COMP 3361 Natural Language Processing

Lecture 11: Attention and Transformers

Spring 2025

Many materials from CSE447@UW (Liwei Jiang), COS 484@Princeton, and CS224n@Stanford with special thanks!

Announcements

- Assignment 2 is out, due on April 1.
  - Written questions resemble the types of questions that could appear on your final exam.

Transformers

Attention Is All You Need

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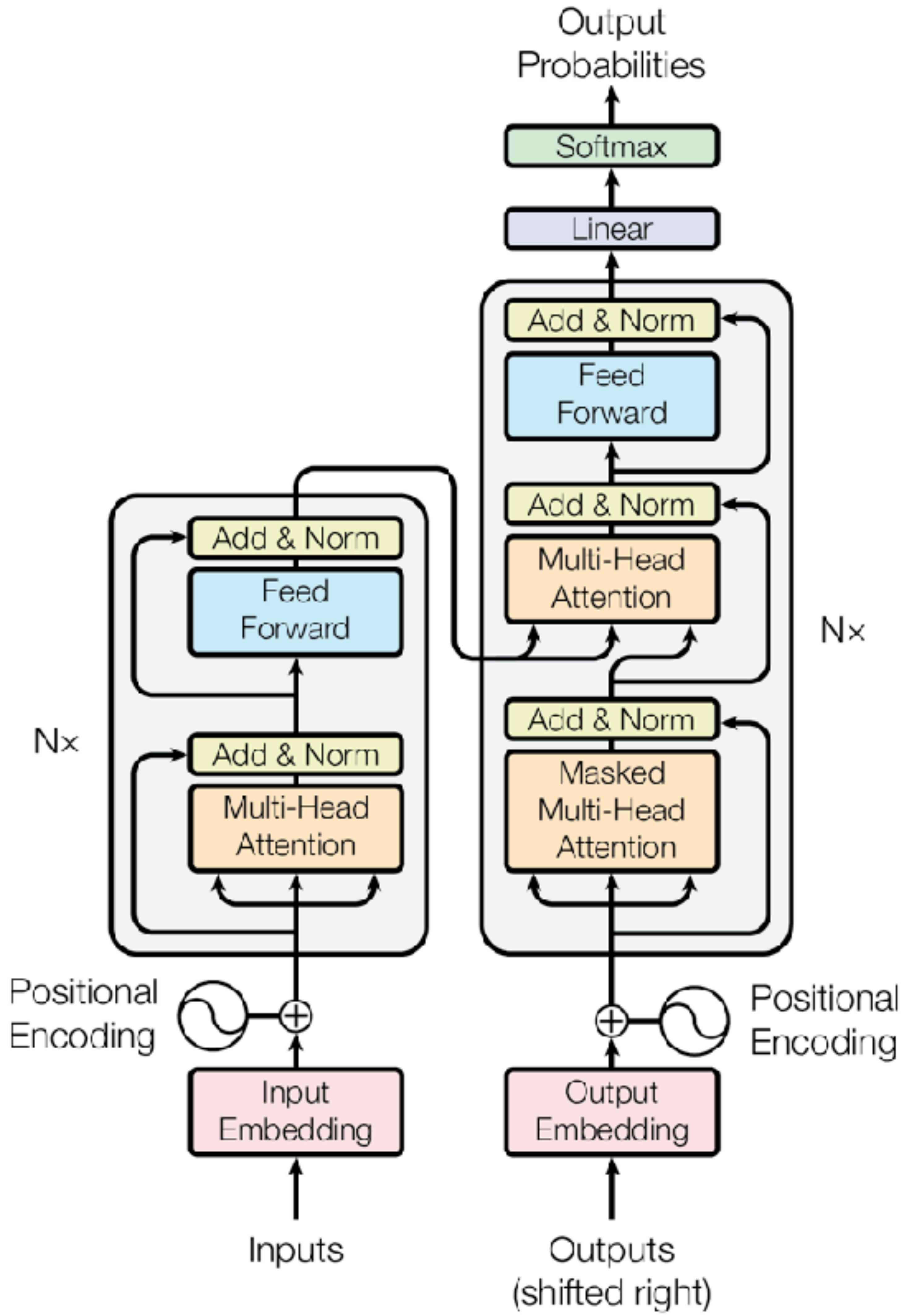
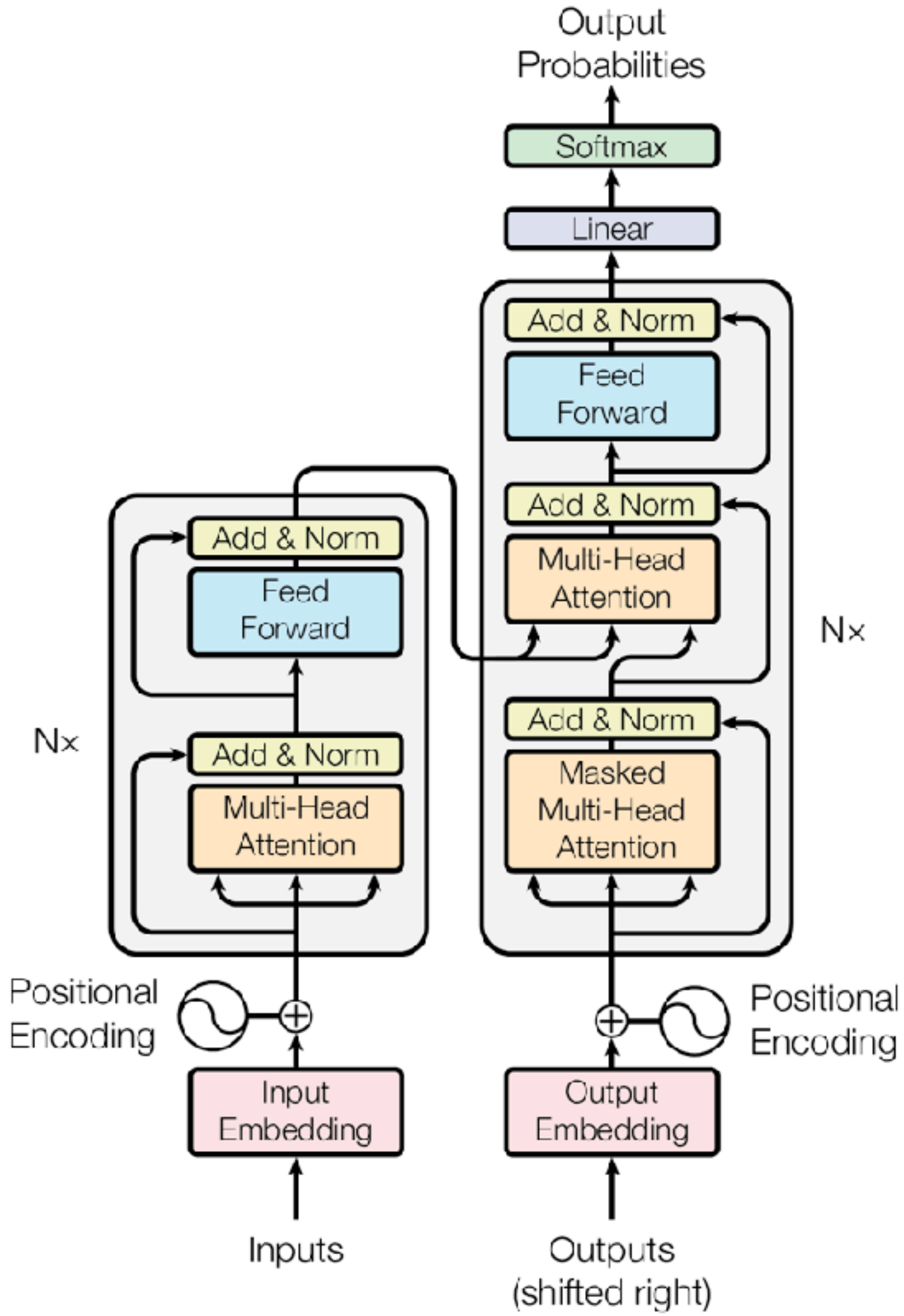
(Vaswani et al., 2017)

Transformer encoder-decoder



- Transformer encoder + Transformer decoder
- First designed and experimented on NMT

Transformer encoder-decoder



- Transformer encoder = a stack of **encoder layers**
- Transformer decoder = a stack of **decoder layers**

Transformer encoder: BERT, RoBERTa, ELECTRA

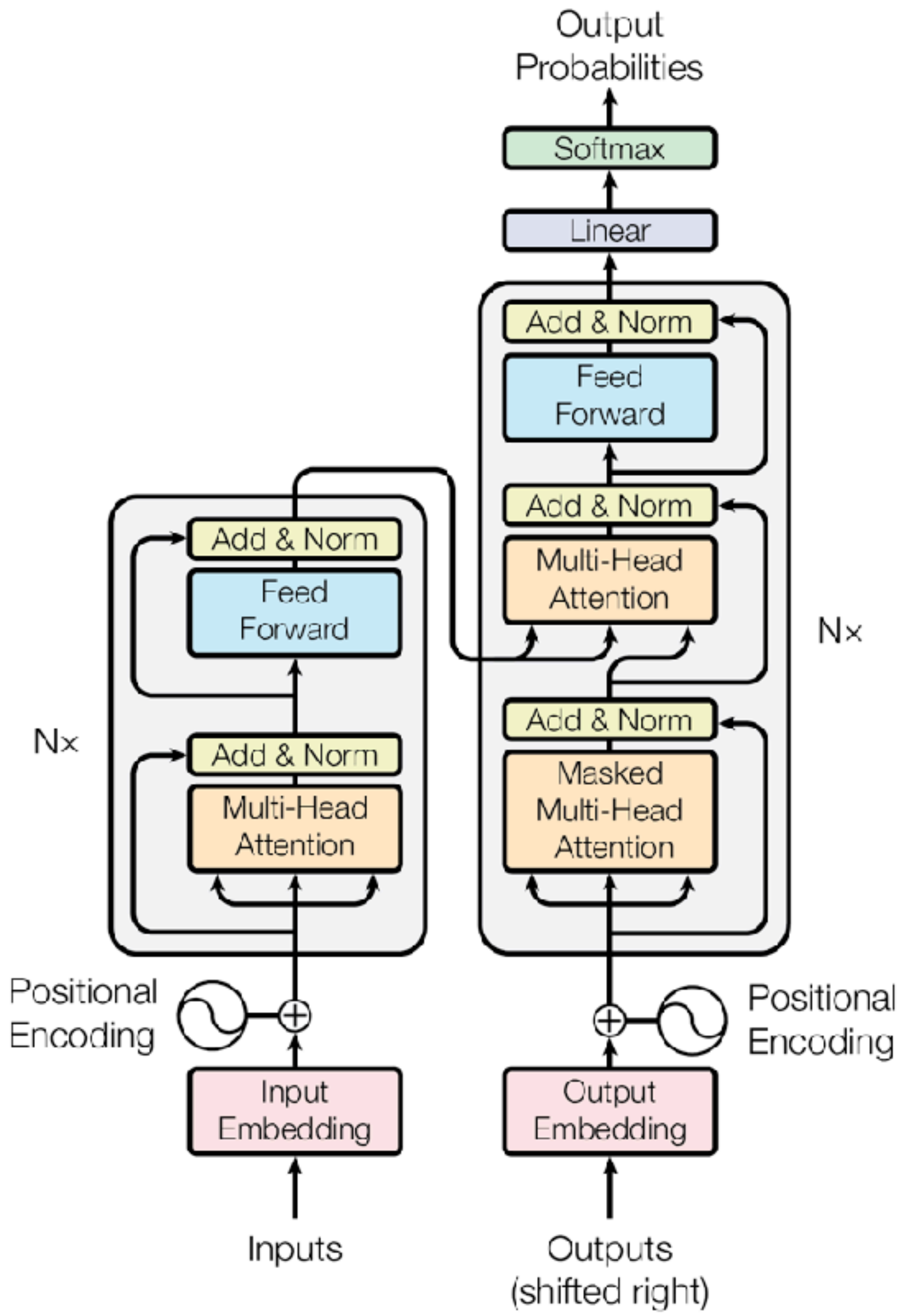
Transformer decoder: GPT-3, ChatGPT, Palm

