COS 484

Natural Language Processing

L14: Transformers (cont'd)

Spring 2025

(Some slides adapted from John Hewitt)

Announcements

- Final project: Princeton AI sandbox - access to LLM through chat interface & API
  1 account per group
  https://researchcomputing.princeton.edu/support/knowledge-base/ai-sandbox

- Final project compute cost reimbursement: $60 per group, details in Ed post

Self-attention

A self-attention layer maps a sequence of input vectors $\mathbf{x}_1, \ldots, \mathbf{x}_n \in \mathbb{R}^{d_1}$ to a sequence of n vectors: $\mathbf{h}_1, \ldots, \mathbf{h}_n \in \mathbb{R}^{d_2}$

Step #1: Transform each input vector into three vectors: query, key, and value vectors

$$\mathbf{q}_i = \mathbf{x}_i \mathbf{W}^Q \in \mathbb{R}^{d_q} \qquad \mathbf{k}_i = \mathbf{x}_i \mathbf{W}^K \in \mathbb{R}^{d_k} \qquad \mathbf{v}_i = \mathbf{x}_i \mathbf{W}^V \in \mathbb{R}^{d_v}$$

$$\mathbf{W}^Q \in \mathbb{R}^{d_1 \times d_q} \qquad \mathbf{W}^K \in \mathbb{R}^{d_1 \times d_k} \qquad \mathbf{W}^V \in \mathbb{R}^{d_1 \times d_v}$$

Step #2: Compute pairwise similarities between keys and queries; normalize with softmax

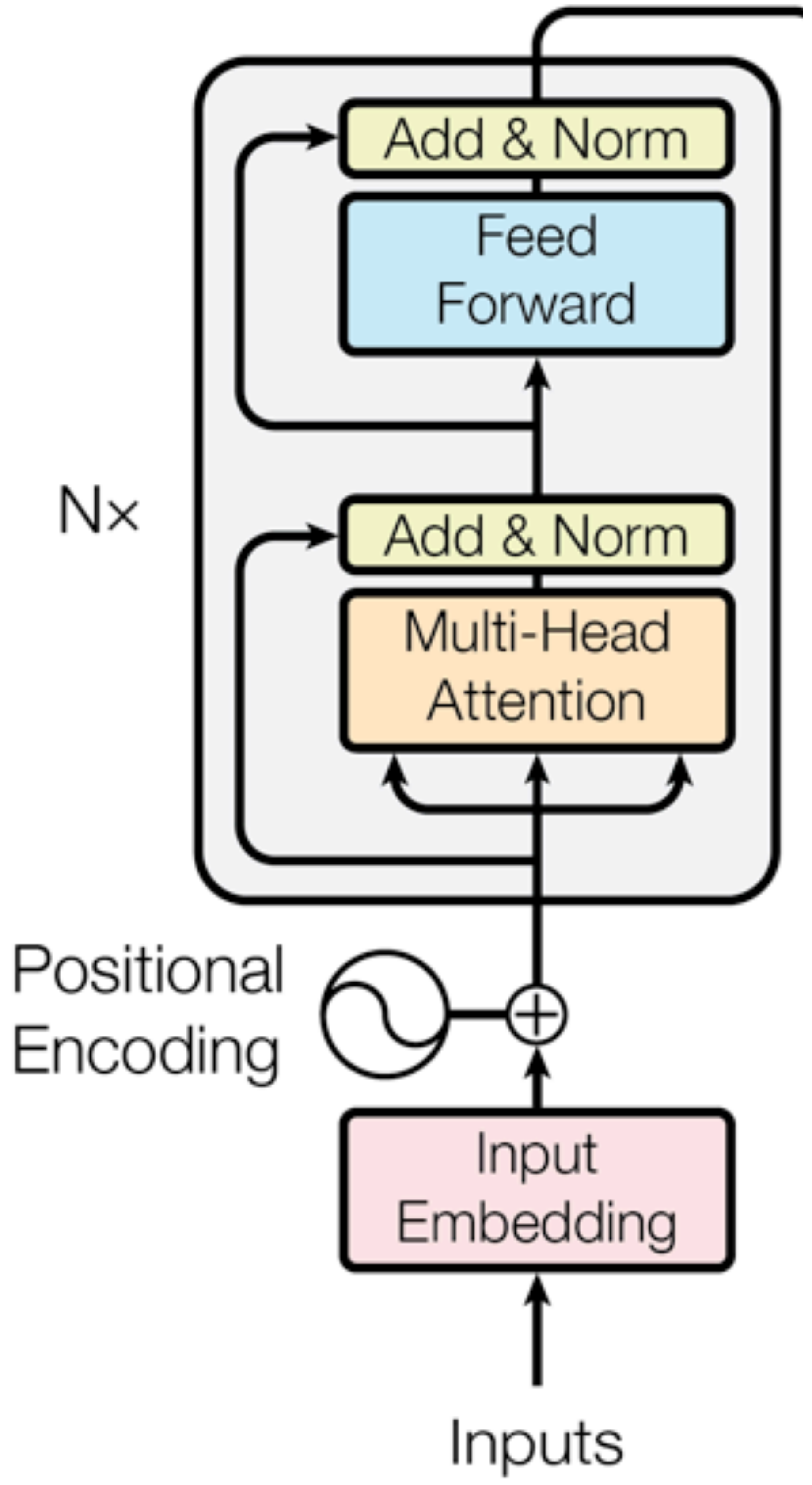
For each $\mathbf{q}_i$, compute attention scores and attention distribution:

$$e_{i,j} = \frac{\mathbf{q}_i \cdot \mathbf{k}_j}{\sqrt{d_k}}, \forall j = 1, \ldots, n$$

$$\alpha_i = \mathrm{softmax}(\mathbf{e}_i)$$

$$\alpha_{i,j} = \frac{\exp(e_{i,j})}{\sum_{k=1}^{n} \exp(e_{i,k})}$$

Transformer encoder: let's put things together



From the bottom to the top:

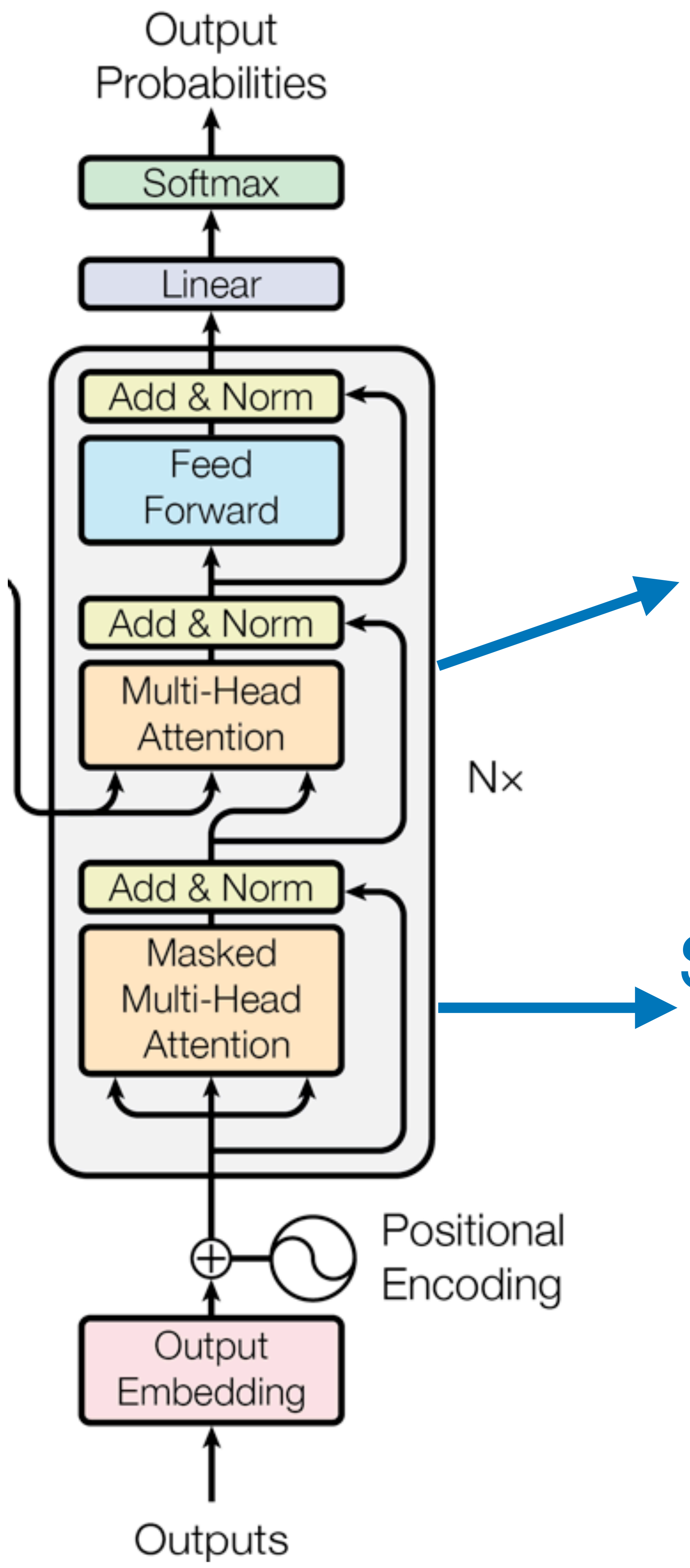
- Input embedding
- Positional encoding
- A stack of Transformer encoder layers

Transformer encoder is a stack of N layers, which consists of two sub-layers:

- Multi-head attention layer
- Feed-forward layer

$$\mathbf{x}_1, \ldots, \mathbf{x}_n \in \mathbb{R}^{d_1} \longrightarrow \mathbf{h}_1, \ldots, \mathbf{h}_n \in \mathbb{R}^{d_2}$$

Transformer decoder



Cross-attention between source and target sequence

Self-attention within target sequence

From the bottom to the top:

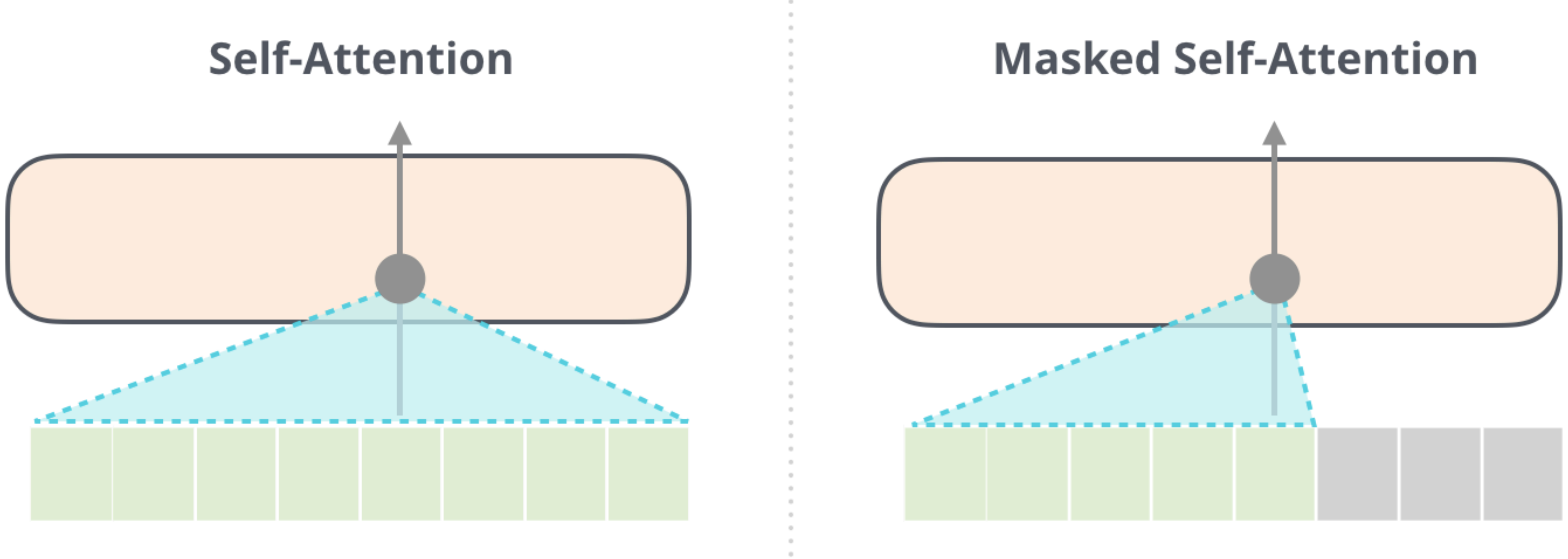
- Output embedding
- Positional encoding
- A stack of Transformer decoder layers
- Linear + softmax

Transformer decoder is a stack of N layers, which consists of three sub-layers:

- Masked multi-head attention
- Multi-head cross-attention
- Feed-forward layer
- (W/ Add & Norm between sub-layers)

Masked (casual) self-attention

- Key: You can’t see the future text for the decoder!



- Solution: for every $\mathbf{q}_i$, only attend to $\{(\mathbf{k}_j, \mathbf{v}_j)\}, j \leq i$

How to implement this? Masking!

