CSCI 544: Applied Natural Language Processing

Self-attention & Transformer

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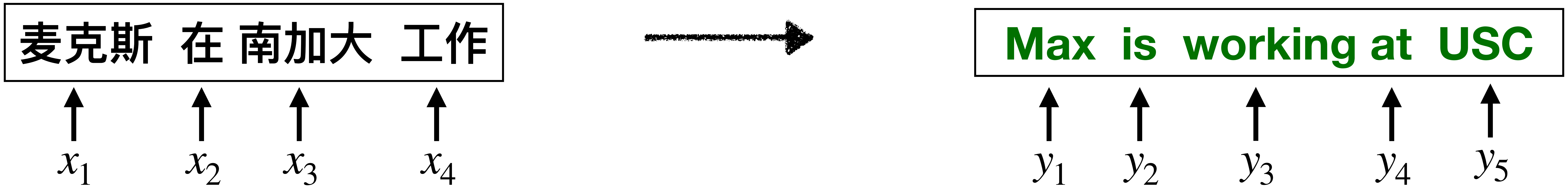
Logistic Points

- **Midterm:**
  - In-person unless approved to participate remotely
  - Remote students: sign up in this Google Sheet https://docs.google.com/spreadsheets/d/1BjmjBs6tceW5RHLj1-nskg9m79Iimq2BzJFVxDYRXcE/edit#gid=0
  - We will email questions to students only in this list
  - Camera and microphone should be open with no virtual background (please find a quite location)
  - Please follow the discussions on the Slack channel, which are sometimes useful

Recap: Seq2seq Generation

- **Sequence-to-Sequence (Seq2seq) Generation**
  - Input: $X = \{x_1, x_2, \ldots, x_L\}, x_i \in \mathcal{X}$
  - Output: $Y = \{y_1, y_2, \ldots, y_T\}, y_i \in \mathcal{Y}$
  - Model: $p_\theta(Y|X)$
- **Difference from Sequence Labeling**
  - The length of Y can be different from the length of X
  - The size of $\mathcal{Y}$ is often much larger



Recap: Autoregressive Seq2seq Generation

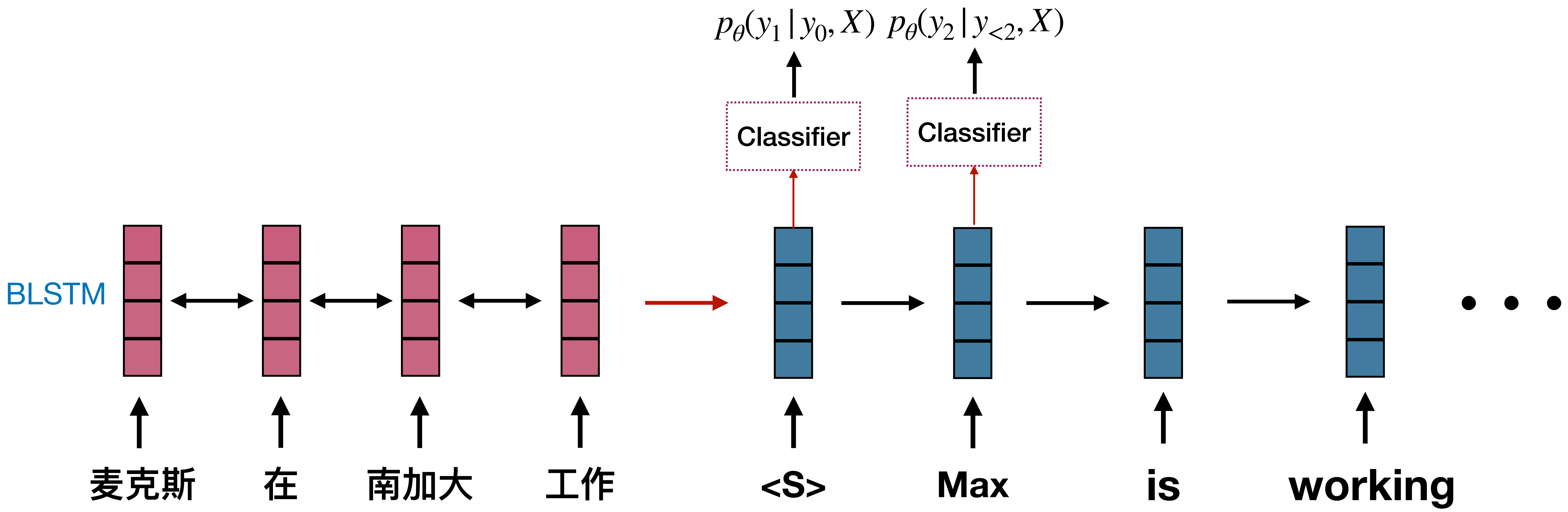
- **Autoregressive Factorization:**

$$p_\theta(Y|X) = \prod_{t=1}^{T} p_\theta(\underbrace{y_t}_{\text{Next Token}} \,|\, \underbrace{y_{\boxed{<t}}}_{\text{history}}, X)$$

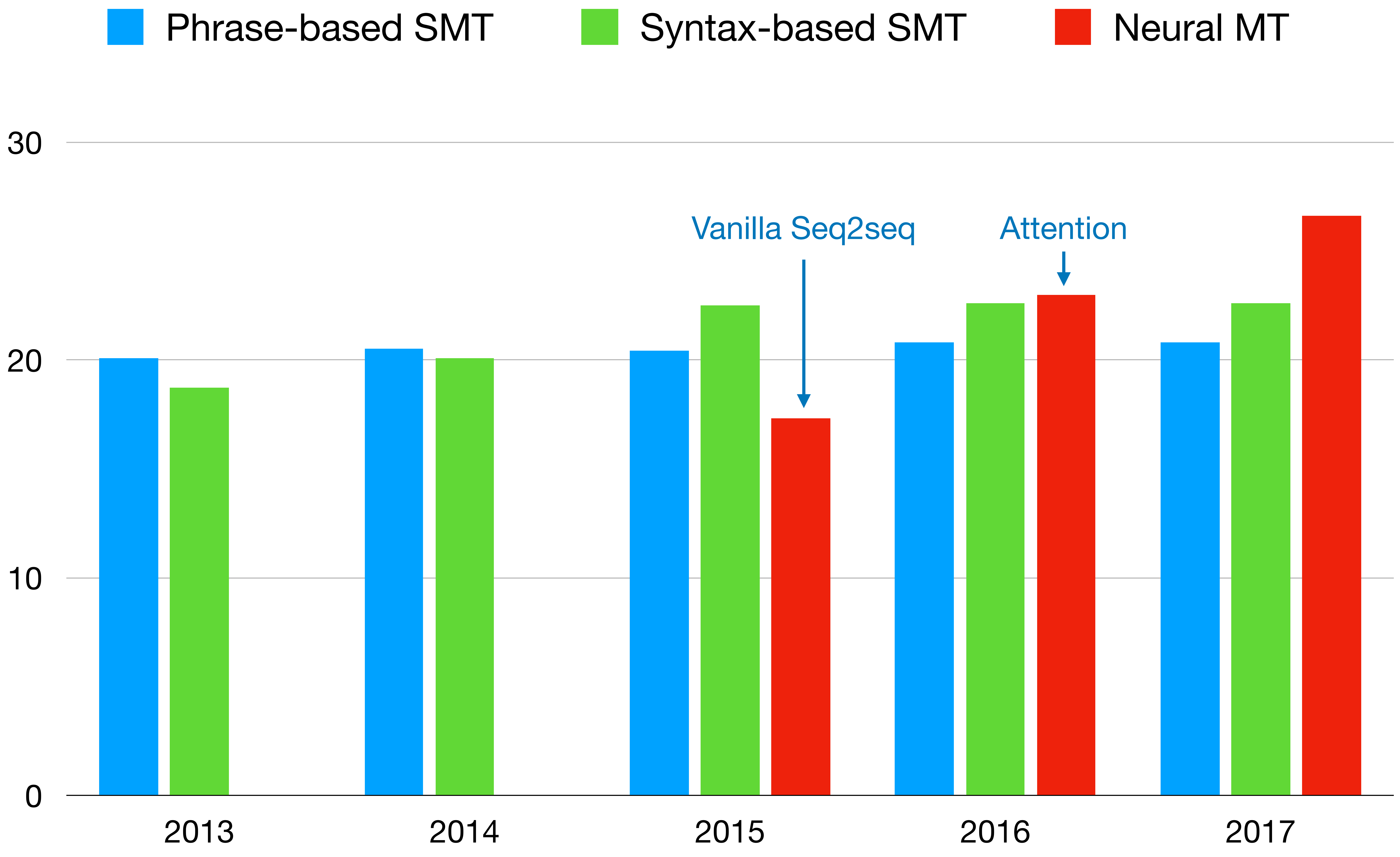
- Autoregressive factorization is just chain-rule (HMMs, MEMMs)
- Autoregressive factorization does NOT assume any independence
- With autoregressive factorization, we need to model each $p_\theta(y_t \,|\, y_{<t}\ , X)$

Recap: Encoder-Decoder Architecture

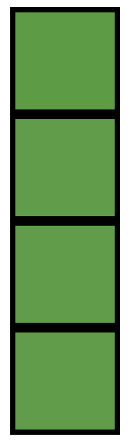
- **Two Components:**
  - Encoder: Convert input sequence into a sequence of vectors
  - Decoder: Convert encoding into a sequence in the output space



Recap: MT Progress

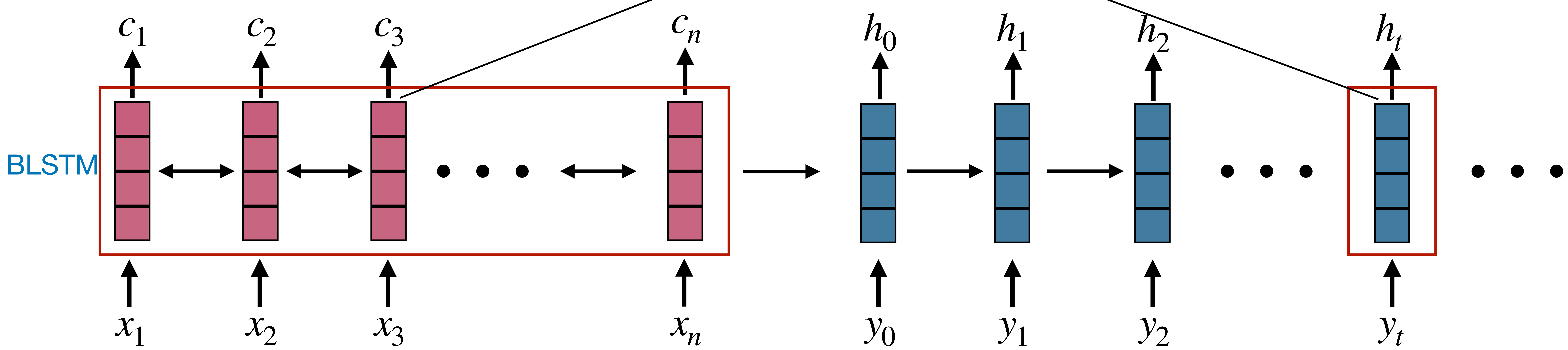


Recap: Attention Mechanism

 $= \mathrm{attn}([c_1, c_2, \ldots, c_n], h_t) = \sum_{j=1}^{n} a_j^t c_j \in \mathbb{R}^d$ Attention output

$a^t = \mathrm{softmax}(e^t) \in \mathbb{R}^n$ Attention distribution

$e_j^t = \mathrm{sim}(c_j, h_t), \ \forall j \in \{1, \ldots, n\}$ Attention scores



Recap: Types of Attention

- **Dot-product attention** (assumes equal dimensions for c and h)

$$\mathrm{sim}(c_j, h_t) = c_j^T h_t$$

- **Multiplicative attention**

$\mathrm{sim}(c_j, h_t) = c_j^T W h_t$, where W is learnable weight matrix

- **Additive attention**

$$\mathrm{sim}(c_j, h_t) = v^T \tanh(W_c c_j + W_h h_t)$$

where W_c and W_h are learnable weight matrices and v is a learnable weight vector

RESEARCH › PUBLICATIONS ›

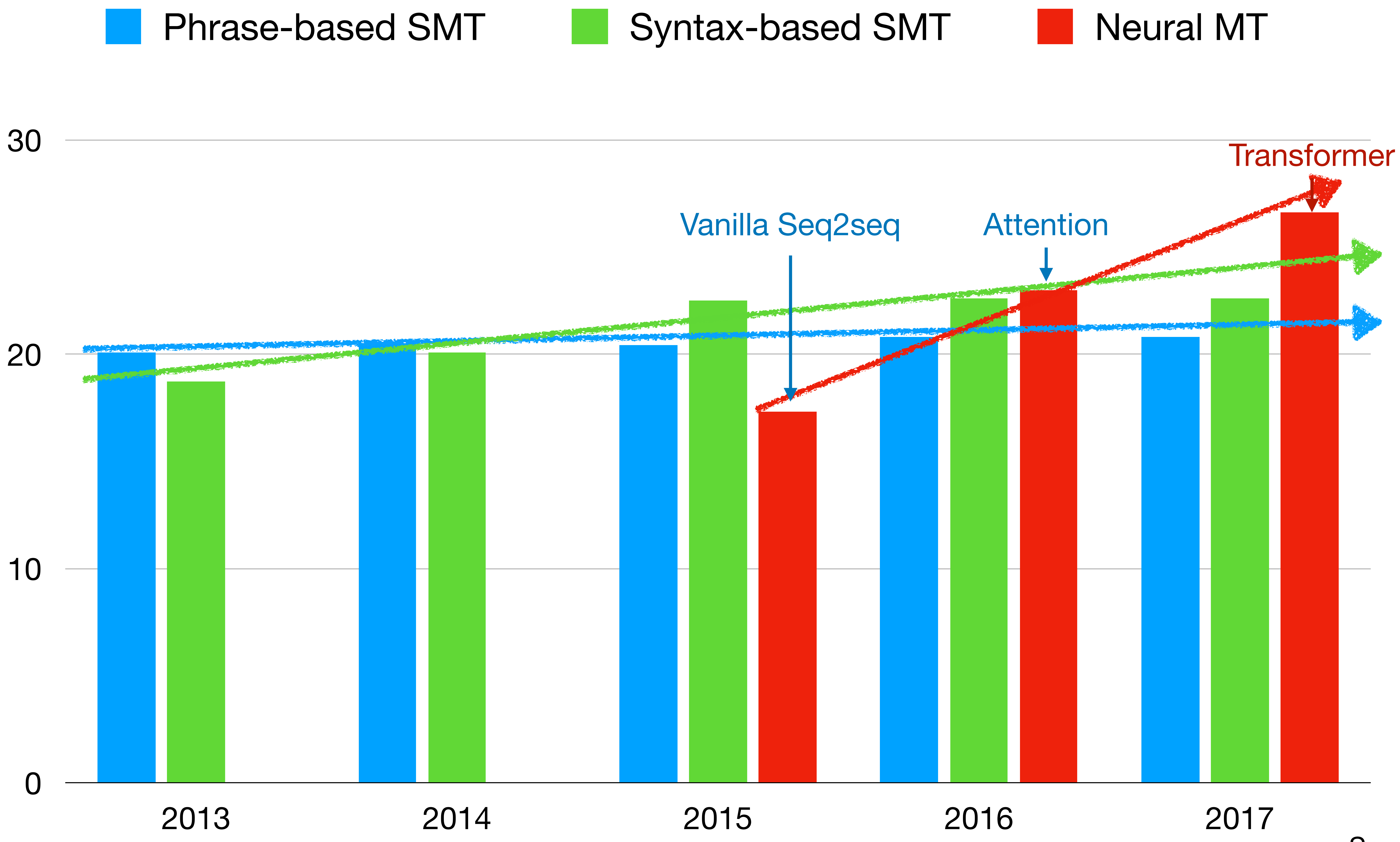
Google's Neural Machine Translation System: Bridging the Gap between Human and Machine Translation

Table 10: Mean of side-by-side scores on production data

	PBMT	GNMT	Human	Relative Improvement
English $\rightarrow$ Spanish	4.885	5.428	5.504	87%
English $\rightarrow$ French	4.932	5.295	5.496	64%
English $\rightarrow$ Chinese	4.035	4.594	4.987	58%
Spanish $\rightarrow$ English	4.872	5.187	5.372	63%
French $\rightarrow$ English	5.046	5.343	5.404	83%
Chinese $\rightarrow$ English	3.694	4.263	4.636	60%

(Wu et al., 2016)

