Transformer Model

Credit to: Prof. Jongwuk Lee, SKKU

References

Online Courses

- Natural Language Processing with Deep Learning (Stanford)
  - Transformer Networks and Convolution Neural Networks
  - http://web.stanford.edu/class/cs224n/lectures/lecture12.pdf
- The Illustrated Transformer
  - http://jalammar.github.io/illustrated-transformer/

Papers

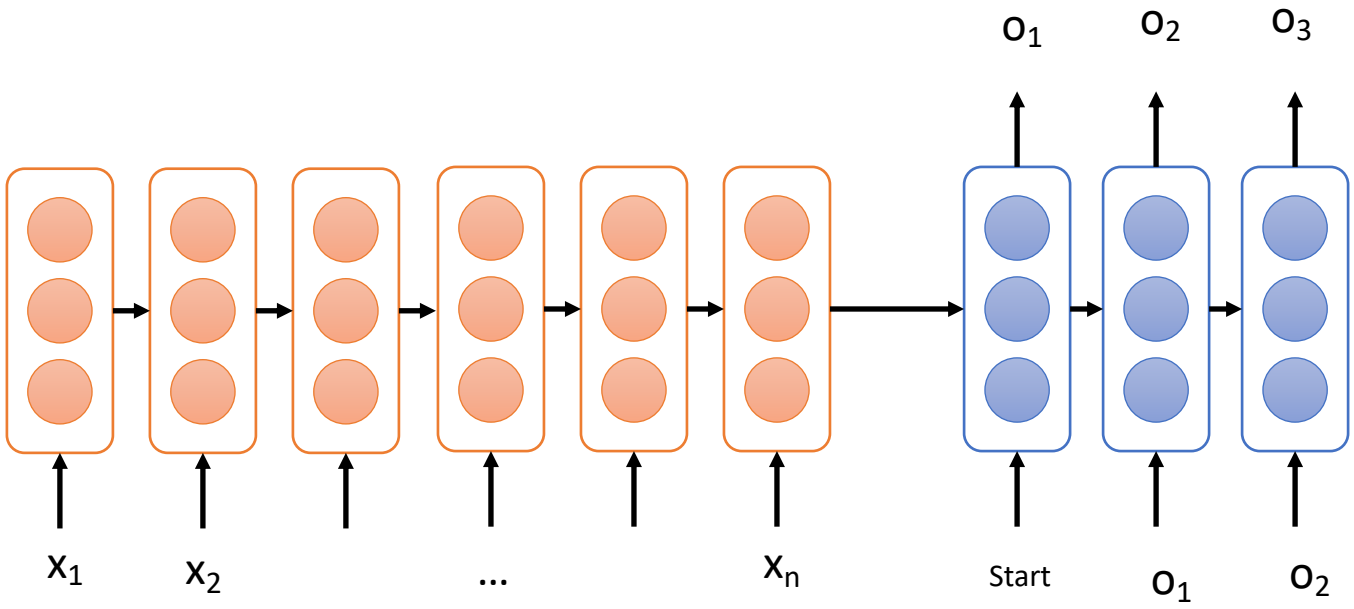
- Ashish Vaswani, Noam Shazeer, Niki Parmar, Jakob Uszkoreit, Llion Jones, Aidan N. Gomez, Łukasz Kaiser, Illia Polosukhin, "Attention Is All You Need," NIPS 2018

Sequence Generator

- It would take a sentence in source language, and output its translation in another.

Problems with RNN

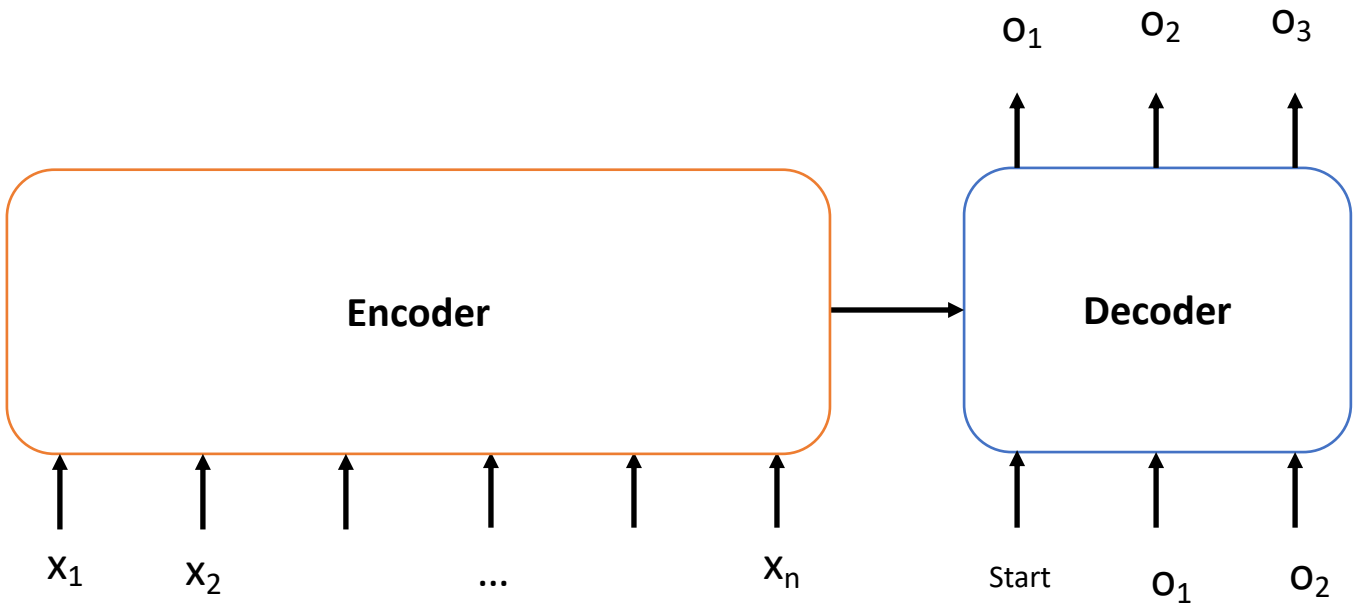
- Sequential computation prevents **parallelization**.



- Despite GRUs and LSTMs, RNNs still need attention mechanism to deal with long range dependencies.
- Can we parallelize the encoding process?

Problems with RNN

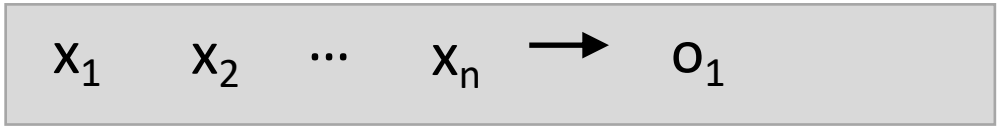
- Why Encoder & Decoder Sequential?

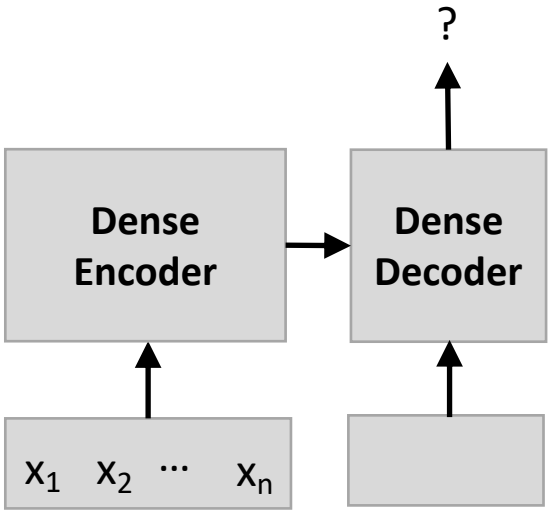


- Let's replace RNNs to fully connected networks

Problems with RNN

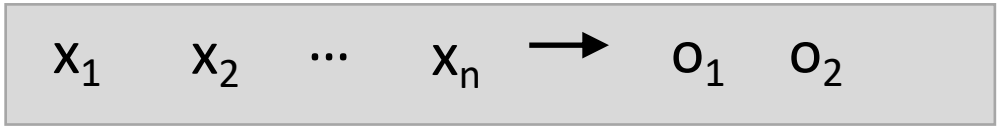
- **Without Sequential Encoder & Decoder**

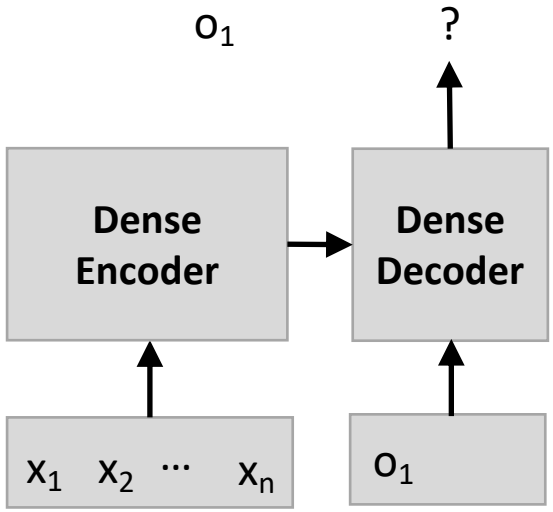




Problems with RNN

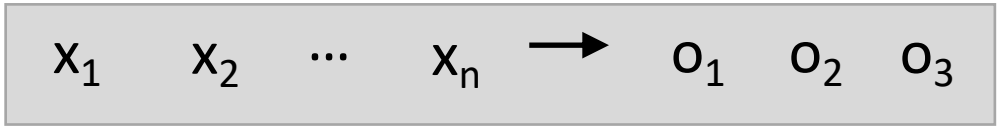
- **Without Sequential Encoder & Decoder**

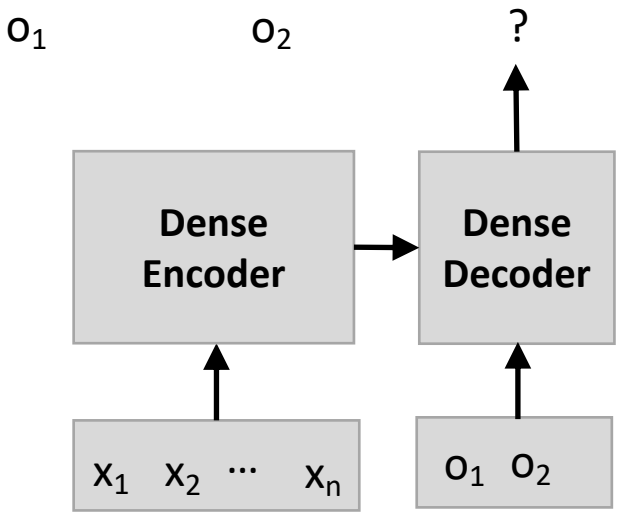




Problems with RNN

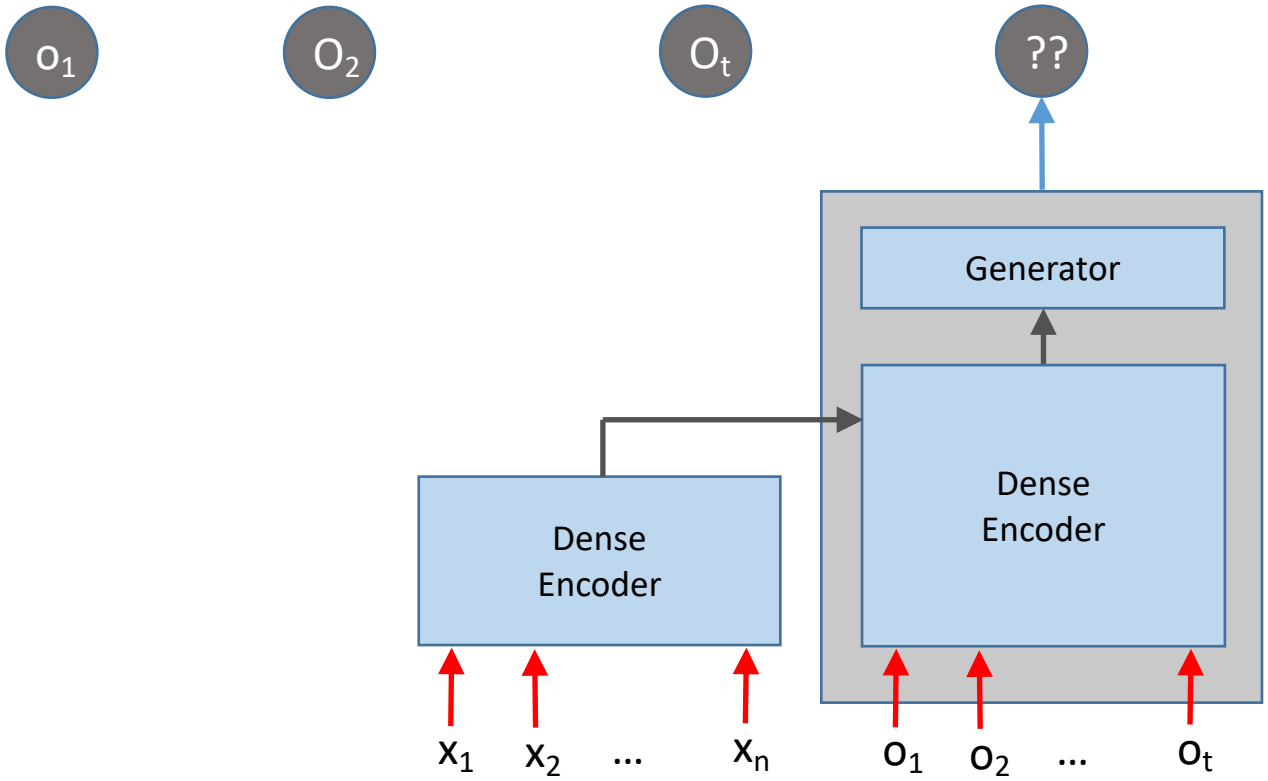
- **Without Sequential Encoder & Decoder**