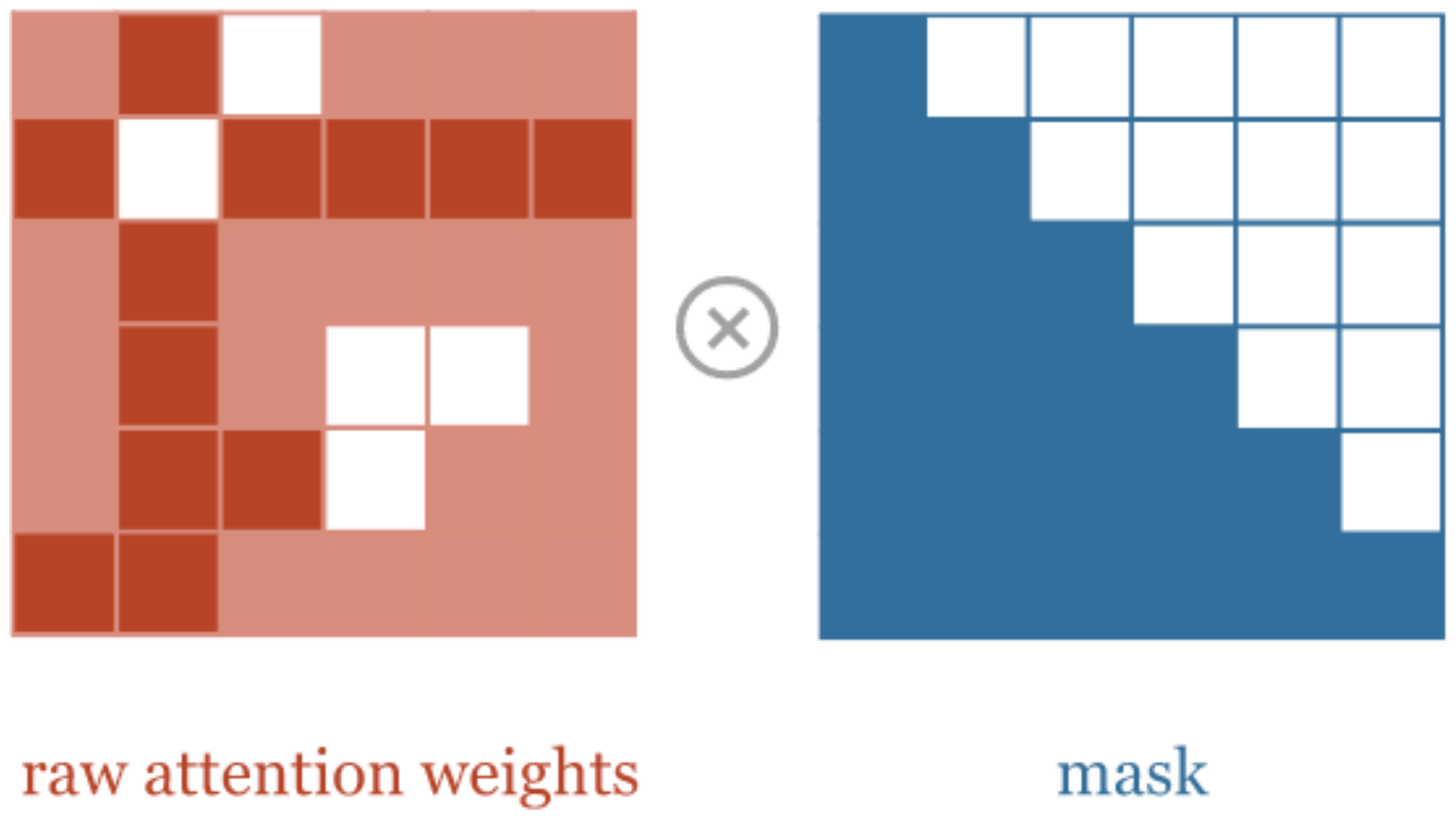
https://jalammar.github.io/illustrated-gpt2/

Masked multi-head attention

$$\mathbf{q}_i = \mathbf{x}_i \mathbf{W}^Q, \mathbf{k}_i = \mathbf{x}_i \mathbf{W}^K, \mathbf{v}_i = \mathbf{x}_i \mathbf{W}^V$$

$$e_{i,j} = \frac{\mathbf{q}_i \cdot \mathbf{k}_j}{\sqrt{d_k}}, \forall j = 1, \ldots, n$$

$$\alpha_i = \mathrm{softmax}(\mathbf{e}_i)$$



Implementation: compute attention as we normally do, mask out attention to future words by setting attention scores to $-\infty$

```
dot = torch.bmm(queries, keys.transpose(1, 2))

indices = torch.triu_indices(t, t, offset=1)
dot[:, indices[0], indices[1]] = float('-inf')

dot = F.softmax(dot, dim=2)
```

http://peterbloem.nl/blog/transformers

Masked (multi-head) attention

The following matrix denotes the values of $\frac{\mathbf{q}_i \cdot \mathbf{k}_j}{\sqrt{d_k}}$ for $1 \leq i \leq n, 1 \leq j \leq n \ (n = 4)$

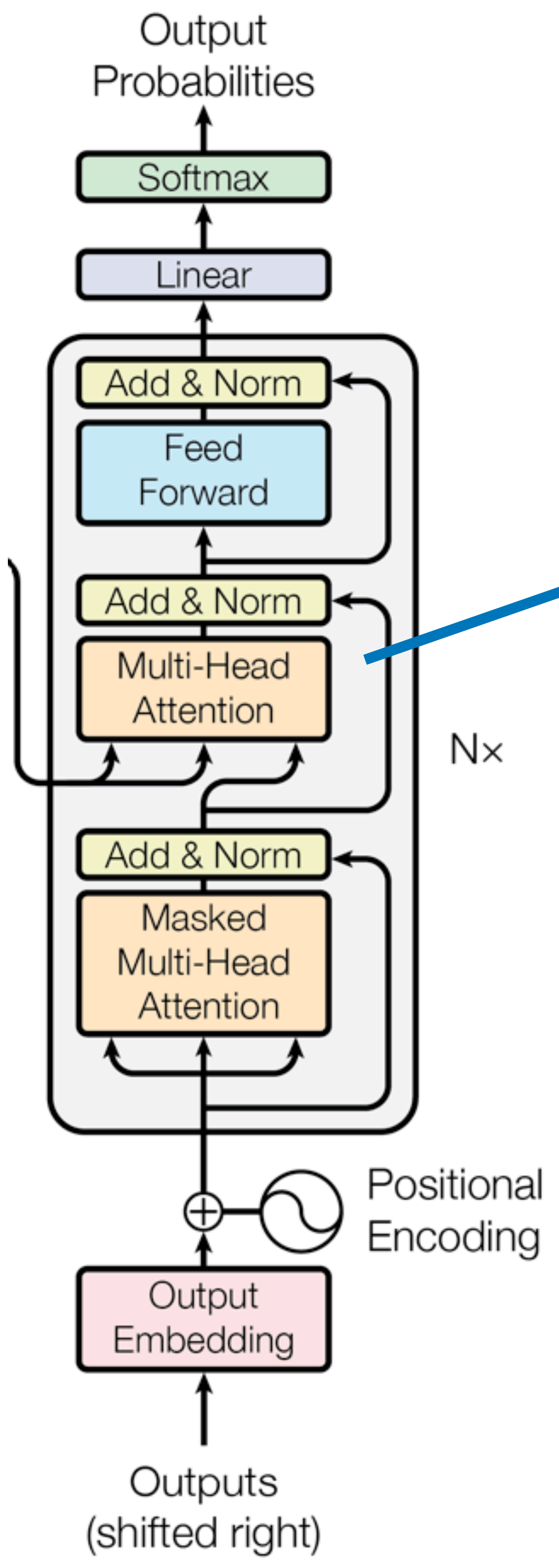
1	0	-1	-1
1	1	-1	0
0	1	1	-1
-1	-1	2	1

What should be the value of $\alpha_{2,2}$ in masked attention?

(A) 0
(B) 0.5
(C) $\frac{e}{2e + e^{-1} + 1}$
(D) 1

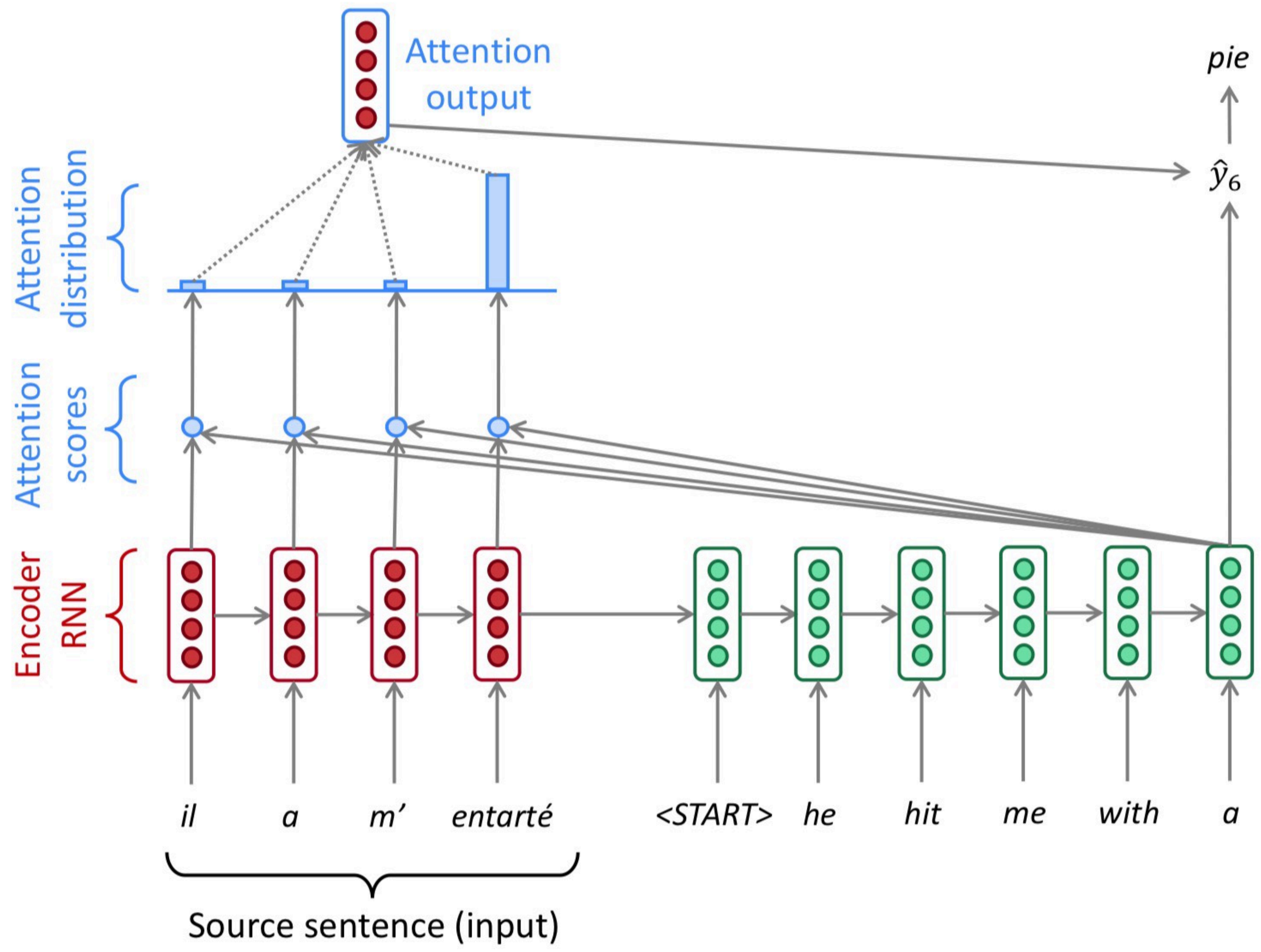
The correct answer is (B)

Multi-head cross-attention



Cross-attention between source and target sequence

Similar as the attention we learned in the previous lecture



Multi-head cross-attention

Self-attention:

$$\mathbf{q}_i = \mathbf{x}_i \mathbf{W}^Q, \mathbf{k}_i = \mathbf{x}_i \mathbf{W}^K, \mathbf{v}_i = \mathbf{x}_i \mathbf{W}^V$$

$$e_{i,j} = \frac{\mathbf{q}_i \cdot \mathbf{k}_j}{\sqrt{d_k}}, \forall j = 1, \ldots, n$$

$$\alpha_i = \mathrm{softmax}(\mathbf{e}_i)$$

$$\mathbf{h}_i = \sum_{j=1}^{n} \alpha_{i,j} \mathbf{v}_j$$

Cross-attention:

(always from the top layer)

