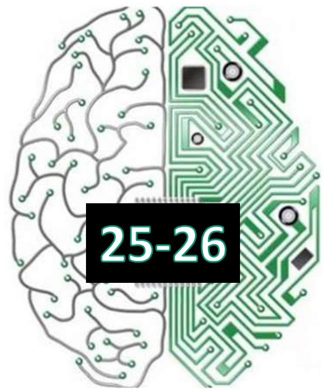
Open Elective Course [OE]
Course Code: CSO507
Winter 2023-24

Lecture#



Deep Learning

Unit-5: Sequence Modeling with Recurrent Neural Network (RNN) Part-VI&VII, Attention Mechanism, Transformer (Part-I)

Course Instructor:
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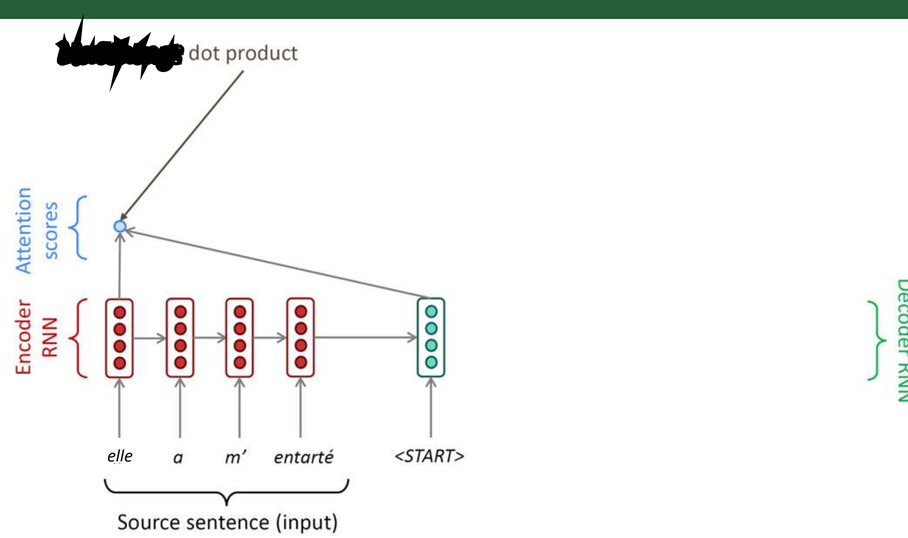
Indian Institute of Technology (Indian School of Mines) Dhanbad, Jharkhand 826004, India

Attention Mechanism



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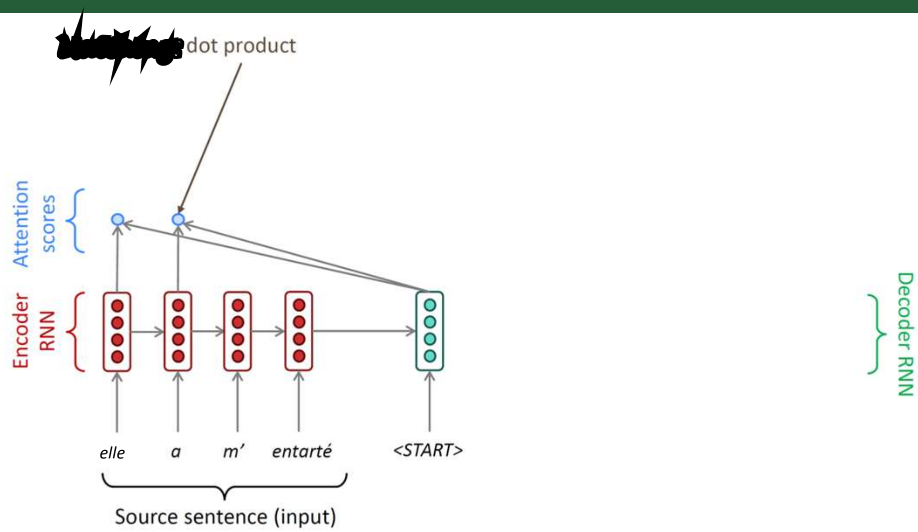

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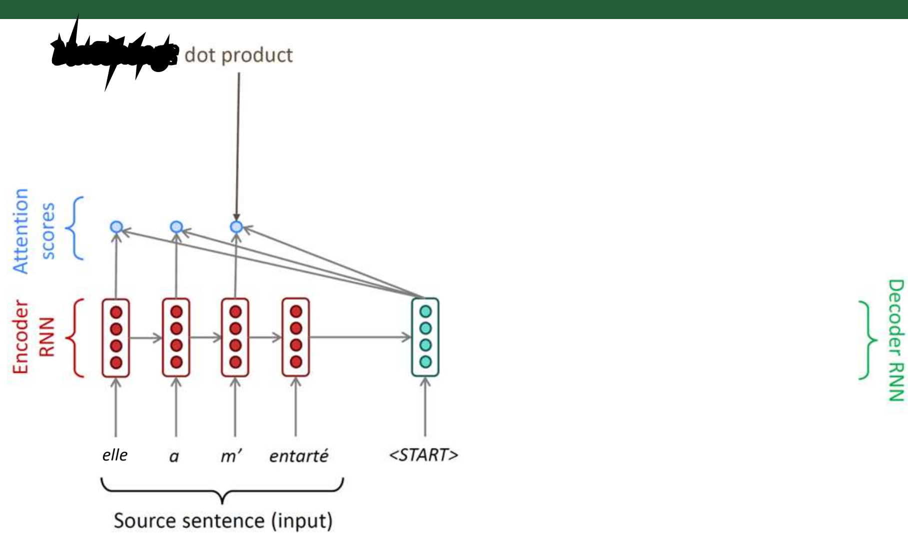
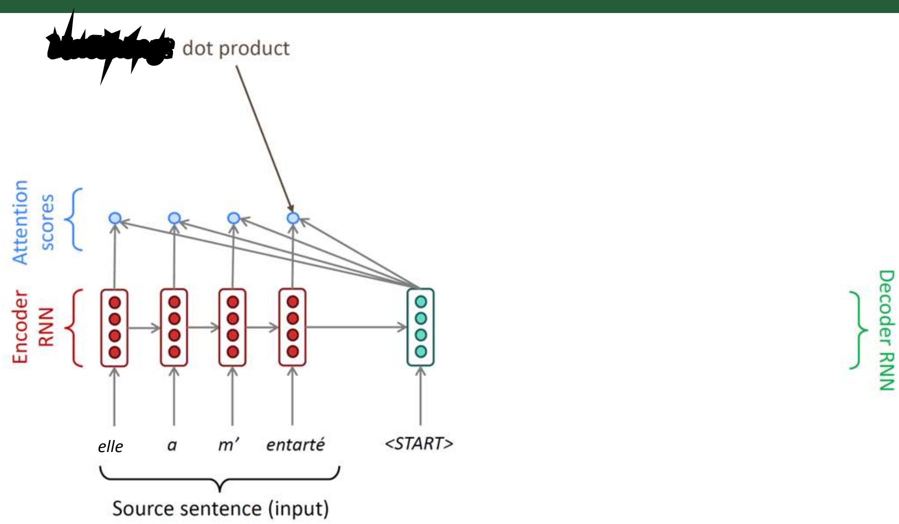


