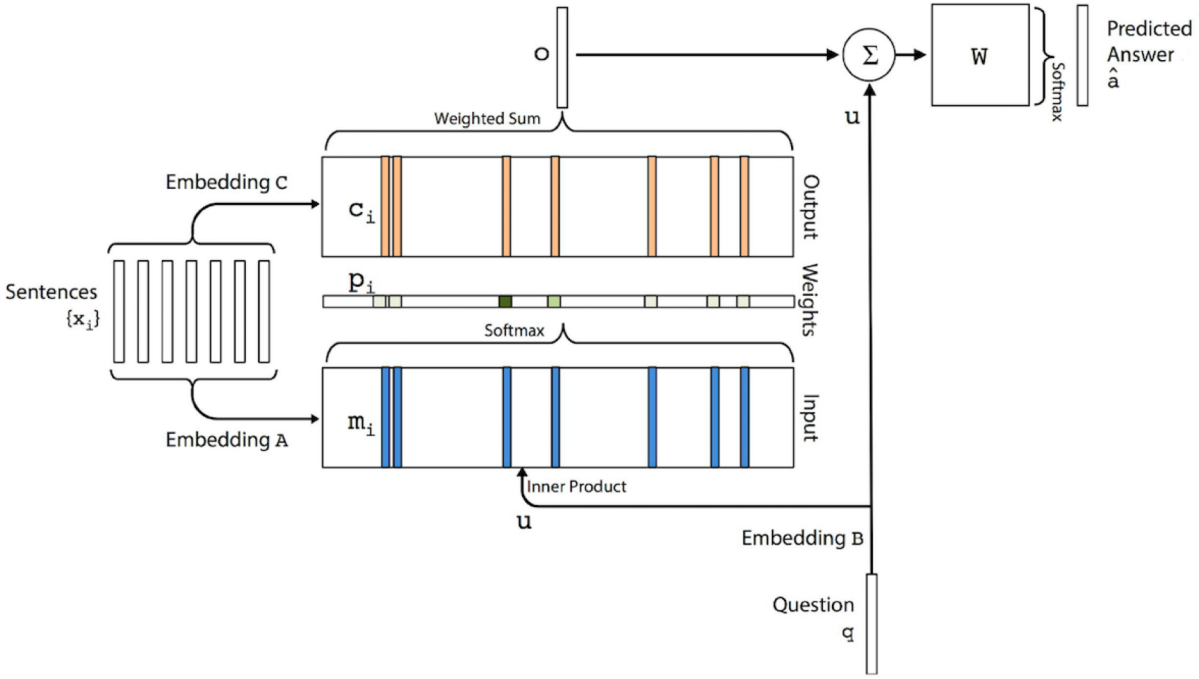


Sukhbaatar et al. End-To-End Memory Networks. NIPS 2015

# End-to-End Memory Networks

Neural networks (RNN) + explicit storage + attention

- Input $\{x_i\}$ are embedded by $A, B$ into $m_i, c_i$ (See the paper)
- Embedding matrices $A, B, C, W$ are learned during training




(1) Query embedding
$u = Bq$

(2) Attention in memory
$p_i = \text{softmax}(u^T m_i)$

(3) Memory output
$o = \sum_i p_i c_i$

(4) Answer selection
$\hat{a} = \text{softmax}(W(o + u))$

# Outline

- Attention
- Self-attention
- Transformer

# Representation Learning of Sequential Data

Basic building block of sequence-to-sequence learning

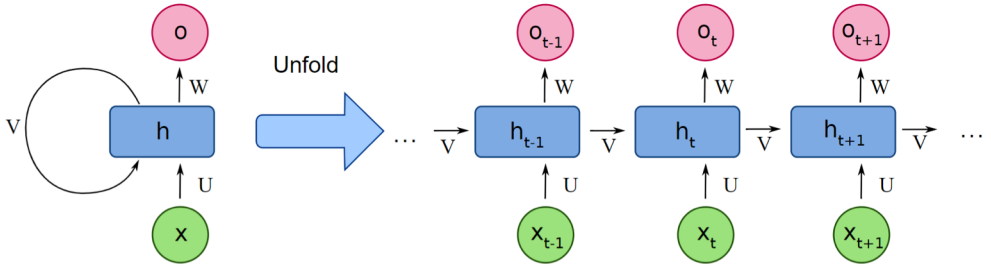
- Neural machine translation, summarization, QA, …