$\tilde{\mathbf{x}}_1, \ldots, \tilde{\mathbf{x}}_m$: hidden states from encoder

$\mathbf{x}_1, \ldots, \mathbf{x}_n$: hidden states from decoder

$$\mathbf{q}_i = \mathbf{x}_i \mathbf{W}^Q \quad i = 1,2,\ldots,n$$

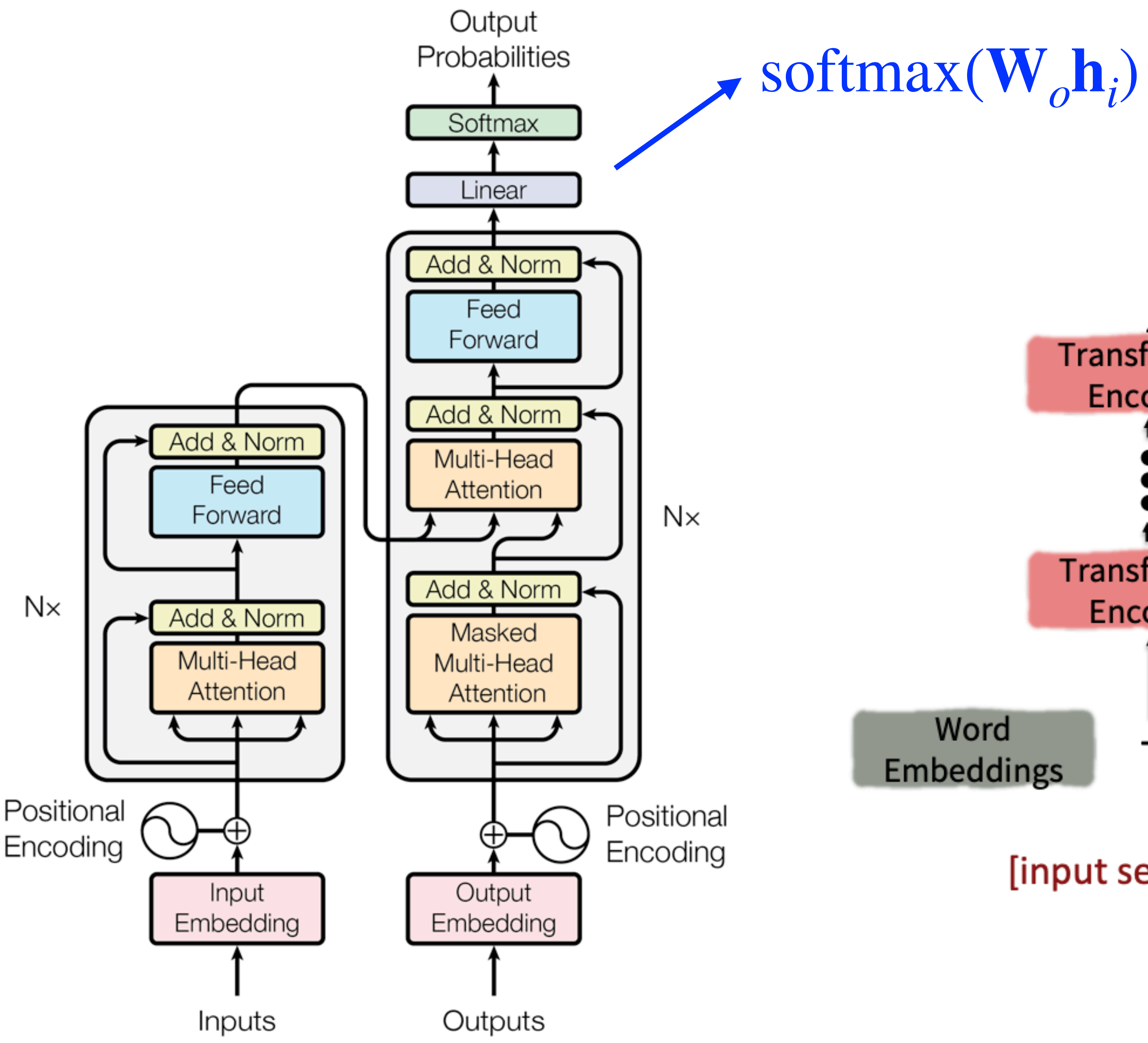
$$\mathbf{k}_j = \tilde{\mathbf{x}}_j \mathbf{W}^K, \mathbf{v}_j = \tilde{\mathbf{x}}_j \mathbf{W}^V \quad \forall j = 1,2,\ldots,m$$

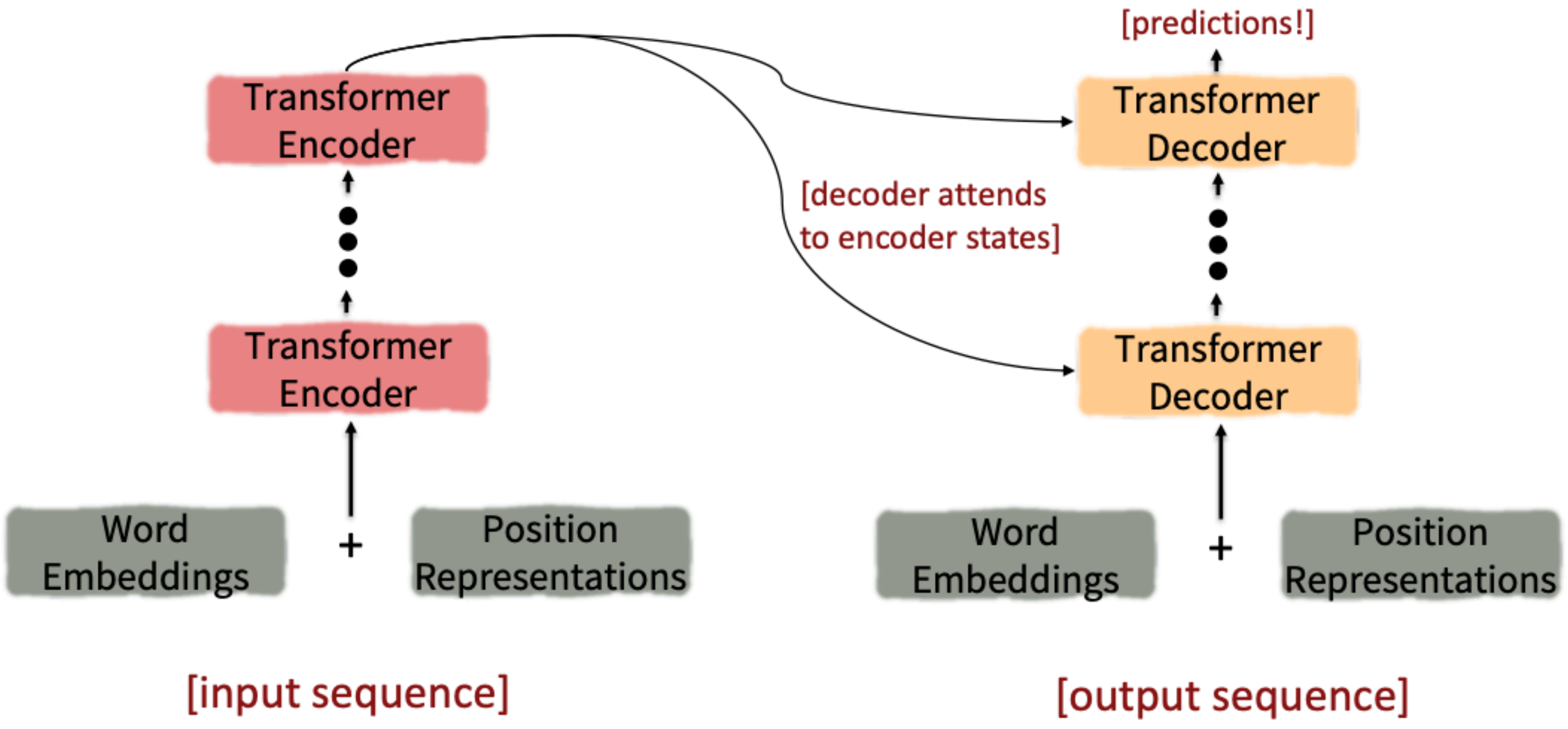
$$e_{i,j} = \frac{\mathbf{q_i} \cdot \mathbf{k}_j}{\sqrt{d_k}}, \forall j = 1, \ldots, m$$

$$\alpha_i = \mathrm{softmax}(\mathbf{e}_i)$$

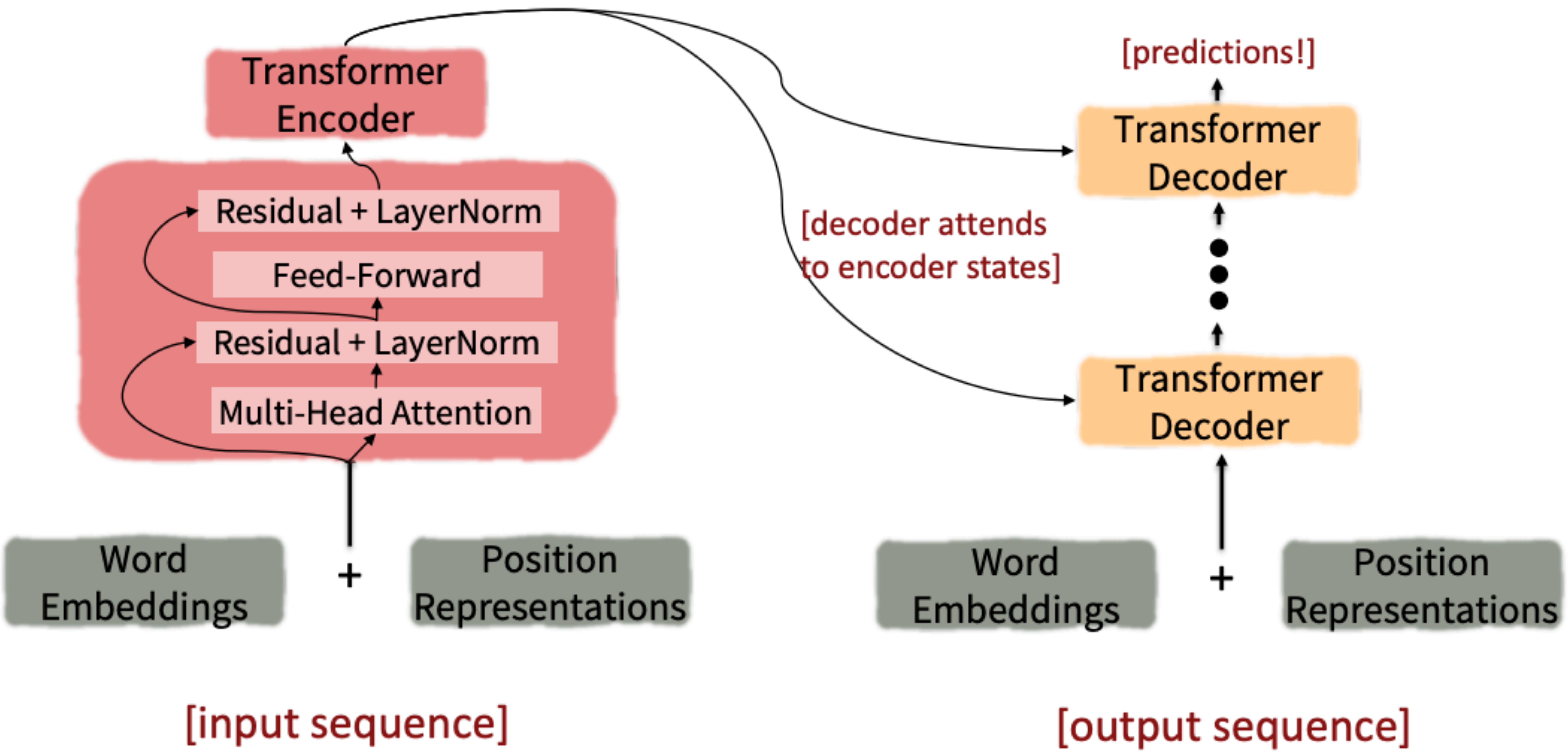
$$\mathbf{h}_i = \sum_{j=1}^{m} \alpha_{i,j} \mathbf{v}_j$$

Transformer encoder-decoder



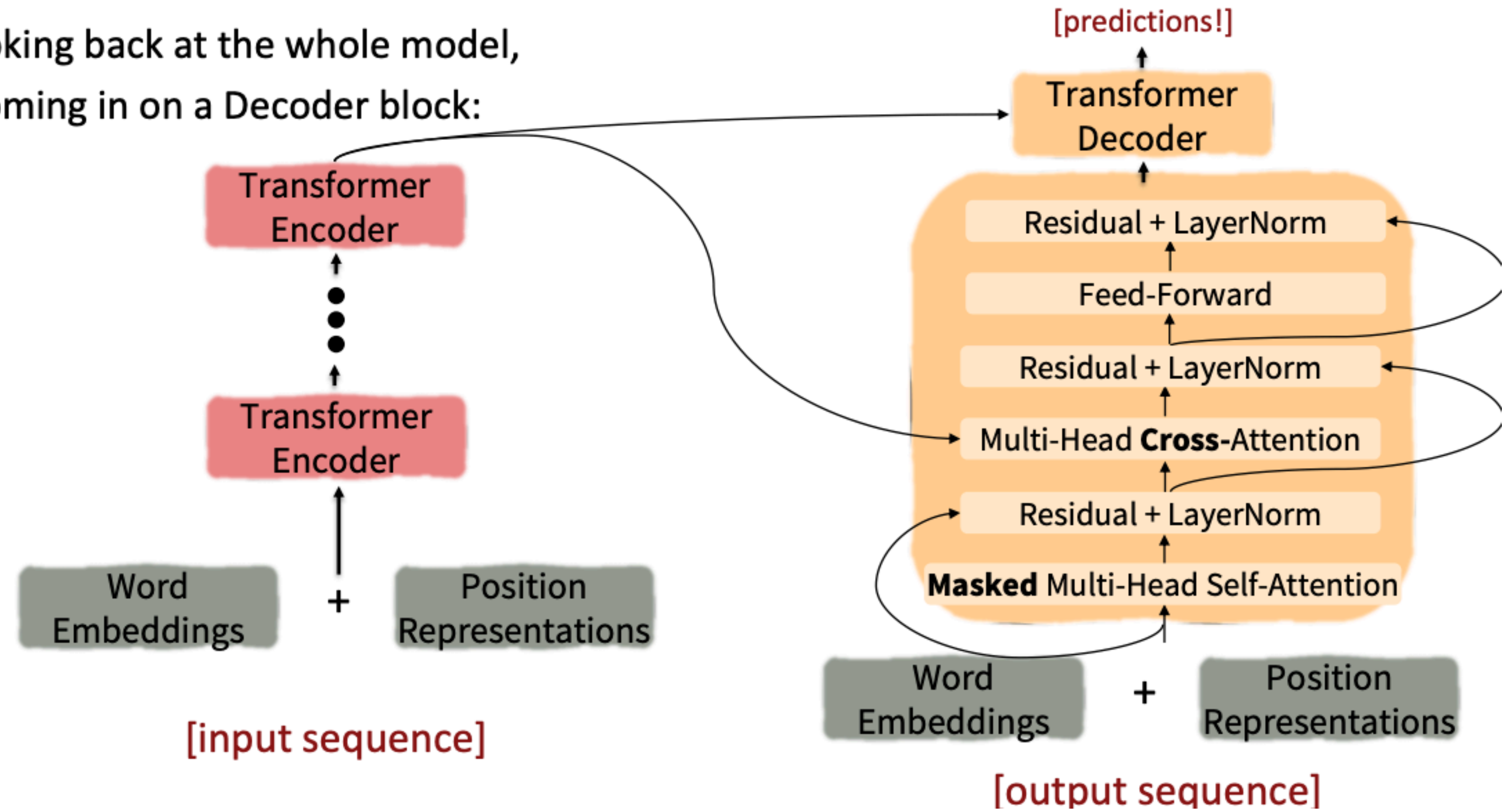


Transformer encoder-decoder



Transformer encoder-decoder

Looking back at the whole model, zooming in on a Decoder block:



Training Transformer encoder-decoder models

The same as the way that we train seq2seq models before!

