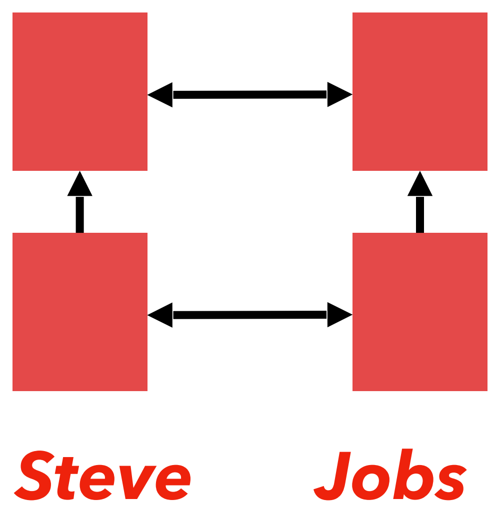
Transformers

CS6120: Natural Language Processing
Northeastern University

David Smith
with slides from John Hewitt, Hung-yi Lee, and Liwei Jiang

Drawbacks of RNNs: **Linear Interaction Distance**

- RNNs are unrolled left-to-right.
  - Linear locality is a useful heuristic: nearby words often affect each other's meaning!



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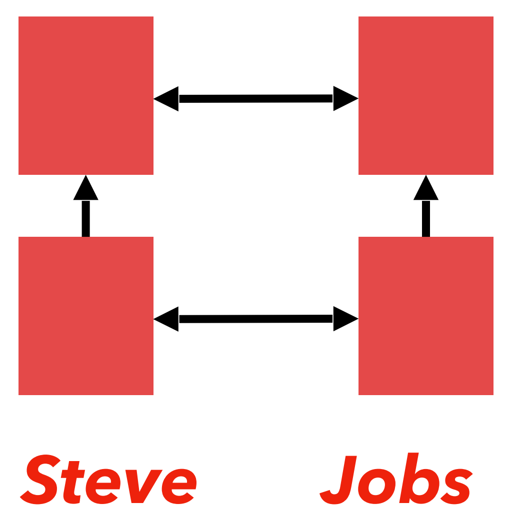
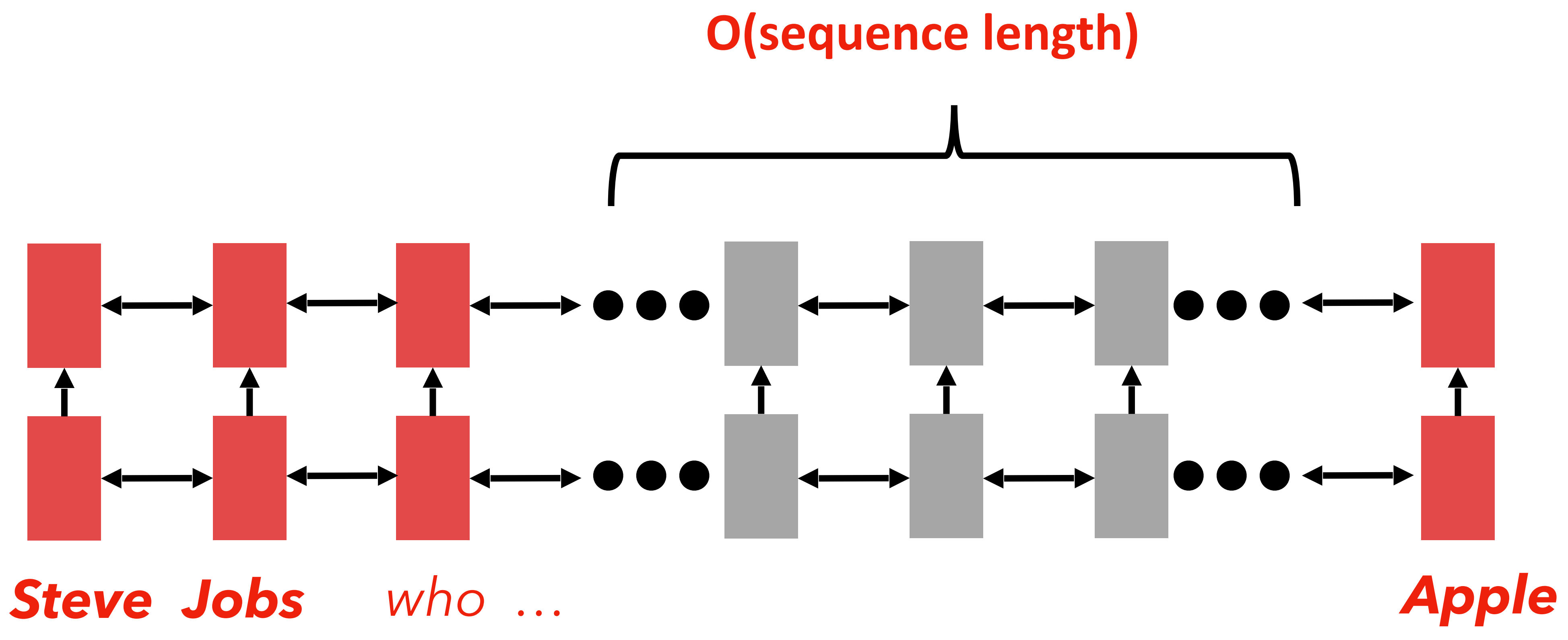


- **However, there's the vanishing gradient problem for long sequences.**
  - **The gradients that are used to update the network become extremely small or "vanish" as they are backpropogated from the output layers to the earlier layers.**



Failing to capture long-term dependences.

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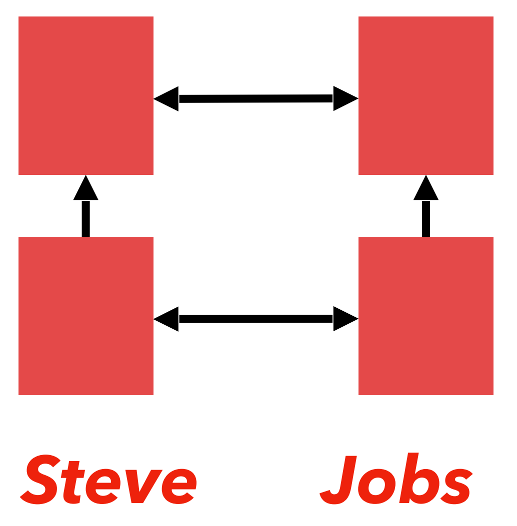

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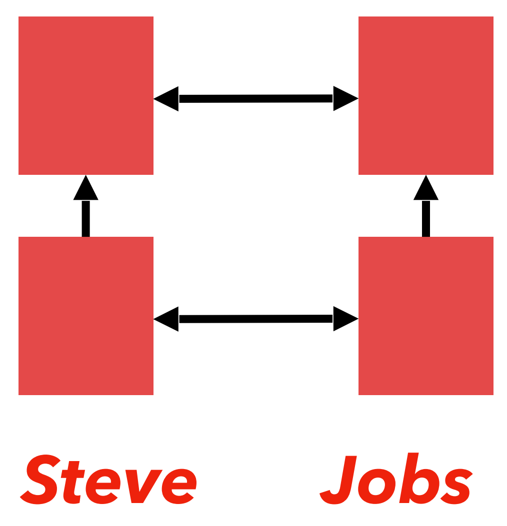

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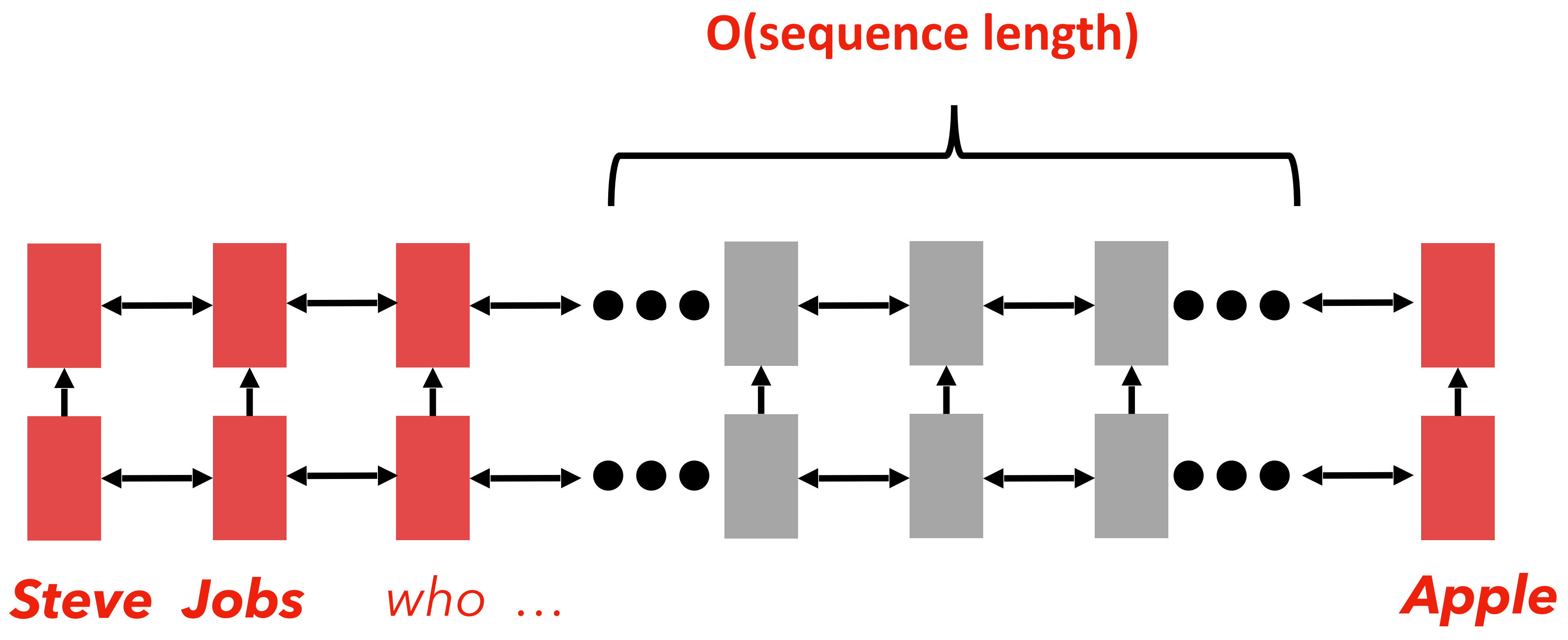
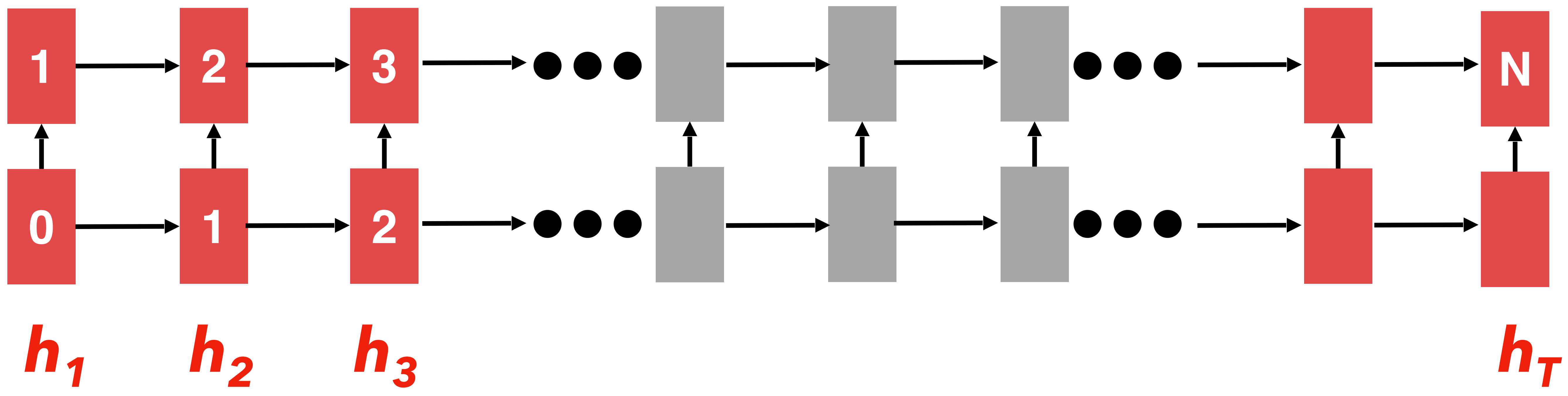


Failing to capture long-term dependences.

Drawbacks of RNNs: **Lack of Parallelizability**

- Forward and backward passes have O(sequence length) unparallelizable operations
  - GPUs can perform many independent computations (like addition) at once!
  - But future RNN hidden states can't be computed in full before past RNN hidden states have been computed.
  - Training and inference are slow; inhibits on very large datasets!



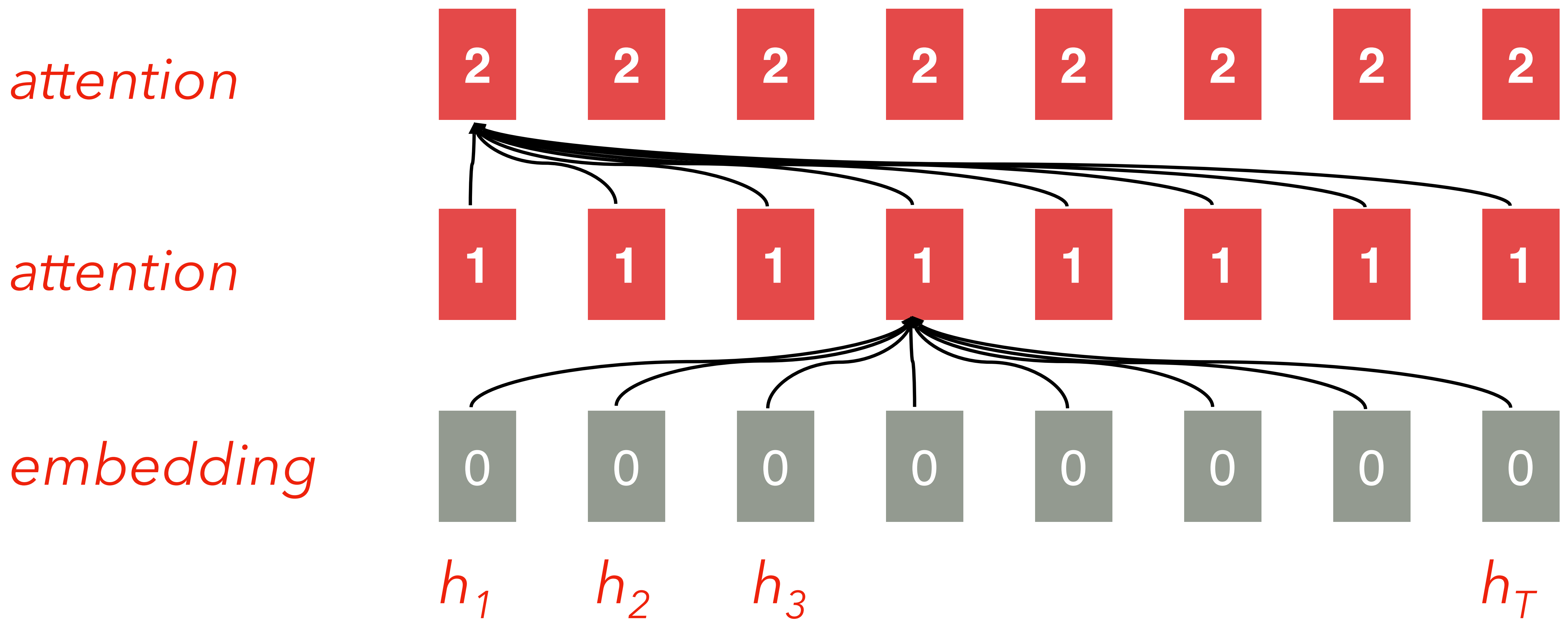
Numbers indicate min # of steps before a state can be computed

Drawbacks of RNNs

- Complicated memory and gating structures
- Backprop through time can't be parallelized
- Is linear order always the most important structure to model? (No, but people do incremental interpretation.)
- Instead, let's **learn** which parts of the context to pay **attention** to

Building the Intuition of **Attention**

- Attention treats each token's representation as a query to access and incorporate information from a set of values.
  - Today we look at attention within a single sequence.
- Number of unparallelizable operations does NOT increase with sequence length.
- Maximum interaction distance: O(1), since all tokens interact at every layer!



All tokens attend to all tokens in previous layer; most arrows here are omitted

Attention Is All You Need (NeurIPS 2017)

Attention Is All You Need

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Attention as a soft, averaging lookup table

We can think of **attention** as performing **fuzzy lookup** in a key-value store.

Attention as a soft, averaging lookup table

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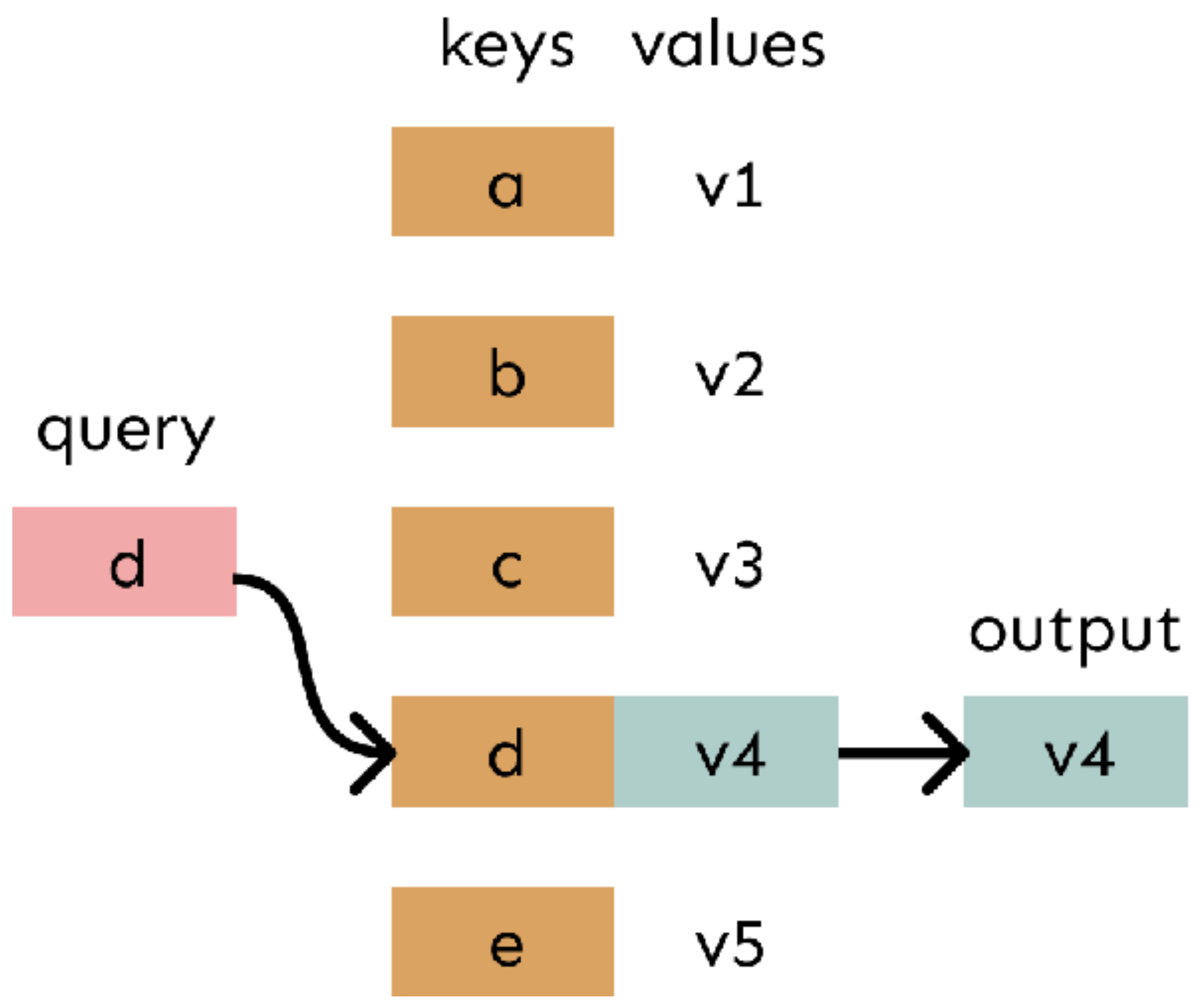
In a **lookup table**, we have a table of **keys** that map to **values**. The **query** matches one of the keys, returning its value.



Attention as a soft, averaging lookup table

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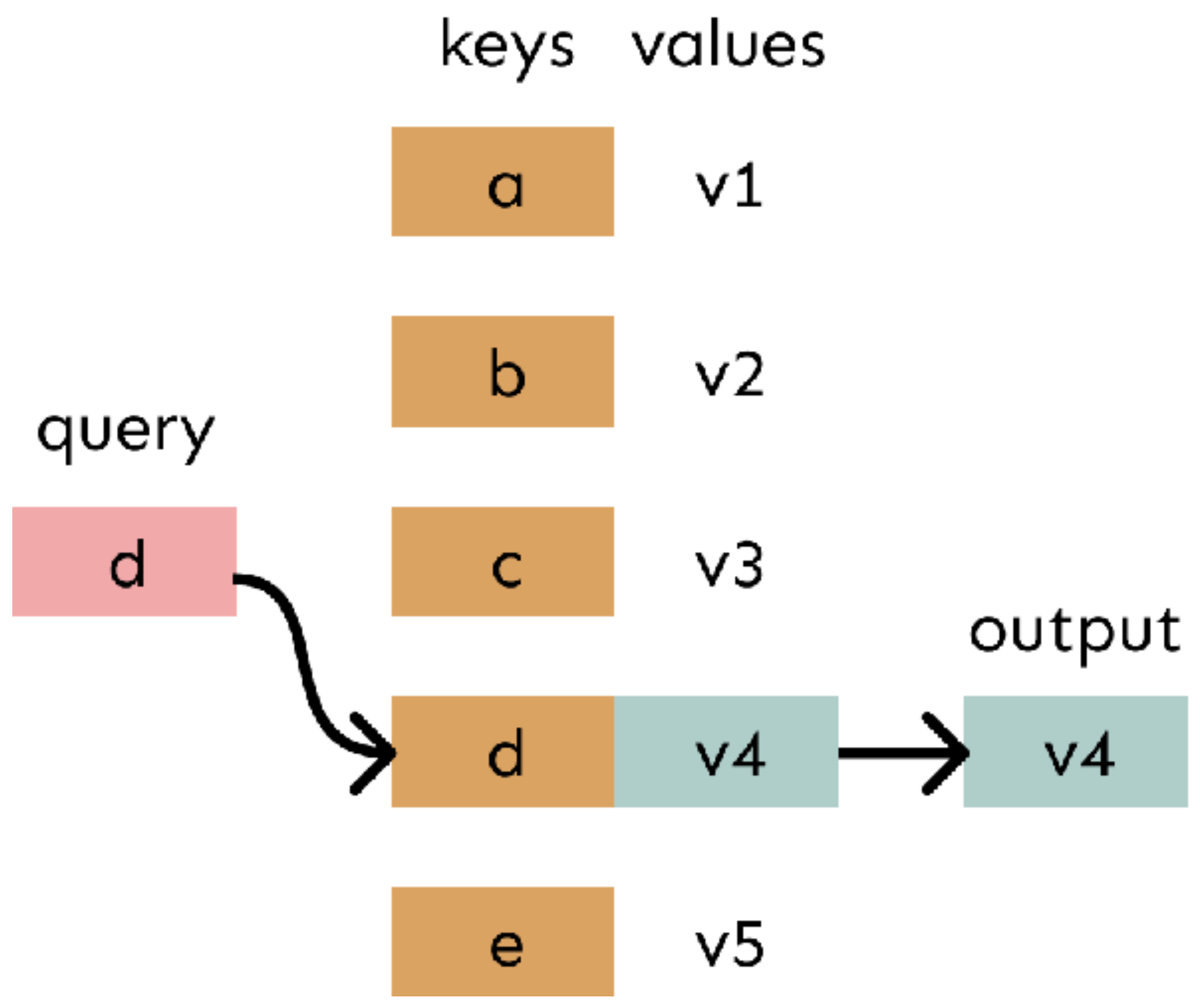
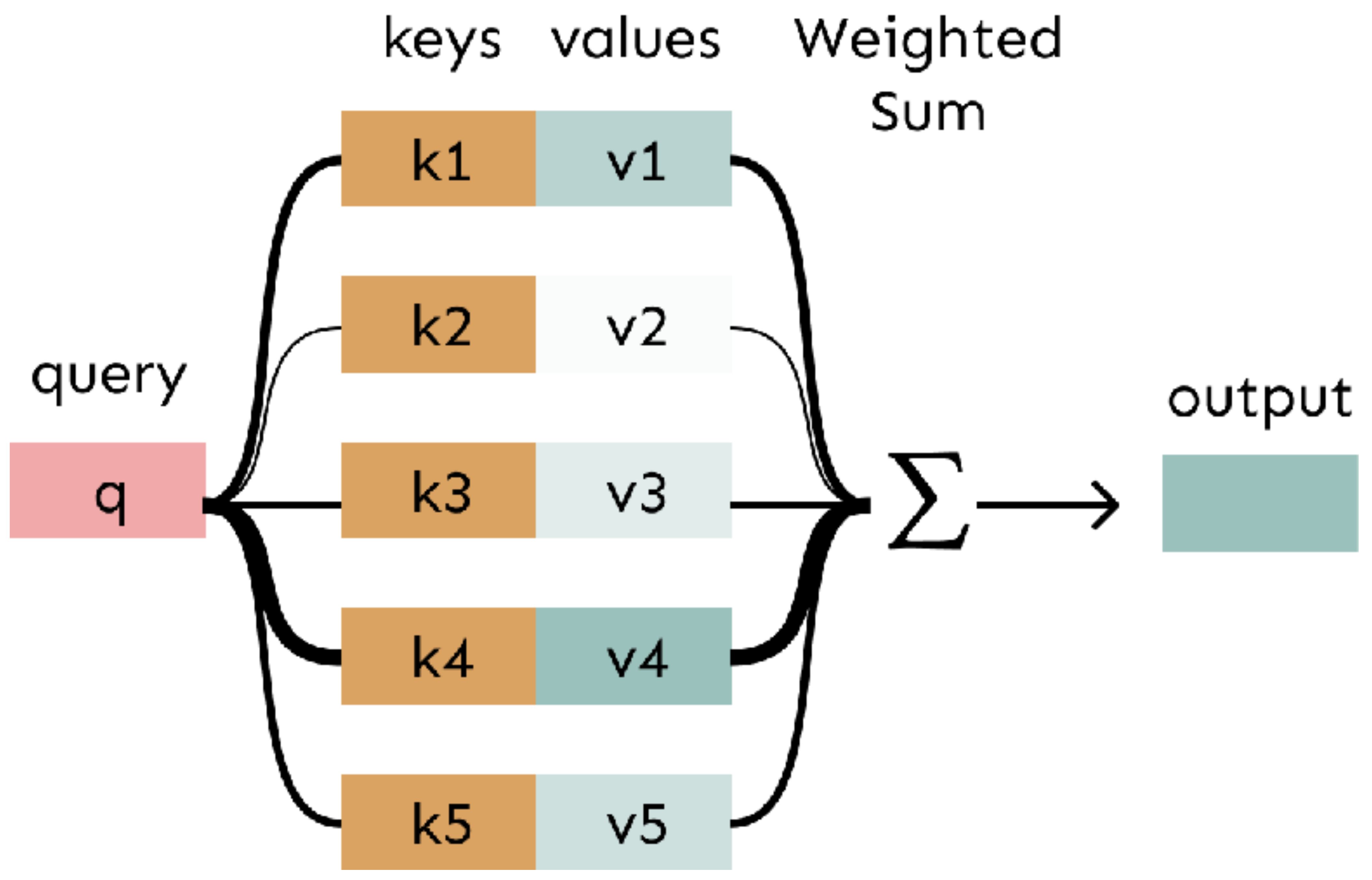


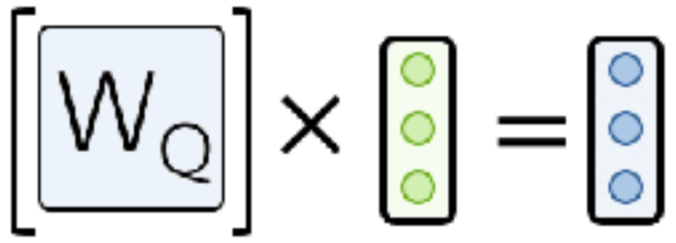
In **attention**, the **query** matches all **keys** *softly*, to a weight between 0 and 1. The keys' **values** are multiplied by the weights and summed.



Self-Attention: Basic Concepts

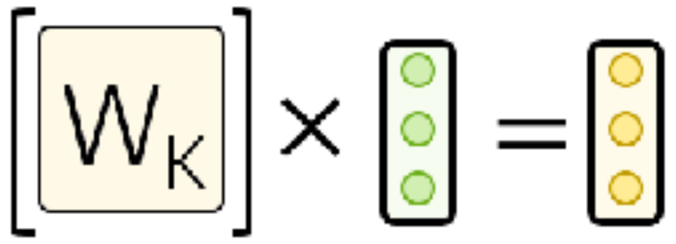
[Lena Viota Blog]

Each vector receives three representations ("roles")



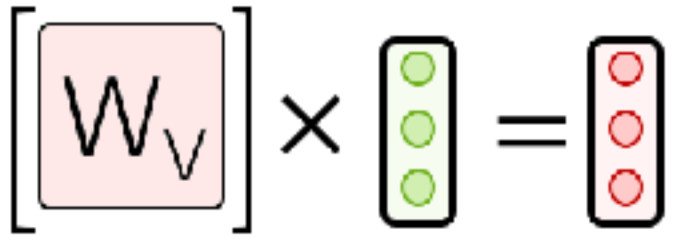
Query: vector from which the attention is looking

"Hey there, do you have this information?"



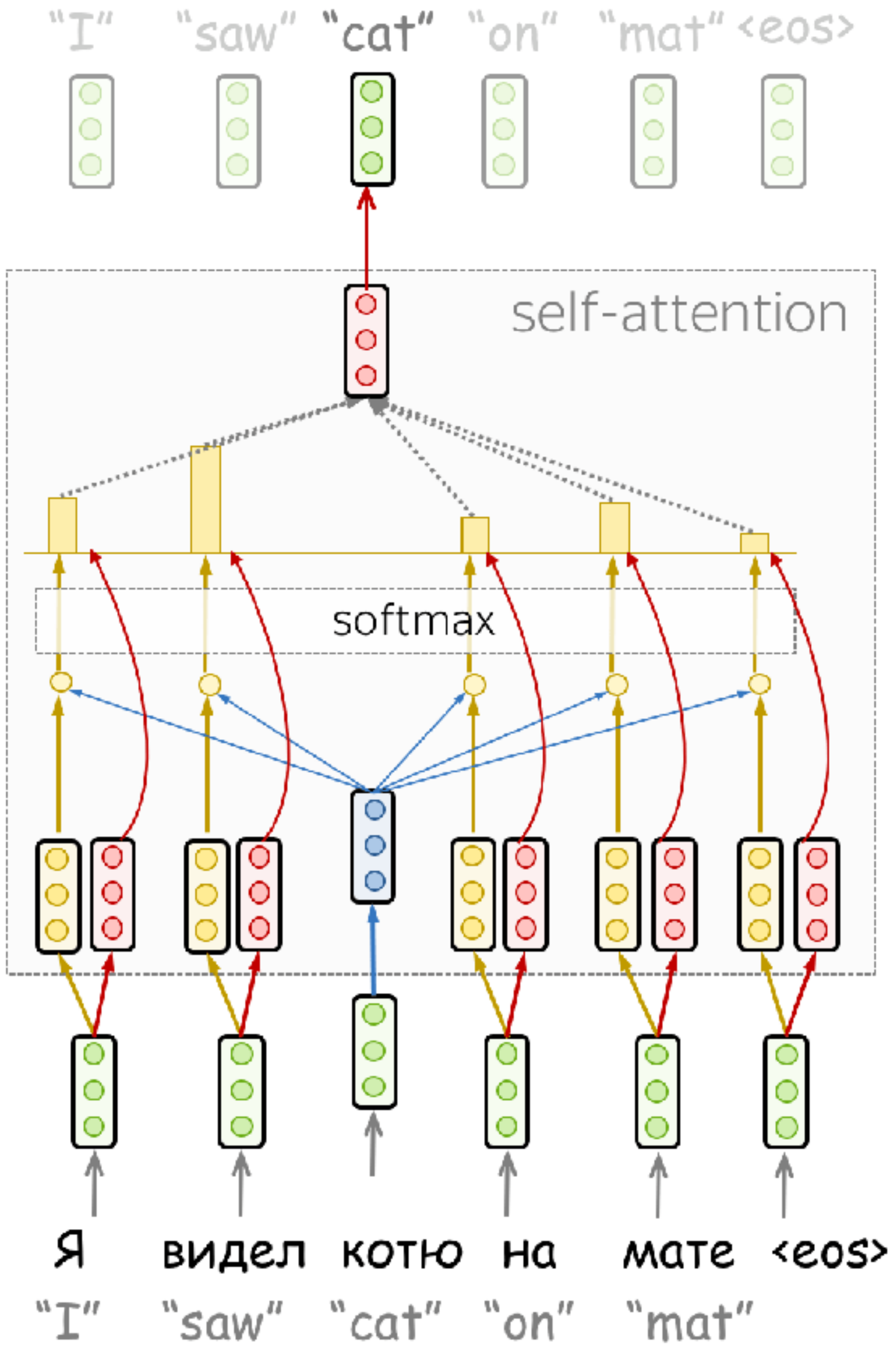
Key: vector at which the query looks to compute weights

"Hi, I have this information – give me a large weight!"



Value: their weighted sum is attention output

"Here's the information I have!"

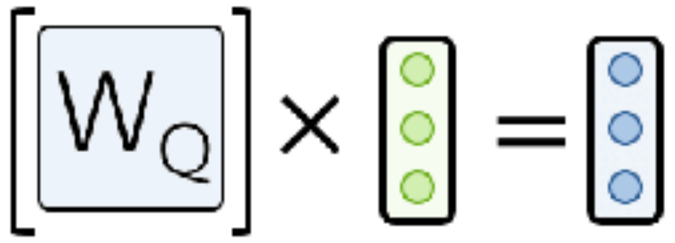


Self-Attention: Basic Concepts

[Lena Viota Blog]

Query: asking for information

Each vector receives t



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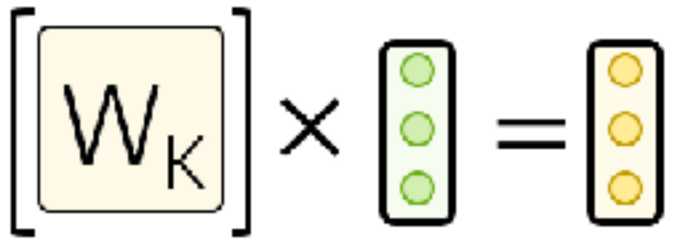

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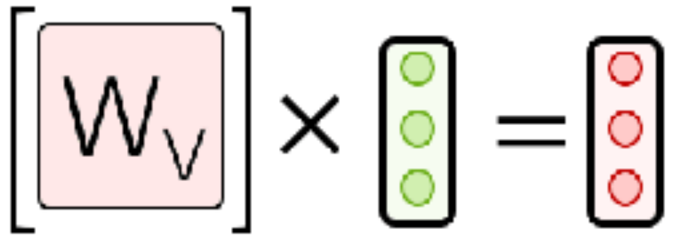

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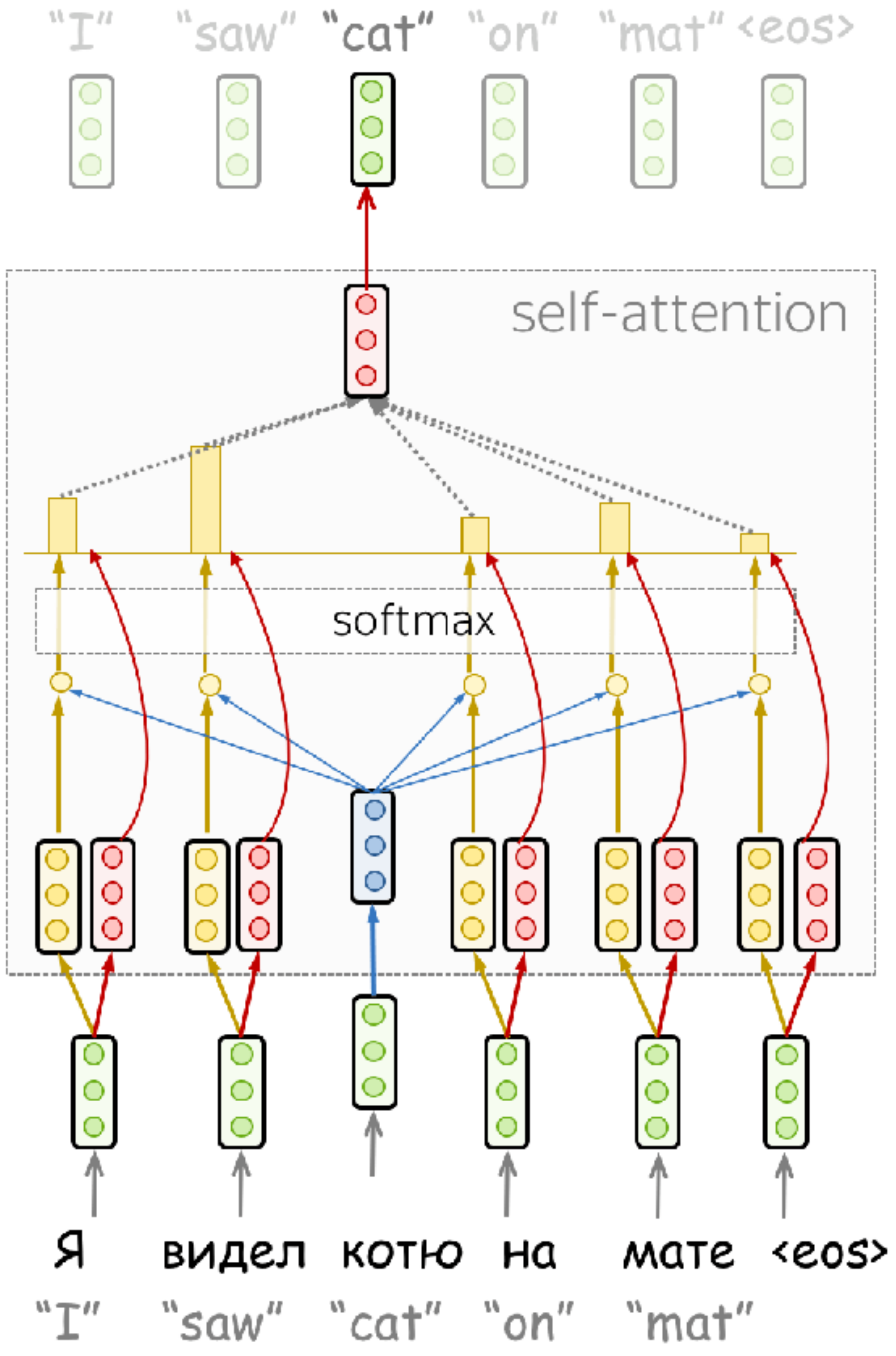


Self-Attention: Basic Concepts

[Lena Viota Blog]

Each vector receives t

Query: asking for information

$[W_Q] \times$ [green vector] = [blue vector]

Que... vector from which the atte...

"Hey there, do you have

Key: saying that it has some information

$[W_K] \times$ [green vector] = [yellow vector]

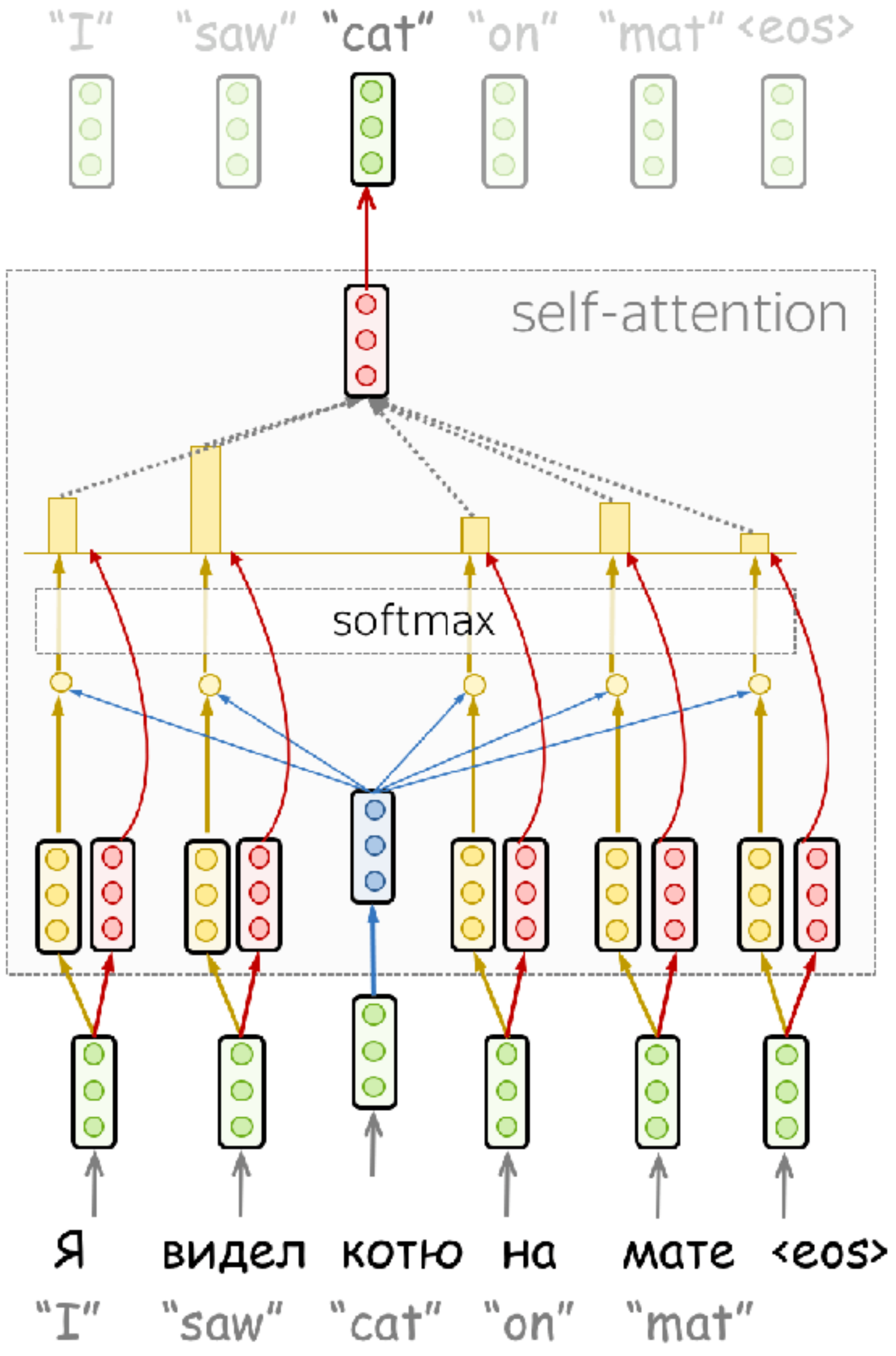
Key: ... looks to compute weights

"Hi, I have this information – give me a large weight!"

$[W_V] \times$ [green vector] = [red vector]

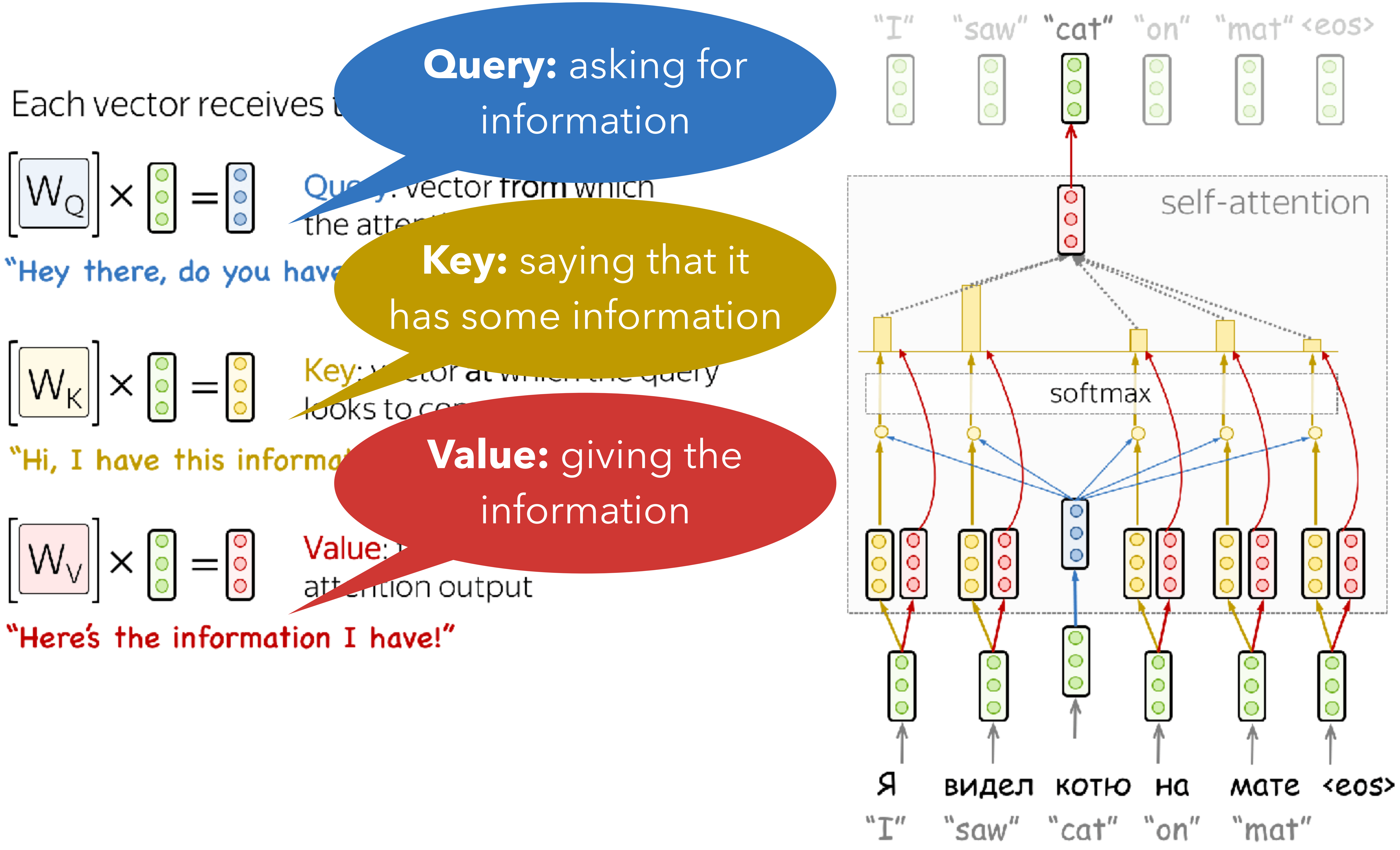
Value: their weighted sum is attention output

"Here's the information I have!"

