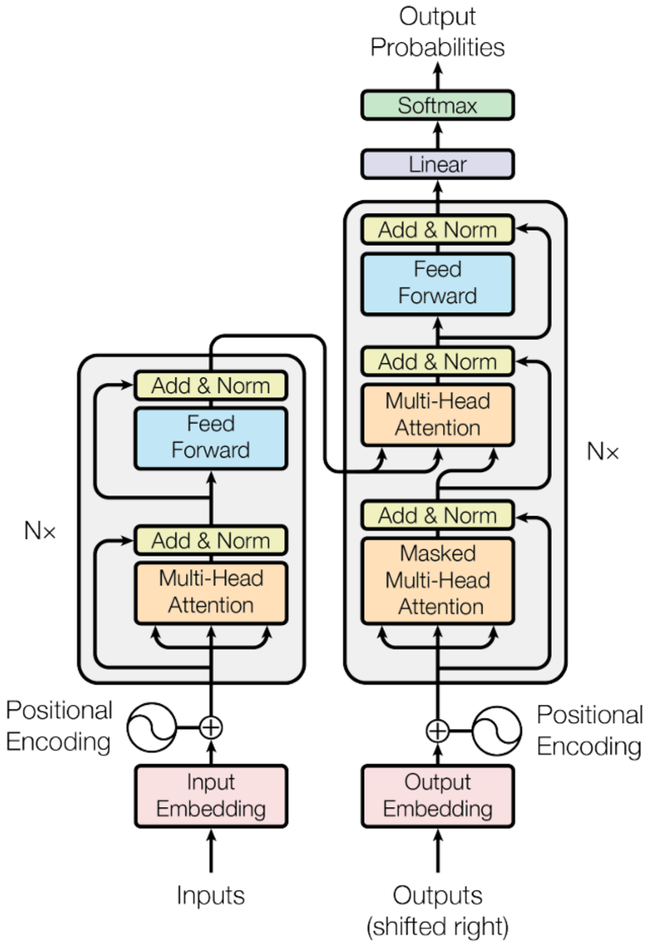
Machine Learning I
60629A

Attention and Transformers
— Week #10


Output Probabilities
Softmax
Linear
Add & Norm
Feed Forward
Add & Norm
Multi-Head Attention
Add & Norm
Masked Multi-Head Attention
N×
Add & Norm
Feed Forward
Add & Norm
Multi-Head Attention
N×
Positional Encoding
Positional Encoding
Input Embedding
Output Embedding
Inputs
Outputs (shifted right)

Transformers

- A deep learning model
  - Introduced in 2017 (Google researchers)
    - Quickly adopted for modelling sequential data (text and images)—architecture behind LLMs
  - Uses the *attention mechanism*

* Most of the slides/figures/narrative are from David Berger (you might see them again in ML #2).

Today’s plan

- Refresh our understanding of RNNs and bidirectional ones
- Introduce *attention*
- Transformer block
- Examples of transformers in practice (more on that next week)

- For concreteness, I will think of our data as a sequence of words
- And I use words and tokens synonymously
- In practice, tokens are sub-words (e.g., a few letters)
  - Tokenization is a topic beyond today's class

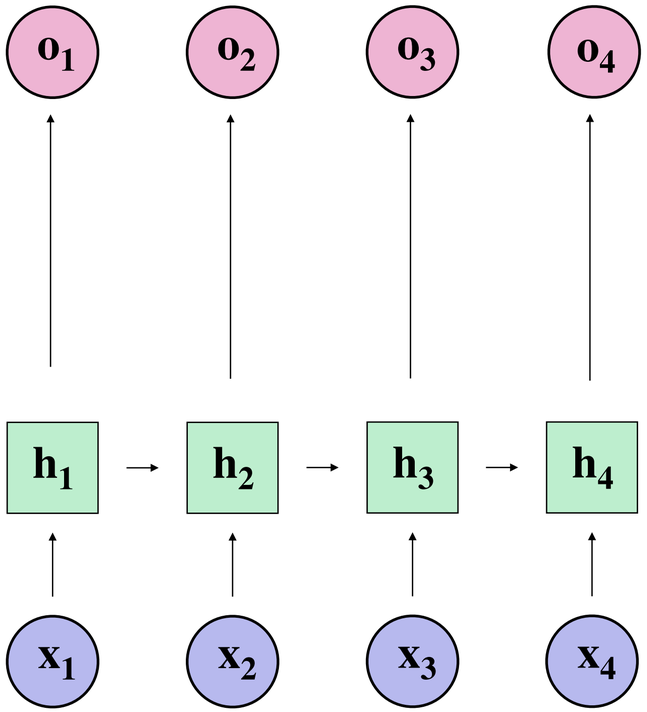
RNNs

For one time step

x_i Data

h_i Hidden layer (Left to right)

o_i Prediction



The hidden state at each timestep (h_t)
Must contain all useful information up to time t.

Bidirectional RNNs

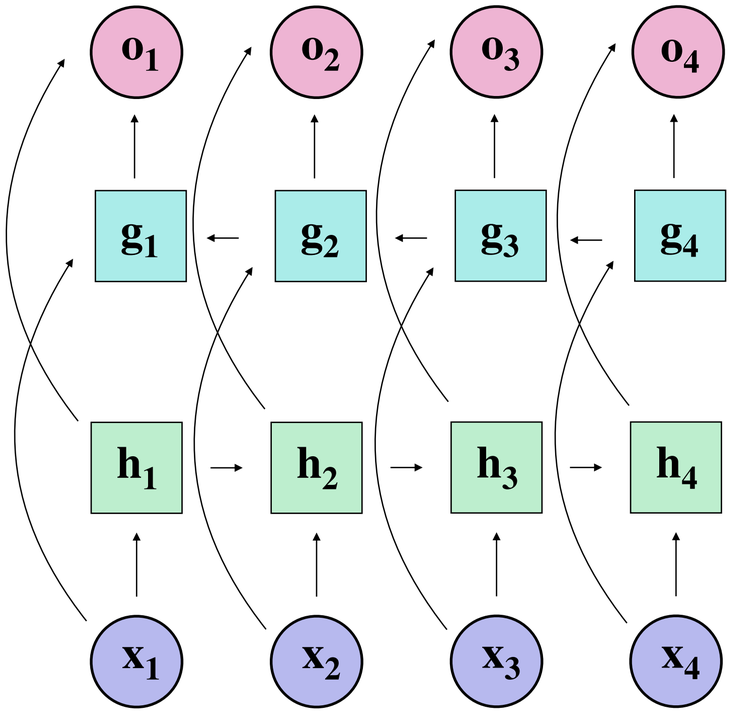
For one time step

x_i Data

h_i Hidden layer (Left to right)

g_i Hidden layer (Right to left)

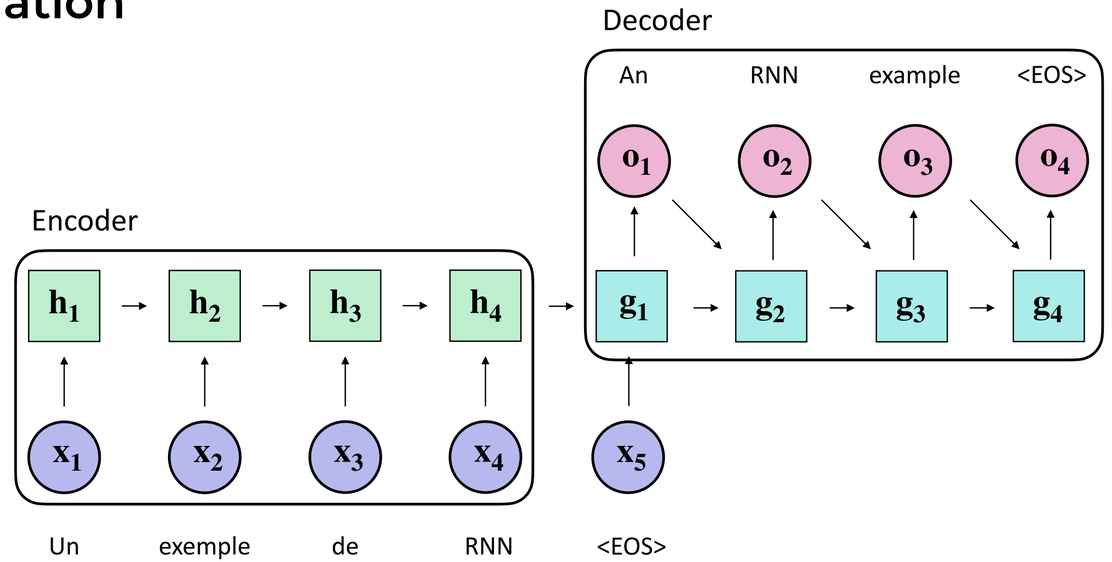
o_i Prediction



- The hidden state h_t must contain all useful information from to t
- The hidden state g_t must contain all useful information from the end (T) to t.
- Difficulties:
  - Exploding & vanishing gradients
    - Predictions will tend to use information from close neighbours

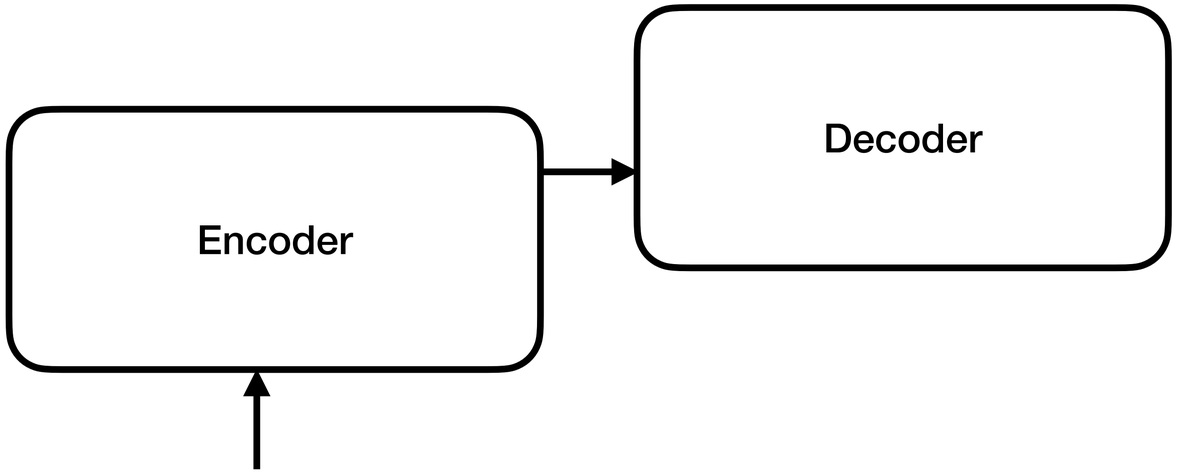
Encoder-Decoder
(Also known as Sequence to Sequence — Seq2Seq)