- Training data: parallel corpus $\{(\mathbf{w}_i^{(s)}, \mathbf{w}_i^{(t)})\}$
- Minimize cross-entropy loss:

$$\sum_{t=1}^{T} -\log P(y_t \mid y_1, \ldots, y_{t-1}, \mathbf{w}^{(s)})$$

(denote $\mathbf{w}^{(t)} = y_1, \ldots, y_T$)

- Back-propagate gradients through both encoder and decoder

12M sentence pairs

French: bonjour le monde .

English: hello world .

Masked self-attention is the key!

This can enable parallelizable operations while NOT looking at the future

Empirical results with Transformers

Model	BLEU		Training Cost (FLOPs)	
	EN-DE	EN-FR	EN-DE	EN-FR
ByteNet [15]	23.75			
Deep-Att + PosUnk [32]		39.2		$1.0 \cdot 10^{20}$
GNMT + RL [31]	24.6	39.92	$2.3 \cdot 10^{19}$	$1.4 \cdot 10^{20}$
ConvS2S [8]	25.16	40.46	$9.6 \cdot 10^{18}$	$1.5 \cdot 10^{20}$
MoE [26]	26.03	40.56	$2.0 \cdot 10^{19}$	$1.2 \cdot 10^{20}$
Deep-Att + PosUnk Ensemble [32]		40.4		$8.0 \cdot 10^{20}$
GNMT + RL Ensemble [31]	26.30	41.16	$1.8 \cdot 10^{20}$	$1.1 \cdot 10^{21}$
ConvS2S Ensemble [8]	26.36	**41.29**	$7.7 \cdot 10^{19}$	$1.2 \cdot 10^{21}$
Transformer (base model)	27.3	38.1	$\mathbf{3.3 \cdot 10^{18}}$	
Transformer (big)	**28.4**	**41.0**	$2.3 \cdot 10^{19}$	

(Vaswani et al., 2017)

Test sets: WMT 2014 English-German and English-French

Empirical results with Transformers

Model	Test perplexity	ROUGE-L
seq2seq-attention, $L = 500$	5.04952	12.7
Transformer-ED, $L = 500$	2.46645	34.2
Transformer-D, $L = 4000$	2.22216	33.6
Transformer-DMCA, no MoE-layer, $L = 11000$	2.05159	36.2
Transformer-DMCA, MoE-128, $L = 11000$	1.92871	37.9
Transformer-DMCA, MoE-256, $L = 7500$	1.90325	38.8

ED: encoder-decoder, D: decoder

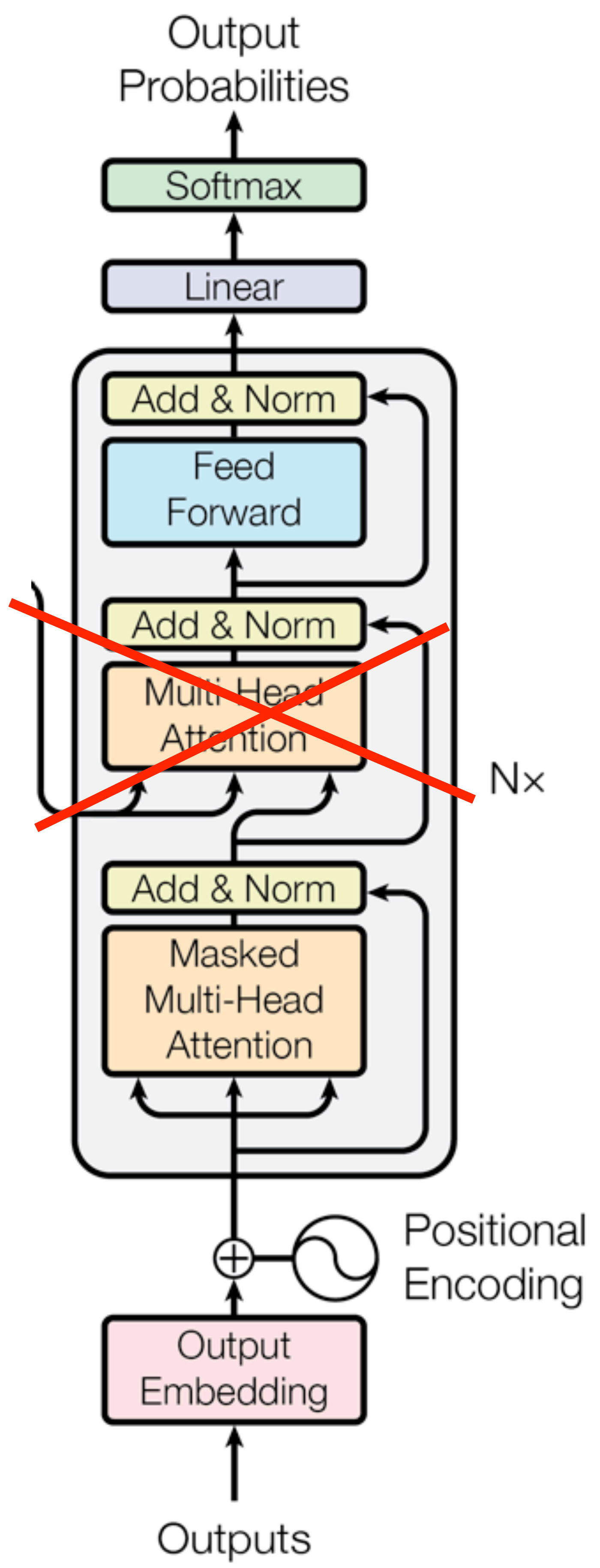
DMCA: decoder with memory-compressed attention

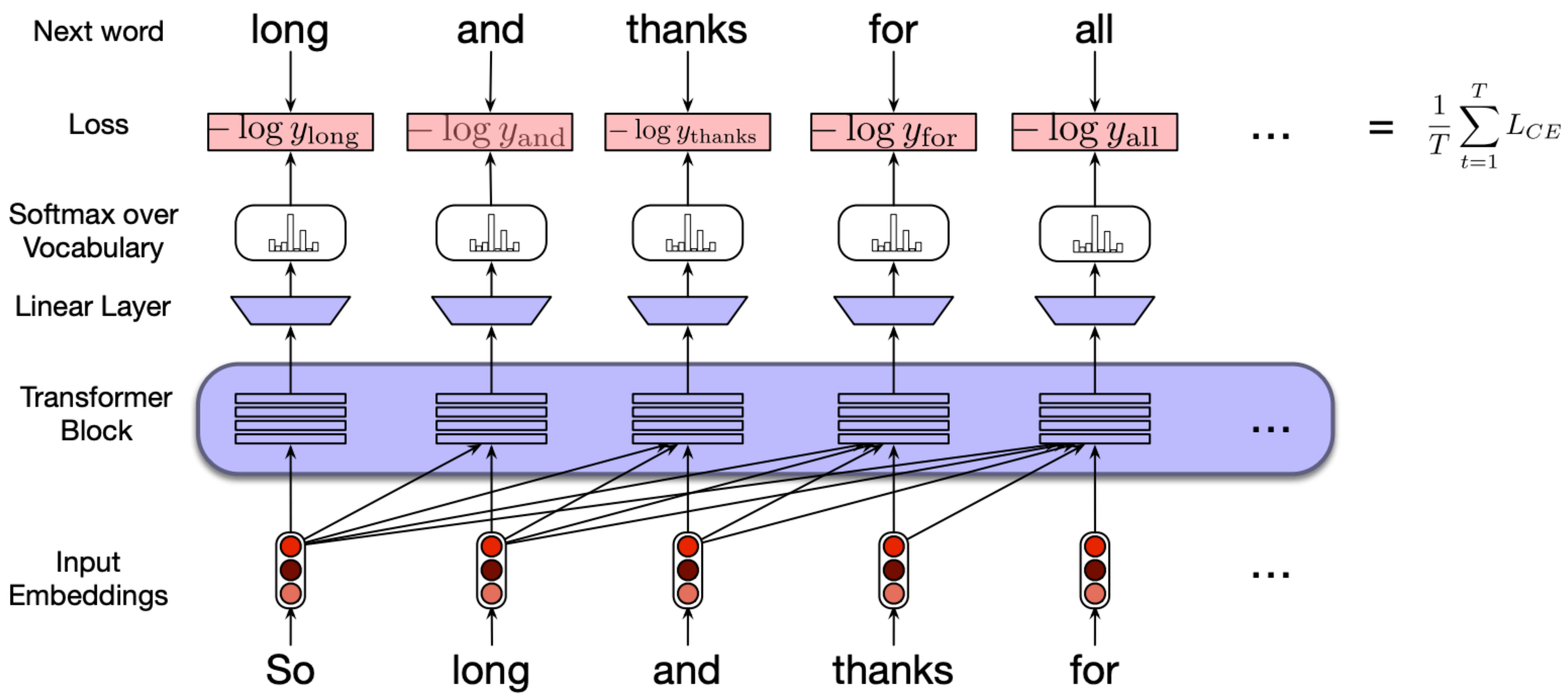
MoE: mixture of experts

(Liu et al., 2018): Generating Wikipedia by Summarizing Long Sequences

Transformer-based language models

- The model architecture of GPT-3, ChatGPT, …





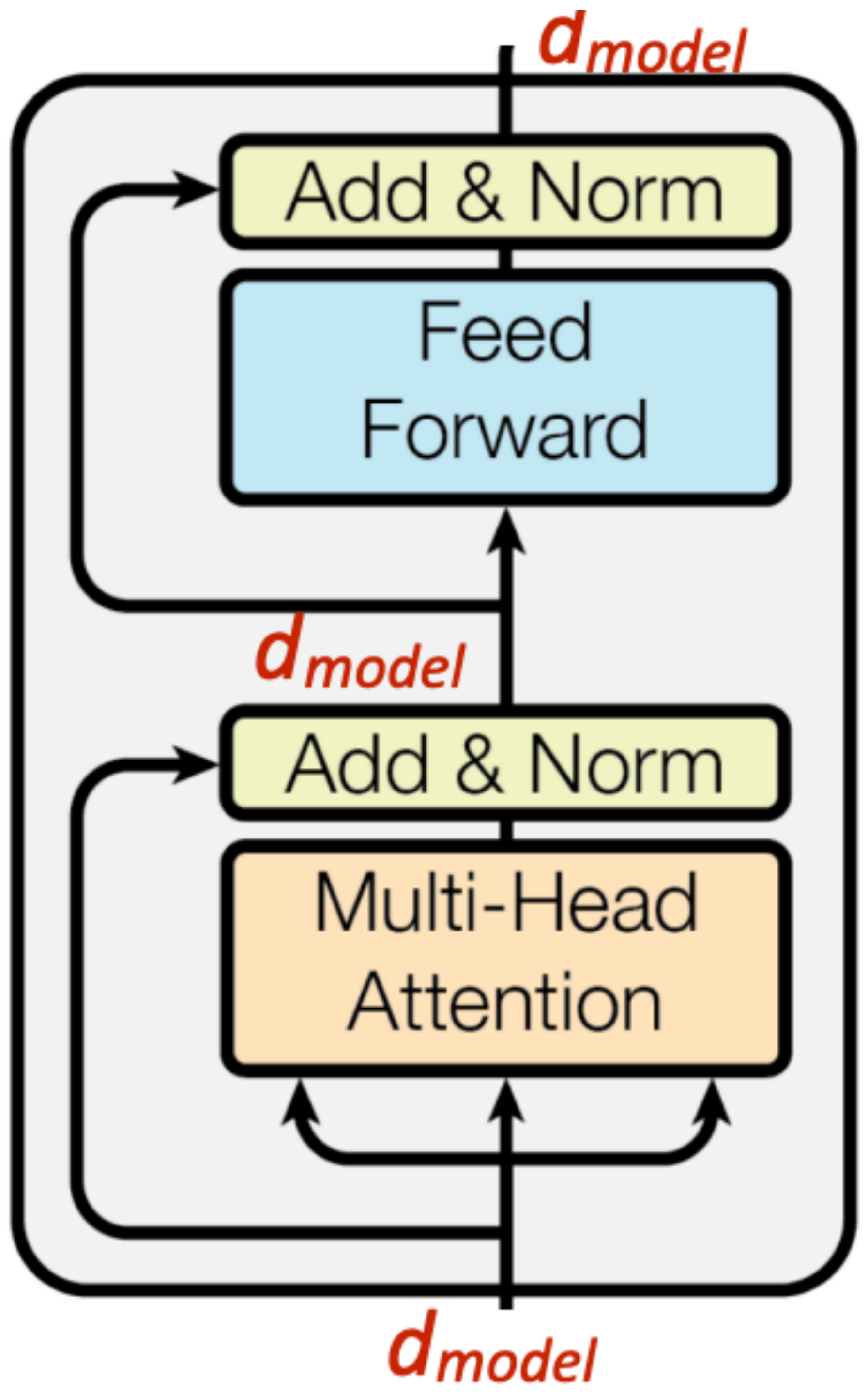
Transformer architecture specifications

	N	d_{model}	d_{ff}	h	d_k	d_v
base	6	512	2048	8	64	64

- From Vaswani et al.

