CS388: Natural Language Processing
Lecture 7: Transformers

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Administrivia

- Project 2 due on Feb 13 (one week); autograder fixed
  - d_internal vs. d_model: d_internal in the code is d_k in the slides
- Final project spec posted Thursday

Recap: Attention

Step 1: Compute scores for each key

keys k_i

[1, 0] [1, 0] [0, 1] [1, 0]

query: q = [0, 1] (we want to find 1s)

0 0 1 0

$s_i = k_i^T q$

0 0 1 0

Step 2: softmax the scores to get probabilities α

0 0 1 0 => (1/6, 1/6, 1/2, 1/6) if we assume e=3

Step 3: compute output values by multiplying embs. by alpha + summing

result = sum($\alpha_i e_i$) = 1/6 [1, 0] + 1/6 [1, 0] + 1/2 [0, 1] + 1/6 [1, 0] = [1/2, 1/2]

Recap: Self-Attention

$$E = \begin{pmatrix} 1 & 0 \\ 1 & 0 \\ 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$$W^Q = \begin{matrix} 0 & 1 \\ 0 & 1 \end{matrix} \qquad W^K = \begin{matrix} 10 & 0 \\ 0 & 10 \end{matrix}$$

$$Q = E\,(W^Q) = \begin{pmatrix} 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \end{pmatrix} \qquad K = E\,(W^K) = \begin{pmatrix} 10 & 0 \\ 10 & 0 \\ 0 & 10 \\ 10 & 0 \end{pmatrix}$$

Scores $S = QK^T$ $\quad S_{ij} = q_i \cdot k_j$

len x len = (len x d) x (d x len)

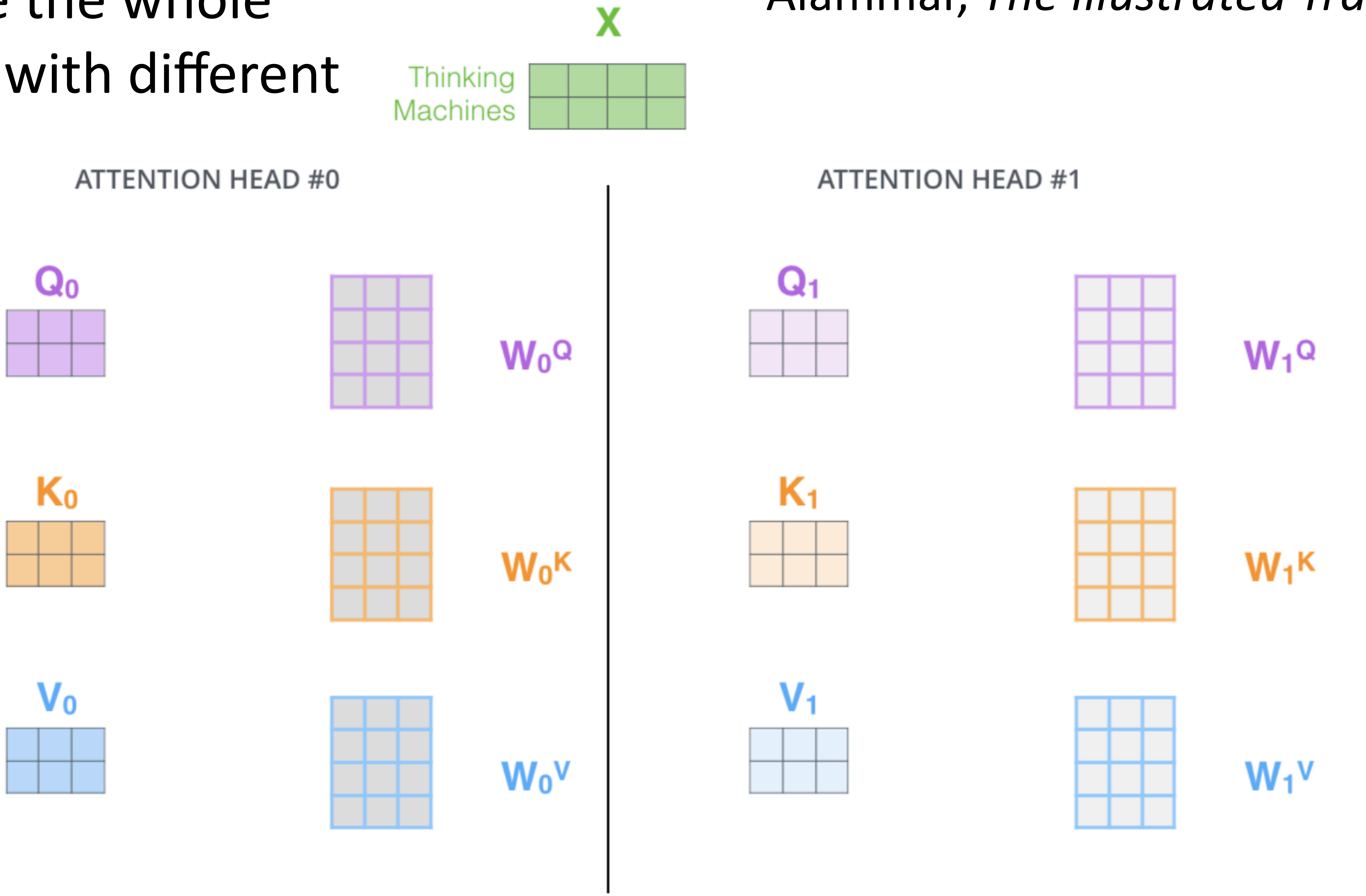
Final step: softmax to get attentions A, then output is AE

*technically it's $A\,(EW^V)$, using a values matrix $V = EW^V$

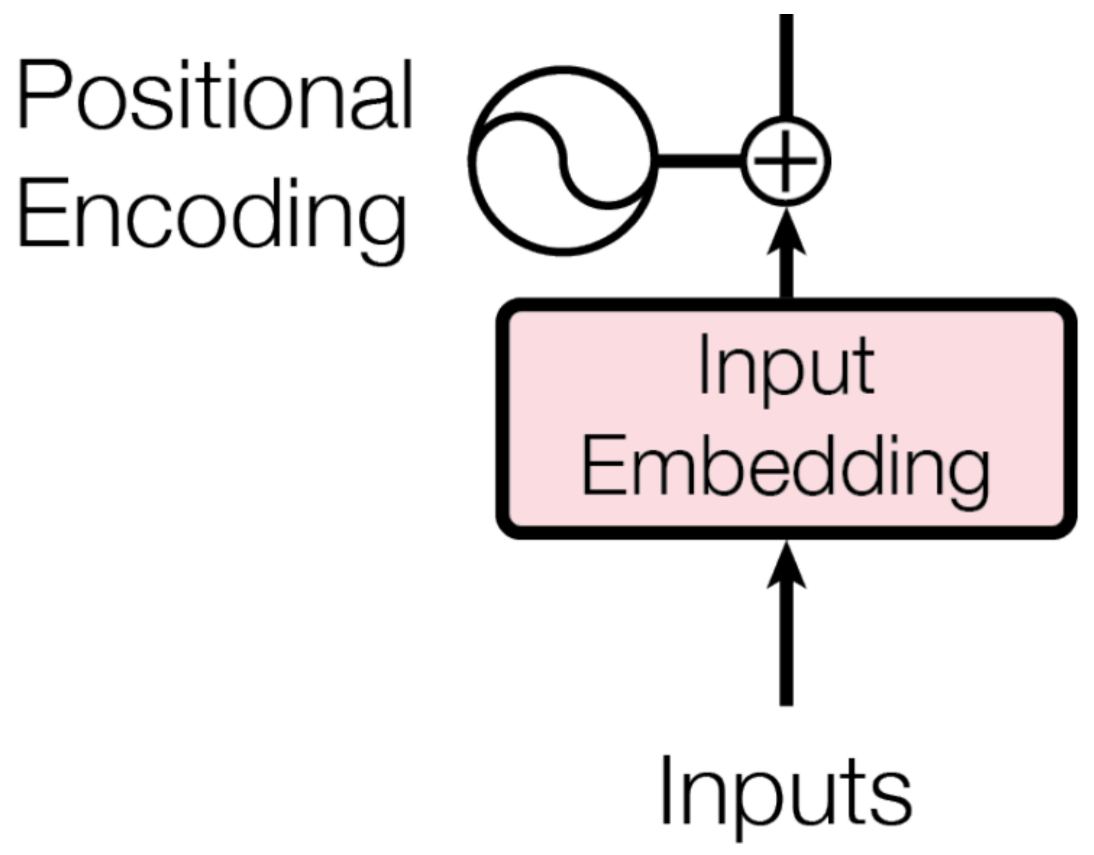
Recap: Multi-head Self-Attention

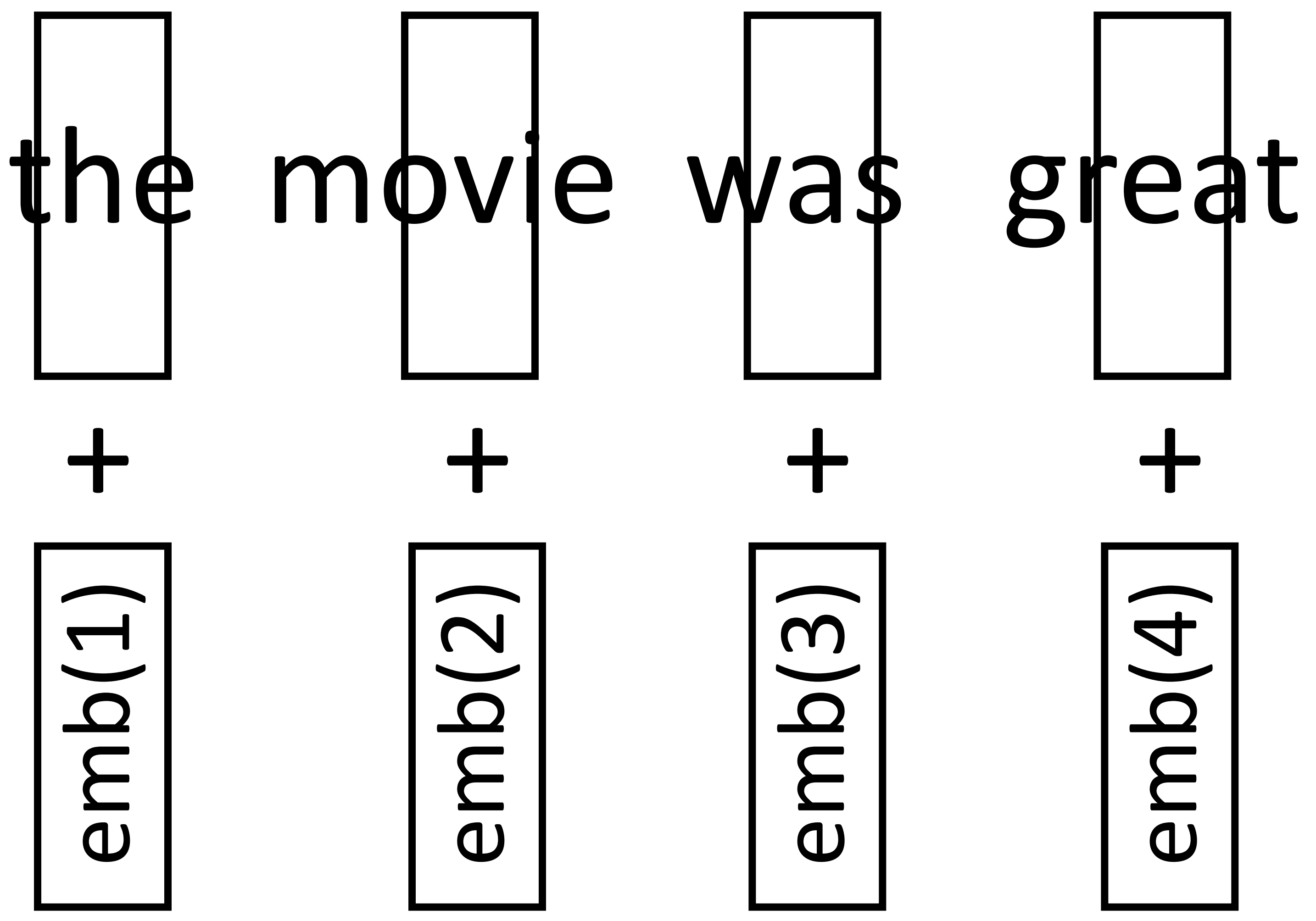
Just duplicate the whole computation with different weights:

Alammar, *The Illustrated Transformer*



Recap: Positional Encodings



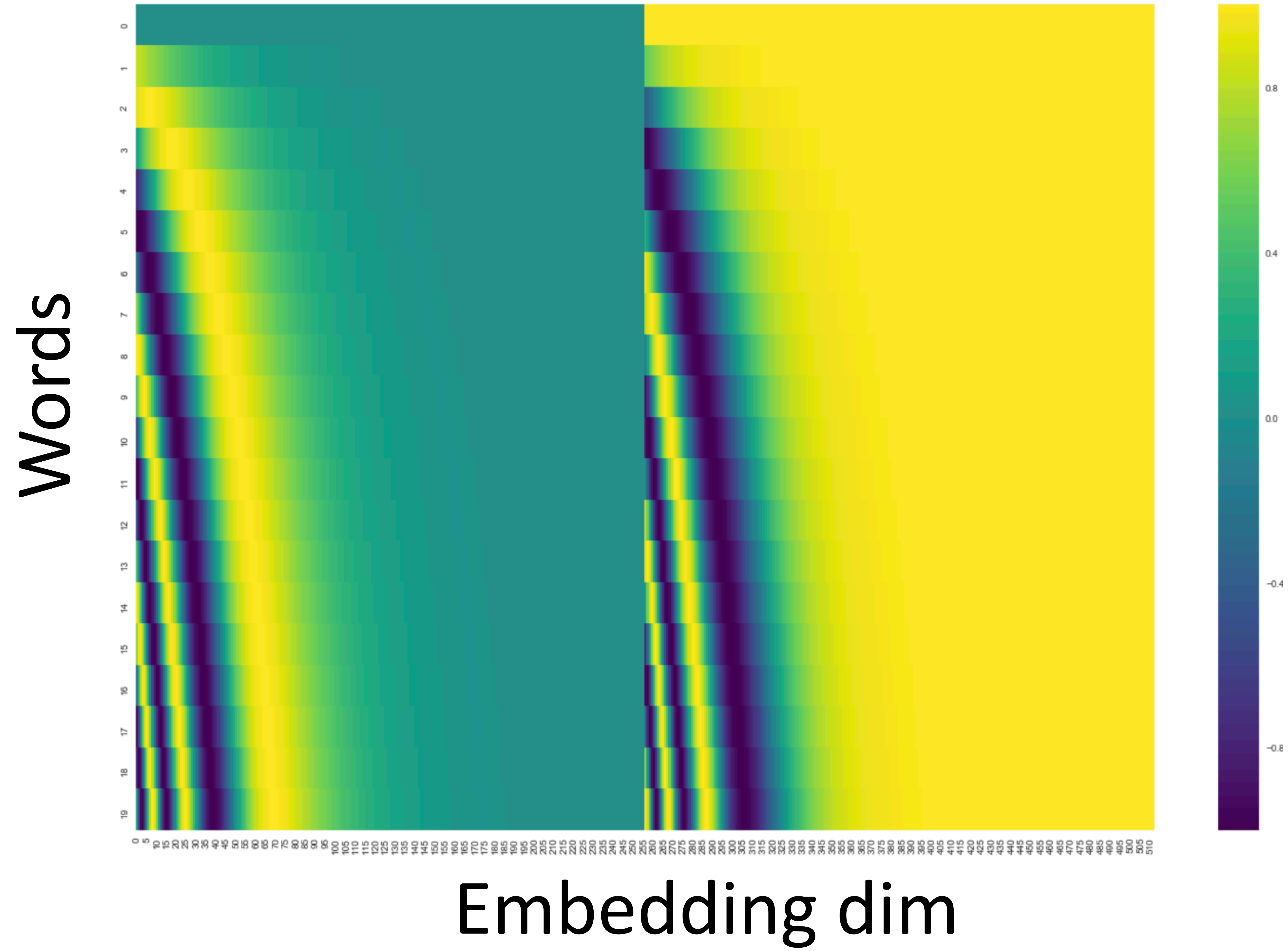


- Encode each sequence position as an integer, add it to the word embedding vector

Recap: Positional Encodings

Alammar, *The Illustrated Transformer*

- Alternative from Vaswani et al.: sines/cosines of different frequencies (closer words get higher dot products by default)



Transformers

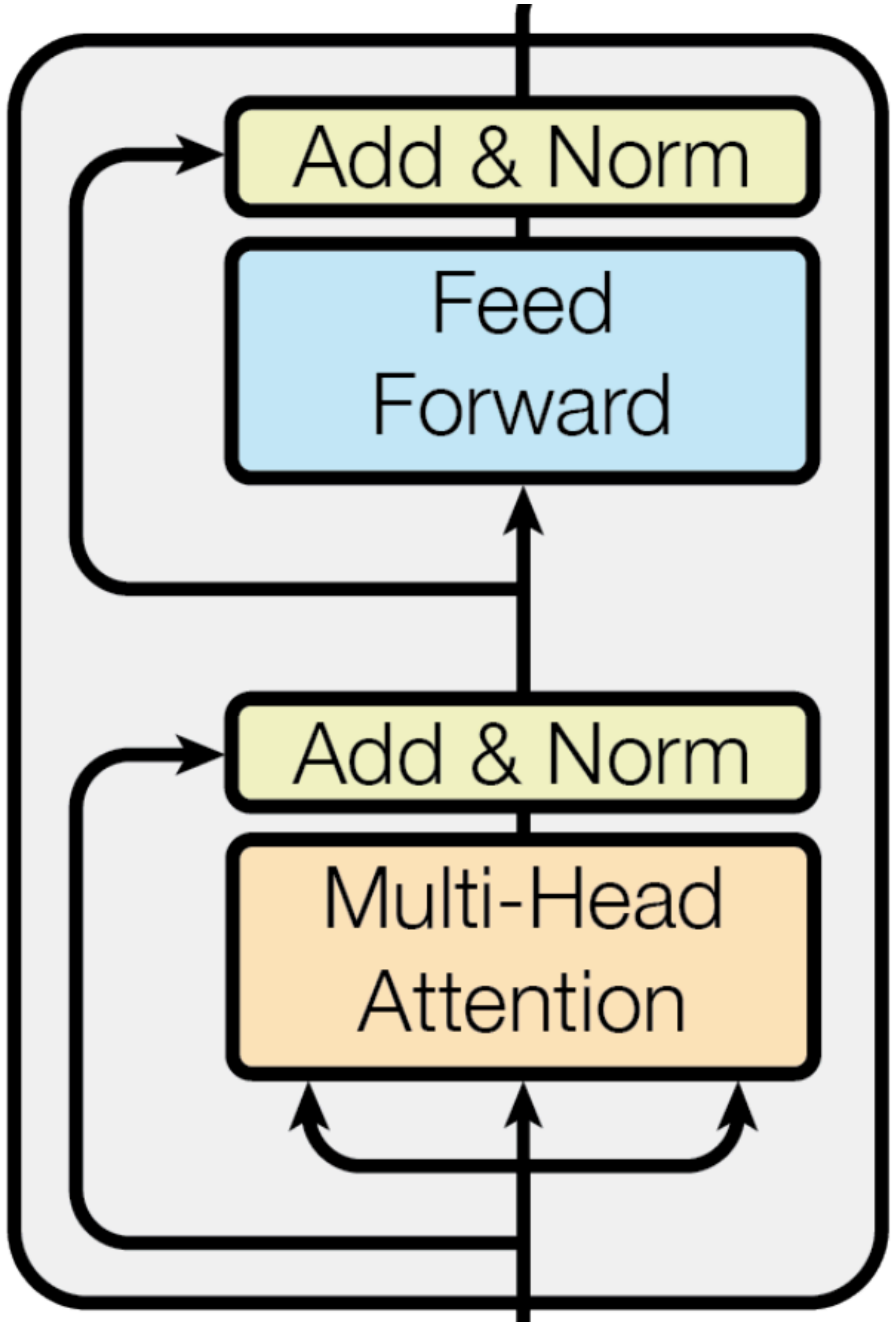
Architecture

- Alternate multi-head self-attention with feedforward layers that **operate over each word individually**

$$\mathrm{FFN}(x) = \max(0, xW_1 + b_1)W_2 + b_2$$

  - These feedforward layers are where most of the parameters are

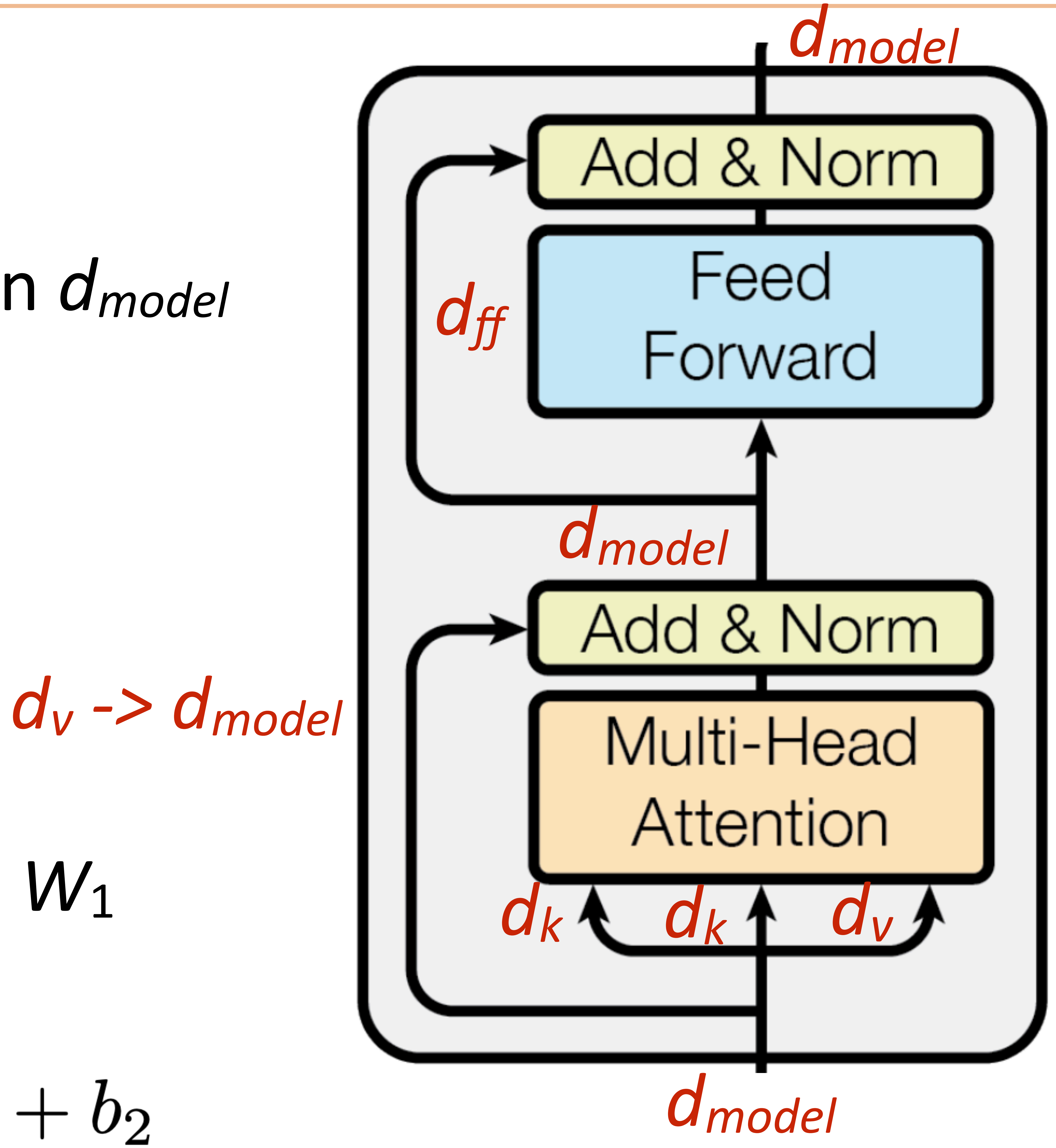
- Residual connections in the model: input of a layer is added to its output
- Layer normalization: controls the scale of different layers in very deep networks (not needed in the assignment)



Dimensions

- Vectors: d_{model}
- Queries/keys: d_k, always smaller than d_{model}
- Values: separate dimension d_v, output is multiplied by W^O which is $d_v \times d_{model}$ so we can get back to d_{model} before the residual
- FFN can explode the dimension with W_1 and collapse it back with W_2

$$\mathrm{FFN}(x) = \max(0, xW_1 + b_1)W_2 + b_2$$



Vaswani et al. (2017)

