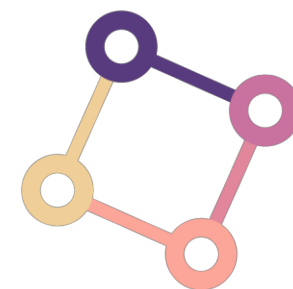


How Transformer Model Works

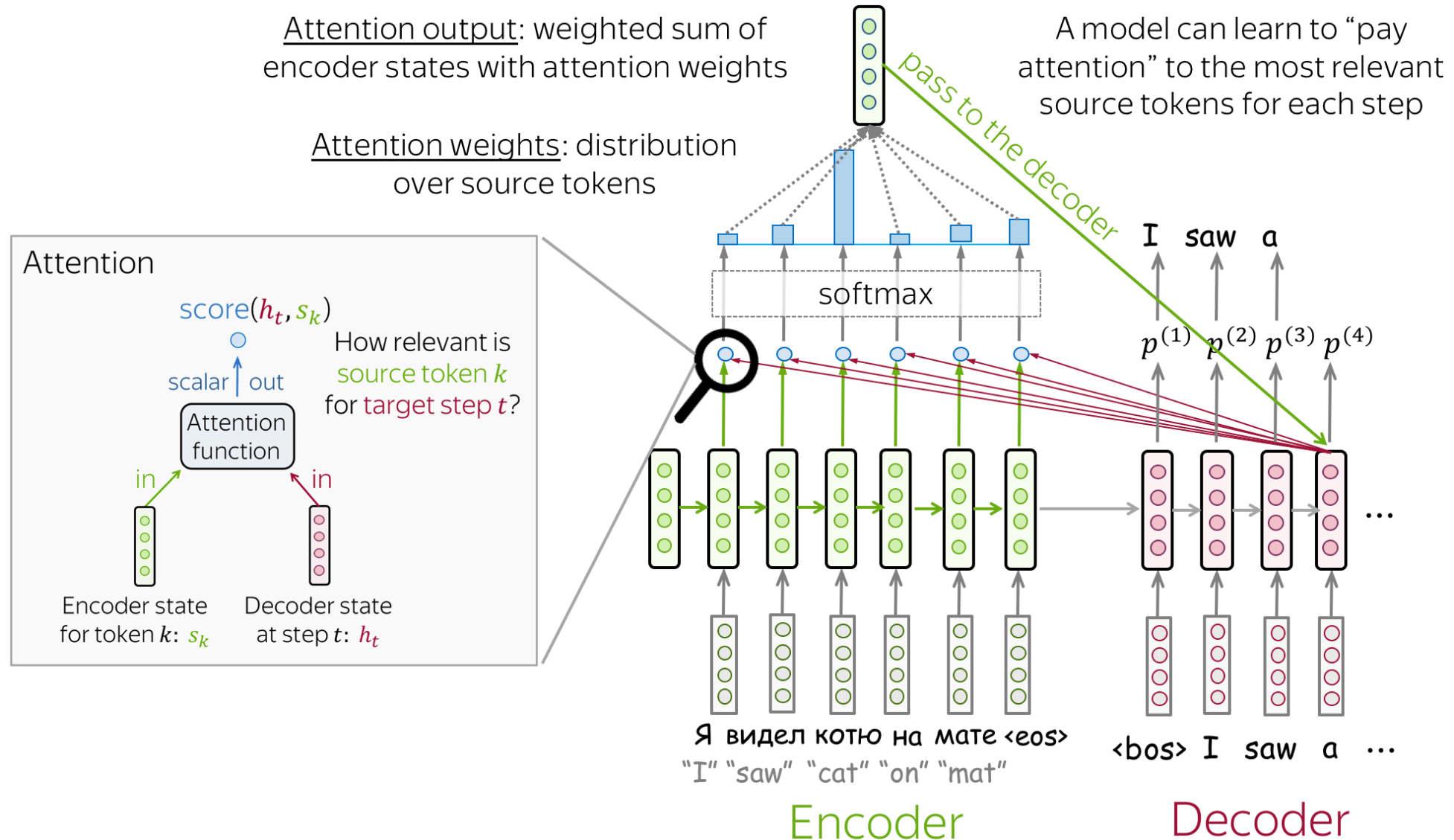
주재걸 교수

KAIST 김재철AI대학원



DAVIAN
Data and Visual Analytics Lab

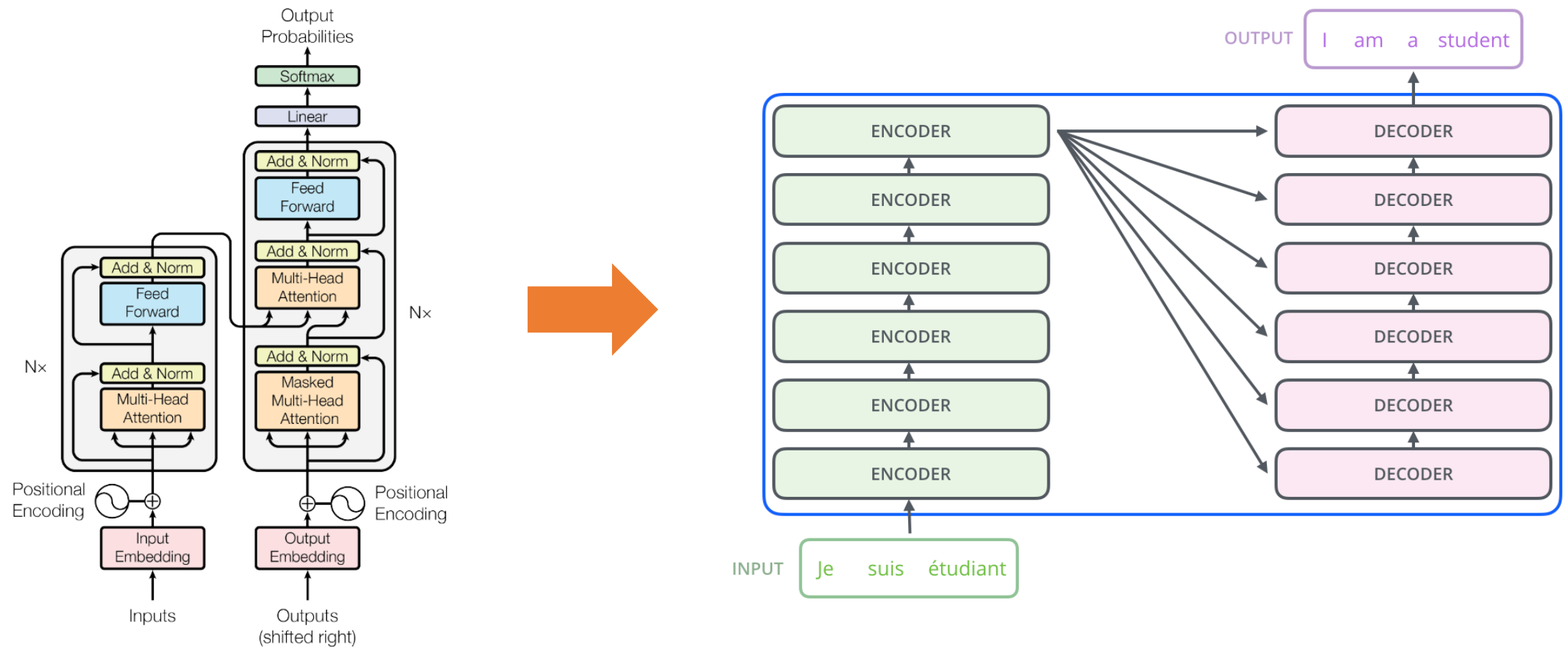
Review: Seq2Seq with Attention ← RNN 기반



Seq2Seq attention 14/11

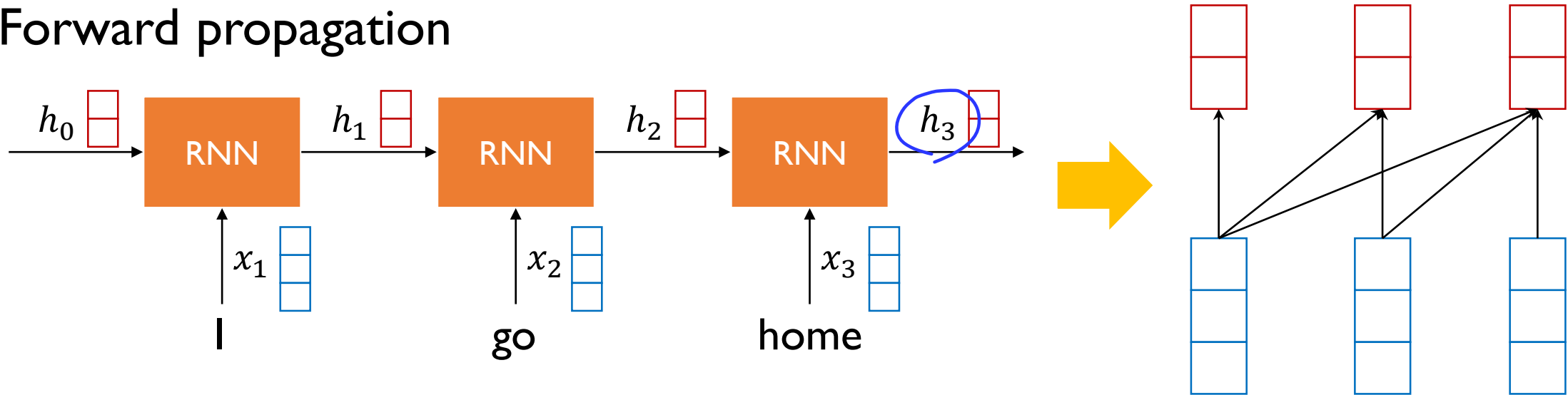
Transformer: High-level View

- Attention module can work as both a sequence encoder and a decoder in seq2seq with attention.
- In other words, RNNs or CNNs are no longer necessary, but all we need is attention modules.