Model Name	n_{params}	n_{layers}	d_{model}	n_{heads}	d_{head}
GPT-3 Small	125M	12	768	12	64
GPT-3 Medium	350M	24	1024	16	64
GPT-3 Large	760M	24	1536	16	96
GPT-3 XL	1.3B	24	2048	24	128
GPT-3 2.7B	2.7B	32	2560	32	80
GPT-3 6.7B	6.7B	32	4096	32	128
GPT-3 13B	13.0B	40	5140	40	128
GPT-3 175B or "GPT-3"	175.0B	96	12288	96	128

- From GPT-3; d_{head} is our d_k



The Annotated Transformer

The Annotated Transformer

Attention is All You Need

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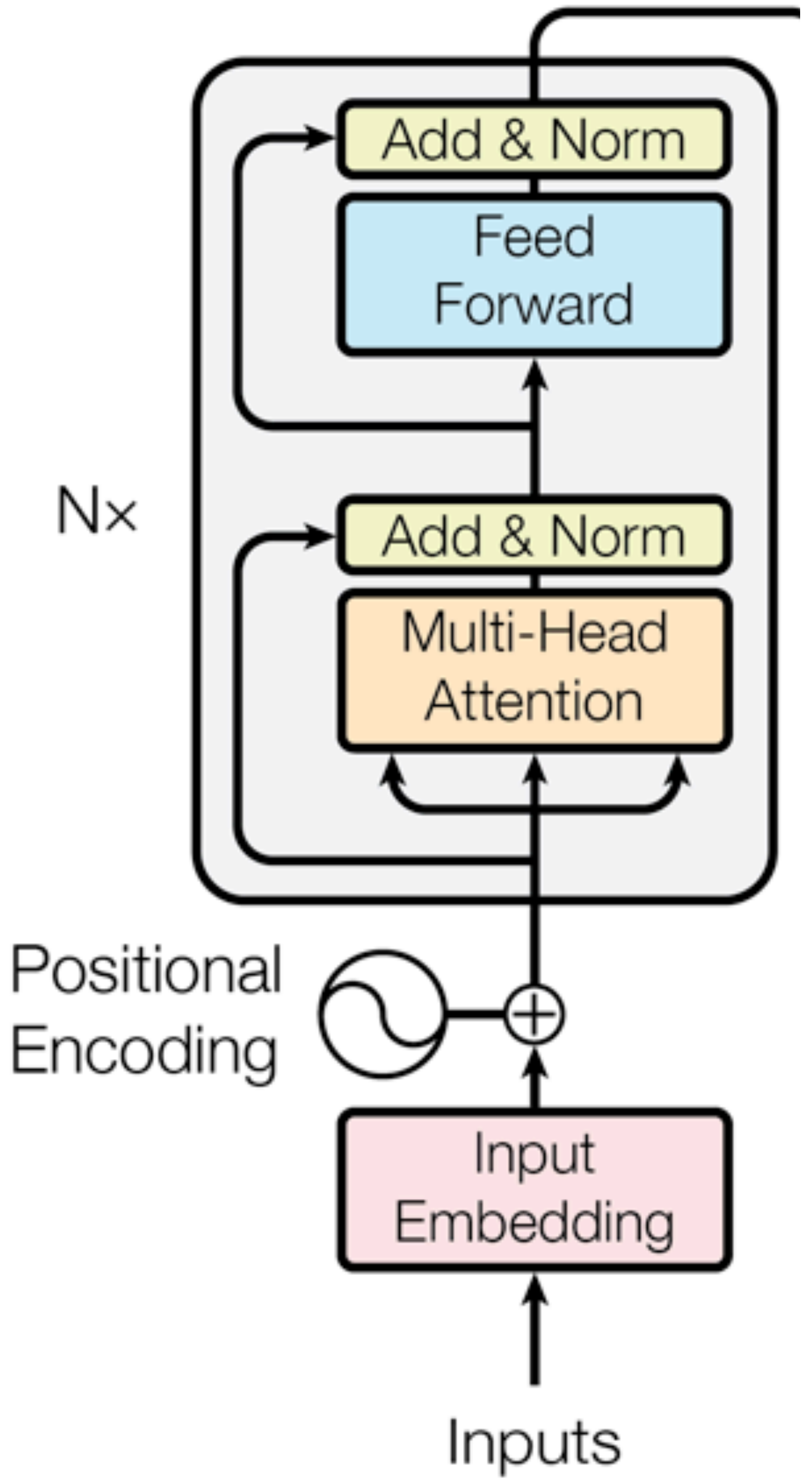
http://nlp.seas.harvard.edu/annotated-transformer/

Understanding Transformers



Which of the following is CORRECT?

(A) Multi-head attention is more computationally expensive than feedforward layers

(B) Multi-head attention is more computationally expensive than single-head attention

(C) It is hard to apply Transformers to sequences that are longer than the pre-defined max_seq_length L

(D) We can easily scale Transformers to long sequences

The correct answer is (C)

Transformers: pros and cons

- **Easier to capture long-range dependencies**: we draw attention between every pair of words!
- **Easier to parallelize:**

$$Q = XW^Q \qquad K = XW^K \qquad V = XW^V$$

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

- **Are positional encodings enough to capture positional information?**

Otherwise self-attention is an unordered function of its input

- **Quadratic computation in self-attention**

Can become very slow when the sequence length is large

Quadratic computation as a function of sequence length

$Q = XW^Q \qquad K = XW^K \qquad V = XW^V$

$$\boxed{\mathrm{Attention}(Q, K, V) = \mathrm{softmax}(\frac{\overbrace{Q}^{n \times d_q}\overbrace{K^T}^{d_k \times n}}{\sqrt{d_k}})\underbrace{V}_{n \times d_v}}$$

Need to compute n^2 pairs of scores (= dot product) O(n^2d)

RNNs only require $O(nd^2)$ running time:

$$\mathbf{h}_t = g(\mathbf{W}\mathbf{h}_{t-1} + \mathbf{U}\mathbf{x}_t + \mathbf{b})$$

(assuming input dimension = hidden dimension = d)

Motivation: Modeling Long Sequences

Enable New Capabilities

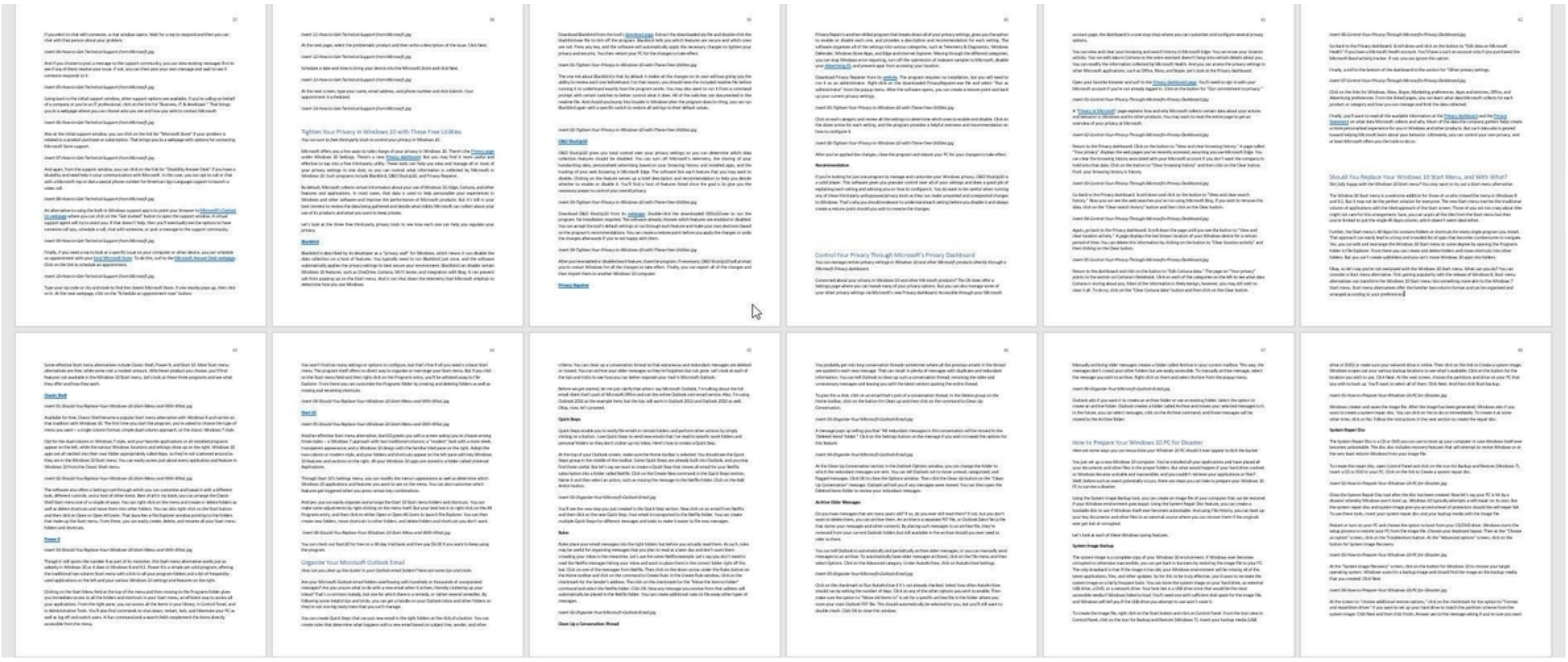
NLP: Large context required to understand books, plays, codebases.

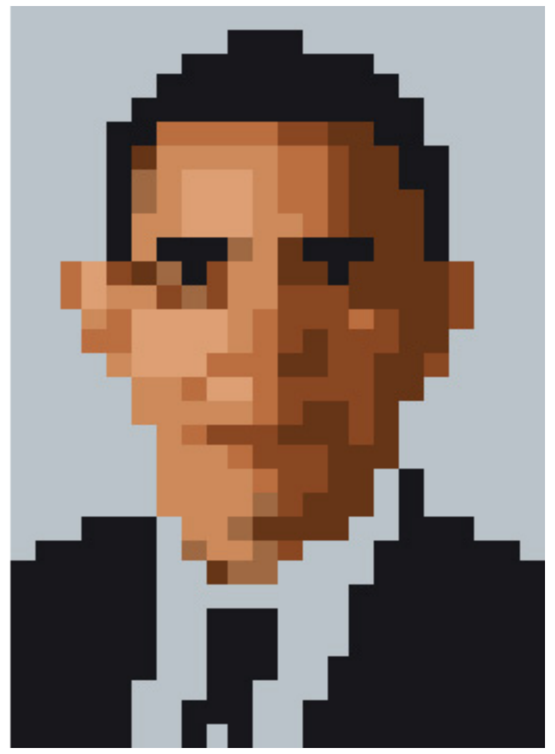
Close Reality Gap

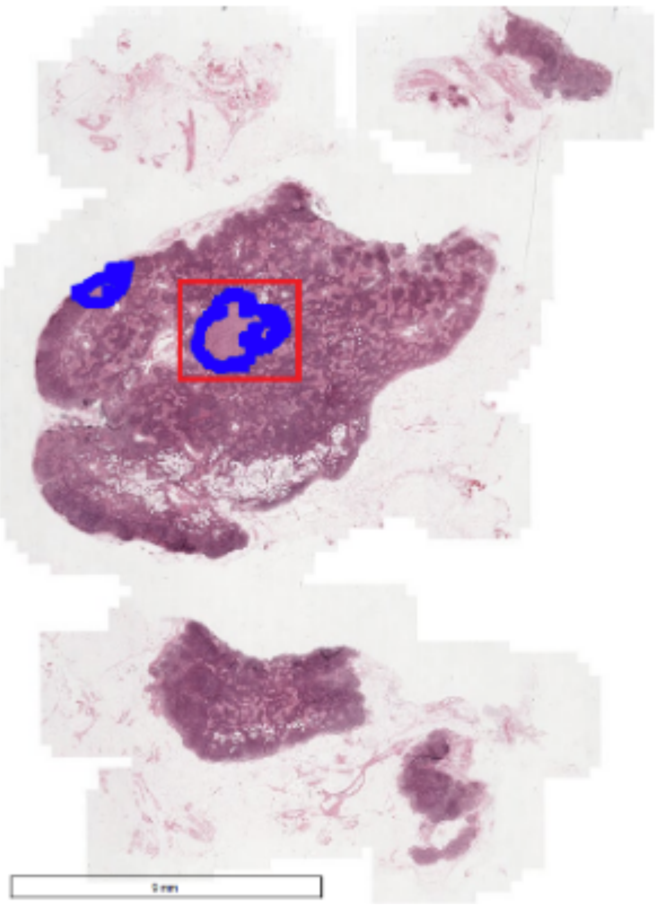
Computer vision: higher resolution can lead to better, more robust insight.

Open New Areas

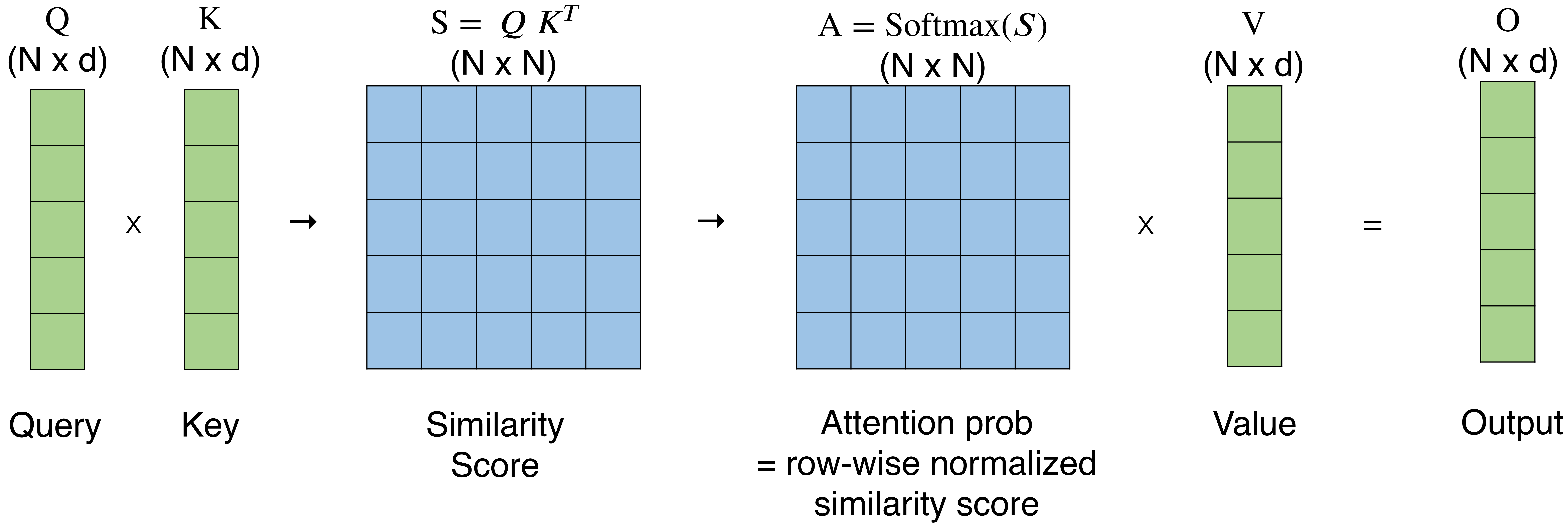
Time series, audio, video, medical imaging data naturally modeled as sequences of millions of steps.