Recurrent Neural Networks (LSTMs, GRUs and variants)

- Natural fit for sentences and sequences of pixels

However,

- Sequential computation inhibits parallelization
- No explicit modeling of long and short range dependencies
- No model hierarchy



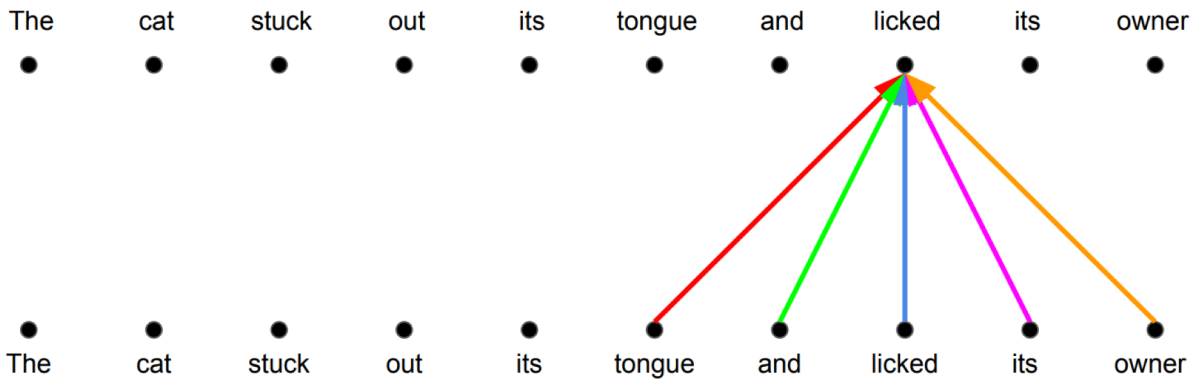
# Representation Learning of Sequential Data

Convolutional neural networks

- Trivial to parallelize (per layer)
- Exploits local dependencies
- ‘Interaction distance’ between positions linear or logarithmic …

However,

- Long-distance dependencies require many layers



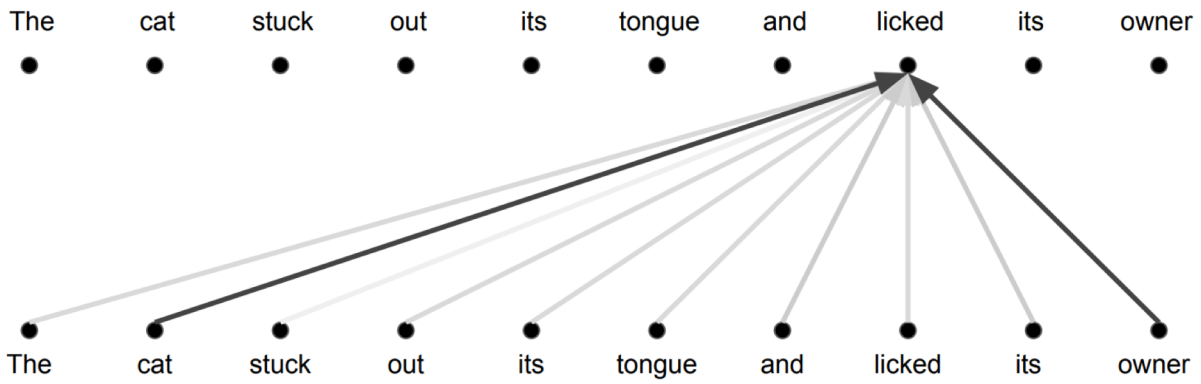
# Self-Attention

Why not use attention for representations?