Transformer encoder-decoder: T5, BART

- Key innovation: **multi-head, self-attention**
- Transformers don't have any recurrence structures!

$$\mathbf{h}_t = f(\mathbf{h}_{t-1}, \mathbf{x}_t) \in \mathbb{R}^h$$

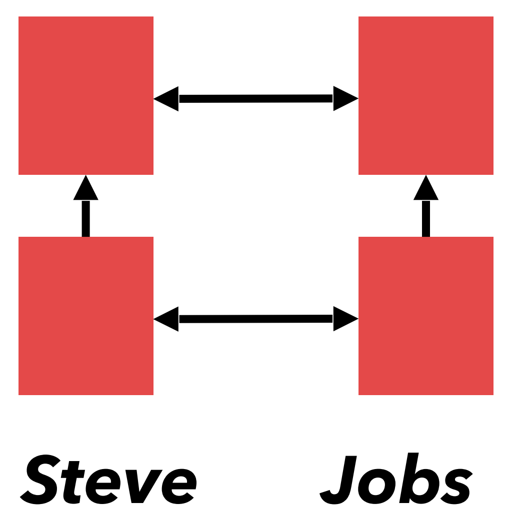
Transformers: roadmap



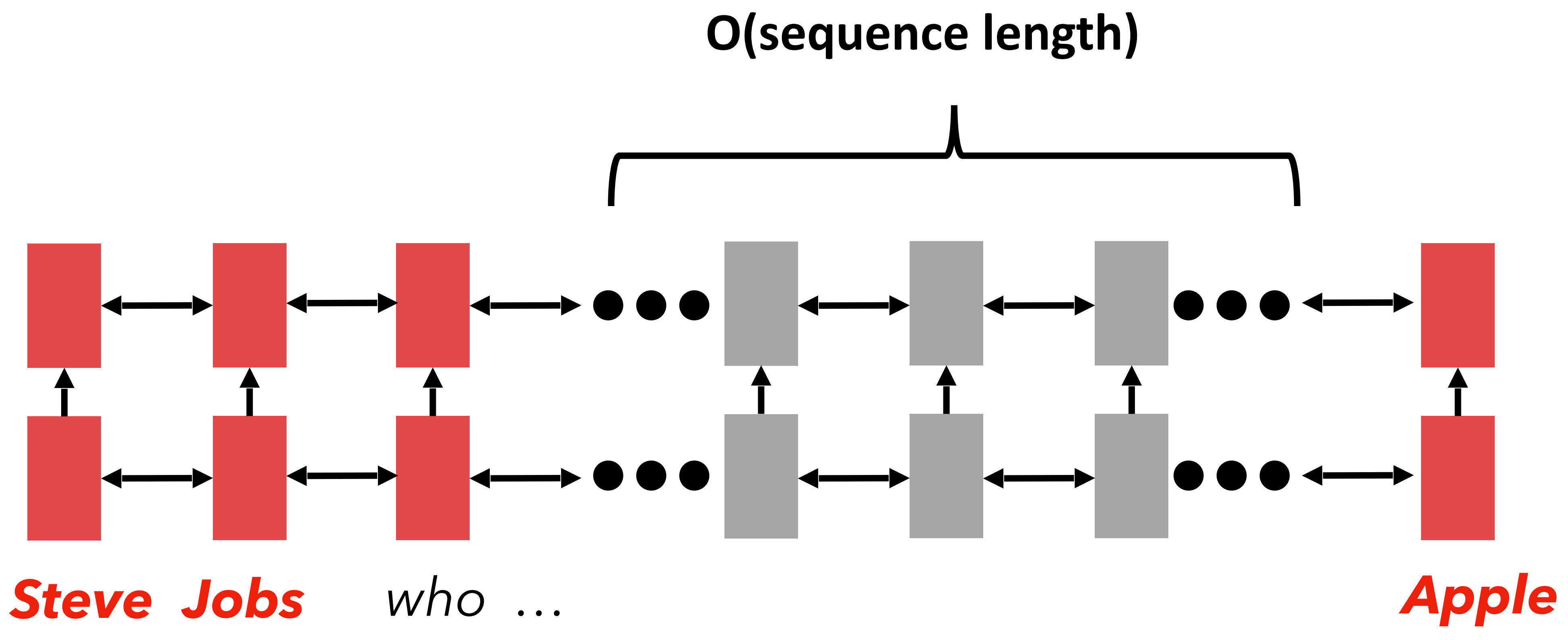
- From attention to self-attention
- From self-attention to multi-head self-attention
- Feedforward layers
- Positional encoding
- Residual connections + layer normalization
- Transformer encoder vs Transformer decoder

Issues with RNNs: Linear Interaction Distance

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



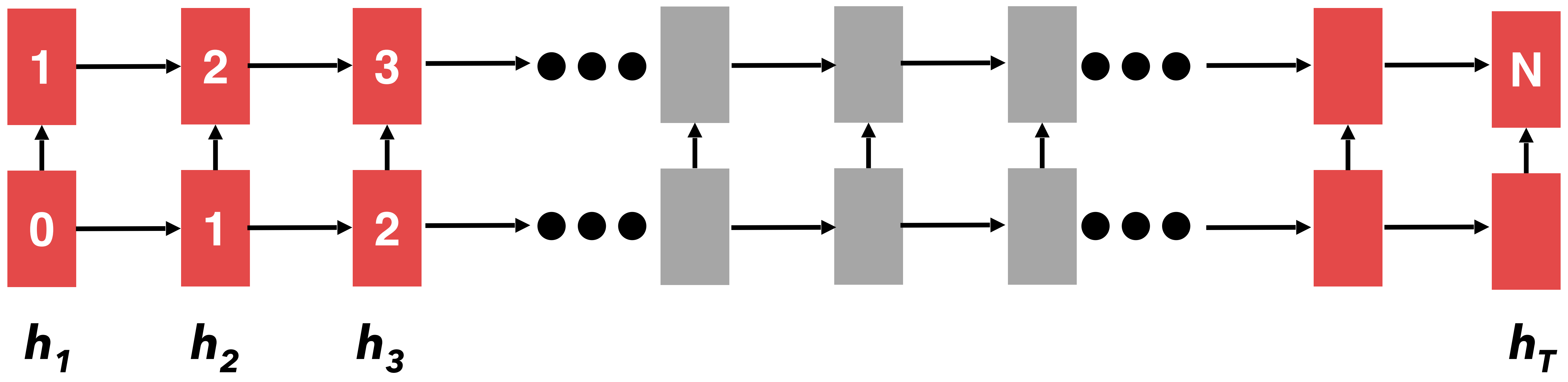
- However, there's the **vanishing gradient problem** for long sequences.
  - The gradients that are used to update the network become extremely small or "vanish" as they are backpropogated from the output layers to the earlier layers.



Failing to capture **long-term dependences**.

Issues with RNNs: Lack of Parallelizability

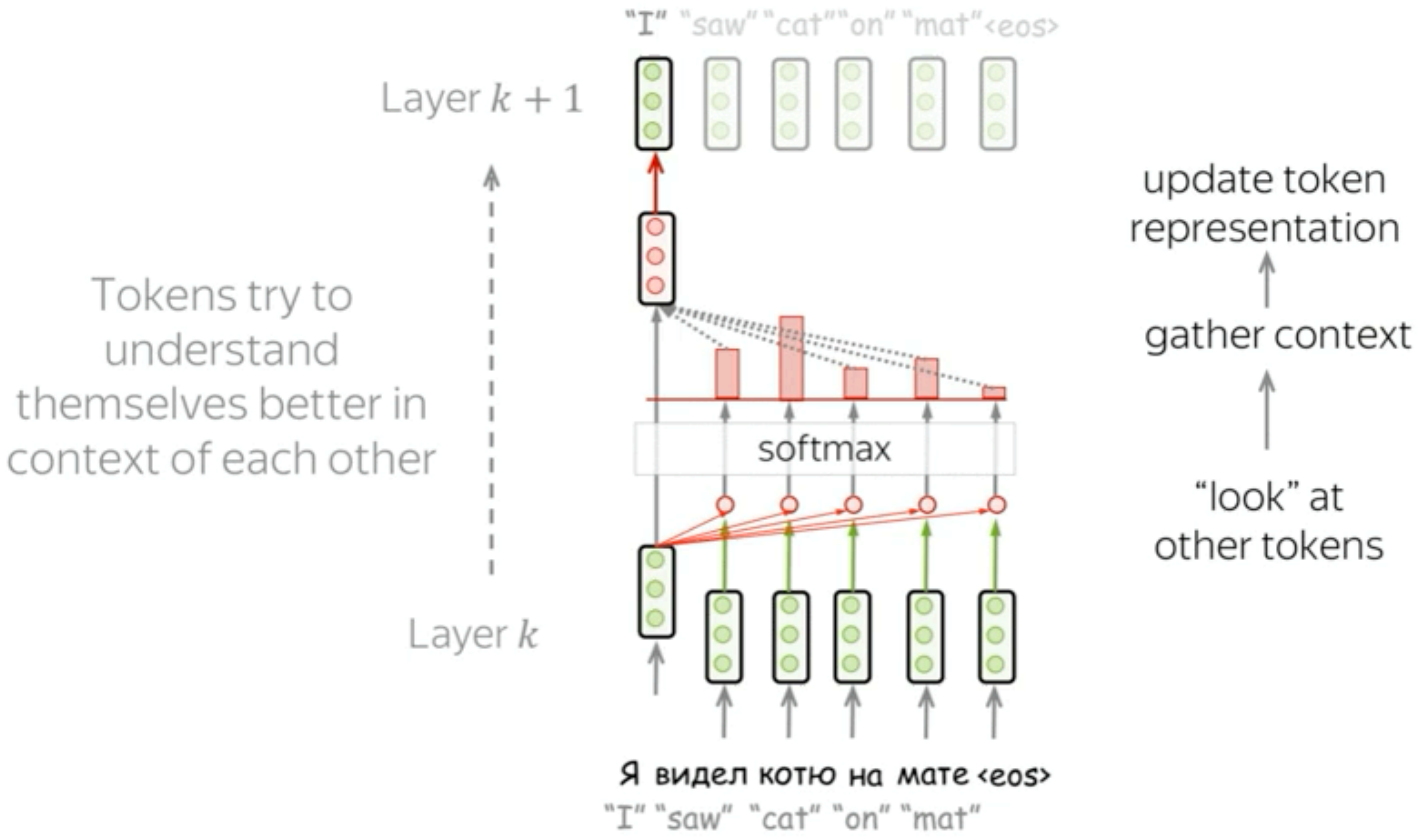
- Forward and backward passes have **O(sequence length)** **unparallelizable** operations
  - GPUs can perform many independent computations (like addition) at once!
  - But future RNN hidden states can't be computed in full before past RNN hidden states have been computed.
  - Training and inference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