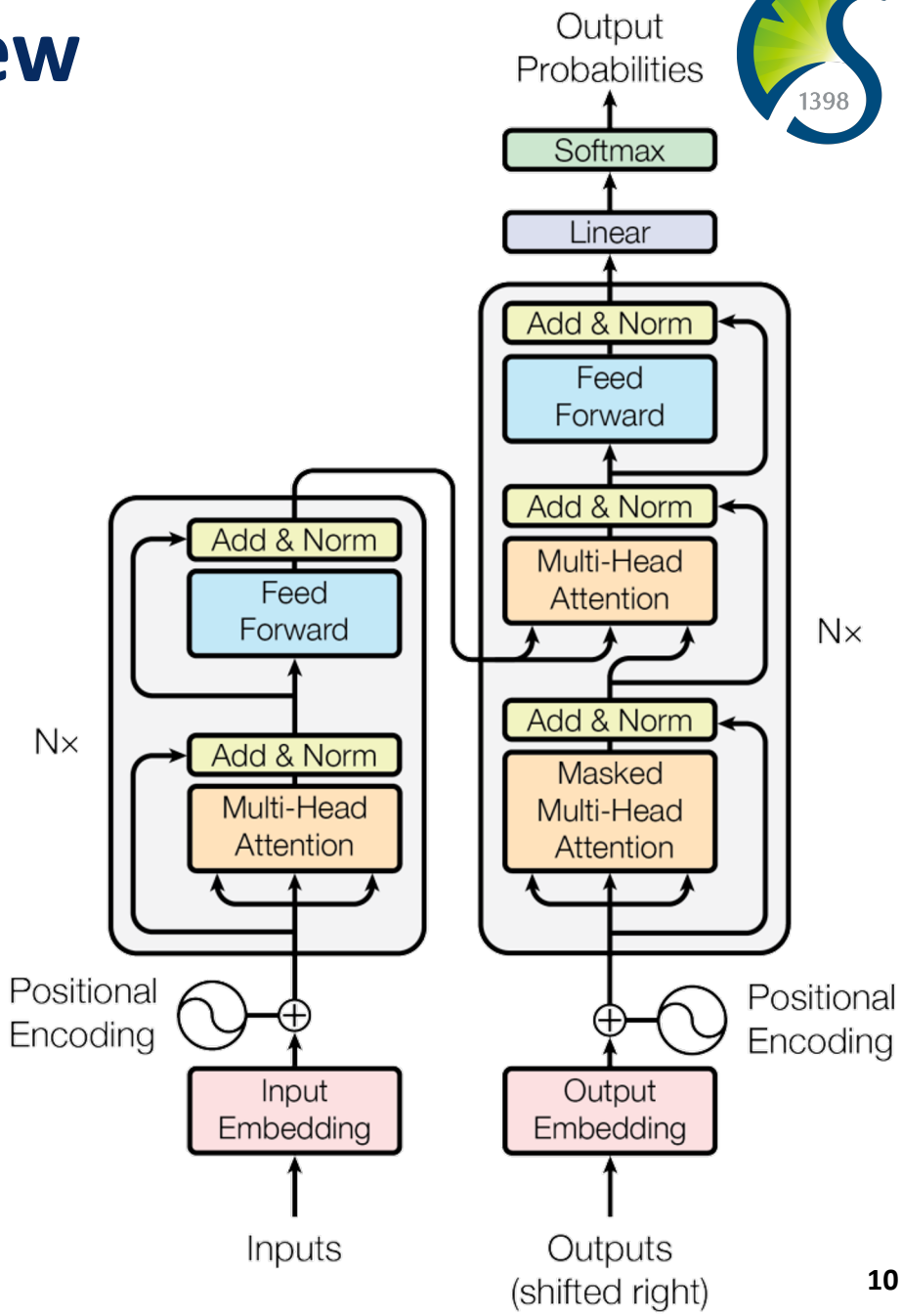
Problems with RNN

- Sequential computation prevents **parallelization**.

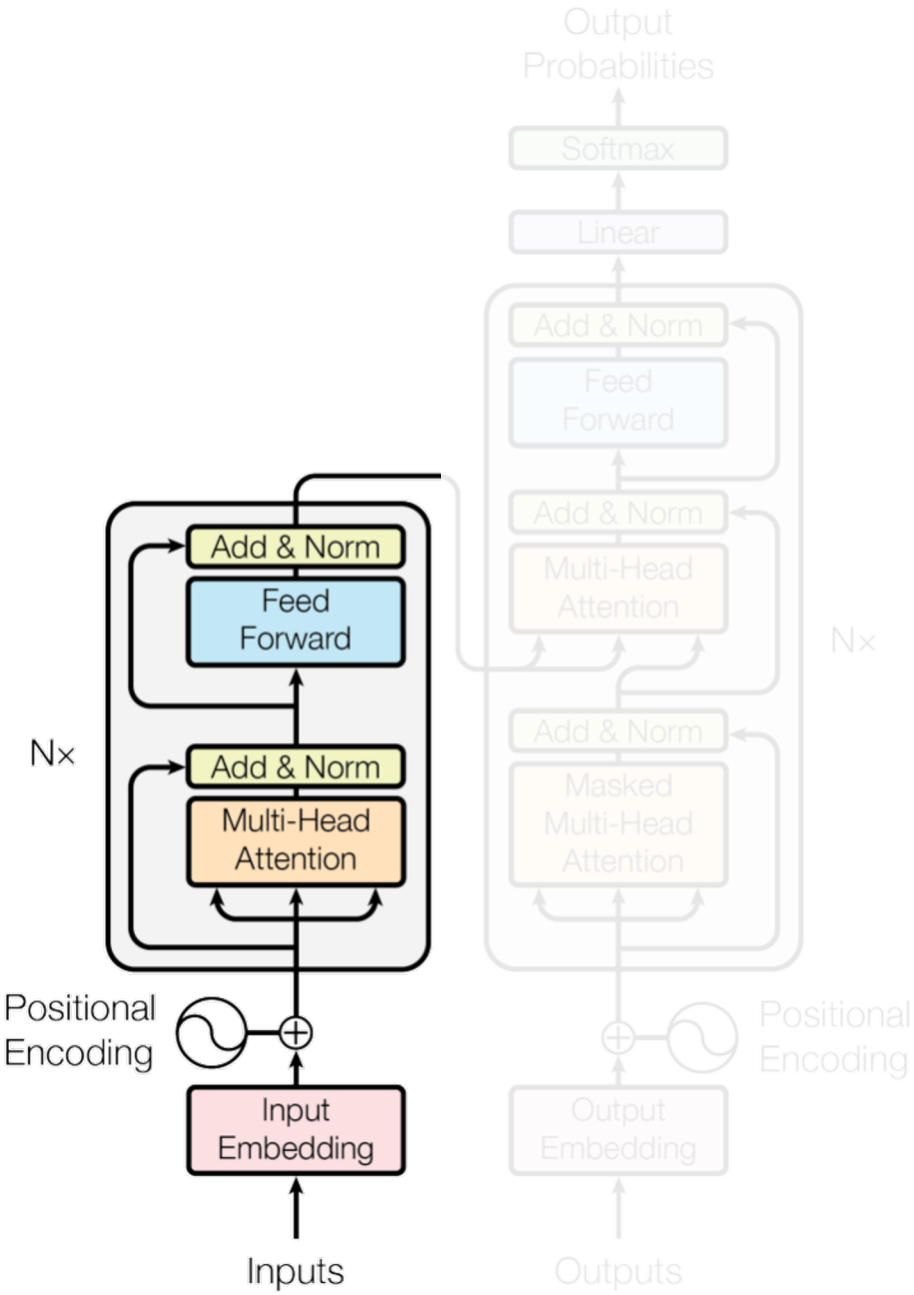


Transformer Overview

- **Encoder-Decoder approach**
- **Task: machine translation with parallel corpus**
- **Predict each translated word.**

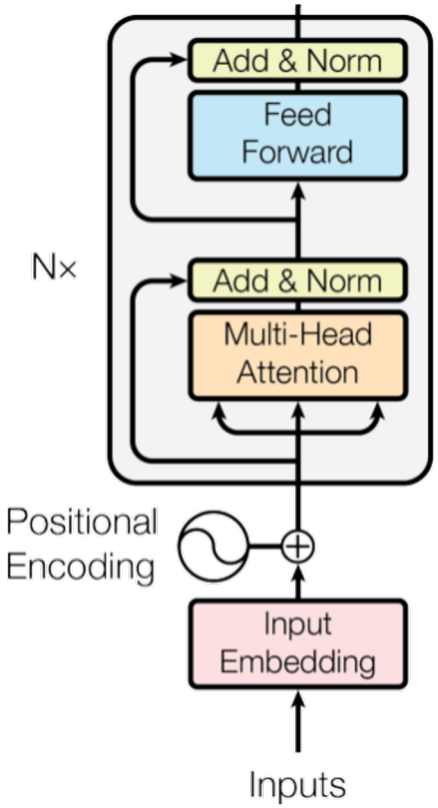


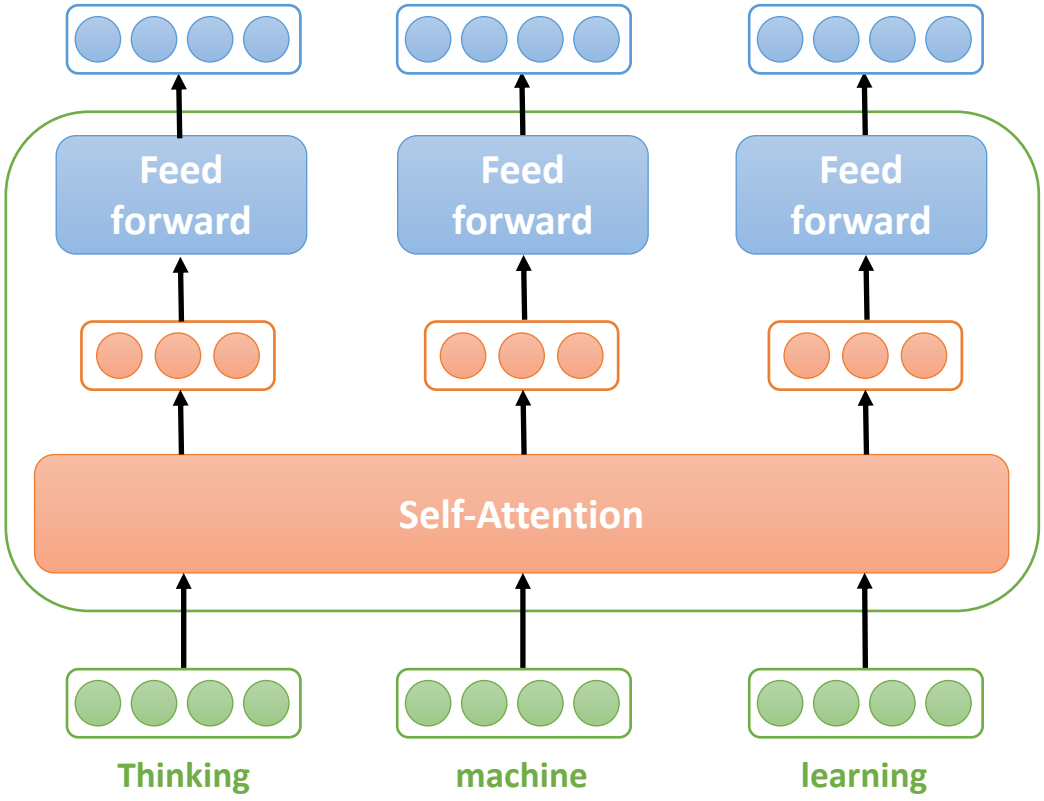
Encoder


Output Probabilities
Softmax
Linear
Add & Norm
Feed Forward
Add & Norm
Multi-Head Attention
Add & Norm
Masked Multi-Head Attention
Nx
Positional Encoding
Output Embedding
Outputs
Add & Norm
Feed Forward
Add & Norm
Multi-Head Attention
Nx
Positional Encoding
Input Embedding
Inputs

Encoder Internals

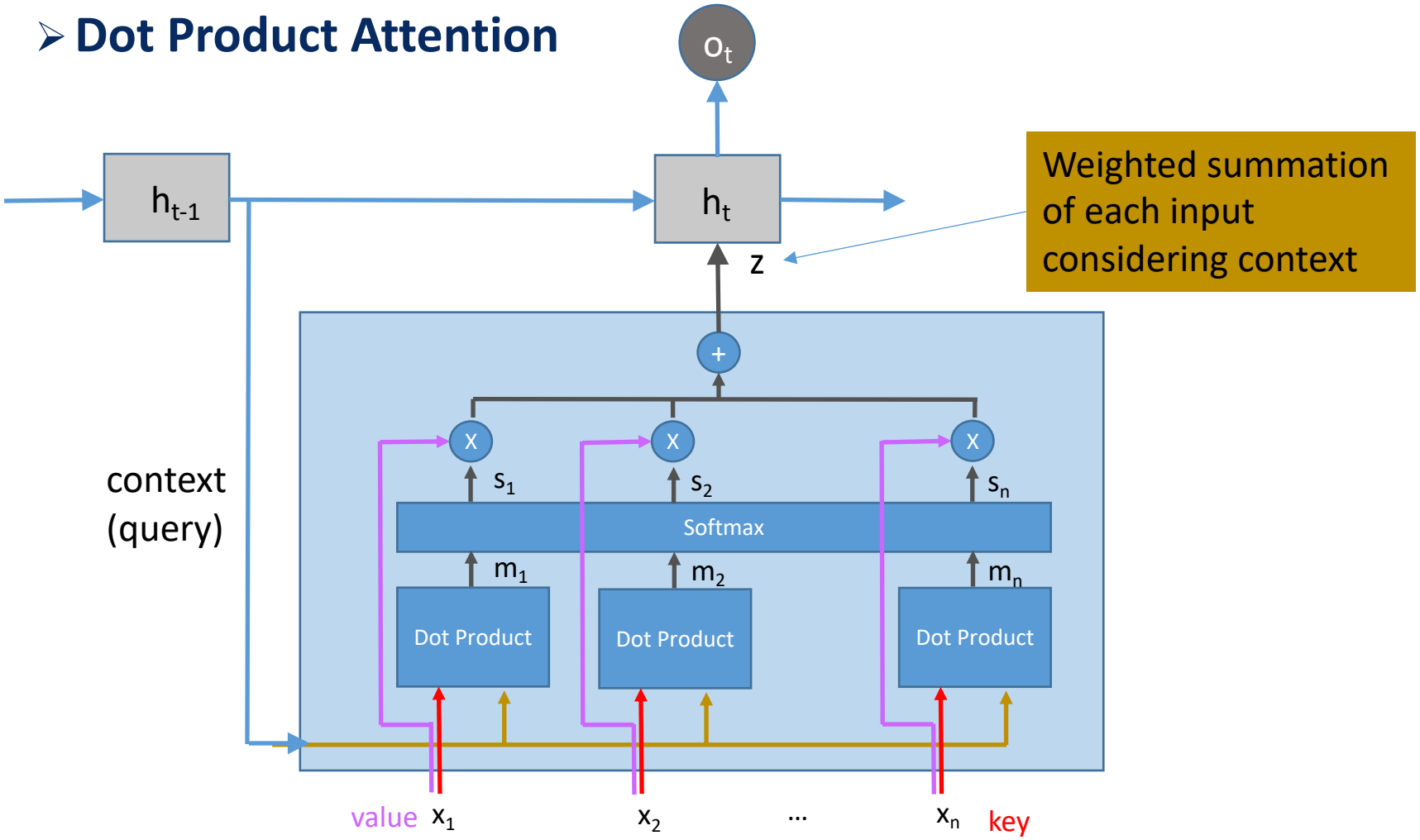
- After embedding the words in the input sentence, each of them flows through the two layers of the encoder.





