CIS 6930 Topics in Computing for Data Science
Week 8: Transformers (1)+(2)

10/21/2021

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2pm-3:20pm

Week 8: Transformers

- **Week 8: Transformers**
- **Week 9: Pre-trained Language Models**
- Week 10: More Machine Learning Techniques
- Week 11: More Deep Learning Techniques for NLP (Text generation, Text summarization, Information Extraction etc.)
- Week 12: Advanced Techniques and Challenges
- Week 13: Final project presentations

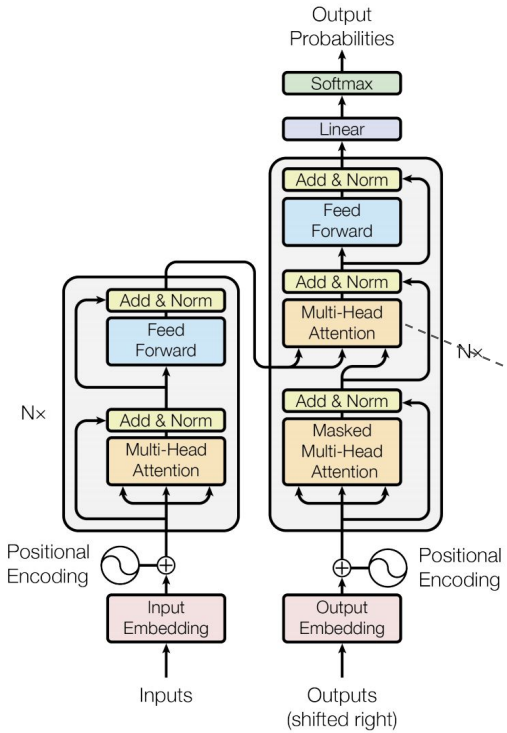
Attention!

- Today’s content is extremely important for understanding modern Deep Learning techniques

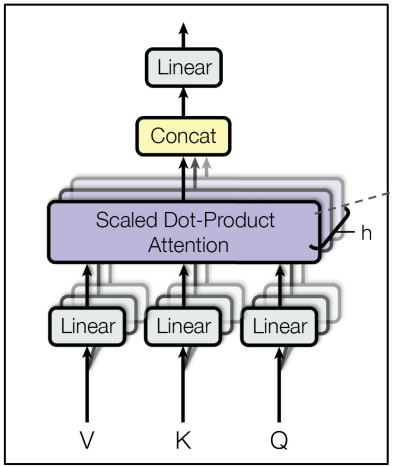
- The content might be technically difficult and complicated 
  - Don’t worry. The concept is relatively simple

- Please make sure that you follow the explanation of each step
  - Don’t hesitate to interrupt and ask questions if you don’t

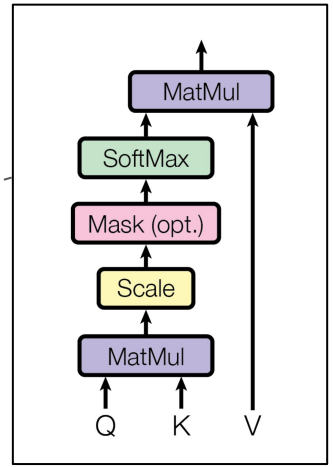
This Week's Goal:
Understanding the Transformer Architecture



Model Architecture



Multi-Head Attention

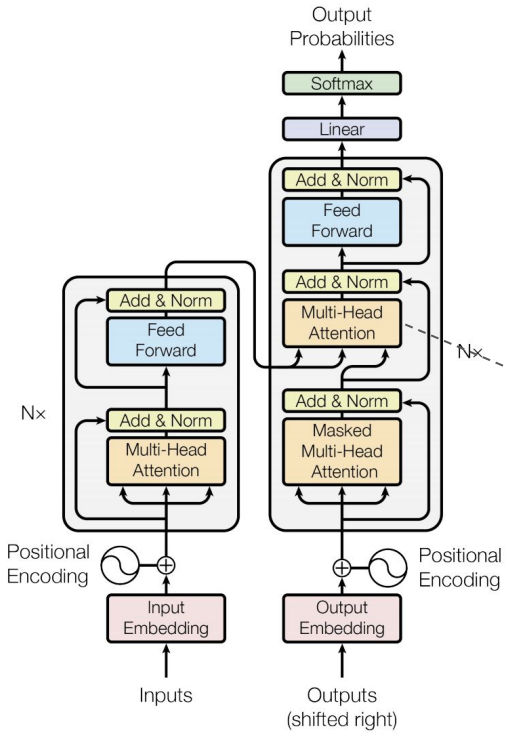


Scaled Dot-Product Attention

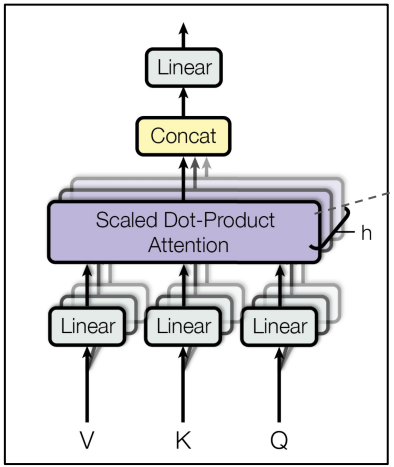
The Transformer: Basic Concepts

The figures and explanations are from the following excellent blog article (highly recommended)
The Illustrated Transformer – Jay Alammar – Visualizing machine learning one concept at a time.

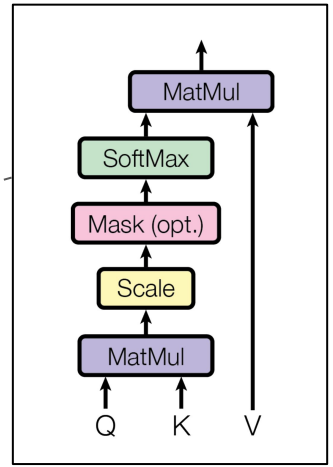
The Transformer



Model Architecture



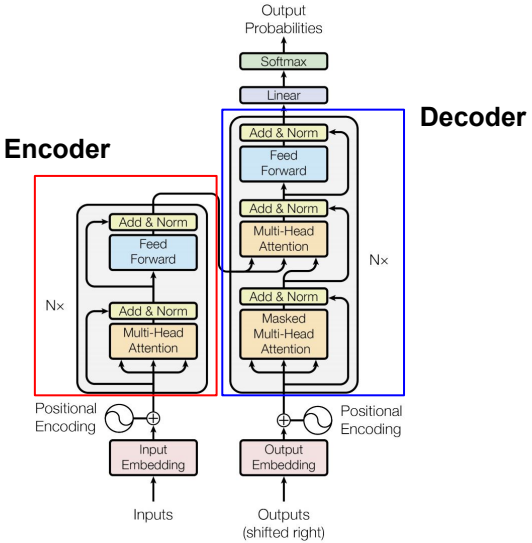
Multi-Head Attention



Scaled Dot-Product Attention

What is the Transformer?

- Transformer is an **Encoder-Decoder model!**
  - Can be used for any sequence-to-sequence generation tasks
- Transformer = **Transformer Encoder** + **Transformer Decoder**



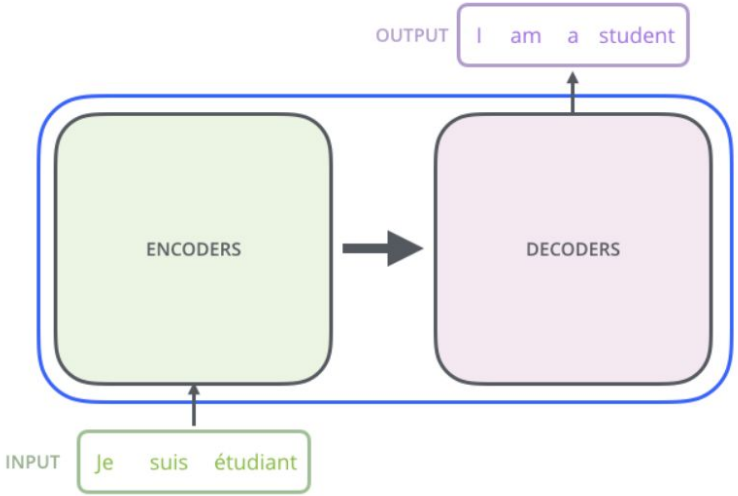
Transformer

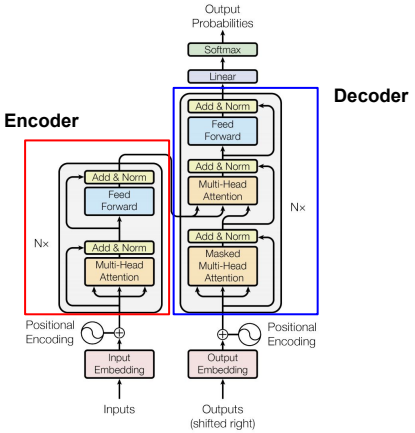
100%

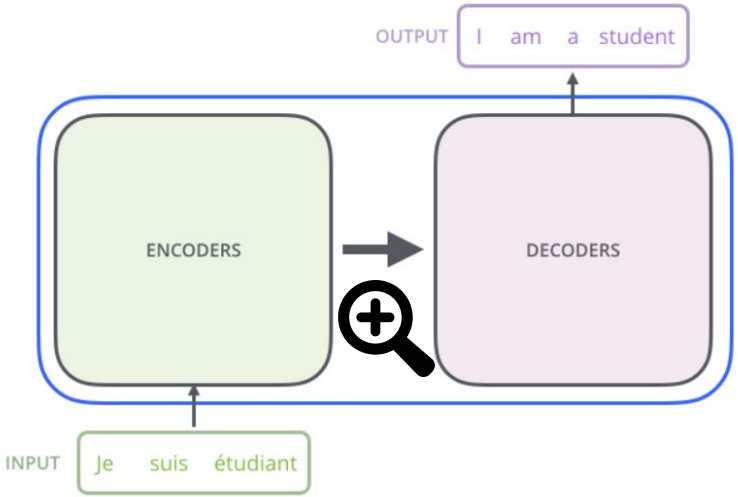
Transformer

100%

150%

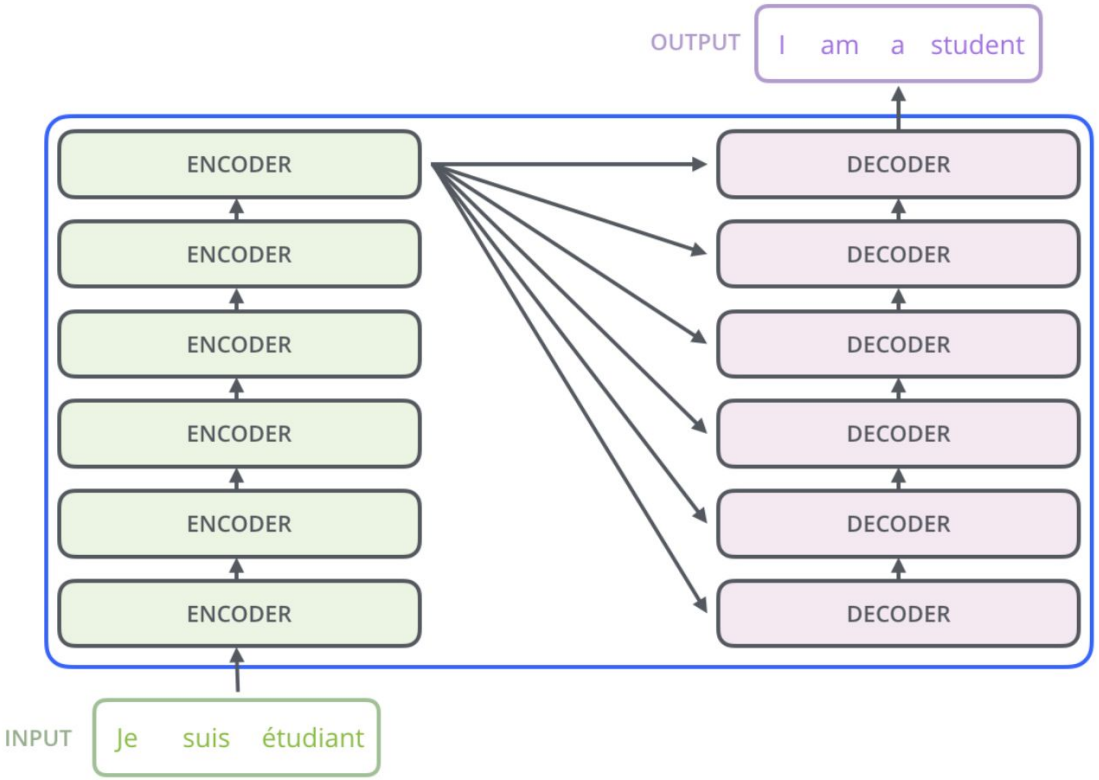

OUTPUT
I am a student
ENCODERS
DECODERS
INPUT
Je suis étudiant

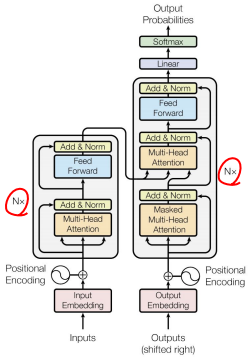

Output Probabilities
Softmax
Linear
Encoder
Decoder
Add & Norm
Feed Forward
Add & Norm
Multi-Head Attention
Add & Norm
Masked Multi-Head Attention
Add & Norm
Feed Forward
Add & Norm
Multi-Head Attention
N×
N×
Positional Encoding
Positional Encoding
Input Embedding
Output Embedding
Inputs
Outputs (shifted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


OUTPUT
I am a student
ENCODERS
DECODERS
INPUT
Je suis étudiant

Encoder/Decoder
= Stack of Encoder/Decoder Blocks

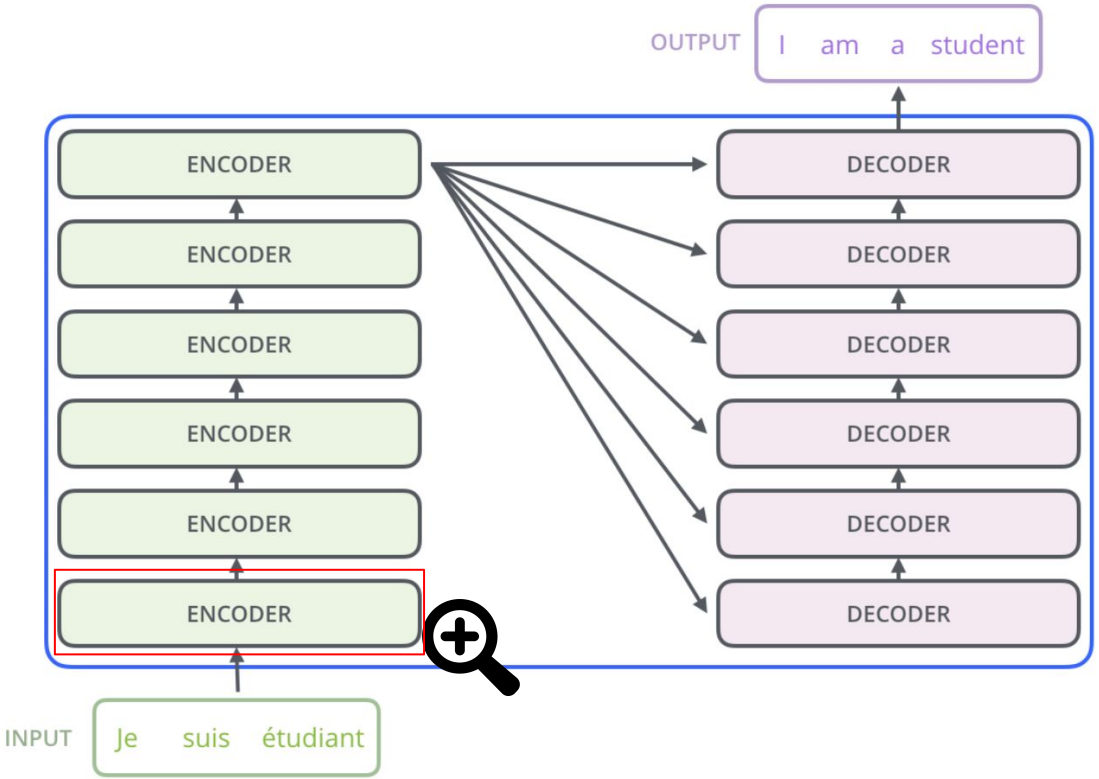
300%



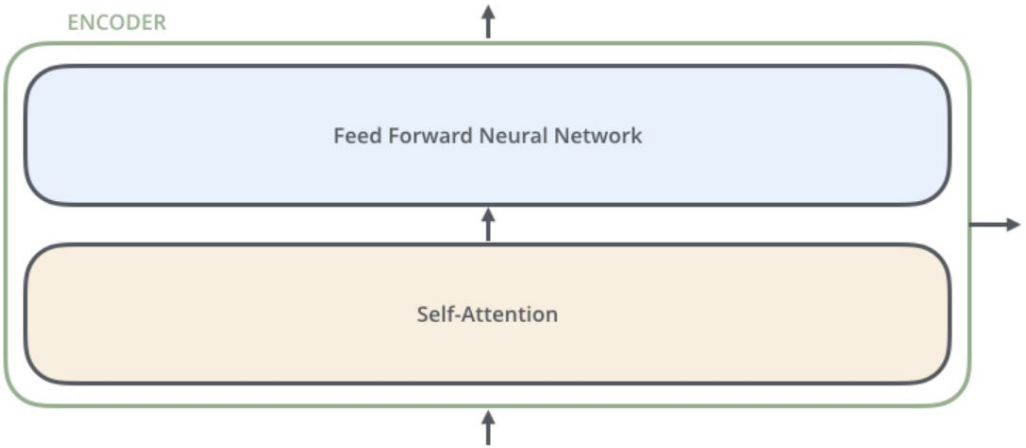


Encoder/Decoder
= Stack of Encoder/Decoder Blocks

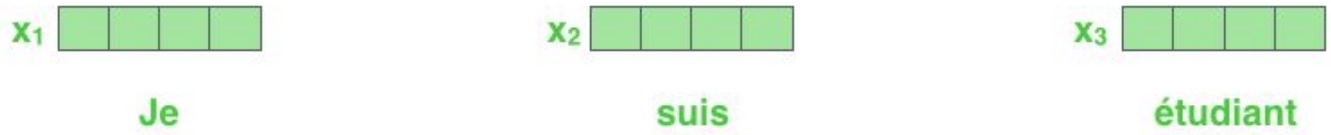
300%



Encoder Block
= Self-Attention + Feed Forward NN

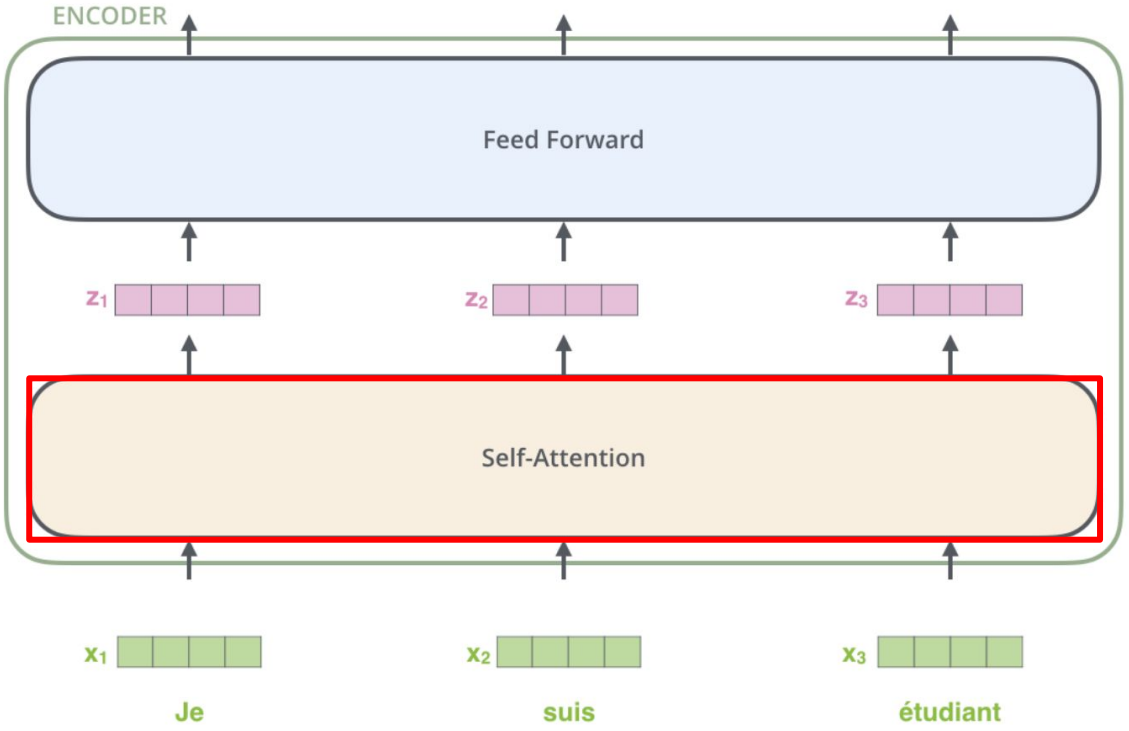


Step 1: Input Tokens → Token Embeddings



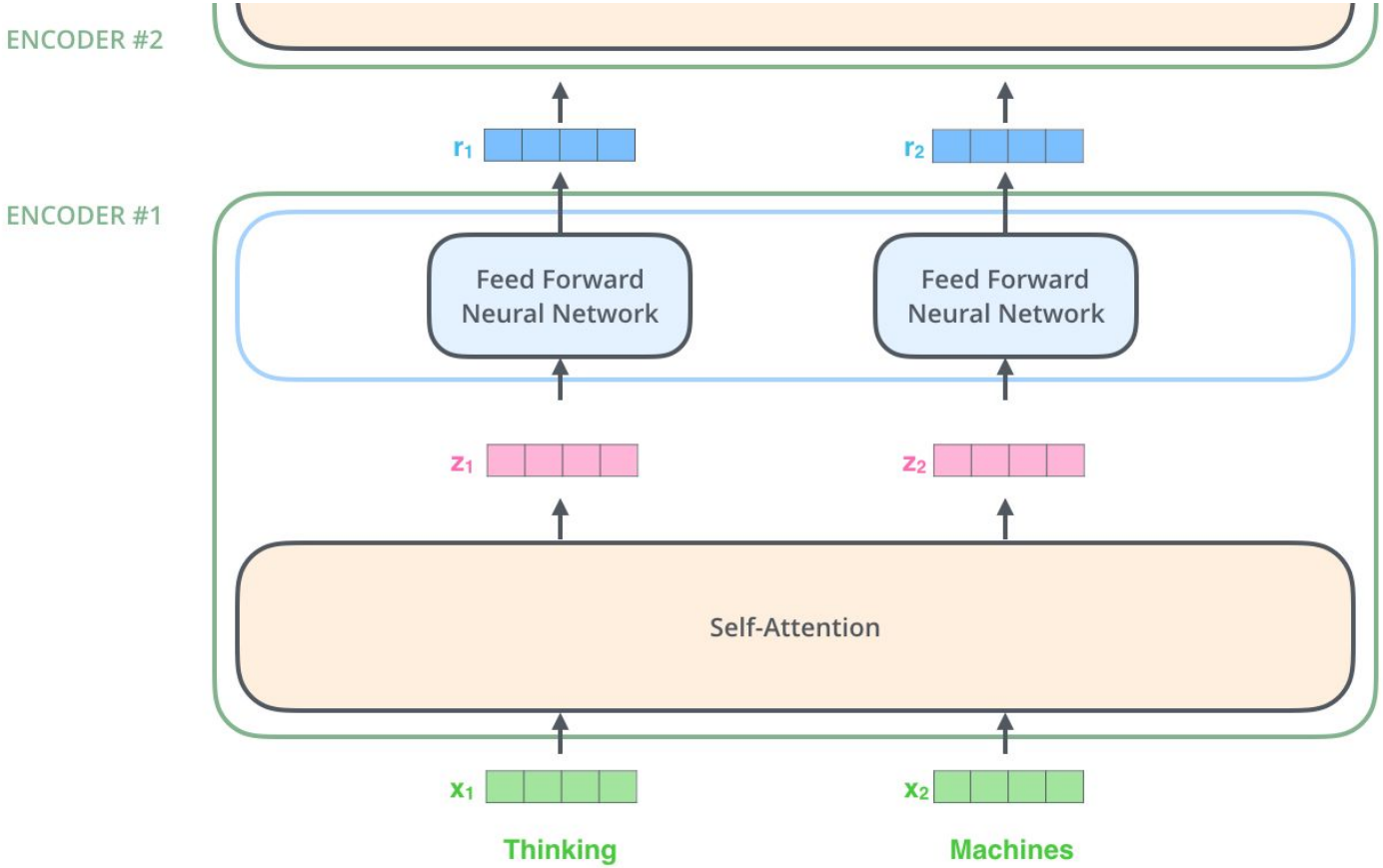
Will come back to the positional encoding later