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

The New De Facto Method: Attention

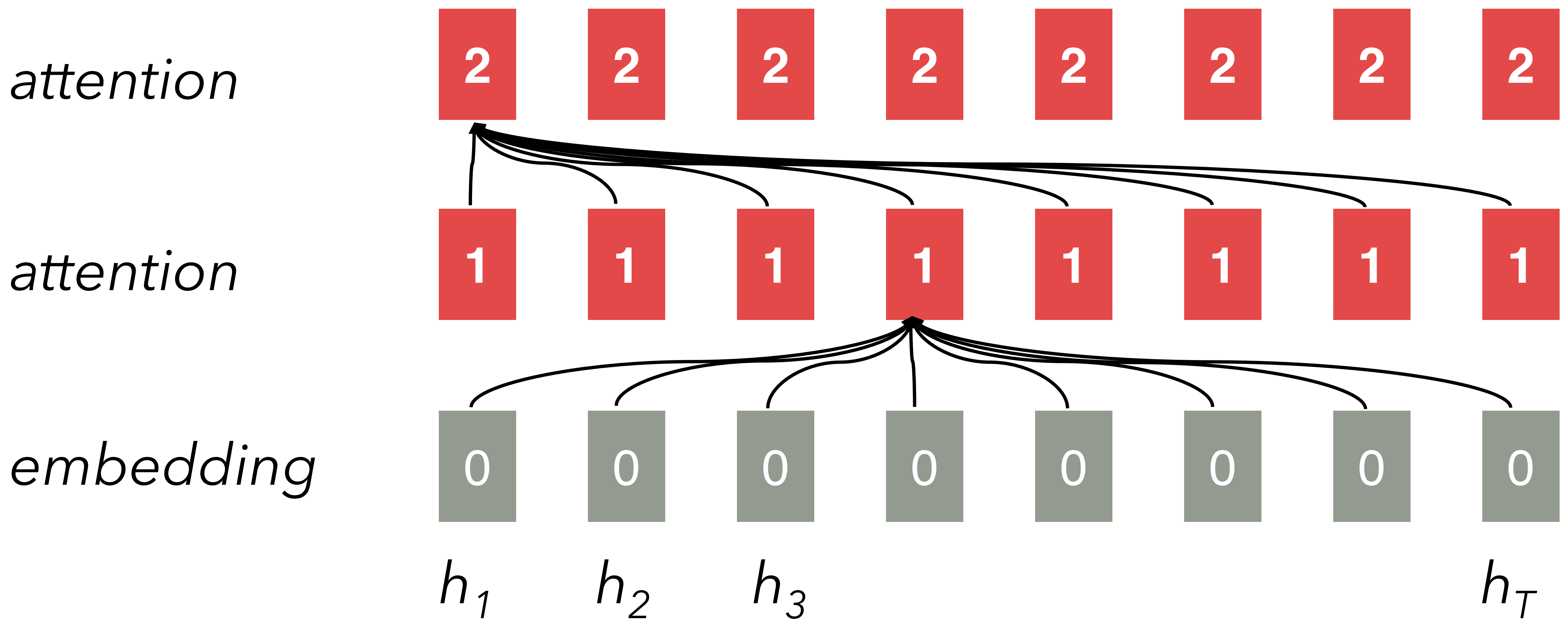
Instead of deciding the next token solely based on the previously seen tokens, **each token will "look at" all input tokens at the same to decide which ones are most important** to decide the next token.



In practice, the actions of all tokens are done in parallel!

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!

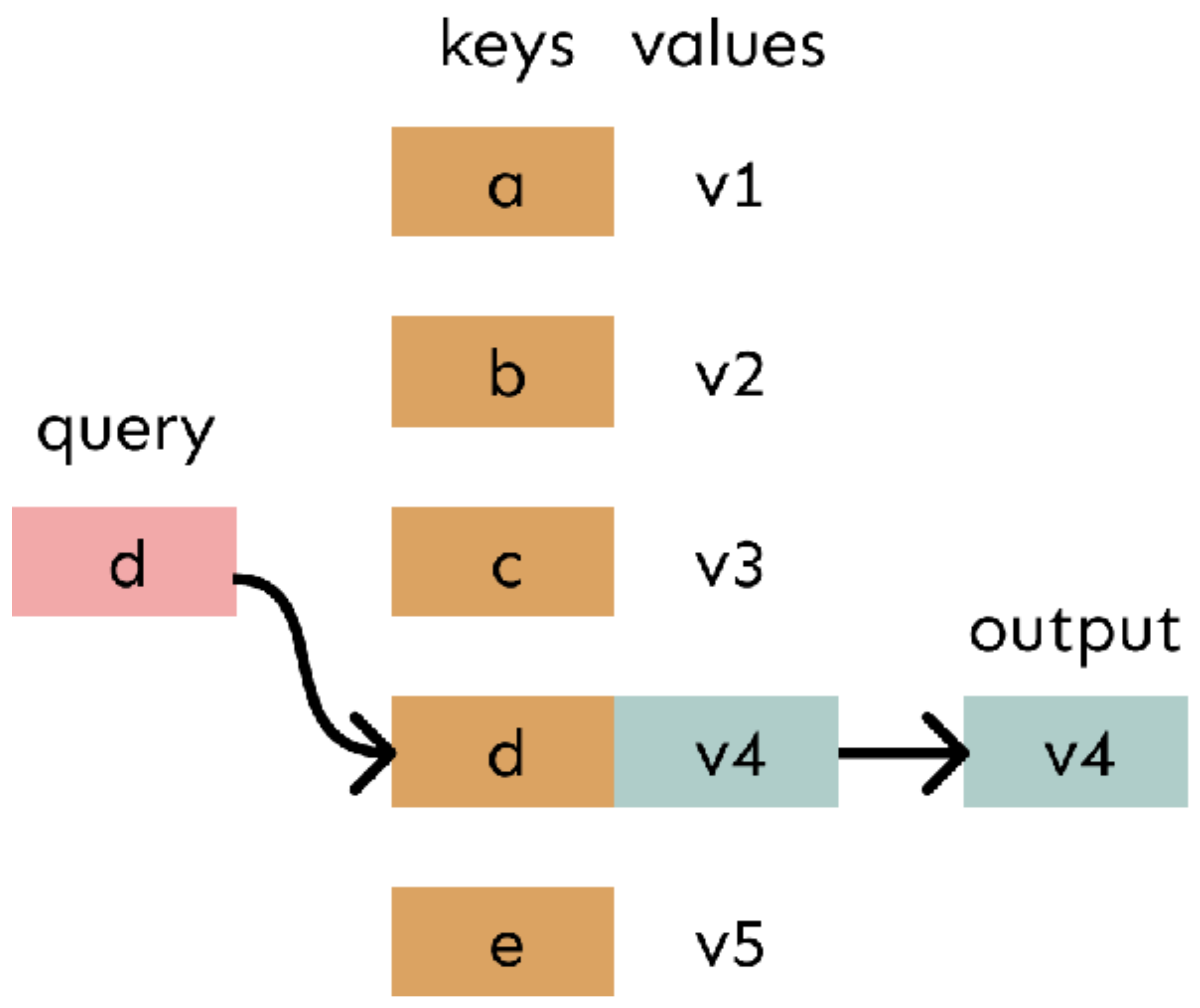


All tokens attend to all tokens in previous layer; most arrows here are omitted

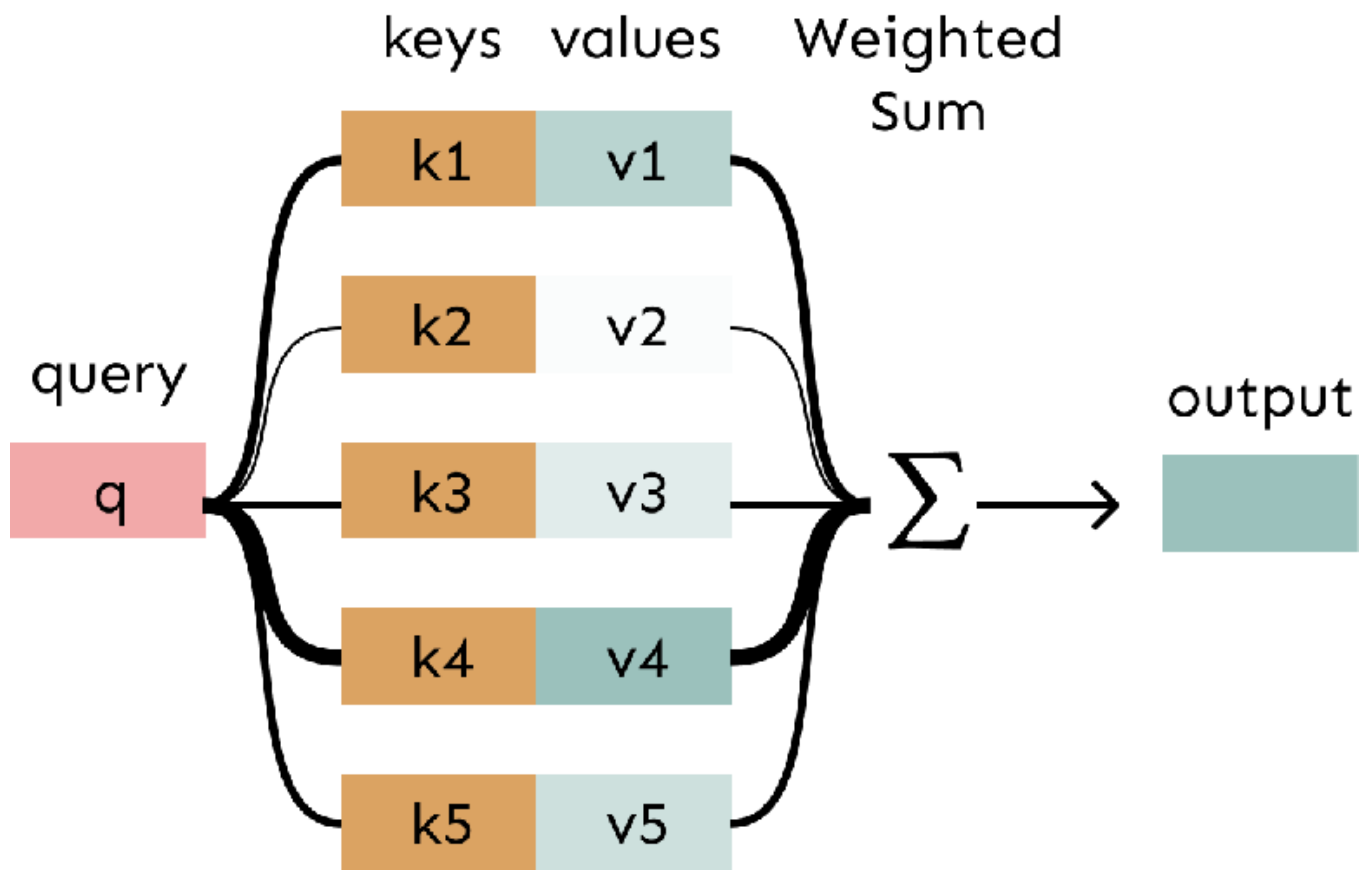
Attention as a soft, averaging lookup table