Attention Mechanism



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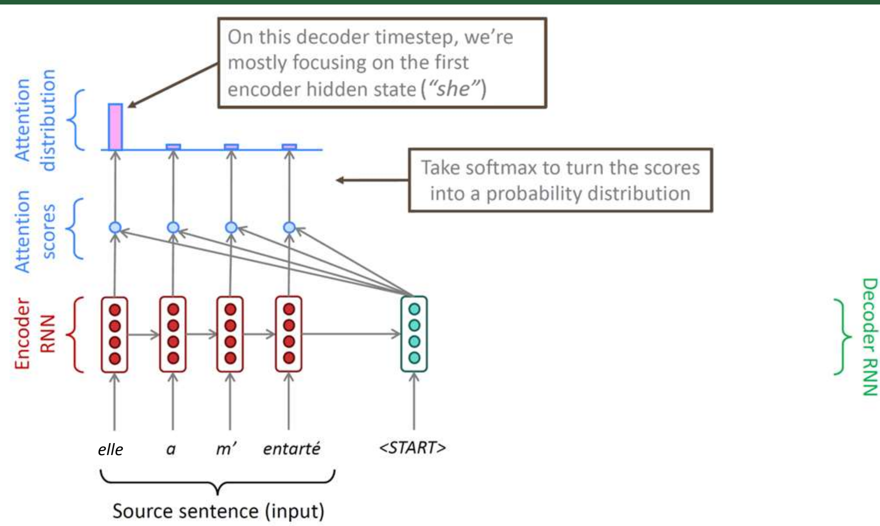
Attention Mechanism



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Attention Mechanism

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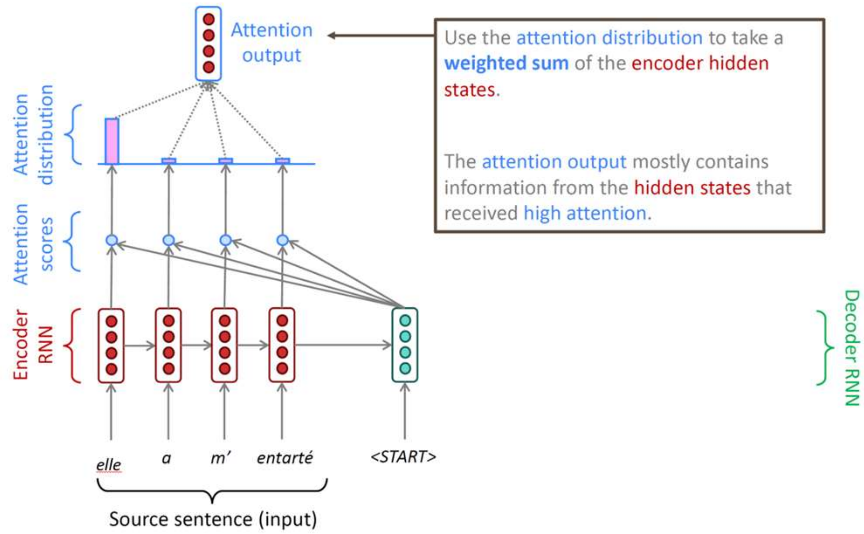

Use the attention distribution to take a **weighted sum** of the encoder hidden states.

The attention output mostly contains information from the hidden states that received high attention.

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Attention Mechanism

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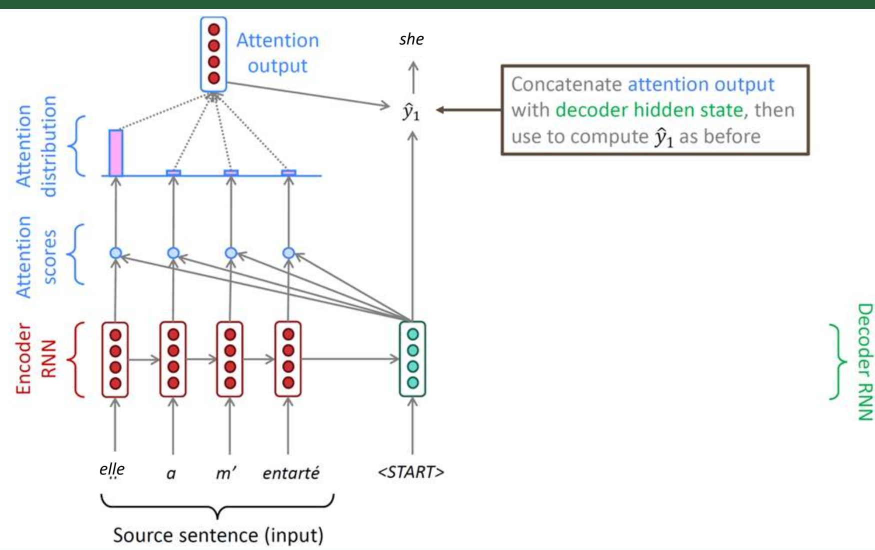

Concatenate attention output with decoder hidden state, then use to compute $\hat{y}_1$ as before