Step 2: Token Embeddings → Attention Vectors

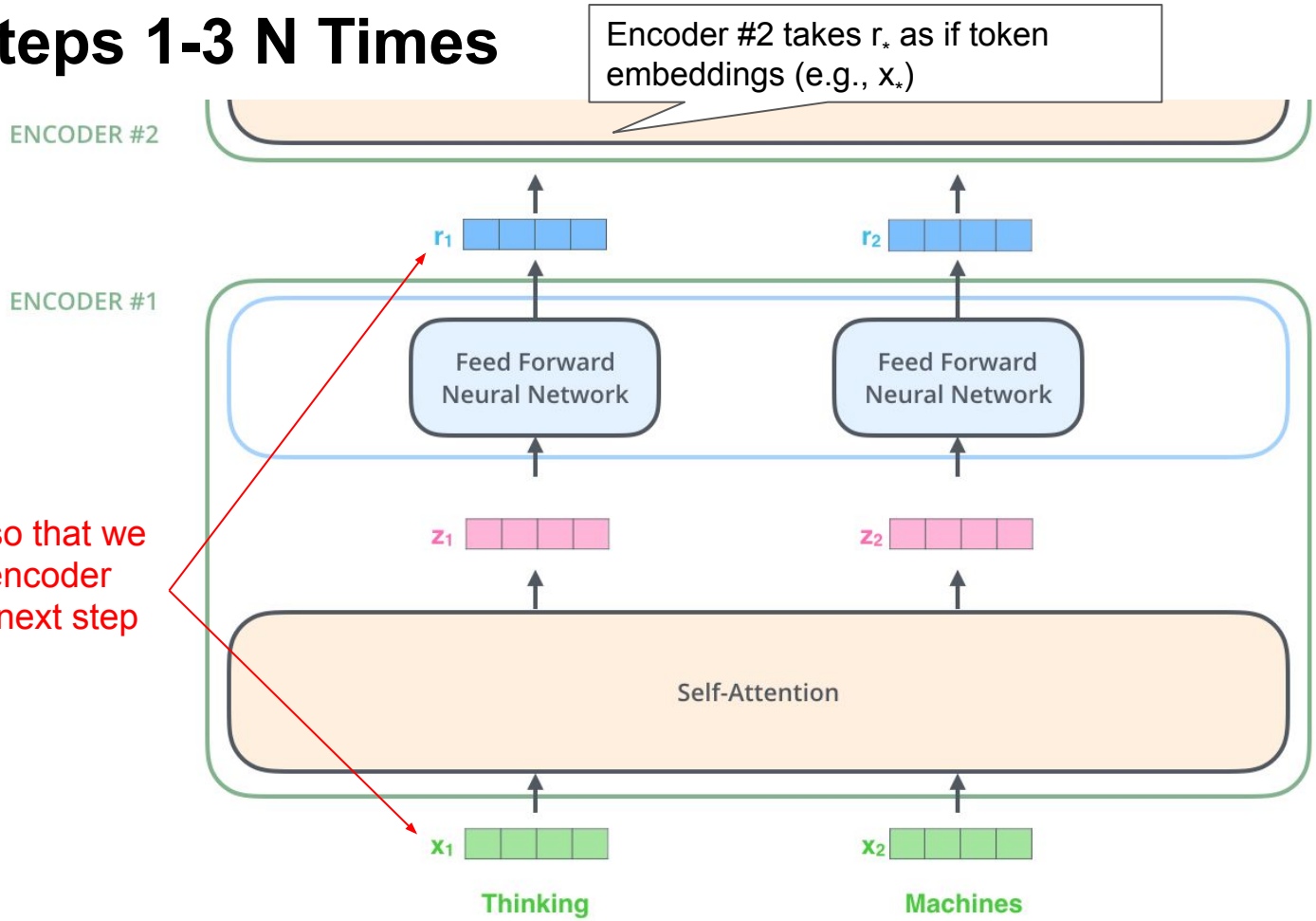


← Attention vectors

Step 3: Attention Vectors → Output Vectors



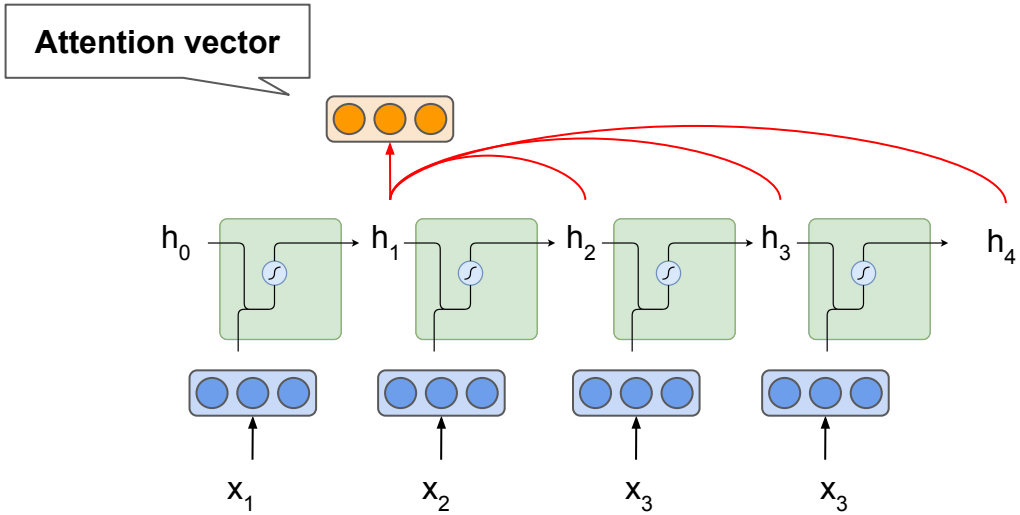
Repeat Steps 1-3 N Times



Same dimensions so that we can use the same encoder architecture as the next step

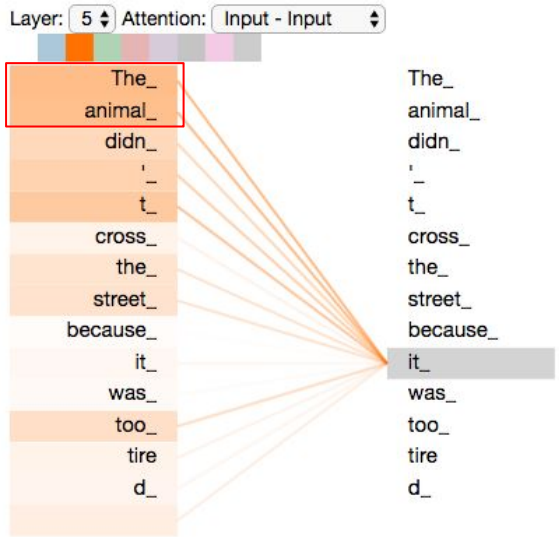
Self-Attention in Detail

Recap: Self-Attention for RNNs



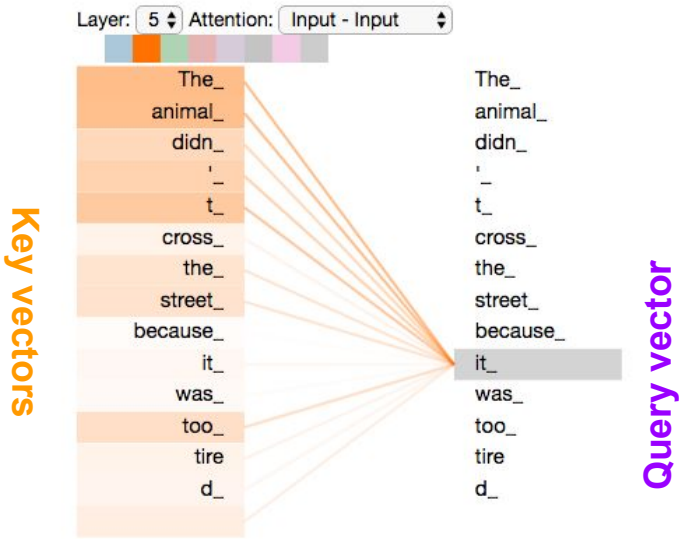
Self-Attention: Key Idea

- Self-Attention looks at **all tokens** in the input sequence to calculate **the target token embedding** based on the context
- Example: “The animal didn’t cross the street because **it** was too tired.”



Self-Attention: Key, Query, Value Vectors

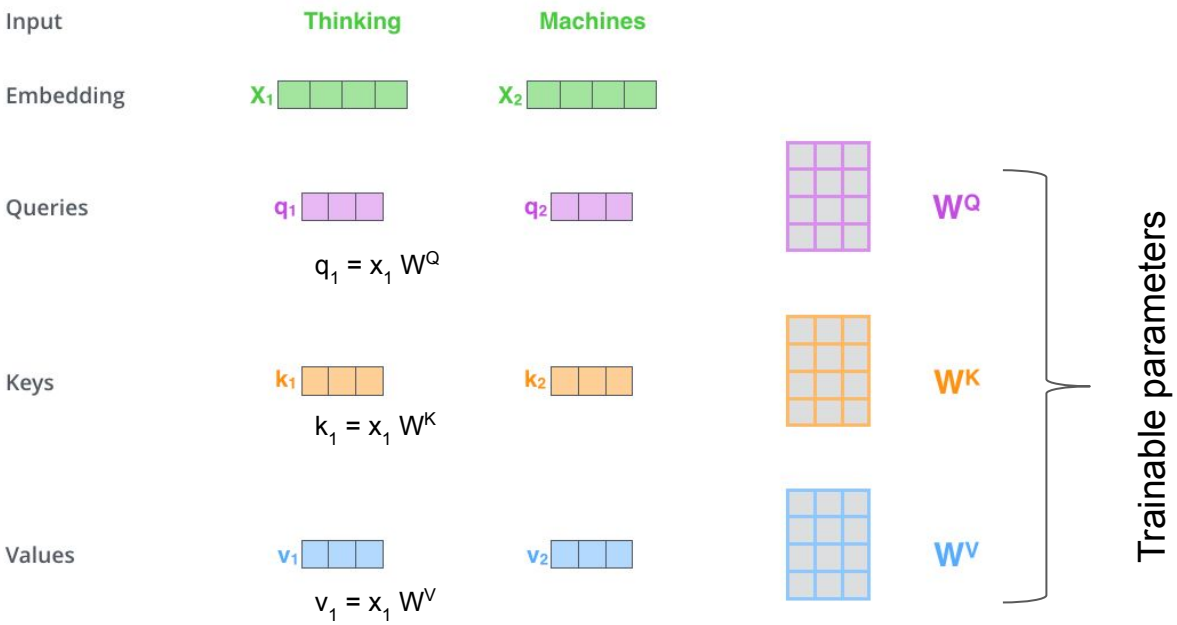
- The Self-Attention Layer encodes token embeddings by averaging **Value vectors** of input tokens based on the similarities between **Key vectors** of input tokens and **Query vector** of the target token



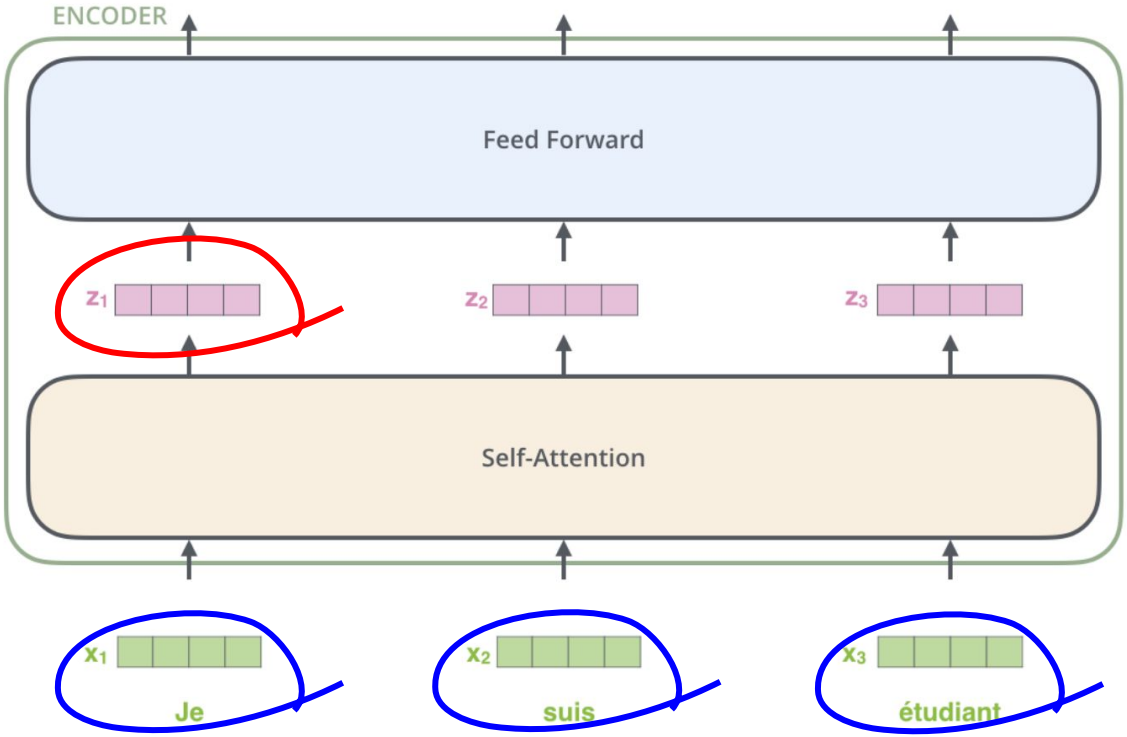
x **Value vectors** **= Attention vector**

Token Embeddings → Query, Key, Value Vectors

- Self-attention layer has **transformation matrices** for Query, Key, and Value vectors



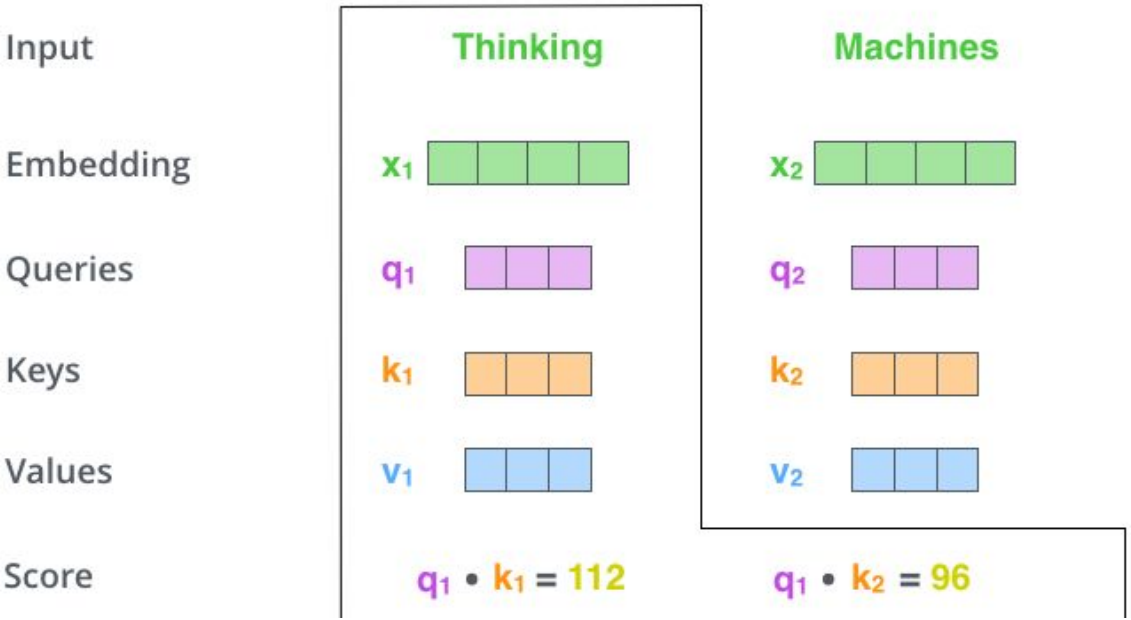
Calculating z_1 from Input Token Embeddings x_{1-3}



Example: Calculating Attention Vector for “Thinking”

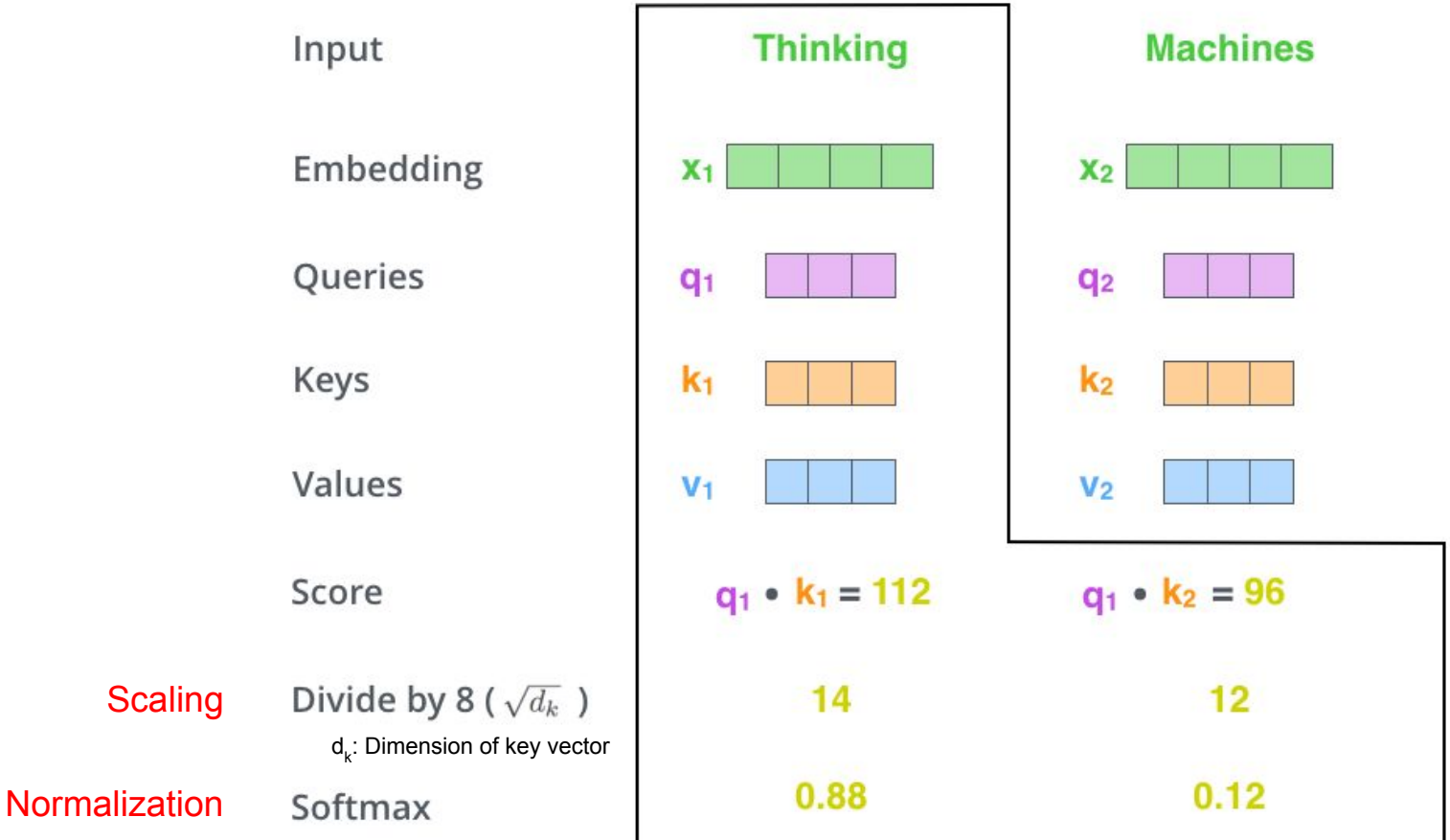
Step 1: Query-Key Similarity Calculation

