Transformers and Large Language Models

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Thanks to Boyuan Chen for the original slides

Pre-words

- The slides were adapted from Stanford CS224N, Natural Language Processing

- You should know deep learning basics

Outline

Part 1: Transformer

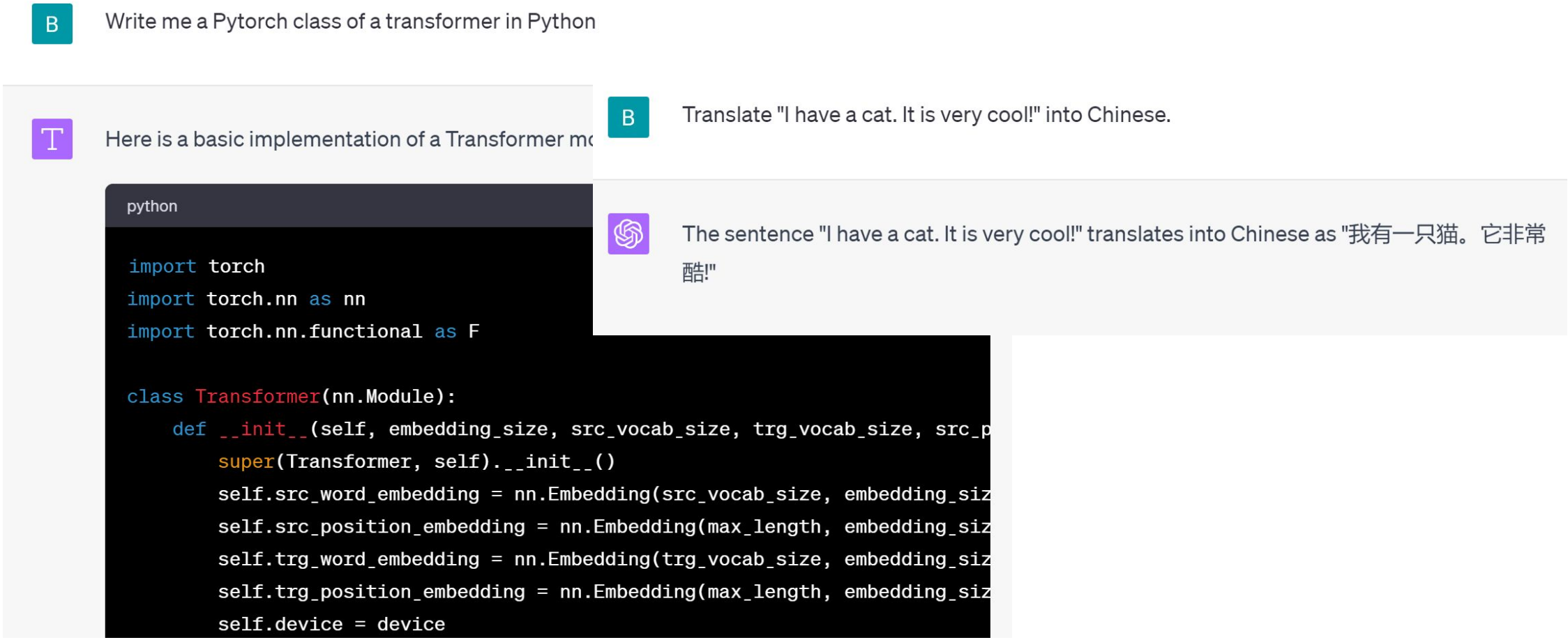
- What can transformers do
- Different types of transformer
- Why is transformer better than RNN
- Attention mechanism
  - General Structure
  - Query, Key & Value
  - Multi-Head Attention
  - Self-Attention

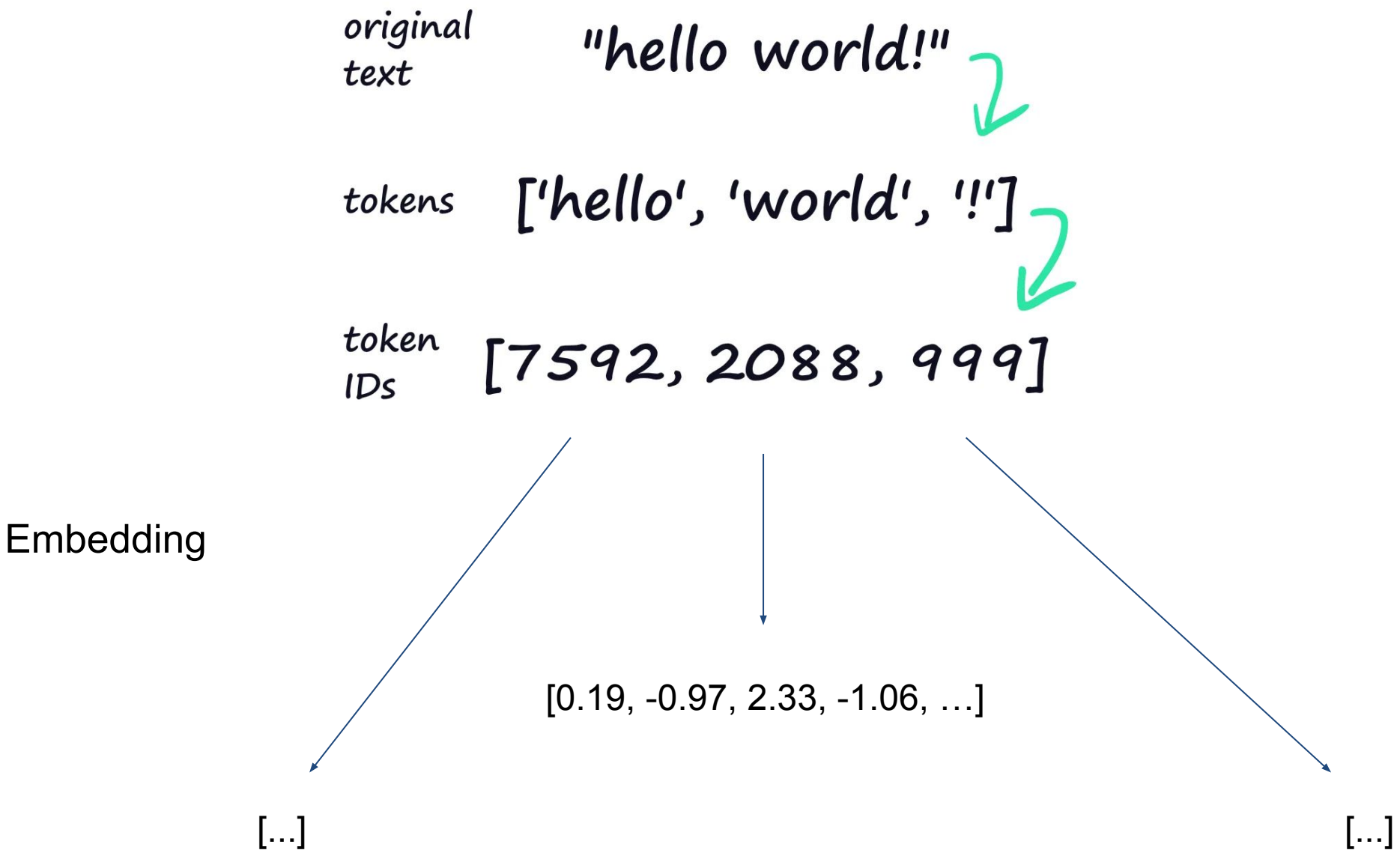
Part 2: Large Language Models

- Introduction to Language Models and Large Language Models
- Common architecture of LLMs
  - Autoencoding
  - Autoregressive
  - Sequence to sequence
- Application of LLMs
- Training a LLM

What can transformers do?

- Text Generation




original text
"hello world!"
tokens
['hello', 'world', '!']
token IDs
[7592, 2088, 999]
Embedding
[0.19, -0.97, 2.33, -1.06, …]
[...]
[...]

How are transformers trained?

- Text Generation (Training)

Input (English): I have a cat.

Output (French): J’ai un ___

label: chat

Each token is represented as an [embedding]-dimensional vector. For example, if your embedding is 5, then the “chat” token might be represented as [0.53, 1.2, 0.01, 0.275, 0.90]. It is converted using a **tokenizer** that comes along with the model.

What can transformers do?

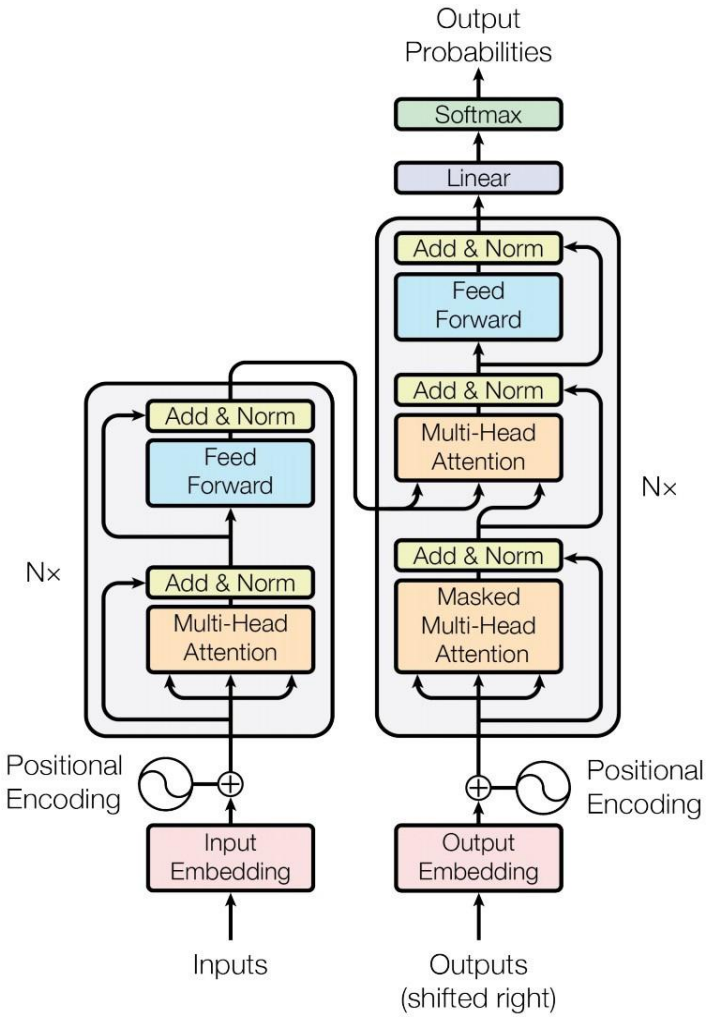
- Text Classification

```
Positive tweets:
RT @JohnGGalt: Amazing—after years of attacking Donald
Trump the media managed
to turn #InaugurationDay into all about themselves.
#MakeAme…
```

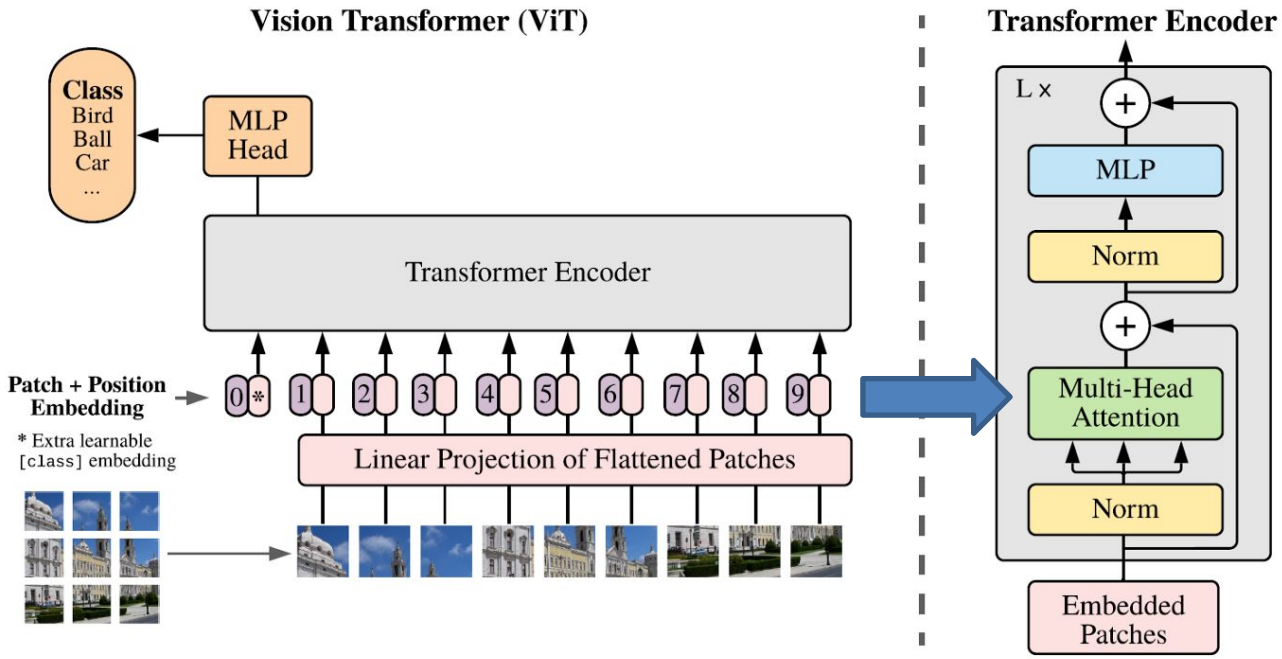
```
Negative tweets:
RT @Slate: Donald Trump’s administration: “Government by
the worst men.”
RT @RVAwonk: Trump, Sean Spicer, etc. all lie for a
reason.
```

What can transformers do?

- **<u>NLP: Machine Translation</u>**



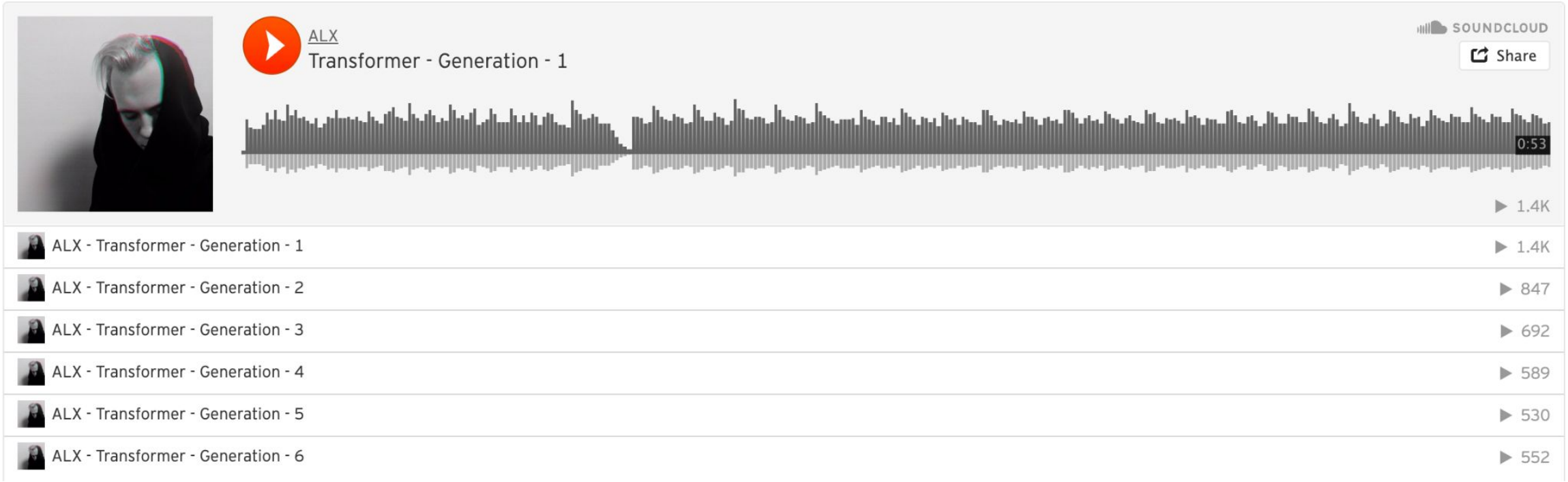
- CV: Classifier / Object Detection



What can transformers do?

- Audio Generation

https://alxmamaev.medium.com/generating-music-with-ai-or-transformers-go-brrrr-3a3ac5a04126



Image, video, movements, etc… We call it **multimodal**.

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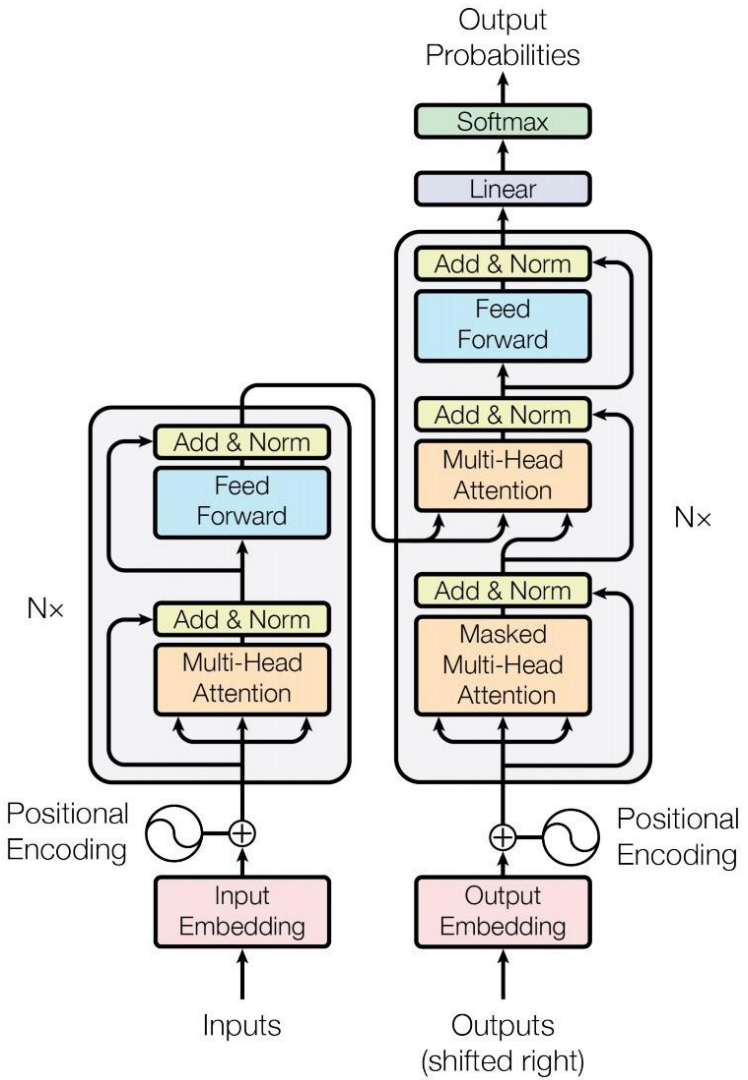
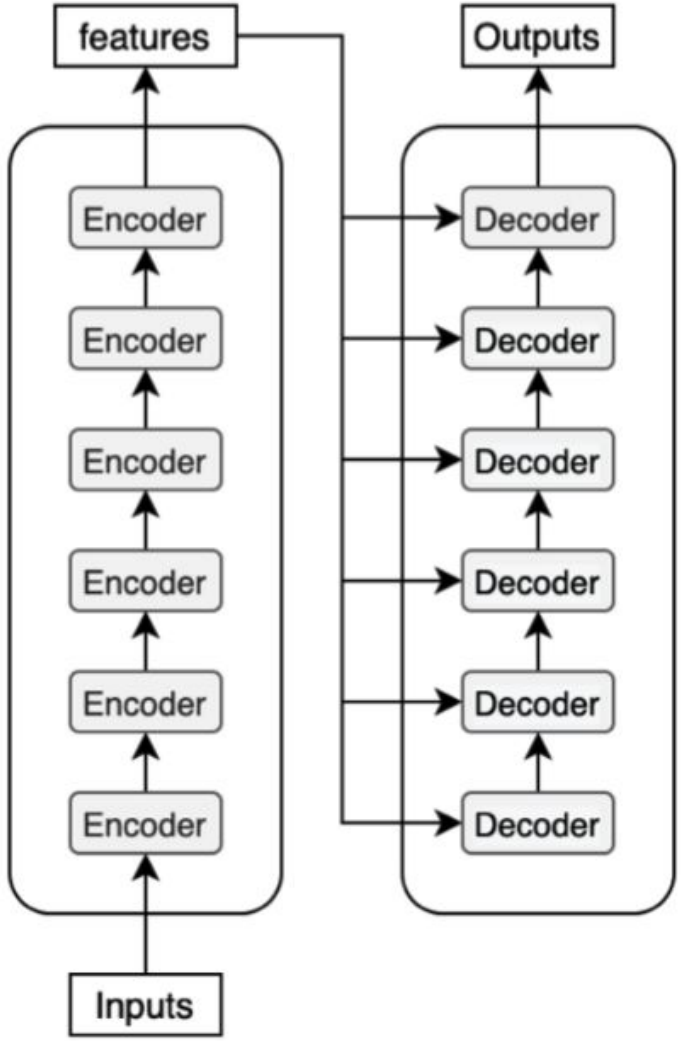
Different Types of Transformers

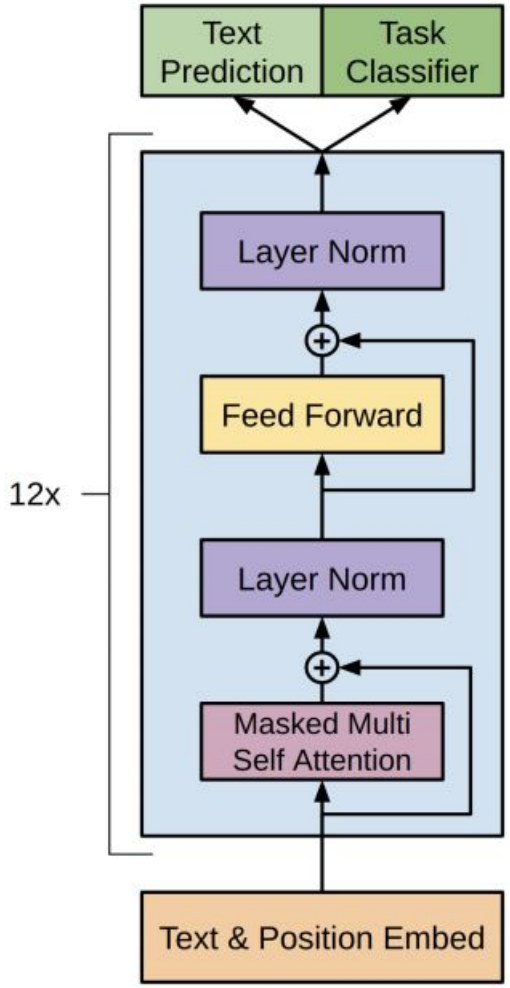
- Encoder-Decoder (2017)



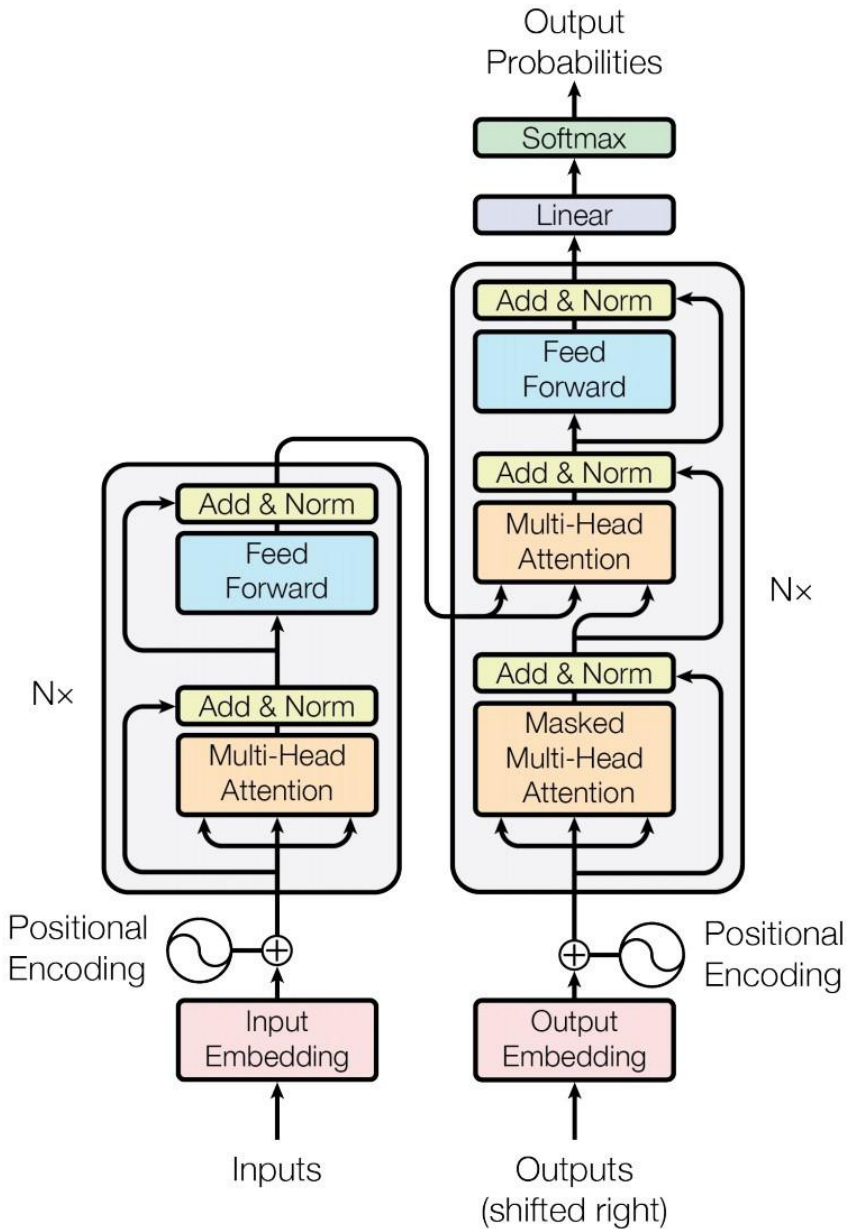


Different Types of Transformers

- Decoder-Only (Openai GPT-2, 2019)
- Encoder-Only (BERT, 2018)



Encoder-Decoder Transformer Architecture



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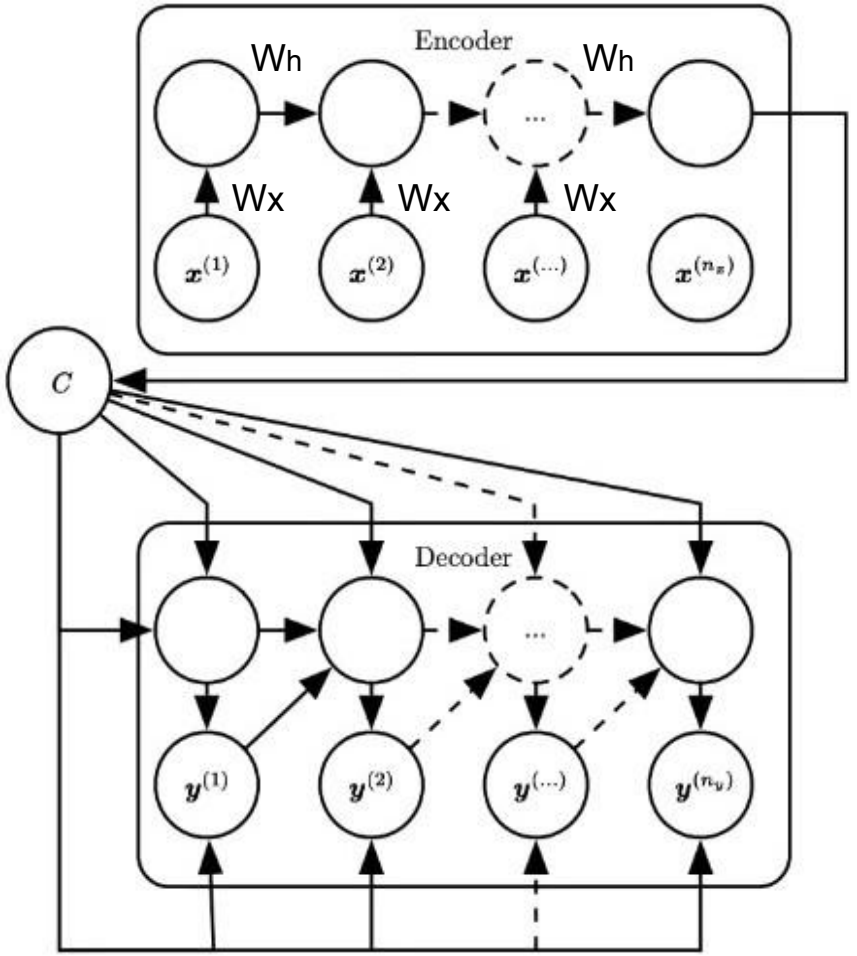
Why is transformer better than RNN?

