# From Attention to Transformers

Antoine Bosselut

# Outline

- **Transformers**:
  - self-attention
  - multi-headed attention
  - masked attention
  - position embeddings

Some slides adapted from Danqi Chen, Mohit Iyyer, Emma Strubell

# Attention Recap

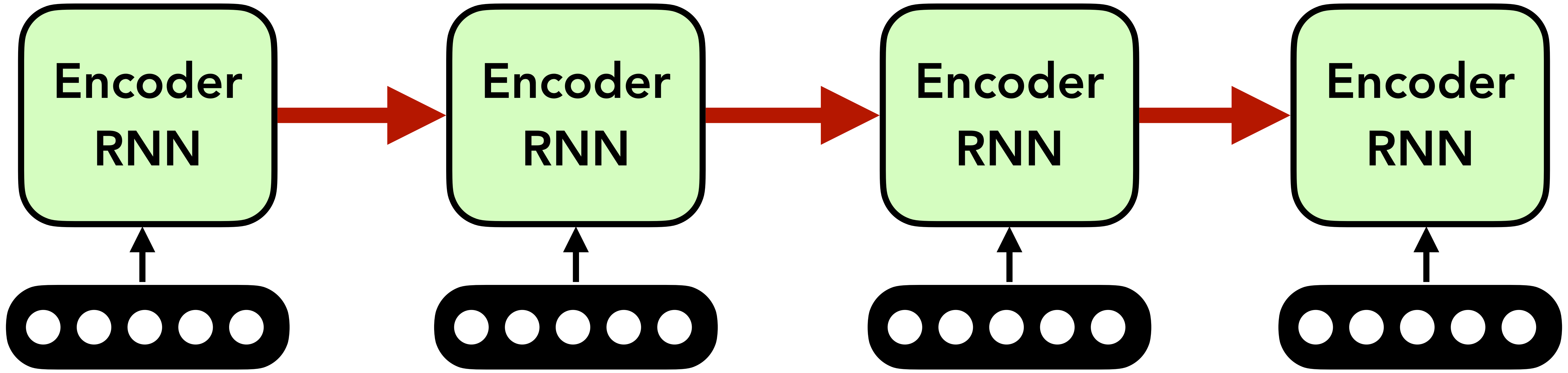
- **Main Idea:** Decoder computes a weighted sum of encoder outputs
  - Compute pairwise score between each encoder hidden state and initial decoder hidden state
- Many possible functions for computing scores (dot product, bilinear, etc.)
- **Temporal Bottleneck Fixed! Direct link** between decoder and encoder states
  - Helps with vanishing gradients and modelling long-term dependencies!
- Attention is **agnostic** to the type of RNN used in the encoder and decoder!

# Question

Do any other inefficiencies remain in our sequence-to-sequence pipelines?

# Encoder is still Recurrent

- **Encoder:** Recurrent functions can't be parallelized because previous state needs to be computed to encode next one



- **Problem: Encoder hidden states must still be computed in series**

# Encoder is still Recurrent

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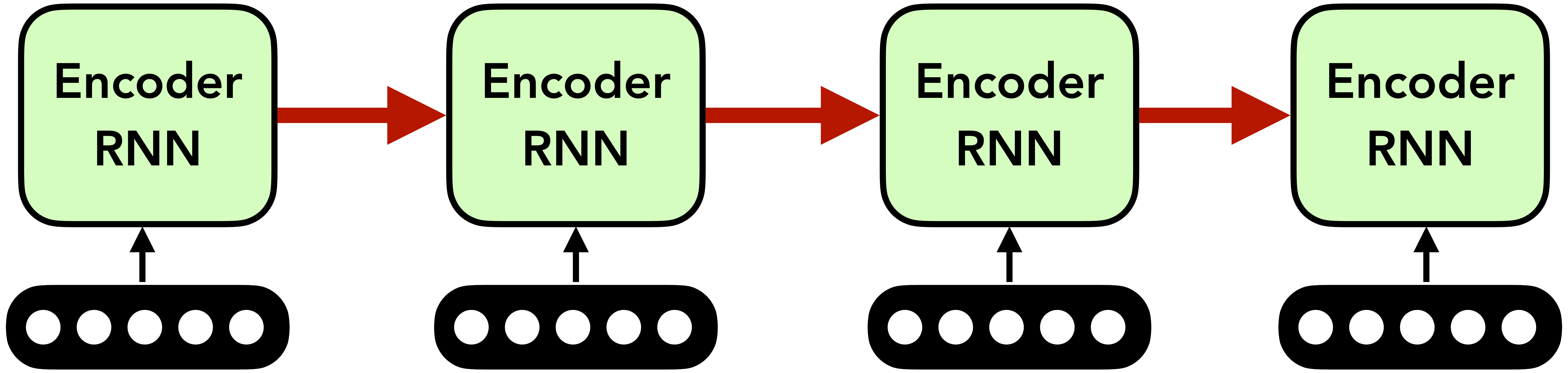


- **Problem: Encoder hidden states must still be computed in series**

**Who can think of a task where this might be a problem?**

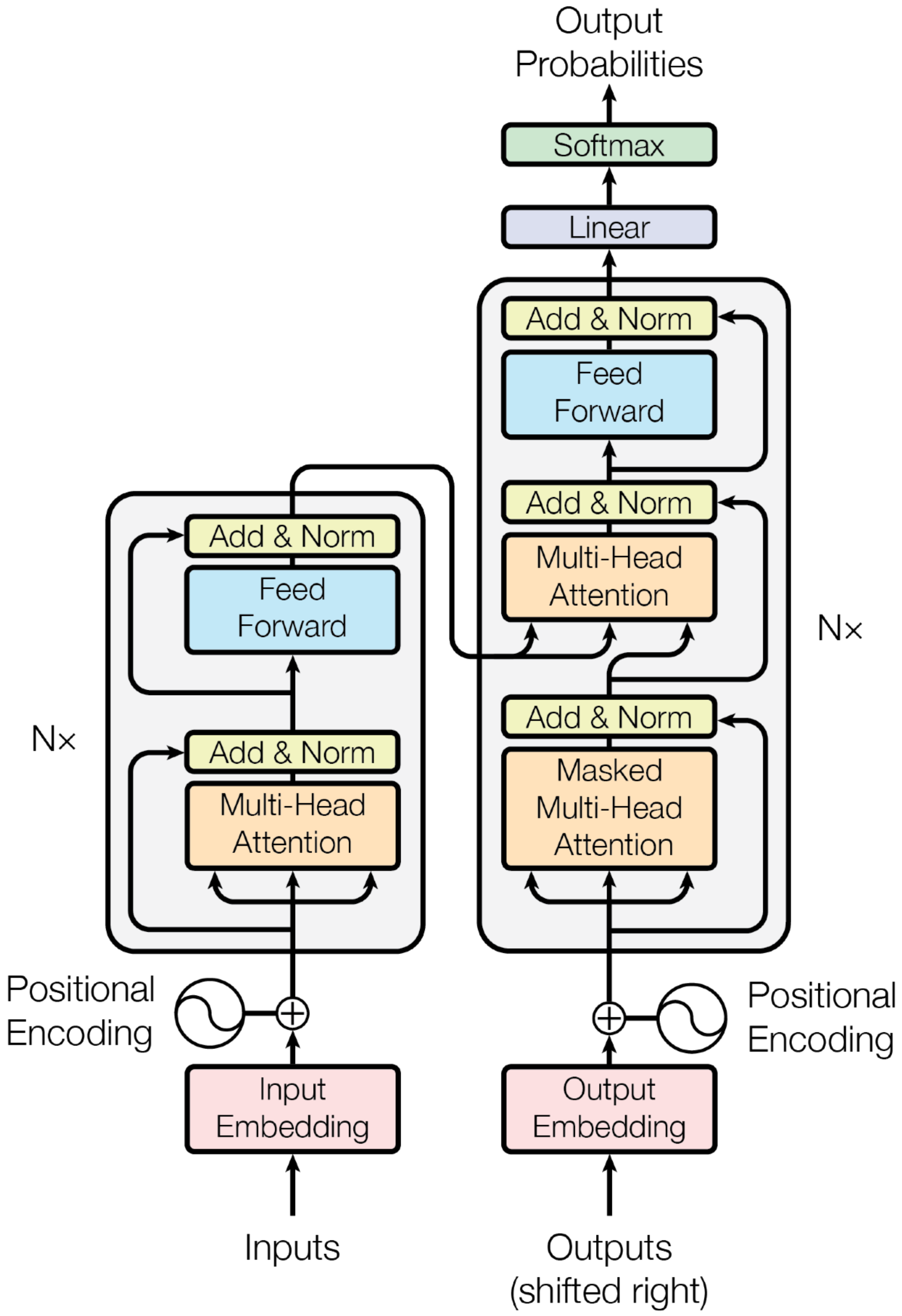
Solution:

**Transformers!**

# Full Transformer

- Made up of encoder and decoder
- Both encoder and decoder made up of multiple cascaded transformer blocks
  - slightly different architecture in encoder and decoder transformer blocks
- Blocks generally made up **multi-headed attention** layers (self-attention) and **feedforward** layers
- No recurrent computations!

**Encode sequences with self-attention**



(Vaswani et al., 2017)

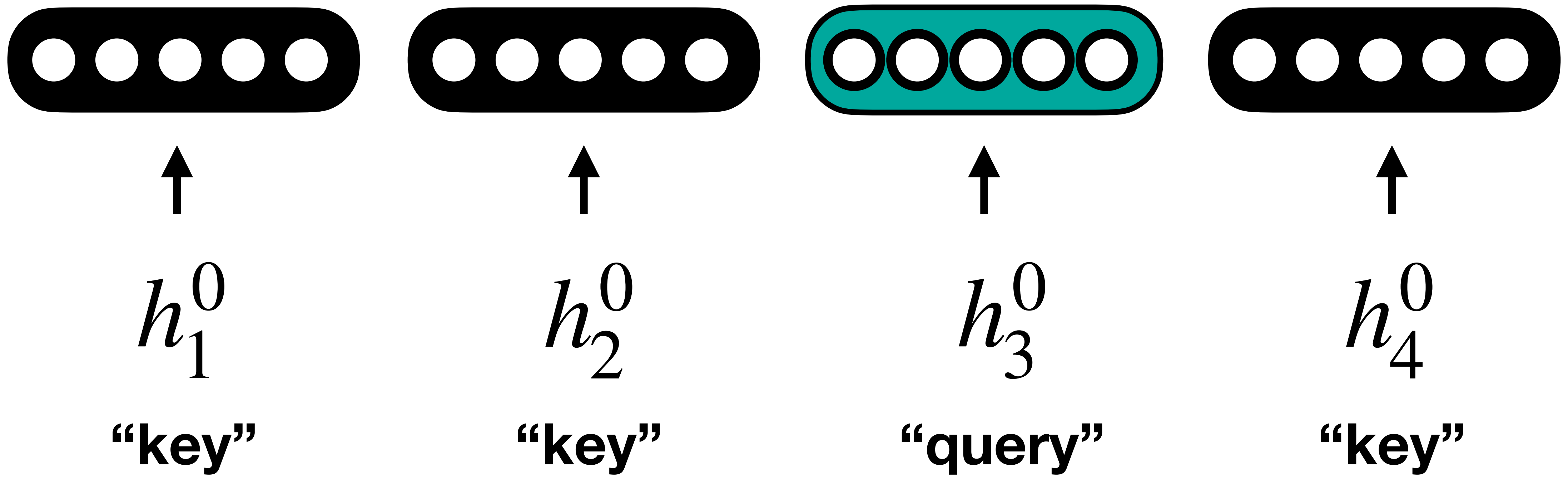
# Self-Attention

- **Original Idea:** Use decoder hidden state to compute attention distribution over encoder hidden states

- **New Idea:** **Could we use encoder hidden states to compute attention distribution over themselves?**

- **Ditch recurrence** and compute encoder state representations in parallel!

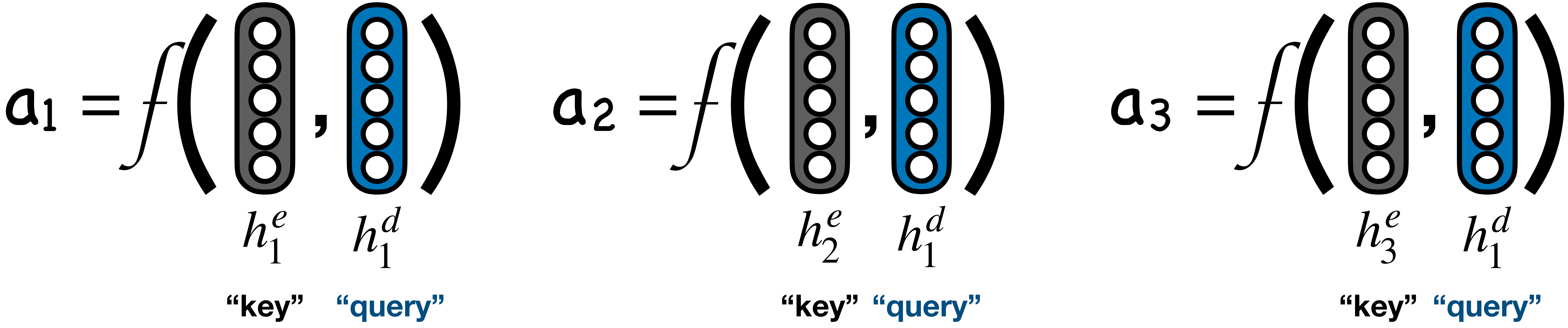
$h_t^\ell$ = encoder hidden state at time step *t* at layer $\ell$



**Note:** Subscripts of *h* have switched back to *t*

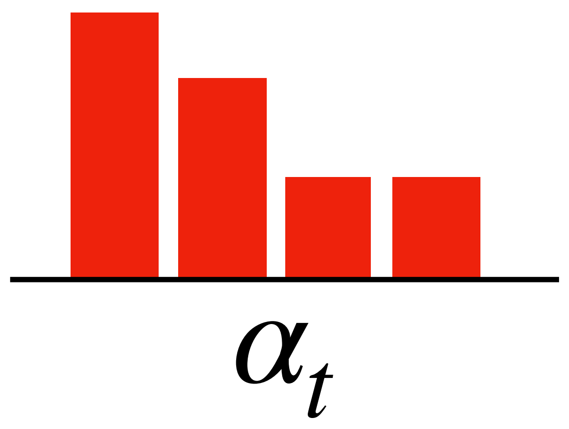
# Recap: Attention with Seq2Seq

- **Compute** pairwise similarity between each encoder hidden state and decoder hidden state ("idea of what to decode")



- **Convert** pairwise similarity scores to probability **distribution** (using softmax!) over encoder hidden states and compute weighted average:

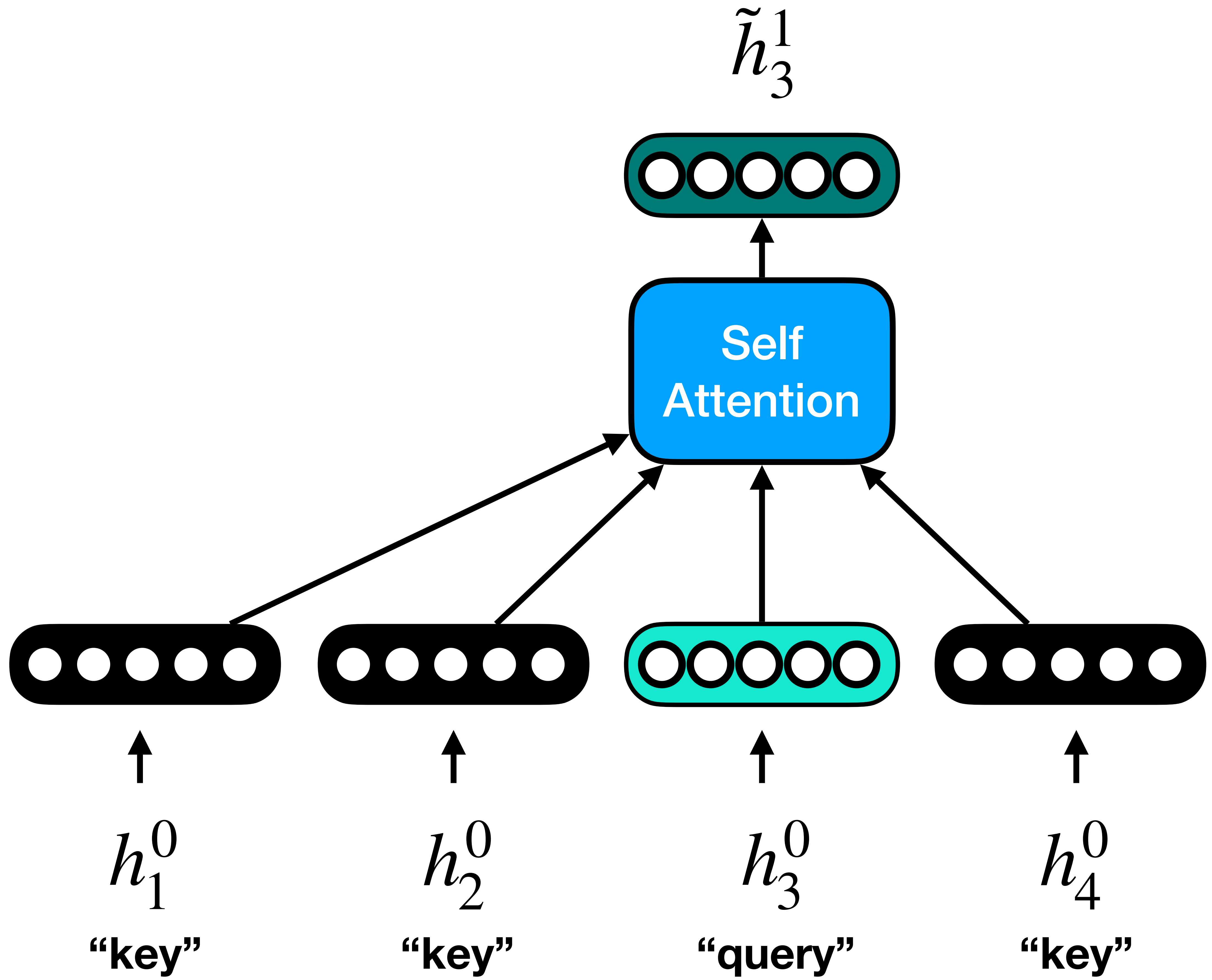
Softmax! $$\boxed{\alpha_t = \frac{e^{a_t}}{\sum_j e^{a_j}}} \rightarrow$$



$$\rightarrow \tilde{h}^d_1 = \sum_{t=1}^{T} \alpha_t h^e_t$$

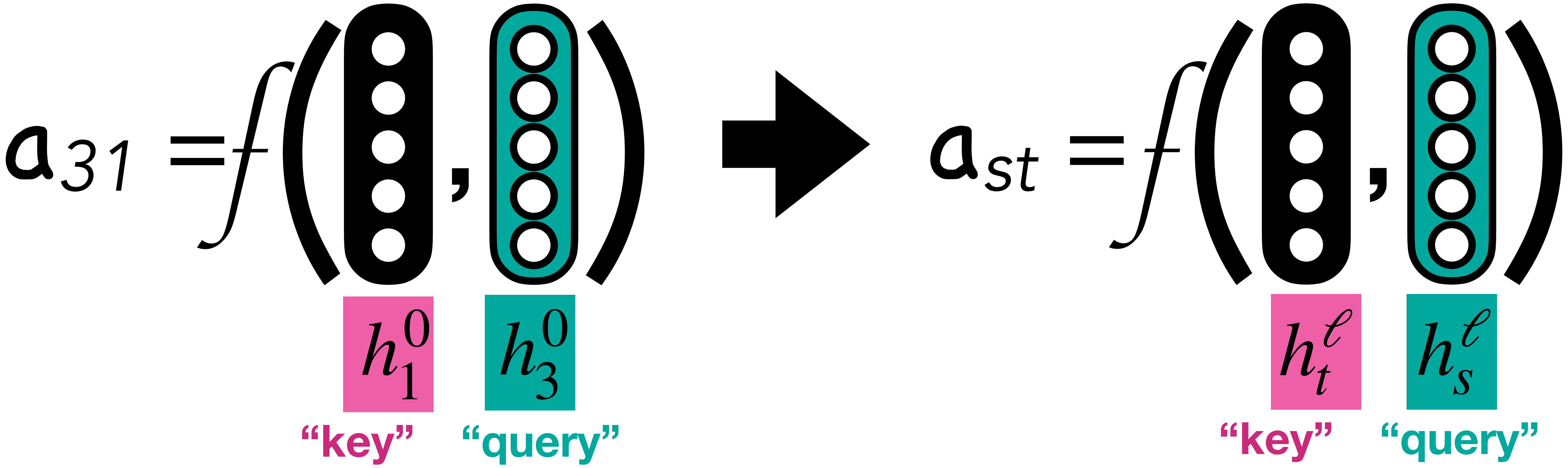
**Here $h^e_t$ is known as the "value"**