- What if the output is a different length than the input? E.g., translation



- h_4 must contain ("summarize") information from the input
  - It's a bottleneck. Its size (num. neurons) is an important hyperparameter

Problem



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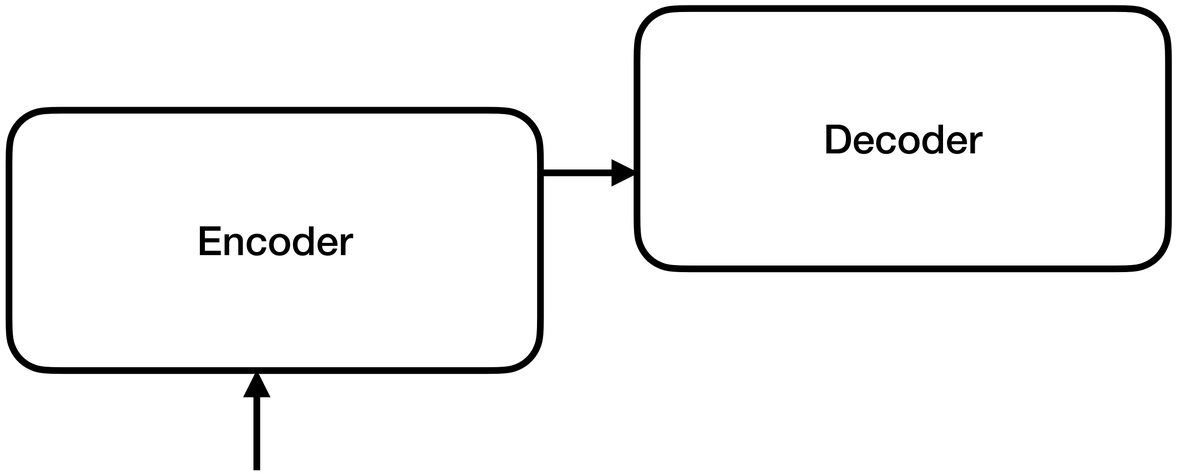
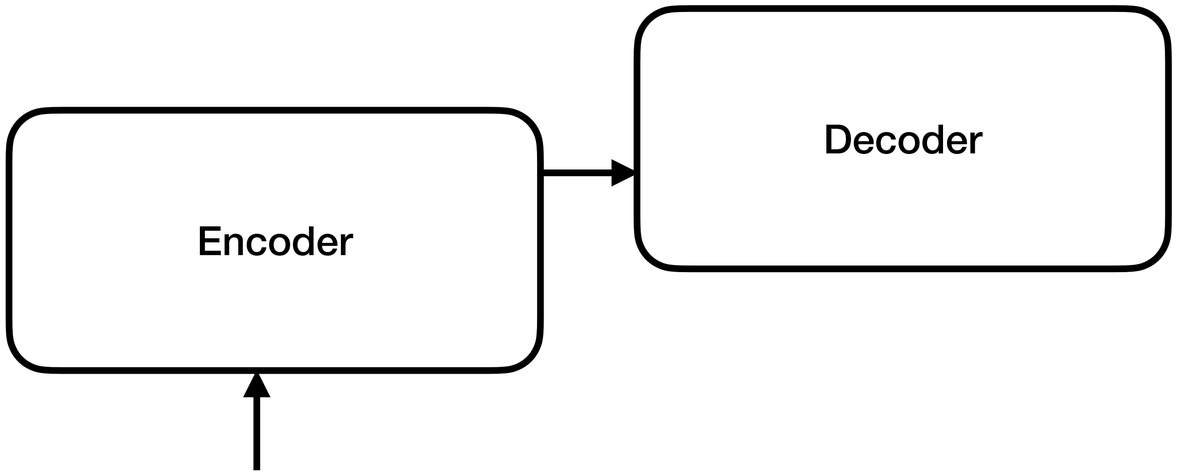


- **Challenging to encode vast amounts of information**

Problem



- **Challenging to encode vast amounts of information**
- **Could try to divide your input (e.g. sentence by sentence)**

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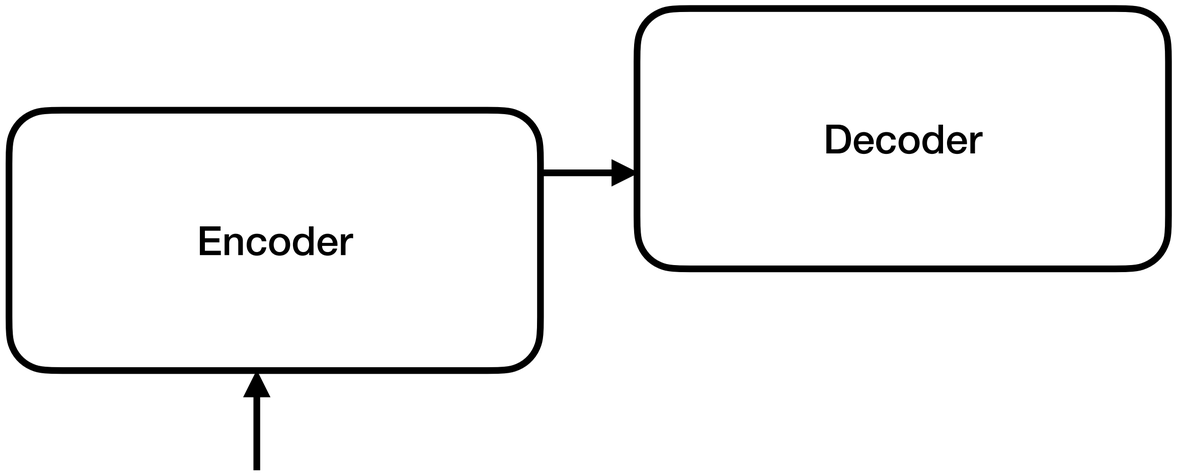

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  - Tasks (e.g. translation) can require *local* and *global* coherence

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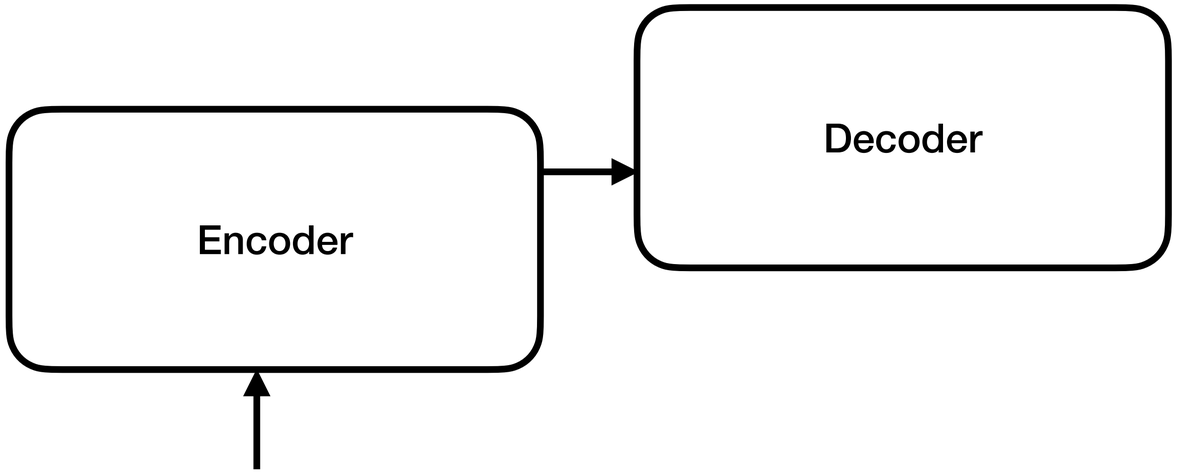
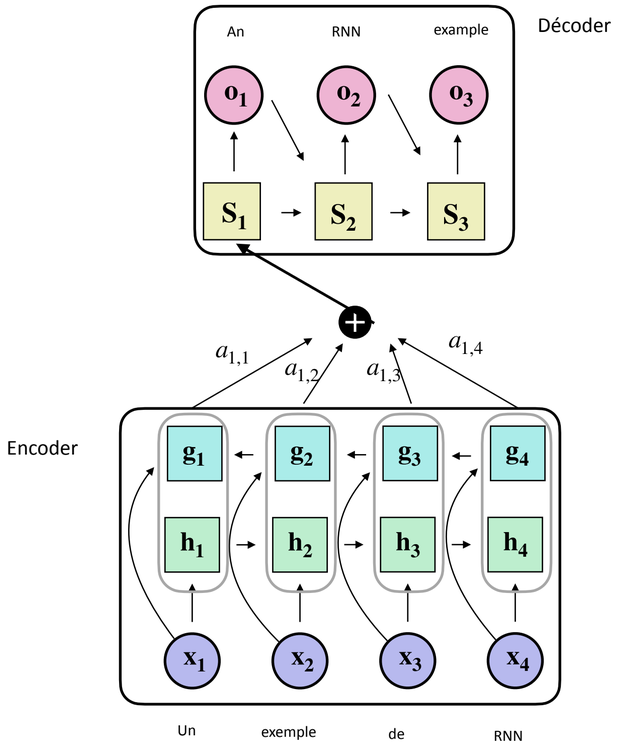


- Challenging to encode vast amounts of information
- Could try to divide your input (e.g. sentence by sentence)
  - Tasks (e.g. translation) can require *local* and *global* coherence
- Instead, decode word by word by focusing on the relevant different parts of the input