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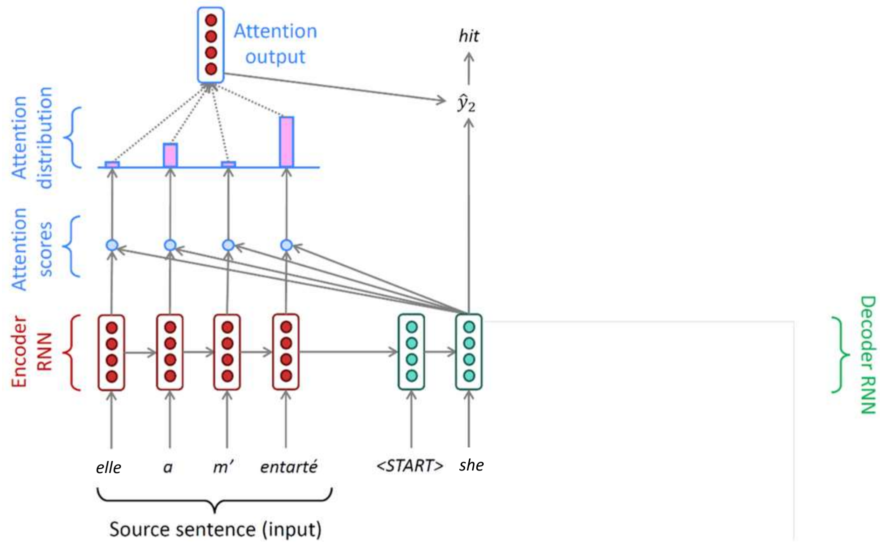
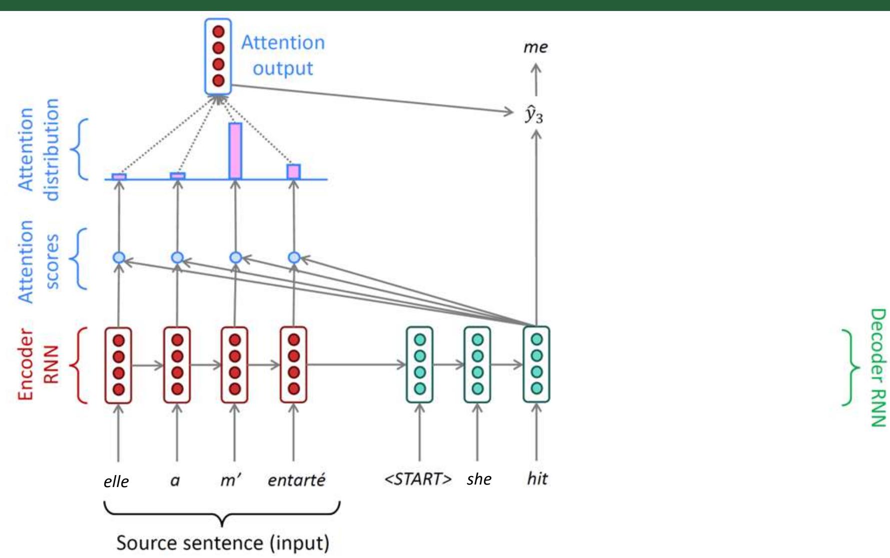
Attention Mechanism



Attention Mechanism



Attention Mechanism

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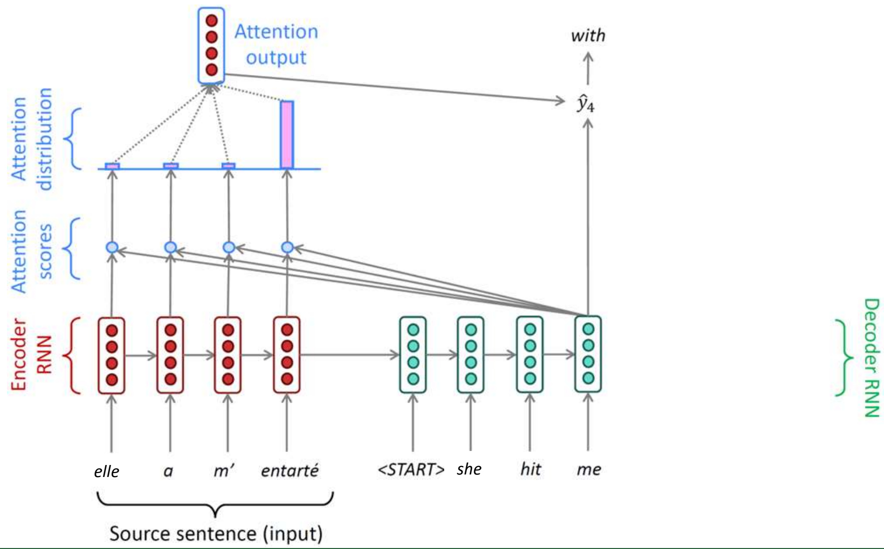

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Attention Mechanism

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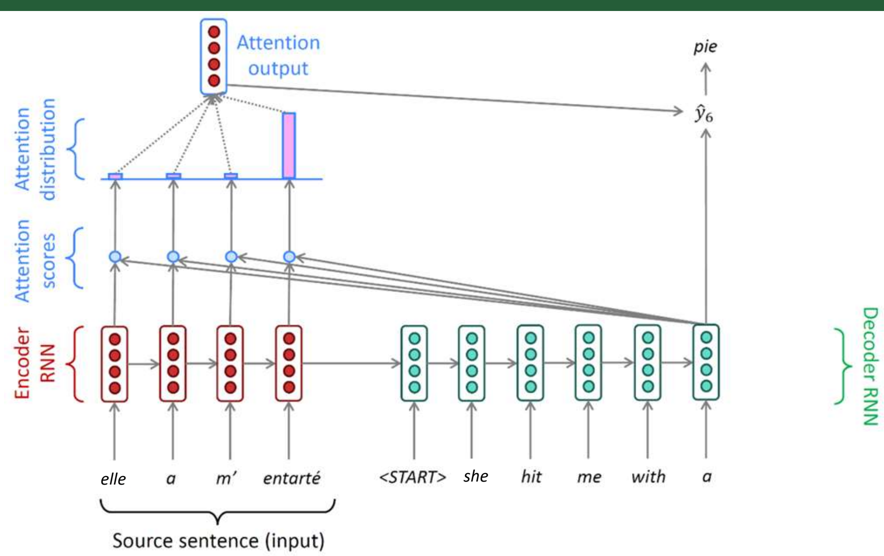