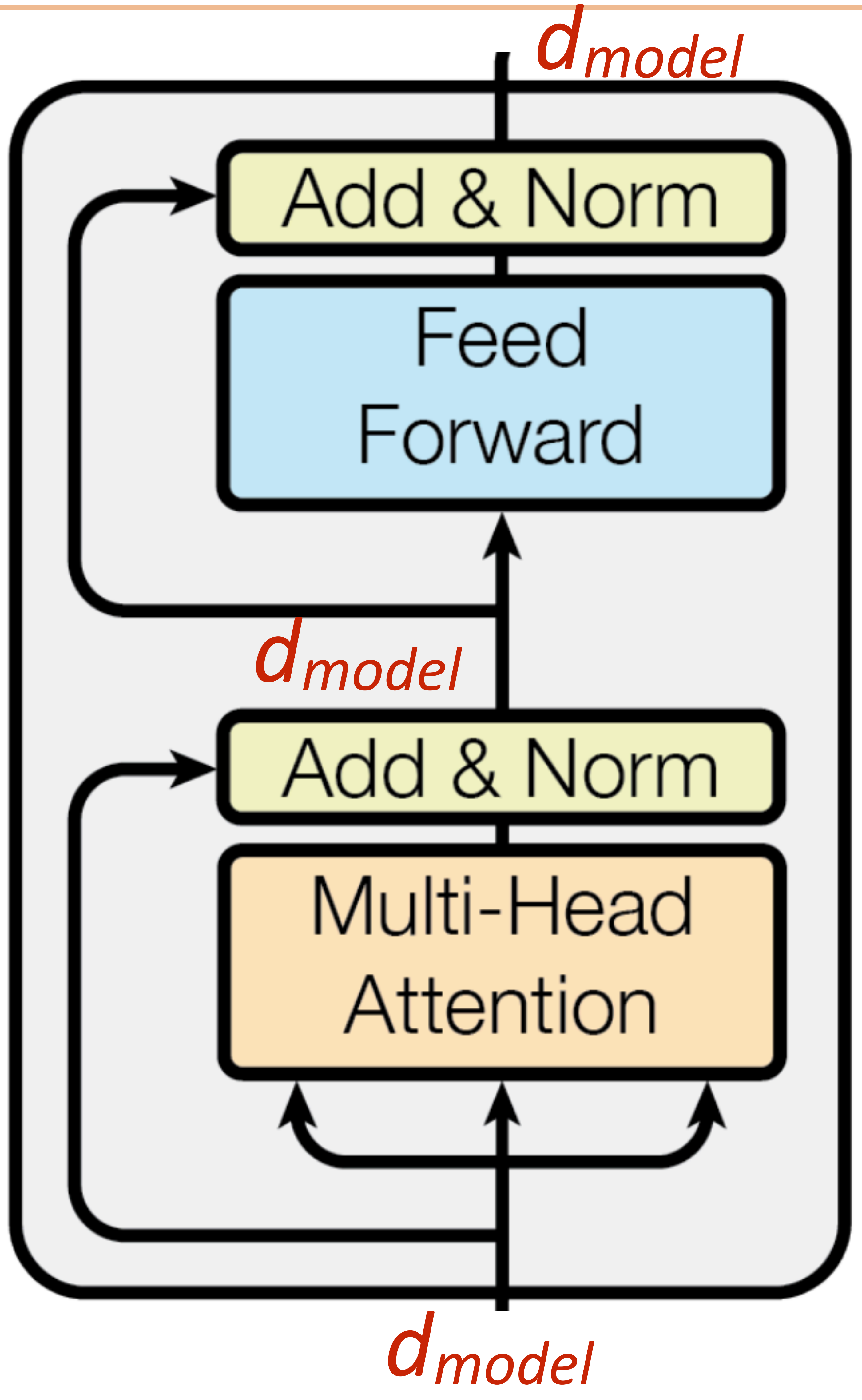
Transformer Architecture

	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



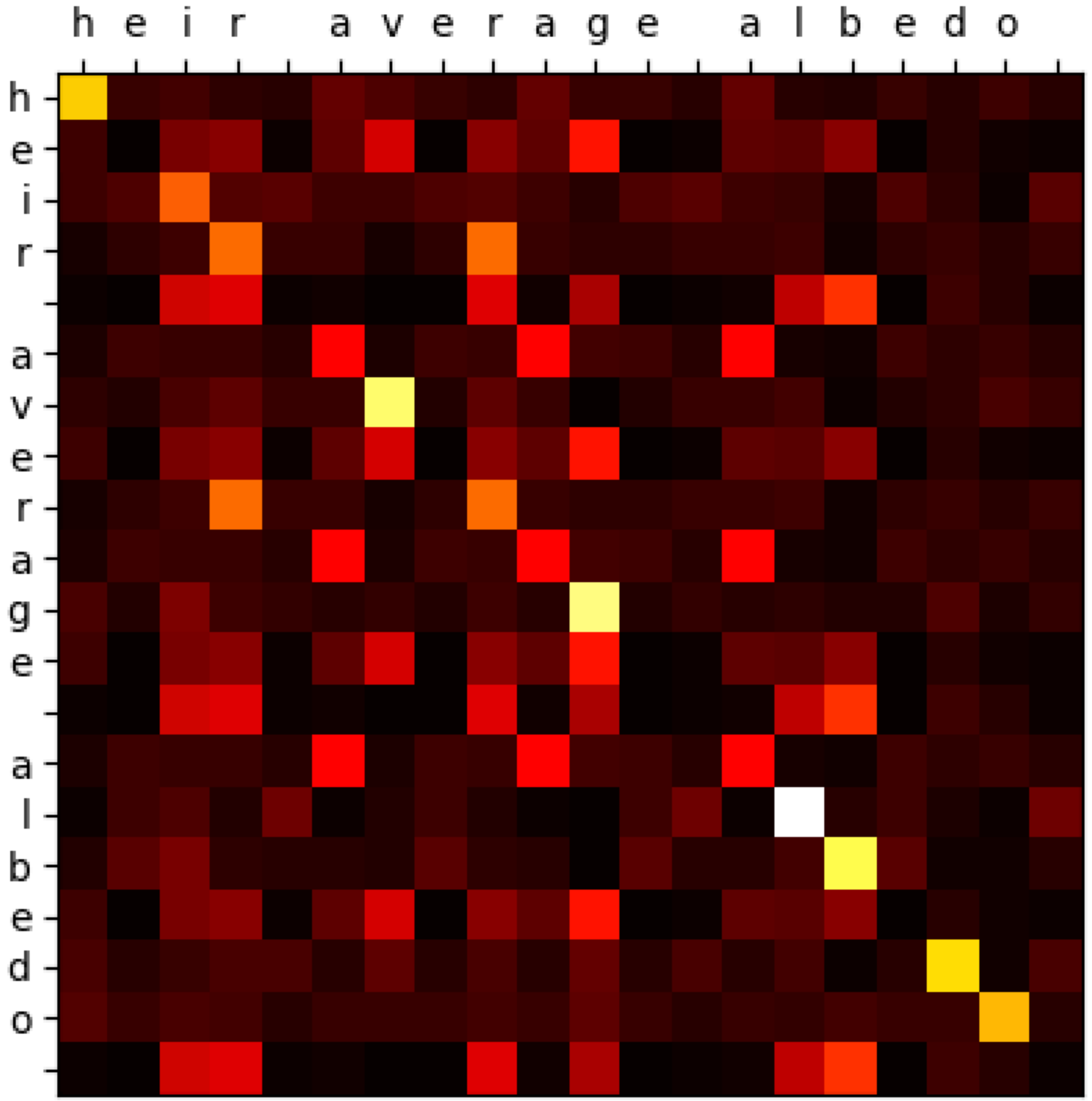
Transformer Architecture

1	description	FLOPs / update	% FLOPS MHA	% FLOPS FFN	% FLOPS attn	% FLOPS logit
8	OPT setups					
9	760M	4.3E+15	35%	44%	14.8%	5.8%
10	1.3B	1.3E+16	32%	51%	12.7%	5.0%
11	2.7B	2.5E+16	29%	56%	11.2%	3.3%
12	6.7B	1.1E+17	24%	65%	8.1%	2.4%
13	13B	4.1E+17	22%	69%	6.9%	1.6%
14	30B	9.0E+17	20%	74%	5.3%	1.0%
15	66B	9.5E+17	18%	77%	4.3%	0.6%
16	175B	2.4E+18	17%	80%	3.3%	0.3%

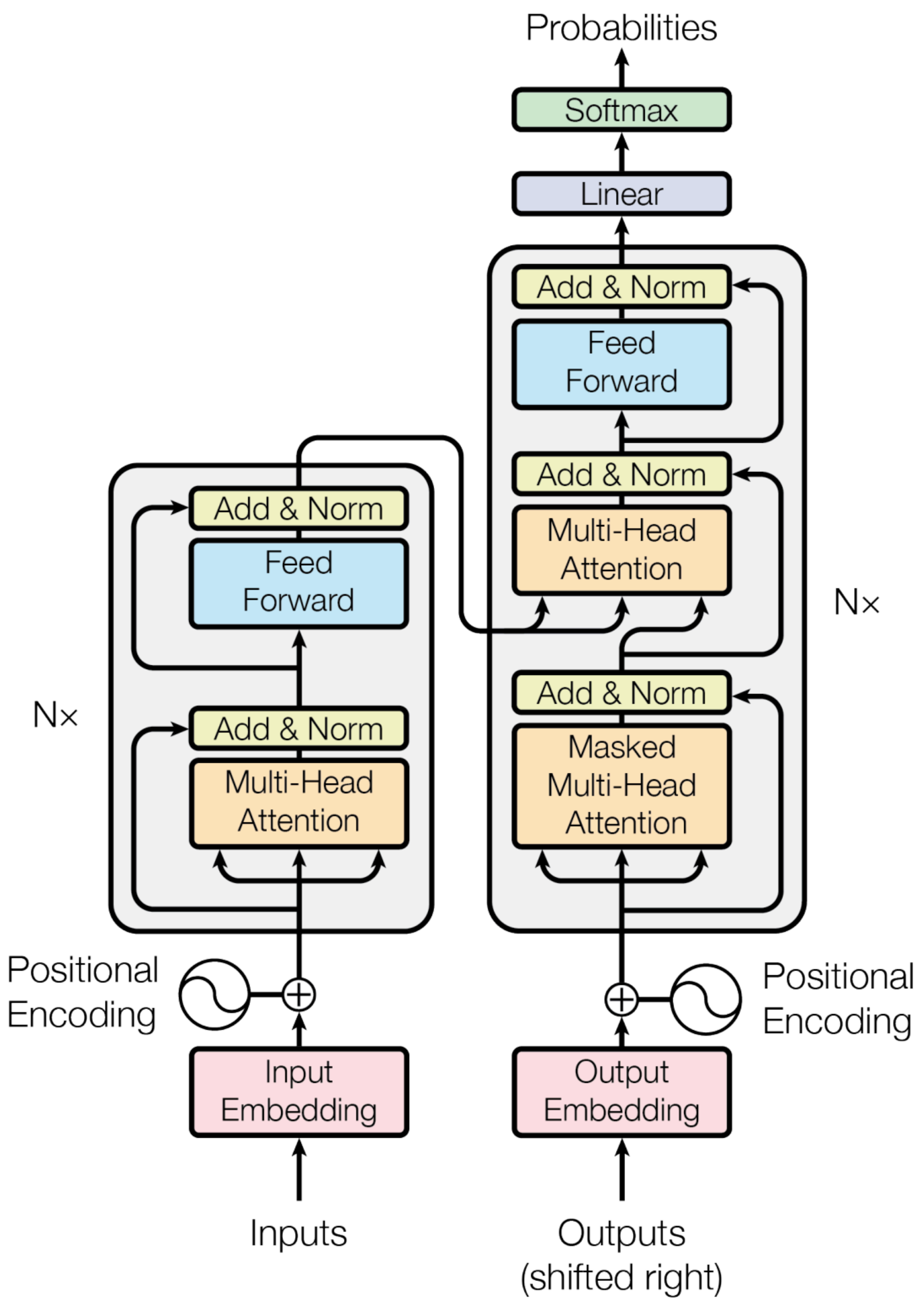
Credit: Stephen Roller on Twitter

Attention Maps

- Example visualization of attention matrix A (from assignment)
- Each row: distribution over what that token attends to. E.g., the first "v" attends very heavily to itself (bright yellow box)
- **On the HW: look to see if the attentions make sense!**



Transformers: Complete Model

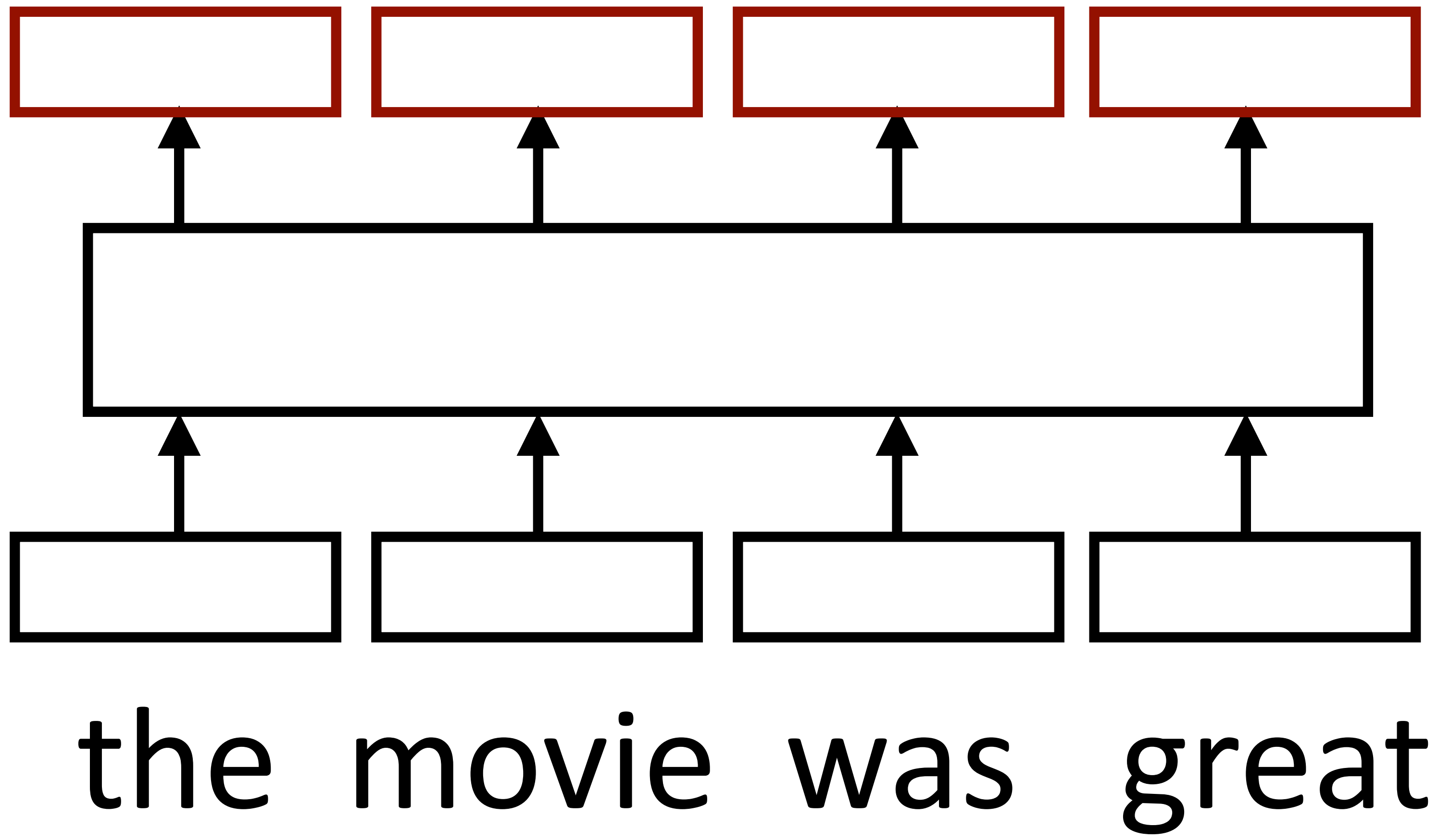


- Original Transformer paper presents an **encoder-decoder** model
- Right now we don't need to think about both of these parts — will return in the context of MT
- Can turn the encoder into a decoder-only model through use of a triangular causal attention mask (only allow attention to previous tokens)