MT Progress

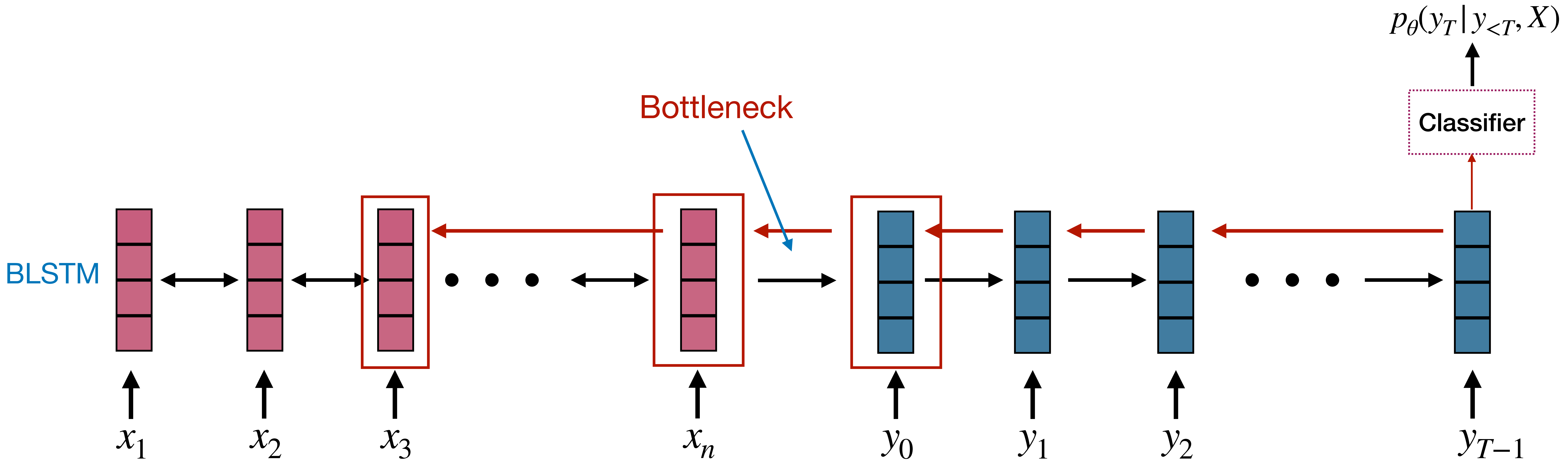


Source: Rico Sennrich

Self-Attention & Transformer

Revisit: Motivation of Attention Mechanism

- A single encoding vector needs to capture **all the information** about source sentence
- Longer sequences can lead to **vanishing gradients**

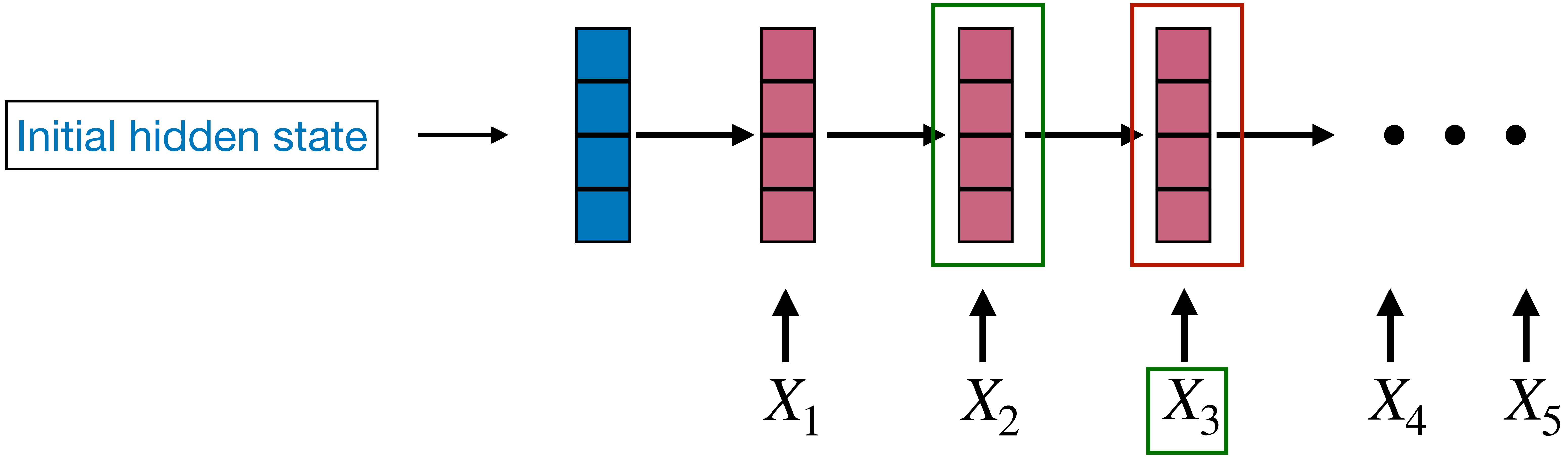


Issues with RNN!

Issues with RNNs

- **One vector** to memorize all historical information

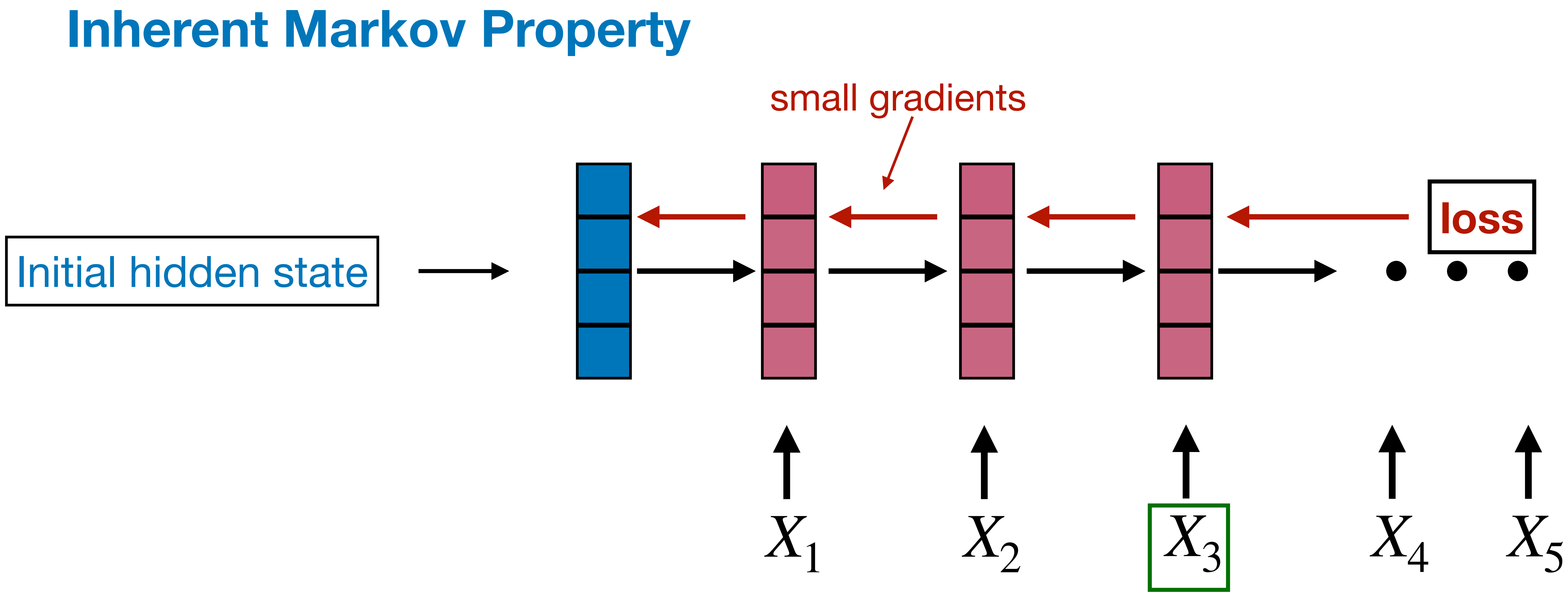
Inherent Markov Property



Issues with RNNs

- **One vector** to memorize all historical information
- **Hard to capture long-distance information: vanishing gradients**

Attention is the key to solve the problem!



This Lecture

- Do we really need RNNs to model the arbitrary context?
- Maybe attention is all you need!

Attention Is All You Need

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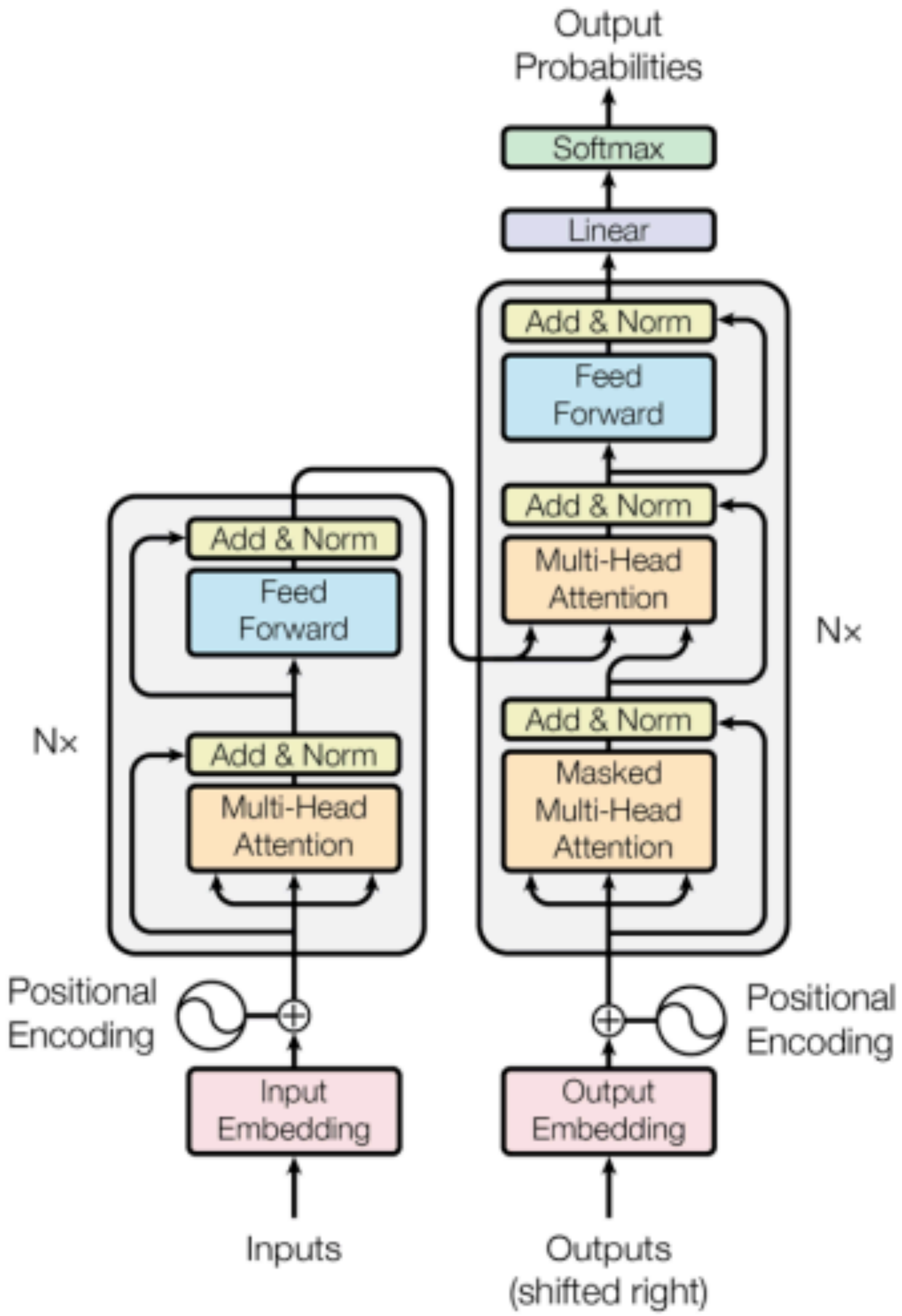
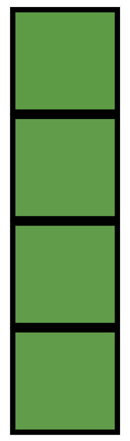
Transformers



- Consists of an encoder and a decoder
- Originally proposed for neural machine translation and later adapted for almost all the NLP tasks
  - For example, BERT only uses the **encoder** of the Transformer architecture (next lecture)
- Both encoder and decoder consist of N layers
  - Each encoder layer has two sub-layers
  - Each decoder layer has three sublayers
  - Key innovation: **multi-head self-attention**

Vaswani et al., 2017: Attention Is All You Need

Recap: Attention Mechanism



$$= \mathrm{attn}([c_1, c_2, \ldots, c_n], h_t) = \sum_{j=1}^{n} a_j^t c_j \in \mathbb{R}^d$$

Attention output

$$a^t = \mathrm{softmax}(e^t) \in \mathbb{R}^n$$

Attention distribution

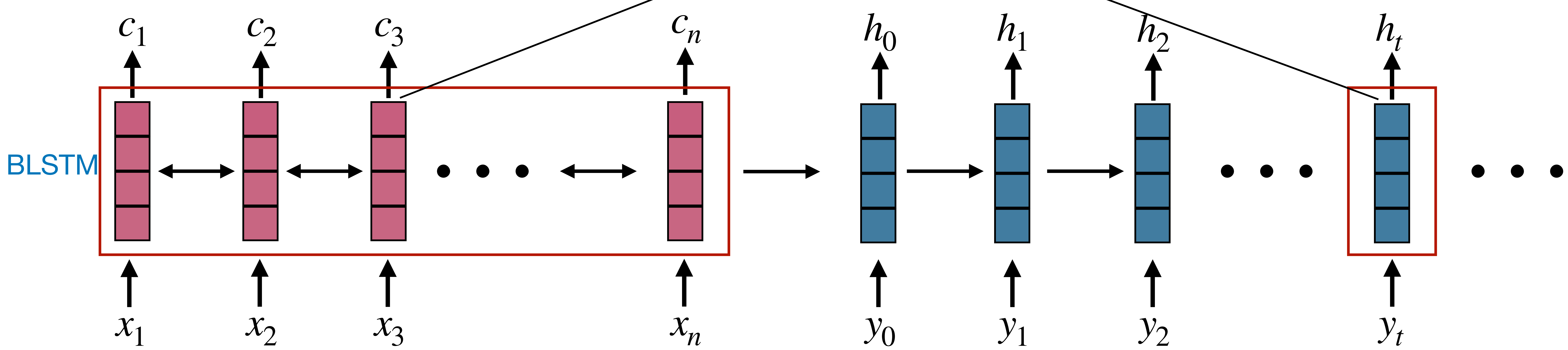
$$e_j^t = \mathrm{sim}(c_j, h_t), \ \forall j \in \{1, \ldots, n\}$$

Attention scores

Why we need LSTM?