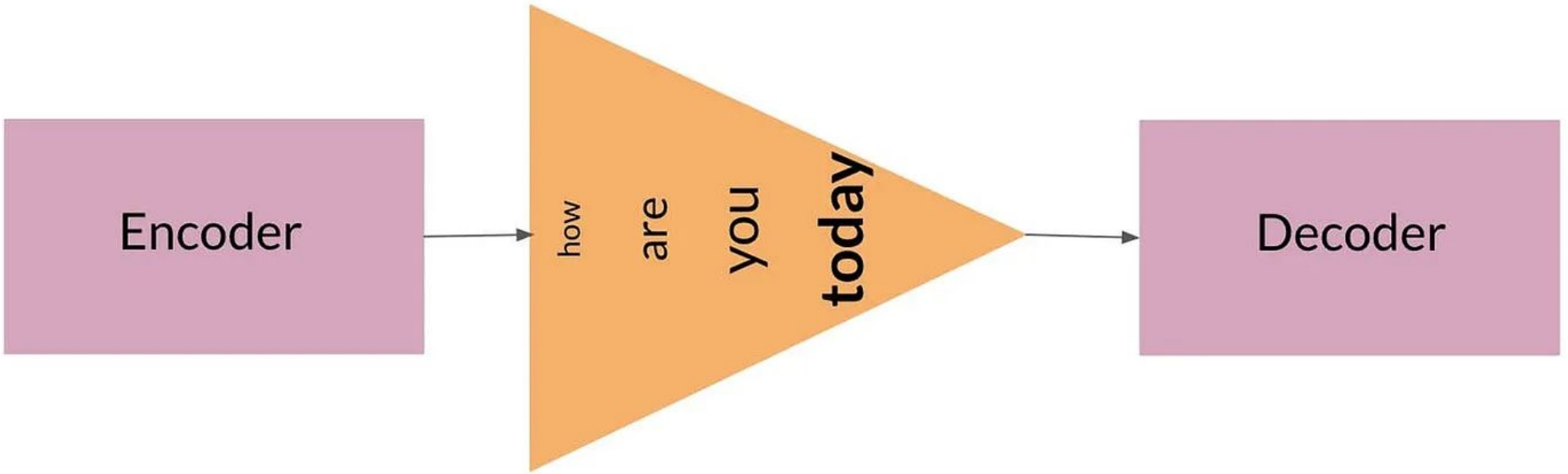
Les pauvres sont démunis
(French)

Decoder-Encoder Model



The poor do not have any money
(English)

Information Bottleneck



Forgets about the early tokens

Gradient vanishing and gradient explosion

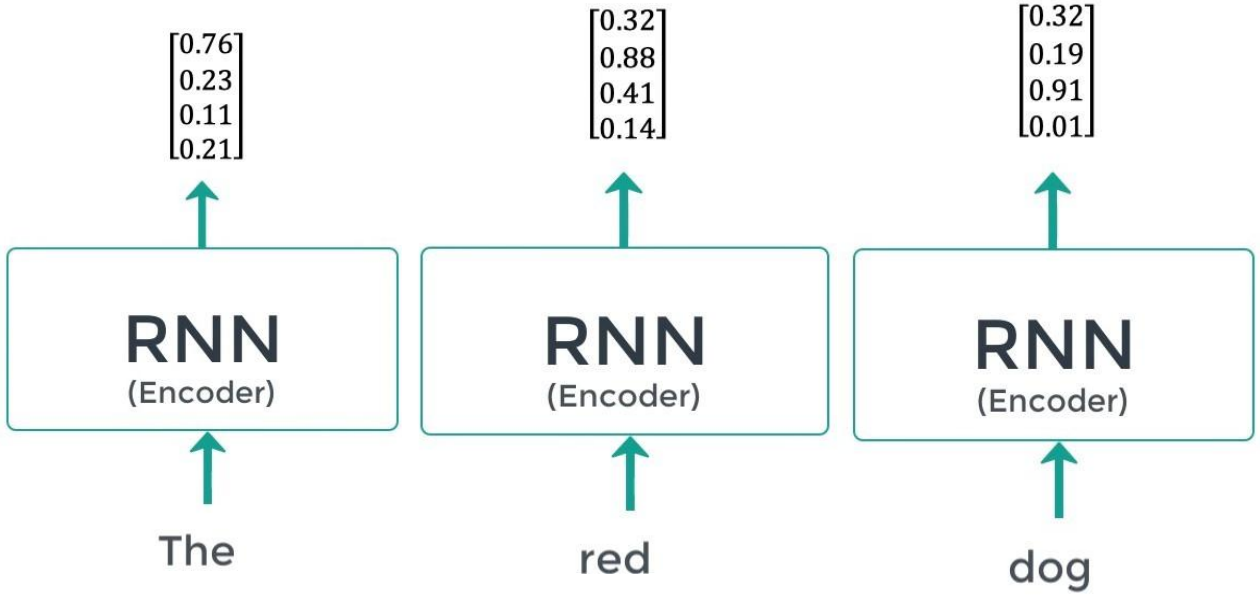
Motivations of Attention

RNNs

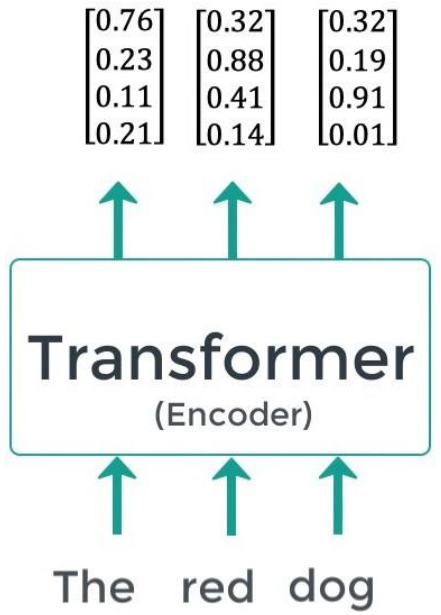
1. Long-range Dependencies
2. Gradient Vanishing/Exploding
3. Large #Training Steps
4. Recurrence prevents Parallel computation

Transformers

1. Facilitate Long-range dependencies
2. No Gradient Vanishing/Exploding
3. Fewer #Training Steps
4. Parallelization



VS



Attention Mechanism

Solution to the bottleneck problem: *Attention*

Key idea: On each step of the decoder, *focus on a particular part* of the source sequence

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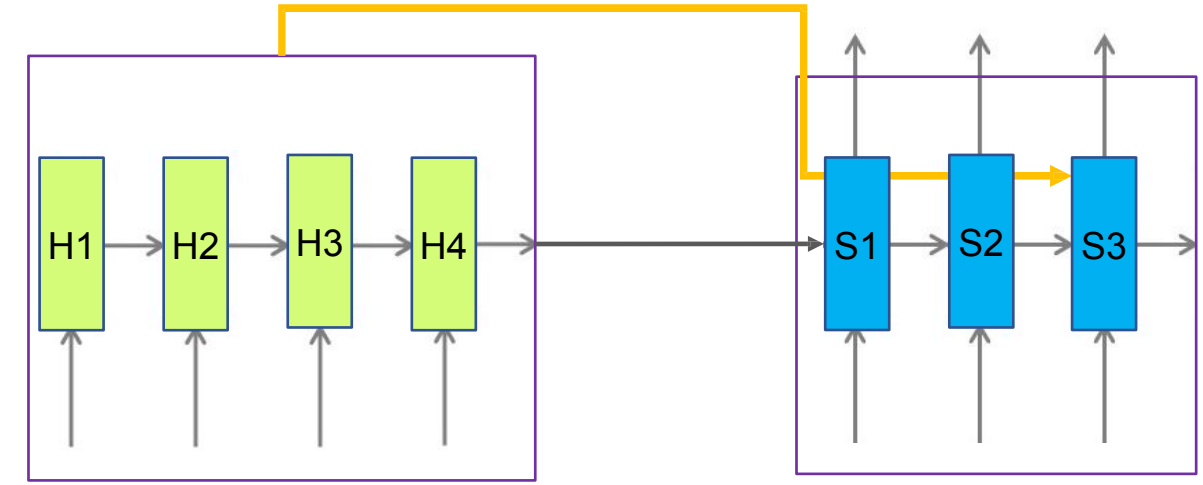
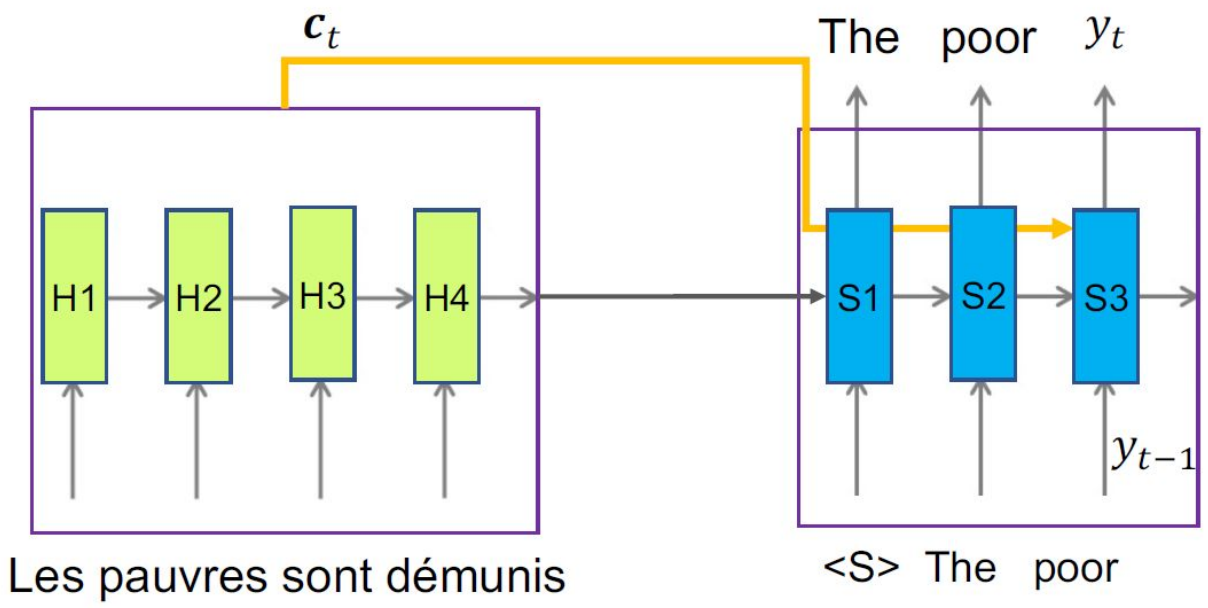
Attention Mechanism



Random Access Memory: Retrieve as Needed

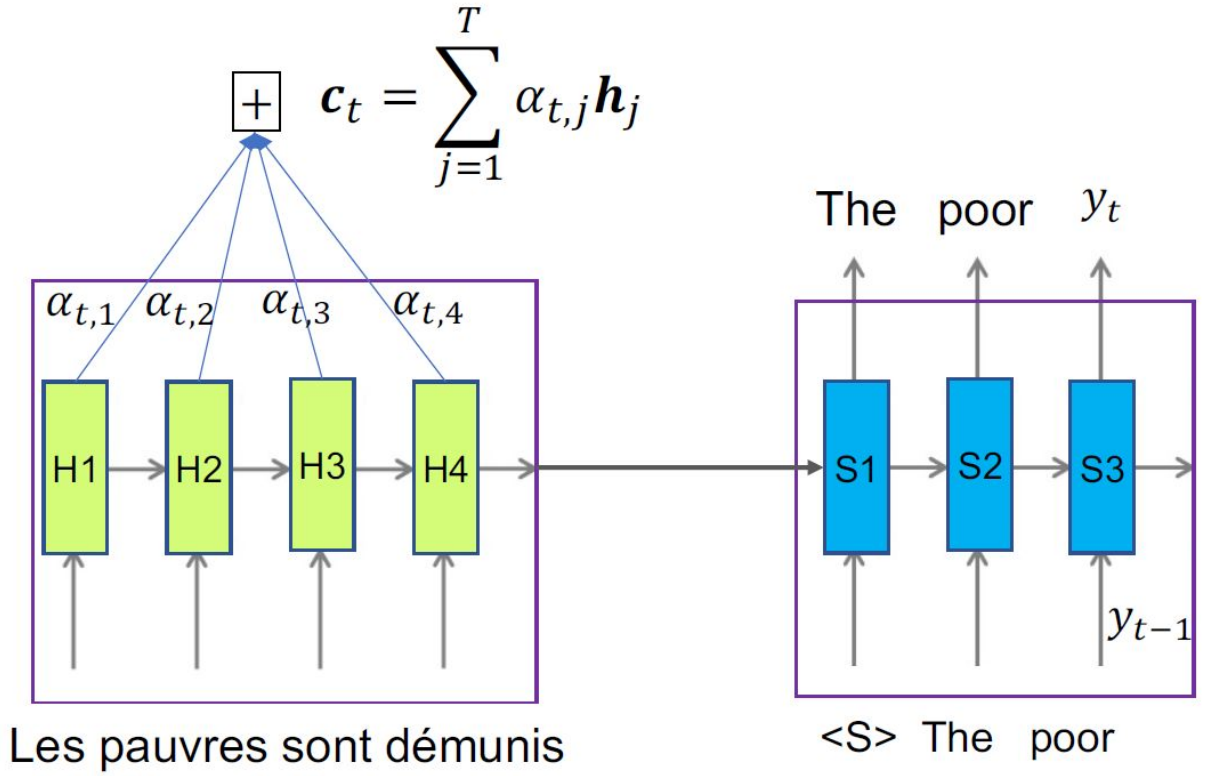
Attention Mechanism



$$p(y_t|y_{t-1}, \dots, y_1, \boldsymbol{x}) = f(y_{t-1}, \boldsymbol{s}_t, \boldsymbol{c}_t)$$

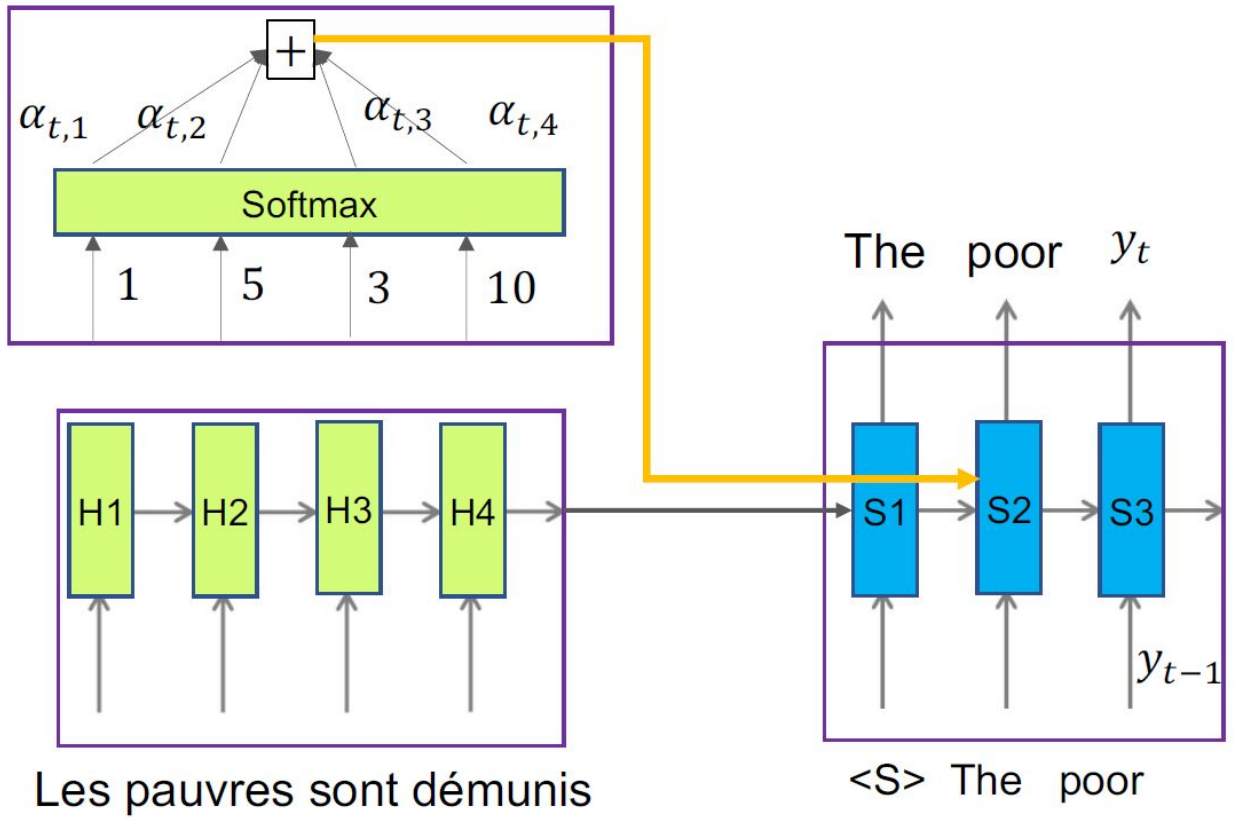
Attention Mechanism

Get weighted sum



Attention Mechanism

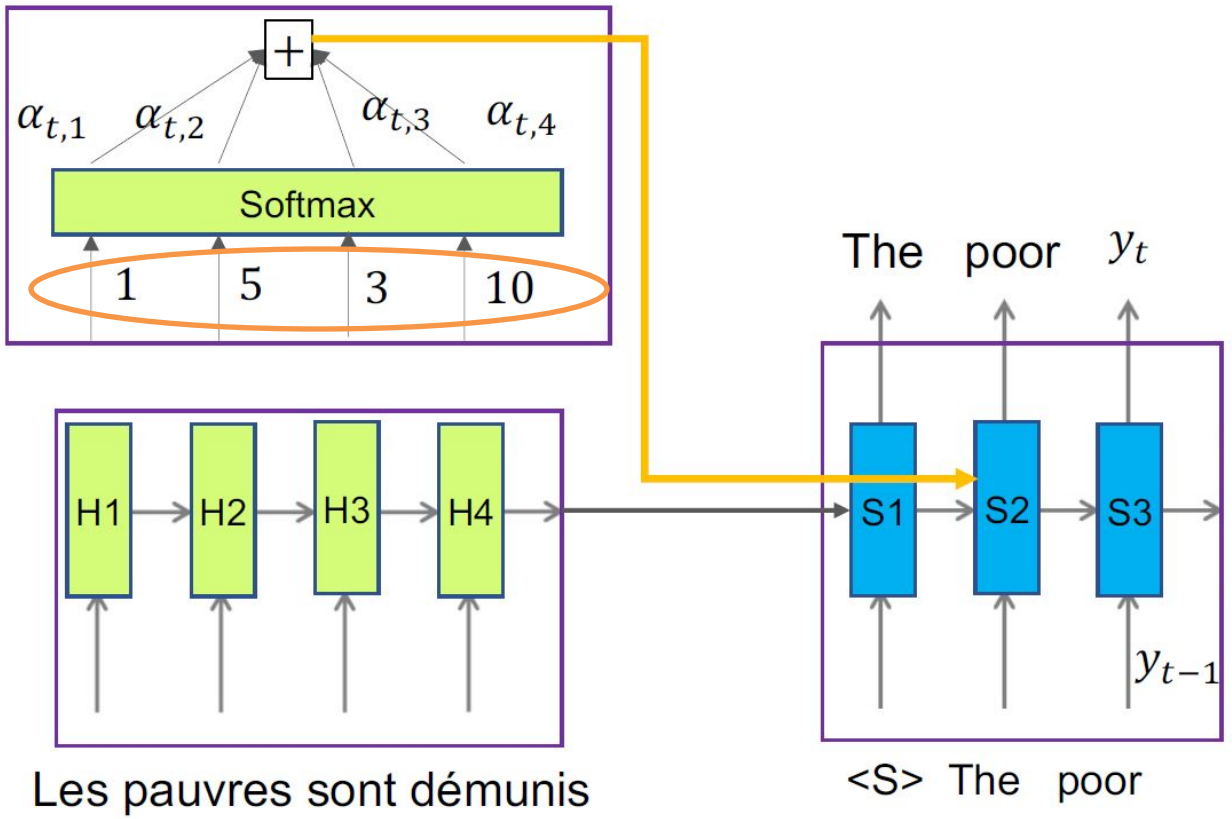
$$\alpha_{t,j} = \frac{\exp(Score_{t,j})}{\sum_{k=1}^{T} \exp(Score_{t,k})} = \text{Softmax (scores)}$$



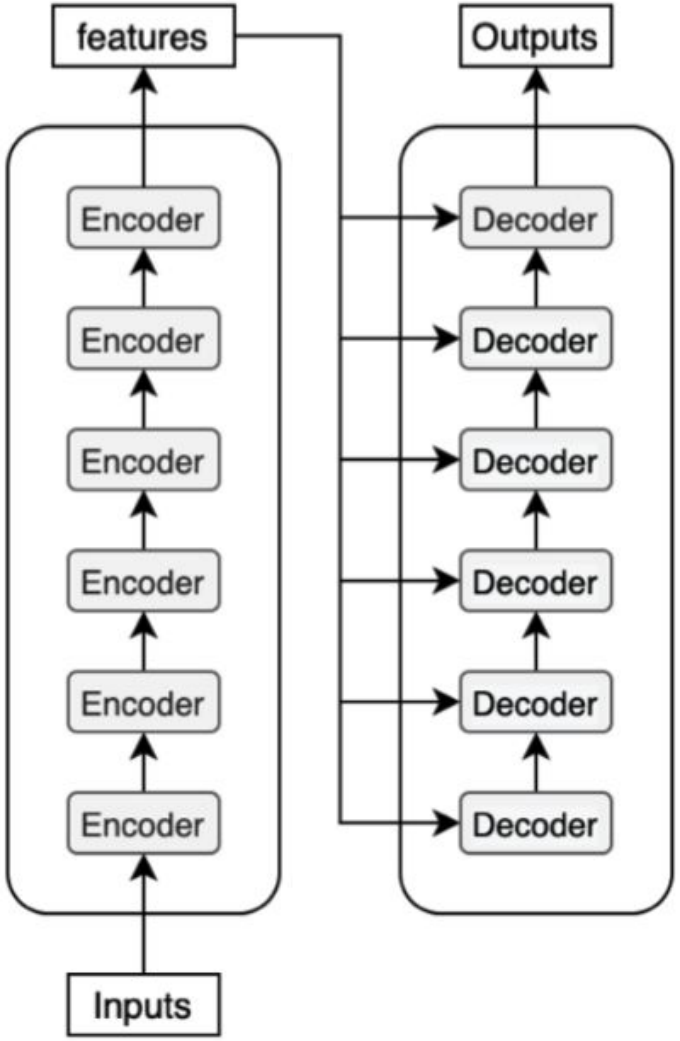
Attention Mechanism

How are the weights calculated?

$$\alpha_{t,j} = \frac{\exp(Score_{t,j})}{\sum_{k=1}^{T} \exp(Score_{t,k})} = \text{Softmax (scores)}$$



Attention Mechanism



All the ↑ are passing a hidden state (h). It is of shape
[batch size, text length, embedding]

text length is the input length for encoder; output length for decoder.

Example:
Input: Les pauvres sont démunis
Output: The poor do __
Batch size = 1, embedding = 1024. What is the hidden states' shape for encoder and decoder?