- The inner product of q_1 and k_*



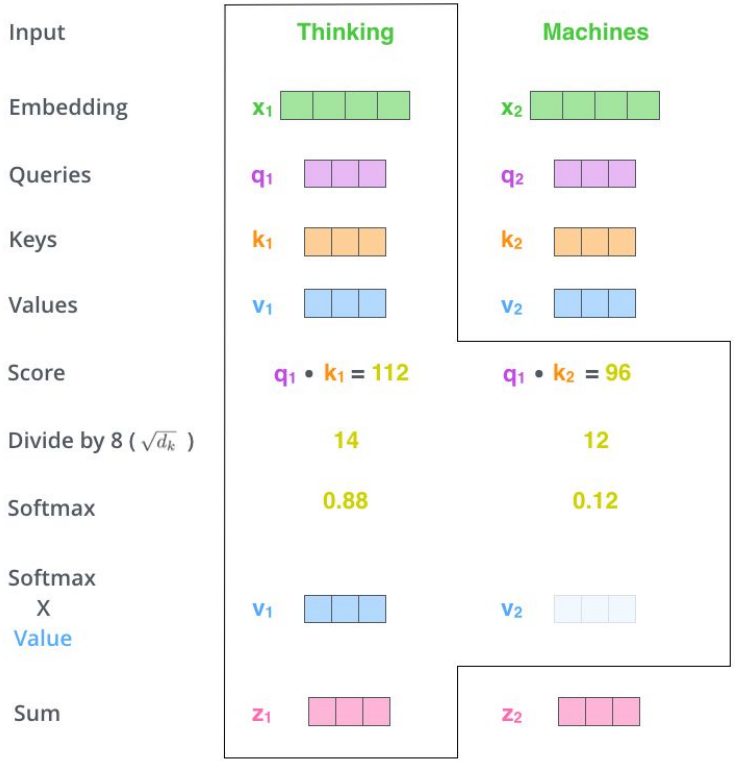
Example: Calculating Attention Vector for “Thinking”

Step 2: Scaling and normalization



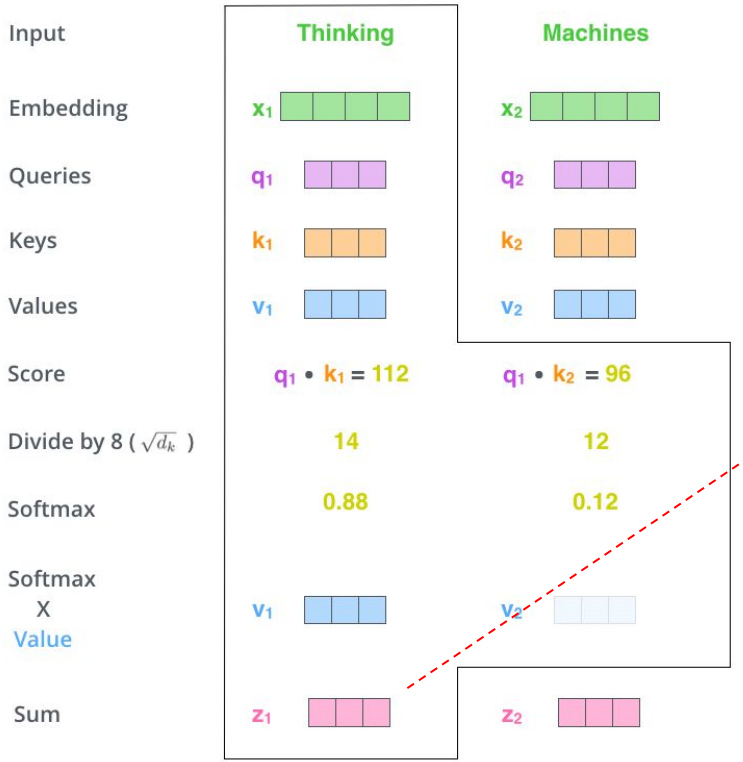
Example: Calculating Attention Vector for “Thinking”

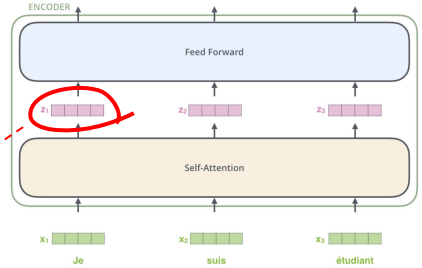
Step 3: Weighted Average of Value Vectors



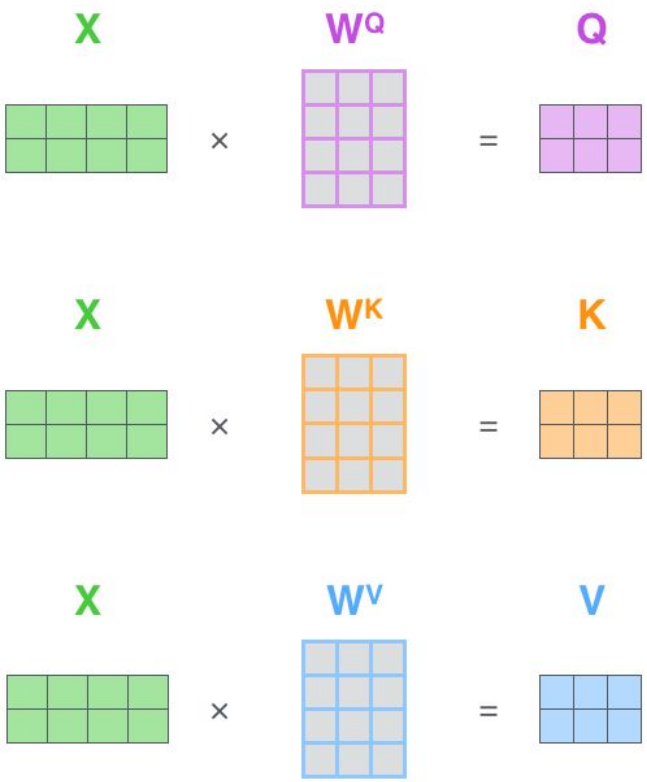
Example: Calculating Attention Vector for “Thinking”

Step 3: Weighted Average of Value Vectors



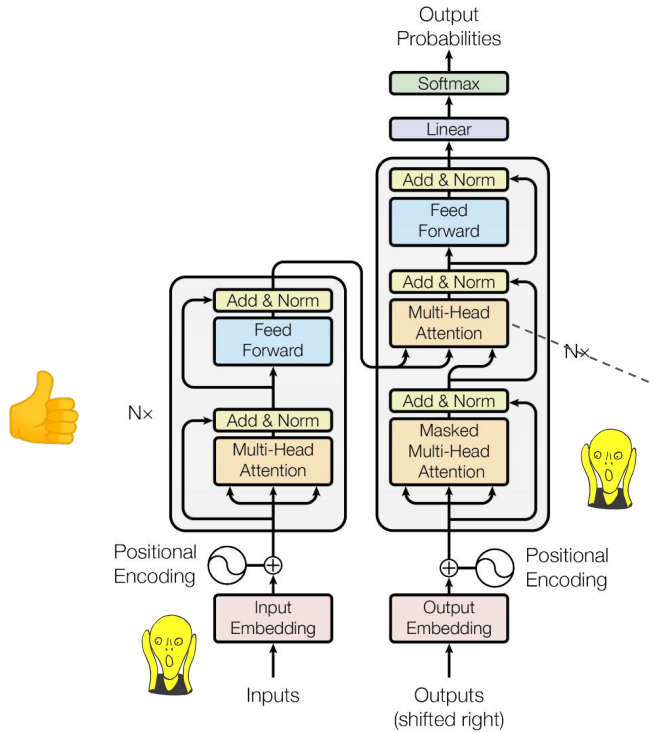


Understanding Self-Attention in Matrix Calculation

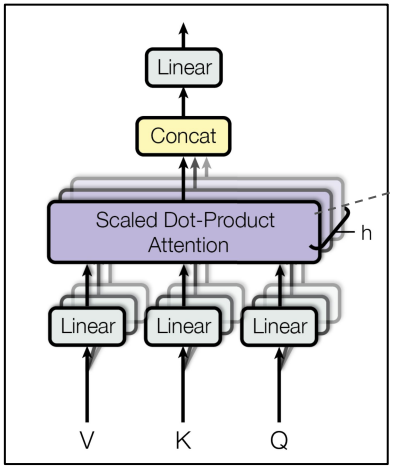


$$\text{softmax}\left(\frac{Q \times K^T}{\sqrt{d_k}}\right) V = Z$$

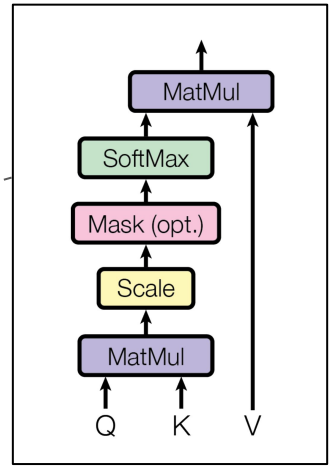
The Transformer



Model Architecture



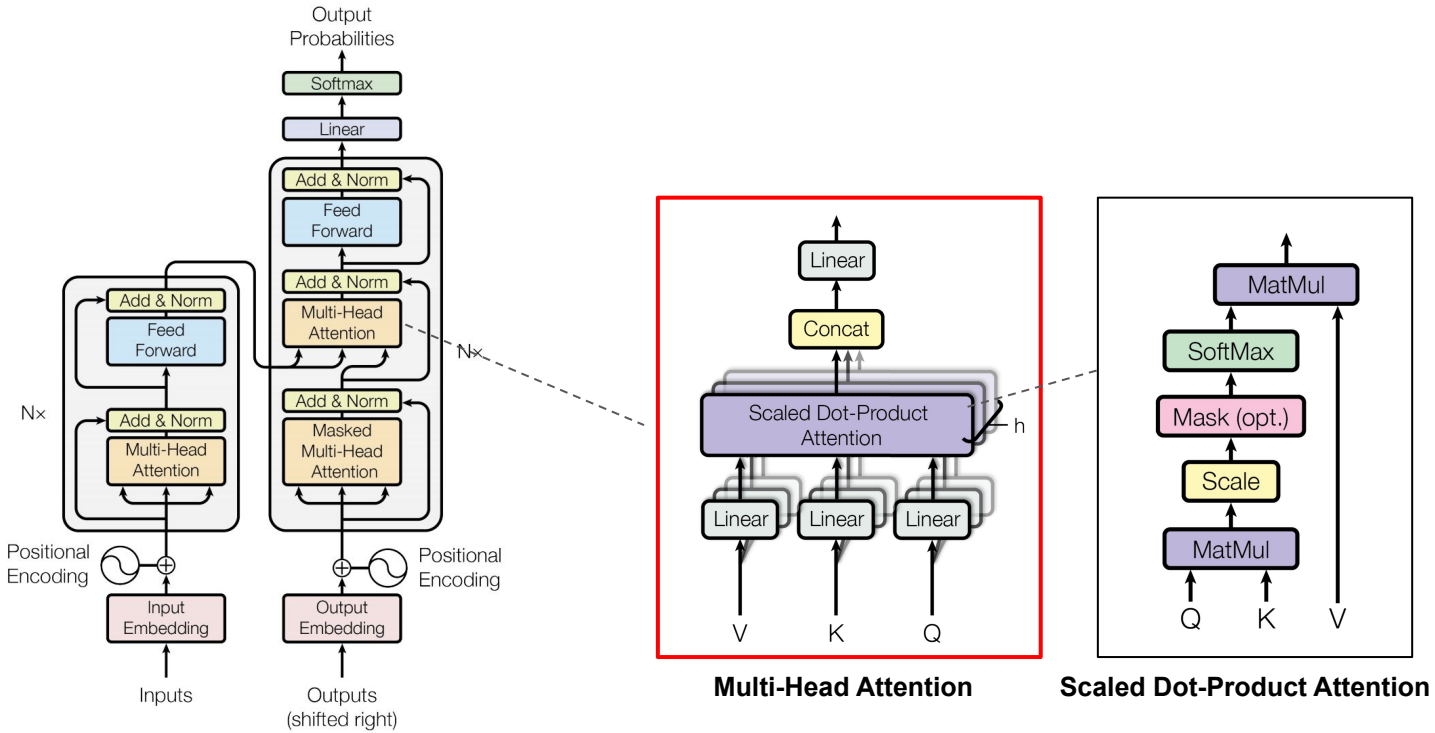
Multi-Head Attention



Scaled Dot-Product Attention

Multi-head Attention!

Multi-head Attention for Multiple K, Q, V Representations

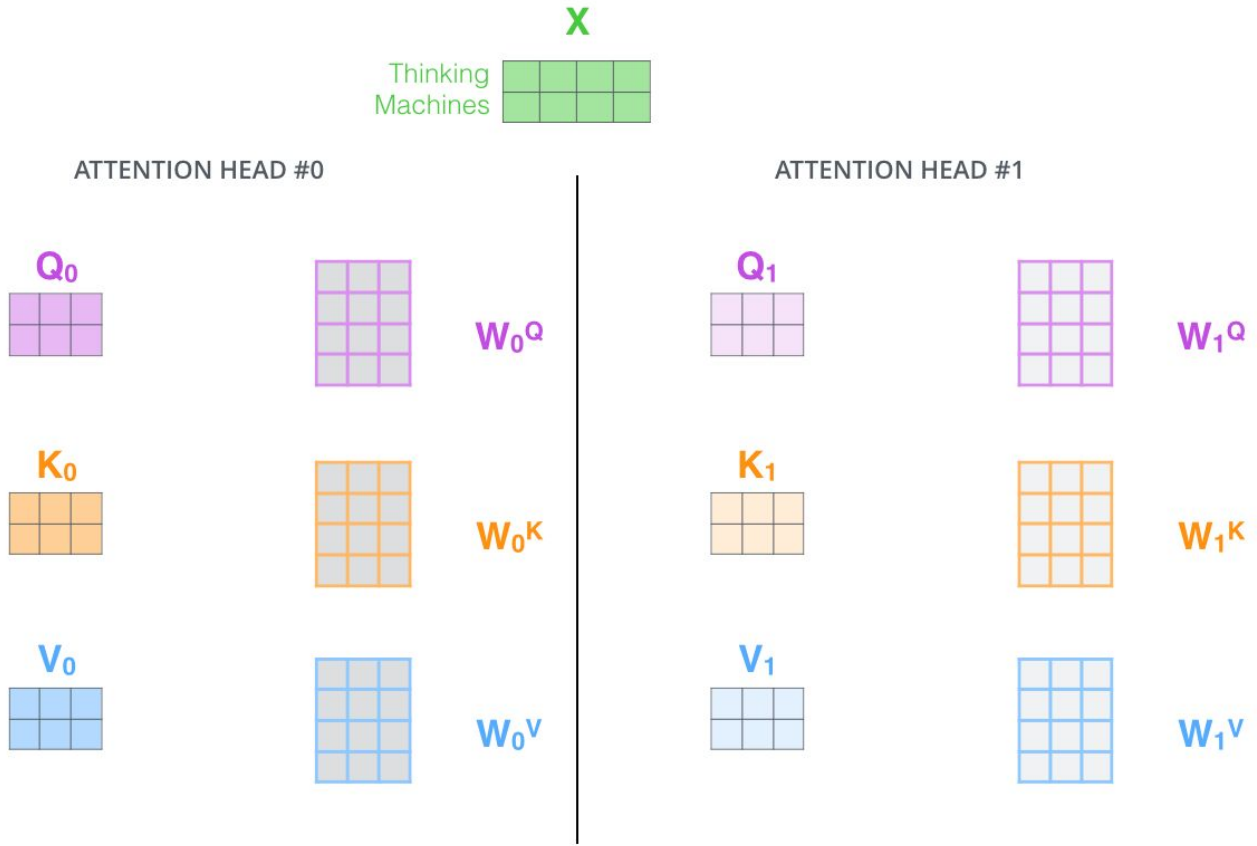


Model Architecture

Multi-Head Attention

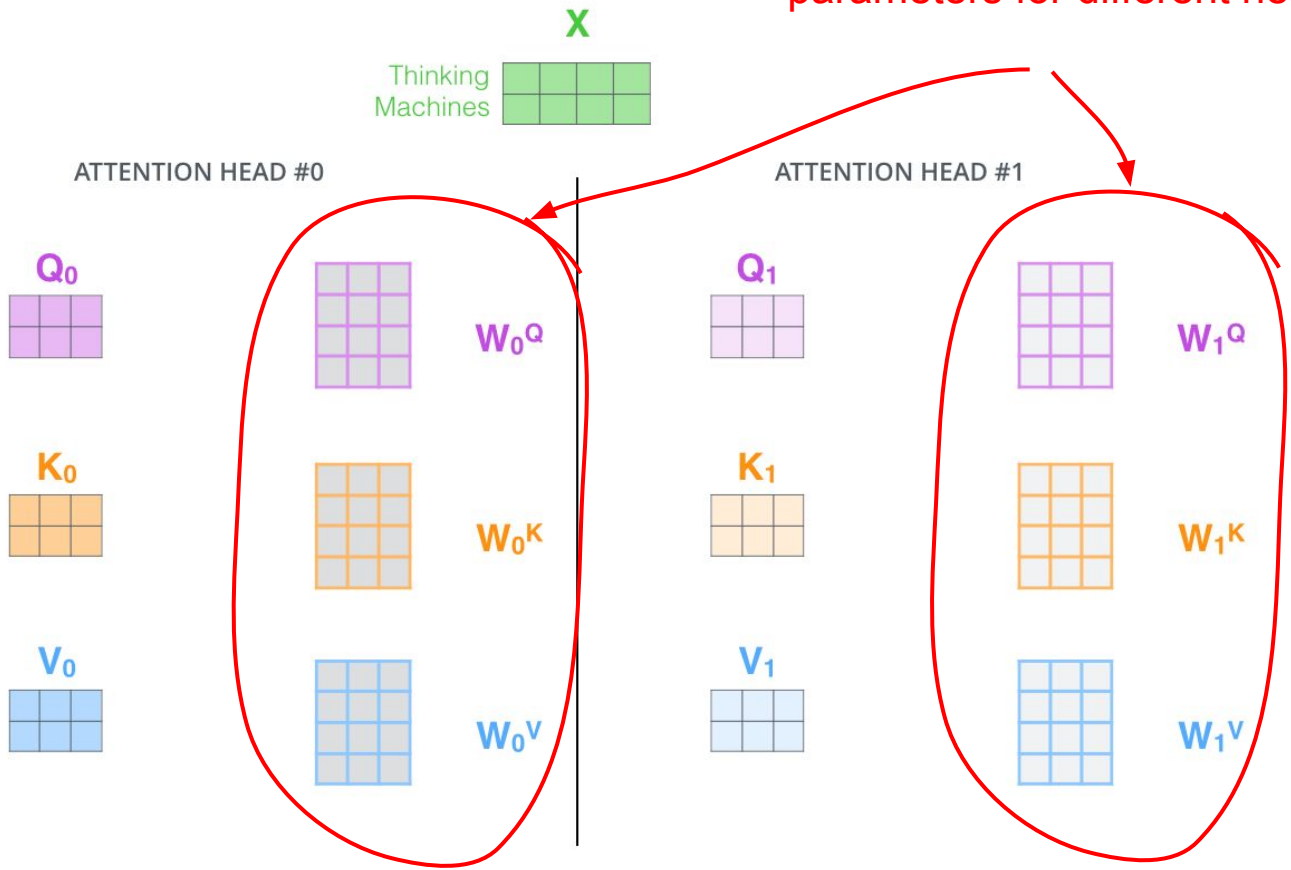
Scaled Dot-Product Attention

2-head Self-Attention

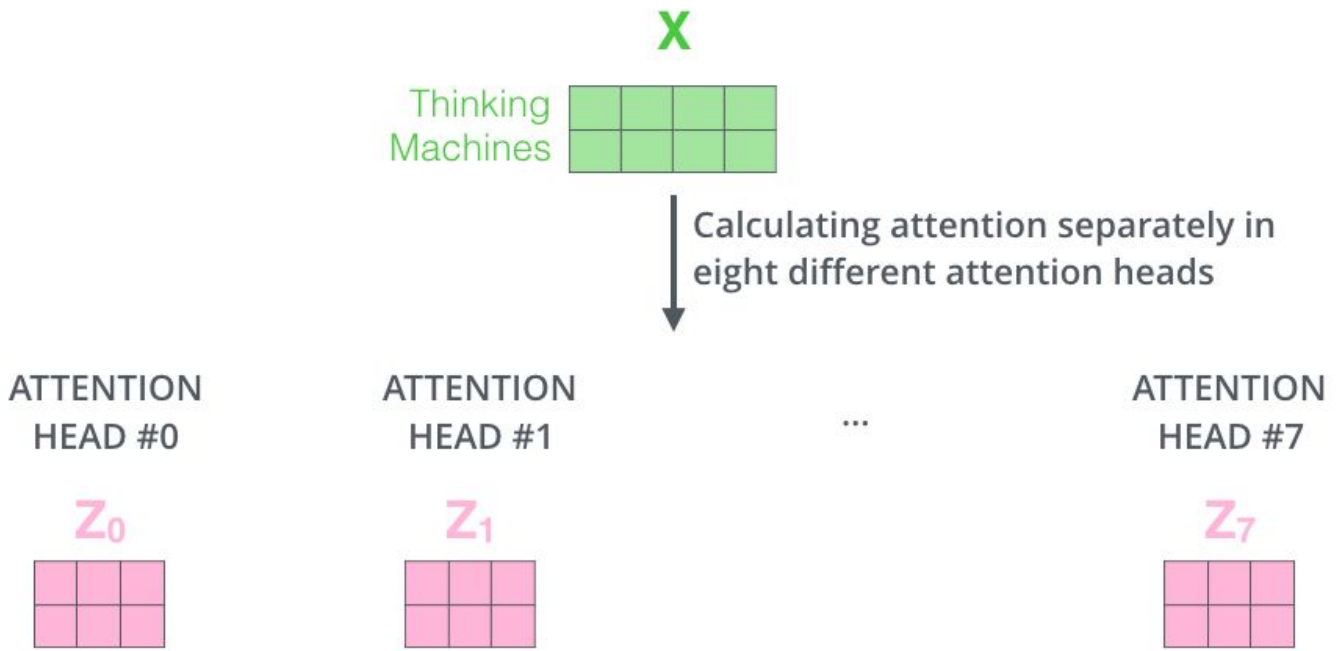


2-head Self-Attention

[Important!] Different trainable parameters for different heads

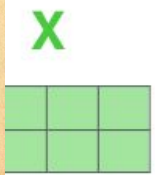


8-head Self-Attention = 8 Attention Vectors



8 Attention Vectors

Yamata no orochi (やまたのおろち八岐大蛇)
A legendary 8-head 8-tail Japanese dragon
https://en.wikipedia.org/wiki/Yamata_no_Orochi



Calculating attention separately in eight different attention heads

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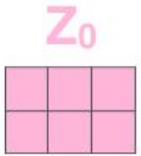
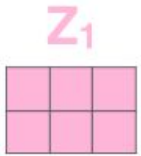
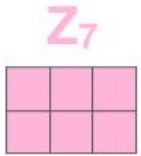
ATTENTION HEAD #7







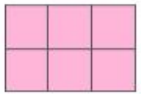
8

A

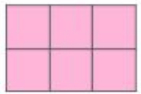
Yamata no Orochi (やまたのおろち 八岐大蛇)
A legendary 8-head 8-tail Japanese dragon
https://en.wikipedia.org/wiki/Yamata_no_Orochi

cf. Hydra (Greek myth)
Multi-head serpent
https://en.wikipedia.org/wiki/Lernaean_Hydra