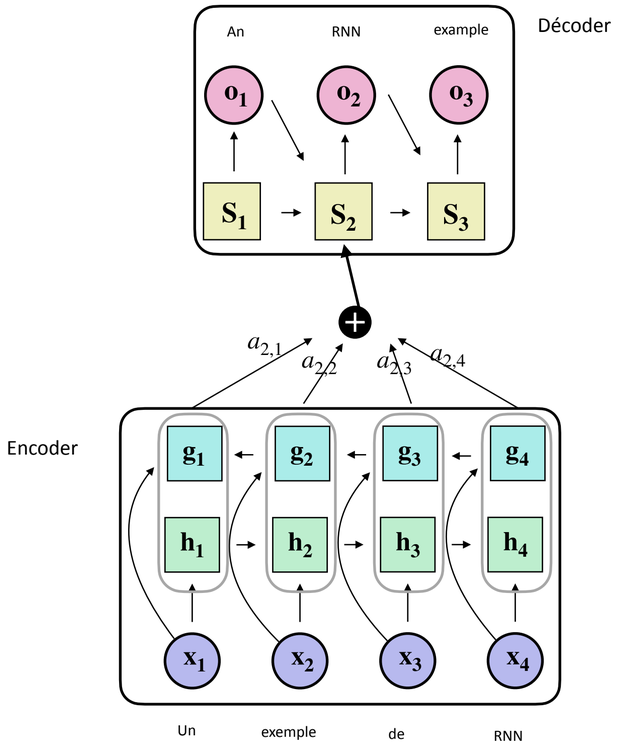
(Soft) Attention



a_{tj} : how much should decoder word t, "use" (attend to) on encoder word j

$$\sum_j a_{tj} = 1 \quad \forall t$$

(Soft) Attention



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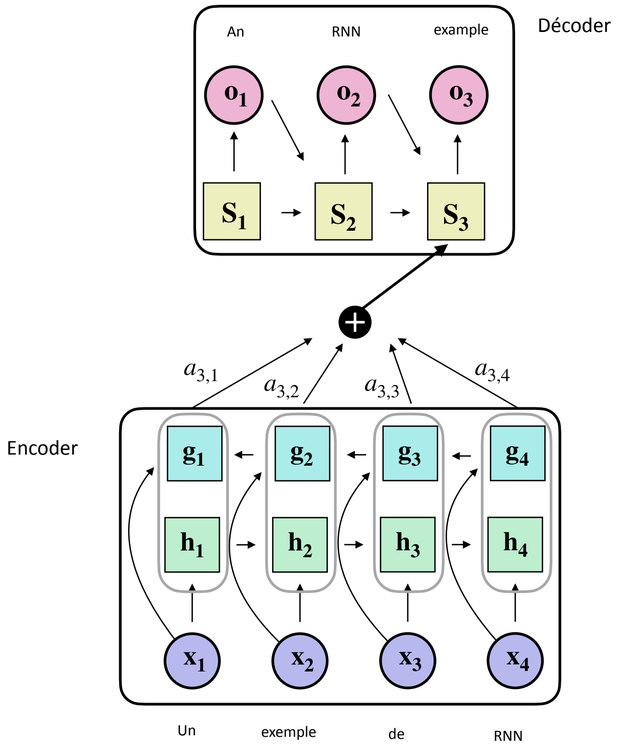

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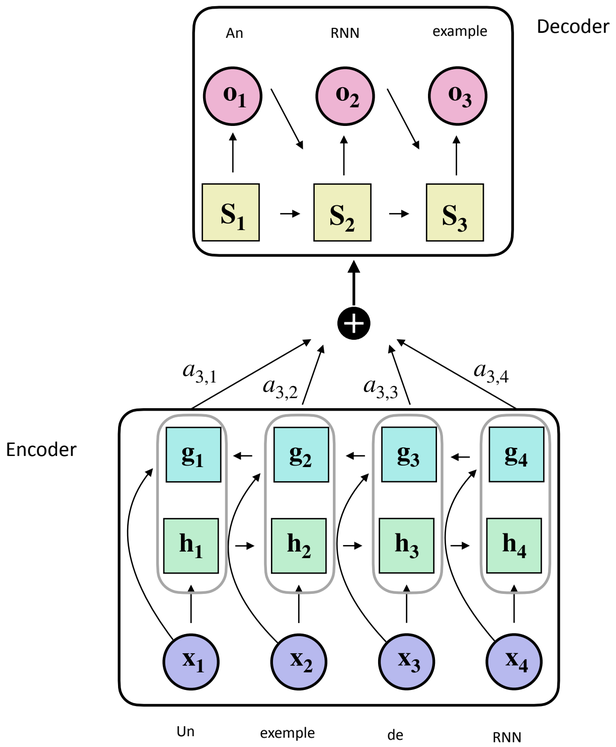
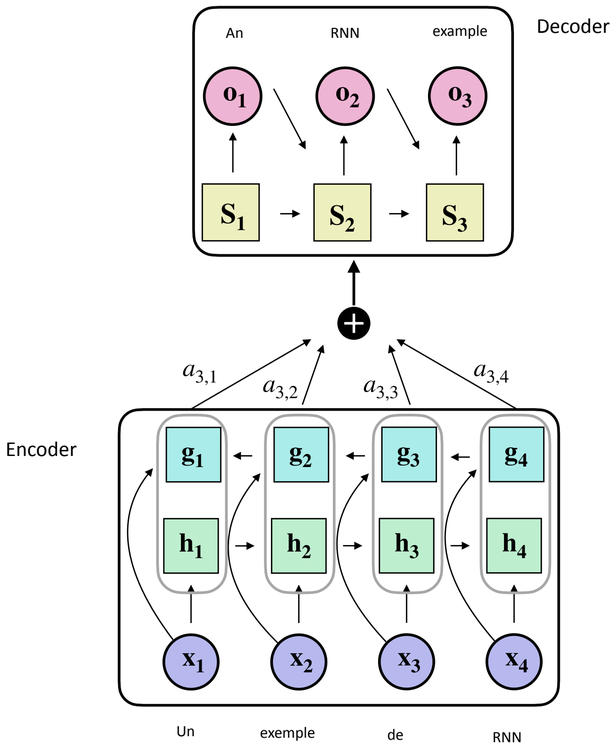


Advantages:

- *No more bottleneck*
- The decoder can consider different representations (information)
- The latent representation is now proportional to the length of the sequence.
- Shortcuts between the encoder and decoder
- Can model longer dependencies



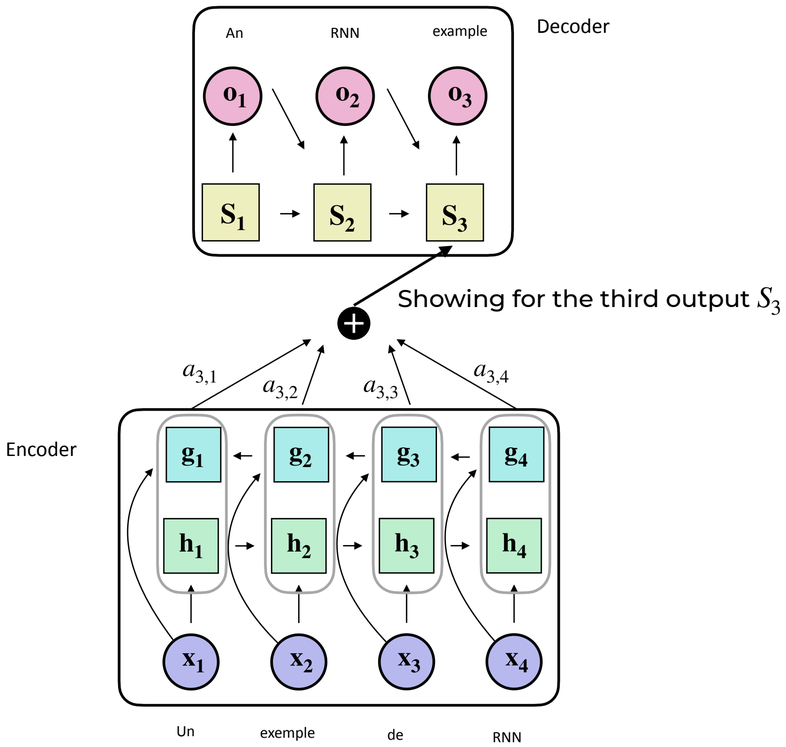
Mathematical details:

$$\mathbb{P}(\mathbf{o_t} \mid \mathbf{o_{1:t-1}}, \mathbf{x_{1:T}}) = f(\mathbf{s_t}, \mathbf{c_t}),$$

where

$$\mathbf{c_t} = \sum_{\mathbf{j=1}}^{\mathbf{T_x}} \mathbf{a_{t,j}} \cdot [\mathbf{g_j}, \mathbf{h_j}]$$

Attention
- Timestep t (output)
- Hidden representation j (input)



Mathematical details:

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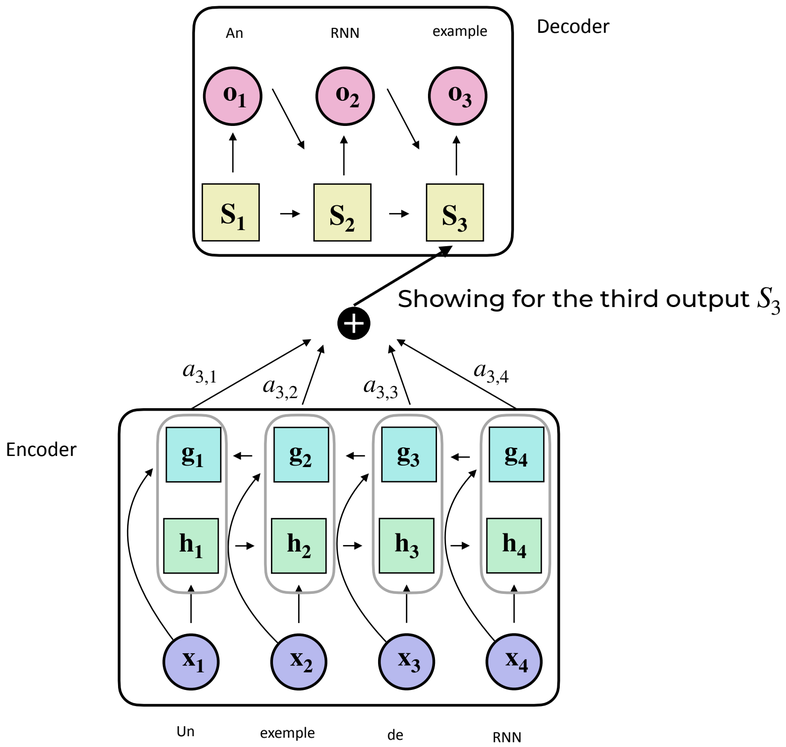