Recap: Attention Mechanism

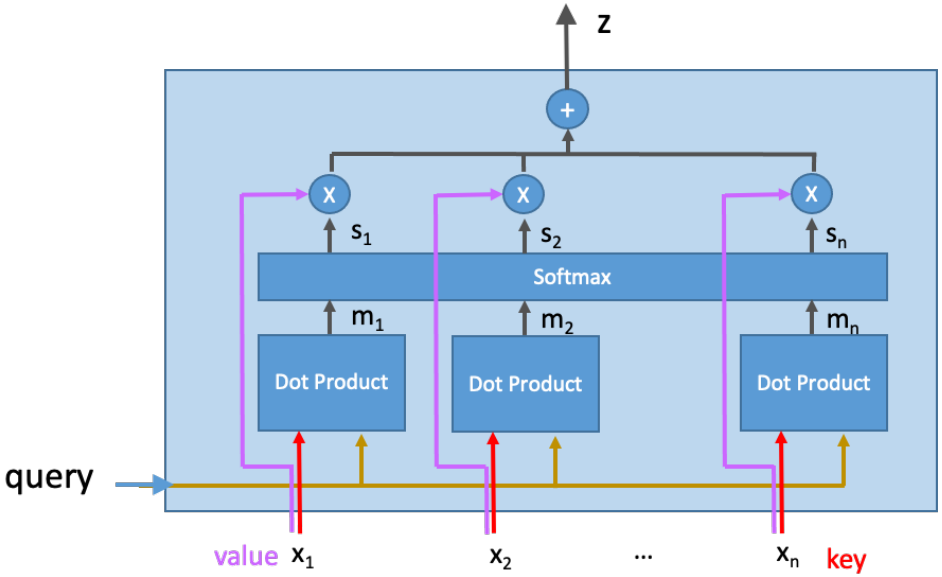
➢ **Dot Product Attention**



Recap: Attention Mechanism

➢ Dot Product Attention

$$z = A(q, K, V)$$



q =

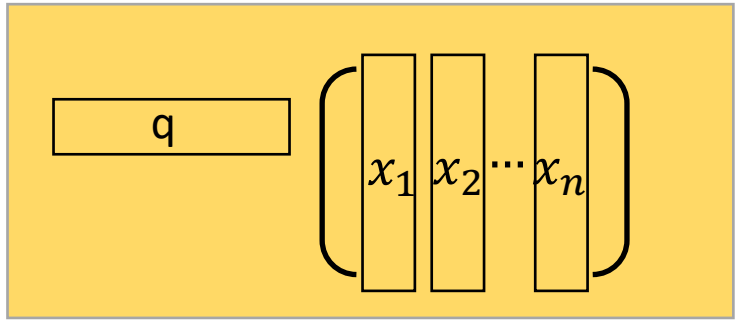
V = $\begin{bmatrix} x_1 \\ x_2 \\ \dots \\ x_n \end{bmatrix}$

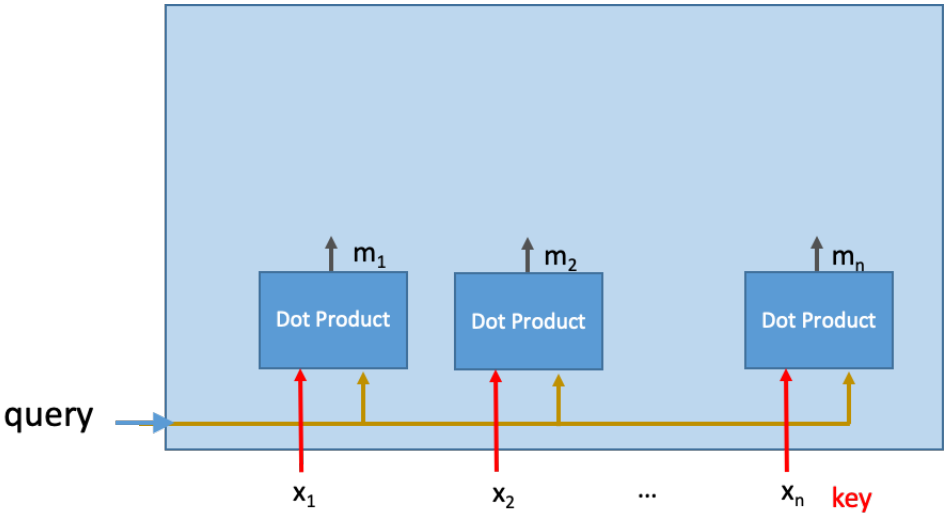
K = $\begin{bmatrix} x_1 \\ x_2 \\ \dots \\ x_n \end{bmatrix}$

Recap: Attention Mechanism

➢ Dot Product Attention

$$(m_1, m_2, \dots, m_n) = (q \cdot x_1, q \cdot x_2, \dots, q \cdot x_n) = qK^T$$





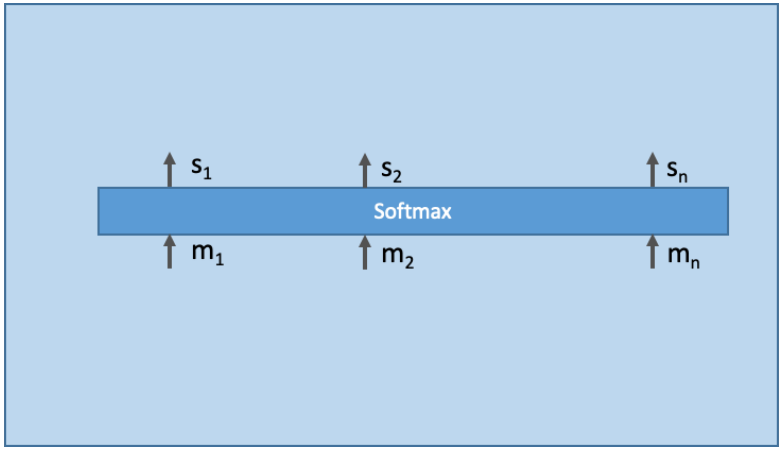
K = $\begin{pmatrix} x_1 \\ x_2 \\ \dots \\ x_n \end{pmatrix}$

Recap: Attention Mechanism

- **Dot Product Attention**

$$(s_1, s, \dots, s_n) = \text{Softmax}(m_1, m_2, \dots, m_n)$$

$$(m_1, m_2, \dots, m_n) = qK^T$$



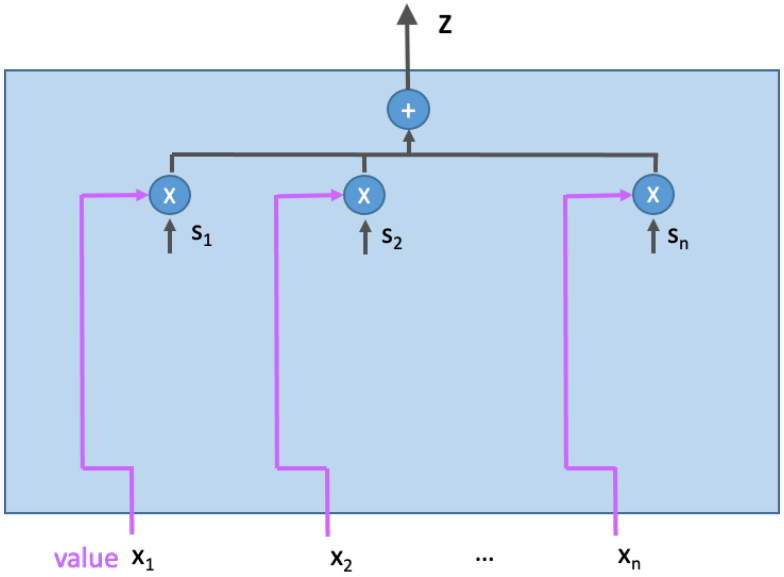
Recap: Attention Mechanism

➢ Dot Product Attention

$$z = s_1 \cdot x_1 + s_2 \cdot x_2 + \cdots + s_n \cdot x_n = (s_1, s, \dots, s_n) \cdot V$$

$$(s_1, s, \dots, s_n) = \text{Softmax}(m_1, m_2, \dots, m_n)$$

$$(m_1, m_2, \dots, m_n) = qK^T$$



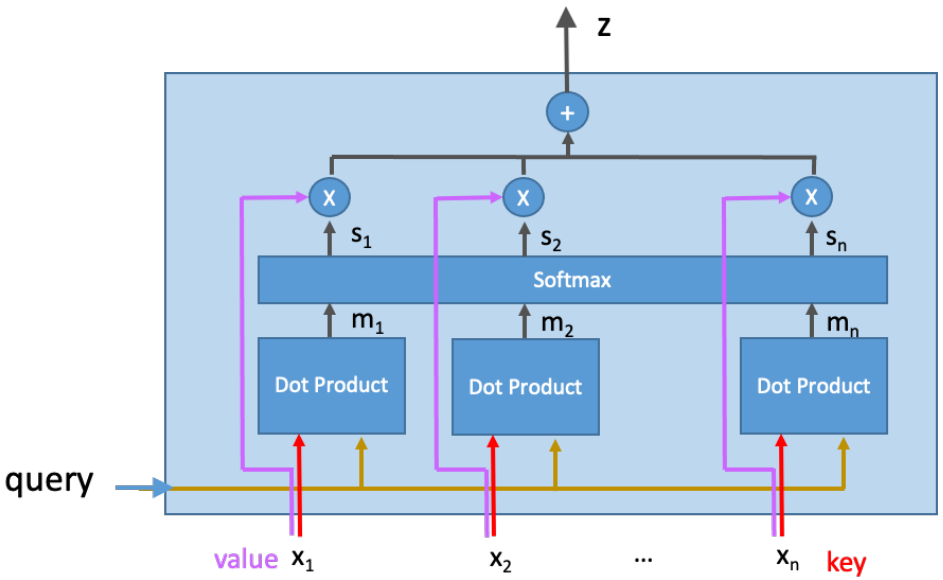
$(s_1, s, \dots, s_n)$ $\begin{pmatrix} x_1 \\ x_2 \\ \dots \\ x_n \end{pmatrix}$

V = $\begin{pmatrix} x_1 \\ x_2 \\ \dots \\ x_n \end{pmatrix}$

Recap: Attention Mechanism

➢ Dot Product Attention

$$z = A(q, K, V) = \text{Softmax}(qK^T)V$$



q =

V = $\begin{bmatrix} x_1 \\ x_2 \\ \dots \\ x_n \end{bmatrix}$

K = $\begin{bmatrix} x_1 \\ x_2 \\ \dots \\ x_n \end{bmatrix}$

Recap: Attention Mechanism

- **Dot Product Attention**

$$z = A(q, K, V) = \text{Softmax}(qK^T)V$$

$$z_1 = A(q_1, K, V)$$
$$z_2 = A(q_2, K, V)$$
$$\dots$$
$$z_m = A(q_m, K, V)$$

$$Z = \begin{pmatrix} z_1 \\ z_2 \\ \dots \\ z_m \end{pmatrix}$$

$$Q = \begin{pmatrix} q_1 \\ q_2 \\ \dots \\ q_m \end{pmatrix}$$

Recap: Attention Mechanism

- **Dot Product Attention**

$$Z = A(Q, K, V) = \text{Softmax}(QK^T)V$$

$$\begin{pmatrix} z_1 \\ z_2 \\ \vdots \\ z_m \end{pmatrix} = \begin{pmatrix} \text{Softmax}(q_1K^T)V \\ \text{Softmax}(q_2K^T)V \\ \vdots \\ \text{Softmax}(q_mK^T)V \end{pmatrix} = \begin{pmatrix} \text{Softmax}(q_1K^T) \\ \text{Softmax}(q_2K^T) \\ \vdots \\ \text{Softmax}(q_mK^T) \end{pmatrix} V$$

$$= \text{Softmax}\begin{pmatrix} q_1K^T \\ q_2K^T \\ \vdots \\ q_mK^T \end{pmatrix} V = \text{Softmax}\left(\begin{pmatrix} q_1 \\ q_2 \\ \vdots \\ q_m \end{pmatrix} K^T\right) V = \text{Softmax}(QK^T)V$$

Recap: Attention Mechanism

➢ **Dot Product Attention**

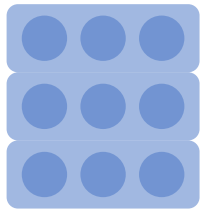
$$Z = A(Q, K, V) = \text{Softmax}(QK^T)V$$

$$Z = \begin{pmatrix} z_1 \\ z_2 \\ \dots \\ z_m \end{pmatrix} \qquad V = \begin{pmatrix} x_1 \\ x_2 \\ \dots \\ x_n \end{pmatrix}$$

$$Q = \begin{pmatrix} q_1 \\ q_2 \\ \dots \\ q_m \end{pmatrix} \qquad K = \begin{pmatrix} x_1 \\ x_2 \\ \dots \\ x_n \end{pmatrix}$$

Recap: Attention Mechanism

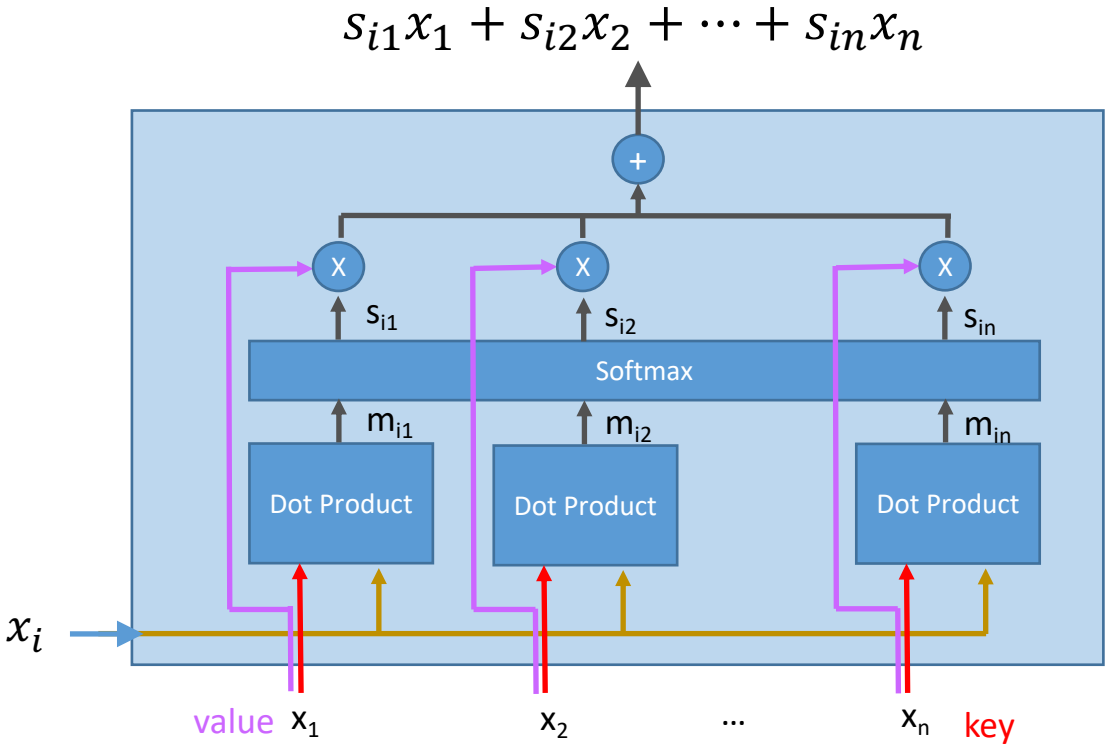
$$\text{softmax}\left(\frac{\boldsymbol{Q} \cdot \boldsymbol{K^T}}{\sqrt{|k|}}\right) \cdot \boldsymbol{V}$$



As $|k|$ gets large, the variance of QK^T increases.
→ Some values inside the softmax get **large**.
→ The softmax get very **peaked**.
→ Its gradient gets **smaller**.

