

01 Transformer

- 1) Encoder-Decoder
- 2) Transformer Structure
- 3) Usage of Encoder-Decoder

02 Transformer Decoder

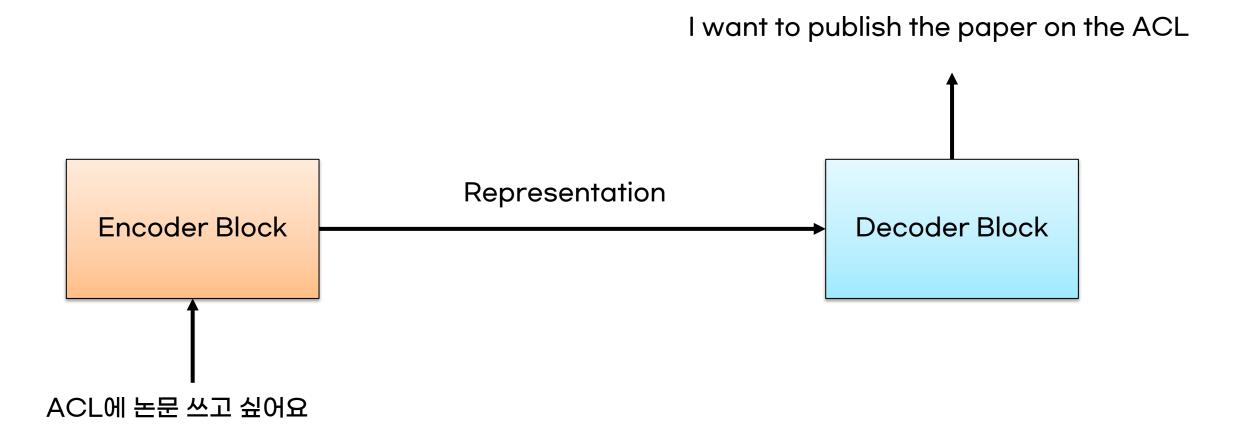
- 1) Masked Multi-Head Attention
- 2) Multi-Head Attention
- 3) Add & Norm
- 4) Linear & Softmax

Contents



01 Encoder-Decoder Structure

- Transformer Encoder-Decoder Architecture: Without Bottleneck
 - ✓ The size of input and output embedding are the same size
 - ✓ Since it encodes via self-attention, it does not seem to require a bottleneck.



02 Transformer Structure

- Tokenize the input sentence through a tokenizer, convert it to a
 token embedding, and combine the position embedding and token
 embedding to inject information about the position of the token into
 the encoder.
- Encoders and decoders consist of a stack of encoder layers and decoder layers, similar to the stack of convolutional layers in computer vision.
- The output of the encoder is injected into each decoder layer, and the decoder predicts the next most likely token in the sequence, predicts the <EOS> token, or repeats until the maximum length is reached.
- The transformer architecture is designed for seq2seq operations, but the encoder and decoder blocks are independent models.

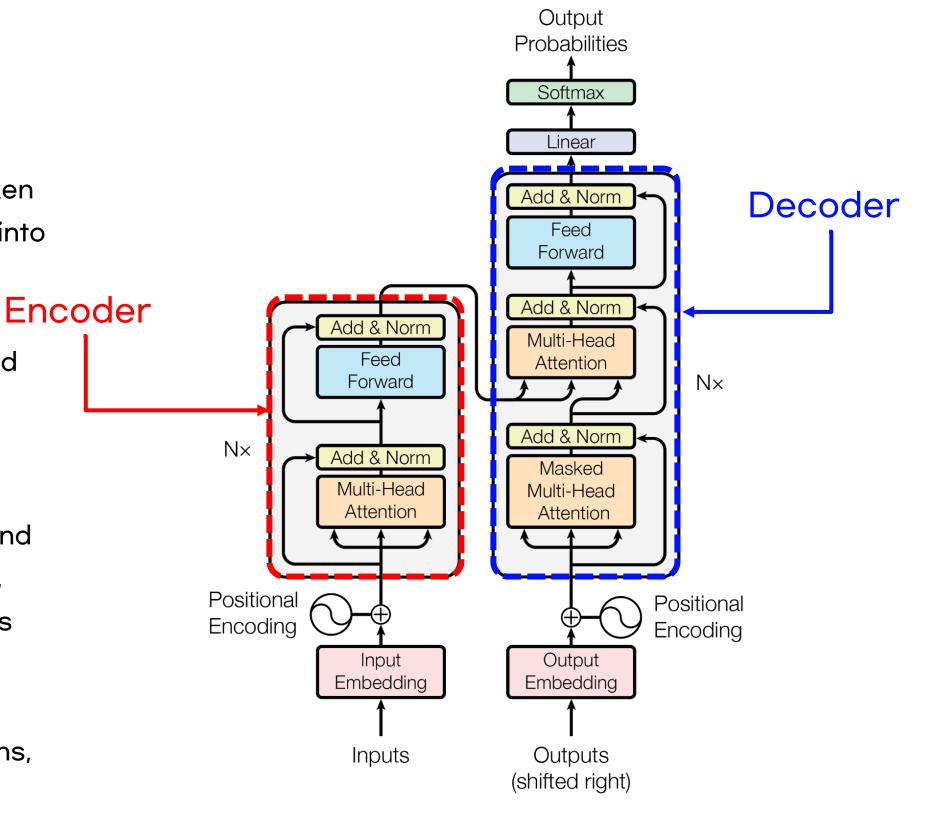


Figure 1: The Transformer - model architecture.

03 Usage of Encoder-Decoder

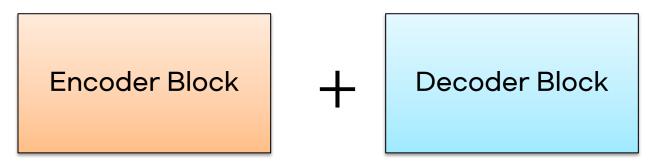
Transformer Encoder-Decoder Architecture.



> Encoder block: BERT Series Models for QA, text classification

Decoder Block

Decoder block: GPT-like models for Chatbot, NLG, QA



> Encoder block + Decoder block : BART, T5 for Machine Translation and Summarization

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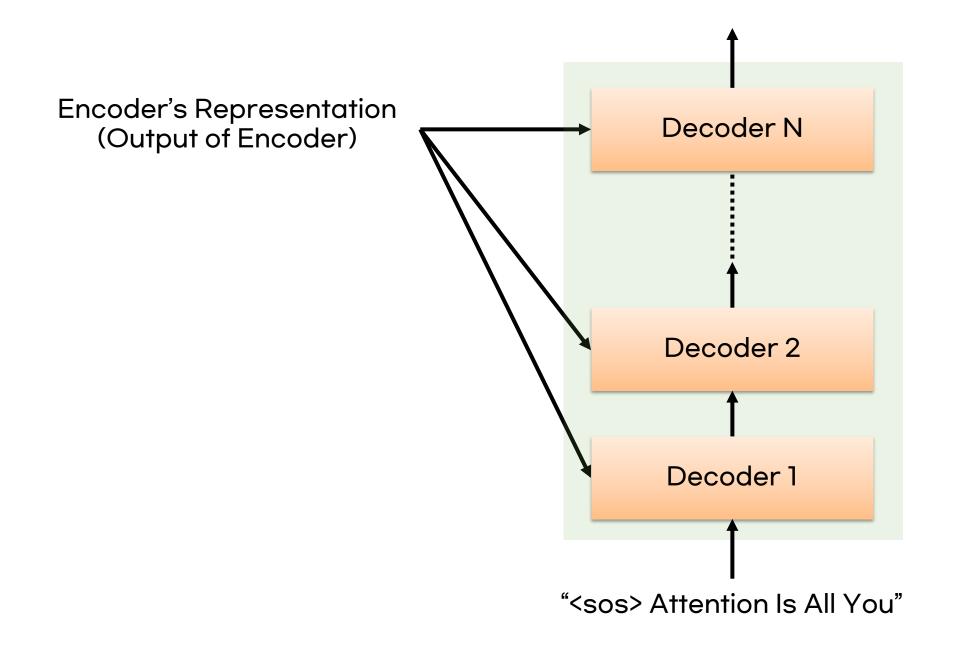
02 Transformer Decoder