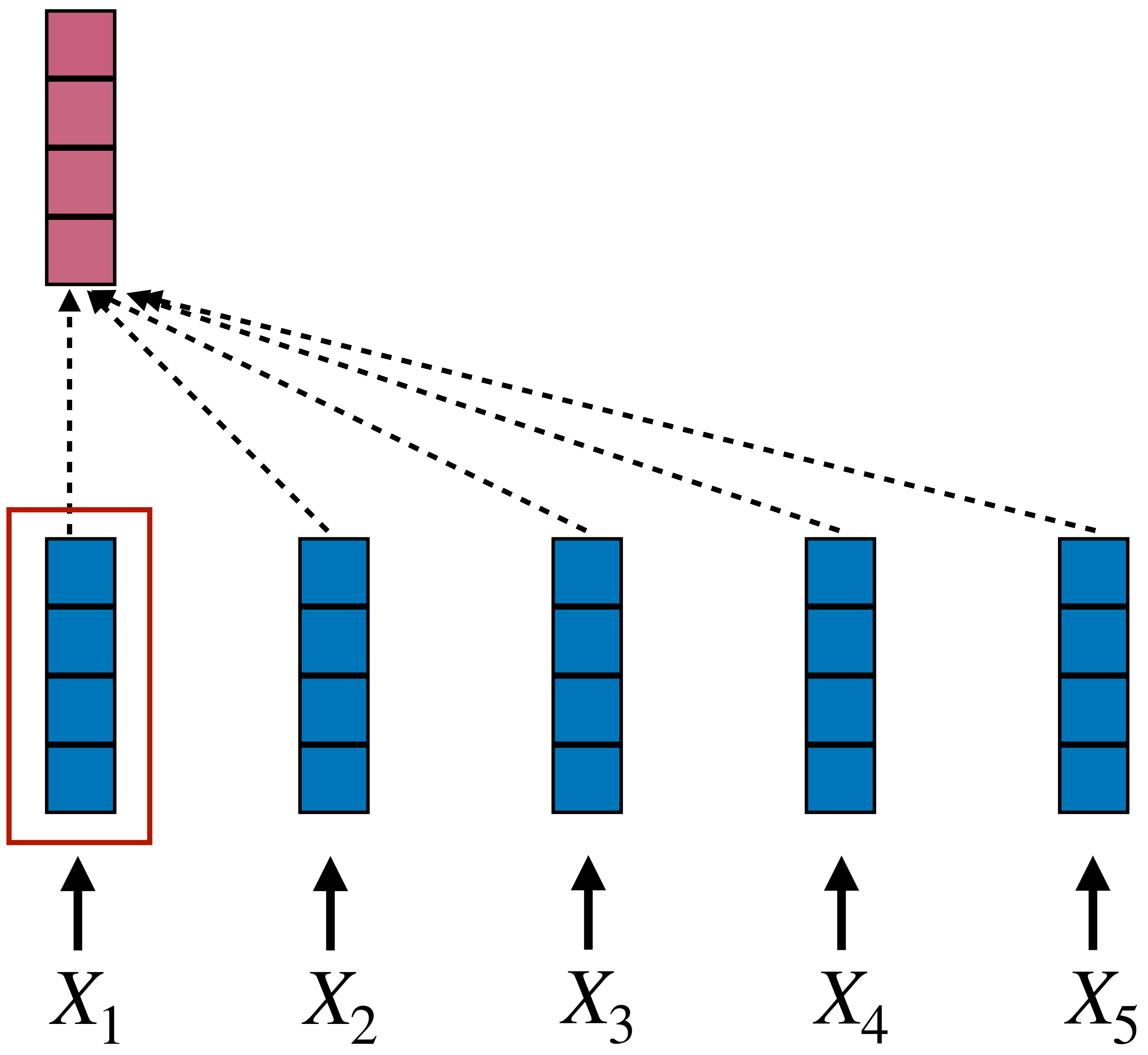
Modeling contextual information in both source and target languages

Contextual information via attention?



Self-Attention

- **Self-attention: attention within on single sequence**
  - Contexts and queries are drawn from the same source
- **Contextual information via self-attention**



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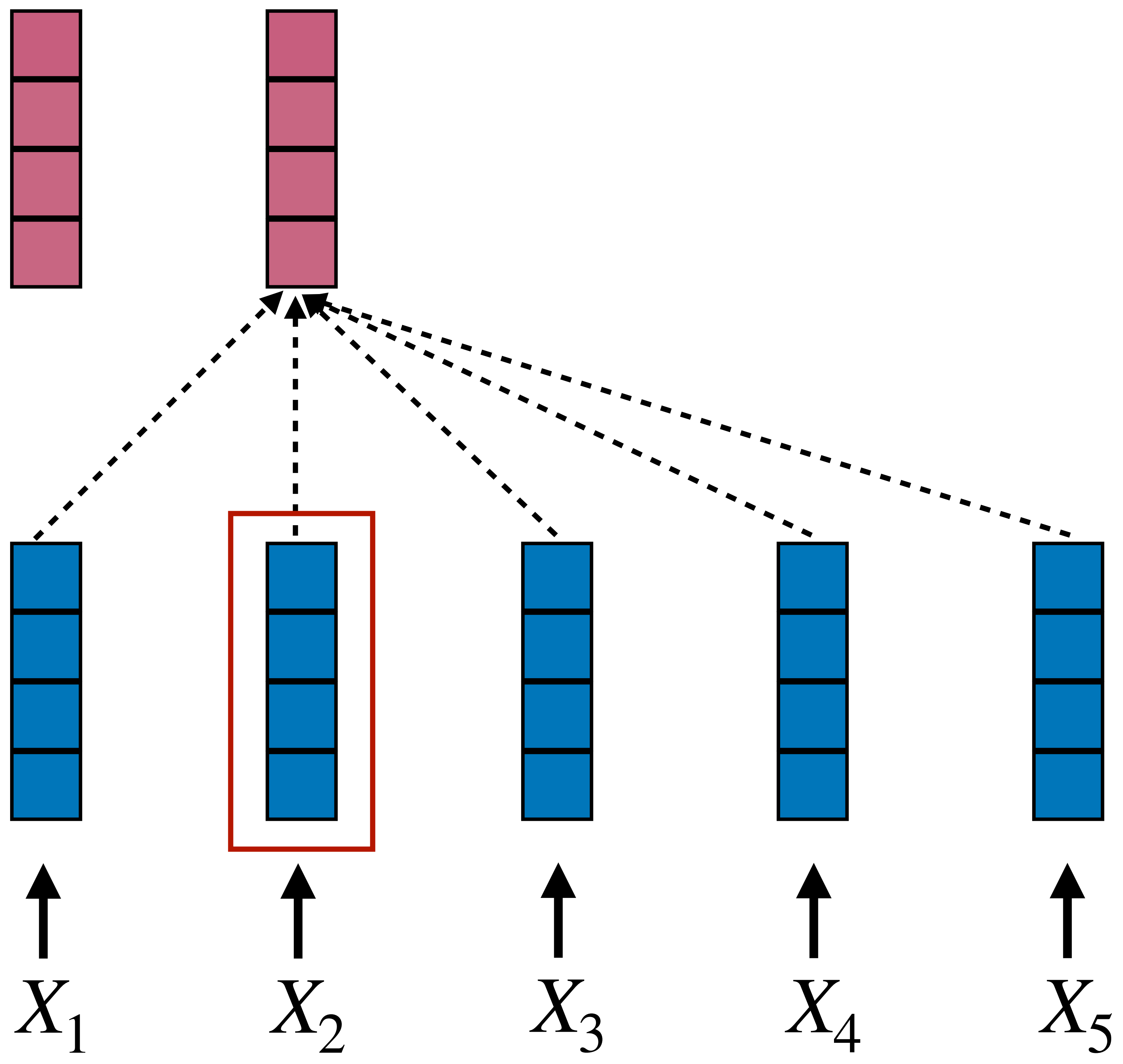

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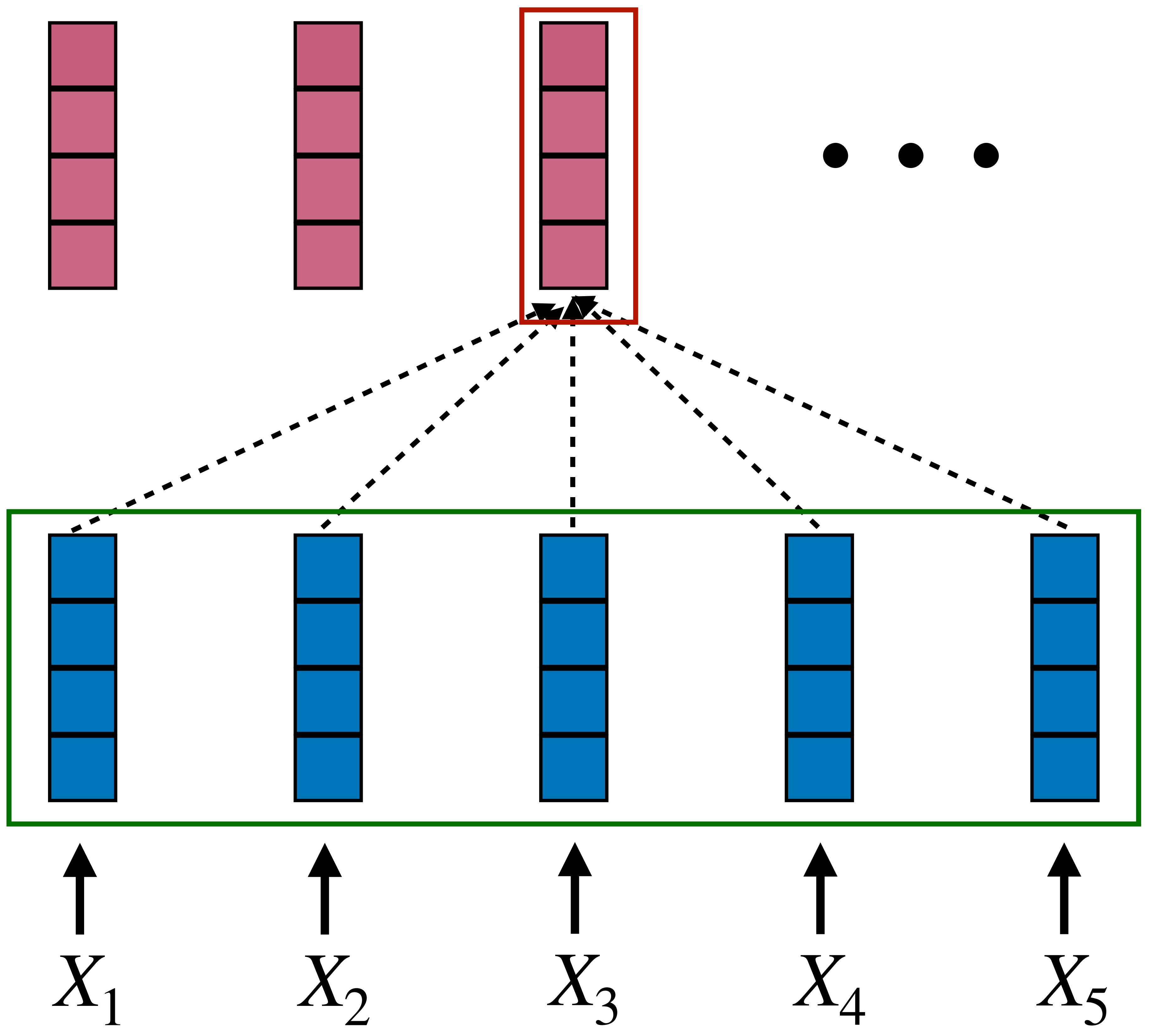

- **Capturing long-distance dependencies**
- **No gradient vanishing**

Self-attention in equations

- A sequence of input vectors $x_1, \ldots, x_n \in \mathbb{R}^d$
- First, construct a set of queries, keys and values:

$$q_i = W_Q x_i,\ k_i = W_K x_i,\ v_i = W_V x_i$$

- Second, for each q_i, compute attention scores and attention distributions:

$$a_{i,j} = \mathrm{softmax}(\frac{q_i^T k_j}{\sqrt{d}})$$

aka. "scaled dot product"

- Finally, compute the weighted sum:

$$y_i = \sum_{j=1}^{n} a_{i,j} v_j$$

Why *Scaled* Dot Product?

- **Softmax is sensitive to scale**

If $[x_1, x_2] = [0.1, 0.5], \alpha = 10$

$$\text{softmax}([x_1, x_2]) = \left[\frac{e^{x_1}}{e^{x_1} + e^{x_2}}, \frac{e^{x_2}}{e^{x_1} + e^{x_2}}\right]$$

$[0.4013, 0.5987]$

$$\text{softmax}([\alpha x_1, \alpha x_2]) = \left[\frac{e^{\alpha x_1}}{e^{\alpha x_1} + e^{\alpha x_2}}, \frac{e^{\alpha x_2}}{e^{\alpha x_1} + e^{\alpha x_2}}\right]$$

$[0.0180, 0.9820]$

Self-attention in equations

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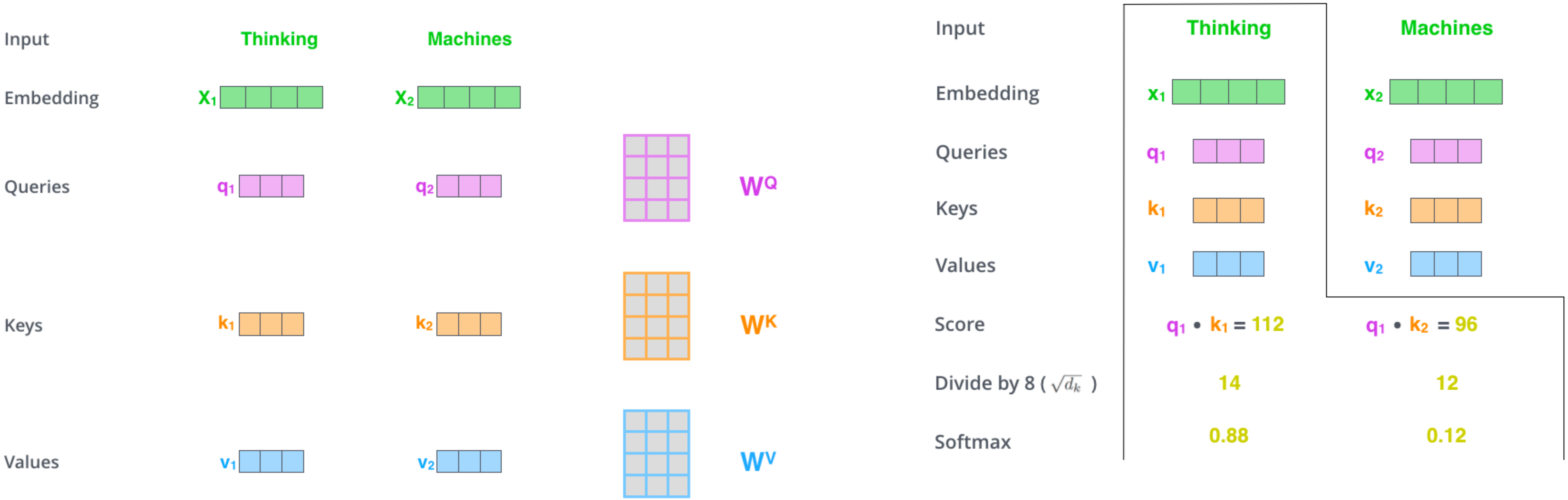
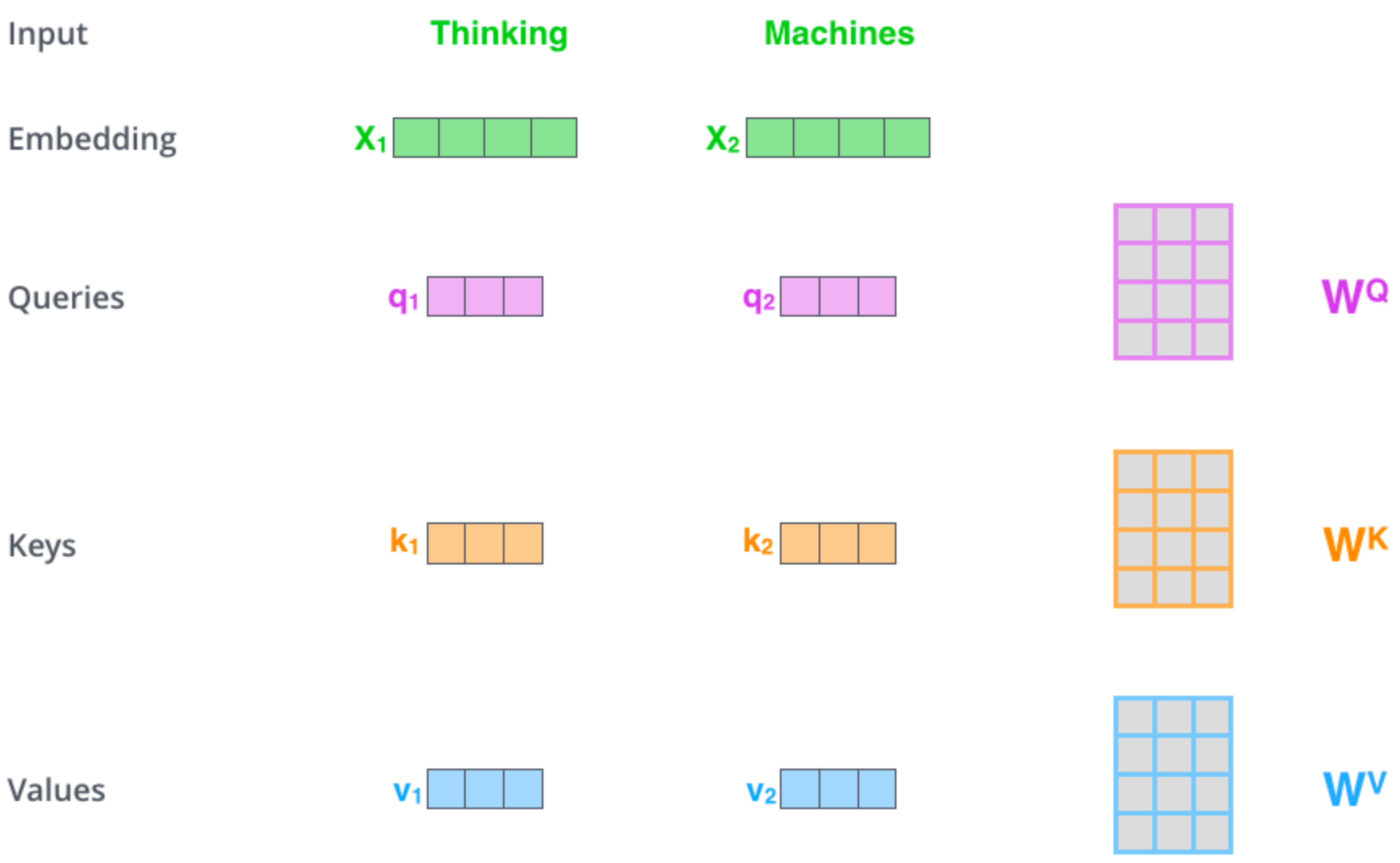
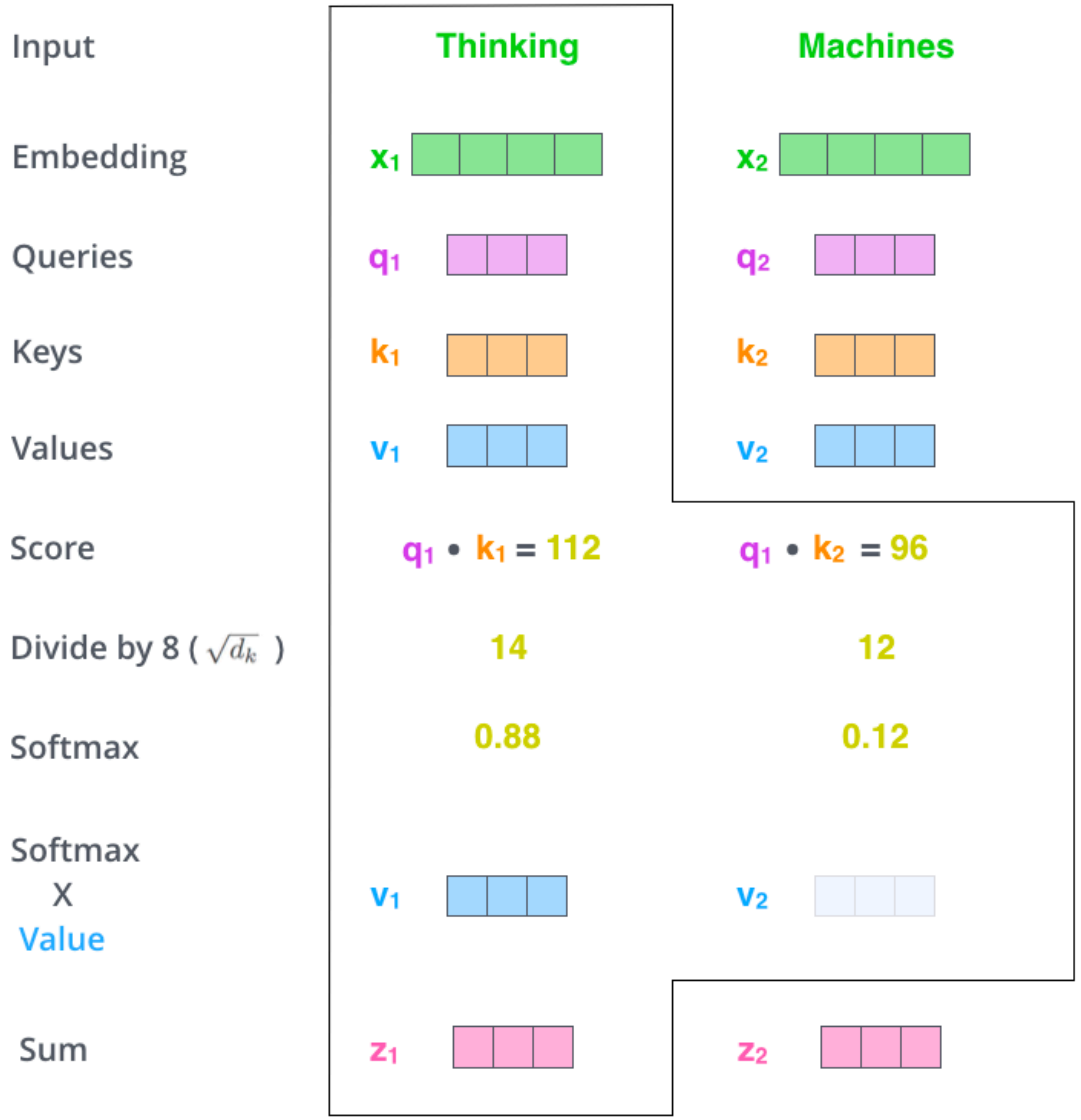
Self-attention: Illustration