Self-Attention

➢ **Definition:** $A(x_i, X, X)$



$$A(x_i, X, X) = s_{i1}x_1 + s_{i2}x_2 + \cdots + s_{in}x_n = x_i'$$

Self-Attention

- **Definition:** $A(x_i, X, X)$

$$A(x_i, X, X) = s_{i1}x_1 + s_{i2}x_2 + \cdots + s_{in}x_n = x_i'$$

Similarity of x_i to x_1

Similarity of x_i to x_2

Similarity of x_i to x_n

Re-description of x_i considering long-term dependency in input

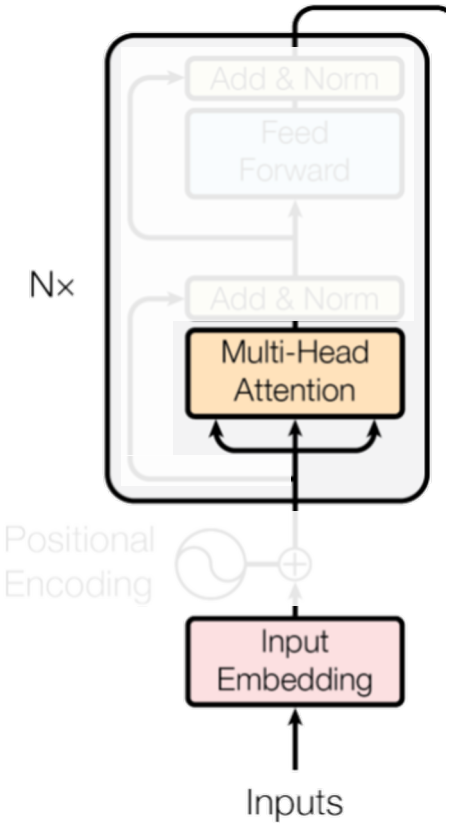
Self-Attention

- **Definition:**

$$A(X, X, X) = \begin{pmatrix} s_{11}x_1 + s_{12}x_2 + \cdots + s_{1n}x_n \\ s_{21}x_1 + s_{22}x_2 + \cdots + s_{2n}x_n \\ \dots \\ s_{n1}x_1 + s_{n2}x_2 + \cdots + s_{nn}x_n \end{pmatrix} = X'$$

Multi-headed Attention

- **Refine the self-attention layer by adding a mechanism called "multi-headed" attention.**
  - It expands the model's ability to focus on different positions.
  - It gives the attention layer **multiple representation subspaces**.



Multi-headed Attention

➢ Attention

$$A(Q,K,V) = softmax(QK^T)V$$

$$Q: |Q| \times k, \qquad K: |K| \times k, \qquad V: |V| \times k$$

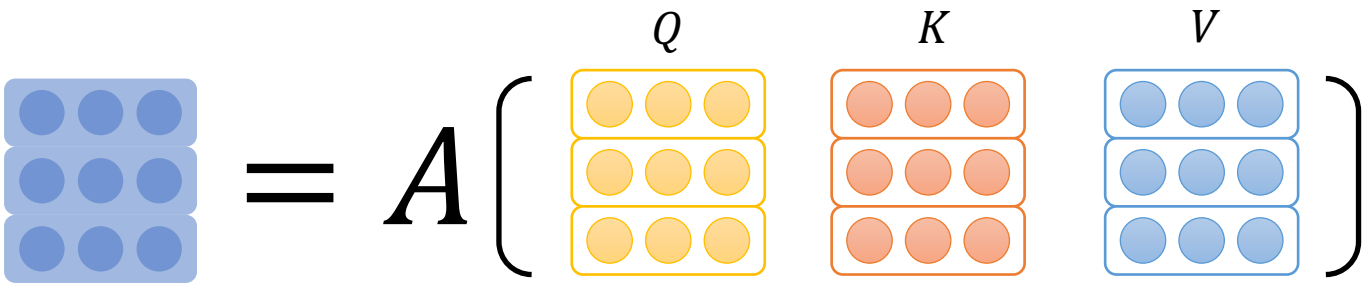
➢ What is 'headed'?

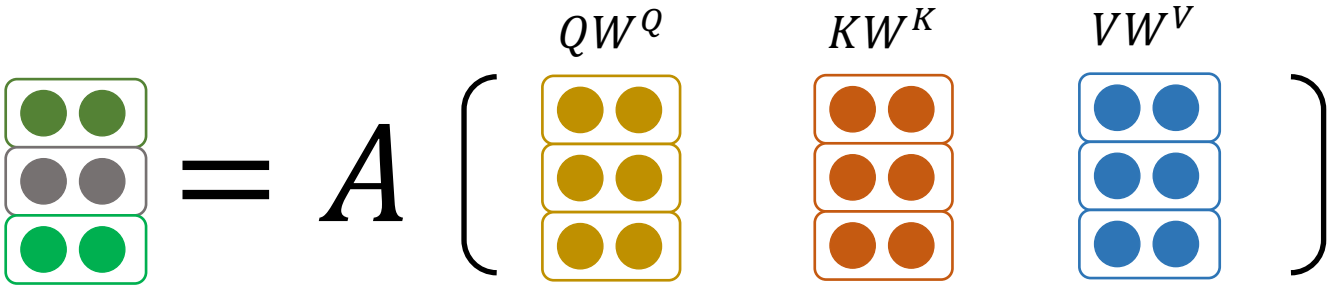
- Linear Transformed: $W^Q, W^K, W^V \ (= k \times m)$

$$A(QW^Q, KW^K, VW^V)$$

Multi-headed Attention

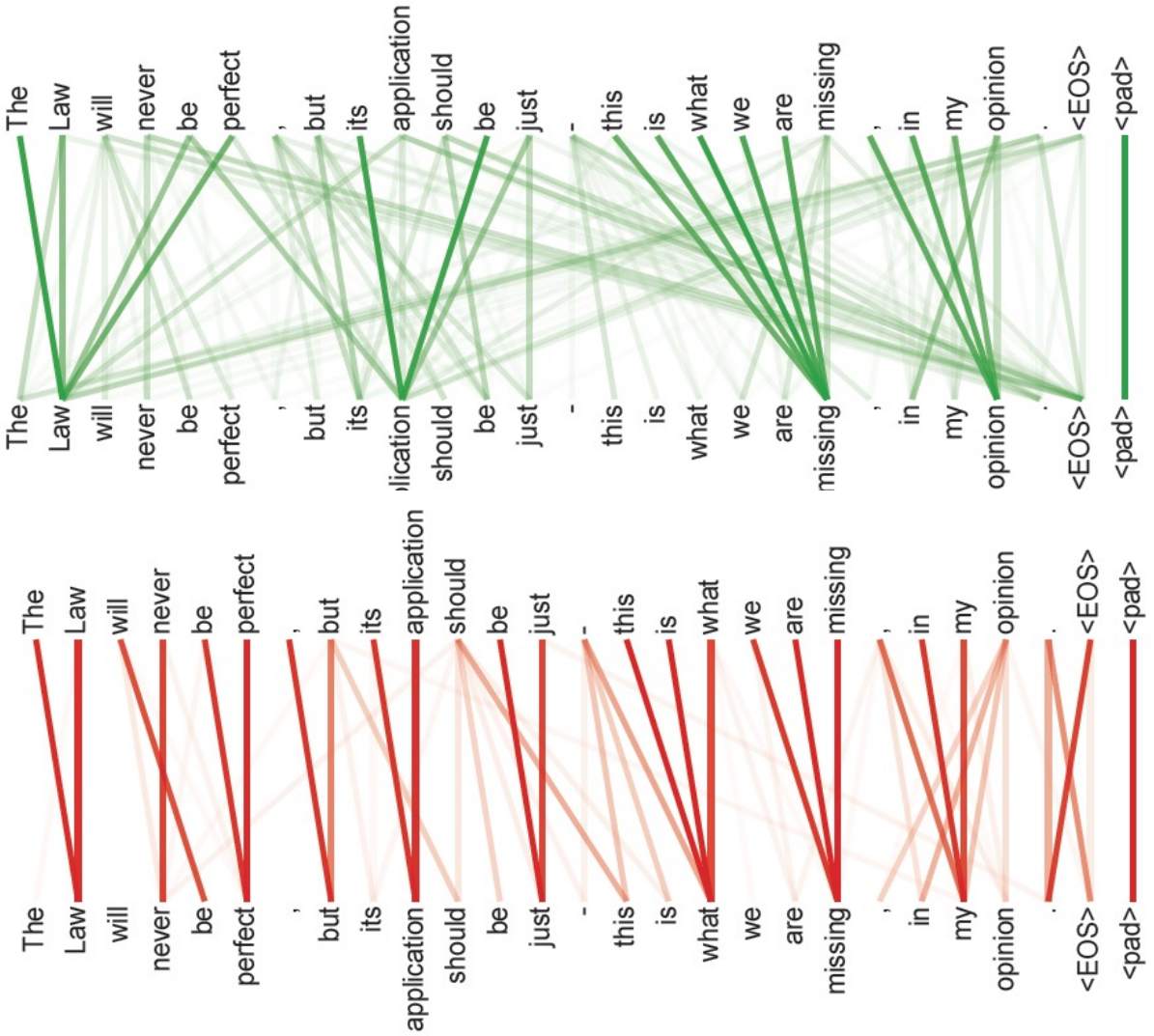
$$A(QW^Q, KW^K, VW^V)$$





Multi-headed Attention

- **Head: A viewpoint of similarity**

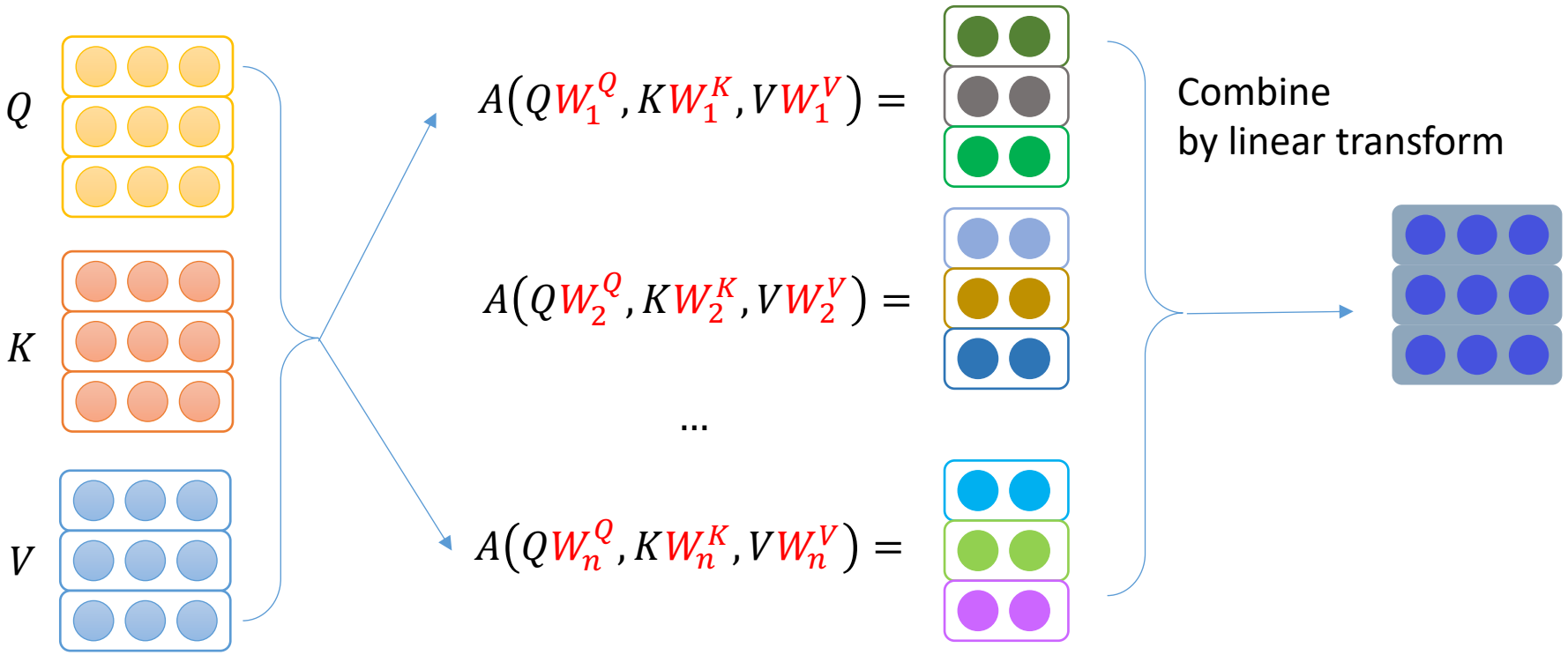


The encoder self-attention at layer 5 and 6.

The heads clearly learned to perform different tasks.