- Self-attention directly models relationships between all words in a sentence, regardless of their respective position

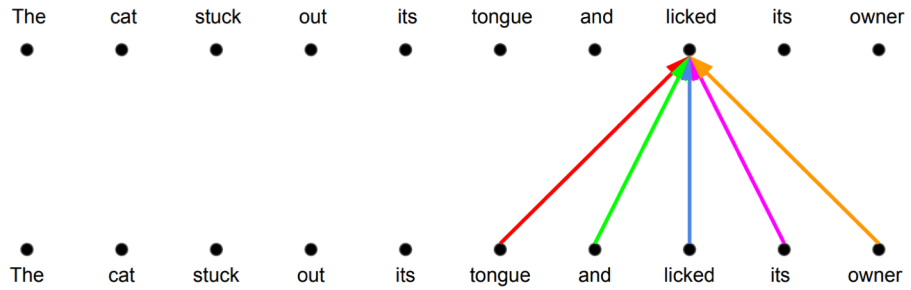
*I arrived at the bank after crossing the river*

- For representation of "*bank*", use a weighted average of all words' representations (the attention scores are used as weights)
- Trivial to parallelize (per layer)
- Constant 'path length' between any two positions

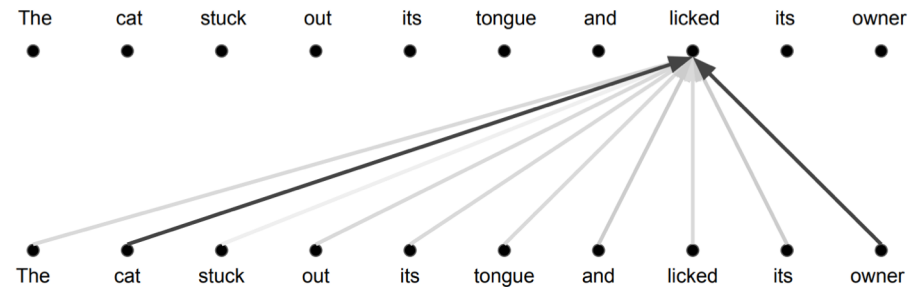


# Convolution vs Attention

Convolution: different linear transformations by relative position



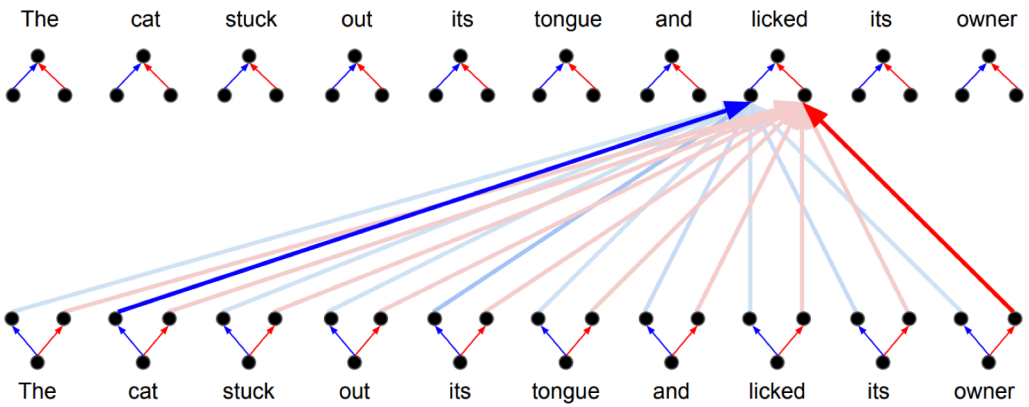

Convolution: a weighted average for all inputs



# Multi-head Attention

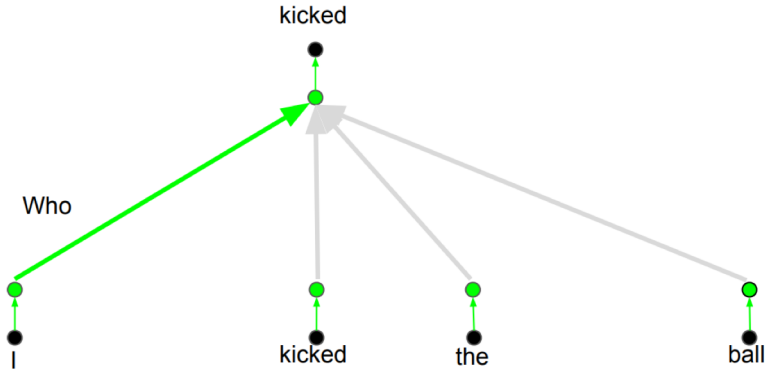
Parallel attention layers with different linear transformations on input and output