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

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

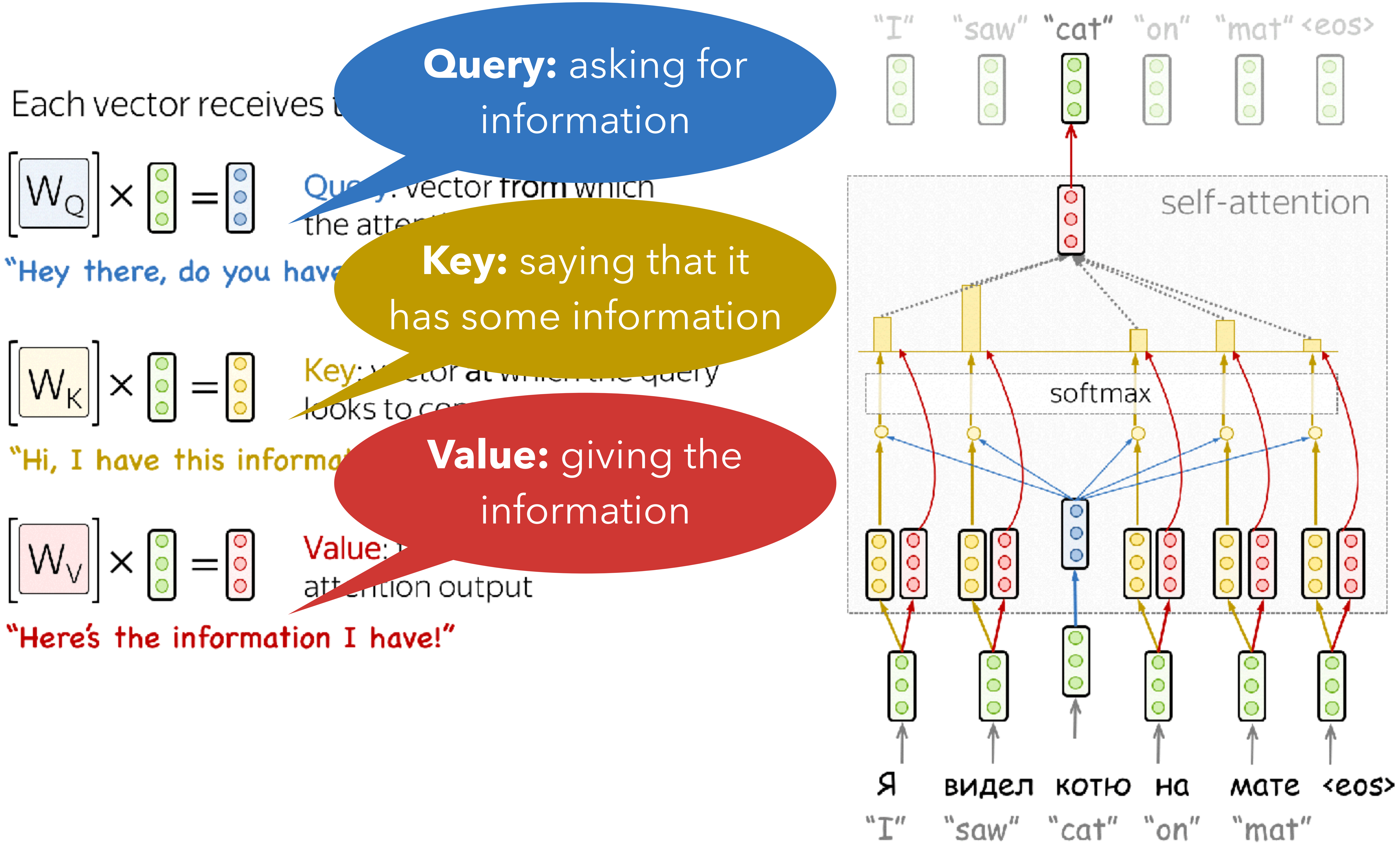


In **attention**, the **query** matches all **keys** *softly*, to a weight between 0 and 1. The keys' **values** are multiplied by the weights and summed.

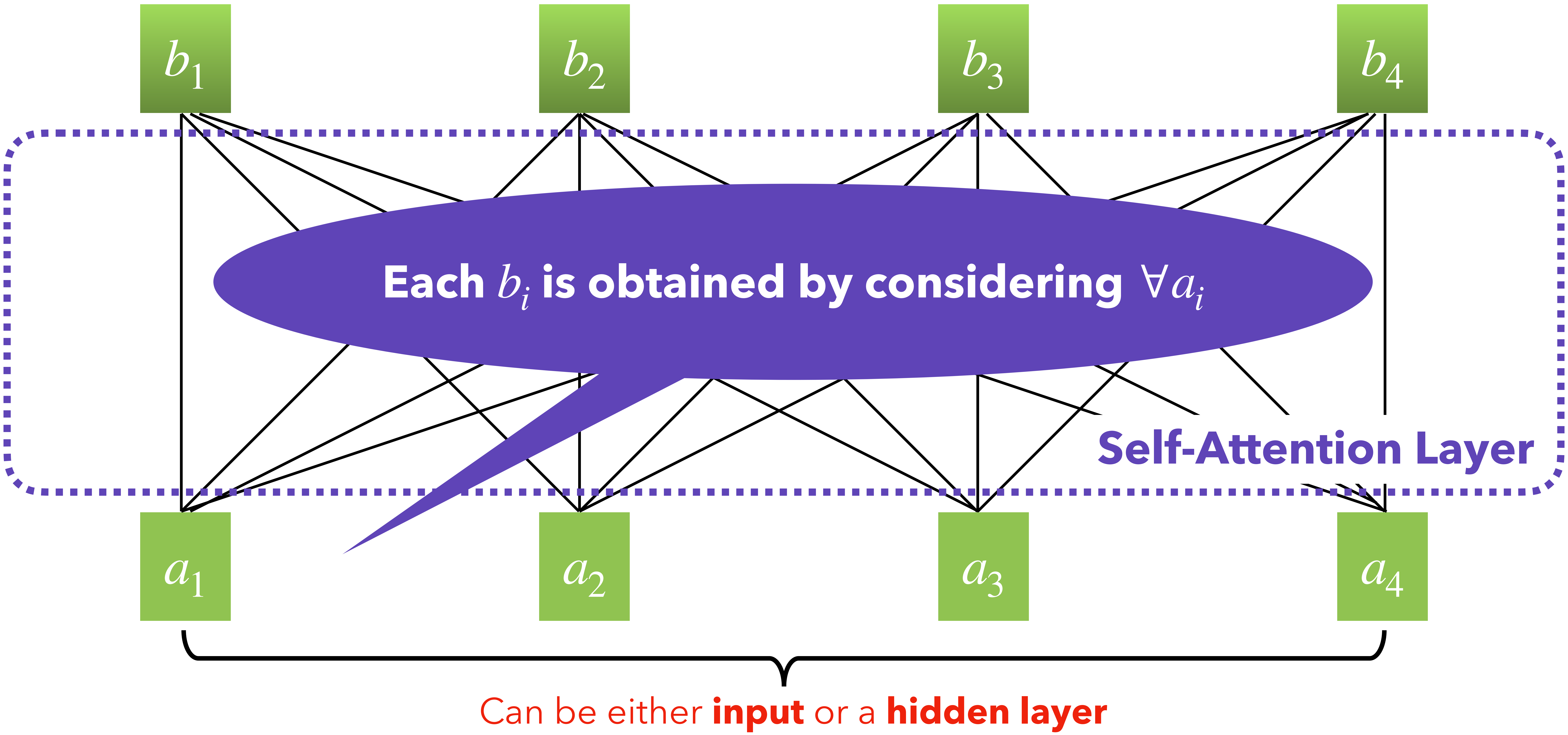


Self-Attention: Basic Concepts

[Lena Viota Blog]