http://jalammar.github.io/illustrated-transformer/

Self-attention: Illustration





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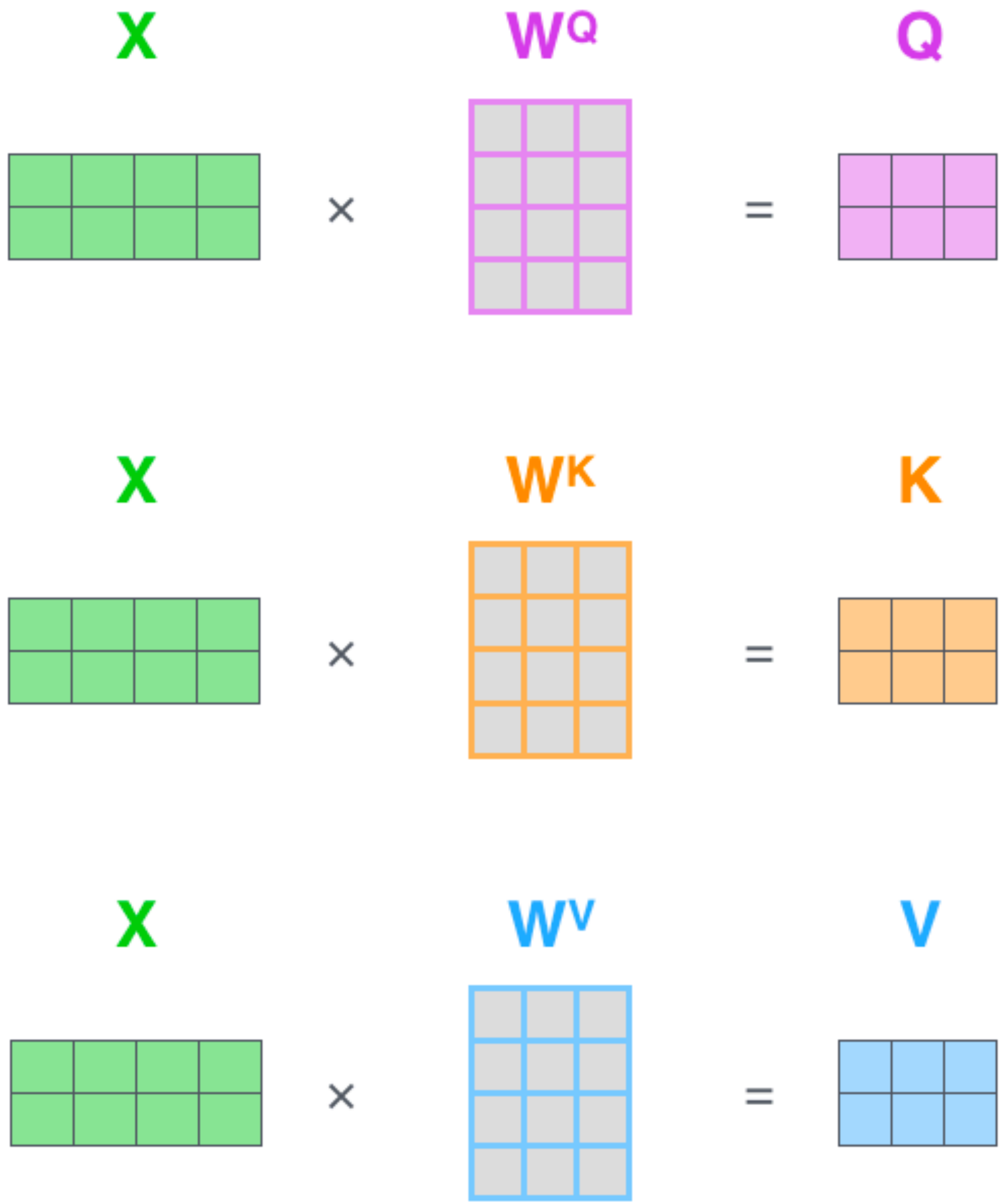
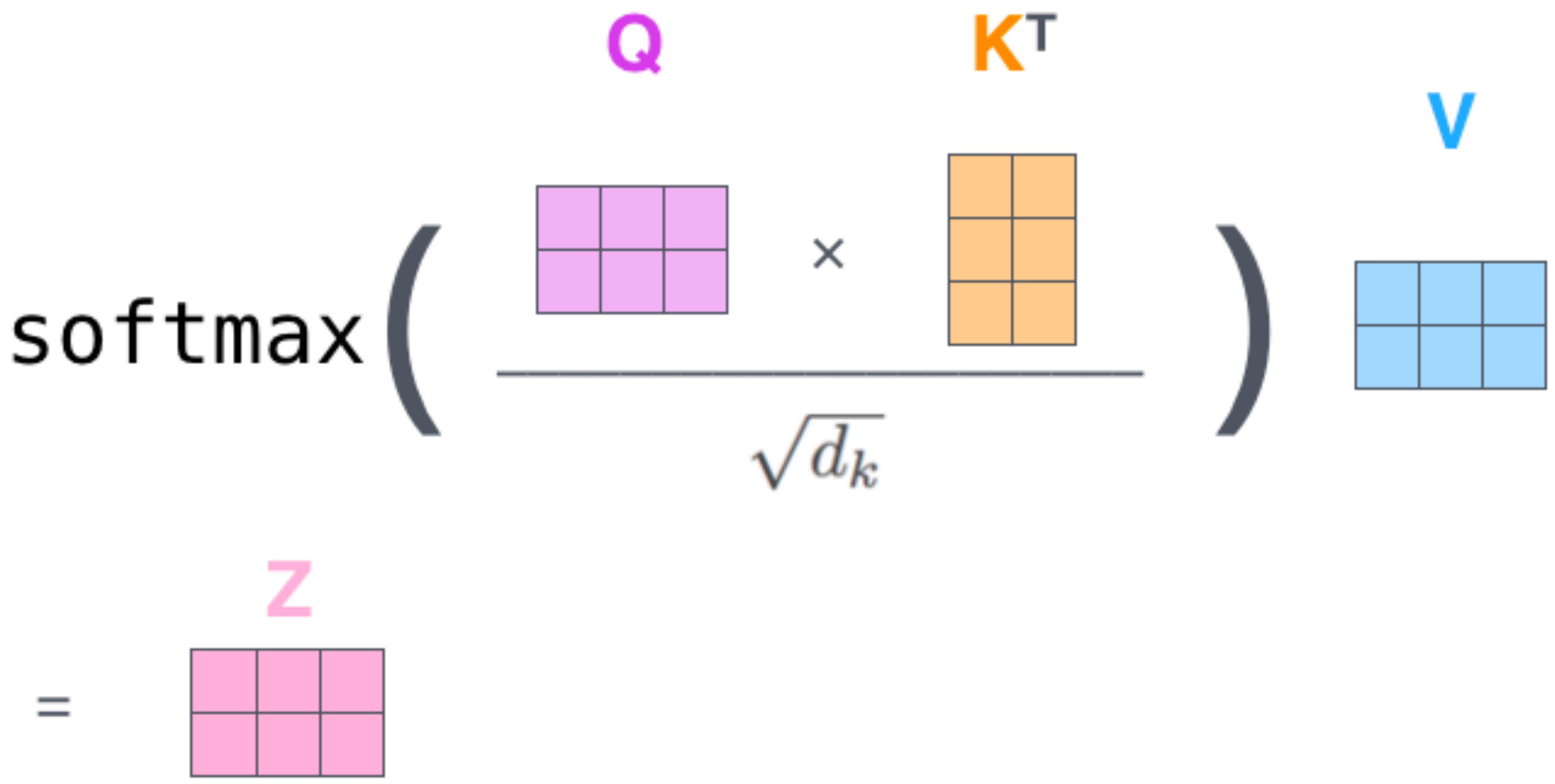
Self-attention: matrix notations



Self-attention: matrix notations

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



Self-attention: matrix notations

hardmaru
@hardmaru

The most important formula in deep learning after 2018

Self-Attention

What is self-attention? Self-attention calculates a weighted average of feature representations with the weight proportional to a similarity score between pairs of representations. Formally, an input sequence of n tokens of dimensions d, $X \in \mathbf{R}^{n \times d}$, is projected using three matrices $W_Q \in \mathbf{R}^{d \times d_q}$, $W_K \in \mathbf{R}^{d \times d_k}$, and $W_V \in \mathbf{R}^{d \times d_v}$ to extract feature representations Q, K, and V, referred to as query, key, and value respectively with $d_k = d_q$. The outputs Q, K, V are computed as

$$Q = XW_Q, \quad K = XW_K, \quad V = XW_V. \qquad (1)$$

So, self-attention can be written as,

$$S = D(Q, K, V) = \mathrm{softmax}\left(\frac{QK^T}{\sqrt{d_q}}\right)V, \qquad (2)$$

where softmax denotes a *row-wise* softmax normalization function. Thus, each element in S depends on all other elements in the same row.

9:08 PM · Feb 9, 2021 · Twitter Web App

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Attention is *General*

- **Given a set of key and value vectors, and a query vector, attention is a technique to compute a weighted sum of the value vectors, dependent on the query and keys**
  - We sometimes say that the query attends to the values via keys
  - In the NMT vase, each decoder hidden state (query) attends to all the encoder hidden states (keys and values)
- **Intuition**
  - The weighted sum is a *selective summary* of the information contained in the values, where the query and keys determines which values to focus on
  - Attention is a way to obtain a *fixed-size representation* of an arbitrary set of representations (the values), dependent on some other representation (the query)

$$\boxed{\mathrm{attn}(Q, K, V) = \mathrm{softmax}(\frac{QK^T}{\sqrt{d}})V}$$

Multi-head Attention

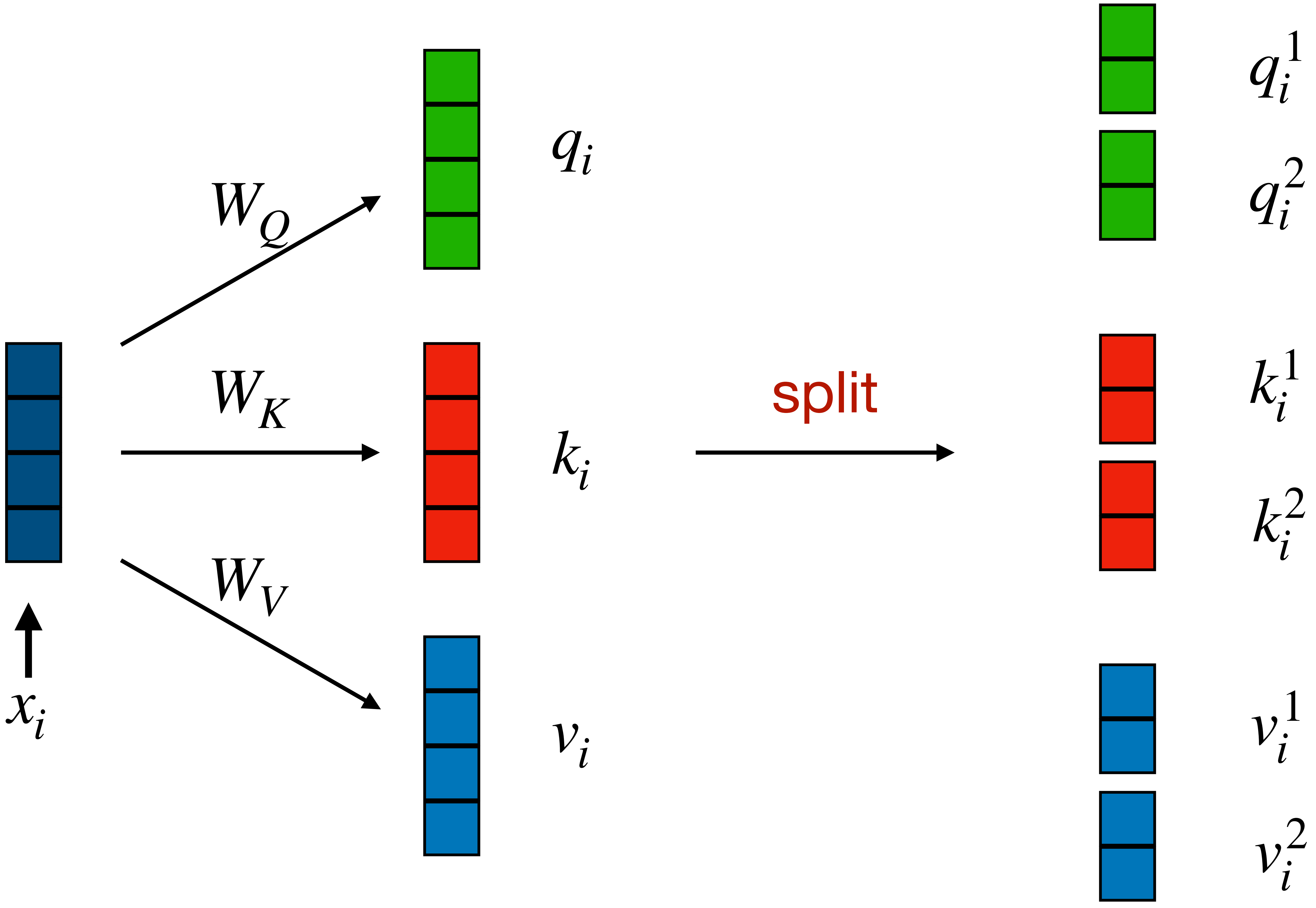
- **Problem with self-attention?**

$$y_i = \sum_{j=1}^{n} a_{i,j} v_j$$

one set of attention weights a_i

- **It is better to use multiple attention weights instead of one!**
  - Each attention can focus on different positions
- **How to do this? Splits queries, keys, values to multiple heads!**