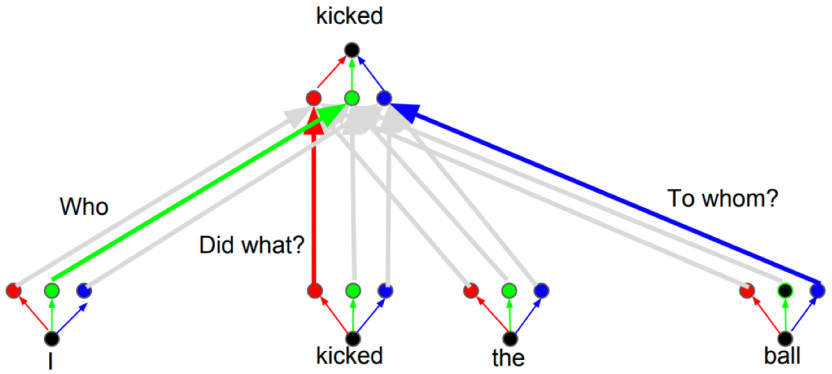
- It turns out that multiple different attentions are helpful



# Multi-head Attention

Can combine the knowledge explored by multiple heads or agents instead of doing it by one



# Comparison with Other Architectures

Self-attention connects all positions with a constant number of sequentially executed operations

- Moreover, $n \ll d$ usually

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

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

The amount of computation that can be parallelized

The maximum path length between any two input/output



Image Credit: Vaswani et al. Attention Is All You Need. NIPS 2017

# Outline

- Attention
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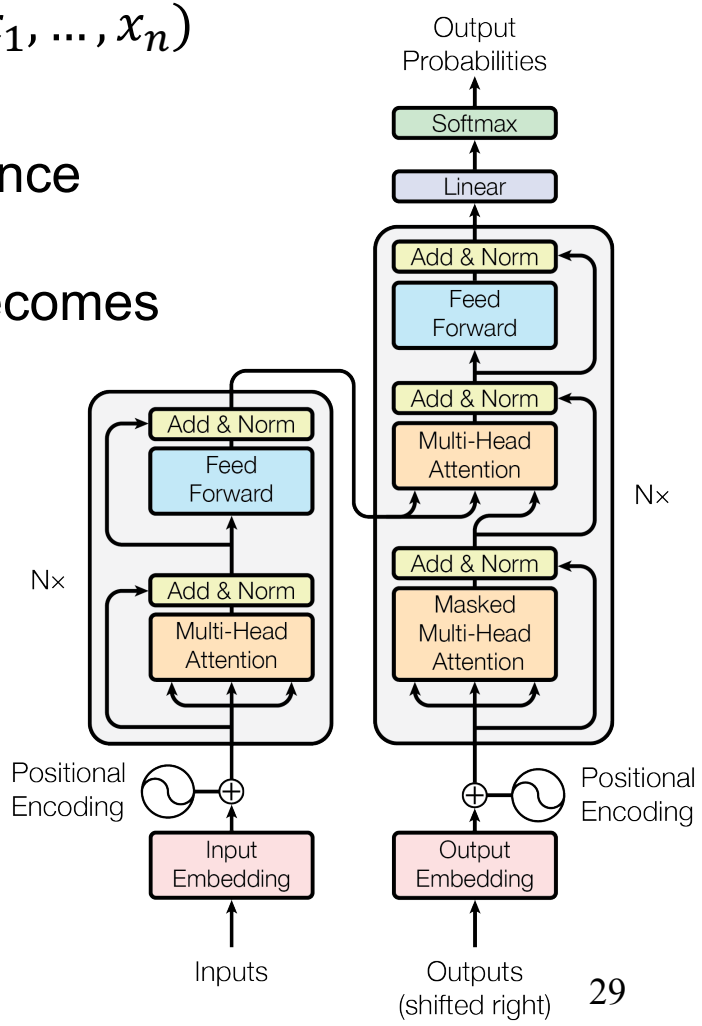
- Transformer