Answer:
Input: [<start>, 'Les', ' pauvres', ' sont', ' démunis', <end>]
[1, 6, 1024]
Output: [<start>, 'The', ' poor', ' do']
[1, 4, 1024]

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Attention Mechanism

Mimics *Retrieval Process* in a database:

- Query
- Key
- Value

Quer y

```
-- Find any employee born in October
SELECT *
FROM employee
WHERE birth_date LIKE '____-10%';
```

Value Value Value Key Value Value Value Value

Employee

emp_id	first_name	last_name	birth_date	sex	salary	super_id	branch_id
100	David	Wallace	1967-11-17	M	250,000	NULL	1
101	Jan	Levinson	1961-05-11	F	110,000	100	1
102	Michael	Scott	1964-03-15	M	75,000	100	2
103	Angela	Martin	1971-06-25	F	63,000	102	2
104	Kelly	Kapoor	1980-02-05	F	55,000	102	2
105	Stanley	Hudson	1958-02-19	M	69,000	102	2
106	Josh	Porter	1969-09-05	M	78,000	100	3
107	Andy	Bernard	1973-07-22	M	65,000	106	3
108	Jim	Halpert	1978-10-01	M	71,000	106	3

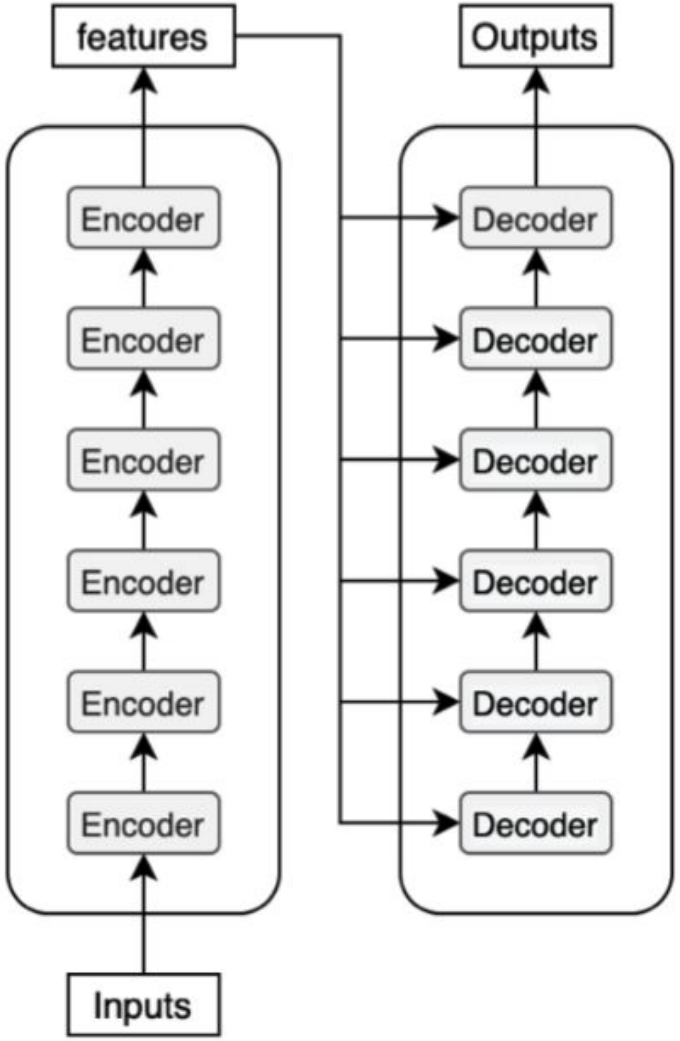
Success
1 rows

Explore | SQL | Data | Chart | Export

5:47 PM
0.045 seconds

emp_id	first_name	last_name	birth_date	sex	salary	super_id	branch_id
108	Jim	Halpert	1978-10-01	M	71000	106	3

Attention Mechanism



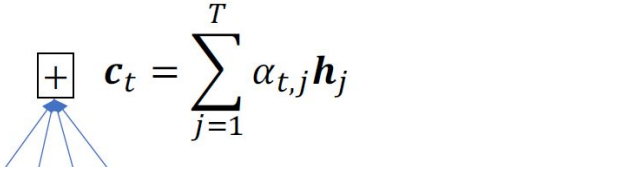
Q = HiddenStates x W_q

K = HiddenStates x W_k

V = HiddenStates x W_v

Each is of shape [batch size, text length, qkv-embedding]

$$Attention(Query, Key, Value) = \sum_i Similarity(Query, Key_i) * Value_i$$

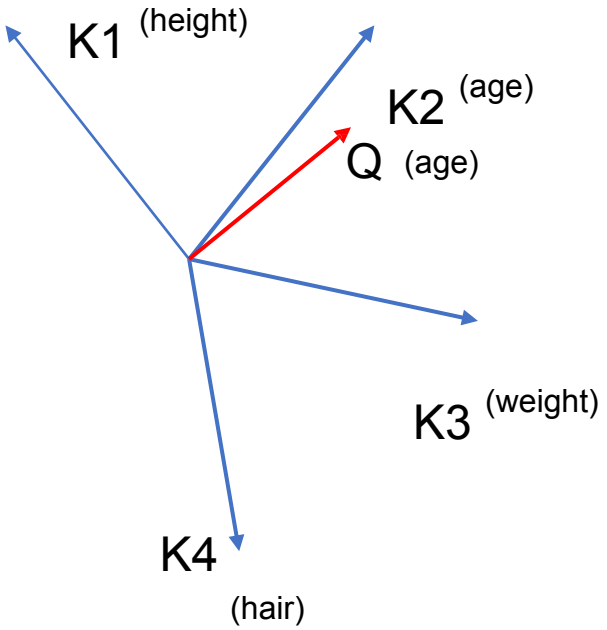


Attention = Q K^T V, with a little twist…

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

Attention Mechanism

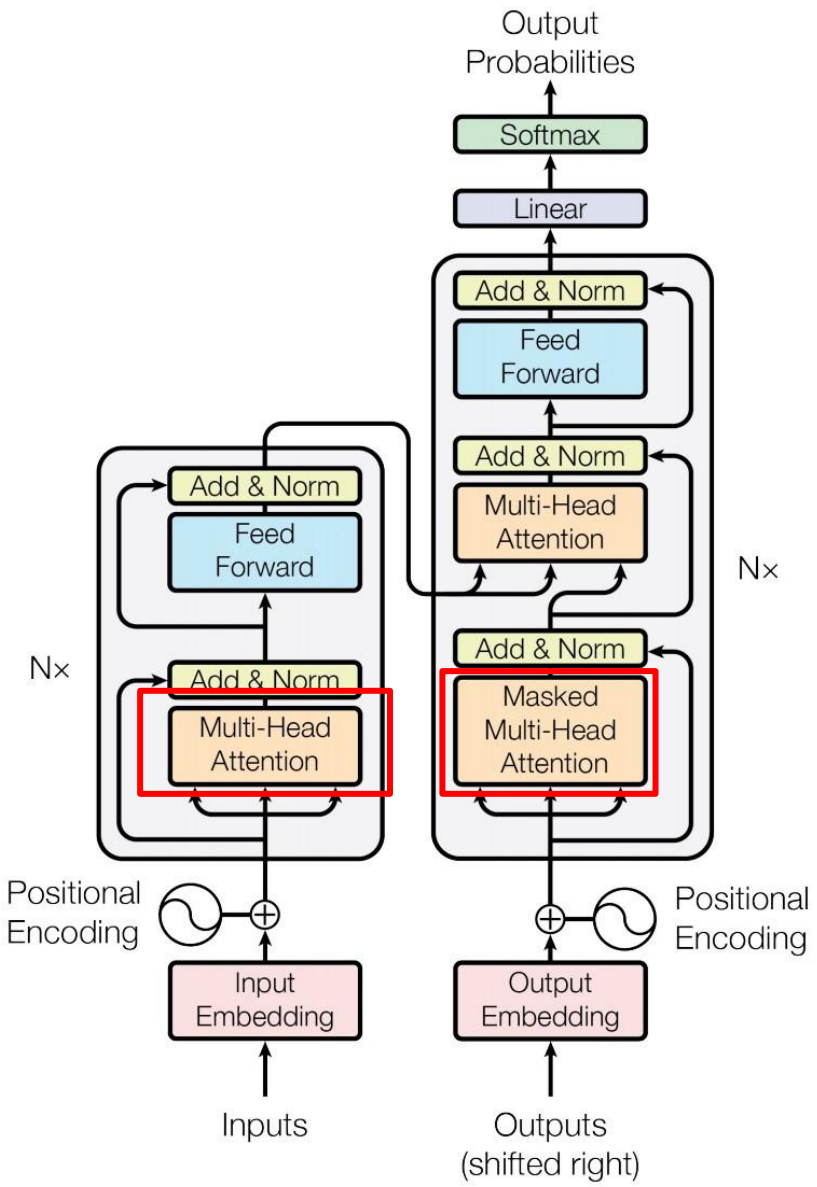
$$Attention(Query, Key, Value) = \sum_i Similarity(Query, Key_i) * Value_i$$

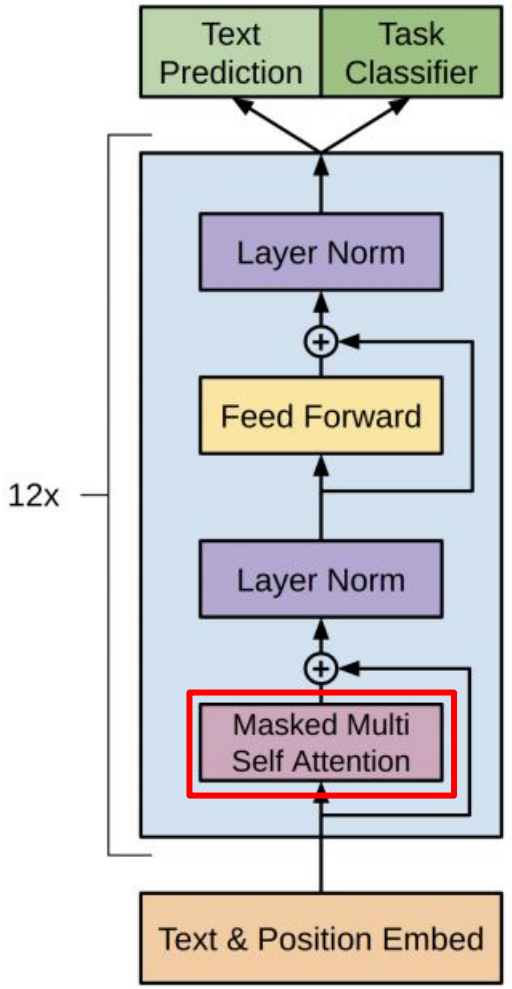


<Q,K>		V		
0.1		171		17.1
0.9	x	23	=	20.7
0.2		130		26
0.1		1		0.1

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

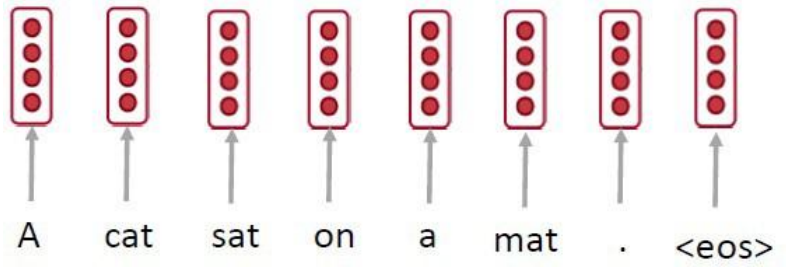
Self Attention

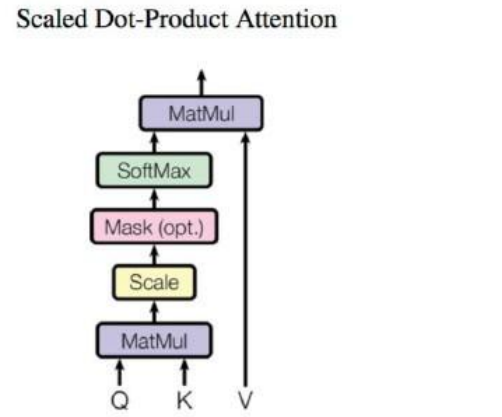




Self-Attention: Running Example

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





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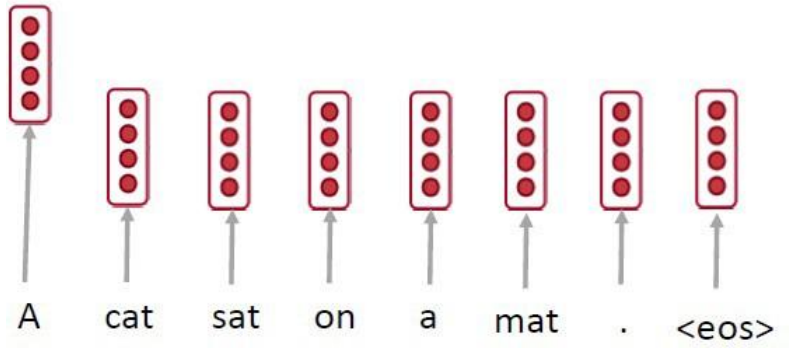

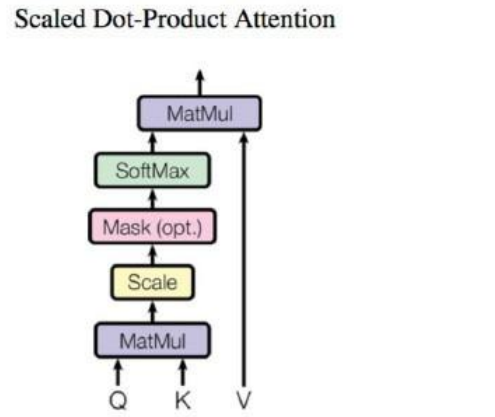

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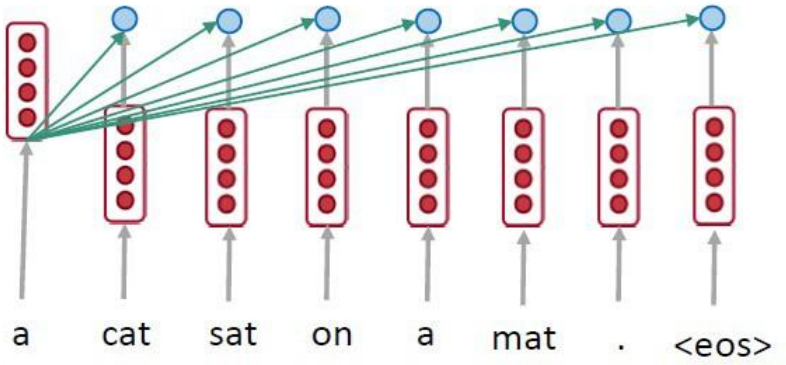

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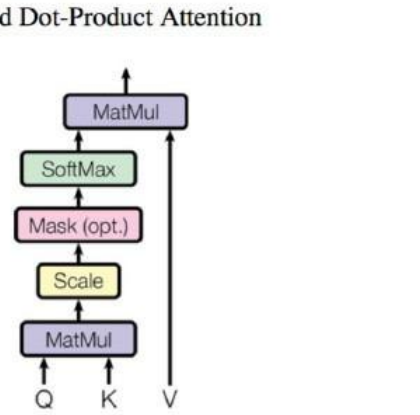

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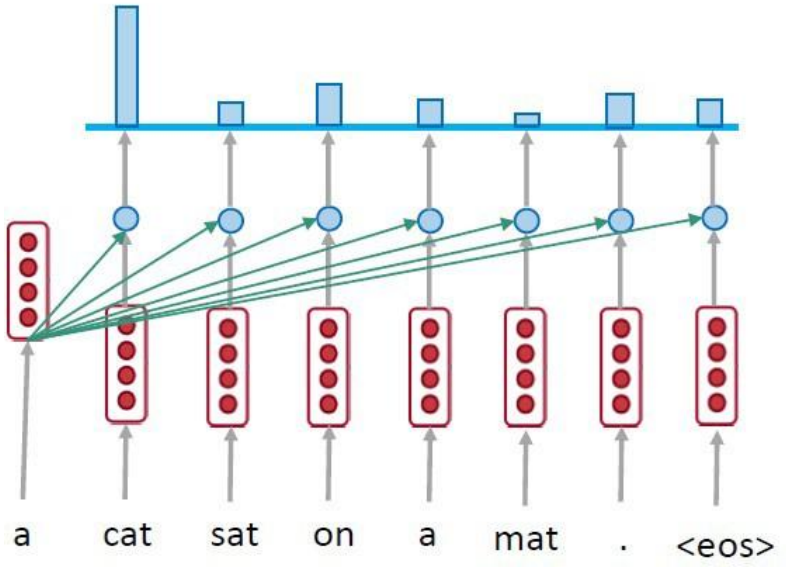

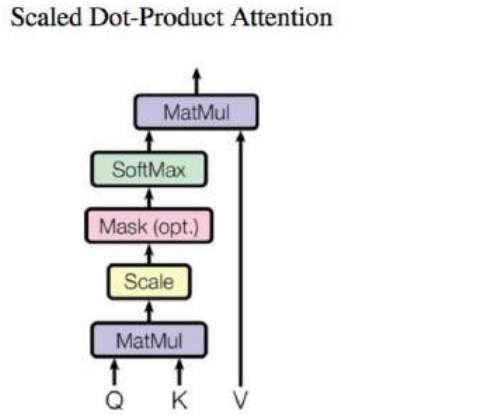

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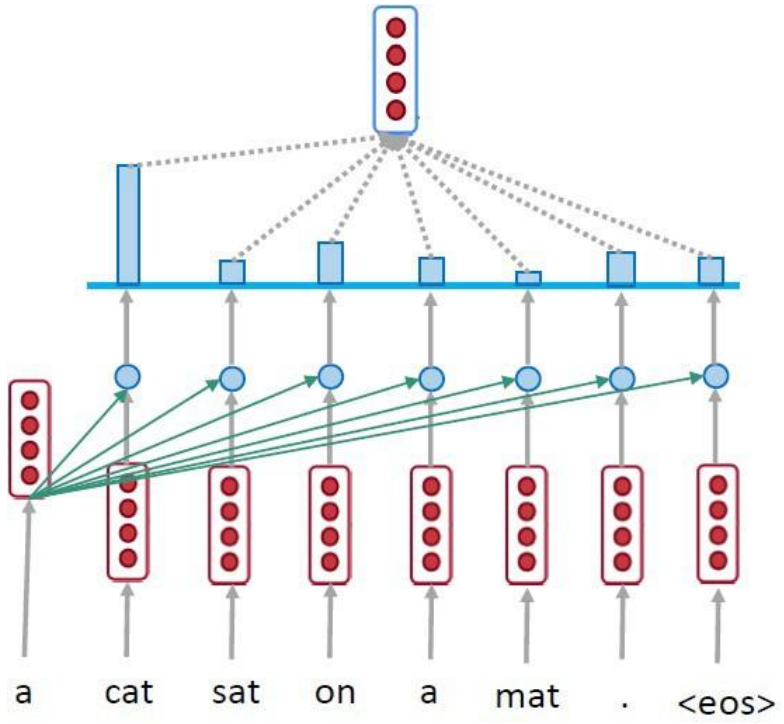

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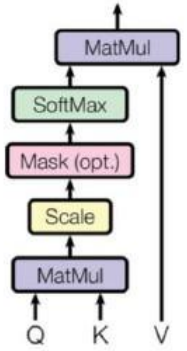
Scaled Dot-Product Attention



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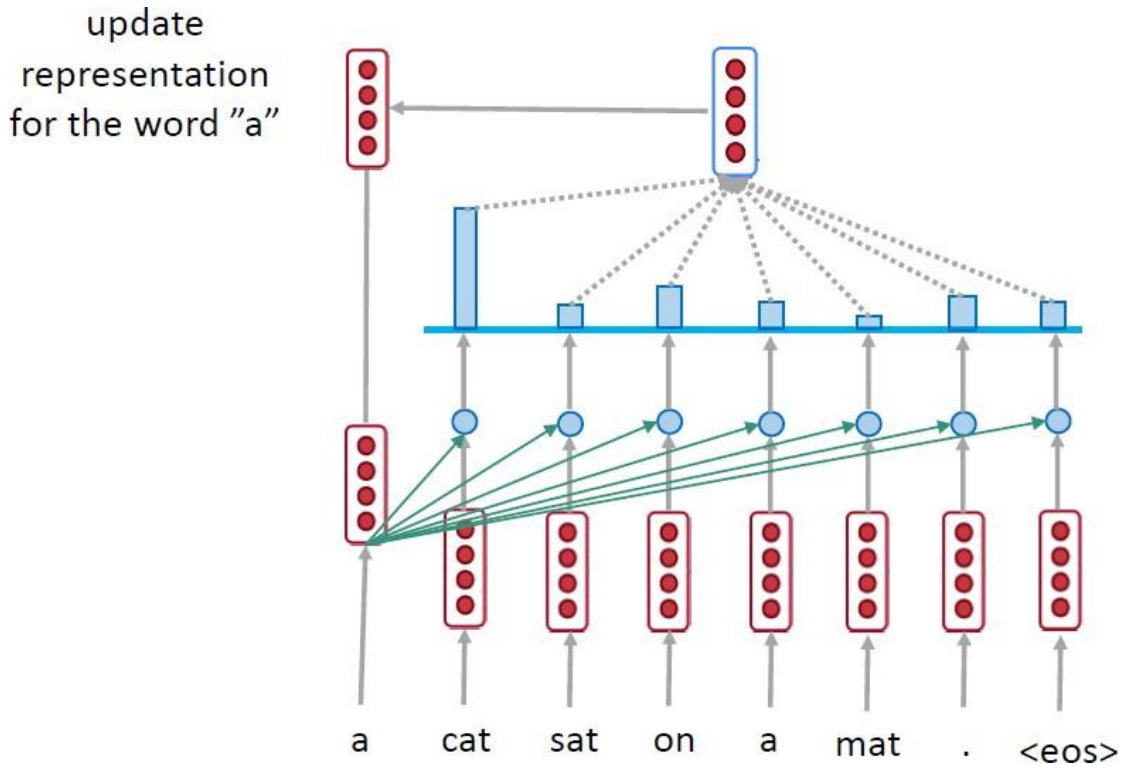

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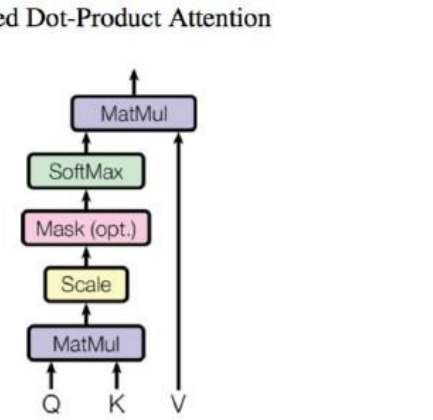
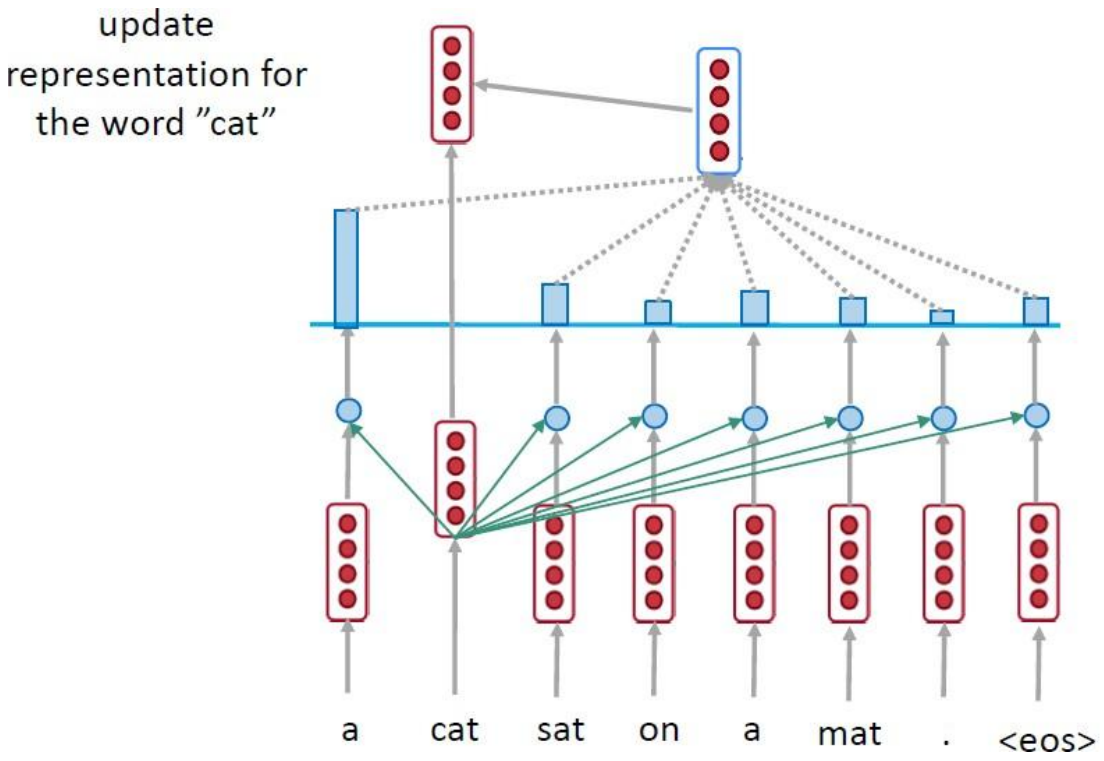
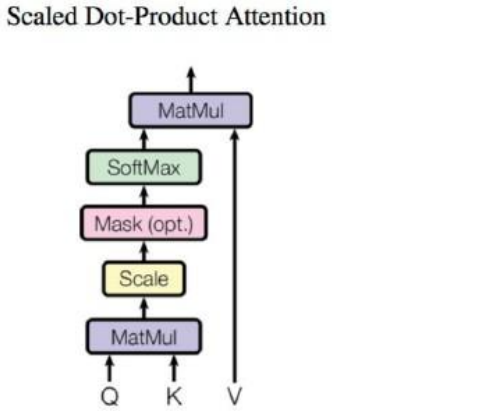


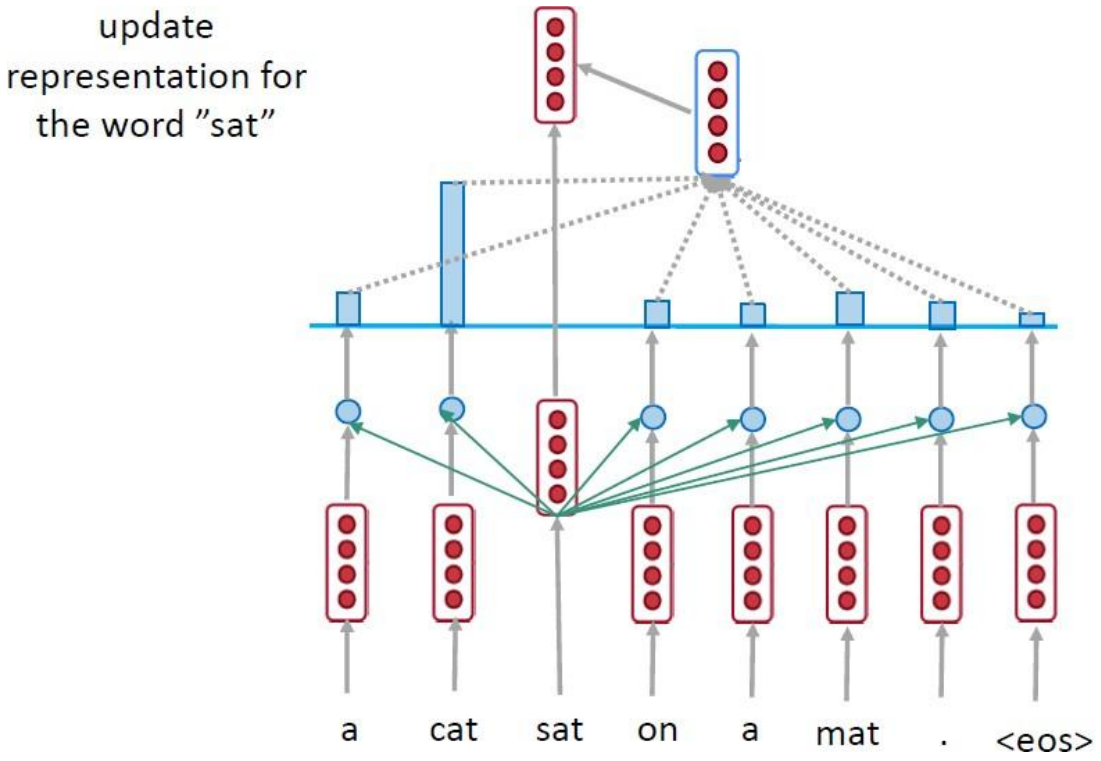
Self-Attention: Running Example



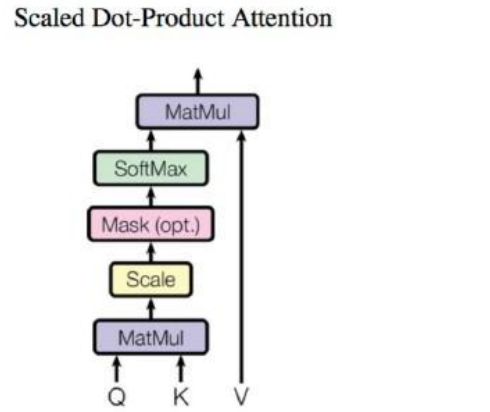
$$\text{Attention}(Q, K, V) = \text{softmax}(\frac{QK^T}{\sqrt{d_k}})V$$