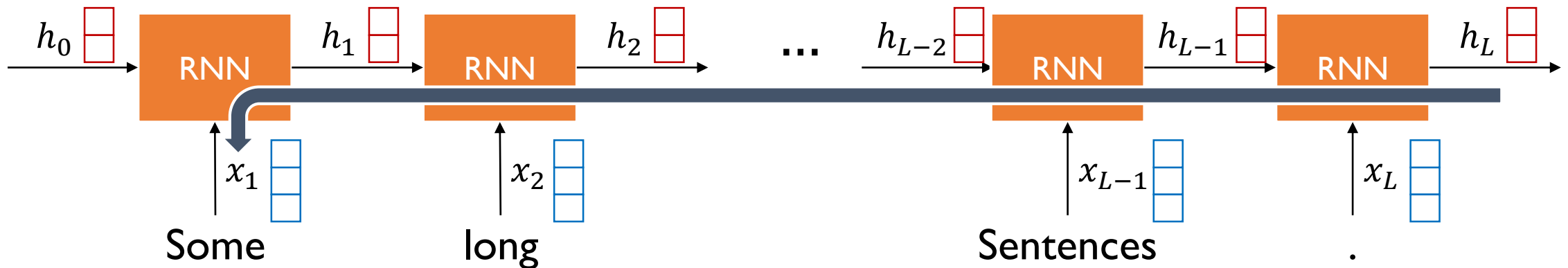


Long-term Dependency Issue of RNN Models

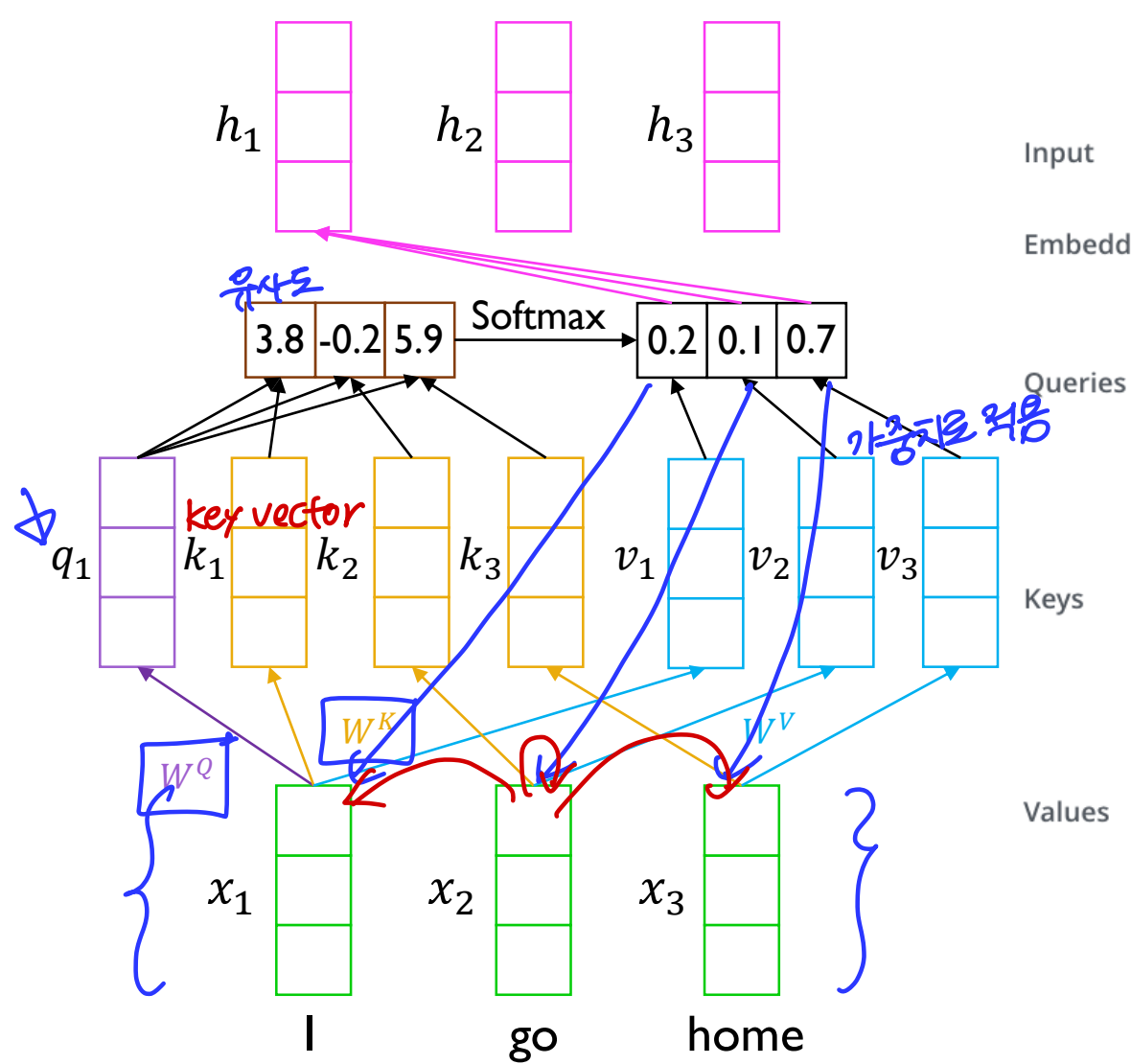
Forward propagation



Backpropagation



Transformer: Solving Long-term Dependency Problem



★ self-attention

Input

Thinking

Machines

Embedding

x_1

x_2

x

산정 변환

Q

Queries

q_1

q_2

x

W^Q

Q

Keys

k_1

k_2

x

W^K

K

key

Values

v_1

v_2

x

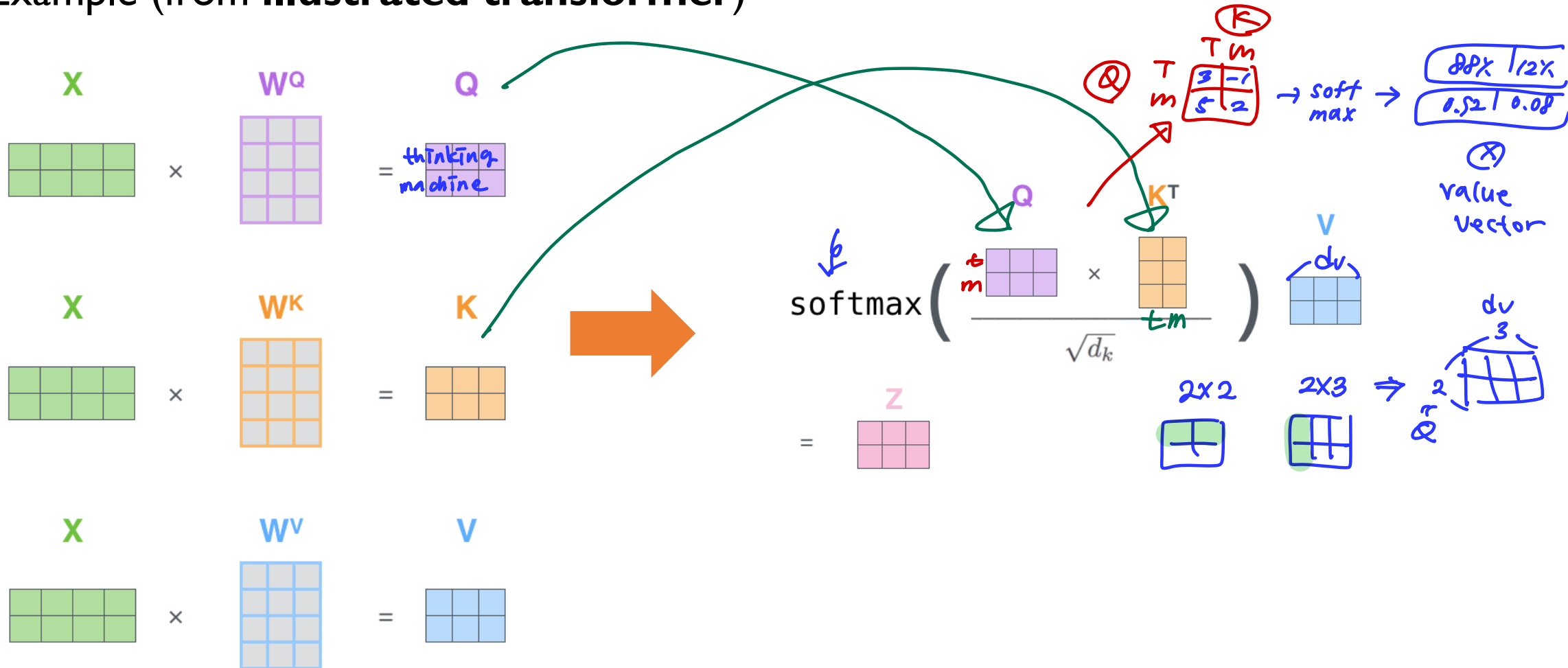
W^V

V

value

Transformer: Scaled Dot-product Attention

- Example (from **illustrated transformer**)



