

Self Attention (Intra Attention) Networks **Transformers**



- The Transformer (Vaswani et al., 2017) is an architecture that uses attention for information flow: "Attention is all you need"
- It was originally designed for machine translation and has two parts:
 - an encoder that "summarizes" an input sentence
 - a decoder (a conditional LM) that generates an output, based on the input

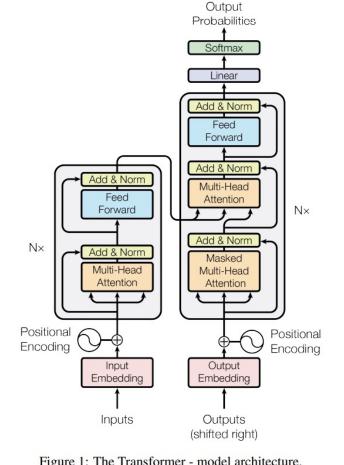


Figure 1: The Transformer - model architecture.

Self Attention (Intra Attention) Networks Transformers



- It is an approach to sequence processing that eliminates recurrent connections and returns to architectures reminiscent of the fully connected networks.
- Transformers map sequences of input vectors $(x_1,...,x_n)$ to sequences of output vectors $(y_1,...,y_n)$ of the same length.

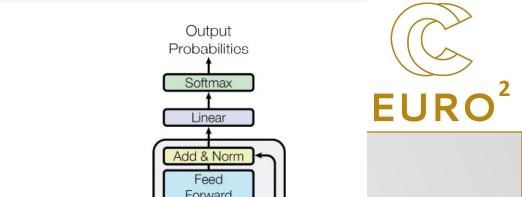


Self Attention (Intra Attention) Networks Transformers



- Transformers are made up of stacks of network layers consisting of simple linear layers, feedforward networks, and custom connections around them.
- The key innovation of transformers is the use of self-attention layers.

Vanilla Transformer: Embedding



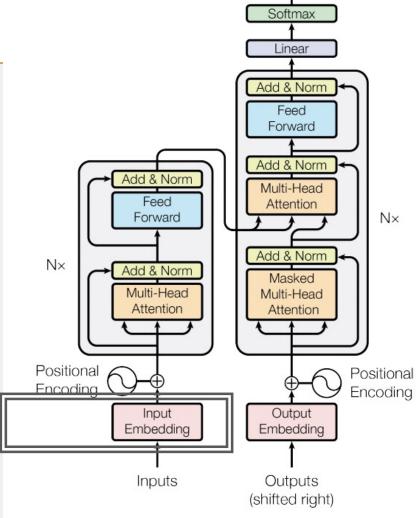


Figure 1: The Transformer - model architecture.

Input and Word Embedding



- They use learned embeddings to convert the input tokens and output tokens to vectors of dimension d_{model} .
- They use the usual learned linear transformation and softmax function to convert the decoder output to predicted next-token probabilities.

Vanilla Transformer: Positional Encoding

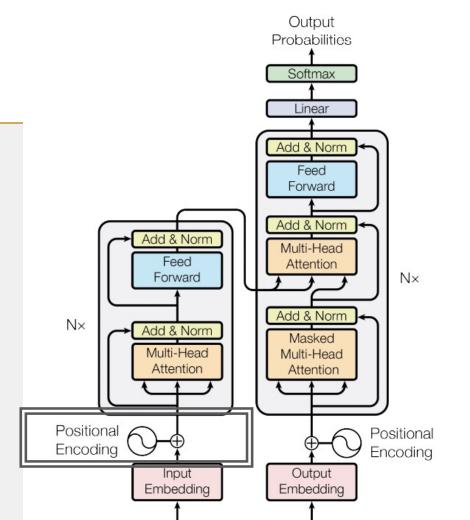


Figure 1: The Transformer - model architecture.

Inputs

Outputs

(shifted right)





- The order in the RNN is inherently encoded in the model itself.
- This is not true for transformers.
 - If you scramble the order of inputs in the attention computation illustrated earlier you get exactly the same answer.
 - To address this issue, Transformer inputs are combined with positional embeddings specific to each position in an input sequence.



• The positional encodings have the same dimension d_{model} as the embeddings, so that the two can be summed:

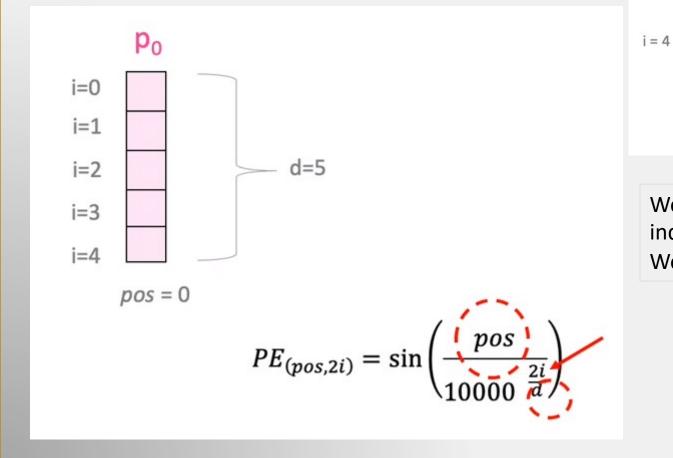
$$PE_{(pos,2i)} = sin(pos/10000^{2i/d_{\text{model}}})$$