Vaswani et al. (2017)

Using Transformers

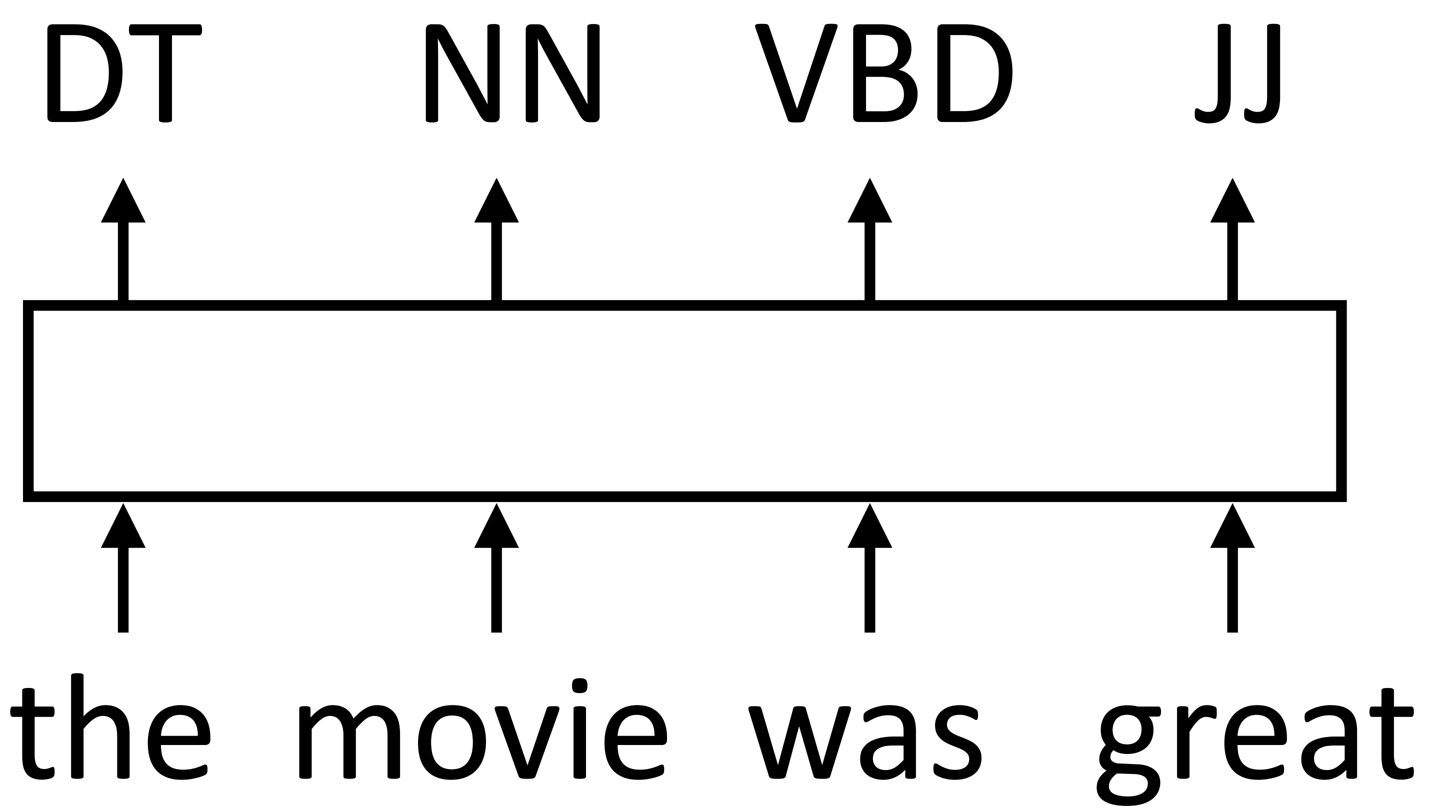
What do Transformers produce?



- Encoding of each word — can pass this to another layer to make a prediction (like predicting the next word for language modeling)
- Like RNNs, Transformers can be viewed as a transformation of a sequence of vectors into a sequence of context-dependent vectors

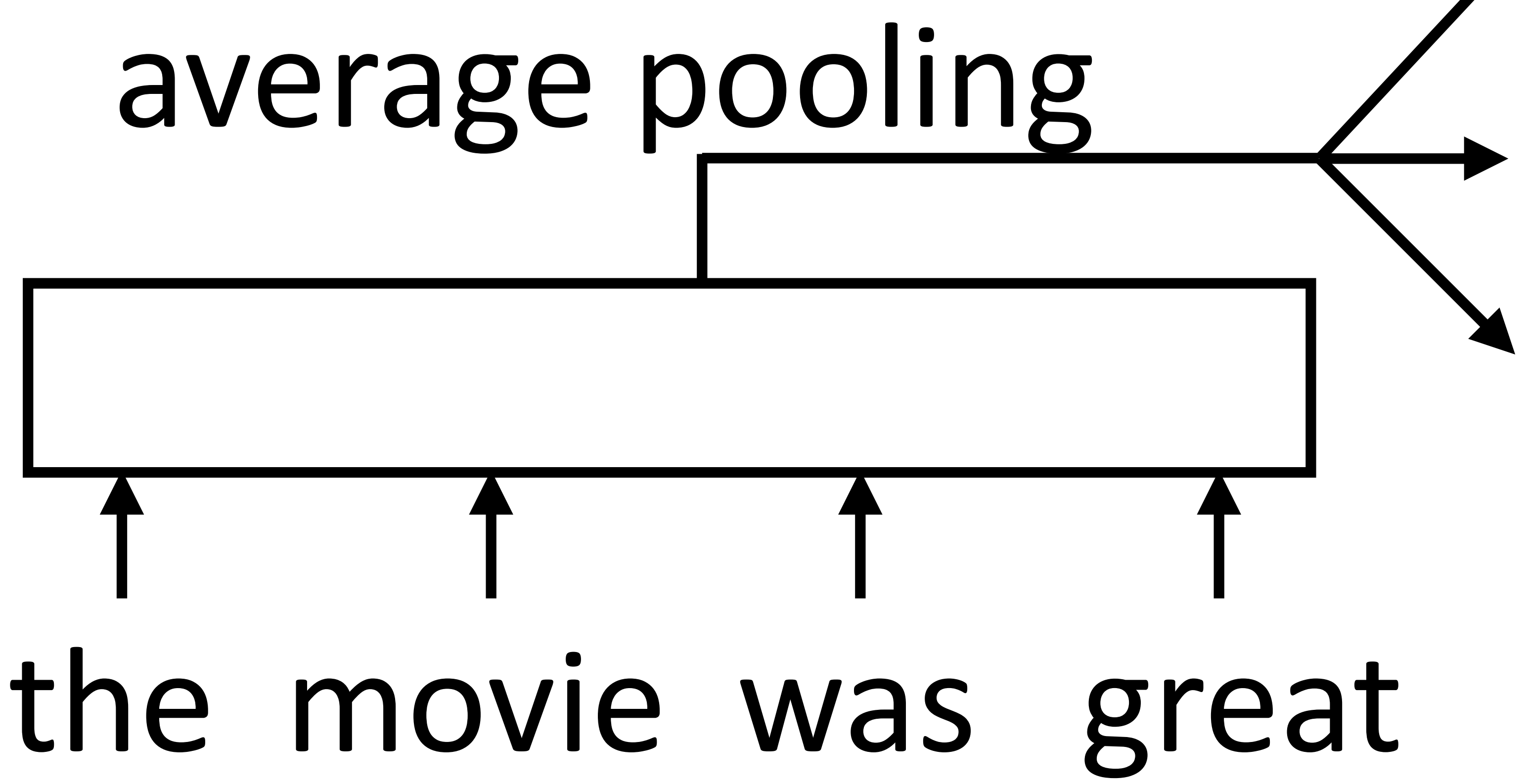
Transformer Uses

- Transducer: make some prediction for each element in a sequence



output **y** = score for each tag, then softmax

- Classifier: encode a sequence into a fixed-sized vector and classify that

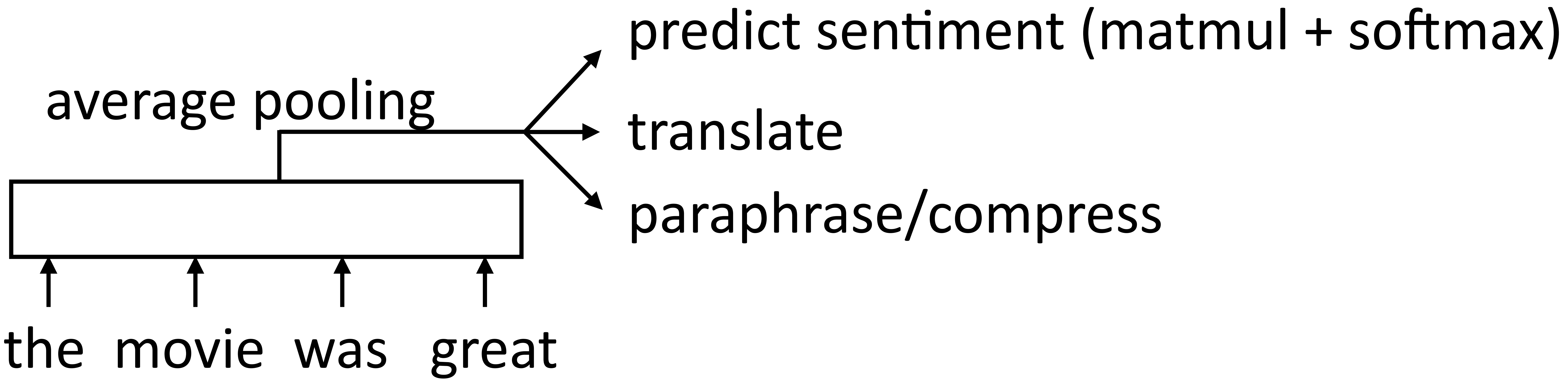


predict sentiment (matmul + softmax)

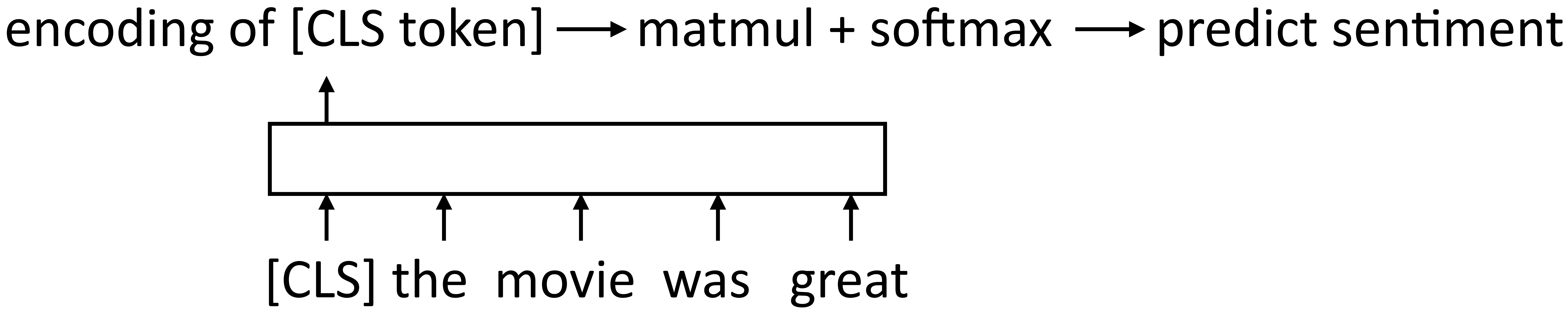
translate

paraphrase/compress

Transformer Uses

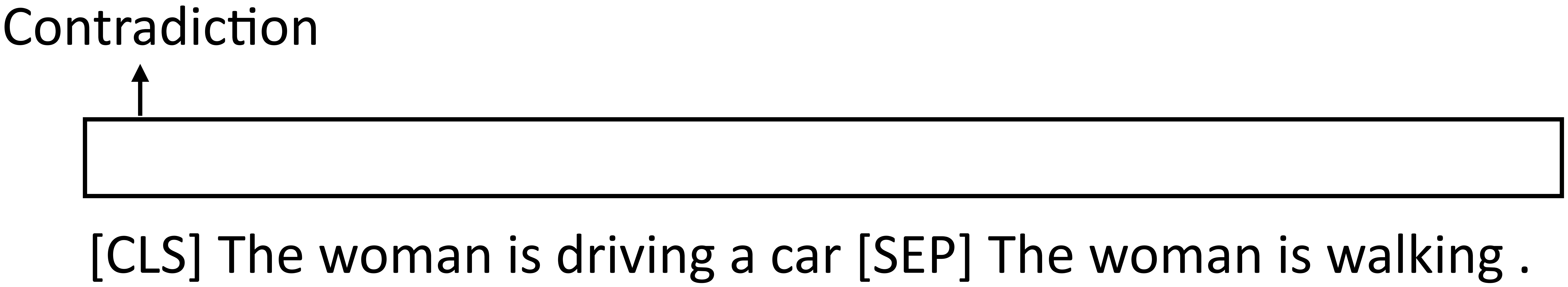


- Alternative: use a placeholder [CLS] token at the start of the sequence. Because [CLS] attends to everything with self-attention, it can do the pooling for you!