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Attention Mechanism

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- Input sequence X, encoder f_{enc}, and decoder f_{dec}
- $f_{enc}\,(X)$ produces hidden states $h_1^{enc}, h_2^{enc}, \ldots, h_N^{enc}$
- On time step t, we have decoder hidden state h_t
- Compute attention score $\alpha_i = h_t^T h_i^{enc}$ //dot product attention
- Compute attention distribution $\hat{\alpha}_i = P_{att}(X_i) = softmax(\alpha_i)$
- Attention output: $h_{att}^{enc} = \sum_i \hat{\alpha}_i h_i^{enc}$
- $Y_t \sim g(h_t, h_{att}^{enc}; \theta)$
  - Sample an output using both

Attention Mechanism

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- Attention solves the bottleneck problem
  - Attention allows decoder to look directly at source; bypass bottleneck
- Attention helps with vanishing gradient problem
  - Provides shortcut to faraway states
- Attention provides some interpretability
  - By inspecting attention distribution, we can see what the decoder was focusing on

Self Attention

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“I am going to the bank to deposit the cheque”
“The boat went down the river bank”

The vector representation used as input to RNN cannot differentiate context

Problems with RNNs: **Sequential computation inhibits parallelization**

Self Attention

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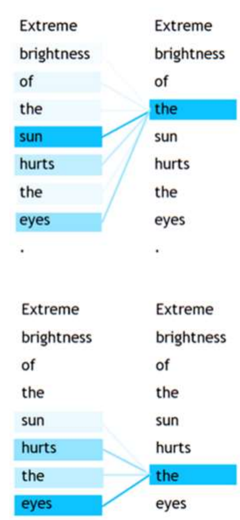
- **Self attention**
  - Re-express representation in terms of the context the word occurs in

  - Construct Probability distribution of importance - Dot product and normalization with only the input

  - Re-express word vectors weighted by the probabilities as weights



Self Attention

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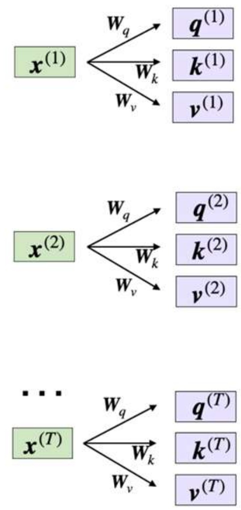
- **Defining the Weight Matrices**
  - Three matrices serve to project the inputs into ***query, key***, and ***value*** components



- Query sequence: $\mathbf{q}^{(i)} = \mathbf{W}_q \mathbf{x}^{(i)}$ for $i \in [1, T]$
- Key sequence: $\mathbf{k}^{(i)} = \mathbf{W}_k \mathbf{x}^{(i)}$ for $i \in [1, T]$
- Value sequence: $\mathbf{v}^{(i)} = \mathbf{W}_v \mathbf{x}^{(i)}$ for $i \in [1, T]$

Self Attention

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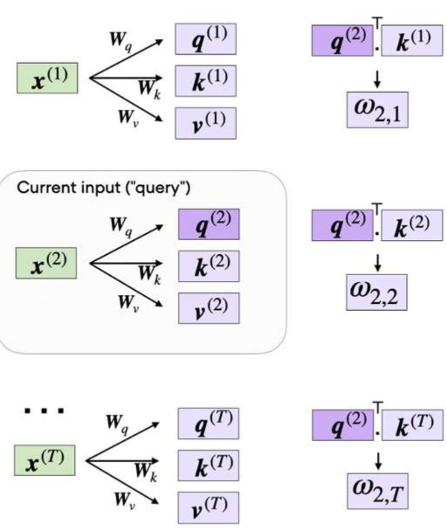
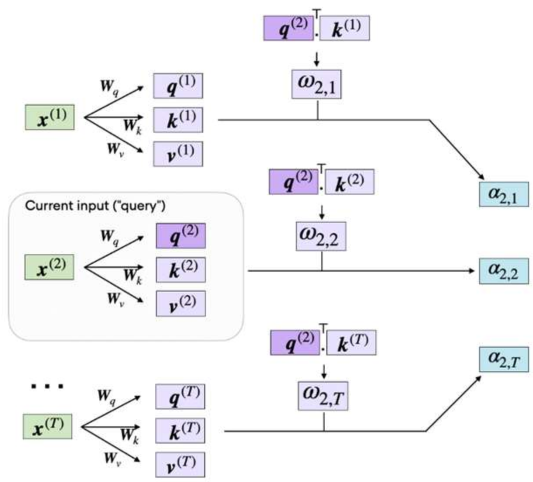
- **Computing the Unnormalized Attention Weights**



Self Attention

- **Computing the Attention Scores**

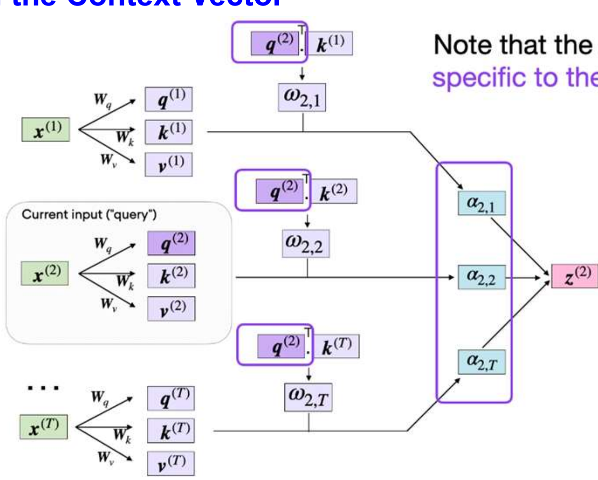


where $\alpha_{2,i} = \text{softmax}\left(\frac{\omega_{2,i}}{\sqrt{d_k}}\right)$