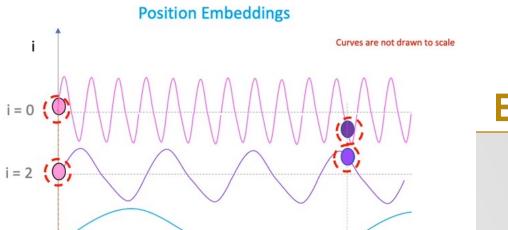
 $PE_{(pos,2i+1)} = cos(pos/10000^{2i/d_{\text{model}}})$

• where *pos* is the position and *i* is the dimension. That is, each dimension of the positional encoding corresponds to a sinusoid.

How does it work?

We work with frequencies!







We generate a different sinusoidal curve for each index.

We locate each pos on each sinusoidal curve.

word position

How does it work?

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

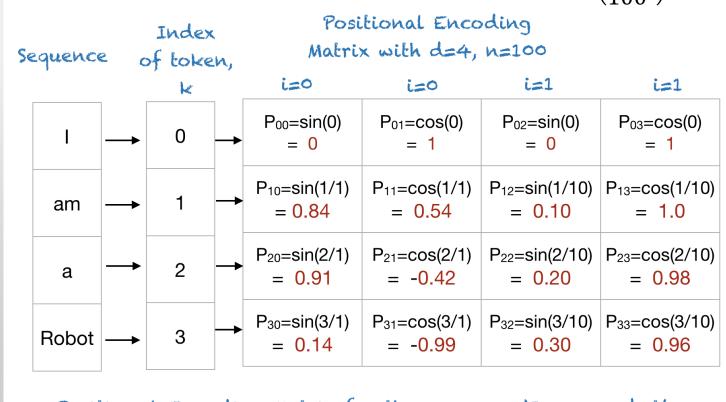
 $PE_{(pos,2i+1)} = cos(pos/10000^{2i/d_{\text{model}}})$

EURO²

• A toy example:

$$PE(0,0) = \sin\left(\frac{0}{100^0}\right) = \sin(0) = 0$$

 $PE(0,1) = \cos\left(\frac{0}{100^0}\right) = \cos(0) = 0$



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

In Python

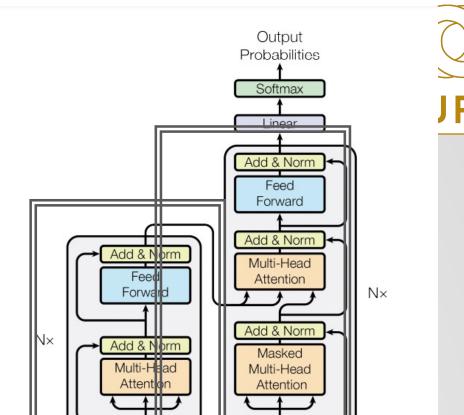


```
def position_encode(pos):
    input_sequence_length=4
    pe=[0]*input_sequence_length
    d_model=4
    n=100
    for i in range(0,input_sequence_length,2):
        pe[i]=math.sin(pos/(n**((2*i)/d_model)))
        pe[i+1]=math.cos(pos/(n**((2*i)/d_model)))
    return pe
```

Position scar import soutation

```
In Pytho pos0=position_encode(0)
          print(f'pos0:{pos0}')
          pos1=position encode(1)
          print(f'pos1:{pos1}')
          pos2=position_encode(2)
          print(f'pos2:{pos2}')
          pos3=position_encode(3)
          print(f'pos3:{pos3}')
          result 1=1-spatial.distance.cosine(pos0,pos1)
          result 2=1-spatial.distance.cosine(pos0,pos2)
          result 3=1-spatial.distance.cosine(pos0,pos3)
          print(f'Similarity between position 0 and 1 is {result 1}')
          print(f'Similarity between position 0 and 2 is {result_2}')
          print(f'Similarity between position 0 and 3 is {result 3}')
          pos0:[0.0, 1.0, 0.0, 1.0]
          pos1:[0.8414709848078965, 0.5403023058681398, 0.009999833334166664, 0.9999500004166653]
          pos2:[0.9092974268256817, -0.4161468365471424, 0.01999866669333308, 0.9998000066665778]
          pos3:[0.1411200080598672, -0.9899924966004454, 0.02999550020249566, 0.9995500337489875]
          Similarity between position 0 and 1 is 0.7701261531424025
          Similarity between position 0 and 2 is 0.2918265850597177
          Similarity between position 0 and 3 is 0.004778768574271064
```

Vanilla Transformer: Encoder and Decoder Stacks



Positional

Encoding

Output

Embedding

Outputs

(shifted right)

Figure 1: The Transformer - model architecture.