Attention Mechanism



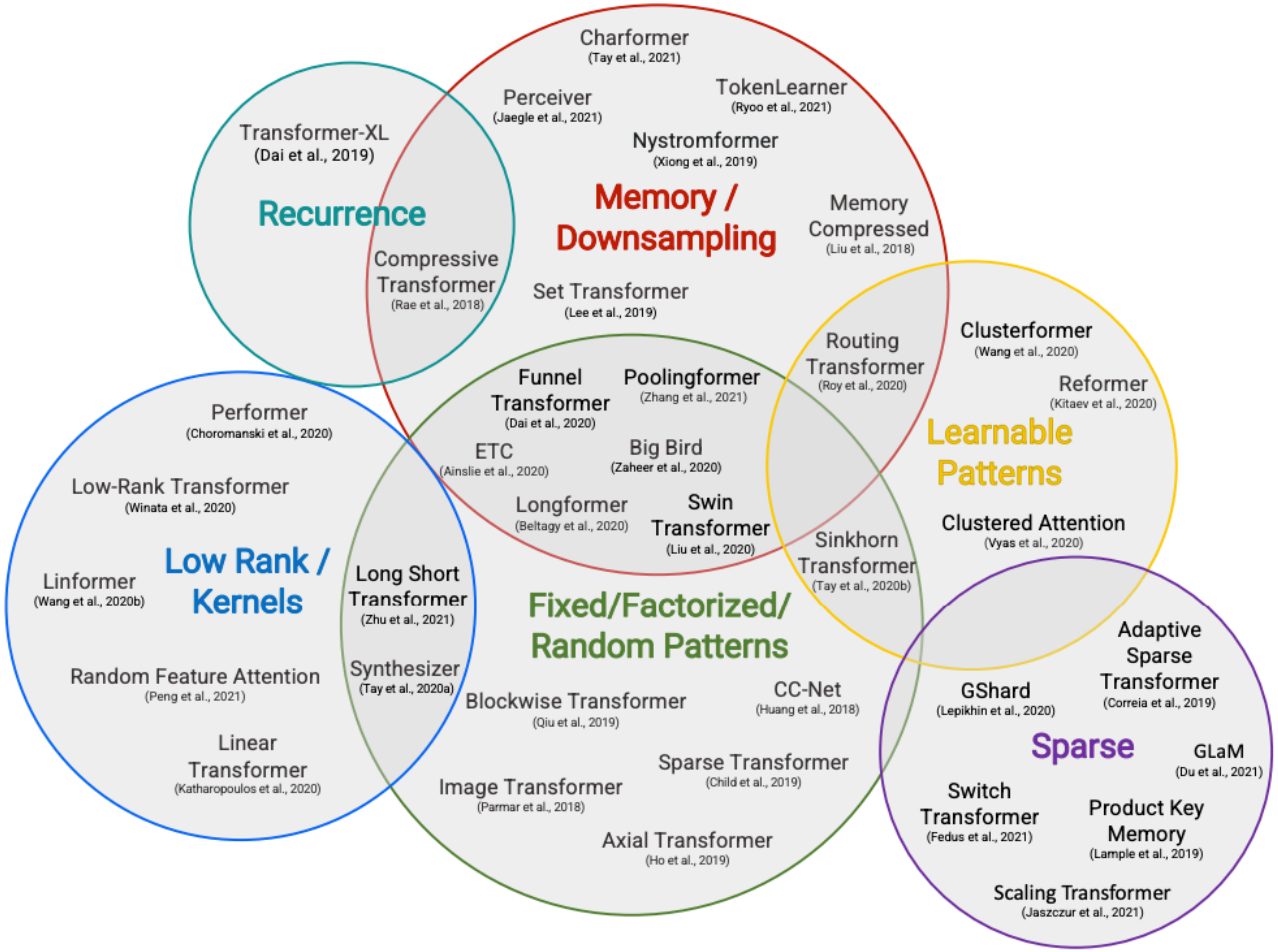
Typical sequence length N: 1K – 8K
Head dimension d: 64 – 128

$$\text{Softmax}\left(\left[s_1,\ \cdots,\ s_N\right]\right) = \left[\frac{e^{s_1}}{\sum_i e^{s_i}}, \cdots, \frac{e^{s_N}}{\sum_i e^{s_i}}\right]$$

$$O = \text{Softmax}(QK^T)V$$

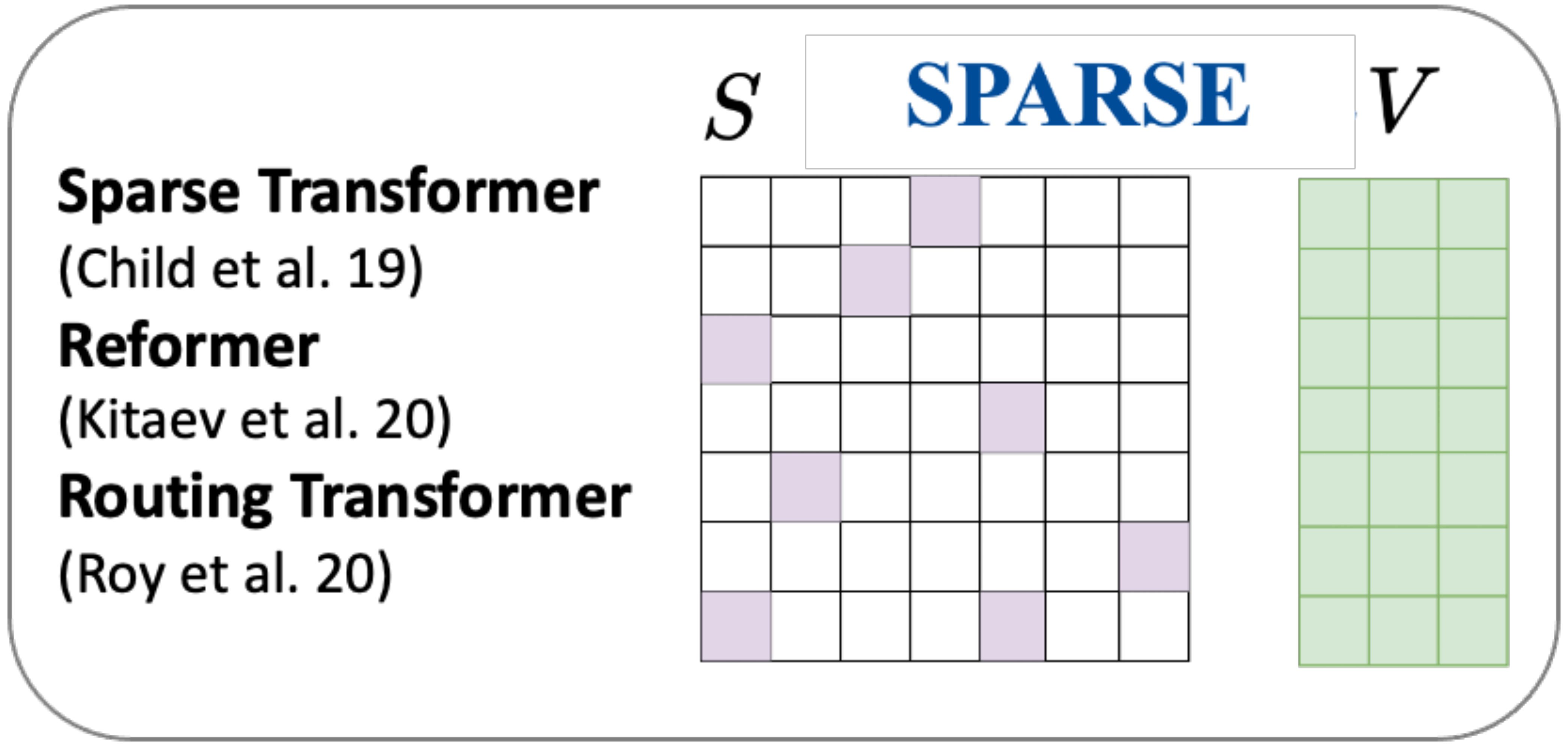
Attention scales quadratically in sequence length N

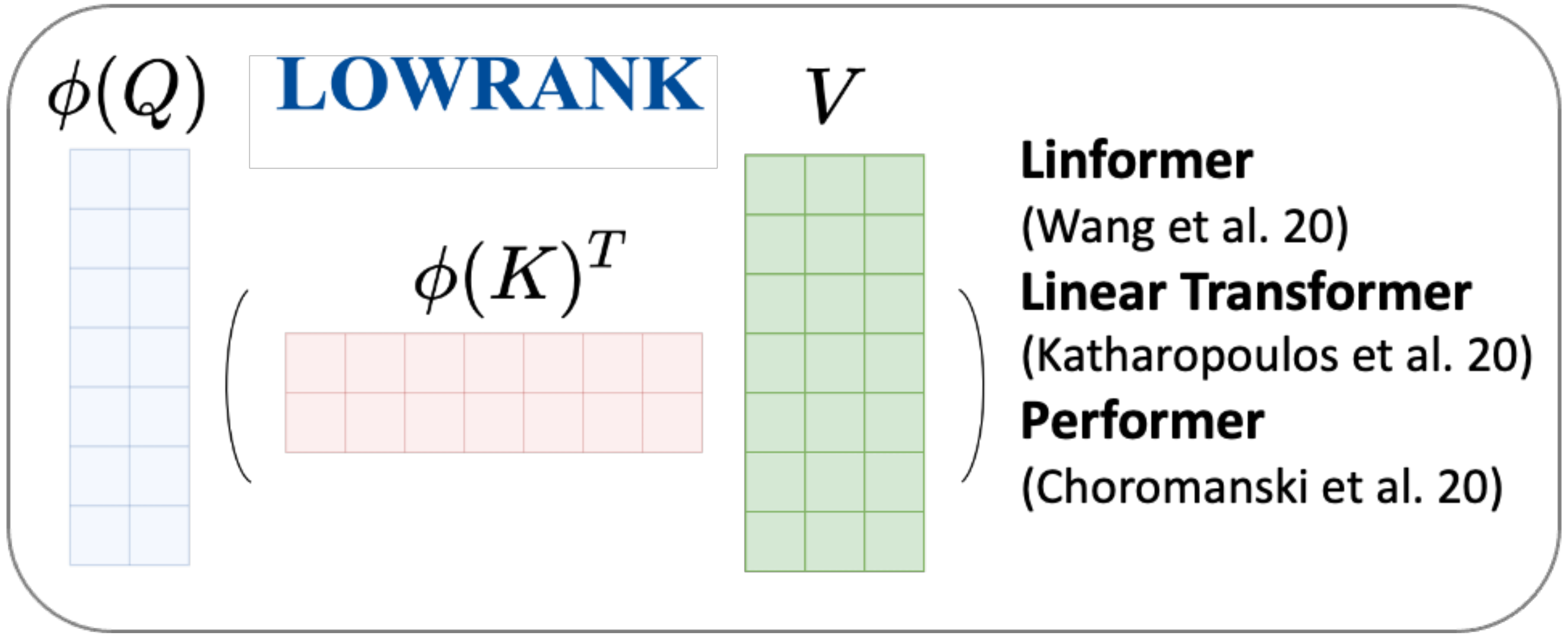
Efficient Transformers



(Tay et al., 2020): Efficient Transformers: A Survey

Approximate Attention

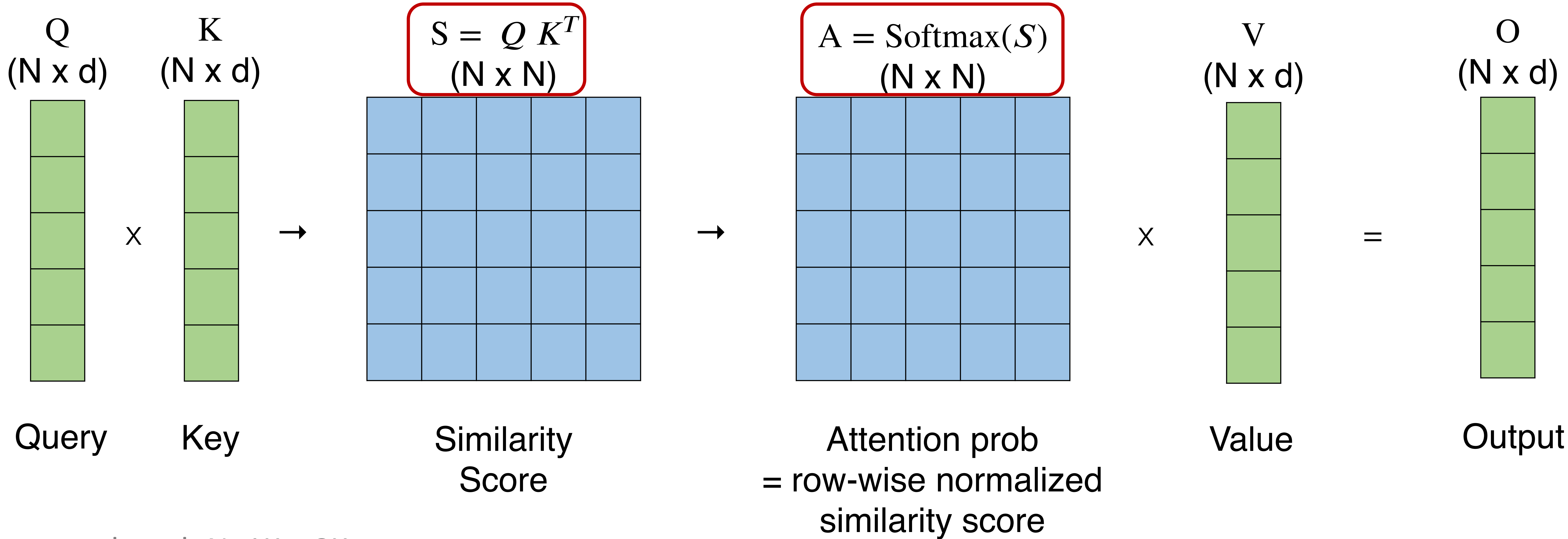




Approximate attention: tradeoff quality for fewer FLOPS

Survey: *Tay et al. Long Range Arena : A Benchmark for Efficient Transformers.* ***ICLR 2020.***