A. Vaswani, N. Shazeer N. Parmar, J. Uszkoreit, L. Jones, A. N. Gomez, Ł. Kaiser I. Polosukhin . Attention is All you Need. NeurIPS 2017

# Transformer

An encoder-decode structure

- Encoder maps an input sequence $(x_1, \ldots, x_n)$ to a latent sequence $(z_1, \ldots, z_n)$
- Decoder generates an output sequence $(y_1, \ldots, y_n)$ from $\boldsymbol{z}$ autoregressively (i.e. previously generated outputs becomes an input to generating a next output)



# Transformer

## Encoding

- Start initial representations for each word (unfilled circles)
- Using self-attention, it aggregates information from all of the other words, generating a new representation per word informed by the entire context (filled balls)
- This step is then repeated multiple times in parallel

## Decoding

- The decoder generates one word at a time from left to right
- It attends not only to the other previously generated words, but also to the final representations by the encoder

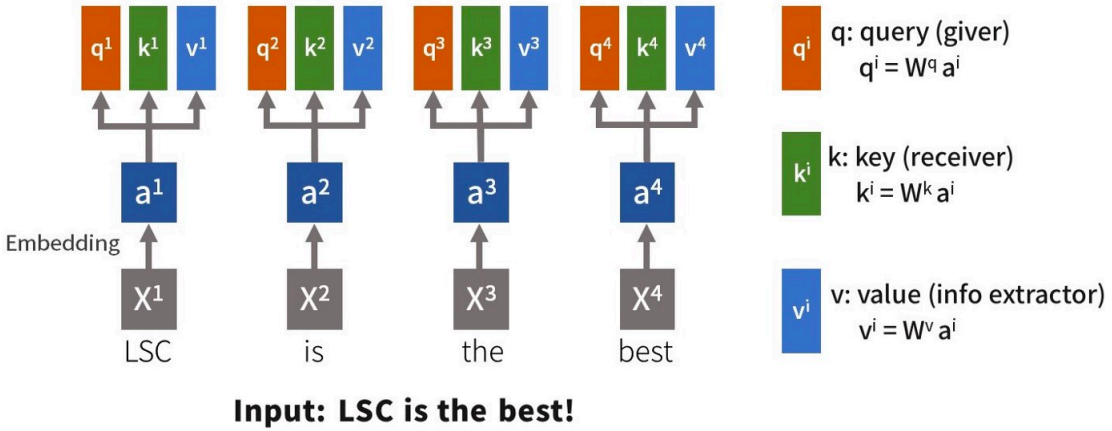


Image Credit: https://ai.googleblog.com/2017/08/transformer-novel-neural-network.html

# Self-Attention Layer

For every input word $x_i$

- First encode into a vector $x_i$ and then obtain query $q_i$, key $k_i$ value $v_i$ as
- $q_i = W_q a_i$, $k_i = W_k a_i$, $v_i = W_v a_i$ where $W_*$ are learnable parameters