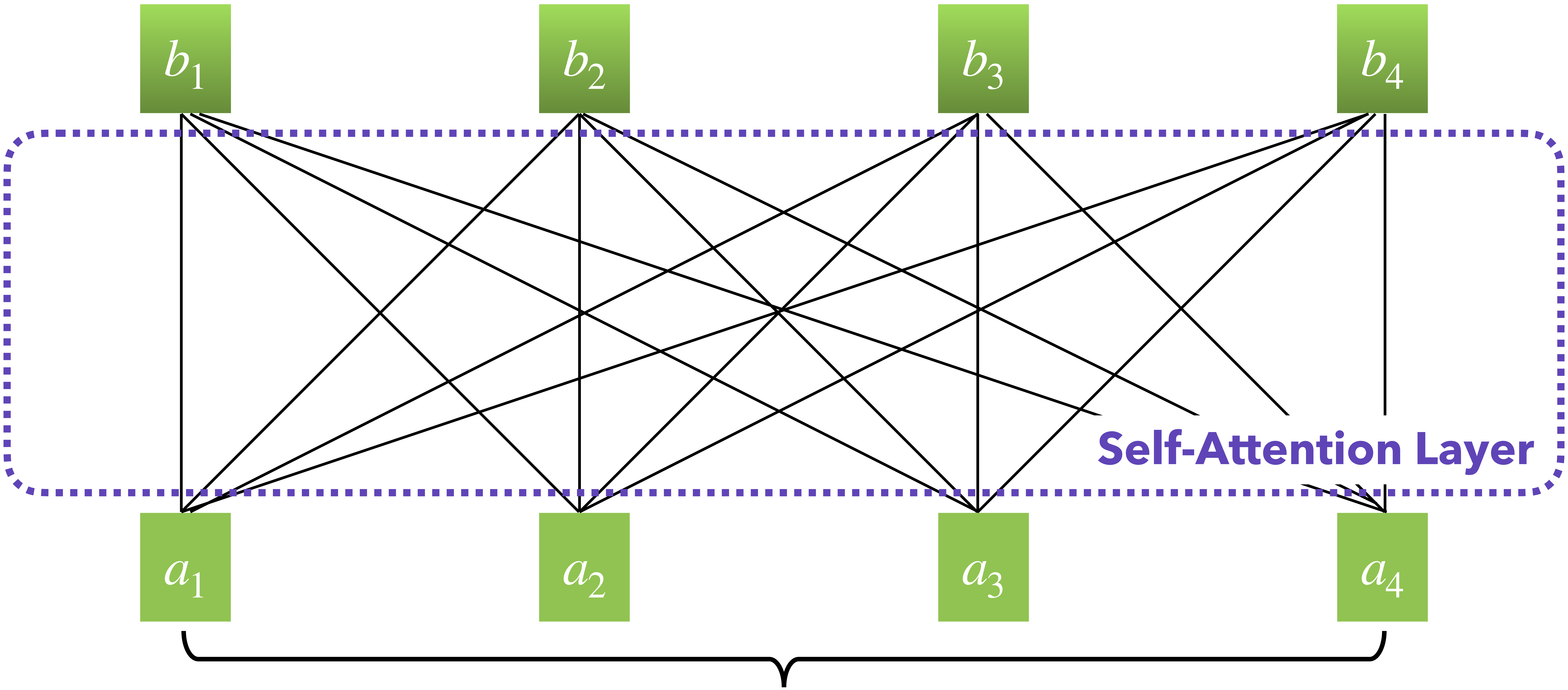


Self-Attention: Basic Concepts

[Lena Viota Blog]

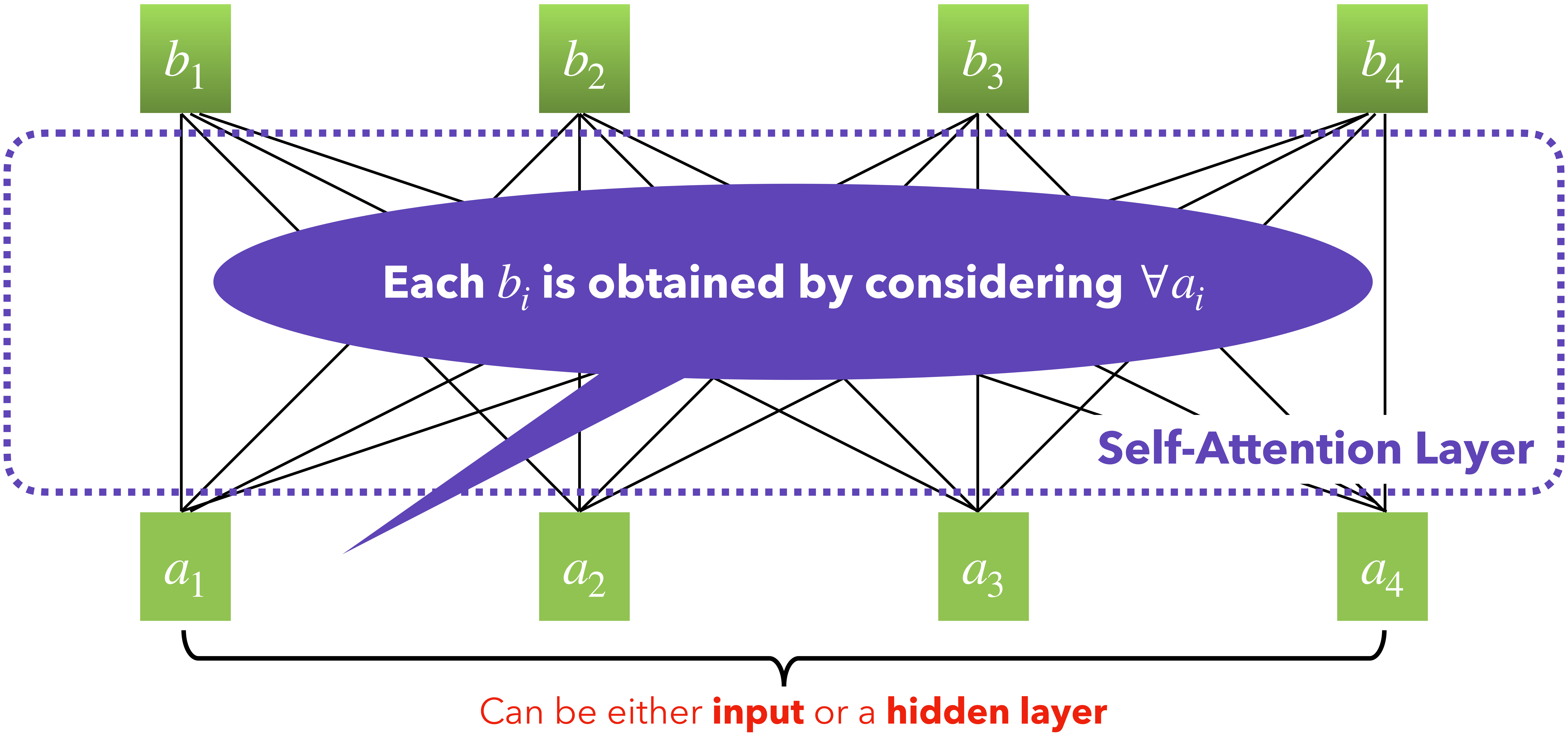


Self-Attention: Walk-through



Can be either **input** or a **hidden layer**

Self-Attention: Walk-through



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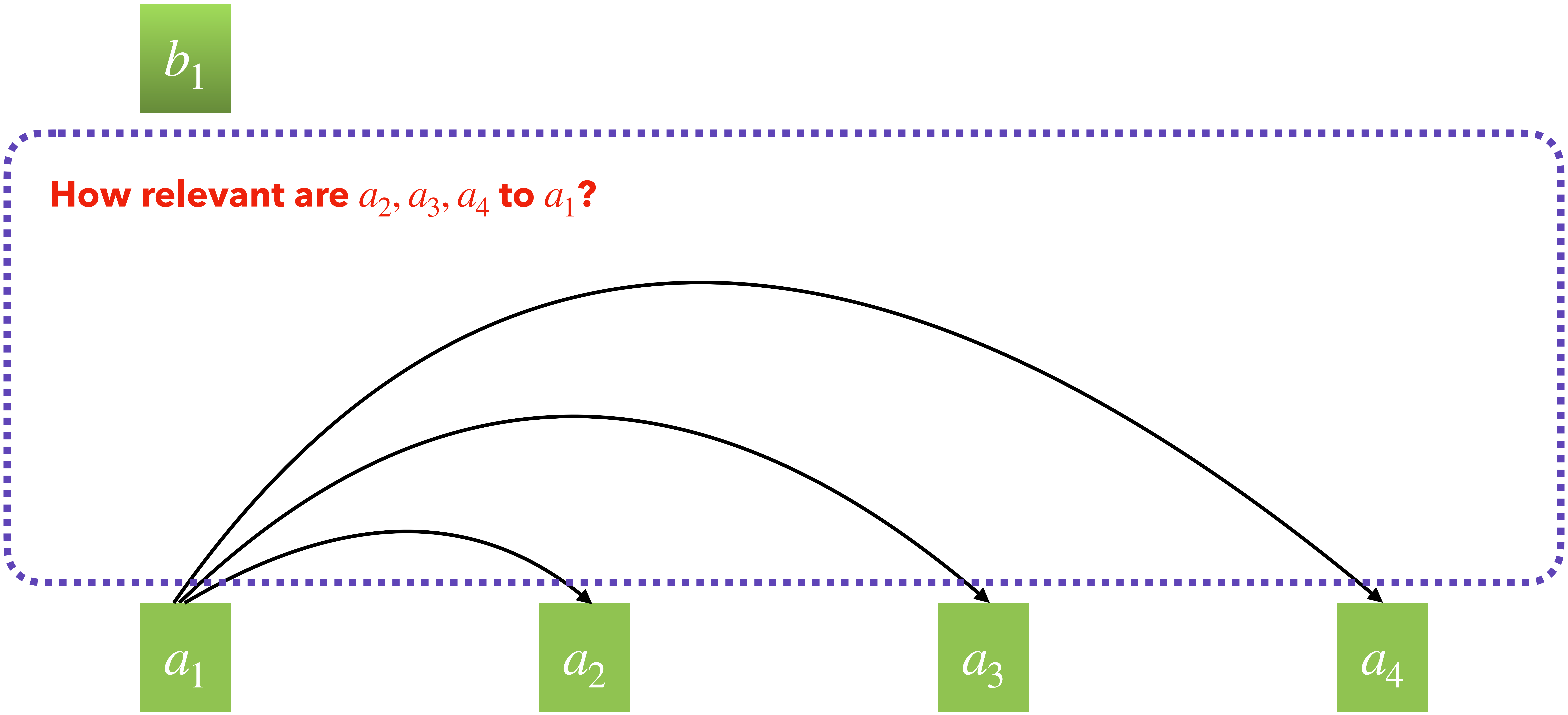

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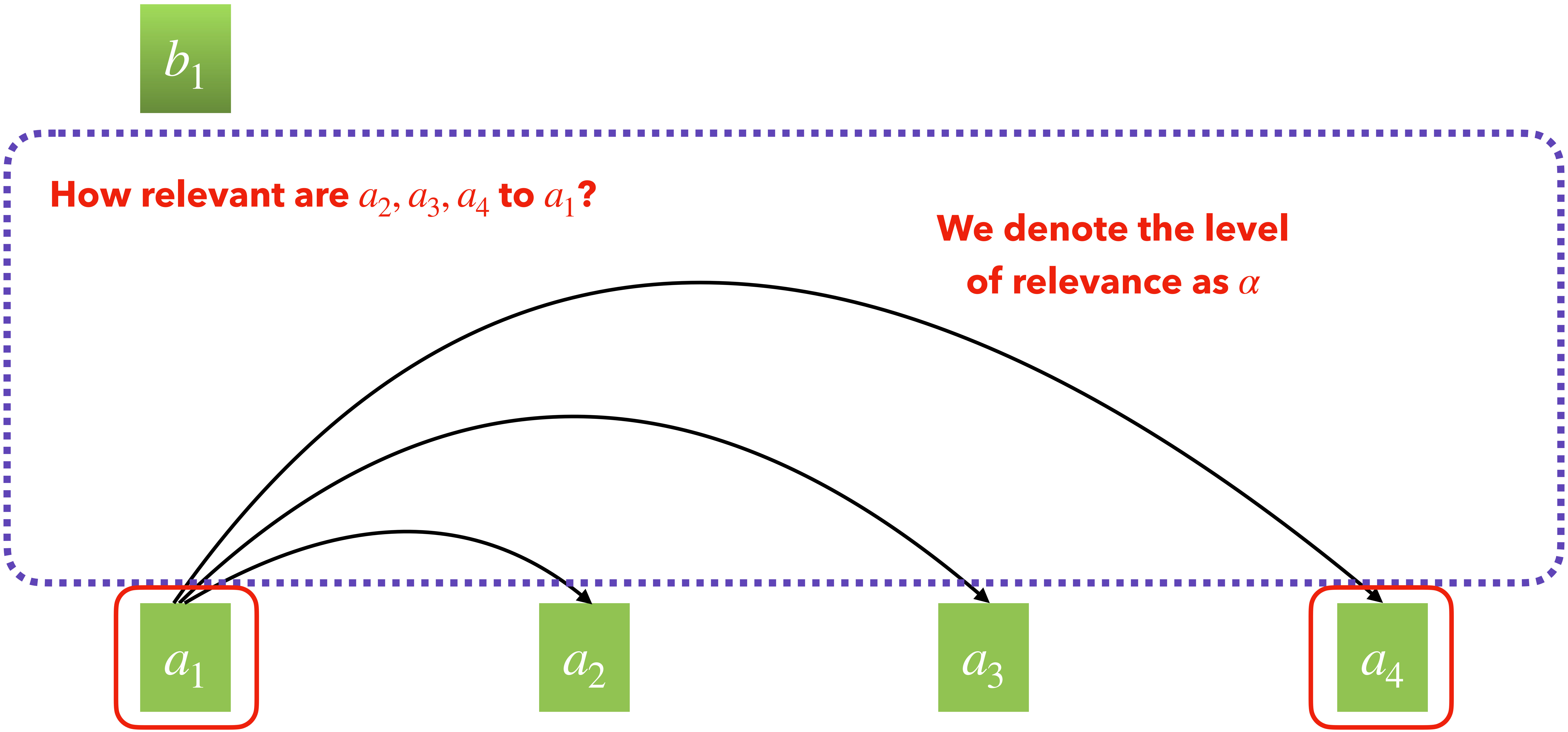
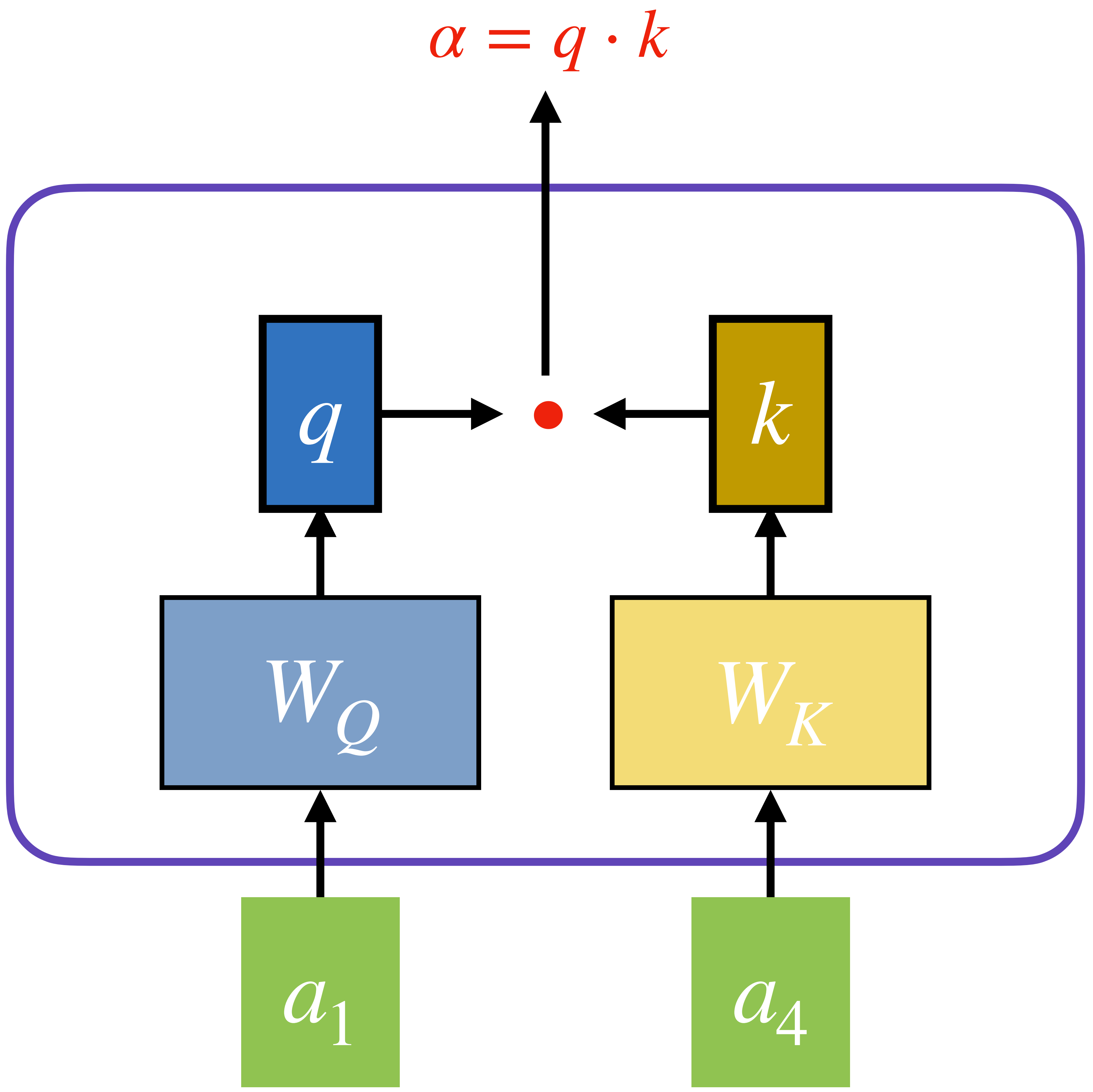
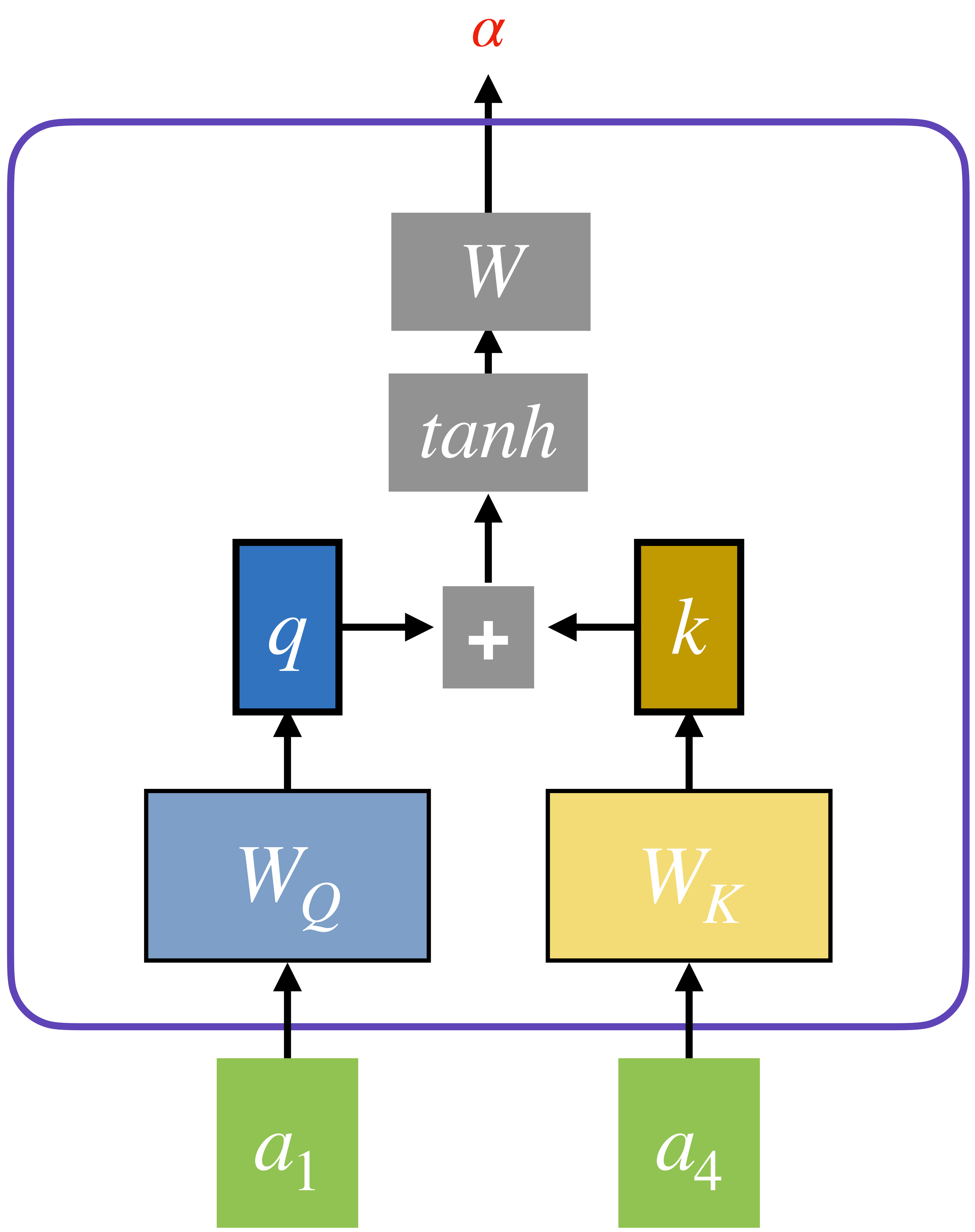


How to compute α?



Method 1 **(most common): Dot product**



Method 2: **Additive**

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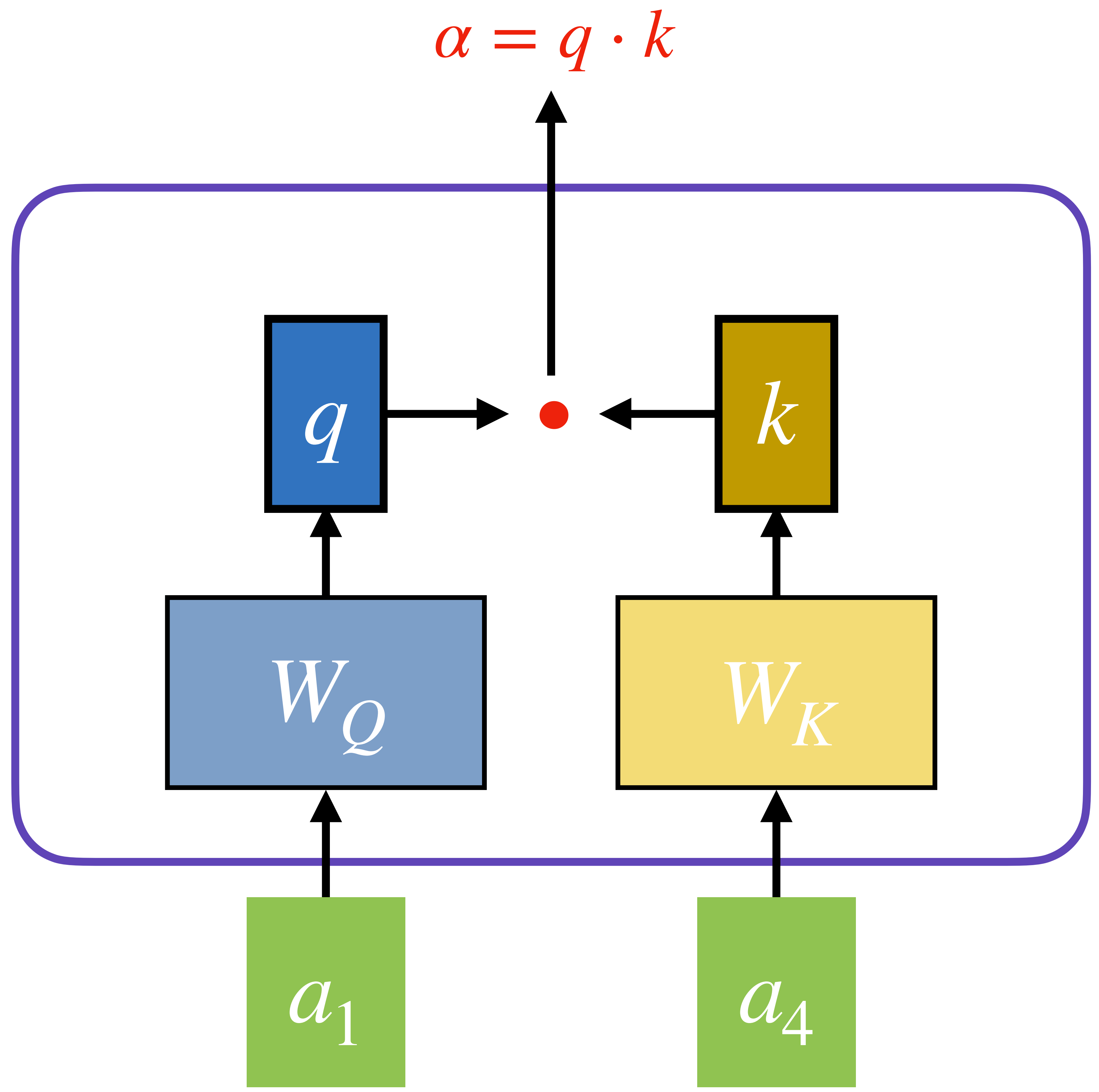
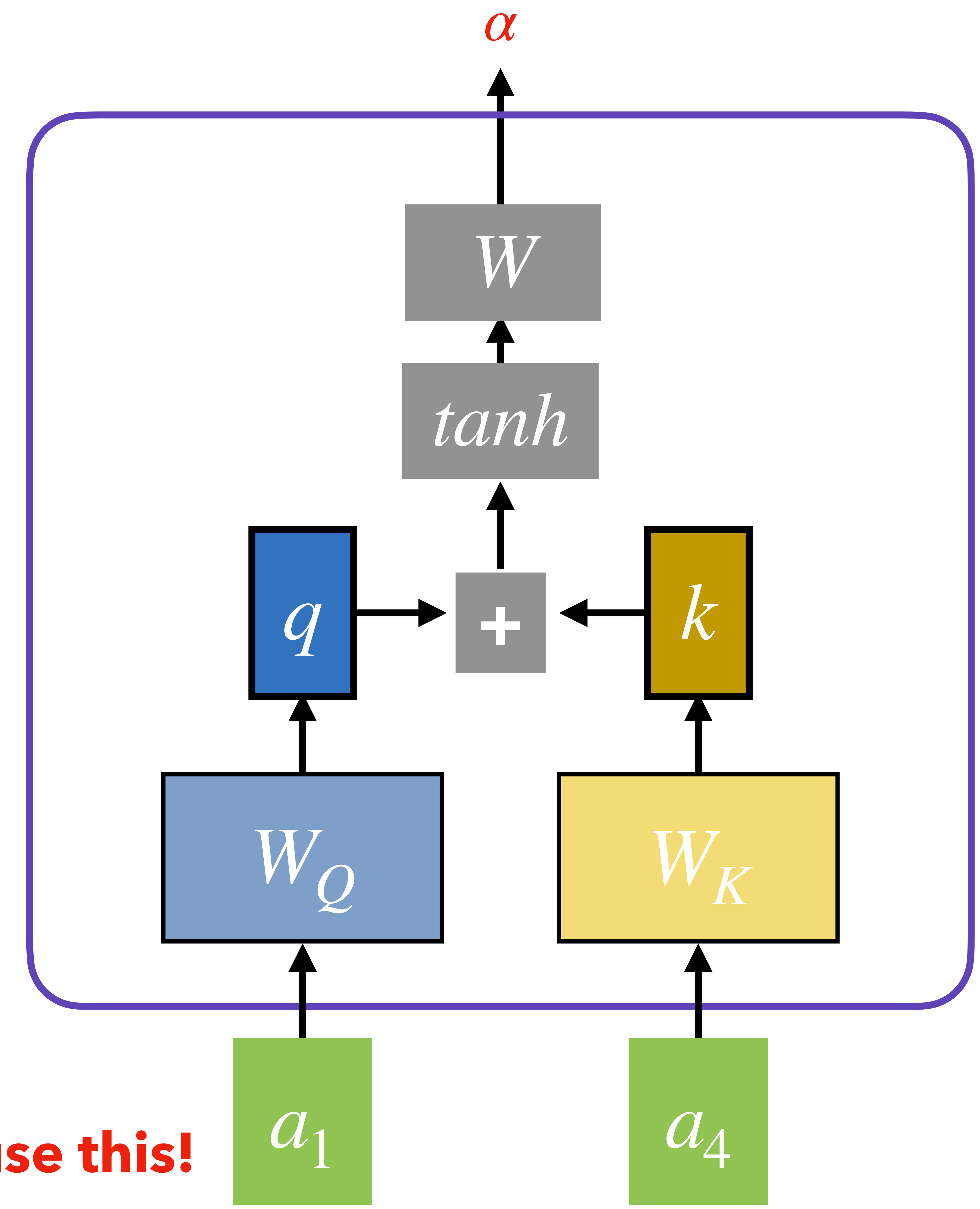


Method 1 **(most common): Dot product**

We'll use this!



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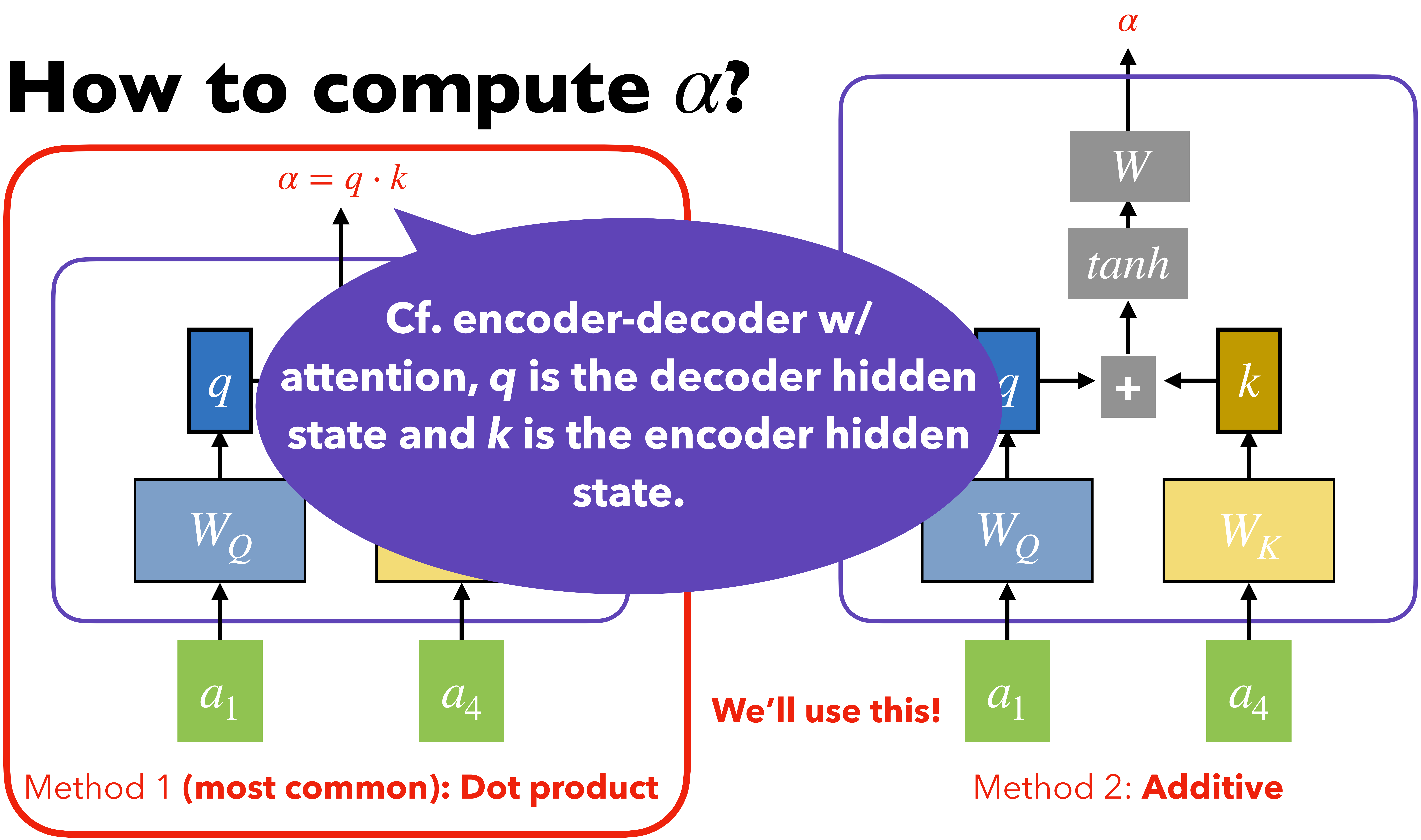

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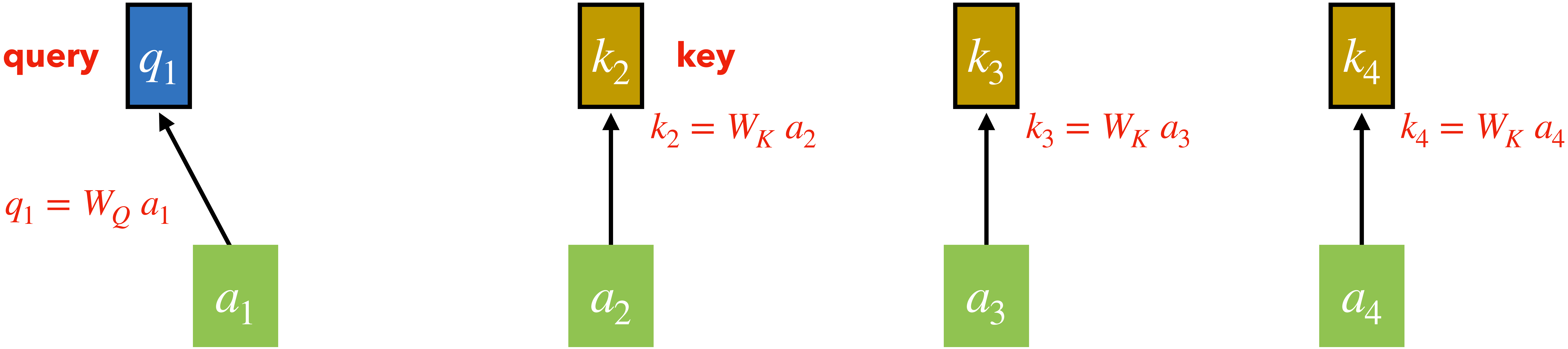

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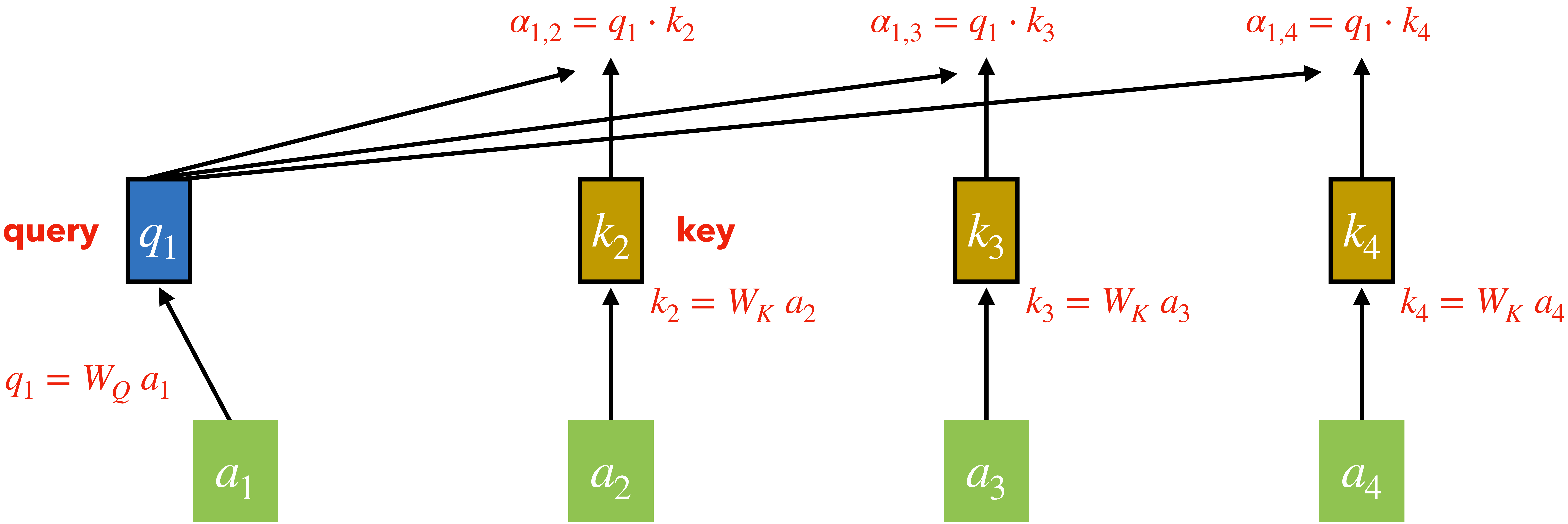

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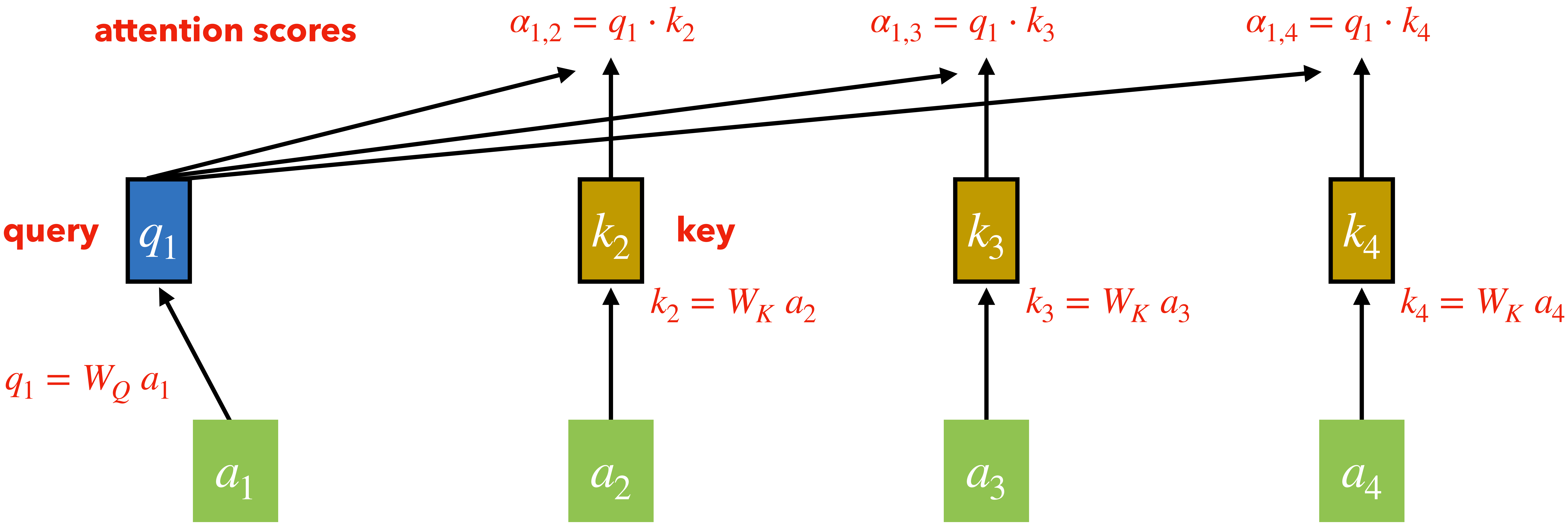
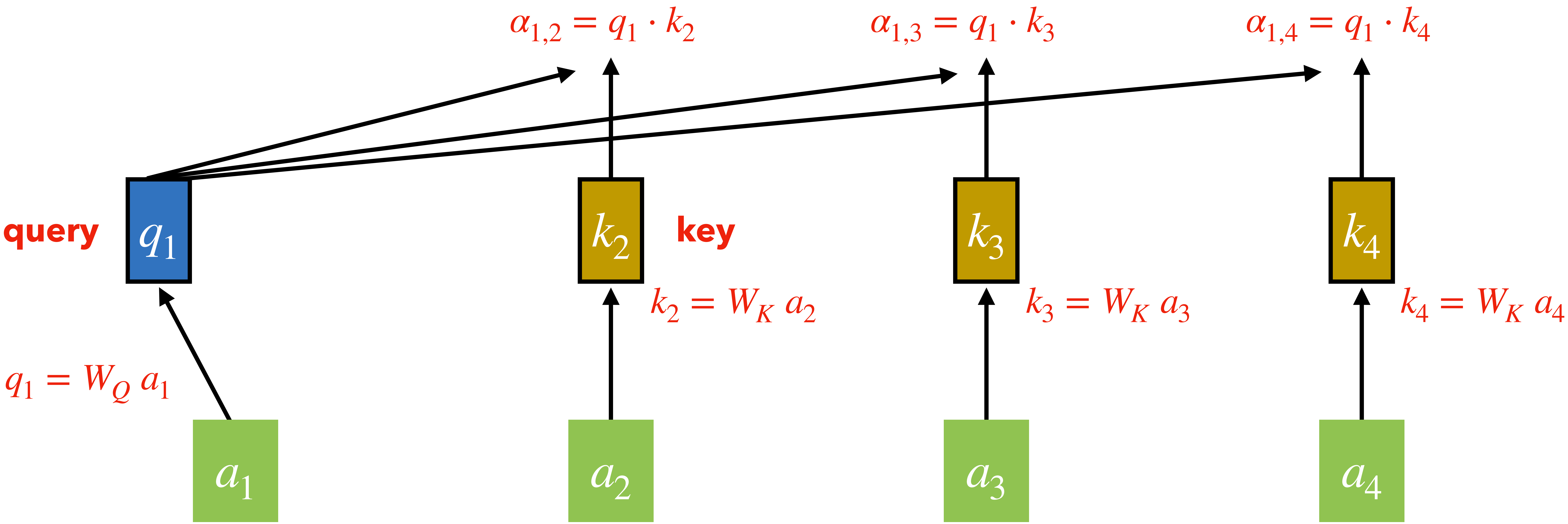
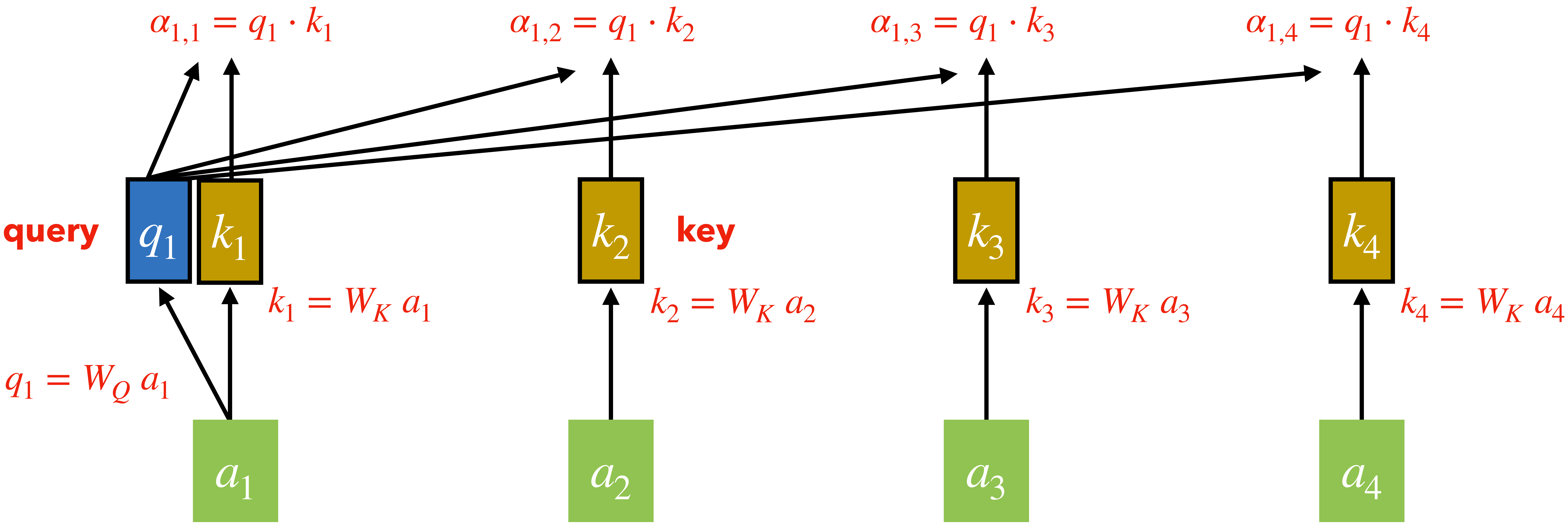