Transformer Uses

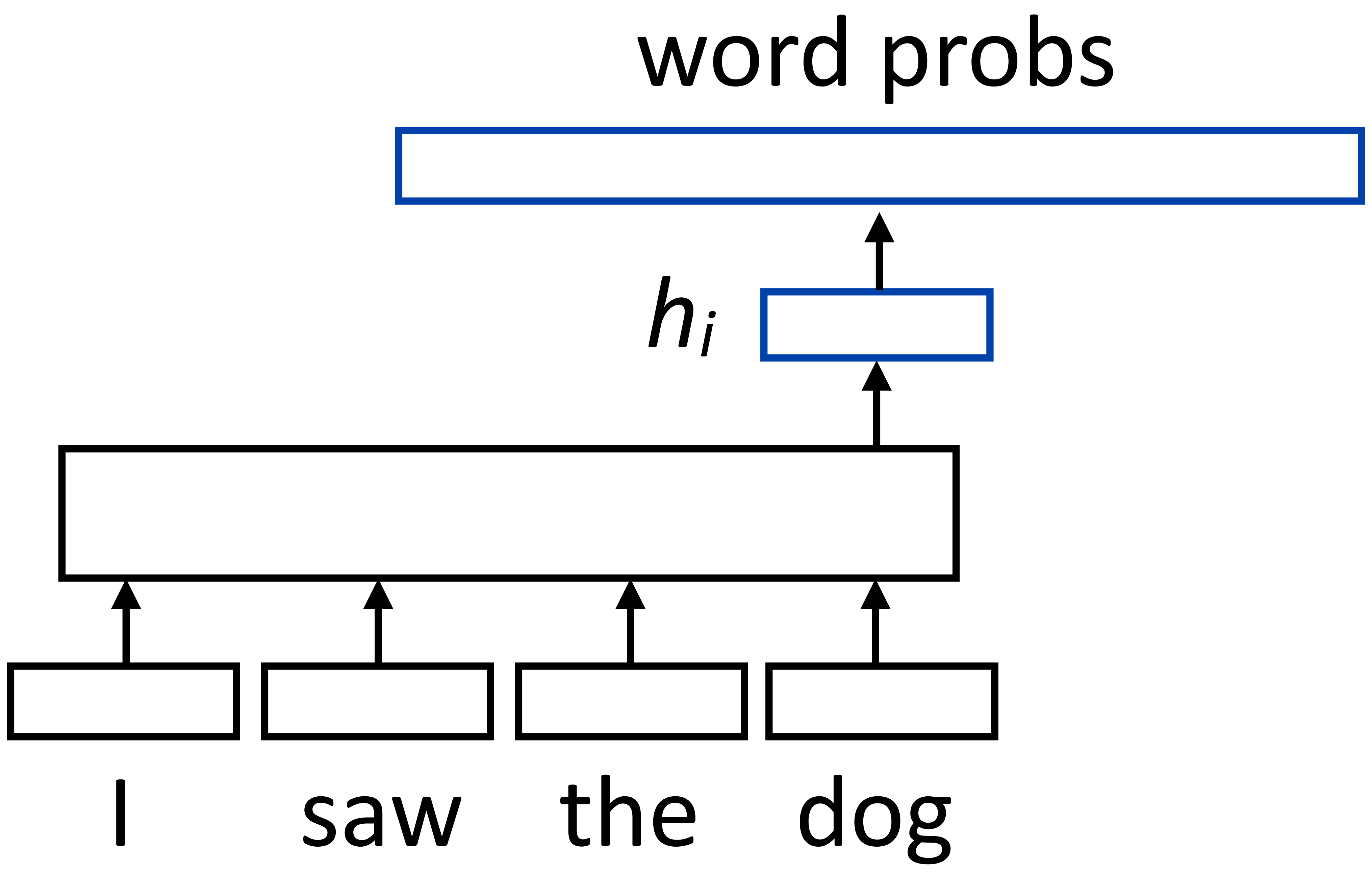
- Sentence **pair** classifier: feed in two sentences and classify something about their relationship



- Why might Transformers be particularly good at sentence **pair** tasks compared to something like a DAN?

Transformer Language Modeling

Transformer Language Modeling



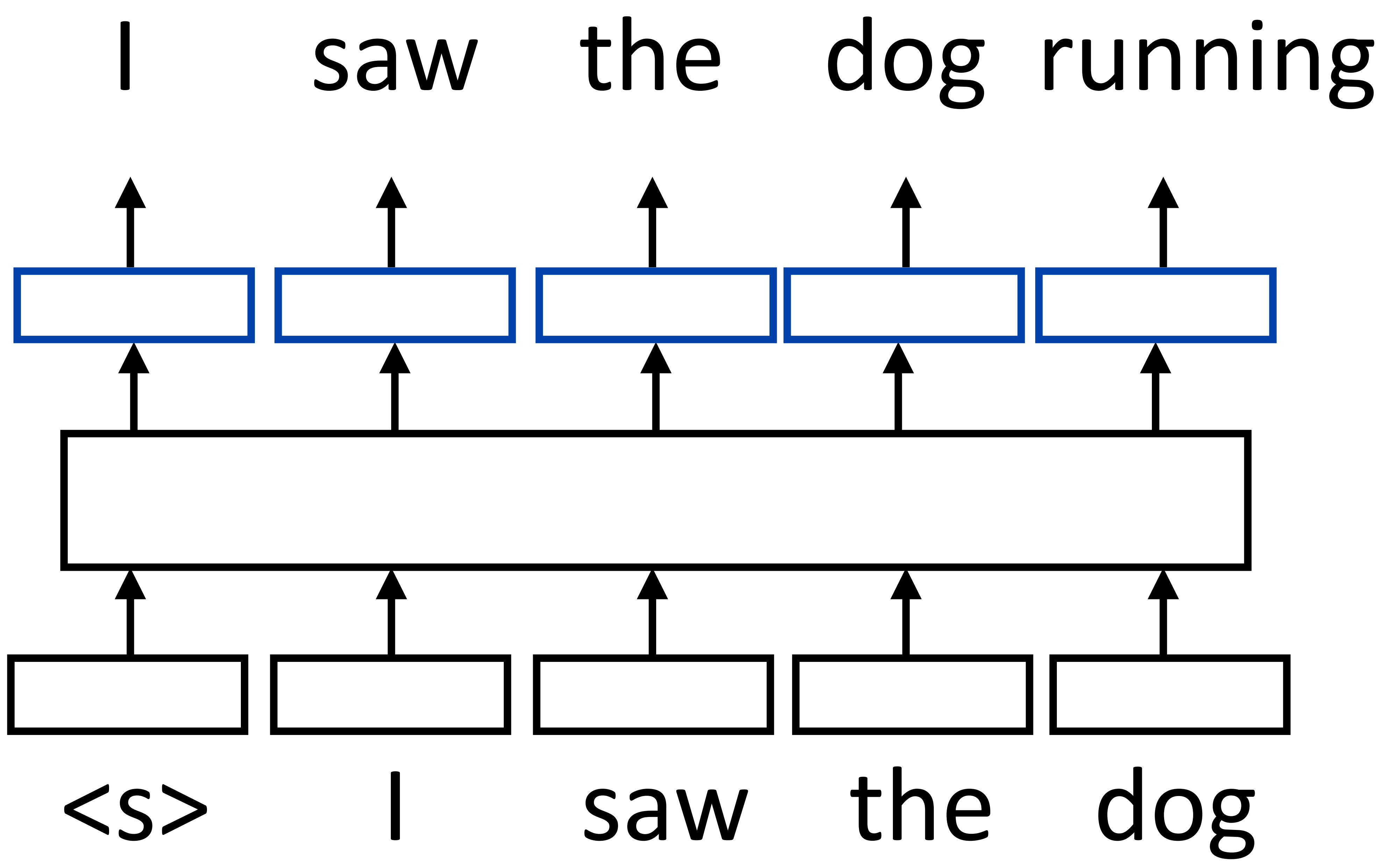
$$P(w|\text{context}) = \frac{\exp(\mathbf{w} \cdot \mathbf{h_i})}{\sum_{w'} \exp(\mathbf{w'} \cdot \mathbf{h_i})}$$

equivalent to

$$P(w|\text{context}) = \text{softmax}(W\mathbf{h}_i)$$

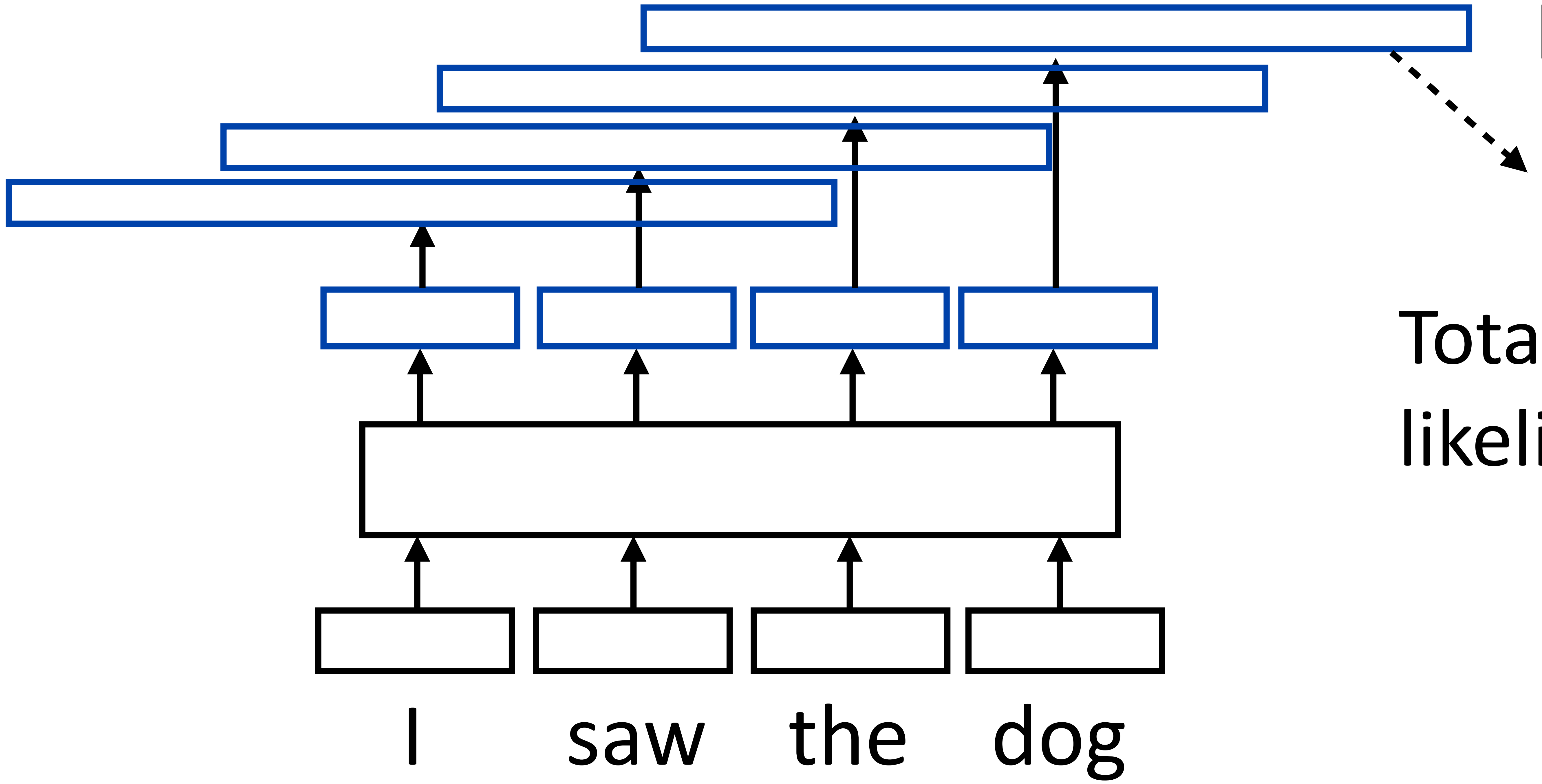
- *W* is a (vocab size) x (hidden size) matrix; linear layer in PyTorch (rows are word embeddings)