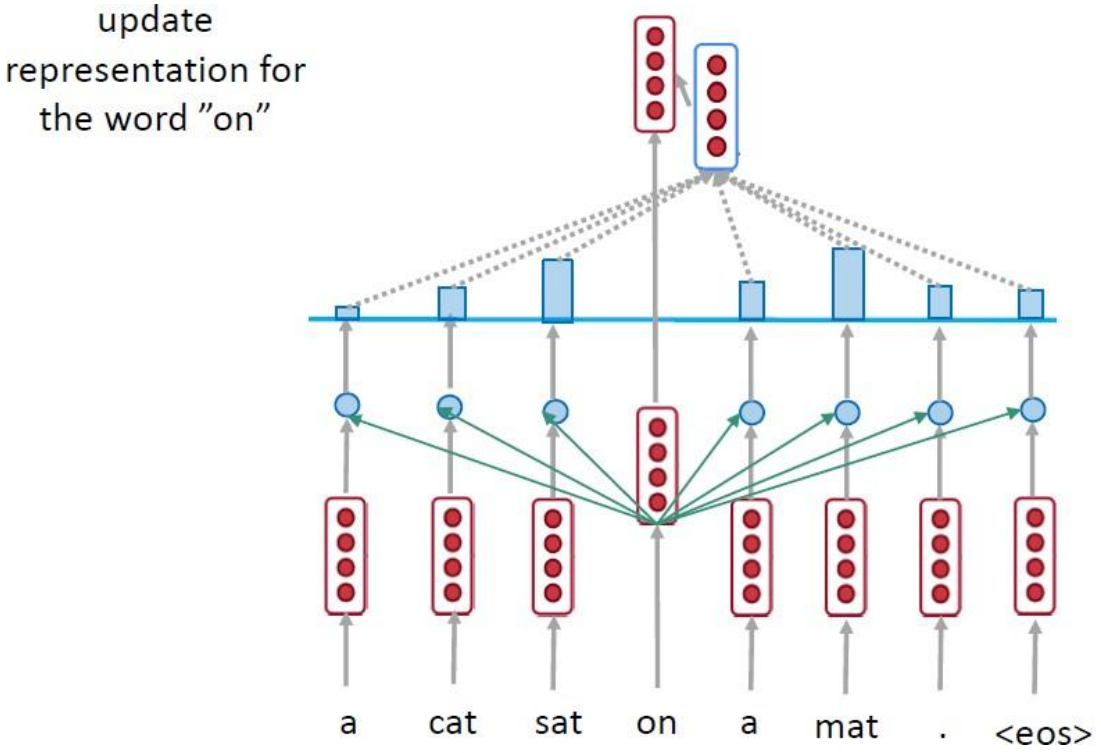
Self-Attention: Running Example



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

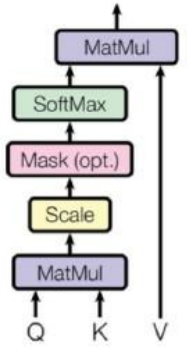


Self-Attention: Running Example



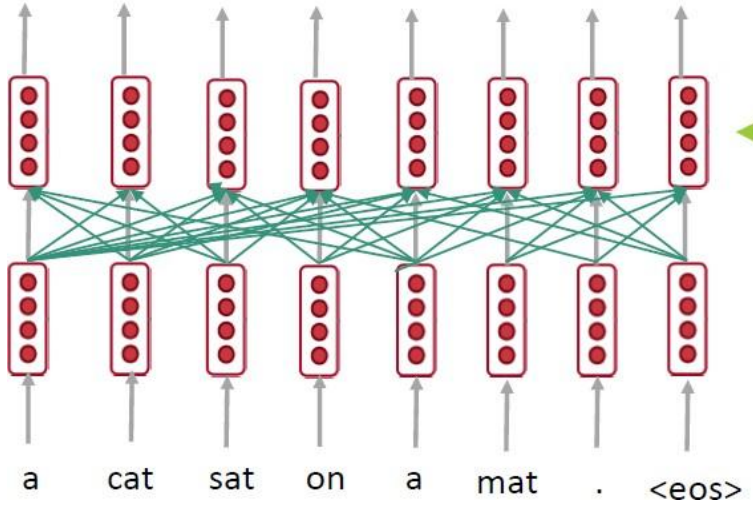
$$\text{Attention}(Q, K, V) = \text{softmax}(\frac{QK^T}{\sqrt{d_k}})V$$

Scaled Dot-Product Attention



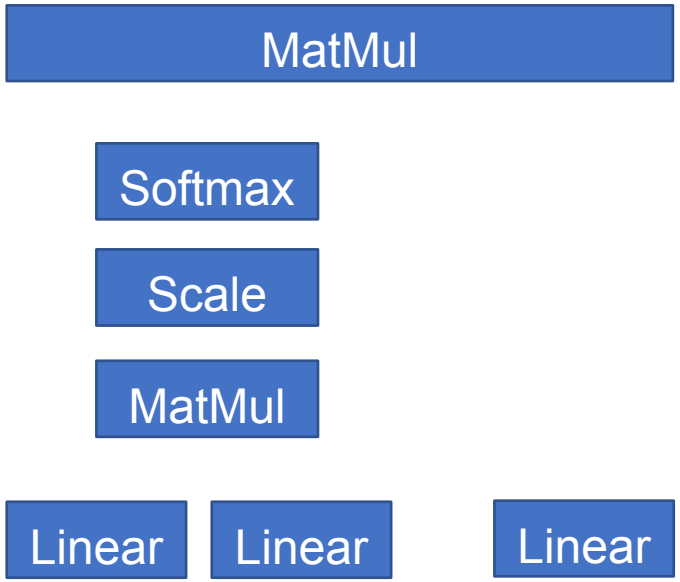
Self-Attention: Running Example

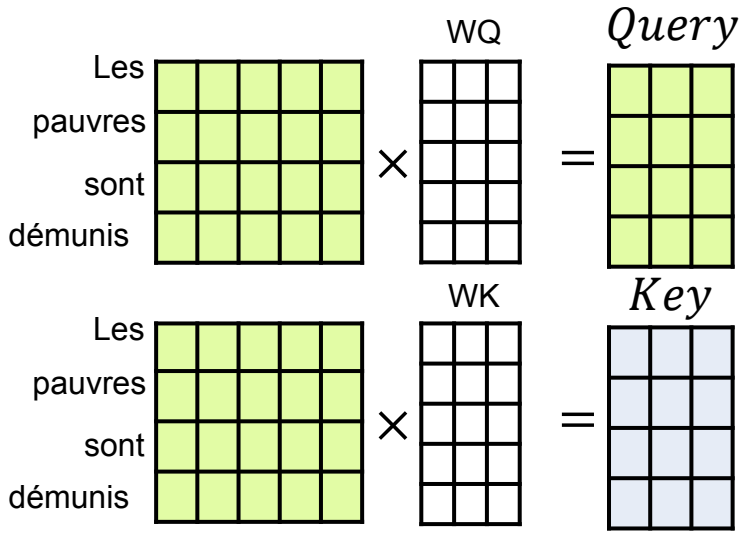
$$\text{Attention}(Q, K, V) = \text{softmax}(\frac{QK^T}{\sqrt{d_k}})V$$



Updated representations for each word (one layer)

Self-Attention

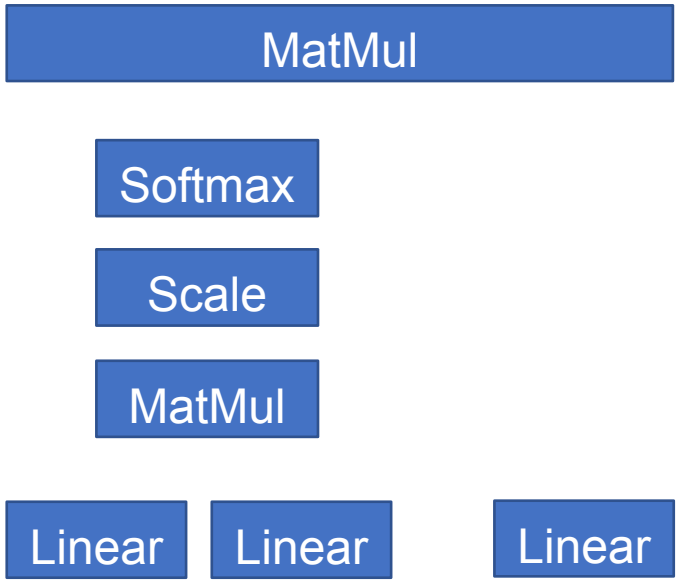


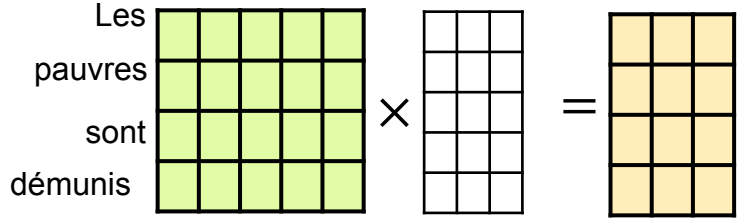


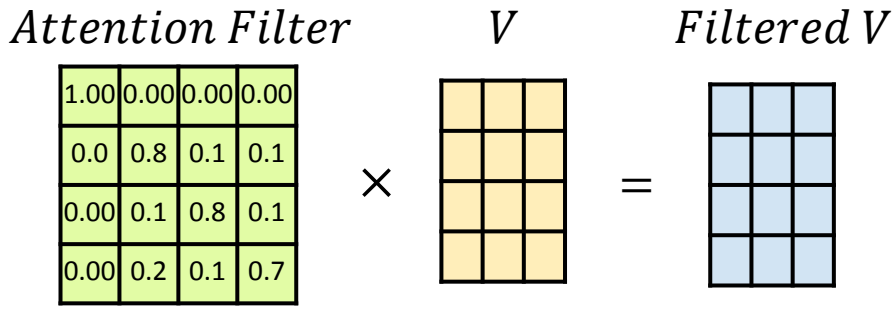
Attention Filter

1.00	0.00	0.00	0.00
0.0	0.8	0.1	0.1
0.00	0.1	0.8	0.1
0.00	0.2	0.1	0.7

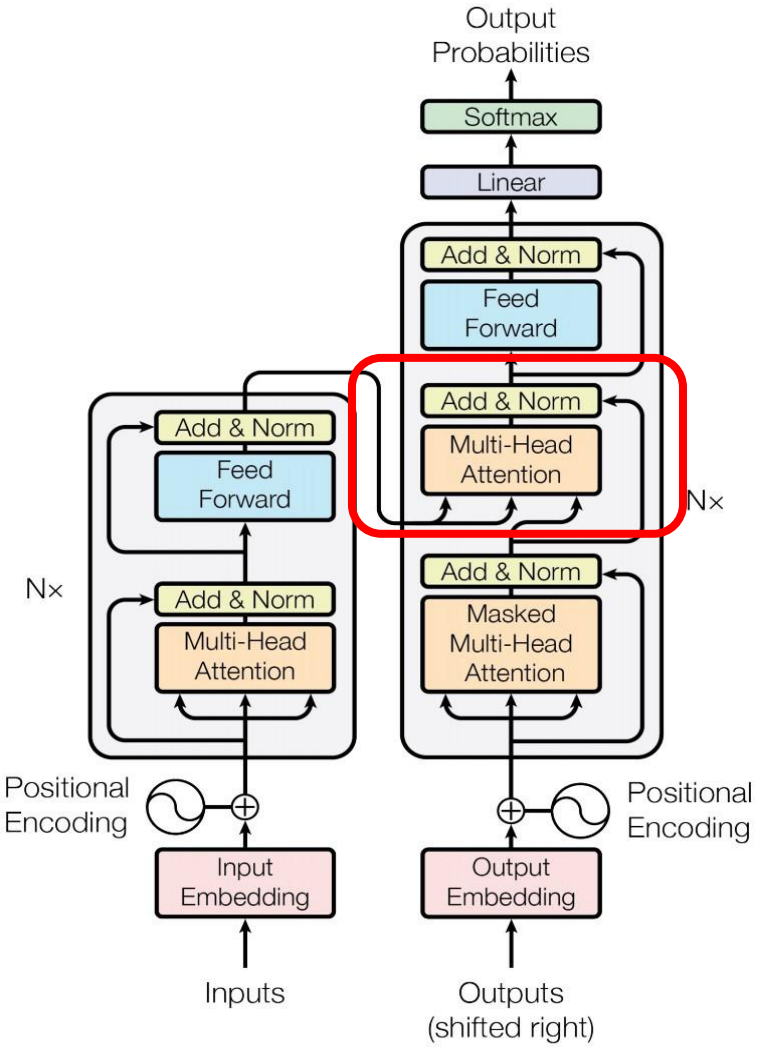
Self-Attention

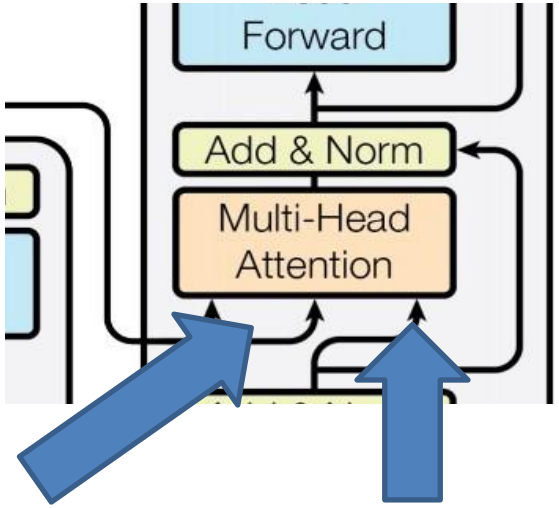






Cross Attention





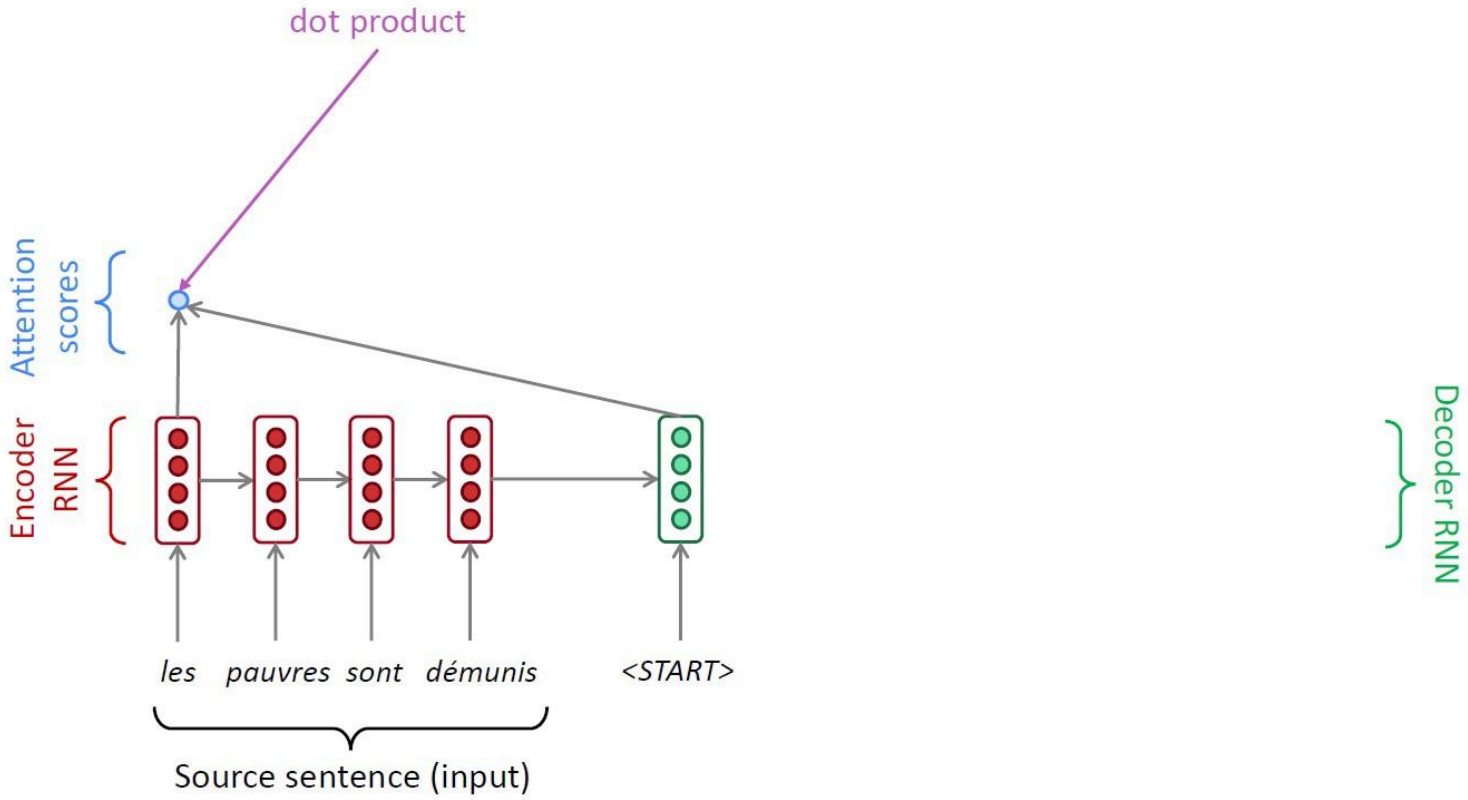
Key & Value shape: [input length, qkv-embedding]

Query shape: [output length, qkv-embedding]

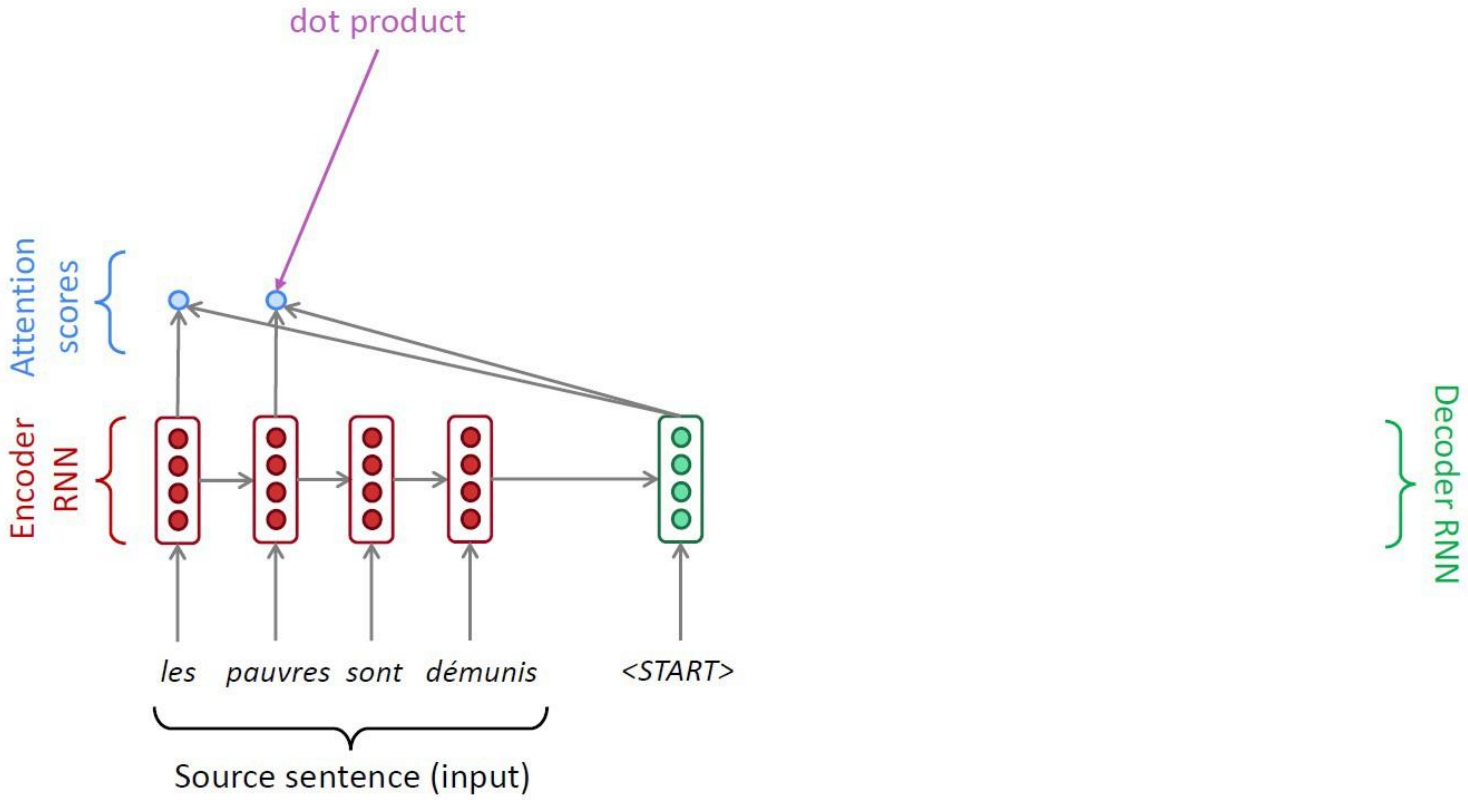
$$Attention(Query, Key, Value) = \sum_i Similarity(Query, Key_i) * Value_i$$

$$\boxplus \quad \boldsymbol{c}_t = \sum_{j=1}^{T} \alpha_{t,j} \boldsymbol{h}_j$$