$\alpha_{1,2} = q_1 \cdot k_2$
$\alpha_{1,3} = q_1 \cdot k_3$
$\alpha_{1,4} = q_1 \cdot k_4$
query
q_1
k_2
key
k_3
k_4
$k_2 = W_K\, a_2$
$k_3 = W_K\, a_3$
$k_4 = W_K\, a_4$
$q_1 = W_Q\, a_1$
a_1
a_2
a_3
a_4



$\alpha_{1,1} = q_1 \cdot k_1$
$\alpha_{1,2} = q_1 \cdot k_2$
$\alpha_{1,3} = q_1 \cdot k_3$
$\alpha_{1,4} = q_1 \cdot k_4$
query
q_1
k_1
k_2
key
k_3
k_4
$k_1 = W_K\, a_1$
$k_2 = W_K\, a_2$
$k_3 = W_K\, a_3$
$k_4 = W_K\, a_4$
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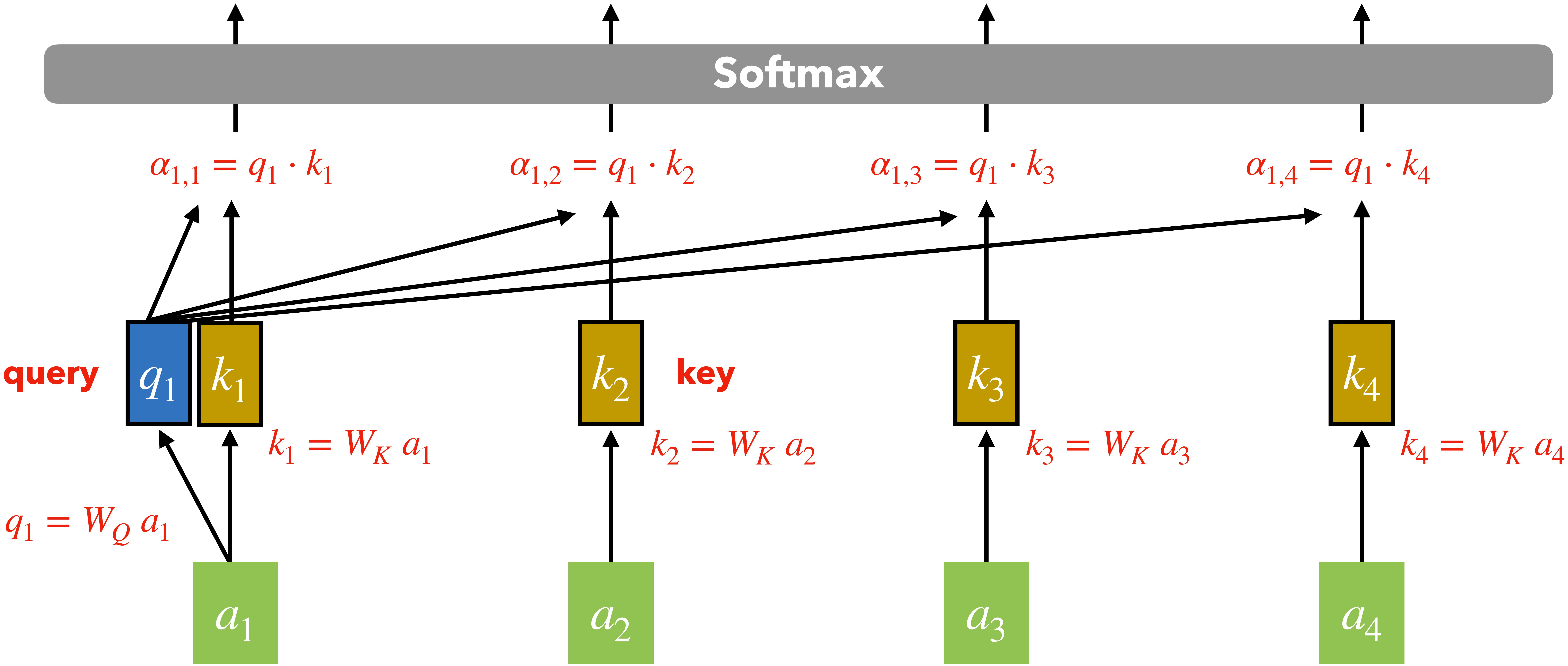
a_1
a_2
a_3
a_4


Softmax
$\alpha_{1,1} = q_1 \cdot k_1$
$\alpha_{1,2} = q_1 \cdot k_2$
$\alpha_{1,3} = q_1 \cdot k_3$
$\alpha_{1,4} = q_1 \cdot k_4$
query
q_1
k_1
k_2
key
k_3
k_4
$k_1 = W_K\, a_1$
$k_2 = W_K\, a_2$
$k_3 = W_K\, a_3$
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a_1
a_2
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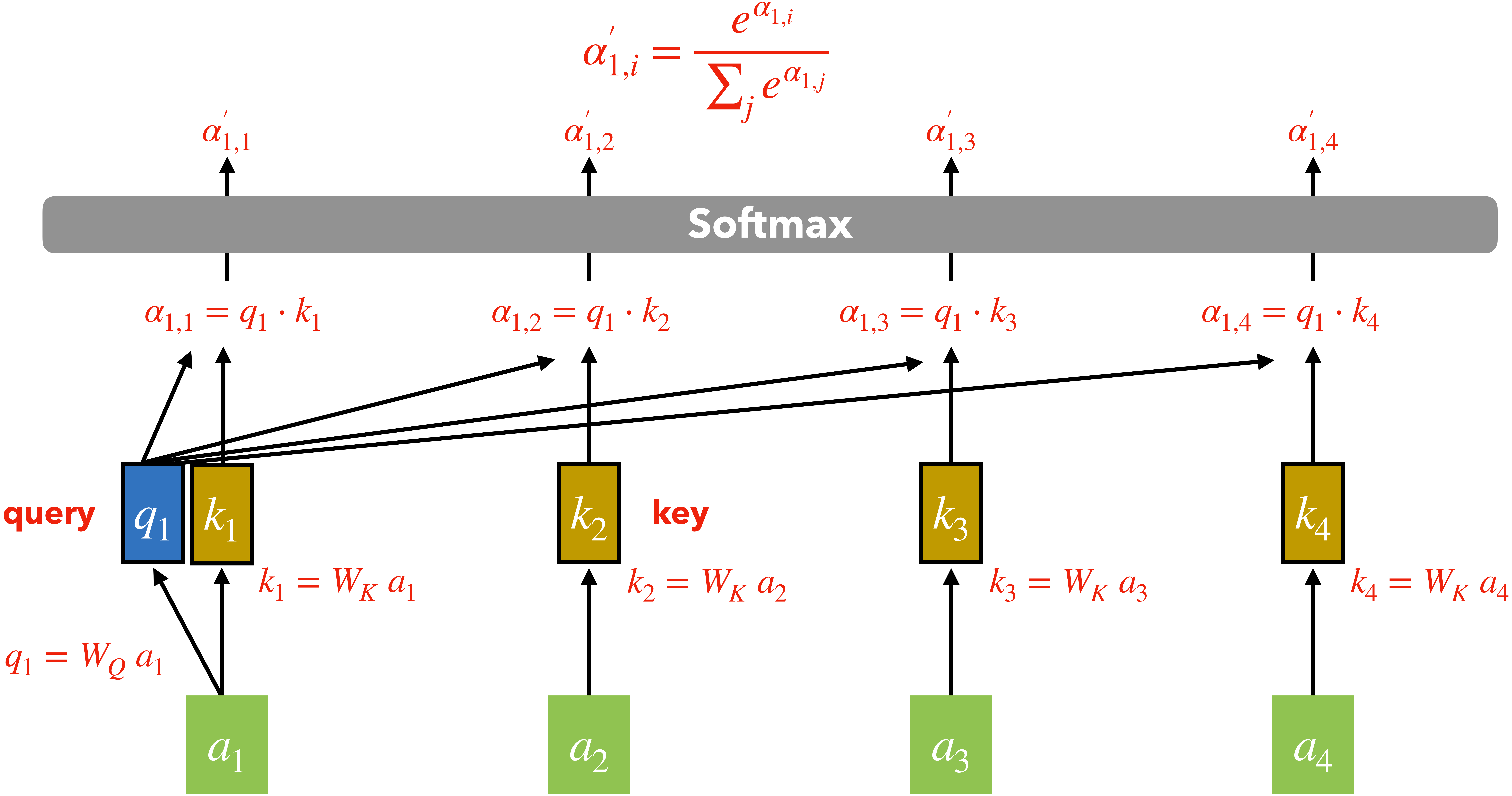

$\alpha'_{1,i} = \frac{e^{\alpha_{1,i}}}{\sum_j e^{\alpha_{1,j}}}$
$\alpha'_{1,1}$
$\alpha'_{1,2}$
$\alpha'_{1,3}$
$\alpha'_{1,4}$
Softmax
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k_2
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$k_1 = W_K\, a_1$
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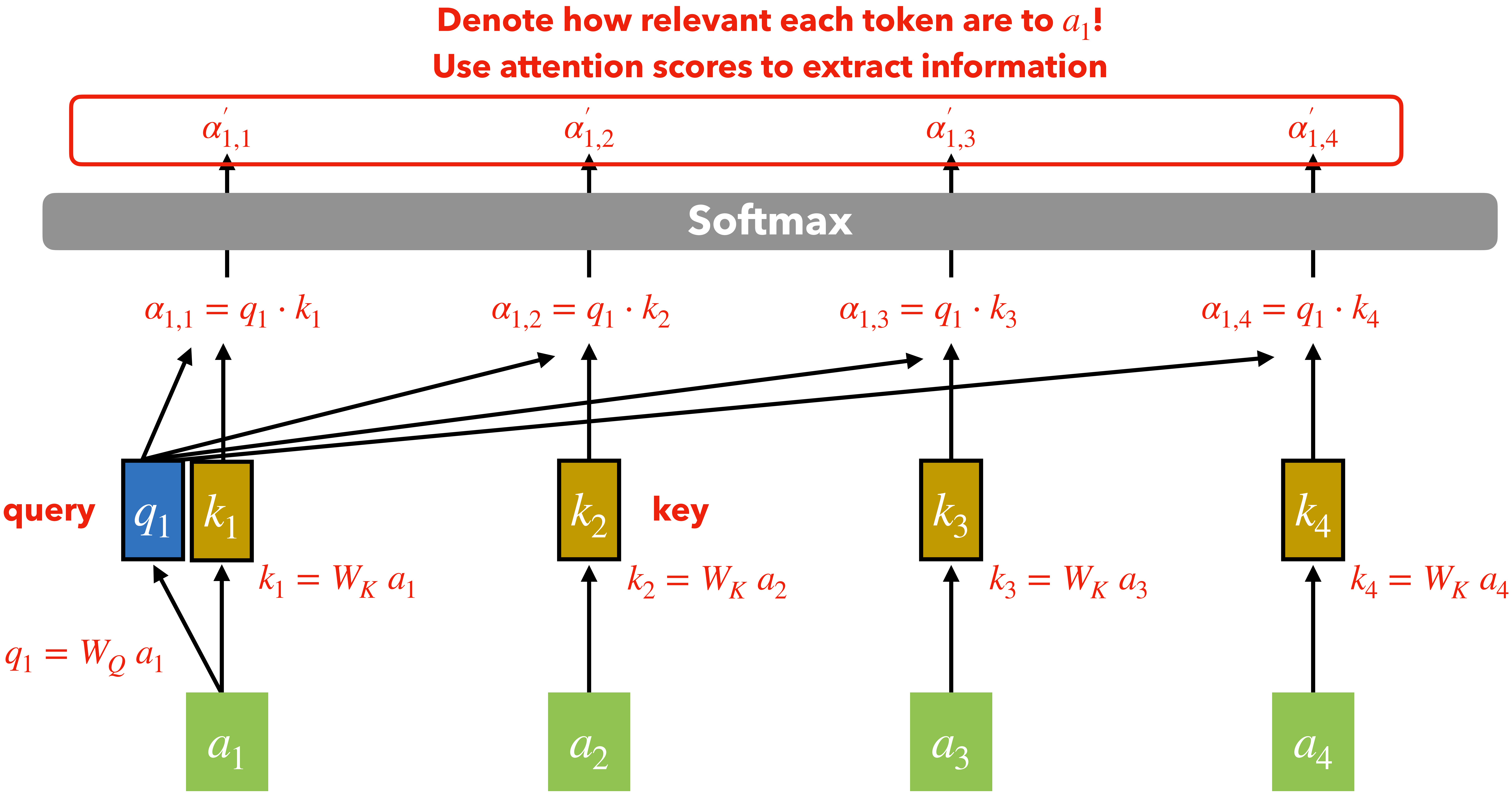

Denote how relevant each token are to a_1!
Use attention scores to extract information
$\alpha'_{1,1}$
$\alpha'_{1,2}$
$\alpha'_{1,3}$
$\alpha'_{1,4}$
Softmax
$\alpha_{1,1} = q_1 \cdot k_1$
$\alpha_{1,2} = q_1 \cdot k_2$
$\alpha_{1,3} = q_1 \cdot k_3$
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k_1
k_2
key
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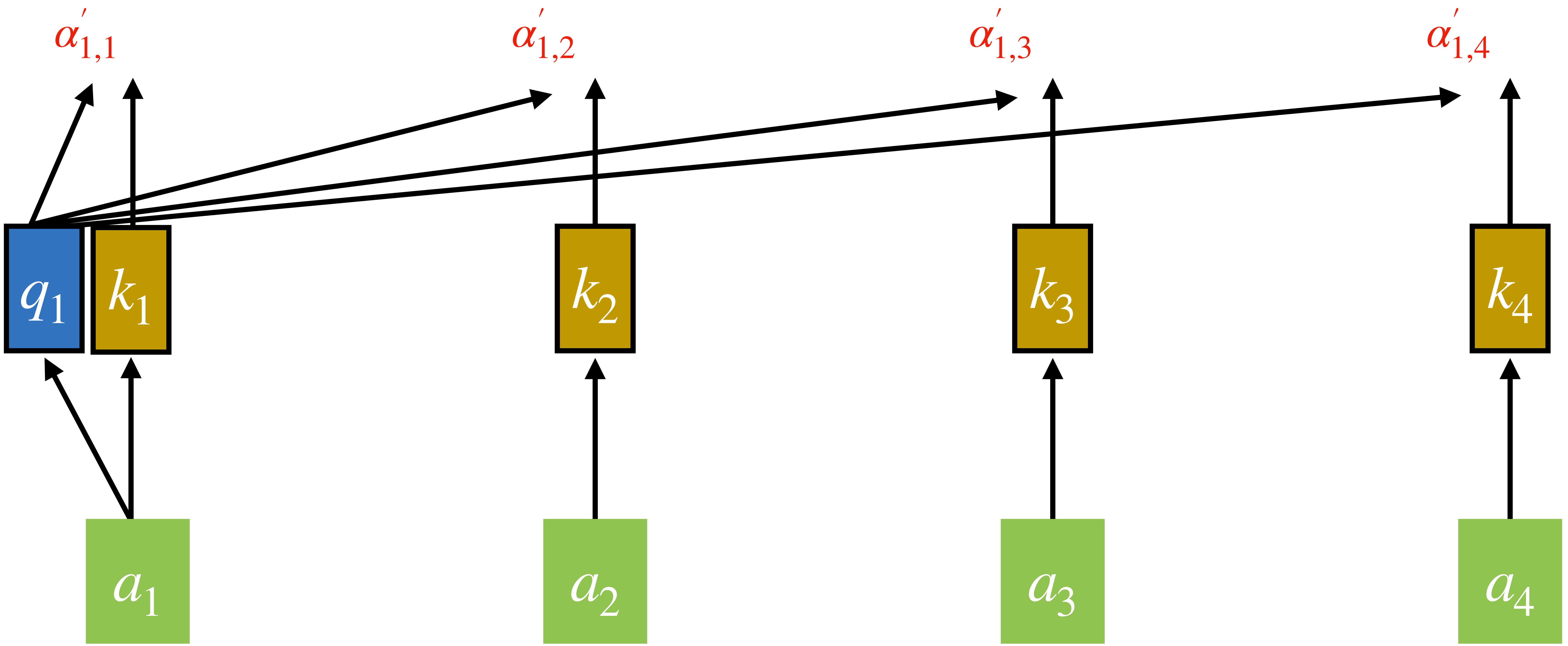
$k_1 = W_K\, a_1$
$k_2 = W_K\, a_2$
$k_3 = W_K\, a_3$
$k_4 = W_K\, a_4$
$q_1 = W_Q\, a_1$
a_1
a_2
a_3
a_4

Use attention scores to extract information



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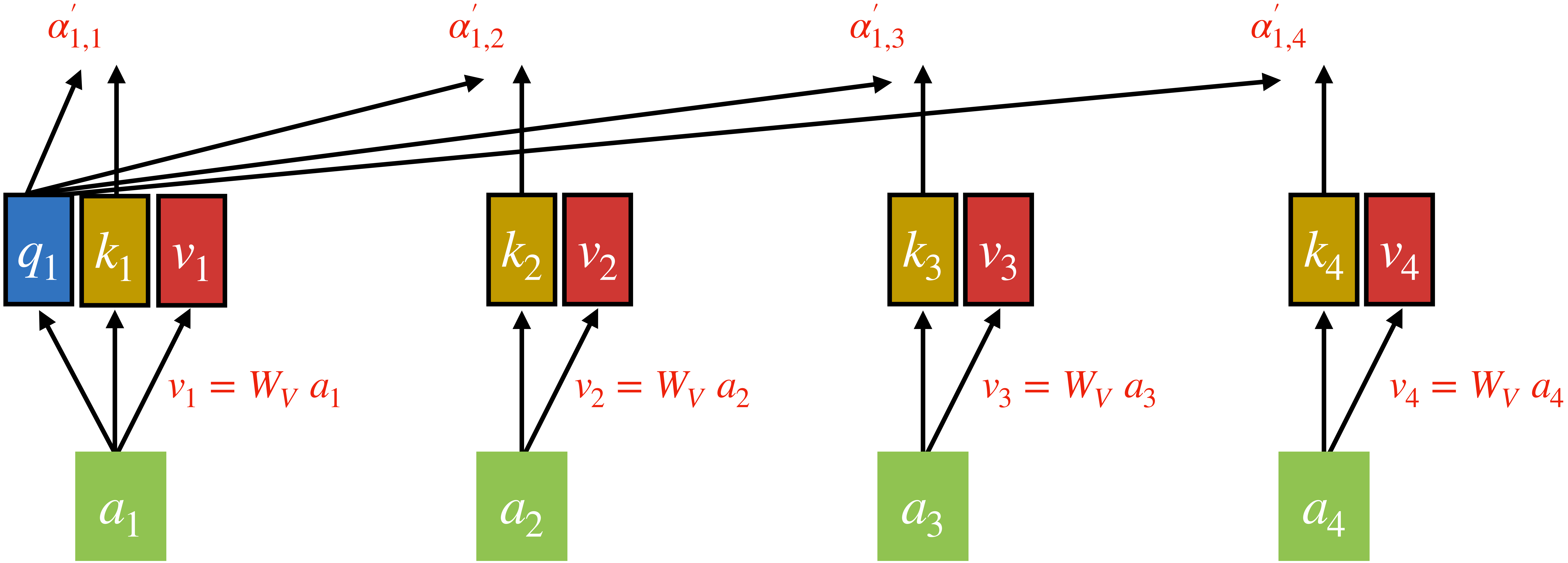

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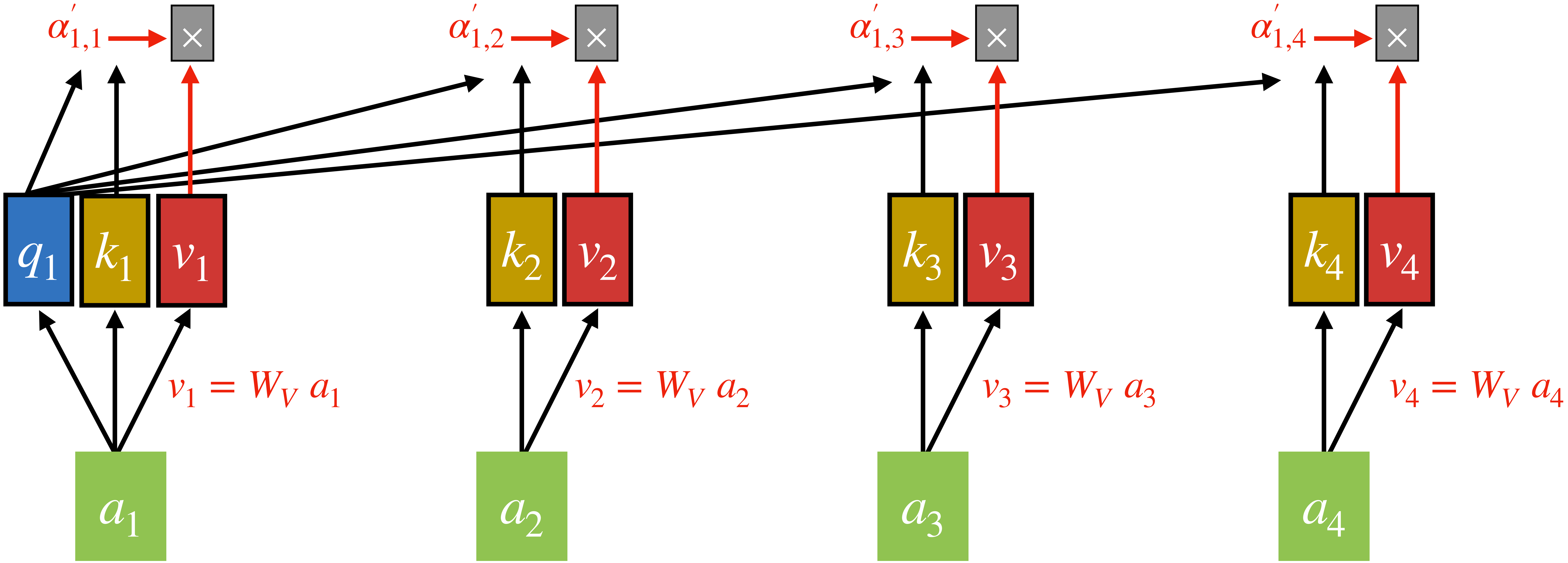
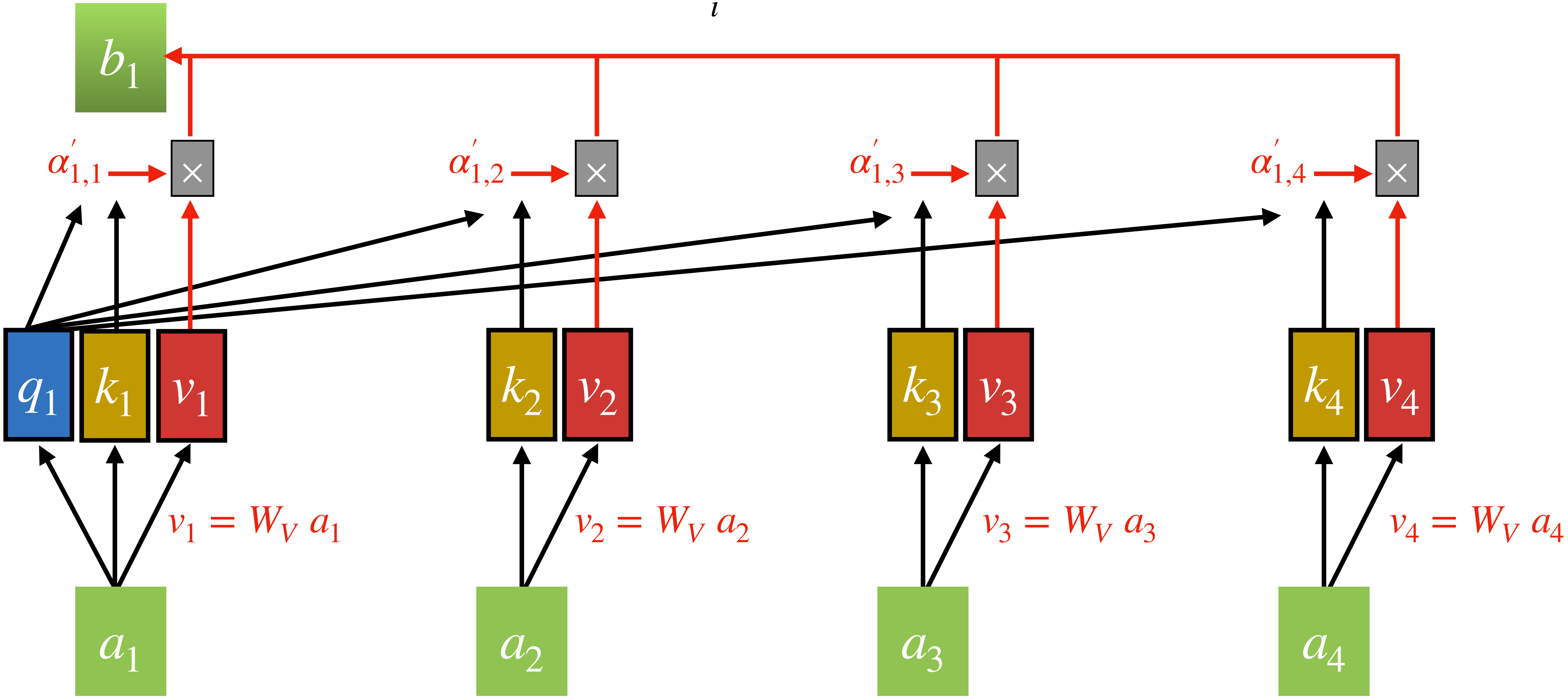


Use attention scores to extract information

$$b_1 = \sum_i \alpha'_{1,i} \, v_i$$



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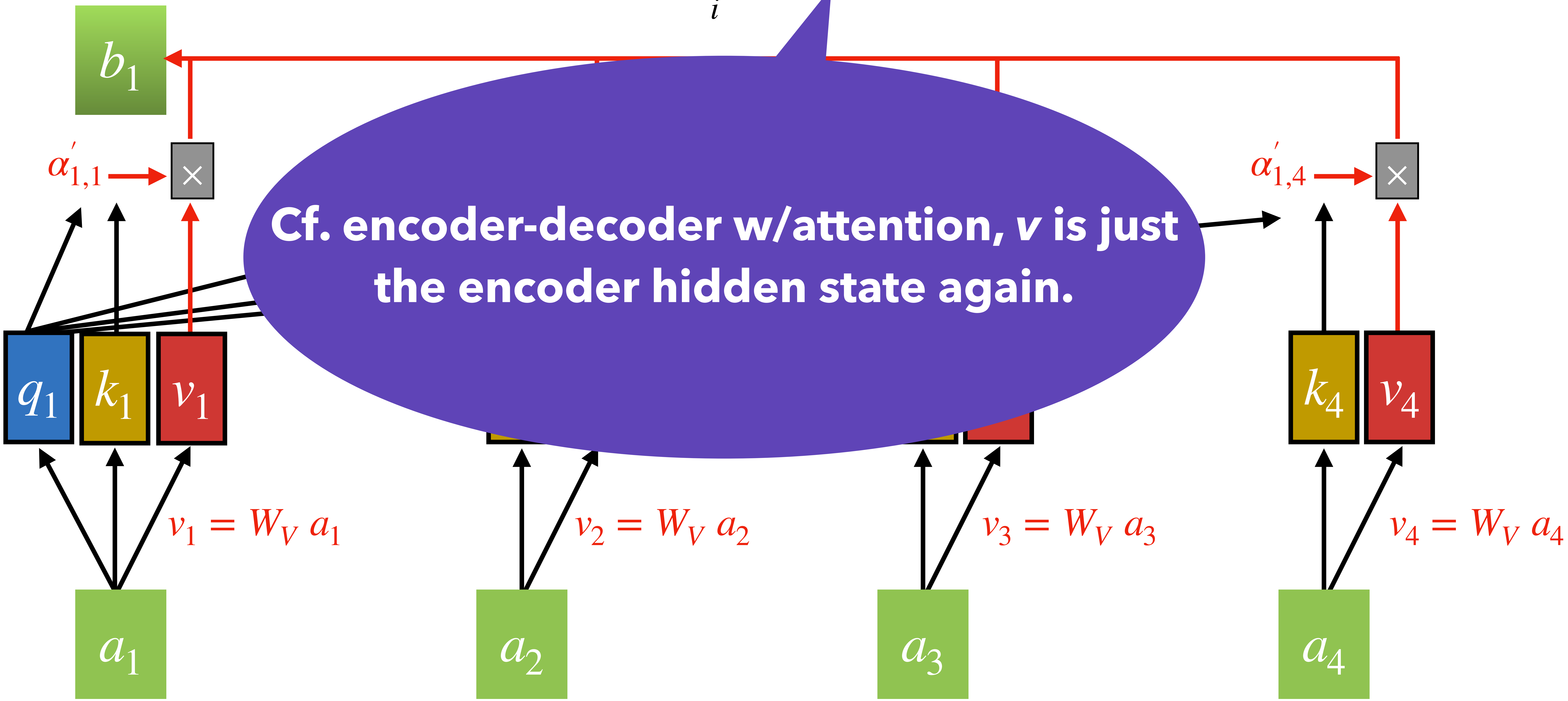

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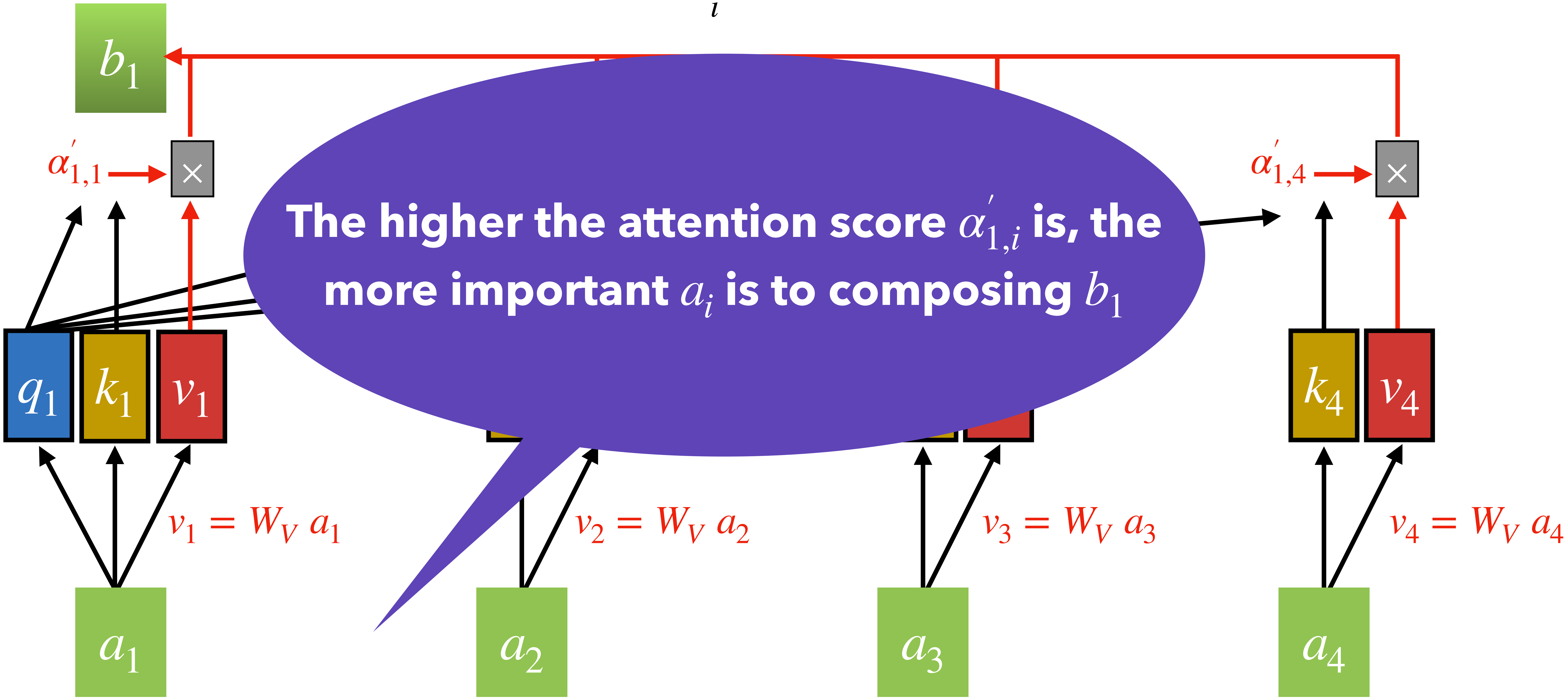
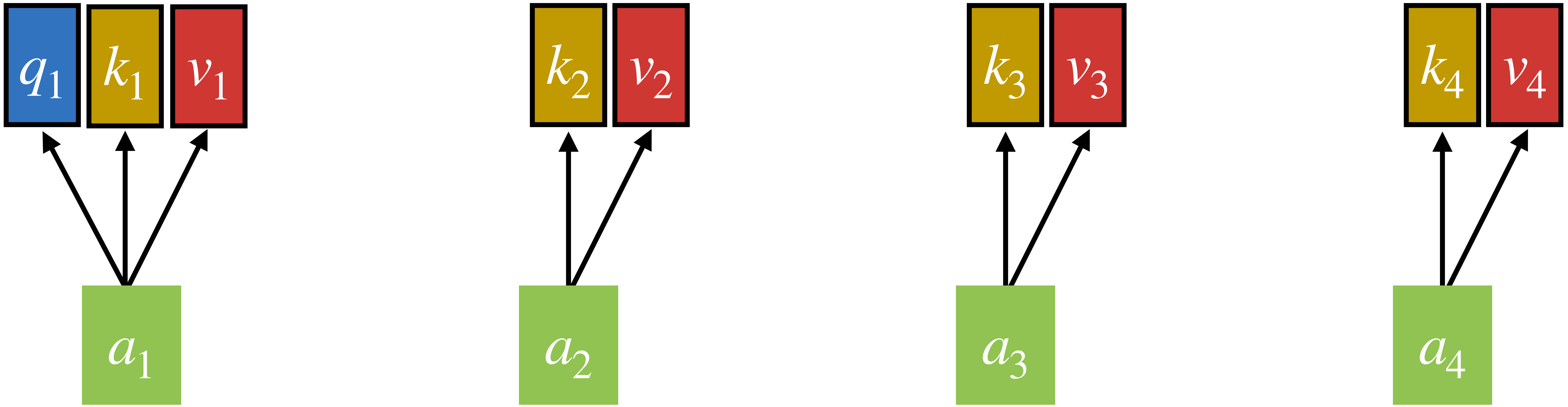


Repeat the same calculation for all a_i to obtain b_i



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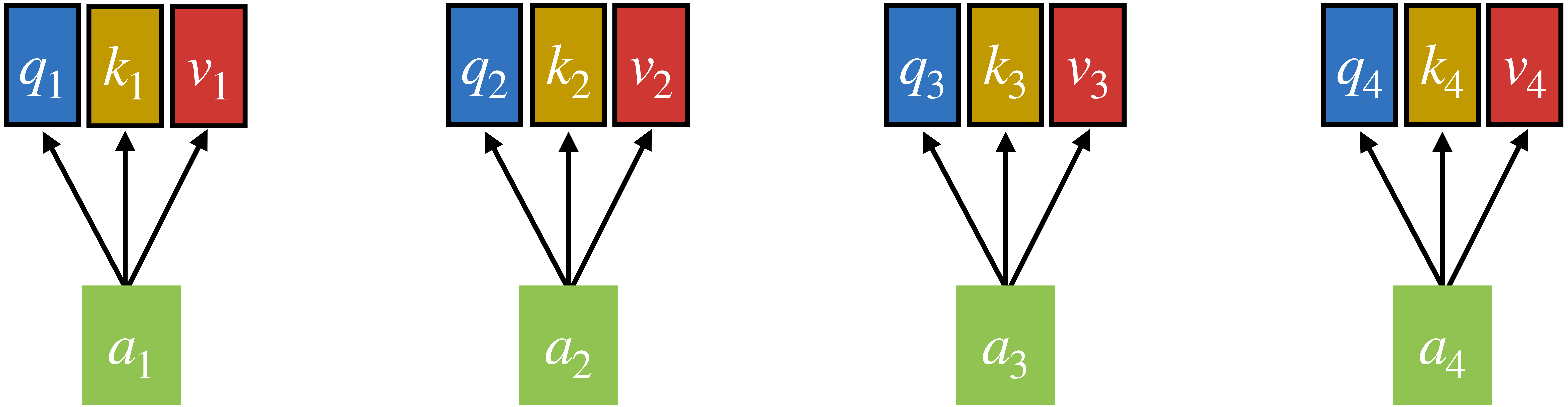

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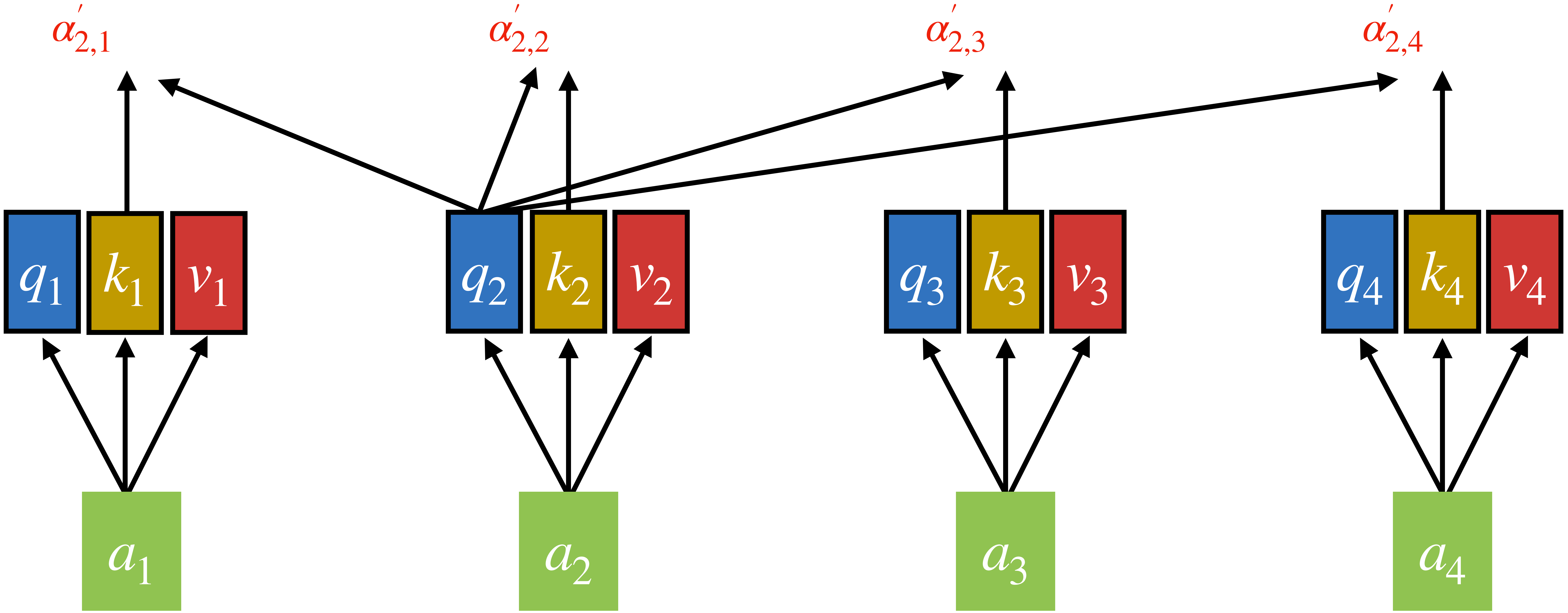

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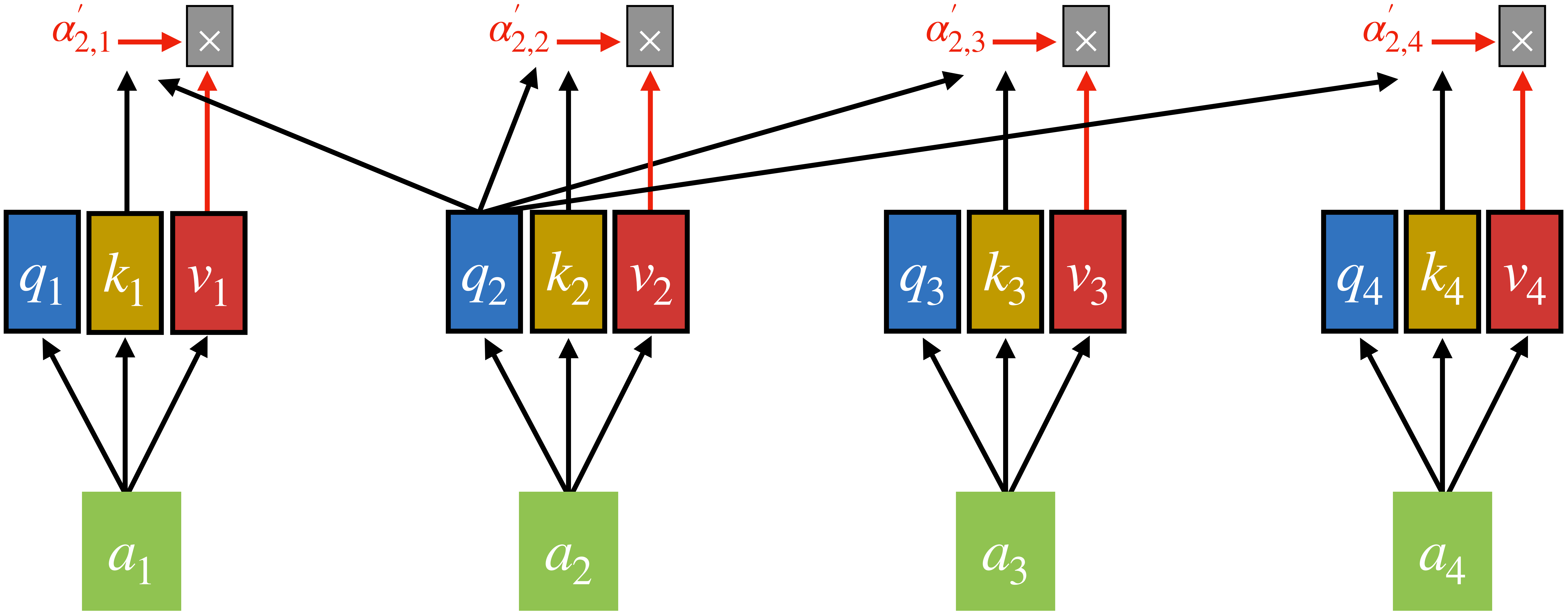
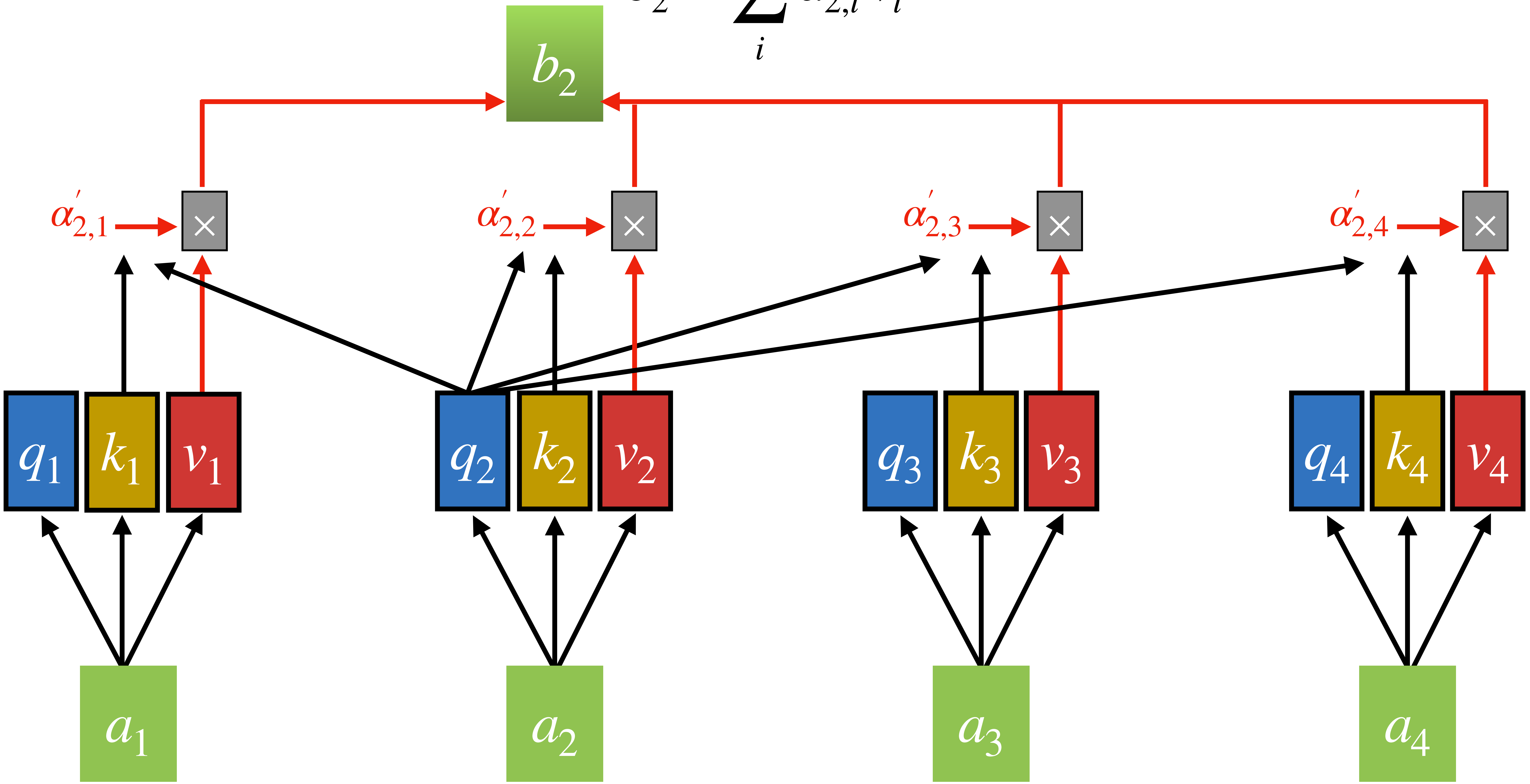


Repeat the same calculation for all a_i to obtain b_i

$$b_2 = \sum_i \alpha'_{2,i} v_i$$



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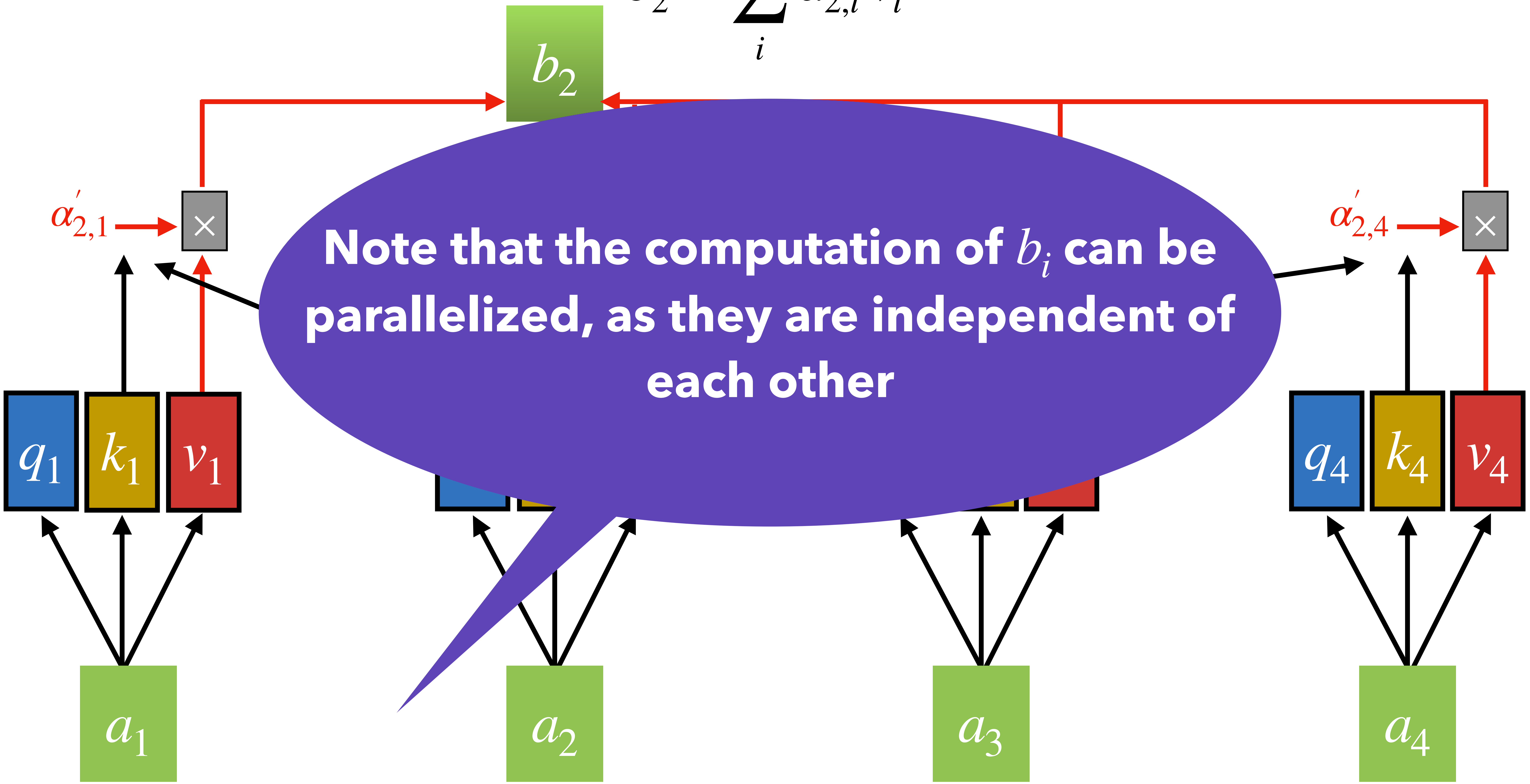

Parallelize the computation!