- 1) Masked Multi-Head Attention
- 2) Multi-Head Attention
- 3) Add & Norm
- 4) Linear & Softmax

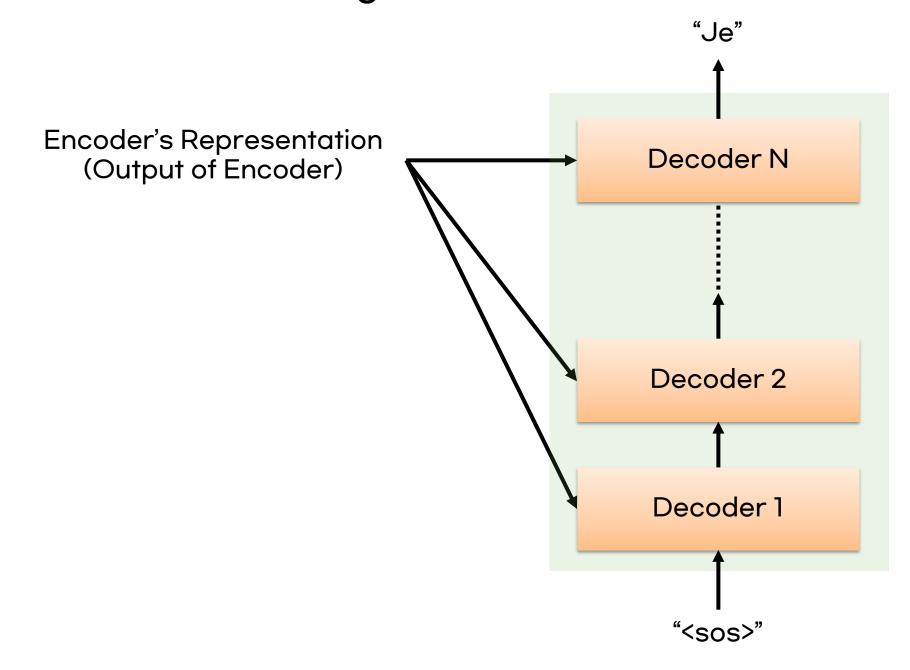
Contents



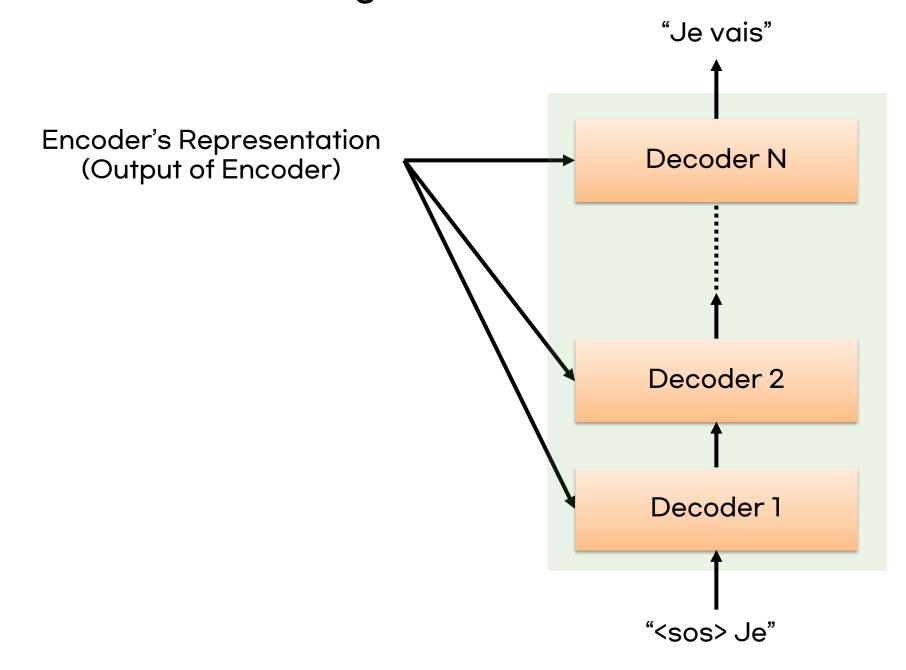
- Use N decoders as a stacked structure
- The Decoder takes as input the output of the previous Decoder and the representation of the Encoder.



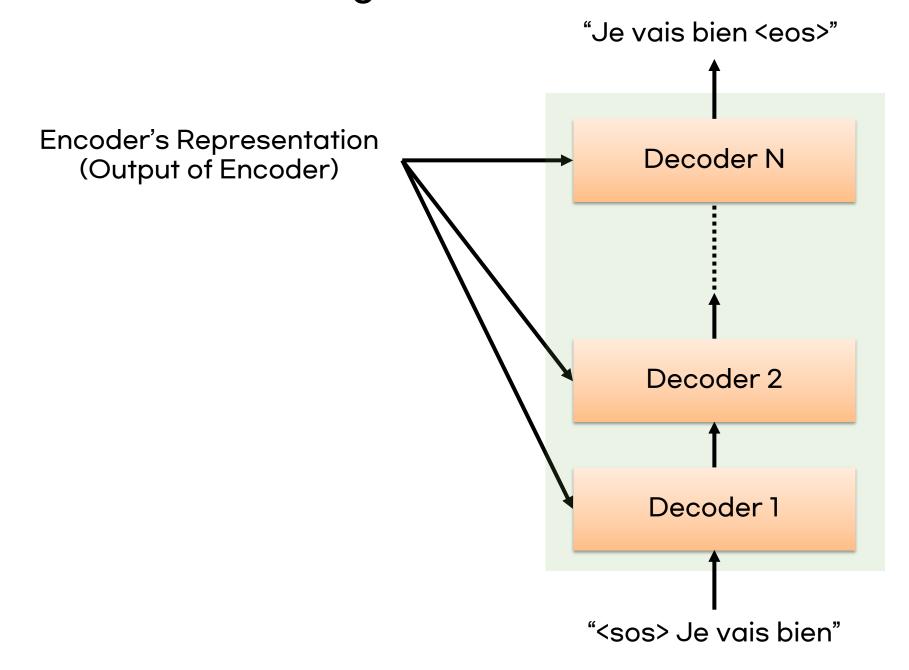
- How the Decoder Works?
- Example of generating the French sentence "Je vais bien" from the English sentence "I am good".