Transformer: Scaled Dot-product Attention

• Problem

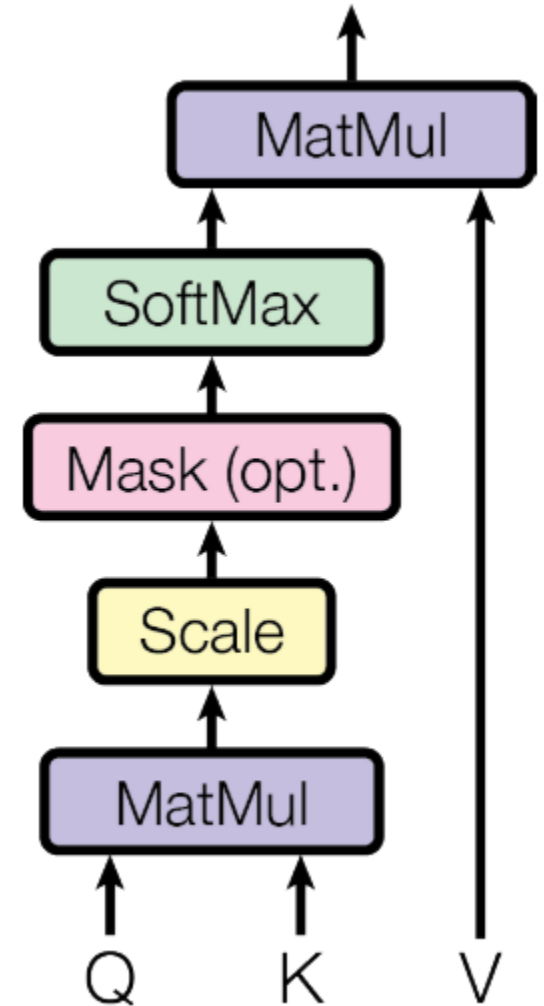
- As d_k gets large, the variance of $q^T k$ increases.
 dimension이 커질수록 더 많은 숫자相加 → 분산 증가 → softmax 특성상 한 값이 100% 될아름. (0 → (0, 5), 1000 → (0, 200))
- Some values inside the softmax get large.
 gradient 작아짐
- The softmax gets very peaked.
- Hence its gradient gets smaller.

• Solution

- Scaled by the length of query / key vectors:

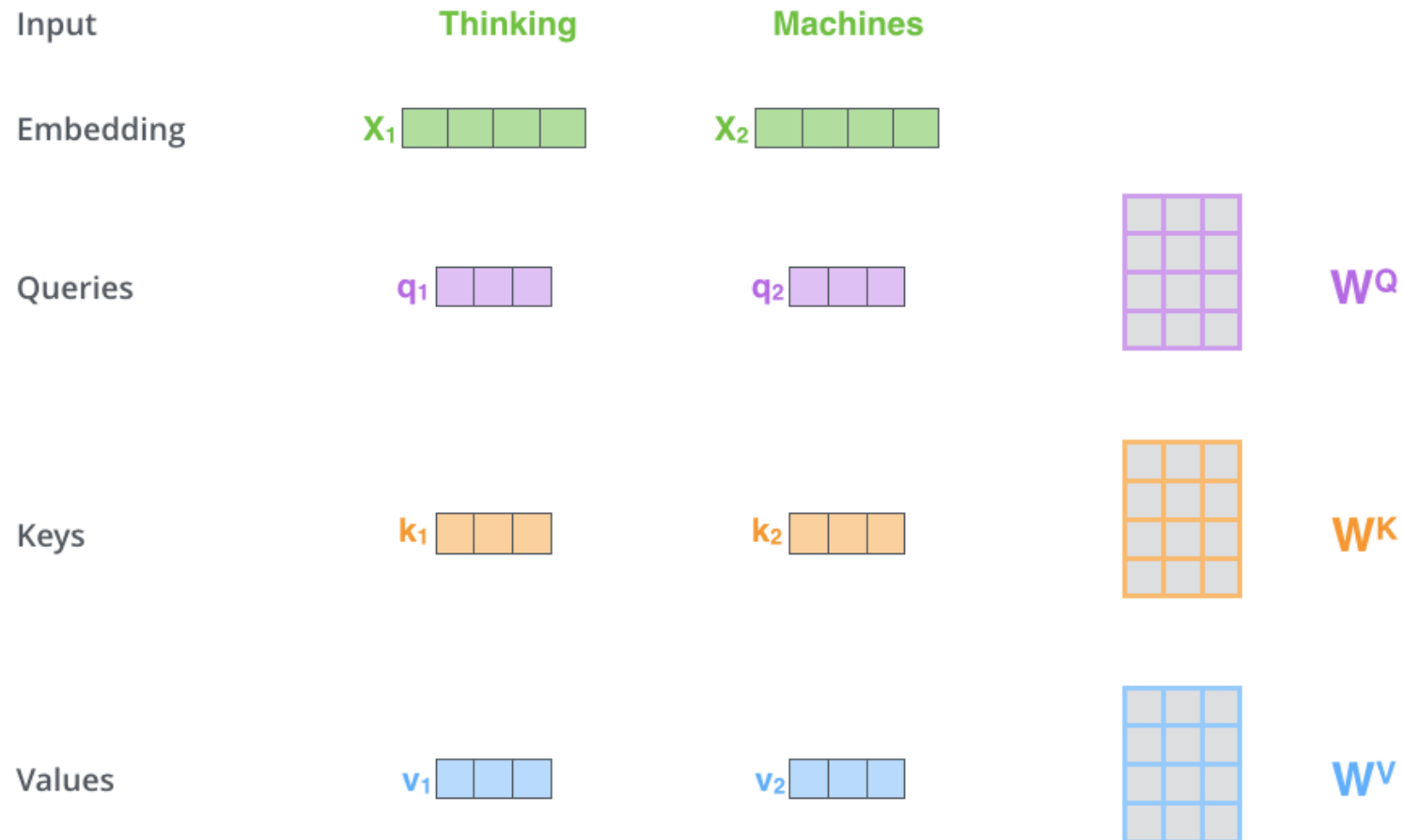
$$A(Q, K, V) = \text{softmax}\left(\frac{QK^T}{\sqrt{d_k}}\right)V$$

인정하는 분산감소 정도를



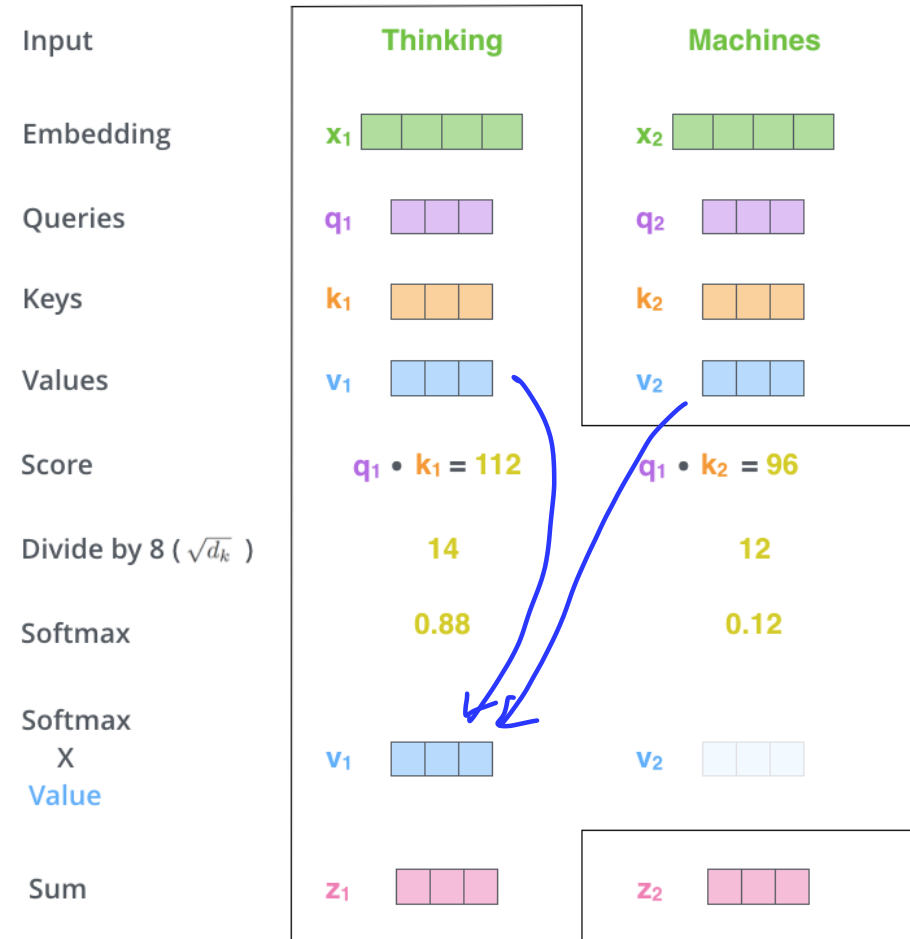
Transformer: Scaled Dot-product Attention