QKV

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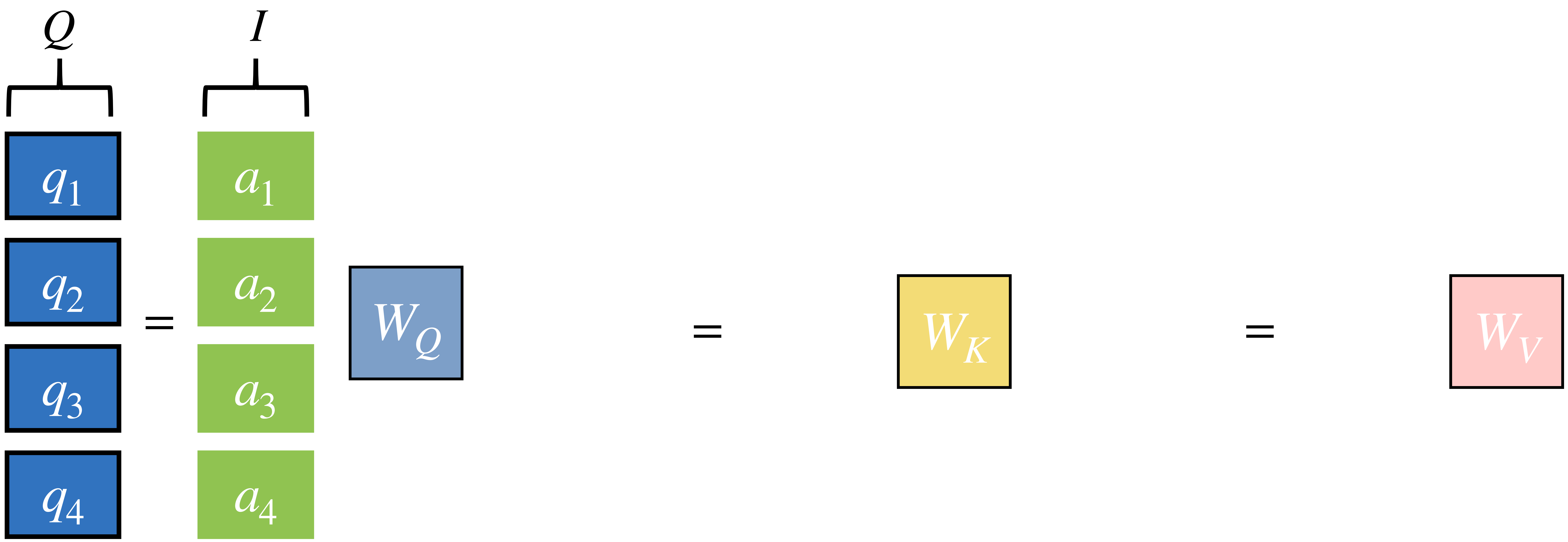

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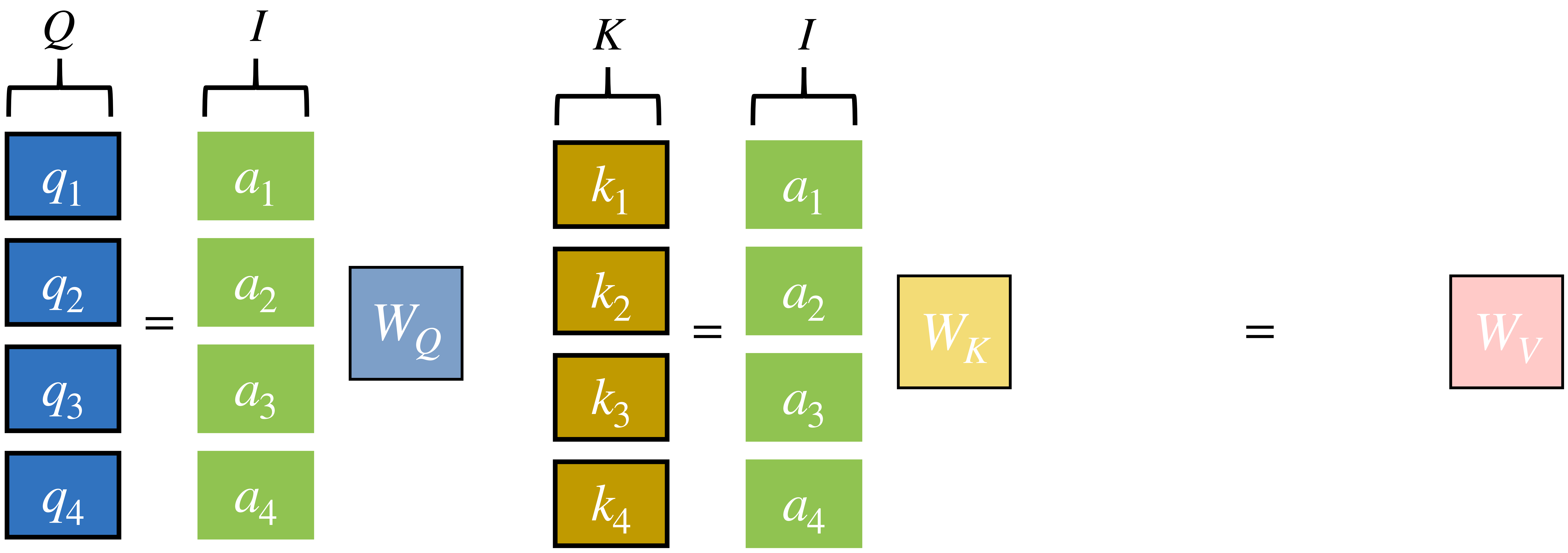

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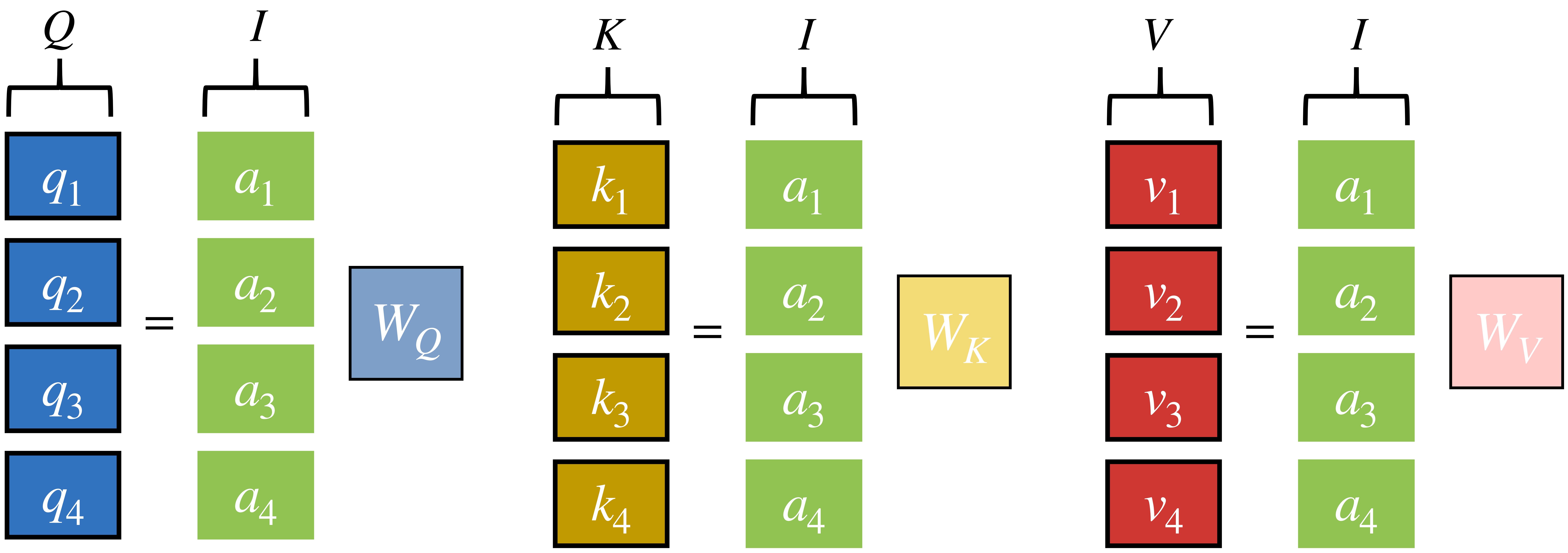

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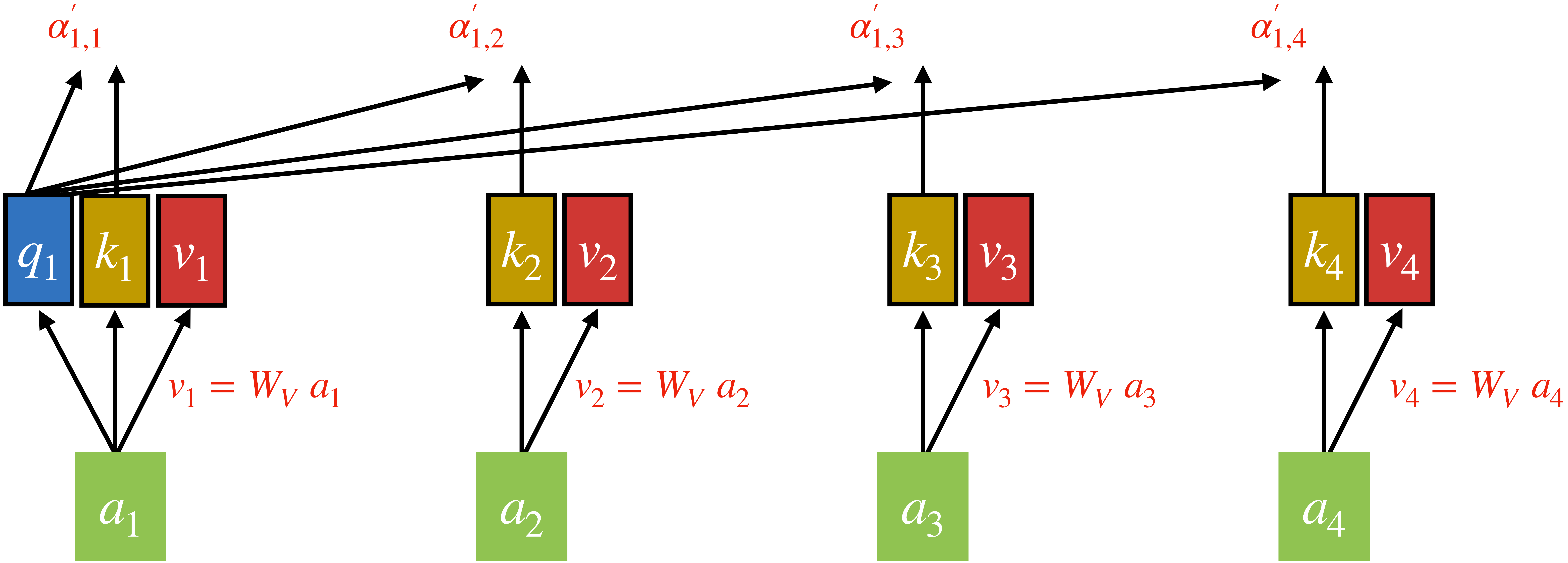

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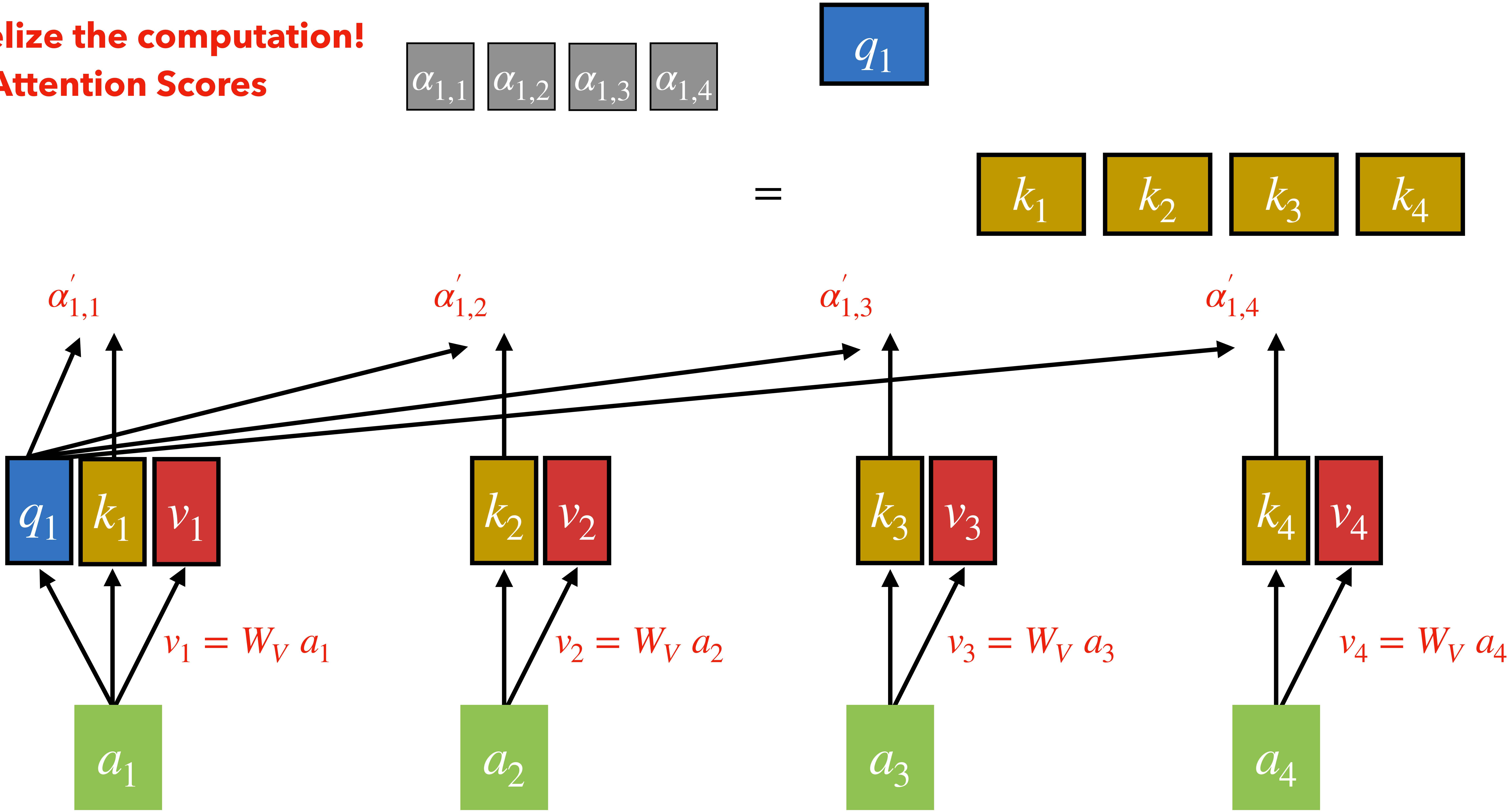

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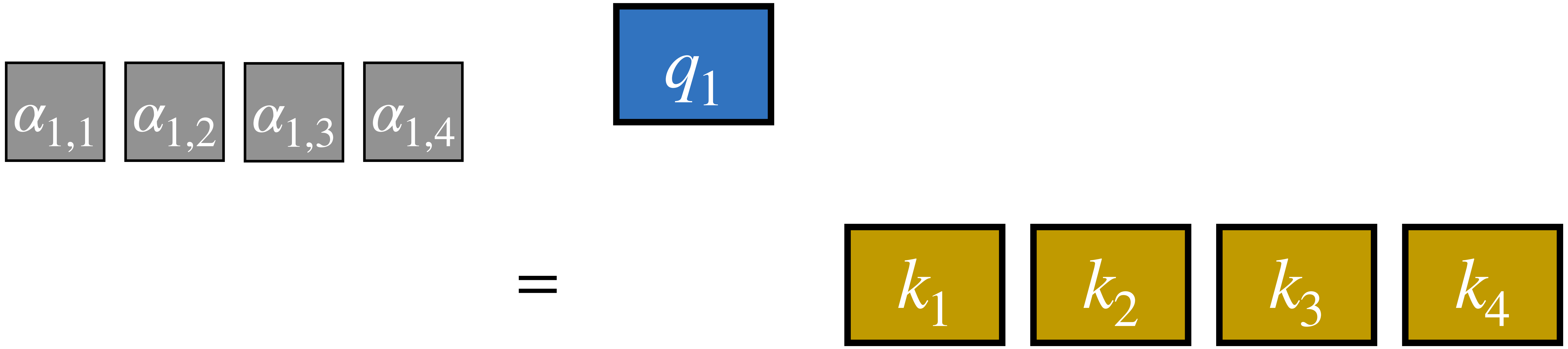

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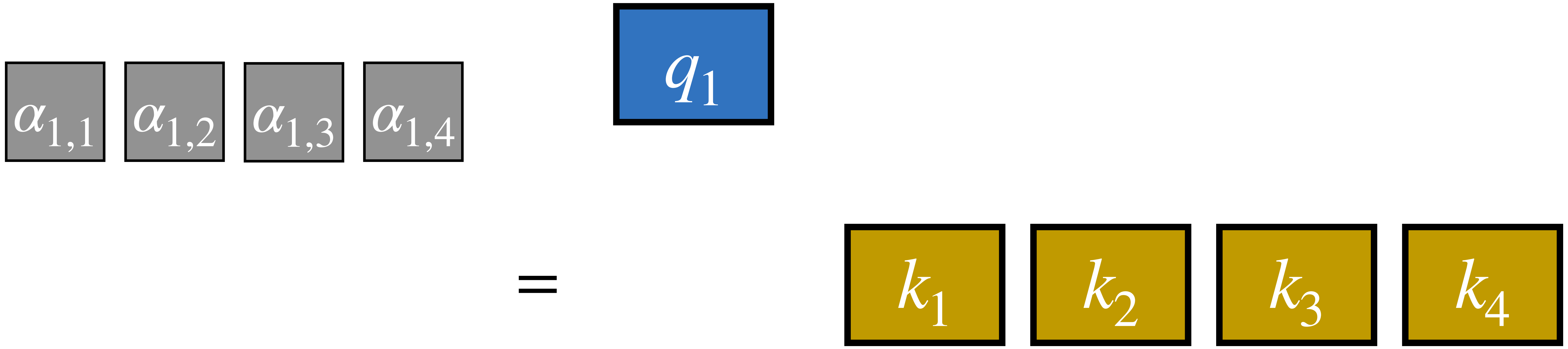

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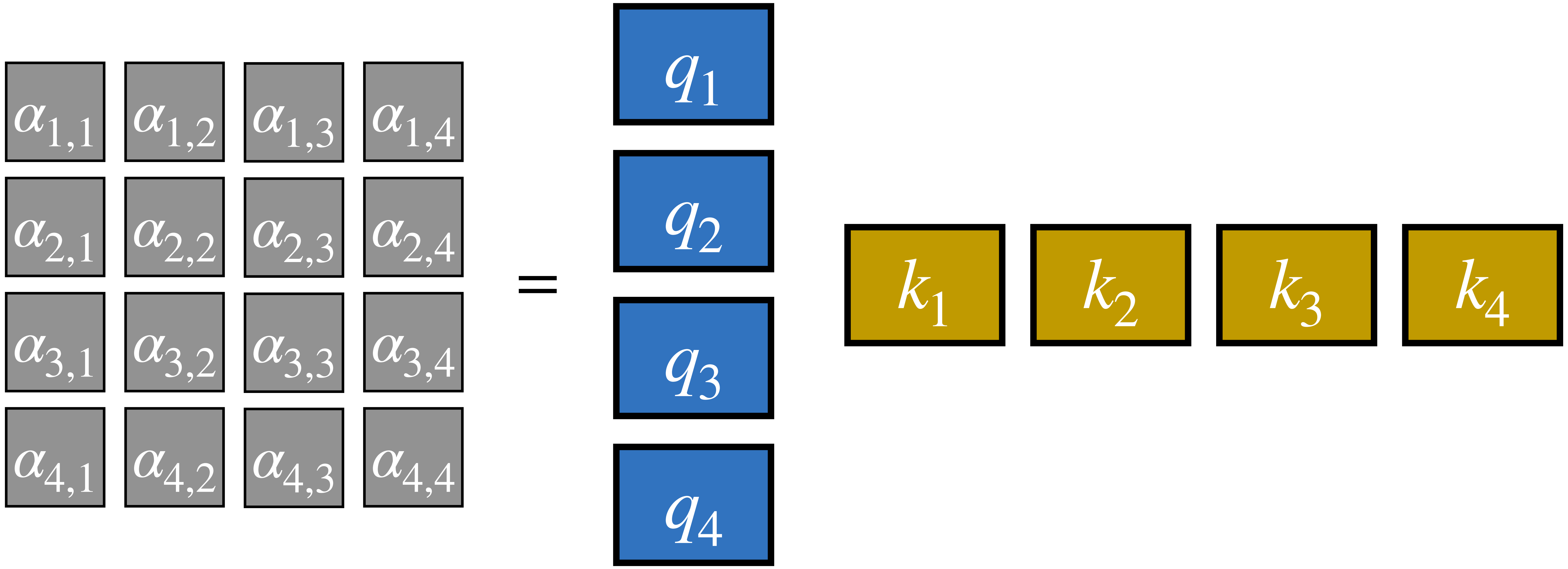

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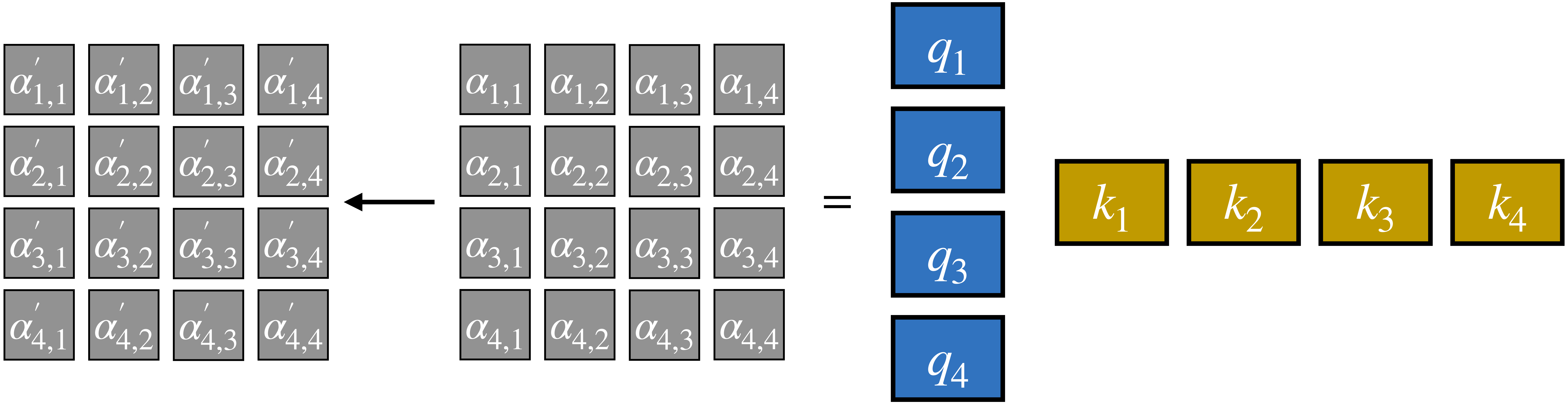

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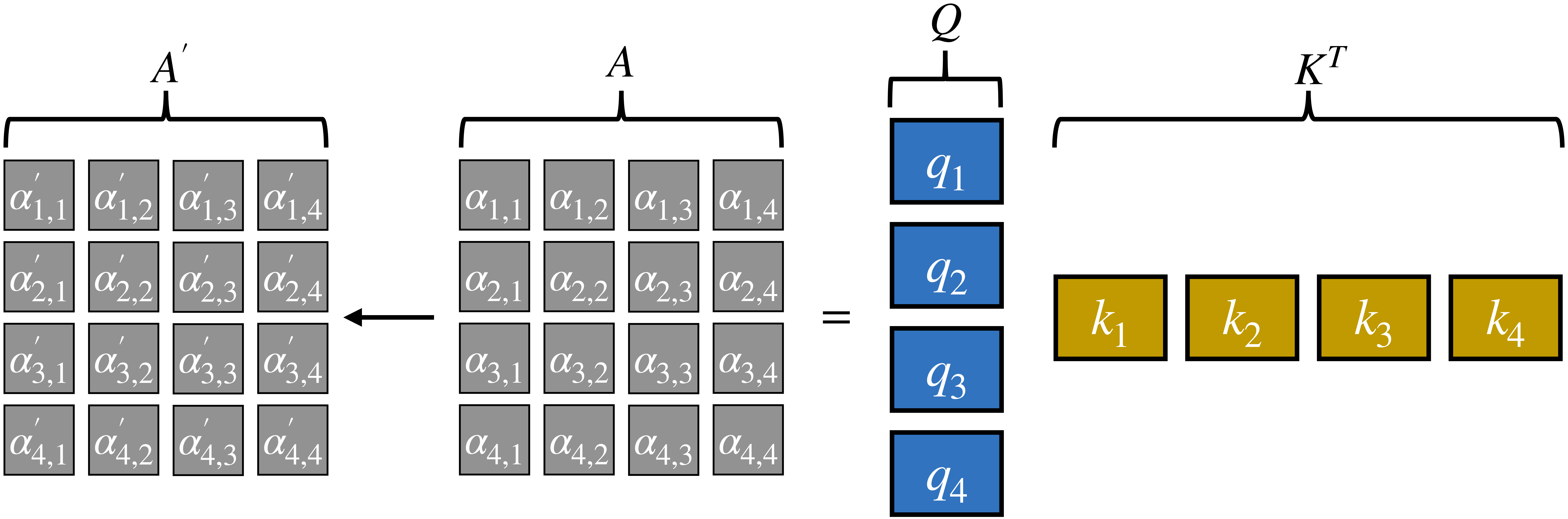

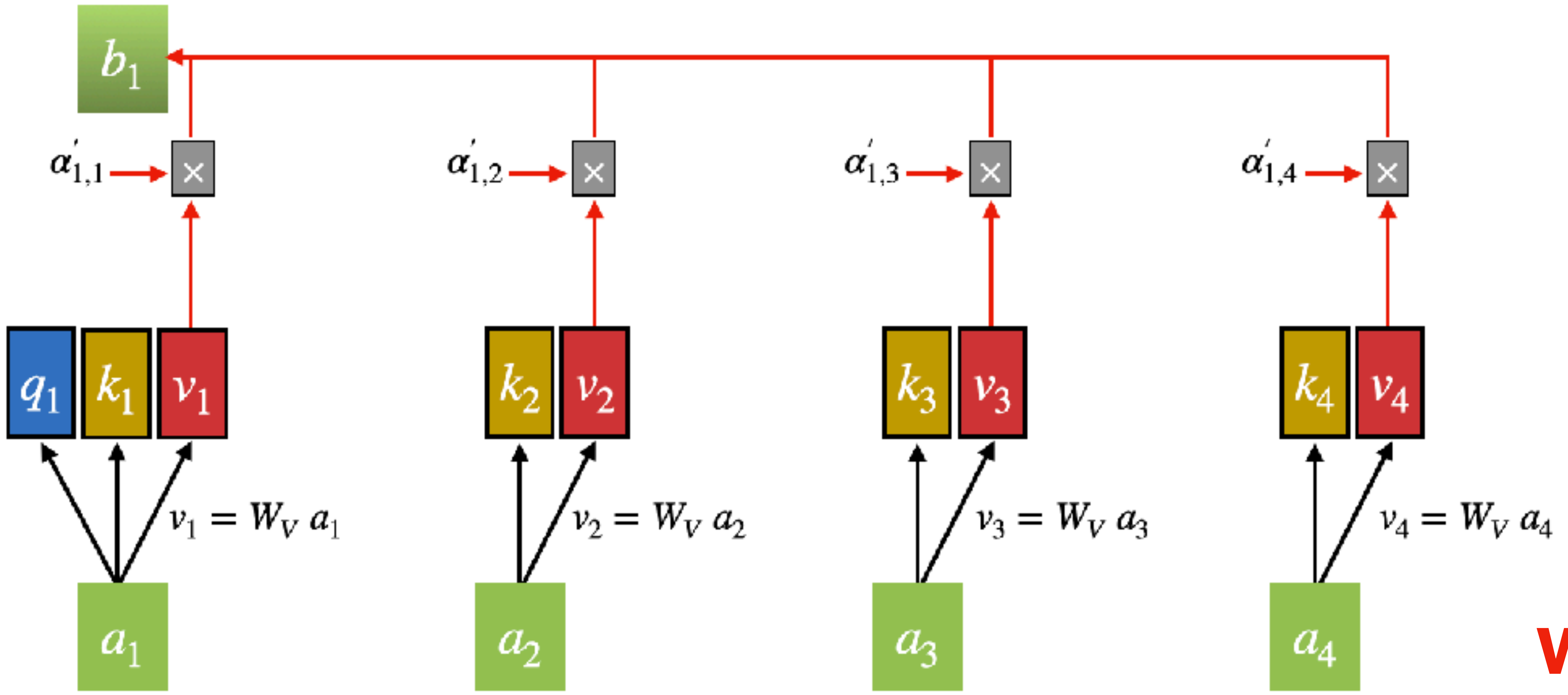

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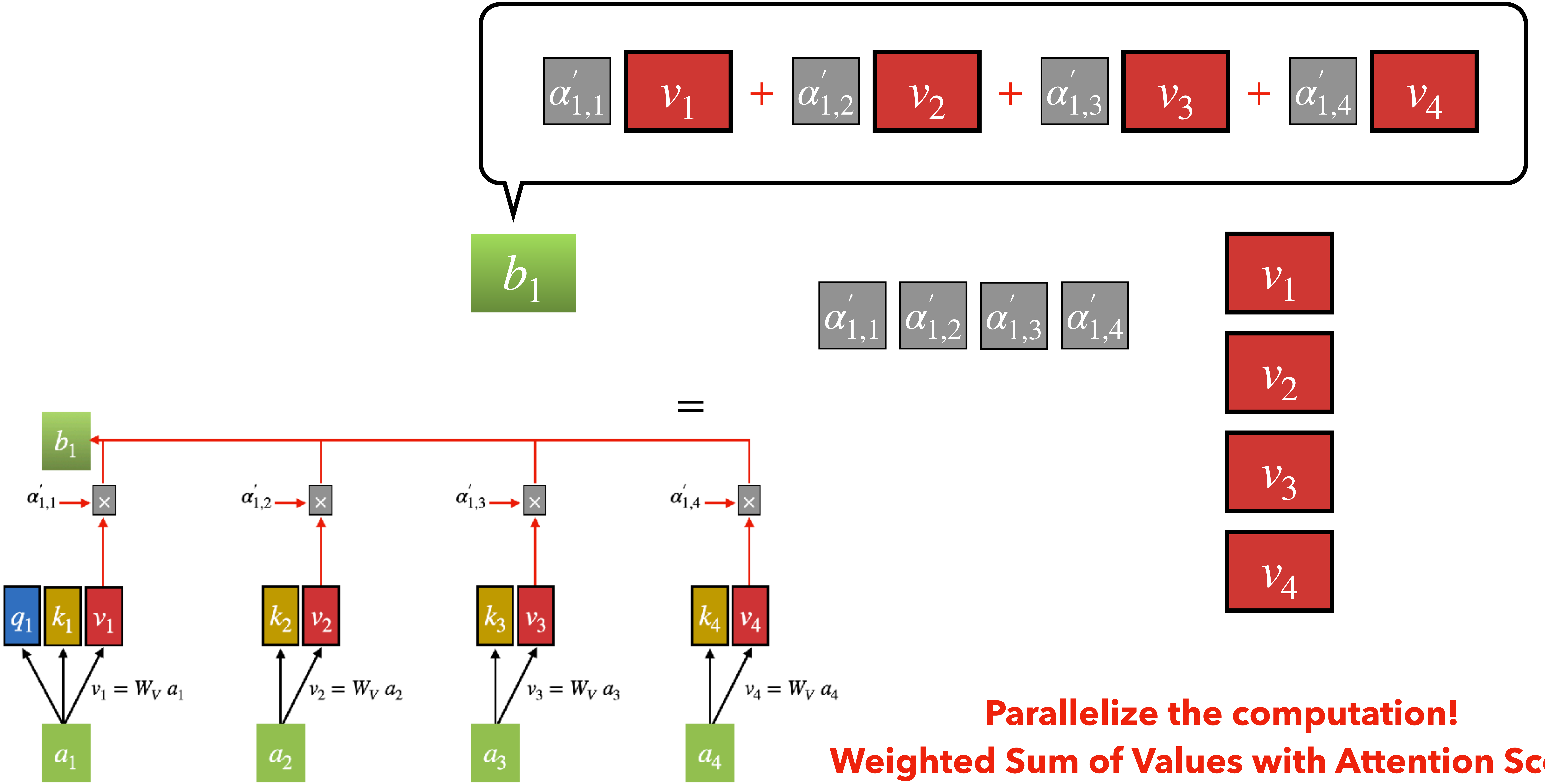

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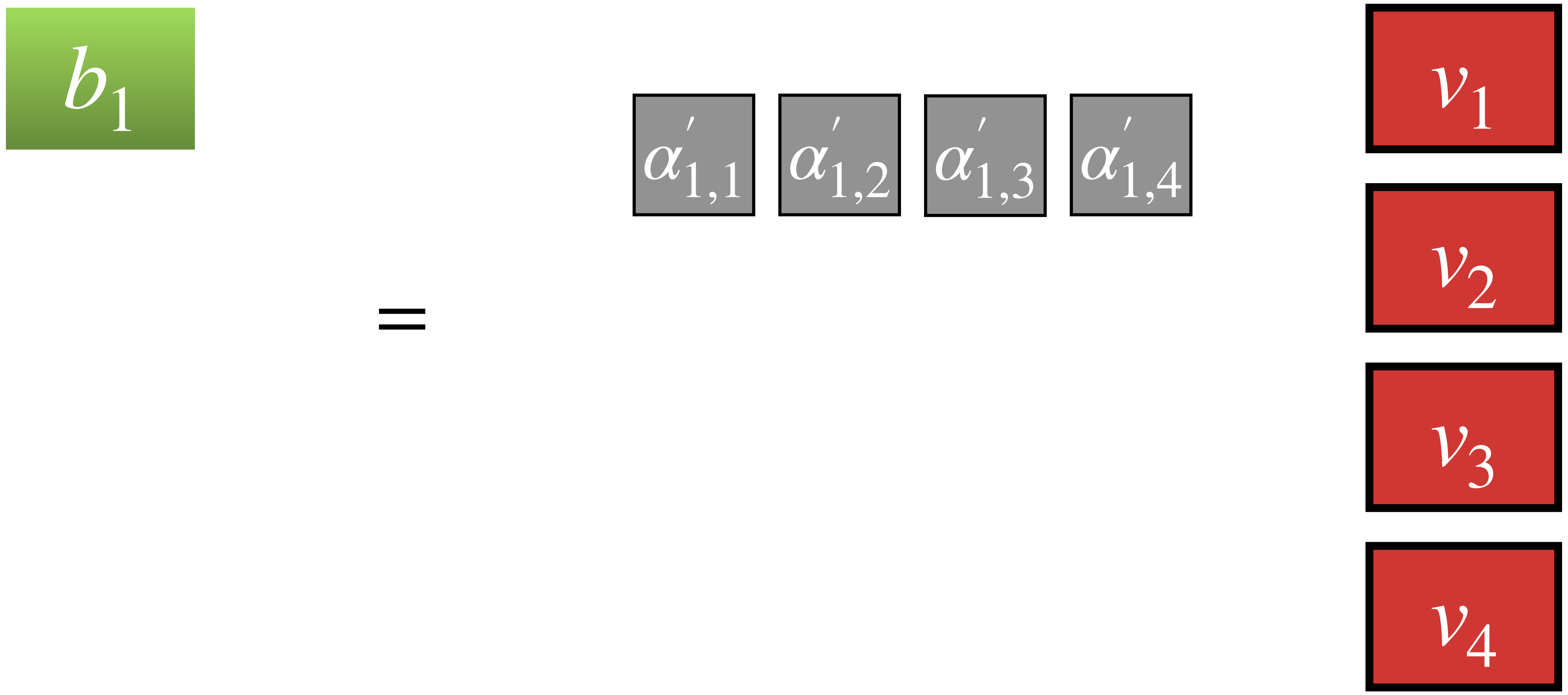

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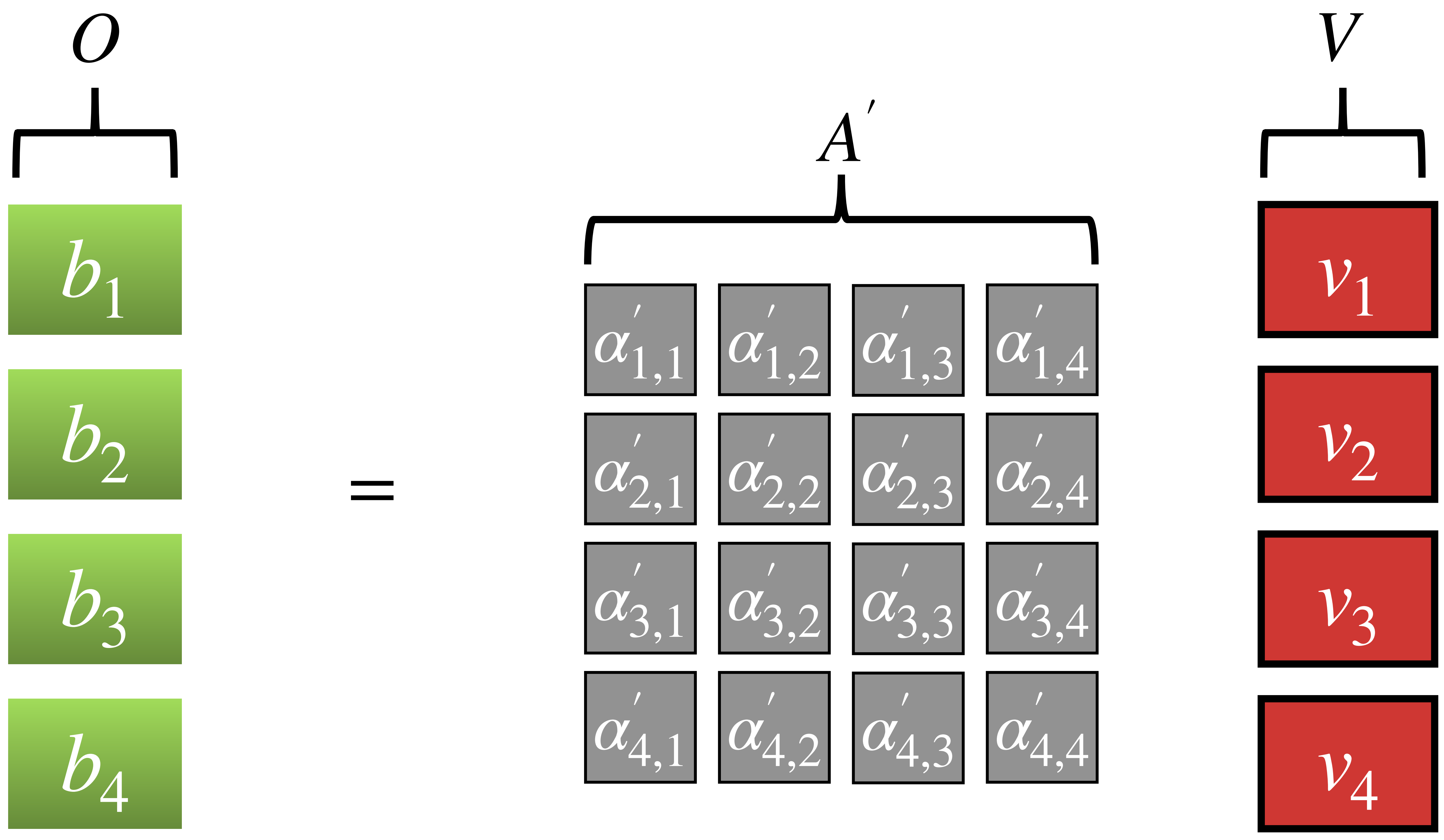