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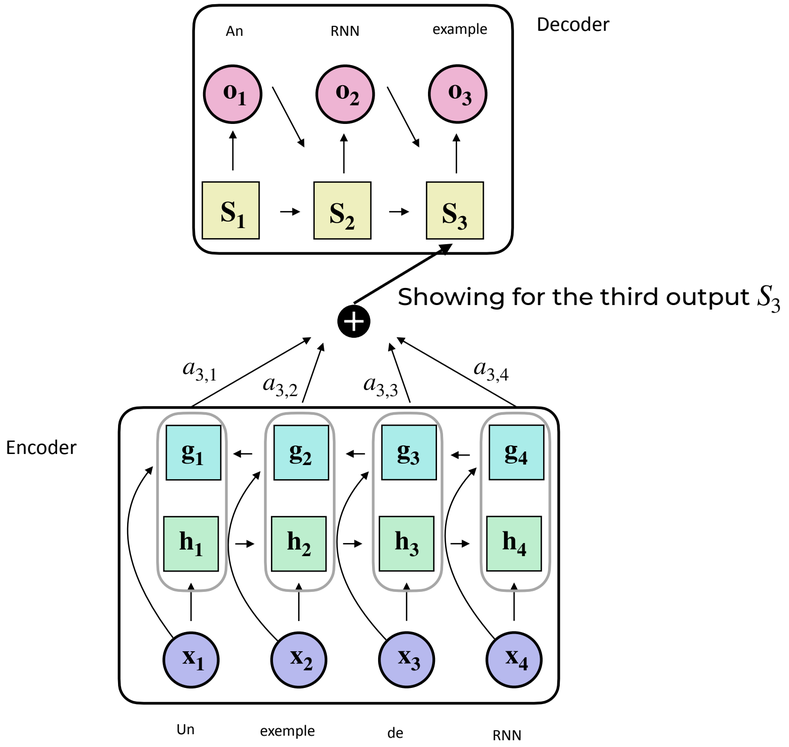
Function models the similarity between input and output representations



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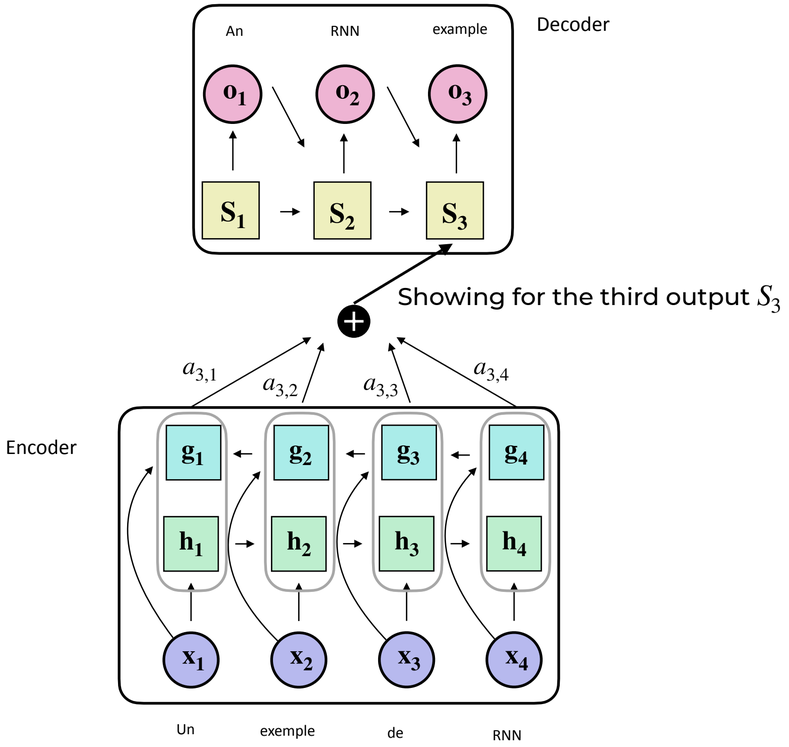

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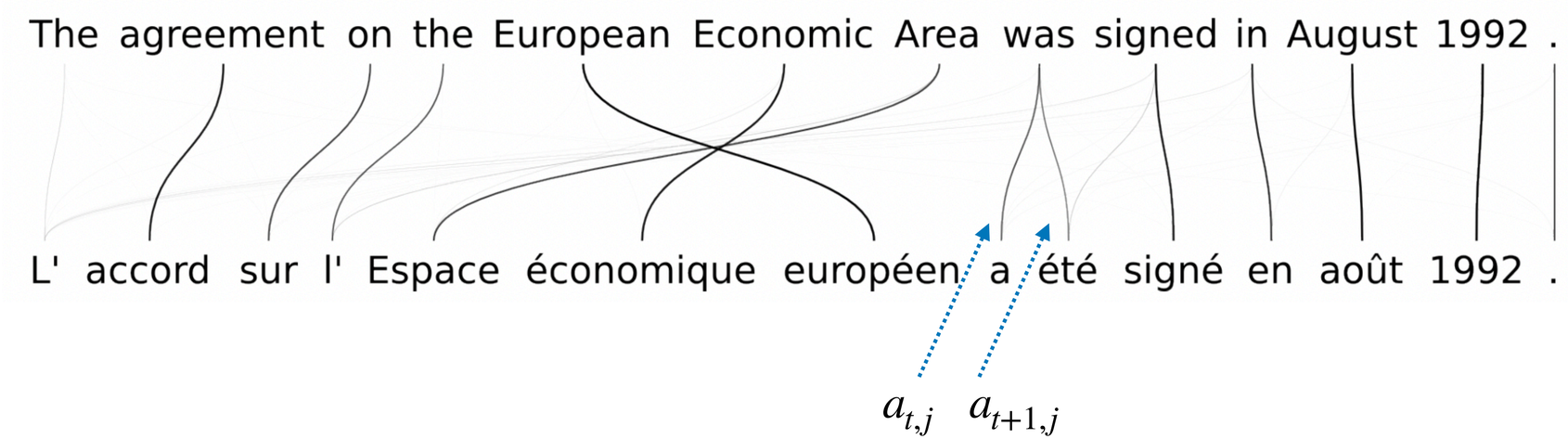
Visualizing attention

Translation task (EN -> FR)



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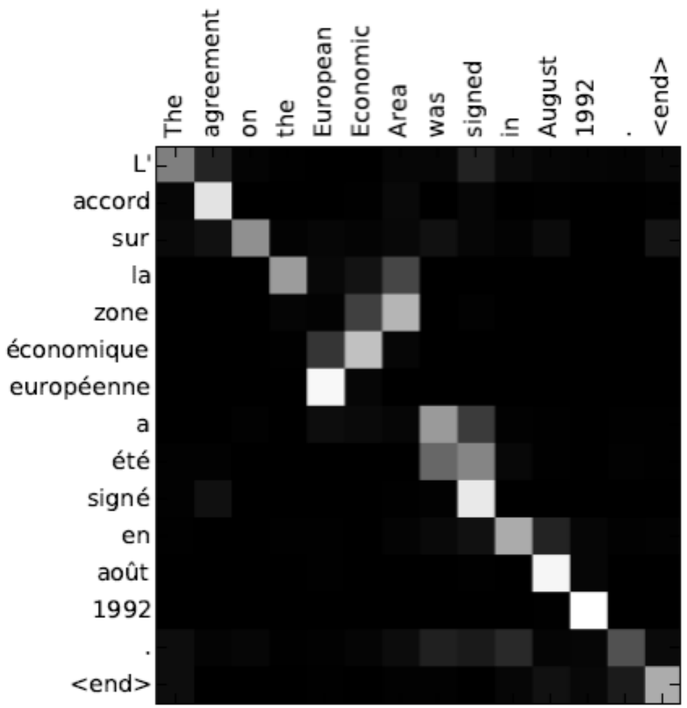

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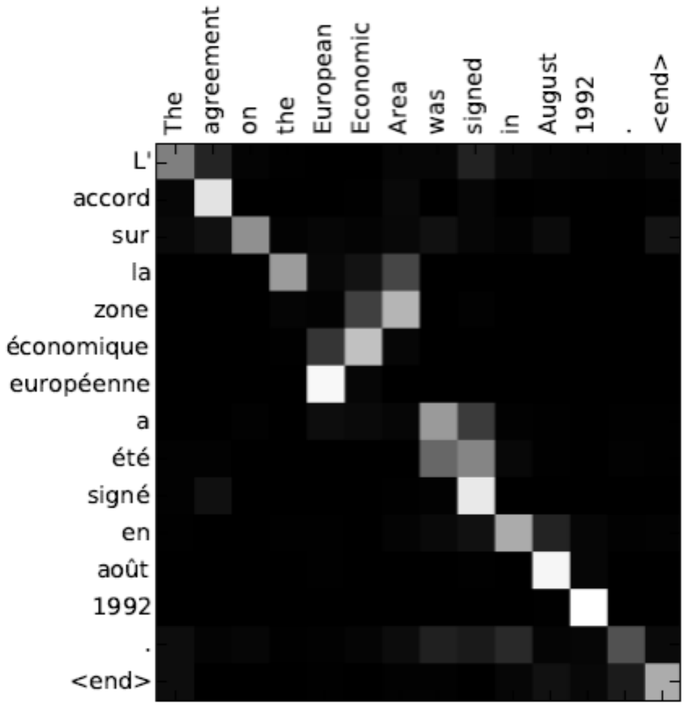
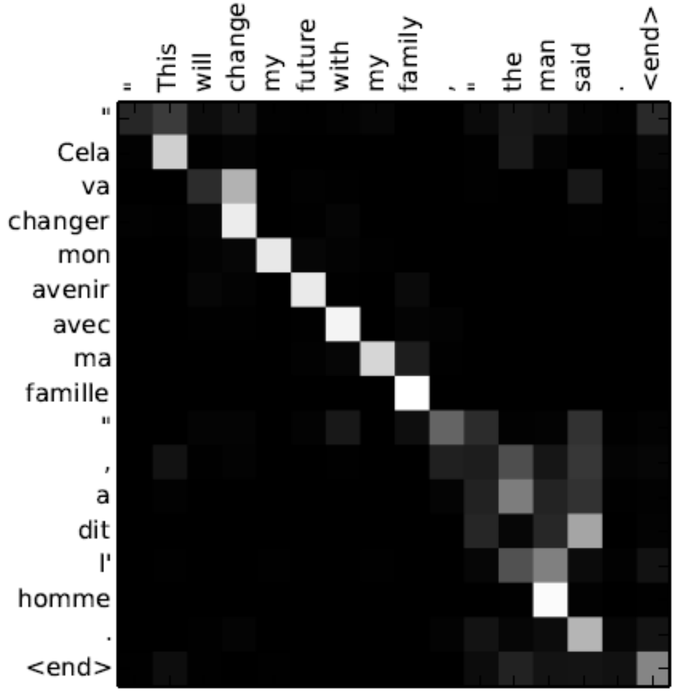
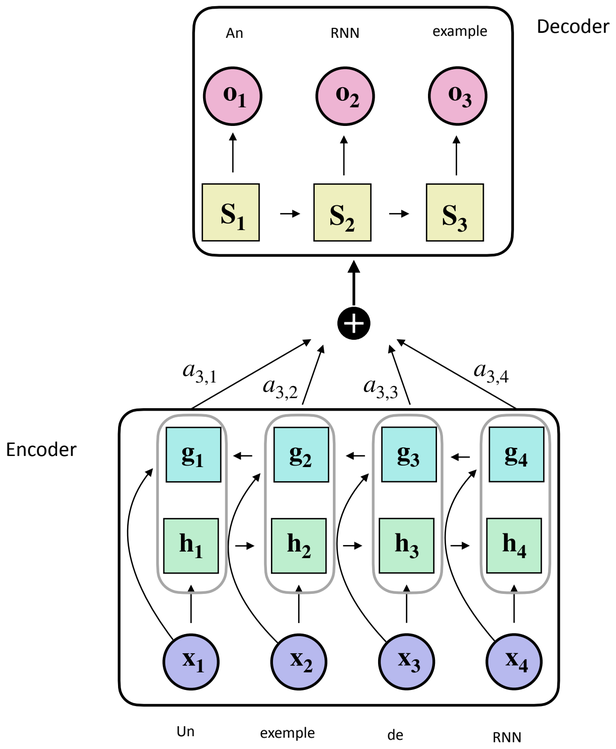