Self-Attention: Walk-through



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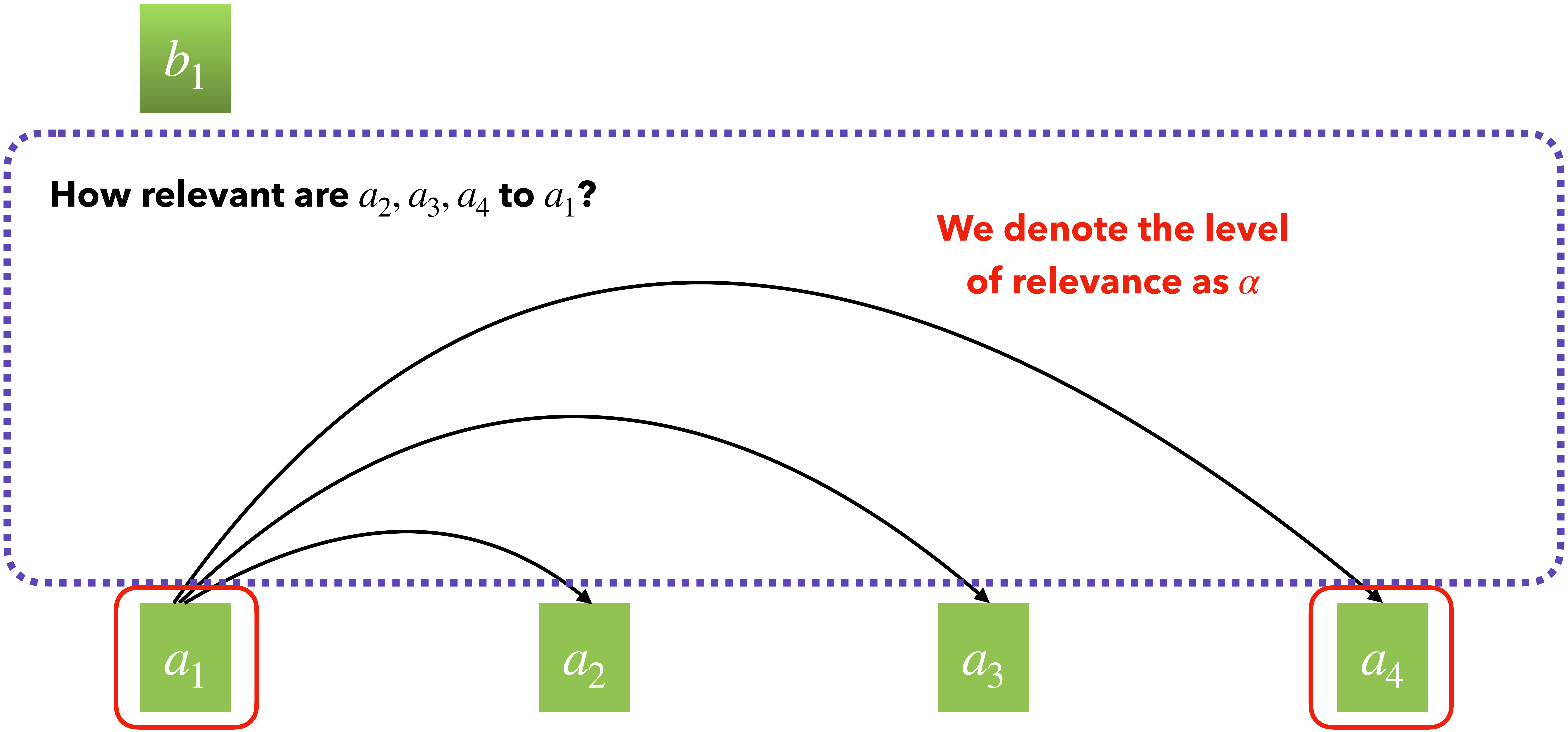
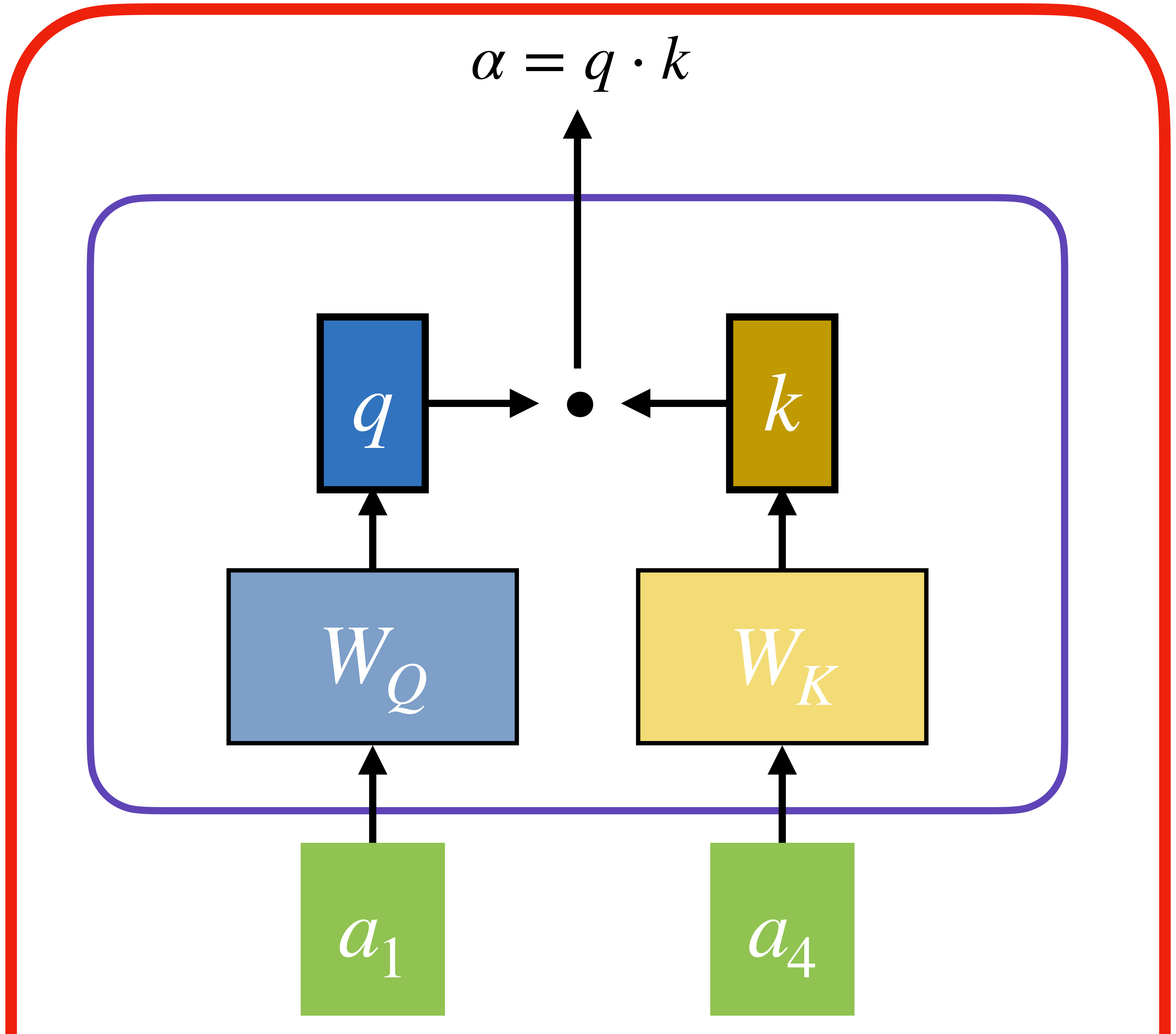
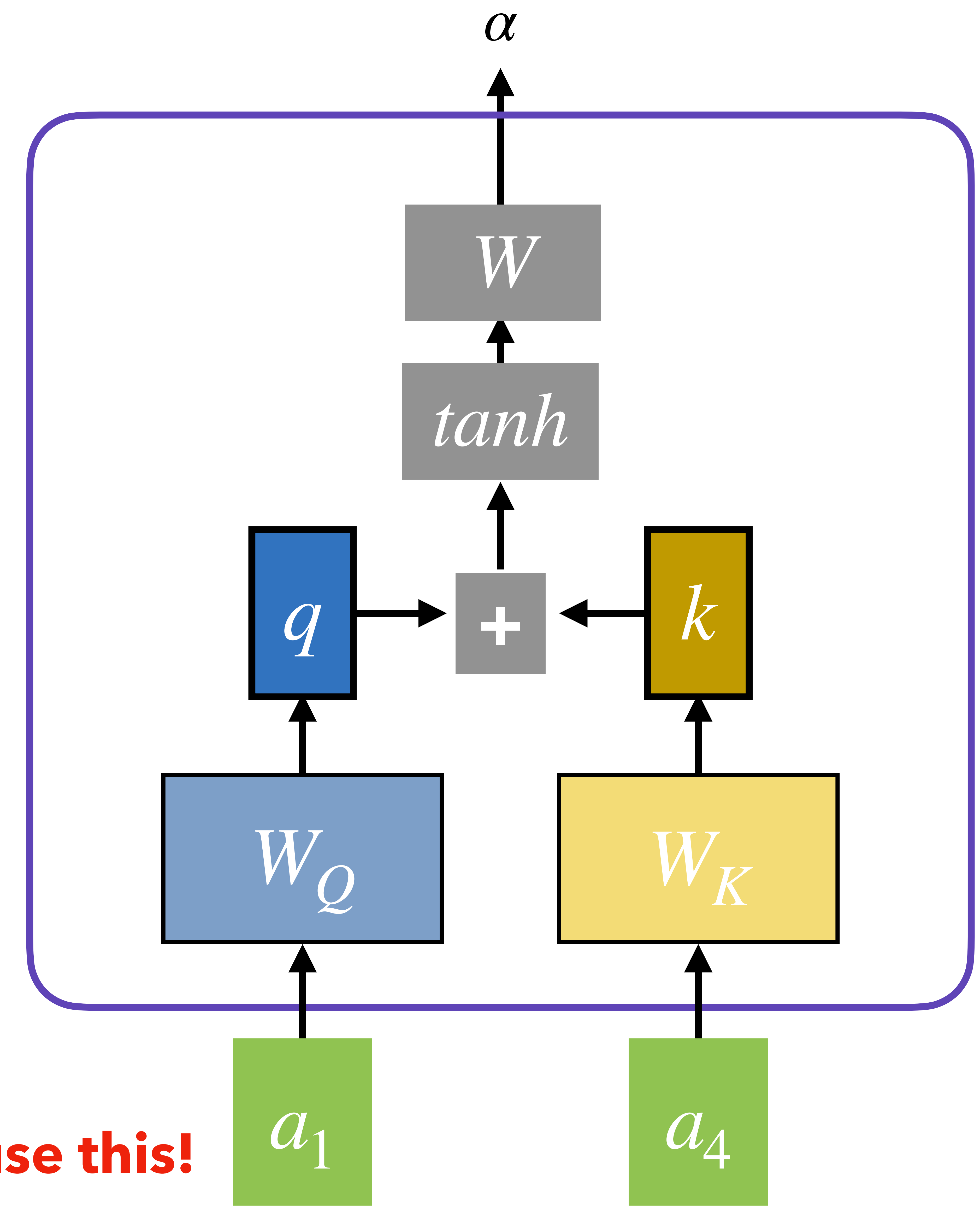


How to compute α?



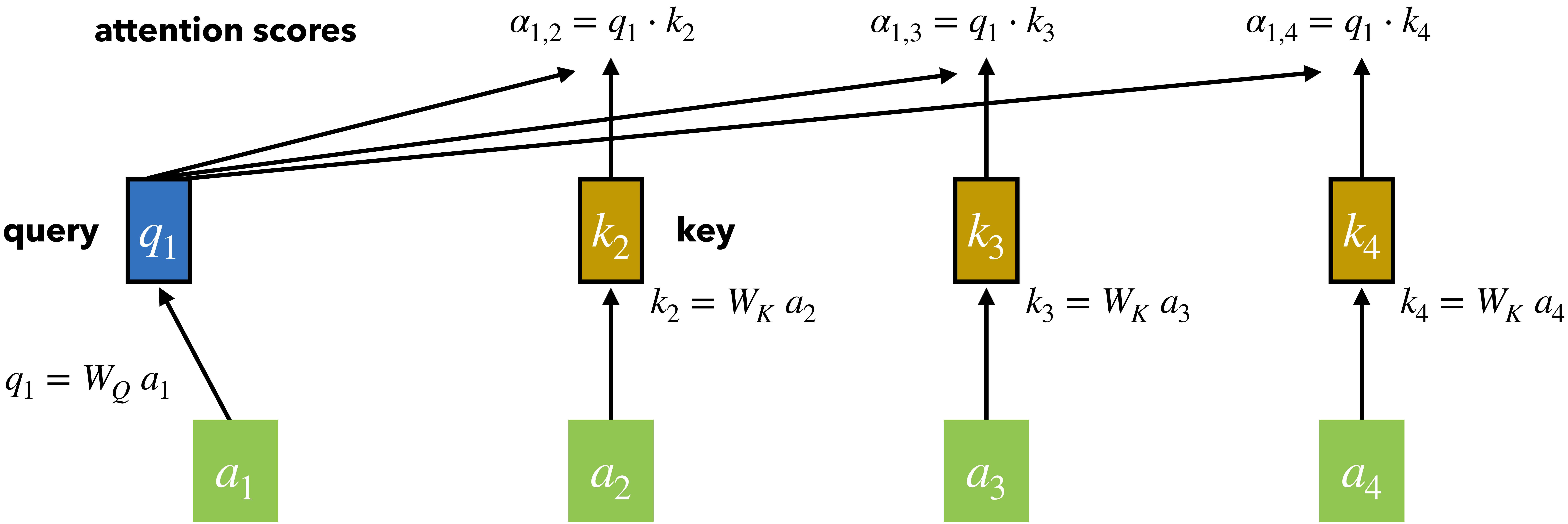
Method 1 **(most common): Dot product**

We'll use this!