Training Transformer LMs



- Input is a sequence of words, output is those words shifted by one,
- Allows us to train on predictions across several timesteps simultaneously (similar to batching but this is NOT what we refer to as batching)

Training Transformer LMs



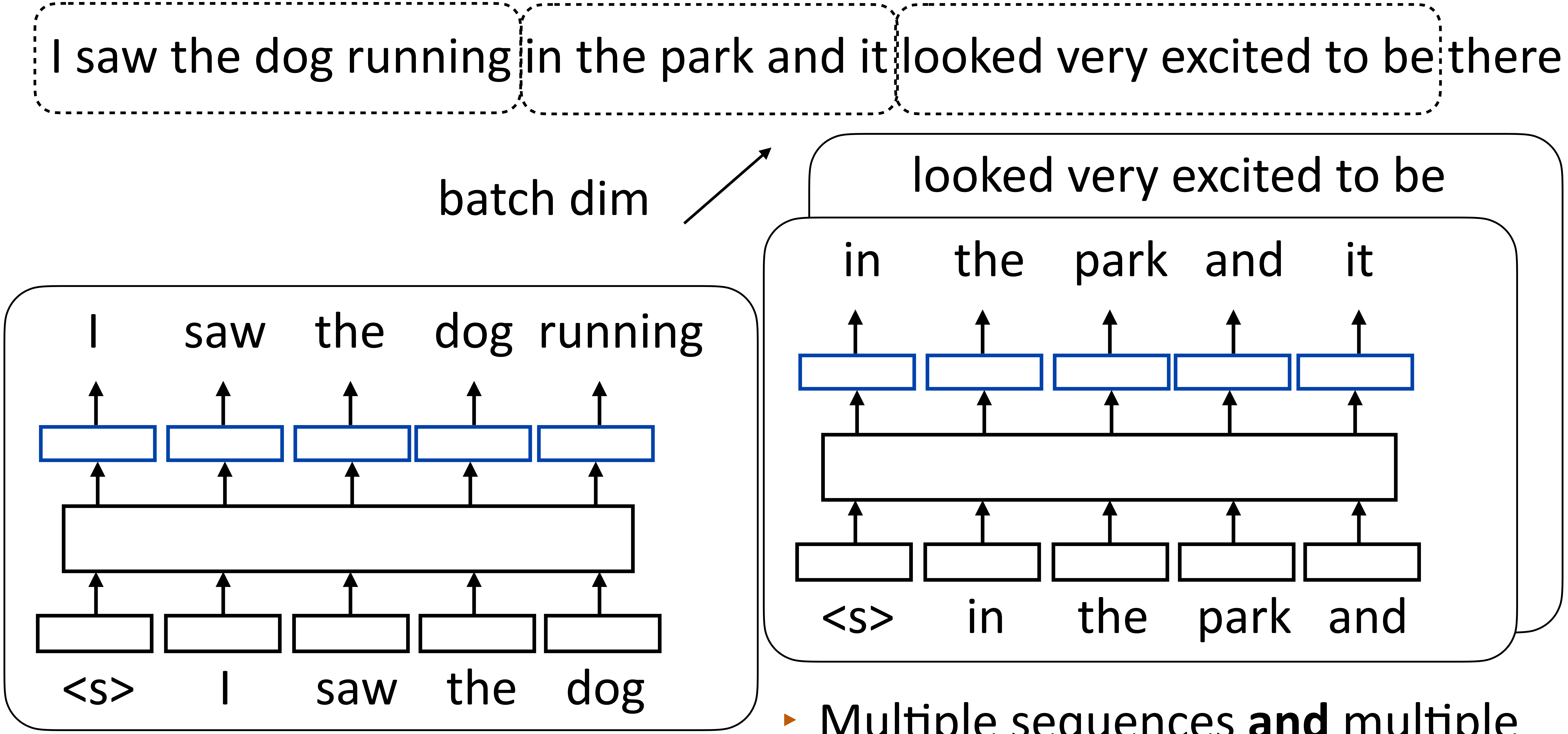
Total loss = sum of negative log likelihoods at each position

```
loss_fcn = nn.NLLLoss()
loss += loss_fcn(log_probs, ex.output_tensor)
```

[seq len, num output classes]   [seq len]

- Batching is a little tricky with NLLLoss: need to collase [batch, seq len, num classes] to [batch * seq len, num classes]. You do not need to batch

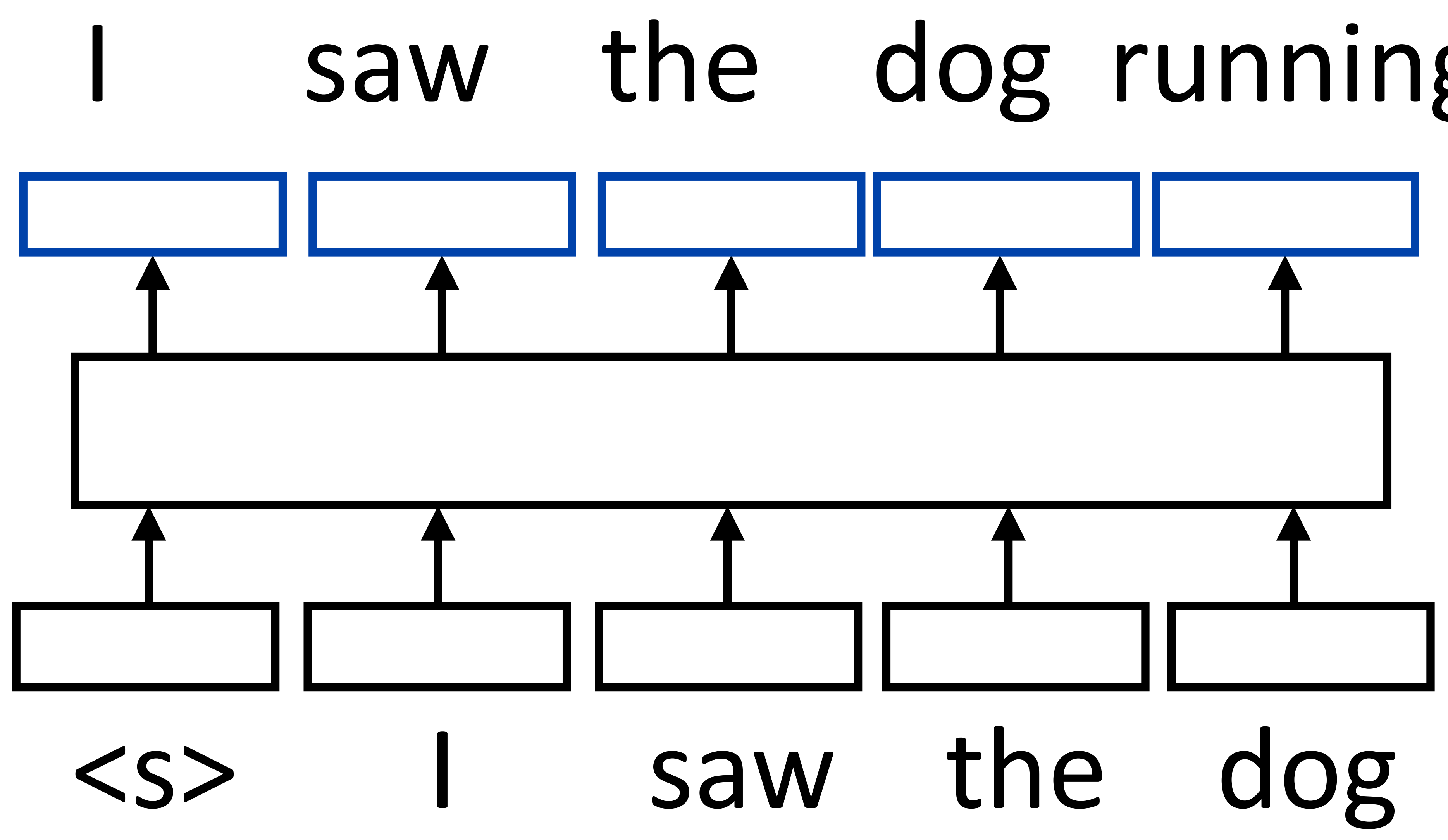
Batched LM Training



- Multiple sequences **and** multiple timesteps per sequence

A Small Problem with Transformer LMs

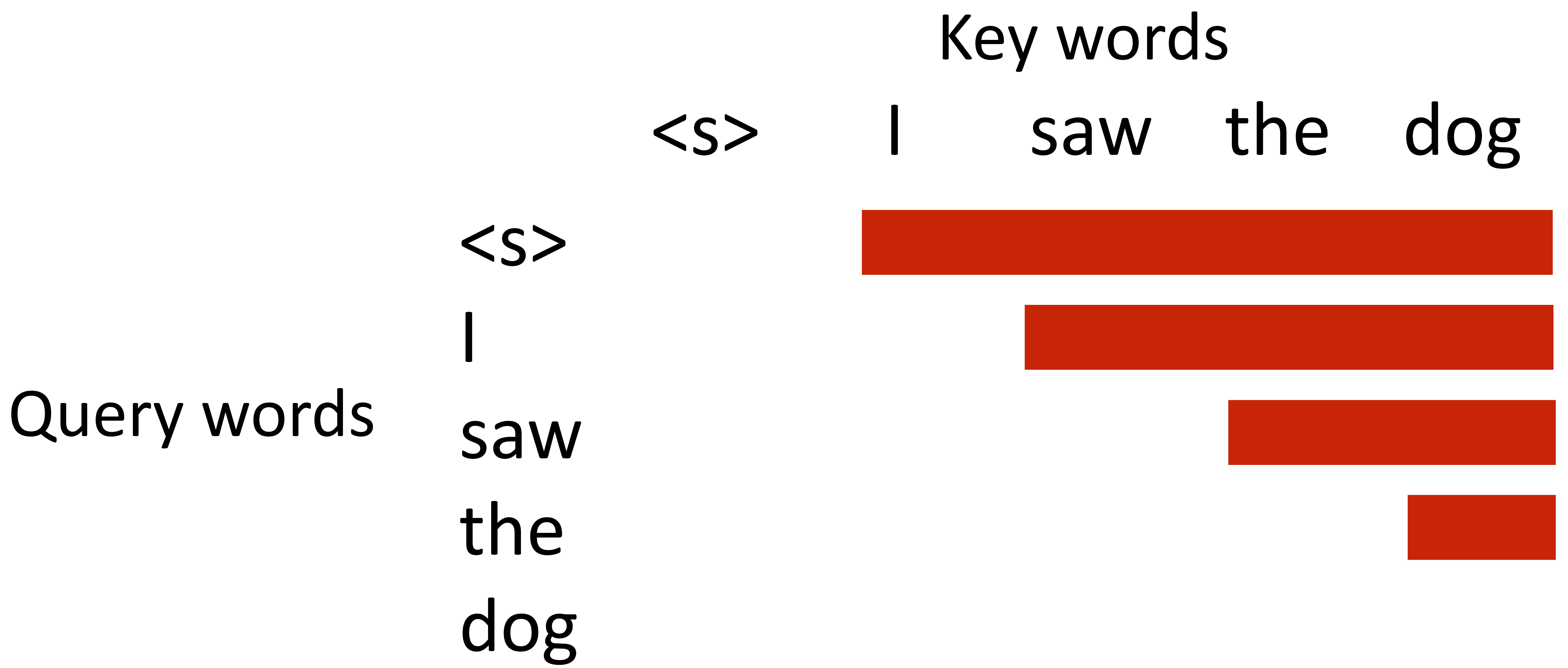
- This Transformer LM as we've described it will *easily* achieve perfect accuracy. Why?



- With standard self-attention: "I" attends to "saw" and the model is "cheating". How do we ensure that this doesn't happen?

Attention Masking

- What do we want to prohibit?