Attention is Bottlenecked by Memory Reads/Writes



Typical sequence length N: 1K – 8K
Head dimension d: 64-128

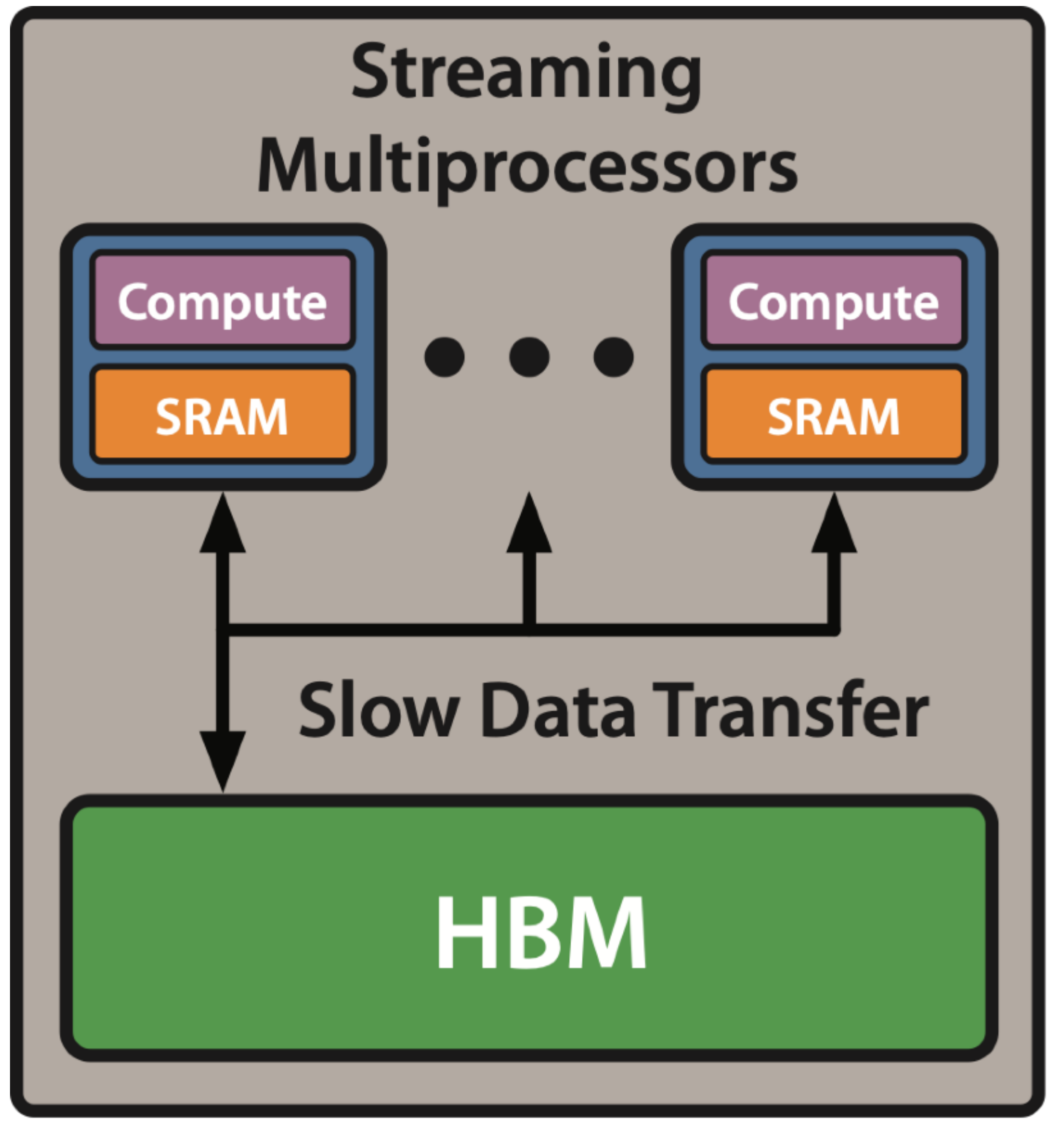
The biggest cost is in moving the bits!
Standard implementation requires repeated R/W from slow GPU memory

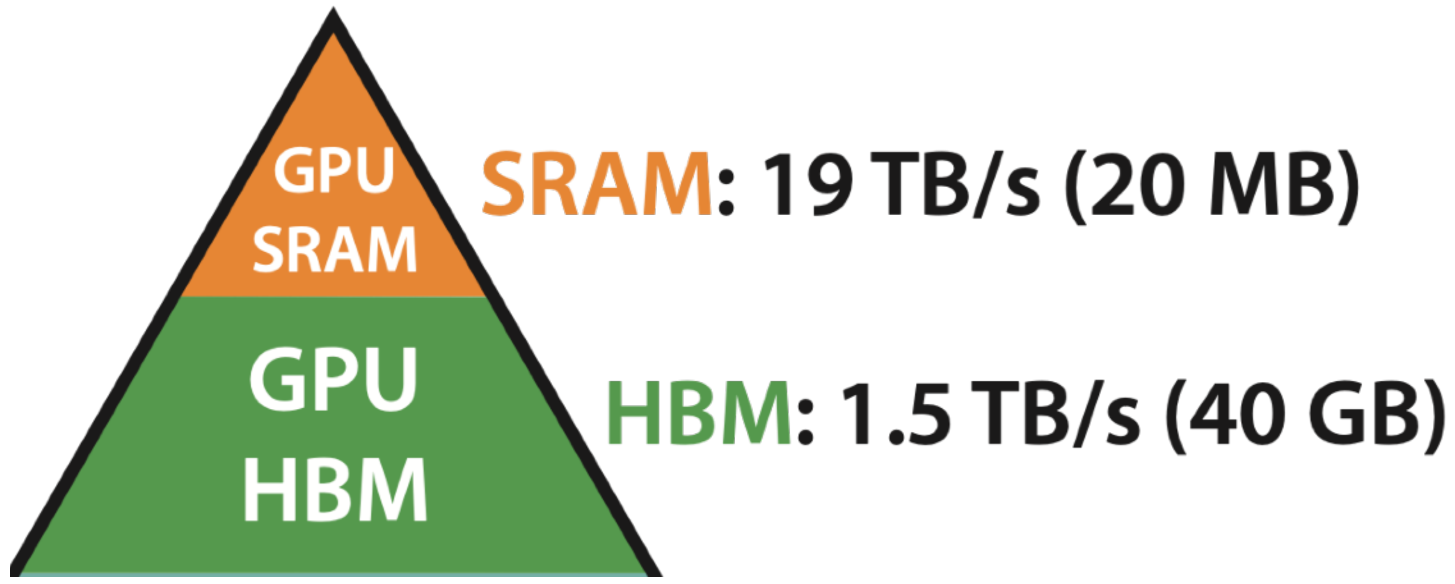
Background: GPU Compute Model & Memory Hierarchy

2. Data moved to compute units & SRAM for computation

1. Inputs start out in HBM (GPU memory)

3. Output written back to HBM





Blogpost: Horace He, Making Deep Learning Go Brrrr From First Principles.

Can we exploit the memory asymmetry to get speed up?
With IO-awareness (accounting for R/W to different levels of memory)

FlashAttention: Reduce HBM Reads/Writes - Compute by Blocks

Challenges:

(1) Compute softmax normalization without access to full input.

(2) Backward without the large attention matrix from forward.

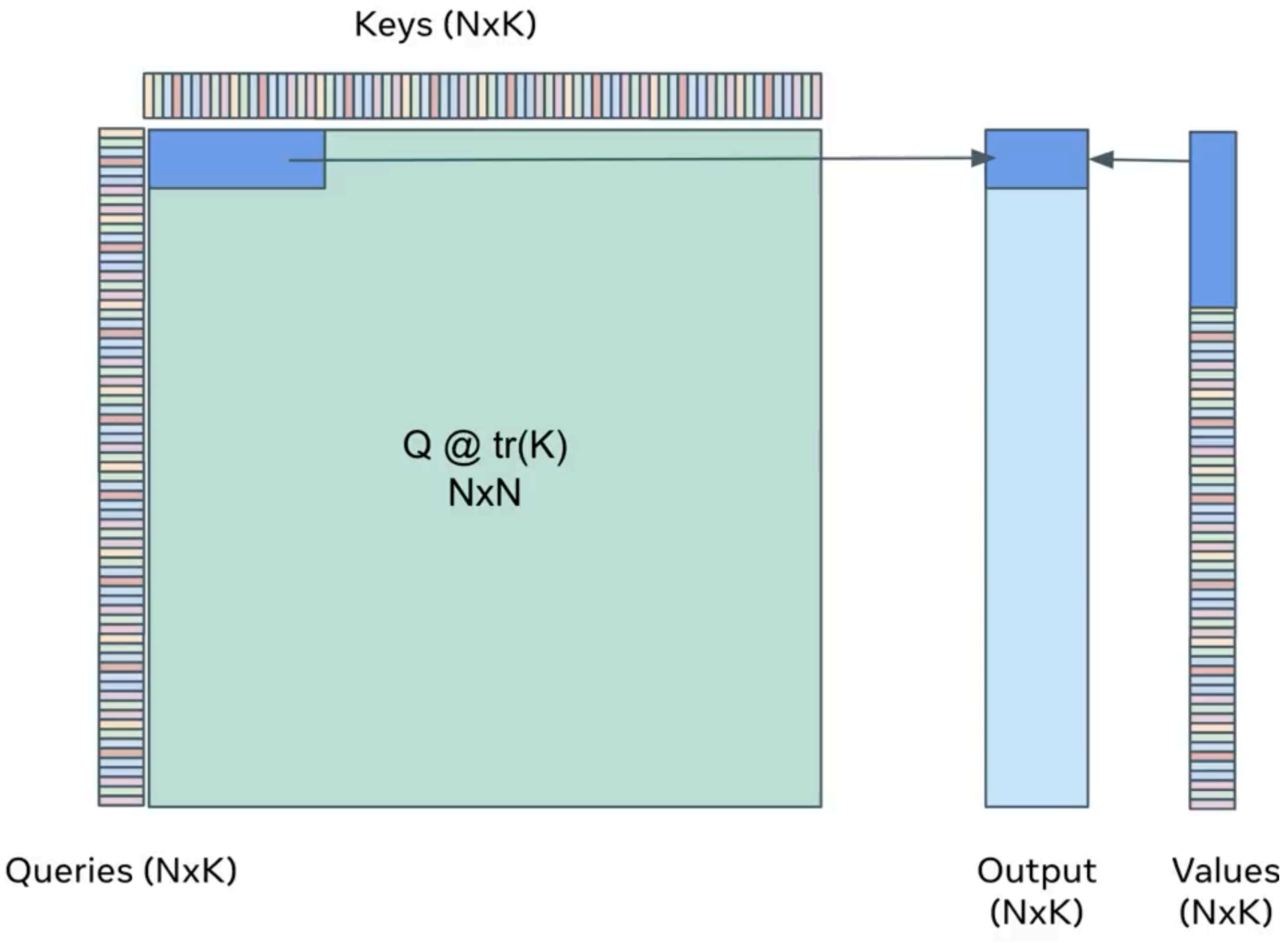
Approaches:

(1) Tiling: Restructure algorithm to load block by block from HBM to SRAM to compute attention.

(2) Recomputation: Don't store attn. matrix from forward, recompute it in the backward.