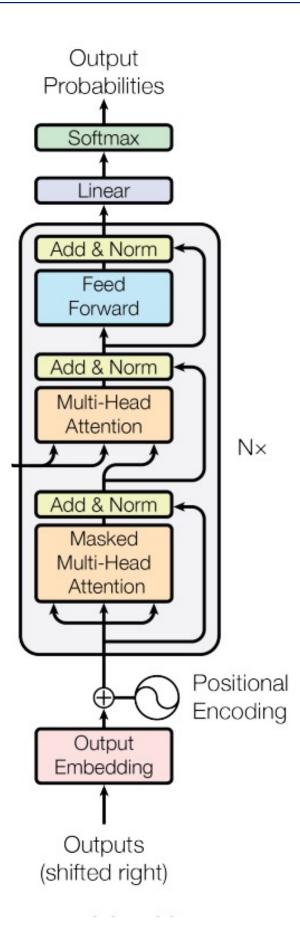
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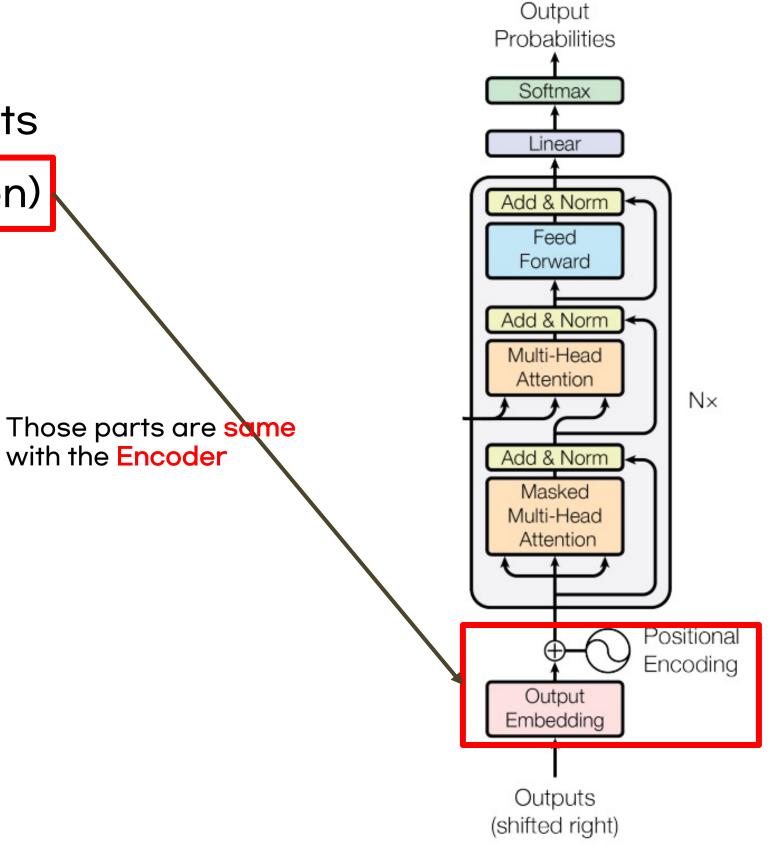
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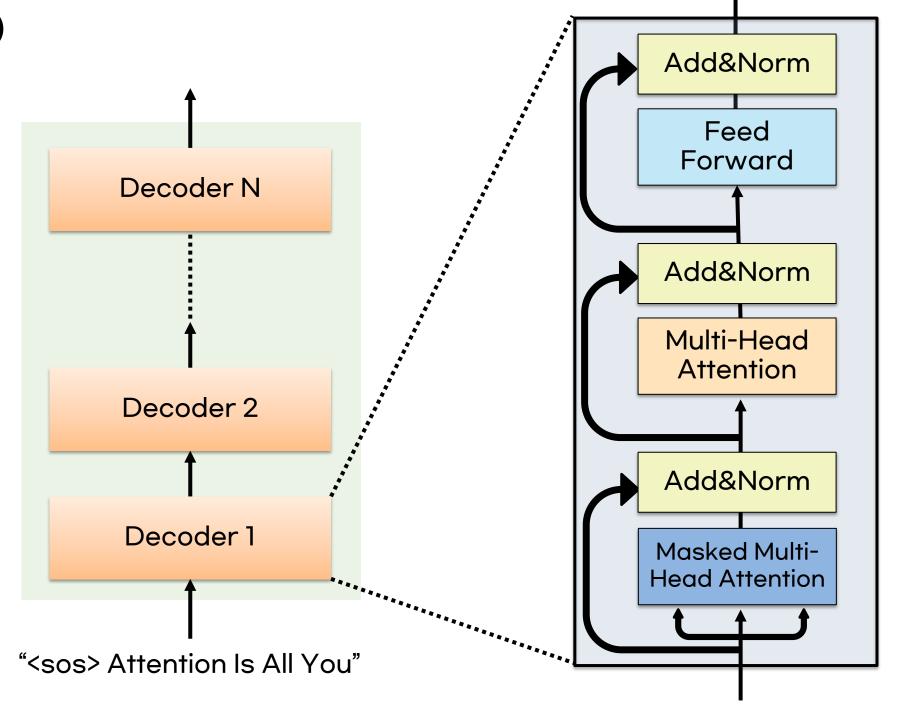
- Transformer Decoder Components
 - ✓ Embedding layer (Word, Position)
 - ✓ Masked Multi-Head Attention
 - ✓ Multi-Head Attention
 - ✓ Feed-Forward
 - ✓ Add & Norm



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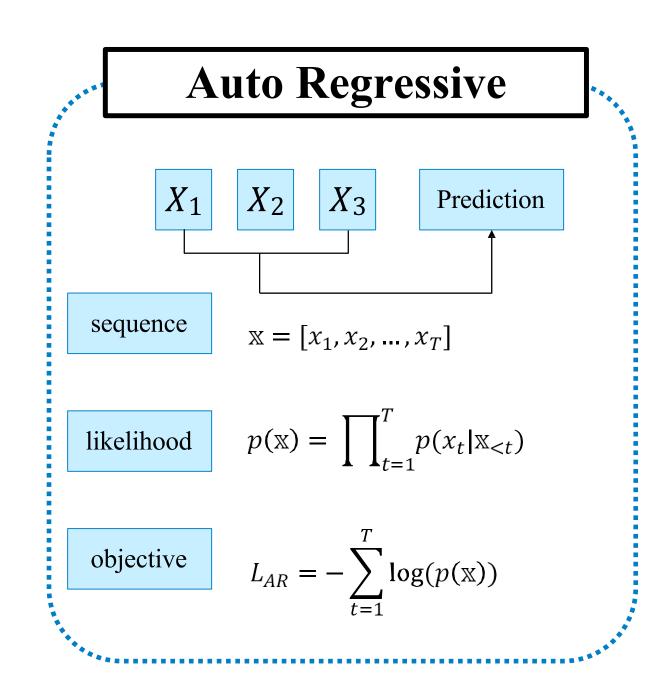


Transformer Decoder Architecture

Introduction of Masked Multi-Head Attention

- When the decoder generates a sentence, it only puts the words generated in the previous step into the input sentence.
 - ex) input : [<sos>, 'Je'], output : ['Je', 'vais']
- Decoder Characteristics + self-attention = Masked Multi-Head Attention
 - the characteristic is about Auto-Regressive
 - Auto-Regressive: Predicting the next token based on all previous tokens

Auto-Regressive: Predicting the next token based on all previous tokens



```
Sentence: I have a dream

- <SOS> I

- <SOS> I have

- <SOS> I have a
```

Can we compute multi-head attention parallelly in the Auto-regressive model?

Masking the un sheet next to you! == masked multi-head attention

<sos></sos>	Je	vais	bien
<sos></sos>	Je	vais	bien
<sos></sos>	Je	vais	bien
<sos></sos>	Je	vais	bien



<sos></sos>	mask	mask	mask
<sos></sos>	Je	mask	mask
<sos></sos>	Je	vais	mask
<sos></sos>	Je	vais	bien

Masked Multi-Head Attention - Process

- 1. Extract embeddings from a sentence: create an embeddings matrix
- 2. Create Key, Query, Value from Embedded Matrix
- 3. Calculate the similarity between Query and Key : $Q \cdot K^T$
- 4. Scaling and Softmax (normalization) \rightarrow score matrix : $softmax \left(\frac{Q \cdot K^T}{\sqrt{d_k}} \right)$
- 5. Multiply by Value to obtain Attachment matrix M