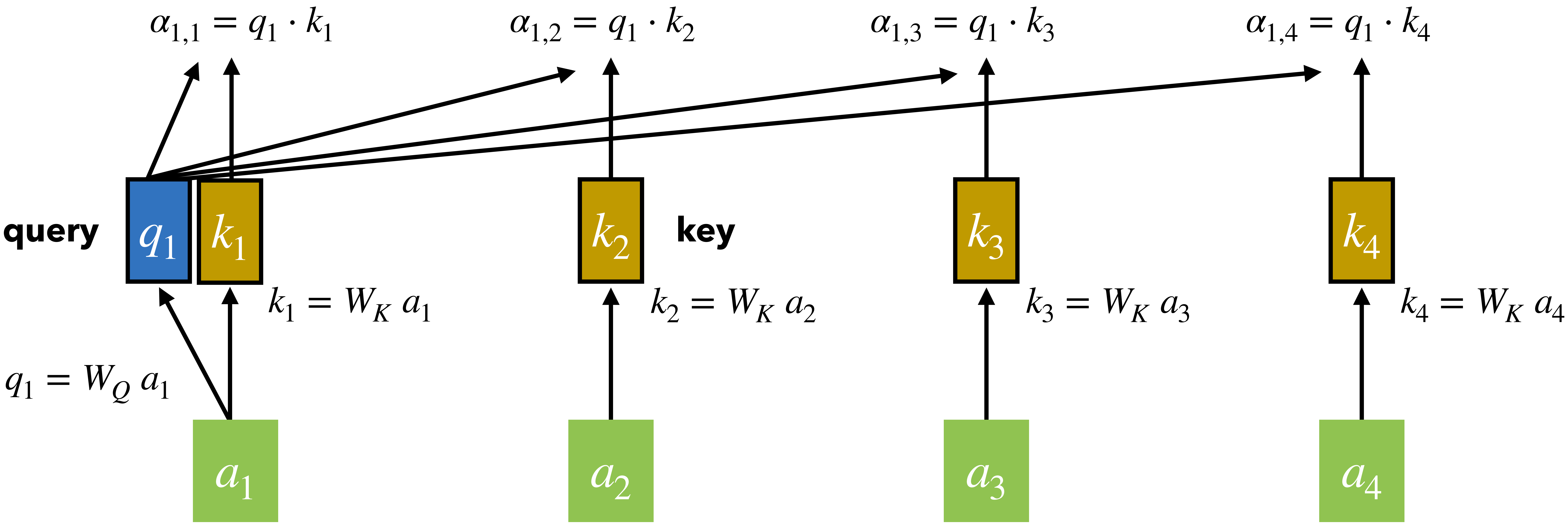


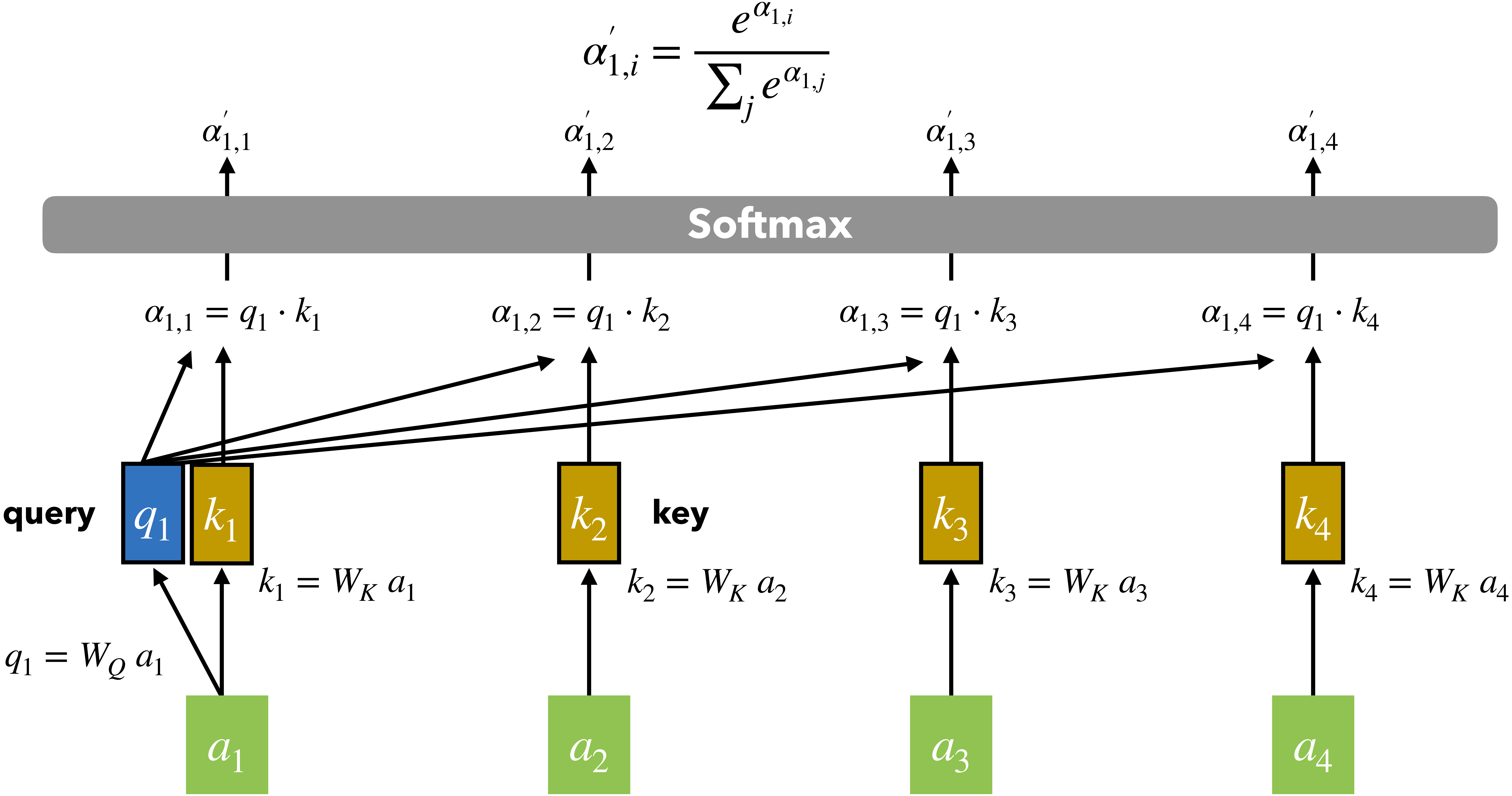
Method 2: **Additive**

Self-Attention: Walk-through



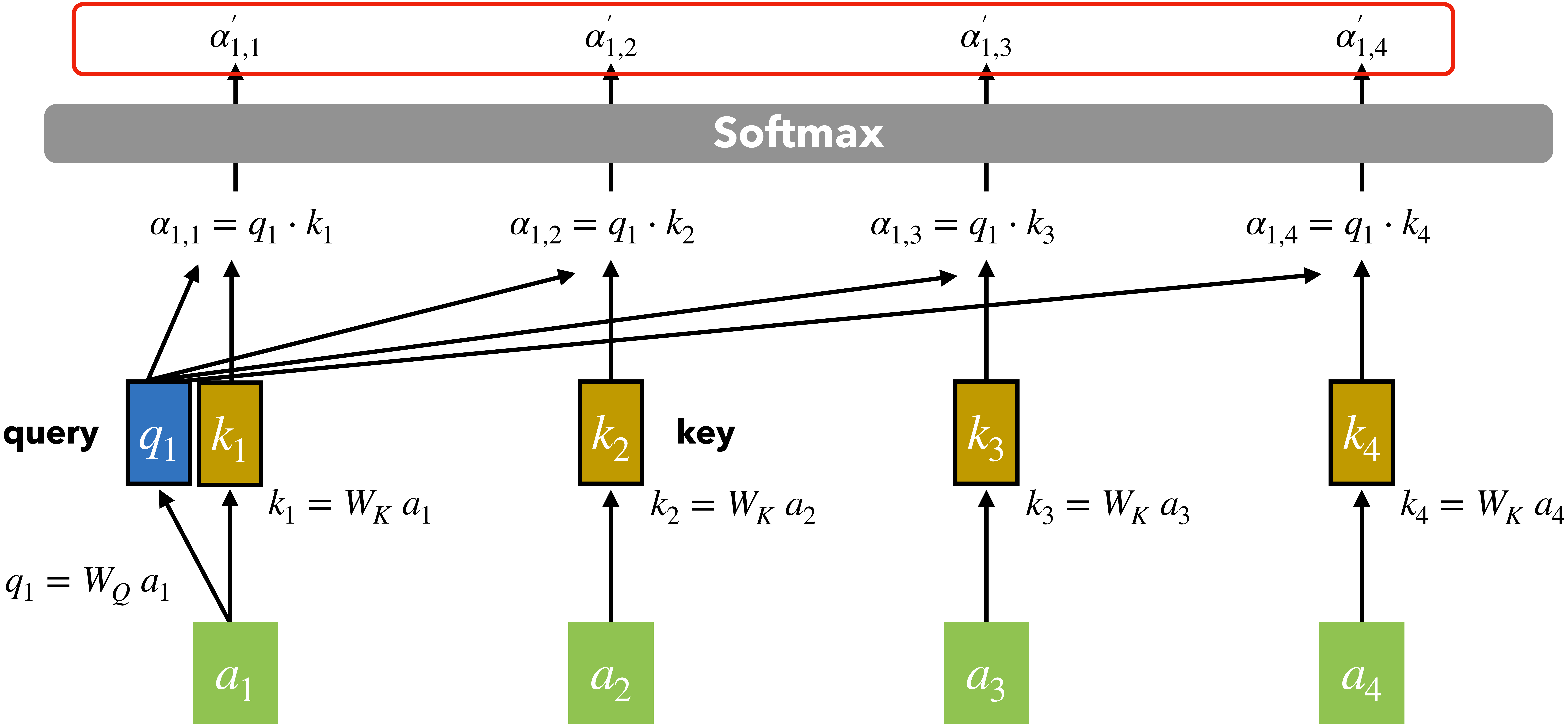
Self-Attention: Walk-through




$\alpha'_{1,i} = \frac{e^{\alpha_{1,i}}}{\sum_j e^{\alpha_{1,j}}}$
$\alpha'_{1,1}$
$\alpha'_{1,2}$
$\alpha'_{1,3}$
$\alpha'_{1,4}$
Softmax
$\alpha_{1,1} = q_1 \cdot k_1$
$\alpha_{1,2} = q_1 \cdot k_2$
$\alpha_{1,3} = q_1 \cdot k_3$
$\alpha_{1,4} = q_1 \cdot k_4$
query
q_1
k_1
k_2
key
k_3
k_4
$k_1 = W_K\, a_1$
$k_2 = W_K\, a_2$
$k_3 = W_K\, a_3$
$k_4 = W_K\, a_4$
$q_1 = W_Q\, a_1$
a_1
a_2
a_3
a_4