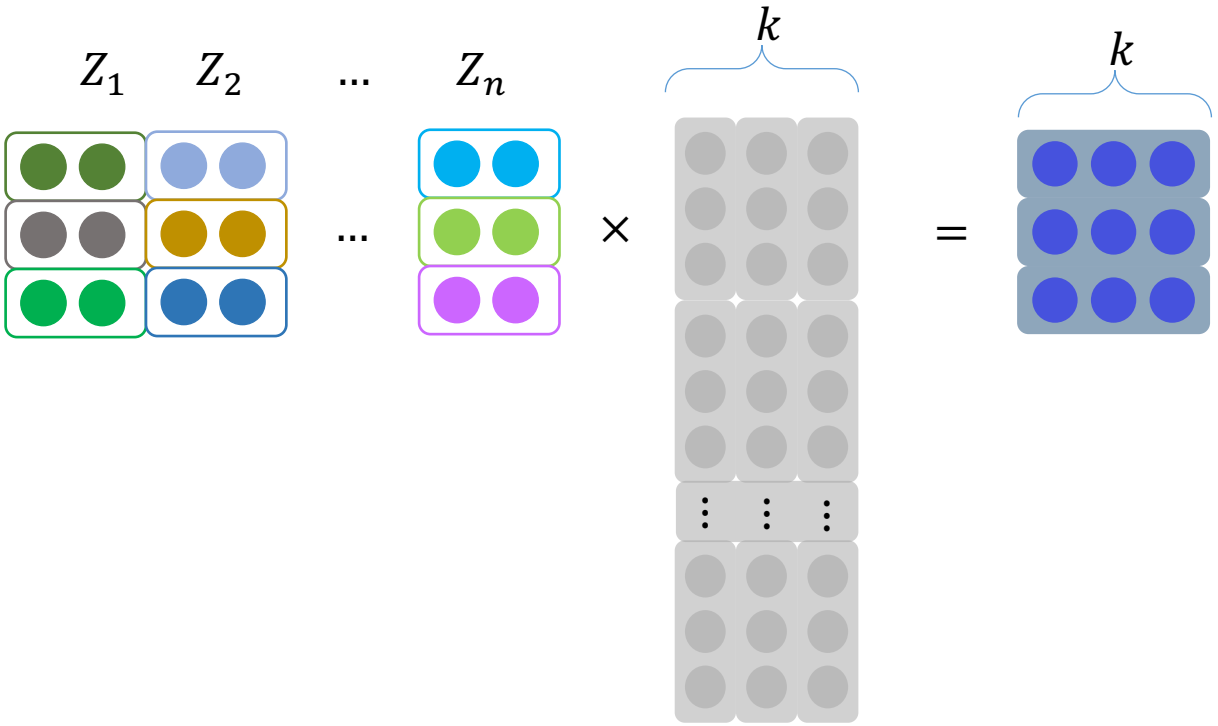
Multi-headed Attention

- Let's use multiple heads to capture various similiarities



Multi-headed Attention

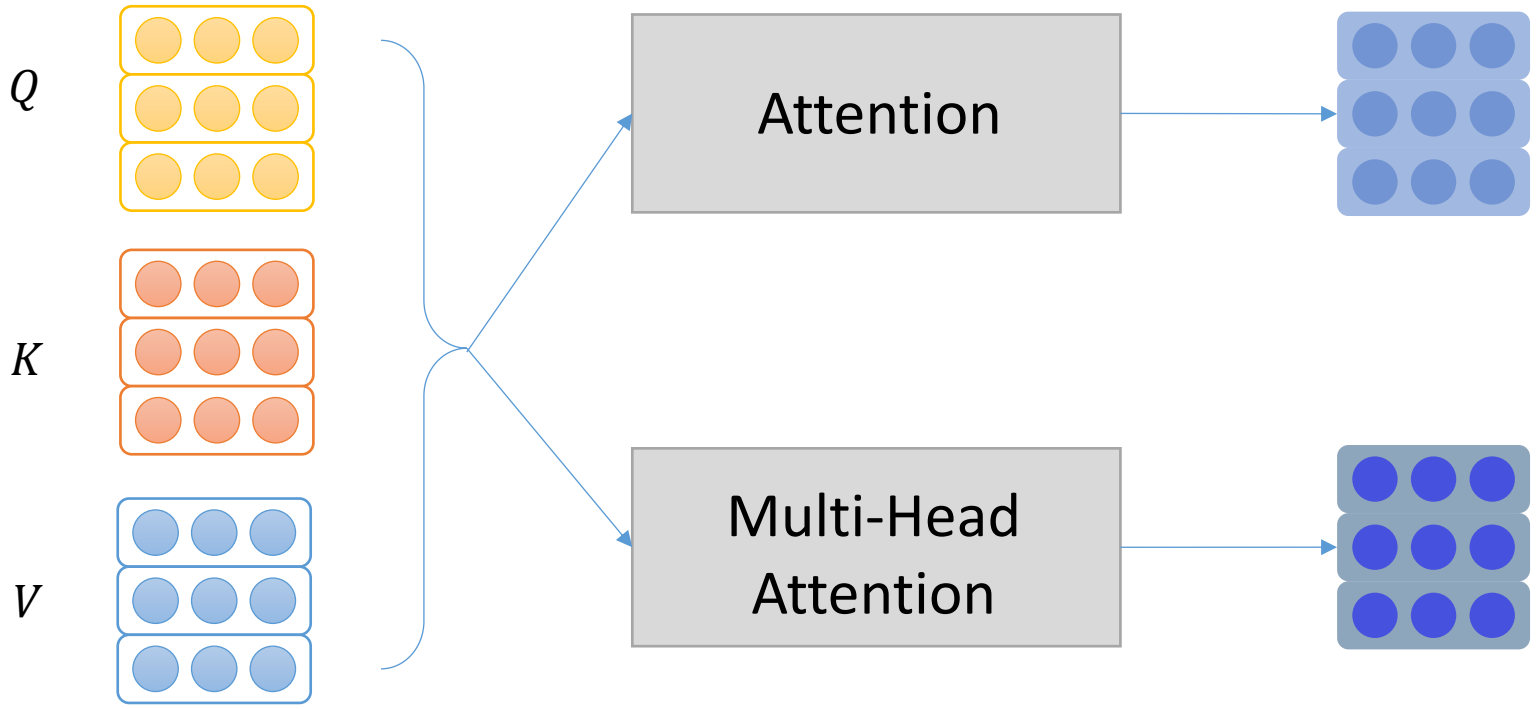
- Let's use multiple heads to capture various similiarities



Transform matrix

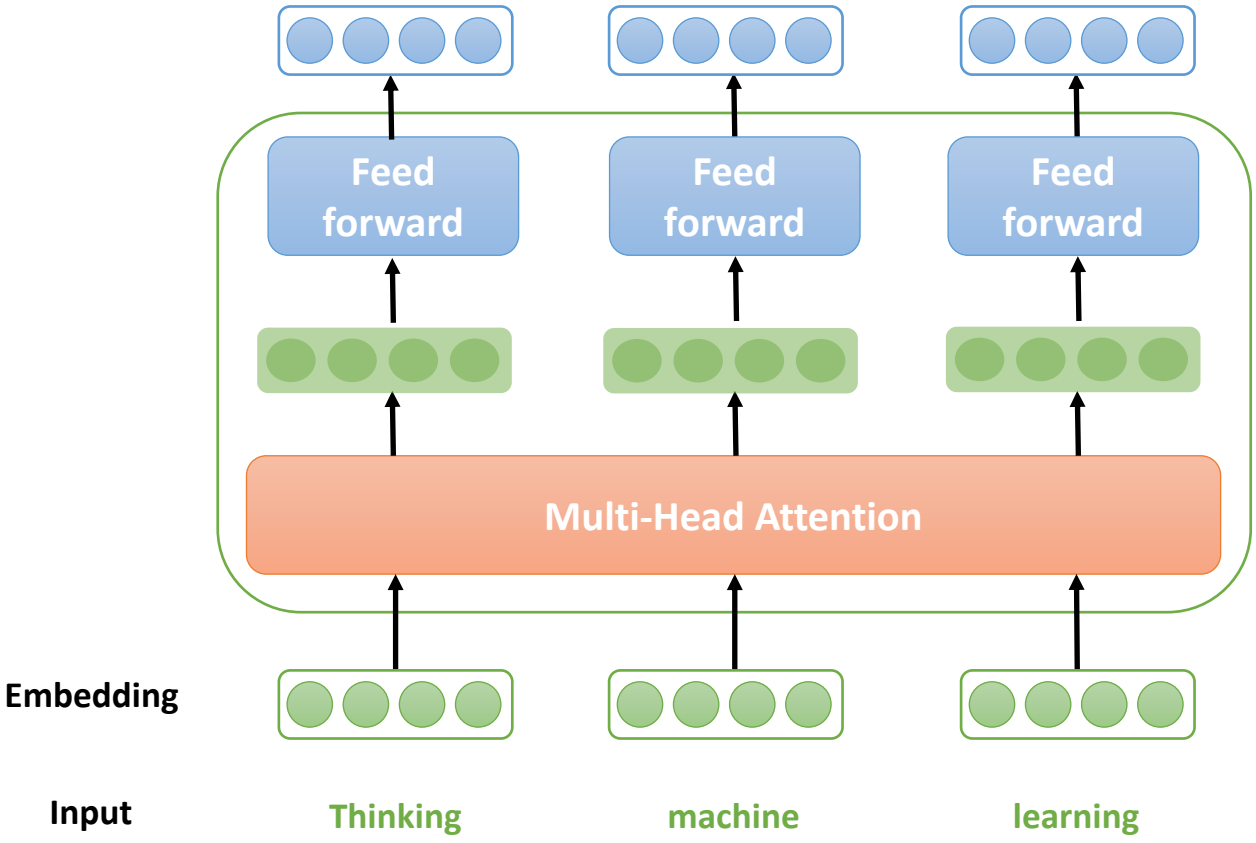
Multi-headed Attention

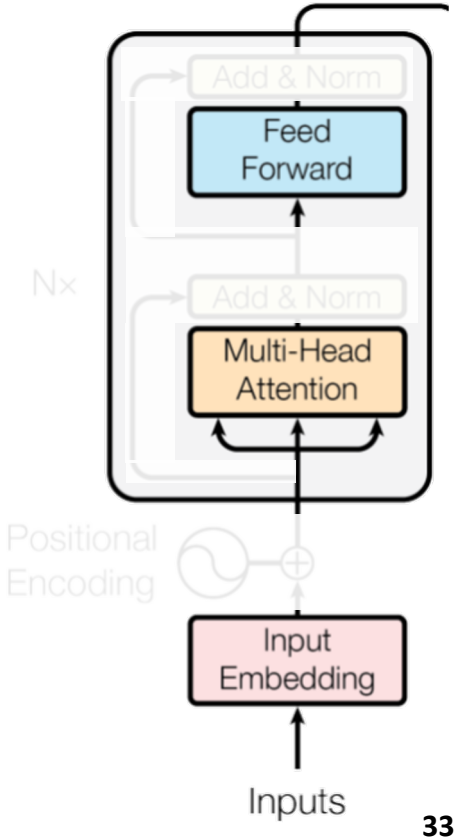
- Let's use multiple heads to capture various similiarities