Input Embedding

Inputs

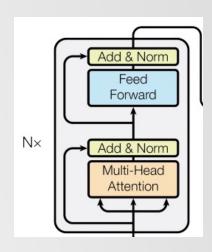
Positional

Encoding

Encoder Stacks: Summary



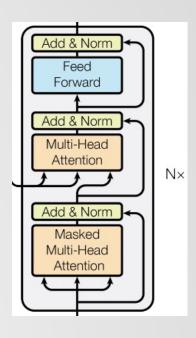
- The encoder is composed of a stack of N = 6 identical layers.
- Each layer has two sub-layers:
 - The first is a multi-head self-attention mechanism,
 - The second is a simple, positionwise fully connected feed-forward network.
 - They employ a residual connection around each of the two sub-layers, followed by layer normalization. That is, the output of each sub-layer is LayerNorm(x + Sublayer(x)), where Sublayer(x) is the function implemented by the sub-layer itself.
 - To facilitate these residual connections, all sub-layers in the model, as well as the embedding layers, produce outputs of dimension d_{model} = 512.



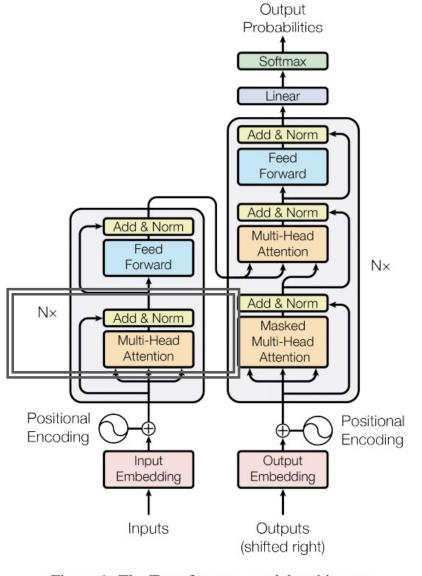
Decoder Stacks: Summary

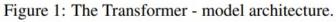


- The decoder is also composed of a stack of N = 6 identical layers
- The decoder also has a third sub-layer, which performs multi-head attention over the output of the encoder stack.
- They employ residual connections around each of the sub-layers, followed by layer normalization.
- They also modify the self-attention sub-layer in the decoder stack to prevent positions from attending to subsequent positions.
 - This masking, combined with fact that the output embeddings are offset by one position, ensures that the predictions for position *i* can depend only on the known outputs at positions less than *i*.



Vanilla Transformer: Attention Layer





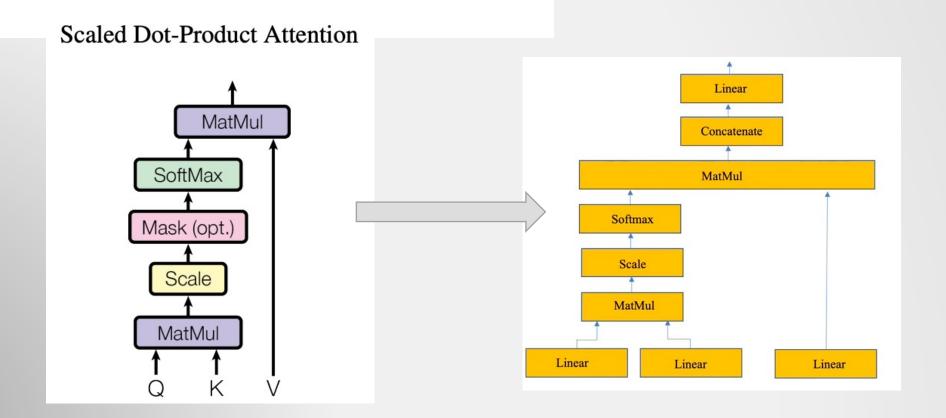




- Self-attention allows a network to directly extract and use information from arbitrarily large contexts without the need to pass it through intermediate recurrent connections as in RNNs.
- When processing each item in the input, the model has access to all the inputs up to an including the one under consideration, but no access to information about inputs beyond the current one.
 - ensures that we can use this approach to create language models and use them for autoregressive generation,
- The computation performed for each item is independent of all the other computations:
 - means that we can easily parallelize both forward inference and training of such models.

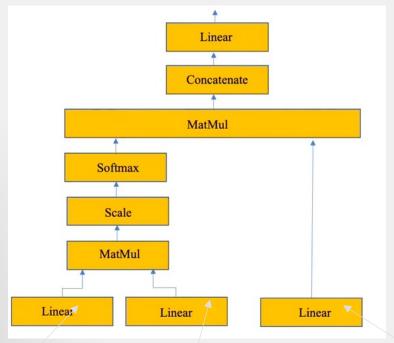


• K, Q and V all connect to a linear layer.