Self Attention

- **Computing the Context Vector**

Note that the attention scores are specific to the current input token



where $z^{(2)} = \sum_{j=1}^{T} \boxed{\alpha_{2,j}}\, v^{(j)}$

Multi-Head Attention

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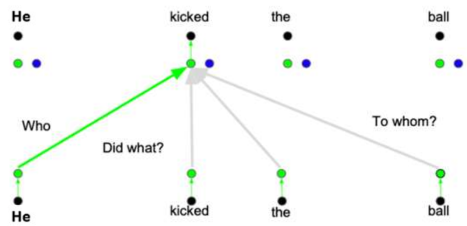
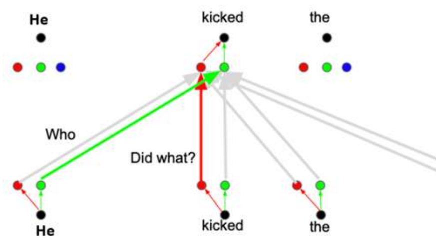
- All similarities do not encode the same aspects
- Multi-head Attention: Each notion of similarity is represented by an attention head

"He kicked the ball"



Aspect: "who"



Aspect: "did what"

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Multi-Head Attention

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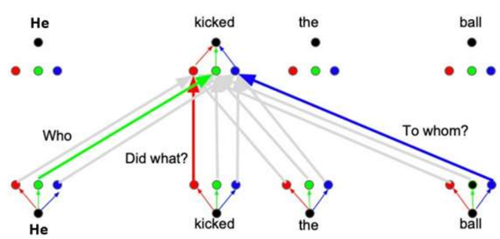
- All similarities do not encode the same aspects
- Multi-head Attention: Each notion of similarity is represented by an attention head

"He kicked the ball"



Aspect: "to whom"

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Multi-Head Attention

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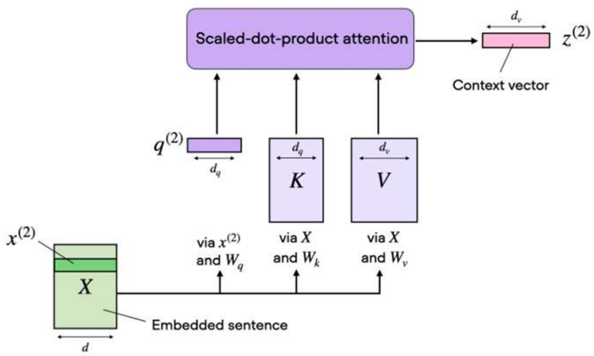

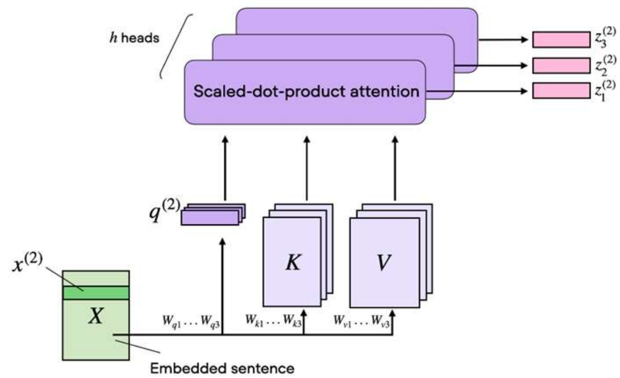

Self Attention: Permutation Invariant!

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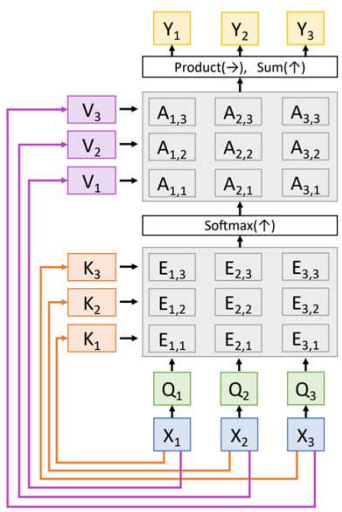
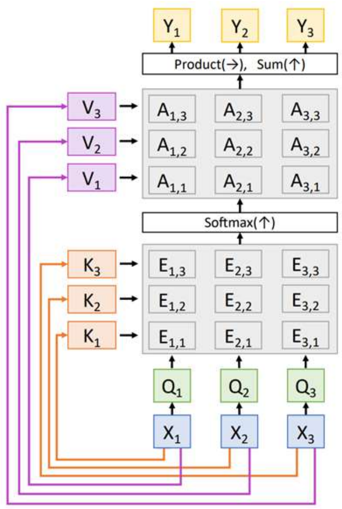
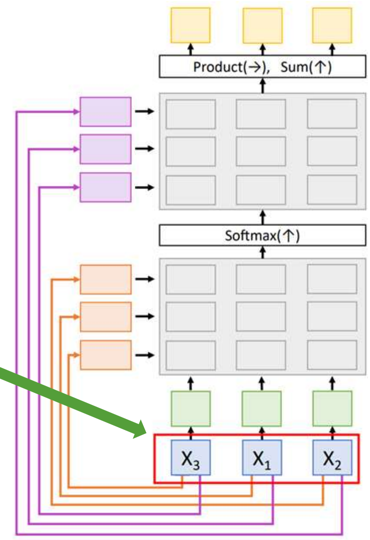


Self Attention: Permutation Invariant!



Consider permutating the input vectors:



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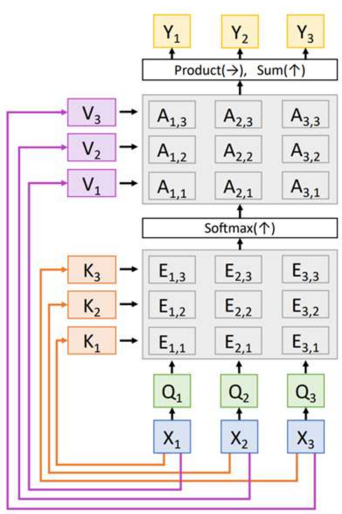

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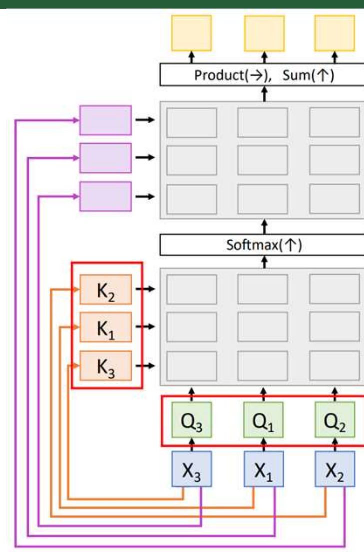

Self Attention: Permutation Invariant!