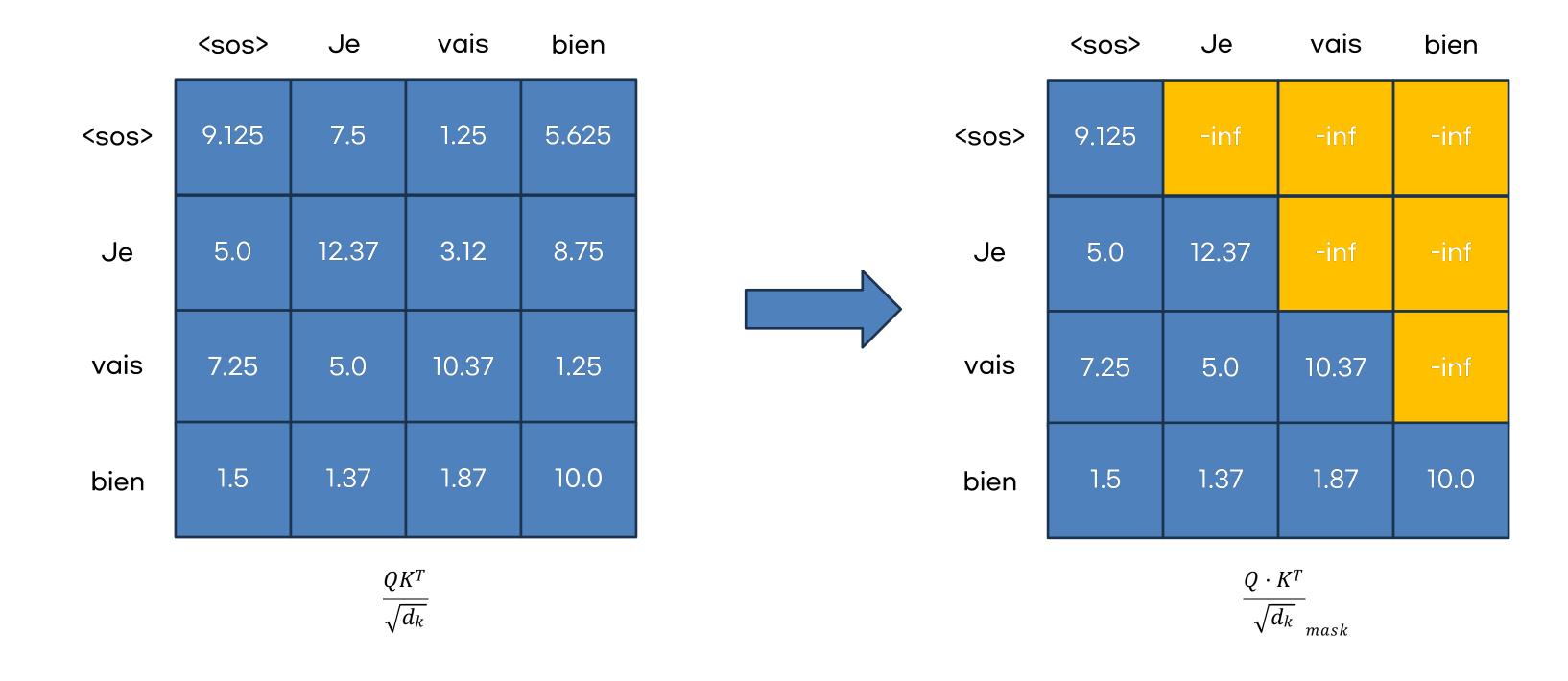
Those parts are same with the Encoder

Masked Multi-Head Attention - Process

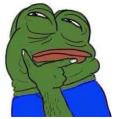
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Those parts are same with the Encoder

4. Scaling and Softmax (normalization)



• Why mask with -inf? • exp(-inf) = 0



$$- exp(-\inf) = 0$$

-
$$softmax\left(\frac{Q \cdot K^T}{\sqrt{d_k}}\right) =$$

	<sos></sos>	Je	vais	bien
<sos></sos>	1	Ο	Ο	Ο
Je	0.37	0.62	Ο	Ο
vais	0.26	0.31	0.43	О
bien	0.21	0.26	0.26	0.27

Masked Multi-Head Attention - Process

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- 5. Multiply by Value to obtain Attachment matrix M

Those parts are same with the Encoder

01 Masked Multi-Head Attention (code)

• Get the score matrix in the same way as the encoder and replace the upper triangular matrix with -inf

Masking effect because the value is zero after passing Softmax

```
def scaled_dot_product_attention(query, key, value, mask=None):
    dim_k = query.size(-1)
    scores = torch.bmm(query, key.transpose(1, 2)) / sqrt(dim_k)
    if mask is not None:
        scores = scores.masked_fill(mask == 0, float("-inf"))
    weights = F.softmax(scores, dim=-1)
    return weights.bmm(value)
```

mask is a half-triangular matrix

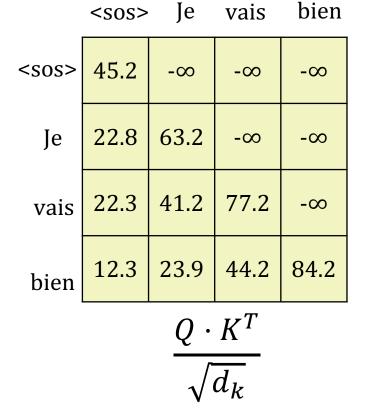
1 0 0

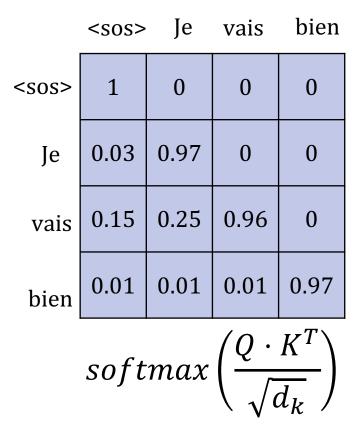
1 1 0 ···

1 1 1

••

	<sos></sos>	Je	vais	bien	
<sos></sos>	45.2	20.1	18.3	17.8	
Je	22.8	63.2	7.3	16.3	
vais	22.3	41.2	77.2	12.2	
bien	12.3	23.9	44.2	84.2	
$Q \cdot K^T$					





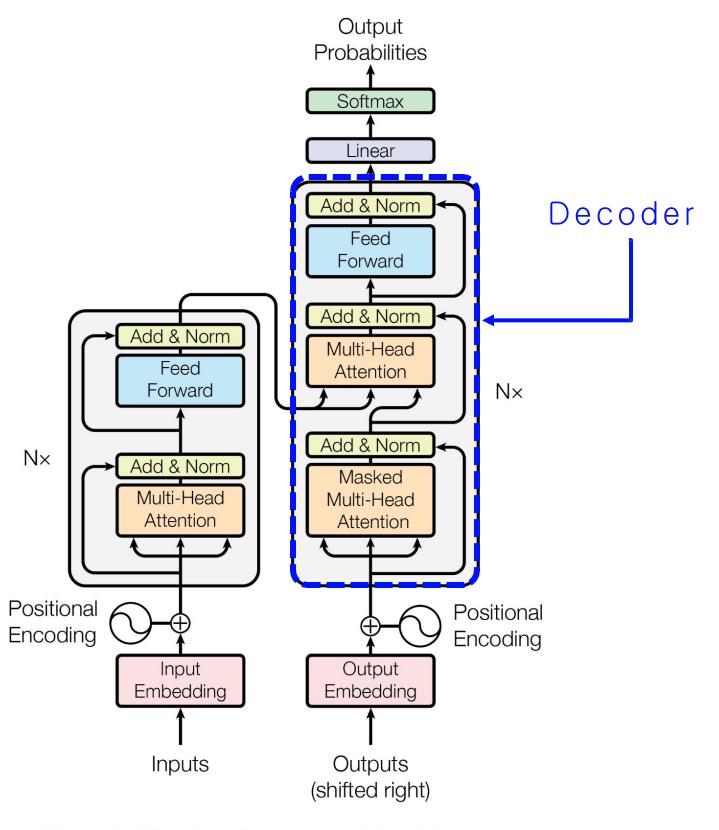
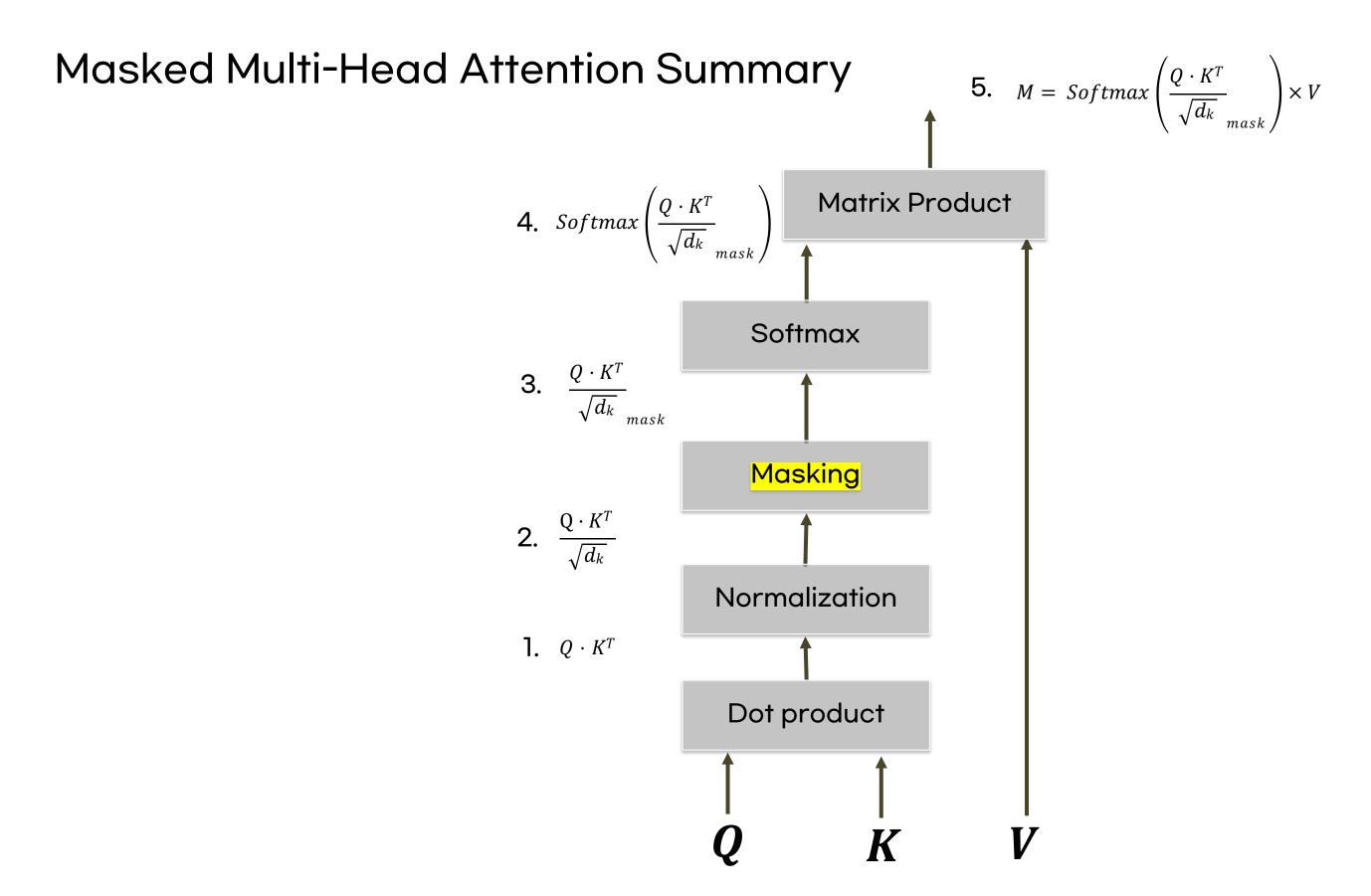