- Consider the example sentence S: "I watched the movie Transformers."
 - the length of the sentence: 5, the embedding dimension: 8

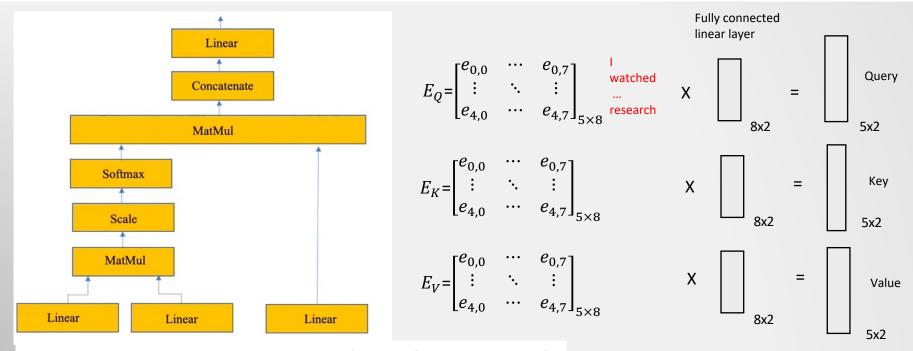


These input vectors (E_Q , E_K , E_V) are same and include embedding+positional embedding.

$$E_{Q} = \begin{bmatrix} e_{0,0} & \cdots & e_{0,7} \\ \vdots & \ddots & \vdots \\ e_{4,0} & \cdots & e_{4,7} \end{bmatrix}_{5 \times 8} \qquad E_{K} = \begin{bmatrix} e_{0,0} & \cdots & e_{0,7} \\ \vdots & \ddots & \vdots \\ e_{4,0} & \cdots & e_{4,7} \end{bmatrix}_{5 \times 8} \qquad E_{V} = \begin{bmatrix} e_{0,0} & \cdots & e_{0,7} \\ \vdots & \ddots & \vdots \\ e_{4,0} & \cdots & e_{4,7} \end{bmatrix}_{5 \times 8}$$



- Consider the example sentence S: "I watched the movie Transformers."
 - the length of the sentence: 5, the embedding dimension: 8



Notice that these new vectors (Key, Query, Value) are smaller in dimension than the embedding vector. Their dimensionality is 2, while the embedding and encoder input/output vectors have dimensionality of 8.

The linear layer here has 2 nodes and each layer has its own weights having a total of 2x8=16 weights.

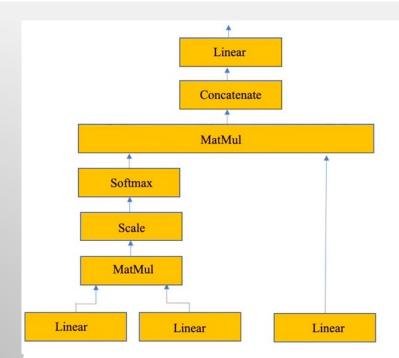
It is directly connected to the embedding (with pos) layer.

- Consider the example sentence S: "I watched the movie Transf
 - the length of the sentence: 5, the embedding dimension: 8

Generally:

Query Size = Embedding Size / Number of heads

Let's set number of heads as 4.



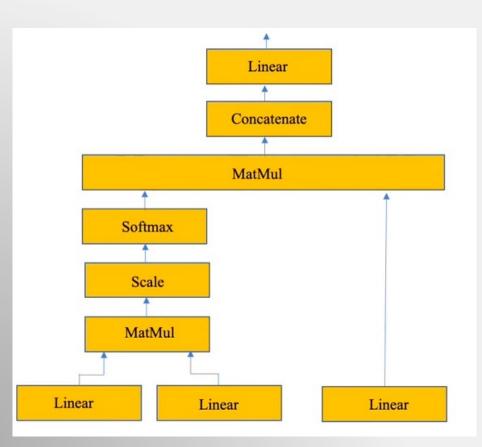
Notice that these new vectors (Key, Query, Value) are smaller in dimension than the embedding vector. Their dimensionality is 2, while the embedding and encoder input/output vectors have dimensionality of 8.

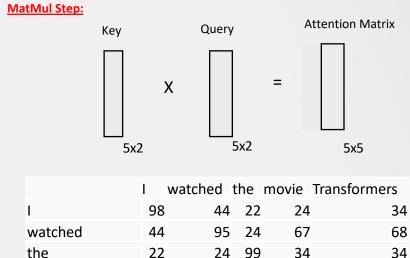
The linear layer here has 2 nodes and each layer has its own weights having a total of 2x8=16 weights.

It is directly connected to the embedding (with pos) layer.