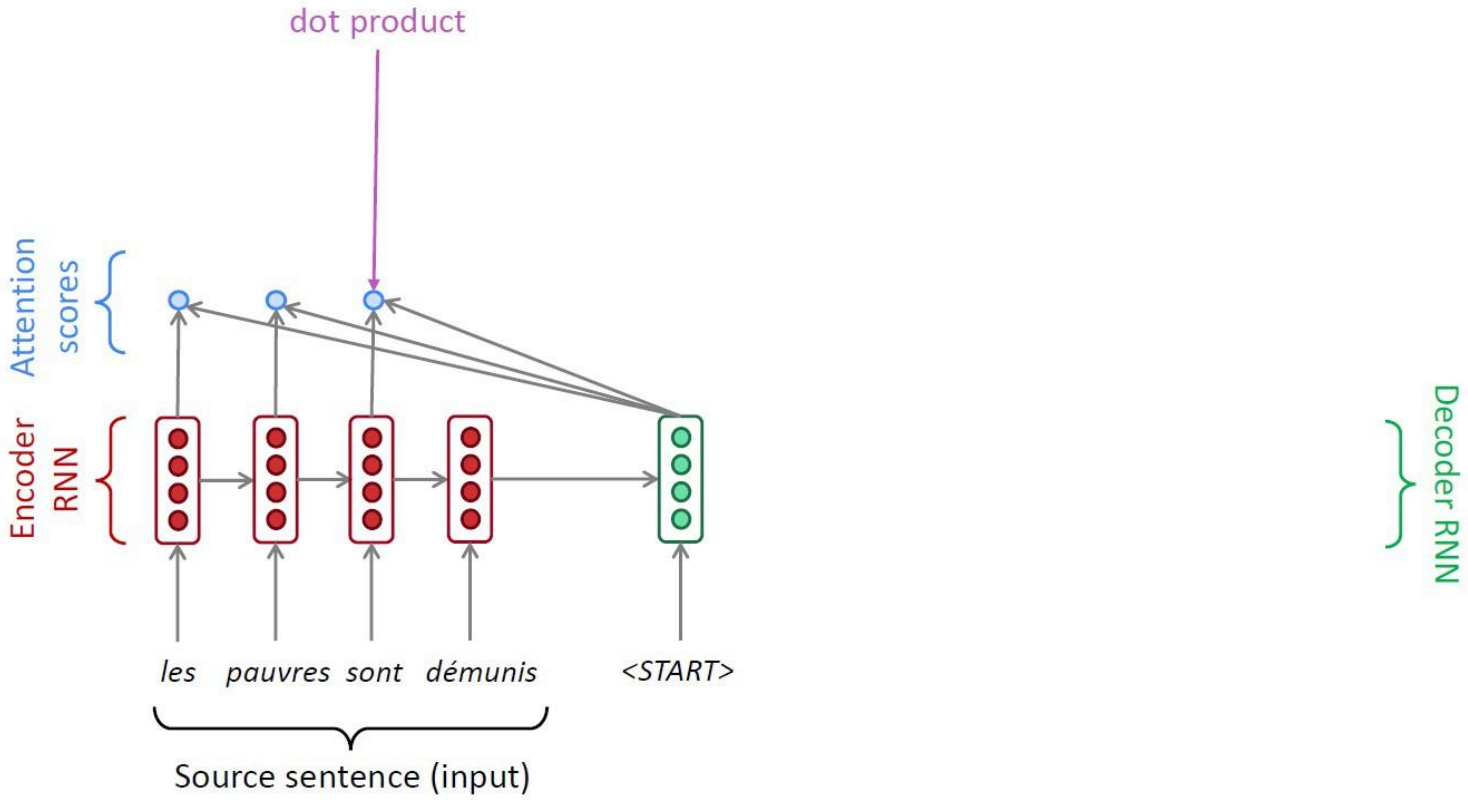
Running Example



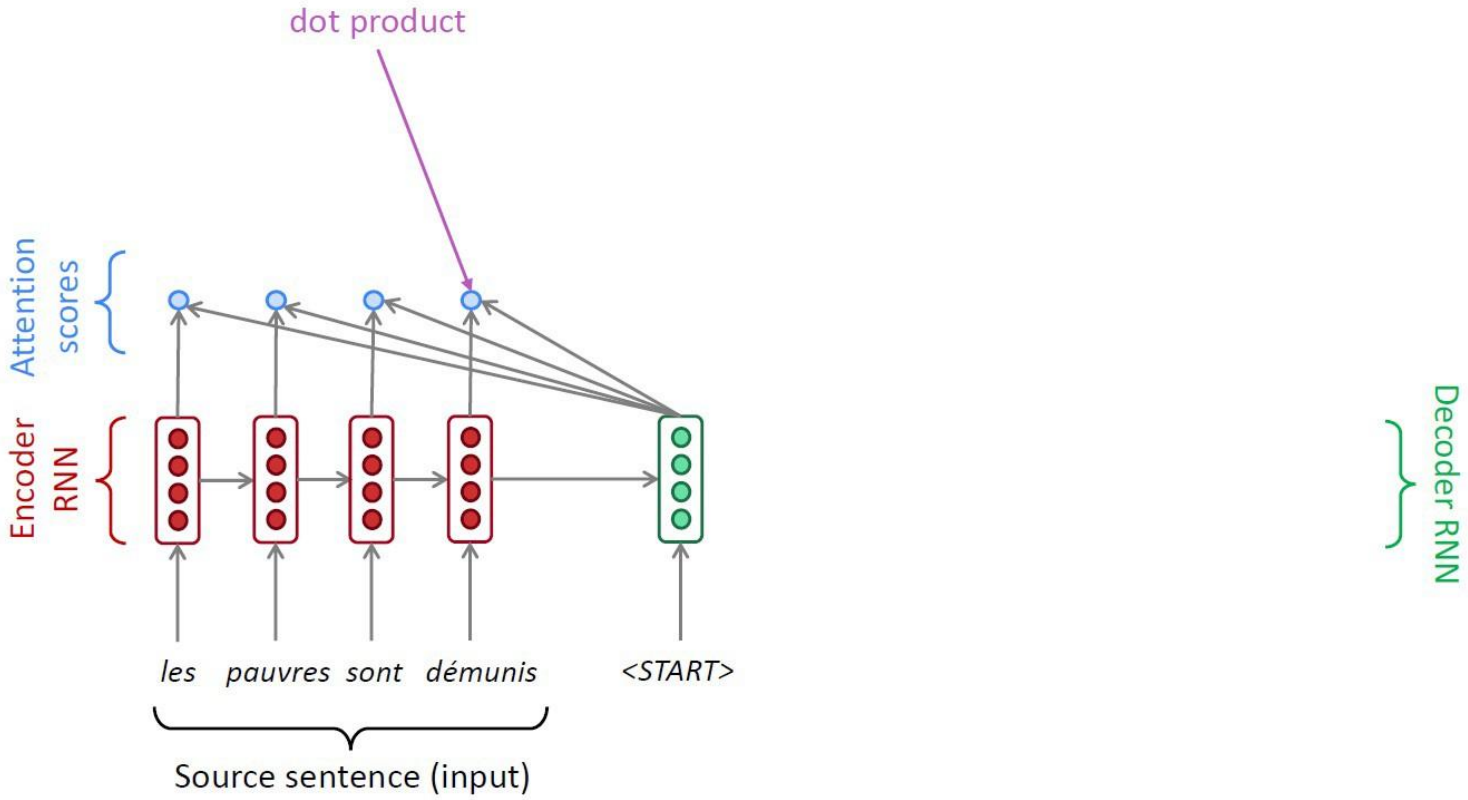
Running Example



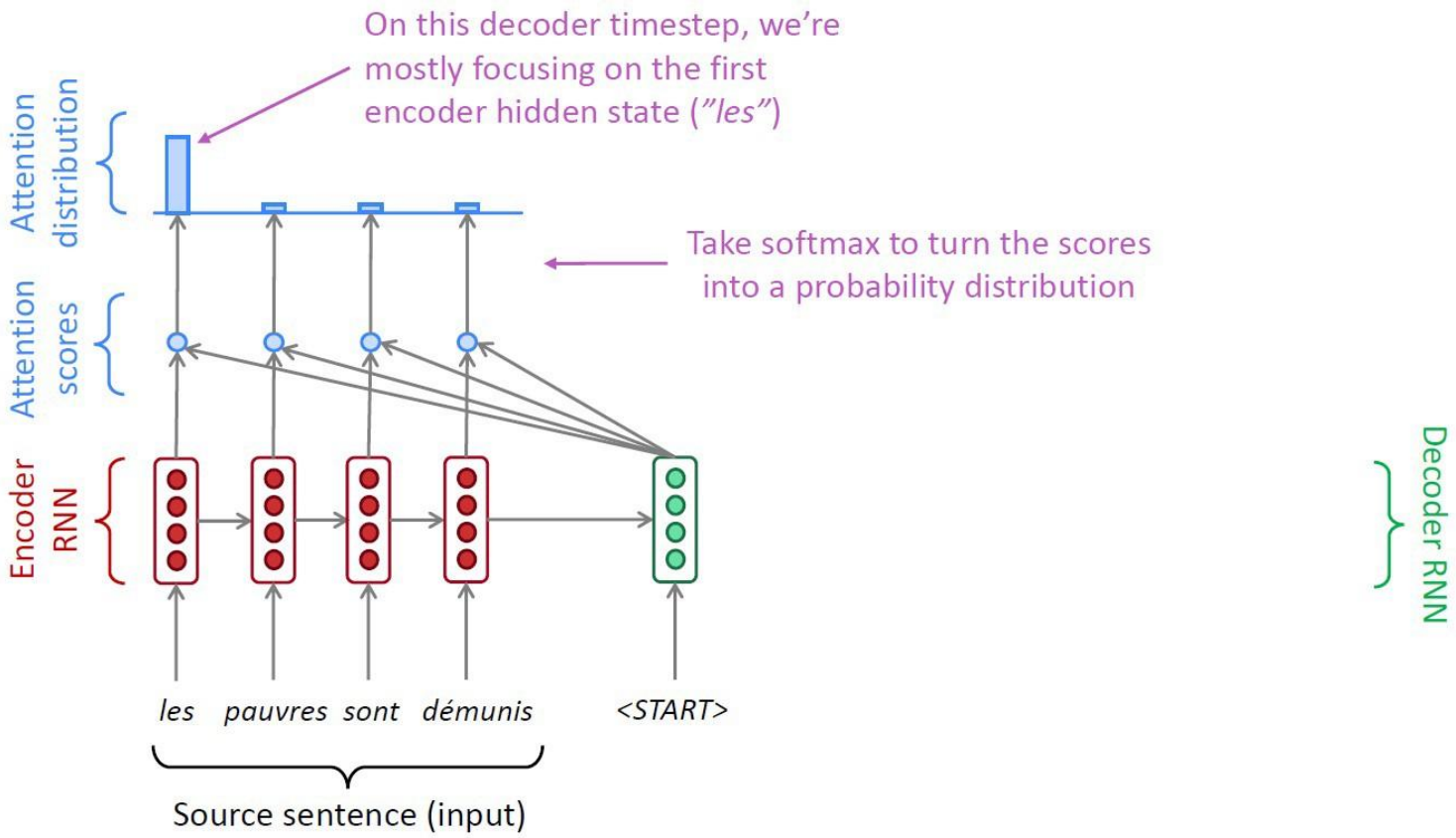
Running Example



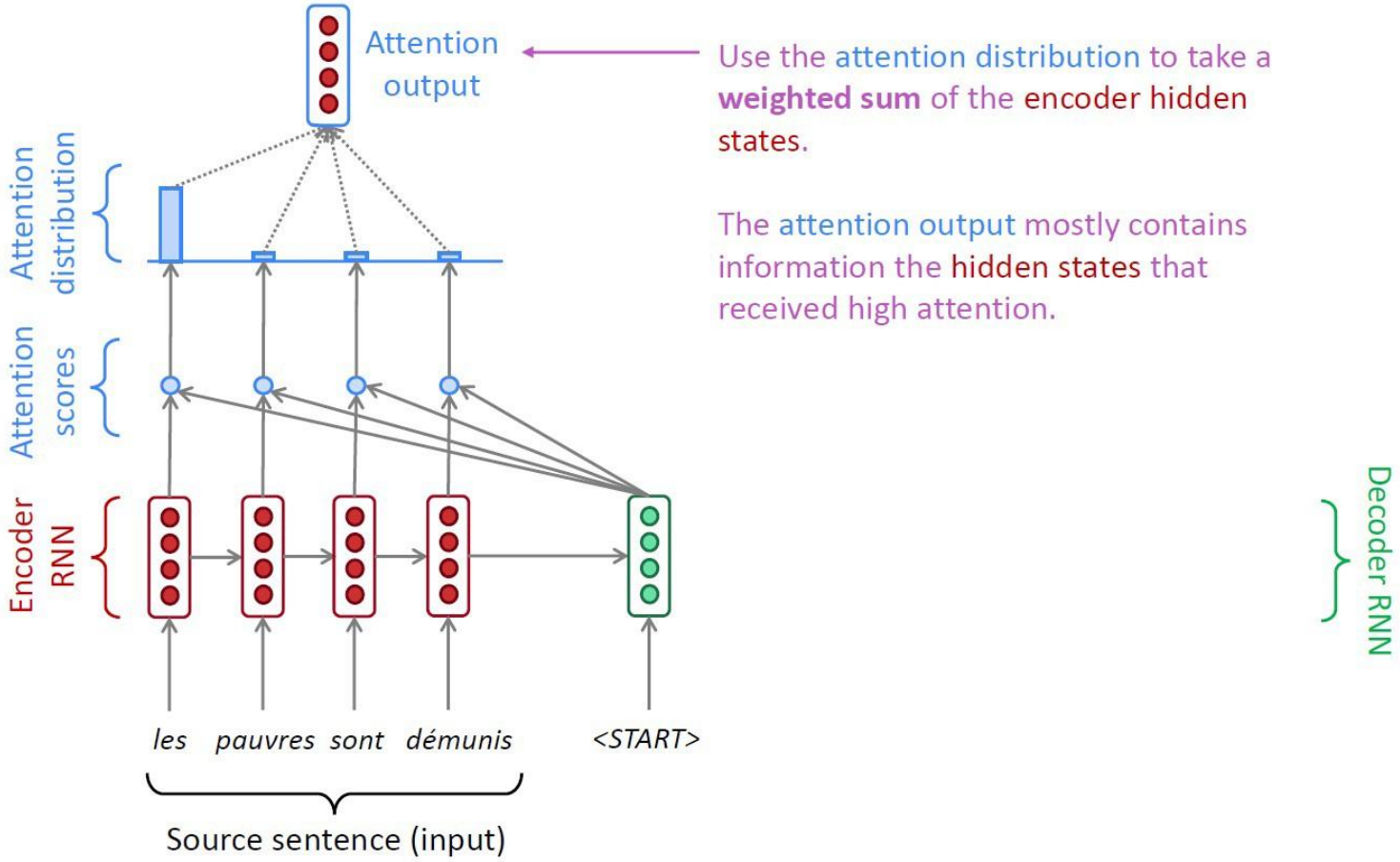
Running Example



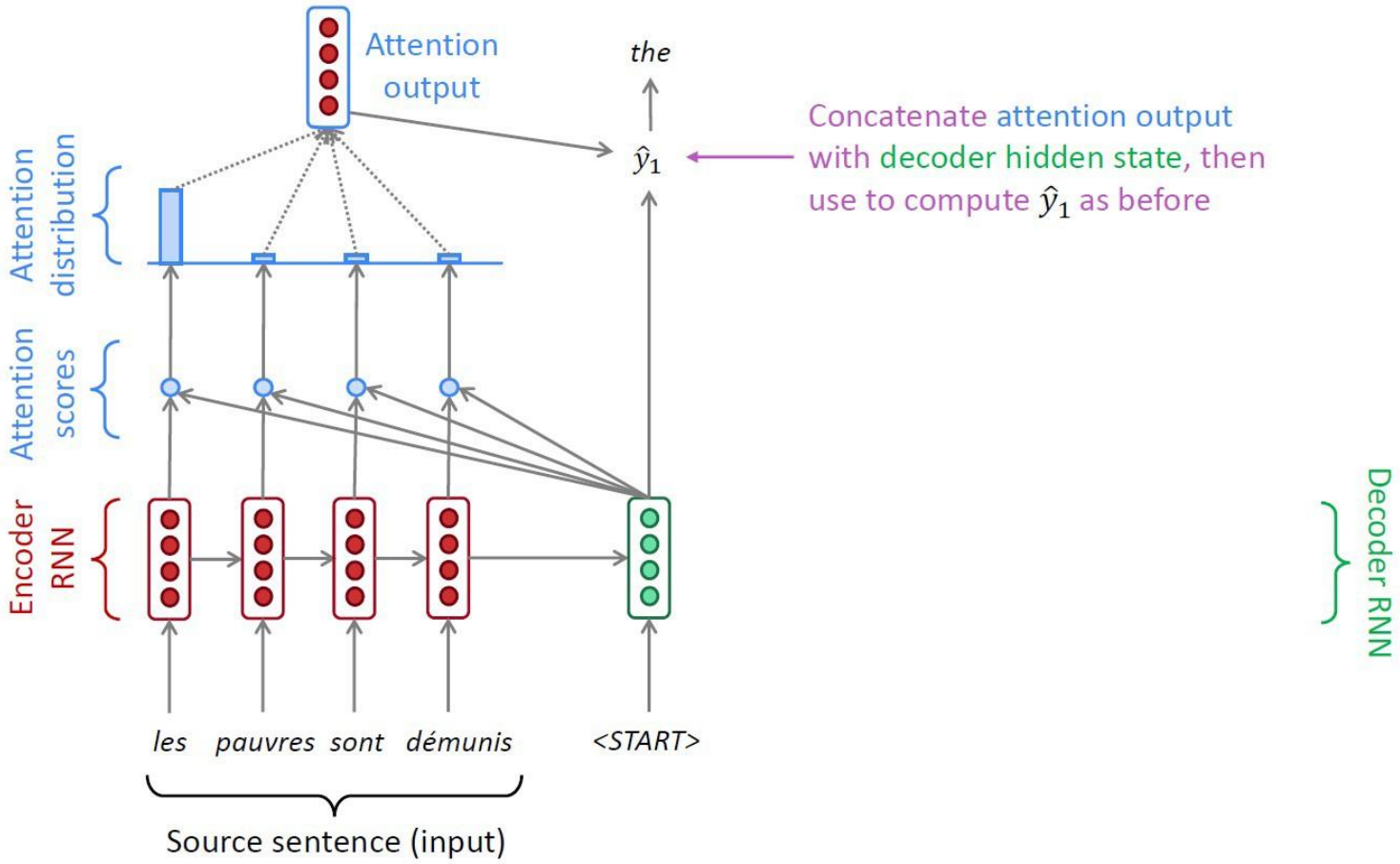
Running Example



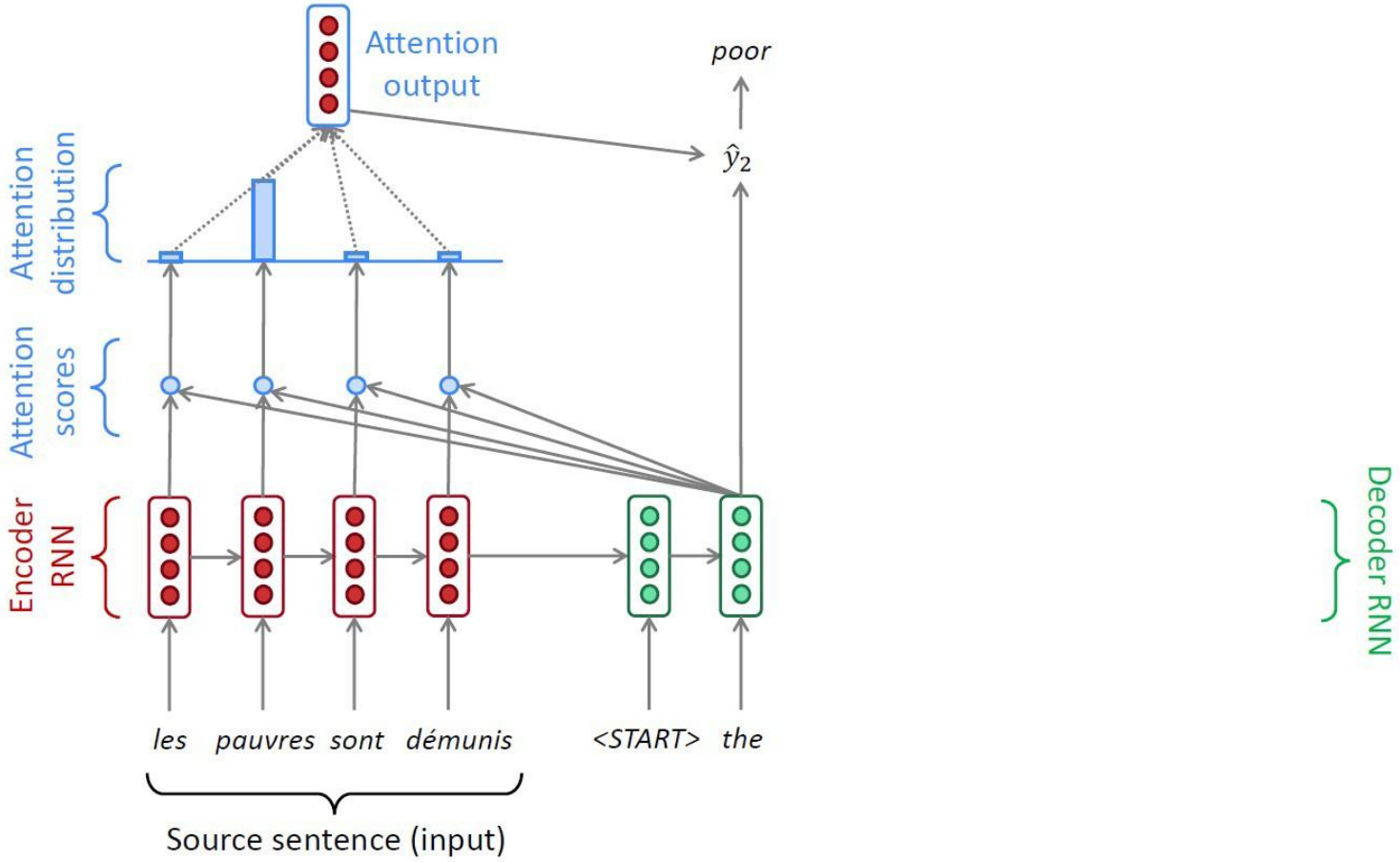
Running Example



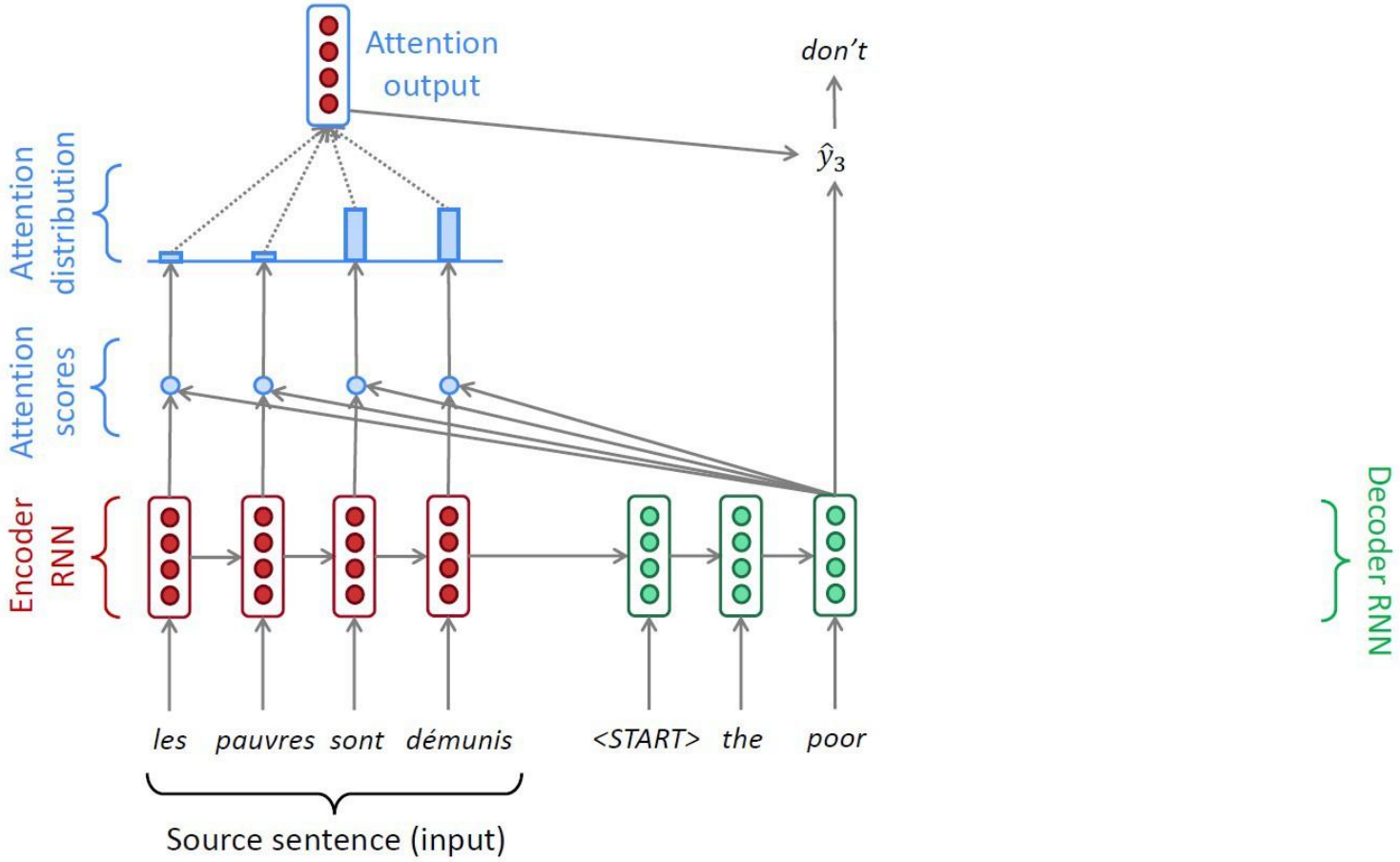
Running Example



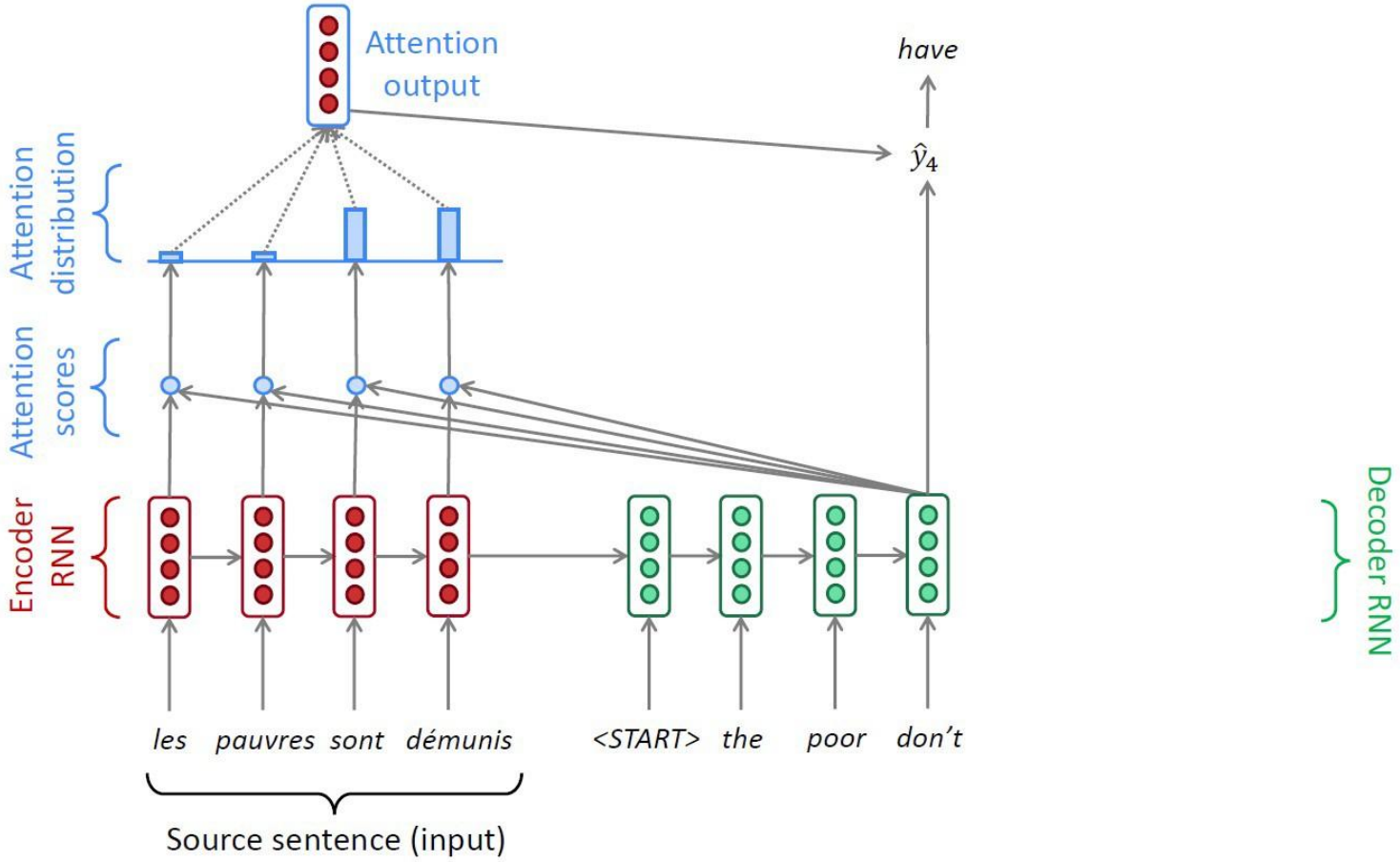
Running Example



Running Example



Running Example



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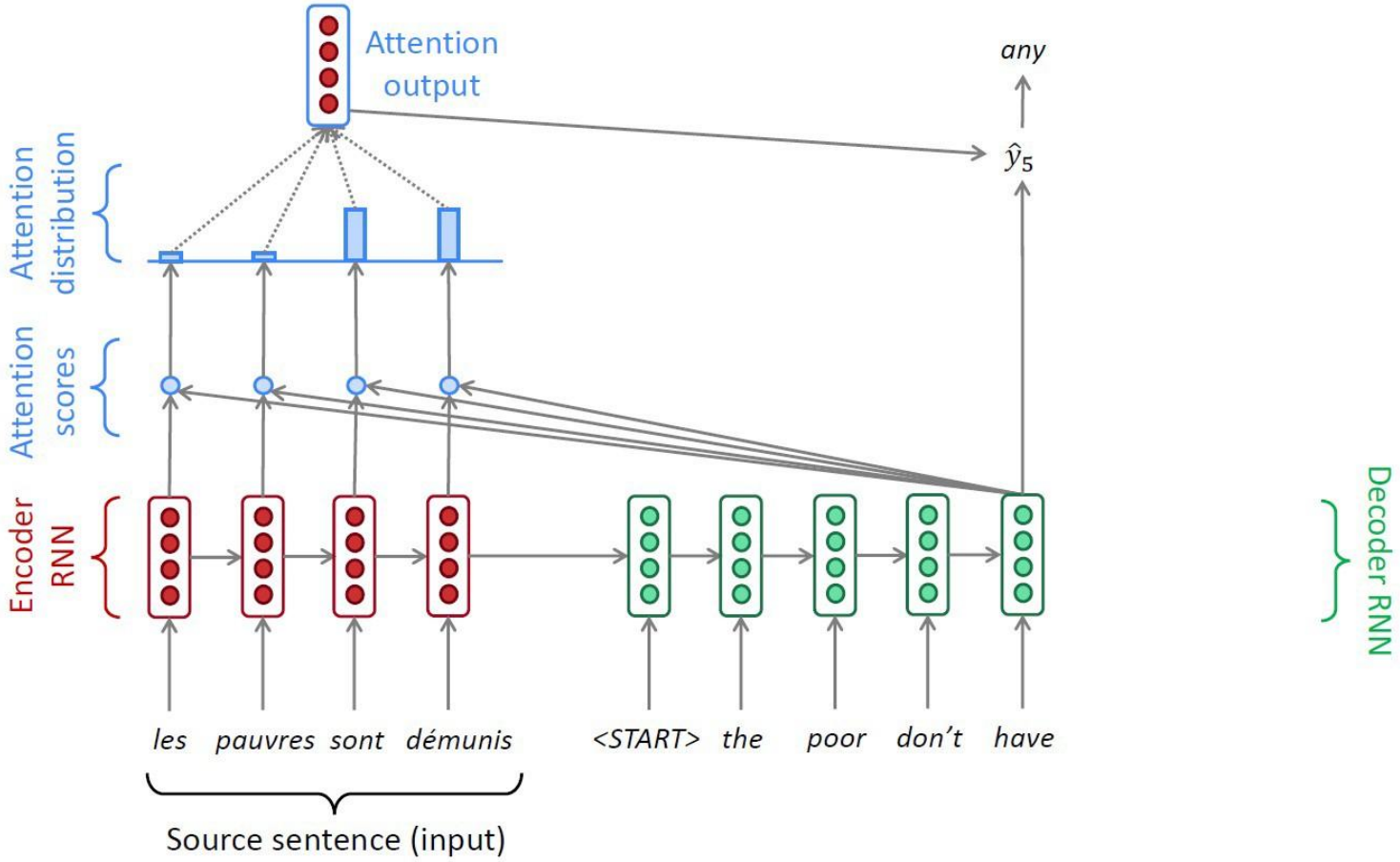