Figure 1: The Transformer - model architecture.



01 Masked Multi-Head Attention (Example)

- Assuming we have two Multi-Head Attention, then the calculation is as follows
- 1. Compute attention heads M_1, M_2
 - 1) Set W_1^Q , W_1^K , W_1^V and compute Q_1 , K_1 , V_1 . Then get $M_1 = \operatorname{softmax}\left(\frac{Q_1K_1^T}{\sqrt{d_k}}\right)V_1$
 - 2) Set W_2^Q , W_2^K , W_2^V and compute Q_2 , K_2 , V_2 . Then get M_2 = softmax $\left(\frac{Q_2K_2^T}{\sqrt{d_k}}\right)V_2$
- 2. Concatenate the obtained Attention Heads and use the Linear Projection concatenate($[M_1, M_2]$)W

Introduction of Multi-Head Attention for Decoder

- Input
 - Output of Masked Multi-Head Attention (Matrix M)
 - Output of Encoder
- Interaction between the results of the encoder and the results of the decoder
 - Called the Encoder-Decoder Attention Layer

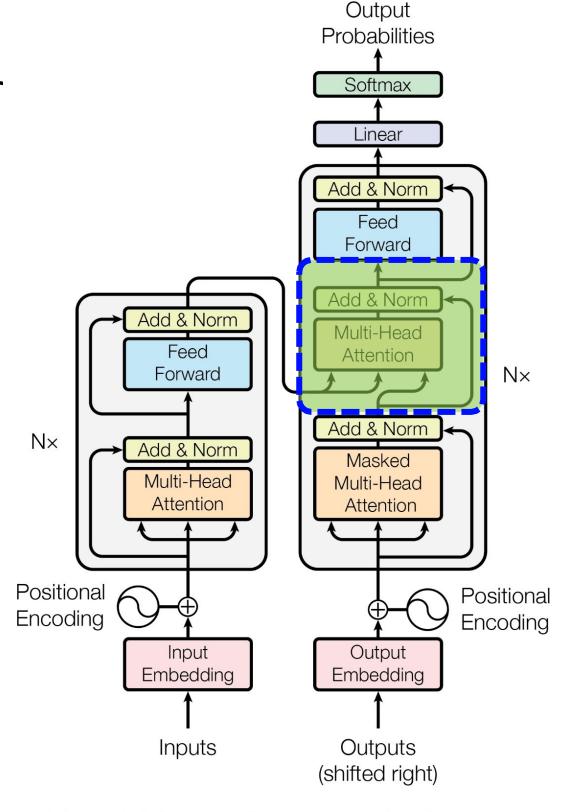
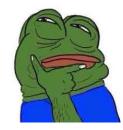
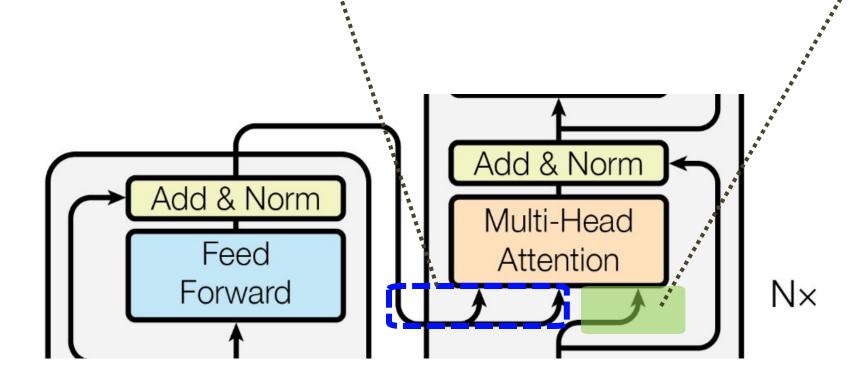


Figure 1: The Transformer - model architecture.

How do encoder results interact with decoder results?



- → Generate the query matrix Q using output of decoder (Attention matrix M)
- → Generate a Key, Value matrix (K, V) using the result of the encoder (representation R)



Multi-Head Attention(in Decoder) - Process

- Generate Query from Attention Matrix (M from Masked), Key and Value from Encoder Representation (R)
- 2. Calculate the similarity between a query and a key : QK^T
- 3. Scaling & Softmax -> score matrix: $softmax \left(\frac{Q \cdot K^T}{\sqrt{d_k}}\right)$
- 4. Multiply by Value to get the Attention matrix Z

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- 4. Multiply by Value to get the Attention matrix Z