- Consider the example sentence *S*: "I watched the movie Transformers.
 - the length of the sentence: 5, the embedding dimension: 8





34

movie

Transformers

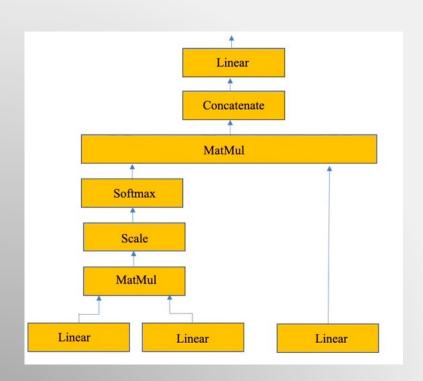
Numbers are randomly selected i.e. co-occurrence number.

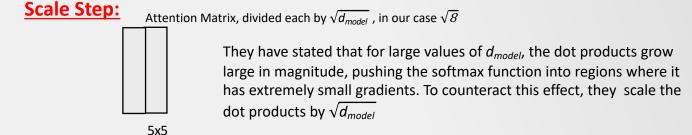
65

98



- Consider the example sentence S: "I watched the movie Transformers."
 - the length of the sentence: 5, the embedding dimension: 8

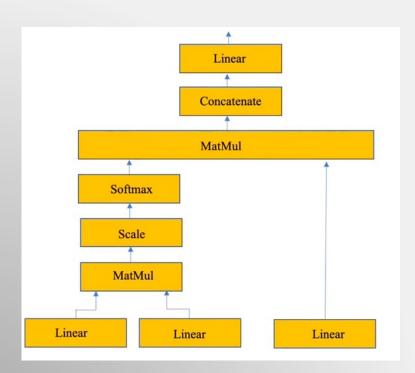




	I	watched	the	movie	Transformers
I	34.65	15.56	7.78	8.49	12.02
watched	15.56	33.59	8.49	23.69	24.04
the	7.78	8.49	35.00	12.02	12.02
movie	8.49	23.69	12.02	32.53	22.98
Transformers	12.02	24.04	12.02	22.98	34.65



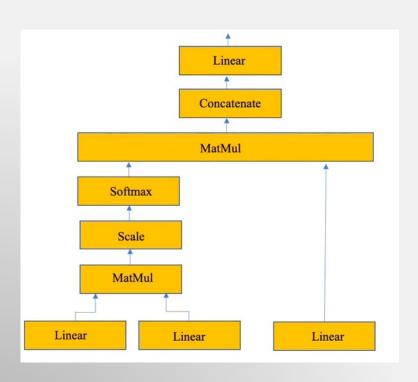
• Consider the example sentence S: "I watched the movie Transformers."



Softmax Step:
$$softmax(x_i) = \frac{\exp(x_i)}{\sum_j \exp(x_j)}$$

	I	watched	the	movie	Transformers
I	1.00	0.00	0.00	0.00	0.00
watched	0.00	1.00	0.00	0.00	0.00
the	0.00	0.00	1.00	0.00	0.00
movie	0.00	0.00	0.00	1.00	0.00
Transformers	0.00	0.00	0.00	0.00	1.00

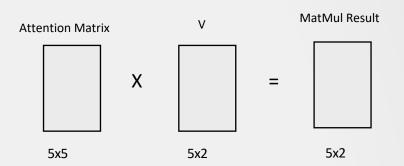




MatMul Step with Value matrix:

We have the scaled attention matrix showing which words are related with which.

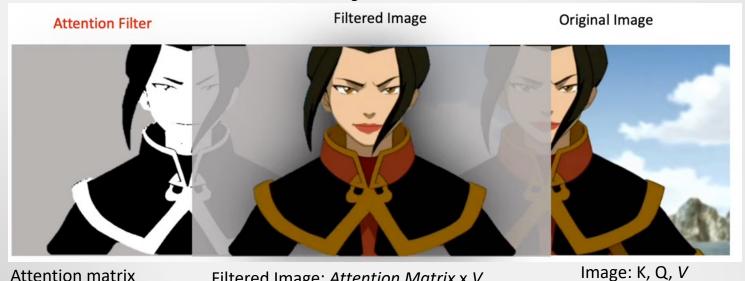
It is like a weight matrix which needs to be multiplied with *V* matrix to get the values from.





MatMul Step with Value matrix:

Intuition from images:



Attention matrix obtained using the following:

$$\operatorname{softmax}(\frac{QK^T}{\sqrt{d_k}})$$

Filtered Image: Attention Matrix x V

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



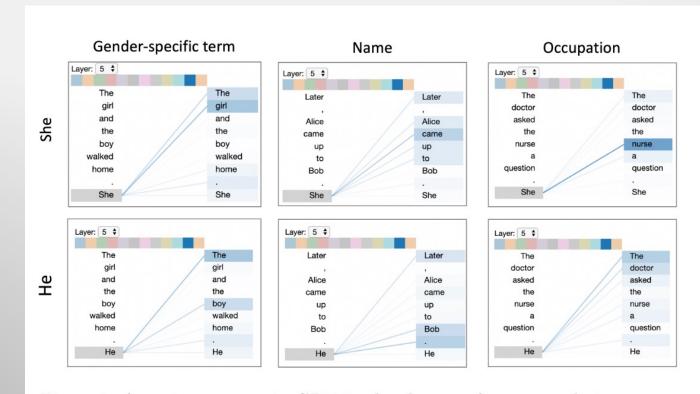


Figure 4: Attention pattern in GPT-2 related to coreference resolution suggests the model may encode gender bias.