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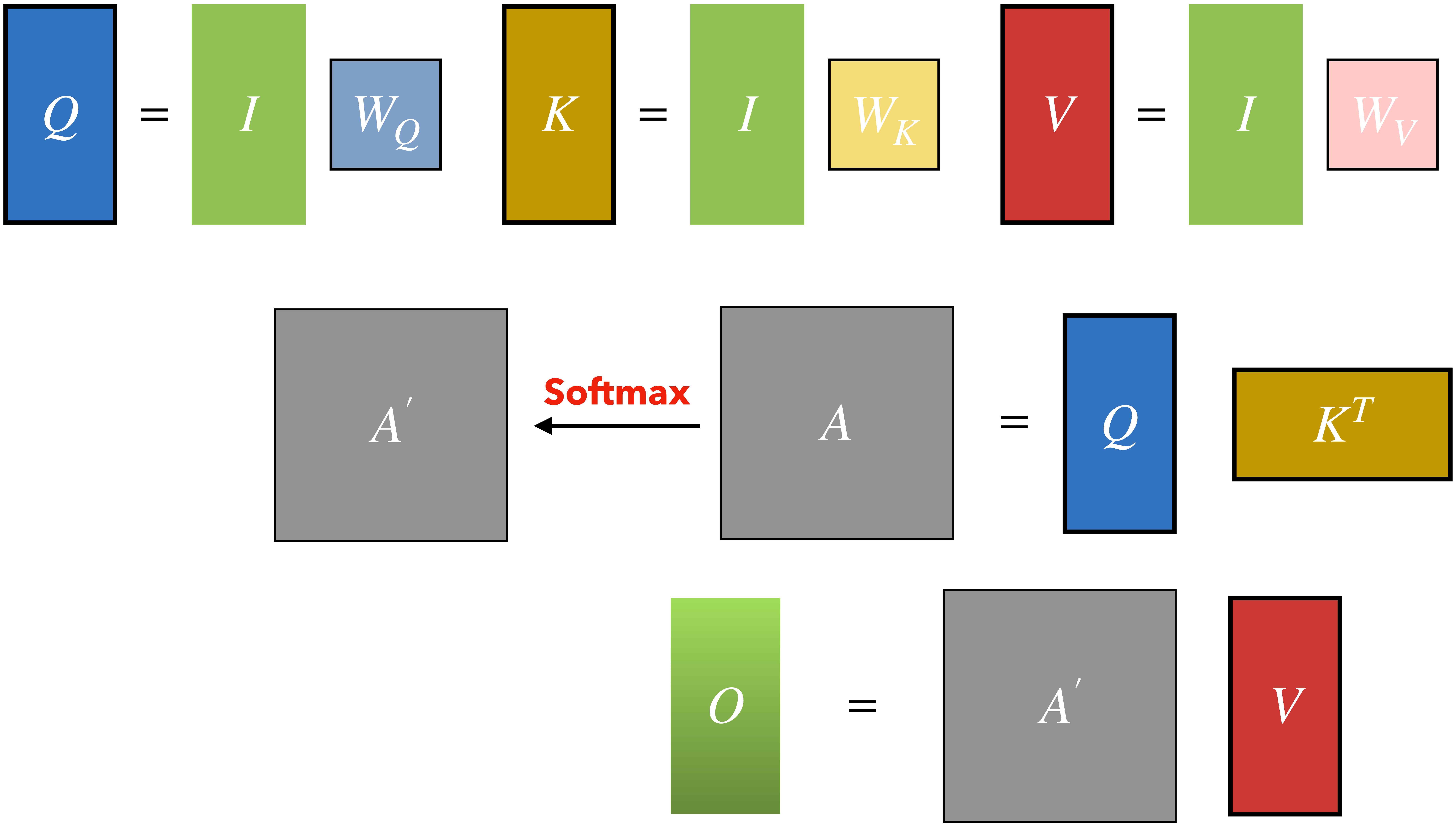
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A' ← Softmax ← A = Q K^T
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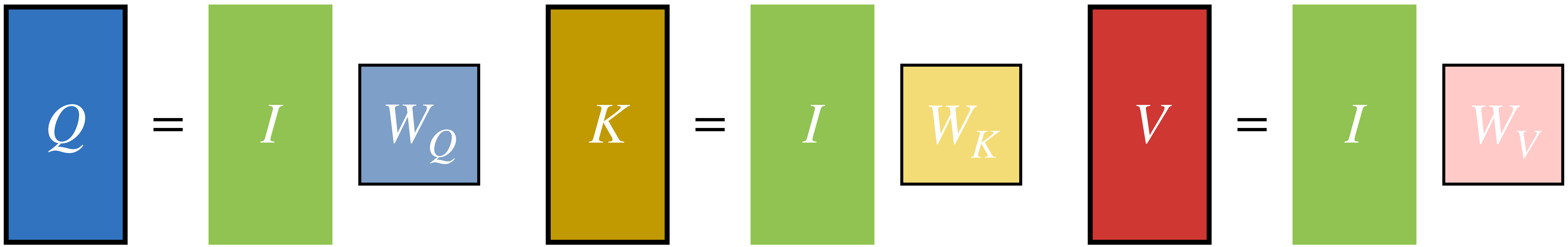

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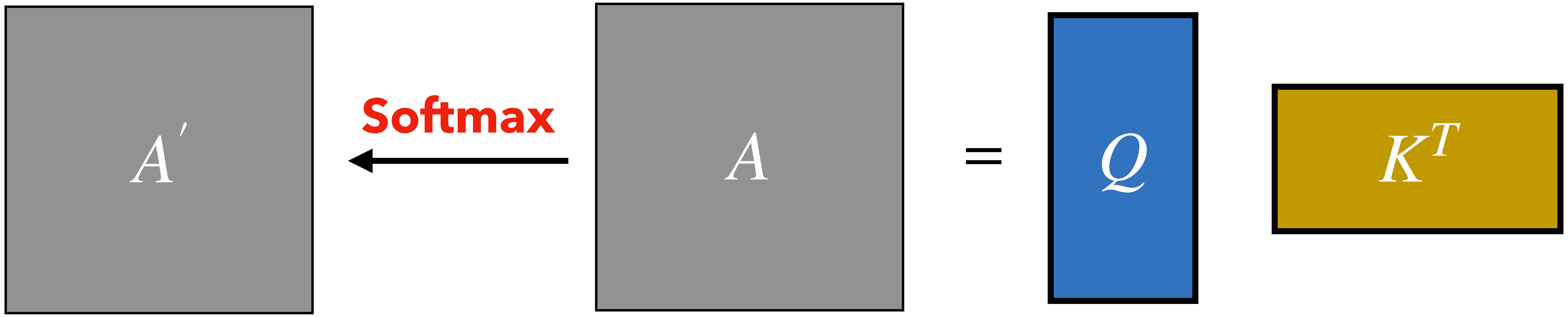

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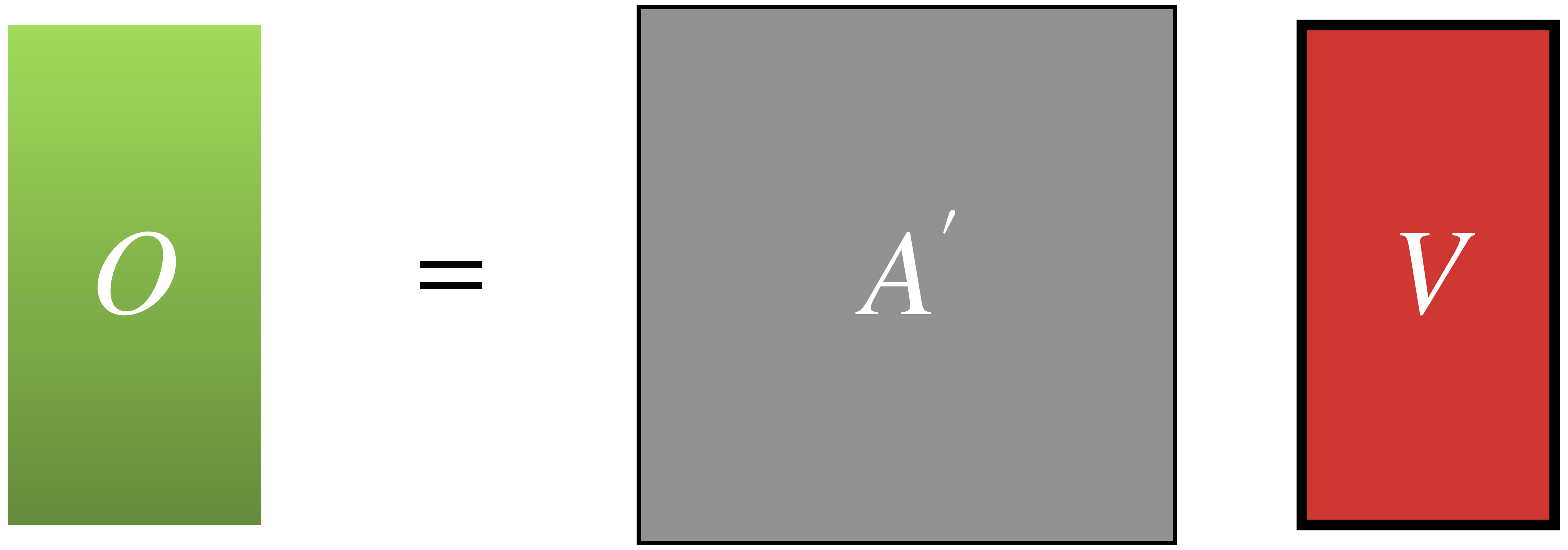

The Matrices Form of Self-Attention

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3. Compute output for each word as weighted sum of values

$$b_i = \sum_j \alpha'_{i,j}\, v_j$$

Limitations and Solutions of Self-Attention

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No Sequence Order

No Nonlinearities

Looking into the Future

Limitations and Solutions of Self-Attention

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Limitations and Solutions of Self-Attention

No Sequence Order	→	Position Embedding
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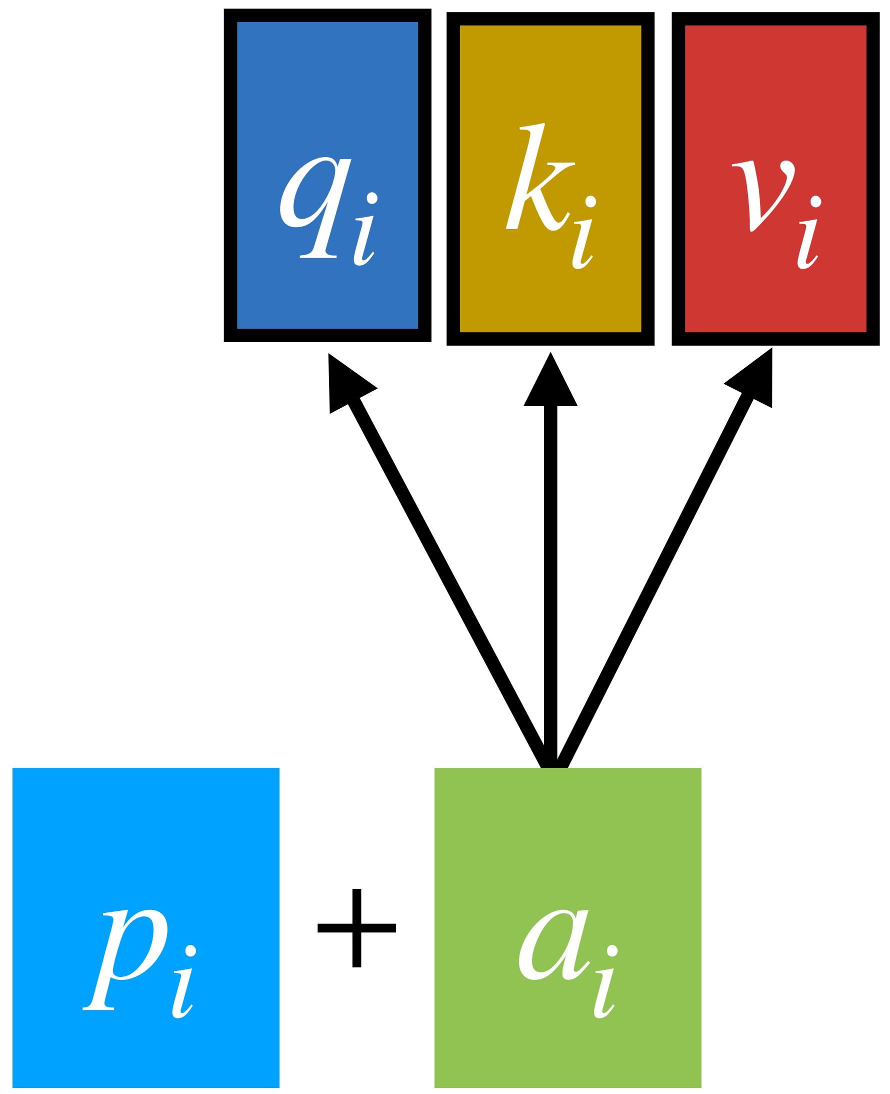
  - **Representing each sequence index as a vector:** $p_i \in \mathbb{R}^d$, for $i \in \{1,...,n\}$
- How to incorporate the position info into the self-attention blocks?
  - Just add the p_i to the input: $\hat{a}_i = a_i + p_i$
  - where a_i is the embedding of the word at index i.
  - In deep self-attention networks, we do this at the **first layer**.
  - We can also concatenate a_i and p_i, but more commonly we add them.



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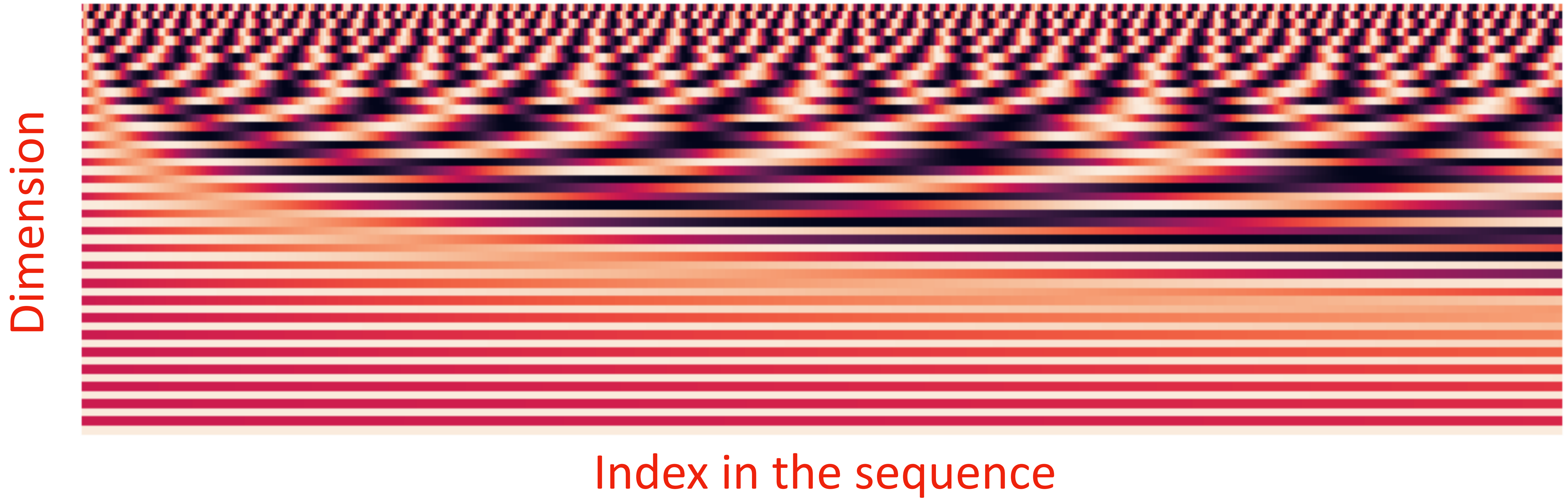

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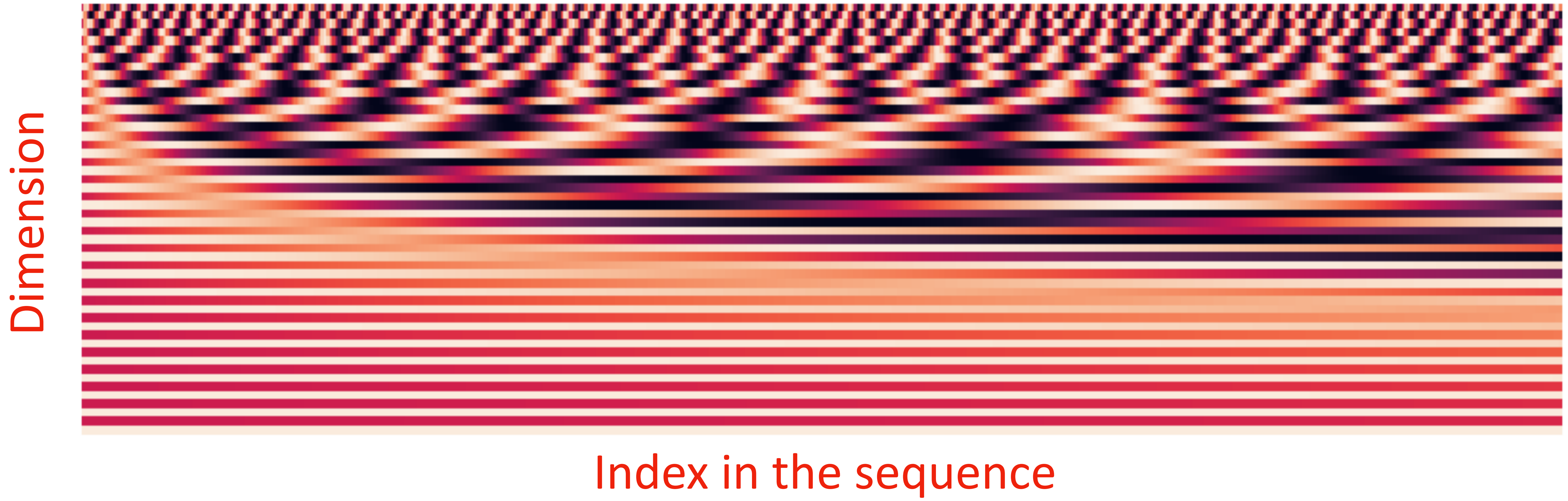

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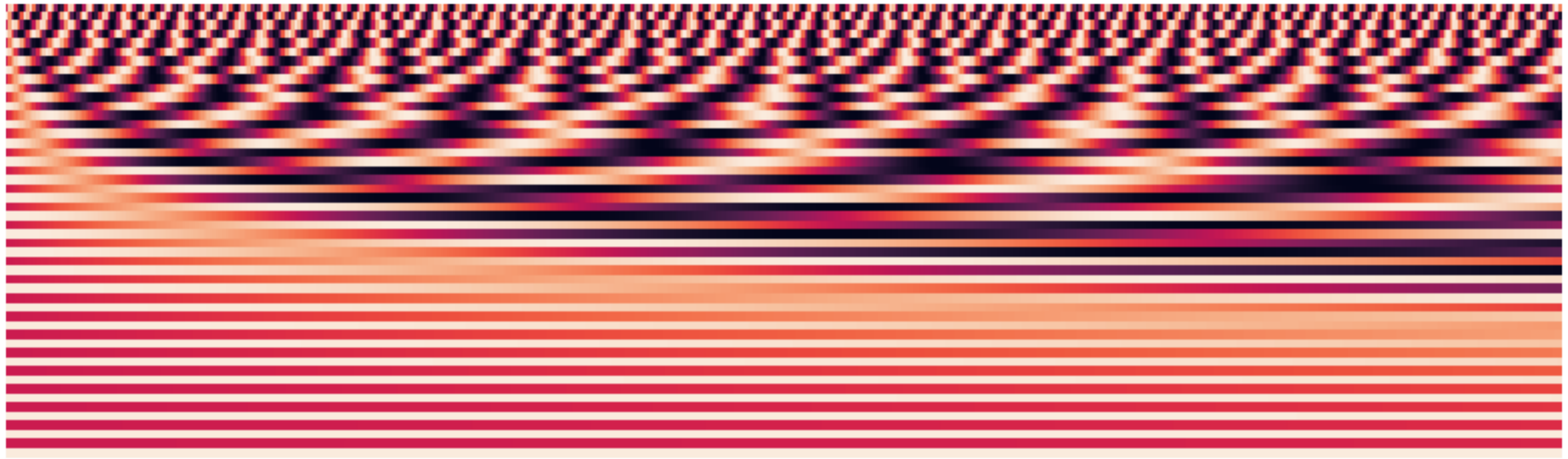

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- **Not learnable; also the extrapolation doesn't really work!**

Learnable Position Representation Vectors

Learned absolute position representations: p_i contains learnable parameters.

- **Learn a matrix $p \in \mathbb{R}^{d \times n}$, and let each p_i be a column of that matrix**
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Sometimes people try more flexible representations of position:

- **Relative linear position attention [Shaw et al., 2018]**
- **Dependency syntax-based position [Wang et al., 2019]**

Limitations and Solutions of Self-Attention

No Sequence Order	→	Position Embedding
No Nonlinearities	→	Adding Feed-forward Networks
Looking into the Future	→	Masking

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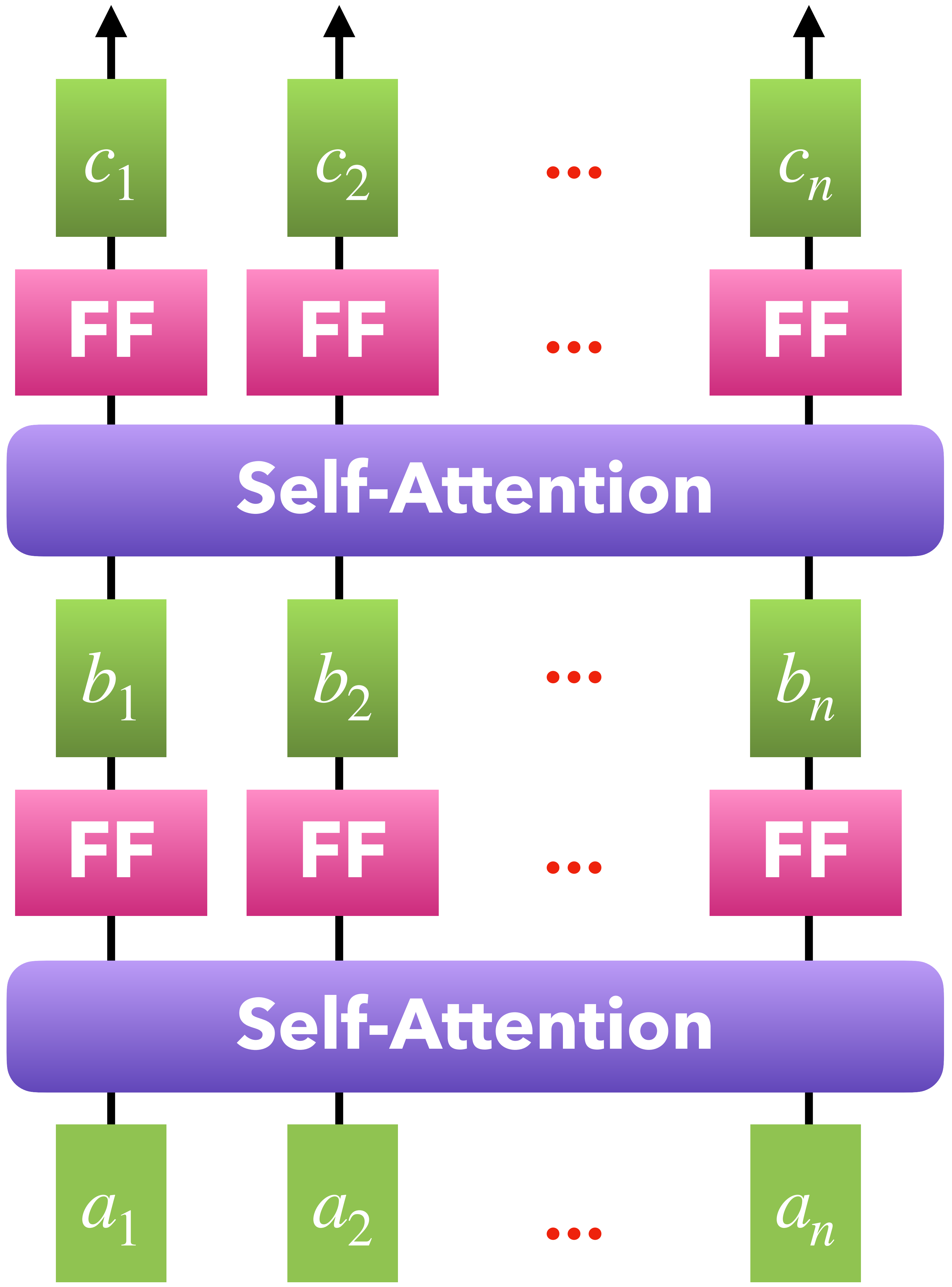
Easy Fix: add a feed-forward network to post-process each output vector.



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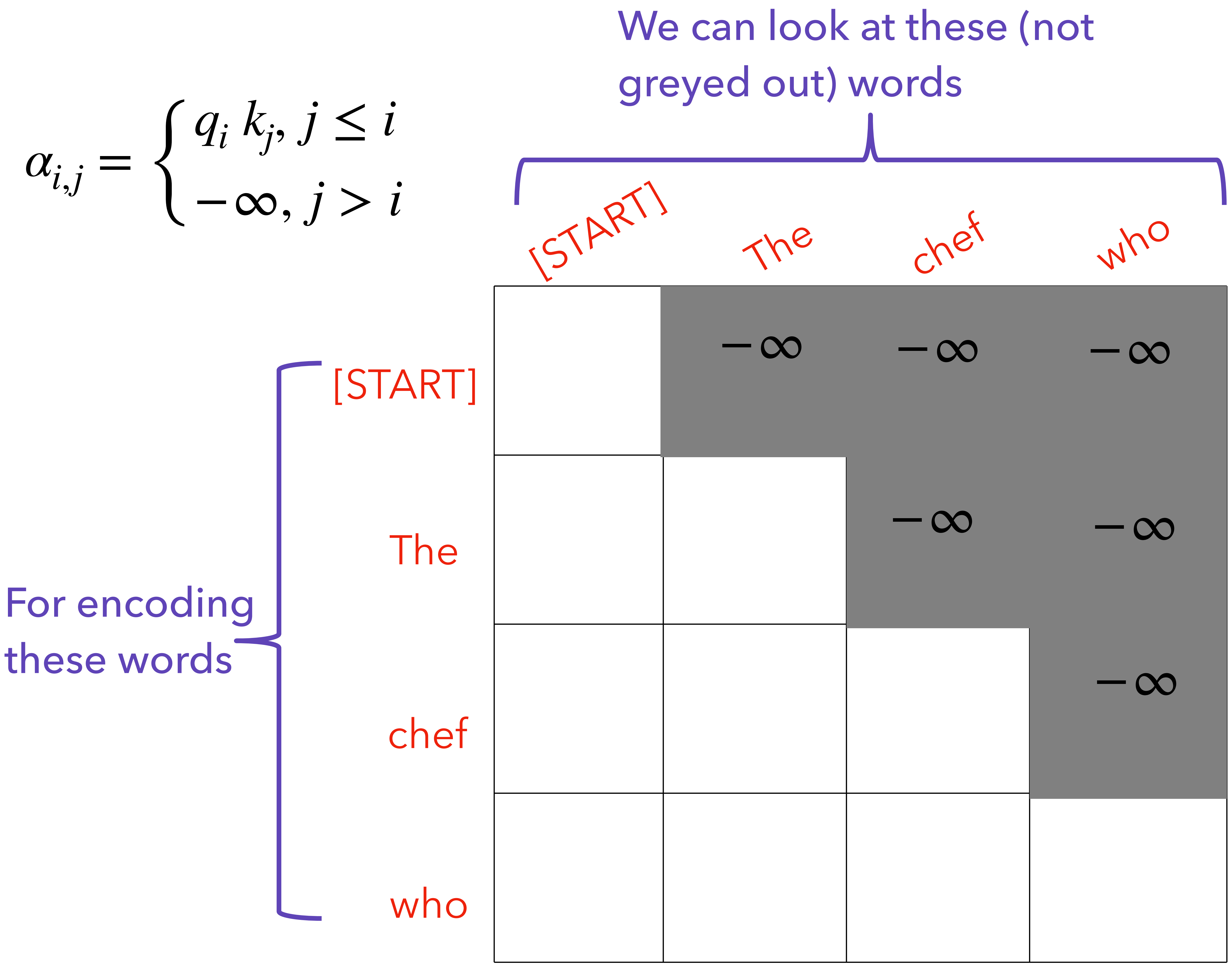
- **To enable parallelization, we mask out attention to future words by setting attention scores to $-\infty$.**

$$\alpha_{i,j} = \begin{cases} q_i k_j, & j \le i \\ -\infty, & j > i \end{cases}$$



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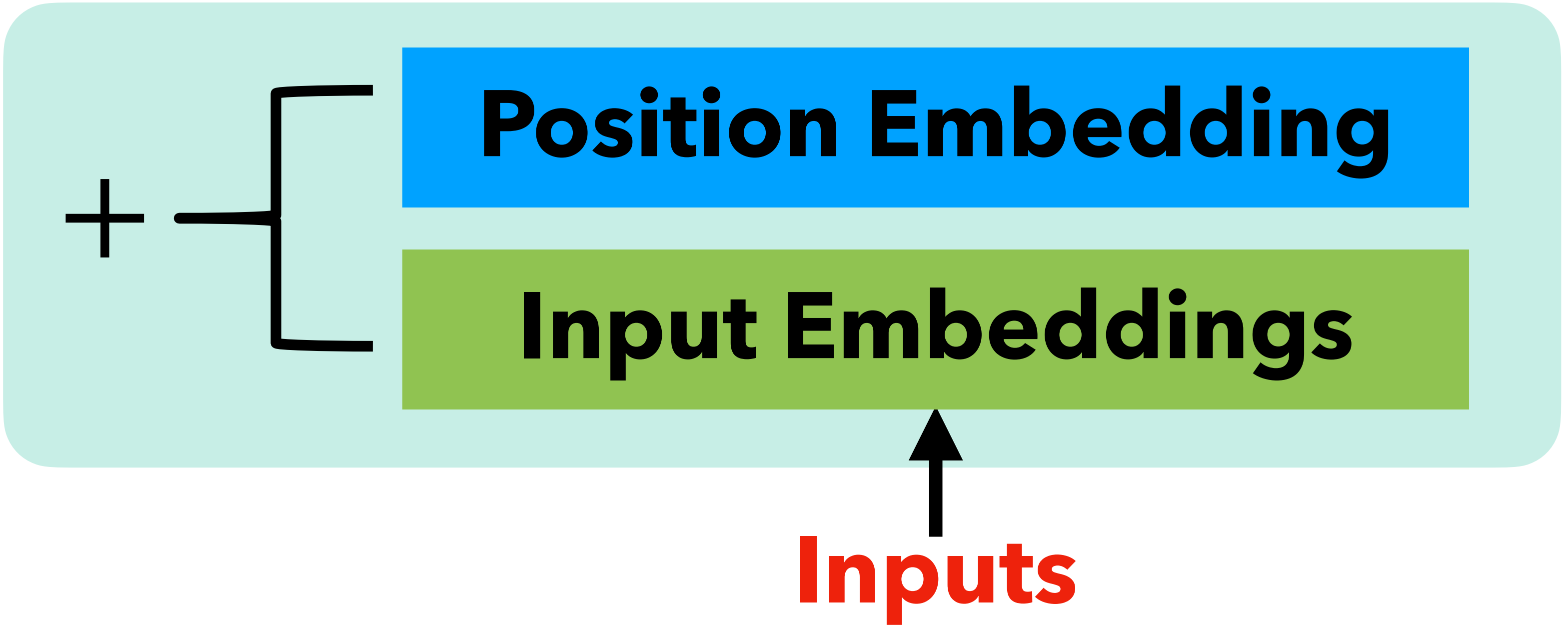

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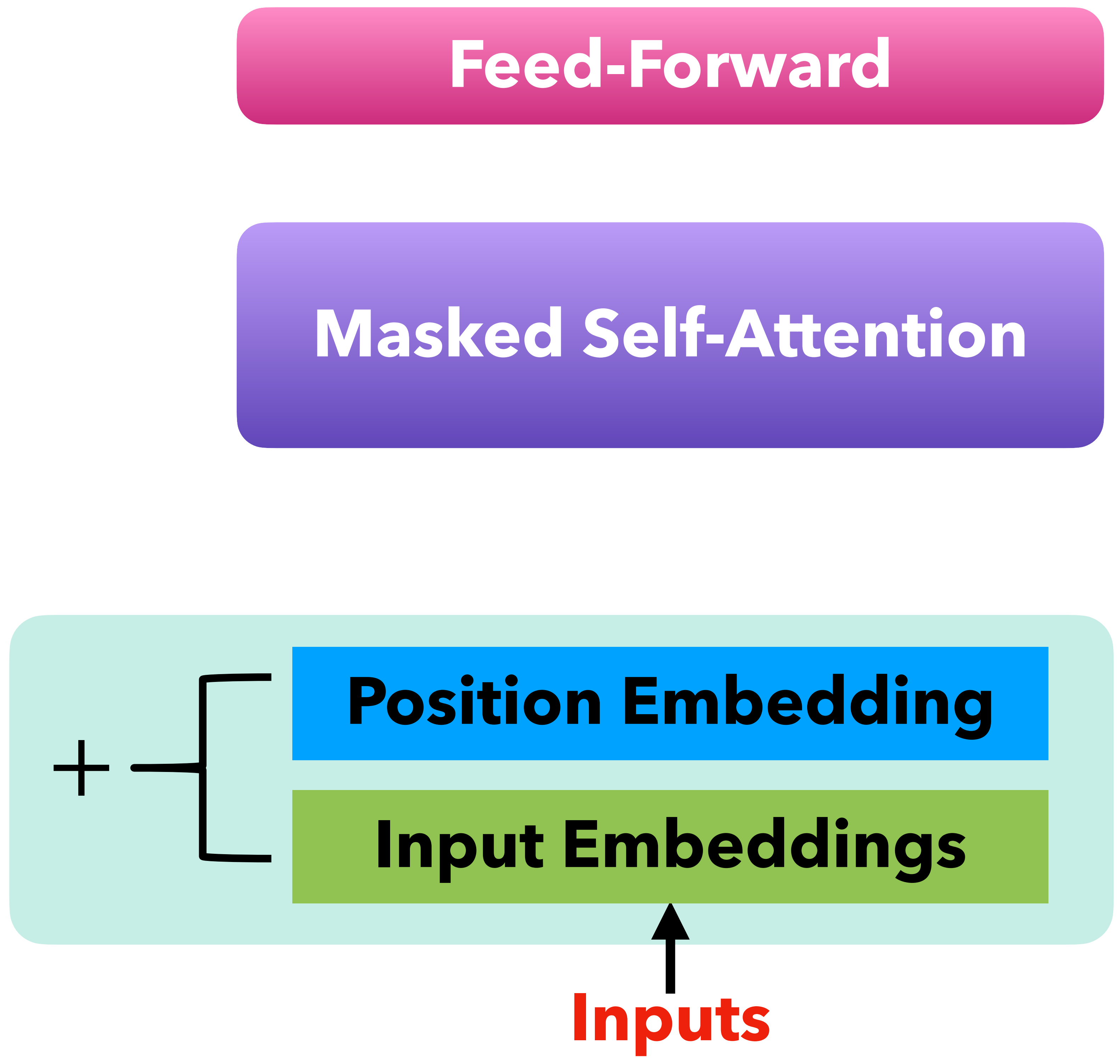

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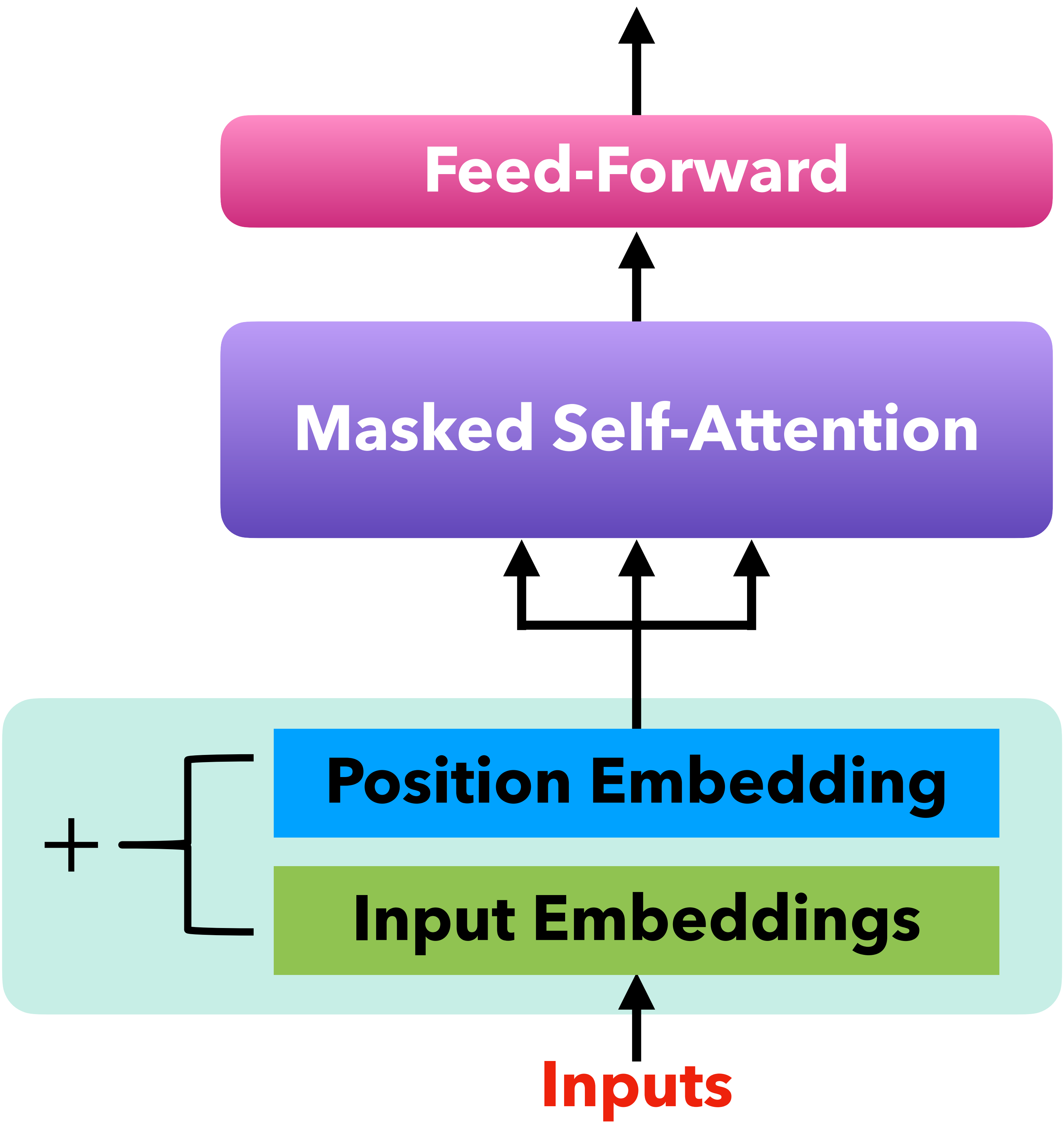

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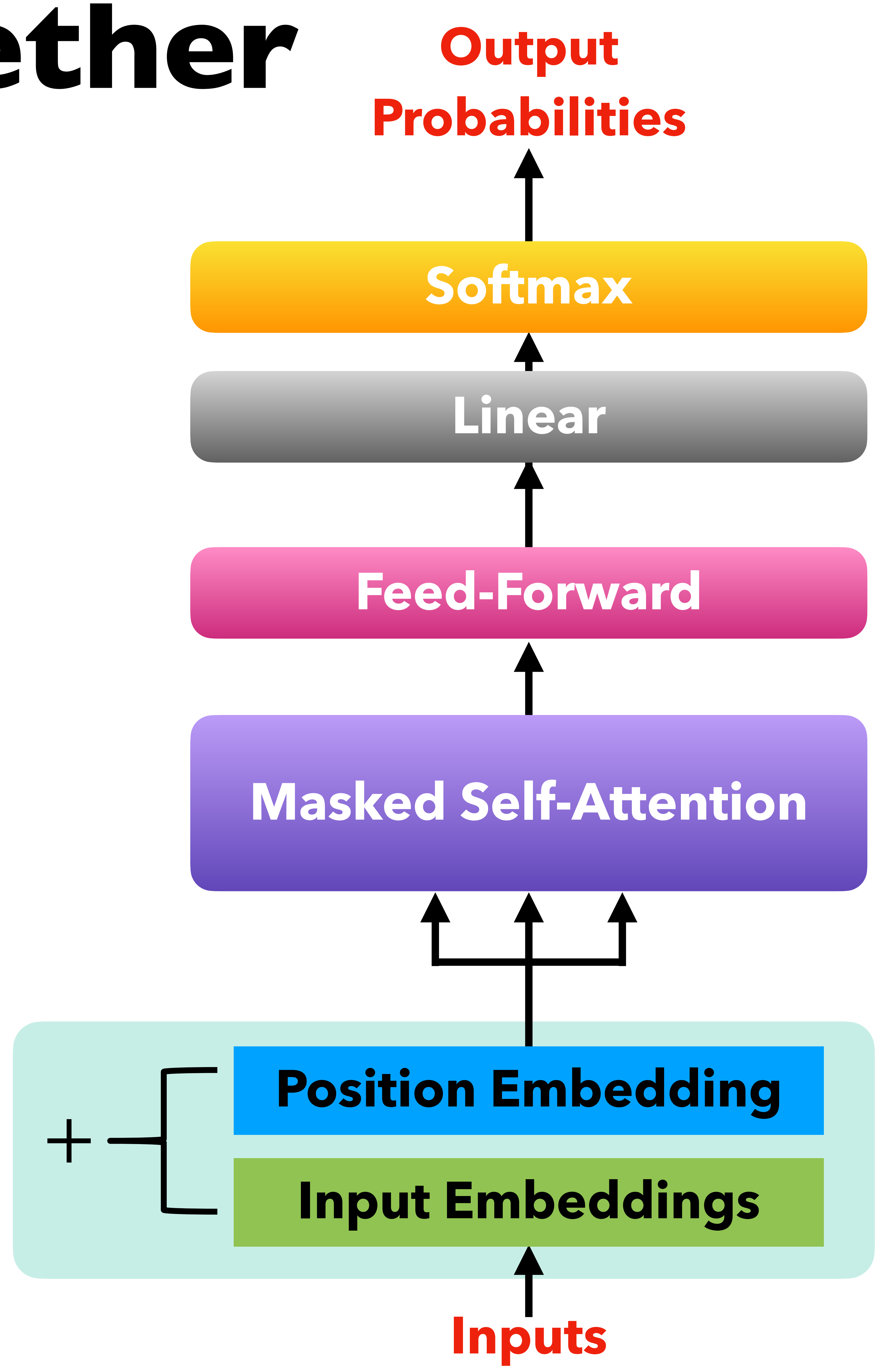

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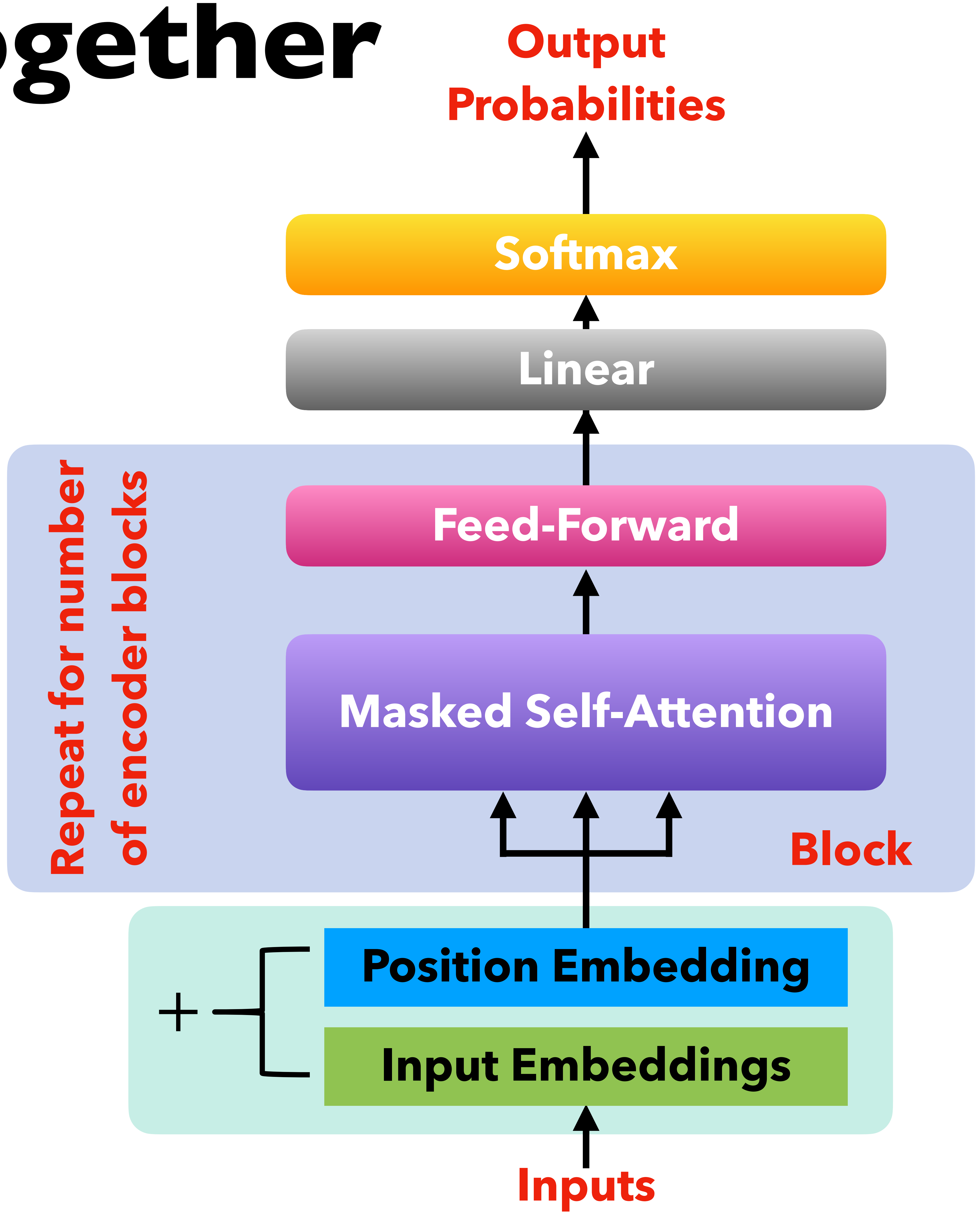