Feed Forward

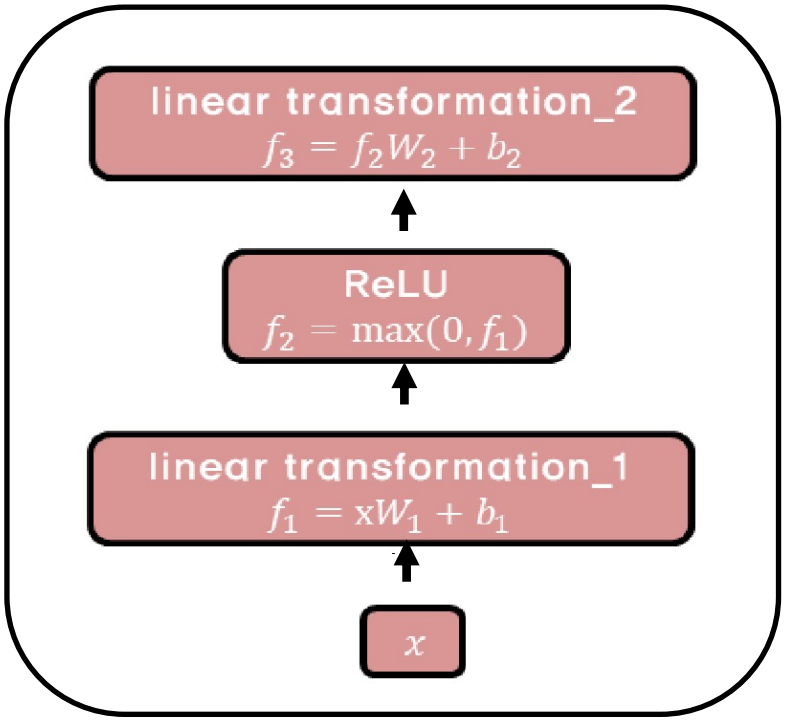
➢ Point-wise Feed Forward

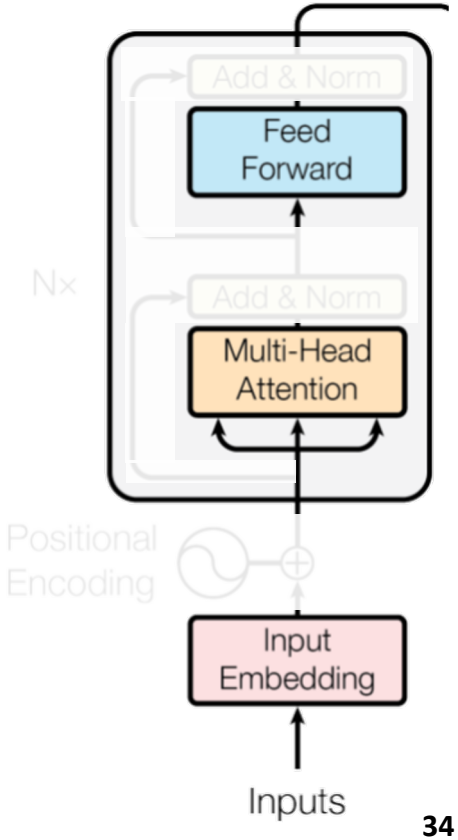




Feed Forward

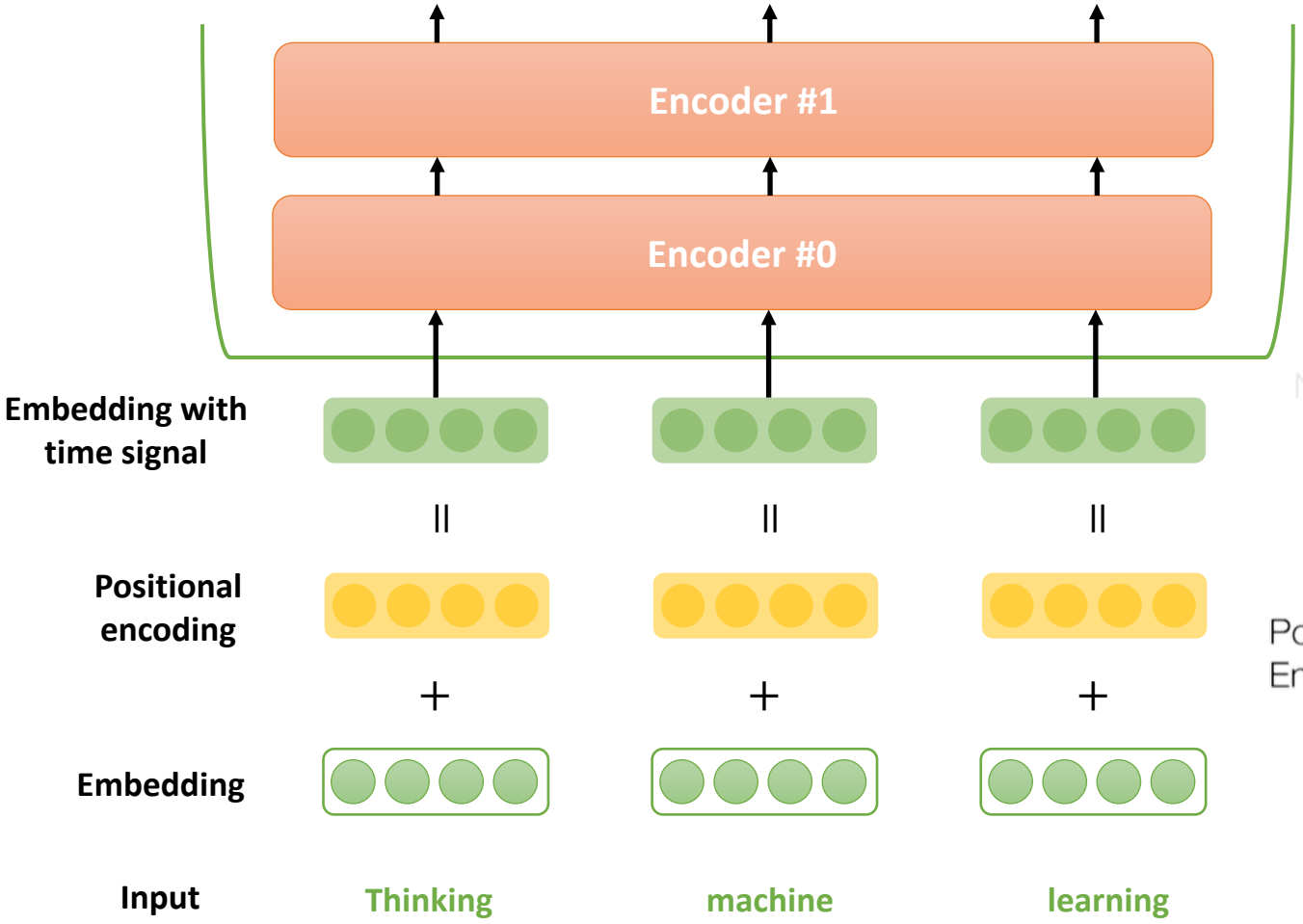
➢ **Point-wise Feed Forward**

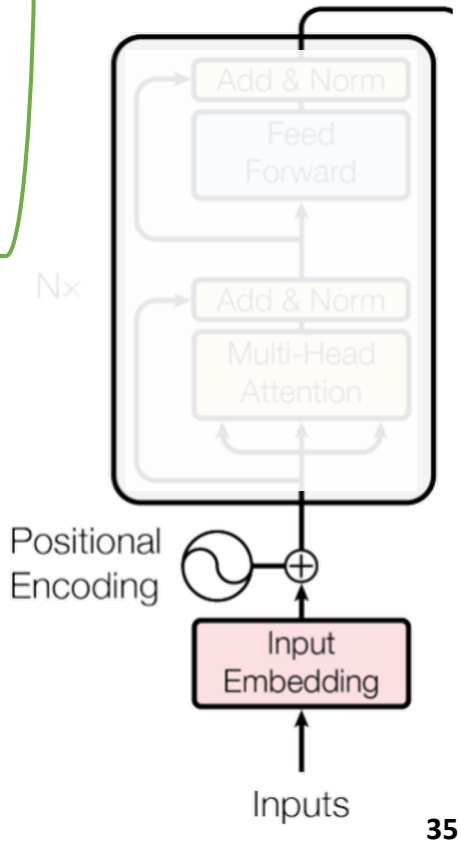




Positional Encoding

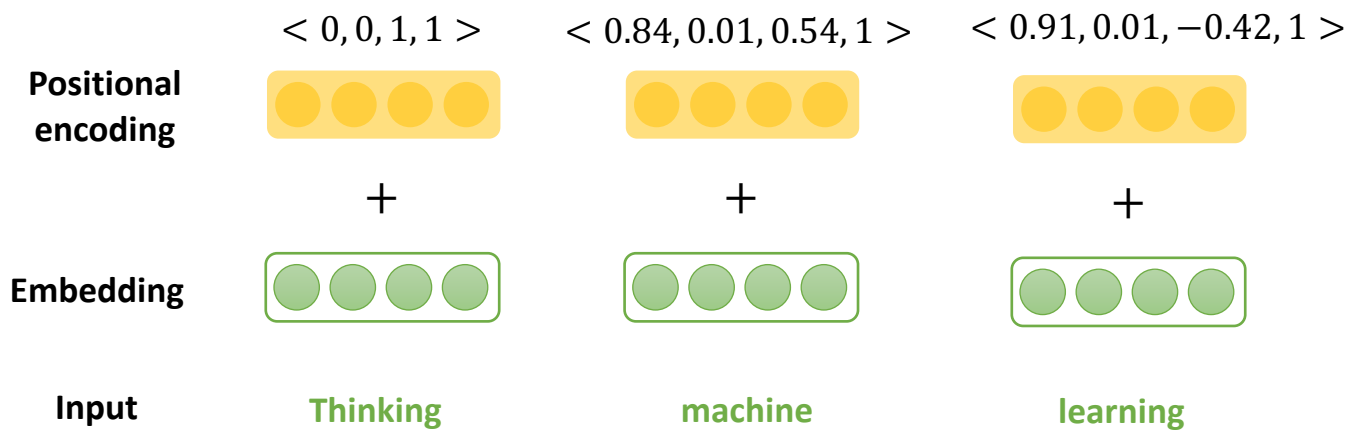
- Need to consider the order of the words in the input sentence.





Positional Encoding

- Assume that embedding has a dimensionality of 4.
- The positional embedding would look like this:
  - Use cosine and sine curves.

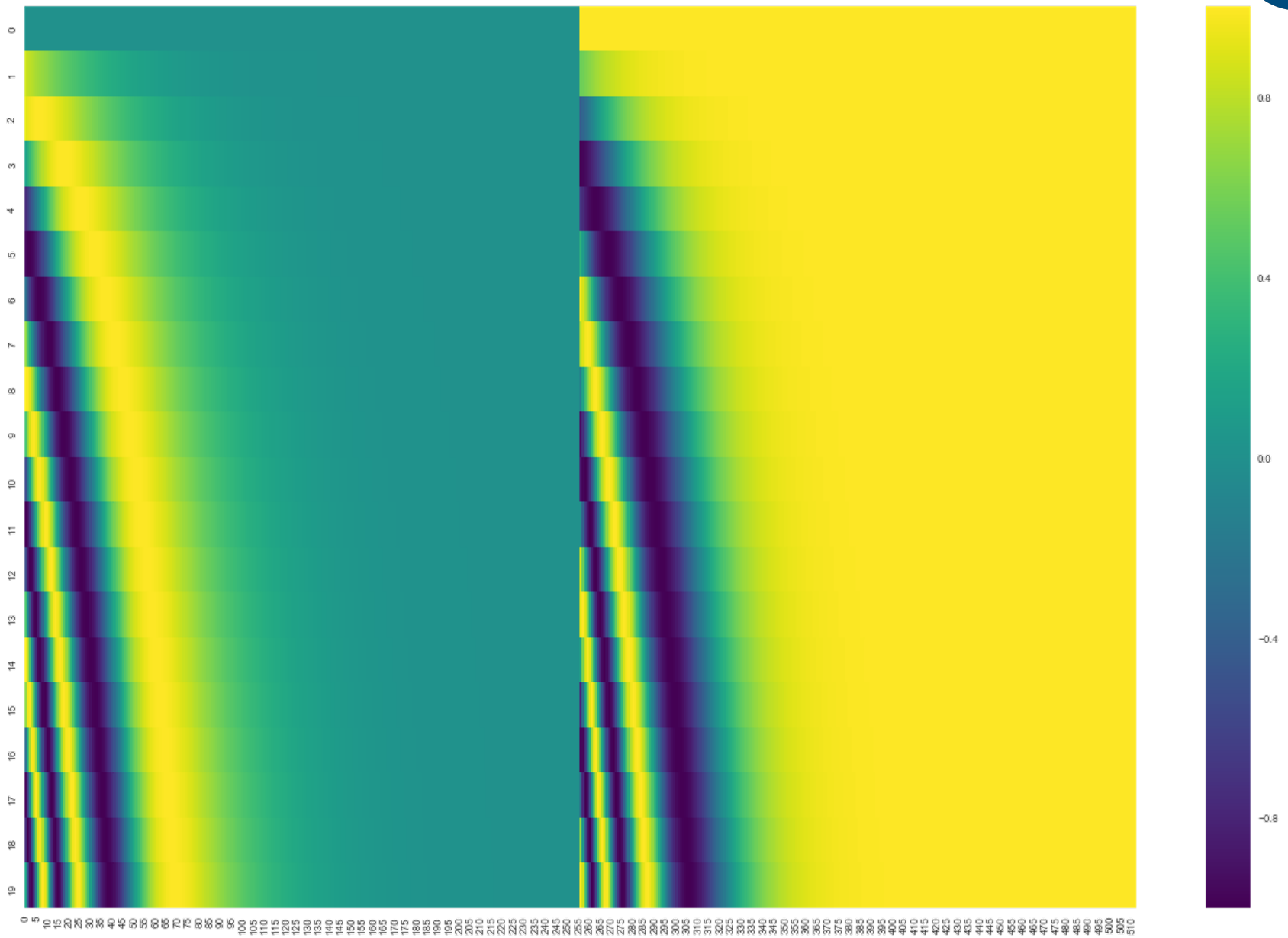


$$PE_{(pos,2i)} = sin(pos/10000^{2i/d_{model}})$$

$$PE_{(pos,2i+1)} = cos(pos/10000^{2i/d_{model}})$$

Positional Encoding

Each row corresponds to the a positional encoding of size 512.

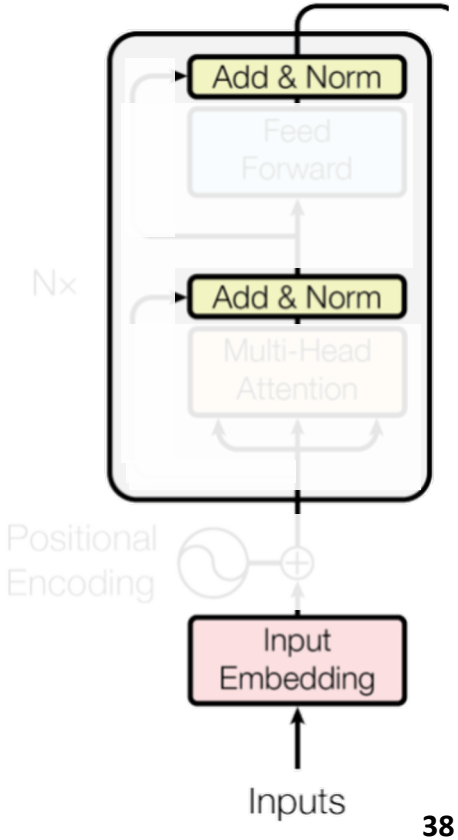


Complete Transformer Block

- **Each block has two sublayers.**
  - Multi-head attention
  - 2 layer feed-forward net (with relu)
- **Each of these two steps also has:**
  - **Residual (short-circuit) connection** and **LayerNorm**:

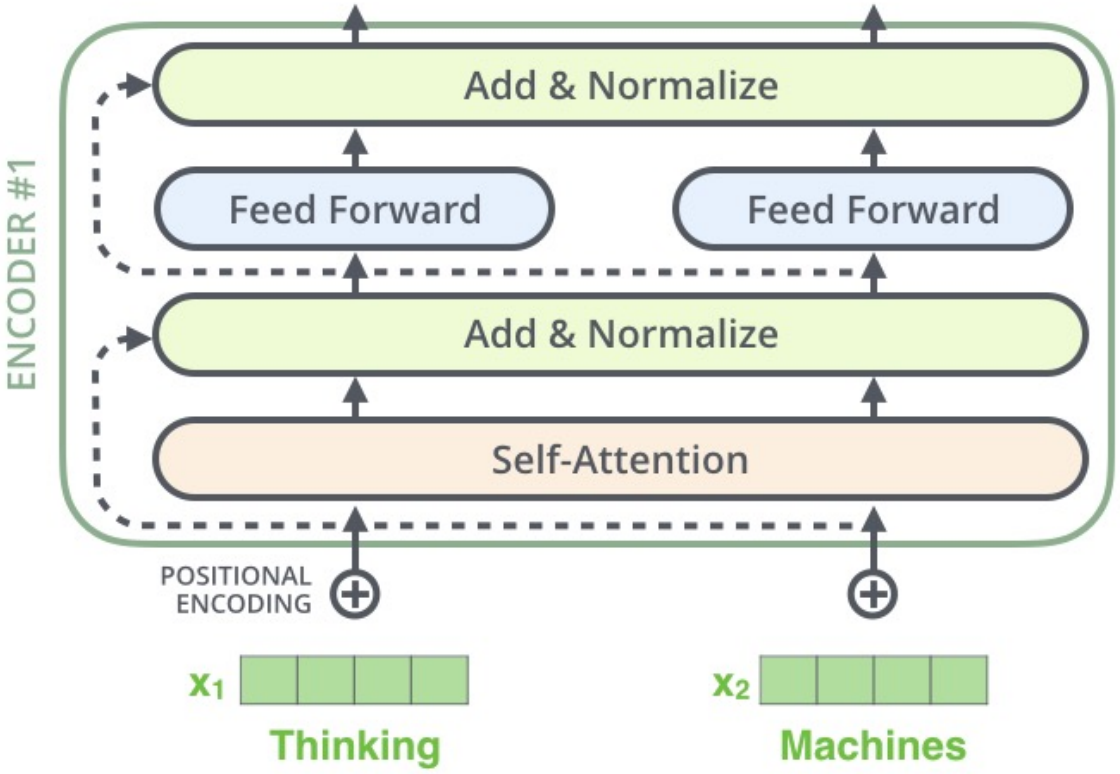
$$LayerNorm(X + Sublayer(X))$$

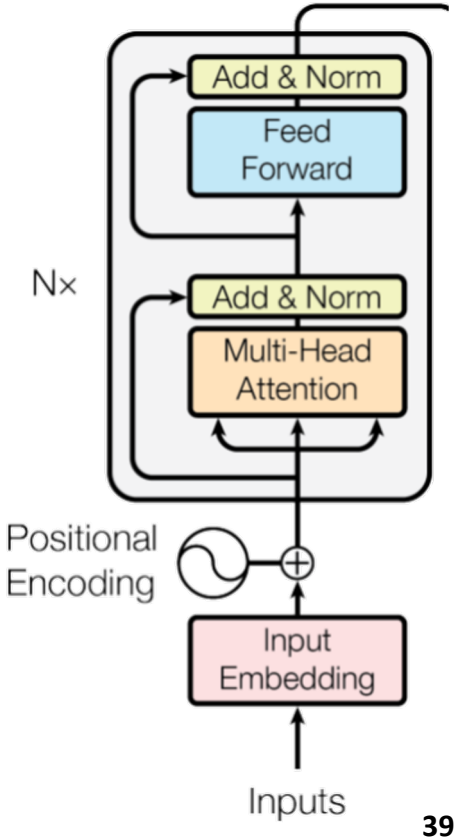
- **Layer normalization**
  - https://arxiv.org/pdf/1607.06450.pdf