# Self-Attention Toy Example



# Self-Attention Toy Example

$h_t^\ell$ = encoder hidden state at time step *t* at layer $\ell$



$$a_{st} = \frac{(\mathbf{W}^Q h_s^\ell)(\mathbf{W}^K h_t^\ell)^T}{\sqrt{d}}$$

Compute pairwise scores

$$\alpha_{st} = \frac{e^{a_{st}}}{\sum_j e^{a_{sj}}}$$

Get attention distribution

$$\tilde{h}_s^\ell = \sum_{t=1}^{T} \alpha_{st}\left(\mathbf{W}^V h_t^\ell\right)$$

Attend to values to get weighted sum

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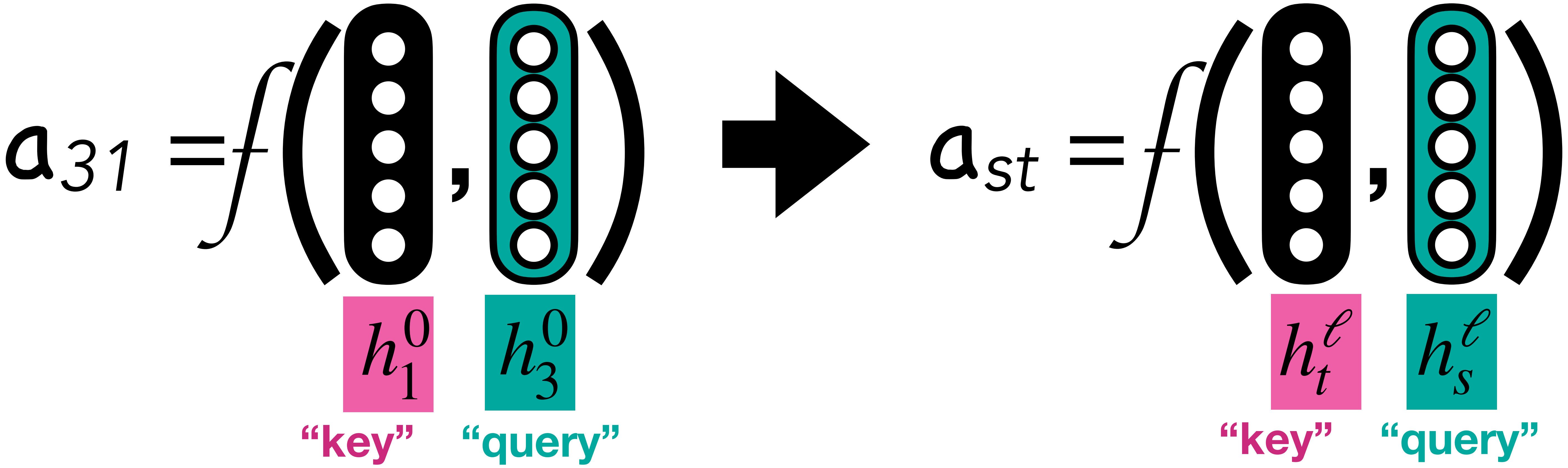

**{1, …, *t*, …, T} includes *s*!**

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**Self-attention!**

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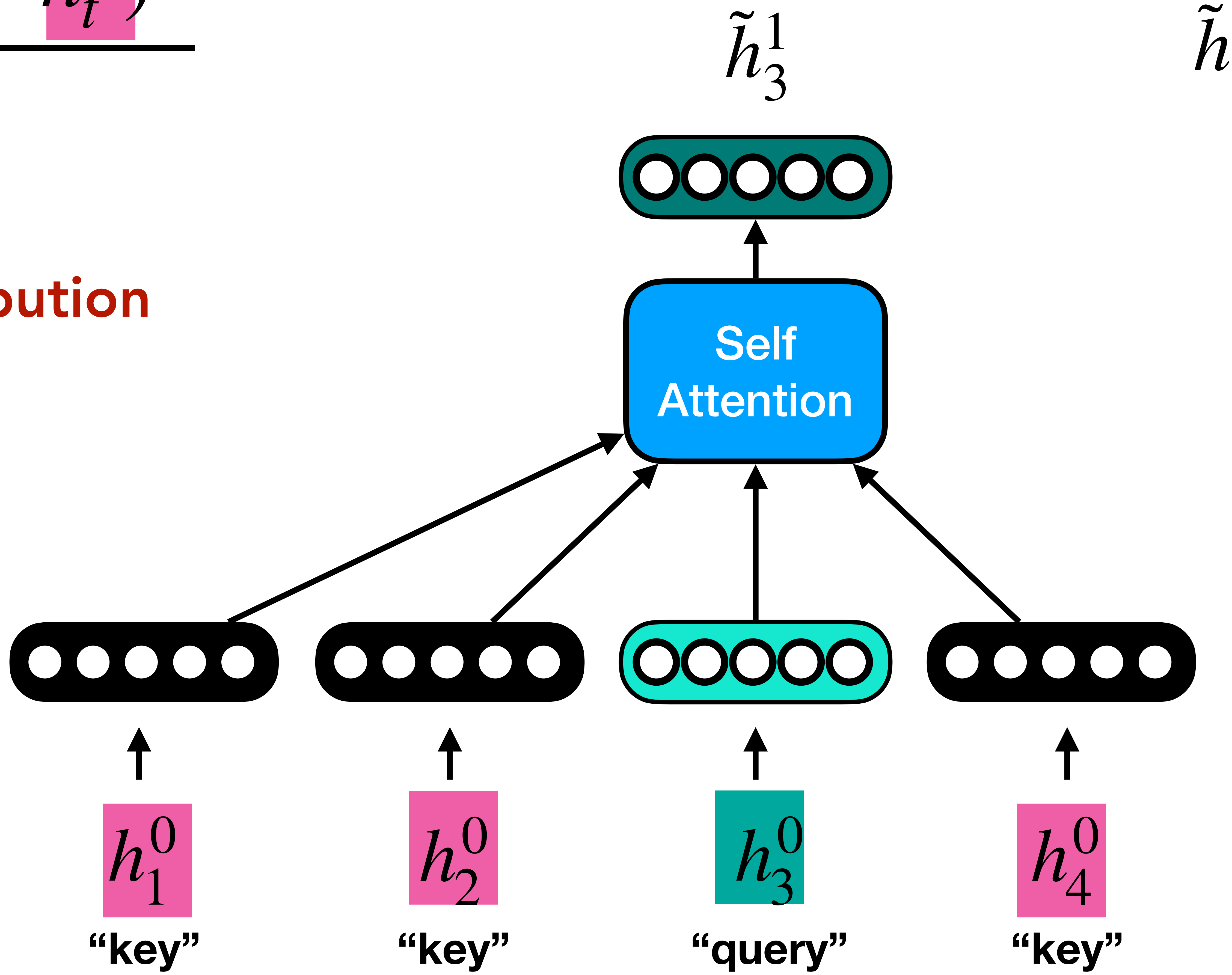


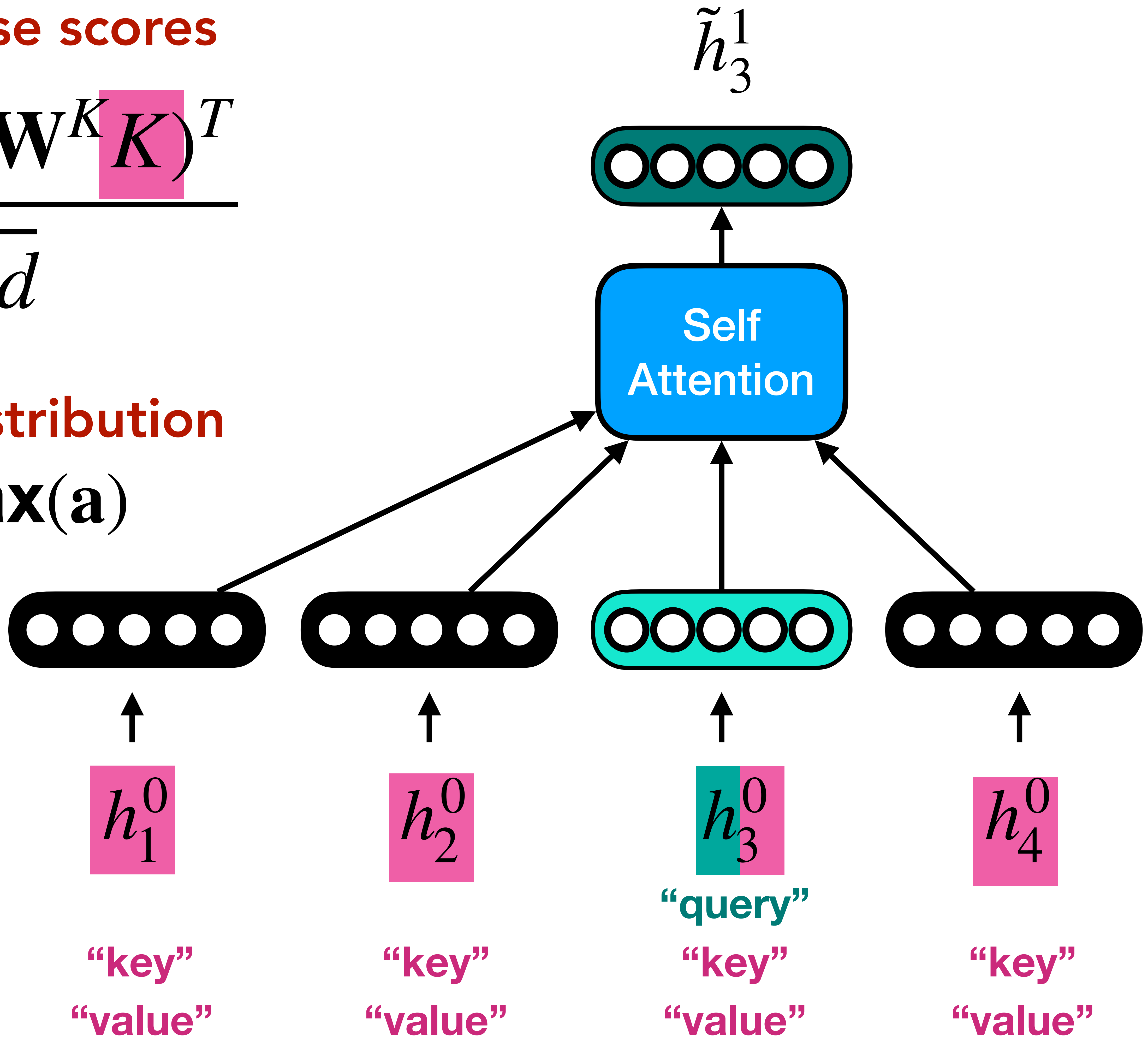
# Self-Attention Toy Example

**Compute pairwise scores**

$$\mathbf{a} = \frac{(\mathbf{W}^Q q)(\mathbf{W}^K K)^T}{\sqrt{d}}$$

**Get attention distribution**

$$\alpha = \textbf{softmax}(\mathbf{a})$$



**Attend to values to get weighted sum**

$$\tilde{h}^\ell = W^O \alpha(V\mathbf{W}^V)$$

"query" $q = h_s^\ell$

"values"

$K = V = \{h_t^\ell\}_{t=0}^T$

"keys"

**For each attention computation, every element is a key and value, and one element is a query**

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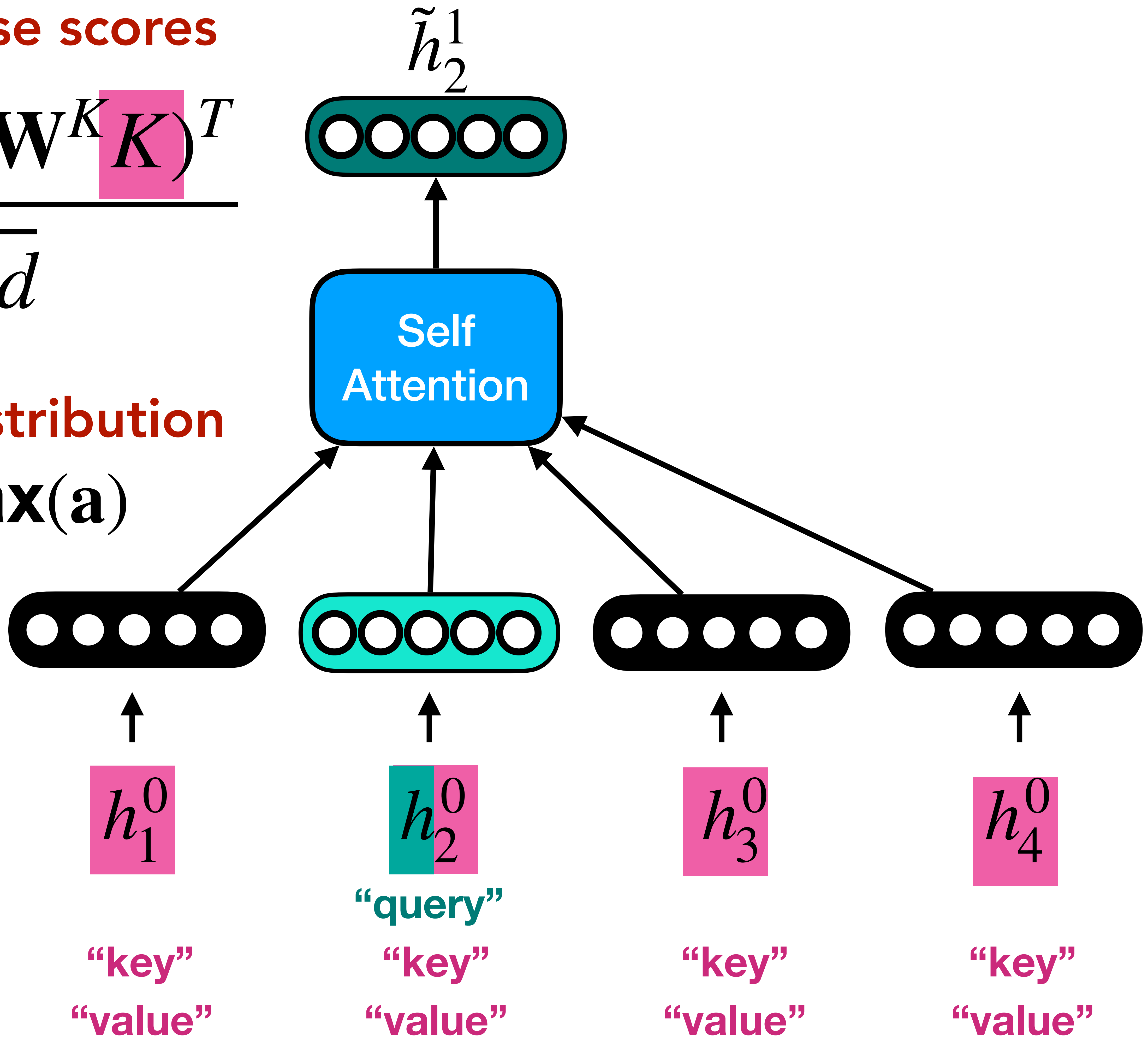

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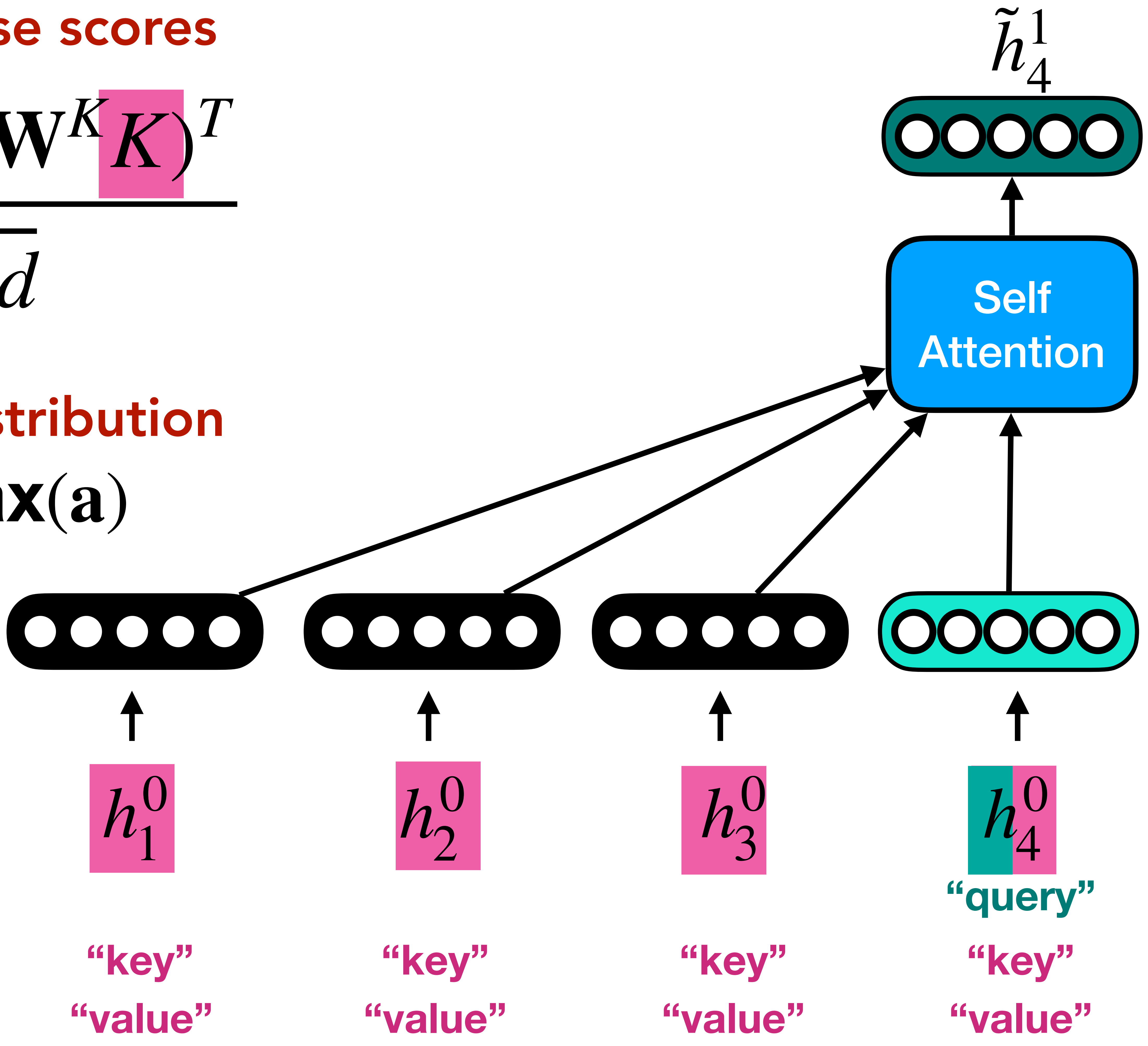