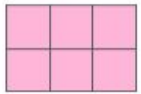
Z_0



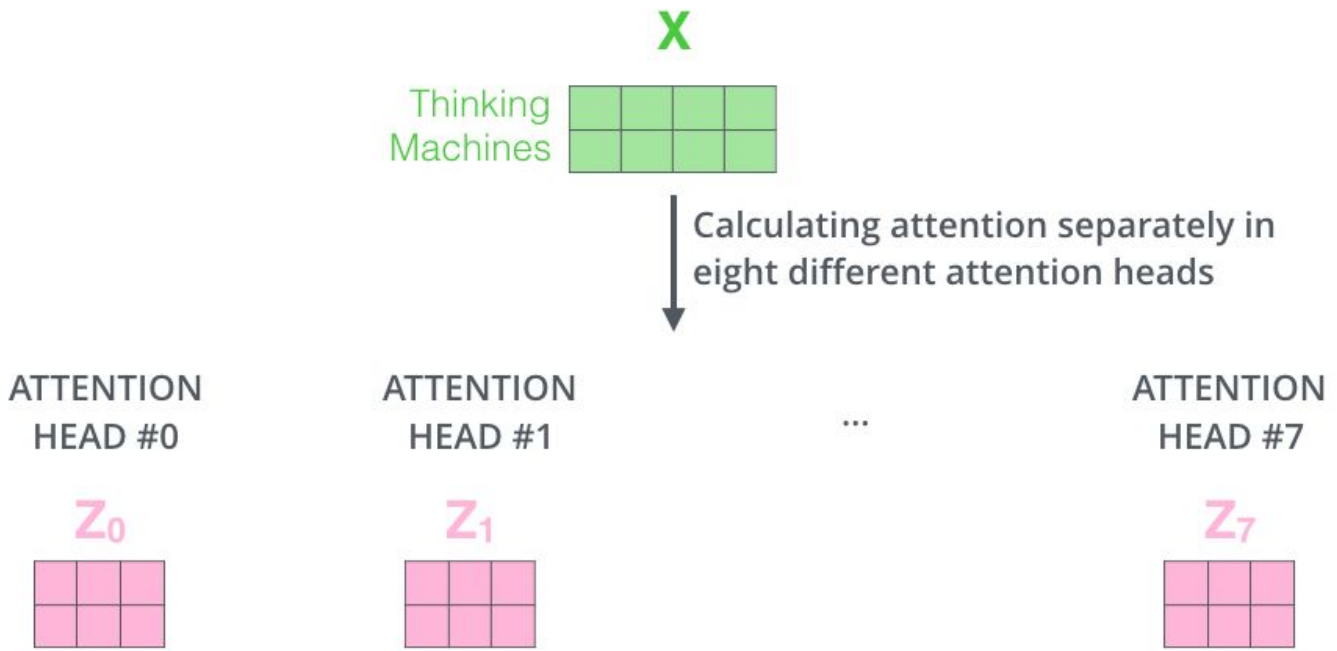
Z_1



Z_7



8-head Self-Attention = 8 Attention Vectors



Q. How do we aggregate them to get a single z_1?

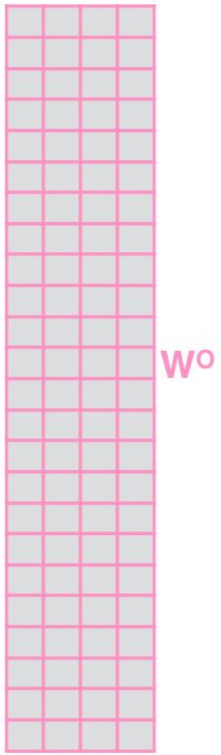
Concatenation & Linear-Transformation

1) Concatenate all the attention heads

(num_tokens, attention_dim*num_heads)

2) Multiply with a weight matrix W^O that was trained jointly with the model

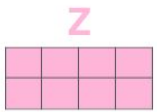
X



(num_heads*attention_dim, attention_dim)

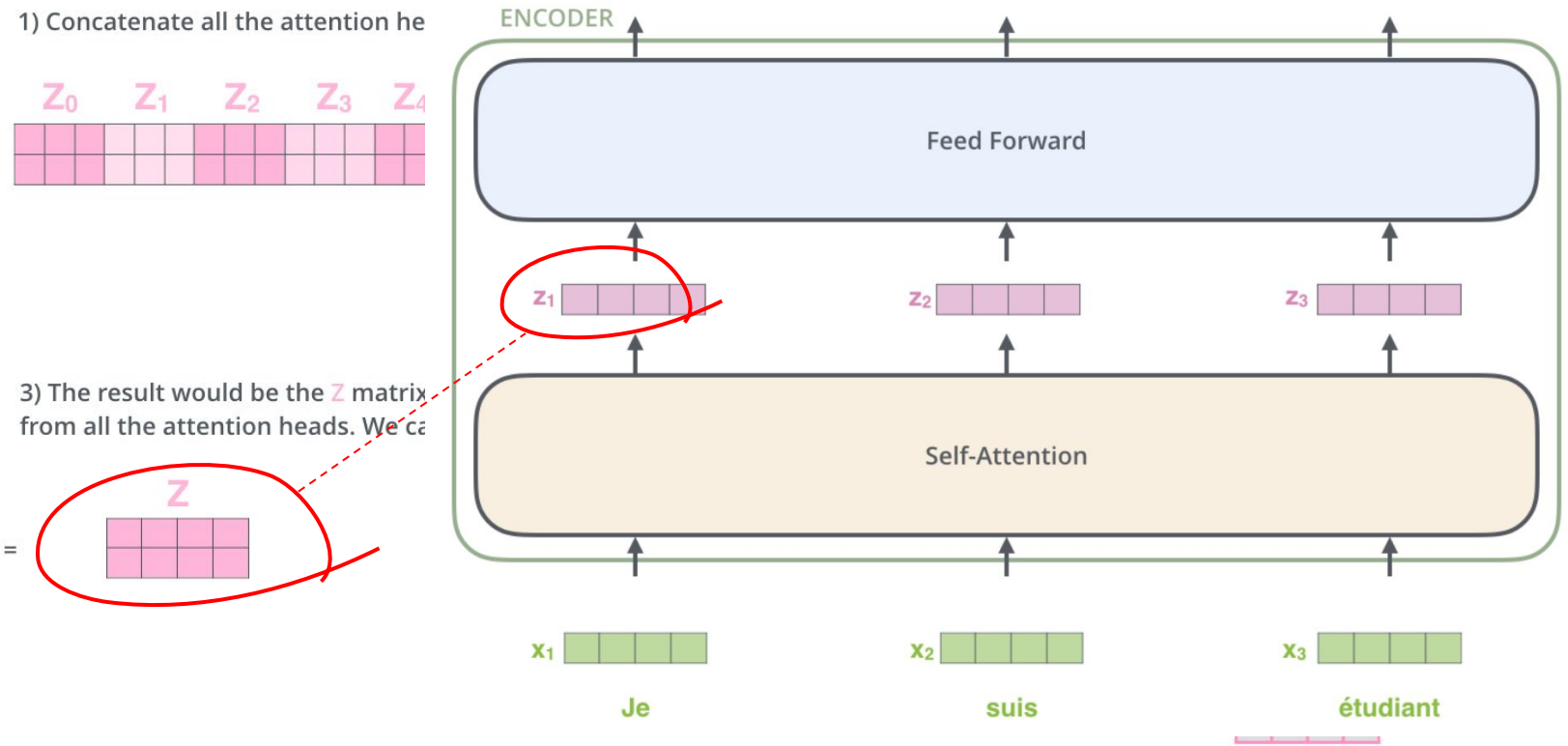
3) The result would be the Z matrix that captures information from all the attention heads. We can send this forward to the FFNN

=

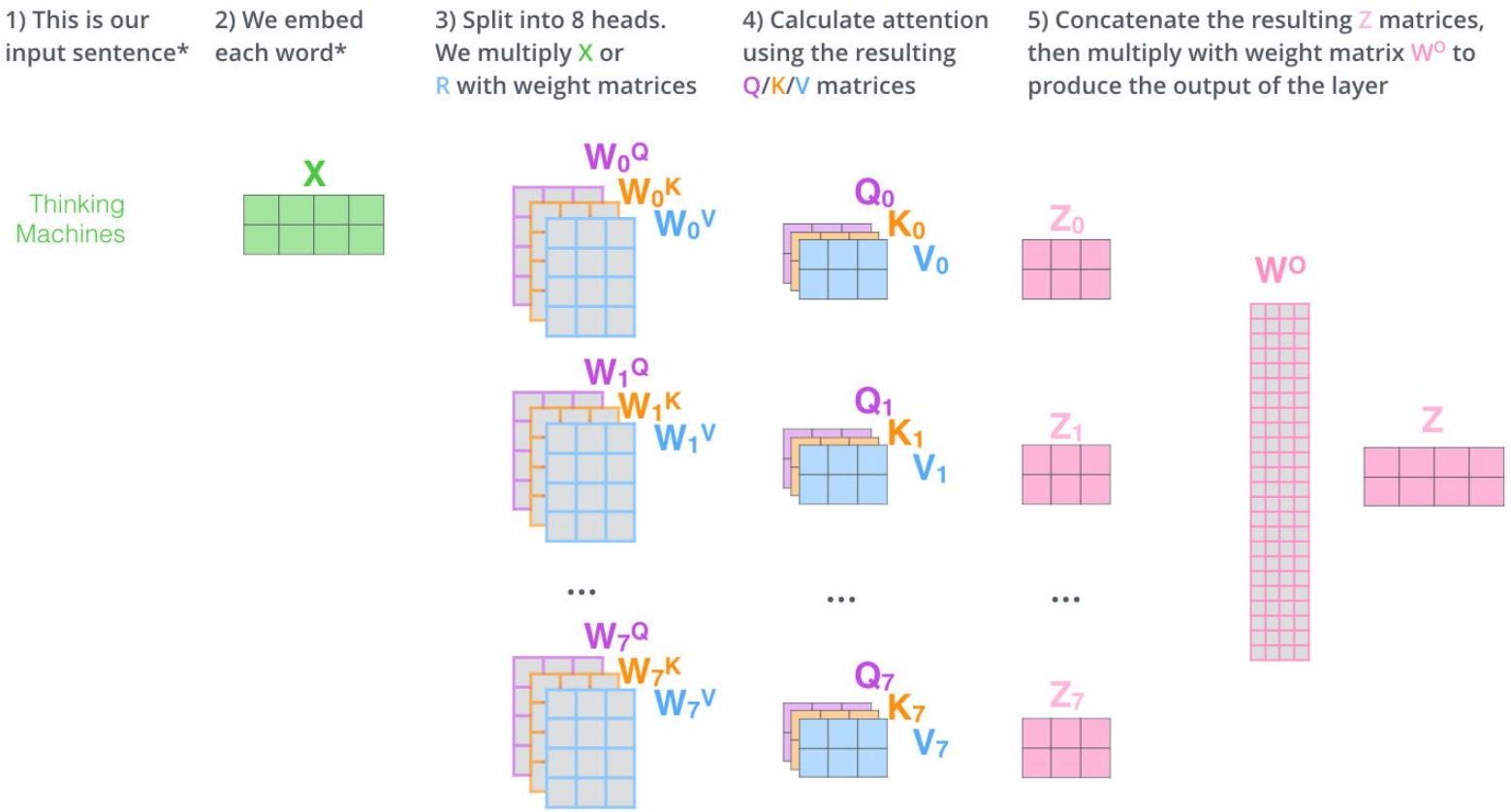


(num_tokens, attention_dim)

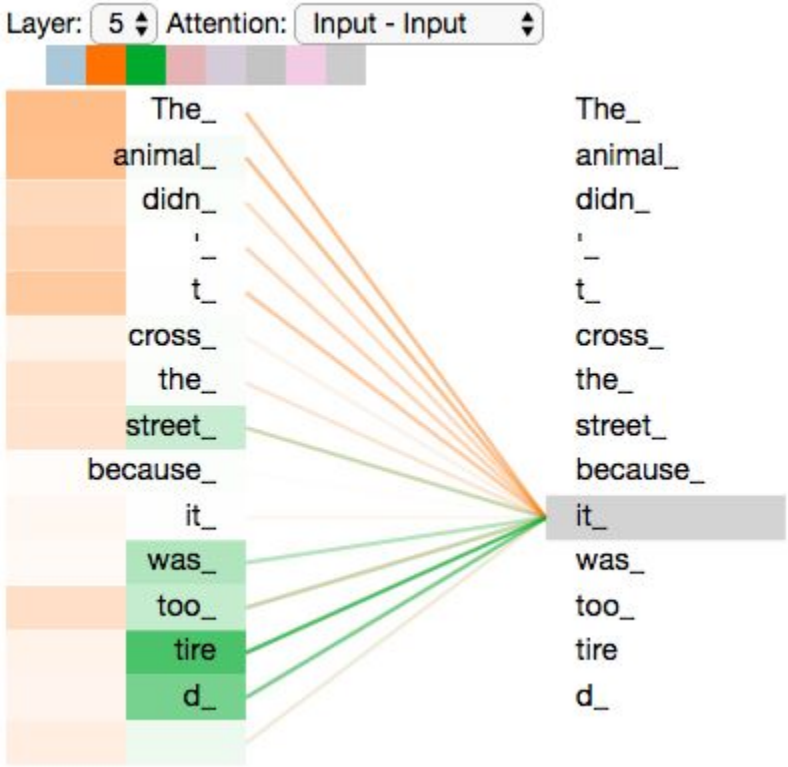
Concatenation & Linear-Transformation



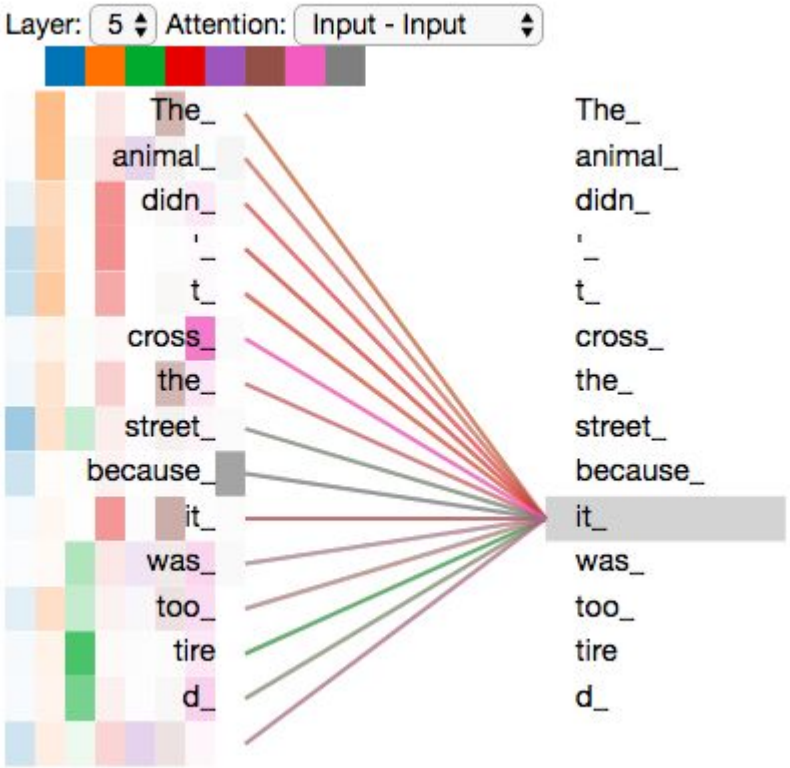
Recap: How Multi-head Self-Attention Works



In Theory: Different Heads Capture Different Types of Contextual Information



In Reality: Multiple Attention Heads are Hard to Interpret



???

Attention is not Explanation

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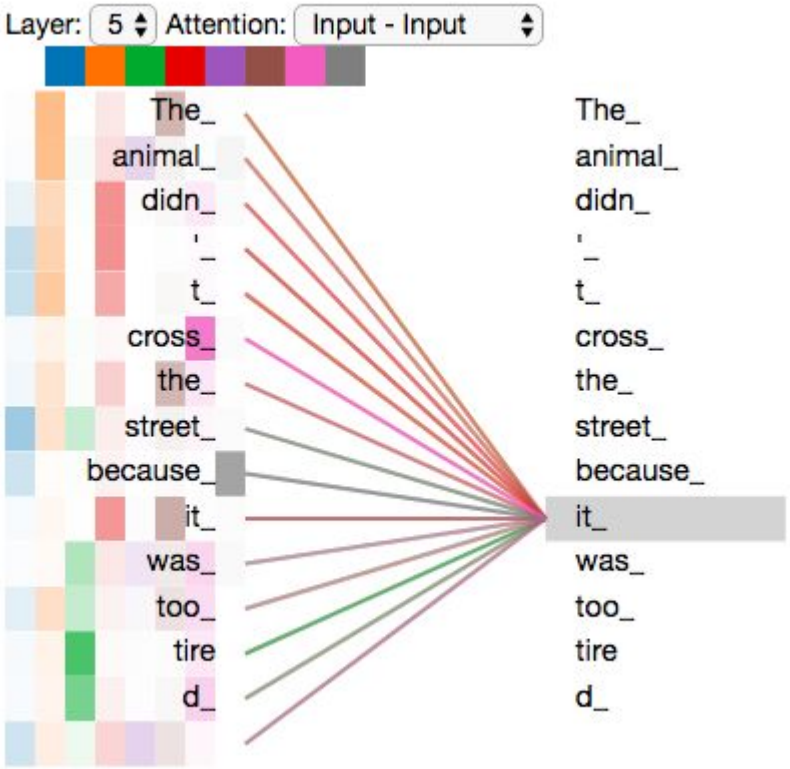
In Reality: Multiple Attention Heads are Hard to Interpret



???

Q. Do we really need so many attention heads?

Q. Do we really need so many attention heads?

- Short answer is **No**

ACL ‘19

Analyzing Multi-Head Self-Attention:
Specialized Heads Do the Heavy Lifting, the Rest Can Be Pruned

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NeurIPS ‘19

Are Sixteen Heads Really Better than One?

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BlackBoxNLP ‘19@ACL ‘19

What Does BERT Look At?
An Analysis of BERT’s Attention

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the simple weighted average. In this paper we make the surprising observation that even if models have been trained using multiple heads, in practice, a large percentage of attention heads can be removed at test time without significantly impacting performance. In fact, some layers can even be reduced to a single head. We further examine greedy algorithms for pruning down models, and

(My opinion)
We could tune the number of heads
But, overshooting may not be that harmful

Note: Conventional Attention Techniques for RNN

- To obtain **context vector c_t** as auxiliary information for the decoder

Similarity

$$\mathbf{c}_t = \sum_{i=1} \alpha_{t,i} \boldsymbol{h}_i \quad ; \text{Context vector for output } y_t$$

$$\alpha_{t,i} = \text{align}(y_t, x_i) \quad ; \text{How well two words } y_t \text{ and } x_i \text{ are aligned.}$$

$$= \frac{\exp(\text{score}(\boldsymbol{s}_{t-1}, \boldsymbol{h}_i))}{\sum_{i'=1}^{n} \exp(\text{score}(\boldsymbol{s}_{t-1}, \boldsymbol{h}_{i'}))} \quad ; \text{Softmax of some predefined alignment score..}$$

Attention? Attention! by Lilian Weng https://lilianweng.github.io/lil-log/2018/06/24/attention-attention.html

Note: Conventional Attention Techniques for RNN

- To obtain **context vector c_t** as auxiliary information for the decoder

Similarity

Value = hidden state of the encoder

$$\mathbf{c}_t = \sum_{i=1} \alpha_{t,i} \boldsymbol{h}_i \quad ; \text{Context vector for output } y_t$$

Query

Key

$$\alpha_{t,i} = \text{align}(y_t, \ldots) \quad ; \text{How well two words } y_t \text{ and } x_i \text{ are aligned.}$$

$$= \frac{\exp(\text{score}(\boldsymbol{s}_{t-1}, \boldsymbol{h}_i))}{\sum_{i'=1}^{n} \exp(\text{score}(\boldsymbol{s}_{t-1}, \boldsymbol{h}_{i'}))} \quad ; \text{Softmax of some predefined alignment score..}$$

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Note: Various Score Functions

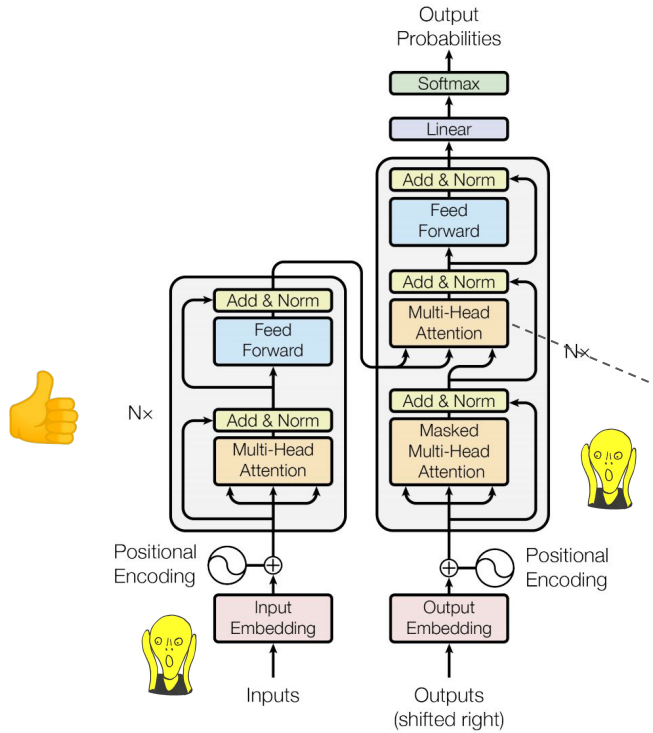
Query

Key

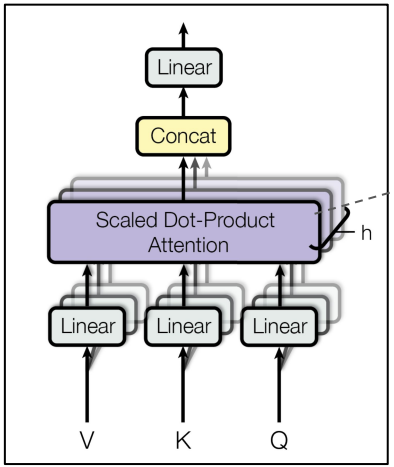
Name	Alignment score function	Citation
Content-base attention	$\text{score}(\boldsymbol{s}_t, \boldsymbol{h}_i) = \text{cosine}[\boldsymbol{s}_t, \boldsymbol{h}_i]$	Graves2014
Additive(*)	$\text{score}(\boldsymbol{s}_t, \boldsymbol{h}_i) = \mathbf{v}_a^\top \tanh(\mathbf{W}_a[\boldsymbol{s}_t; \boldsymbol{h}_i])$	Bahdanau2015
Location-Base	$\alpha_{t,i} = \text{softmax}(\mathbf{W}_a \boldsymbol{s}_t)$ Note: This simplifies the softmax alignment to only depend on the target position.	Luong2015
General	$\text{score}(\boldsymbol{s}_t, \boldsymbol{h}_i) = \boldsymbol{s}_t^\top \mathbf{W}_a \boldsymbol{h}_i$ where $\mathbf{W}_a$ is a trainable weight matrix in the attention layer.	Luong2015
Dot-Product	$\text{score}(\boldsymbol{s}_t, \boldsymbol{h}_i) = \boldsymbol{s}_t^\top \boldsymbol{h}_i$	Luong2015
Scaled Dot-Product(^)	$\text{score}(\boldsymbol{s}_t, \boldsymbol{h}_i) = \frac{\boldsymbol{s}_t^\top \boldsymbol{h}_i}{\sqrt{n}}$ Note: very similar to the dot-product attention except for a scaling factor; where n is the dimension of the source hidden state.	Vaswani2017

Attention? Attention! by Lilian Weng https://lilianweng.github.io/lil-log/2018/06/24/attention-attention.html

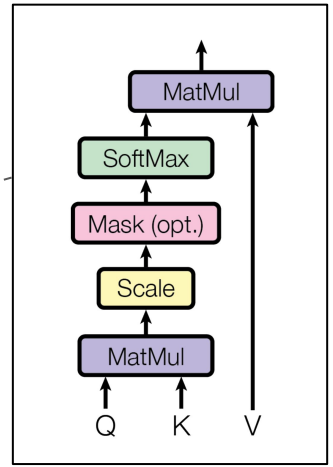
The Transformer



Model Architecture



Multi-Head Attention



Scaled Dot-Product Attention

Remaining Topics

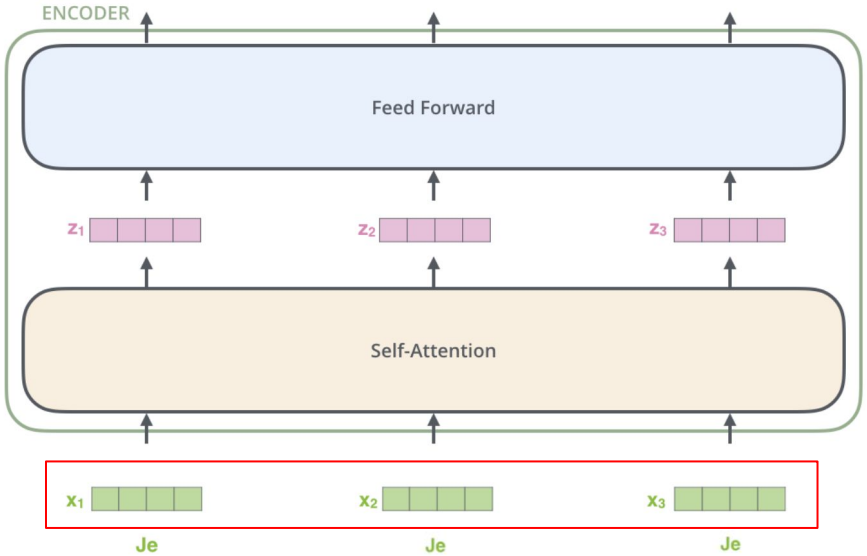
- Positional Encoding
- Residual Connection & Layer normalization
- Transformer Decoder

Remaining Topics

- **Positional encoding**
- **Residual Connection & Layer normalization**
- Transformer Decoder

Why Positional Encoding?