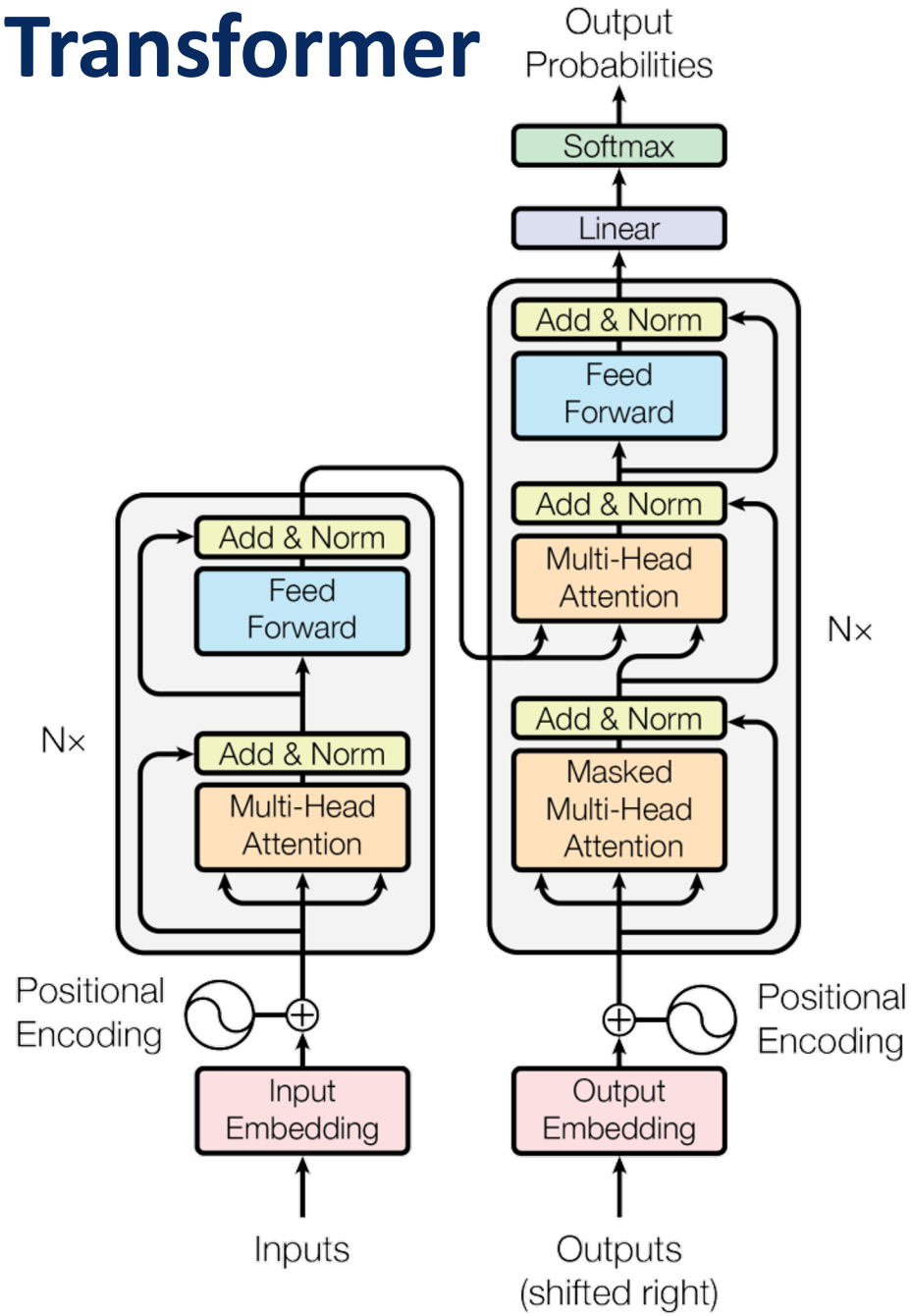
Residual Connection

- **Each sublayer in each encoder has a residual connection.**



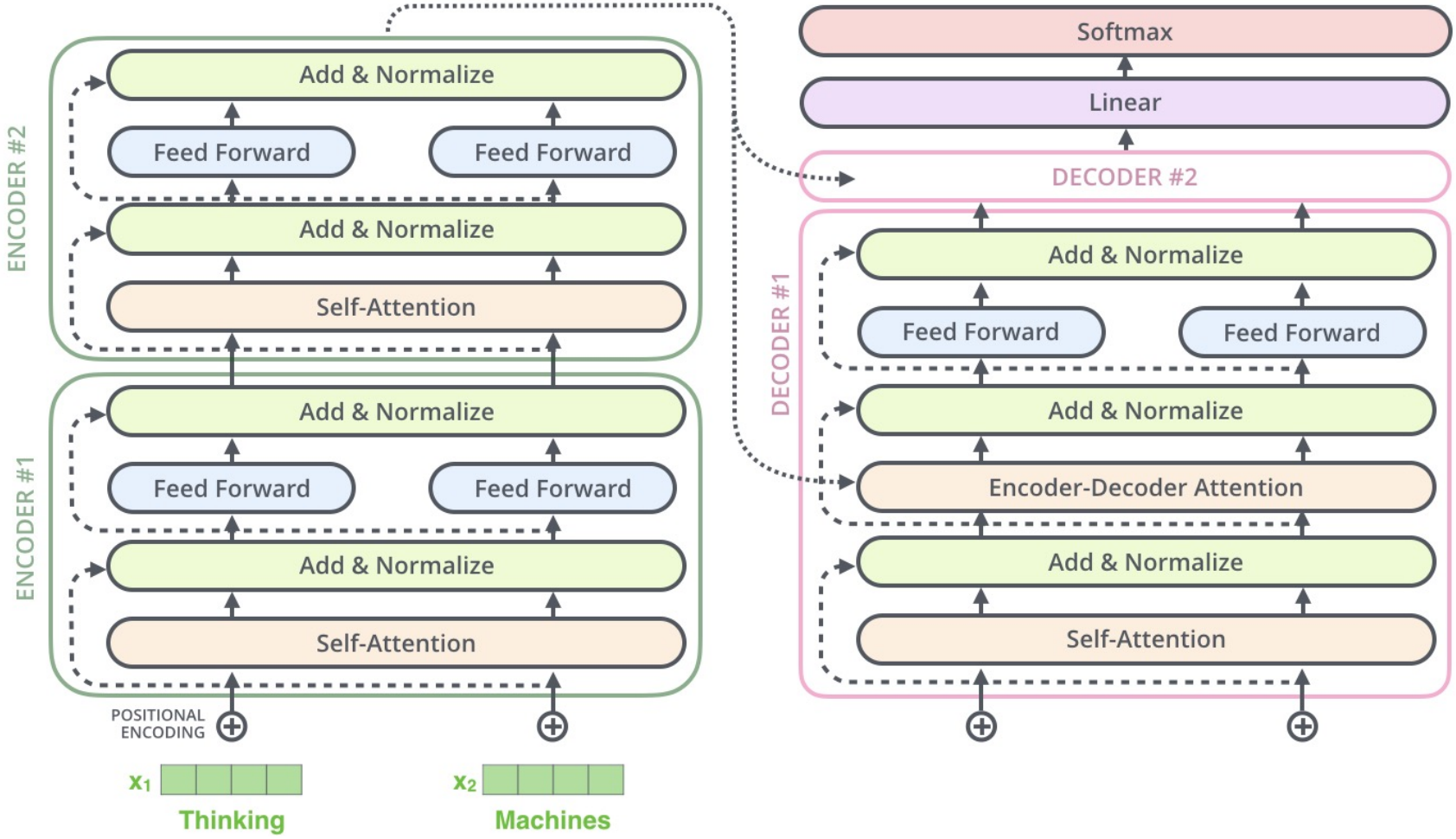


Simplified Transformer



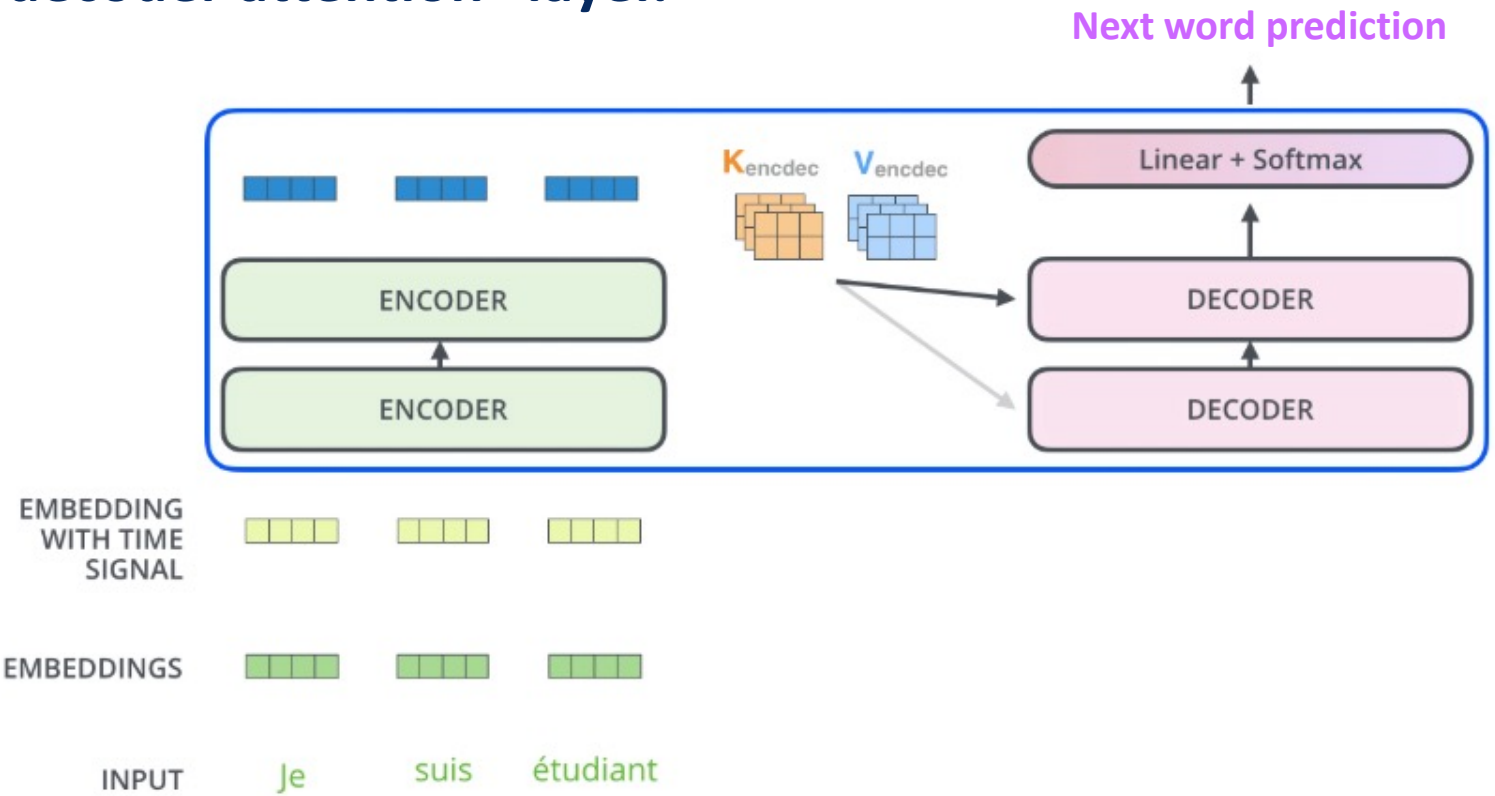
Simplified Transformer

- It consists of 2 stacked encoders and decoders.



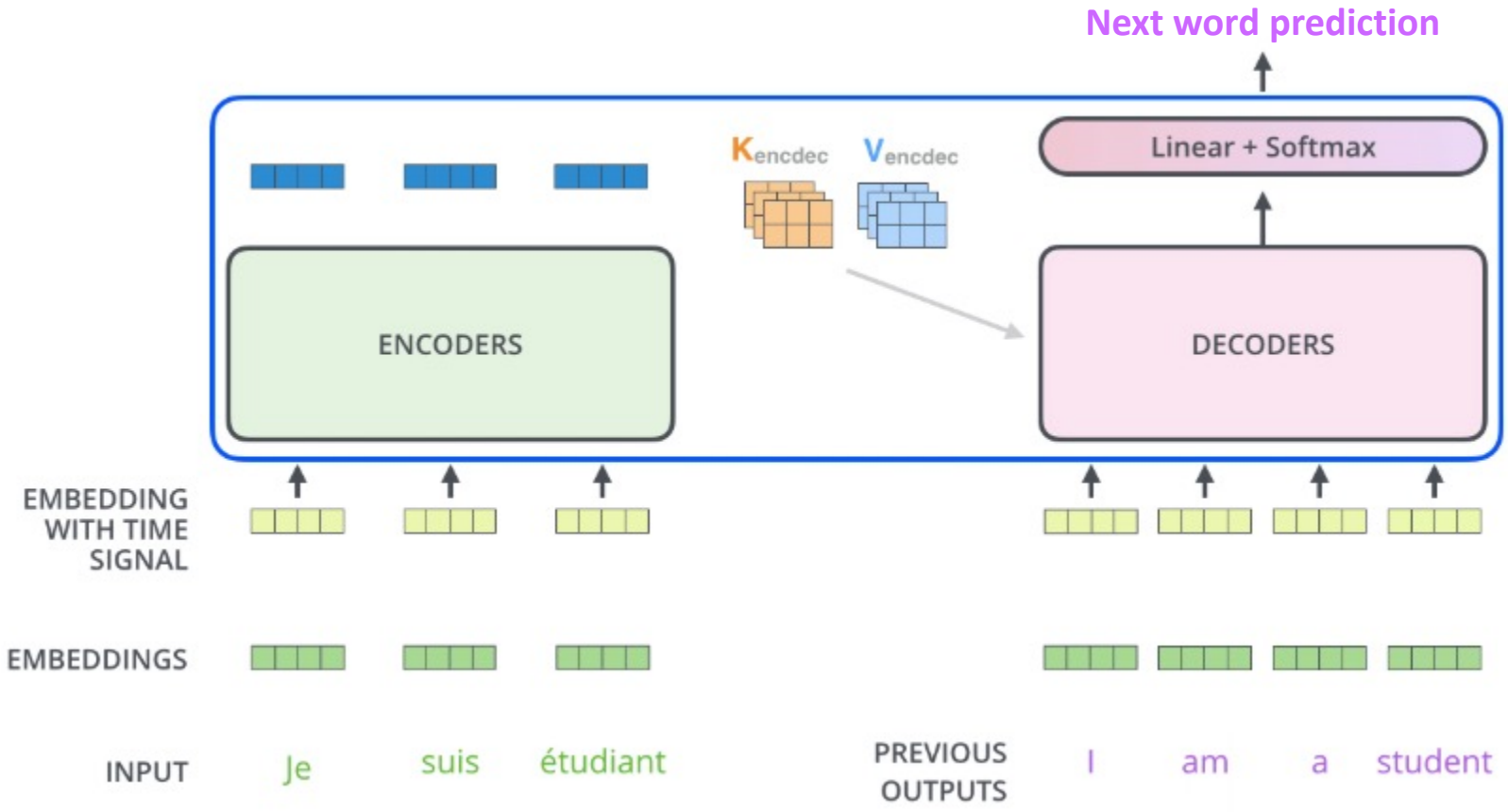
Decoder: Encoder-Decoder Attention

- The output of the top encoder is then transformed into a set of attention vectors K and V.
- These are to be used by each encoder in its "encoder-decoder attention" layer.