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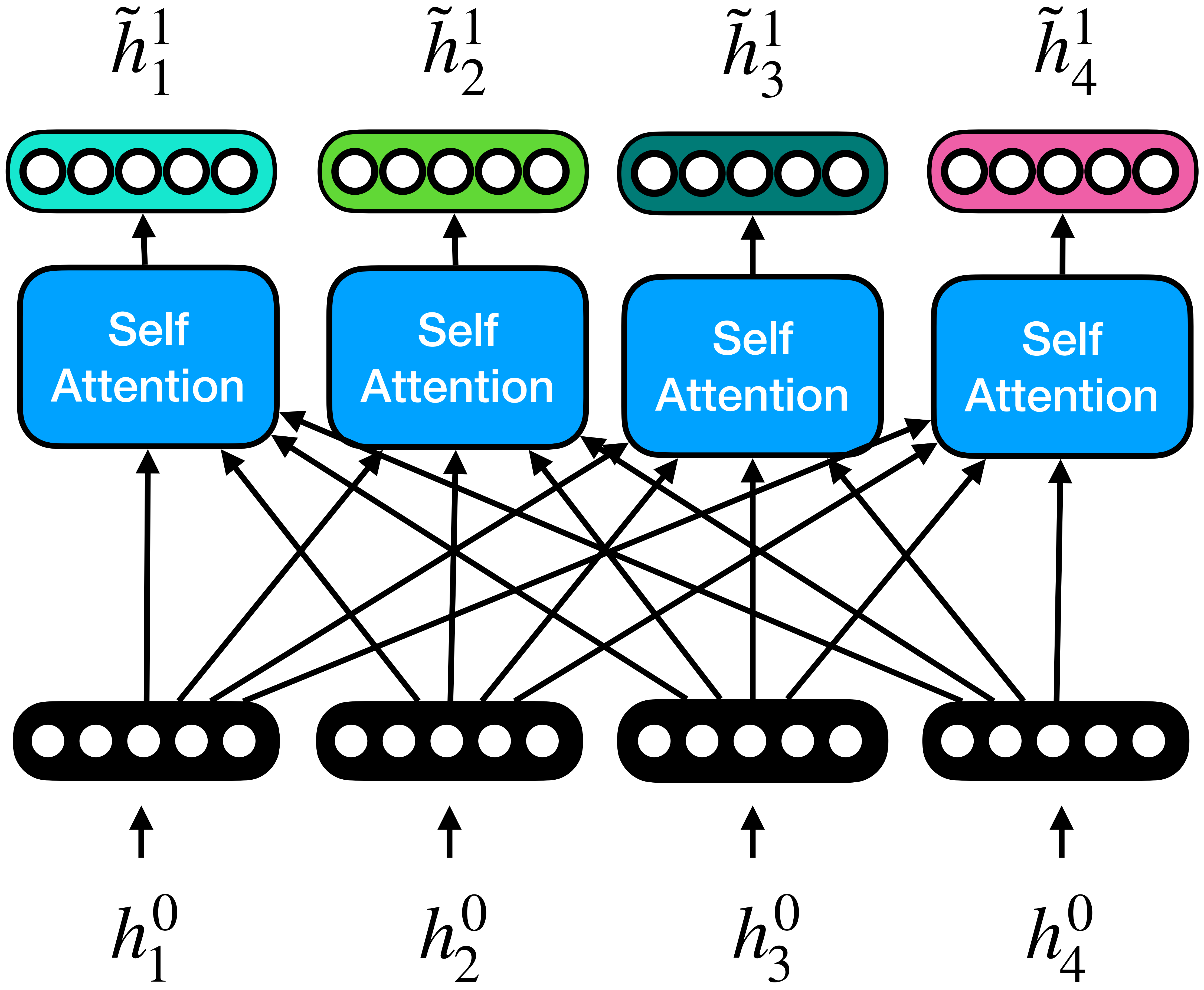


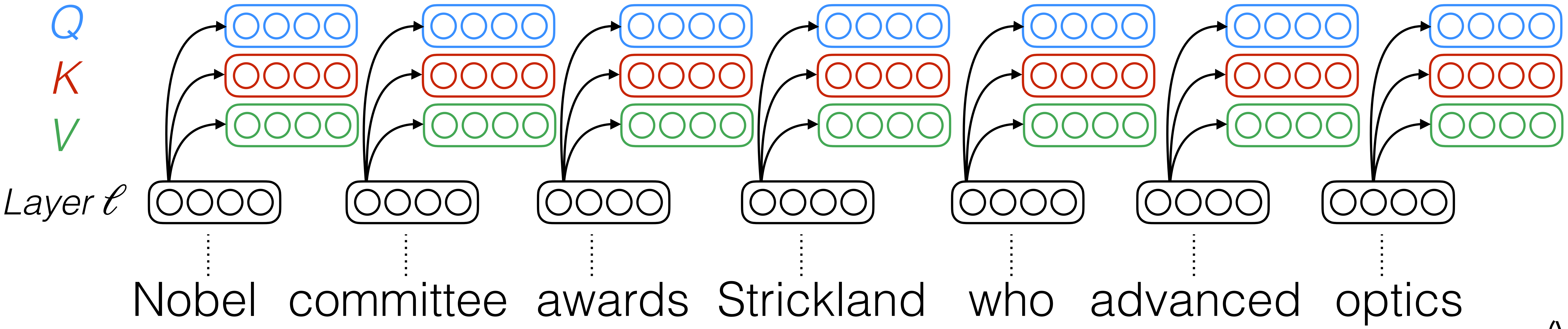
$$\tilde{h}_1^1 = \textbf{Attention}\left(h_1^0, \{h_t^0\}_{t=0}^{t=3}\right)$$

$$\tilde{h}_1^2 = \textbf{Attention}\left(h_2^0, \{h_t^0\}_{t=0}^{t=3}\right)$$

$$\tilde{h}_1^3 = \textbf{Attention}\left(h_3^0, \{h_t^0\}_{t=0}^{t=3}\right)$$

$$\tilde{h}_1^4 = \textbf{Attention}\left(h_4^0, \{h_t^0\}_{t=0}^{t=3}\right)$$

# Self-attention (in encoder)



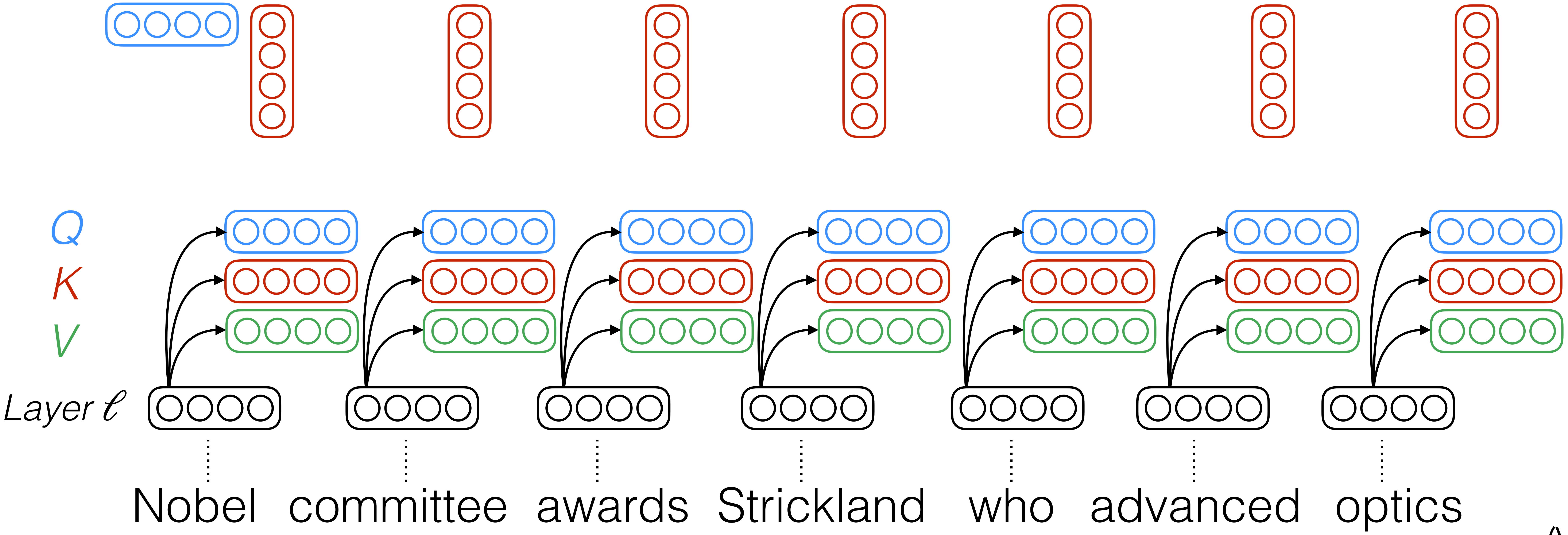
(Vaswani et al., 2017)

# Self-attention (in encoder)

$$\mathbf{a_t} = \frac{(\mathbf{W}^Q Q_t)(\mathbf{W}^K K)^T}{\sqrt{d}}$$

**Keys *K* & values *V* are the same at every time step: Projected token representations**

**Query $Q_t$ changes at every time step since the current token serves as the query**



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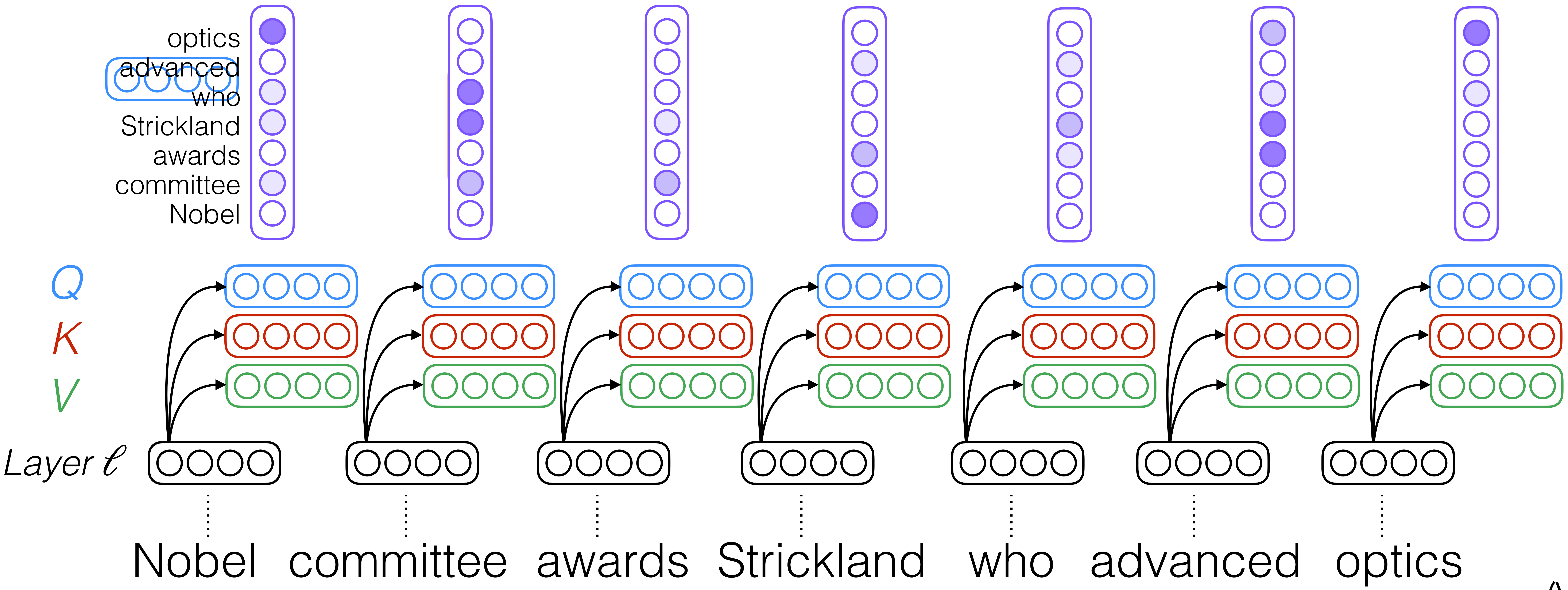

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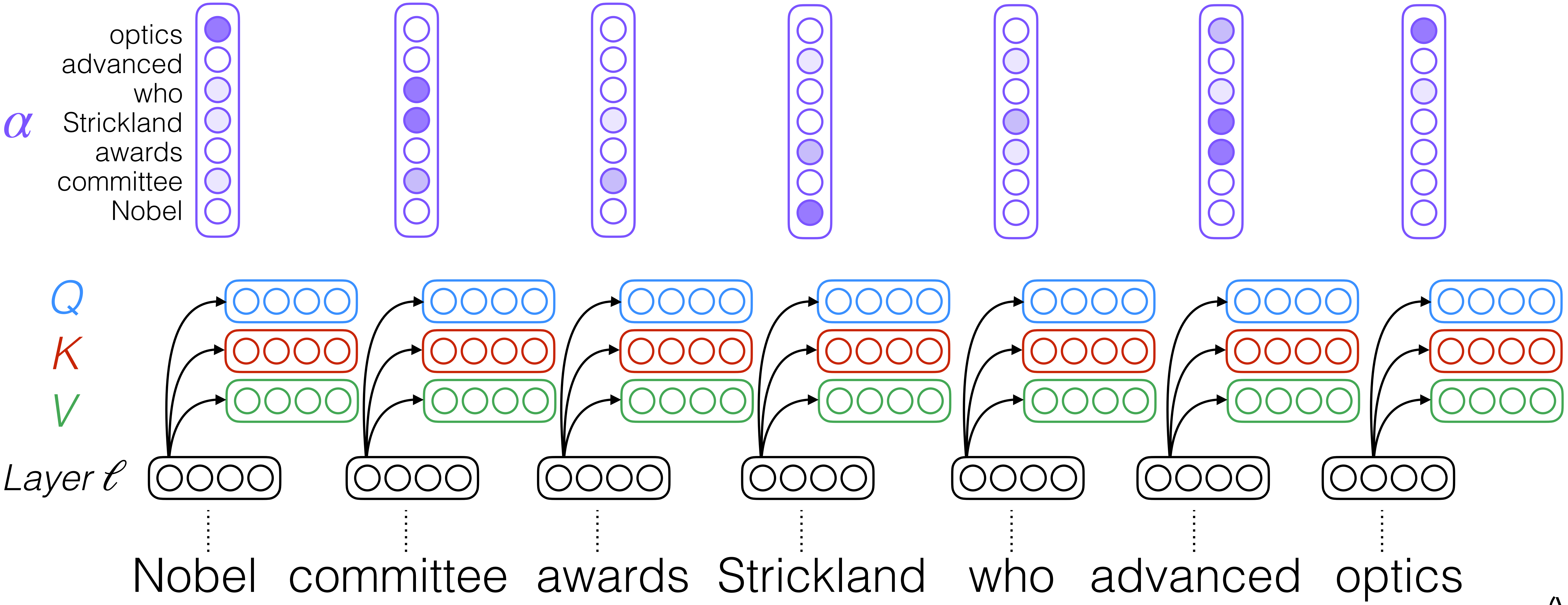

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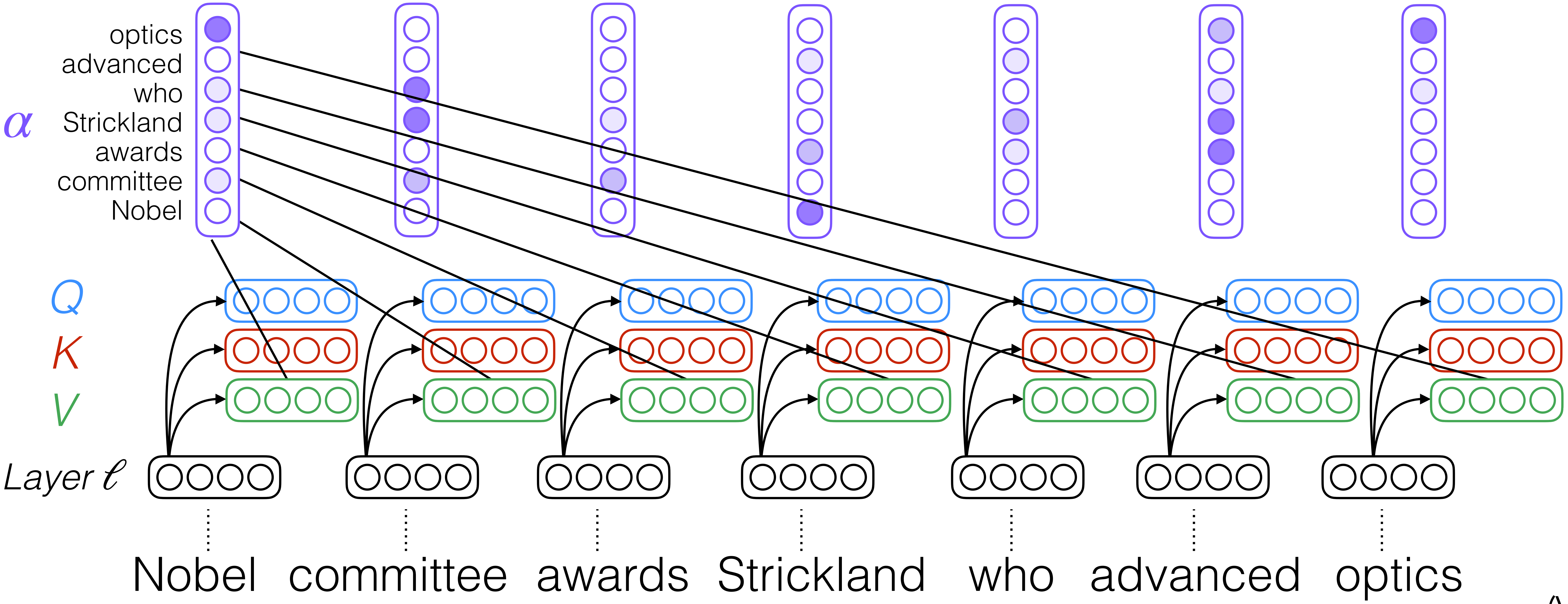