- We want to mask out everything in red (an upper triangular matrix)

Implementing in PyTorch

- nn.TransformerEncoder can be built out of nn.TransformerEncoderLayers, can accept an input and a mask for language modeling:

```
# Inside the module; need to fill in size parameters
layers = nn.TransformerEncoderLayer([...])
transformer_encoder = nn.TransformerEncoder(encoder_layers, num_layers=[...])
[. . .]
# Inside forward(): puts negative infinities in the red part
mask = torch.triu(torch.ones(len, len) * float('-inf'), diagonal=1)
output = transformer_encoder(input, mask=mask)
```

- **You cannot use these for Part 1, only for Part 2**

LM Evaluation

- Accuracy doesn't make sense — predicting the next word is generally impossible so accuracy values would be very low
- Evaluate LMs on the likelihood of held-out data (averaged to normalize for length)

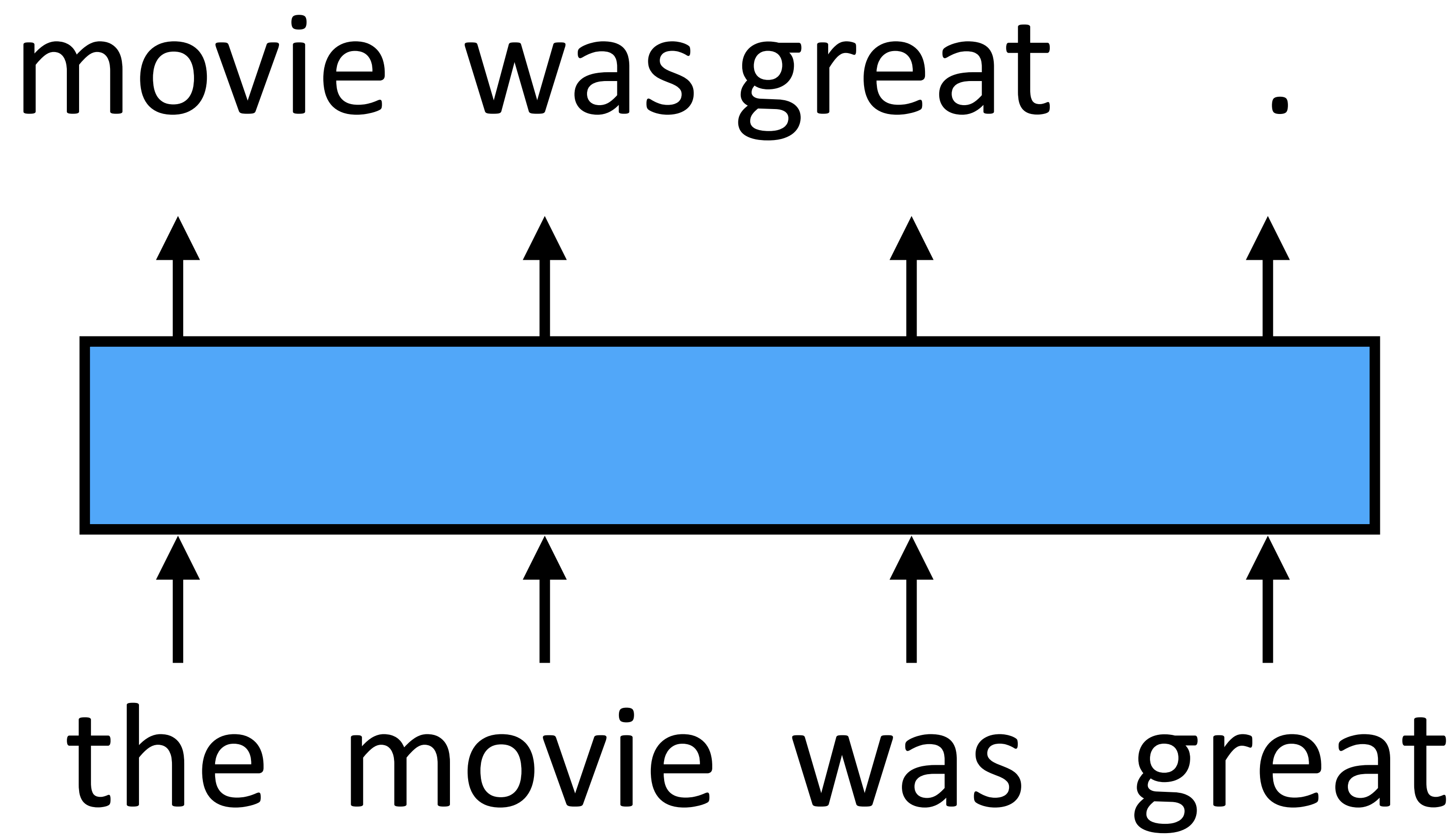
$$\frac{1}{n}\sum_{i=1}^{n}\log P(w_i|w_1,\ldots,w_{i-1})$$

- Perplexity: exp(average negative log likelihood). Lower is better
  - Suppose we have probs 1/4, 1/3, 1/4, 1/3 for 4 predictions
  - Avg NLL (base e) = 1.242   Perplexity = 3.464 <== geometric mean of denominators

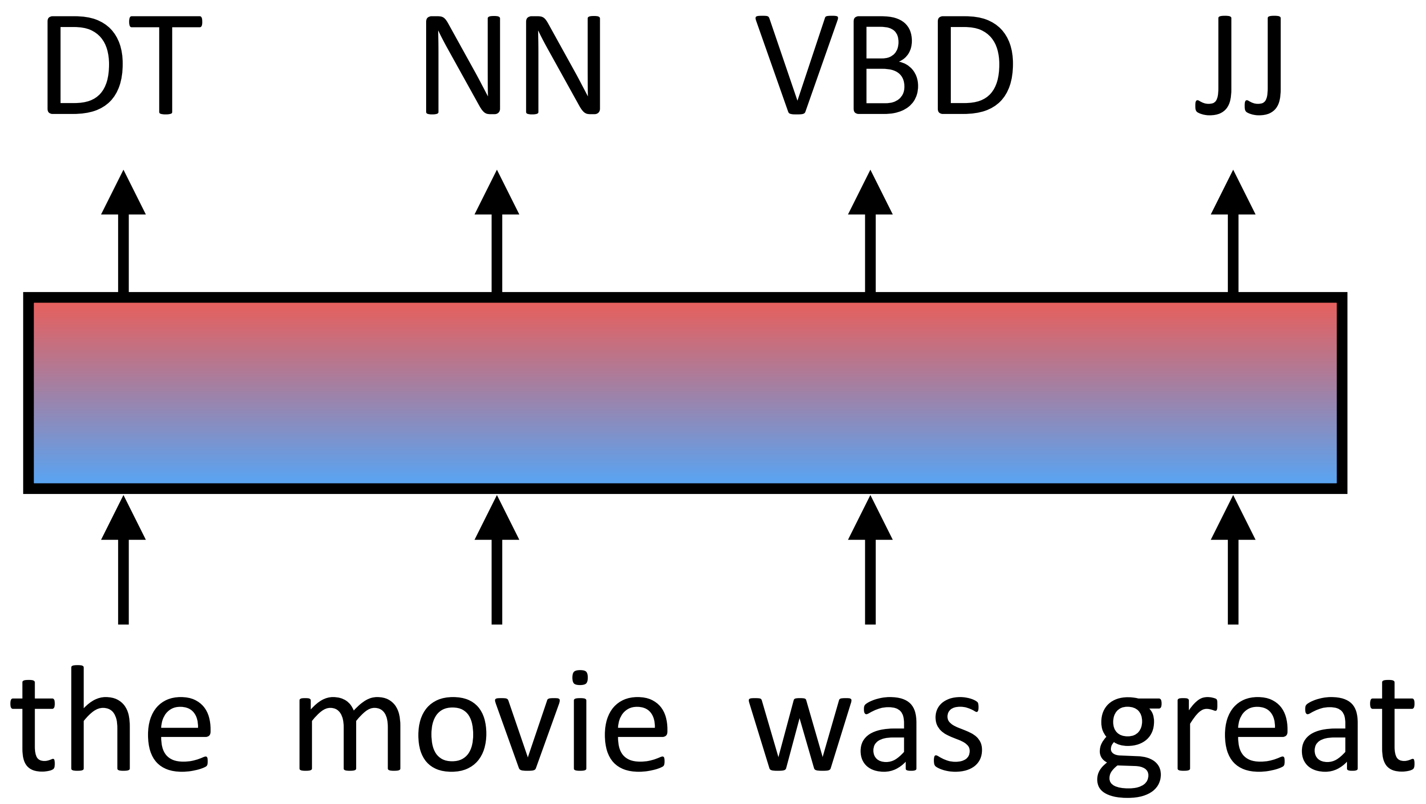
Preview: Pre-training and BERT

- Transformers are usually large and you don't want to train them for each new task

Train on language modeling…



then "fine-tune" that model on your target task with a new classification layer



Transformer Extensions

Scaling Laws

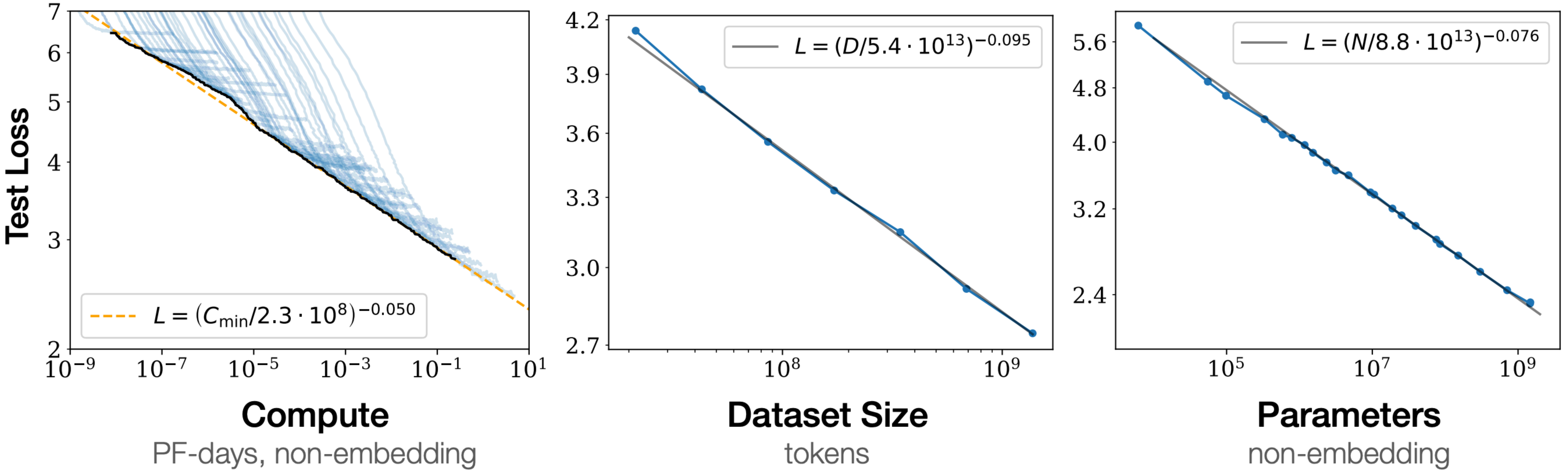


Figure 1 Language modeling performance improves smoothly as we increase the model size, datasetset size, and amount of compute[2] used for training. For optimal performance all three factors must be scaled up in tandem. Empirical performance has a power-law relationship with each individual factor when not bottlenecked by the other two.

- Transformers scale really well!

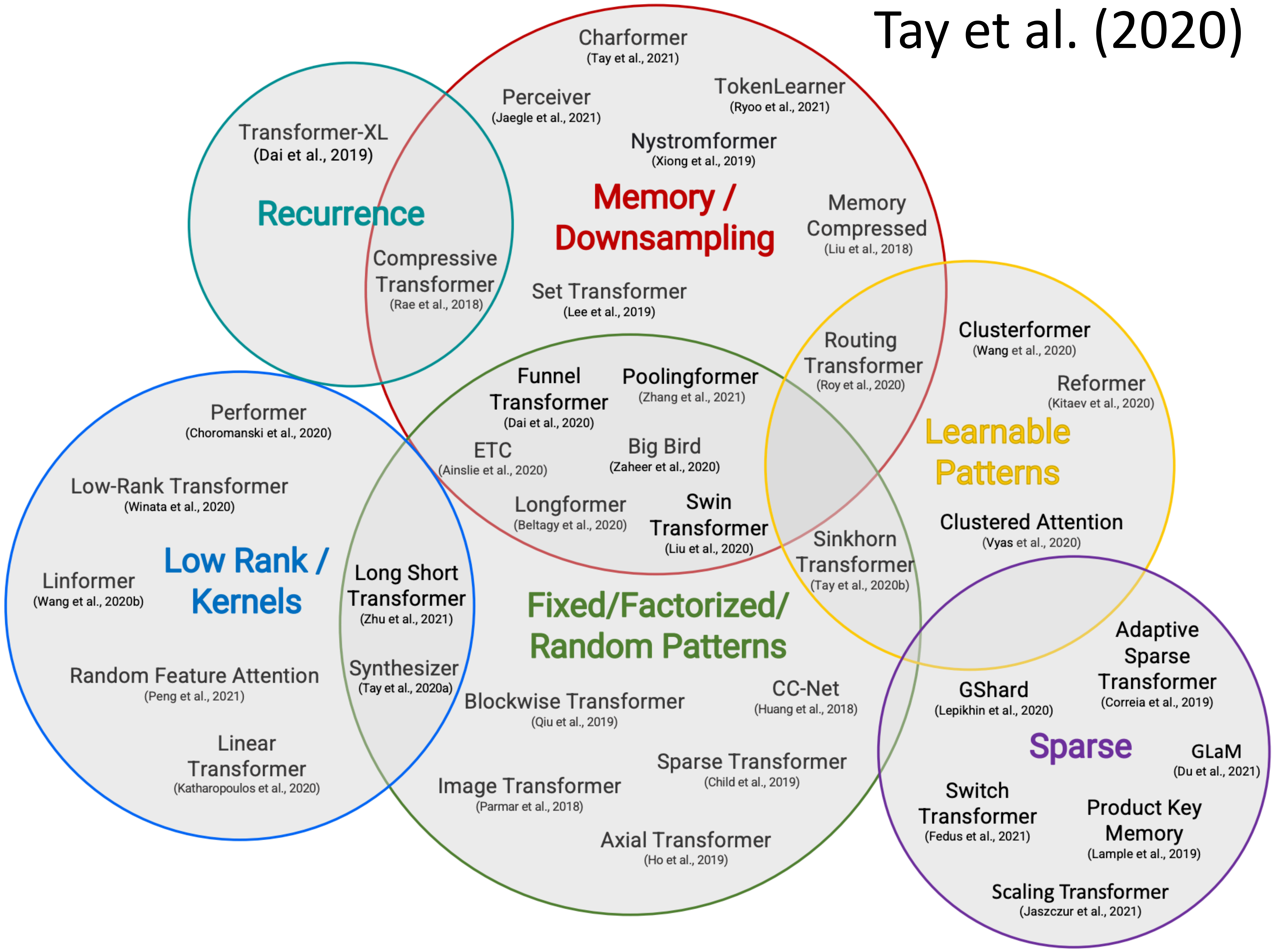
Kaplan et al. (2020)