Multi-head Attention: Head Split

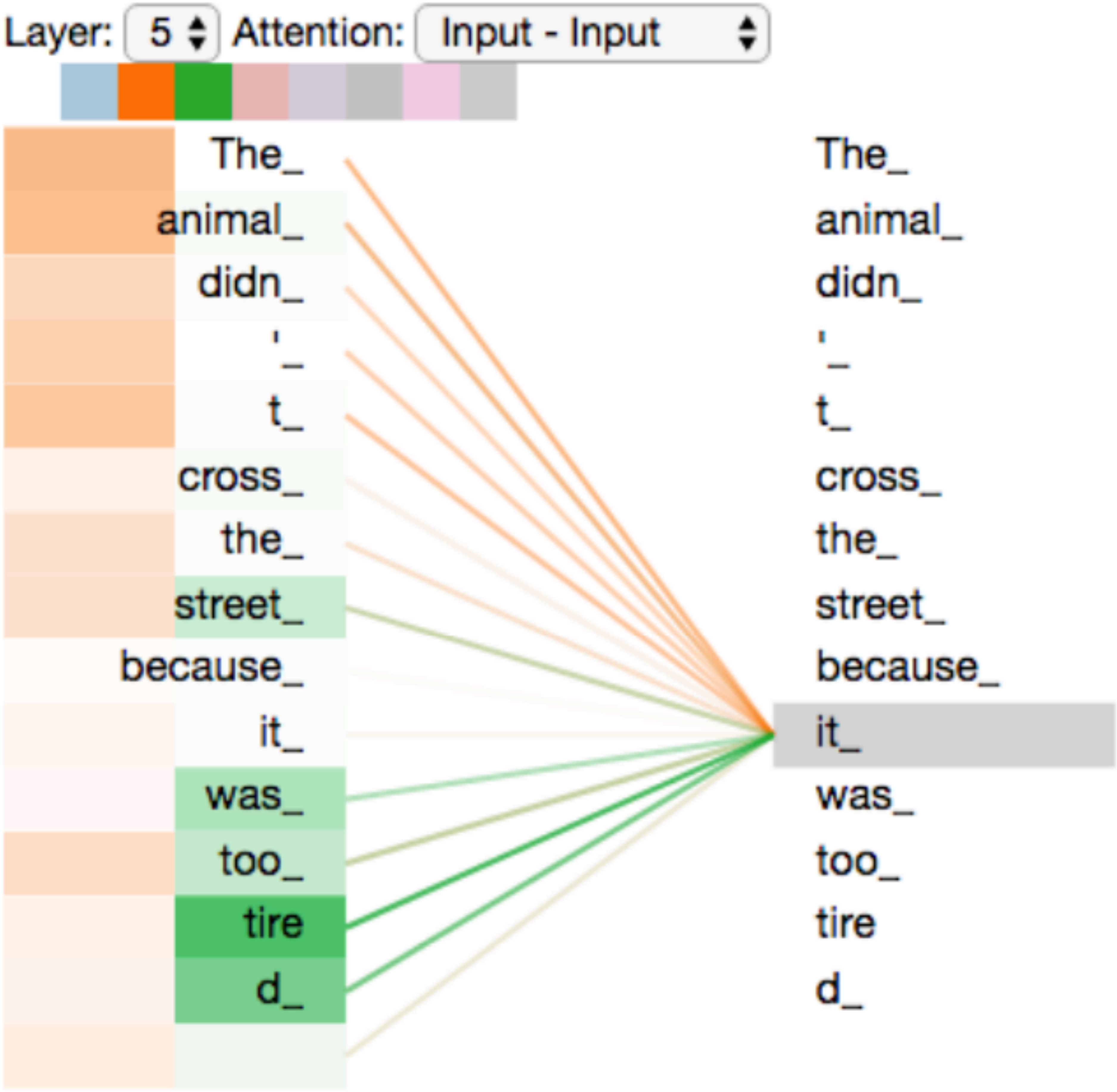


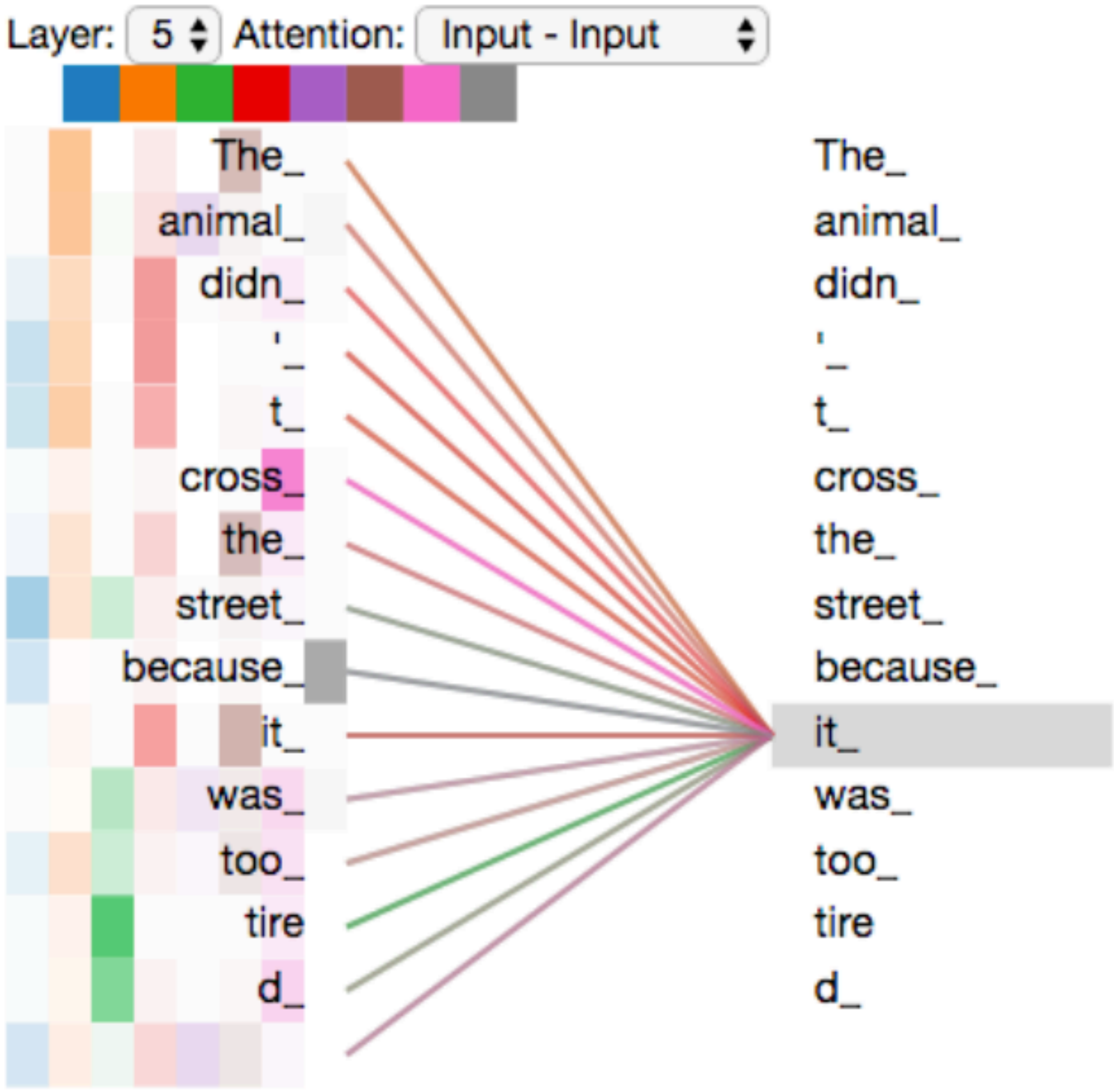
$$h_1 = \text{attn}(Q_1, K_1, V_1) = \text{softmax}(\frac{Q_1 K_1^T}{\sqrt{d/2}})V_1$$

$$h_2 = \text{attn}(Q_2, K_2, V_2) = \text{softmax}(\frac{Q_2 K_2^T}{\sqrt{d/2}})V_2$$

$$Y = \text{concat}(h_1, h_2)W_O$$

What does multi-head attention learn?

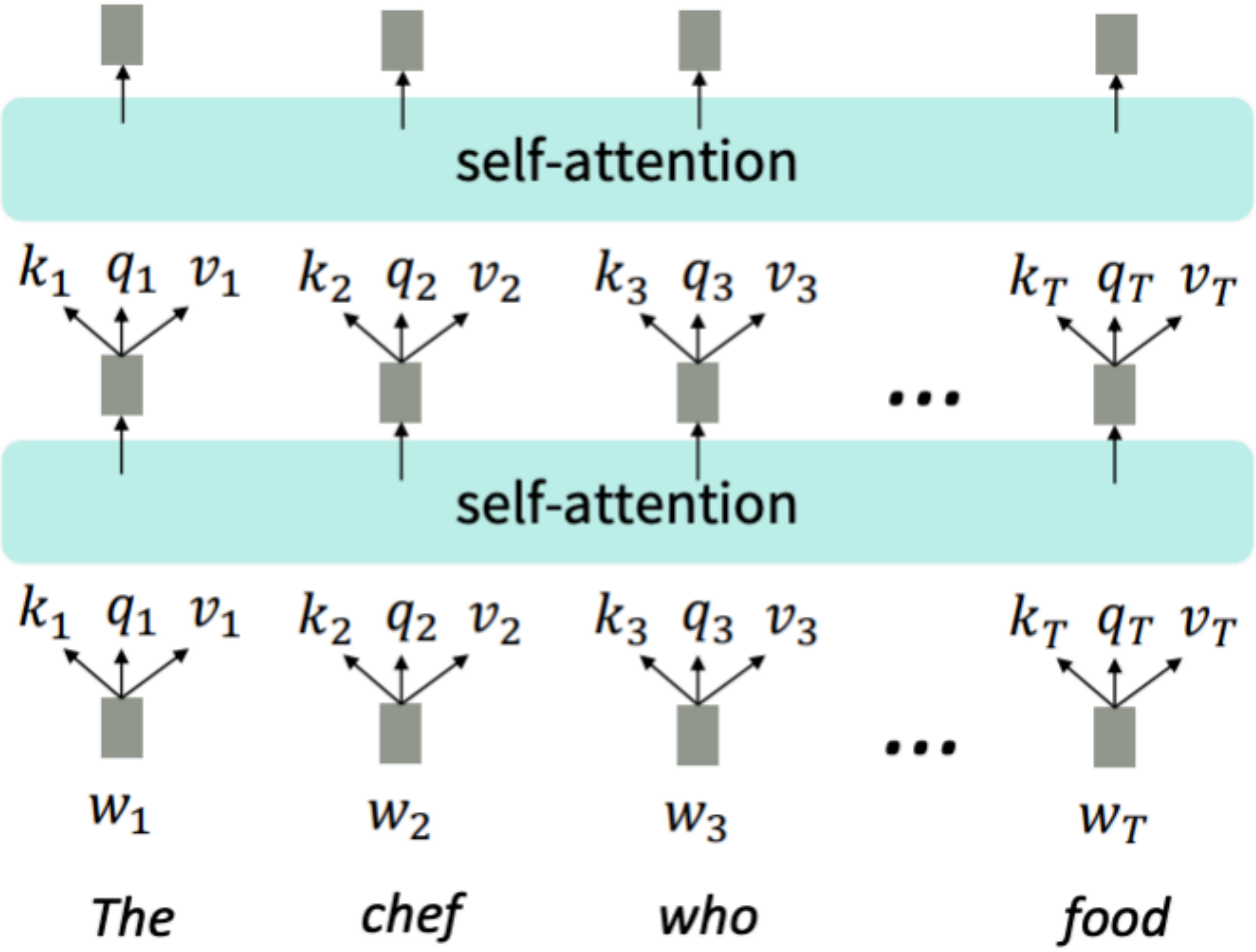




https://github.com/jessevig/bertviz

Transformer Encoder

- **Replacing RNNs with multi-head self-attention**



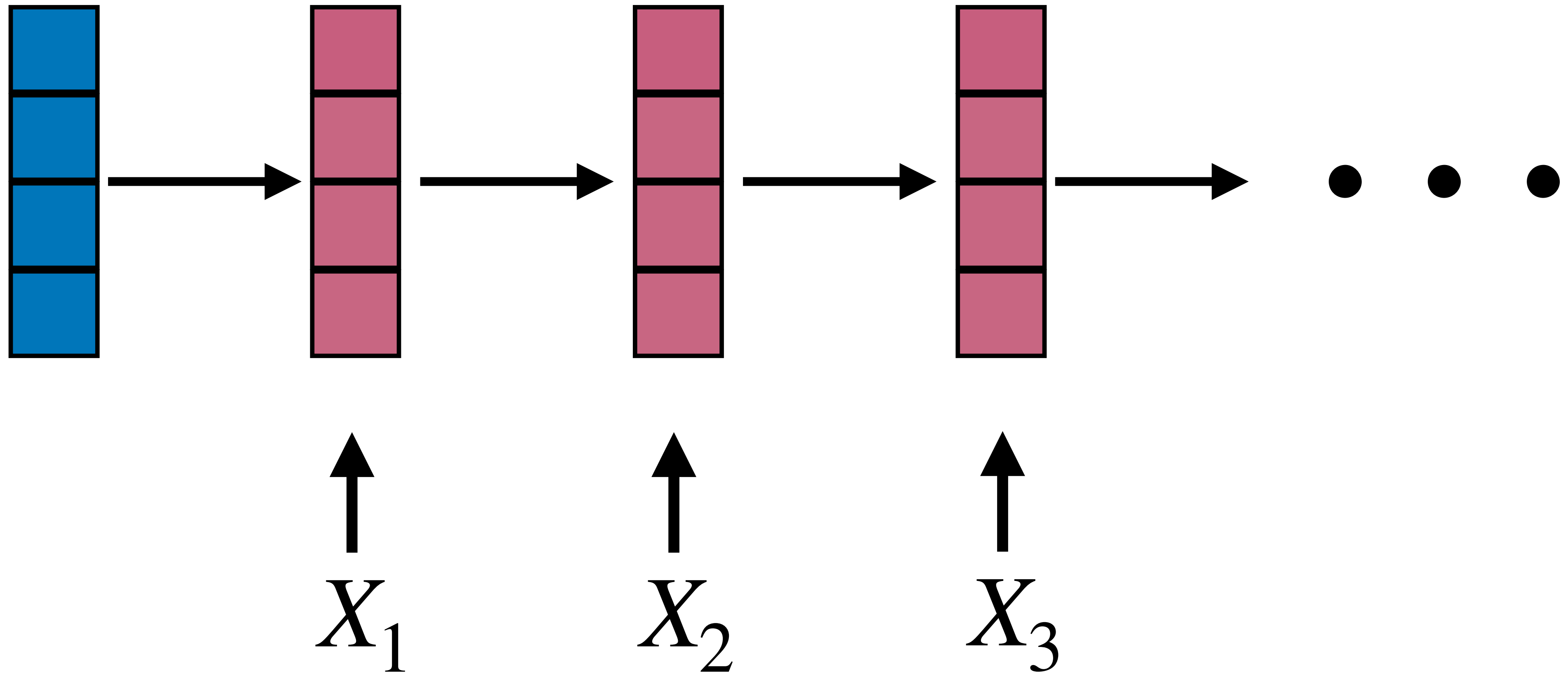
$$\boxed{\begin{gathered}\text{MultiHead}(X) = \text{concat}(h_1, \ldots, h_k)W_O \\ h_i = \text{attn}(Q_i, K_i, V_i) \\ Q_i = (XW_Q)^i, K_i = (XW_K)^i, V_i = (XW_V)^i\end{gathered}}$$