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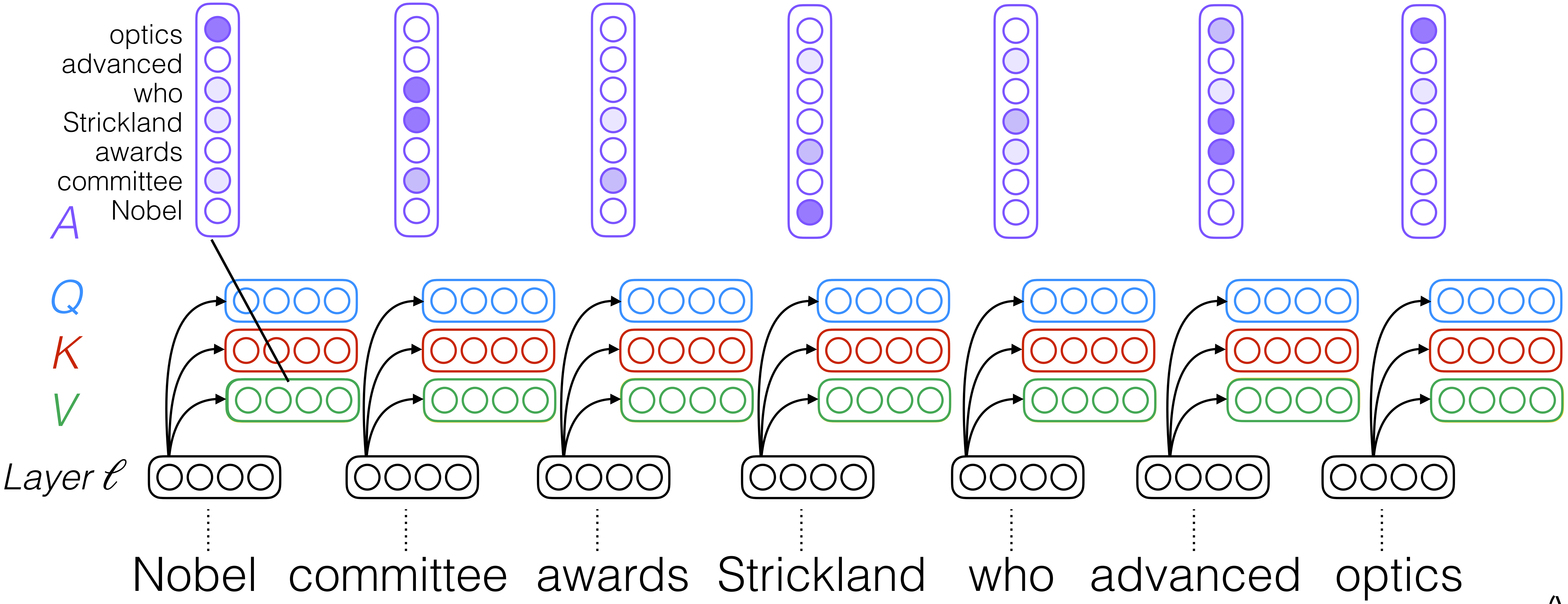

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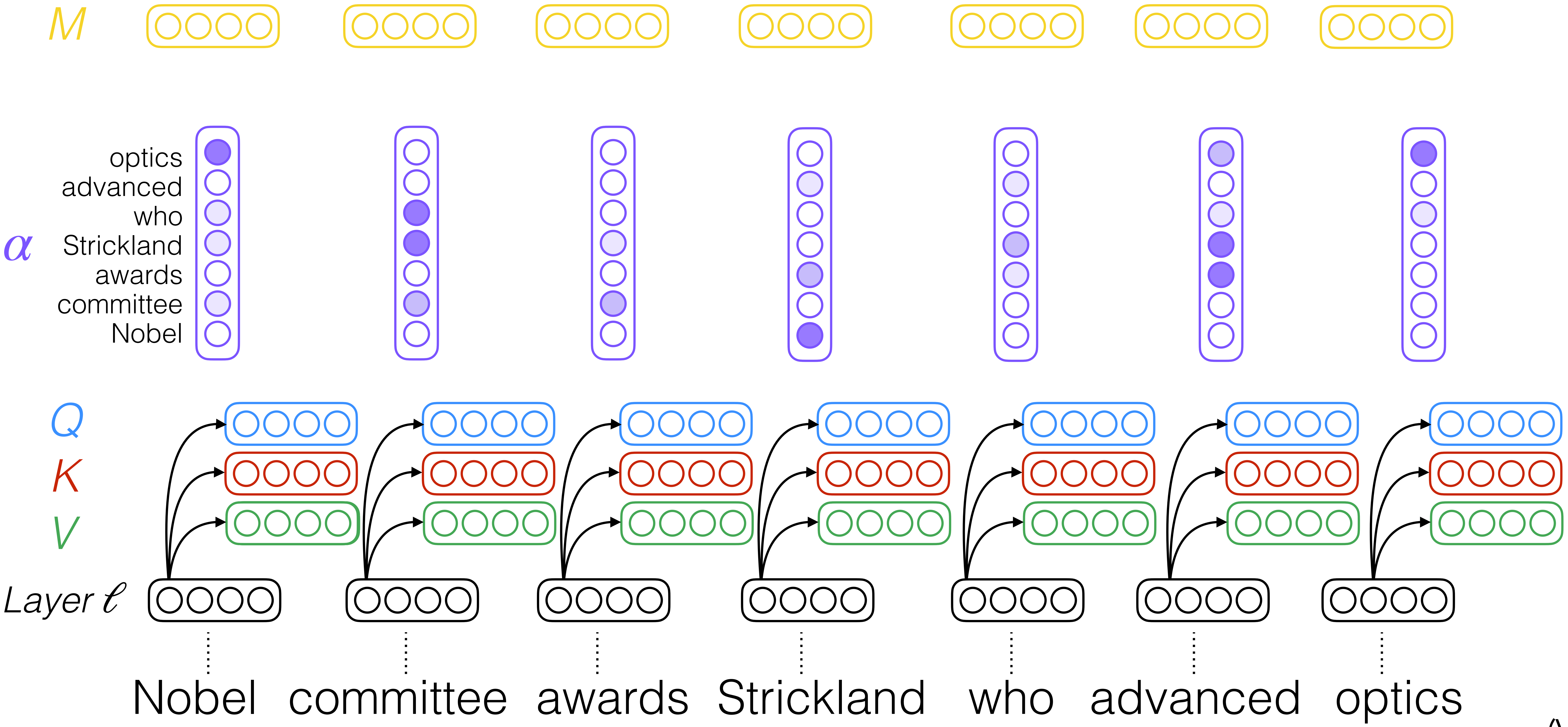

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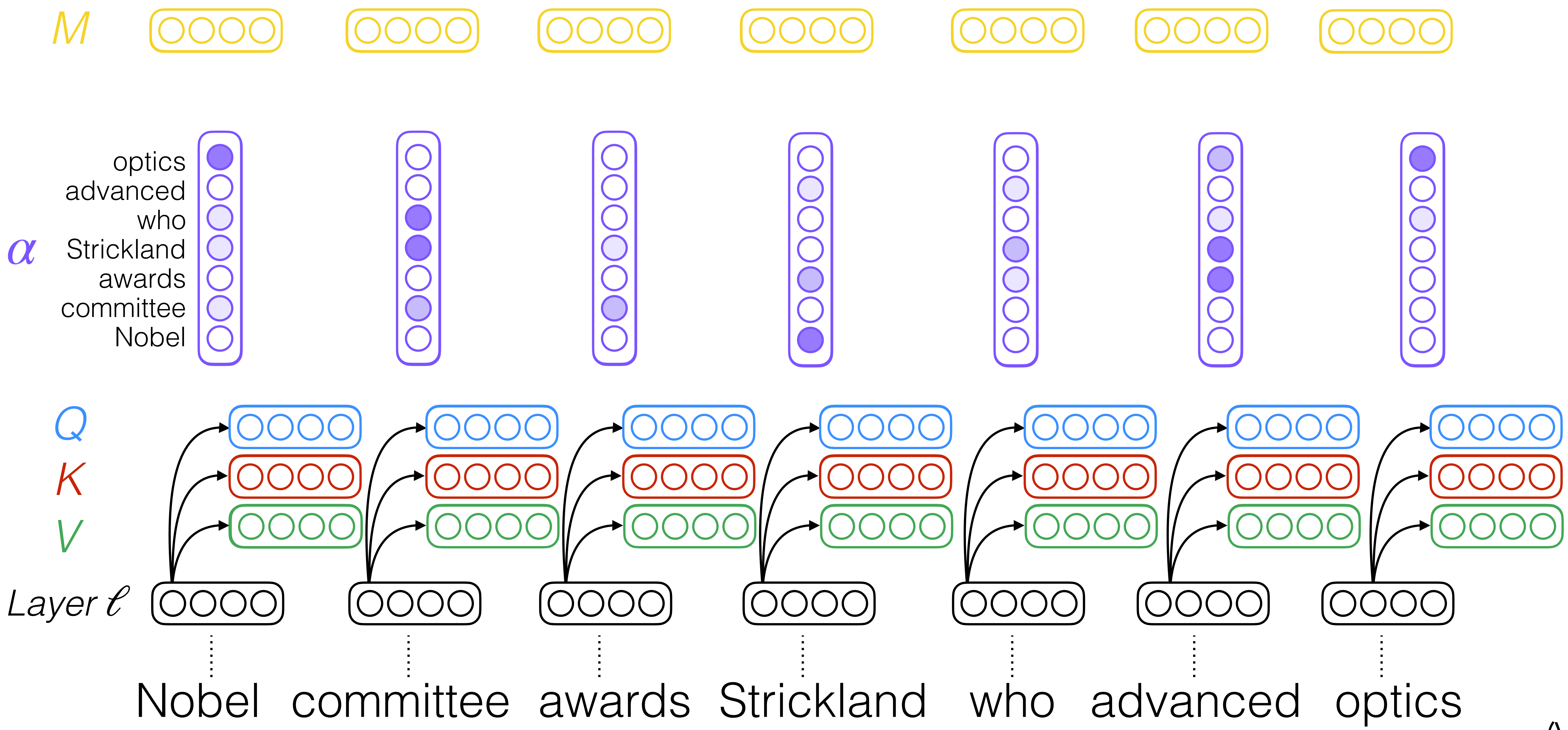

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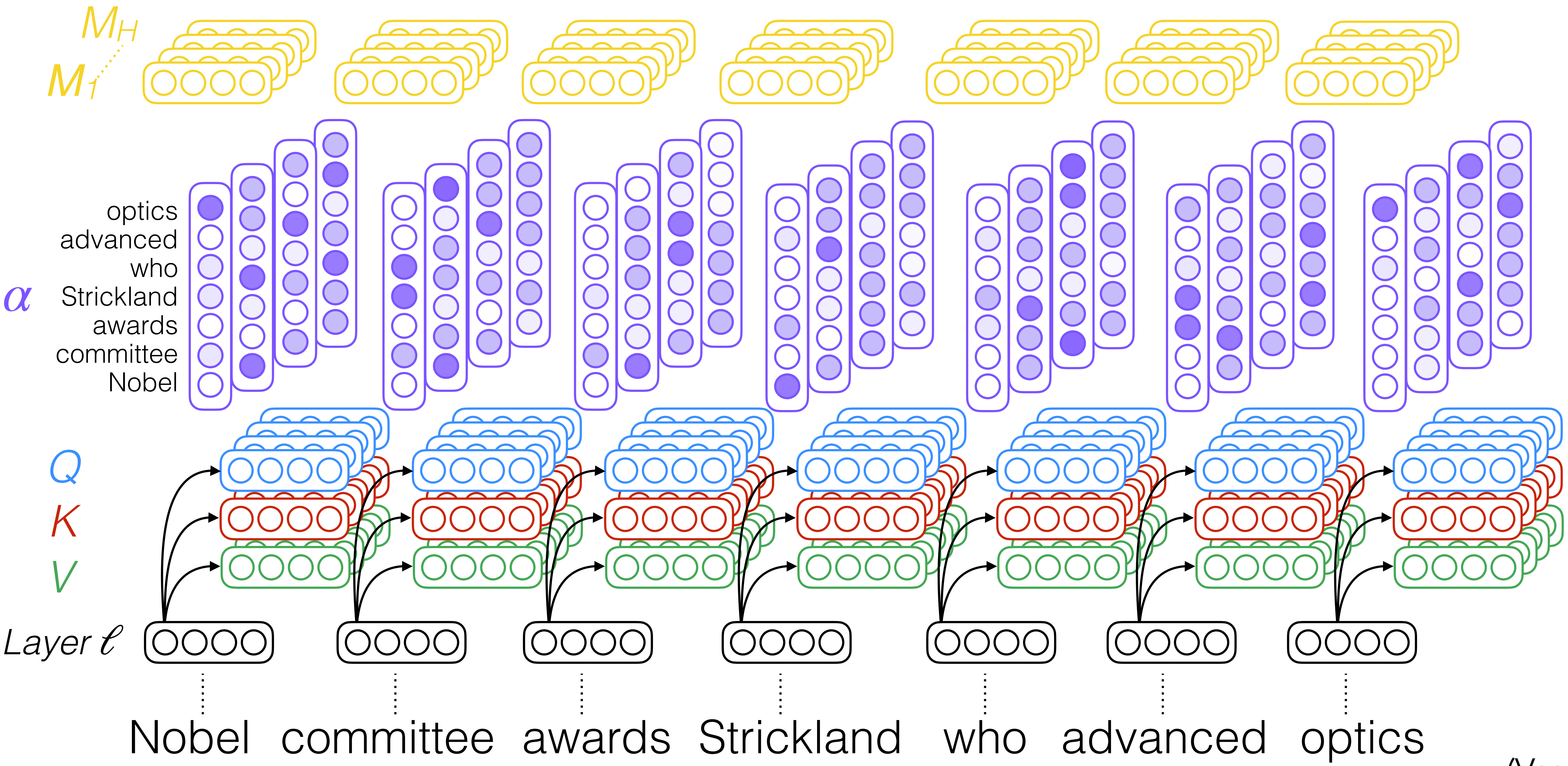
$$\mathbf{a}_{h,t} = \frac{(\mathbf{W}_h^Q Q_t)(\mathbf{W}_h^K K)^T}{\sqrt{d/H}} \qquad \alpha_{h,t} = \mathbf{softmax}(\mathbf{a}_{h,t}) \qquad M_{h,t} = \alpha_{h,t}(V\mathbf{W}_h^V)$$



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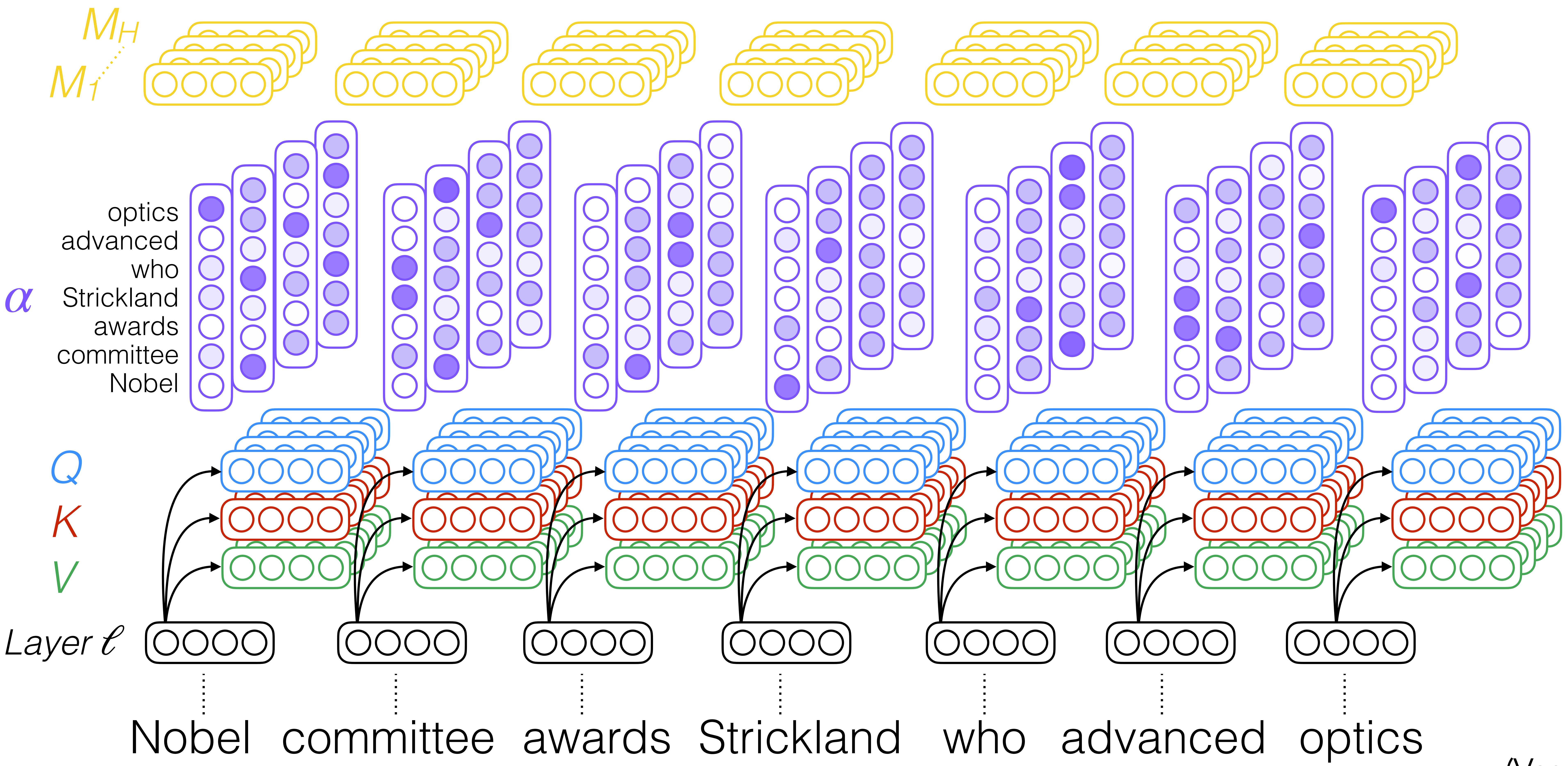