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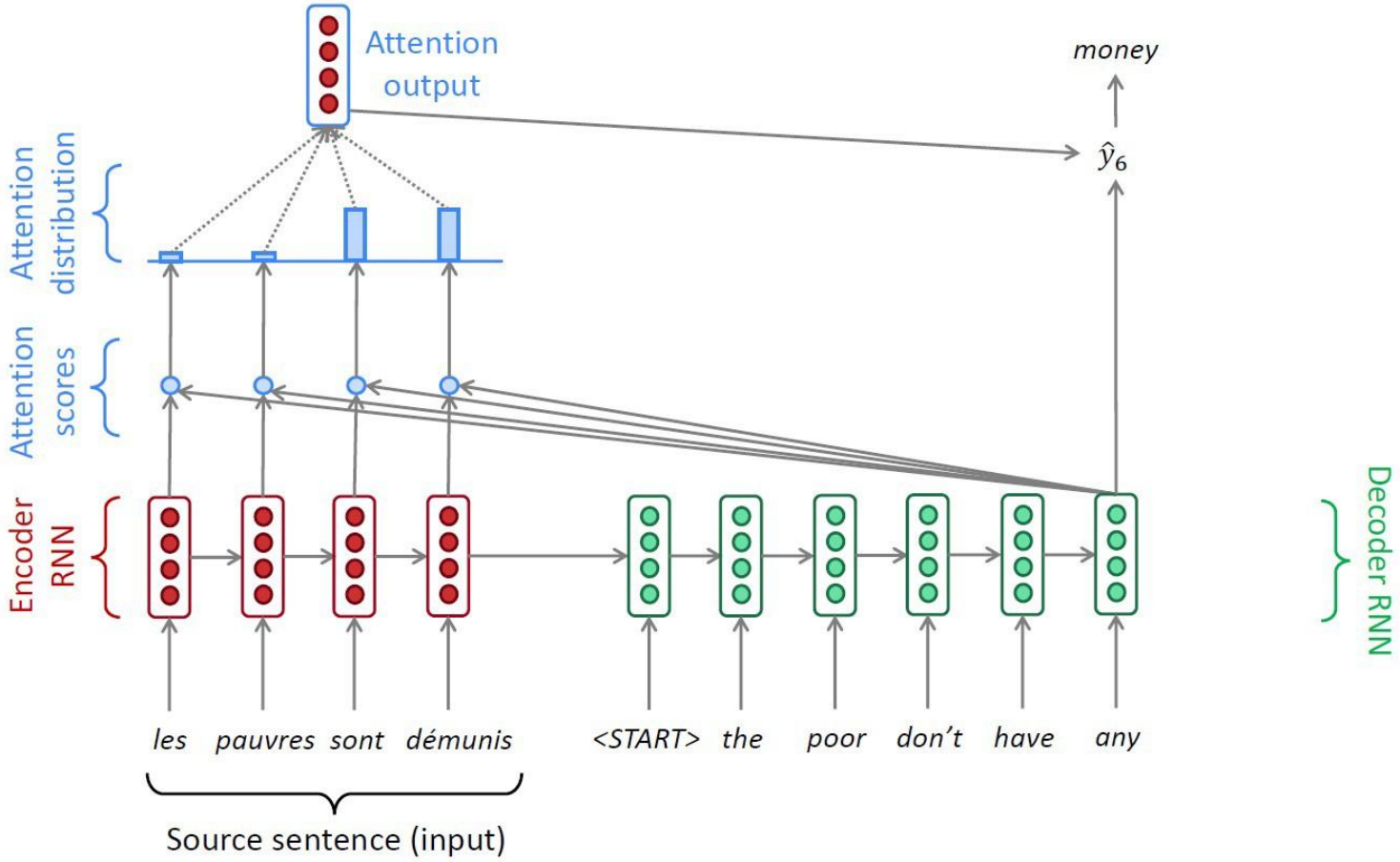
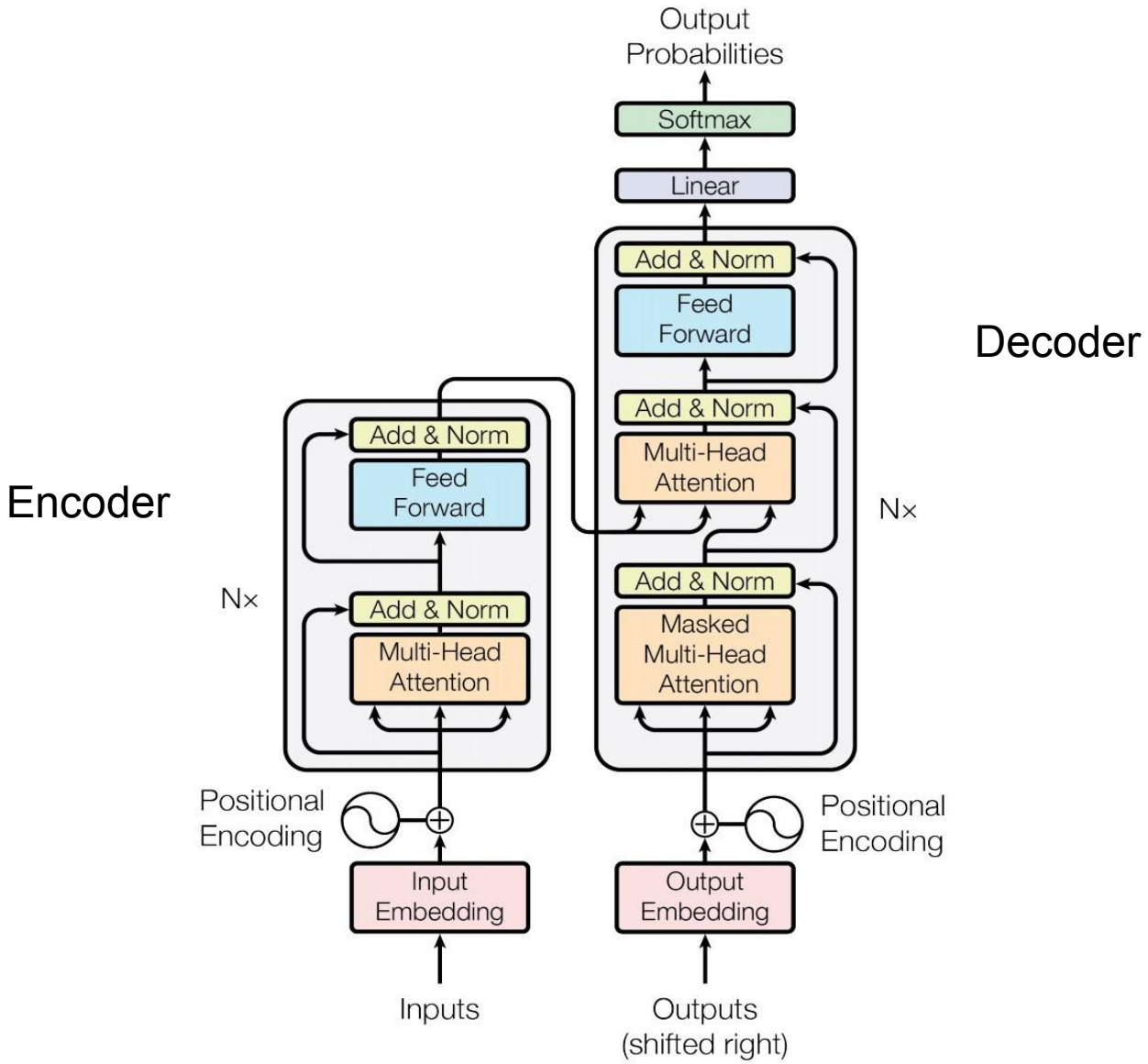
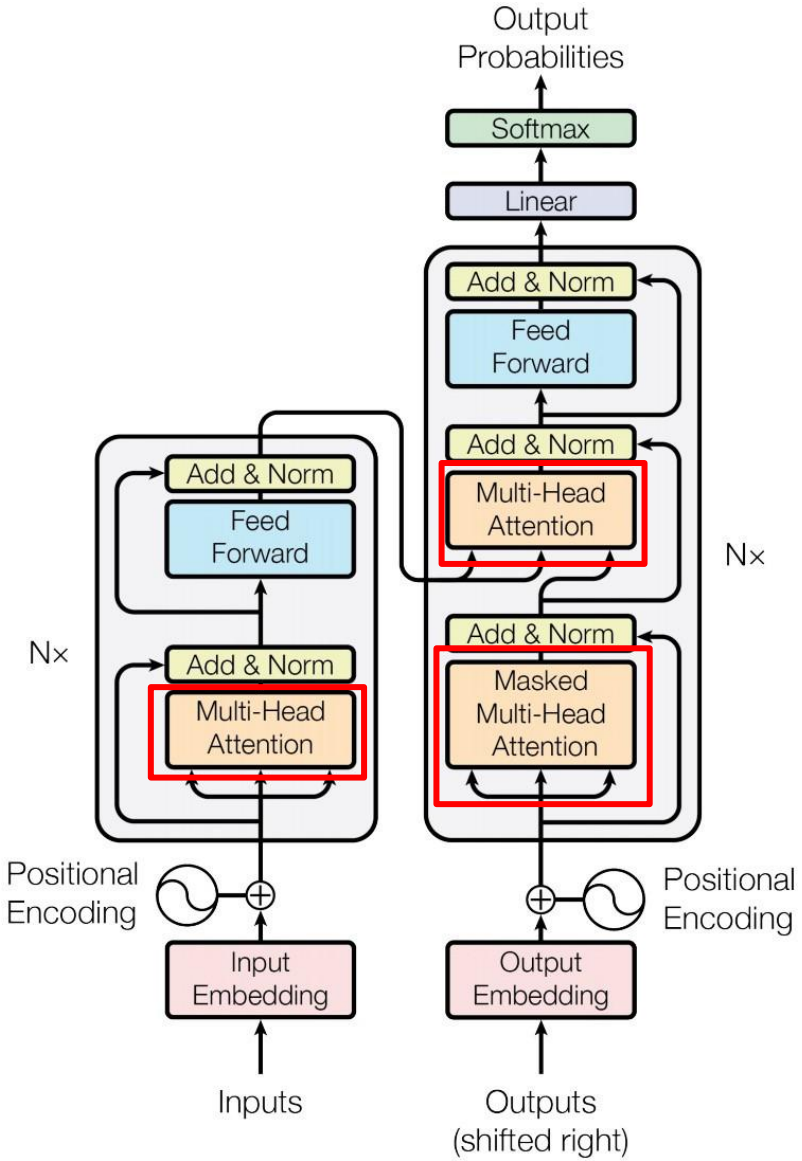


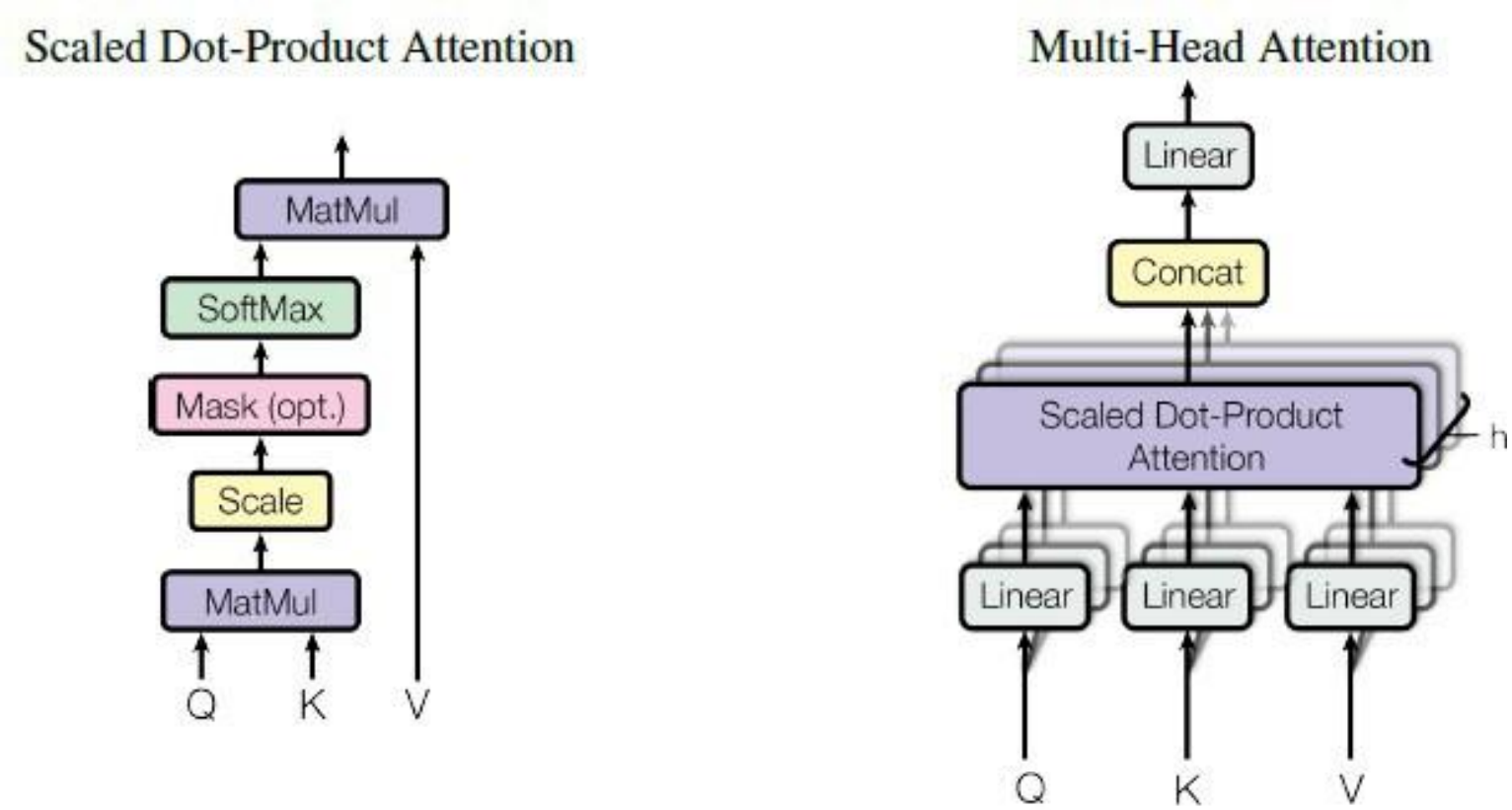
Transformer Architecture





Multi-Head Attention

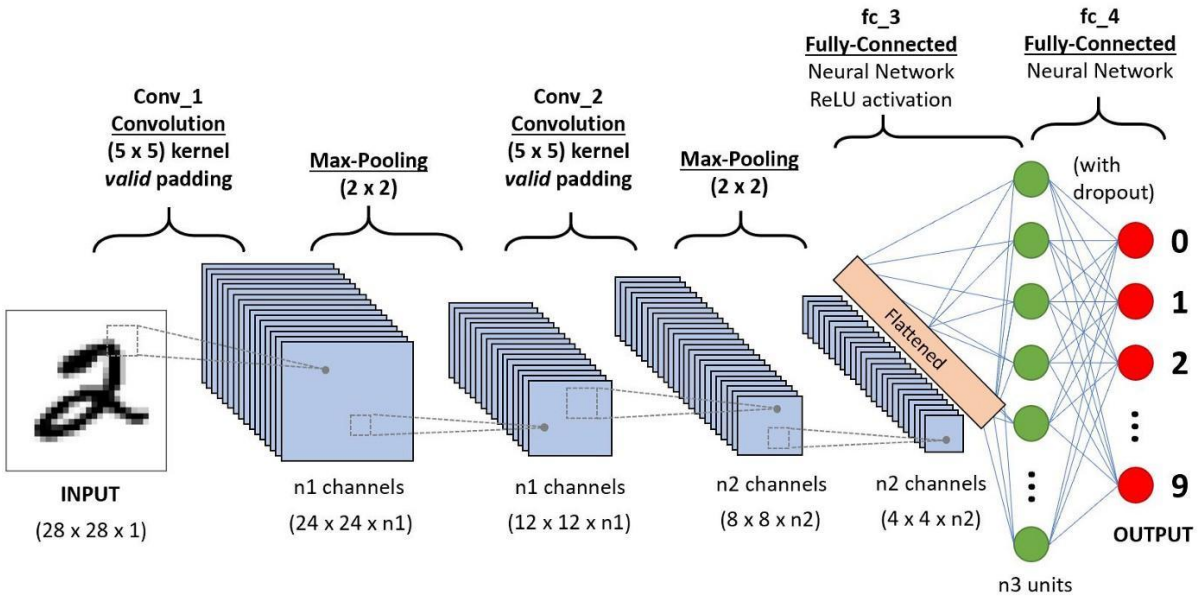
Multi-Head Attention: Summary

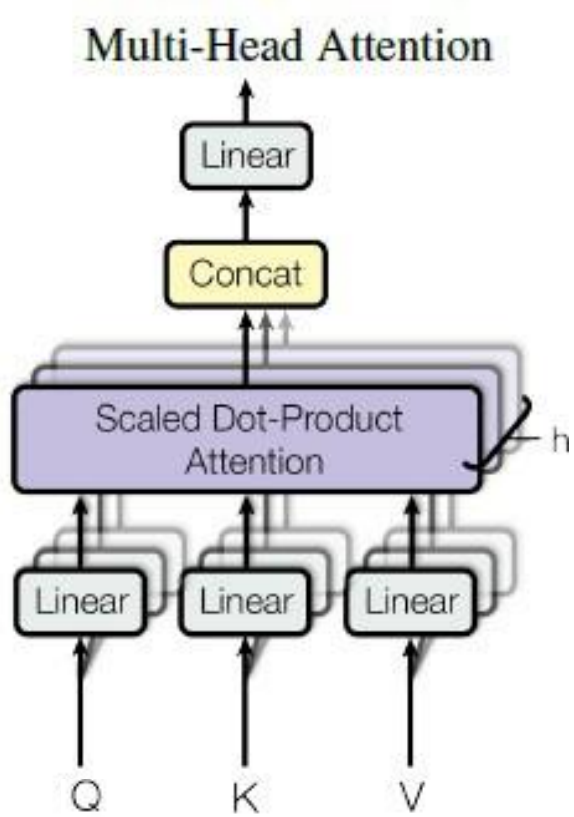


Multi-Head Attention: Intuition

The Encoder:

- Combines pairs of words, pairs of pairs of words, …
- Get the entire sentence
  - Get all words in the input sequence
  - Uses Positional Encoding
- Multiple heads: Similar to the idea of multiple filters in CNN

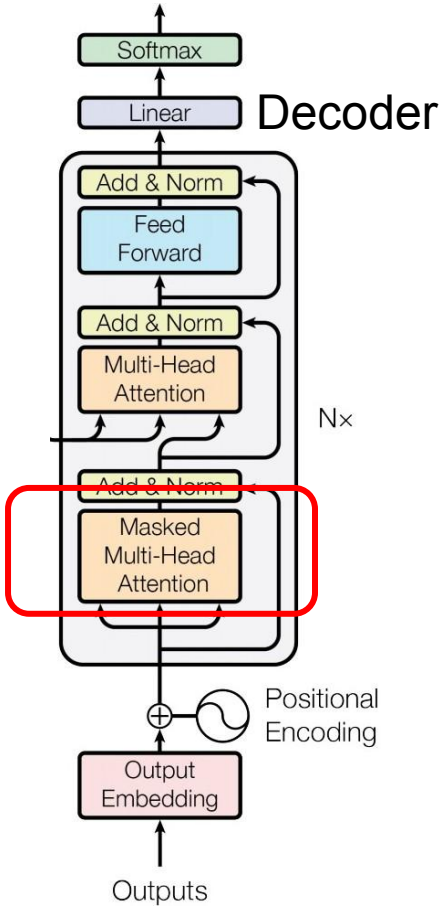




Masked Multi-Head Attention

Les pauvres sont démunis
(French)

The **poor** do not have any money
(English)



Masked Multi-Head Attention

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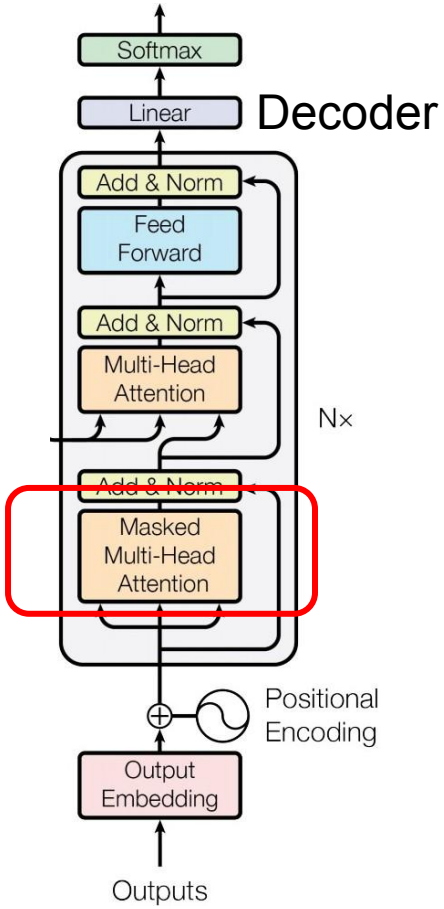


Some of the values should be masked so that we do not use them to make combinations

In Language Translation, when we produce a word:

1. It is fine depend on previously-generated words since we generate them sequentially
2. We cannot depend on the future words since they are not generated yet

Solution: In the decoder, we need to prevent building attention based on future words

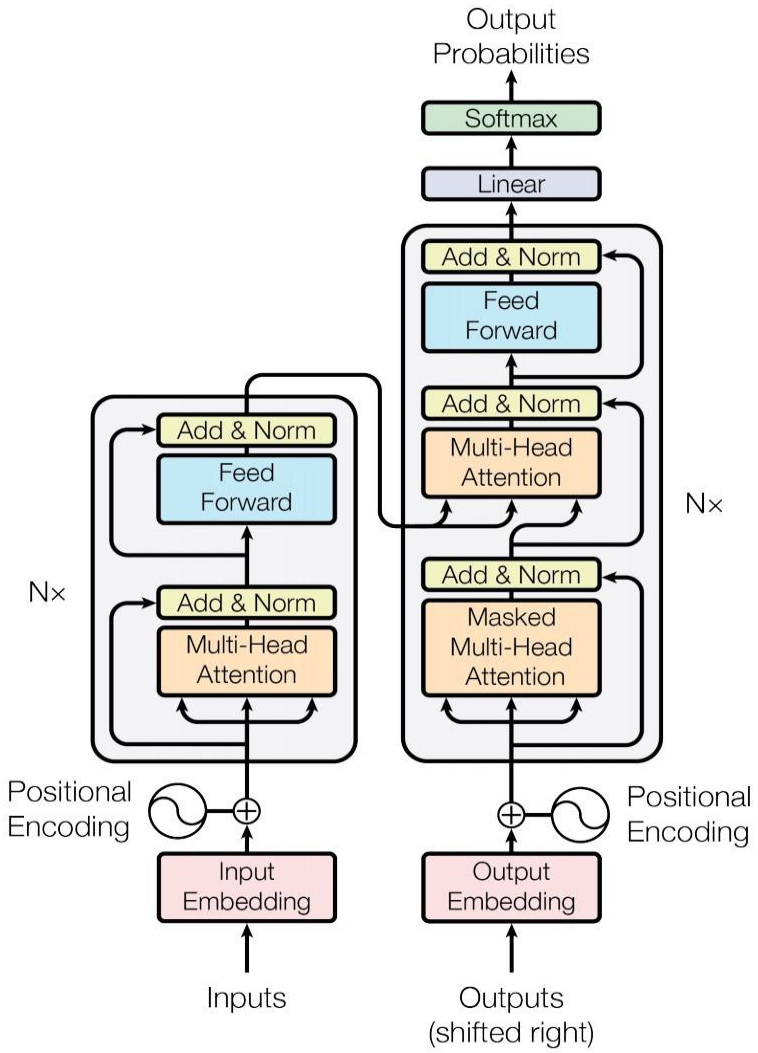
$$Attention(Q,K,V) = Softmax\left(\frac{Q^T K}{\sqrt{d}}\right)V$$

$$MaskedAttention(Q,K,V) = Softmax\left(\frac{Q^T K + M}{\sqrt{d}}\right)V$$

$$M\ Mask\ Matrix\ of\ 0s\ and\ -\infty$$

Attention Mechanism Summary

- Self Attention
- Cross Attention
- Multi-Head
- Masked Attention



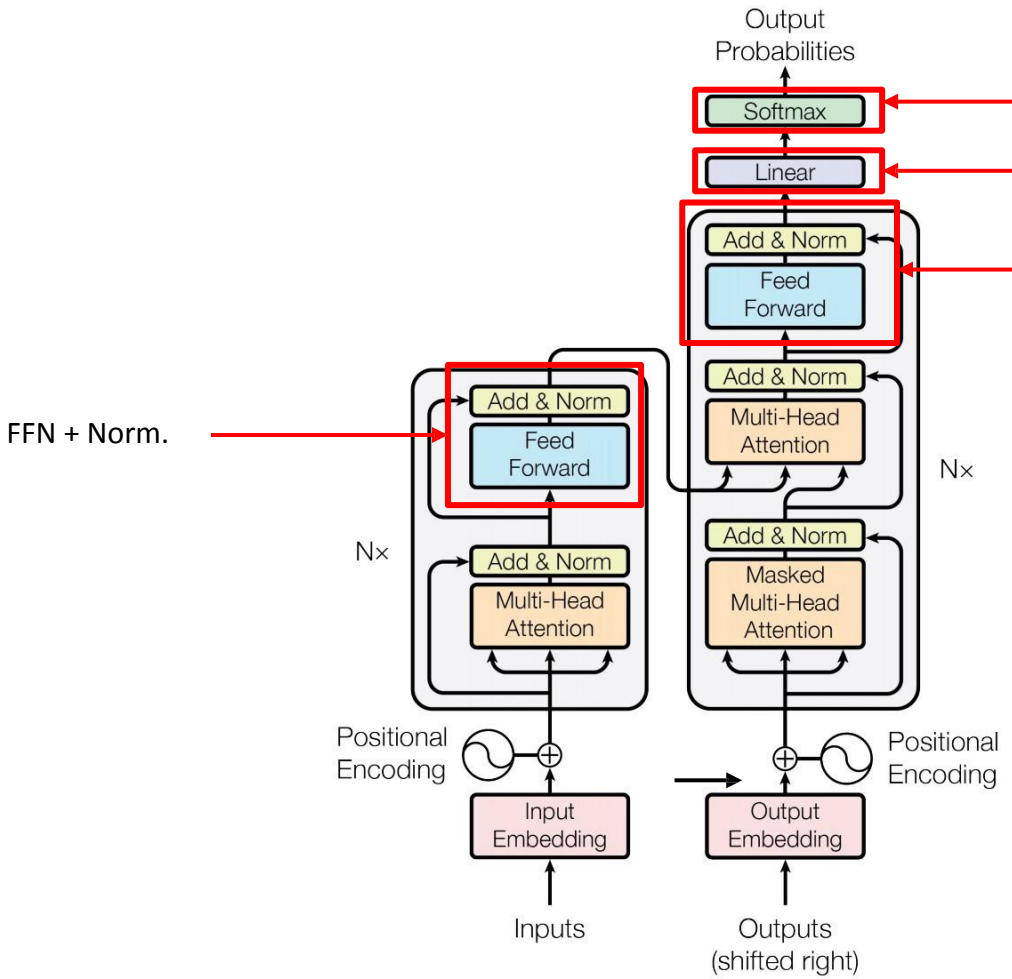
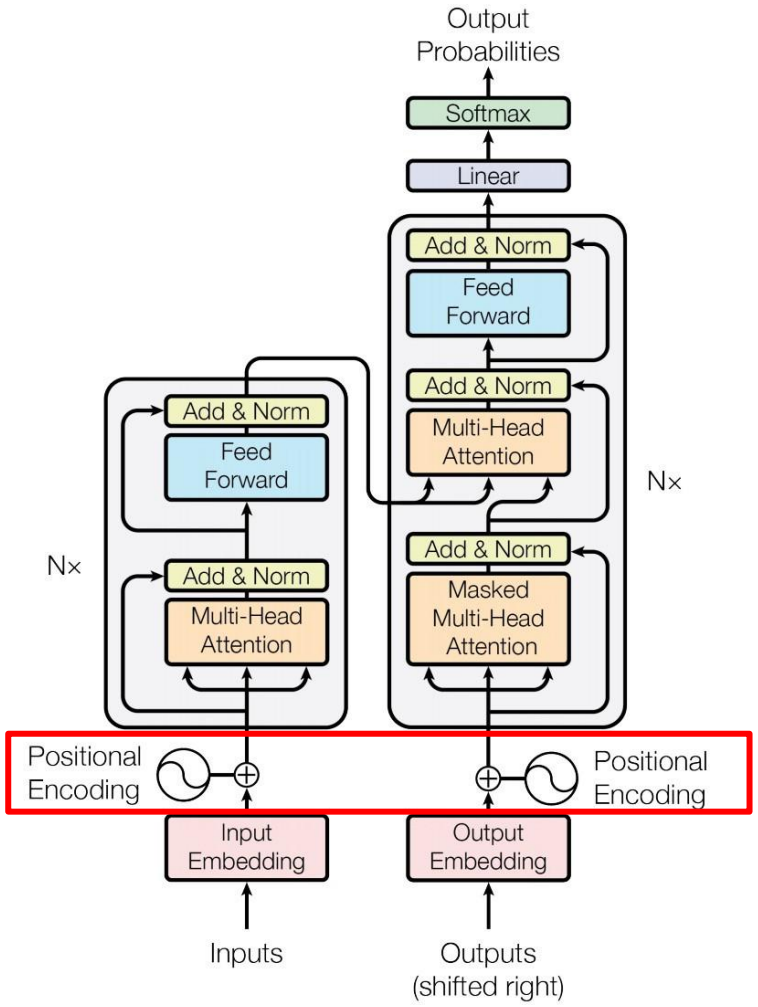
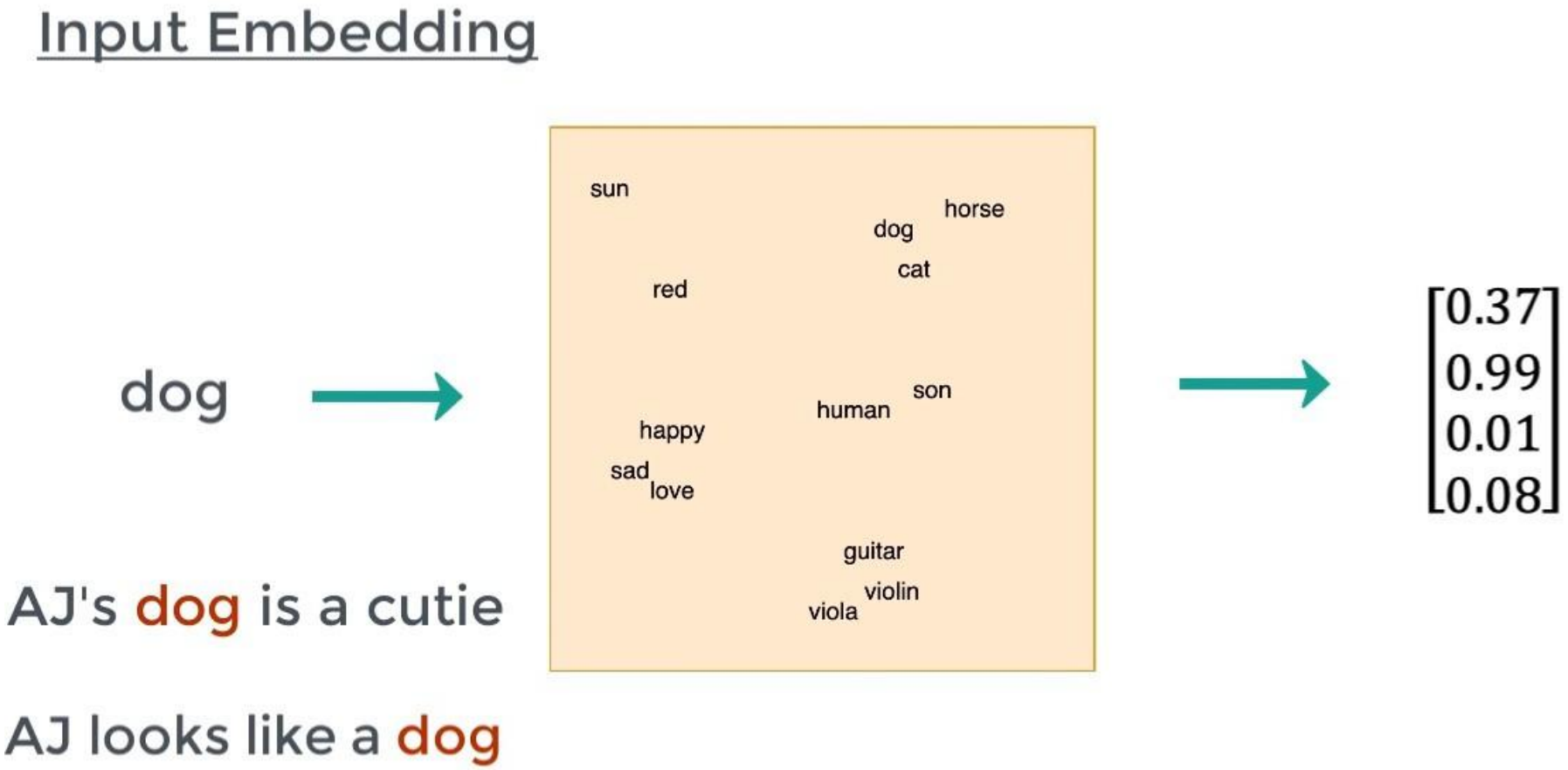


Figure 1: The Transformer - model architecture.