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

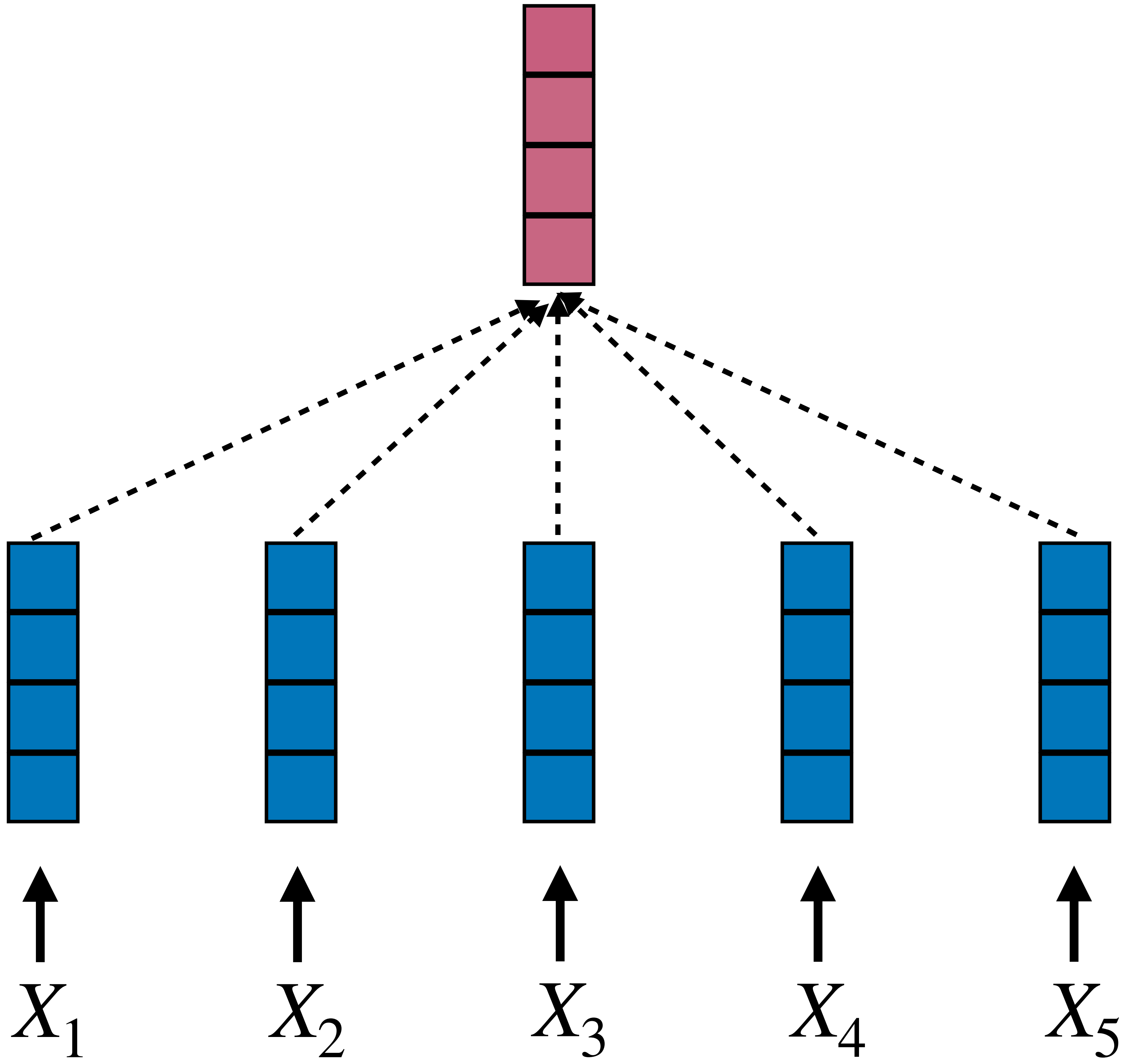
Self-attention does not know the order of the inputs!

Missing Piece: Positional Information

RNN



Self-attention



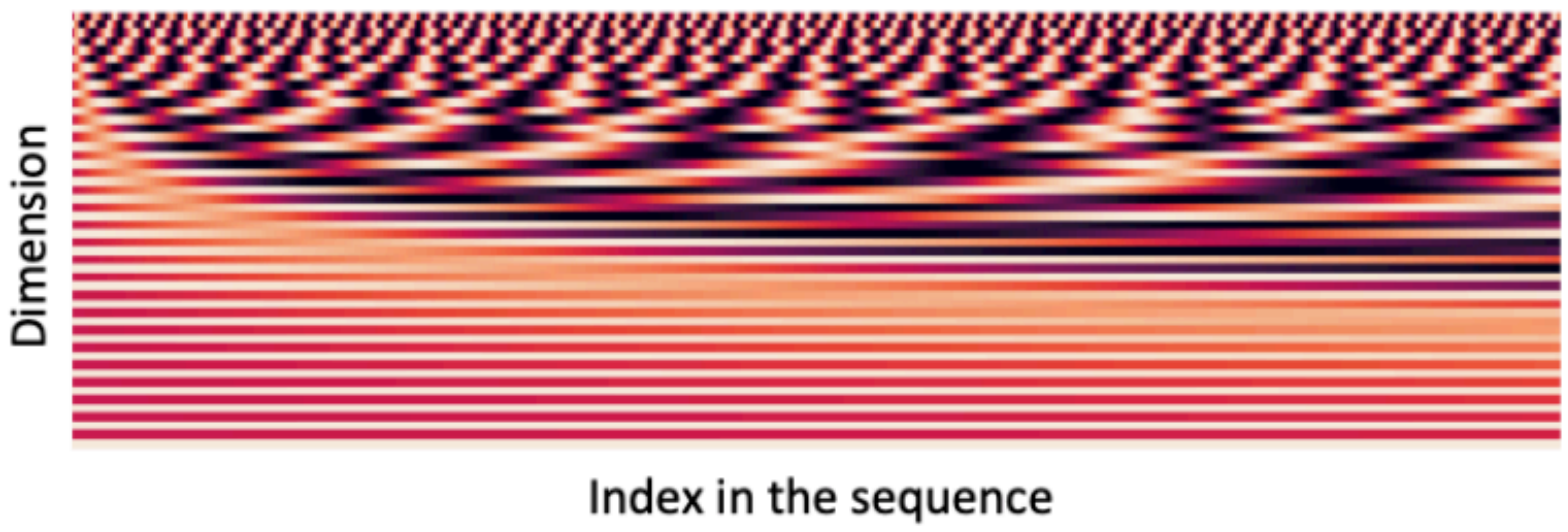
Missing Piece: Positional Information

- **Unlike RNNs, self-attention does not build in order information**
  - Encode the order of the sentence into the input $x_1, \ldots, x_n$
- **Solution: add positional encoding to the input embeddings**

$$x_i \leftarrow x_i + p_i$$

- **Use sine and cosine functions of different frequencies (not learnable)**

$$p_i = \begin{pmatrix} \sin(i/10000^{2*1/d}) \\ \cos(i/10000^{2*1/d}) \\ \vdots \\ \sin(i/10000^{2*\frac{d}{2}/d}) \\ \cos(i/10000^{2*\frac{d}{2}/d}) \end{pmatrix}$$



Adding Nonlinearities

- There is no elementwise nonlinearities in self-attention; stacking more self-attention layers just re-averages value vectors

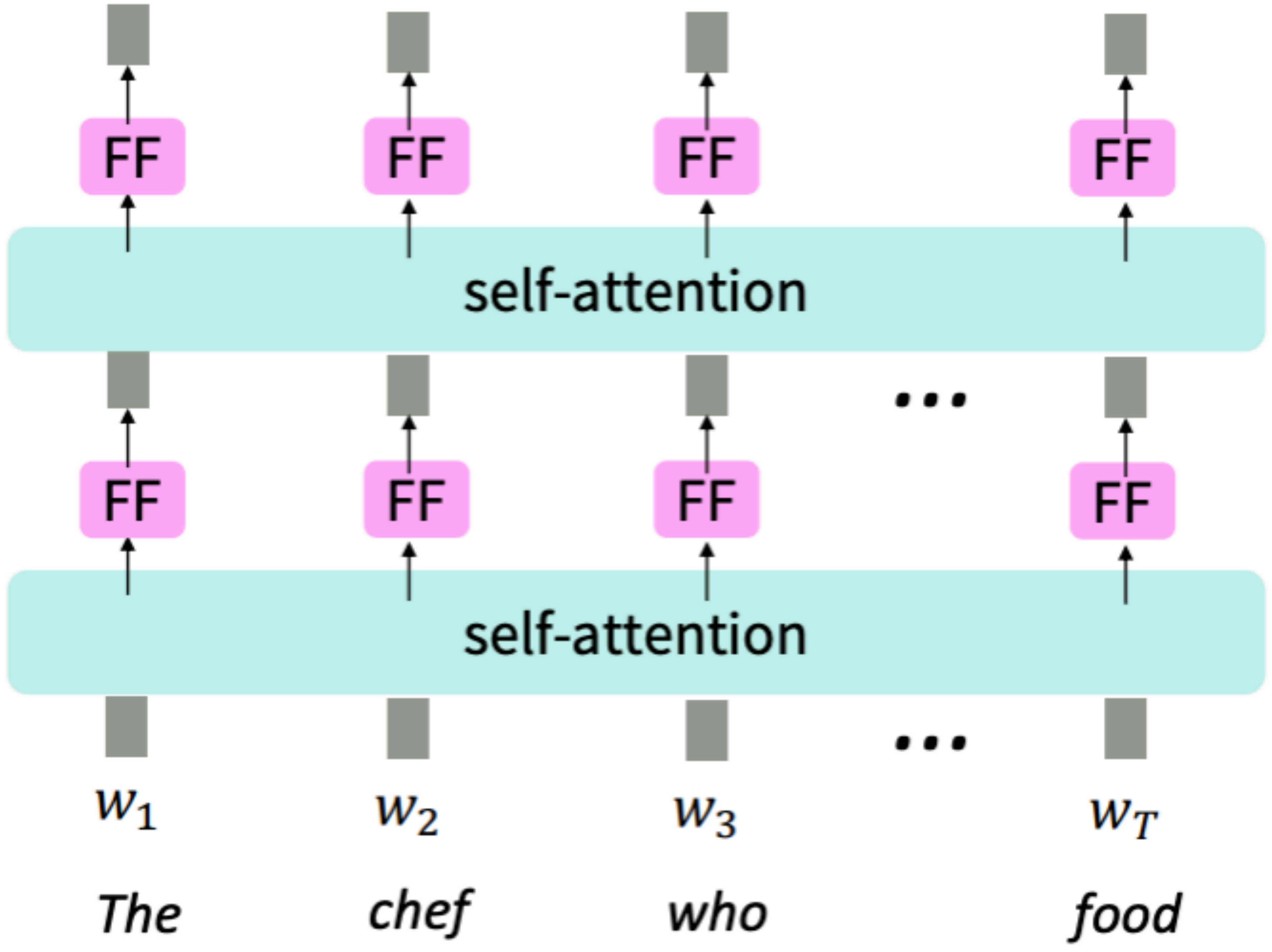
- Simple fix: add a feed-forward network to post-process each output vector

$$\mathrm{FFN}(\mathbf{x}_i) = W_2 \mathrm{ReLU}(W_1 \mathbf{x}_i + \mathbf{b}_1) + \mathbf{b}_2$$

A large number of parameters

$$\boxed{\begin{array}{l} W_1 \in \mathbb{R}^{d_{ff} \times d}, \mathbf{b}_1 \in \mathbb{R}^{d_{ff}} \\ W_2 \in \mathbb{R}^{d \times d_{ff}}, \mathbf{b}_2 \in \mathbb{R}^{d} \end{array}}$$

In practice, they use $d_{ff} = 4d$



Slide credit: Danqi Chen COS 484/584

Feed-Forward Layers

- **Feed-forward layers constitute two-thirds of parameters**
- **Operates as memories of textual patterns** (Gova et al., 2021)

Key	Pattern	Example trigger prefixes
$\mathbf{k}^{1}_{449}$	Ends with "*substitutes*" (shallow)	*At the meeting, Elton said that "for artistic reasons there could be no substitutes* *In German service, they were used as substitutes* *Two weeks later, he came off the substitutes*
$\mathbf{k}^{6}_{2546}$	Military, ends with "*base*"/"*bases*" (shallow + semantic)	*On 1 April the SRSG authorised the SADF to leave their bases* *Aircraft from all four carriers attacked the Australian base* *Bombers flying missions to Rabaul and other Japanese bases*
$\mathbf{k}^{10}_{2997}$	a "part of" relation (semantic)	*In June 2012 she was named as one of the team that competed* *He was also a part of the Indian delegation* *Toy Story is also among the top ten in the BFI list of the 50 films you should*
$\mathbf{k}^{13}_{2989}$	Ends with a time range (semantic)	*Worldwide, most tornadoes occur in the late afternoon, between 3 pm and 7* *Weekend tolls are in effect from 7:00 pm Friday until* *The building is open to the public seven days a week, from 11:00 am to*
$\mathbf{k}^{16}_{1935}$	TV shows (semantic)	*Time shifting viewing added 57 percent to the episode's* *The first season set that the episode was included in was as part of the* *From the original NBC daytime version , archived*

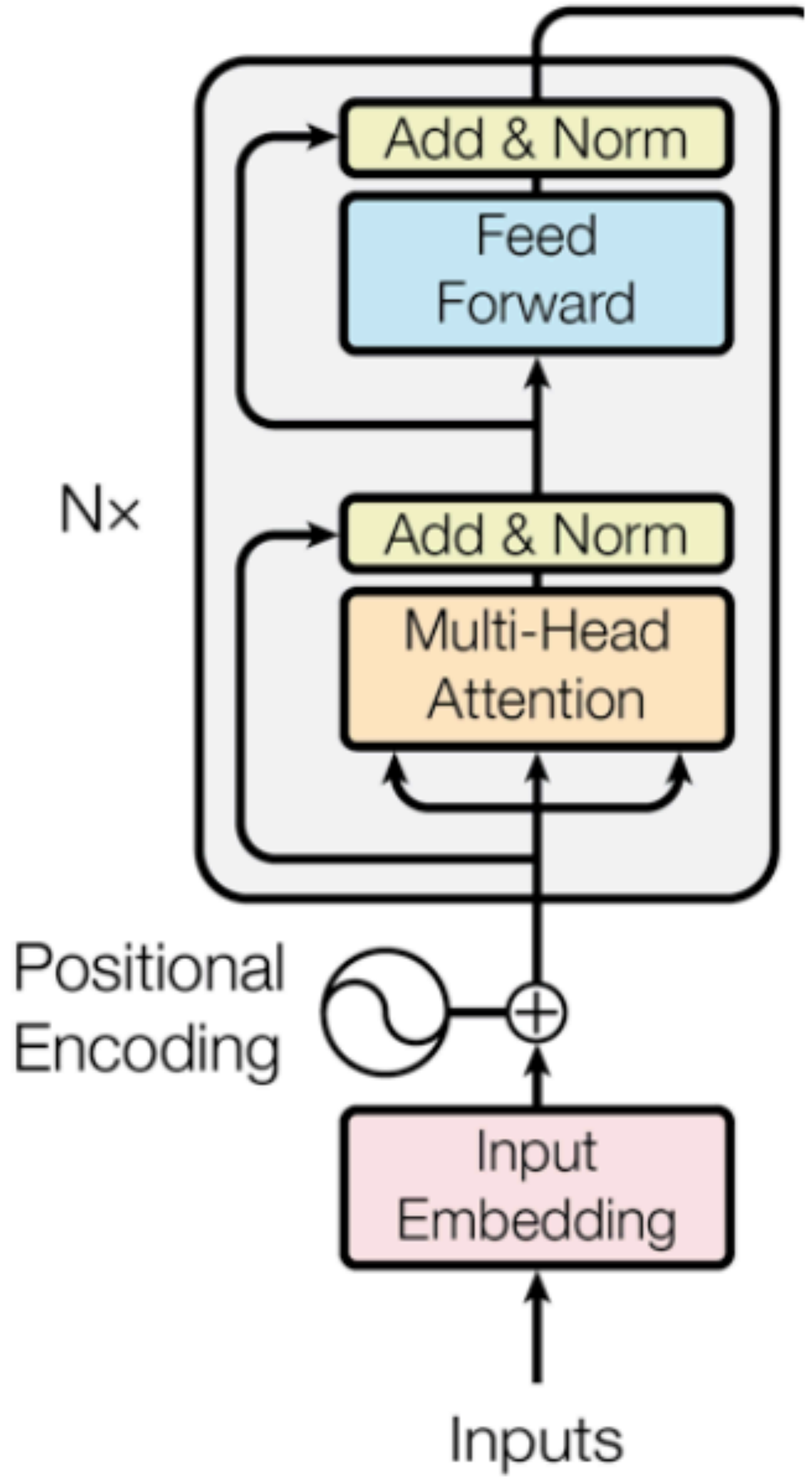
Transformer Encoder

- **Each encoder layer has two sub-layers:**
  - A multi-head self-attention layer
  - A feedforward layer
- **Add & Norm:**
  - Add: Residual connection (He et al., 2016)

$$Y \leftarrow Y + X$$

  - Norm: Layer normalization (Ba et al., 2016)

$$Y = \frac{X - \mathrm{E}[X]}{\sqrt{\mathrm{Var}[X] + \epsilon}} * \gamma + \beta$$



In (Vaswani et al., 2017), N = 6

Question

Which of the following statements is correct?