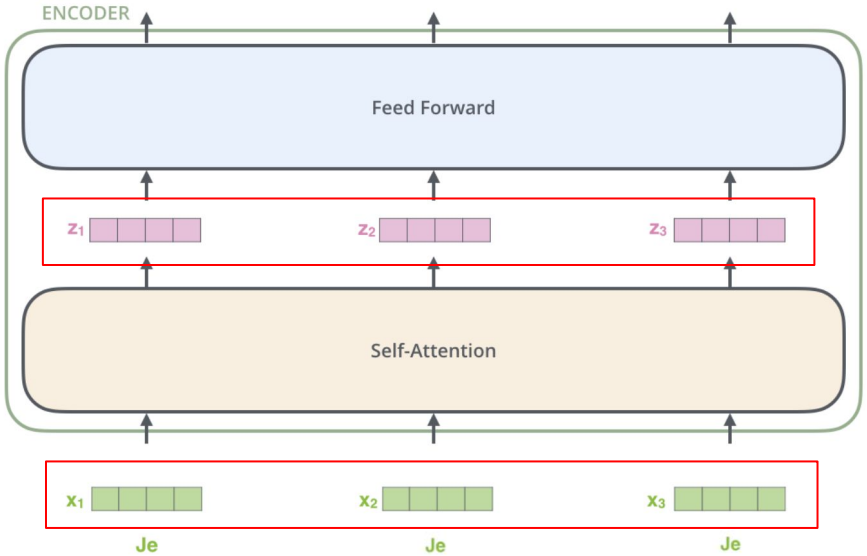
- Transformer Encoder (i.e., self-attention) does **NOT consider any positional information**



If the input token embeddings were the same

Why Positional Encoding?

- Transformer Encoder (i.e., self-attention) does **NOT consider any positional information**
  - In one sense, it can be considered as **"contextualized" bag-of-words** representations

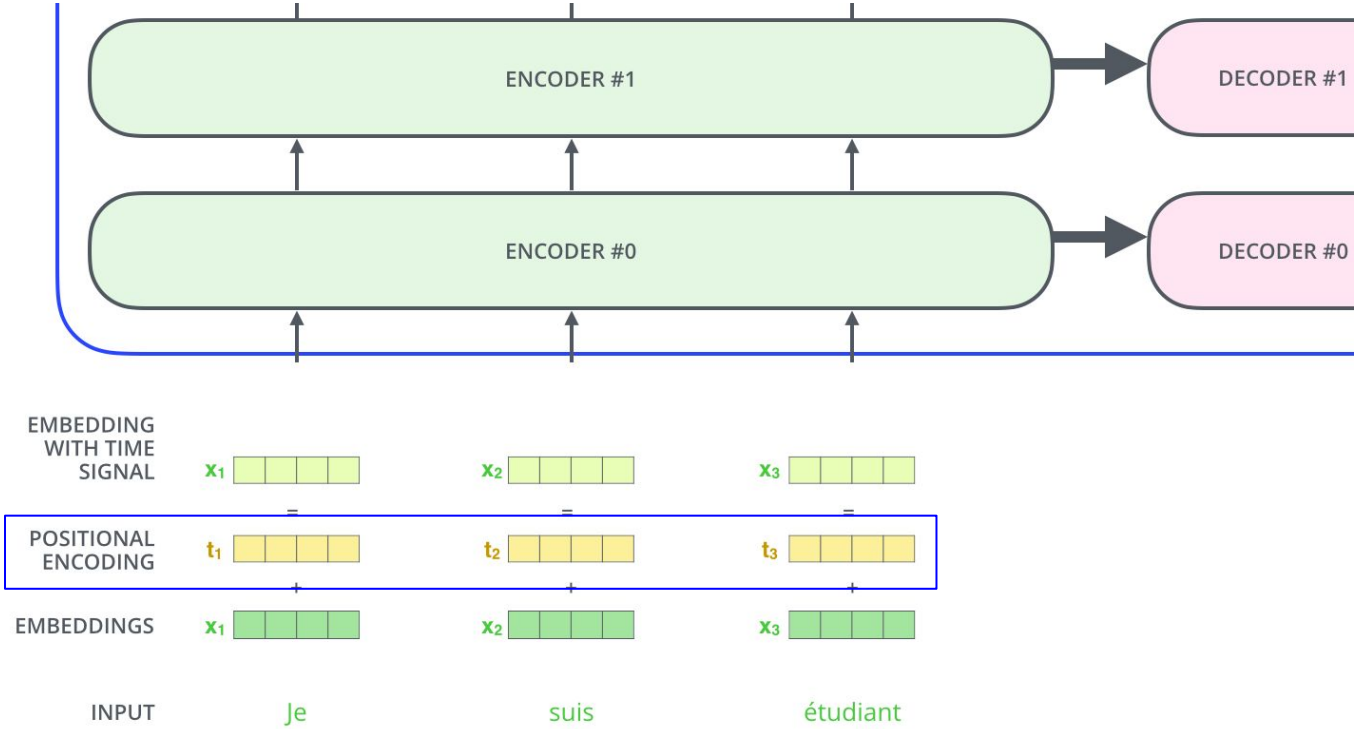


The corresponding attention vectors would become identical

If the input token embeddings were the same

Adding Positional Encoding to Make Position-aware

- Just adding **position information** to input word embeddings

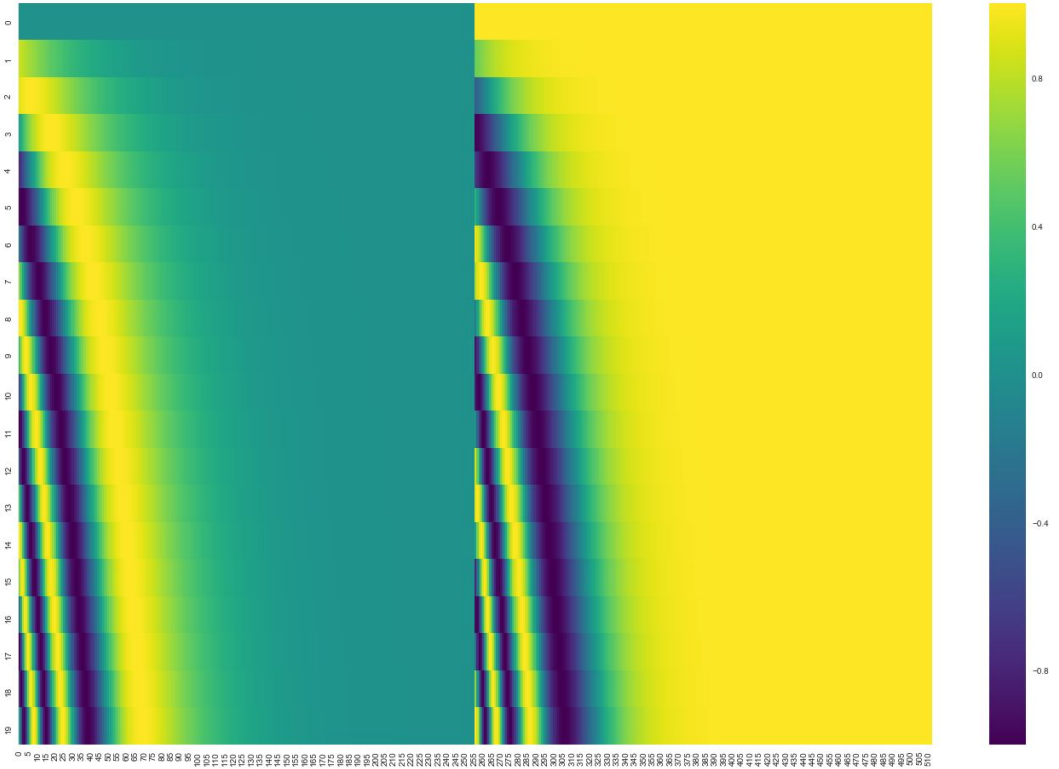


Positional Encoding in Transformer

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

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

How Actual Positional Encoding Values Look Like
20 tokens & embedding size of 512



Input Embedding Layer: Pytorch Example

```python
class TransformerModel(nn.Module):

    def __init__(self, ntoken: int, d_model: int, nhead: int, d_hid: int,
                 nlayers: int, dropout: float = 0.5):
        super().__init__()
        self.model_type = 'Transformer'
        self.pos_encoder = PositionalEncoding(d_model, dropout)
        encoder_layers = TransformerEncoderLayer(d_model, nhead, d_hid, dropout)
        self.transformer_encoder = TransformerEncoder(encoder_layers, nlayers)
        self.encoder = nn.Embedding(ntoken, d_model)
        self.d_model = d_model
        self.decoder = nn.Linear(d_model, ntoken)

        self.init_weights()
```

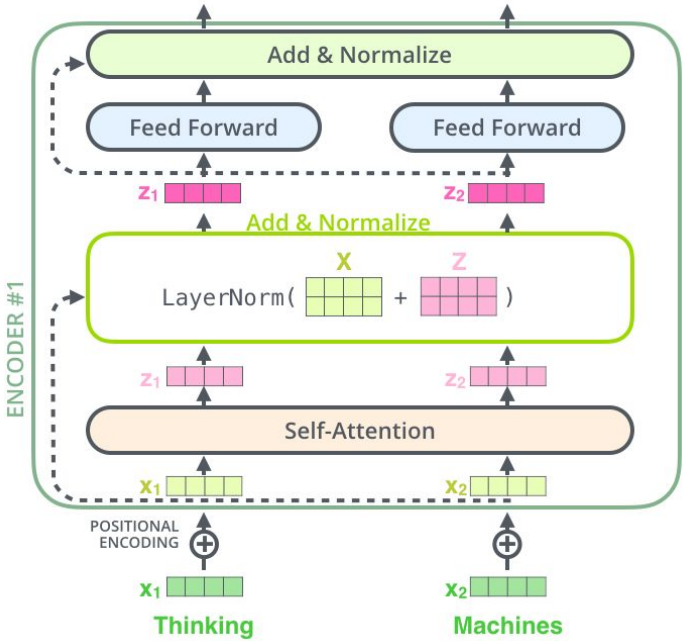
```python
    def forward(self, src: Tensor, src_mask: Tensor) -> Tensor:
        """
        Args:
            src: Tensor, shape [seq_len, batch_size]
            src_mask: Tensor, shape [seq_len, seq_len]

        Returns:
            output Tensor of shape [seq_len, batch_size, ntoken]
        """
        src = self.encoder(src) * math.sqrt(self.d_model)
        src = self.pos_encoder(src)
        output = self.transformer_encoder(src, src_mask)
```

```python
class PositionalEncoding(nn.Module):

    def __init__(self, d_model: int, dropout: float = 0.1, max_len: int = 5000):
        super().__init__()
        self.dropout = nn.Dropout(p=dropout)

        position = torch.arange(max_len).unsqueeze(1)
        div_term = torch.exp(torch.arange(0, d_model, 2) * (-math.log(10000.0) / d_model))
        pe = torch.zeros(max_len, 1, d_model)
        pe[:, 0, 0::2] = torch.sin(position * div_term)
        pe[:, 0, 1::2] = torch.cos(position * div_term)
        self.register_buffer('pe', pe)

    def forward(self, x: Tensor) -> Tensor:
        """
        Args:
            x: Tensor, shape [seq_len, batch_size, embedding_dim]
        """
        x = x + self.pe[:x.size(0)]
        return self.dropout(x)
```

[Language Modeling with nn.Transformer and TorchText — PyTorch Tutorials 1.9.1+cu102 documentation]

Residual Connection & Layer Normalization

- Apply **Residual Connection** (i.e., adding $\mathbf{x}_*$) before **Layer Normalization** (*1)



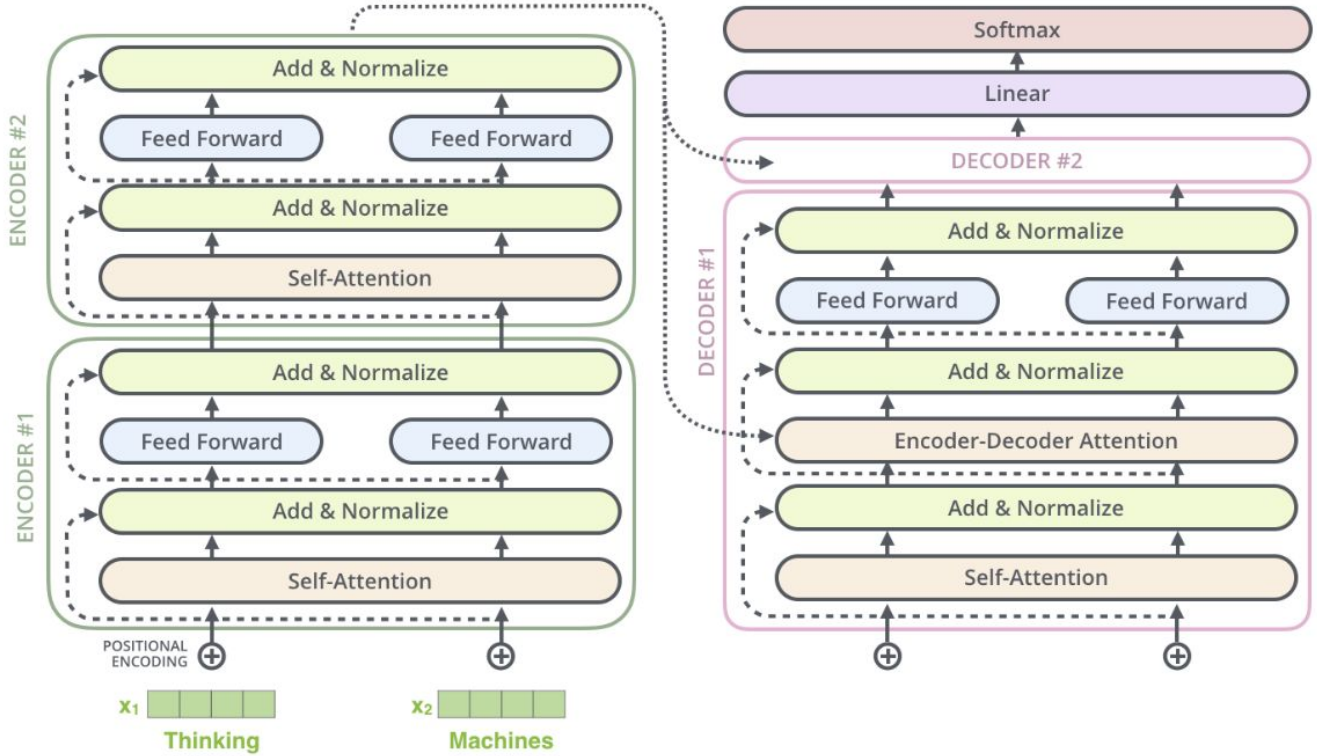
(*1) Layer normalization: Normalization over input tokens (cf. Batch Normalization)

Questions?

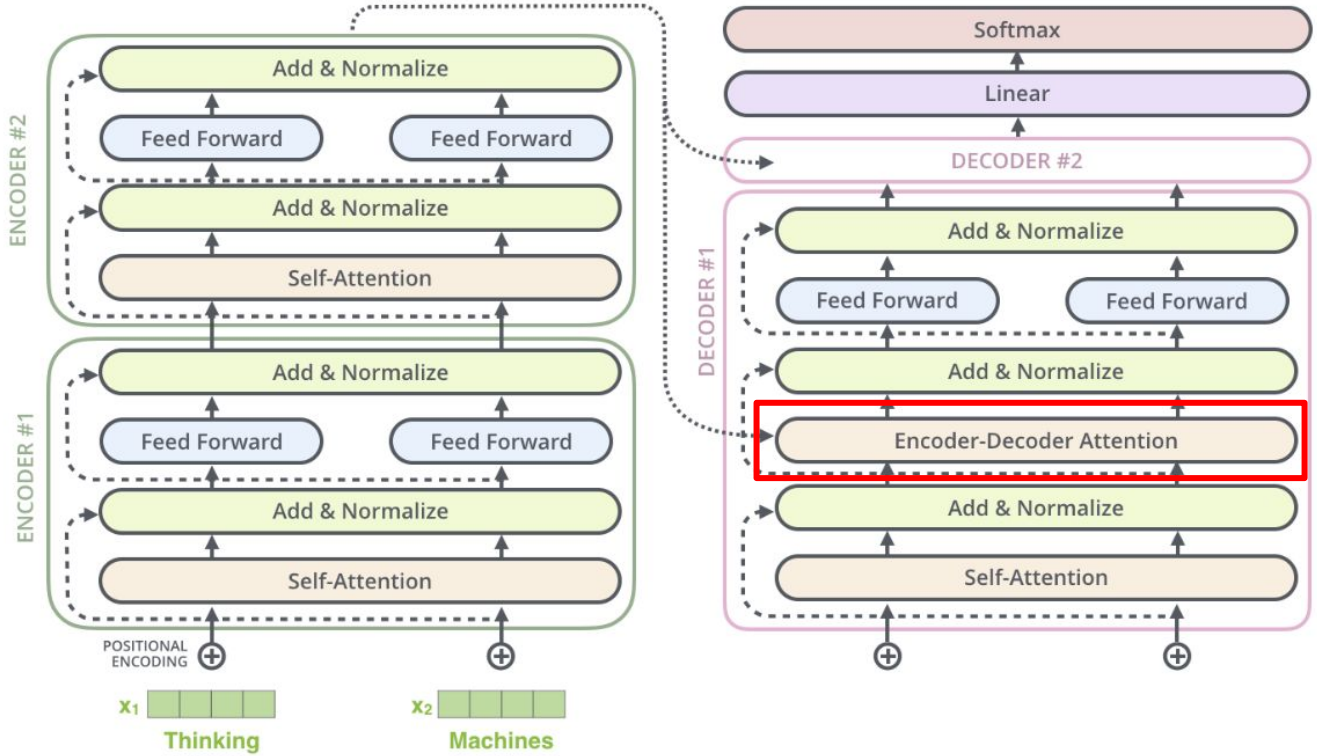
Remaining Topics

- Positional encoding
- Residual Connection & Layer normalization
- **Transformer Decoder**

Transformer (2 Encoders & 2 Decoders)

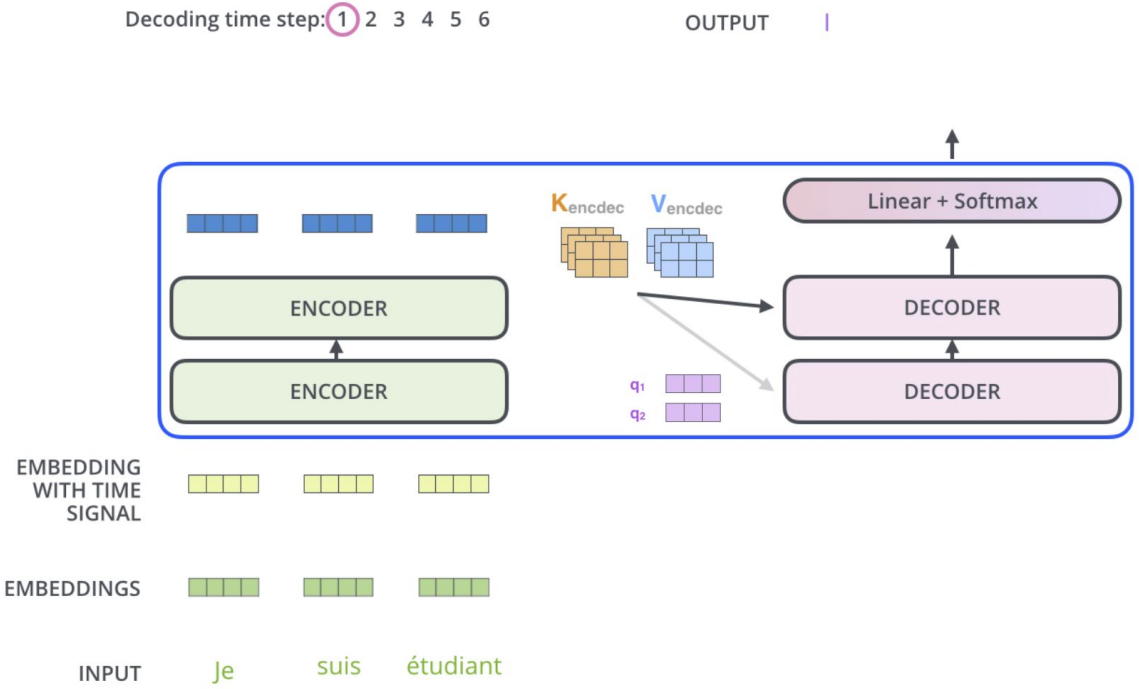


Transformer (2 Encoders & 2 Decoders)