Soft Attention summary

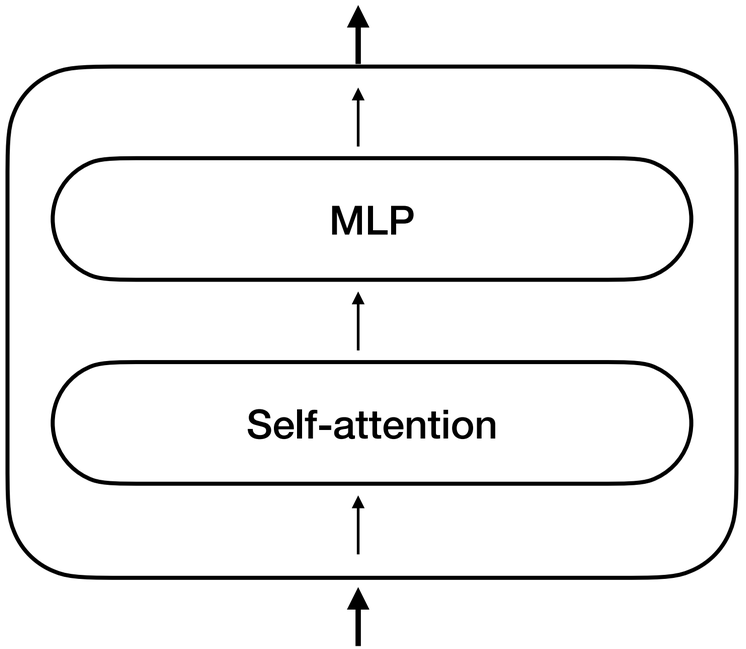
- **Dynamically weights the different contexts.**
- **Empirically: Works for length of up to ~100 time steps**

Toward Transformers



- A mix of sequential (h_i, g_j, S_t) and parallel (attention) processing
  - Expensive computationally
- Could a parallel architecture model sequential data?

Transformer Block



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Word embedding

- Words are categorical and can be encoded using a 1-of-K encoding (i.e., dummies)
- This fails to capture the semantics of words between words (e.g., foot/feet/toe)
- In RNNs/Transformers/etc. words are represented using a vector (of size D)
  - The representation is learned
  - Smaller-dimensional representation (D << K)

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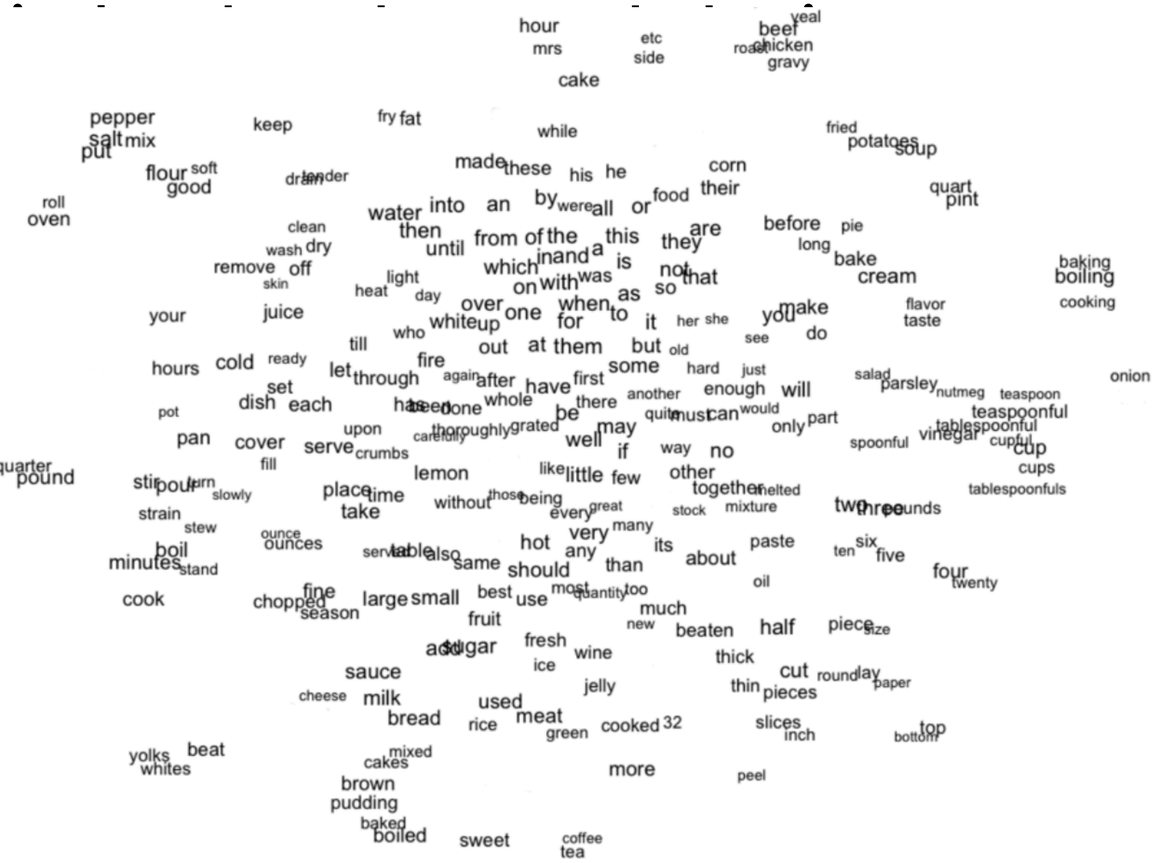
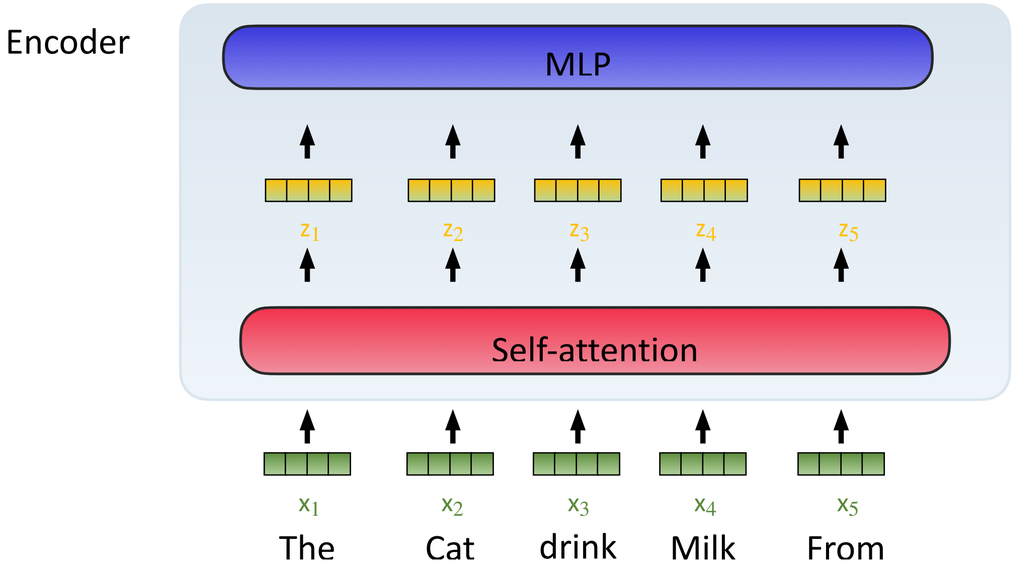


Self-attention

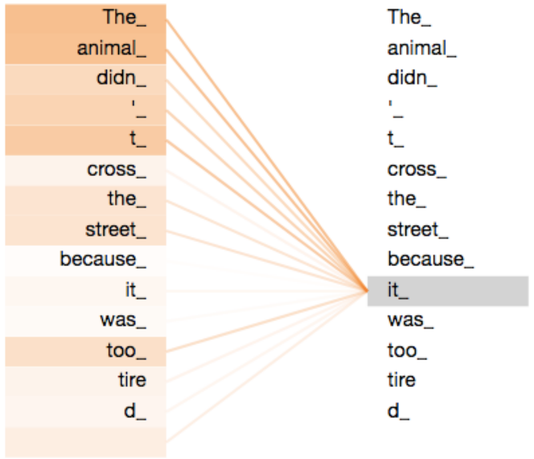


Self-attention

- The representation of each word (token) will be a combination of the representation of other words

Example:

'The animal didn't cross the street because it was too tired



- The procedure is unsupervised (*self*)