The Transformer **Decoder**

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- **A Transformer decoder is what we use to build systems like language models.**
- **It's a lot like our minimal self-attention architecture, but with a few more components.**
  - ***Residual connection ("Add")***
  - ***Layer normalization ("Norm")***

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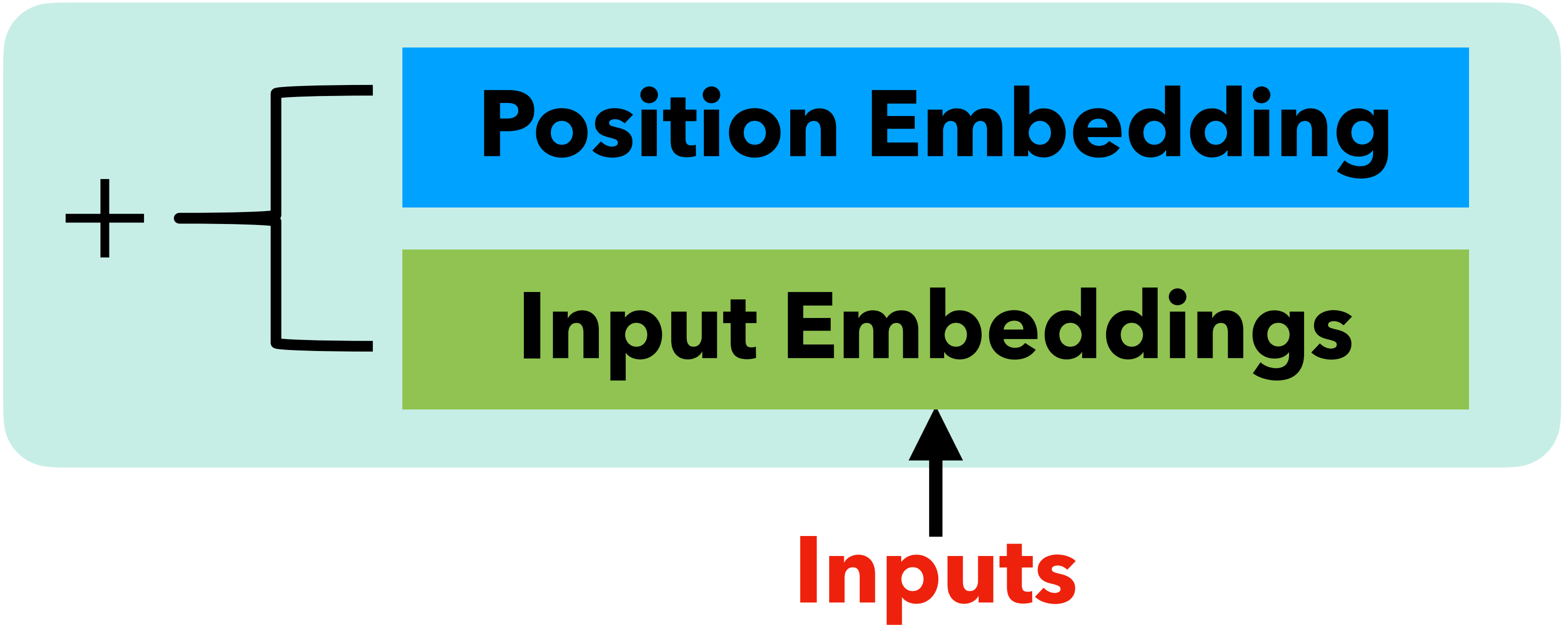

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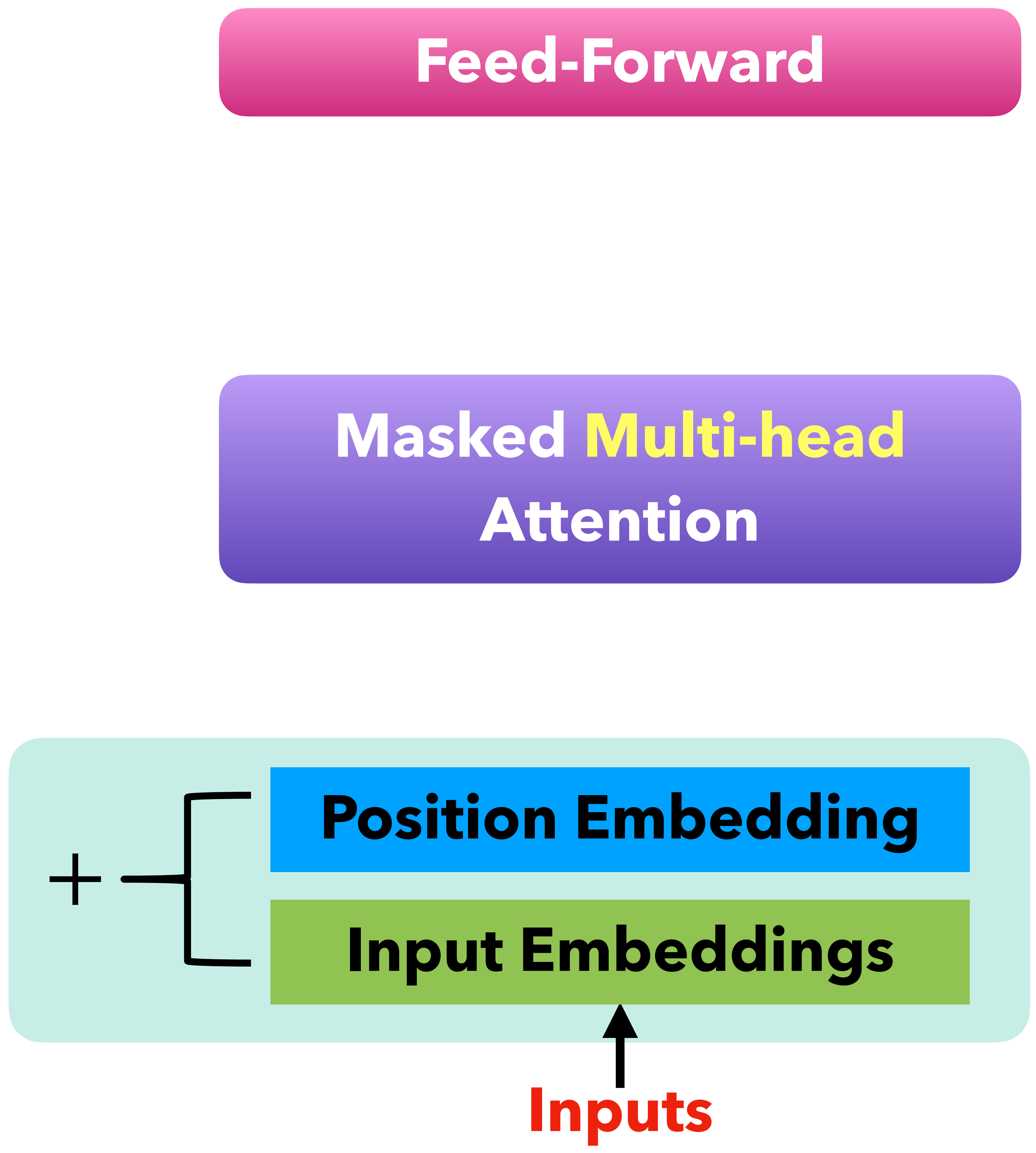

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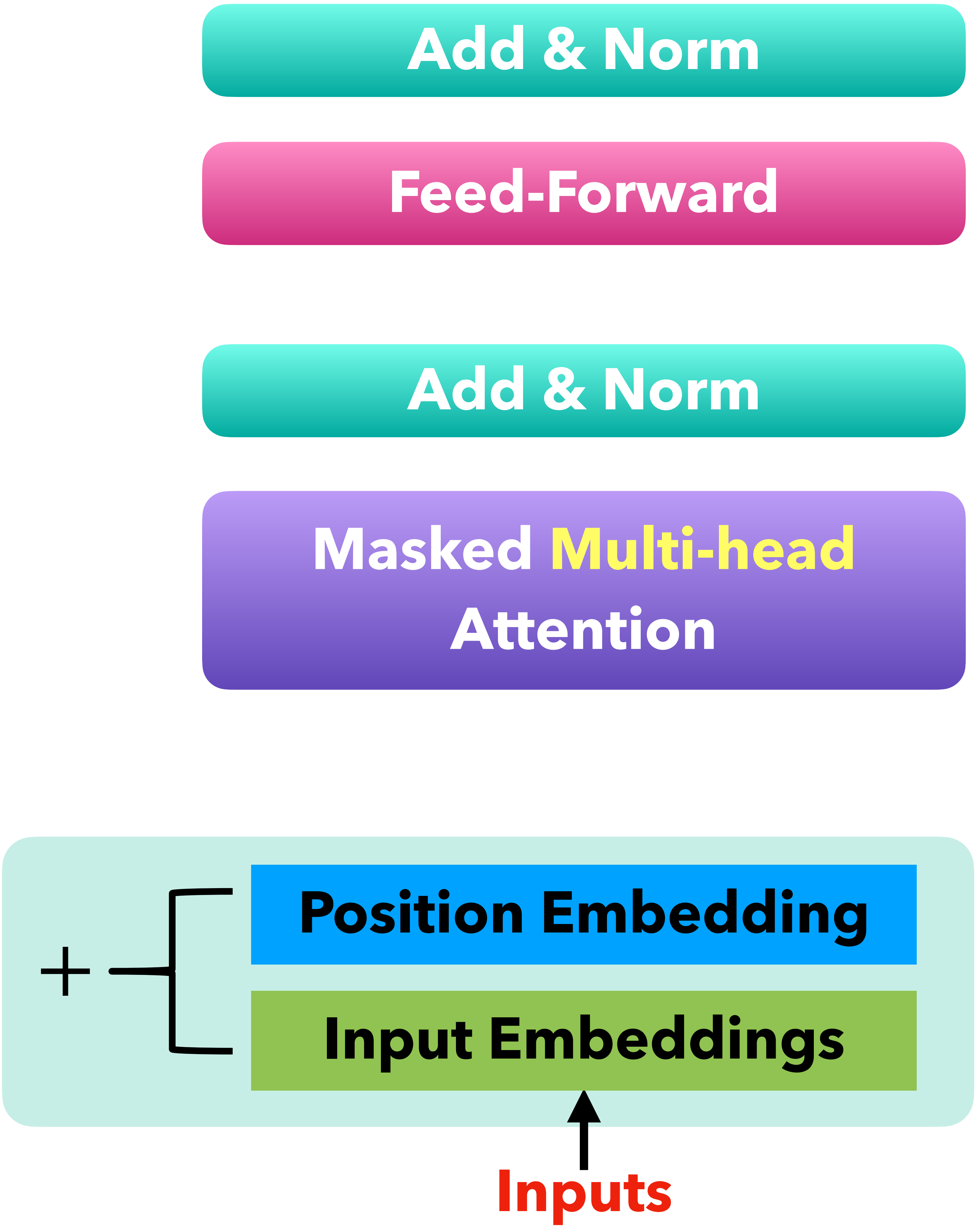

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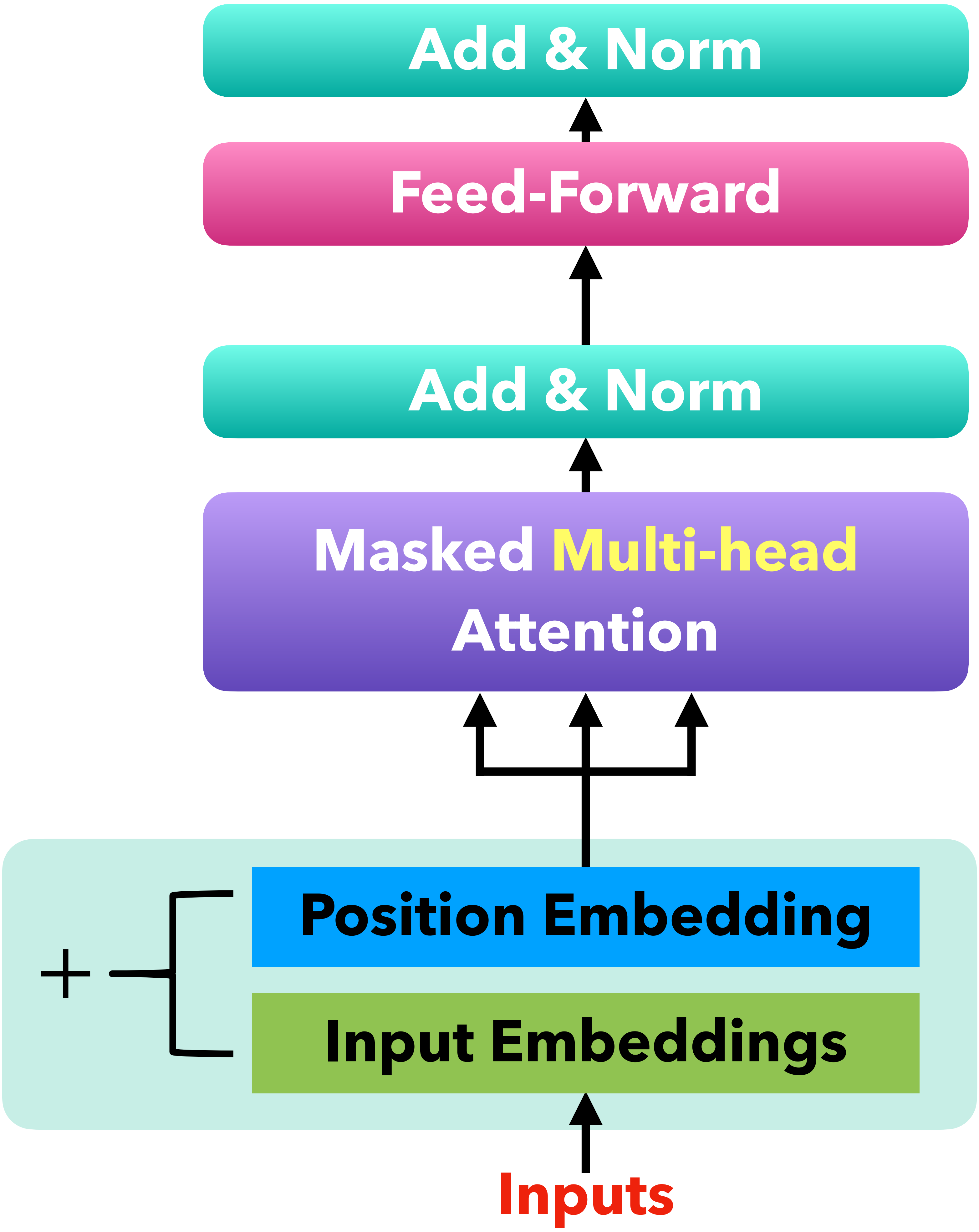

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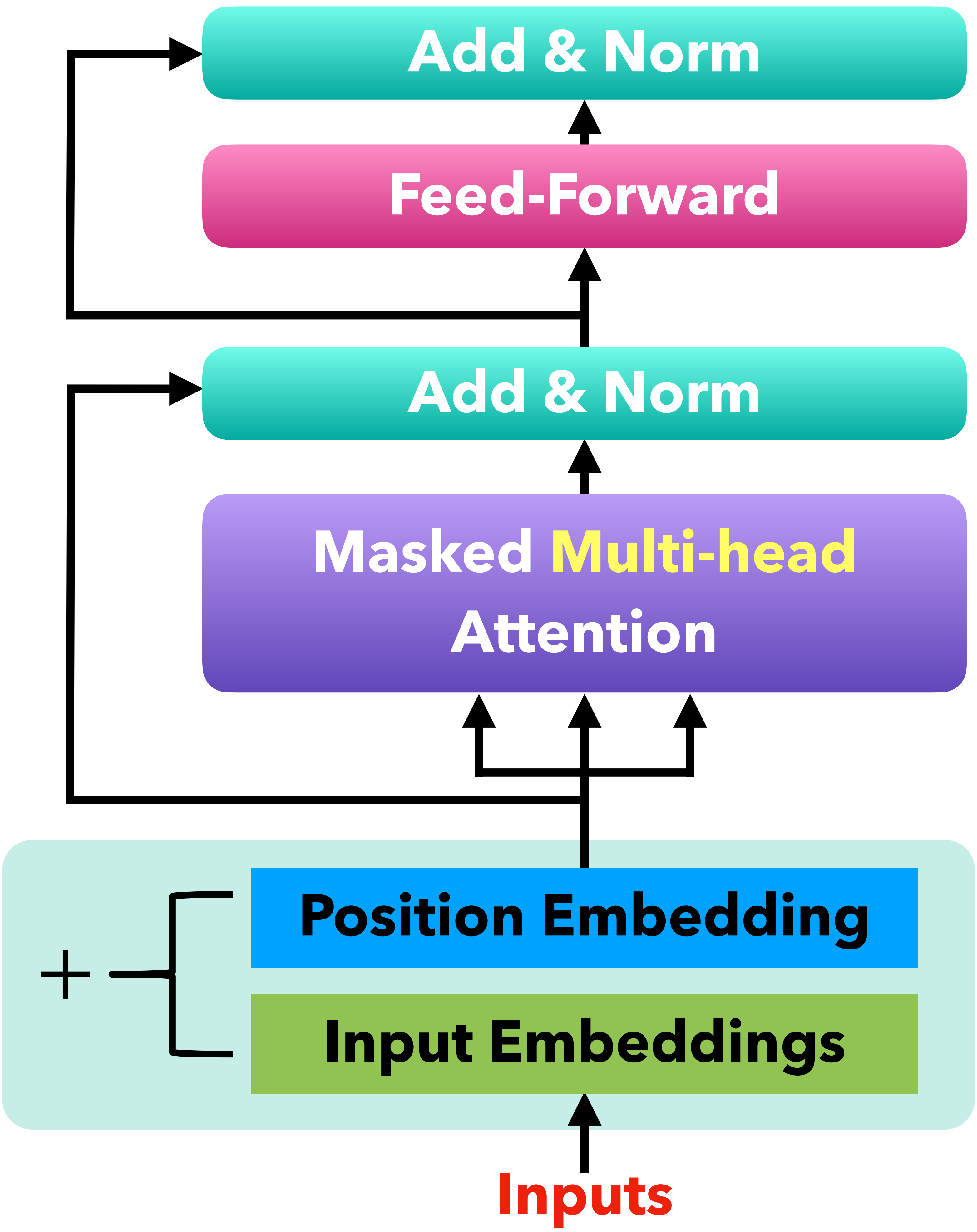

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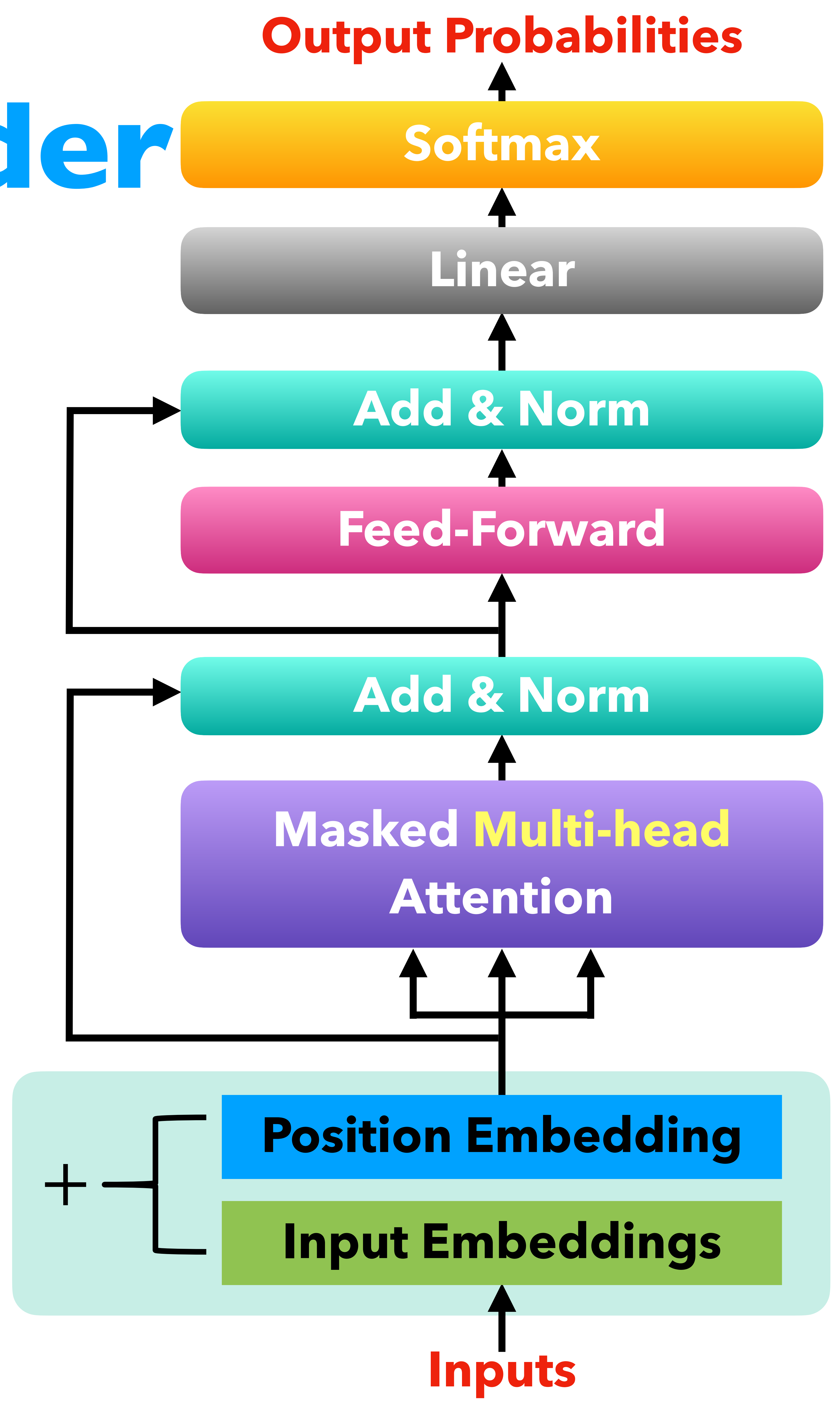

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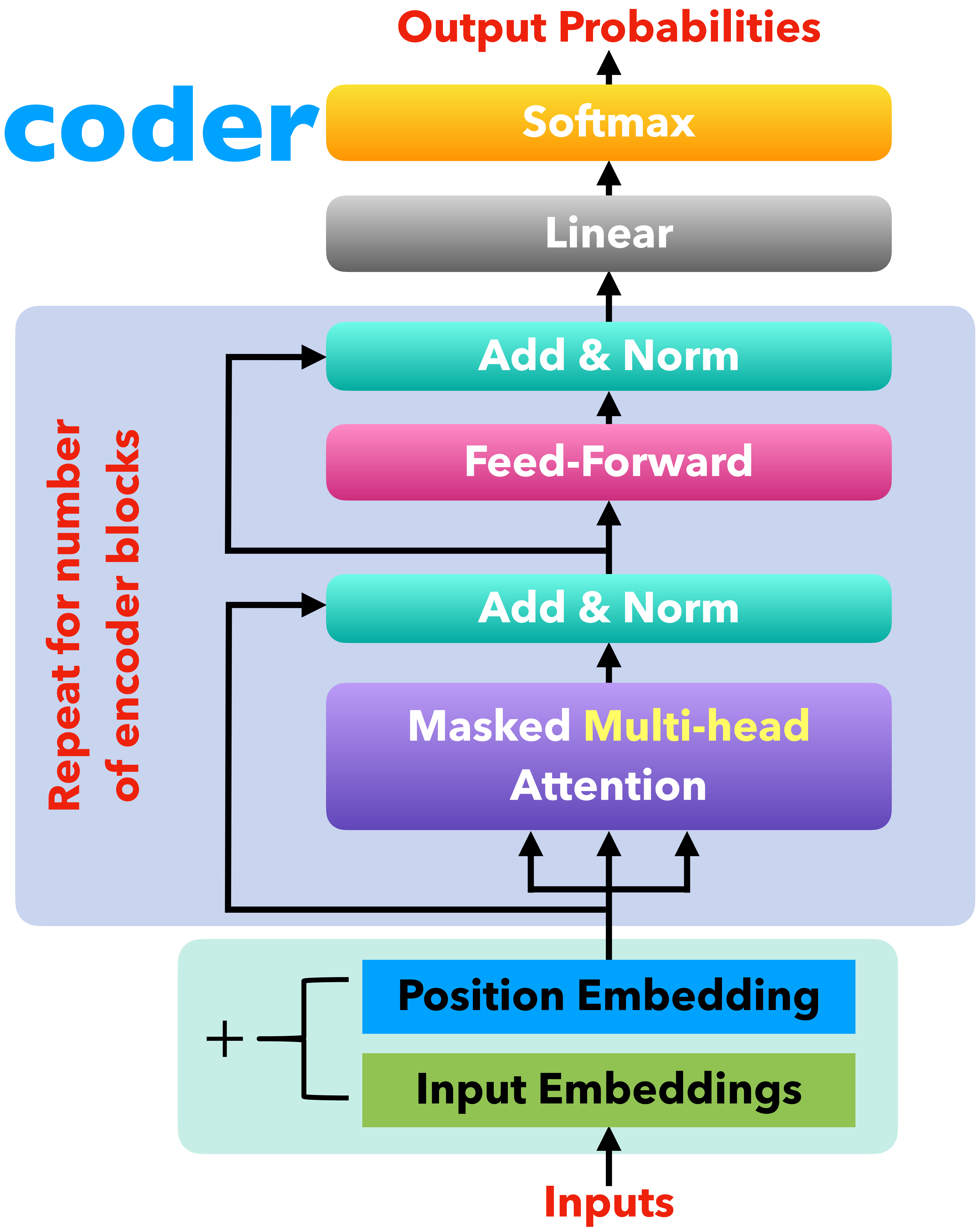

Why Multi-head Attention?

What if we want to look in multiple places in the sentence at once?

?

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What if we want to look in multiple places in the sentence at once?

Instead of having only one attention head, we can create multiple sets of (queries, keys, values) independent from each other!

Multi-Head Attention: Walk-through

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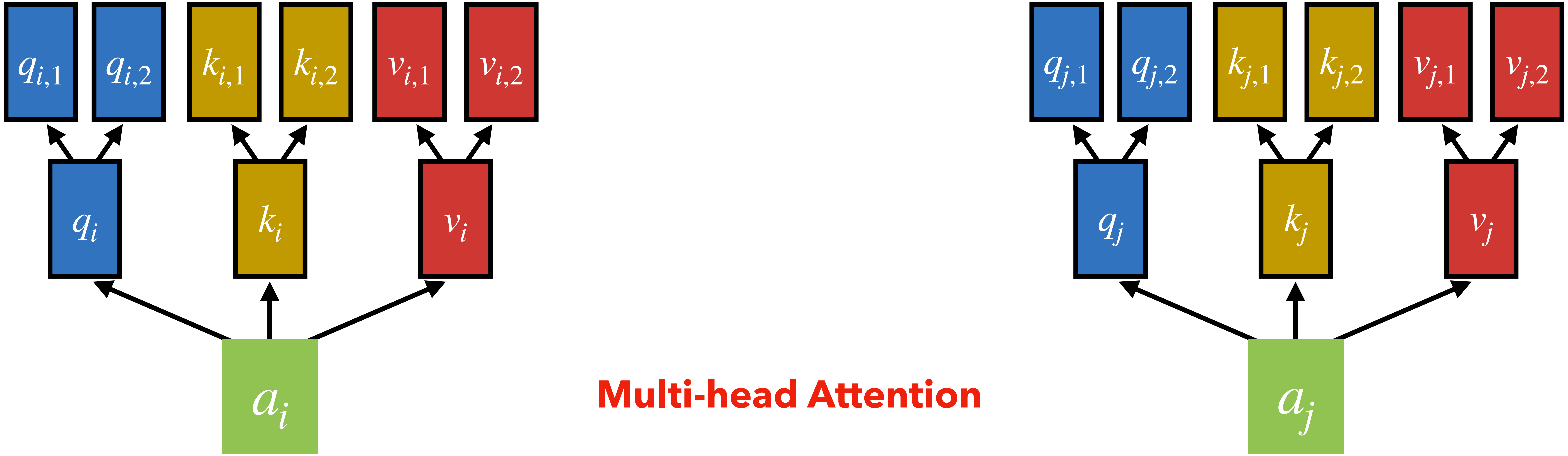

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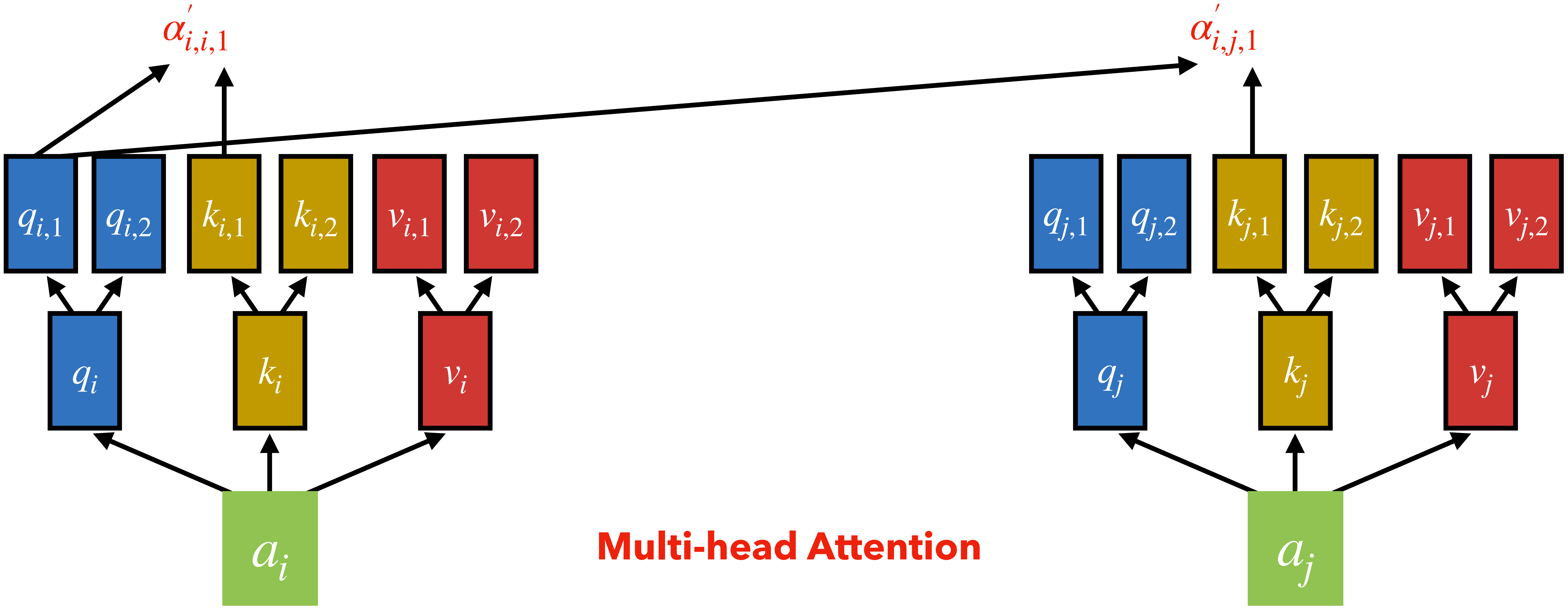

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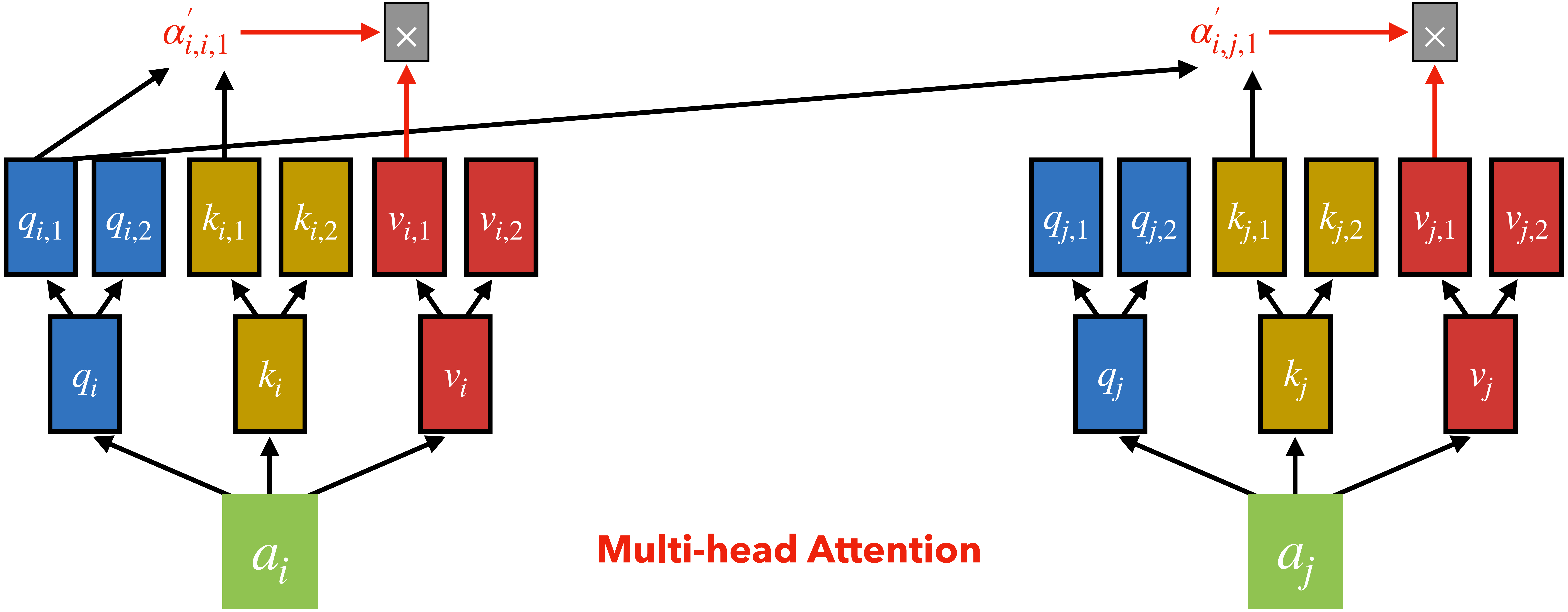

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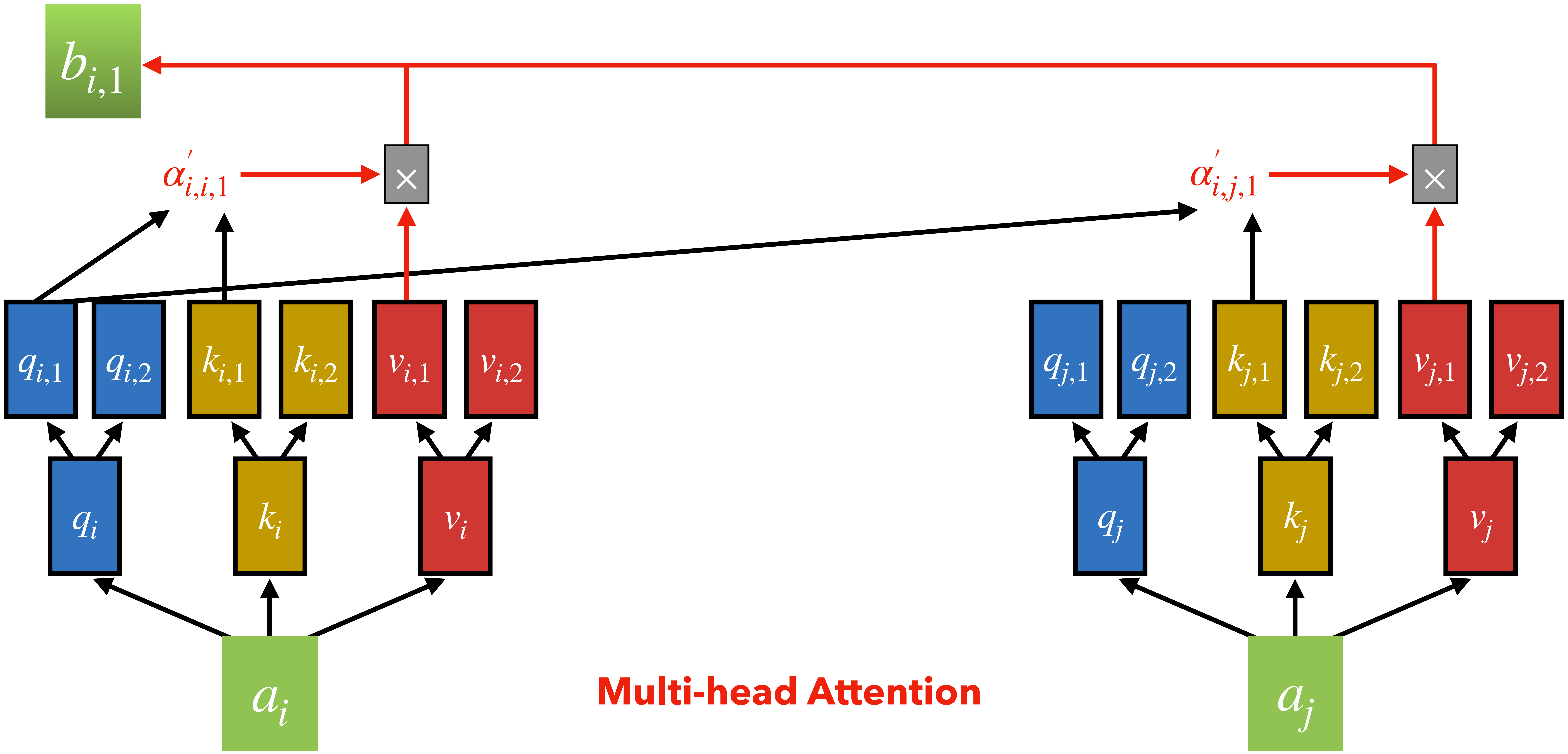

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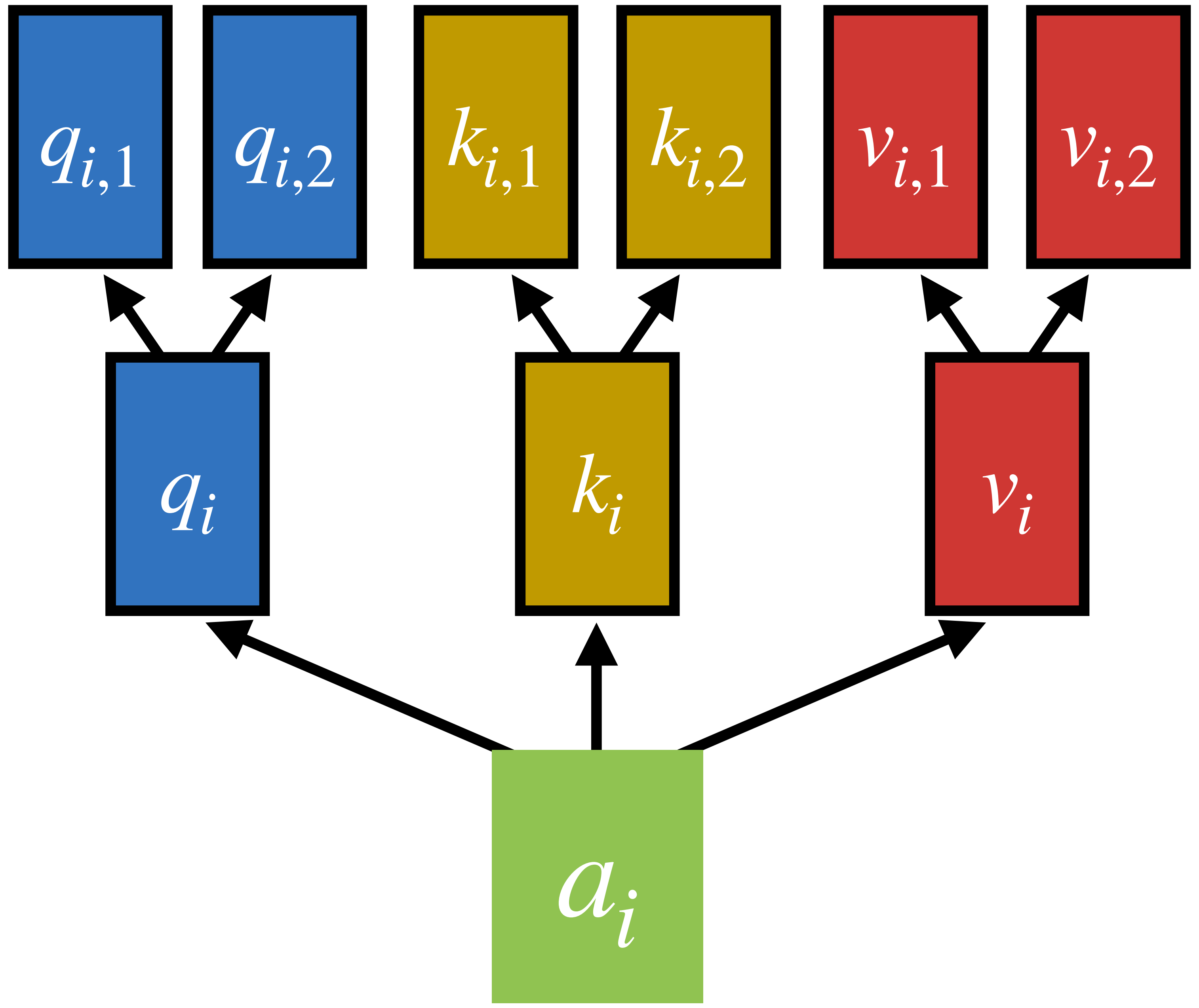

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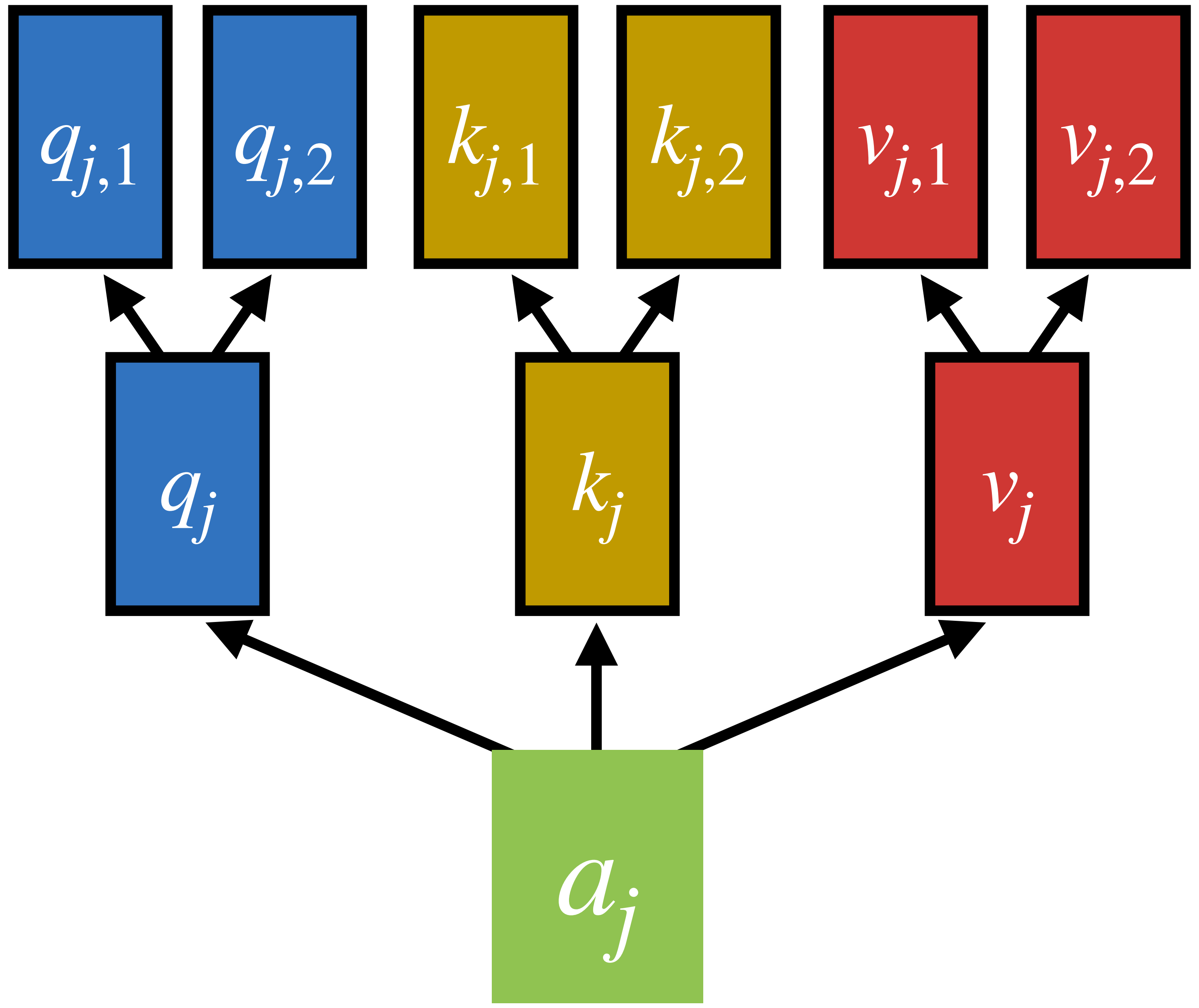