(a) Transformers run faster than LSTMs

(b) Transformers are easier to parallelize compared to LSTMs

(c) Transformers have less parameters compared to LSTMs

(d) Transformers are better at capturing positional information than LSTMs

Transformer: Pros and Cons

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

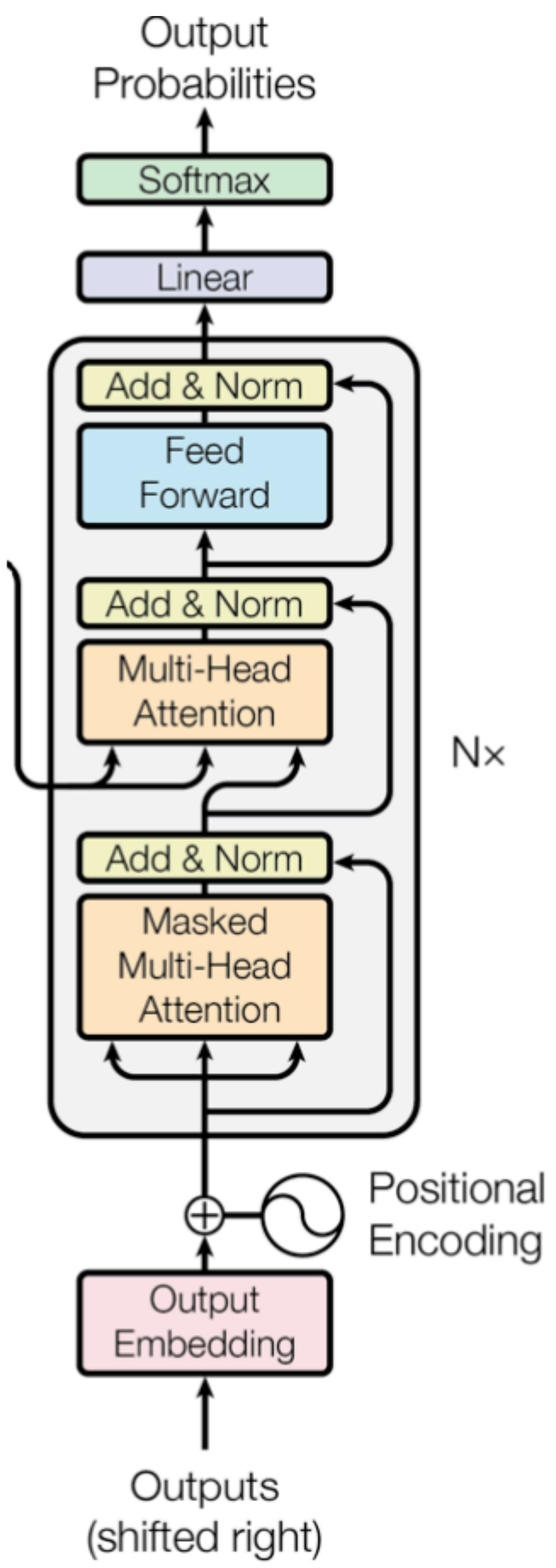
$$\text{MultiHead}(X) = \text{concat}(h_1, \ldots, h_k)W_O$$
$$h_i = \text{attn}(Q_i, K_i, V_i)$$
$$Q_i = (XW_Q)^i, K_i = (XW_K)^i, V_i = (XW_V)^i$$

$$\text{attn}(Q, K, V) = \text{softmax}(\frac{QK^T}{\sqrt{d}})V$$

- **Quadratic computation in self-attention:**
  - Can be very expensive when the sequence is very long
- **Harder to model positional information**

Transformer Decoder

- **Each decoder layer has three sub-layers:**
  - A masked multi-head attention layer
  - A multi-head cross attention layer
  - A feedforward layer
- **Masked multi-head attention**
  - self-attention on the decoder states
- **Multi-head cross attention**
  - Decoder attends to encoder states
  - Encoder: keys/values
  - Decoder: queries



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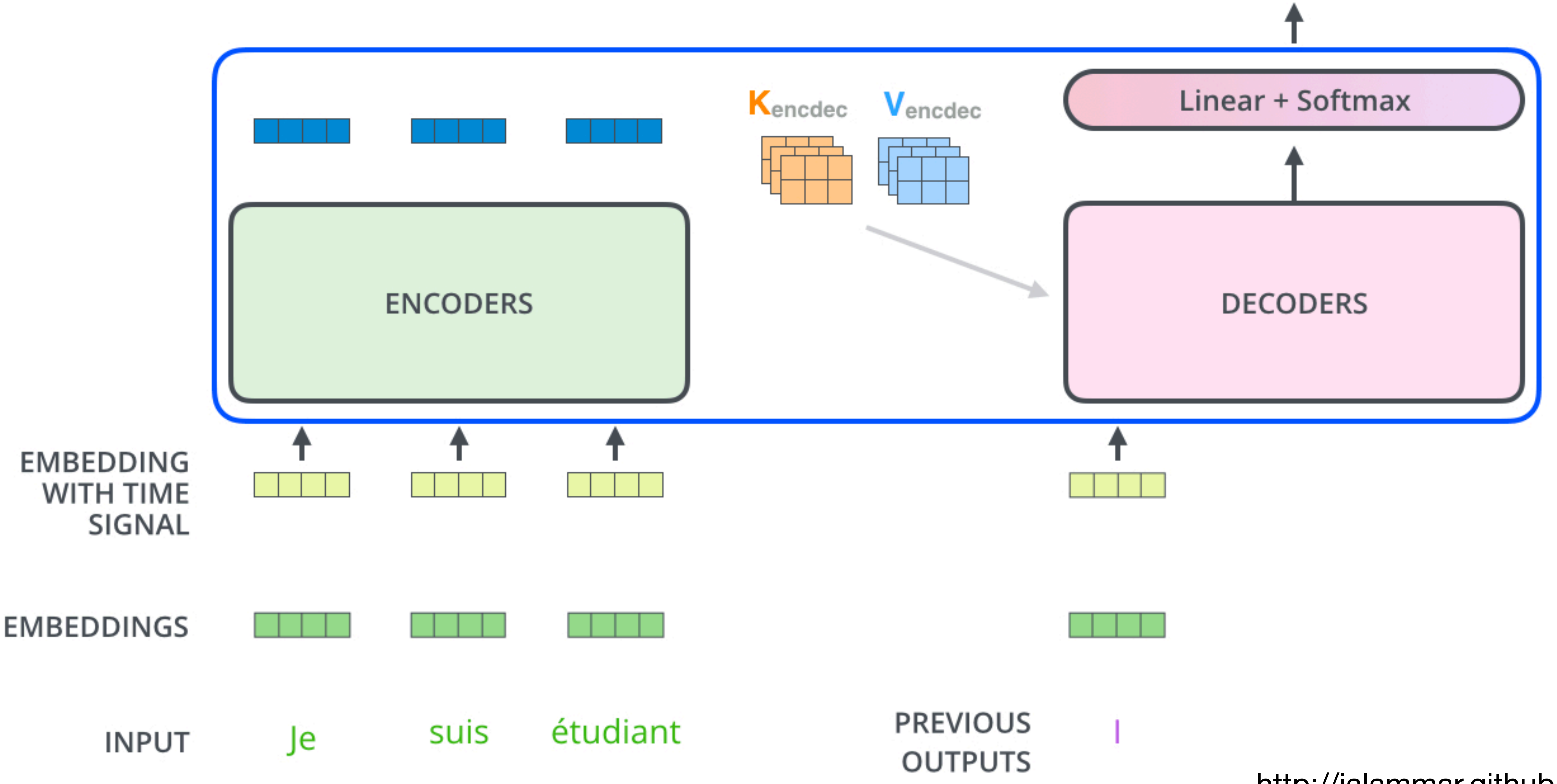
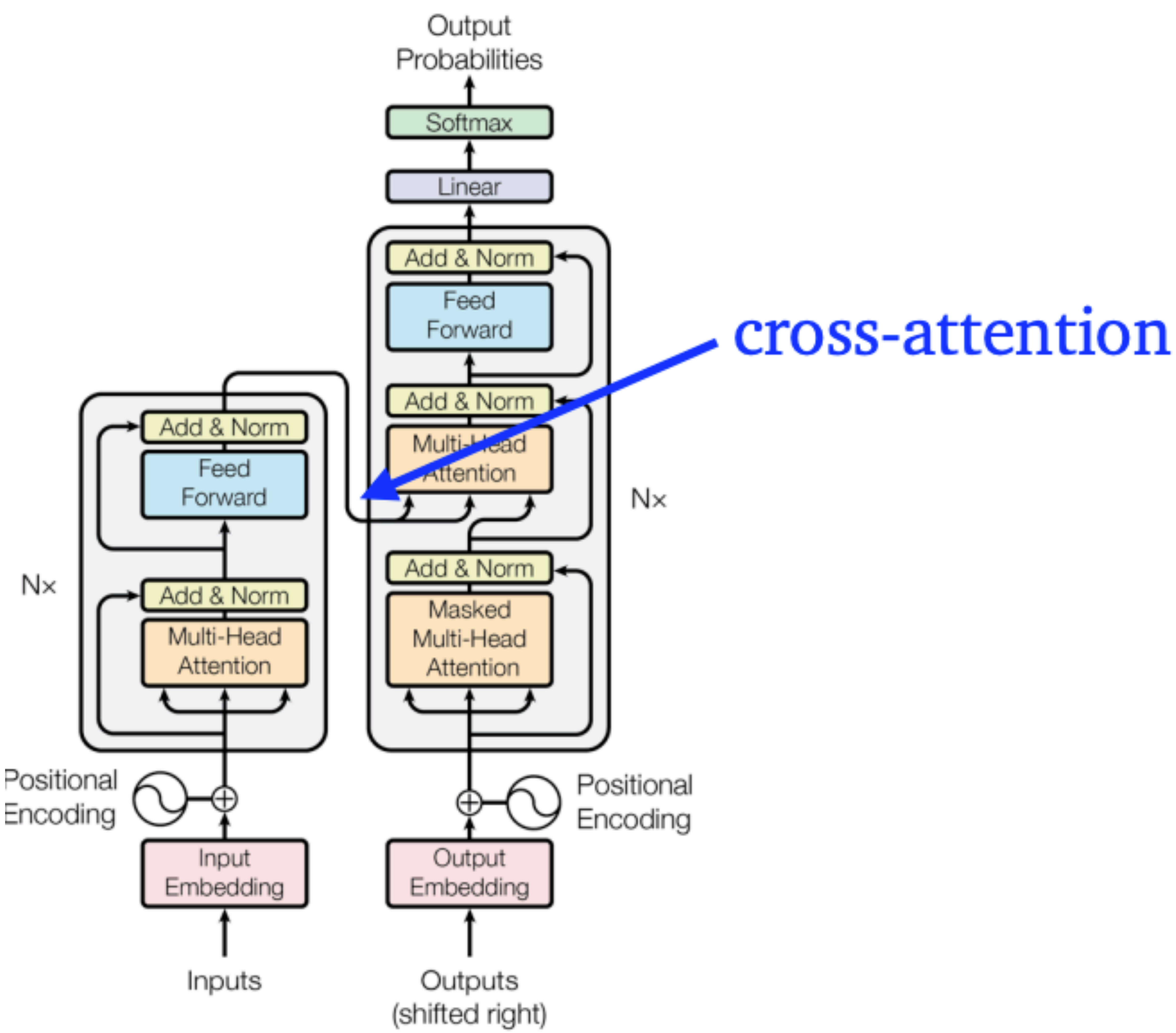
Multi-head Cross Attention

- **Decoder attends to encoder states**
  - Encoder: keys/values
  - Decoder: queries



http://jalammar.github.io/illustrated-transformer/

Multi-head Cross Attention



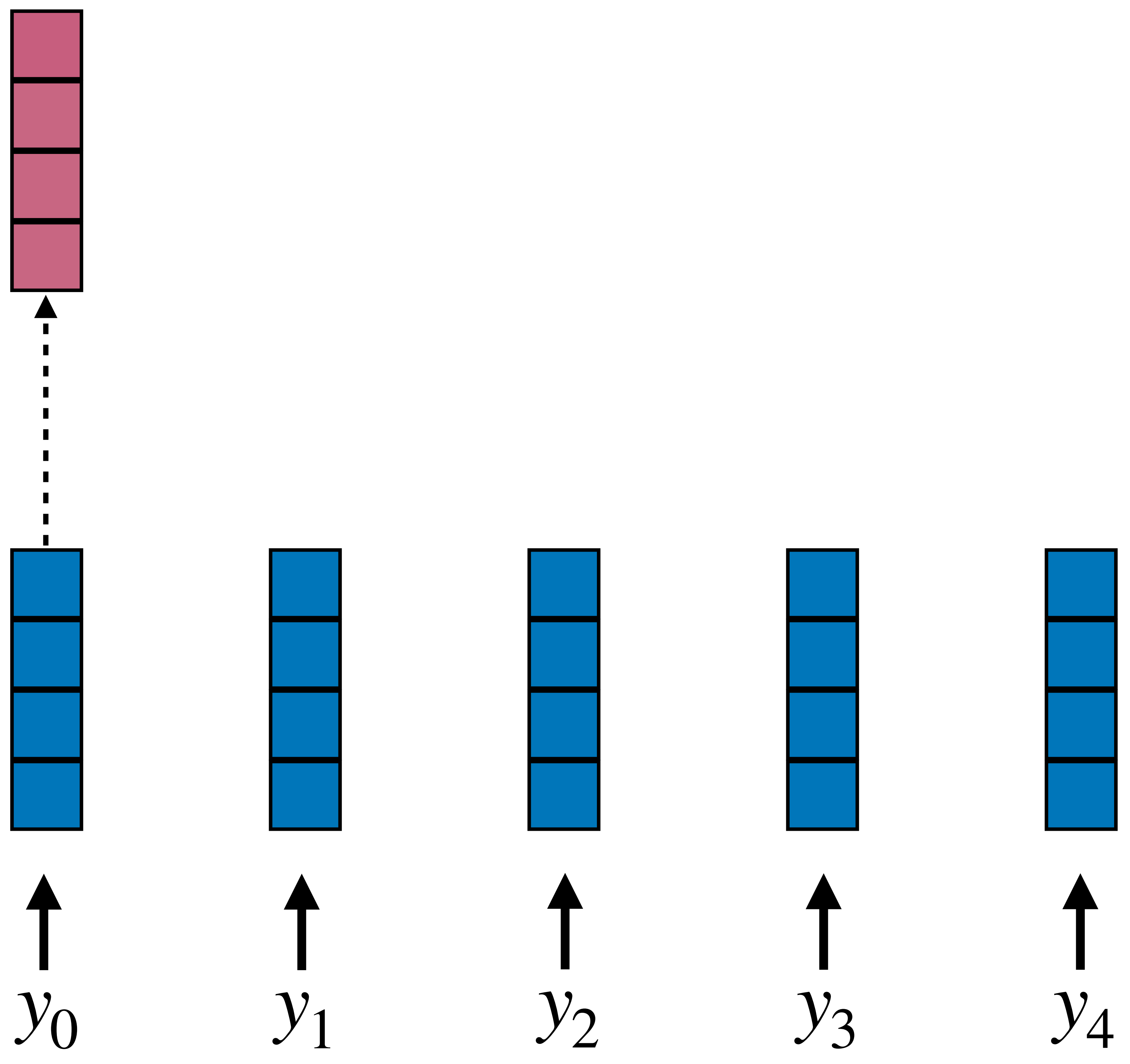
$$q_i = W_Q y_i, \qquad k_i = W_K x_i,\ v_i = W_V x_i$$

$$a_{i,j} = \mathrm{softmax}\left(\frac{q_i^T k_j}{\sqrt{d}}\right)$$

$$y_i' = \sum_{j=1}^{n} a_{i,j} v_j$$

Masked Multi-Head Attention

- **Key point:** we cannot see the future words in decoder
- **Solution:** for every q_i, only attend to $\{(k_j, v_j)\}, j \leq i$