- Generate Query from Attention Matrix (M from Masked), Key and Value from Encoder Representation (R)
- For generating Query(Q) matrix, set W^Q

where $W^Q \in \mathbb{M}^{d_-emb \times d_k}$ are trainable parameters

• Generate Q by dot-product between W^Q and Attention matrix M

$$Q = MW^Q$$

where M is Attention matrix from masked multi head attention

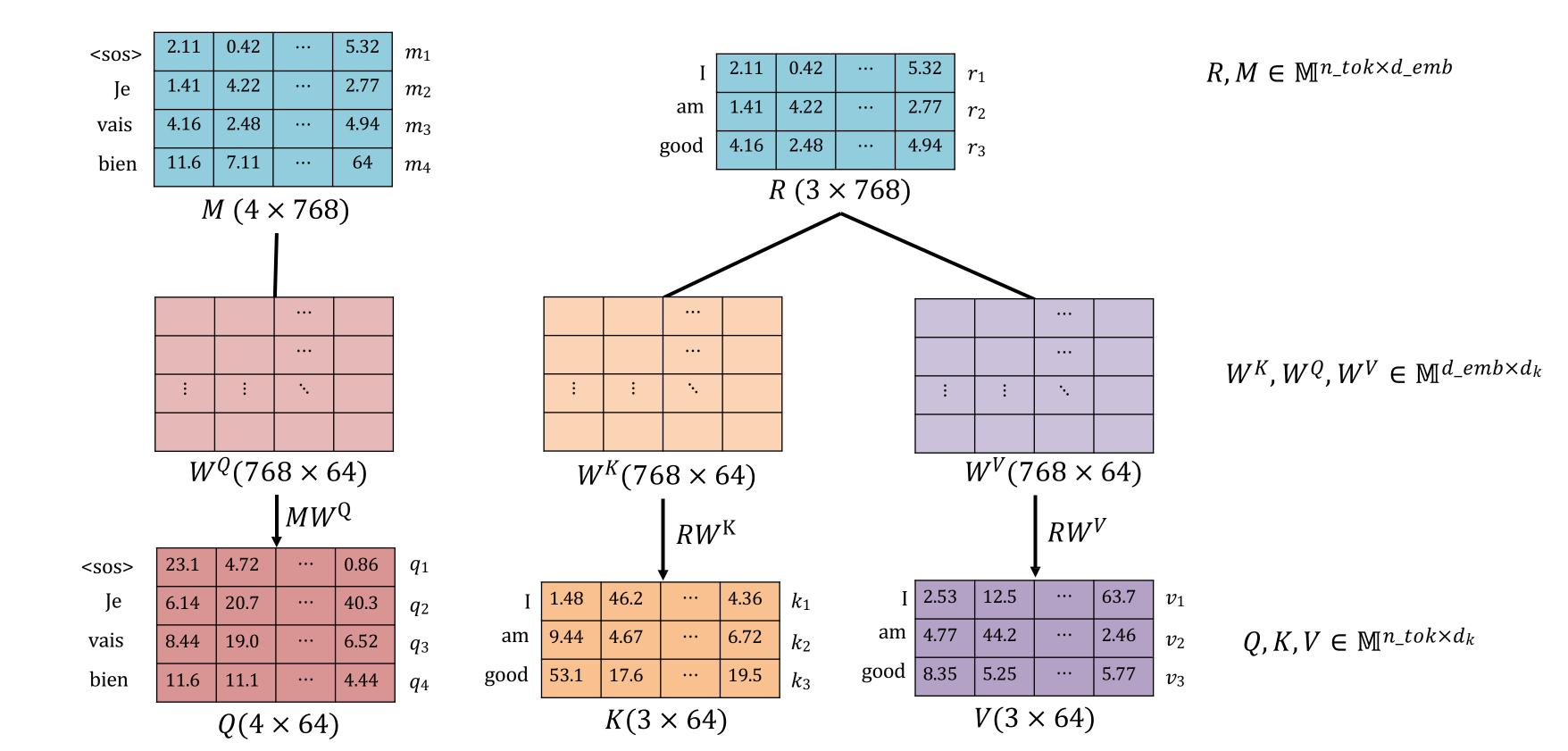
- Generate Query from Attention Matrix (M from Masked), Key and Value from Encoder Representation (R)
- For generating Key (K) and Value(V), set W^K , W^V $where \ W^K, W^V \in \mathbb{M}^{d_emb \times d_k} \ are \ trainable \ parameters$
- Generate K and V by dot-product as follows:

$$K = RW^k$$

$$V = RW^V$$

where R is representation matrix from encoder

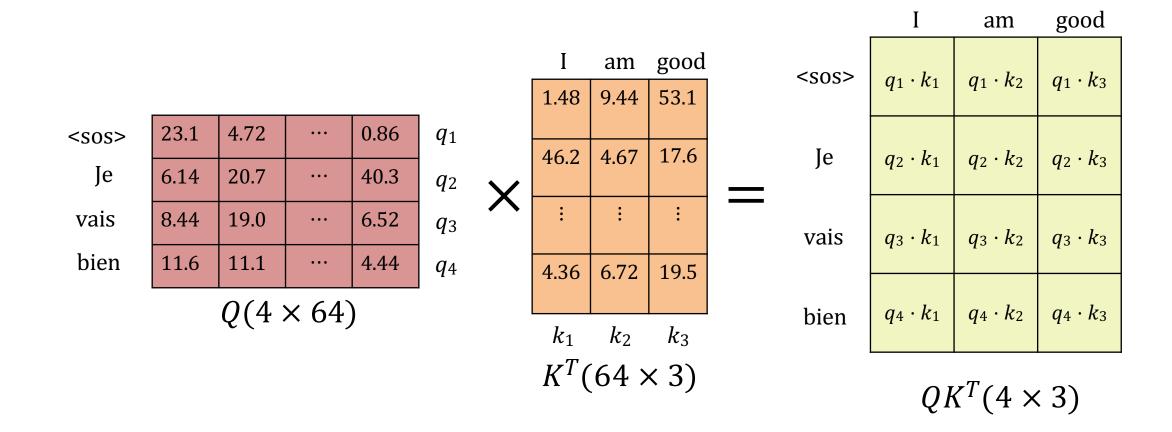
1. Generate Query from Attention Matrix (M from Masked), Key and Value from Encoder output



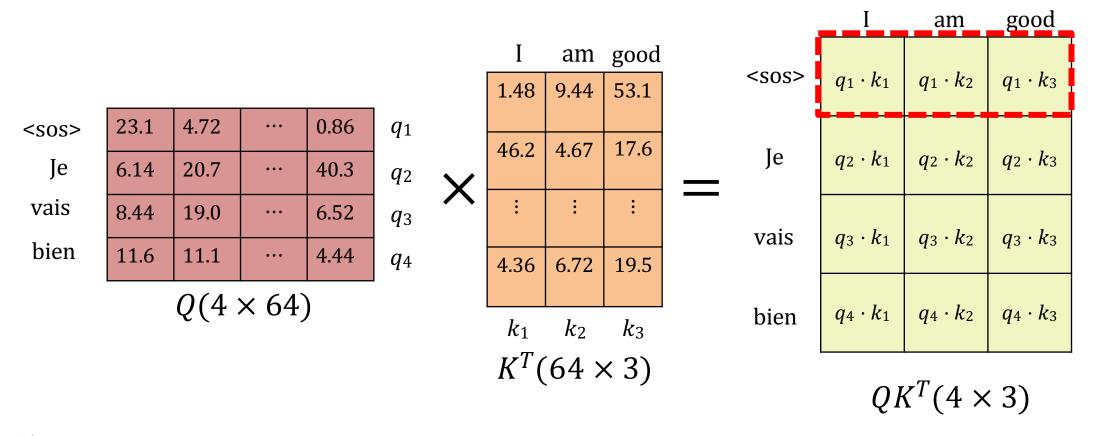
Multi-Head Attention(in Decoder) - Process

- Generate Query from Attention Matrix (M from Masked), Key and Value from Encoder Representation (R)
- 2. Calculate the similarity between a query and a key : QK^T
- 3. Scaling & Softmax -> score matrix: $softmax\left(\frac{Q \cdot K^T}{\sqrt{d_k}}\right)$
- 4. Multiply by Value to get the Attention matrix Z

- 2. Calculate the similarity between a query and a key : QK^T
- Performing the inner product of the Query and Key matrices
- Compute the inner product of two matrices to get the similarity for each token