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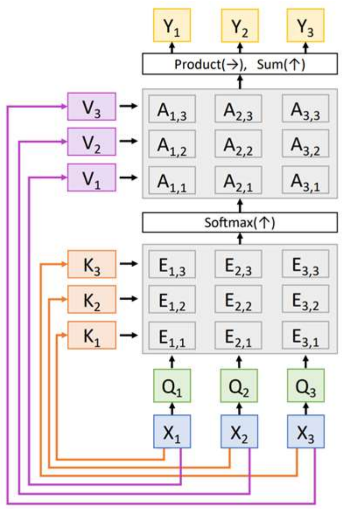

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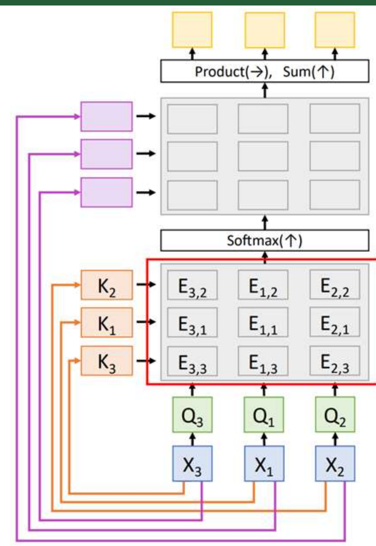

Self Attention: Permutation Invariant!

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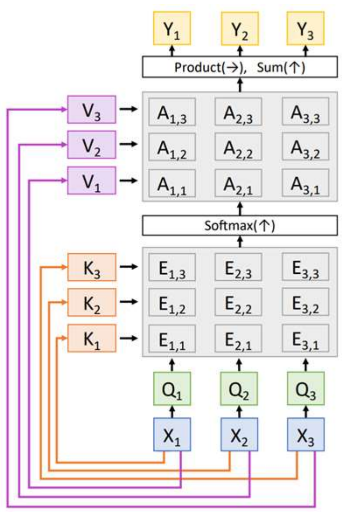

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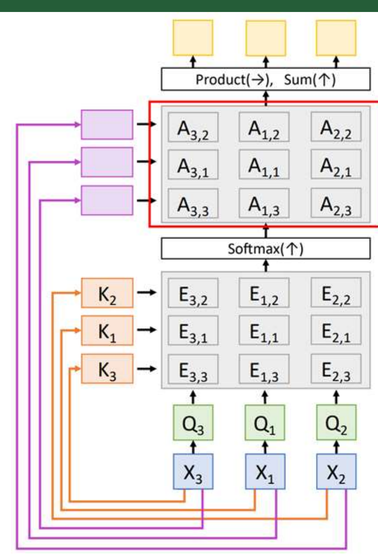

Self Attention: Permutation Invariant!

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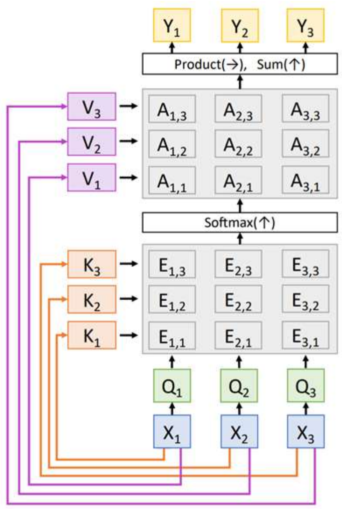

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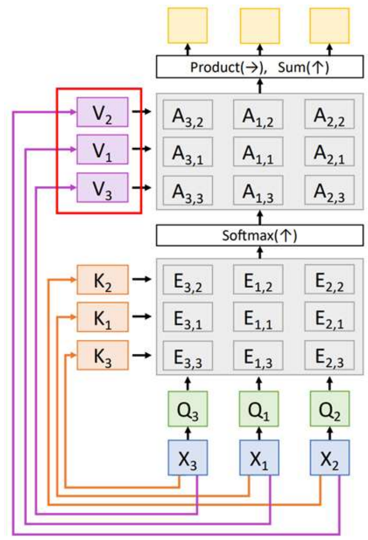

Self Attention: Permutation Invariant!

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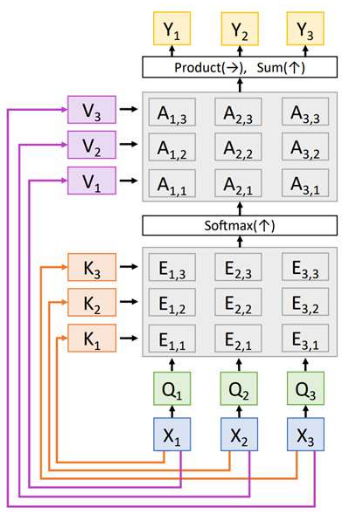
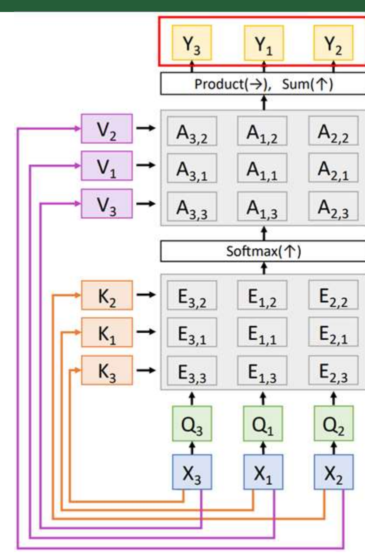


Consider permutating the input vectors:

The output is the same put permuted!



Self Attention: Permutation Invariant!

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- Self attention doesn't "know" the order of the vectors it is processing!
- But what if the ordering of the input vectors conveys information as well?
  - The position of a word in a sentence matters!