Masked Multi-Head Attention

- **Key point:** we cannot see the future words in decoder
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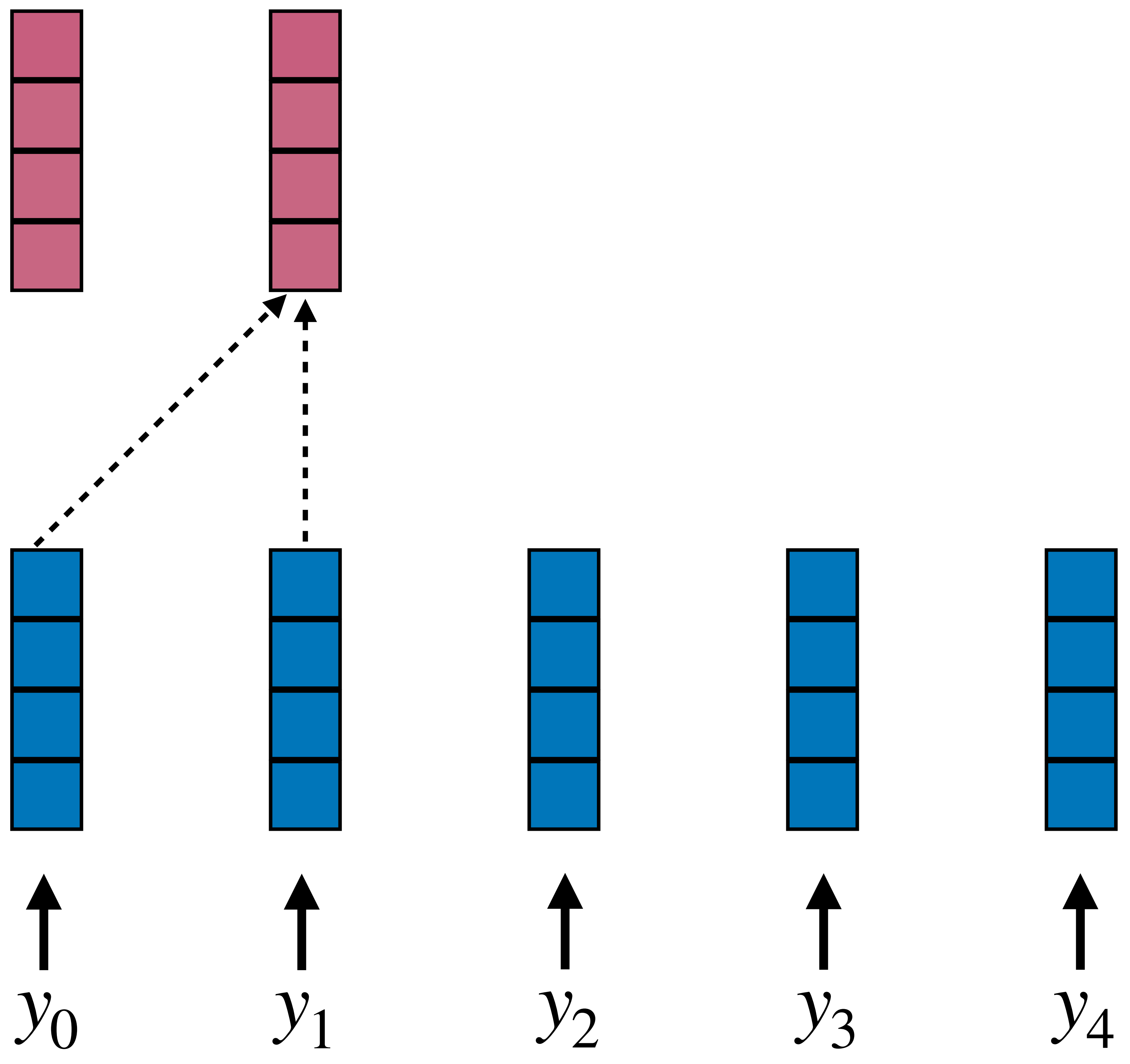
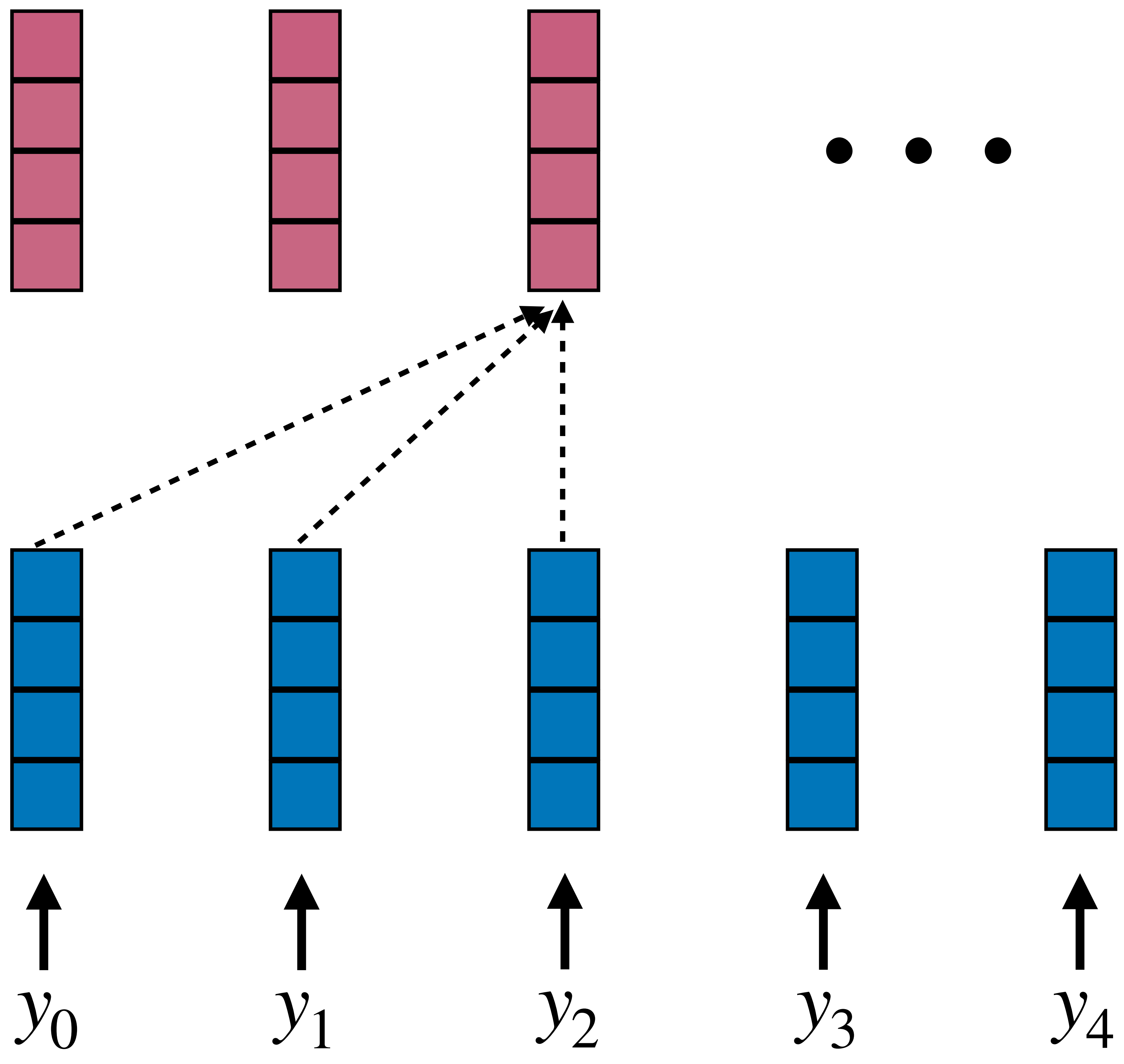


Masked Multi-Head Attention

- **Key point:** we cannot see the future words in decoder
- **Solution:** for every q_i, only attend to $\{(k_j, v_j)\}, j \leq i$

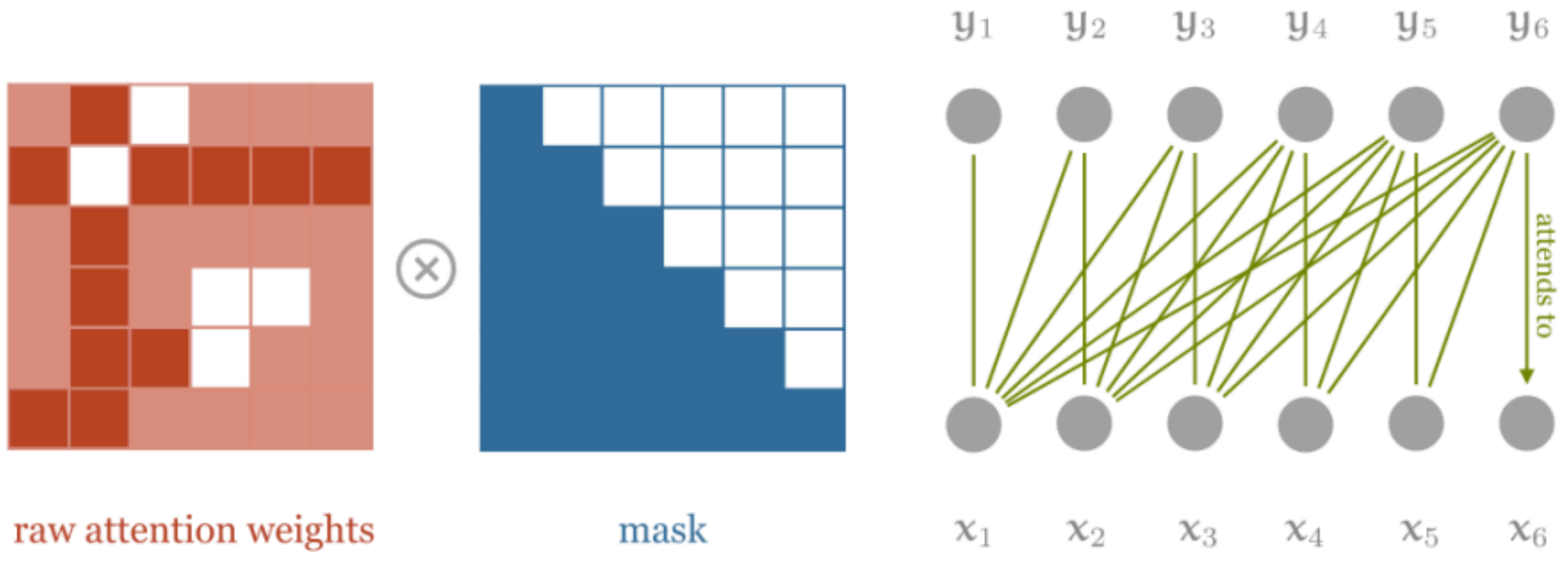


cannot be parallel!

Masked Multi-Head Attention

$$q_i = W_Q x_i,\ k_i = W_K x_i,\ v_i = W_V x_i$$

$$a_{i,j} = \text{softmax}\left(\frac{q_i^T k_j}{\sqrt{d}}\right)$$



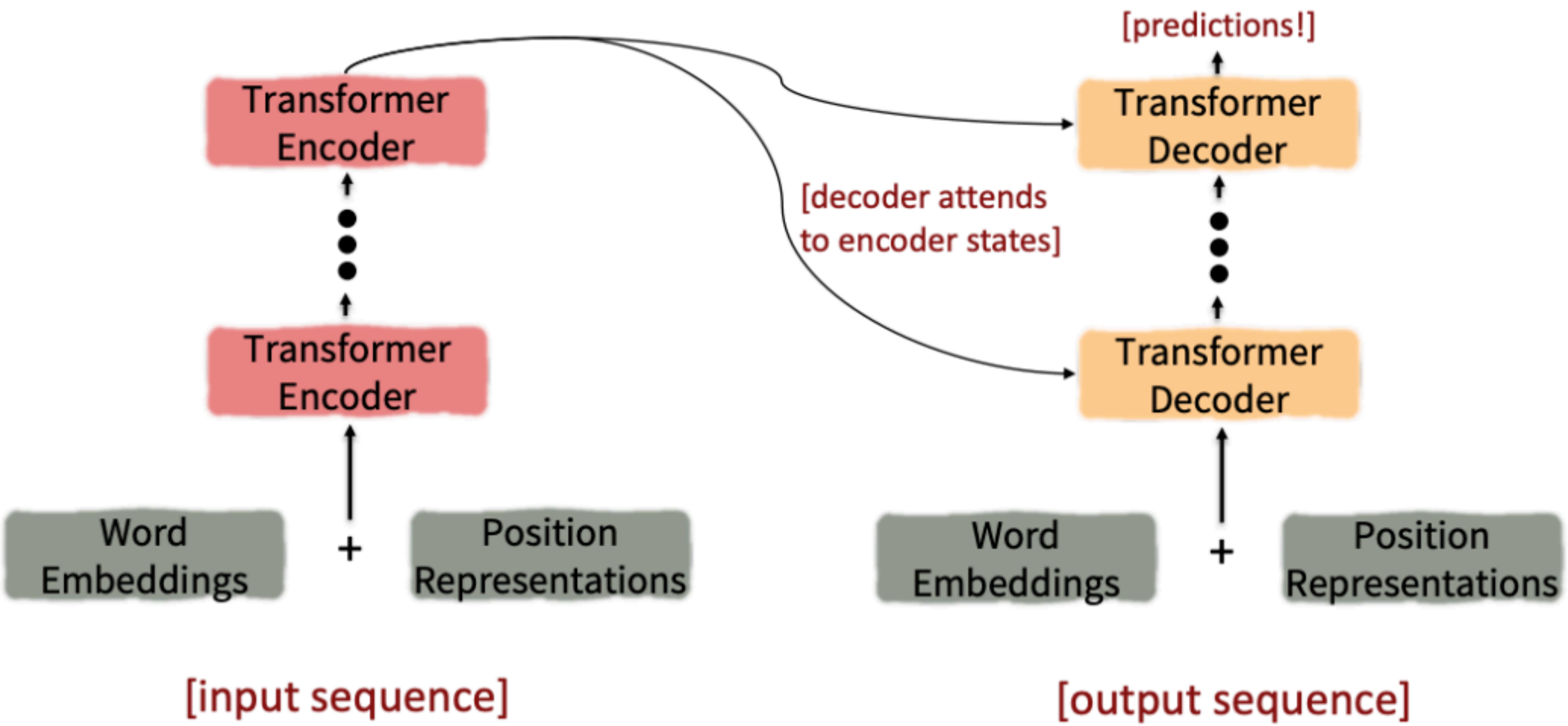
Efficient implementation: compute attention as we normally do, mask out attention to future words by setting attention scores to $-\infty$

```
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

Slide credit: Danqi Chen COS 484/584

Putting the pieces together



Slide credit: Danqi Chen COS 484/584

Transformer: Machine Translation

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	$\mathbf{3.3 \cdot 10^{18}}$	
Transformer (big)	**28.4**	**41.8**	$2.3 \cdot 10^{19}$	

Vaswani et al., 2017: Attention Is All You Need

Transformer: Document Generation

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

Significant gains compared to seq2seq-attention with LSTMs

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