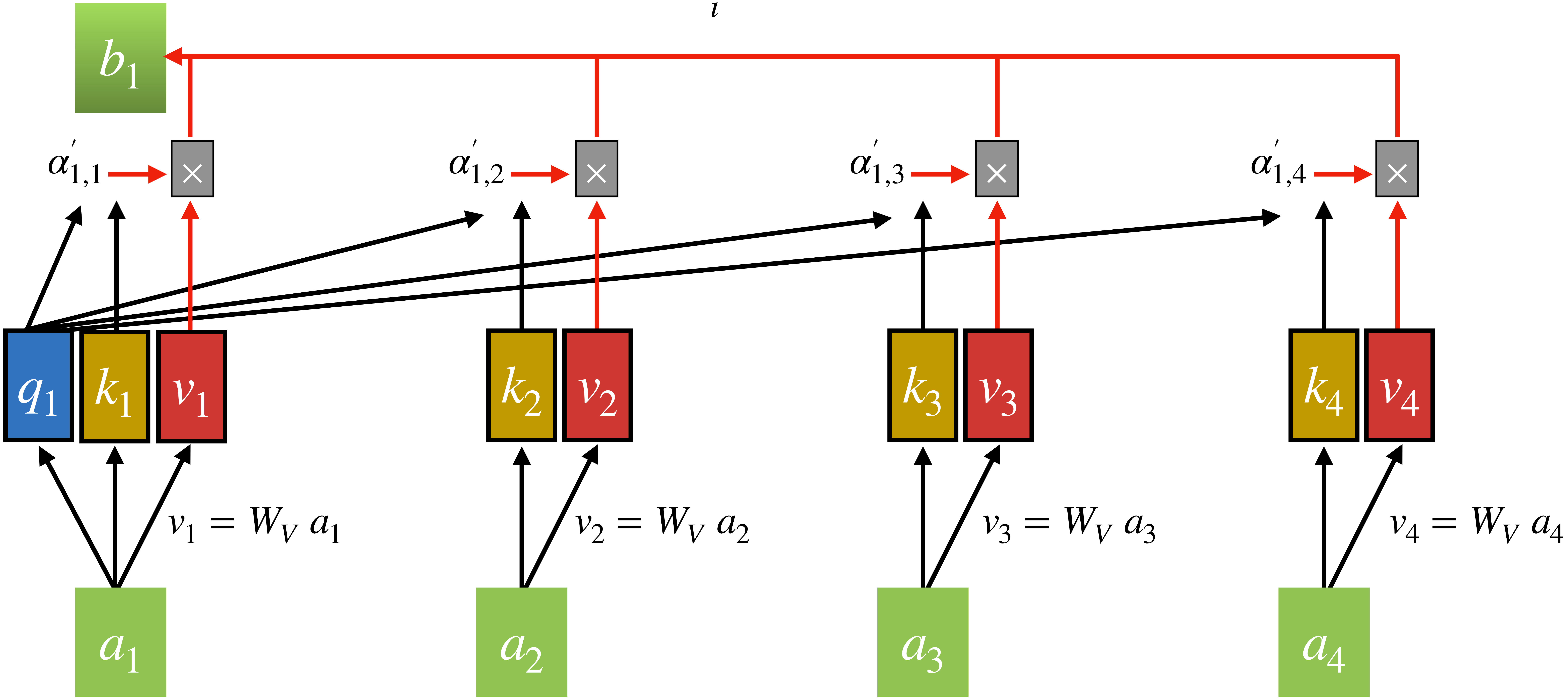
Denote how relevant each token are to a_1!

Use attention scores to extract information



Use attention scores to extract information

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



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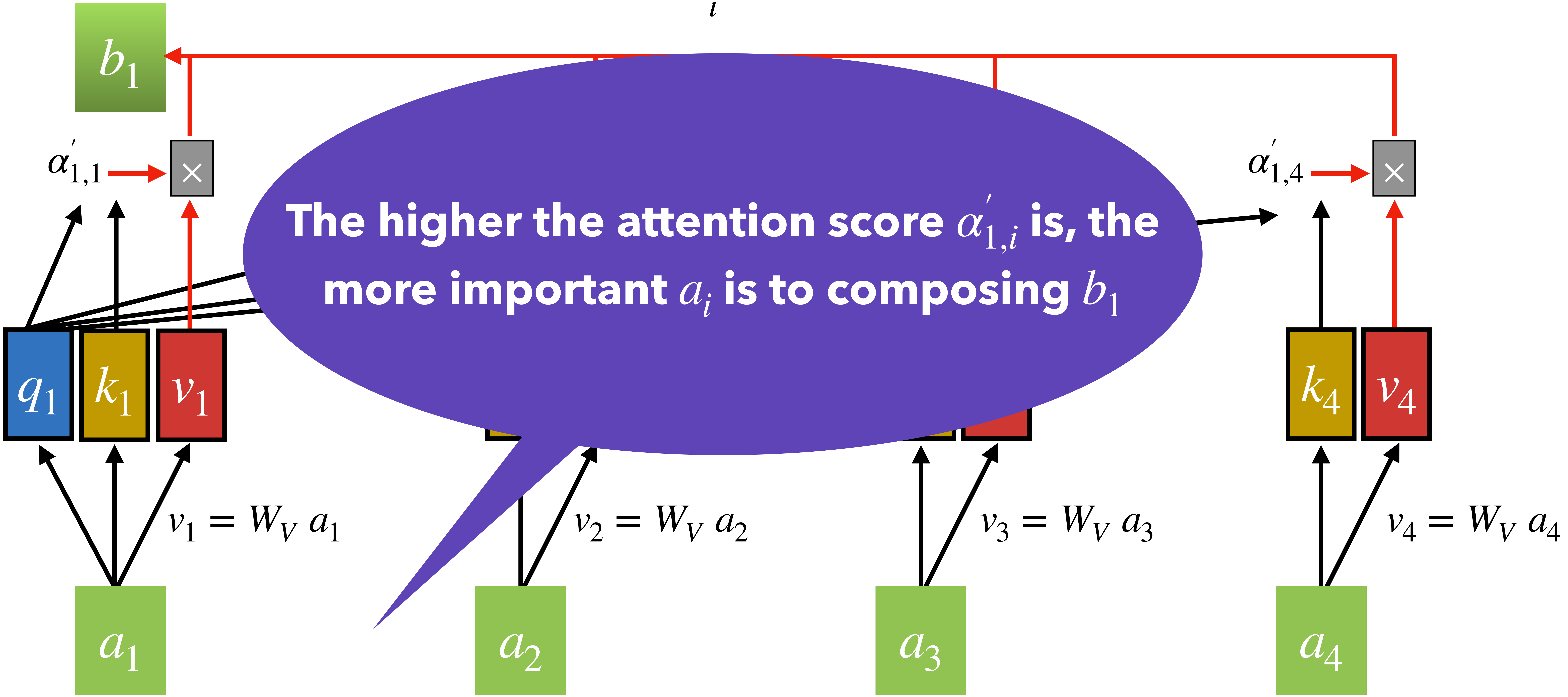
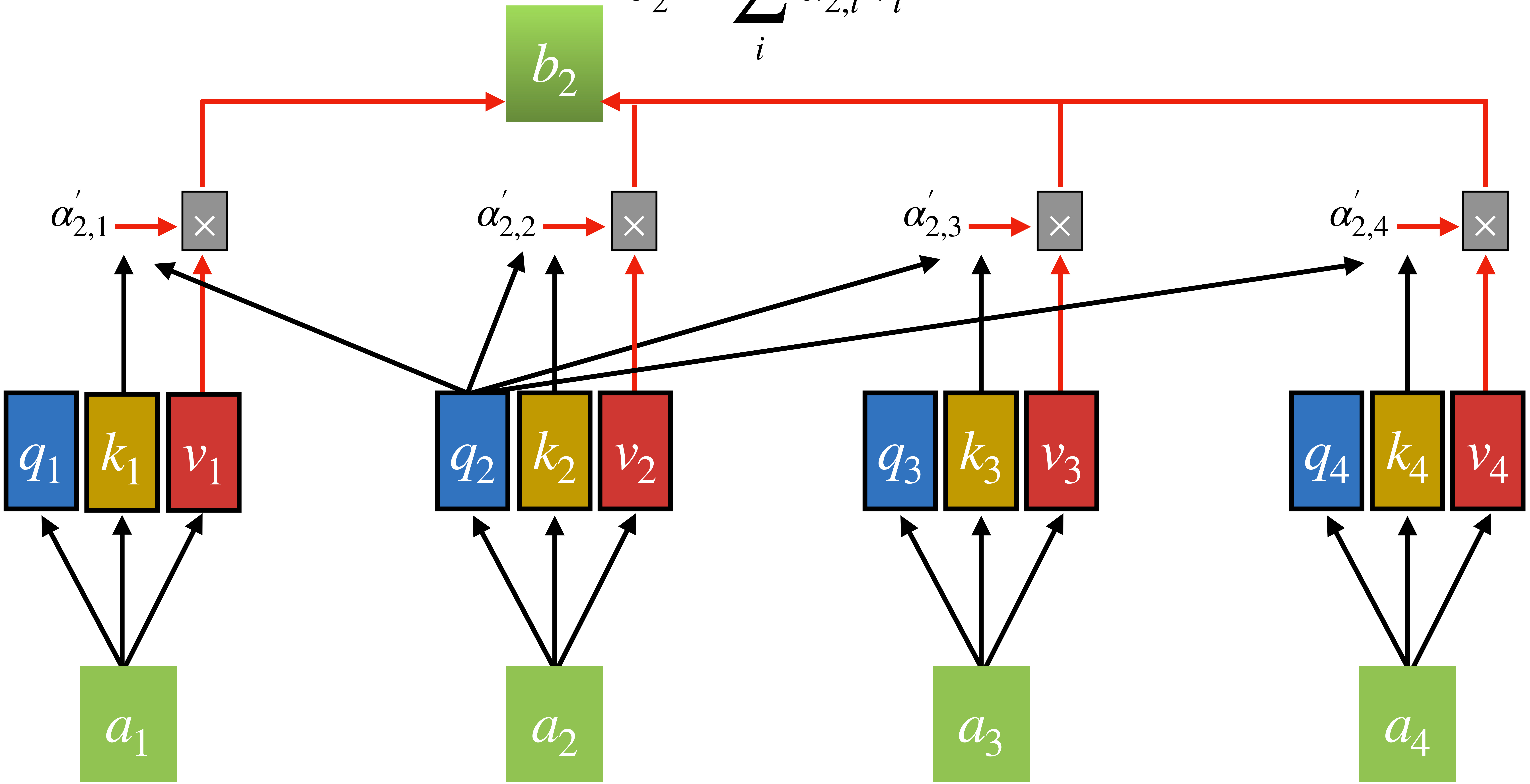