Self-Attention

Mathematical Details

(Recall) Soft attention

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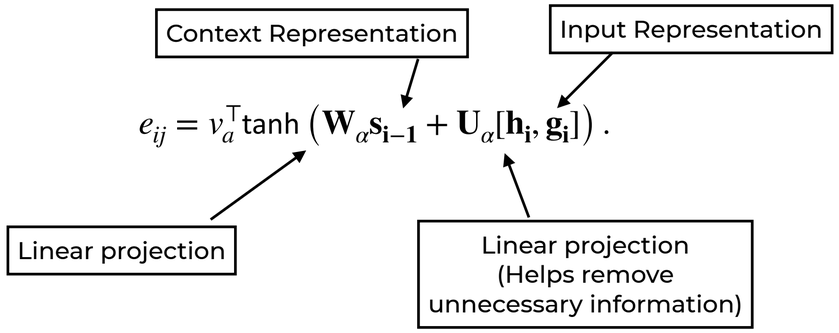

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Context Representation

Input Representation

$$e_{ij} = v_a^\top \tanh\left(\mathbf{W}_\alpha \mathbf{s_{i-1}} + \mathbf{U}_\alpha[\mathbf{h_i}, \mathbf{g_i}]\right).$$

Linear projection

Linear projection
(Helps remove
unnecessary information)

Self attention

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Calculate its output

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x_i: input representation of word i (NxD)
z_j: output representation of word j (1xD)

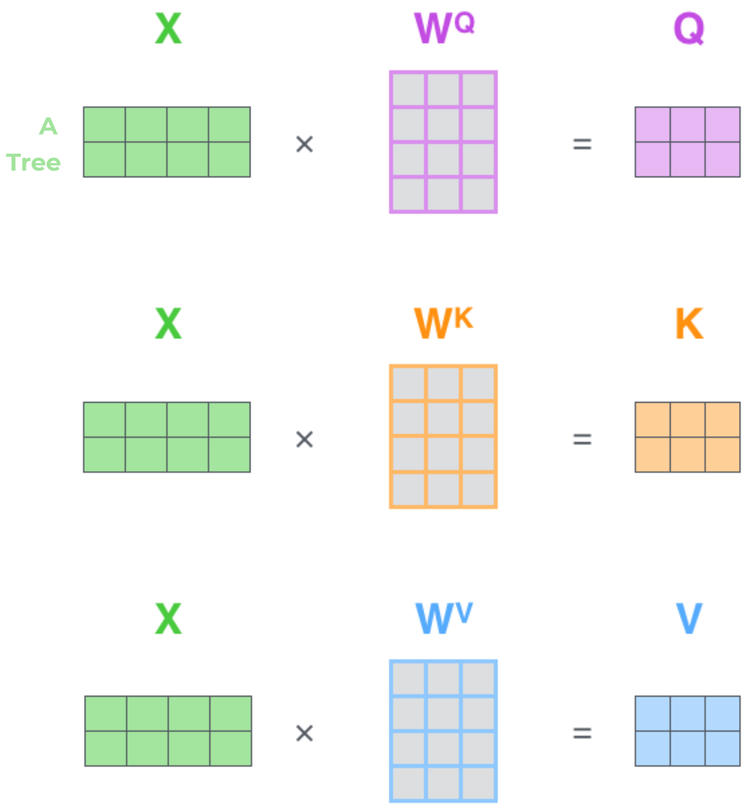
Calculate its output

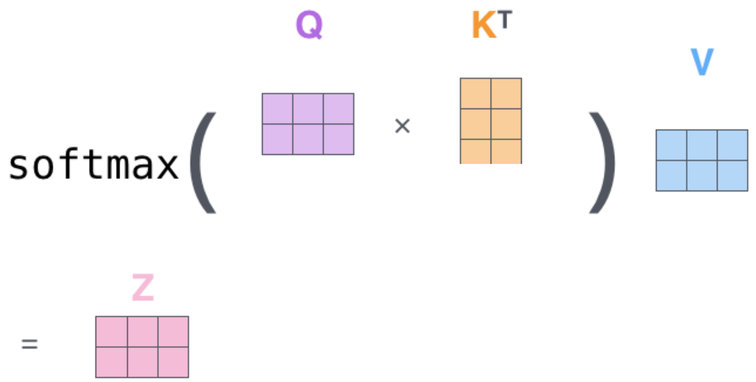
Often referred to as “Key-Query-Value” attention

$$\mathbf{z_j} = \underbrace{(\mathbf{x_i W^v})}_{\text{Value}}\ \mathbf{softmax}(\underbrace{(\mathbf{x_i W^k})}_{\text{Key}}\ \underbrace{(\mathbf{x_j W^q})}_{\text{Query}})$$

Self-Attention

Visual representation
N=2, D=4





*: in practice the value of attention pre-softmax (QK^T) is often normalized by $\sqrt{D}$ for optimisation stability

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

Multi-Head Self-Attention (MHSA)

- Attention captures the similarity between two words
- One may wish to capture several different similarities (e.g., whale and humans are both mammals, whales and sharks live in the water)
- You can learn the parameters for multiple attention mechanisms. Each mechanism is called an attention head:

$$\mathbf{x'_j} = [\mathbf{z_j^1 z_j^2 \cdots z_j^H}]\mathbf{W^0}$$

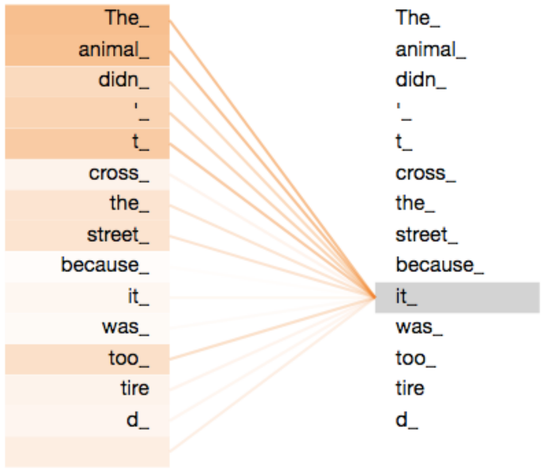
x'_j : the representation of word j after self-attention (D)
z_j^h: the representation of word j from attention head h (D')
H: the number of heads
W^0 : weight matrix (D'H x D)

Multi-Head Self-Attention (MHSA)

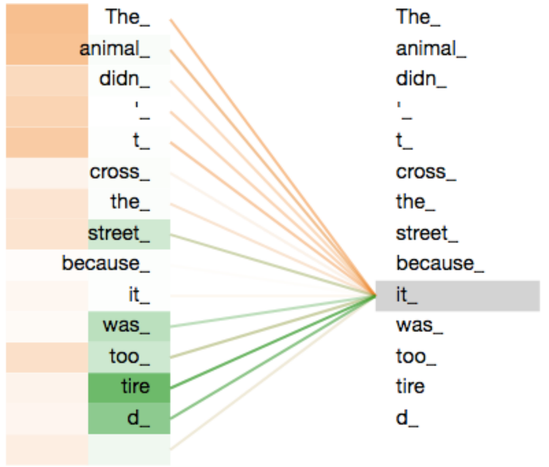
Example:

'The animal didn't cross the street because it was too tired'

One head



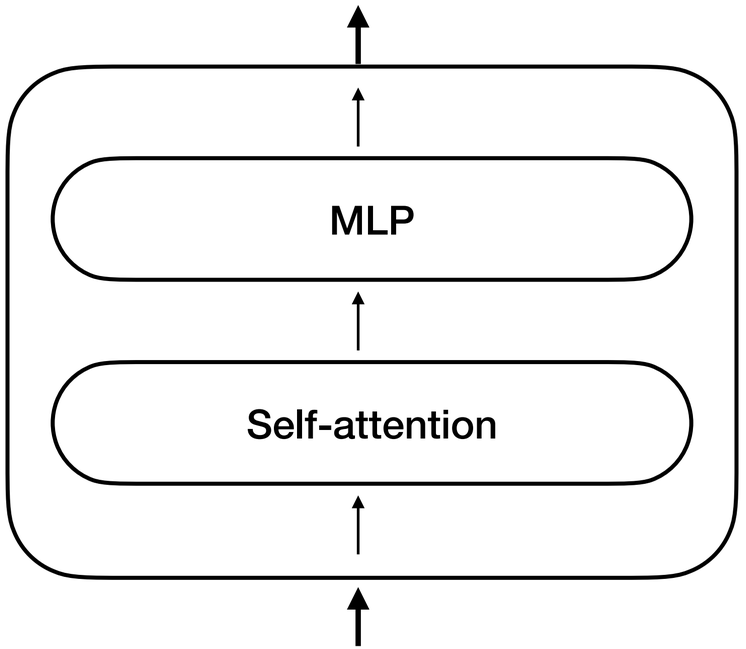
Two heads



Demo

- https://poloclub.github.io/transformer-explainer/
  - Shows attention
  - Sub-word tokens

Transformer Block



Operates across features (D)

(Mostly) Operates across tokens (N)

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Transformers… transform?