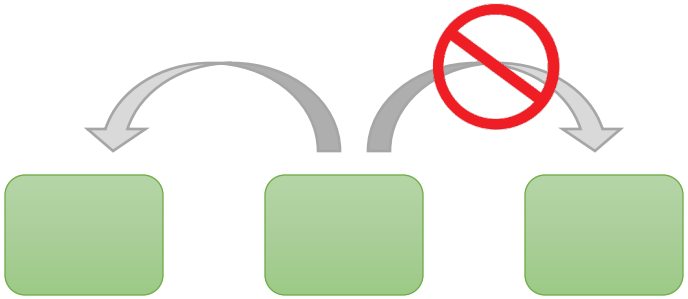
Decoder: Encoder-Decoder Attention

- The self-attention layer in the decoder is only allowed to attend to earlier positions in the output sequence.



Decoder: Encoder-Decoder Attention

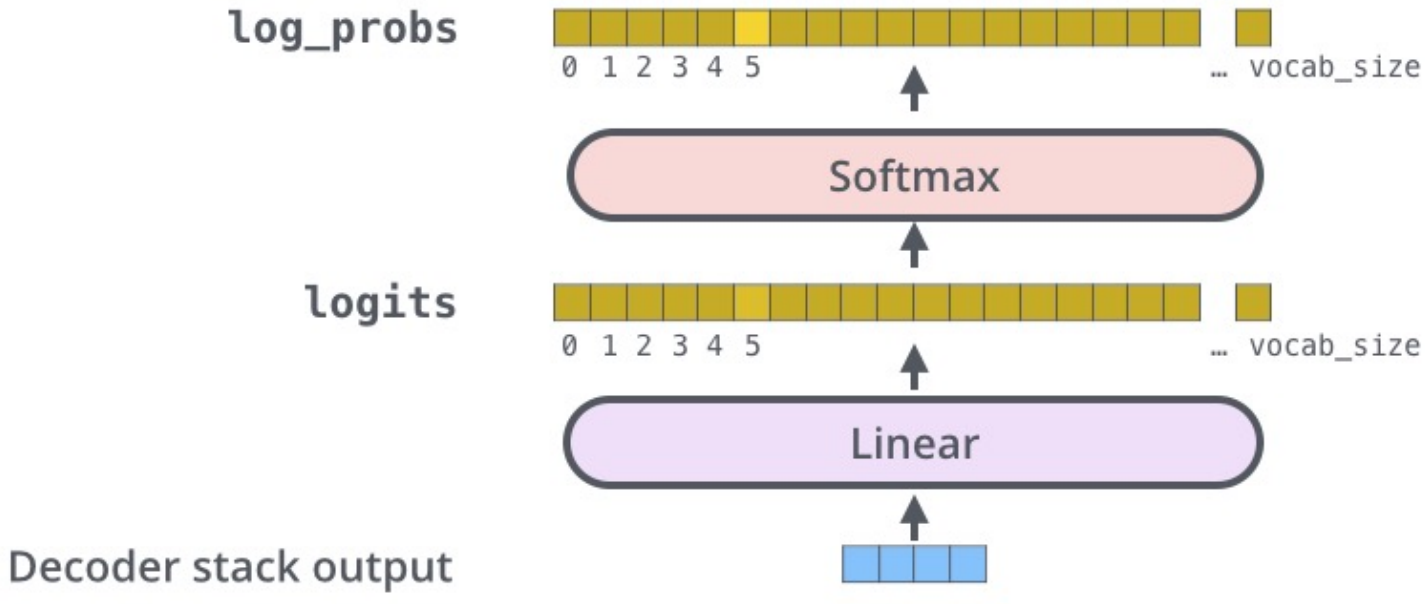
- **2 sublayer changes in decoder.**
- **Masked decoder**
  - Self-attention on previously generated outputs is only used.



- **Encoder-decoder attention**
  - Queries come from previous decoder layer and keys and values come from output of encoder.

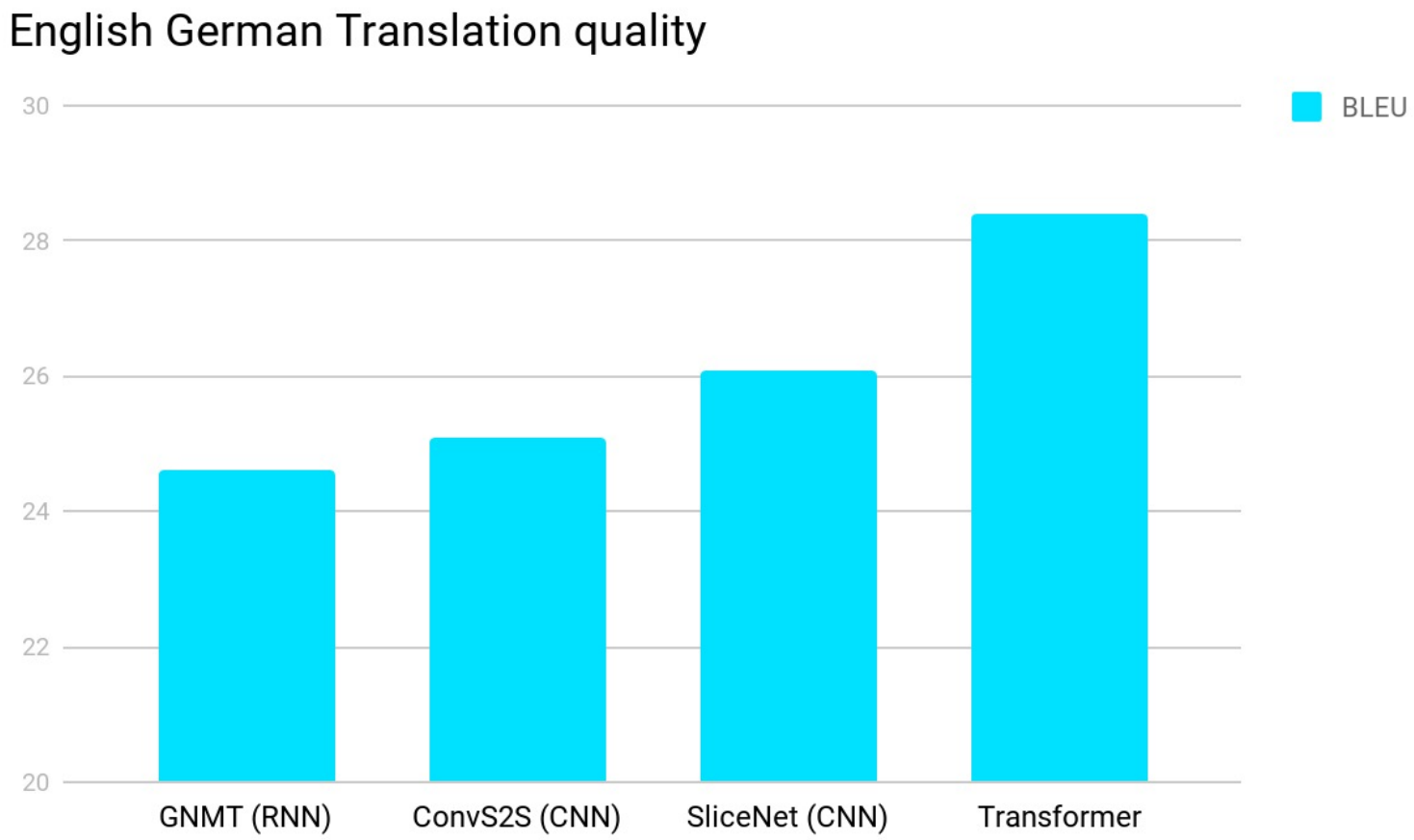
Final Linear and Softmax Layer

- The Linear layer is a simple fully connected neural network that projects the vector produced by the stack of decoders, into a much, much larger vector called a logits vector.
- The softmax layer then turns those scores into probabilities (all positive, all add up to 1.0).



Experimental Results

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



Experimental Results

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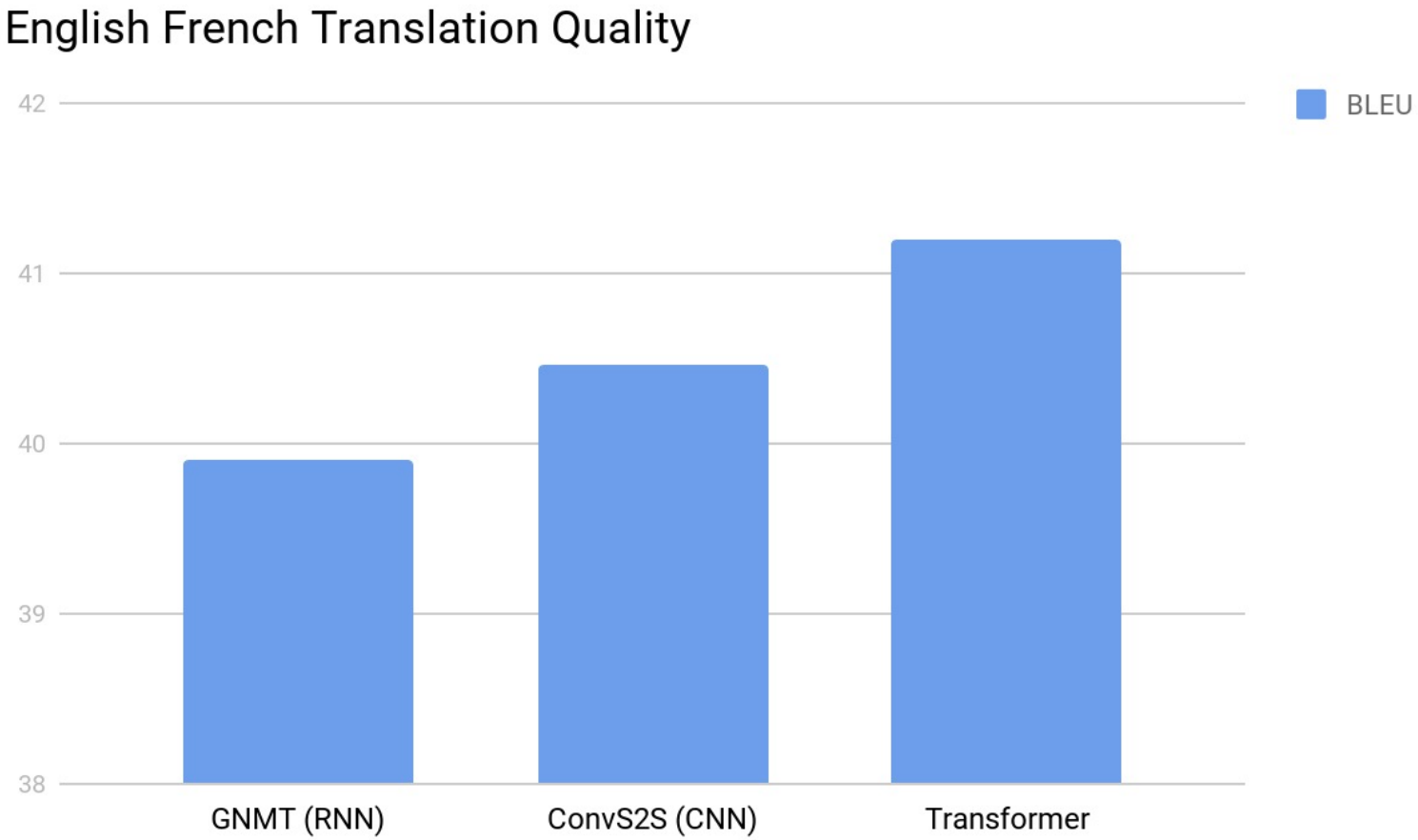

Experimental Results

- **The Transformer achieves better BLEU scores than the previous model, and training cost is much smaller.**

Model	BLEU		Training Cost (FLOPs)	
	EN-DE	EN-FR	EN-DE	EN-FR
ByteNet [18]	23.75			
Deep-Att + PosUnk [39]		39.2		$1.0 \cdot 10^{20}$
GNMT + RL [38]	24.6	39.92	$2.3 \cdot 10^{19}$	$1.4 \cdot 10^{20}$
ConvS2S [9]	25.16	40.46	$9.6 \cdot 10^{18}$	$1.5 \cdot 10^{20}$
MoE [32]	26.03	40.56	$2.0 \cdot 10^{19}$	$1.2 \cdot 10^{20}$
Deep-Att + PosUnk Ensemble [39]		40.4		$8.0 \cdot 10^{20}$
GNMT + RL Ensemble [38]	26.30	41.16	$1.8 \cdot 10^{20}$	$1.1 \cdot 10^{21}$
ConvS2S Ensemble [9]	26.36	**41.29**	$7.7 \cdot 10^{19}$	$1.2 \cdot 10^{21}$
Transformer (base model)	27.3	38.1	**$3.3 \cdot 10^{18}$**	
Transformer (big)	**28.4**	**41.8**	$2.3 \cdot 10^{19}$	

Q&A