- Example (from **illustrated transformer**)



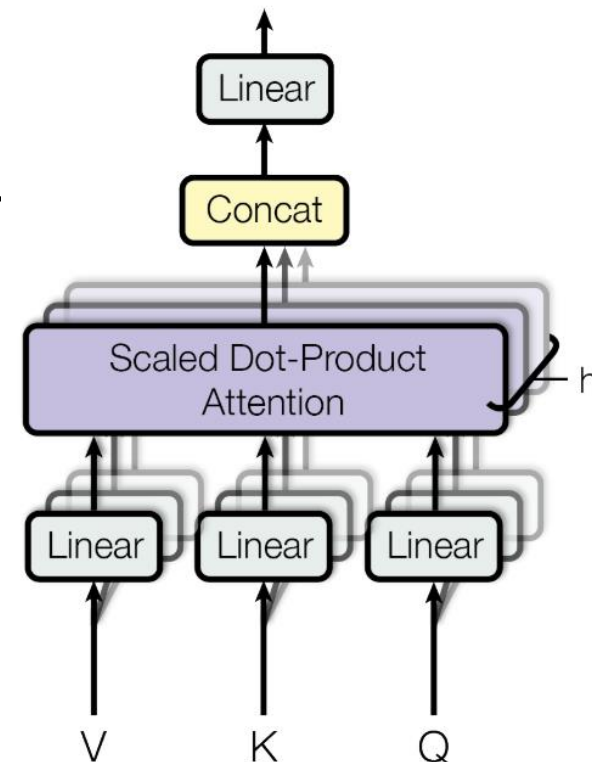
Transformer: Scaled Dot-product Attention

- Example (from **illustrated transformer**)



Transformer: Multi-head Attention

- The input word vectors can be the queries, keys and values.
- In other words, the word vectors themselves select one another.
- **Problem:** only one way for words to interact with one another.
- **Solution:** multi-head attention maps Q , K , and V into the h number of lower-dimensional spaces via W matrices.
- Afterwards, apply attention, then concatenate outputs and pipe through linear layer.



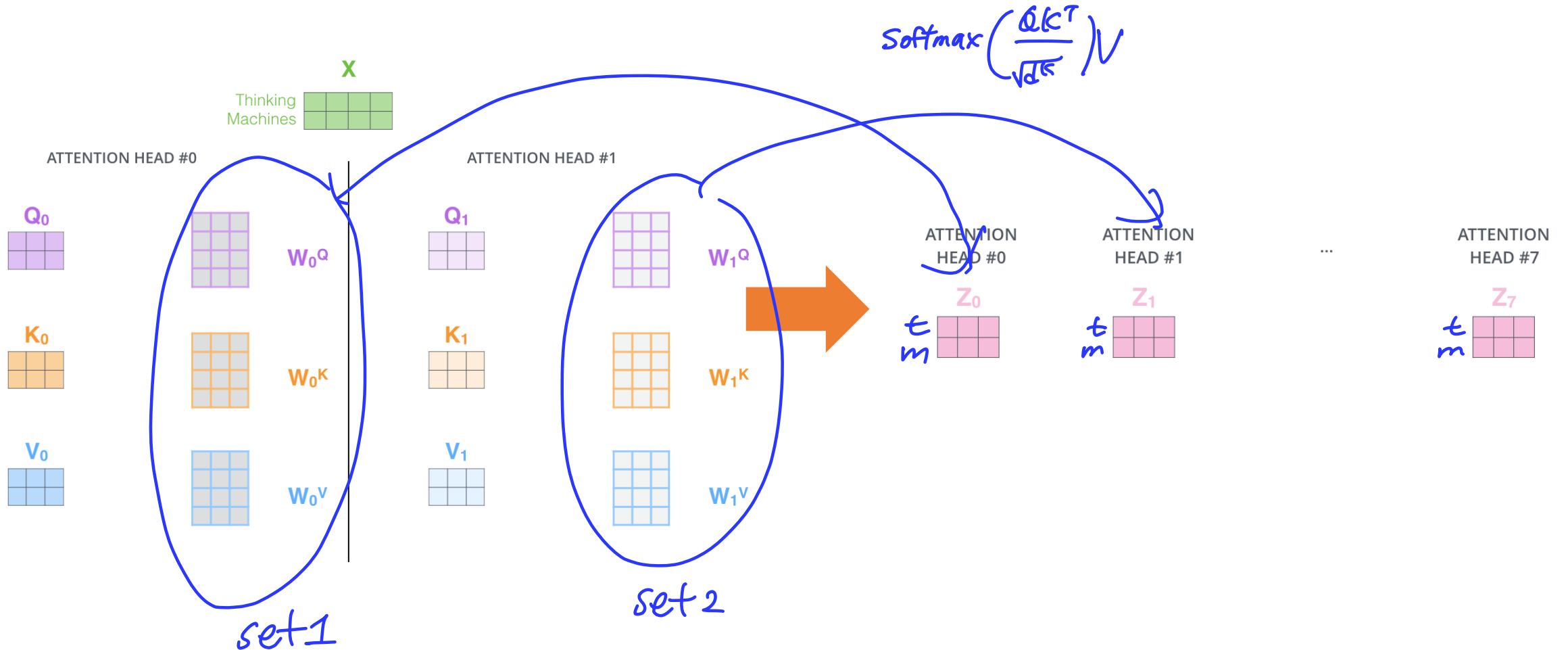
$W^Q W^K W^V$
→ 3개의 선형변환을 곱해서

$$\text{MultiHead}(Q, K, V) = \text{Concat}(\text{head}_1, \dots, \text{head}_h) W^O$$

where $\text{head}_i = \text{Attention}(QW_i^Q, KW_i^K, VW_i^V)$

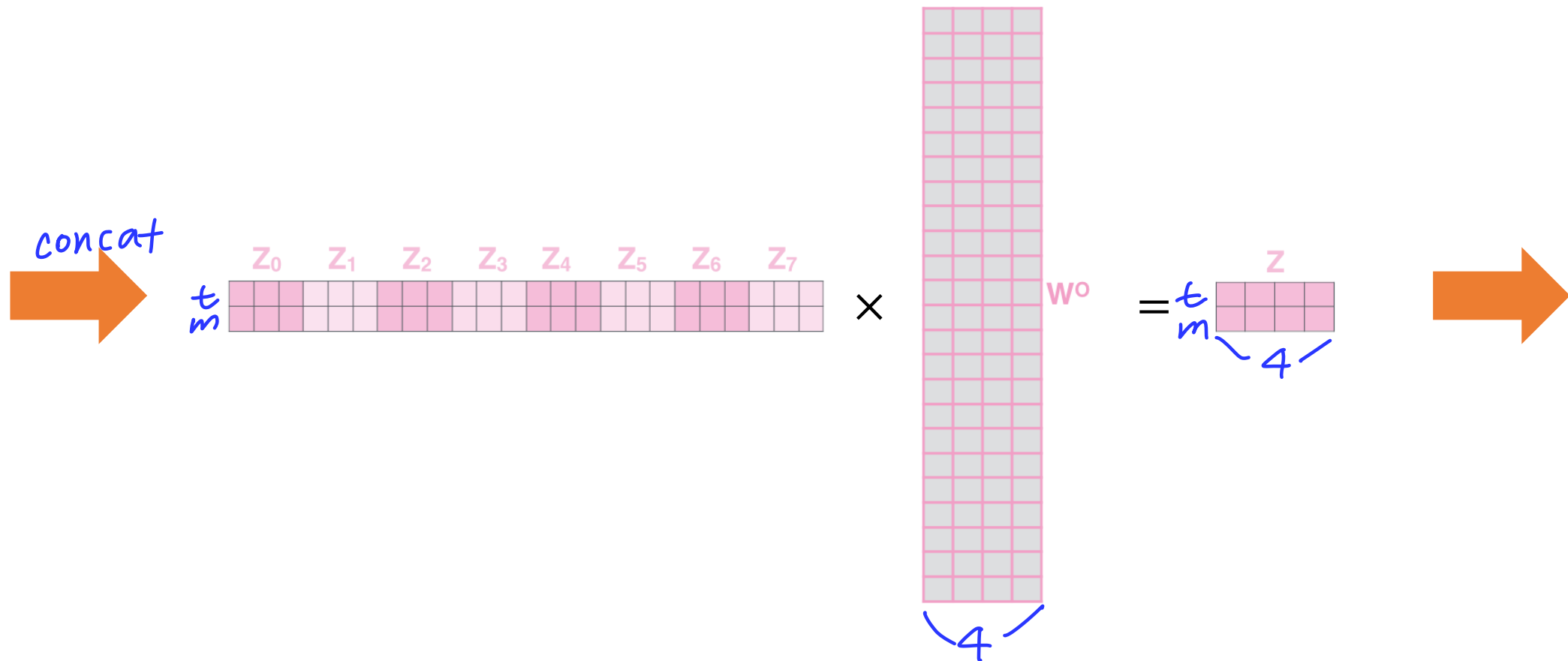
Transformer: Multi-head Attention

- Example (from **illustrated transformer**)