Multi-head Attention



- The different words in a sentence can relate to each other in many different ways simultaneously.
 - For example, distinct syntactic, semantic, and discourse relationships can hold between verbs and their arguments in a sentence.
- Transformers address this issue with multihead self attention layers.
- These are sets of self-attention layers, called heads, that reside in parallel layers at the same depth in a model, each with its own set of parameters.

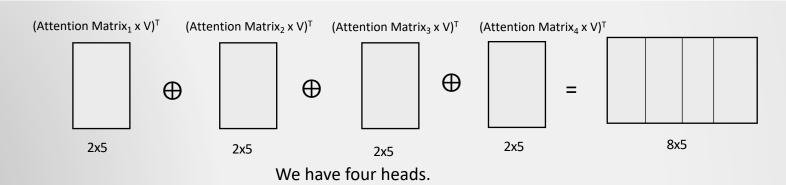
EURO²

Multi-head Attention

 Multi-head attention allows the model to jointly attend to information from different representation subspaces at different positions. With a single attention head, averaging inhibits this.

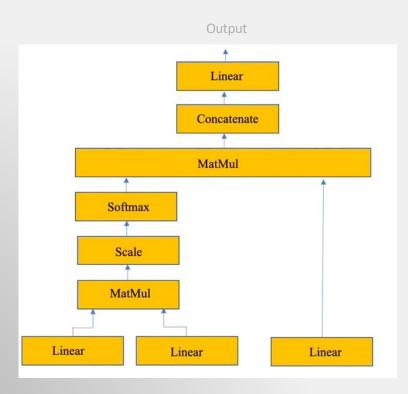
$$\begin{aligned} \text{MultiHead}(Q, K, V) &= \text{Concat}(\text{head}_1, ..., \text{head}_h)W^O \\ \text{where head}_i &= \text{Attention}(QW_i^Q, KW_i^K, VW_i^V) \end{aligned}$$

Where the projections are parameter matrices $W_i^Q \in \mathbb{R}^{d_{\text{model}} \times d_k}$, $W_i^K \in \mathbb{R}^{d_{\text{model}} \times d_k}$, $W_i^V \in \mathbb{R}^{d_{\text{model}} \times d_v}$ and $W^O \in \mathbb{R}^{hd_v \times d_{\text{model}}}$.



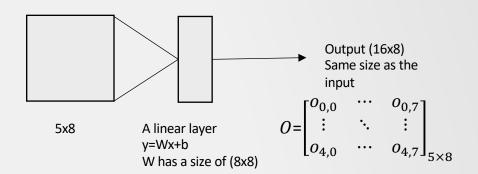


Output:

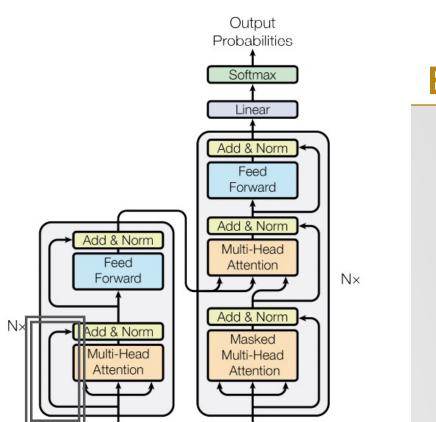


Linear layer at the end shrinks the size of the concatenated matrix.

We don't want to grow it with attention layers.



Vanilla Transformer: Residual Connection



Output

Embedding

Outputs

(shifted right)

Positional

Encoding

Figure 1: The Transformer - model architecture.

Input

Embedding

Inputs

Positional

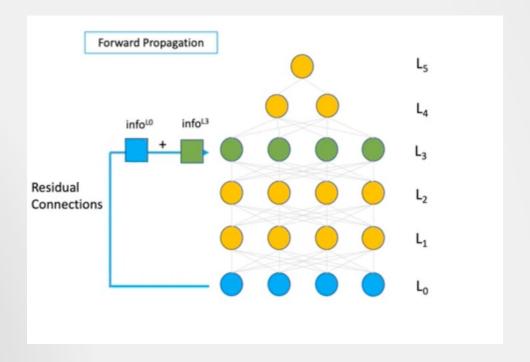
Encoding



Residual Connection

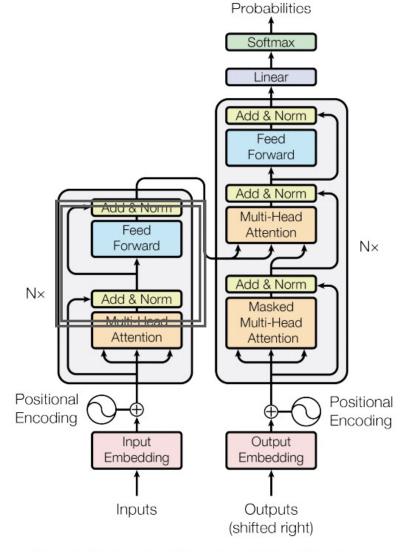


• Information loss at the last hidden layers can be solved with so-called high-ways aka residual connections.