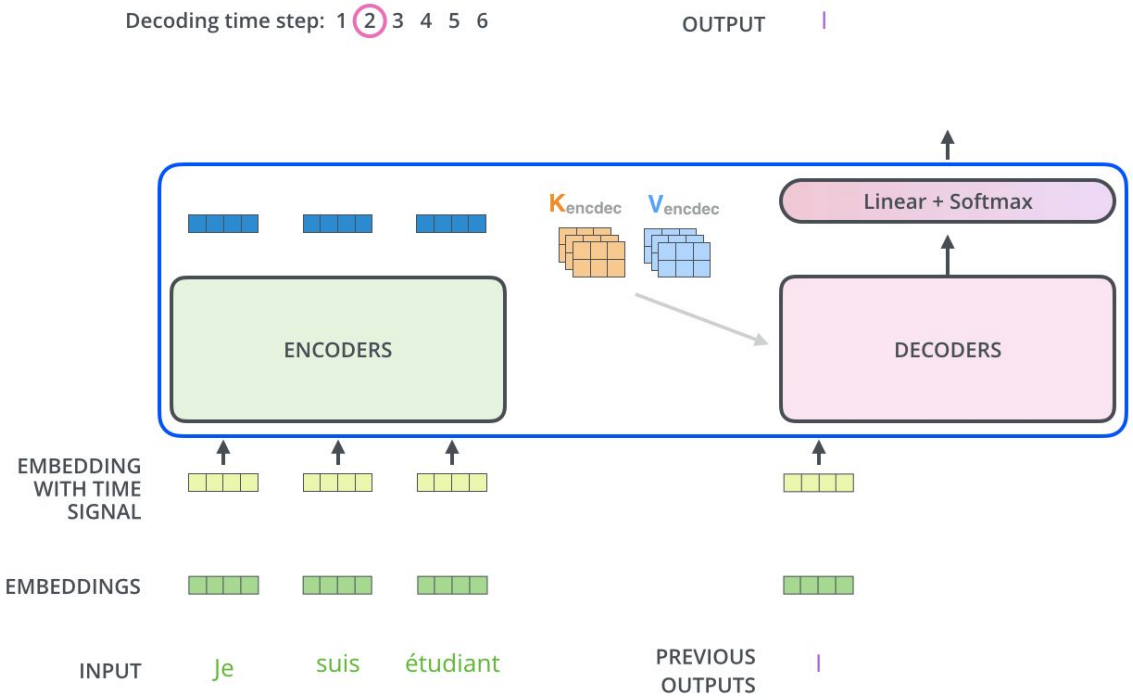
Decoder: Encoder-Decoder Attention

- The same “Query-Key-Value” style attention where **Key** and **Value vectors** are from Encoder and **Query vectors** are from Decoder

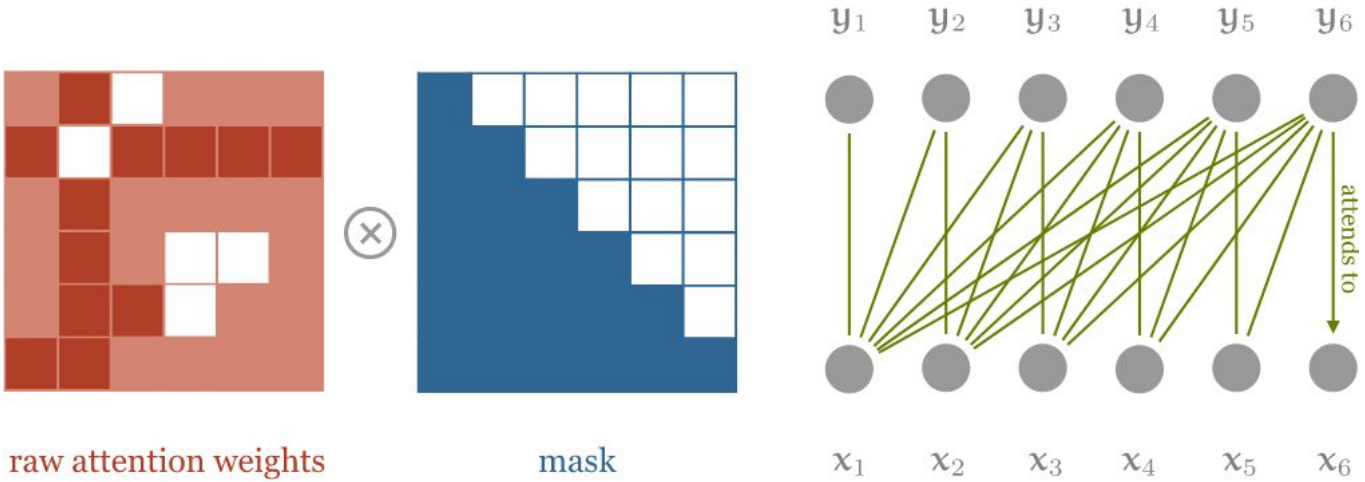


Decoder: “Masked” Self-Attention

- The self-attention layer (in the Decoder) is **only allowed to attend to earlier positions** in the output sequence



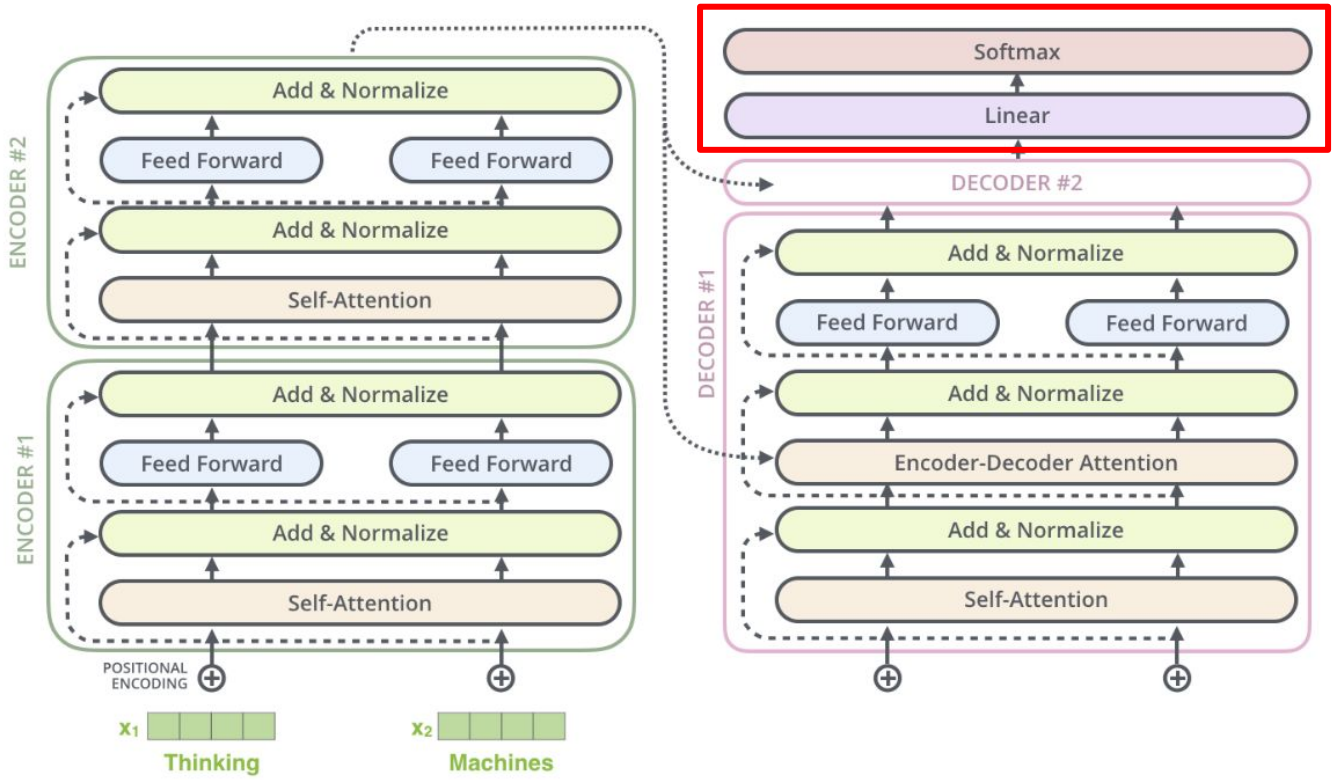
Masked Attention to Prevent “Previous” Step From Attending “Future” Steps



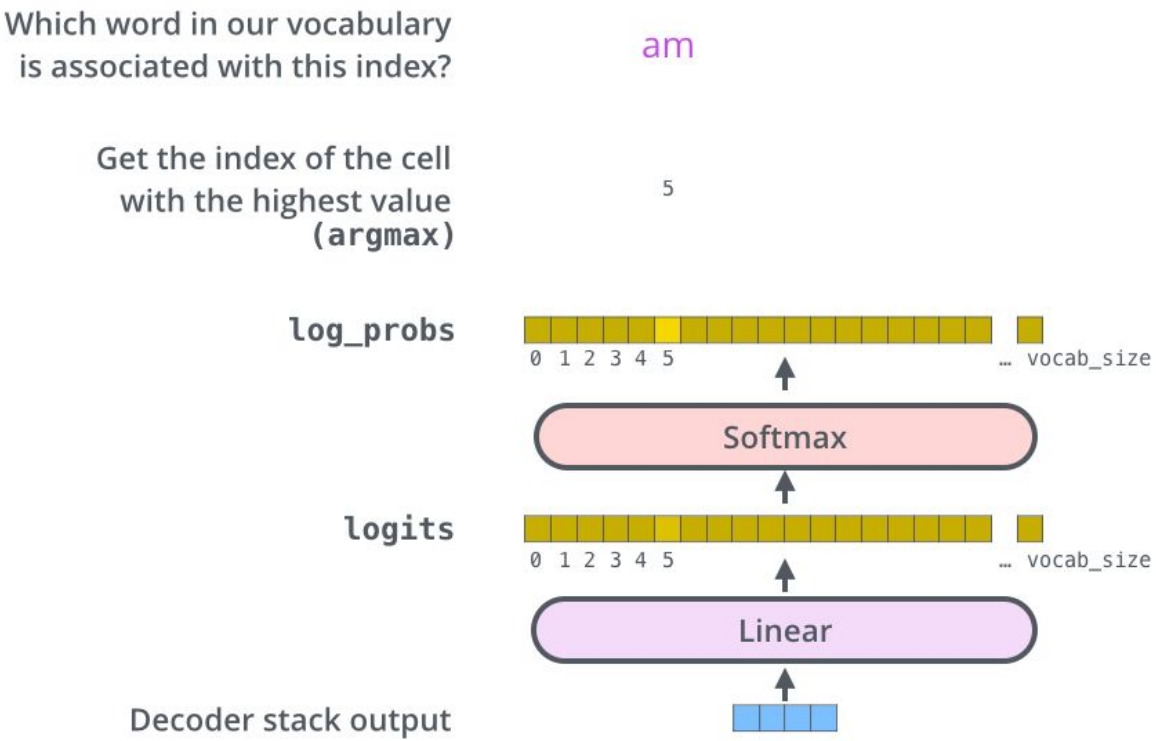
Decoder

[Transformers from scratch | peterbloem.nl]

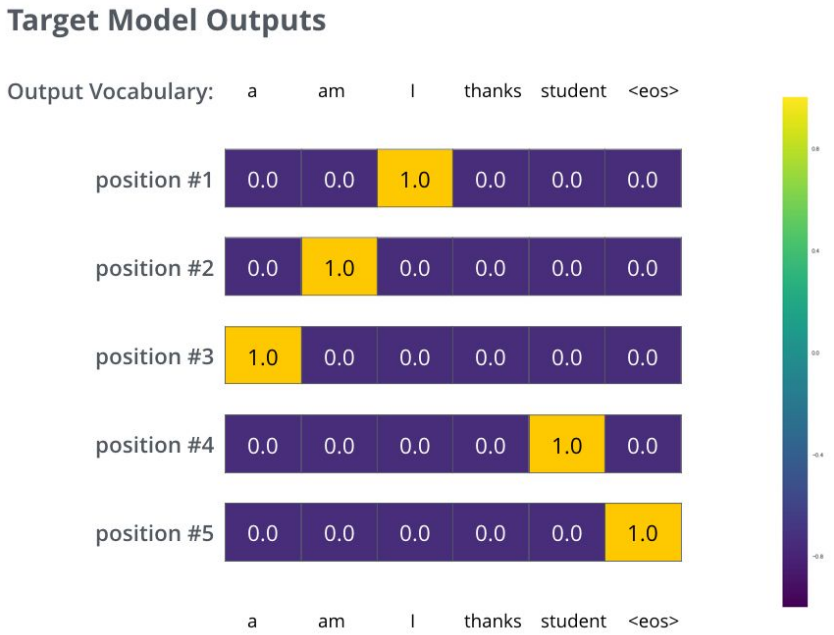
Transformer (2 Encoders & 2 Decoders)

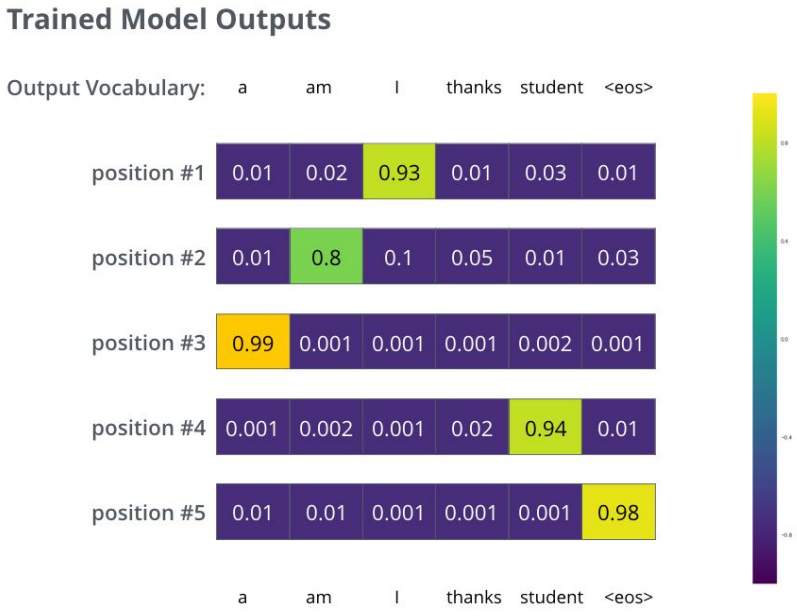


Output Layer



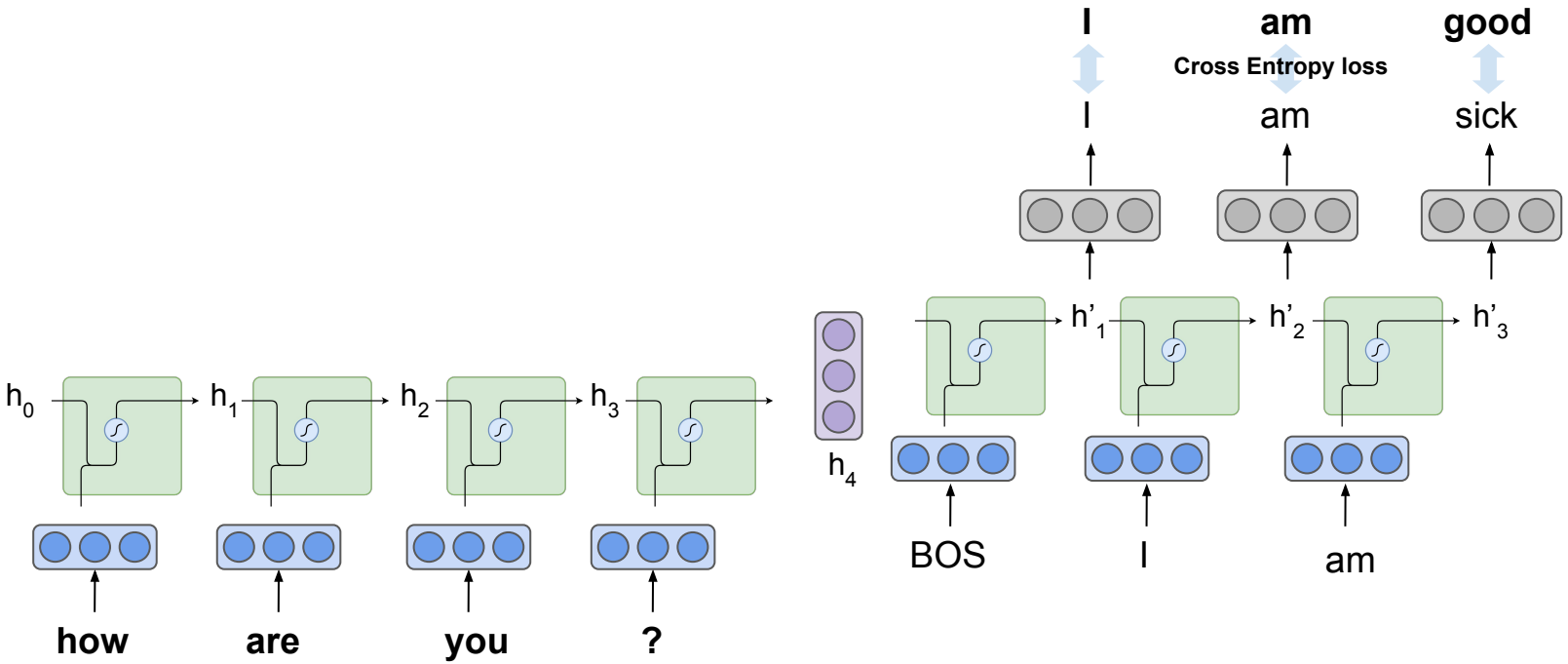
Output Layer: Training with Ground-truth Labels aka Teacher-forcing Training





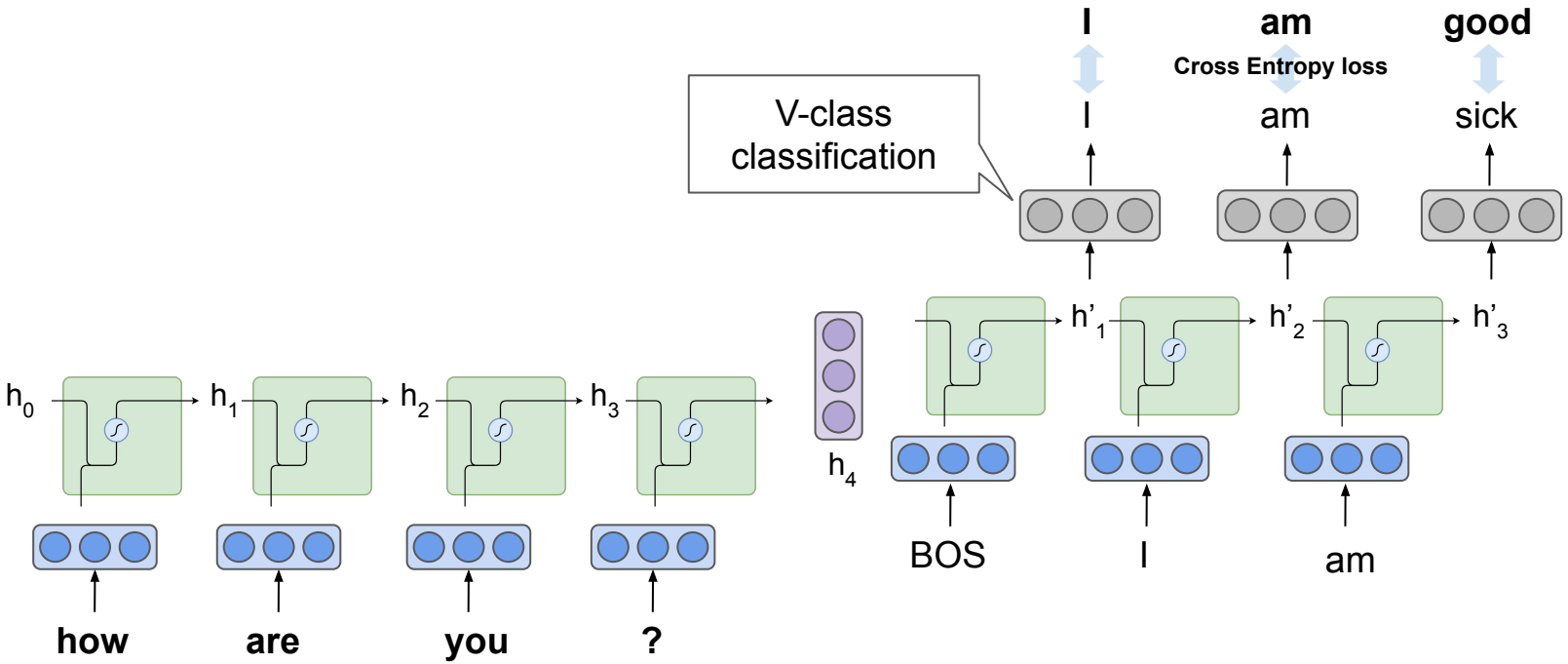
Training Encoder-Decoder Models: Training Data

- Training data: **Pairs of text sequences** (called a **parallel corpus)**
  - e.g., (“How are you?”, “I am good”)



Training Encoder-Decoder Models: “Teacher Forcing”

- Train the model to output **ground-truth outputs**



Note: Transformer Needs Decoding Algorithm

- Any decoding algorithm (e.g., Greedy/Beam Search) can be used
- Again, the Transformer is just an **encoder-decoder model**
- Although the Transformer does not have any recurrent architecture, the decoding procedure is still conducted in an iterative manner