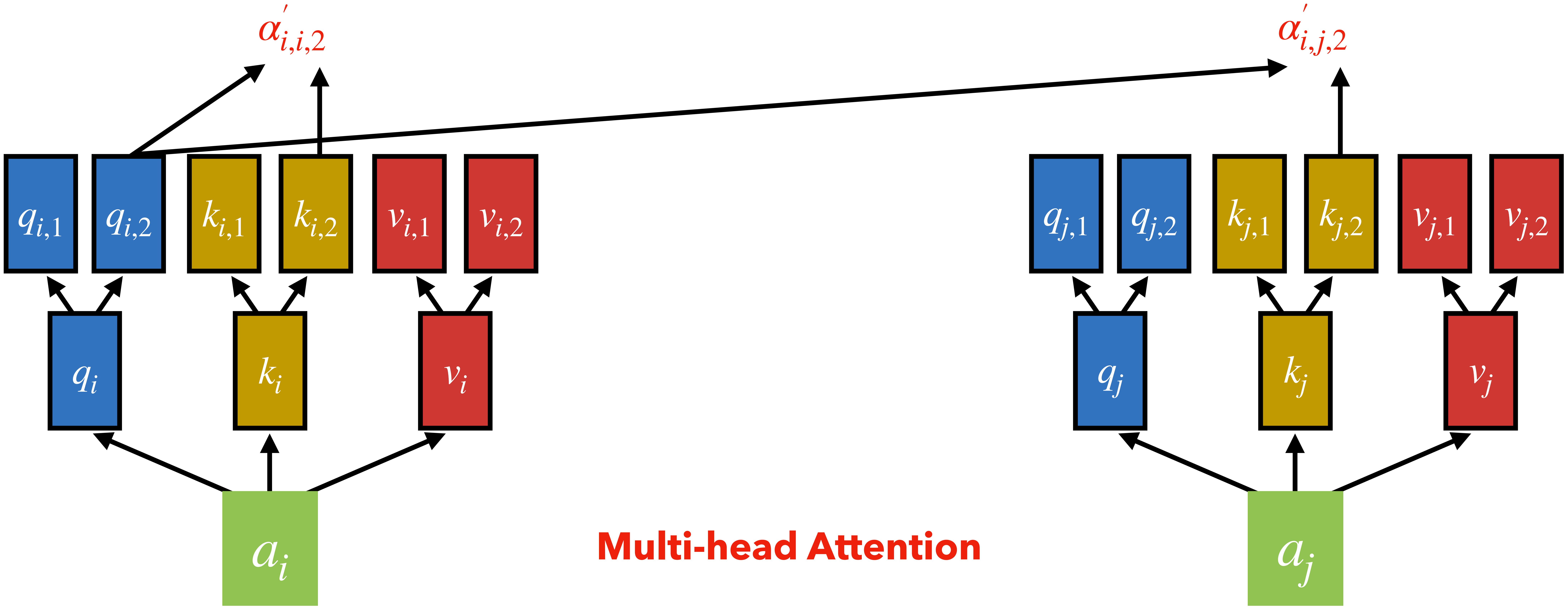

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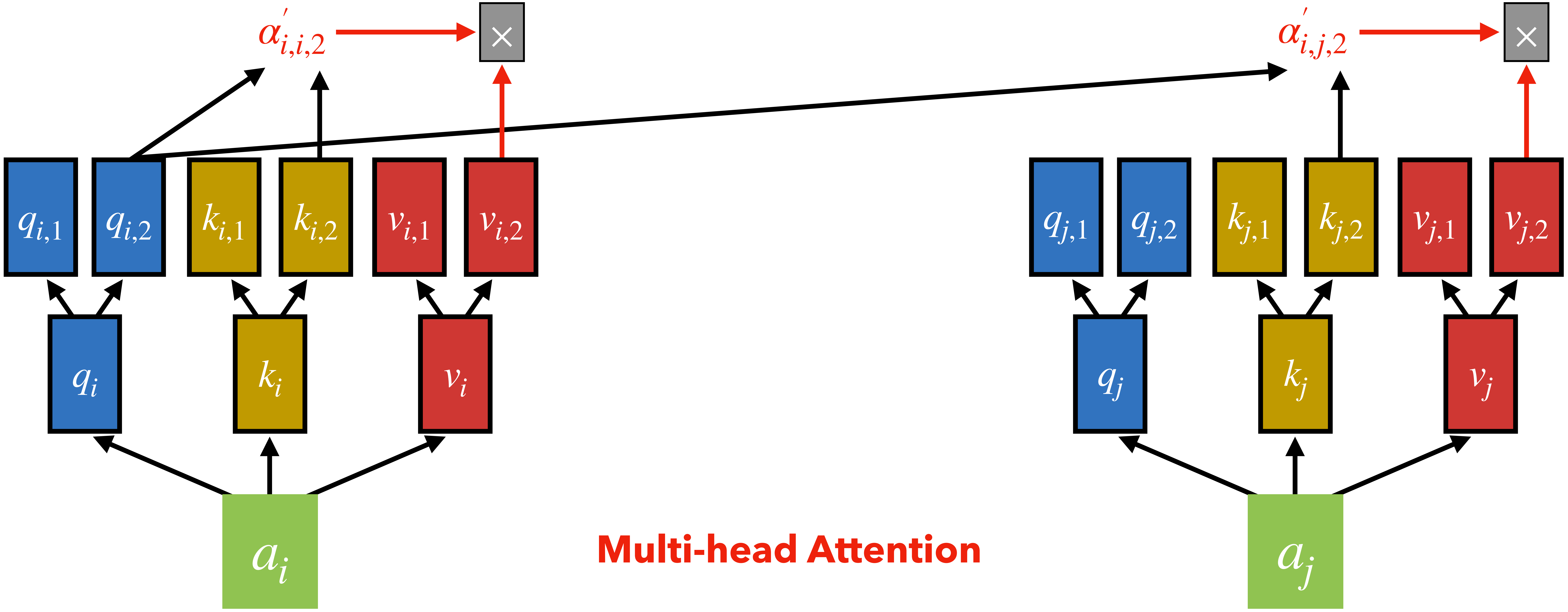

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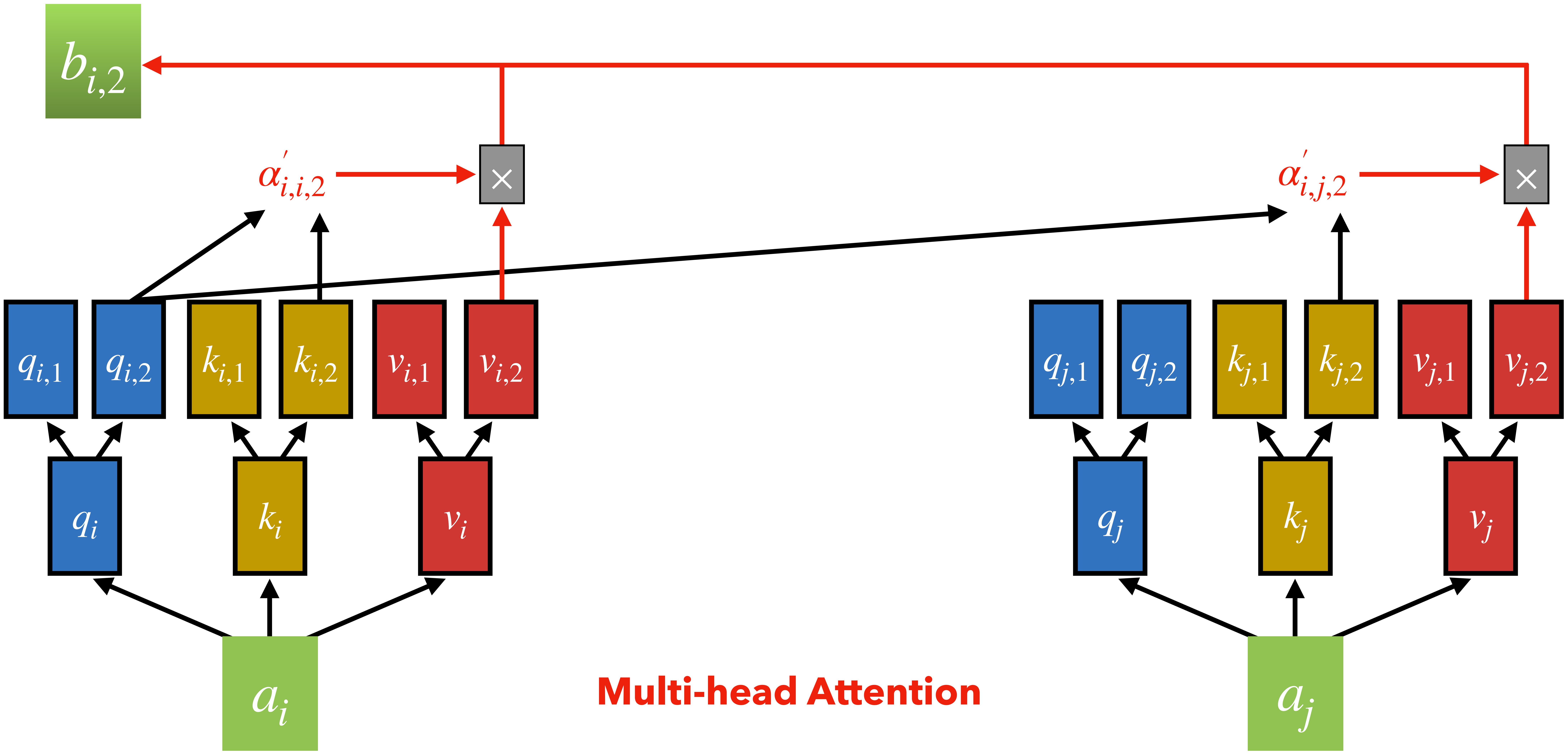

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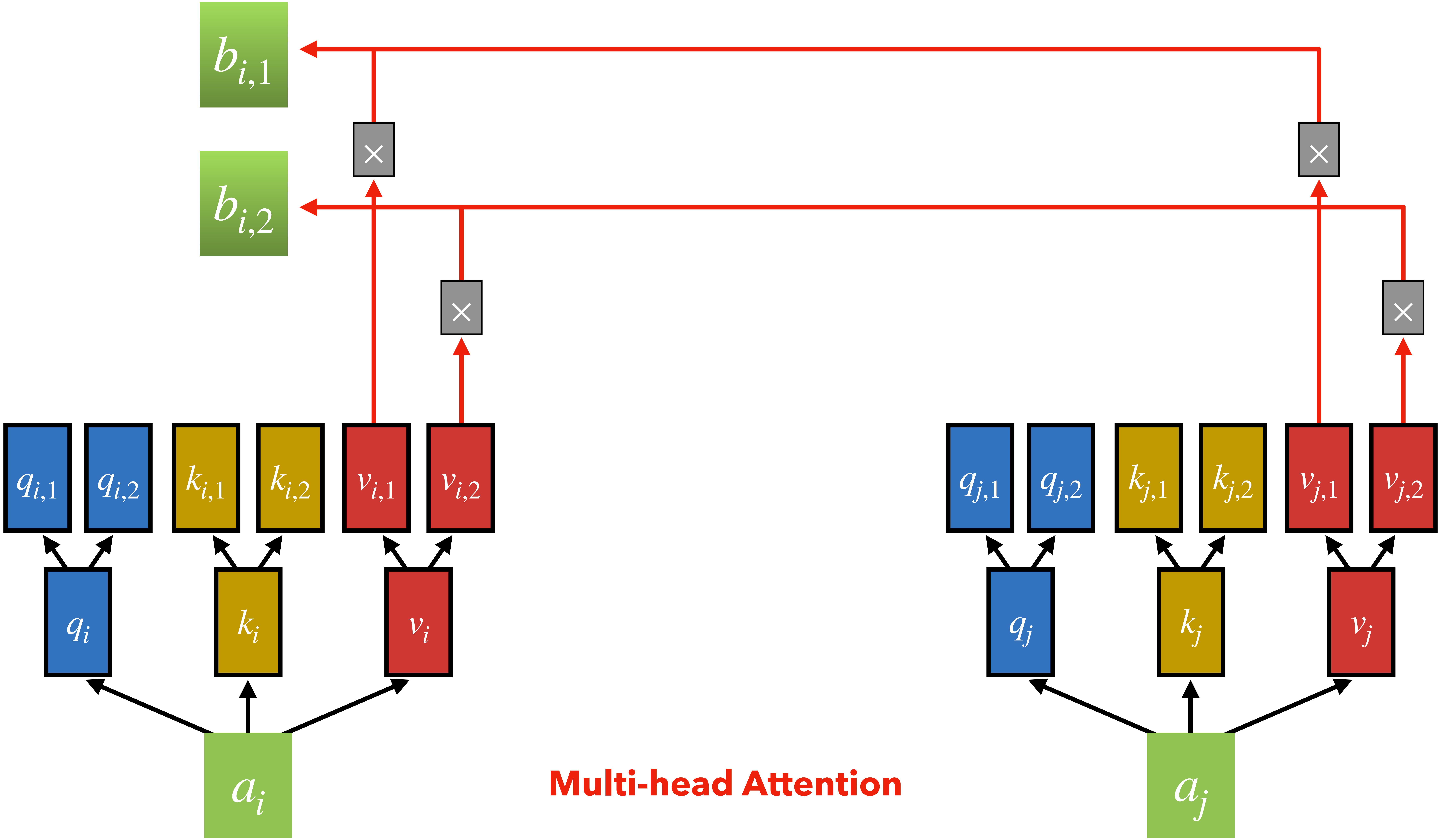

$b_{i,1}$
$b_{i,2}$
×
×
×
×
$q_{i,1}$
$q_{i,2}$
$k_{i,1}$
$k_{i,2}$
$v_{i,1}$
$v_{i,2}$
$q_{j,1}$
$q_{j,2}$
$k_{j,1}$
$k_{j,2}$
$v_{j,1}$
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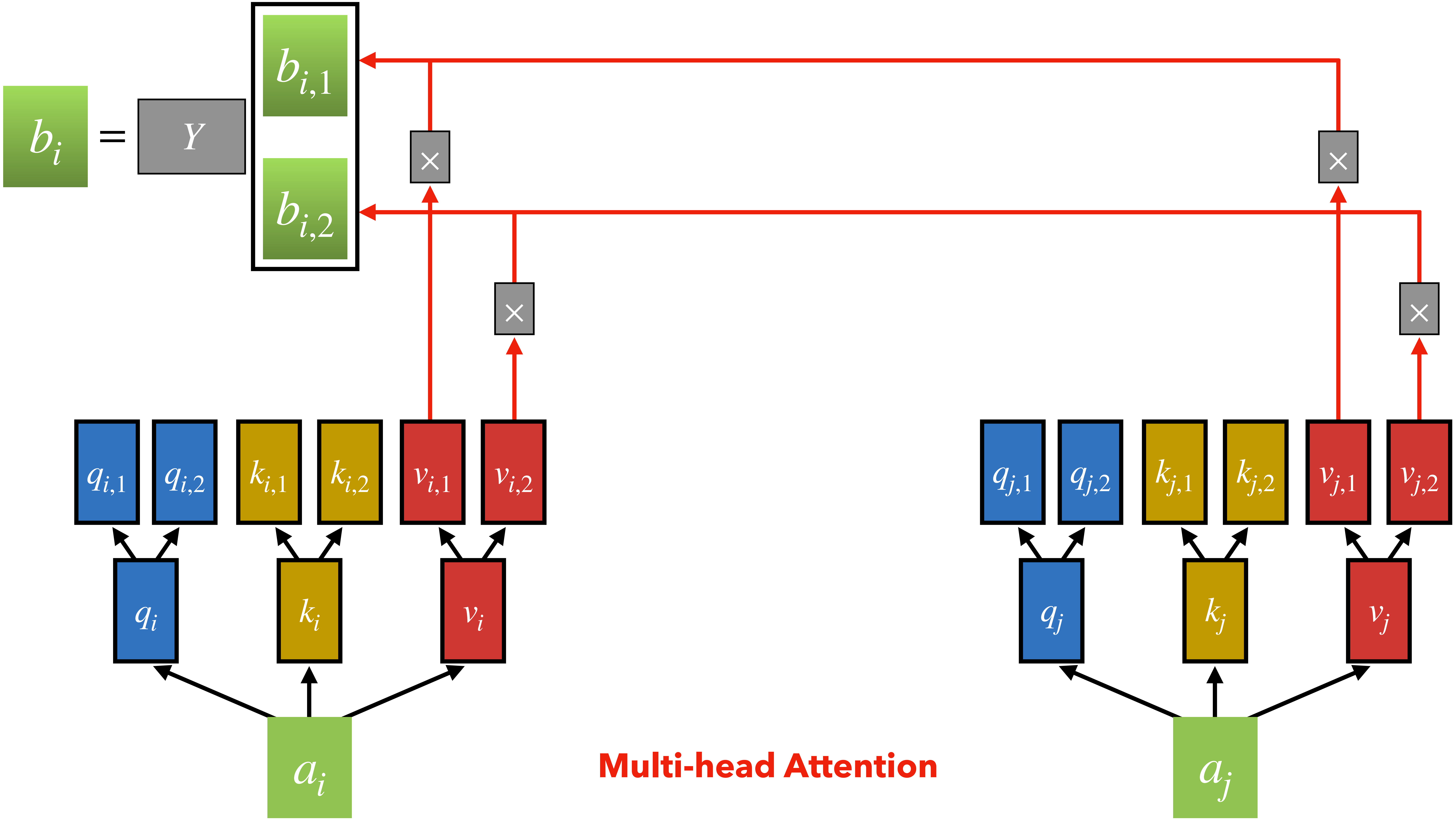
q_i
k_i
v_i
q_j
k_j
v_j
a_i
Multi-head Attention
a_j



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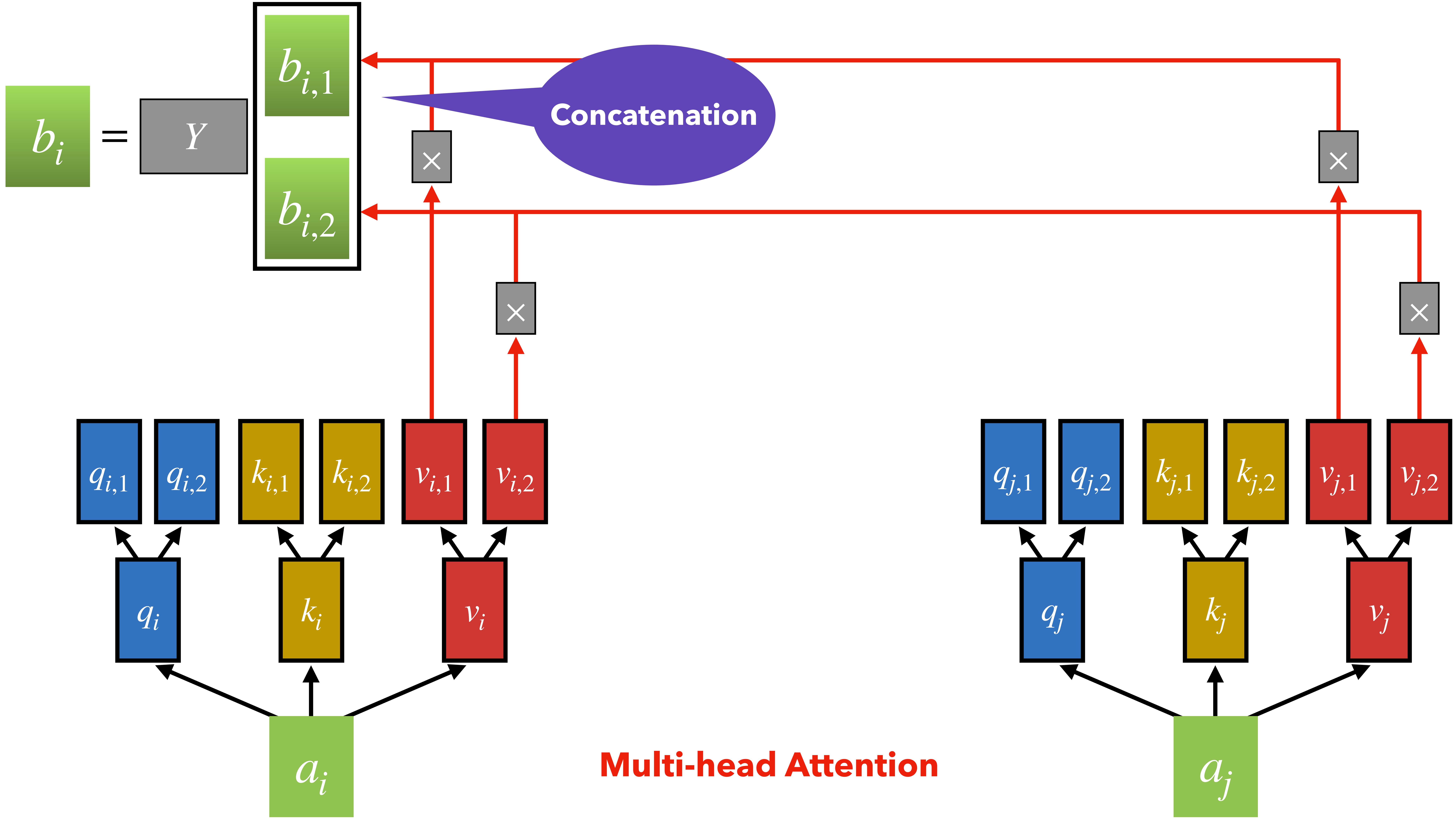
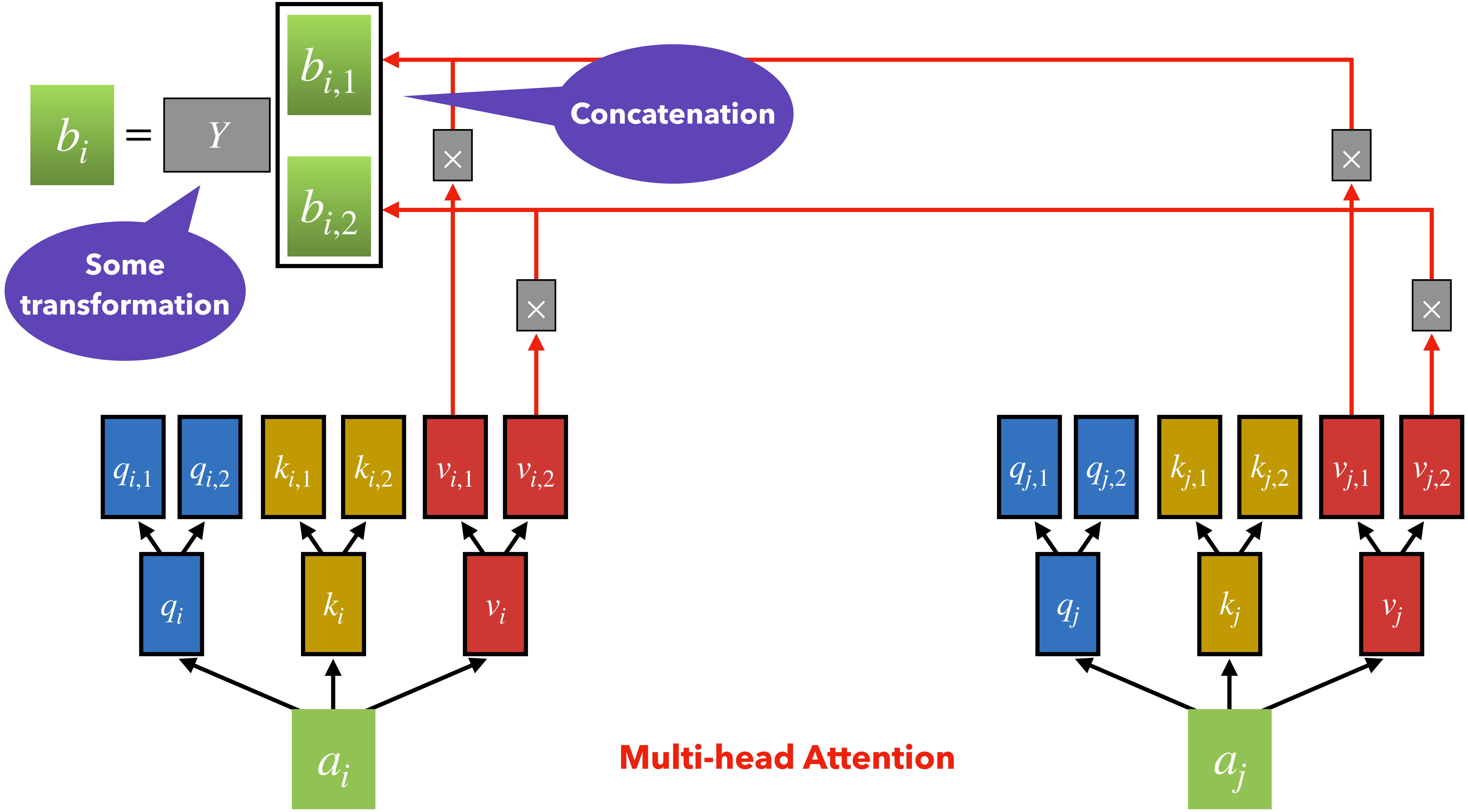

$b_i = Y$
$b_{i,1}$
$b_{i,2}$
Concatenation
$q_{i,1}$ $q_{i,2}$ $k_{i,1}$ $k_{i,2}$ $v_{i,1}$ $v_{i,2}$
q_i k_i v_i
a_i
$q_{j,1}$ $q_{j,2}$ $k_{j,1}$ $k_{j,2}$ $v_{j,1}$ $v_{j,2}$
q_j k_j v_j
a_j
Multi-head Attention



b_i
=
Y
$b_{i,1}$
$b_{i,2}$
Concatenation
Some transformation
×
×
×
×
$q_{i,1}$
$q_{i,2}$
$k_{i,1}$
$k_{i,2}$
$v_{i,1}$
$v_{i,2}$
$q_{j,1}$
$q_{j,2}$
$k_{j,1}$
$k_{j,2}$
$v_{j,1}$
$v_{j,2}$
q_i
k_i
v_i
q_j
k_j
v_j
a_i
Multi-head Attention
a_j

Recall the Matrices Form of Self-Attention

$Q = I\, W_Q$

$K = I\, W_K$

$V = I\, W_V$

$I = \{a_1, \ldots, a_n\} \in \mathbb{R}^{n \times d}$, where $a_i \in \mathbb{R}^d$

$W_Q, W_K, W_V \in \mathbb{R}^{d \times d}$

$Q, K, V \in \mathbb{R}^{n \times d}$

$A = Q\, K^T$

$A = I\, W_Q\, (I\, W_K)^T = I\, W_Q\, W_K^T\, I^T$

$A^{'} = \text{softmax}(A)$

$A^{'}, A \in \mathbb{R}^{n \times n}$

$O = A^{'}\, V$

$O \in \mathbb{R}^{n \times d}$

Multi-head Attention in Matrices

- **Multiple attention "heads" can be defined via multiple W_Q, W_K, W_V matrices**
- **Let $W_Q^l, W_K^l, W_V^l \in \mathbb{R}^{d \times \frac{d}{h}}$, where h is the number of attention heads, and l ranges from 1 to h.**
- **Each attention head performs attention independently:**
  - $O^l = \textbf{softmax}(I\ W_Q^l\ {W_K^l}^T\ I^T)\ I\ W_V^l$
- **Concatenating different O^l from different attention heads.**
  - $O = [O^1; \ldots; O^n]\ Y$**, where** $Y \in \mathbb{R}^{d \times d}$

The Matrices Form of Multi-head Attention

$Q^l = I\,W_Q^l$

$K^l = I\,W_K^l$

$V^l = I\,W_V^l$

- $I = \{a_1, \ldots, a_n\} \in \mathbb{R}^{n \times d}$, where $a_i \in \mathbb{R}^d$
- $W_Q^l, W_K^l, W_V^l \in \mathbb{R}^{d \times \frac{d}{h}}$
- $Q^l, K^l, V^l \in$?

$A^l = Q^l\,K^{l^T}$

$A^{l'} = \text{softmax}(A^l)$

- $A^{l'}, A^l \in \mathbb{R}$?

$O^l = A^{l'}\,V^l$

- $O^l \in \mathbb{R}$?

$O = [O^1; \ldots; O^h]\,Y$

- $Y \in \mathbb{R}^{d \times d}$
- $[O^1; \ldots; O^h] \in$?
- $O \in \mathbb{R}$?

Dimensions?

The Matrices Form of Multi-head Attention

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$Q^l, K^l, V^l \in \mathbb{R}^{n \times \frac{d}{h}}$

$$A^l = Q^l\, K^{l^T}$$
$$A^{l'} = \text{softmax}(A^l)$$

$A^{l'}, A^l \in \mathbb{R}$?

$$O^l = A^{l'}\, V^l$$

$O^l \in \mathbb{R}$?

Dimensions?

$$O = [O^1; \ldots; O^h]\, Y$$

$Y \in \mathbb{R}^{d \times d}$

$[O^1; \ldots; O^h] \in$?

$O \in \mathbb{R}$?

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$$A^l = Q^l\,K^{lT}$$

$$A^{l'} = \text{softmax}(A^l)$$

$A^{l'}, A^l \in \mathbb{R}^{n\times n}$

$$O^l = A^{l'}\,V^l$$

$O^l \in \mathbb{R}$?

$$O = [O^1; \ldots; O^h]\;Y$$

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Dimensions?

Multi-head Attention is Computationally Efficient

- **Even though we compute h many attention heads, it's not more costly.**
  - **We compute $I\,W_Q \in \mathbb{R}^{n\times d}$, and then reshape to $\mathbb{R}^{n\times h\times \frac{d}{h}}$.**
  - **Likewise for $I\,W_K$ and $I\,W_V$.**
  - **Then we transpose to $\mathbb{R}^{h\times n\times \frac{d}{h}}$; now the head axis is like a batch axis.**
  - **Almost everything else is identical. All we need to do is to reshape the tensors!**

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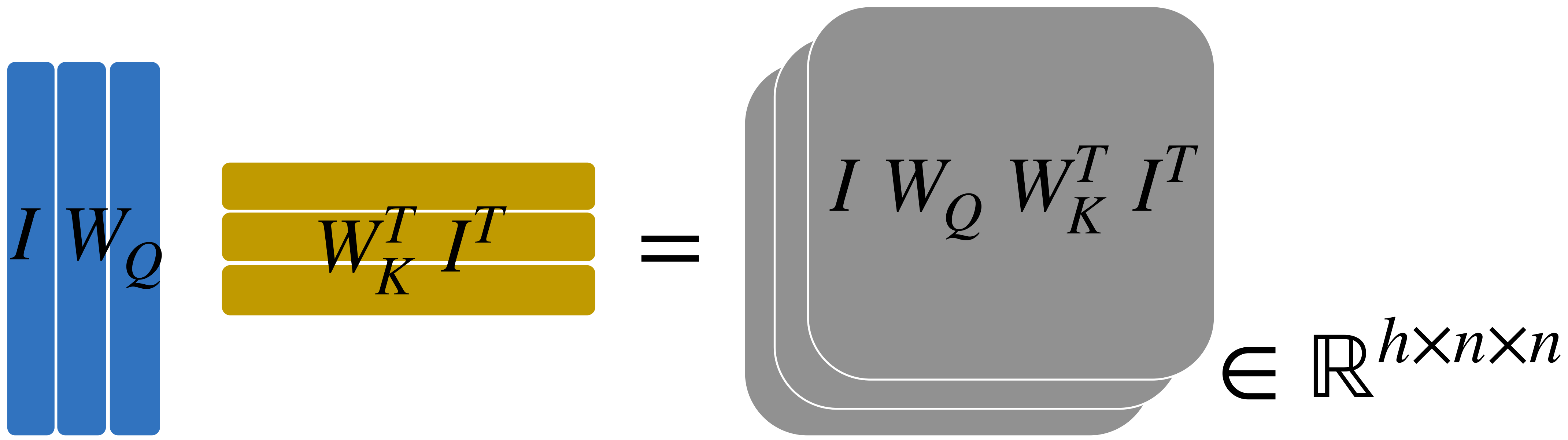

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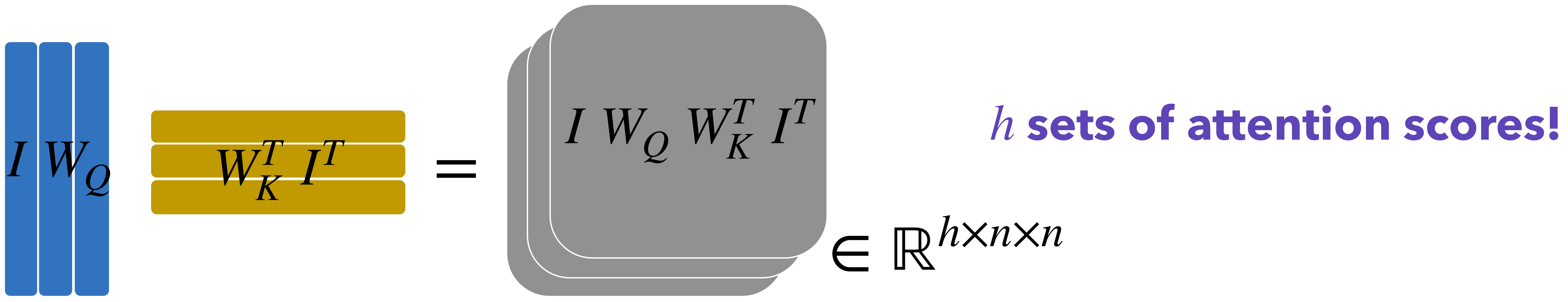

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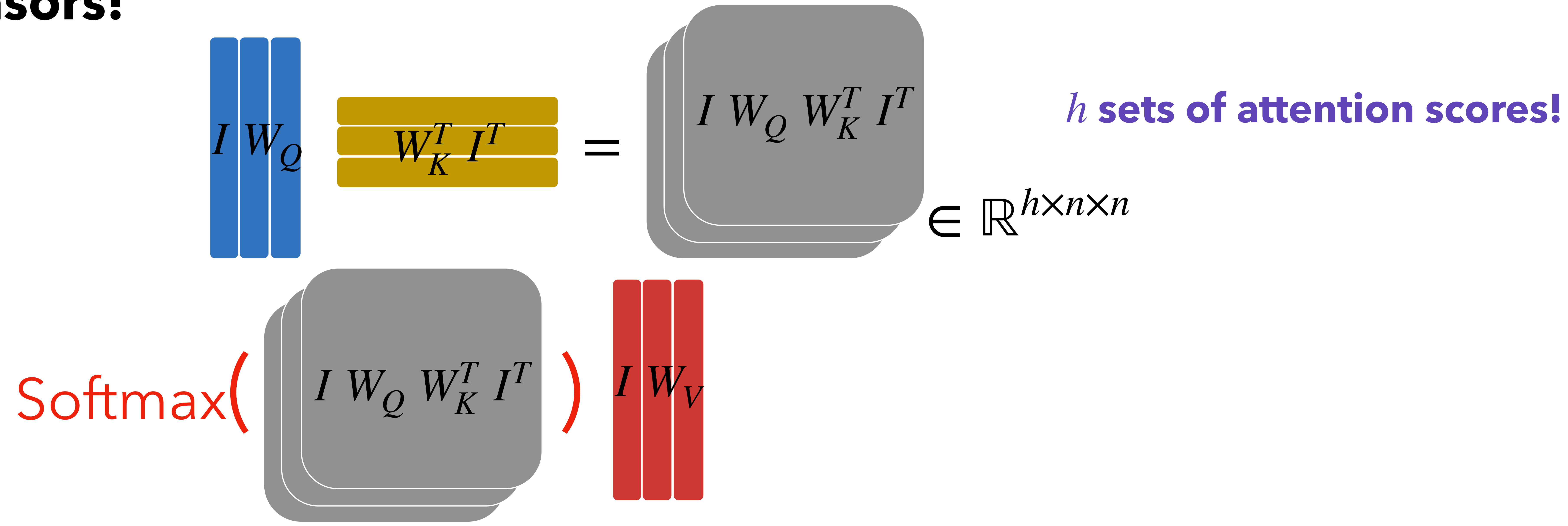

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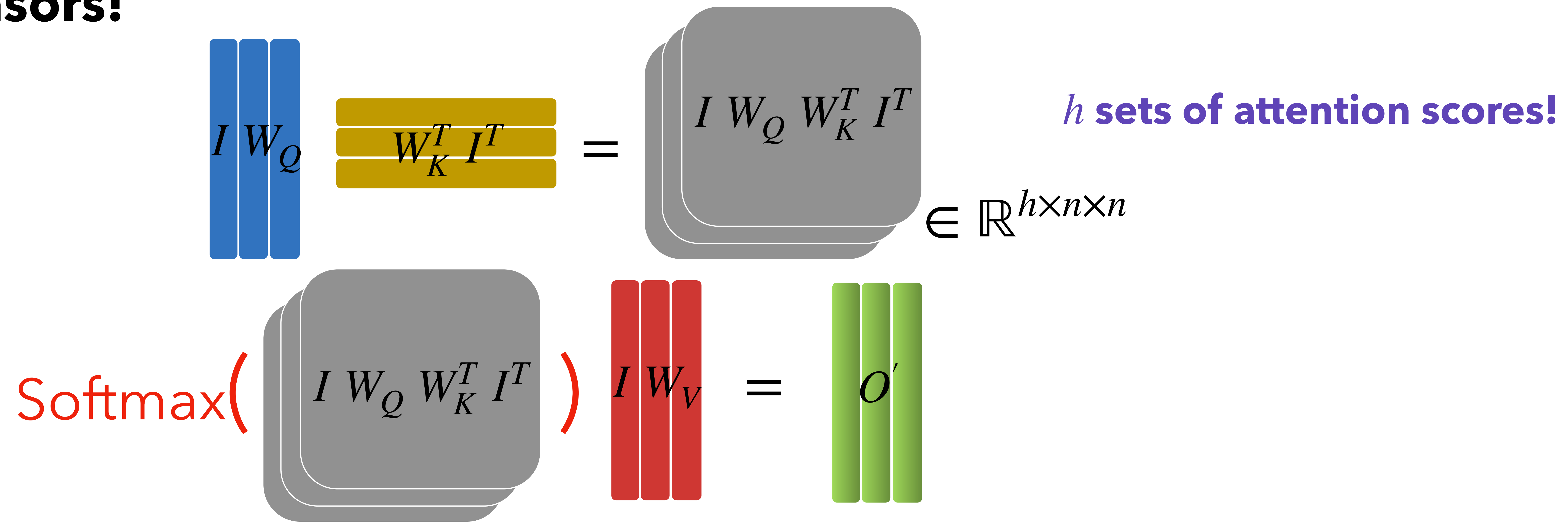

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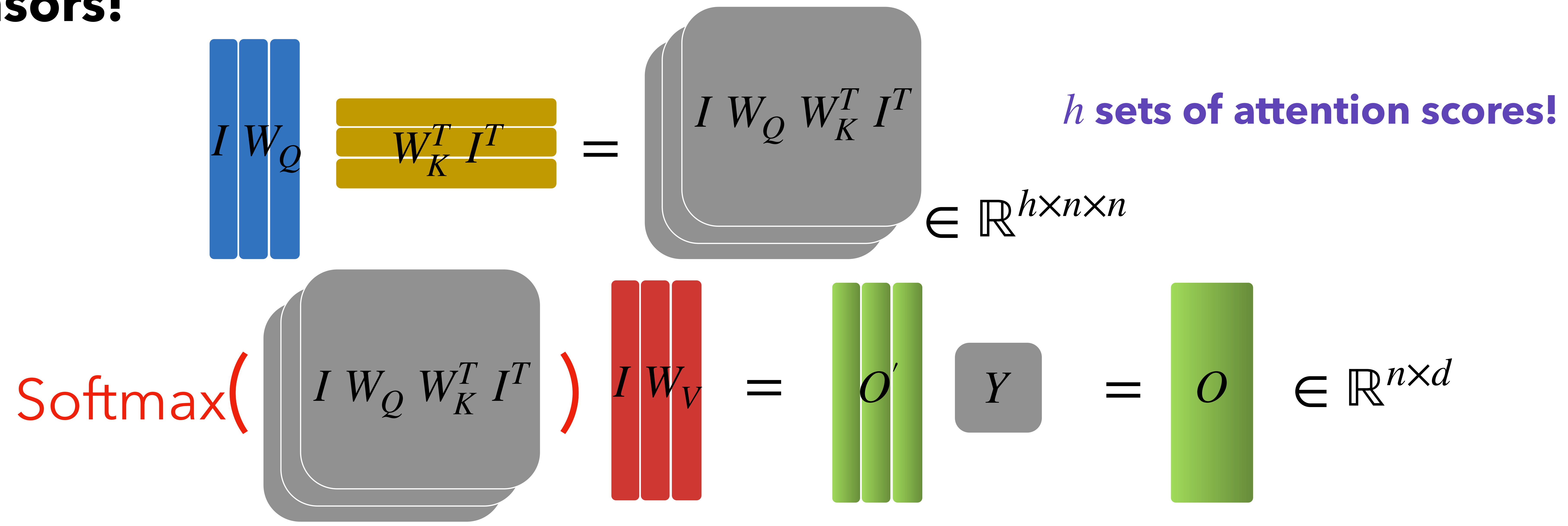

Scaled Dot Product [Vaswani et al., 2017]

- **“Scaled Dot Product” attention aids in training.**
- **When dimensionality d becomes large, dot products between vectors tend to become large.**
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- **Instead of the self-attention function we've seen:**
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- **We divide the attention scores by $\sqrt{d/h}$, to stop the scores from becoming large just as a function of d/h (the dimensionality divided by the number of heads).**

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  - Because of this, inputs to the softmax function can be large, making the gradients small.
- Instead of the self-attention function we've seen:
  - $O^l = \text{softmax}(I\, W_Q^l\, {W_K^l}^T\, I^T)\, I\, W_V^l$
- We divide the attention scores by $\sqrt{d/h}$, to stop the scores from becoming large just as a function of d/h (the dimensionality divided by the number of heads).