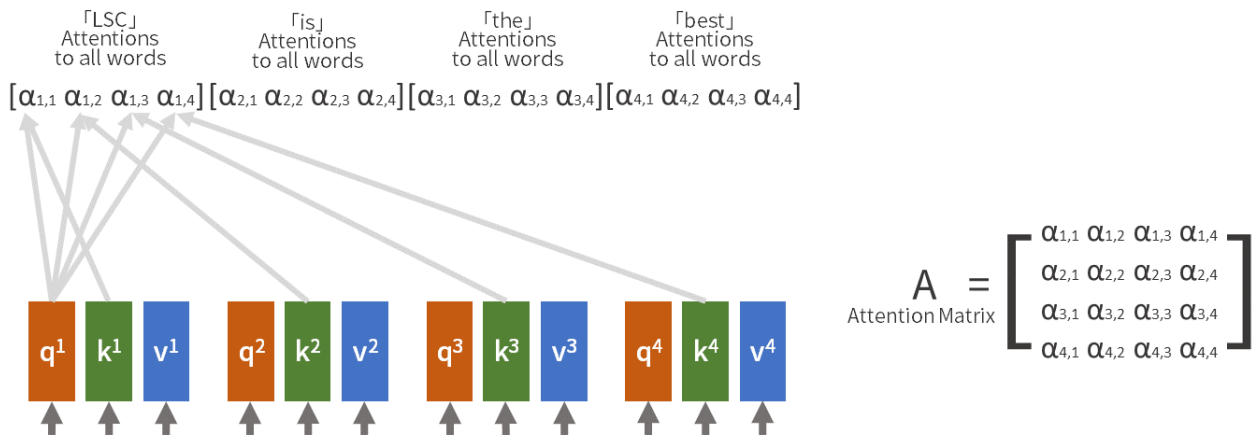

Neil Wu, Introduction of Self-Attention Layer in Transformer

# Self-Attention Layer

Attention $\alpha_{i,j}$

- Defined as inner product of Query $q_i$ and Key $k_j$ divided by square root of its dimensions

$$\alpha_{i,j} = \text{softmax}(\frac{q_i \cdot k_j}{\sqrt{d}})$$



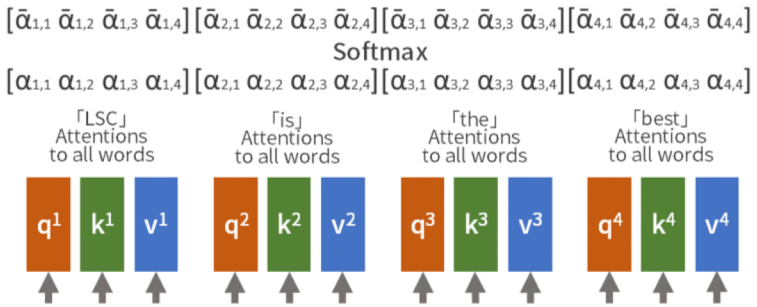

Neil Wu, Introduction of Self-Attention Layer in Transformer

# Self-Attention Layer

Output $b_i$

- Calculated by sum of attentions multiply by extract information from value of each word paid attention to

$$b_i = \sum_j \alpha_{i,j} \cdot v_j$$

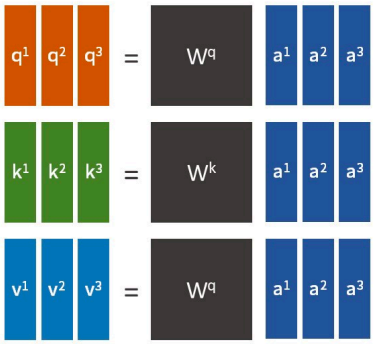


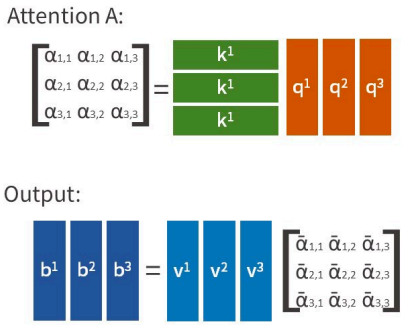



Neil Wu, Introduction of Self-Attention Layer in Transformer

# Self-Attention Layer

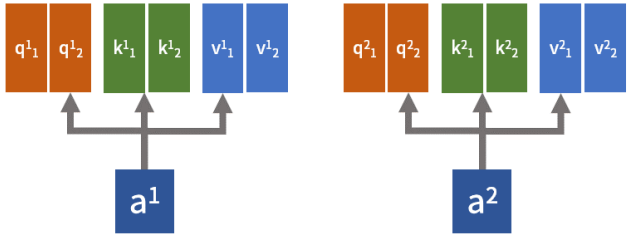
Matricize!