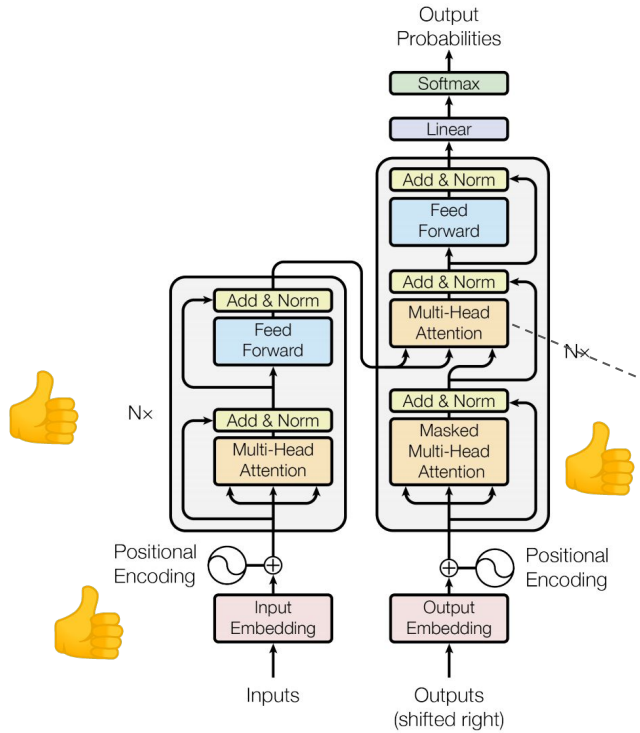
Parameter Initialization: Xavier Initialization

- Sampling initial parameter values from the Normal Distribution, where the standard deviation is **the number of parameters in the previous layer**
  - i.e., More parameters in the prev layer → Lower variance → Smaller absolute values

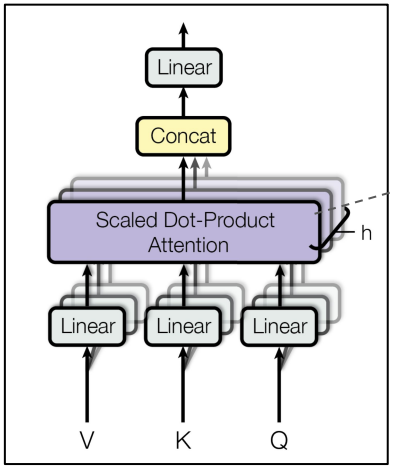
$$W_{i,j}^{[l]} = \mathcal{N}\left(0, \frac{1}{n^{[l-1]}}\right)$$

Detailed derivation: https://cs230.stanford.edu/section/4/

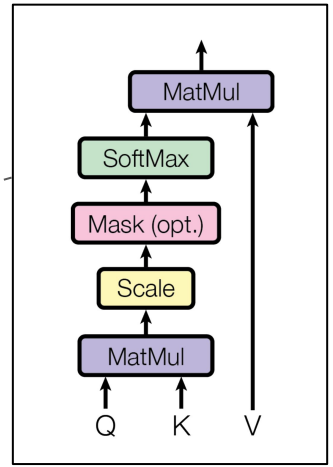
The Transformer 👍



Model Architecture



Multi-Head Attention



Scaled Dot-Product Attention

Key Takeaway

- Model Architecture
  - The Transformer is an **Encoder-Decoder model**
    - Transformer Encoder + Transformer Decoder (not explained yet)
  - Transformer Encoder = Stack of **Transformer Encoder Blocks**
  - Transformer Encoder Block = **Self-Attention Layer** + Feed Forward NN
- **Self-Attention Layer**
  - Token Embeddings → Query, Key, Value Vectors → Attention Vectors
  - Multi-head Attention
- Additional techniques
  - Positional Encoding
  - Residual Connection + Layer Normalization

Let’s Take A Look At The Original Paper

Attention Is All You Need

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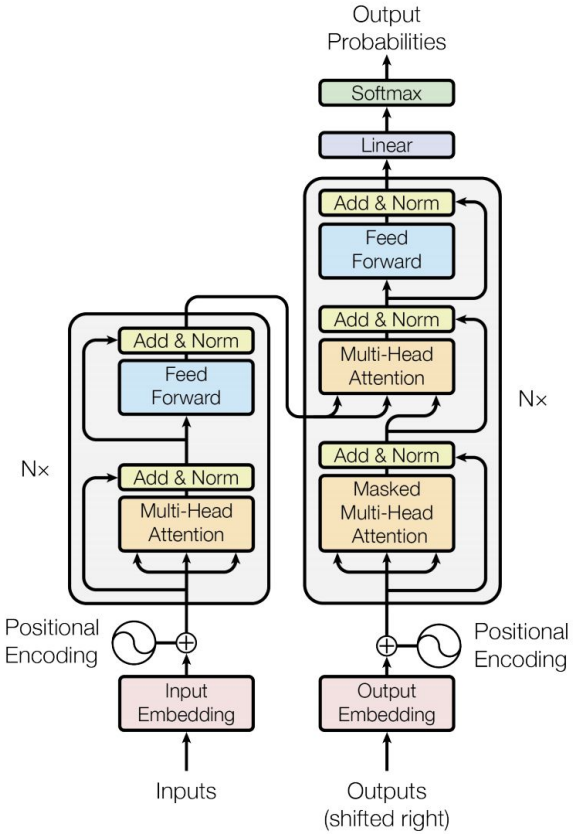
Illia Polosukhin* ‡ illia.polosukhin@gmail.com

Model Descriptions in the Original Paper



3.1 Encoder and Decoder Stacks

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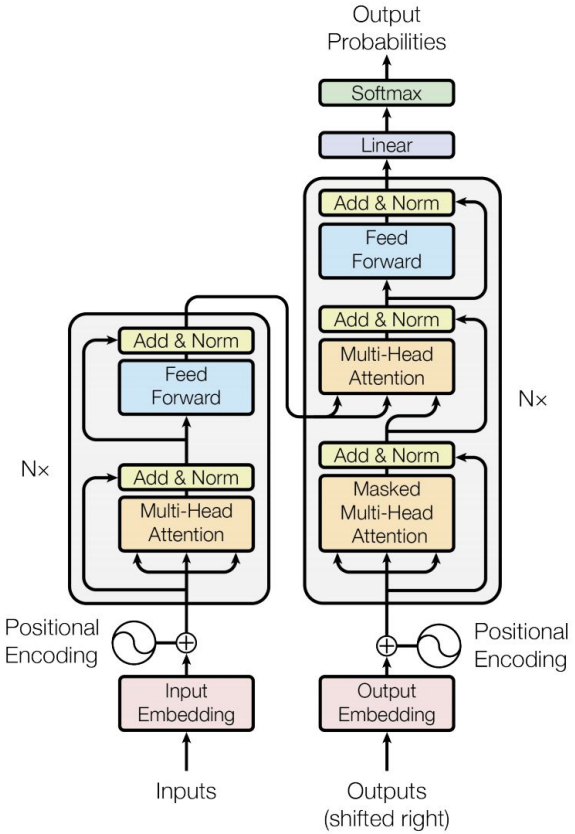

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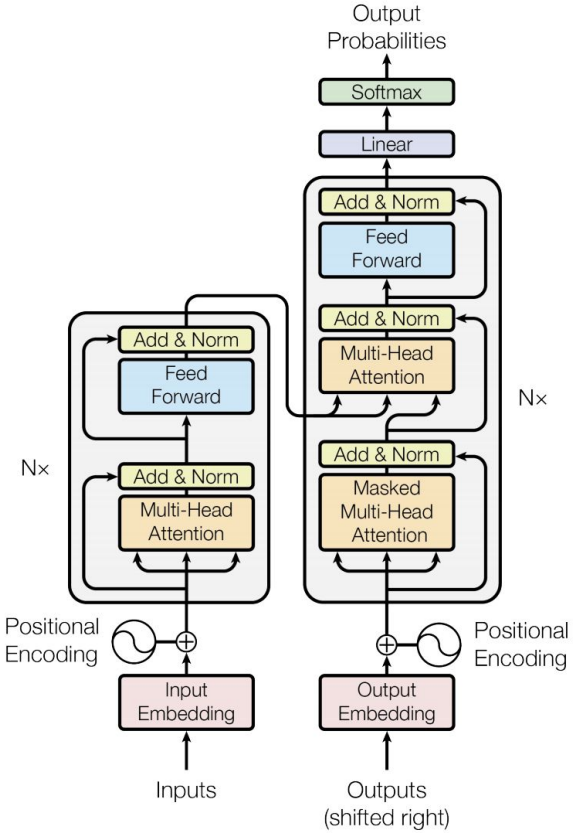

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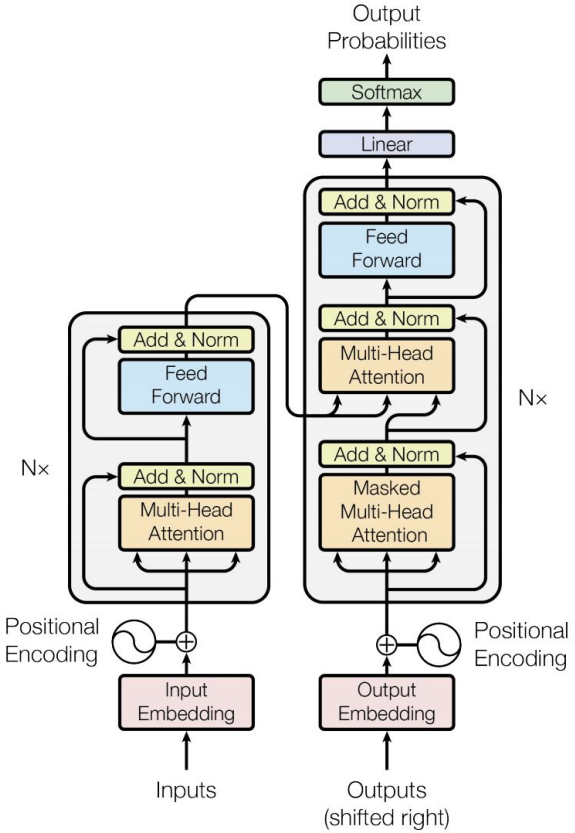

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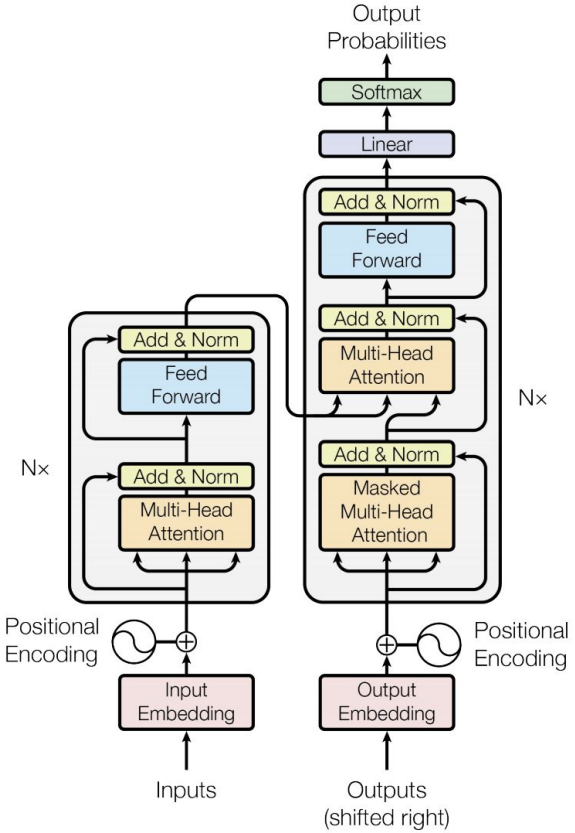

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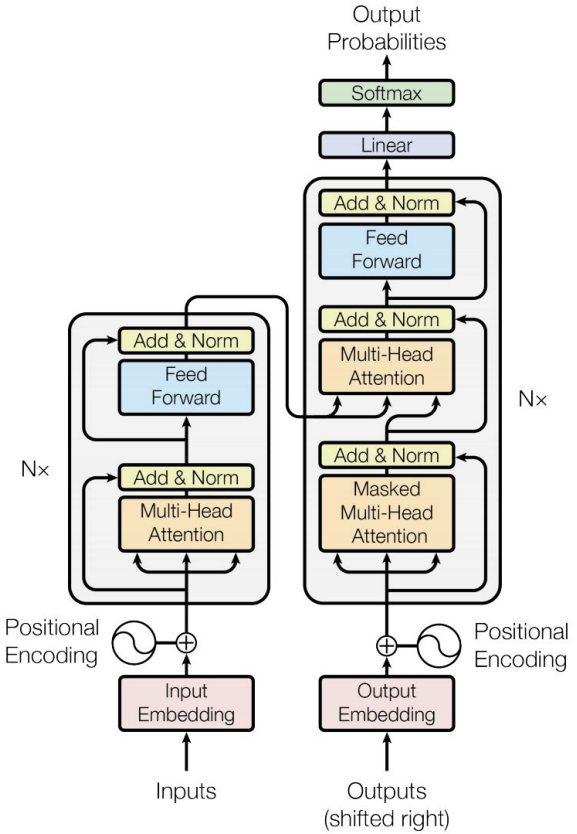

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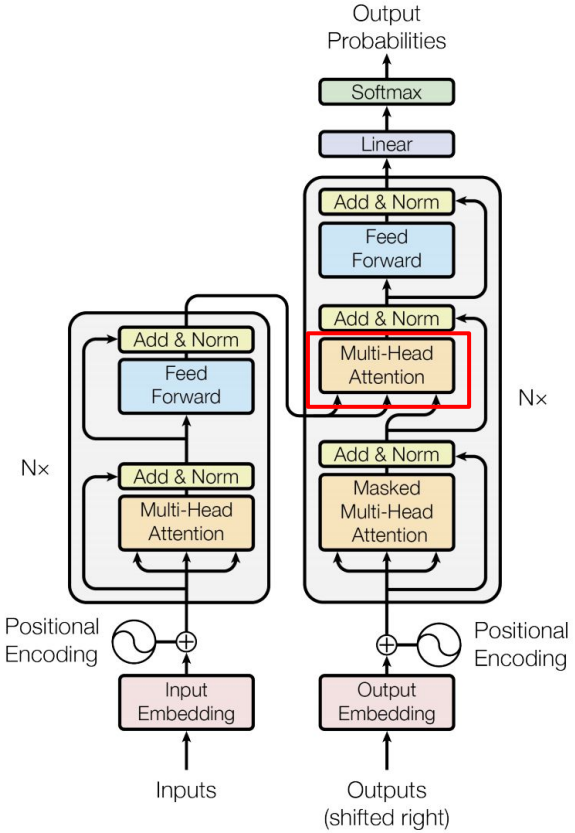

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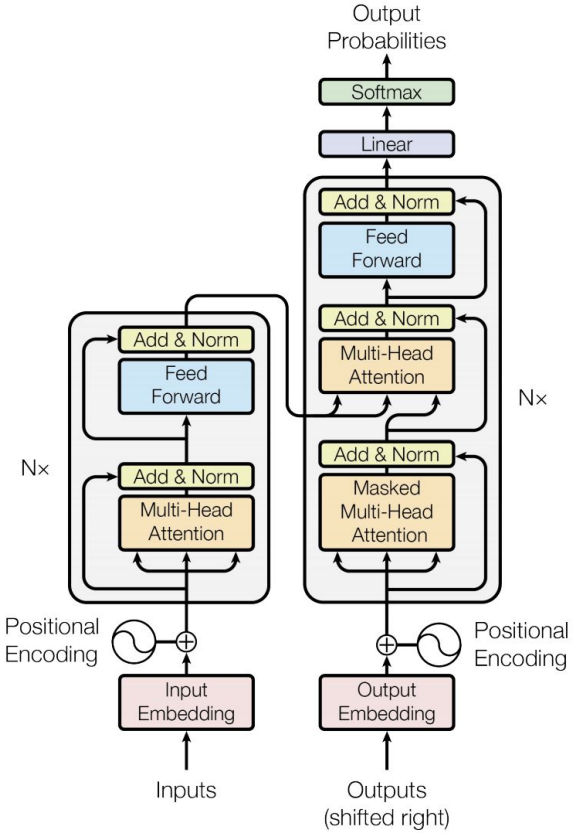

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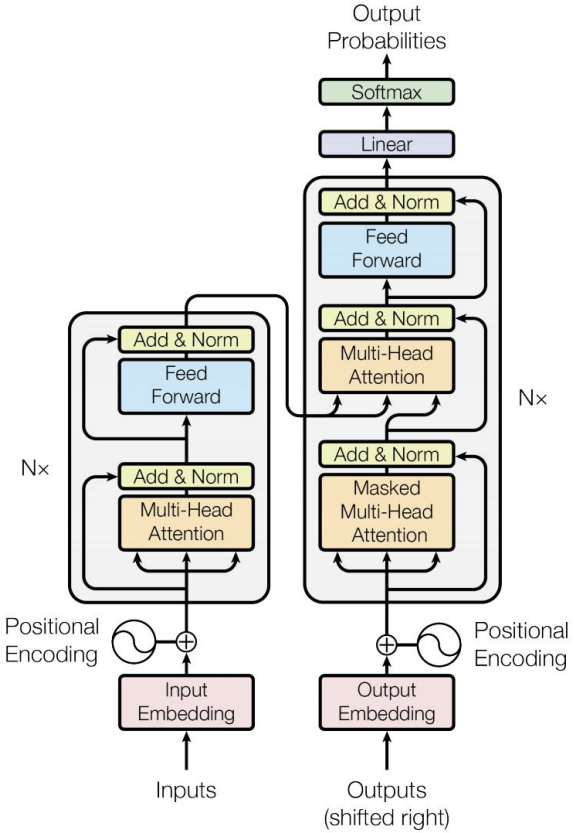

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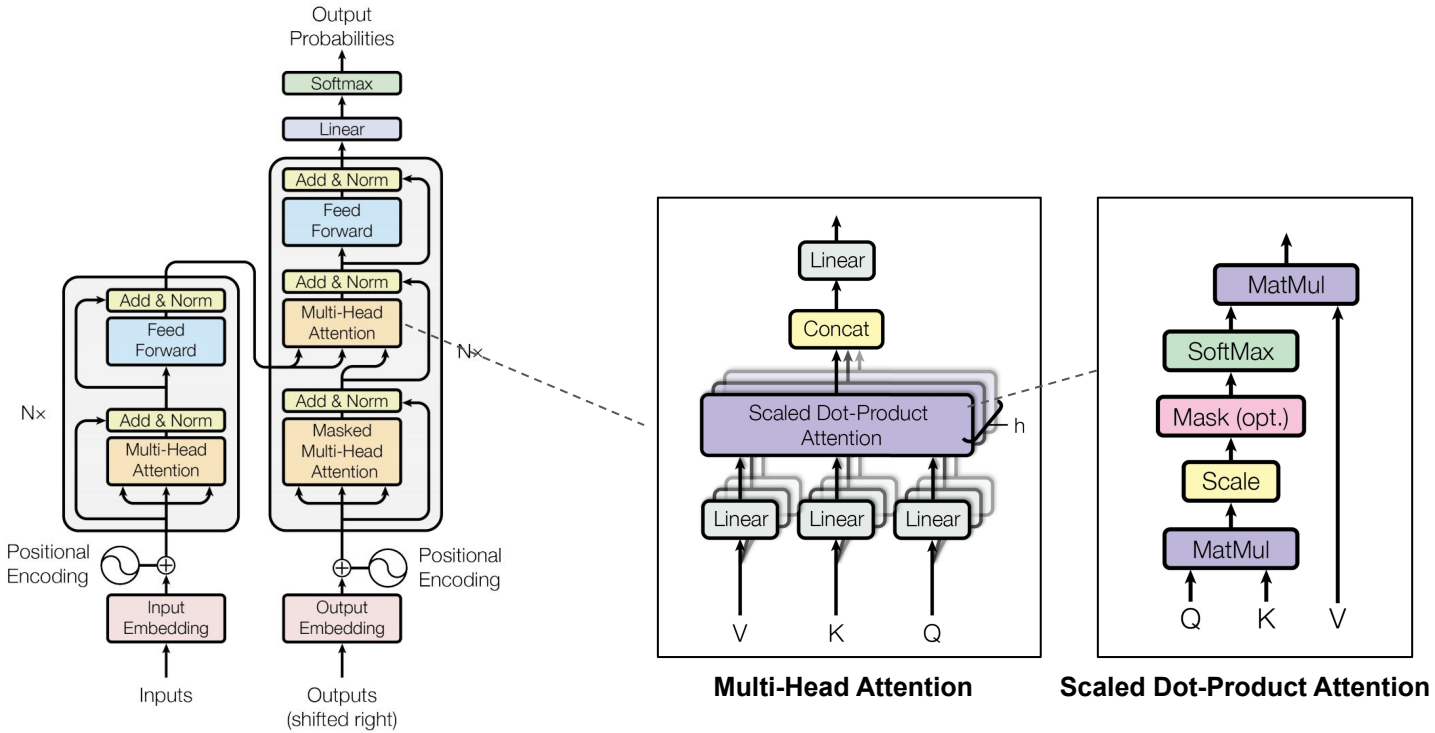
PyTorch Code Reading

- Transformer
- TransformerEncoder
- TransformerEncoderLayer
- MultiheadAttention
- TransformerDecoder
- TransformerDecoderLayer

This Week's Goal:
Understanding the Transformer Architecture 😊



Model Architecture

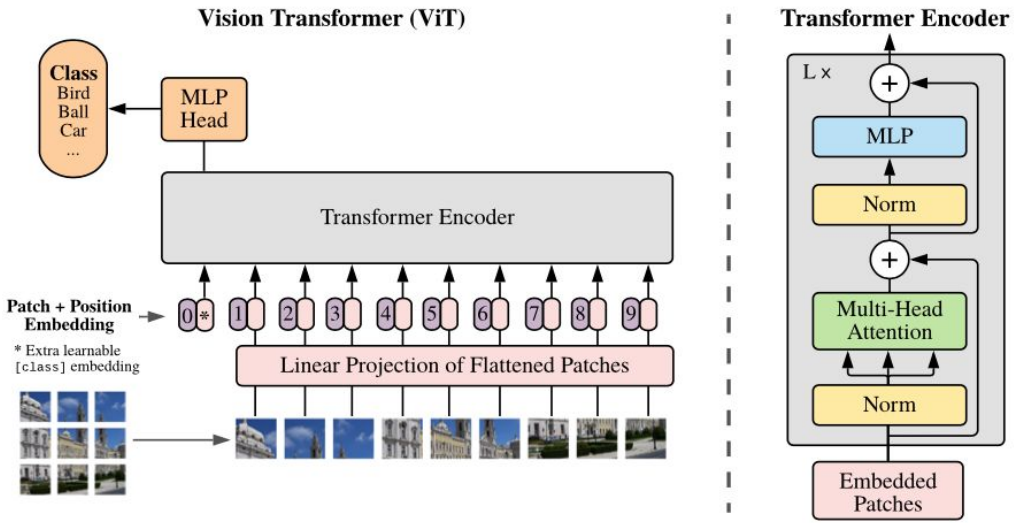
Multi-Head Attention

Scaled Dot-Product Attention

Transformers for Computer Vision

Vision Transformer (ViT) [Dosovitskiy et al. 2021]