Transformer Runtime

- Even though most parameters and FLOPs are in feedforward layers, Transformers are still limited by quadratic complexity of self-attention

- Many ways proposed to handle this

Tay et al. (2020)



Performers

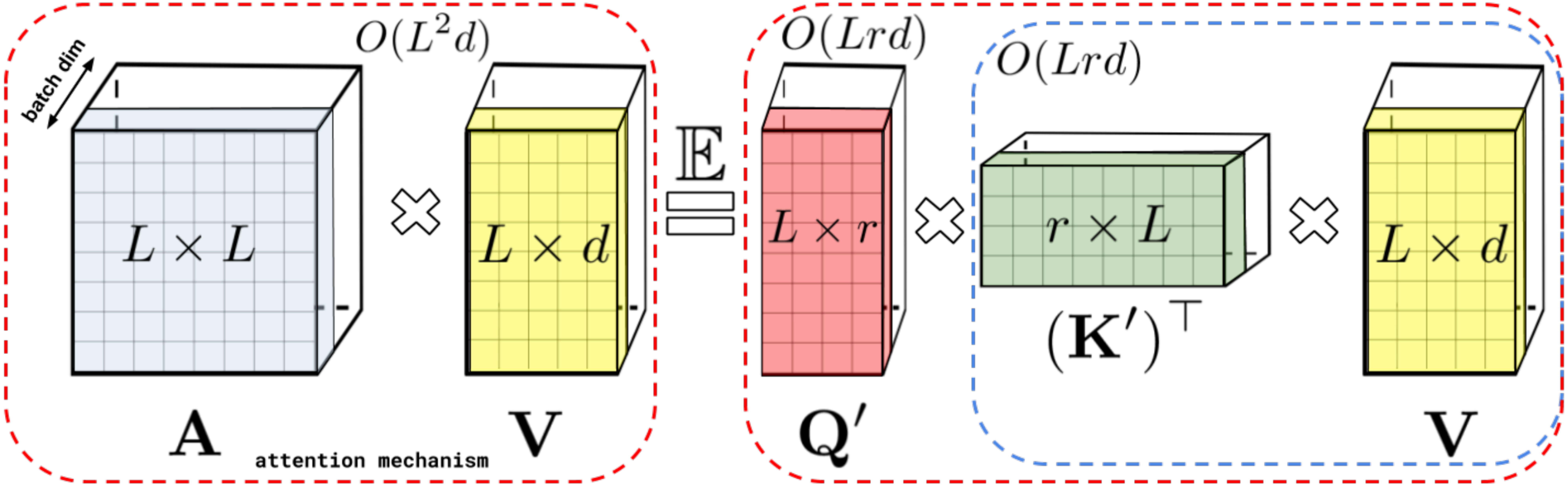


Figure 1: Approximation of the regular attention mechanism **AV** (before $\mathbf{D}^{-1}$-renormalization) via (random) feature maps. Dashed-blocks indicate order of computation with corresponding time complexities attached.

- No more len² term, but we are fundamentally approximating the self-attention mechanism (cannot form **A** and take the softmax)

Choromanski et al. (2020)

Longformer

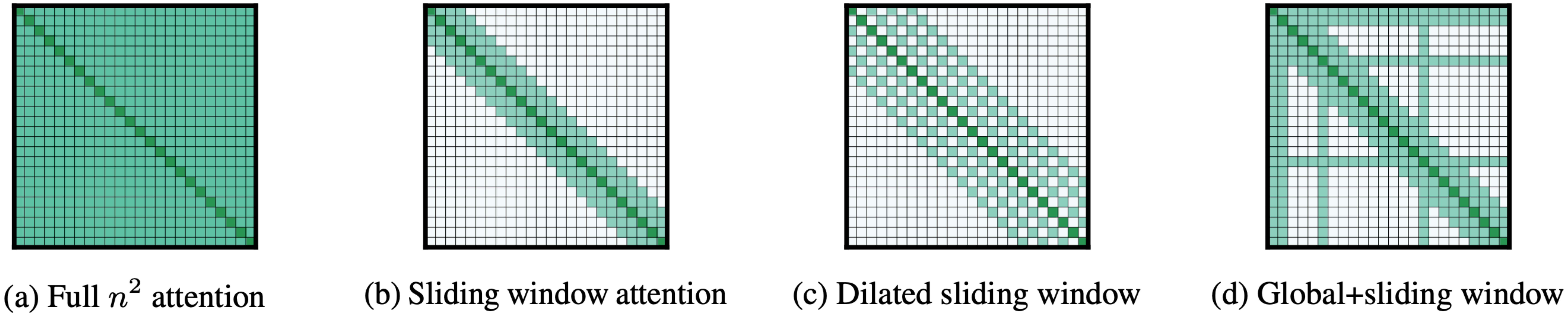
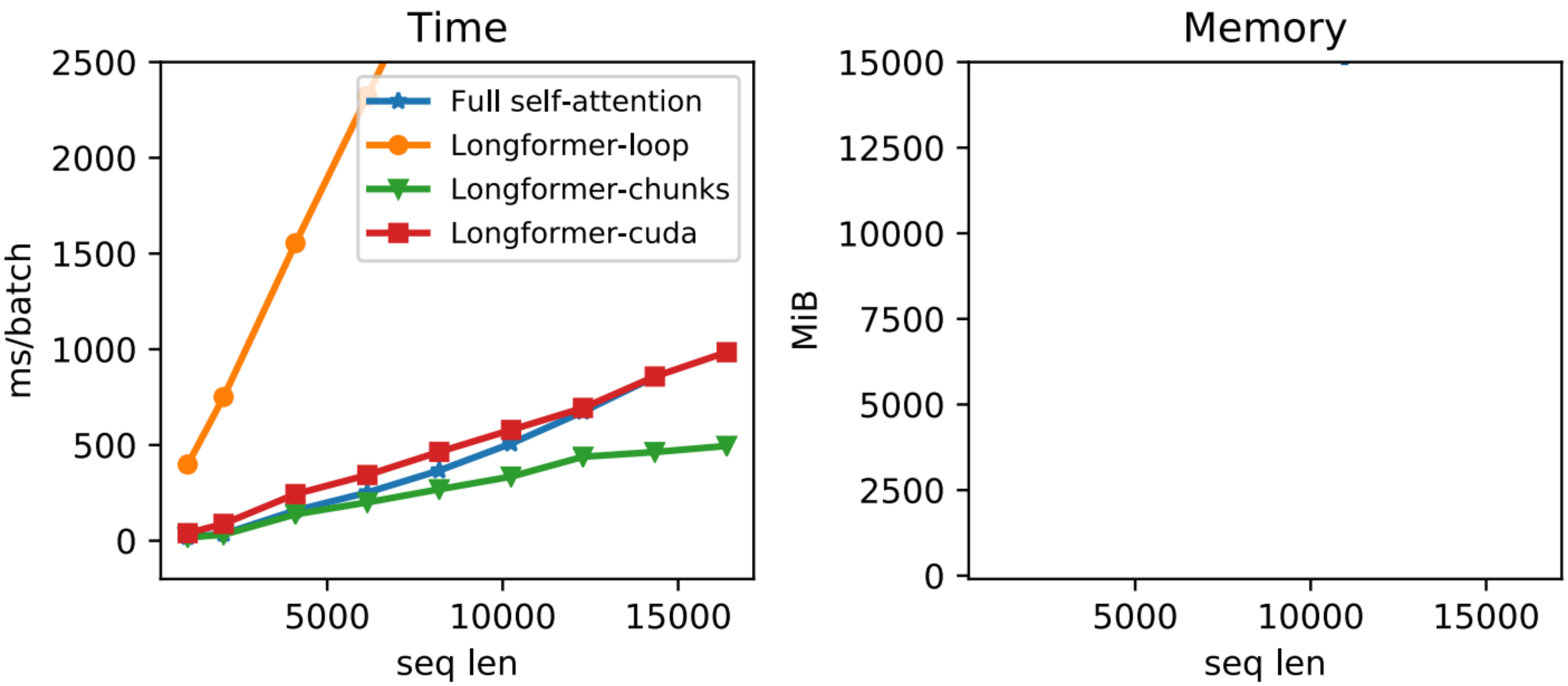


Figure 2: Comparing the full self-attention pattern and the configuration of attention patterns in our Longformer.

- Use several pre-specified self-attention patterns that limit the number of operations while still allowing for attention over a reasonable set of things
- Scales to 4096-length sequences

Beltagy et al. (2021)

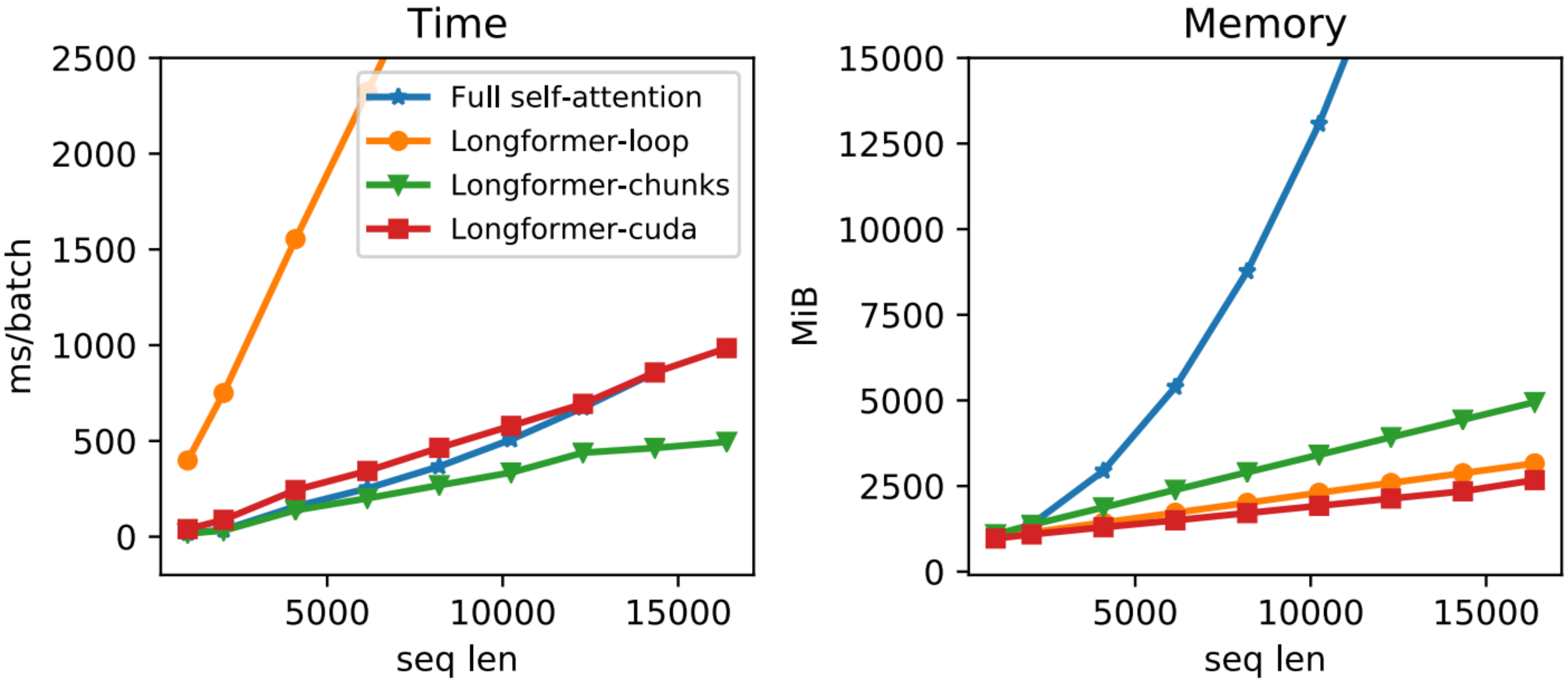
Longformer



- Loop = non-vectorized version

Beltagy et al. (2021)

Longformer



- Loop = non-vectorized version
- Note that memory of full SA blows up but runtime doesn't. Why?

Beltagy et al. (2021)

Frontiers

- Will come back later in the semester when we talk about efficiency in LLMs
- Engineering-based approaches like Flash Attention (which supports the "basic" Transformer) have superseded changing the Transformer model itself

Vision and RL

- DALL-E 1: learns a discrete "codebook" and treats an image as a sequence of visual tokens which can be modeled autoregressively, then decoded back to an image
- Decision Transformer: does reinforcement learning by Transformer-based modeling over a series of actions
- Transformers are now being used all over AI

Ramesh et al. (2021), Chen et al. (2021)

Takeaways

- Transformers are going to be the foundation for the much of the rest of this class and are a ubiquitous architecture nowadays

- Many details to get right, many ways to tweak and extend them, but core idea is the multi-head self attention and their ability to contextualize items in sequences