    "The man ate a fish" **"The fish ate a man""**

- Solution: **Positional Encoding**

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Self Attention: Permutation Invariant!

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- Add positional embeddings to input embeddings
  - Same dimension
  - Can be learned or fixed

Options for *pos*(.)

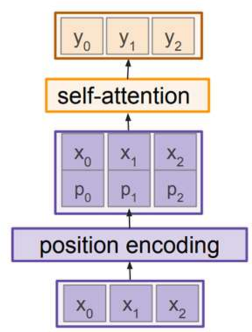
1. Learn a lookup table:
   - Learn parameters to use for *pos*(t) for t ε [0, T)
   - Lookup table contains T x d parameters.
2. Design a fixed function with the desiderata

Desiderata of *pos*(.) :

1. It should output a **unique** encoding for each time-step (word's position in a sentence)
2. **Distance** between any two time-steps should be consistent across sentences with different lengths.
3. Our model should generalize to **longer** sentences without any efforts. Its values should be bounded.
4. It must be **deterministic**.

$$\mathbf{pos(j)} = \begin{bmatrix} \sin(\omega_1 . t) \\ \cos(\omega_1 . t) \\ \\ \sin(\omega_2 . t) \\ \cos(\omega_2 . t) \\ \\ \vdots \\ \\ \sin(\omega_{d/2} . t) \\ \cos(\omega_{d/2} . t) \end{bmatrix}_d$$

where $\omega_k = \frac{1}{10000^{2k/d}}$



Concatenate special positional encoding p_j to each input vector x_j

We use a function *pos*: $N \rightarrow R^d$ to process the position j of the vector into a d-dimensional vector

So, p_j = *pos*(j)

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Masked Self-Attention Layer

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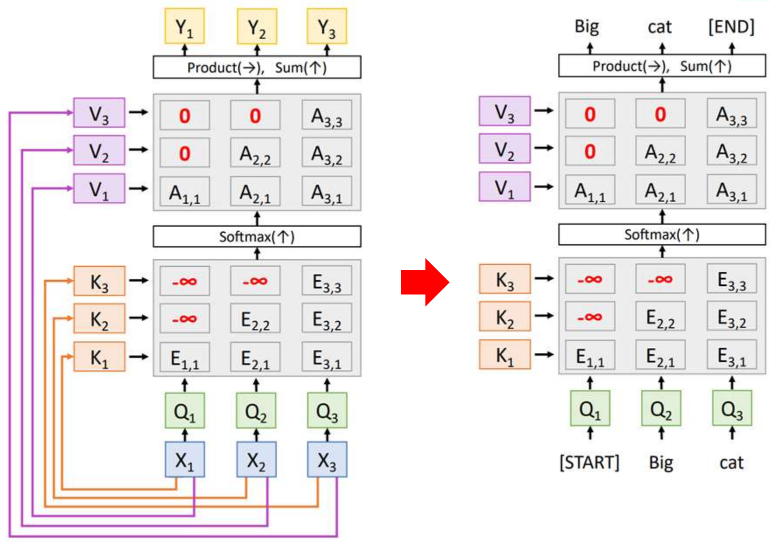
Prevent vectors from looking at future vectors.

Manually set alignment scores to –infinity (−∞)

Used for language modeling (predict next word)



RNN vs. 1D Convolution vs. Self-Attention

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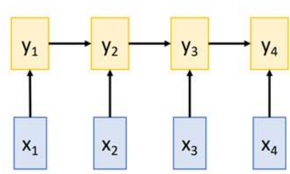
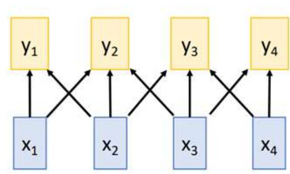
- **Three Ways of Processing Sequences**

Recurrent Neural Network



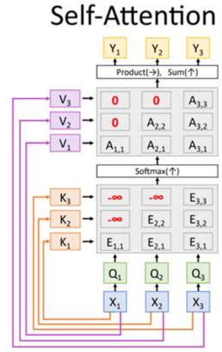
Works on **Ordered Sequences**
(+) Good at long sequences: After one RNN layer, h_T "sees" the whole sequence
(-) Not parallelizable: need to compute hidden states sequentially

1D Convolution



Works on **Multidimensional Grids**
(-) Bad at long sequences: Need to stack many conv layers for outputs to "see" the whole sequence
(+) Highly parallel: Each output can be computed in parallel

Self-Attention



Works on **Sets of Vectors**
(-) Good at long sequences: after one self-attention layer, each output "sees" all inputs!
(+) Highly parallel: Each output can be computed in parallel
(-) Very memory intensive

The Transformer

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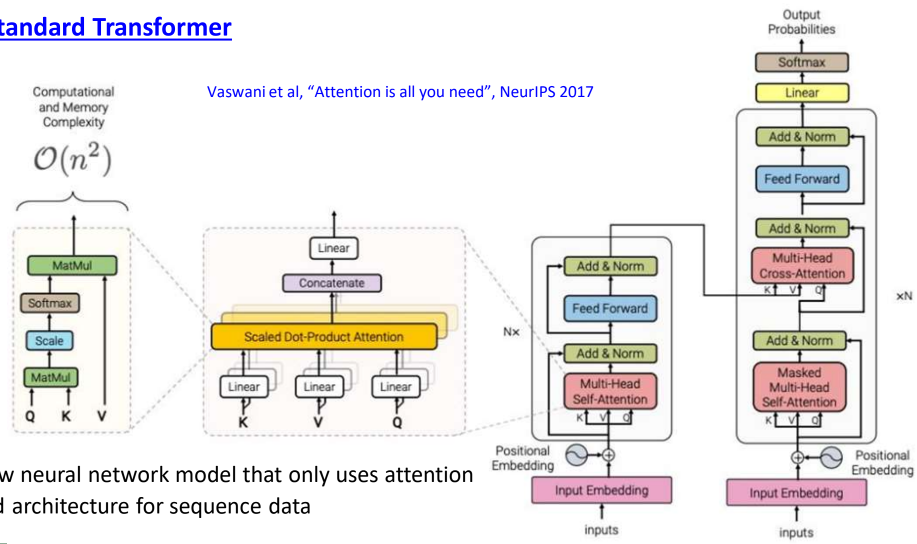
- **[Architecture of a Standard Transformer]**