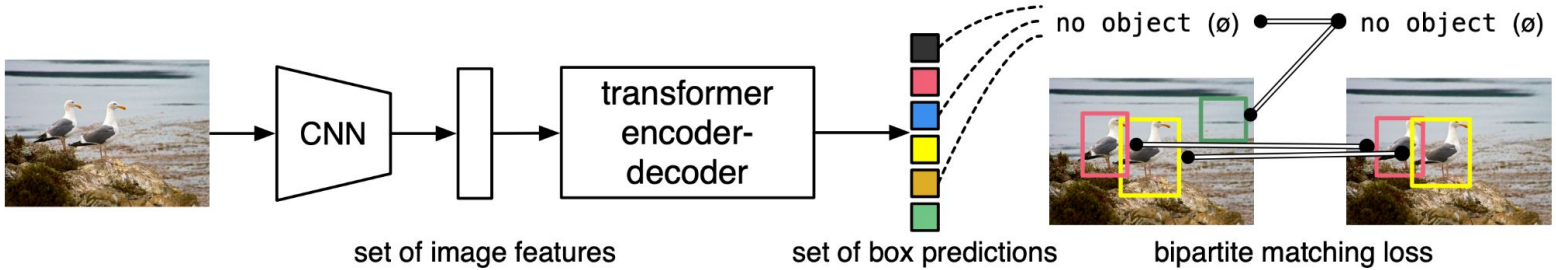
- RGB Image → N Patches → Flattening patches
  - Each patch = (3 * P^2)-dimensional vector



A. Dosovitskiy et al. “An Image is Worth 16x16 Words: Transformers for Image Recognition at Scale”, ICLR ‘21

Detection Transformer (DETR) [Carion et al. 2020]

- CNN + Transformer for object detection



N. Carion et al. “End-to-End Object Detection with Transformers”, arXiv 2020.

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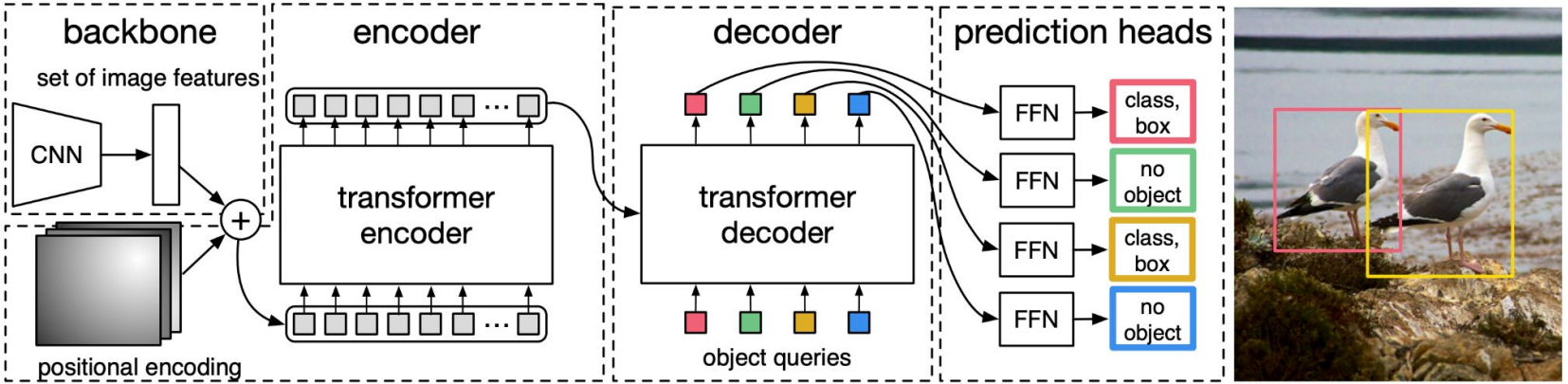

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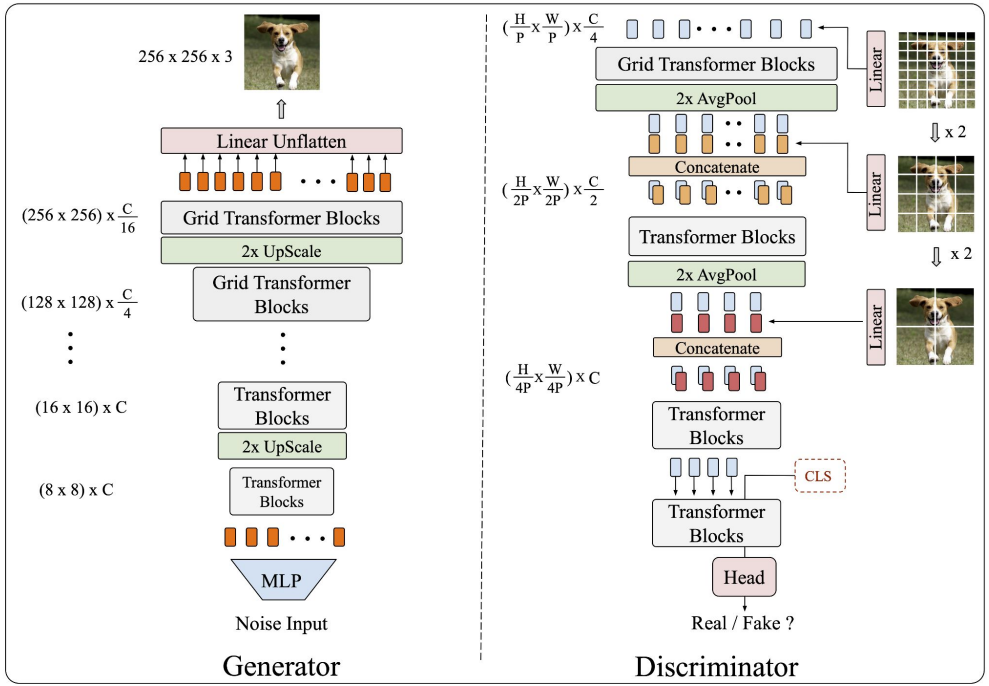
TransGAN [Jian et al. 2021]

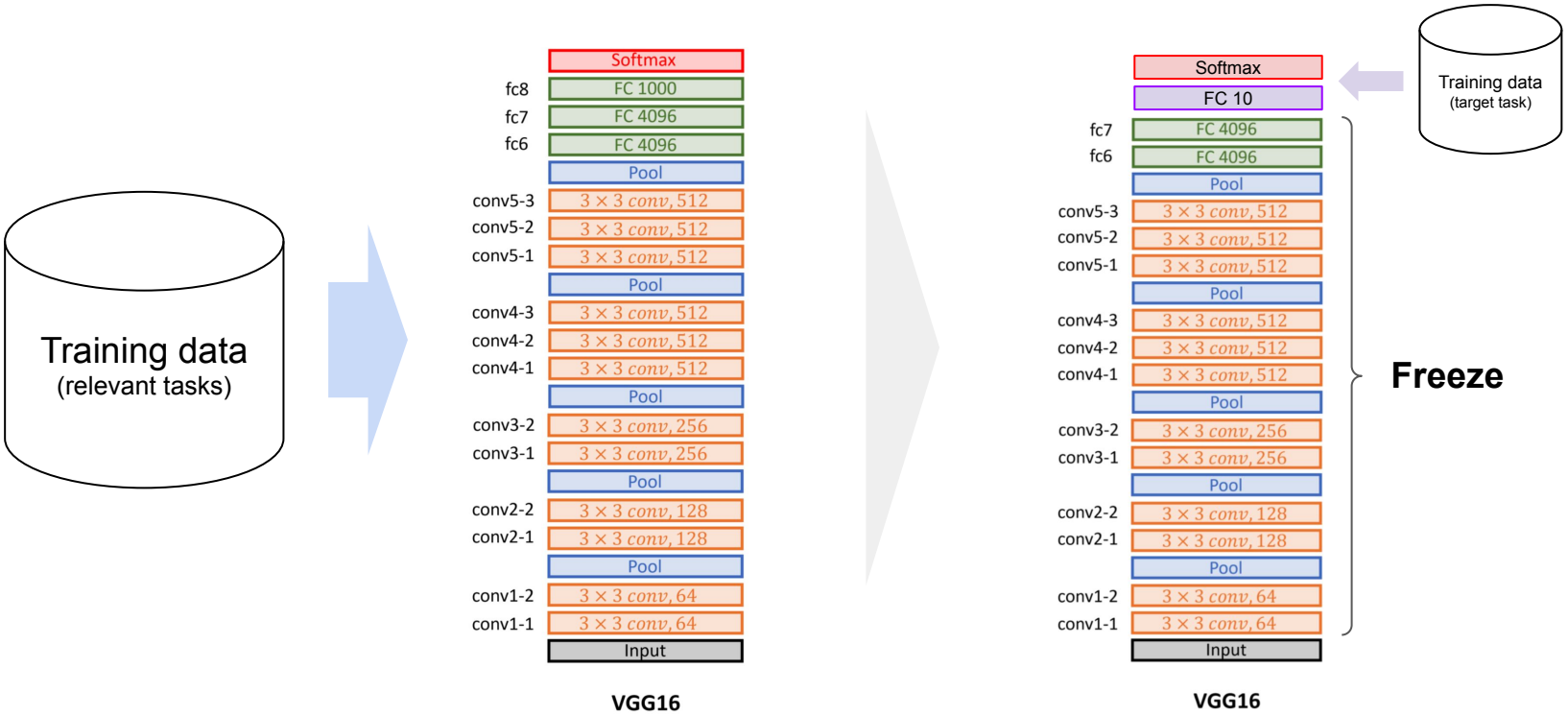


Yifan Jiang, Shiyu Chang, Zhangyang Wang, “TransGAN: Two Pure Transformers Can Make One Strong GAN, and That Can Scale Up”, arXiv 2021.

Pre-trained Language Models

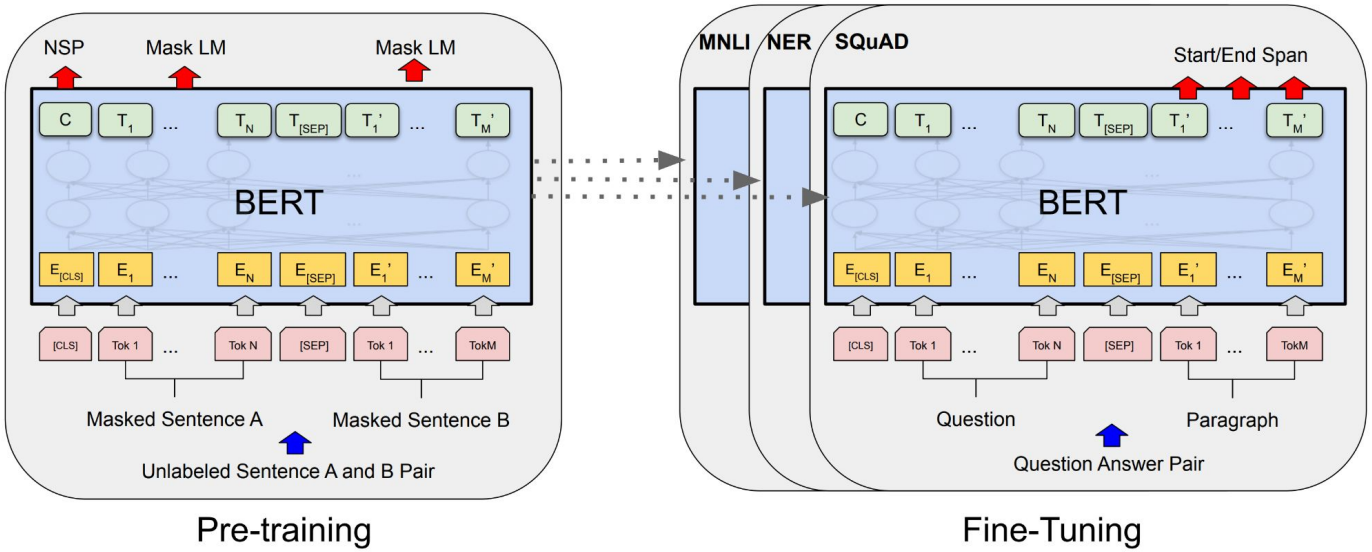
What are Pre-training and Fine-tuning?

- Example for Computer Vision



What are Pre-training and Fine-tuning?

- Example for NLP



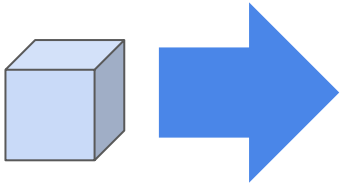
Pre-training & Fine-tuning: Intuition

Pre-training

Pre-training Task 1

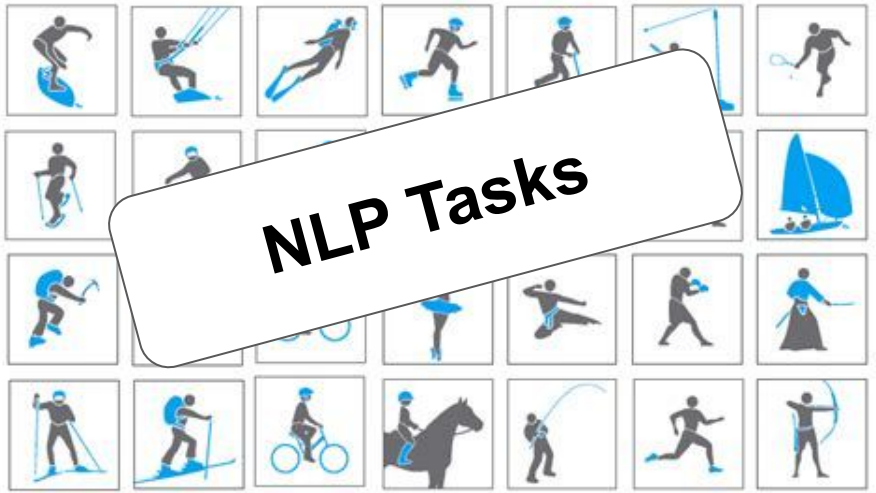
Pre-training Task 2

Fine-tuning



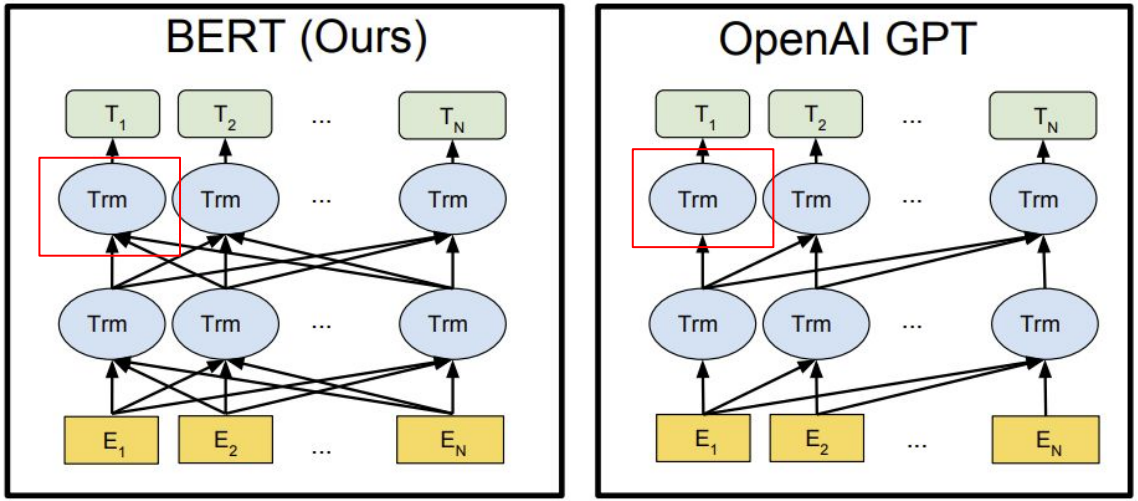
(e.g., BERT)

Downstream tasks



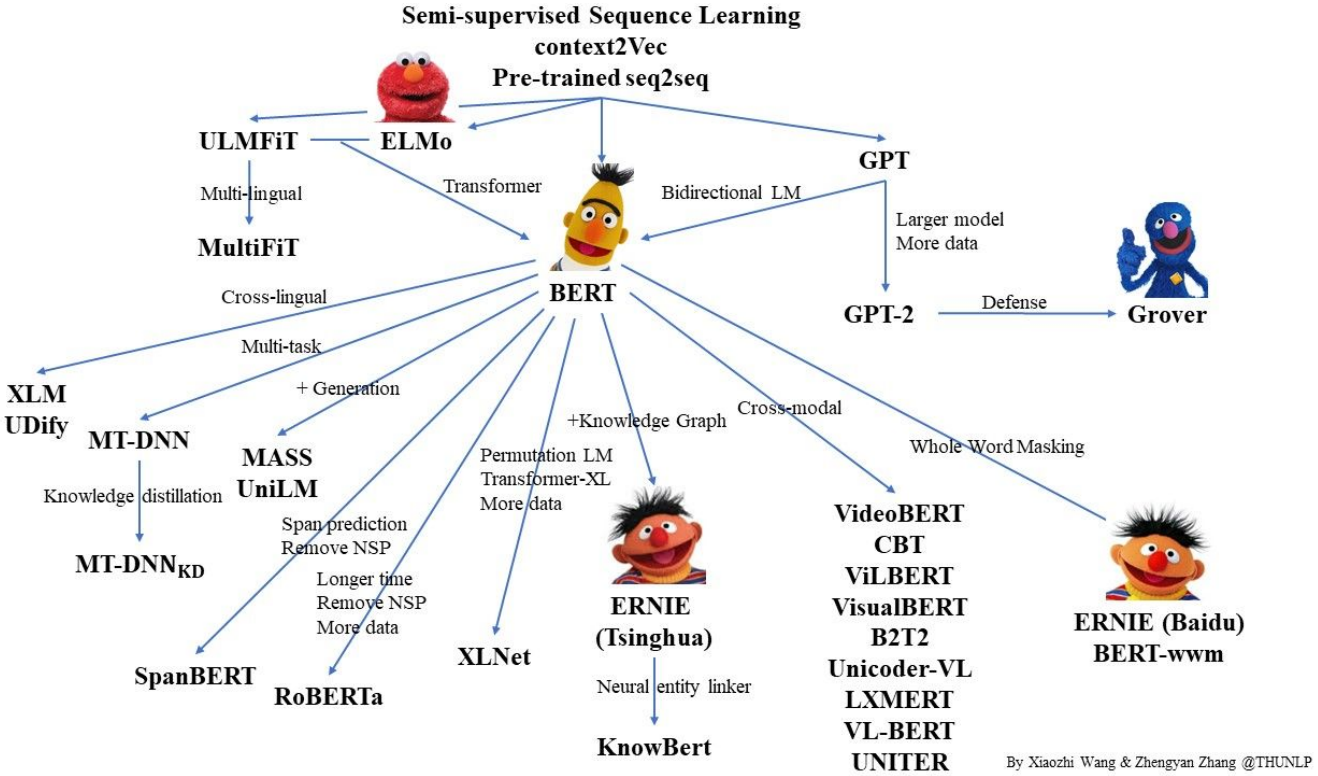
BERT and GPT

- BERT = Bi-directional Transformers (Transformer **Encoder**)
- GPT = left-to-right Transformers (Transformer **Decoder**)



BERT: Pre-training of Deep Bidirectional Transformers for Language Understanding
GPT: Generative Pre-Training

Family Tree of Pre-trained LMs



https://github.com/thunlp/PLMpapers

Pre-trained Model War: Rapid Increase in Model Size

log scale

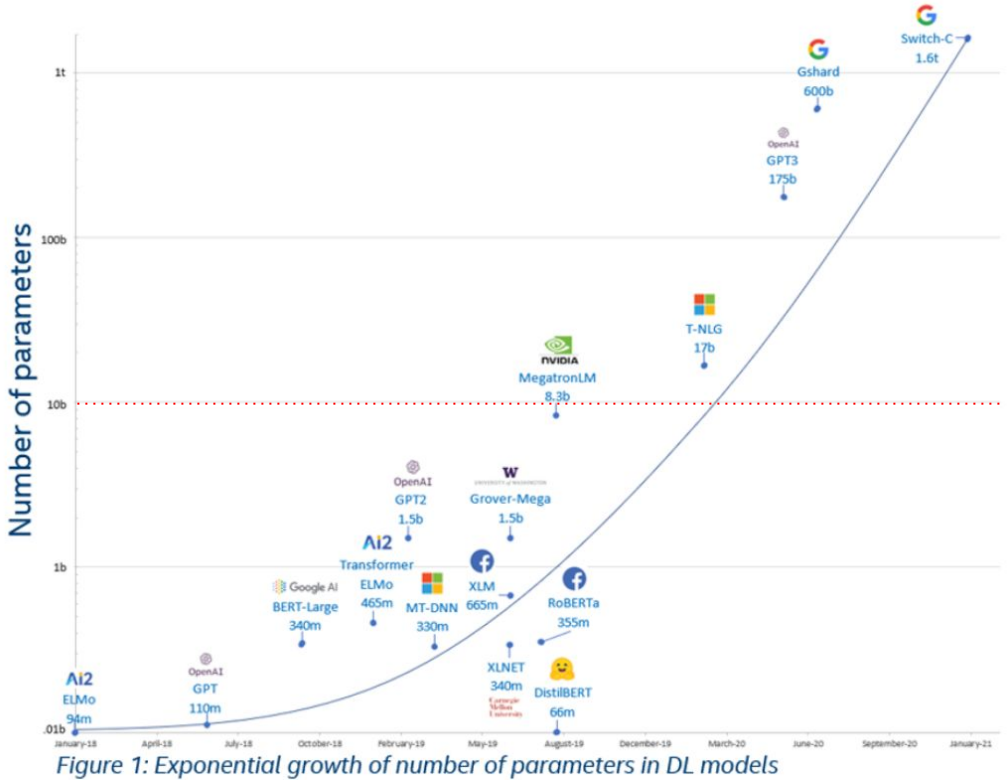


Figure 1: Exponential growth of number of parameters in DL models

2018 2019 2020 2021

Hugging Face's Transformers Library

https://github.com/huggingface/transformers

- You can use a variety of pre-trained language models just with a few lines of Python code

```
>>> from transformers import AutoTokenizer, AutoModel

>>> tokenizer = AutoTokenizer.from_pretrained("bert-base-uncased")
>>> model = AutoModel.from_pretrained("bert-base-uncased")

>>> inputs = tokenizer("Hello world!", return_tensors="pt")
>>> outputs = model(**inputs)
```

Summary

- The Transformer architecture
  - Encoder & Decoder
  - Encoder-decoder attention
- Brief introduction to Transformers for Computer Vision
  - Vision Transformer
  - Detection Transformer
  - TransGAN
- Brief overview of pre-trained Language Models
  - BERT and GPT are Transformer Encoder and Decoder
  - (Almost) all pre-trained models today use the Transformer architecture

Questions?

Further Reading

- The Illustrated Transformer – Jay Alammar – Visualizing machine learning one concept at a time.
- Multi-head attention mechanism: "queries", "keys", and "values," over and over again