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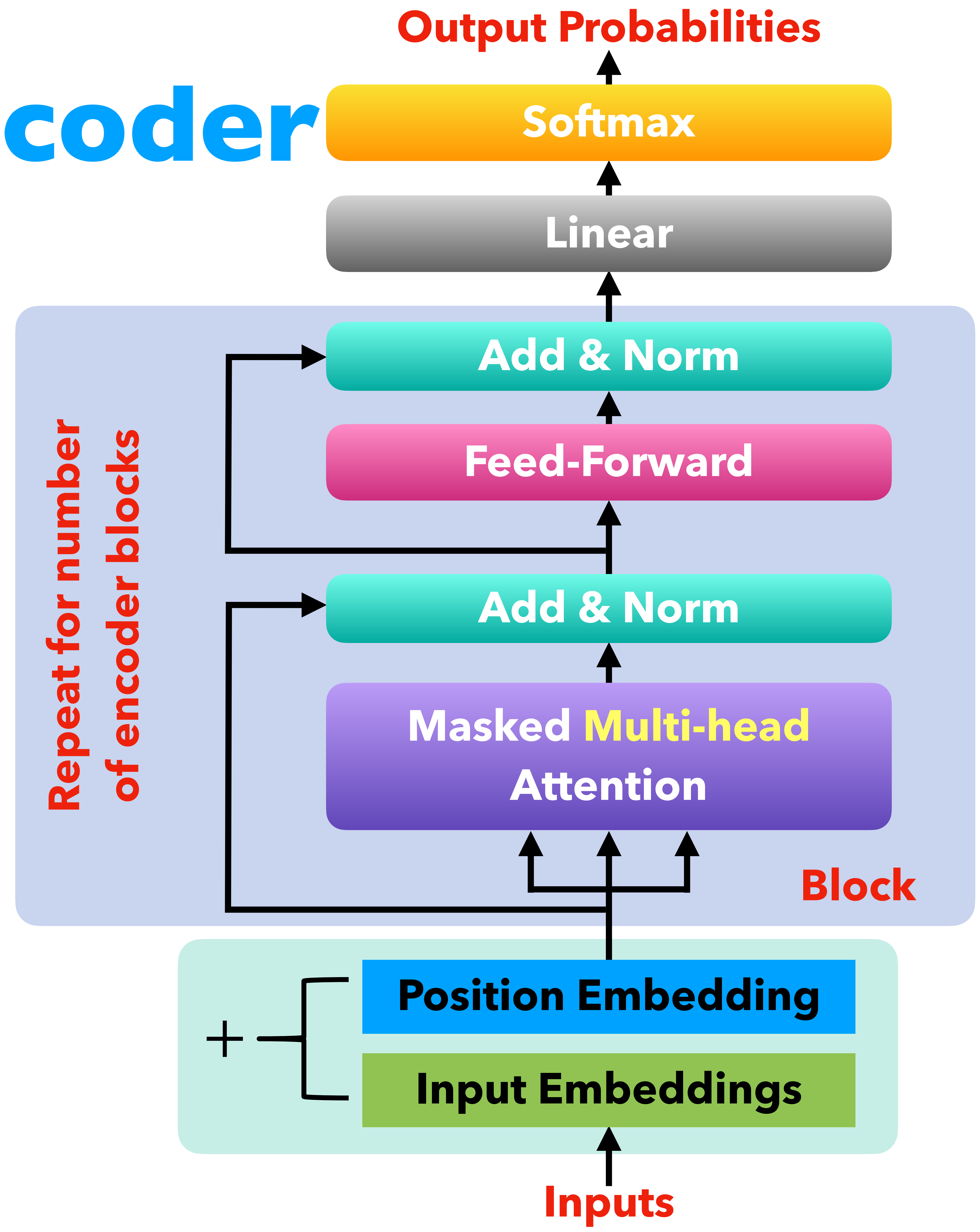
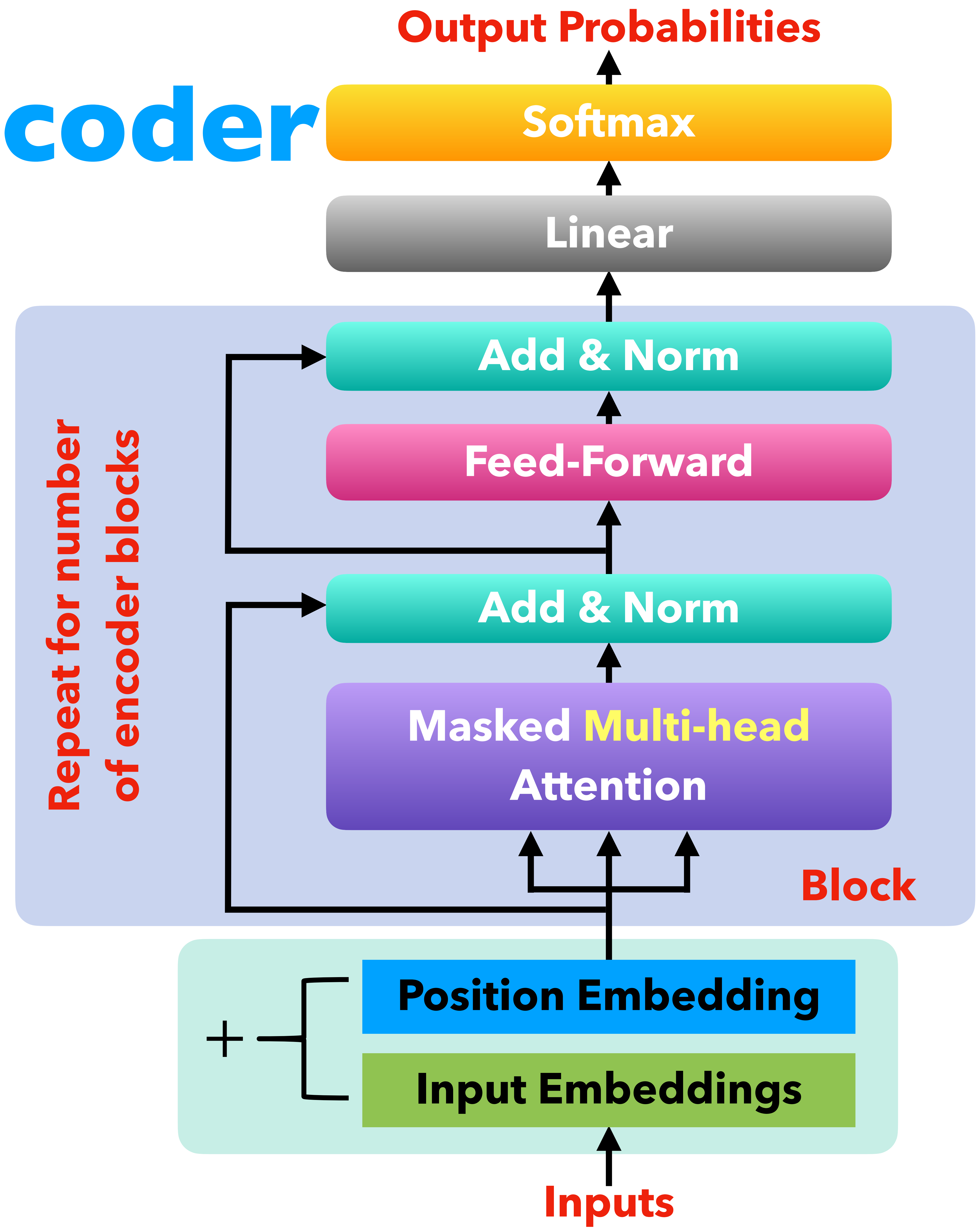
The Transformer Decoder



The Transformer Decoder

- **Now that we've replaced self-attention with multi-head self-attention, we'll go through two optimization tricks:**
  - ***Residual connection ("Add")***
  - ***Layer normalization ("Norm")***



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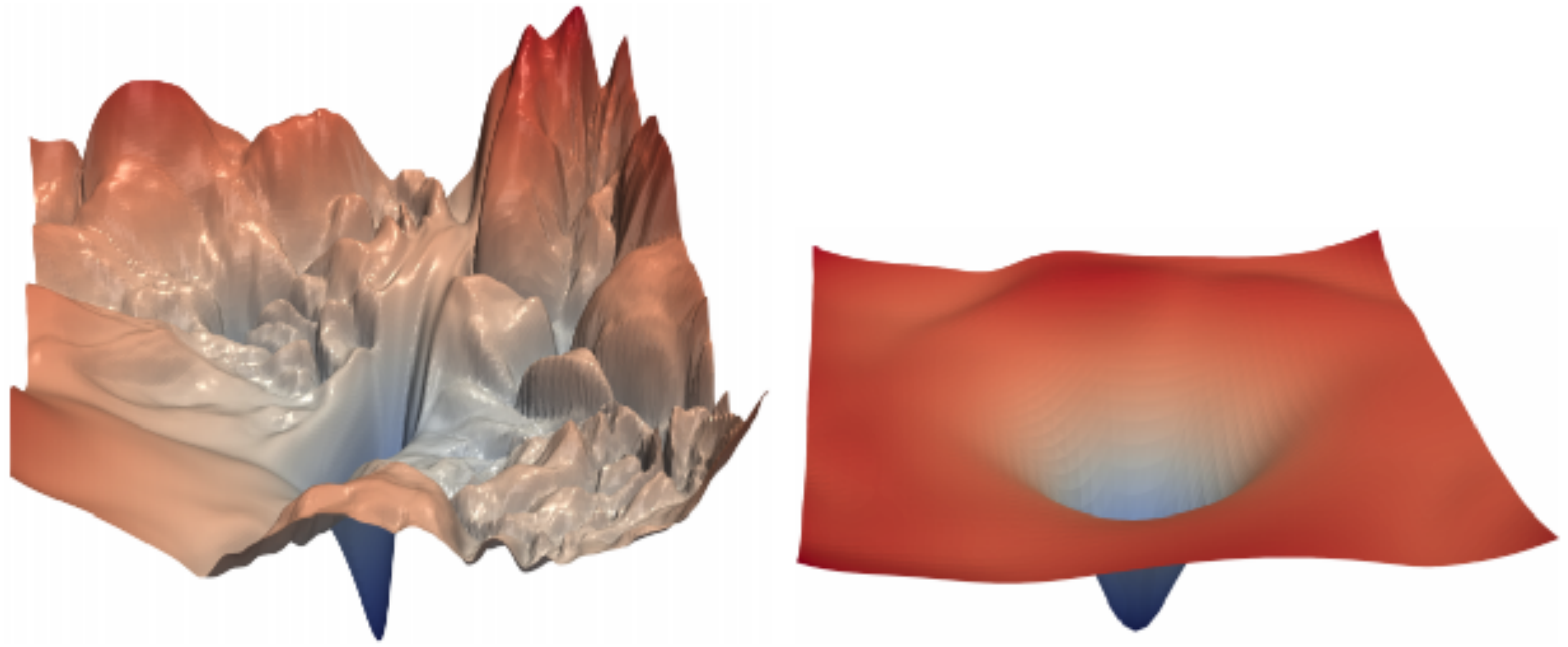

[no residuals] [residuals]

[Loss landscape visualization, Li et al., 2018, on a ResNet]

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Normalize by scalar mean and variance

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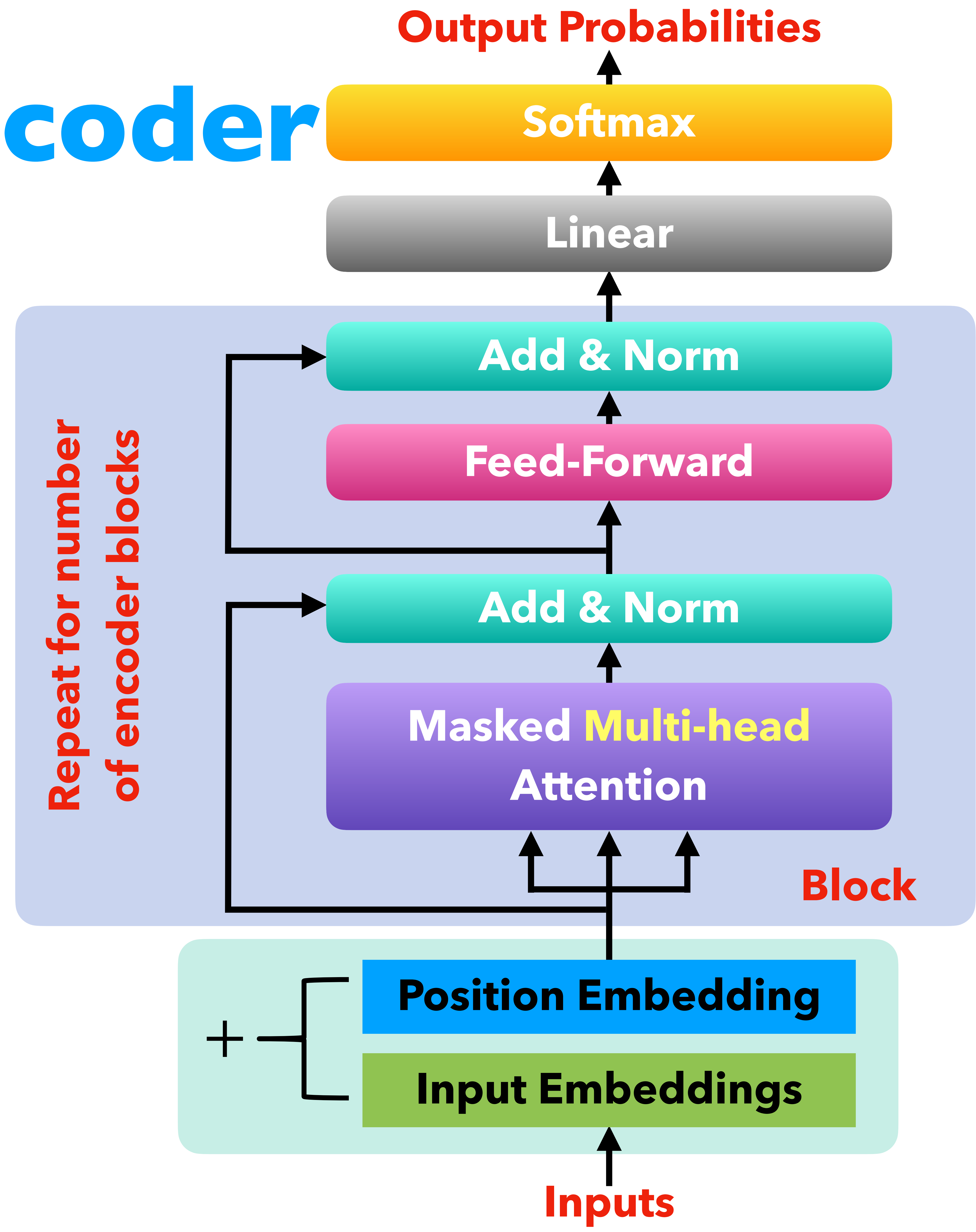
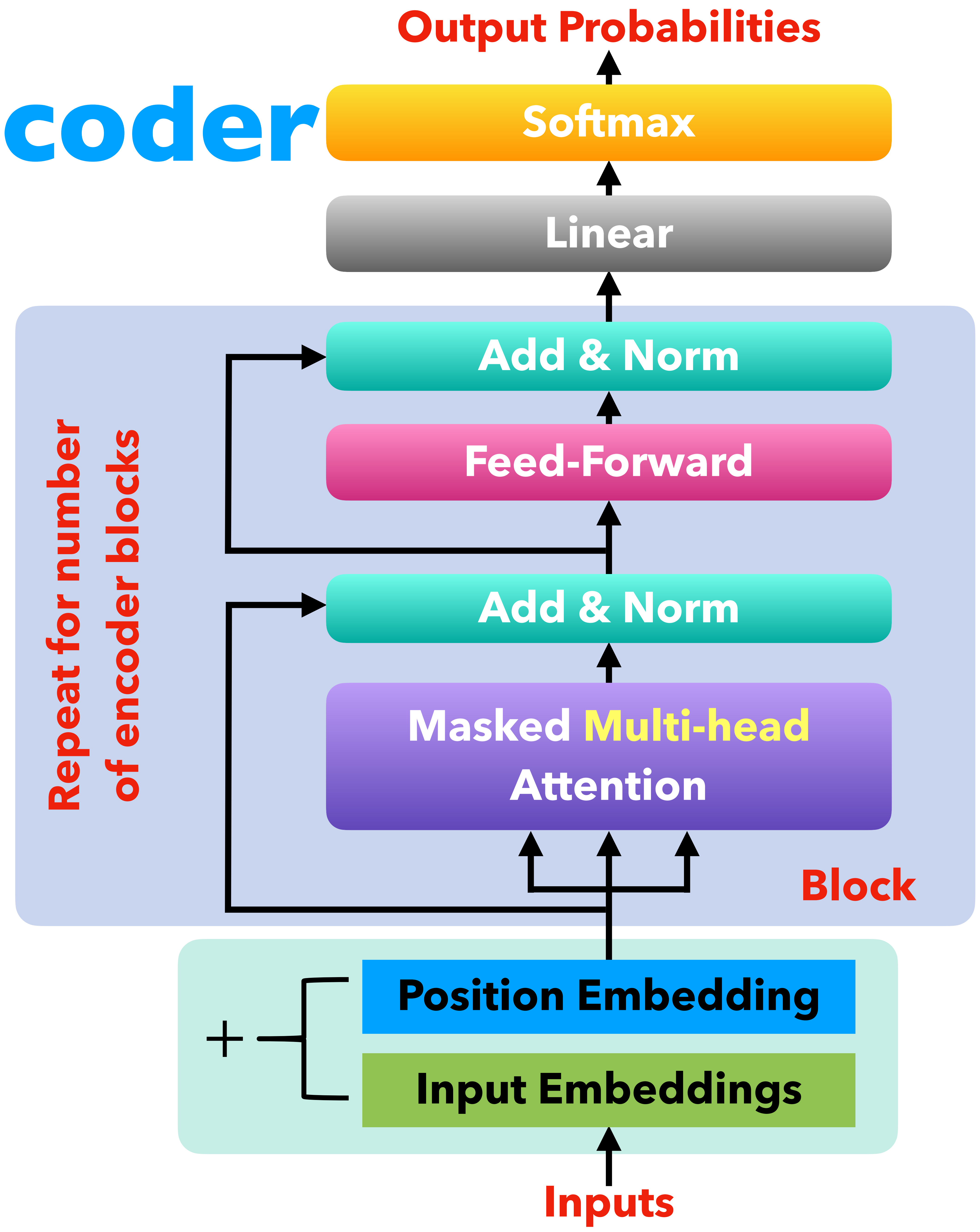
Modulate by learned element-wise gain and bias

The Transformer Decoder



The Transformer Decoder

- The Transformer Decoder is a stack of Transformer Decoder Blocks.
- Each Block consists of:
  - Masked Multi-head Self-attention
  - Add & Norm
  - Feed-Forward
  - Add & Norm



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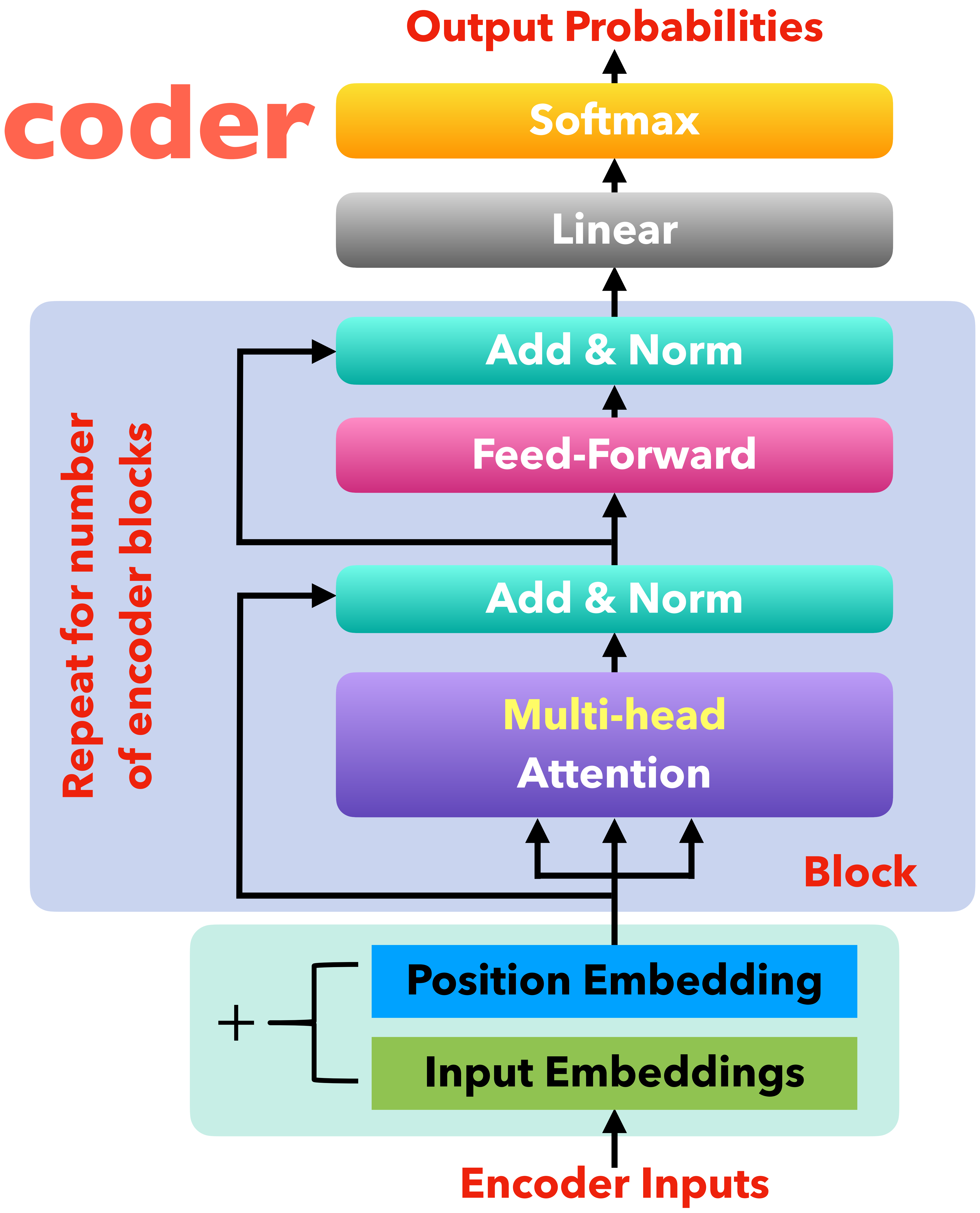

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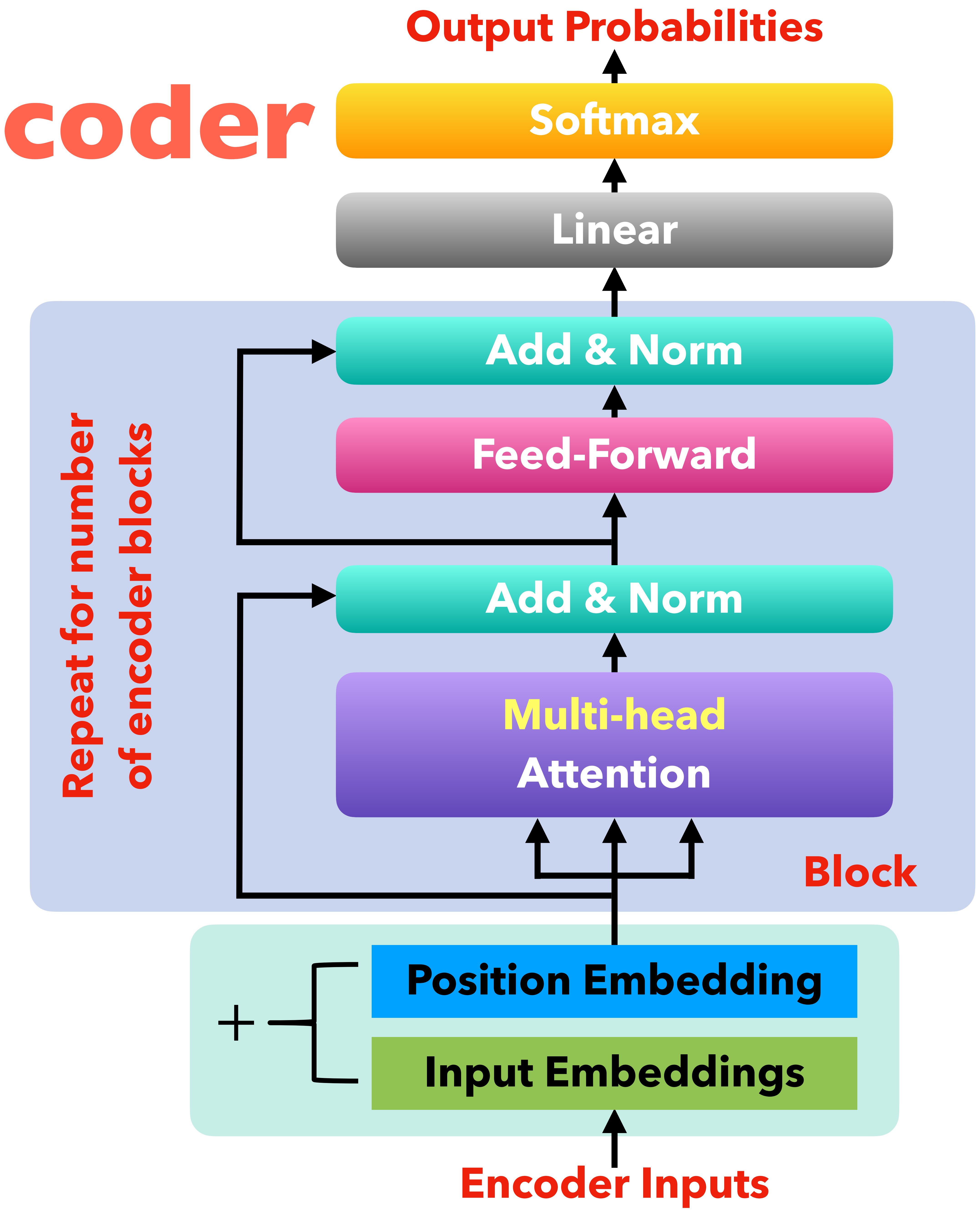

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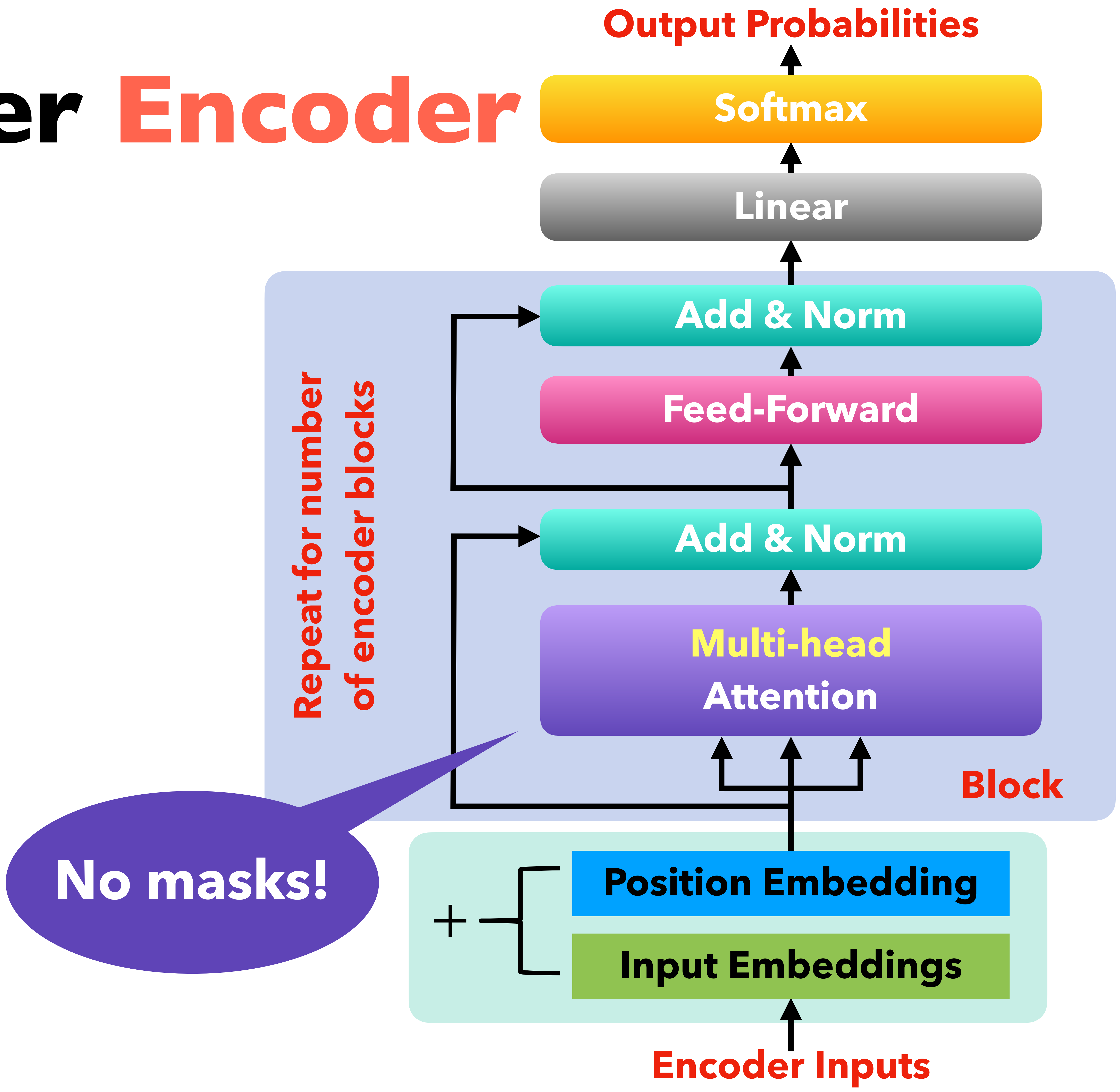
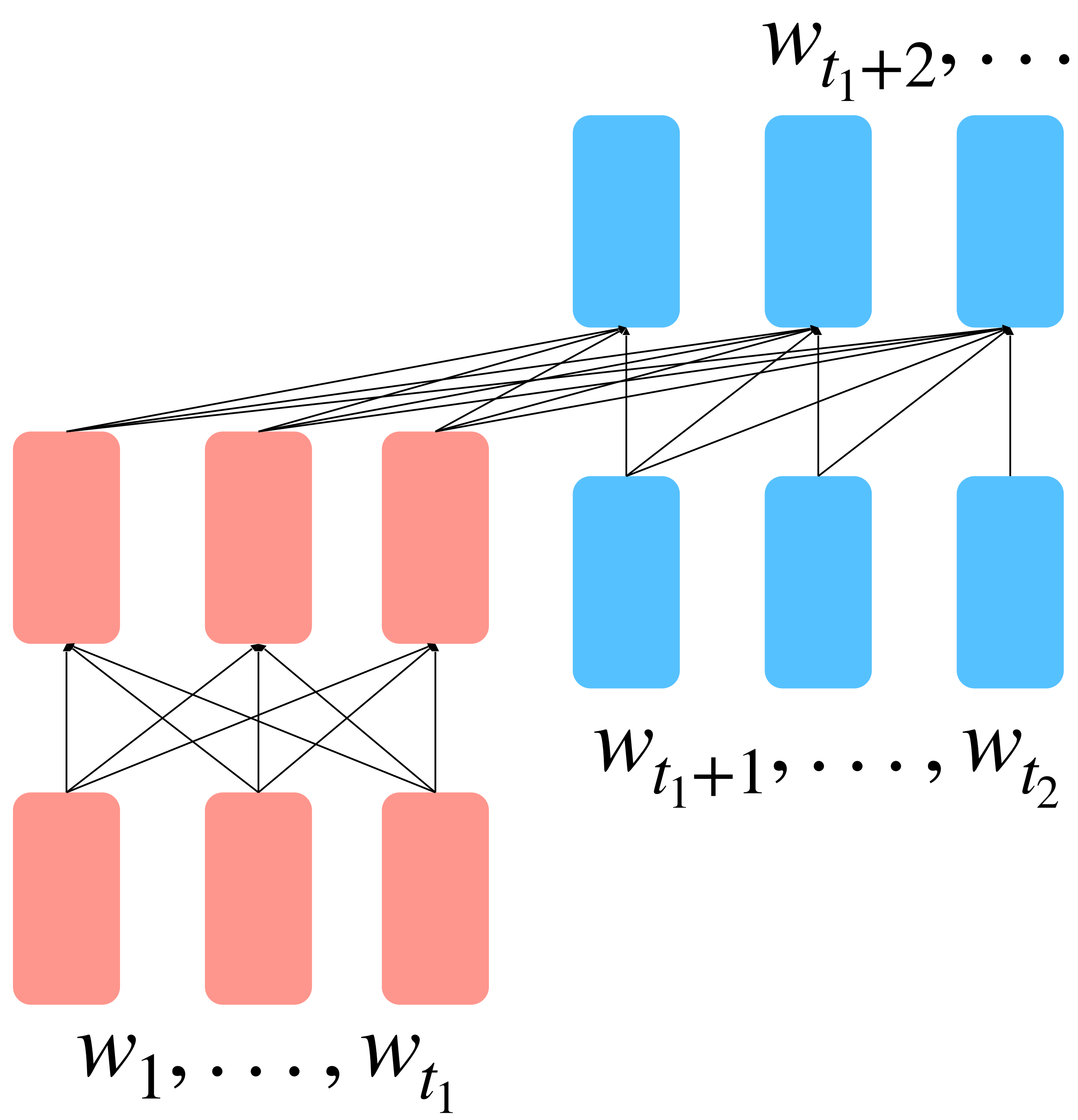
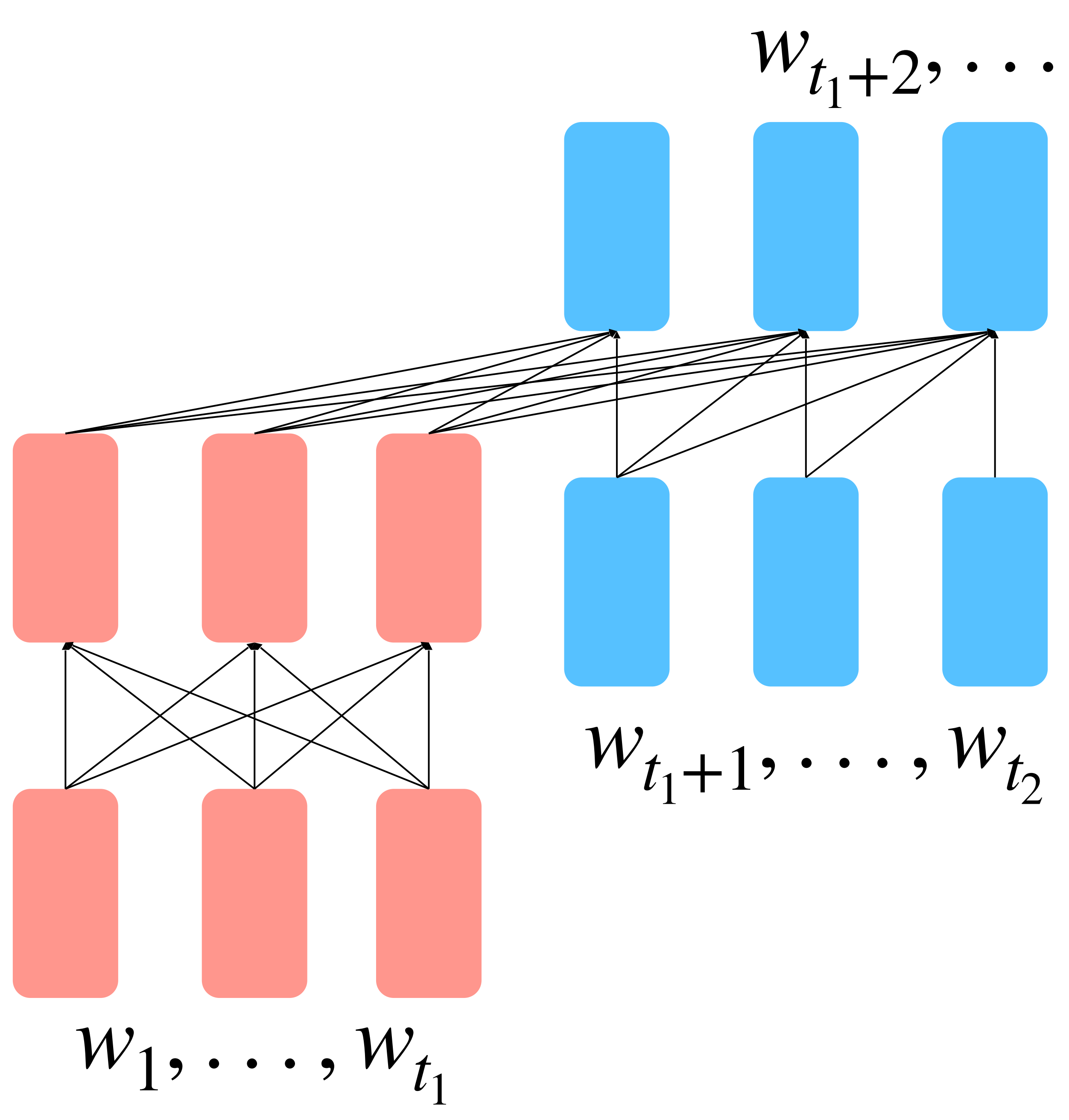


The Transformer Encoder-Decoder

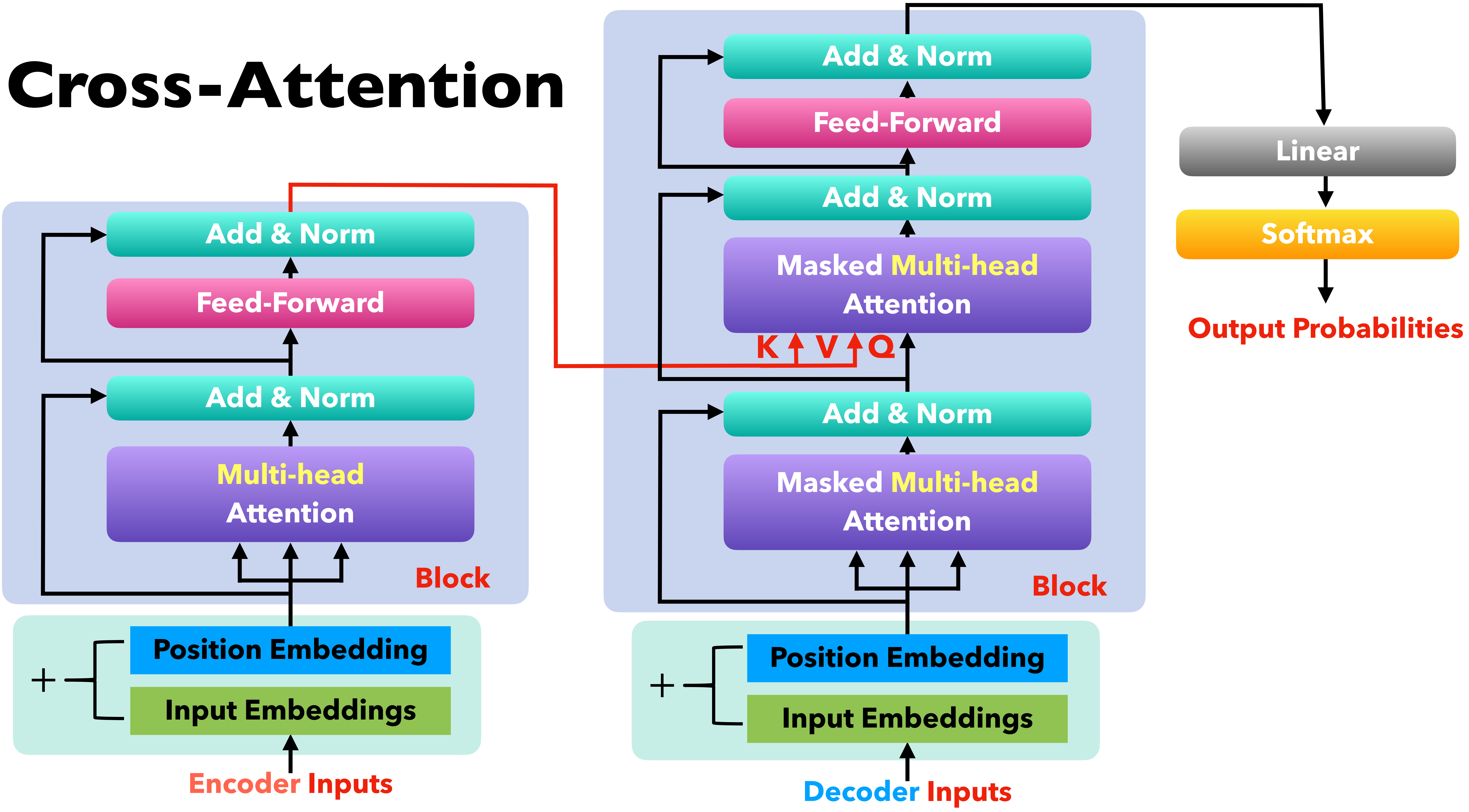


The Transformer Encoder-Decoder

- **More on Encoder-Decoder models will be introduced in future lectures!**
- **Right now we only need to know that it processes the source sentence with a bidirectional model (Encoder) and generates the target with a unidirectional model (Decoder).**
- **The Transformer Decoder is modified to perform cross-attention to the output of the Encoder.**



Cross-Attention



Cross-Attention Details

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- **Self-attention: queries, keys, and values come from the same source.**
- **Cross-Attention: *keys* and *values* are from Encoder (like a memory); *queries* are from Decoder.**
- **Let** $h_1, \ldots, h_n$ **be output vectors from the Transformer encoder,** $h_i \in \mathbb{R}^d$**.**
- **Let** $z_1, \ldots, \ z_n$ **be input vectors from the Transformer decoder,** $z_i \in \mathbb{R}^d$**.**
- **Keys and values from the encoder:**
  - $k_i = W_K \, h_i$
  - $v_i = W_V \, h_i$
- **Queries are drawn from the decoder:**
  - $q_i = W_Q \, z_i$

The Revolutionary Impact of Transformers

- Almost all current-day leading language models use Transformer building blocks.
  - E.g., GPT1/2/3/4, T5, Llama 1/2, BERT, … almost anything we can name
  - Transformer-based models dominate nearly all NLP leaderboards.

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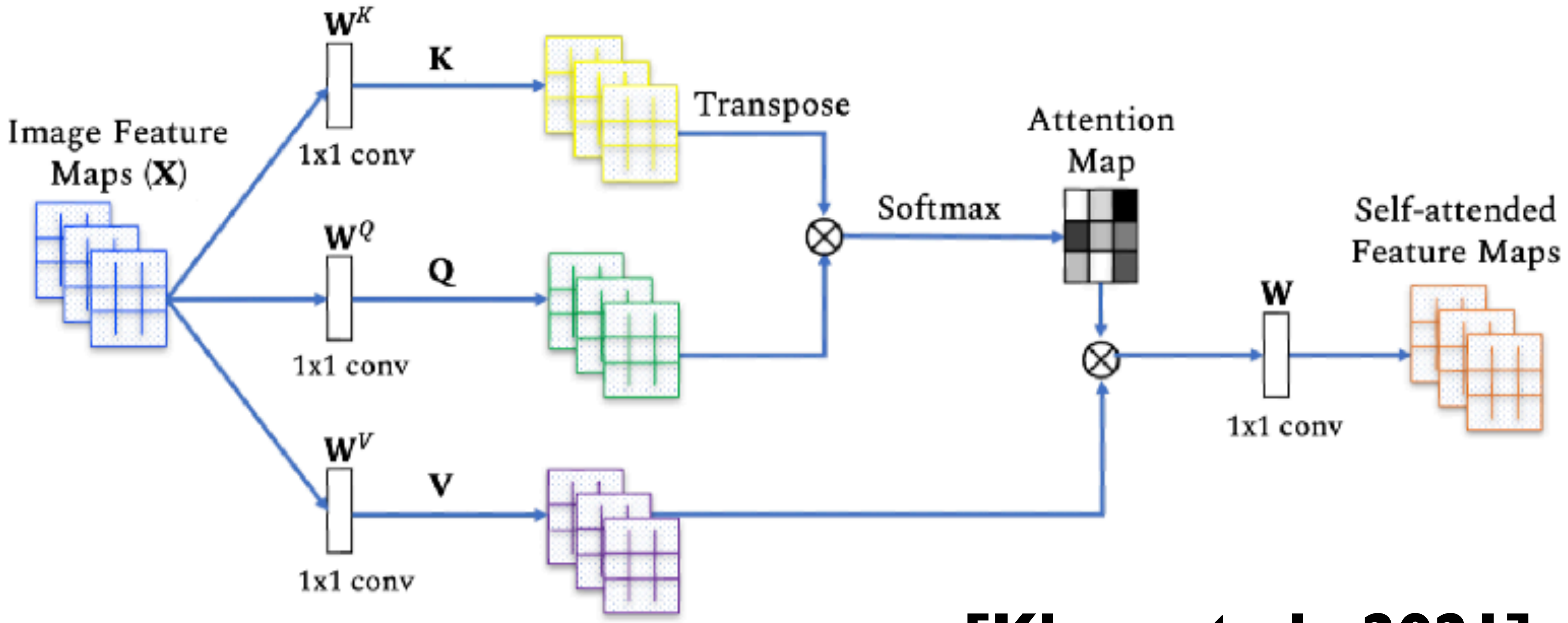

[Khan et al., 2021]

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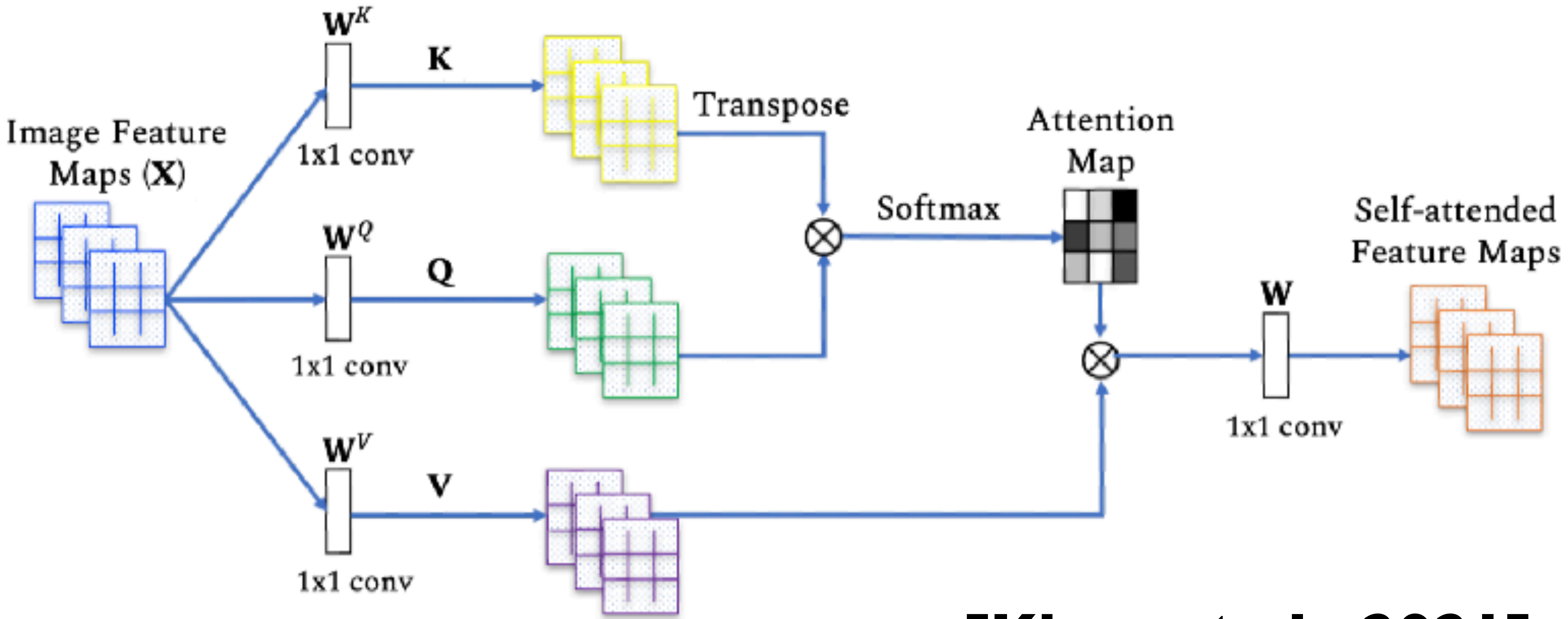

[Khan et al., 2021]

What's next after Transformers?