Tiling

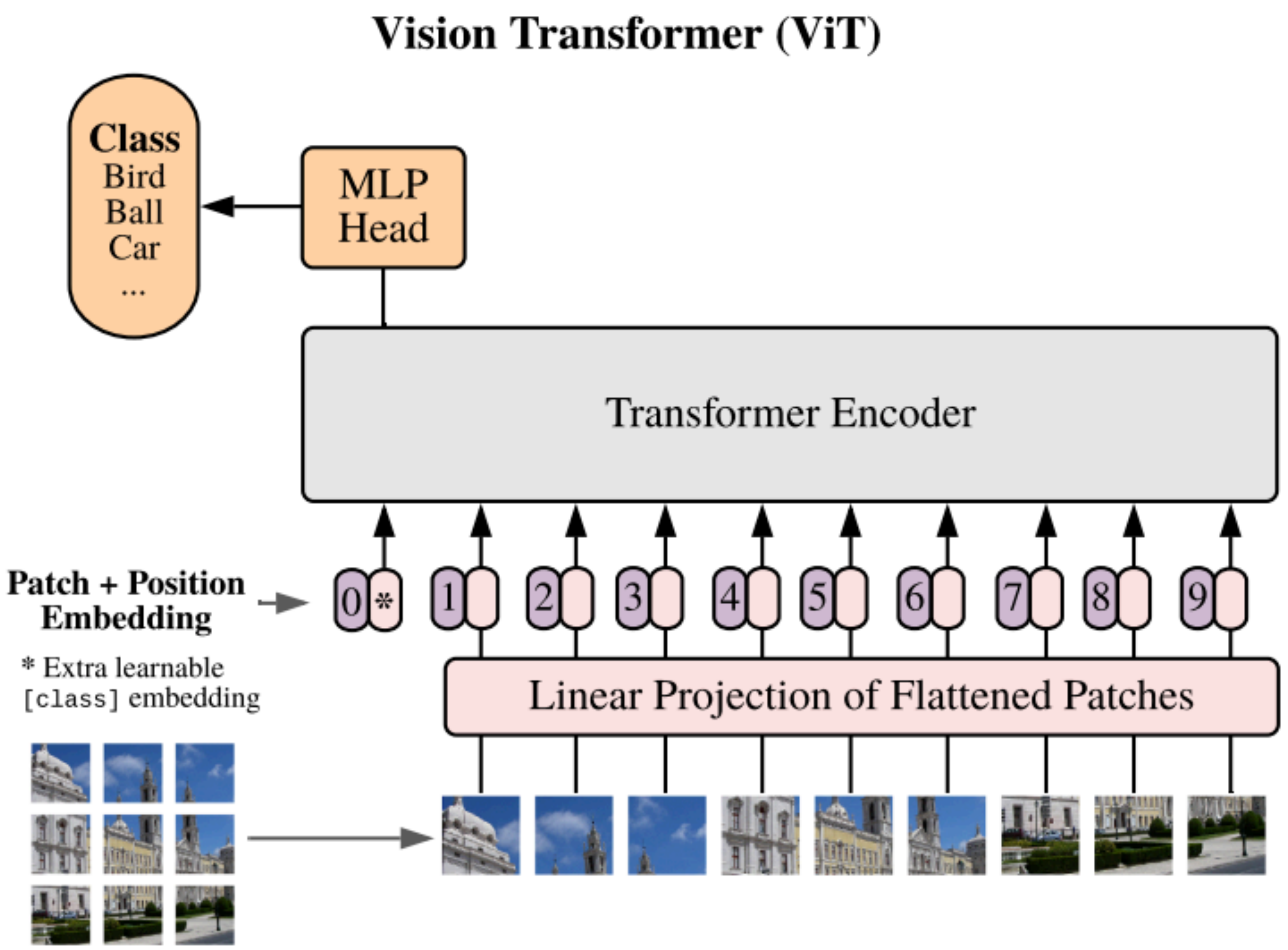
Decomposing large softmax into smaller ones by scaling.

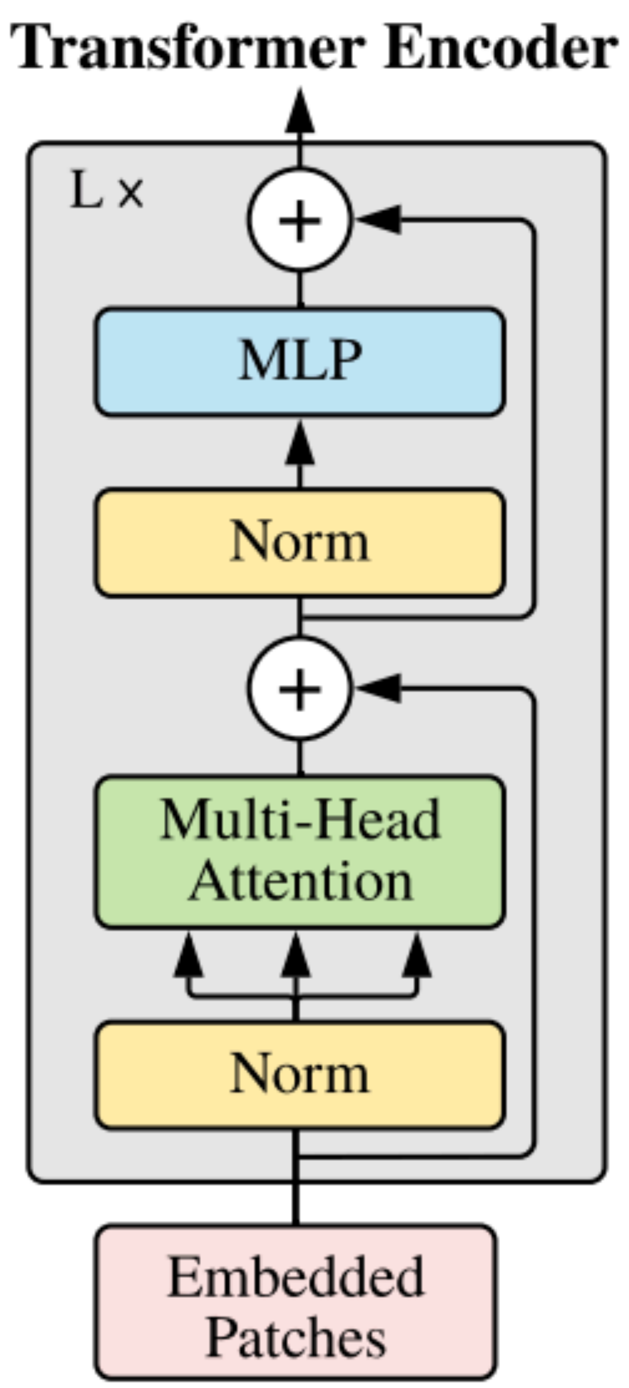


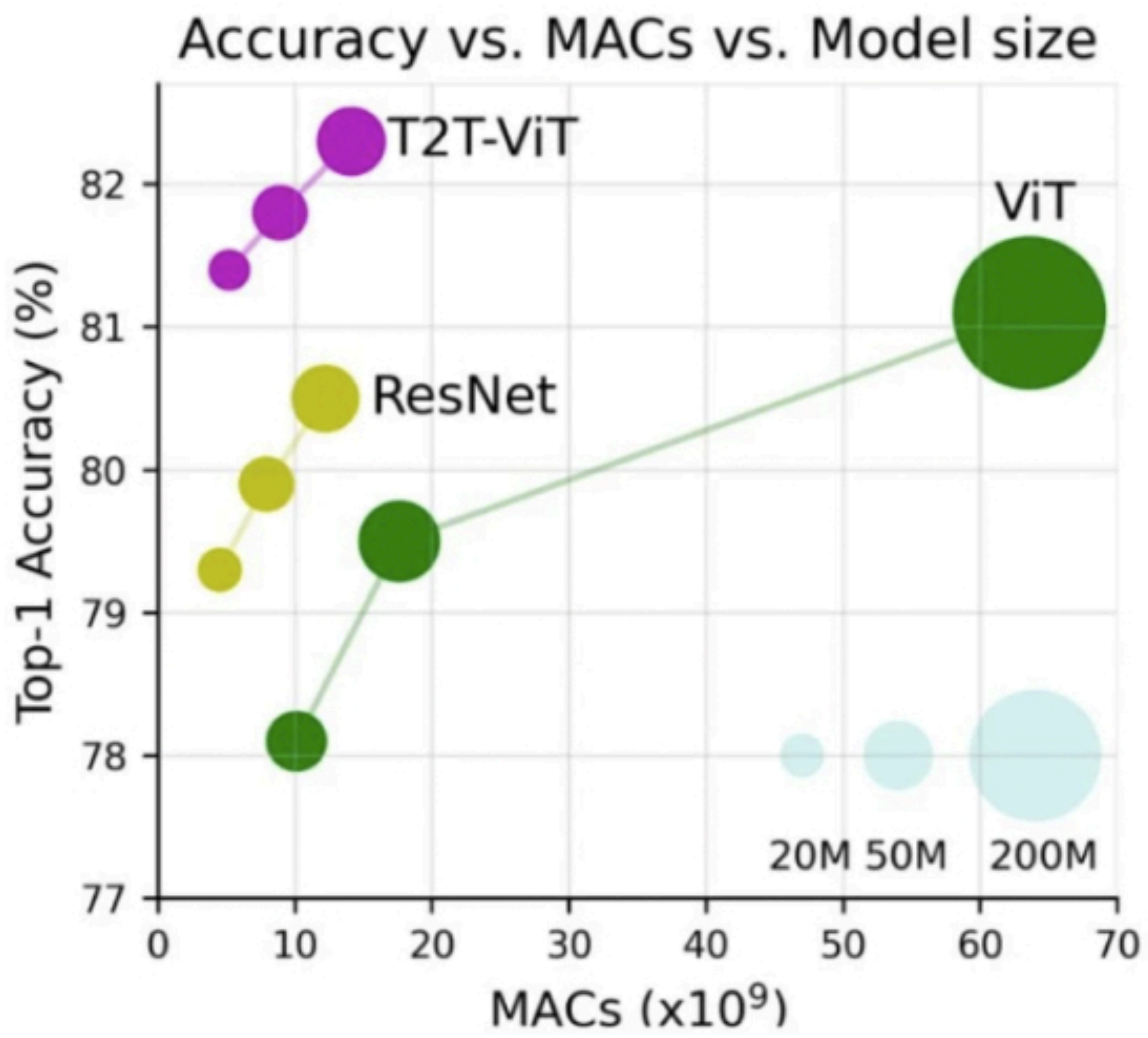
1. Load inputs by blocks from HBM to SRAM.
2. On chip, compute attention output with respect to that block.
3. Update output in HBM by scaling.

Animation credit: Francisco Massa

Vision Transformer (ViT)

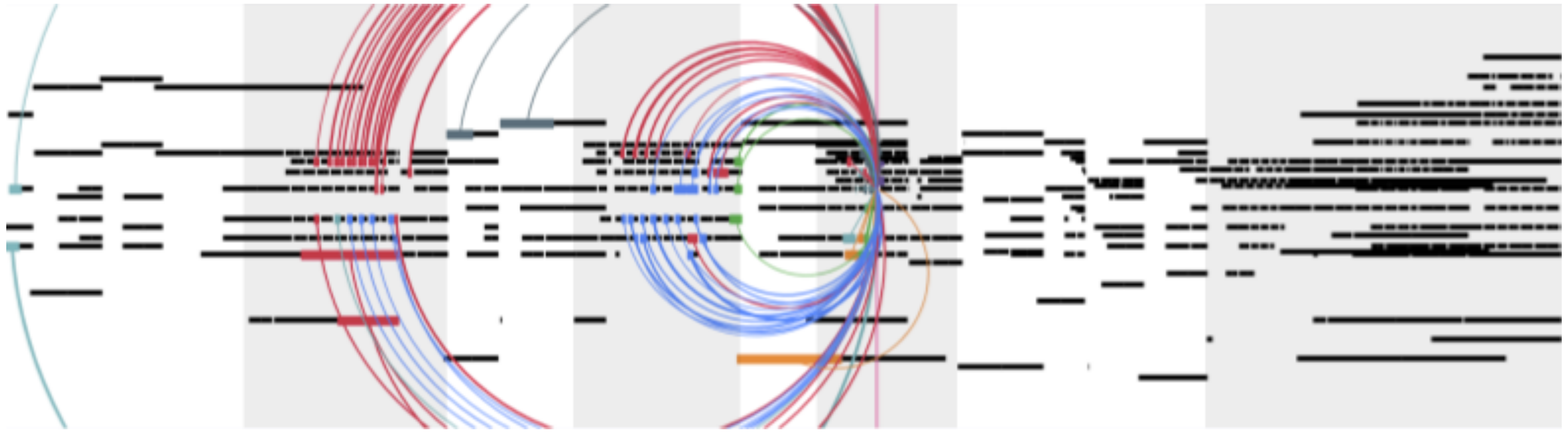


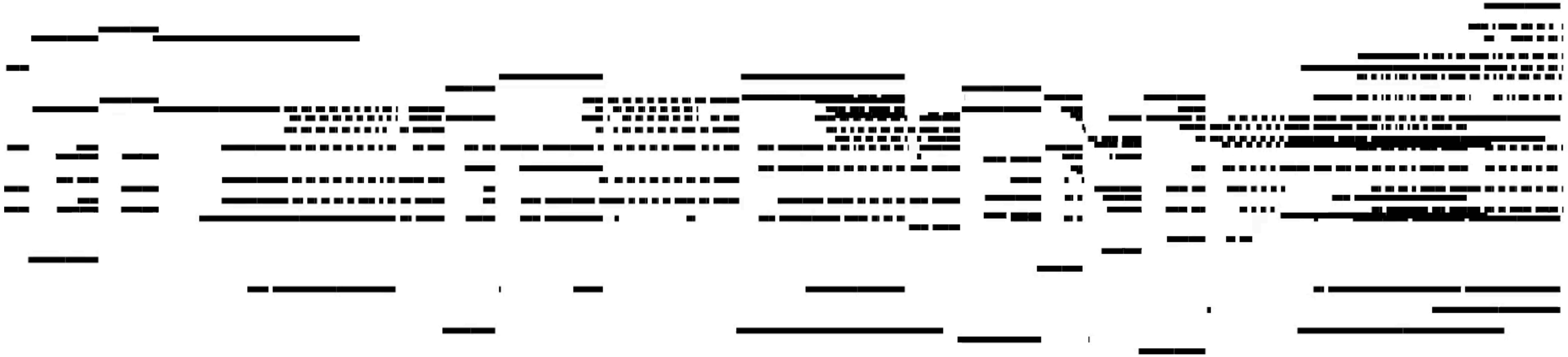




(Dosovitskiy et al., 2021): An Image is Worth 16x16 Words: Transformers for Image Recognition at Scale

Music Transformer





https://magenta.tensorflow.org/music-transformer

(Huang et al., 2018): Music Transformer: Generating Music with Long-Term Structure