Vanilla Transformer: Add&Normalization Layer Feedforward Layer





Output

Figure 1: The Transformer - model architecture.

Add&Normalization Layer



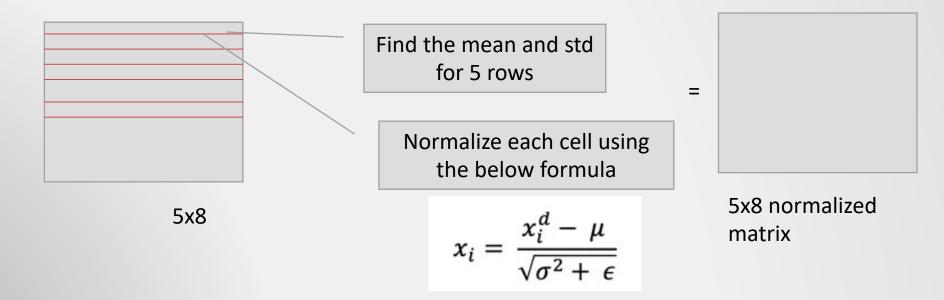
 We simply add the residual connection and the output of multihead attention.

$$E_{Q} = \begin{bmatrix} e_{0,0} & \cdots & e_{0,7} \\ \vdots & \ddots & \vdots \\ e_{4,0} & \cdots & e_{4,7} \end{bmatrix}_{5\times8} \quad \begin{array}{c} \mathbf{I} \\ \text{watched} \\ \cdots \\ \mathbf{I} \\ \end{array} \quad + \quad O = \begin{bmatrix} o_{0,0} & \cdots & o_{0,7} \\ \vdots & \ddots & \vdots \\ o_{4,0} & \cdots & o_{4,7} \end{bmatrix}_{5\times8} \quad = \quad \\ \\ \text{Output of multi-head} \\ \text{attention} \\ \end{array}$$

Add&Normalization Layer



 We simply add the residual connection and the output of multihead attention.

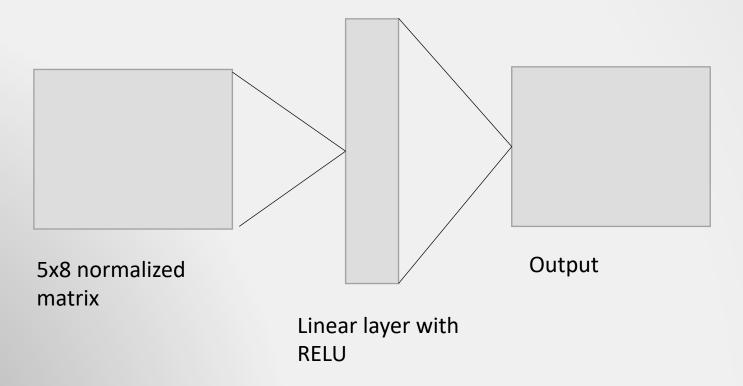


∈ can be set as 0.0001 to make the denominator as non zero

Feedforward Layer

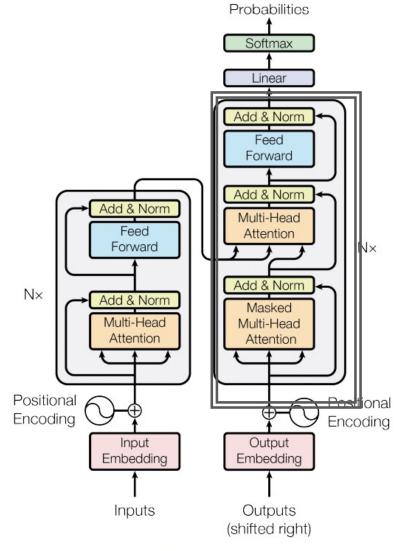


• Linear layers with RELU activation function



Vanilla Transformer: Decoder





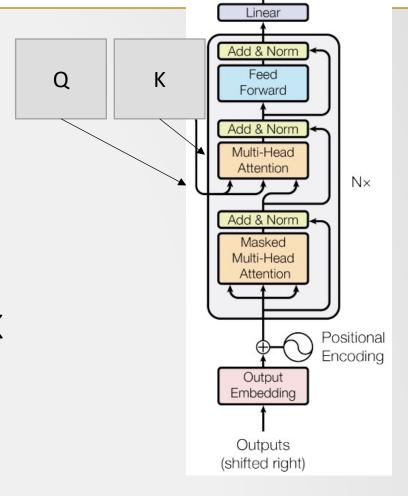
Output

Figure 1: The Transformer - model architecture.