Vaswani et al, "Attention is all you need", NeurIPS 2017



- Transformers are a new neural network model that only uses attention
- a fully attention-based architecture for sequence data

Transformer Block

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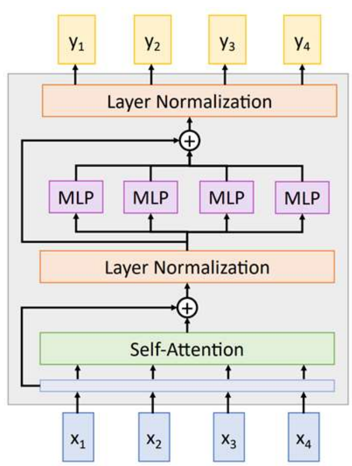
Transformer Block:
Input: Set of vectors x
Output: Set of vectors y

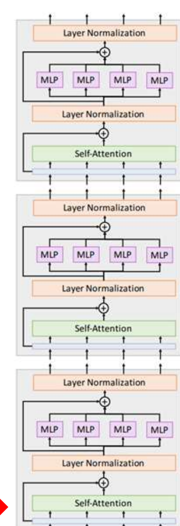
Self-attention is the only interaction between vectors!

Layer norm and MLP work independently per vector

Highly scalable, highly parallelizable



A Transformer is a sequence of transformer blocks



Post-Norm Transformer and Pre-Norm Transformer

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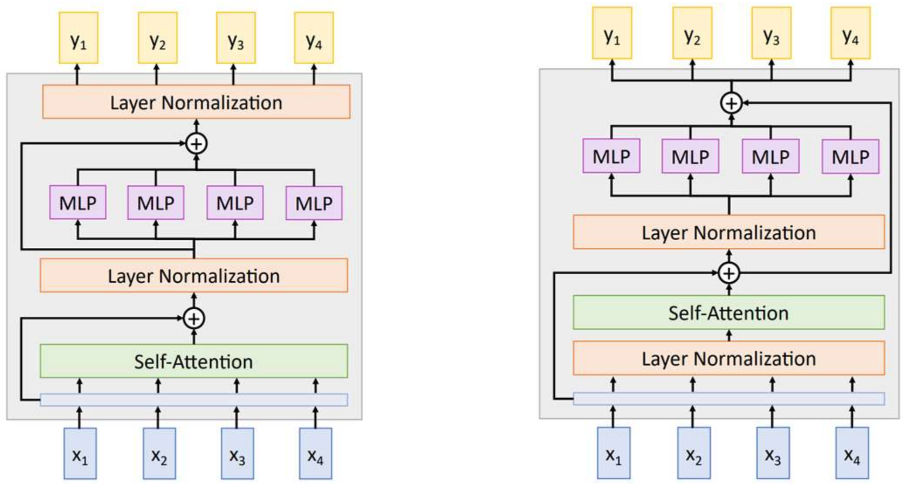

Baevski & Auli, "Adaptive Input Representations for Neural Language Modeling", arXiv 2018

Scaling up Transformers

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Model	Layers	Width	Heads	Params
Transformer-Base	12	512	8	65M
Transformer-Large	12	1024	16	213M
BERT-Base	12	768	12	110M
BERT-Large	24	1024	16	340M
XLNet-Large	24	1024	16	~340M
RoBERTa	24	1024	16	355M
GPT-2	48	1600	?	1.5B
Megatron-LM	72	3072	32	8.3B
Turing-NLG	78	4256	28	17B
GPT-3	96	12,288	96	175B
Gopher	80	16,384	128	280B

Data 10.55 TB | 4096x TPUv3 (38 days) **Training time**

Advantages of Transformers

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- **Great for modelling context**
  - Each token can have access to all other tokens in the sequence
- **A generic architecture:**
  - Operates on any inputs that can be tokenized!
- **Parallelizable**
- **Empirically shown to perform excellently at scale**

Weaknesses of Transformers

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- **Quadratic complexity**
  - Each token attends to every other token
  - N tokens → N2 operations
  - Prohibitive as the number of tokens increases!
- **Most powerful language models are extremely expensive**
- **Large body of work on more efficient transformers.**
- **Transformers can overfit easily on smaller datasets**

RNNs to Transformer

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- **RNNs**
  - **LSTMs work reasonably well for long sequences.**
  - **Expects an ordered sequences of inputs**
  - **Sequential computation: subsequent hidden states can only be computed after the previous ones are done.**
- **Transformer:**
  - **Good at long sequences. Each attention calculation looks at all inputs.**
  - **Can operate over unordered sets or ordered sequences with positional encodings.**
  - **Parallel computation: All alignment and attention scores for all inputs can be done in parallel**
  - **Requires a lot of memory: N x M alignment and attention scalers need to be calculated and stored for a single self-attention head.**

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Transformers for Vision

Image Classification

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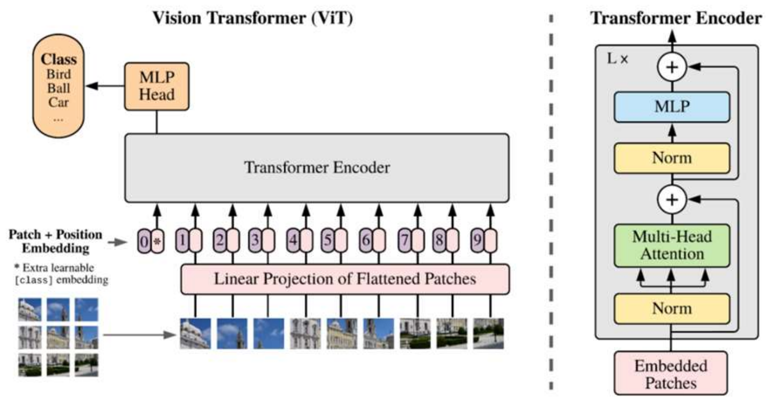
- **Vision Transformer ('21) [ViT]**
  - Decompose an image to NxN patches and then apply transformer encoder



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Questions?