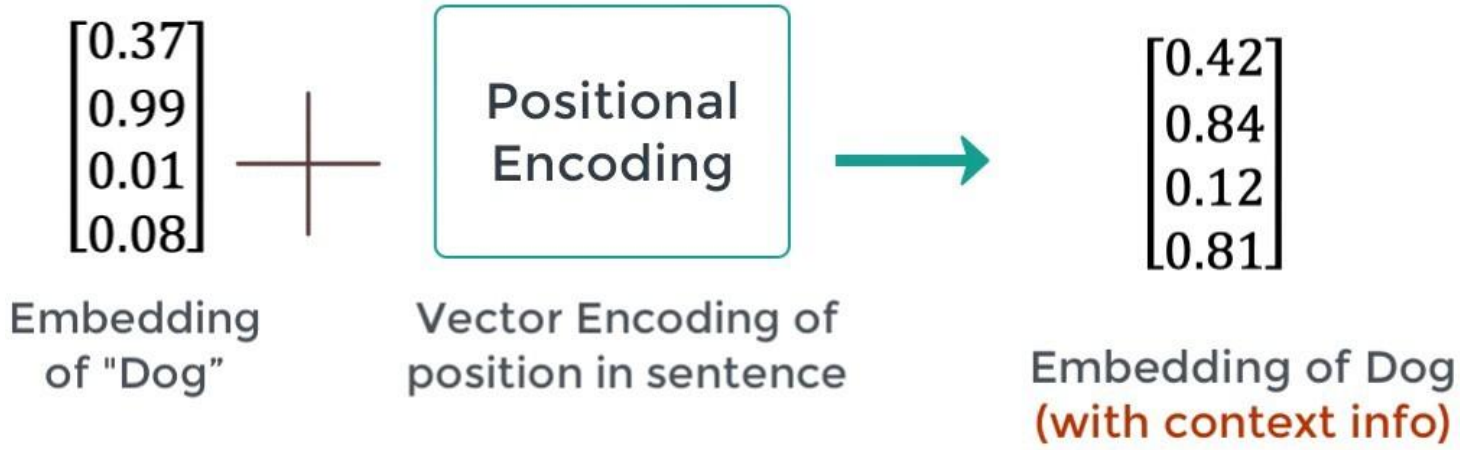


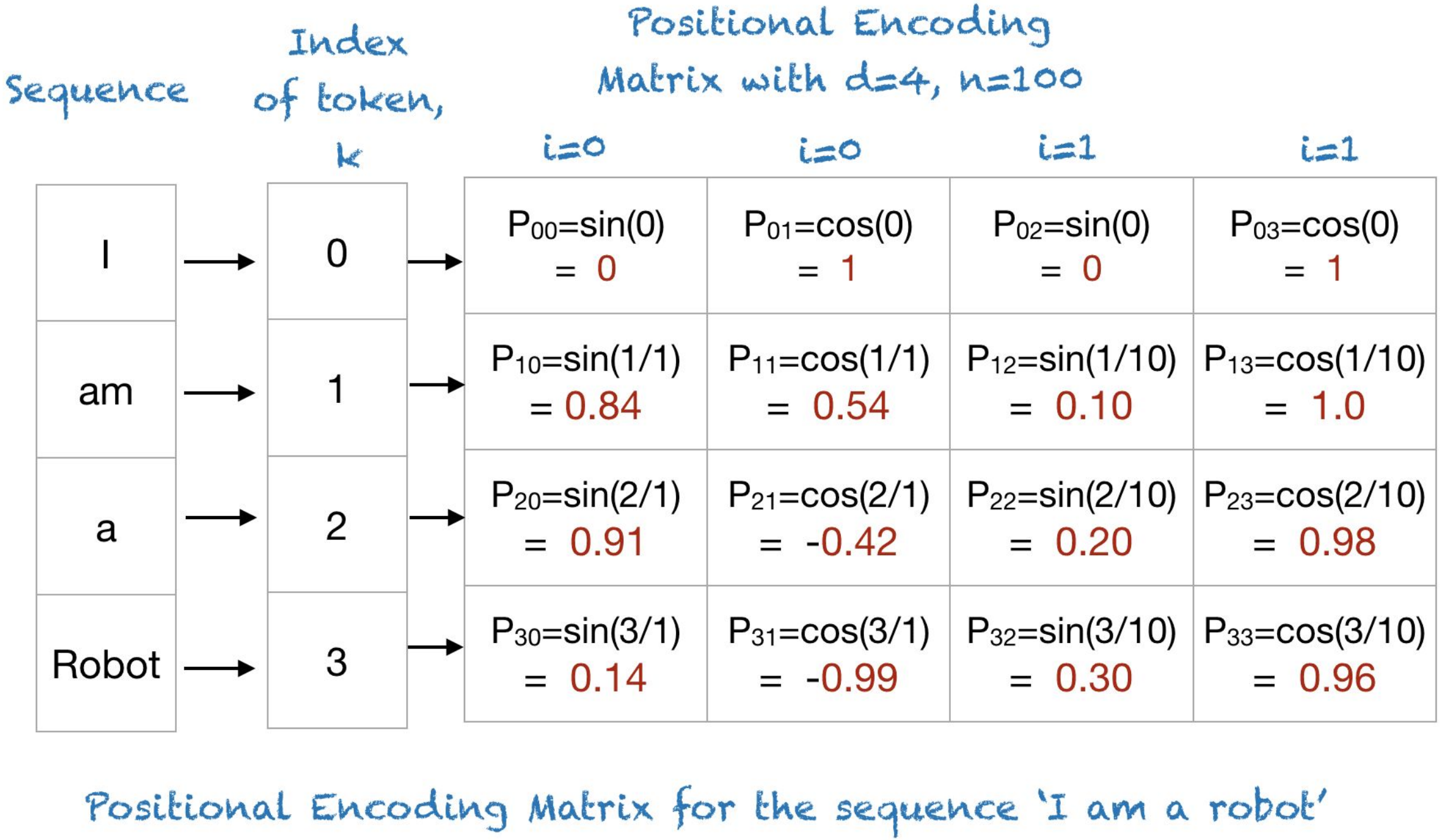
Positional Embedding

Positional Encoding



Positional Encoding





Positional Encoding Matrix for the sequence 'I am a robot'

The Impact of Positional Encoding on Length Generalization in Transformers

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Karthikeyan Natesan Ramamurthy[3], **Payel Das**[3], **Siva Reddy**[1,2,4]
[1]Mila - Québec AI Institute; [2]McGill University;
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Abstract

Length generalization, the ability to generalize from small training context sizes to larger ones, is a critical challenge in the development of Transformer-based language models. Positional encoding (PE) has been identified as a major factor influencing length generalization, but the exact impact of different PE schemes on extrapolation in downstream tasks remains unclear. In this paper, we conduct a systematic empirical study comparing the length generalization performance of decoder-only Transformers with five different position encoding approaches including Absolute Position Embedding (APE), T5's Relative PE, ALiBi, and Rotary, in addition to Transformers without positional encoding (NoPE). Our evaluation encompasses a battery of reasoning and mathematical tasks. Our findings reveal that the most commonly used positional encoding methods, such as ALiBi, Rotary, and APE, are not well suited for length generalization in downstream tasks. More importantly, NoPE outperforms other explicit positional encoding methods while requiring no additional computation. We theoretically demonstrate that NoPE can represent both absolute and relative PEs, but when trained with SGD, it mostly resembles T5's Relative PE attention patterns. Finally, we find that scratchpad is not always helpful to solve length generalization and its format highly impacts the model's performance. Overall, our work suggests that explicit position encodings are not essential for decoder-only Transformers to generalize well to longer sequences.

Research Topics

- Faster Inference
- Mixture of Experts
- Safety Alignment & Attacks
- Replacement of Attention Block

Outline

Part 1: Transformer

- What can transformers do
- Different types of transformer
- Why is transformer better than RNN
- Attention mechanism
  - General Structure
  - Query, Key & Value
  - Multi-Head Attention
  - Self-Attention

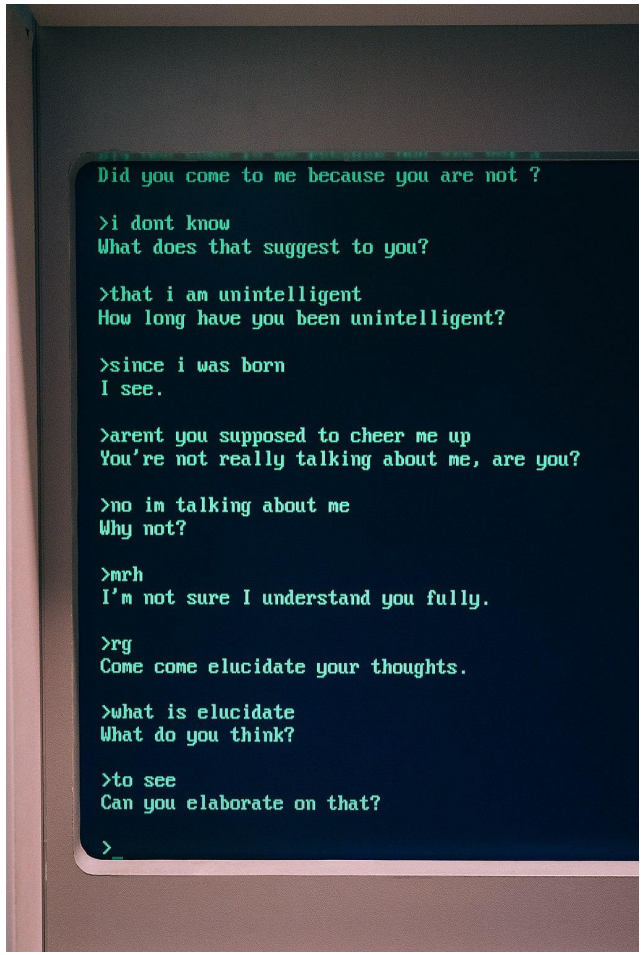
Part 2: Large Language Models

- **Introduction to Language Models and Large Language Models**
- Common architecture of LLMs
  - Autoencoding
  - Autoregressive
  - Sequence to sequence
- Application of LLMs
- Training a LLM

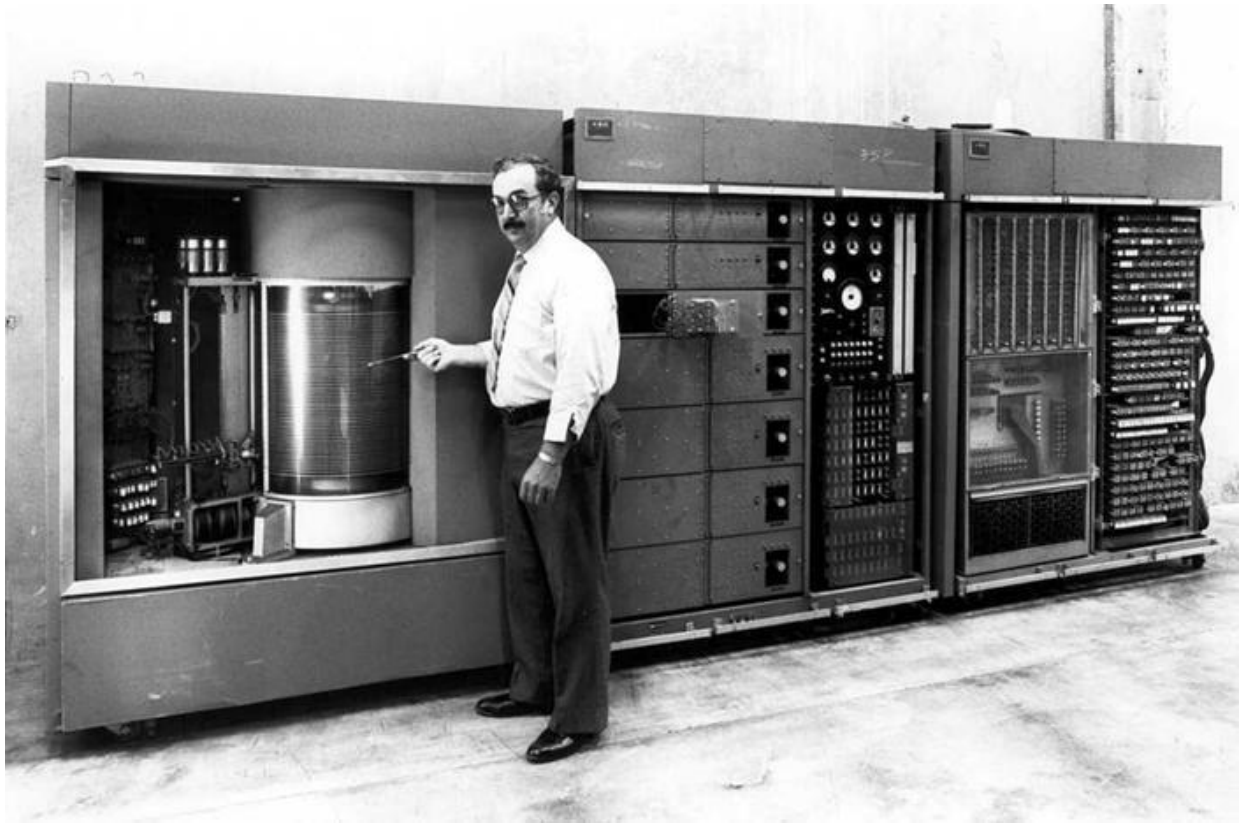
What Are Language Models

A probabilistic model of a natural language that can generate probabilities of a series of words, based on text corpora in one or multiple languages it was trained on.

Applications



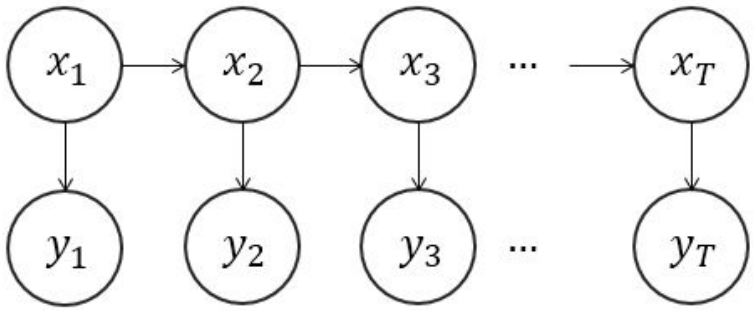
IBM Eliza

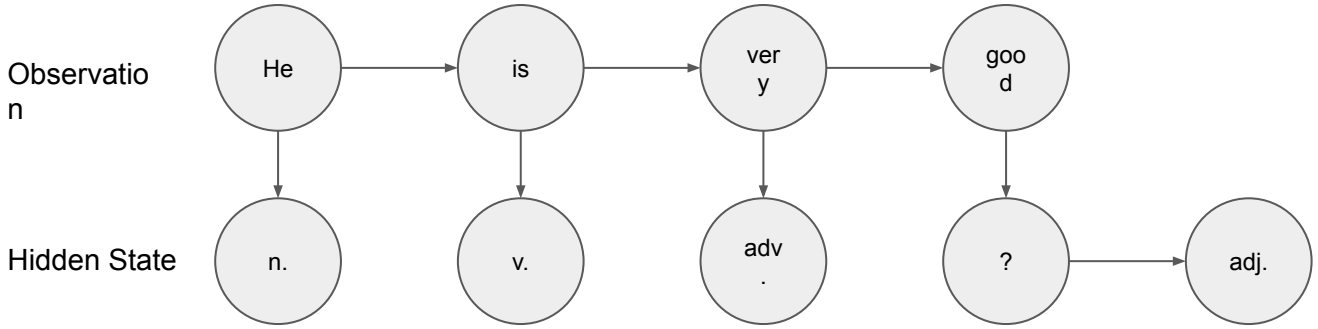


Georgetown-IBM-Experiment

Early Language Model

Statistical Language Models: Hidden Markov Models



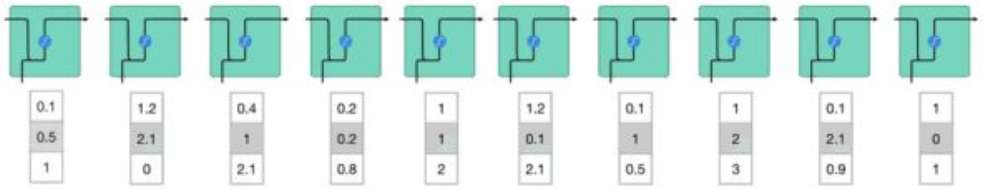


Drawbacks on Early Language Model

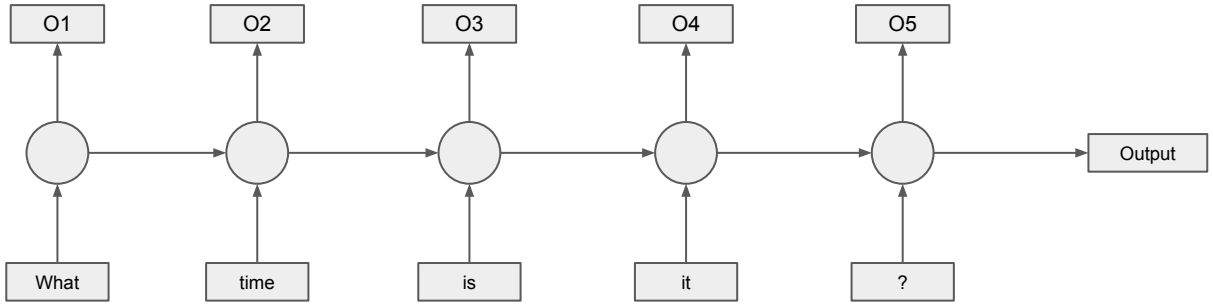
- Slow to compute
- Lack of generalisation
- Data sparsity
- …

Introduction to Neural Network

Neural Network: Recurrent Neural Network

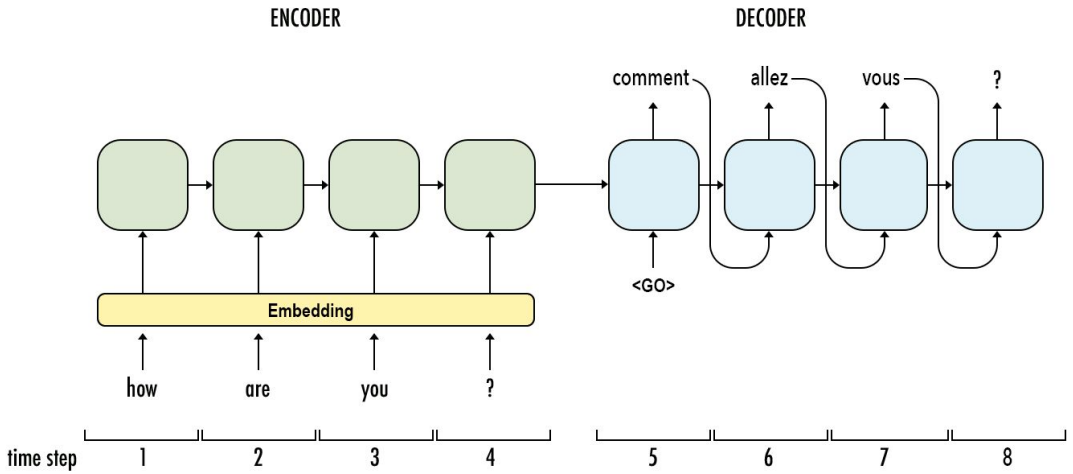


Animation demo of RNN



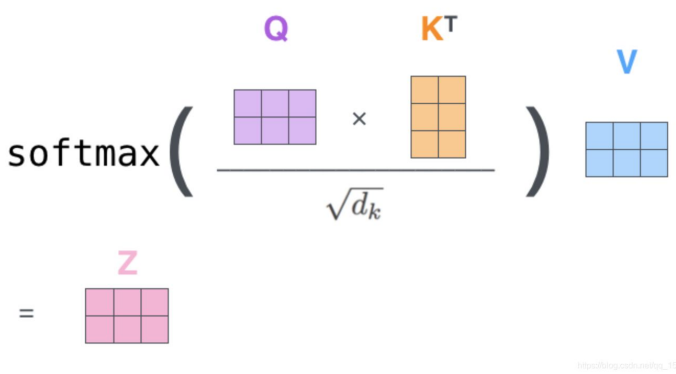
NLP example on semantic understanding

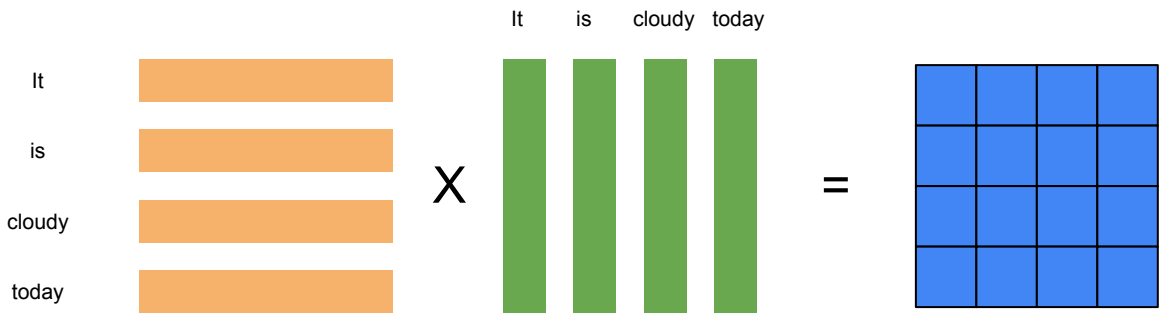
Recap: Why transformer?



In traditional sequence neural networks, sequence were ordered, which means the latter tokens are dependent to the previous sequence, which means both the ability of parallel computation and the ability of model's view is limited

Recap: Why transformer?





In transformer or attention based models, the input sequence was regarded as a whole entity, which means by a simple production, we can get the relationship between any two of the tokens in a single sequence, give the model ability to “see the global status”

Large Language Models

Artificial intelligence (AI) system that has been trained on vast amounts of text data to understand and generate human-like language.

Key characters:

- Deeper architecture
- Larger scale
- Massive data
- Strong capability

Outline

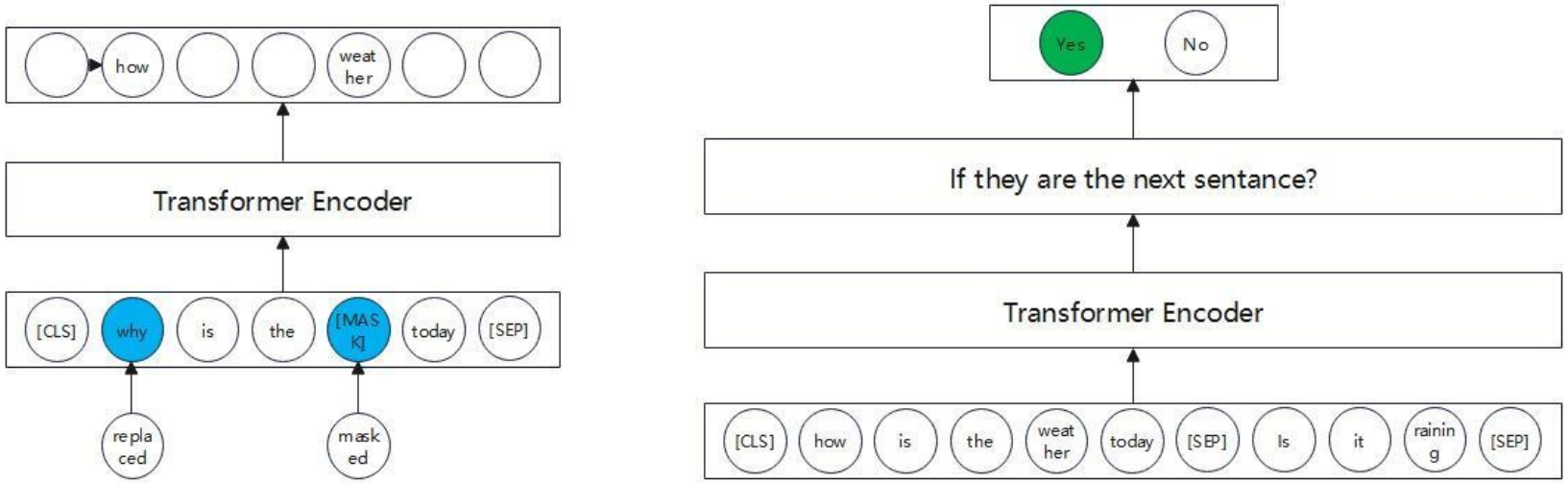
Part 1: Transformer

- What can transformers do
- Different types of transformer
- Why is transformer better than RNN
- Attention mechanism
  - General Structure
  - Query, Key & Value
  - Multi-Head Attention
  - Self-Attention

Part 2: Large Language Models

- Introduction to Language Models and Large Language Models
- **Common architecture of LLMs**
  - Autoencoding
  - Autoregressive
  - Sequence to sequence
- Application of LLMs
- Training a LLM

Autoencoding (Encoder only)

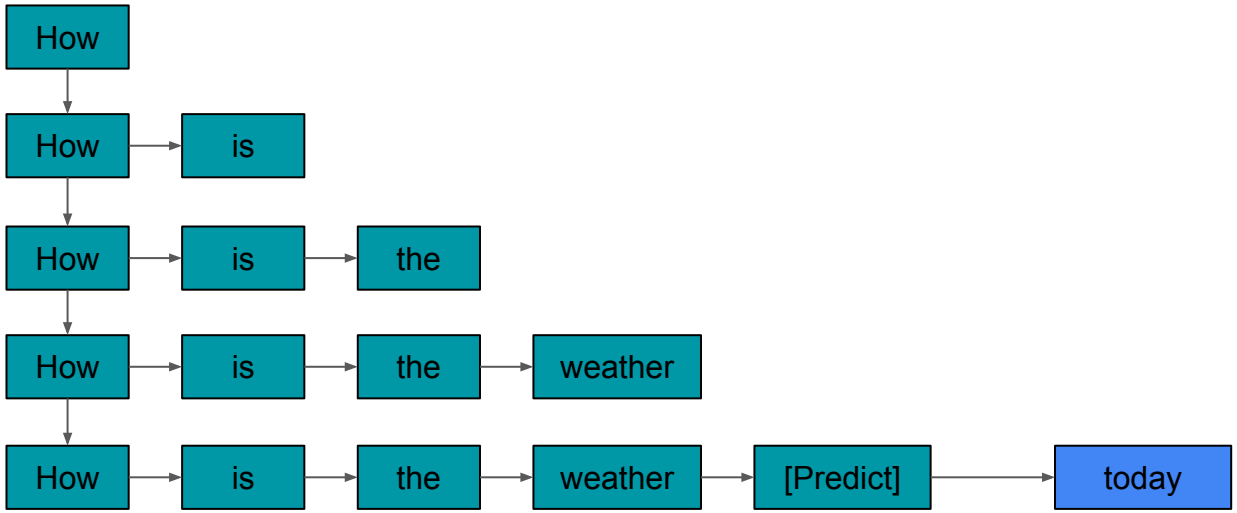


Example of strategy used by BERT

Scenario: Encoders produce contextual representations suitable for natural language understanding tasks, often used to solve reading comprehension, cloze and other problems.