Transformer: Multi-head Attention

- Example (from **illustrated transformer**)



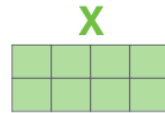
Transformer: Multi-head Attention

- Example (from **illustrated transformer**)

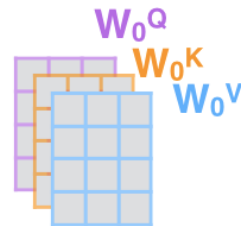
1) This is our input sentence*

Thinking
Machines

2) We embed each word*



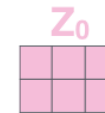
3) Split into 8 heads.
We multiply X or R with weight matrices



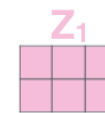
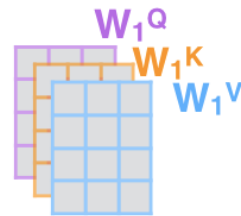
4) Calculate attention using the resulting Q/K/V matrices



5) Concatenate the resulting Z matrices, then multiply with weight matrix W^O to produce the output of the layer



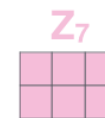
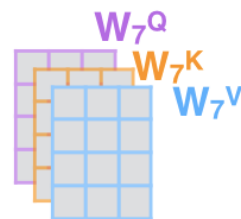
* In all encoders other than #0, we don't need embedding. We start directly with the output of the encoder right below this one



...

...

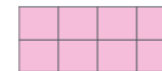
...



W^O



Z



Transformer: Quadratic Memory Complexity

Table 1: Maximum path lengths, per-layer complexity and minimum number of sequential operations for different layer types. n is the sequence length, d is the representation dimension, k is the kernel size of convolutions and r the size of the neighborhood in restricted self-attention.

Layer Type	Complexity per Layer	Sequential Operations	Maximum Path Length
Self-Attention	$O(n^2 \cdot d)$	$O(1)$	$O(1)$
Recurrent	$O(n \cdot d^2)$	$O(n)$	$O(n)$
Convolutional	$O(k \cdot n \cdot d^2)$	$O(1)$	$O(\log_k(n))$
Self-Attention (restricted)	$O(r \cdot n \cdot d)$	$O(1)$	$O(n/r)$

→ 메모리 사용량 증가

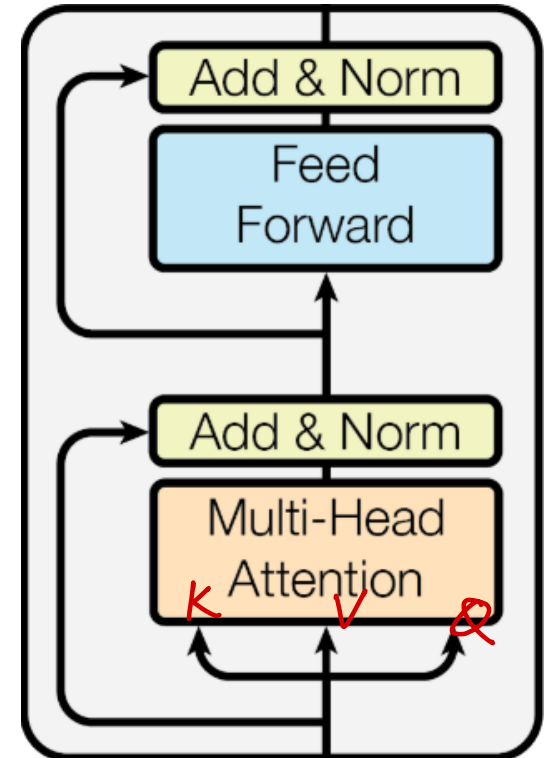
Transformer: Block-Based Model

Each block has two **sub-layers**

- Multi-head attention
- Two-layer feed-forward NN (with ReLU)

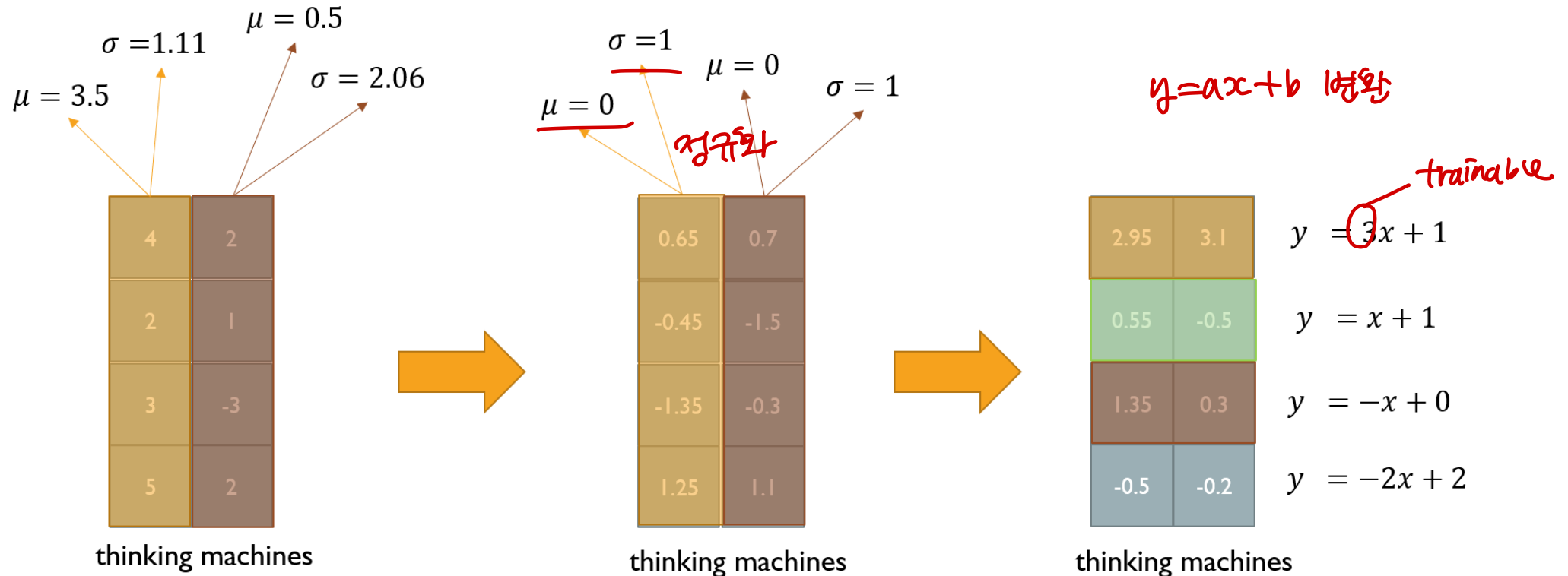
Each of these two steps also has

- Residual connection and layer normalization:
 $\text{LayerNorm}(x + \text{sublayer}(x))$



Layer Normalization

- Layer normalization consists of two steps:
 - Normalization of each word vectors to have zero mean and variance of one.
 - Affine transformation of each sequence vector with learnable parameters.



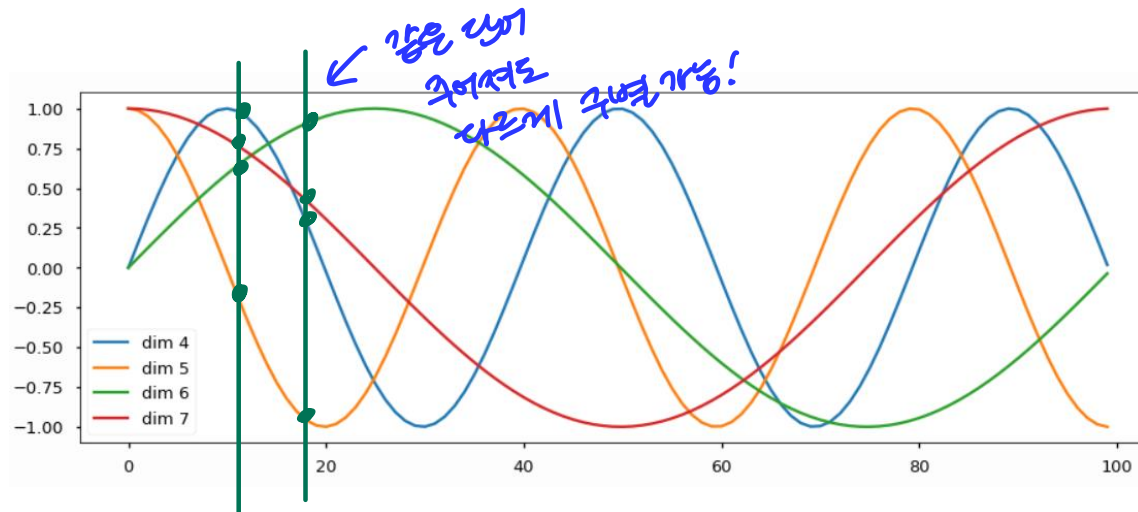
Transformer: Positional Encoding

- Use sinusoidal functions of different frequencies:

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

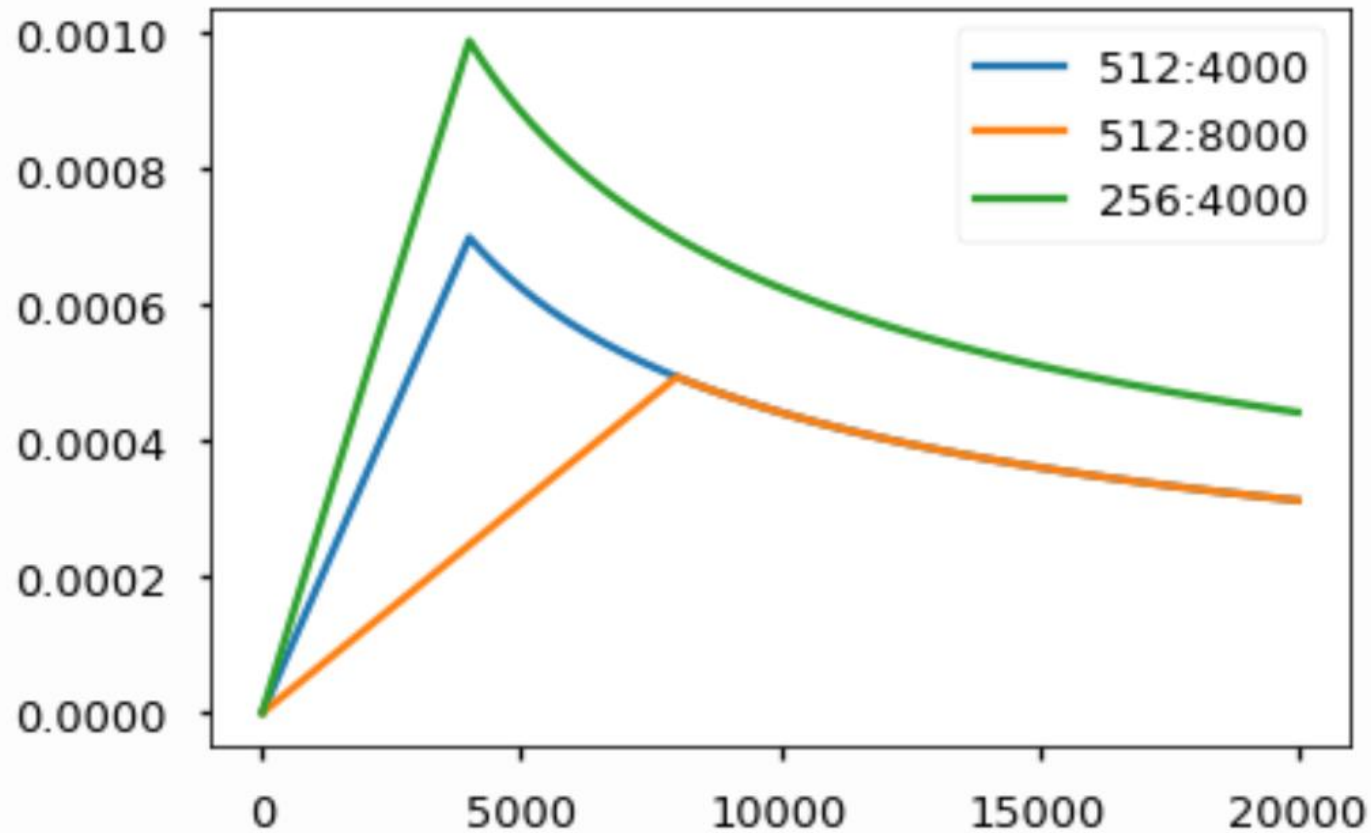


- Easily learn to attend by relative position, since for any fixed offset k , $PE_{(pos+k)}$ can be represented as linear function of $PE_{(pos)}$
- Another positional encoding can also be used (e.g., positional encoding in ConvS2S).



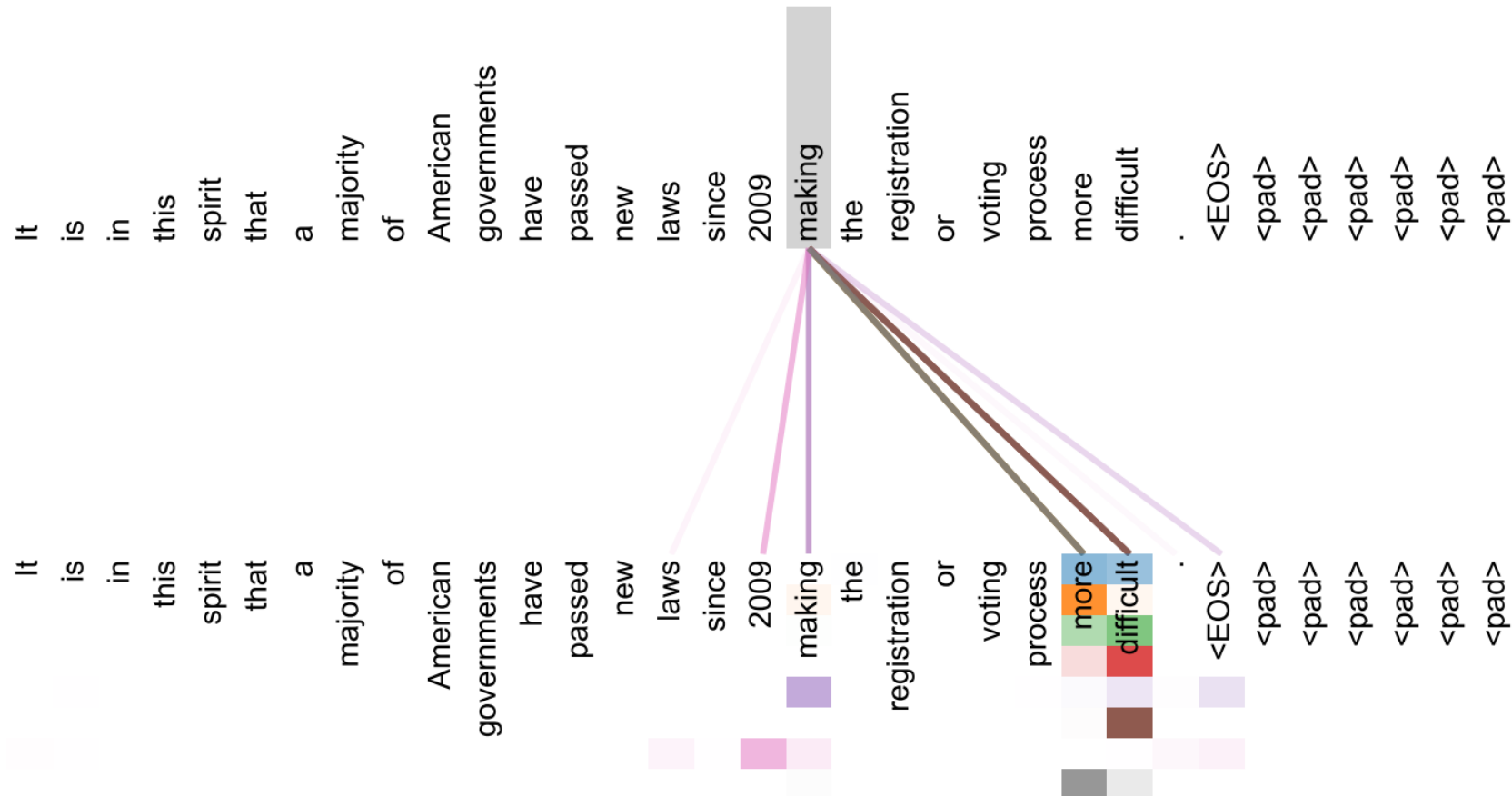
Transformer: Warm-up Learning Rate Scheduler

- learning rate = $d_{\text{model}}^{-0.5} \cdot \min(\text{\#step}^{-0.5}, \text{\#step} \cdot \text{warmup_step}^{-1.5})$



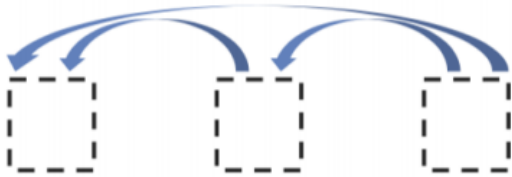
Transformer: Encoder Self-attention Visualization

- Words start to pay attention to other words in sensible ways.