- Transformer blocks rely on attention heads followed by an MLP
- How can we use them for language tasks (e.g., translation)?
- Transformer blocks can be combined and refined
  - Transformer blocks can be used as *encoders* & *decoders*
  - For decoding, a few changes are required

A few other characteristics

- Word embeddings
  - Words are categorical and can be encoded using a 1-of-K encoding (i.e., dummies)
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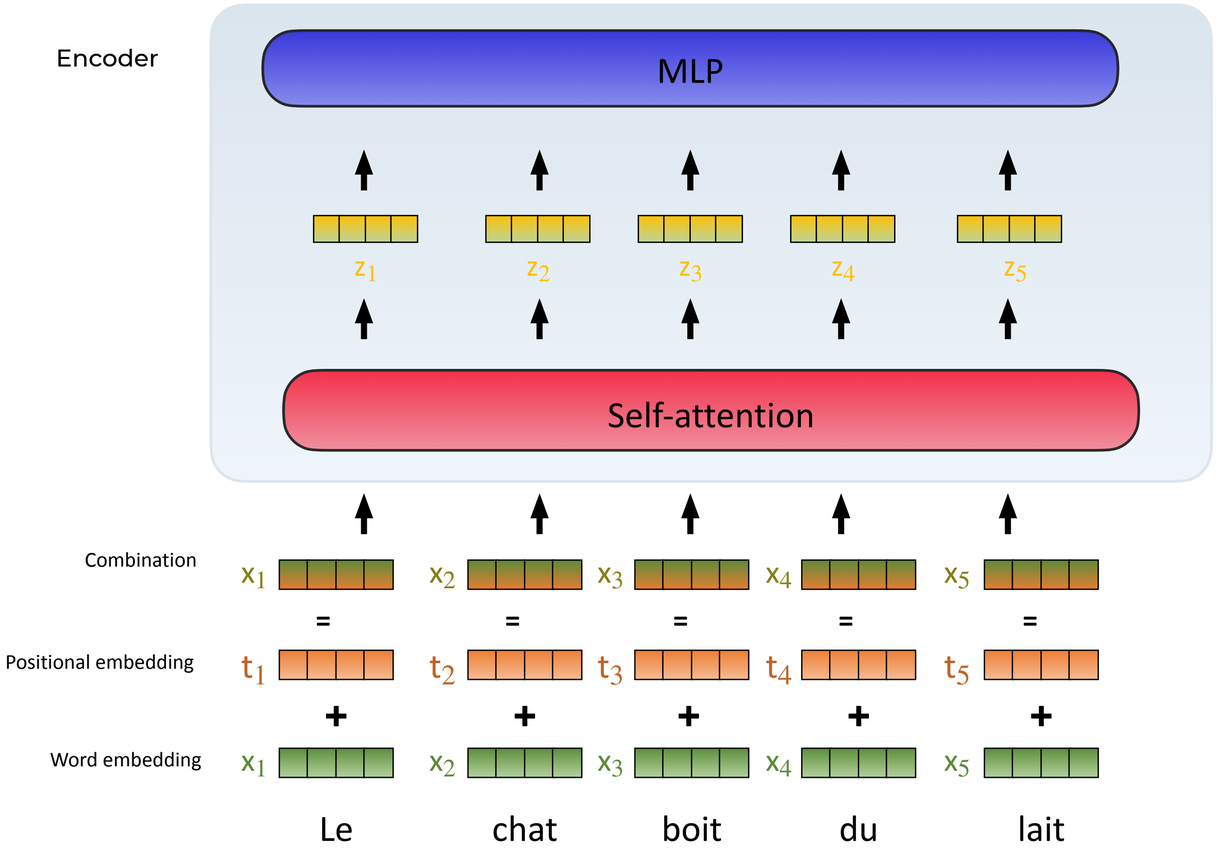
  - In RNNs/Transformers/etc. words are represented using a vector (of size D)

A few other characteristics

- Positional embedding
  - Attention looses the position of words into account
    - In many tasks, position is essential
      - “cat eats plant” is different from “plant eats cat”
  - As a remedy, transformers also learn positional representations
    - Vectors that are specific to the position (can be absolute or relative)

Word + Positional embeddings



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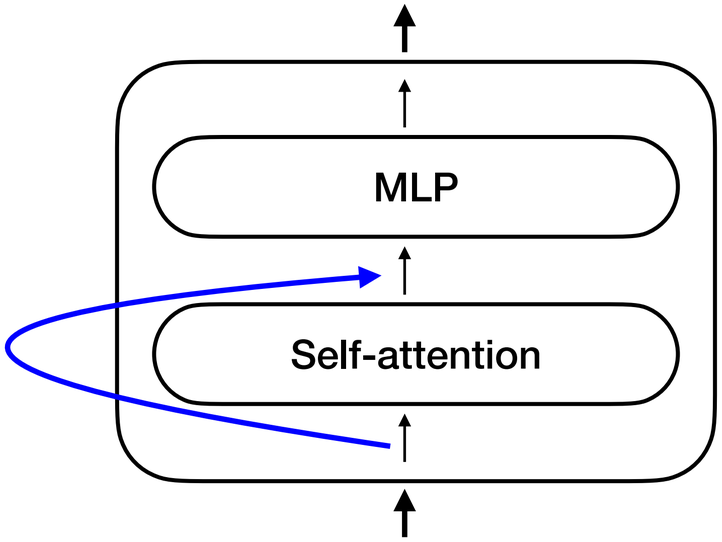
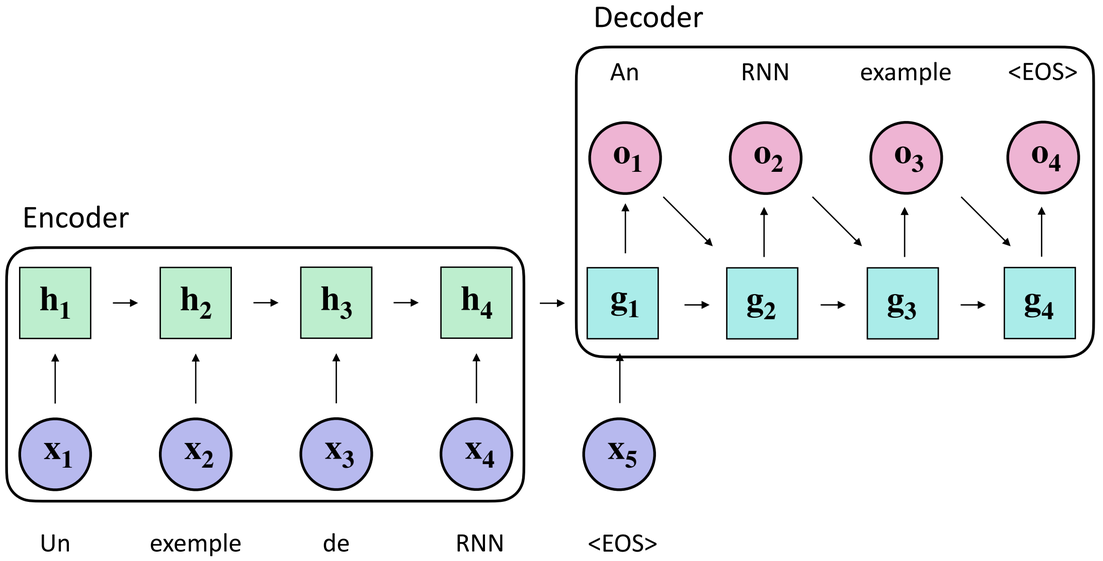
A few other characteristics

- Normalization
  - Layer normalization is often applied. It helps to learn by normalizing each token's dimensions to have 0-mean and 1 standard deviation.
- Residual connections
  - $z_i = \text{Self-Attention}(X) + x_i$
  - Biases learned functions to be "simple", helps to learn
  - Can be used for self-attention & MLP



What about decoding?



What about decoding?

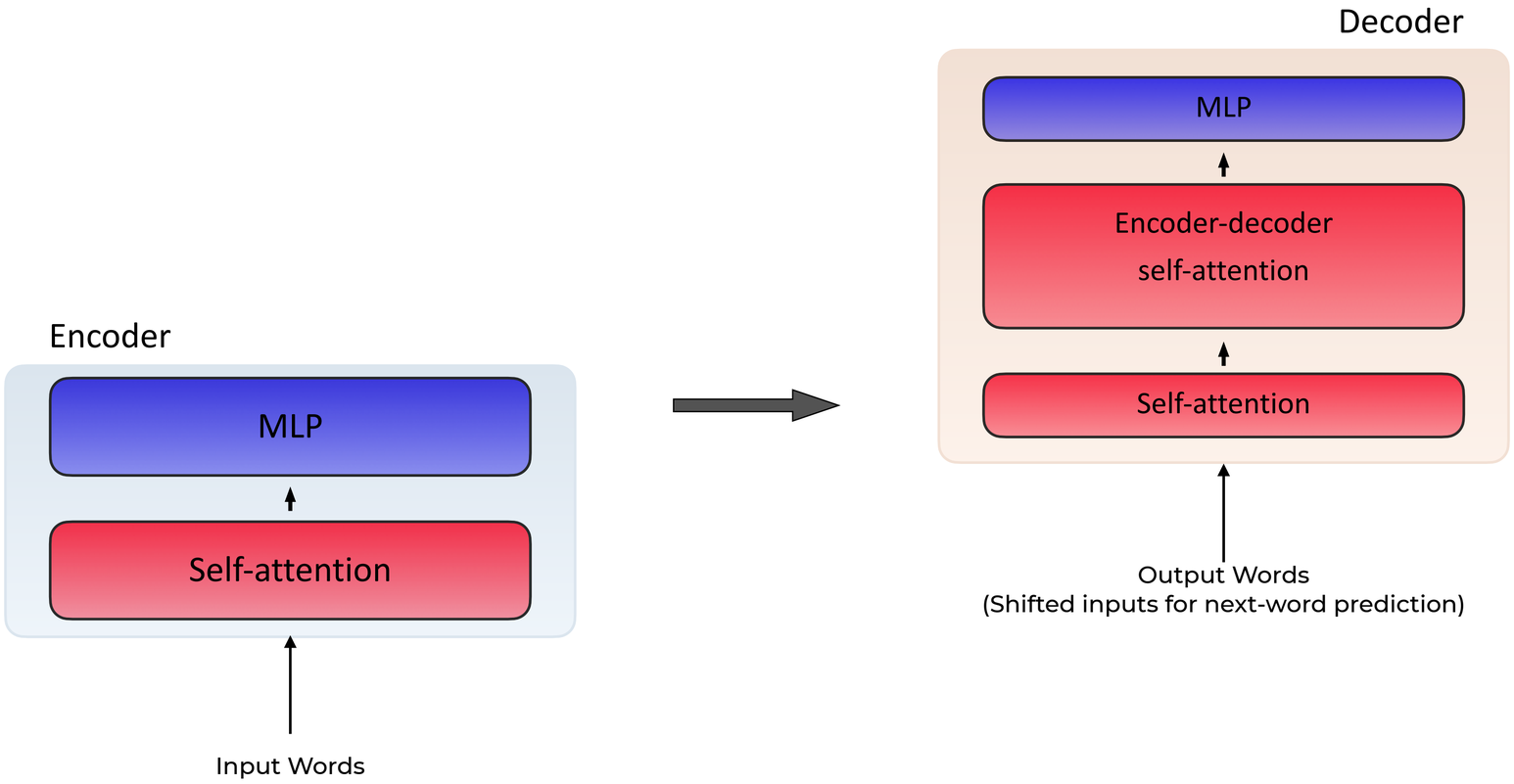
- Transformers transform word representations
  - Decoding requires using these words representations to obtain the following word
  - Add a “softmax”-layer at the end:

$$P(\mathbf{o_n} \mid \mathbf{o_{1:n-1}}) = \frac{\exp(\mathbf{g_w^\top x_{n-1}})}{\sum_{\mathbf{w}}^{\mathbf{W}} \exp(\mathbf{g_w^\top x_{n-1}})}$$

g_w: parameters
W: number of words in the vocabulary

  - You can only attend to previous words
    - Attention matrix is constrained to be (upper) triangular