3. Calculate the similarity between a query and a key : QK^T

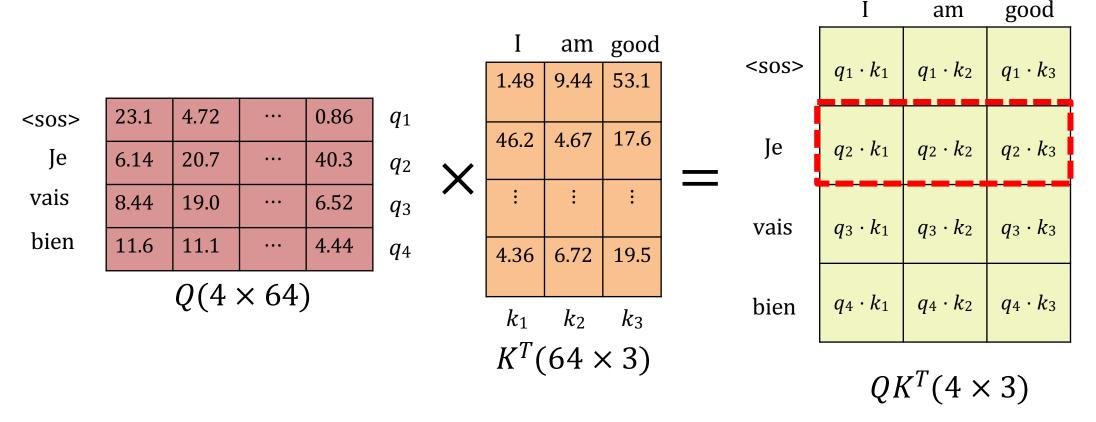


For the first row

Query: <sos>, Key: I, am, good

- -> Compute similarity to all tokens in a sentence for a query
- -> Calculate how similar <sos> is to every word in the input sentence (I, am, good)

3. Query와 Key의 유사도 계산 : $Q \cdot K = QK^T$

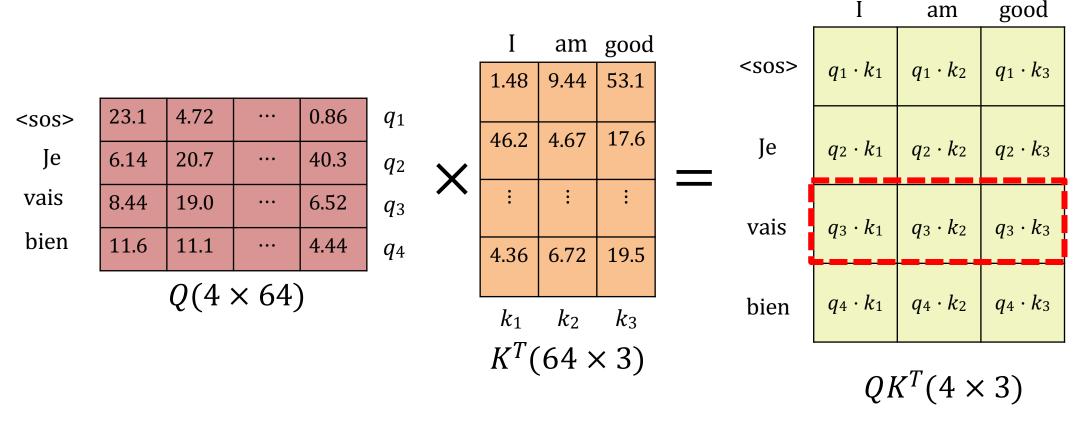


For the second row

Query: Je, Key: I, am, good

- -> Compute similarity to all tokens in a sentence for a query
- -> Compute how similar Je is to every word in the input sentence (I, am, good)

3. Query와 Key의 유사도 계산 : $Q \cdot K = QK^T$

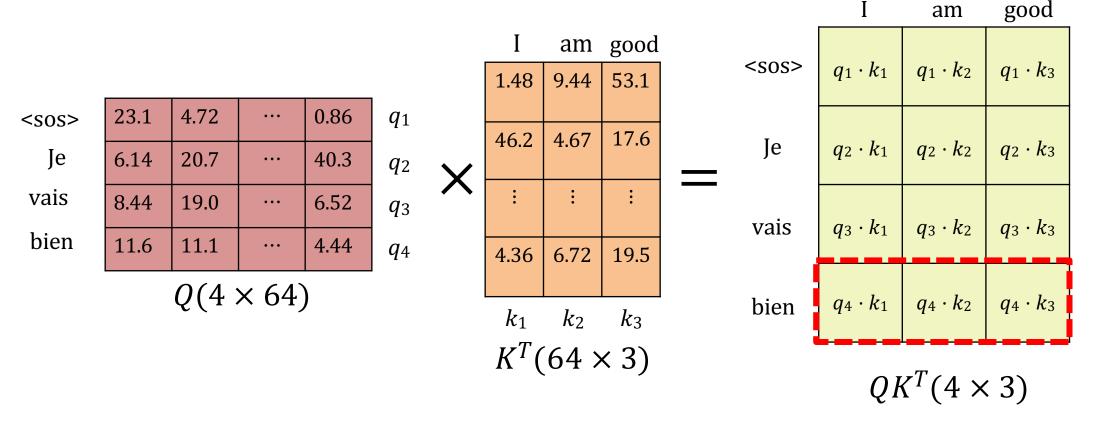


For the third row

Query: vais, Key: I, am, good

- -> Compute similarity to all tokens in a sentence for a query
- -> Compute how similar vais is to every word in the input sentence (I, am, good)

3. Query와 Key의 유사도 계산 : $Q \cdot K = QK^T$



For the fourth row

Query: bien, Key: I, am, good

- -> Compute similarity to all tokens in a sentence for a query
- -> Compute how similar bien is to every word in the input sentence (I, am, good)

Multi-Head Attention(in Decoder) - Process

- Generate Query from Attention Matrix (M from Masked), Key and Value from Encoder Representation (R)
- 2. Calculate the similarity between a query and a key : QK^T
- 3. Scaling & Softmax -> score matrix: softmax $\left(\frac{Q \cdot K^T}{\sqrt{d_k}}\right)$
- 4. Multiply by Value to get the Attention matrix Z