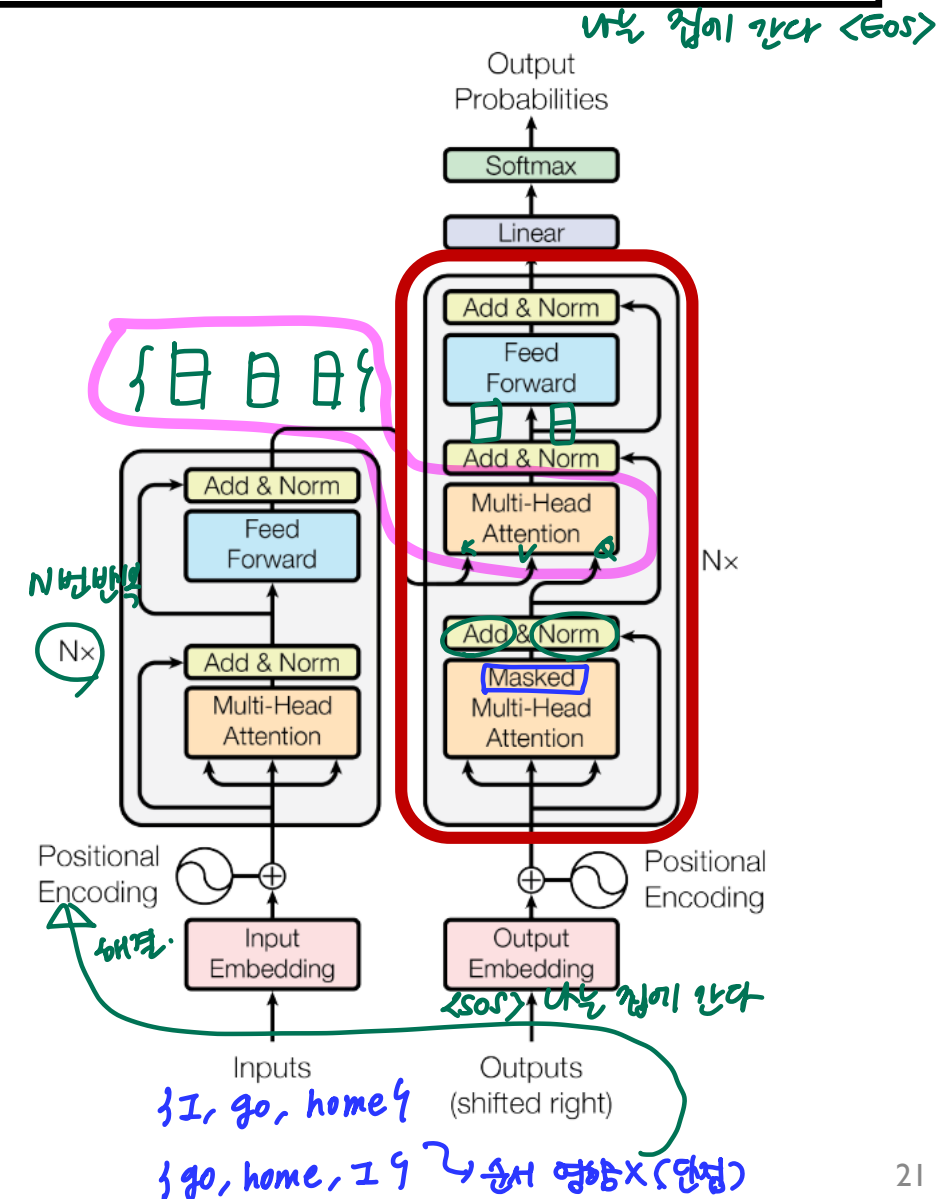
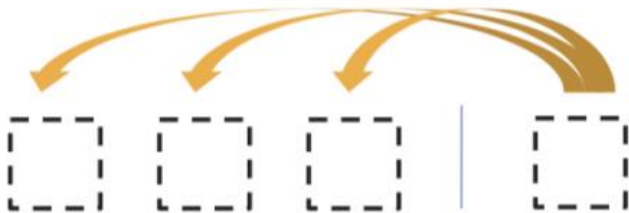


Transformer: Decoder

- Two sub-layer changes in decoder
- Masked decoder self-attention on previously generated outputs:

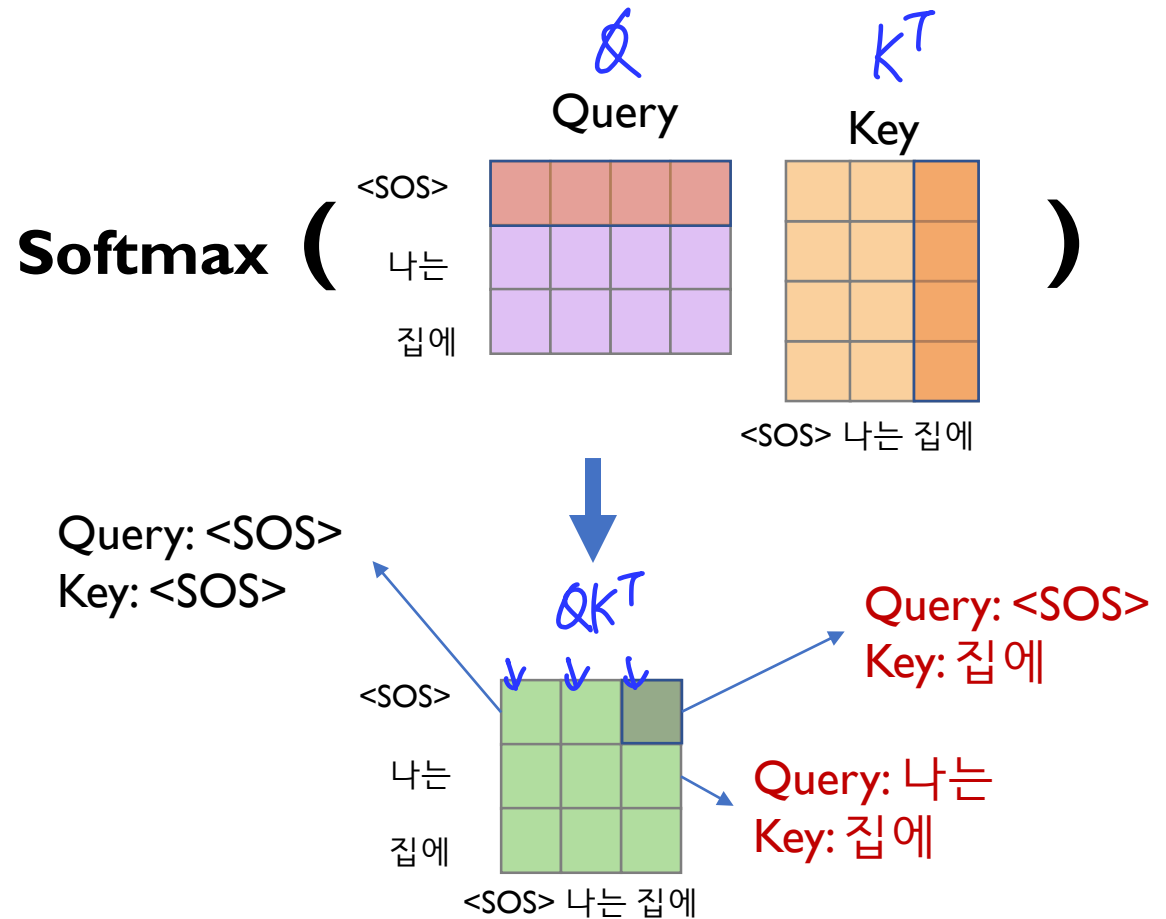
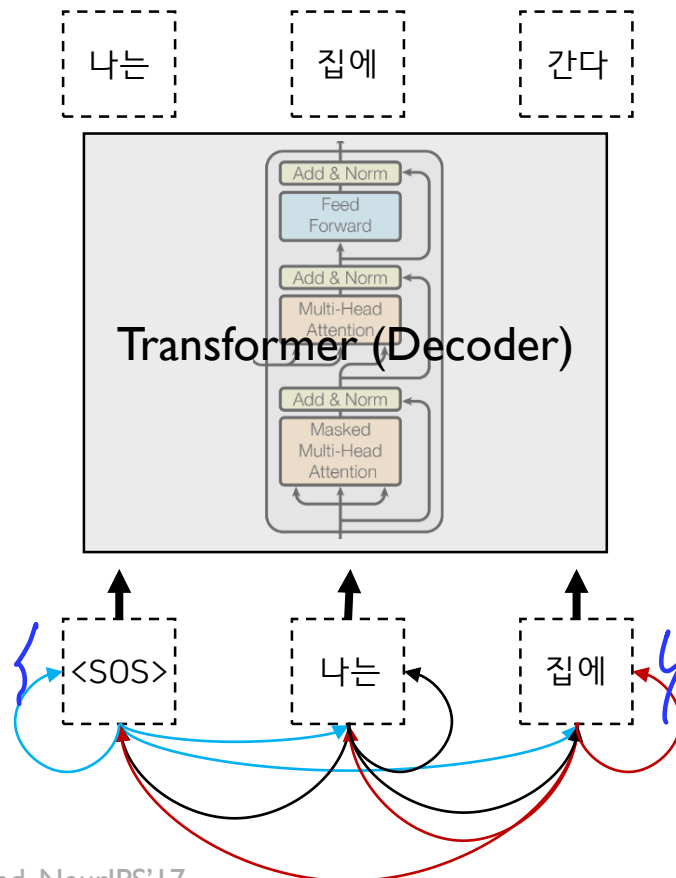


- Encoder-Decoder attention, where queries come from previous decoder layer and keys and values come from output of encoder