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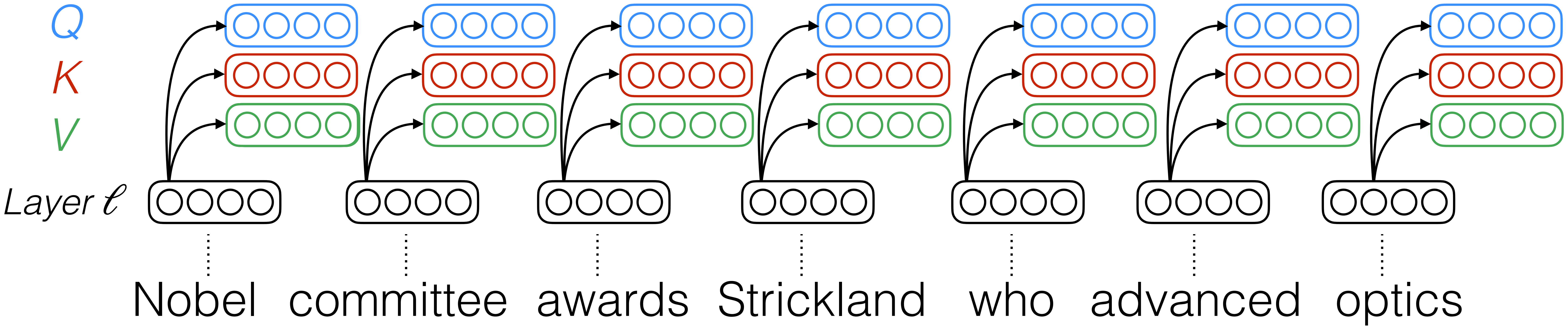
# Single Headed Attention:



$$\mathbf{a_t} = \frac{(\mathbf{W}^Q Q_t)(\mathbf{W}^K K)}{\sqrt{d}}$$

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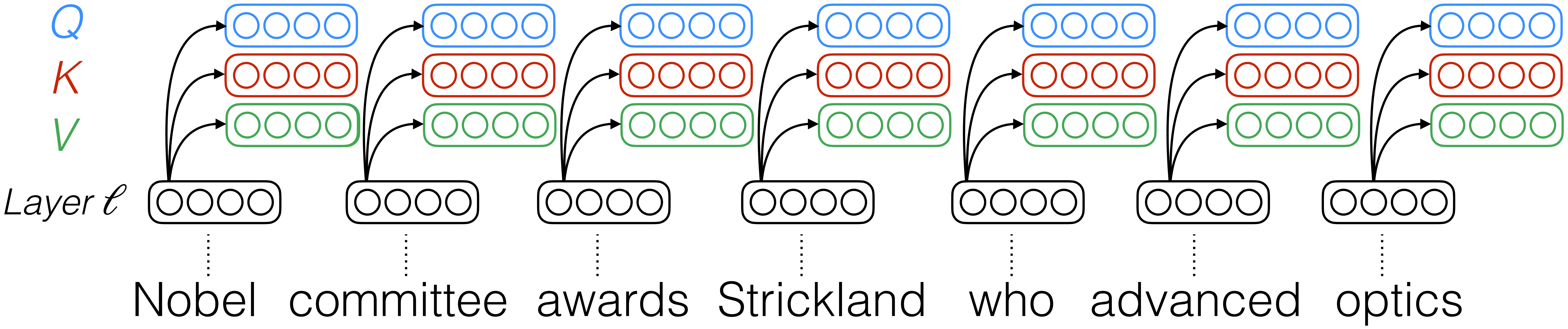

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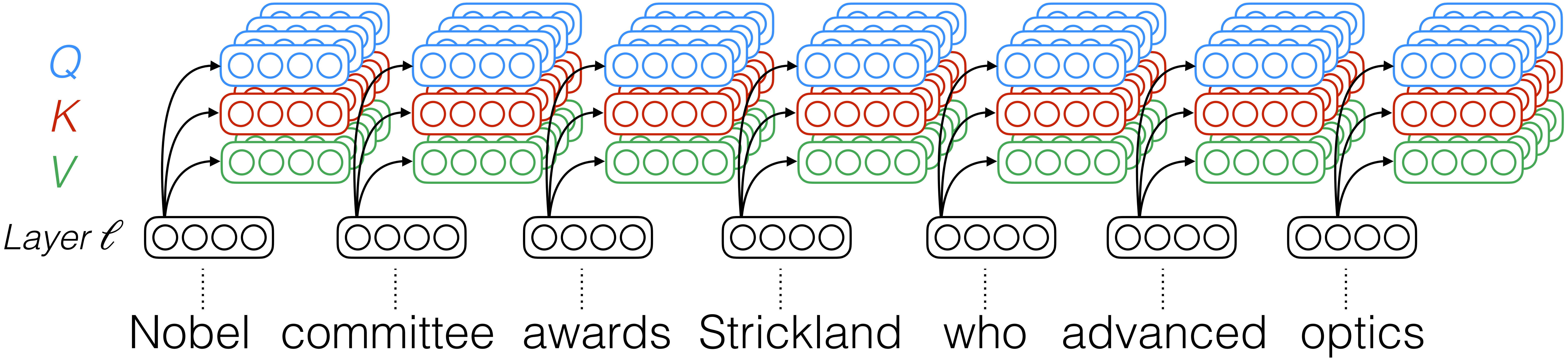

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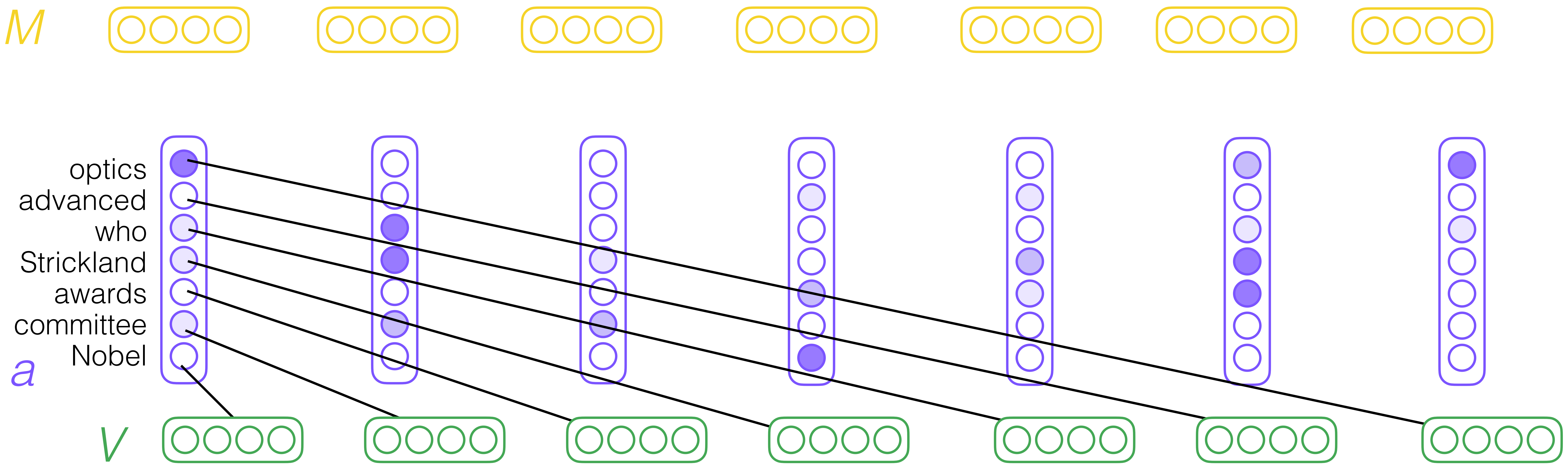

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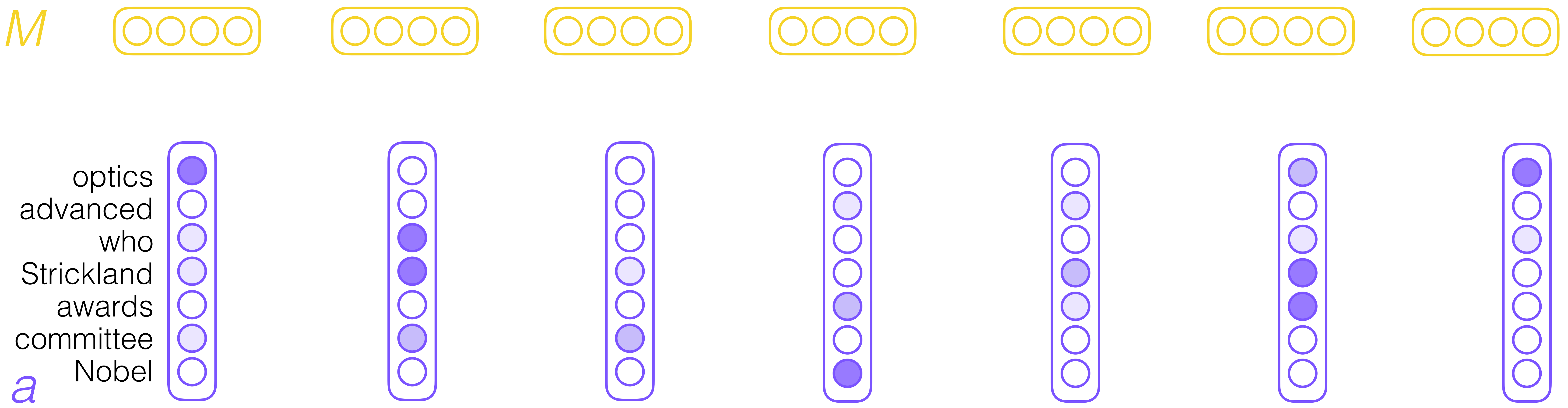

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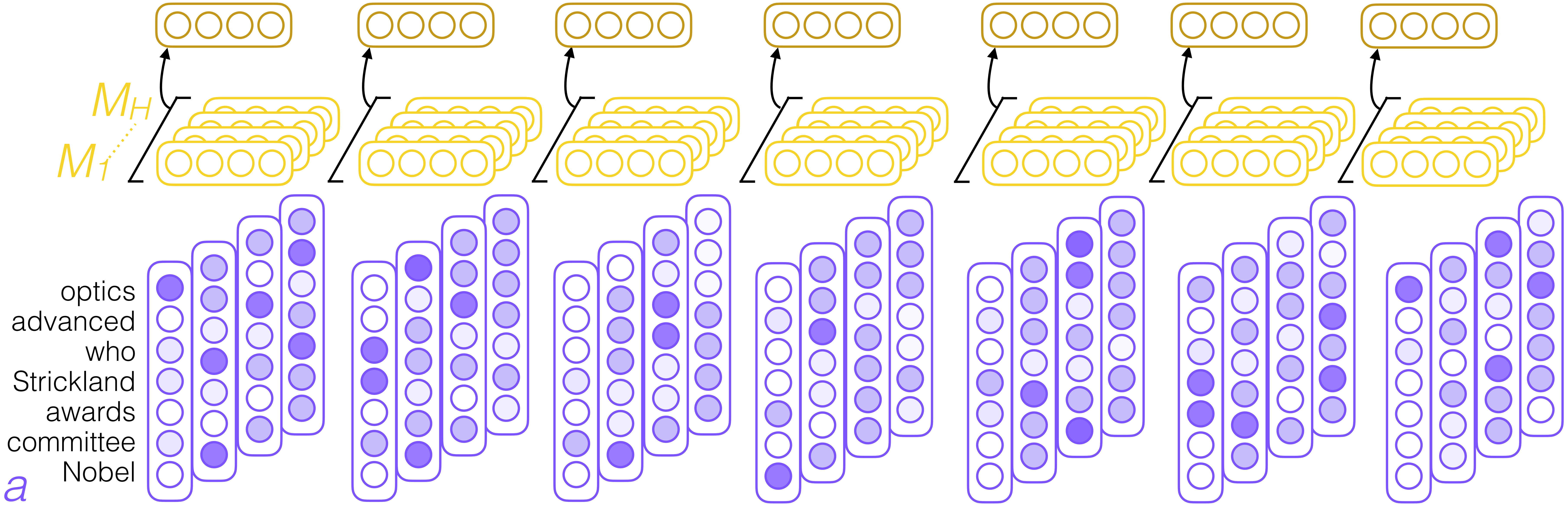

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$$\mathbf{W}_h^V \in \mathbb{R}^{d\times d/H}$$

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# Question

**What are the learnable parameters in these matrices?**

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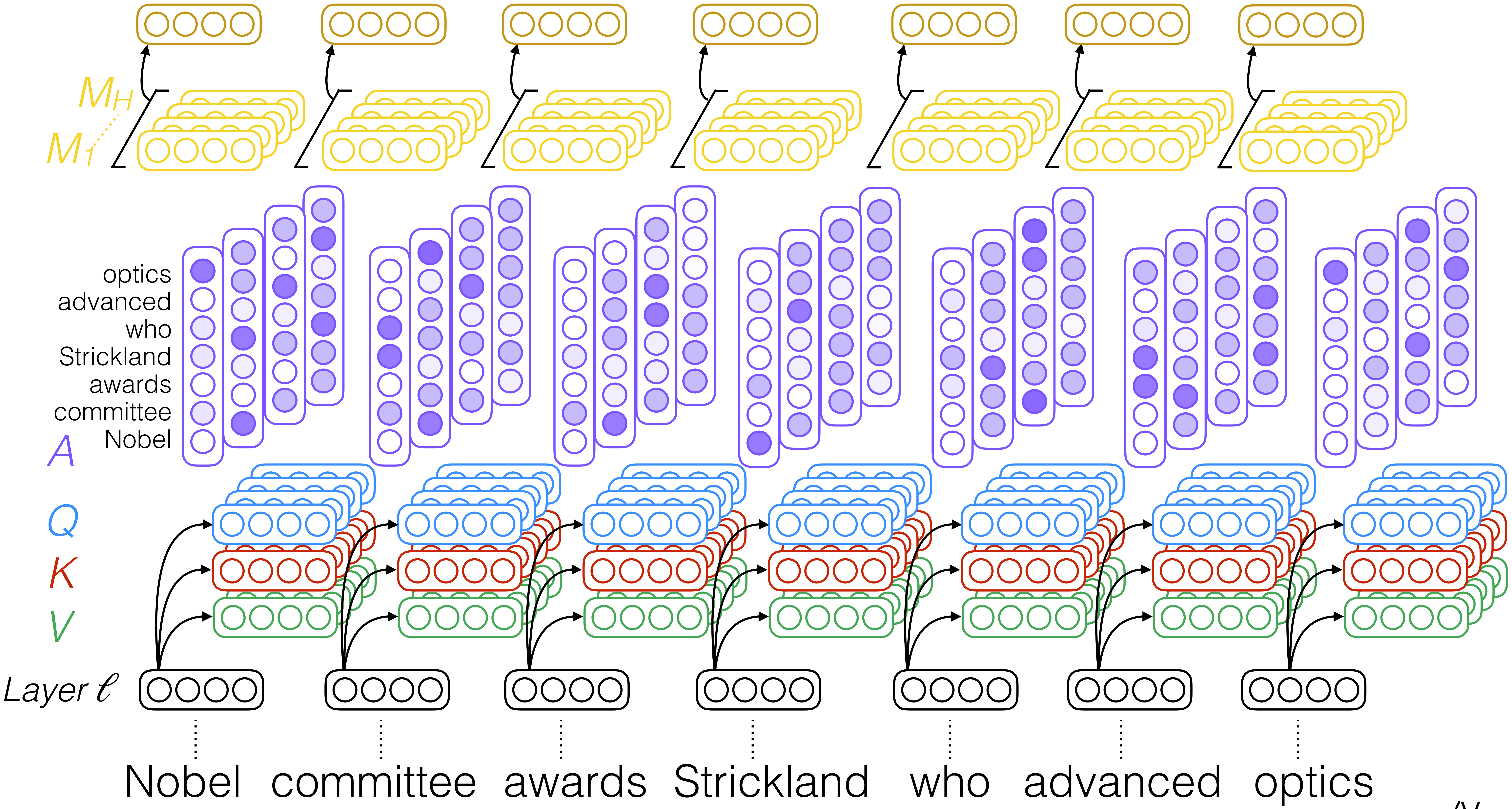


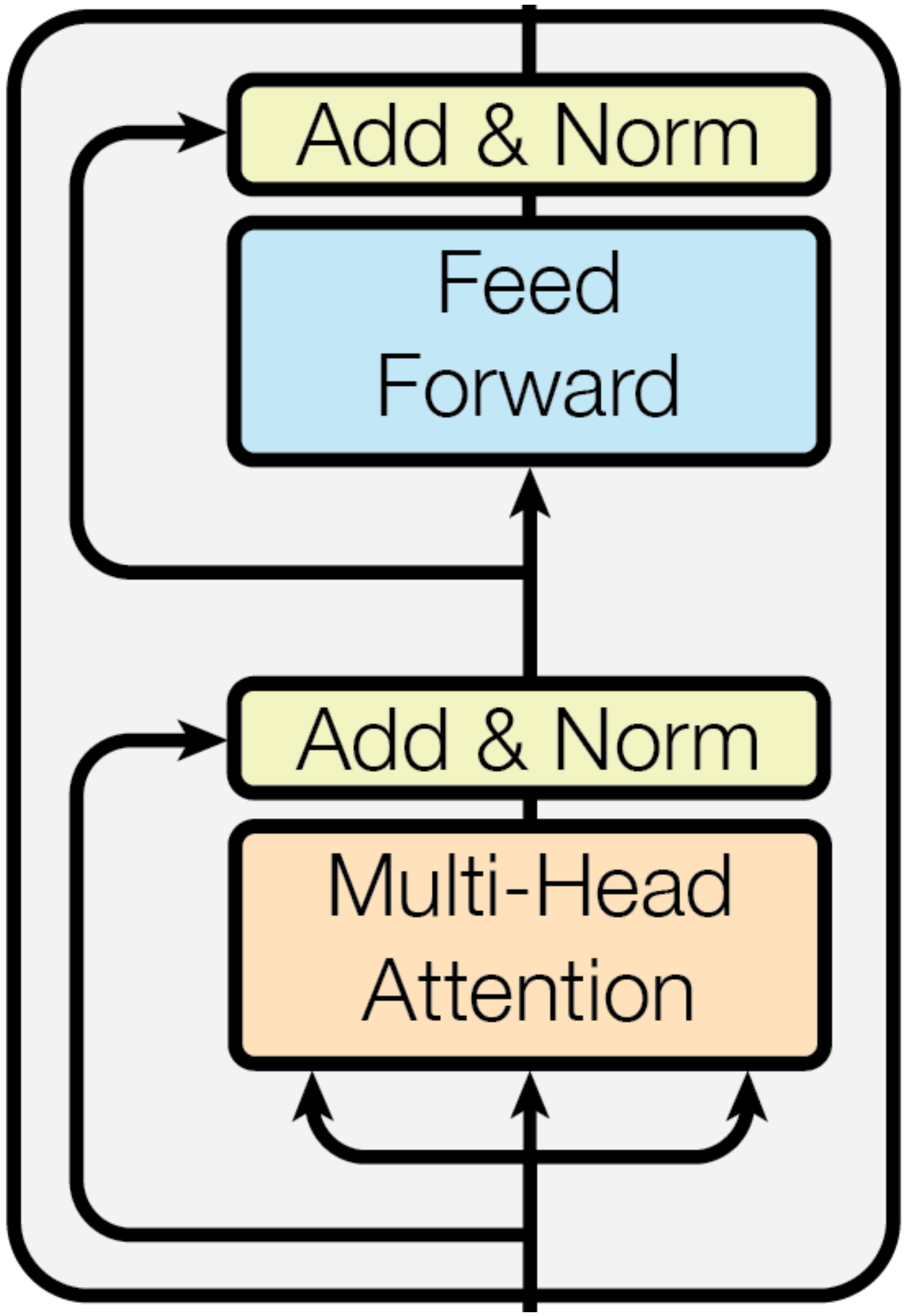
(Vaswani et al., 2017)