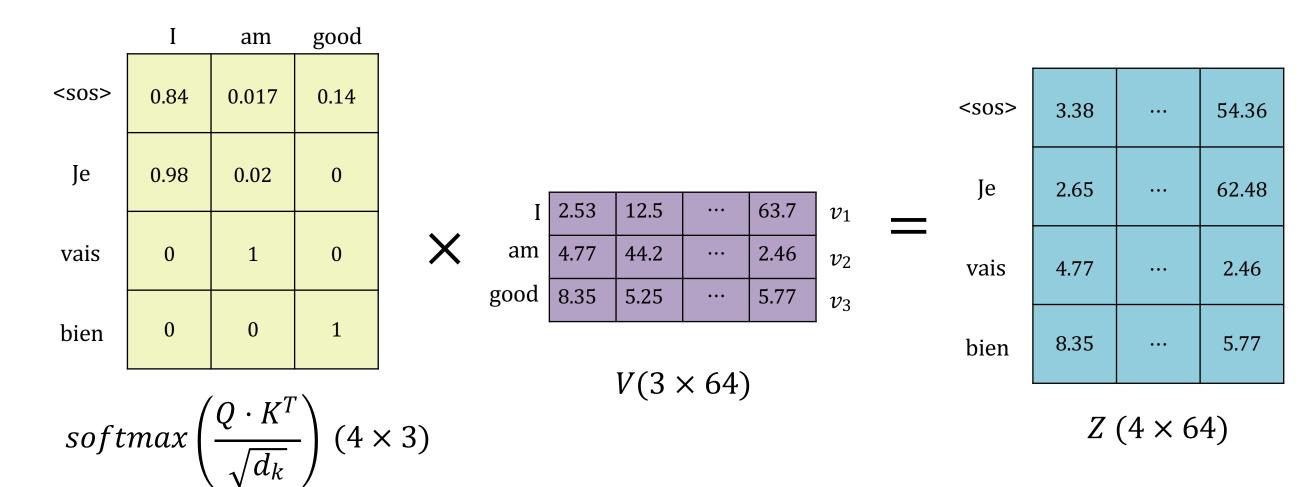
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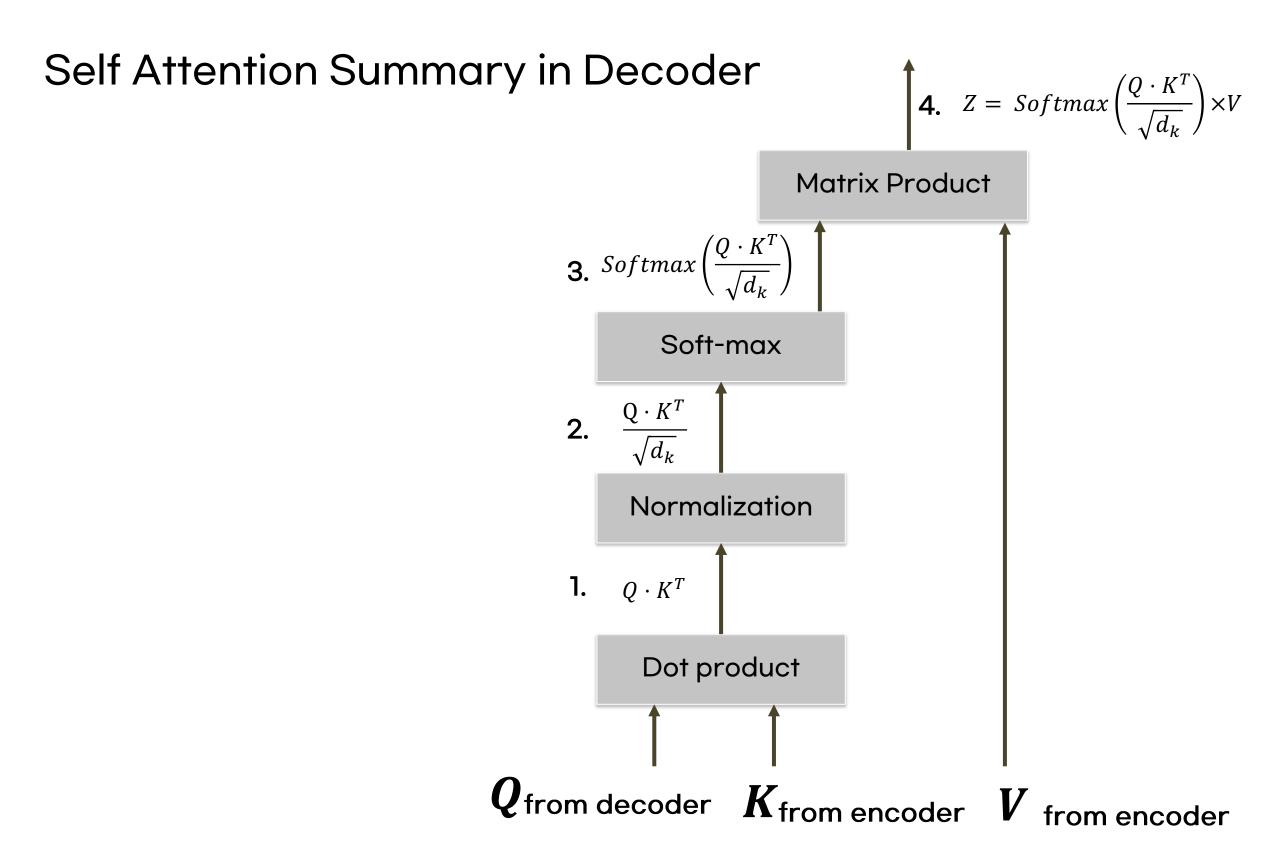
- 4. Scaling and Softmax (normalization) \rightarrow score matrix : $softmax \left(\frac{Q \cdot K^T}{\sqrt{d_k}} \right)$
- Scaling: divide QK^T by the dimension of the key (scaled-dot product)
 - → Scaling values that have become too large due to dot-product
 - → Optimized gradient to be stable when back-propagating

• Softmax : Take the soft-max in $\frac{QK^T}{\sqrt{d_k}}$ and change it to a score matrix

5. Multiply by Value to obtain Attachment matrix Z

- Use the score matrix as a weight to give more weight to highly relevant words
- Multiply the Score matrix and the Value matrix to get the Attention matrix Z.
 - > The model learns which words to focus on in which contexts through an attentional matrix.





02 Multi-Head Attention (code)

• The decoder's attention head generates Q with the decoder's masked multihead attentions, and K and V with the encoder's final representation.

```
def scaled_dot_product_attention(query, key, value, mask=None):
    dim_k = query.size(-1)
    scores = torch.bmm(query, key.transpose(1, 2)) / sqrt(dim_k)
    if mask is not None:
        scores = scores.masked_fill(mask == 0, float("-inf"))
    weights = F.softmax(scores, dim=-1)
    return weights.bmm(value)
```

As the same way decoder concateate all the heads

Concatenate($[Z_1, Z_2, \cdots, Z_h]$) \boldsymbol{W}

03 Add&Norm

- Add: Skip-connection
 Using Skip-Connection to Prevent Vanishing Gradients
- Norm: Layer Normalization
 - Normalizes the sequence to each

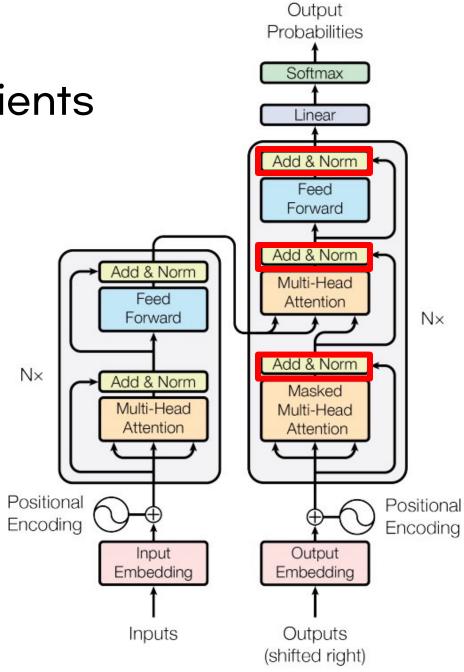


Figure 1: The Transformer - model architecture.

04 Linear & Softmax

Using a Linear Layer as a classifier and the Softmax Function

Output as the word at the index with the highest probability value

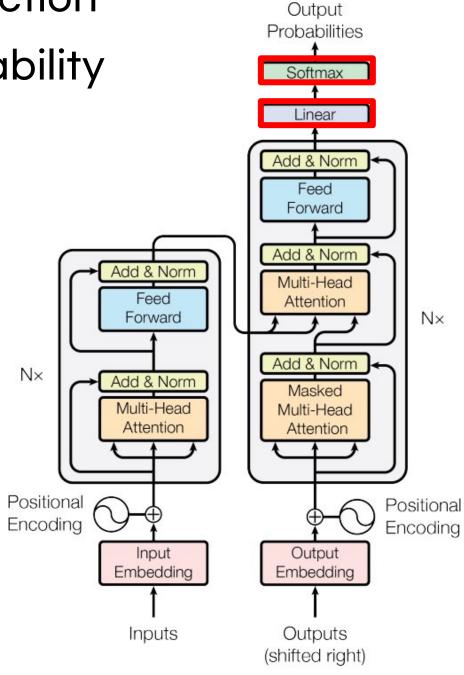


Figure 1: The Transformer - model architecture.

04 Classification head

- Like encoders, decoders are created by stacking layers of decoders.
- The final representation of the decoder has a classification head to predict the next word.

```
class ClassificationHead(nn.Module):

def __init__(self, config):
    super().__init__()
    self.encoder = TransformerEncoder(config)
    self.dropout = nn.Dropout(config.hidden_dropout_prob)
    self.classifier = nn.Linear(config.hidden_size, config.num_labels)

def forward(self, x):
    x = self.encoder(x)[:, -1, :] # 마지막 토큰의 최종 표현 선택
    x = self.dropout(x)
    x = self.classifier(x)
    return x

✓ 0.0s
```

참조 책

구글 BERT의 정석

참조 링크

- https://github.com/bentrevett/pytorch-seq2seq/blob/master/6%20-%20Attention%20is%20All%20You%20Need.ipynb
 - https://towardsdatascience.com/illustrated-guide-to-transformers-step-by-step-explanation-f74876522bc0
- https://stackoverflow.com/questions/58127059/how-to-understand-masked-multi-head-attention-in-transformer/59713254#59713254?newreg=c60d6eca60764bd782a3b453a40ca880

Thank you