Multi-heads

- Create multiple Attention matrices in one layer
- By simply double the Query, Key and Value combinations, and independently calculates attention matrix




$A^1$ = Attention Matrix 1 $\begin{bmatrix} \alpha^1_{1,1} & \alpha^1_{1,2} \\ \alpha^1_{2,1} & \alpha^1_{2,2} \end{bmatrix}$

$A^2$ = Attention Matrix 2 $\begin{bmatrix} \alpha^2_{1,1} & \alpha^2_{1,2} \\ \alpha^2_{2,1} & \alpha^2_{2,2} \end{bmatrix}$



Neil Wu, Introduction of Self-Attention Layer in Transformer

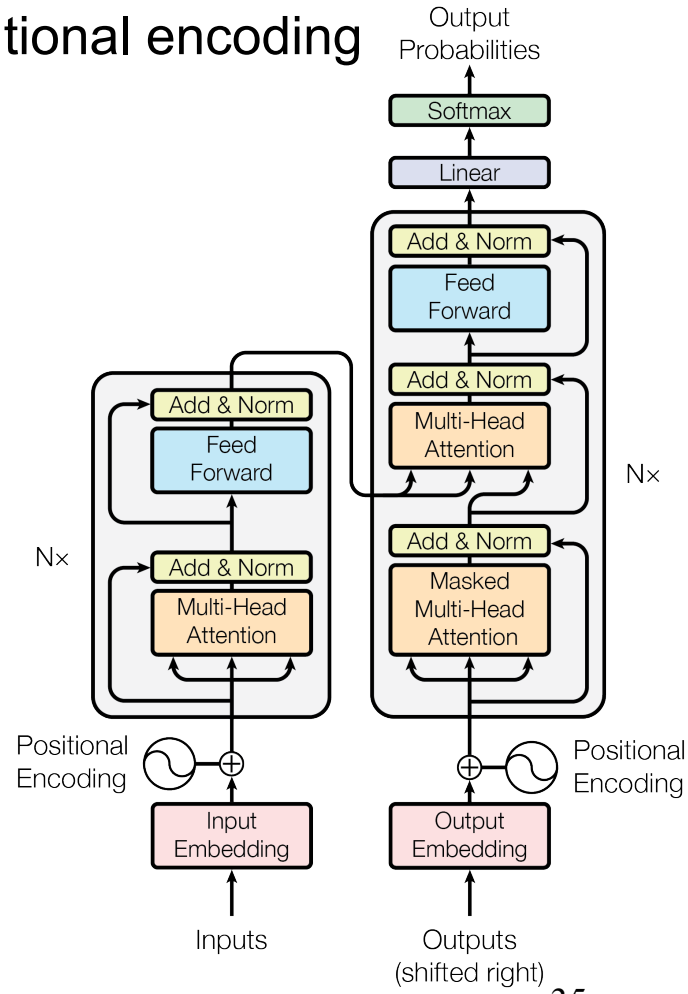
# Transformer Architecture

## Input

- Add the Input embedding and the positional encoding

## Encoder

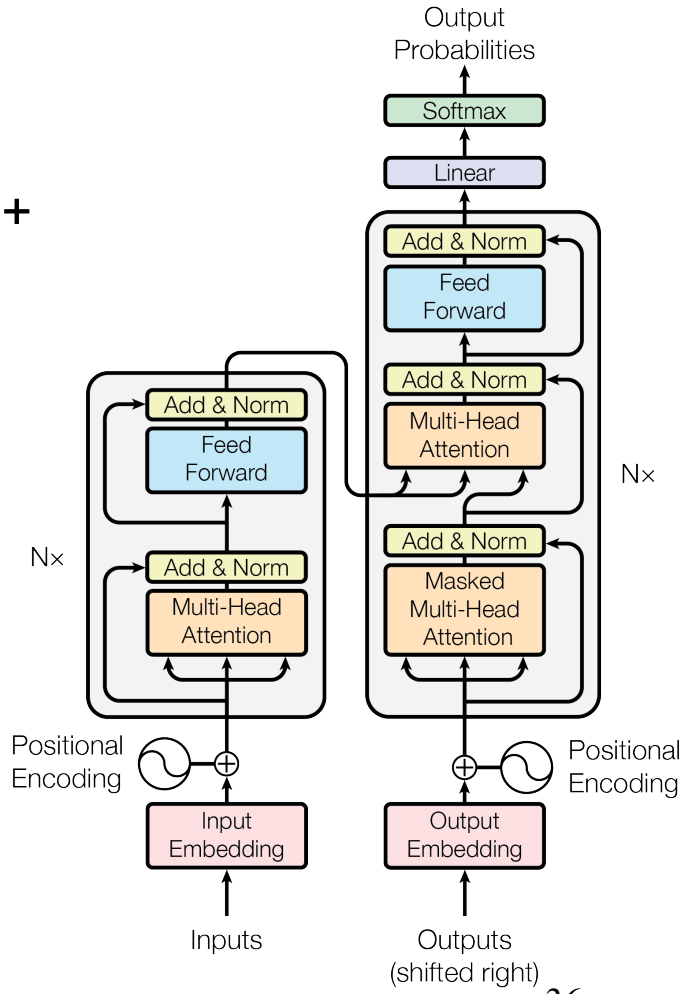
- A stack of *N* (=6) identical layers
- (1) Multi-head attention layer: already discussed!
- (2) Position-wise feedforward neural network: a little FFN has identical parameters for each position
- Dropouts and layer normalization per sublayer



# Transformer Architecture

## Decoder

- Similar to encoder