# Question

**What are two advantages of self-attention over recurrent models?**

# Transformer Block

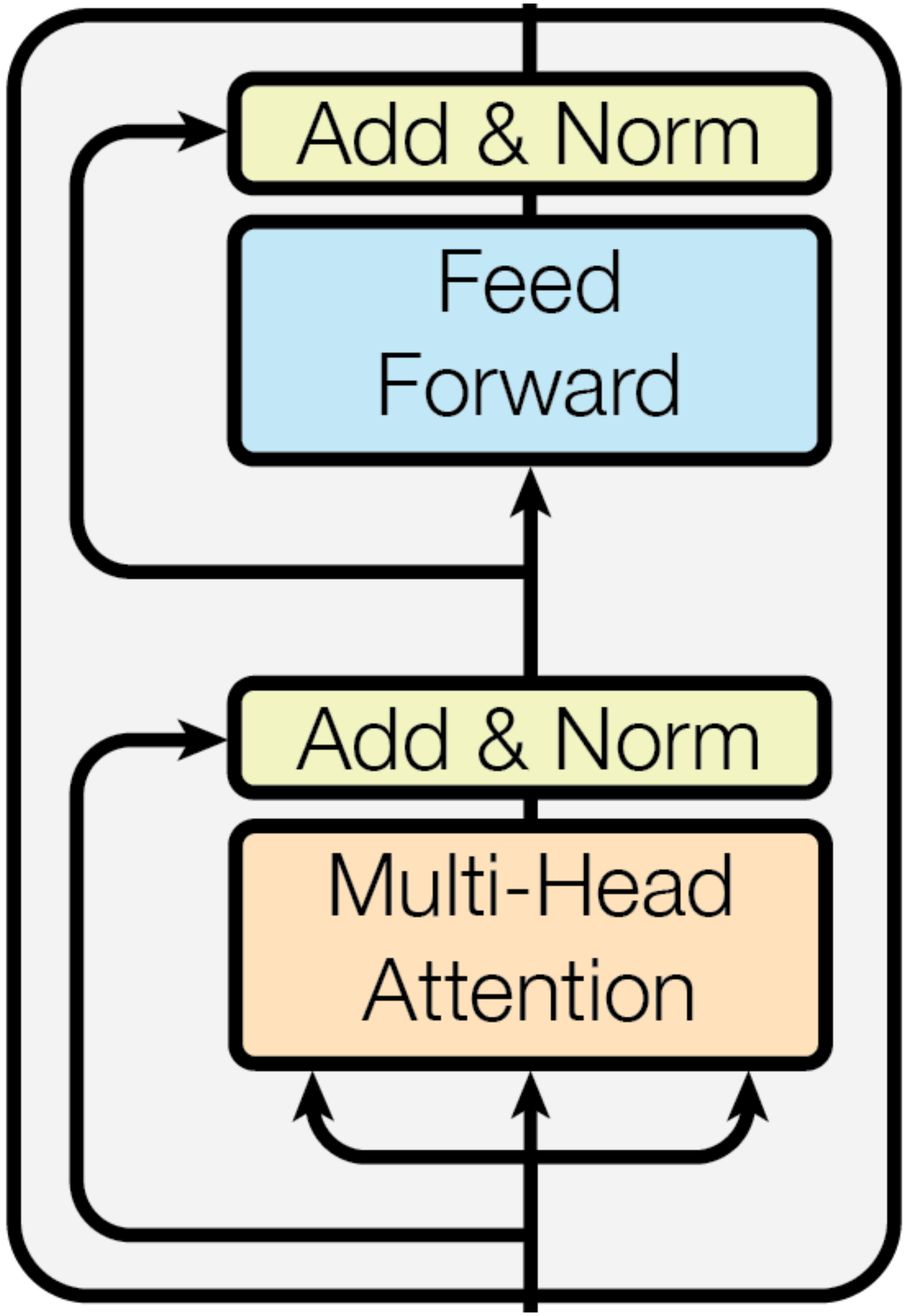
- Multi-headed attention is the main innovation of the transformer model!



Vaswani et al., 2017

# Transformer Block

- Multi-headed attention is the main innovation of the transformer model!
- Each block also composed of:
  - a layer normalisations
  - a feedforward network
  - residual connections



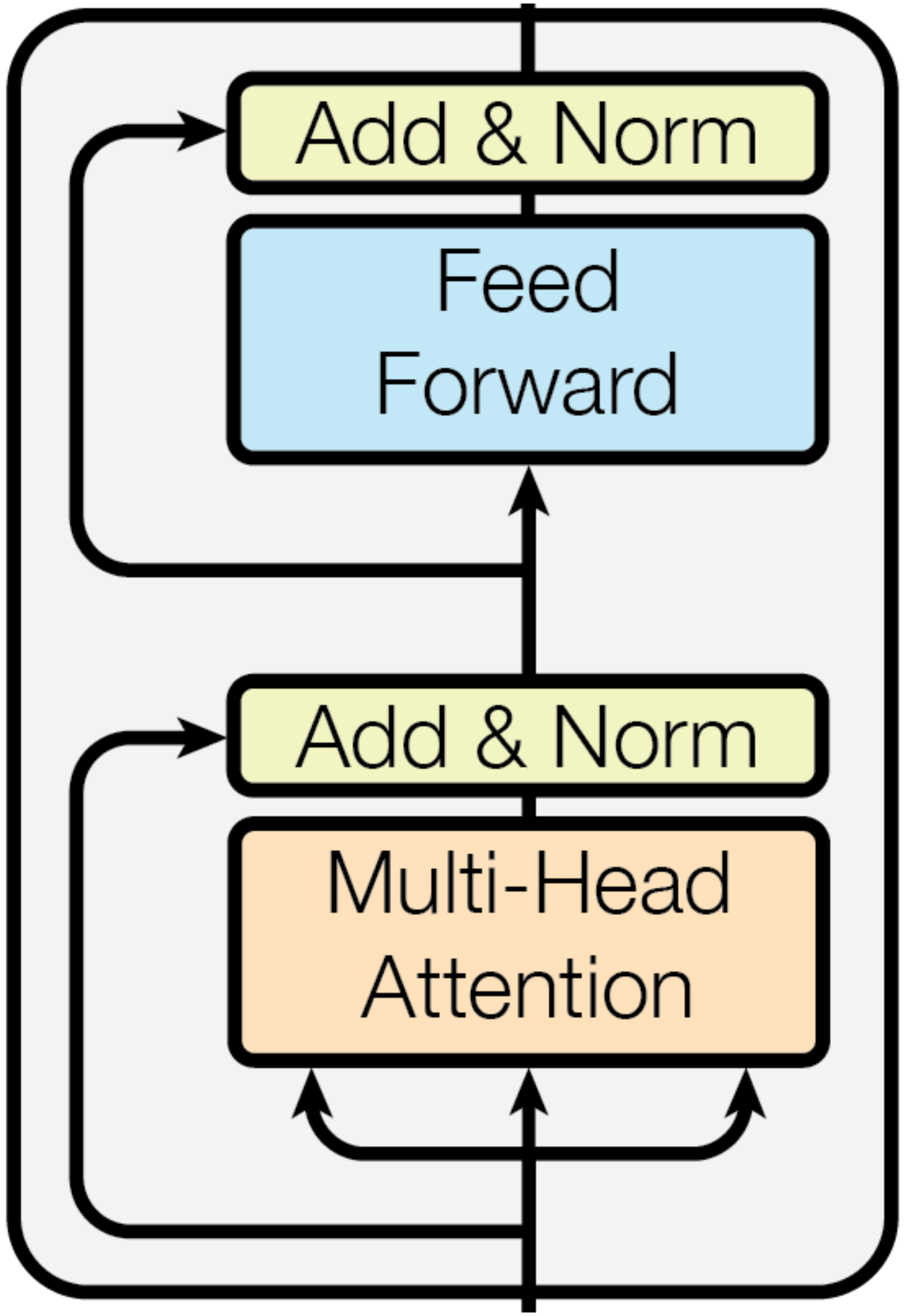
Vaswani et al., 2017

# LayerNorm & Residual Connections

- **Layer Normalisation**
  - Normalize the outputs of different modules

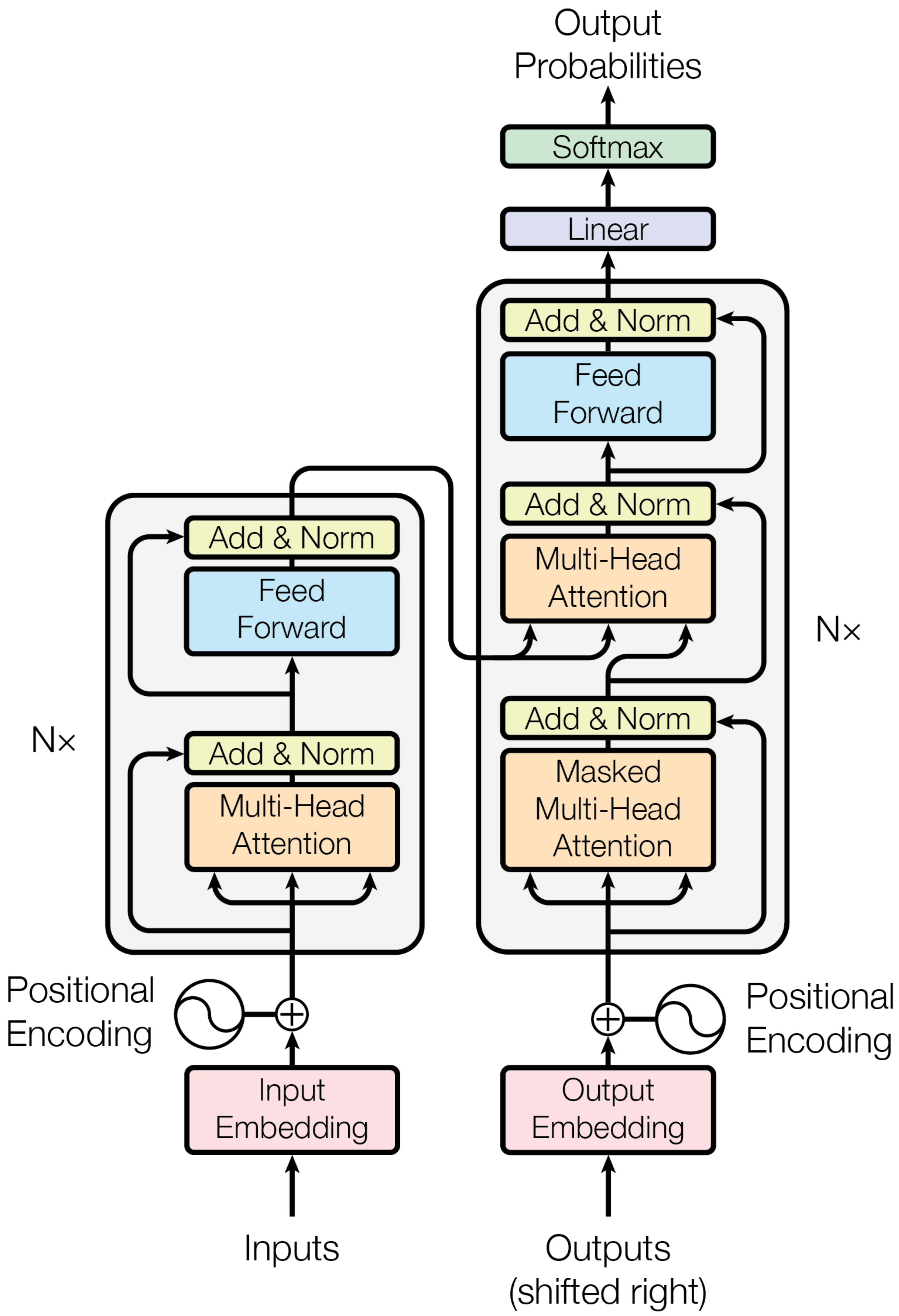
$$y = \frac{x - \mathrm{E}[x]}{\sqrt{\mathrm{Var}[x] + \epsilon}} * \gamma + \beta$$

- **Residual Connections**
  - Add the input of a module to its output
  - $\mathrm{LayerNorm}(x + \mathrm{Sublayer}(x))$



# Full Transformer

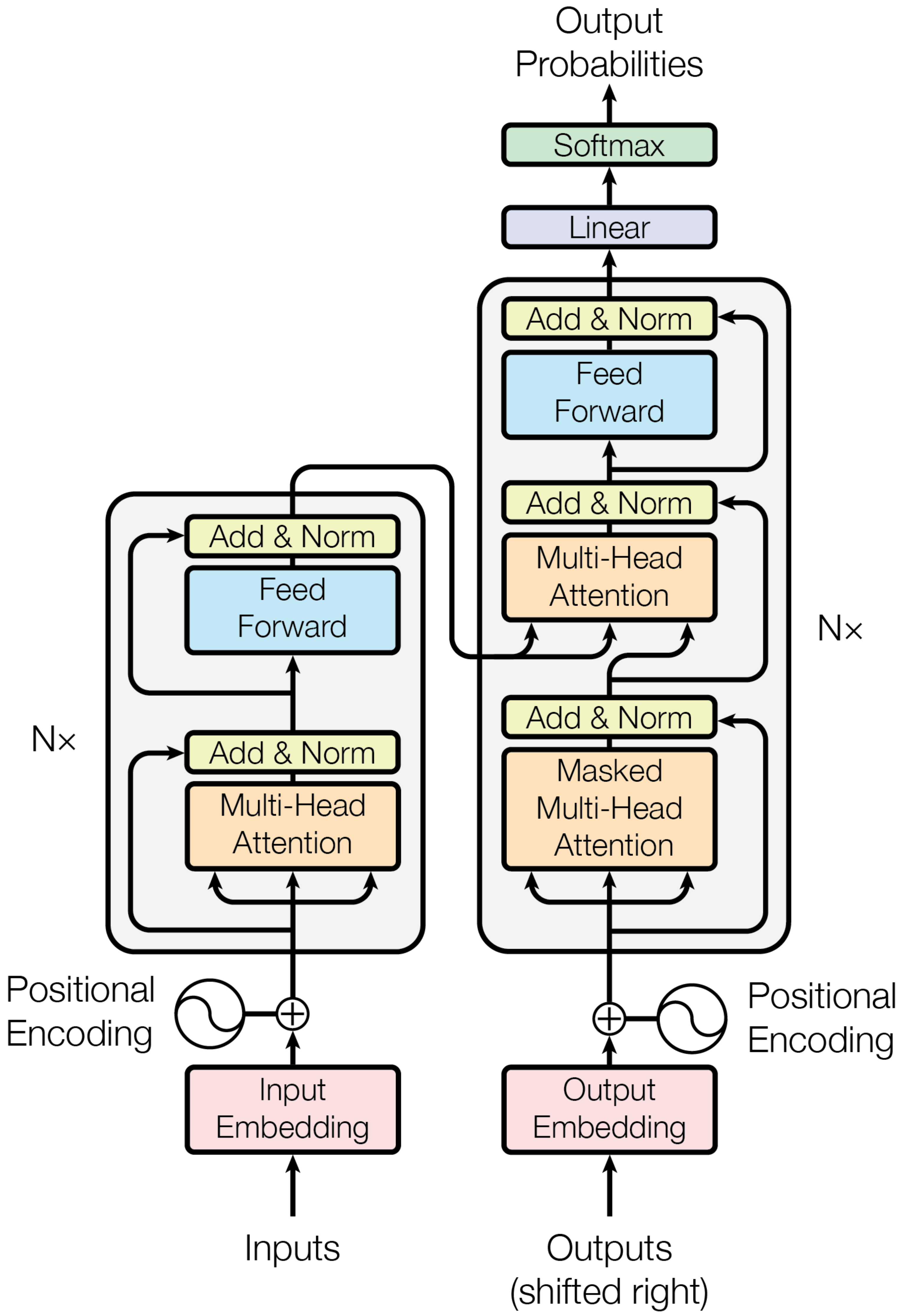
- Full transformer encoder is multiple cascaded transformer blocks
  - **build up compositional representations of inputs**



Vaswani et al., 2017

# Full Transformer

- Full transformer encoder is multiple cascaded transformer blocks
    - **build up compositional representations of inputs**
- Transformer decoder (right) similar to encoder
    - First layer of block is **masked** multi-headed attention
    - Second layer is multi-headed attention over *final-layer* encoder outputs **(cross-attention)**
    - Third layer is feed-forward network



Vaswani et al., 2017

# Question

**What is an issue with self-attention for the decoder?**

# Masked Multi-headed Attention

- Self-attention can attend to any token in the sequence

- For the decoder, **you don't want tokens to attend to future tokens**
  - Decoder used to generate text (i.e., machine translation)

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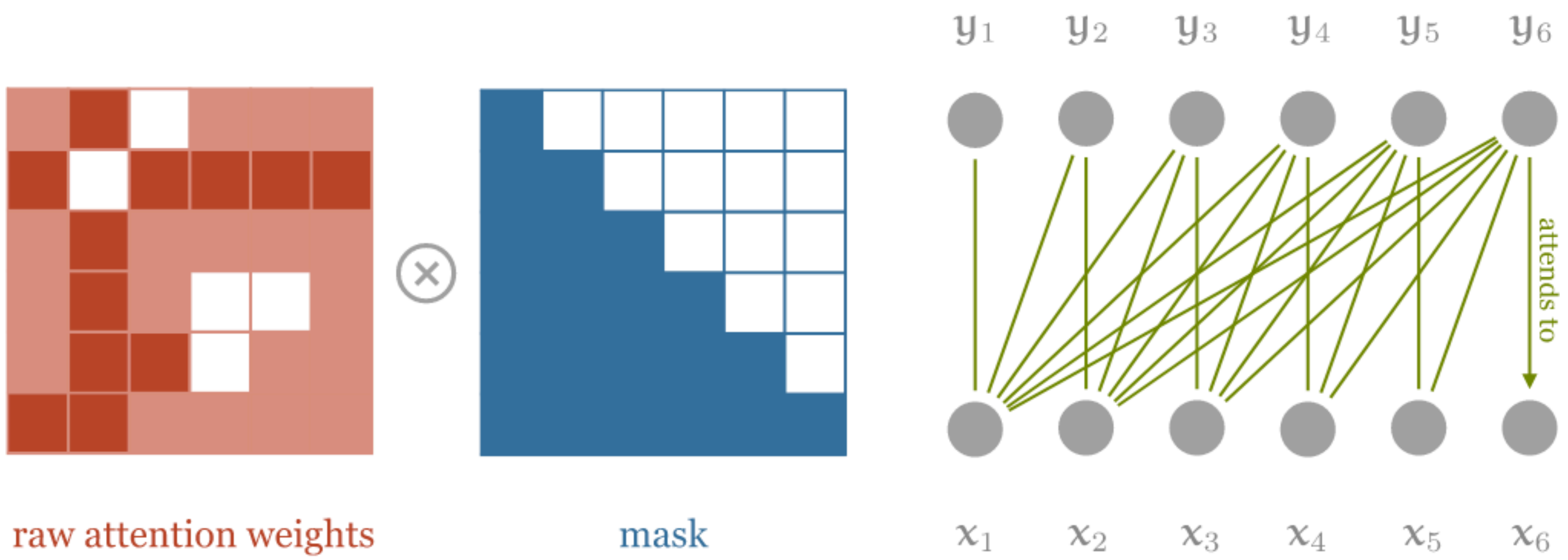