Cons: It can not support the generation of indeterminate length text, and depends on the context before and after, which is very limited to the type of downstream tasks; Generally, it can only be used in downstream tasks after fine-tune, which will also involve a lot of manual operation and model tuning, and the model can not be made too large.

Autoregressive (Decoder model)



Auto-regressive model

Scenario: Suitable for long sequence, zero shot, and generation tasks, Allows the Decoder class model to adapt to various types of downstream tasks without being fine-tuned.

Cons: Unidirectional attention, which makes it impossible to fully capture the dependencies between contexts in NLU tasks. Other tasks can be converted into autoregressive tasks.

Sequence to Sequence (Encoder-Decoder model)

Passage	阅读文章:鲁迅,原名周樟寿,后改名周树人,浙江绍兴人。著名文学家、思想家、革命家、教育家、民主战士,新文化运动的重要参与者,中国现代文学的奠基人之一。早年与厉绥之和钱均夫同赴日本公费留学,于日本仙台医科专门学校肄业。鲁迅,1918年发表《狂人日记》时所用的笔名,也是最为广泛的笔名。鲁迅一生在文学创作、文学批评、思想研究、文学史研究、翻译、美术理论引进、基础科学介绍和古籍校勘与研究等多个领域具有重大贡献。他对于五四运动以后的中国社会思想文化发展具有重大影响,蜚声世界文坛,尤其在韩国、日本思想文化领域有极其重要的地位和影响,被誉为二十世纪东亚文化地图上占最大领土的作家"。请问:鲁迅于1918年发表过什么文章?回答: (Read the article: Lu Xun, formerly known as Zhou Zhangshou, later renamed Zhou Shuren, Zhejiang Shaoxing. He is a famous writer, thinker, revolutionist, educator, democracy fighter, important participant of the New Culture Movement, one of the founders of Chinese modern literature. In his early years, Lu Xun, Li Suizhi and Qian Junfu went to Japan to study abroad at public expense and studied at Sendai Medical School in Japan. Lu Xun, the pen name used when he published Diary of Mad Men in 1918, is also the most widely used pen name. Lu Xun made great contributions in literary creation, literary criticism, ideological research, literary history research, translation, introduction of art theory, introduction of basic science and collation and research of ancient books. He had a great influence on the ideological and cultural development of Chinese society after the May 4th Movement, and was famous in the world literary circles, especially in the ideological and cultural fields of Korea and Japan. He was known as the writer who occupied the largest territory on the cultural map of East Asia in the 20th century. Question: What articles did Lu Xun publish in 1918? Answer:)
PanGu-Σ	鲁迅于1918年发表了《狂人日记》。《狂人日记》是中国现代文学史上最早的一部白话小说,也是中国现代小说的开山之作。 (Lu Xun published the Madman's Diary in 1918. Madman's Diary is the earliest vernacular novel in the history of modern Chinese literature, and is also the beginning of modern Chinese novels.)

Pangu-Σ on bilingual summarisation task

Scenarios: Mainly used for conditional text generation, such as generating summaries and answering questions

Cons: Requires more parameters.

Comparison between LLM and DNN

	Large Language Model	Traditional DNN
Architecture	Typically based on Transformers	Various architecture such as MLP, CNN, RNN, GAN, Diffusion etc
Scale	Hundreds of millions to billions of parameters	May have millions of parameters but not in the billions
Data	Vast and diverse datasets	Domain-specific datasets
Training Strategy	Two-step training process, pre-training and fine-tuning	Task specific supervised or unsupervised training
Application	Natural language understanding and generation tasks	Crossfield, NLP, CV, Audio, Generation etc.

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- Introduction to Language Models and Large Language Models
- Common architecture of LLMs
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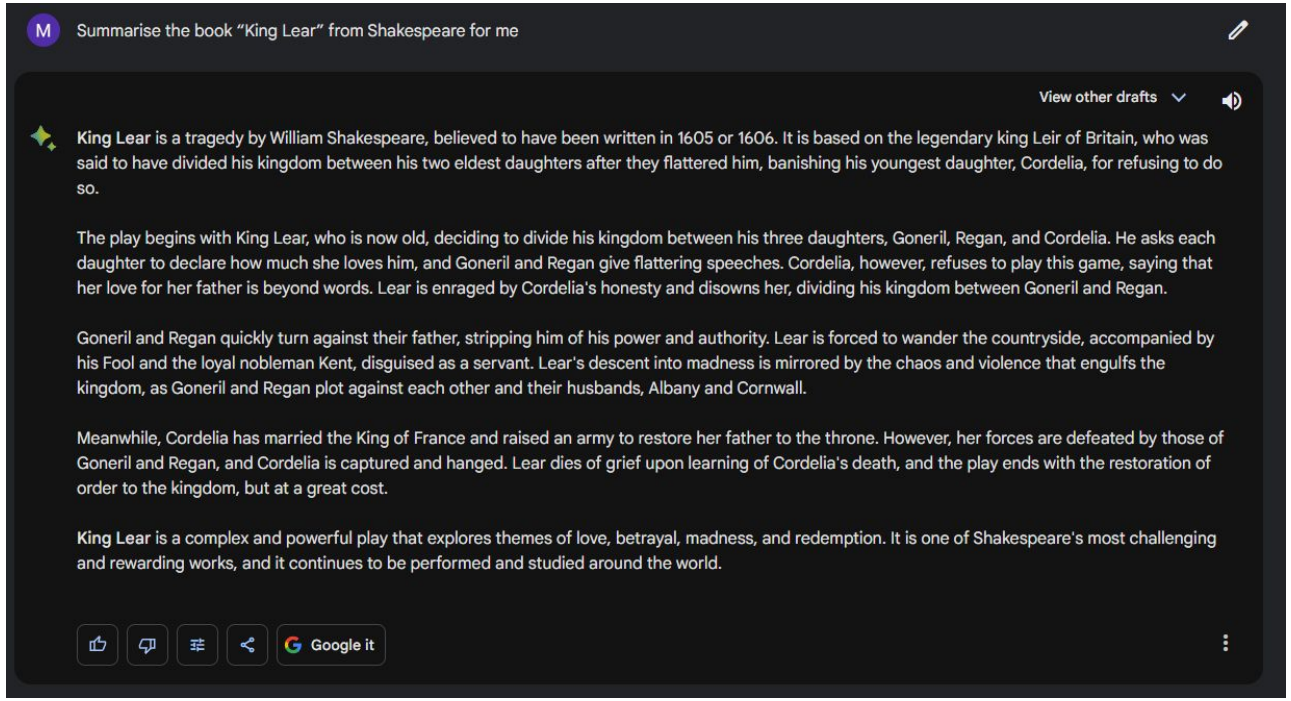
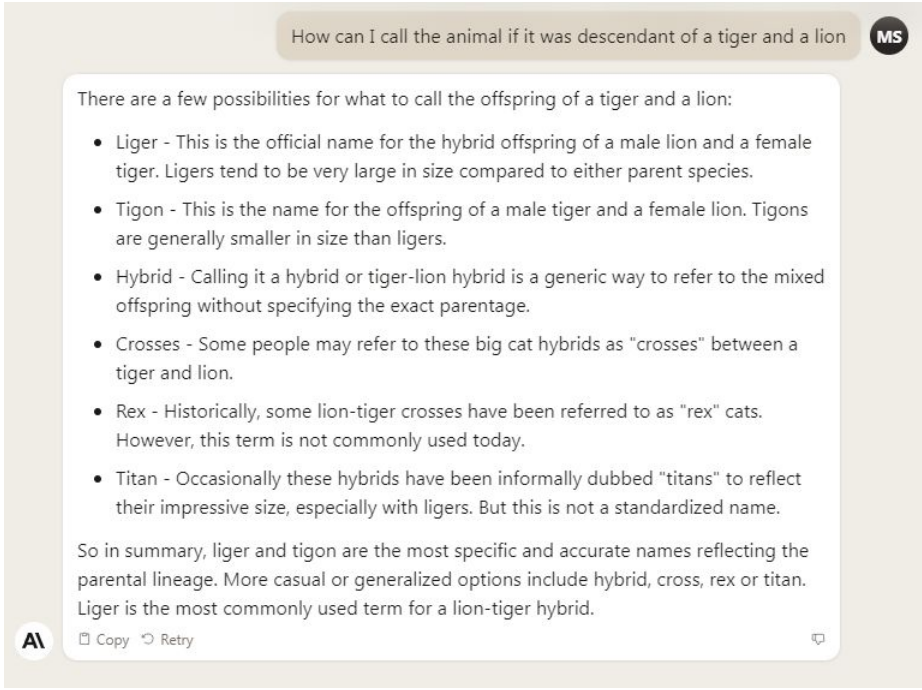
  - Autoregressive
  - Sequence to sequence
- **Application of LLMs**
- Training a LLM

Application of Large Language Model



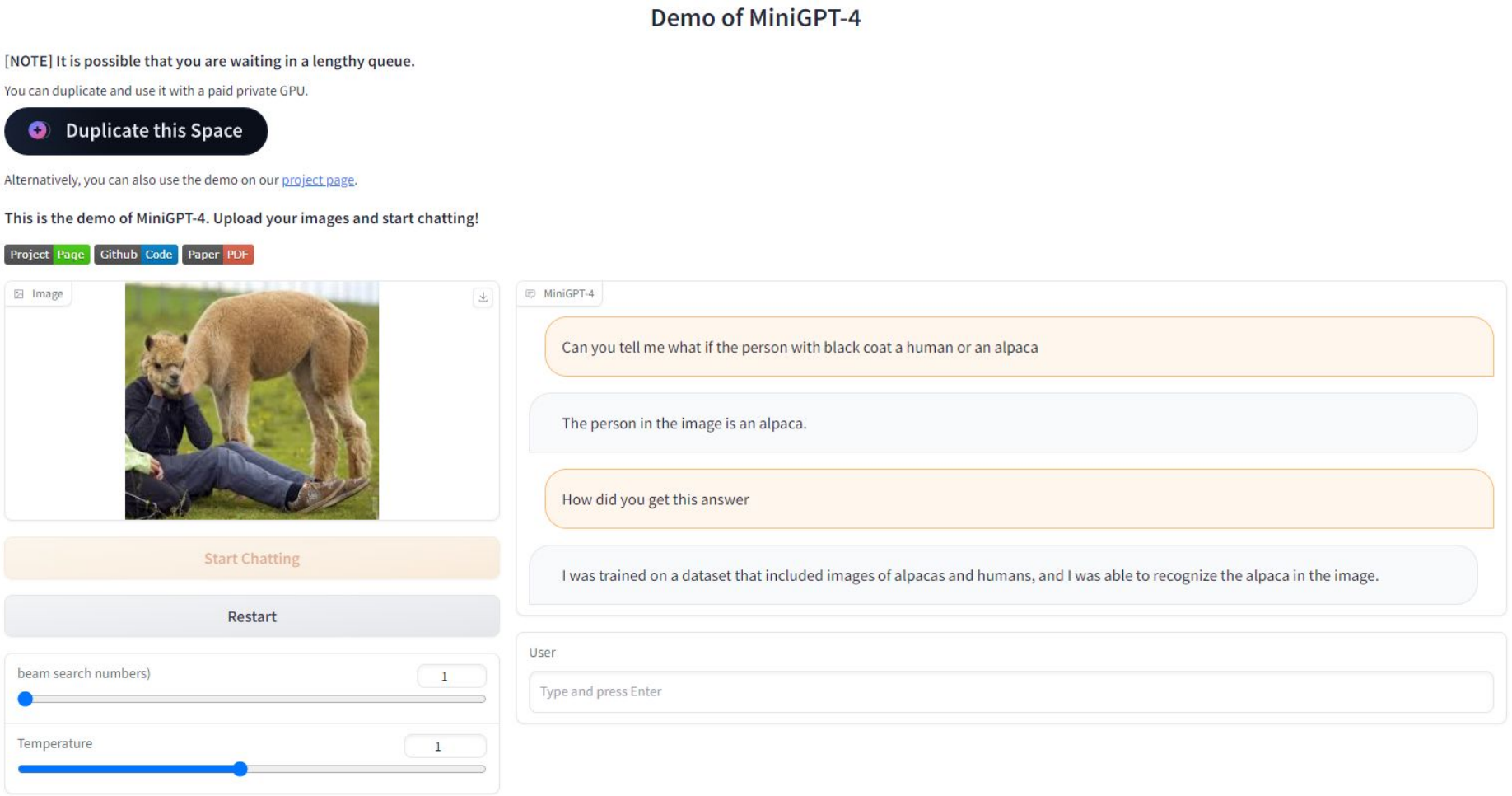
Google Bard on summarisation

Application of Large Language Model



Claude 2 on question answering

Application of Large Language Model



Semantic understanding

Application of Large Language Model

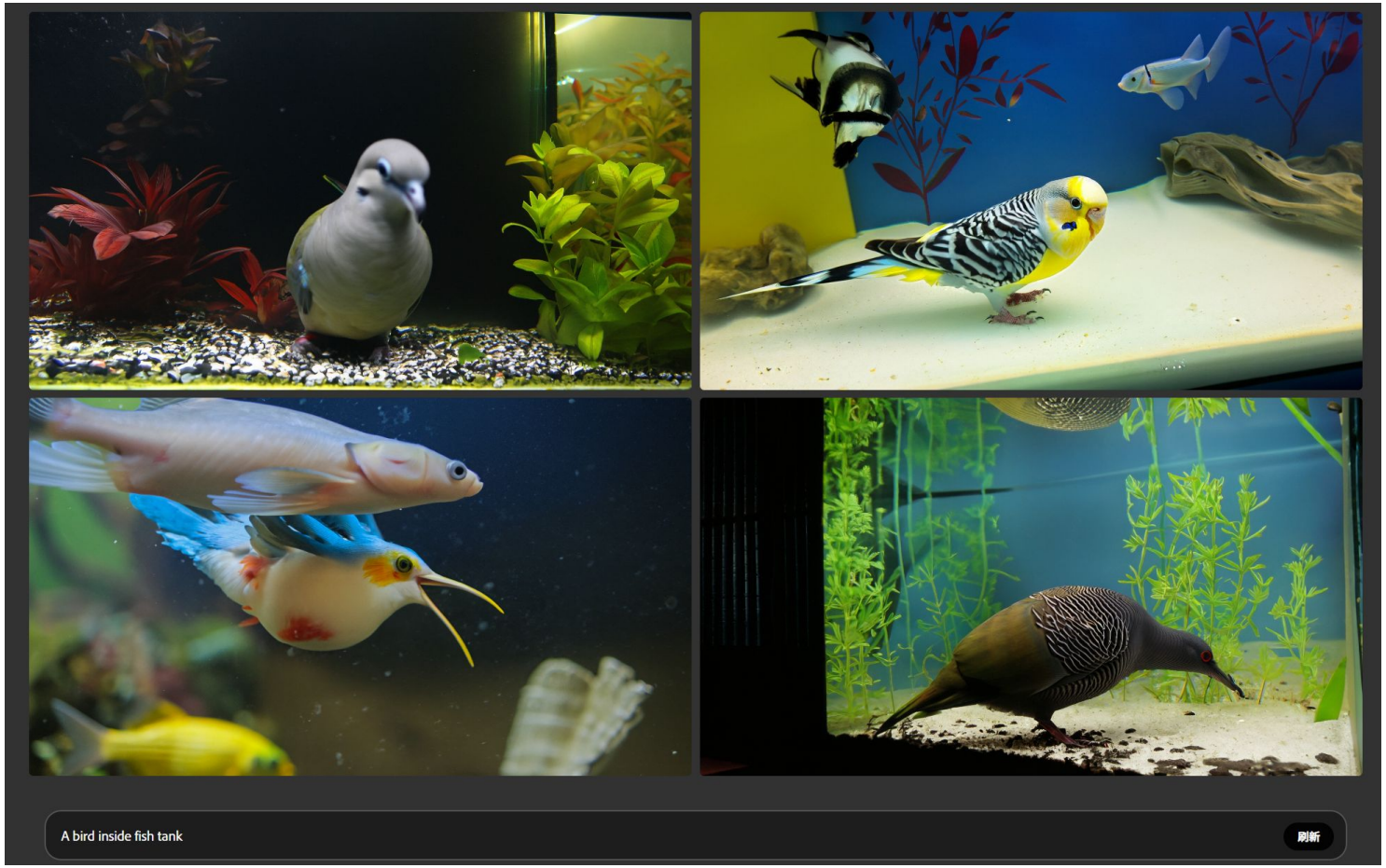
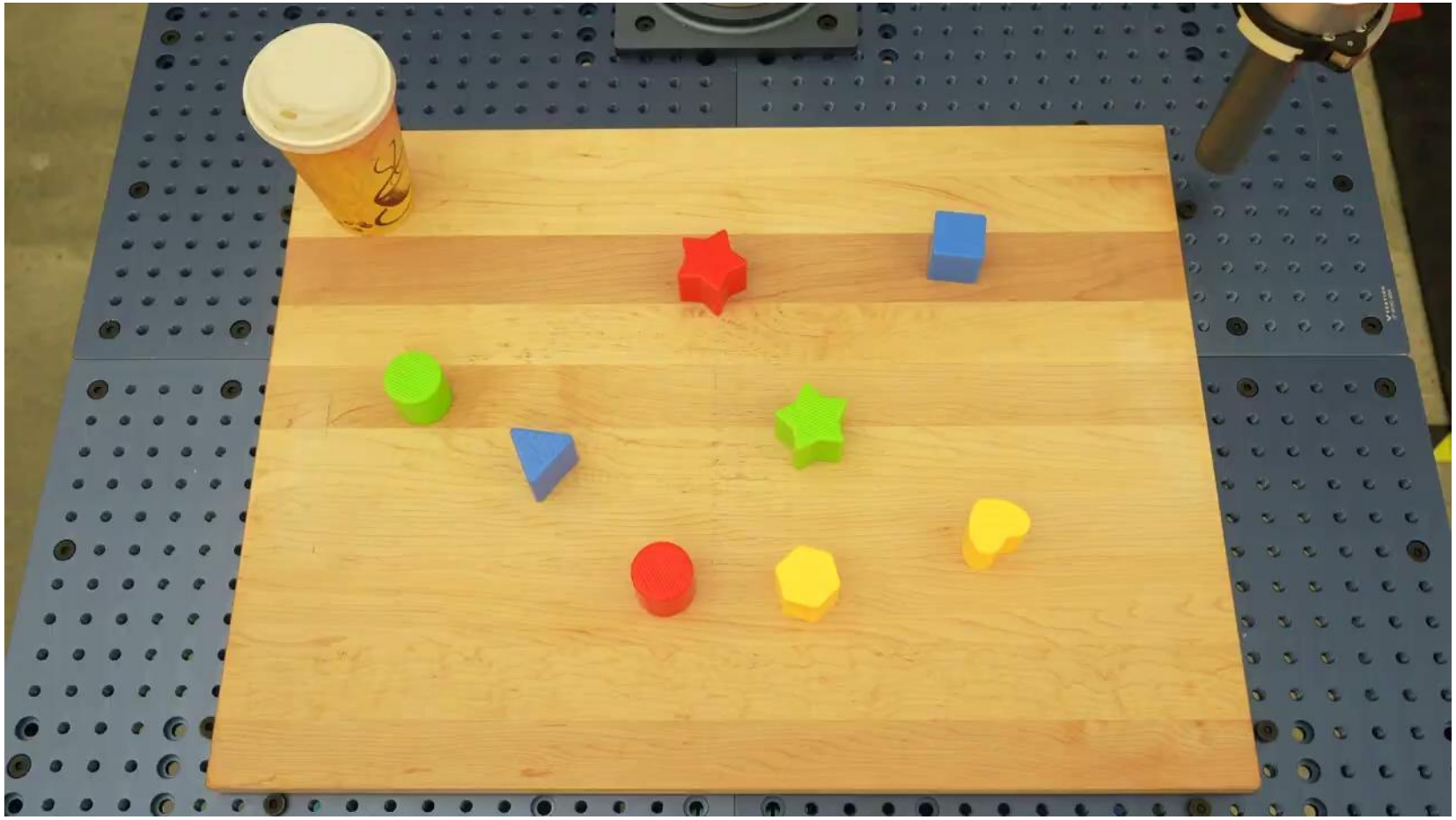


Image generation

Application of Large Language Model



Embodied support of PaLM-E

Outline

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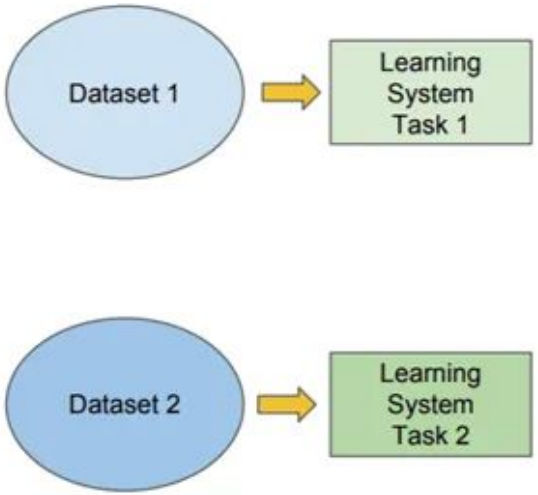
- **Training a LLM**

Training a LLM: Transfer Learning

Traditional ML

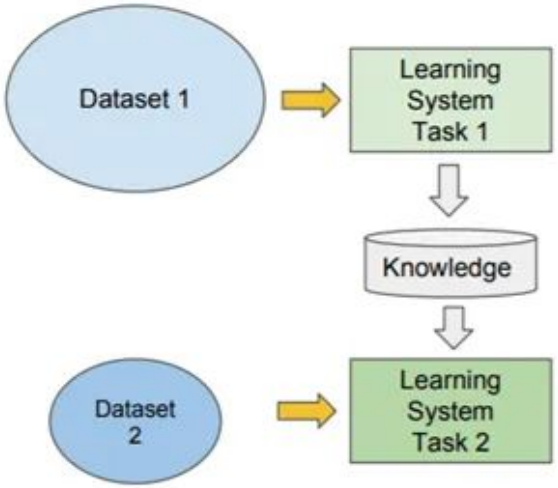
- Isolated, single task learning:
  - Knowledge is not retained or accumulated. Learning is performed w.o. considering past learned knowledge in other tasks



vs

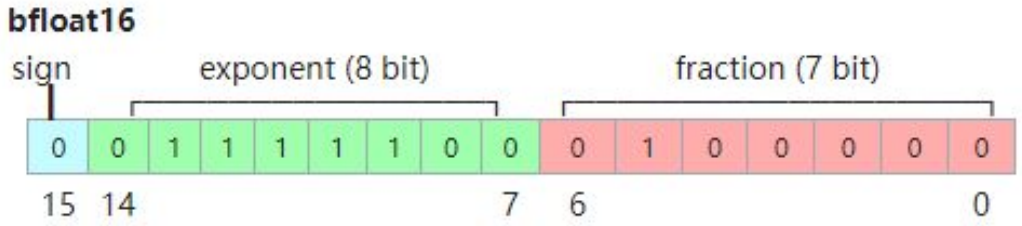
Transfer Learning

- Learning of a new tasks relies on the previous learned tasks:
  - Learning process can be faster, more accurate and/or need less training data



Why it is so hard to train a LLM

LLaMA-6B with bfloat16 (bf16, 16bits, 2 bytes) float format



To train this model we need:

1. Parameter: 6B * 2bytes = 12GB
2. Gradient: 6B * 2bytes = 12GB
3. Optimiser: AdamW normally double of the parameter: 24GB

With LLaMA architecture: hidden_size=4096, intermediate_size=11008, num_hidden_layer=32, context_length=2048

For each sample we need: (4096 + 11008) * 2048 * 32 * 2byte = 1920MB ~ 2GB

With batchsize=50, the total VRAM required to train this model under this configuration is:

48GB + 50 * 2GB = 148GB

Which is larger than a single Nvidia H100 GPU! (one of the best AI chips)

```
training_args = TrainingArguments(
    per_device_train_batch_size=1,
    gradient_accumulation_steps=4,
    gradient_checkpointing=True,
    fp16=True,
    **default_args,
)
```

Why it is so hard to train a LLM

Electronics › Computers & Accessories › Computer Components › Internal Components › Graphics Cards

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How can I get access to the LLMs

- Huggingface (https://huggingface.co/): Include most of open-source models implementation
- GitHub (https://github.com/): Some research groups uploaded the source of the model to GitHub such as LLaMA (https://github.com/facebookresearch/llama)
- API available by AI companies: Such as OpenAI's API (https://openai.com/blog/openai-api)
- Or you can write your own LLM with deep learning frameworks…

Suggested extra tutorials

- Deep Learning: Dive into Deep Learning (https://d2l.ai/)
- PyTorch: Official PyTorch tutorials (https://pytorch.org/tutorials/) and practical code (https://github.com/yunjey/pytorch-tutorial)
- Huggingface: Huggingface NLP course (https://huggingface.co/learn/nlp-course/chapter1/1)

Demonstrations and Assignments

- Transformer Basic: https://drive.google.com/file/d/1_EYvoDVPCNrwGDFbNFq0x8nGcBxw6rdO/view?usp=drive_link
- LLM Inference: https://drive.google.com/file/d/1pqNTiwfixZ7Ee07S1IesH41Ry8cYMfp3/view?usp=drive_link
- LLM Finetuning: https://drive.google.com/file/d/1D-fkUeFPV1ki2VAEd-mRJYDGFVC8HkDh/view?usp=drive_link