Encoder-Decoder Transformer



Putting it all together

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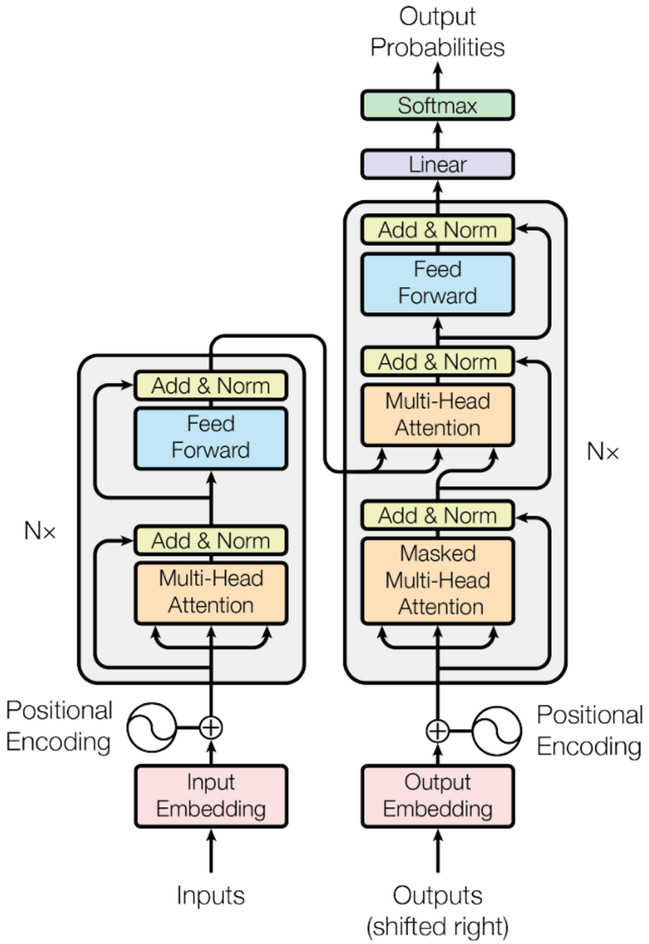
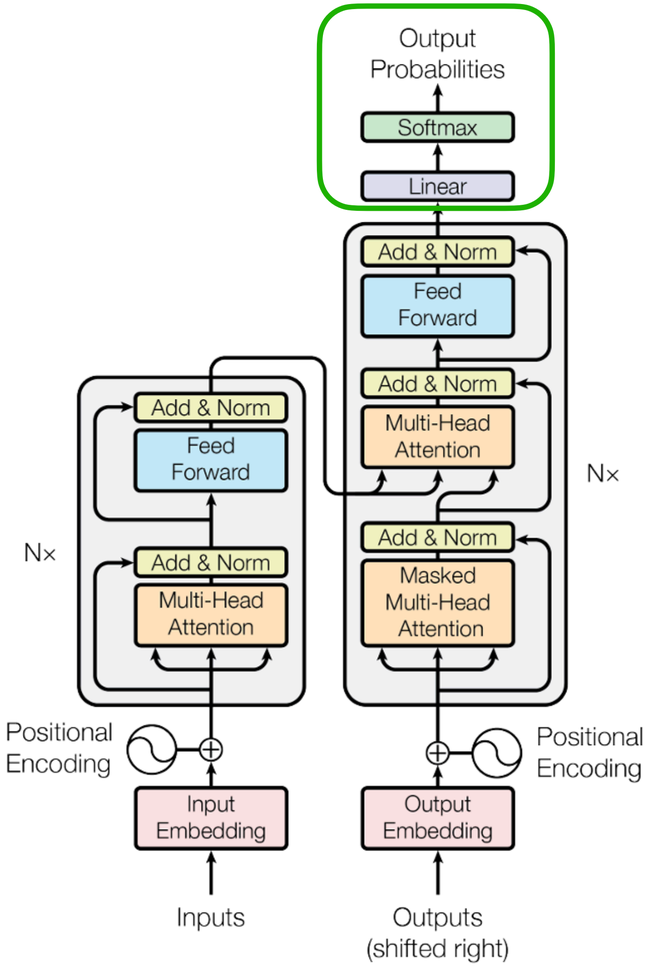


- Self-Attention
- Positional embedding
- Encoder
- Decoder
- Softmax-layer
- Multiple transformer blocks (Nx)

Putting it all together



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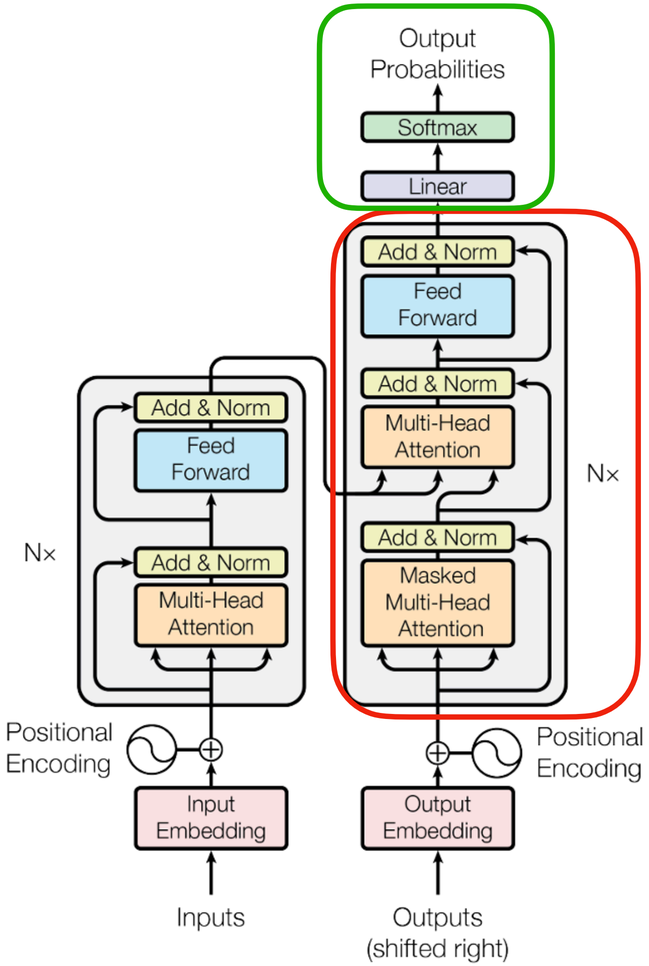

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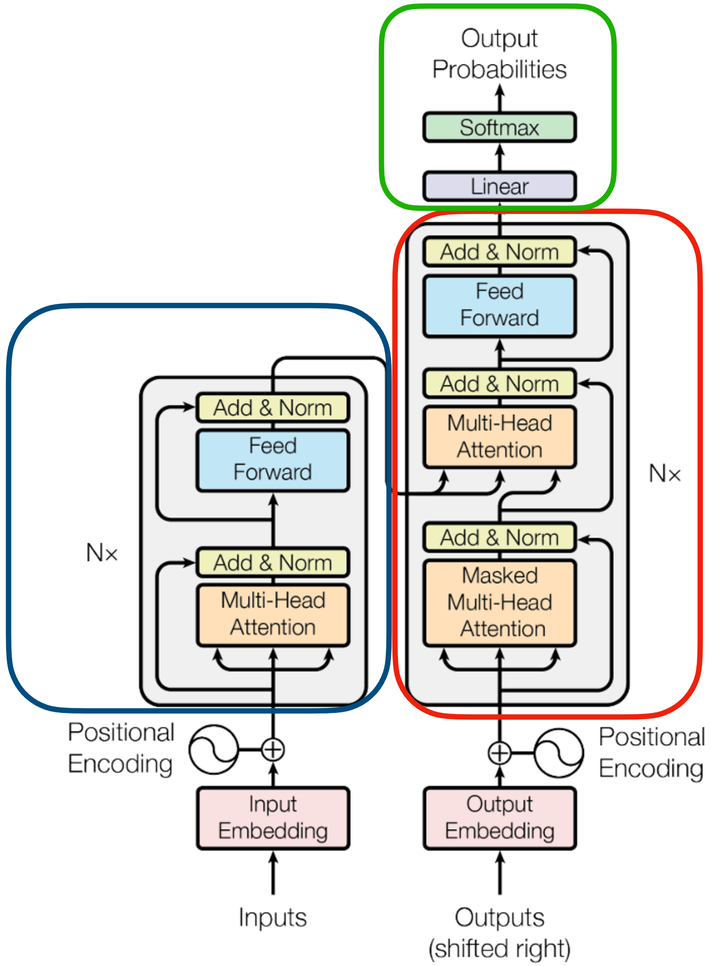
Putting it all together



- Self-Attention
- Positional embedding
- Encoder
- Decoder
- Softmax-layer
- Multiple transformer blocks (Nx)

Objective

- Often in two (or more) stages:
  - **First stage**
    - Next-word prediction
    - Random-word prediction (mask some words in the input/output)
    - Other tasks:
      - Next-sentence prediction
  - **Second stage**
    - Preference and/or downstream task fine-tuning

One of many transformers

- Partial list: https://huggingface.co/docs/transformers/en/index
- Encoder-only models:
  - BERT (RoBERTa), ALBERT
- Encoder-Decoder models:
  - BART
- Decoder-only models:
  - Generative pre-trained transformer (GPT), BLOOM (for code), Llama
- *Most of the above transformers refer to a system that was trained not only an architecture. Many of these models now have tens of billions of parameters (Llama-7B -> 7 billion parameters)
- Also used for image modelling, audio, multi-modalities, etc.

Summary

- Self-attention is the key ingredient
  - Efficient and provides good results
  - Recent LLMs can attend to very long contexts (some refinements of attention)
  - Enables training transformers on much larger-scale datasets (internet size)
- Transformers has become the standard model often surpassing the performance of RNNs/CNNs when trained on enough data

References

- https://jalammar.github.io/illustrated-transformer/
- An Introduction to Transformers, Richard E. Turner, 2024, https://arxiv.org/abs/2304.10557
- Attention Is All You Need, Vaswani et al., 2017, http://arxiv.org/abs/1706.03762