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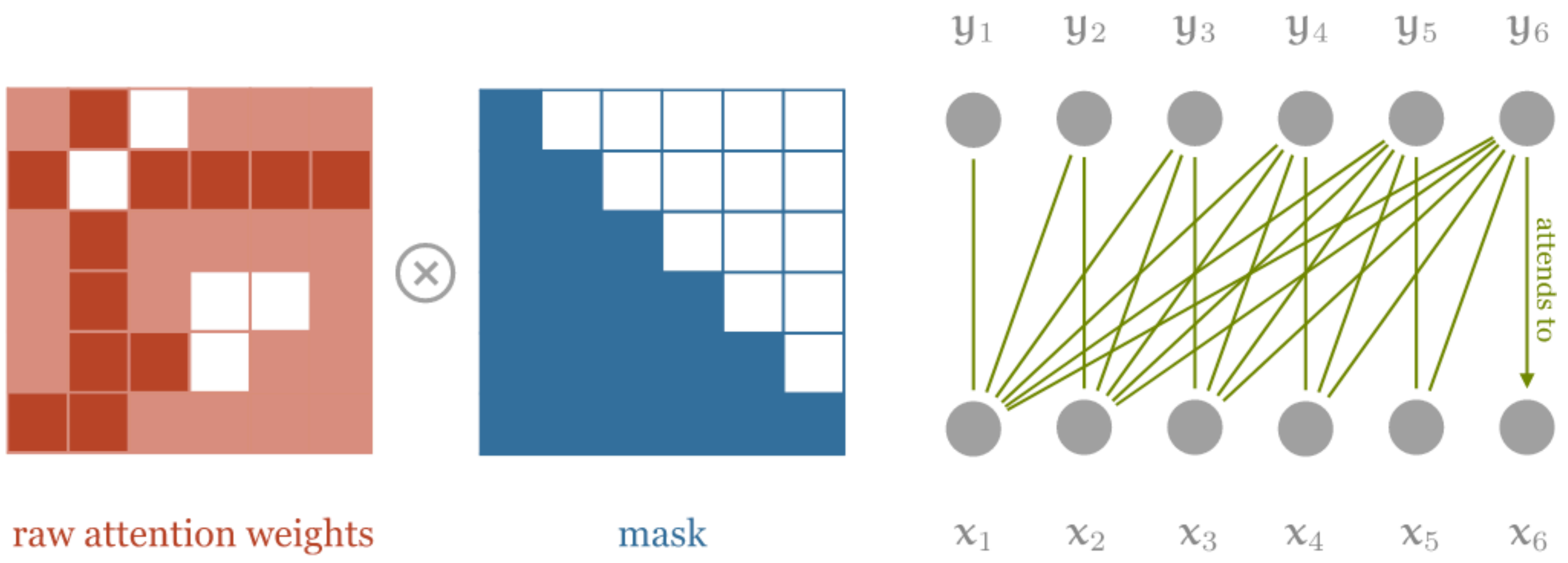
raw attention weights
⊗
mask
$y_1$ $y_2$ $y_3$ $y_4$ $y_5$ $y_6$
attends to
$x_1$ $x_2$ $x_3$ $x_4$ $x_5$ $x_6$

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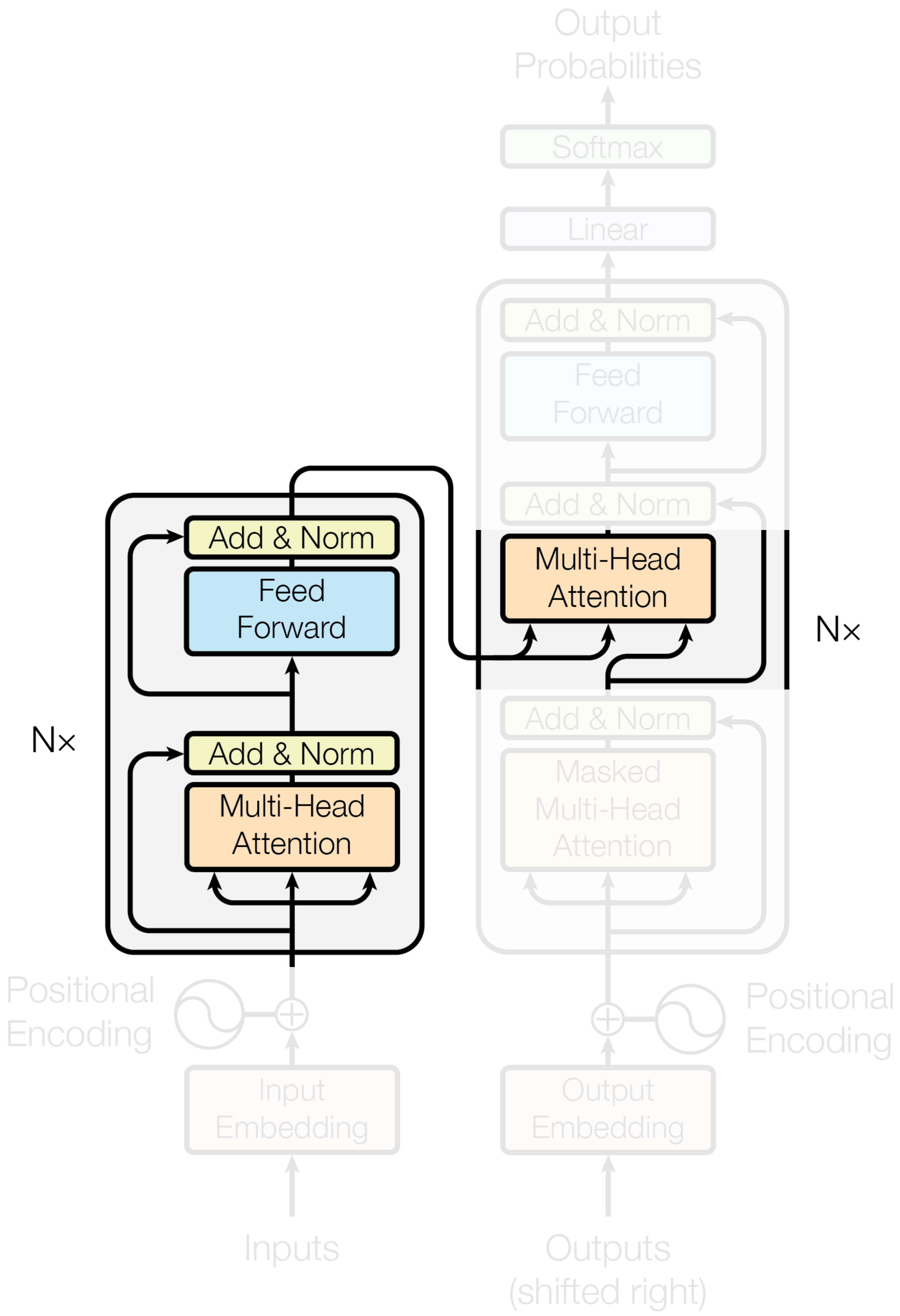
# Cross-attention

- **Cross attention** is the same classical attention as in the RNN encoder-decoder model
- Keys and values are output of **final** encoder block
- Query to the attention function is output of the masked multi-headed attention in the decoder
    - A representation from the decoder is used to **attend** to the encoder outputs



Vaswani et al., 2017

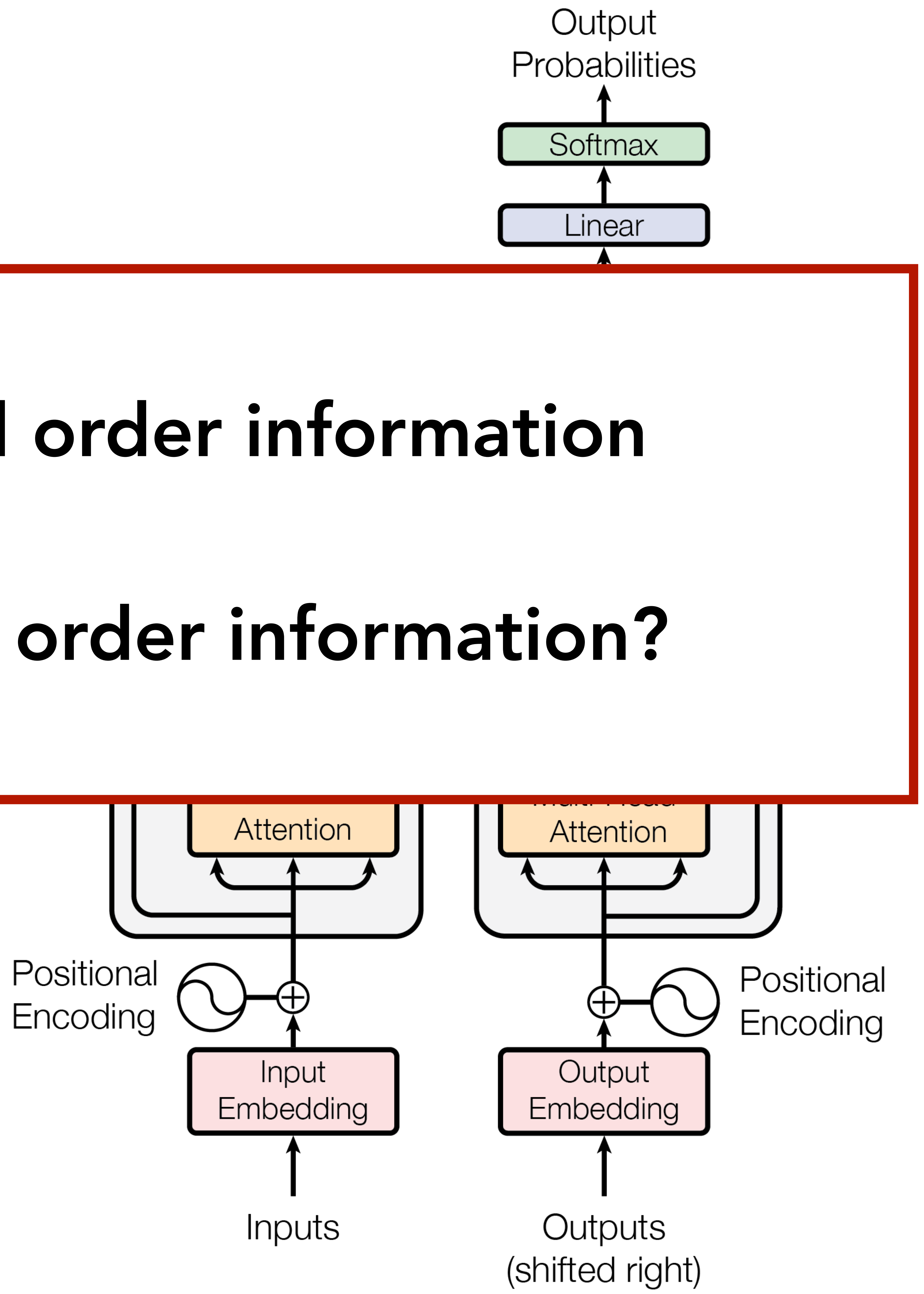
# Full Transformer

- Full transformer encoder is multiple cascaded transformer blocks
- Tr

**Recurrent models provided word order information**

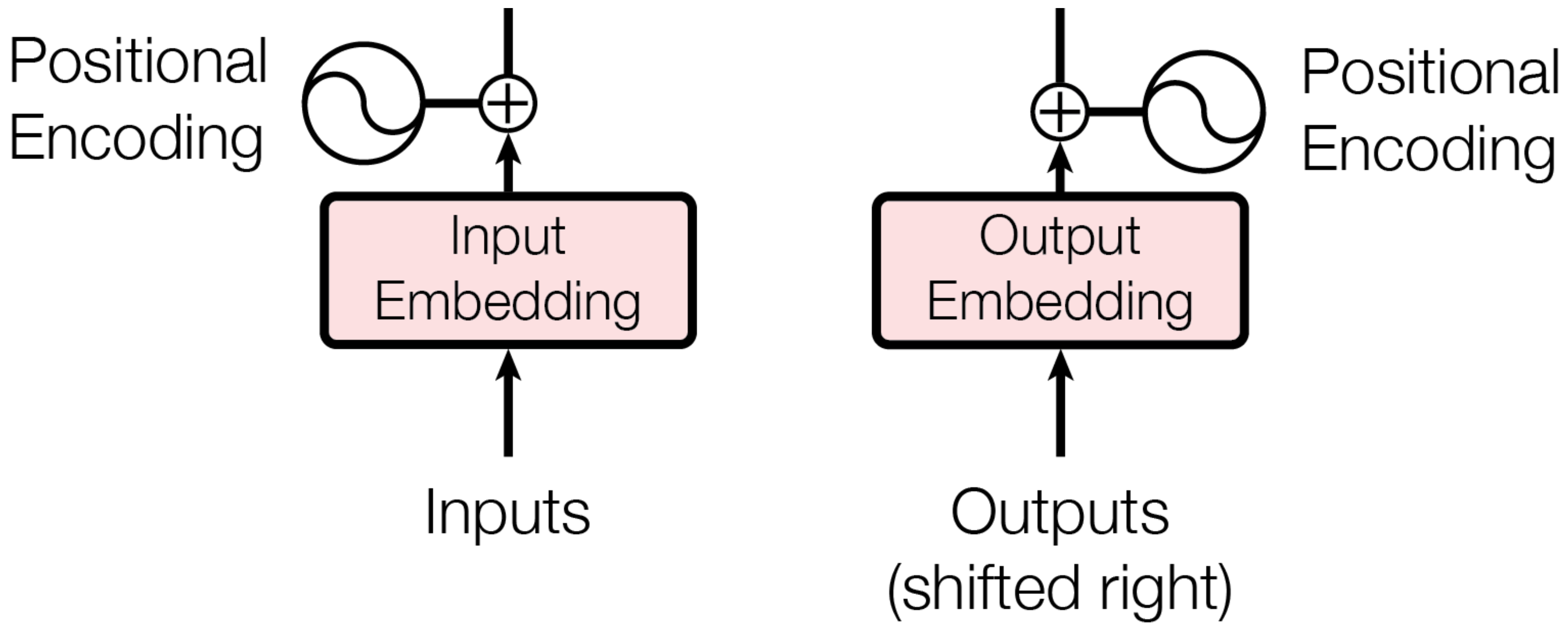
**Does self-attention provide word order information?**

  - Second layer is multi-headed attention over encoder outputs **(cross-attention)**
  - Third layer is feed-forward network