Decoder

EURO²

- Decoder layer takes two inputs:
 - The output of the encoder layer
 - The predicted/generated output so far
- On the other hand, encoder layer takes only inputs
- The output of the encoder layer is copied twice to construct the Q and K matrices.



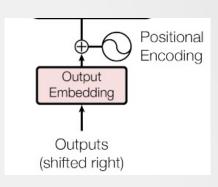
Output

Probabilities

Softmax

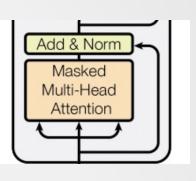


- Step 1:
- The first <s> start of sentence is provided.
- The embedding with its positional embedding is generated.



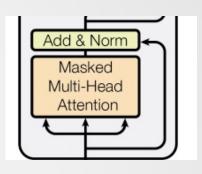


- Step 2:
- During training, the model accepts the input and output as a whole sequence.
- For example:
 - Input:<I watched the movie Transformers.>
 - Output: <Transformers filmini seyrettim.>
- My vocabulary size: 3+2(start and end of sentence tags)





- Step 2:
- Although our input is provided to the encoder, we provide the next sequence items one by one via masked multi-head attention.



Input: < I watched the movie Transformers.>

Next sequence: <Transformers filmini seyrettim.>

Next sequence: <Transformers filmini seyrettim.>

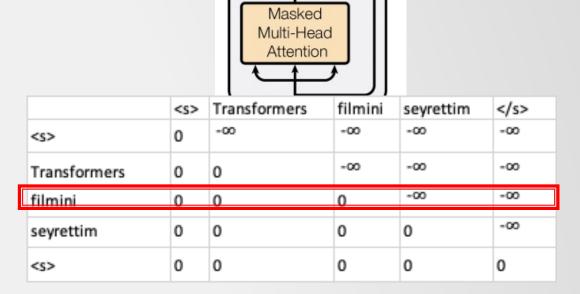
Next sequence: <Transformers filmini seyrettim.>



- Step 2:
- The outputs in the future time steps are masked via -∞ values.

<Transformers filmini seyrettim.>

	<s></s>	Transformers	filmini	seyrettim		
<s></s>	32	4	7	4	1	
Transformers	4	40	7	3	3	
filmini	7	7	31	2	4	+
seyrettim	4	3	2	49	23	
<s></s>	1	3	4	23	0	



Add & Norm

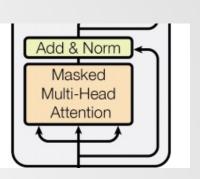
Attention filter

Masked filter

We obtain masked-attention filter at the end.

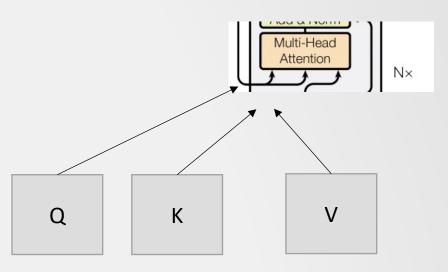


- Step 2:
- The reason of -∞ values is that when we pass it from softmax, they will become zero for the words in the future.
- Don't forget that we use teacher forcing for training.
- We pass it from add&normalization layer to obtain our V matrix.





- Step 3:
- This embedding V together with the previously generated Q and K matrices from the encoding layer is fed to the multi-head attention.

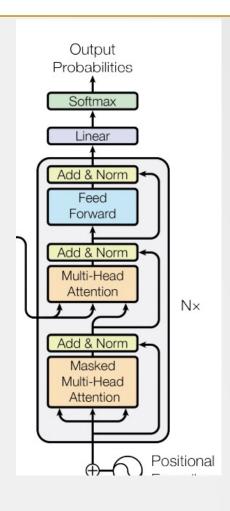


Decoder

Output Embedding



- Step 4:
- The remaining steps feedforward, add&norm, linear layer and softmax steps are same as in the encoding step.
- We produce the probability of each word in our vocabulary.
- We use cross entropy to calculate the loss.



Results

EURO²

Dataset

- WMT 2014 English-German dataset consisting of about 4.5 million sentence pairs are used.
- Sentences were encoded using byte-pair encoding, which has a shared source- target vocabulary of about 37000 tokens.
- For English-French, they used the significantly larger WMT 2014 English-French dataset consisting of 36M sentences and split tokens into a 32000 word-piece vocabulary.
- Sentence pairs were batched together by approximate sequence length.
- Each training batch contained a set of sentence pairs containing approximately 25000 source tokens and 25000 target tokens.

Results



Table 2: The Transformer achieves better BLEU scores than previous state-of-the-art models on the English-to-German and English-to-French newstest2014 tests at a fraction of the training cost.

Model	BLEU		Training Cost (FLOPs)	
Model	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	$2.3\cdot 10^{19}$	



Thanks!





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