- A stack of *N* (=6) identical layers
- Decoder Input: the output Embedding + Positional Encoding up to i-1 outputs
- Masked Multi-Head Attention prevents future words to be part of the attention

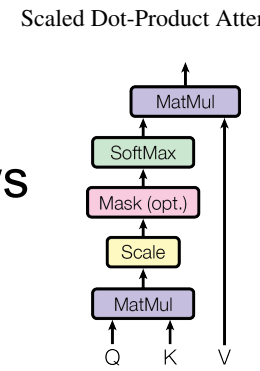


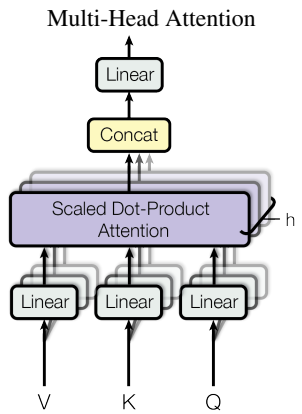
# Transformer Architecture

## Multi-head attention

- The original pictures are as follows

$$\text{Attention}(Q, K, V) = \text{softmax}\left(QK^T/\sqrt{d_k}\right)V$$

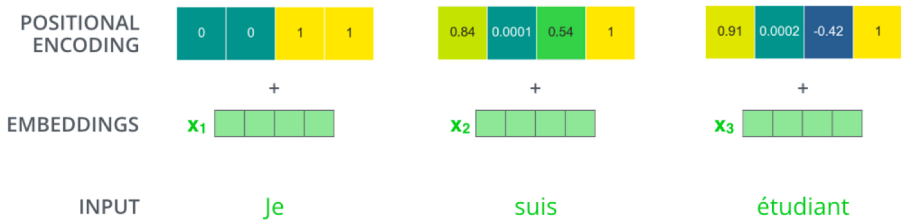



## Position encoding

- Unlike sequential RNNs, the transformer is parallel and non-sequential
- Represent the information on the absolute (or relative) position in a sequence

$$PE_{pos,i} = \begin{cases} \sin\left(\frac{pos}{10000^{\frac{i}{d}}}\right) & \text{if } i \text{ is even} \\ \cos\left(\frac{pos}{10000^{\frac{i}{d}}}\right) & \text{if } i \text{ is odd} \end{cases}$$




where $pos$ is the position and $i$ is the dimension

Jay Alammar, The Illustrated Transformer