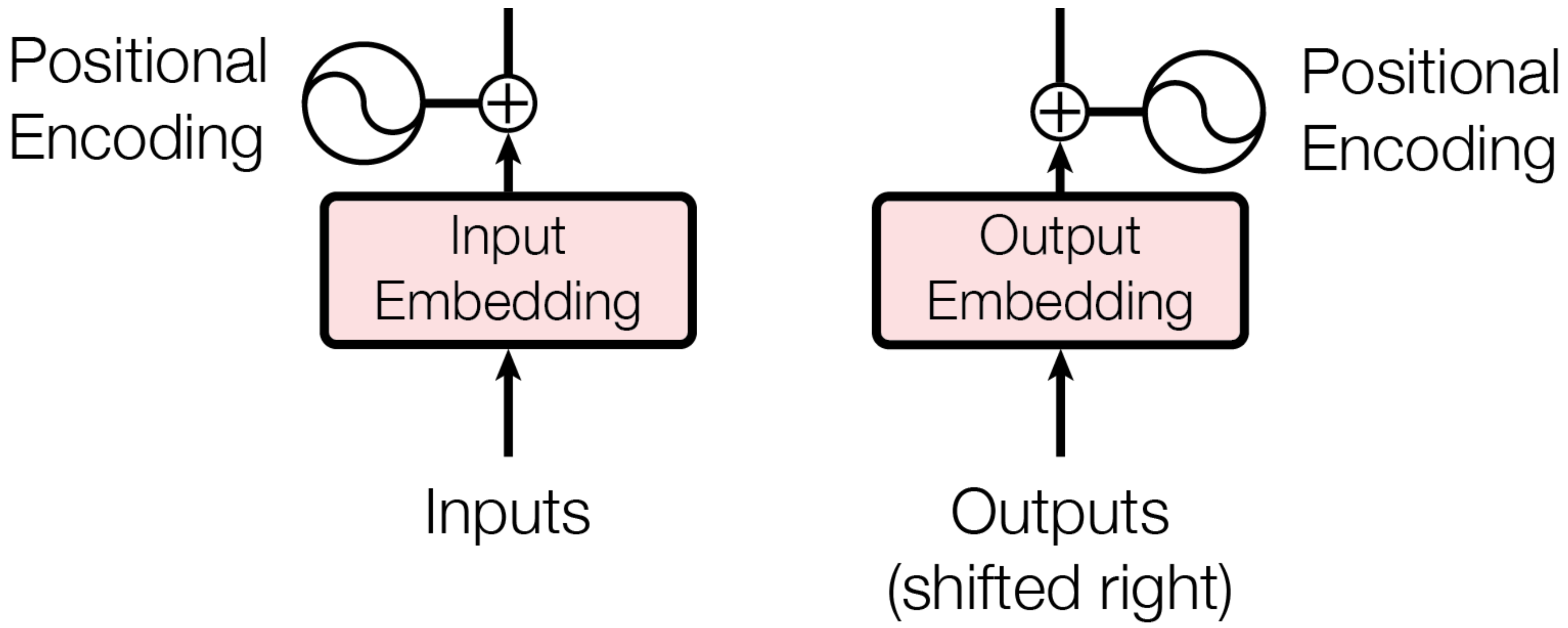
Vaswani et al., 2017

# Position Embeddings



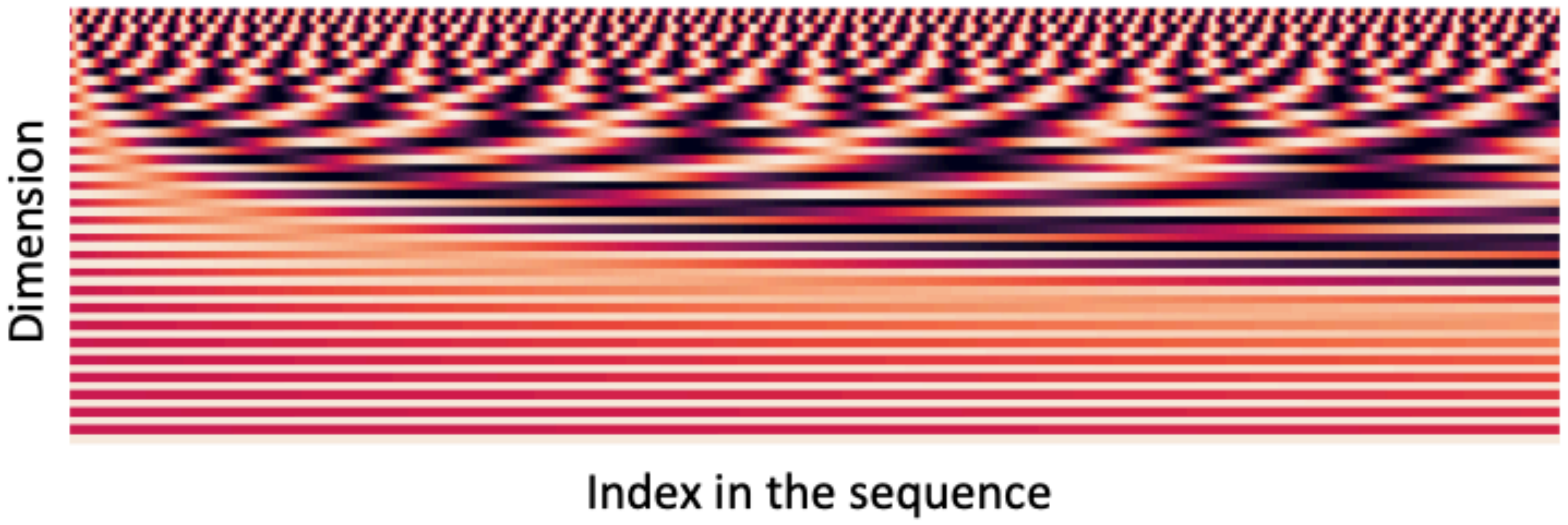
Vaswani et al., 2017

# Position Embeddings



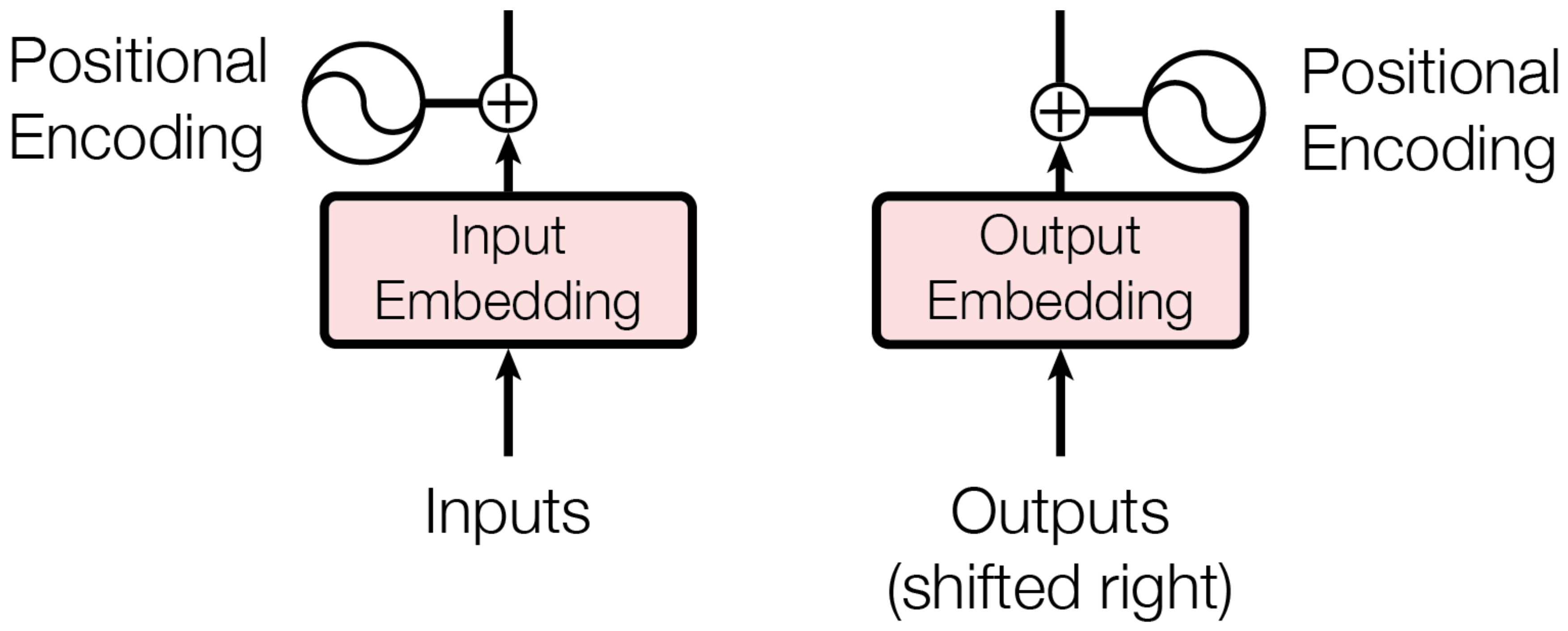
- Early position embeddings encoded a sinusoid function that was offset by a phase shift proportional to sequence position

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



Vaswani et al., 2017

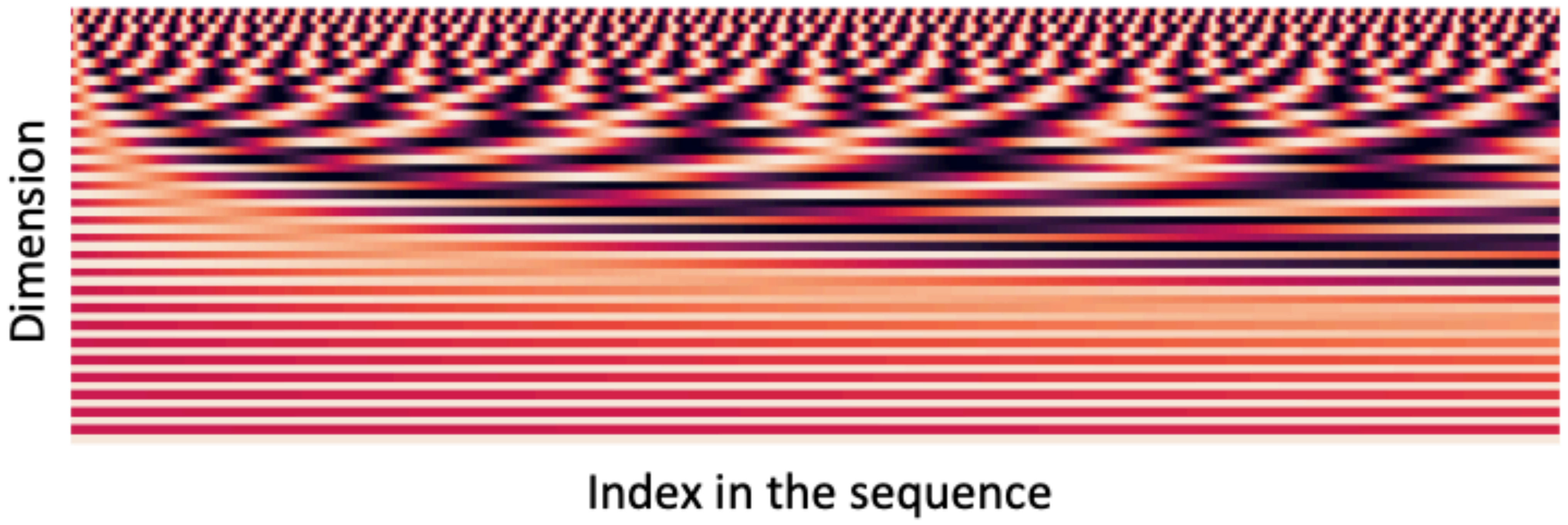
# Position Embeddings



- Early position embeddings encoded a sinusoid function that was offset by a phase shift proportional to sequence position

- **In practice, easiest is to learn position embeddings from scratch**

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



Vaswani et al., 2017

# Question

**What might be a disadvantage of using learned position embeddings?**

Poor generalisation to sequences longer than the maximum position embedding you have learned

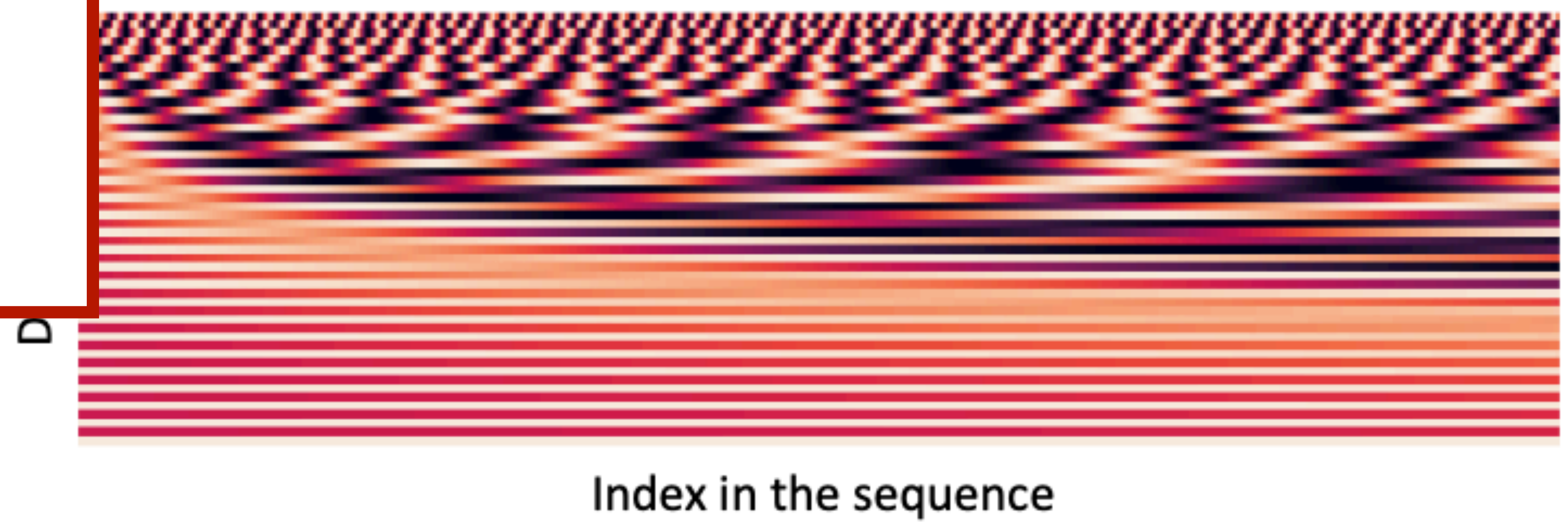
# Position Embeddings

**Lots of potential for new methods that generalise to longer sequences**

**Position embeddings remain an active area of research**

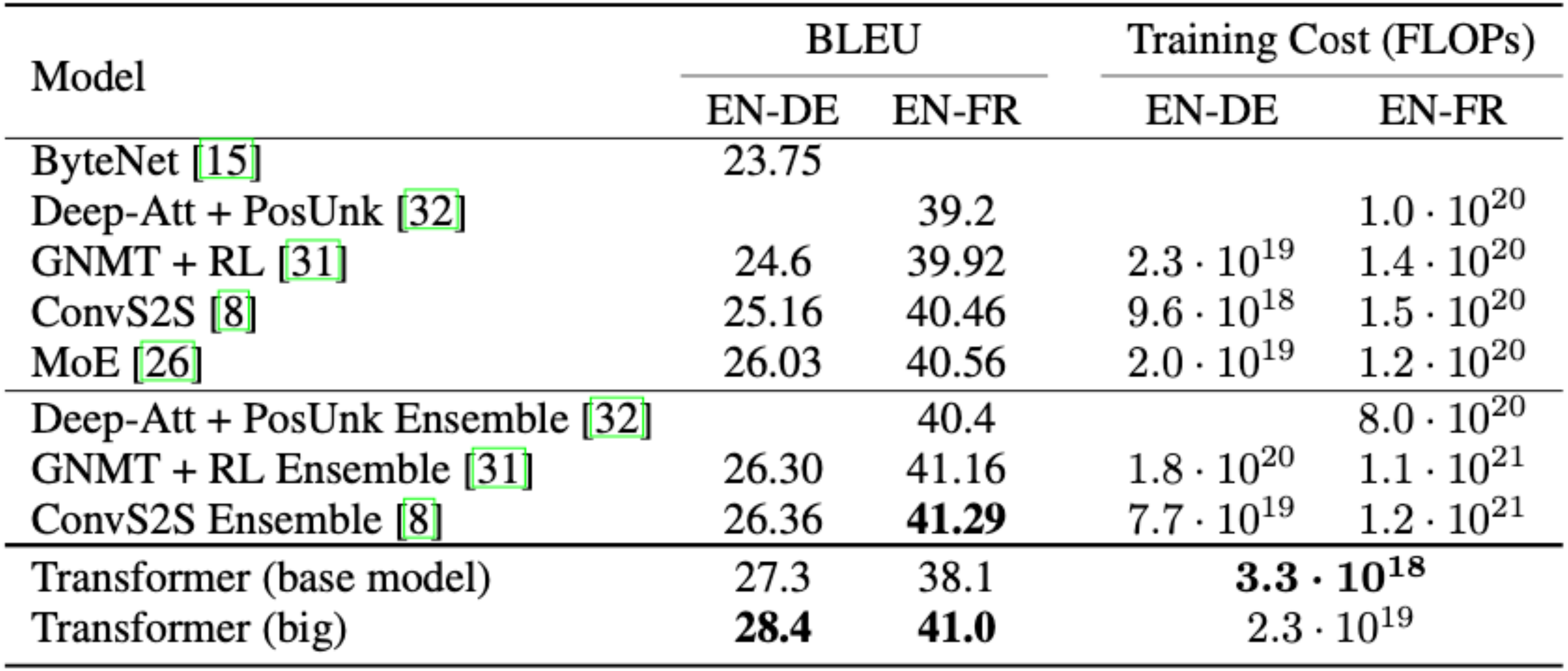
- Early position embeddings encoded a sinusoid function that was offset by a phase shift proportional to sequence position
- **In practice, easiest is to learn position embeddings from scratch**

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



Vaswani et al., 2017

# Performance: Machine Translation

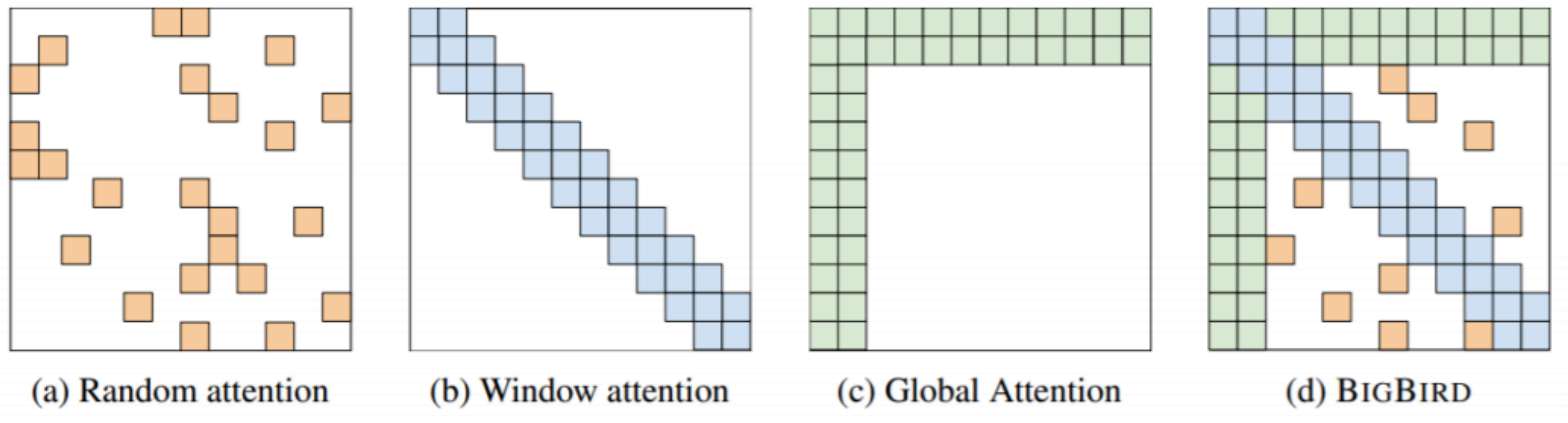


| Model | BLEU | | Training Cost (FLOPs) | |
|---|---|---|---|---|
| | EN-DE | EN-FR | EN-DE | EN-FR |
| ByteNet [15] | 23.75 | | | |
| Deep-Att + PosUnk [32] | | 39.2 | | $1.0 \cdot 10^{20}$ |
| GNMT + RL [31] | 24.6 | 39.92 | $2.3 \cdot 10^{19}$ | $1.4 \cdot 10^{20}$ |
| ConvS2S [8] | 25.16 | 40.46 | $9.6 \cdot 10^{18}$ | $1.5 \cdot 10^{20}$ |
| 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)

# Question

**What could be a disadvantage of transformers over RNNs?**



(a) Random attention (b) Window attention (c) Global Attention (d) BIGBIRD

# Other Resources of Interest

- The Annotated Transformer
  - https://nlp.seas.harvard.edu/2018/04/03/attention.html
- The Illustrated Transformer
  - https://jalammar.github.io/illustrated-transformer/
- Only basics presented here today! Many modifications to initial transformers exist

# Recap

- **Temporal Bottleneck**: **Vanishing gradients** stop many RNN architectures from learning **long-range dependencies**

- **Parallelisation Bottleneck:** RNN states depend on previous time step hidden state, so must be **computed in series**

- **Attention**: Direct connections between output states and inputs (solves temporal bottleneck)

- **Self-Attention**: Remove recurrence, allowing parallel computation

- Modern **Transformers** use attention, but require position embeddings to capture sequence order

# References

- Bahdanau, D., Cho, K., & Bengio, Y. (2014). Neural Machine Translation by Jointly Learning to Align and Translate. *CoRR, abs/1409.0473*.
- Vaswani, A., Shazeer, N.M., Parmar, N., Uszkoreit, J., Jones, L., Gomez, A.N., Kaiser, L., & Polosukhin, I. (2017). Attention is All you Need. *ArXiv, abs/1706.03762*.
- Wu et al., Google's Neural Machine Translation System: Bridging the Gap between Human and Machine Translation. arxiv 2016