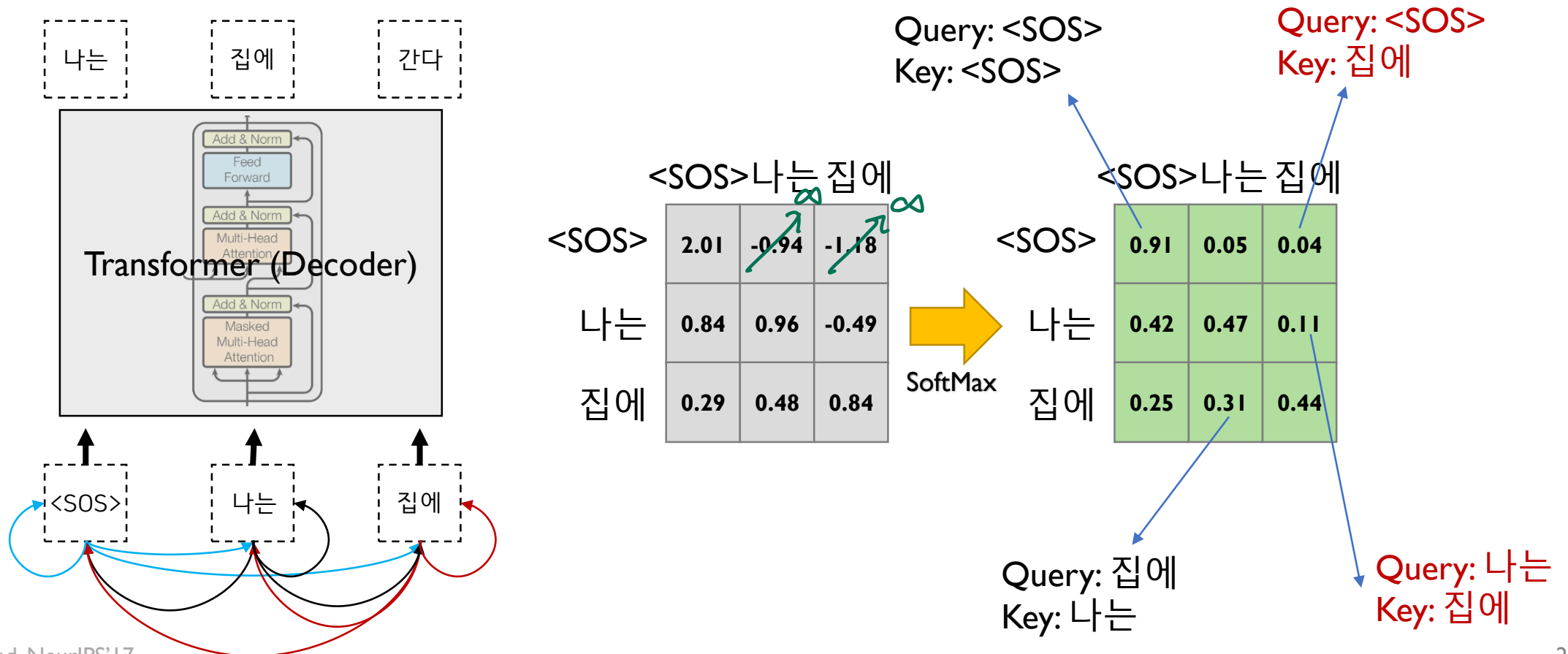
Transformer: Masked Self-attention

- Those words not yet generated cannot be accessed during the inference time.
- Renormalization of softmax output prevents the model from accessing not yet generated words.



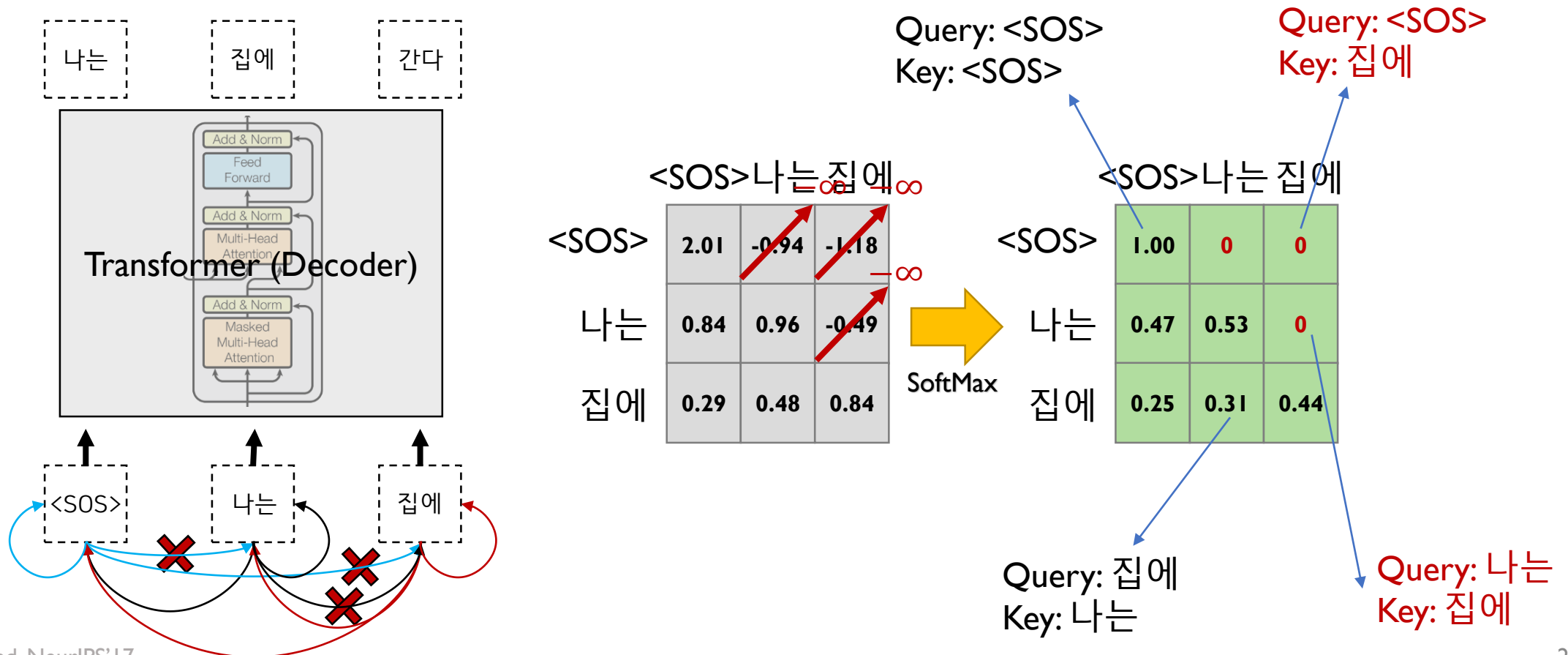
Transformer: Masked Self-attention

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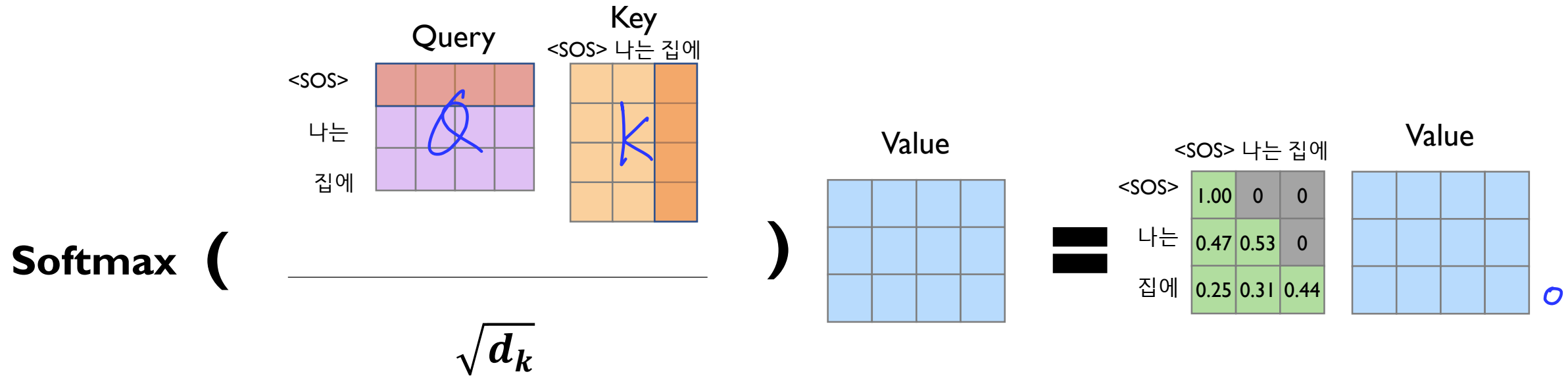
Transformer: Masked Self-attention

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Transformer: Masked Self-attention

- Those words not yet generated cannot be accessed during the inference time.
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Transformer: Experimental Results

- Results on English-German/French translation (newstest2014)

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	$2.3 \cdot 10^{19}$	

Recent Trends

- Transformer model and its self-attention block has become a general-purpose sequence (or set) encoder in recent NLP applications as well as in other areas.
- Training deeply stacked Transformer models via a self-supervised learning framework has significantly advanced various NLP tasks via transfer learning, e.g., BERT, GPT-2, GPT-3, XLNet, ALBERT, RoBERTa, Reformer, T5, ...
- Other applications are fast adopting the self-attention architecture and self-supervised learning settings, e.g., computer vision, recommender systems, drug discovery, and so on
- As for natural language generation, self-attention models still require a greedy decoding of words one at a time.

References

- [Harvard NLP - The Annotated Transformer](#)
- [Stanford University CS224n – Deep learning for Natural Language Processing](#)
- [Fully-parallel text generation for neural machine translation](#)
- [Convolution Sequence to Sequence](#)
- [The Illustrated Transformer \(Eng\)](#)
- [The Illustrated Transformer \(Kor\)](#)