Repeat the same calculation for all a_i to obtain b_i

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



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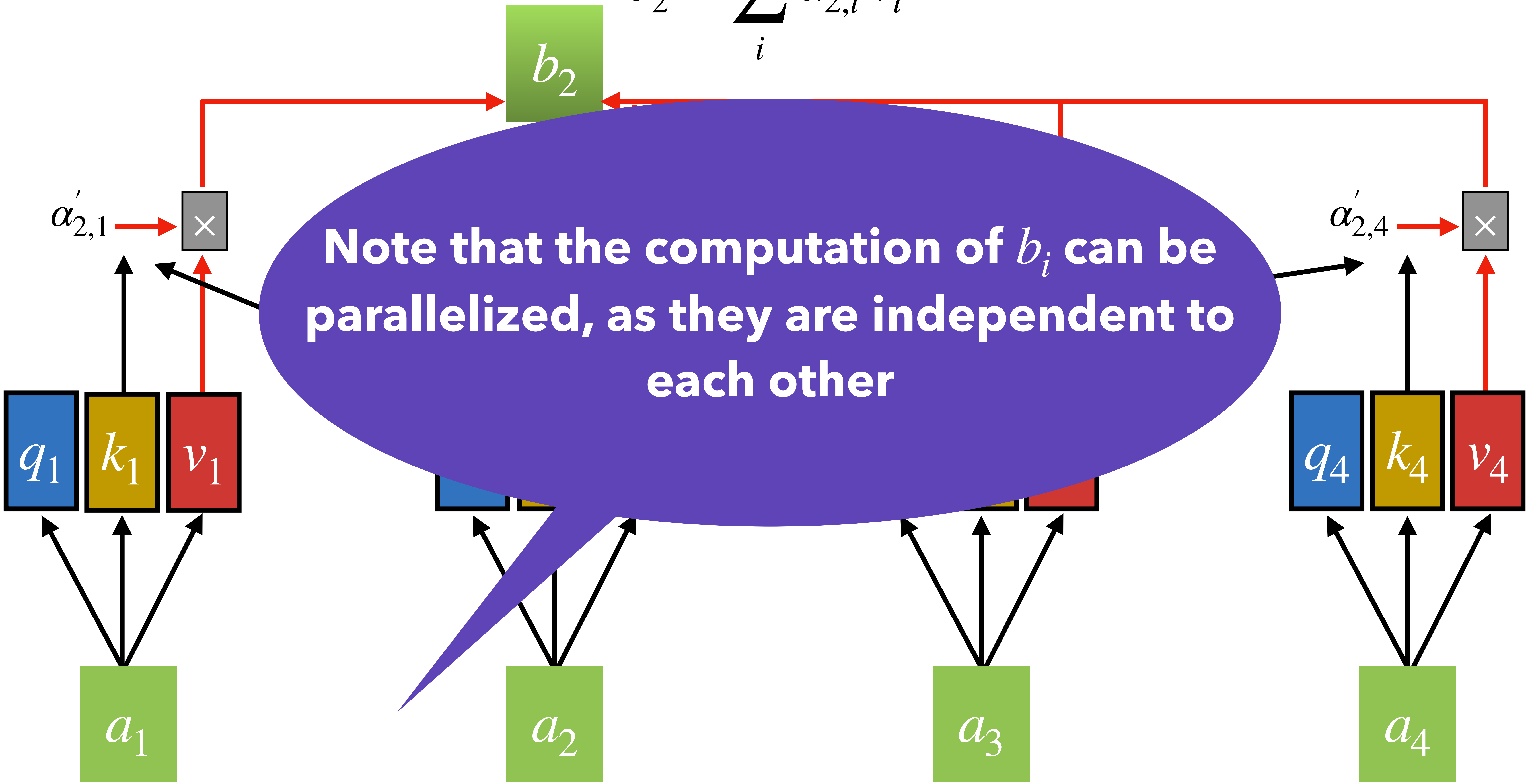
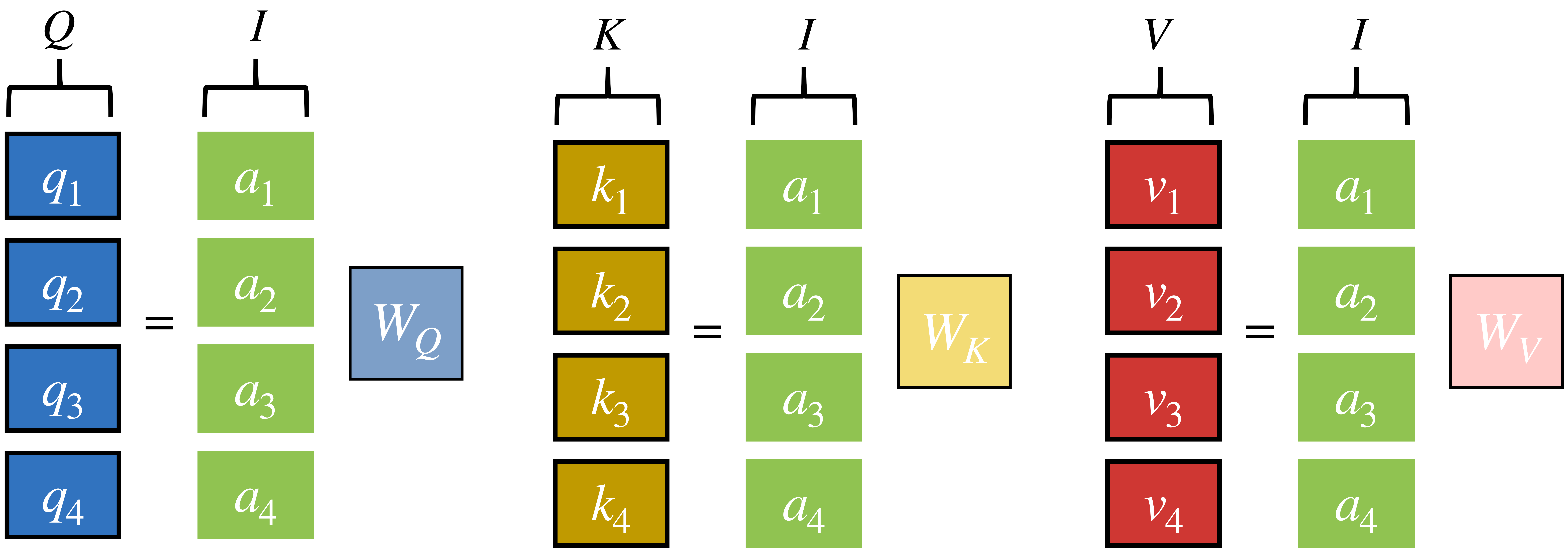
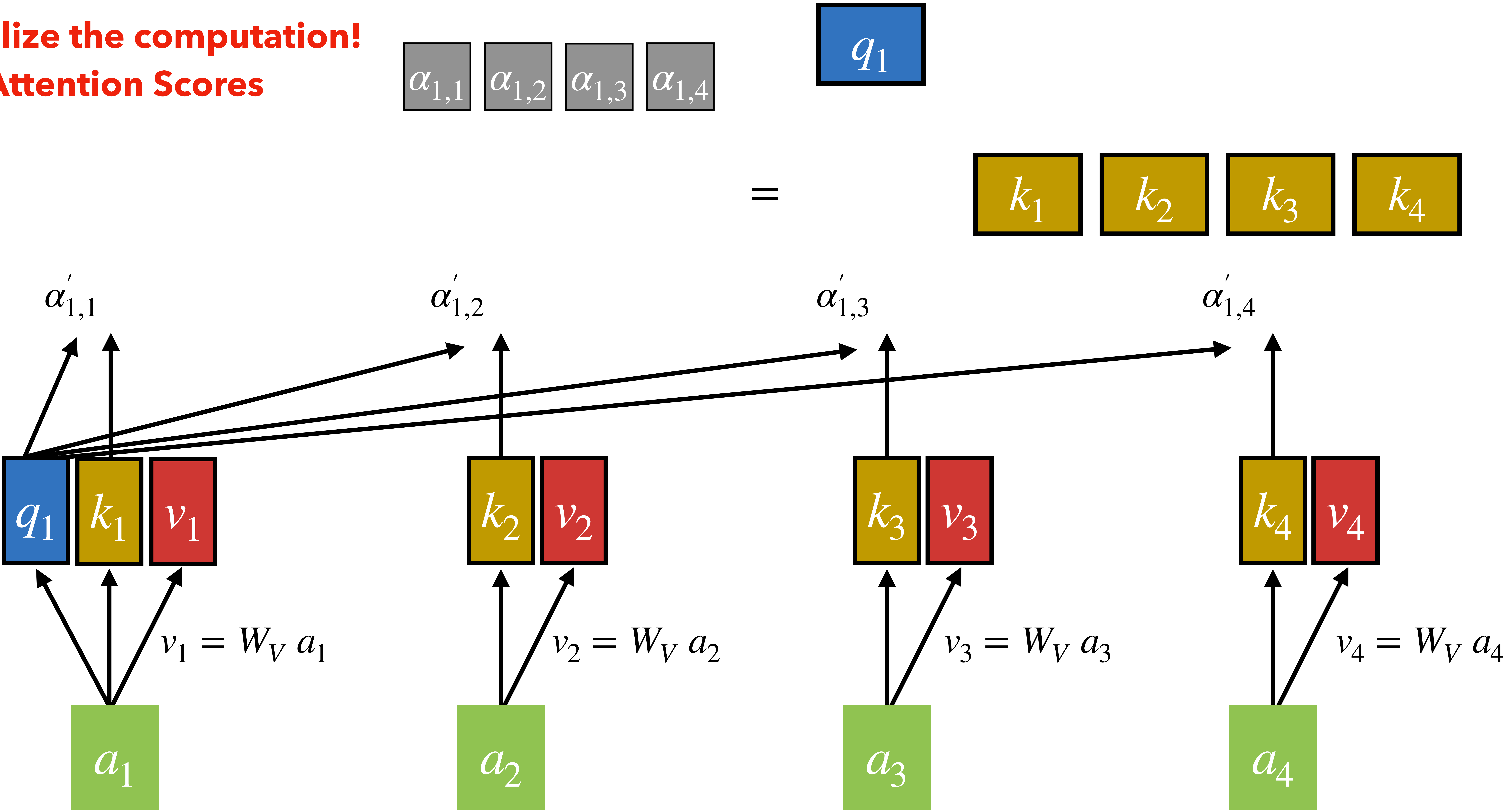


Parallelize the computation!
QKV

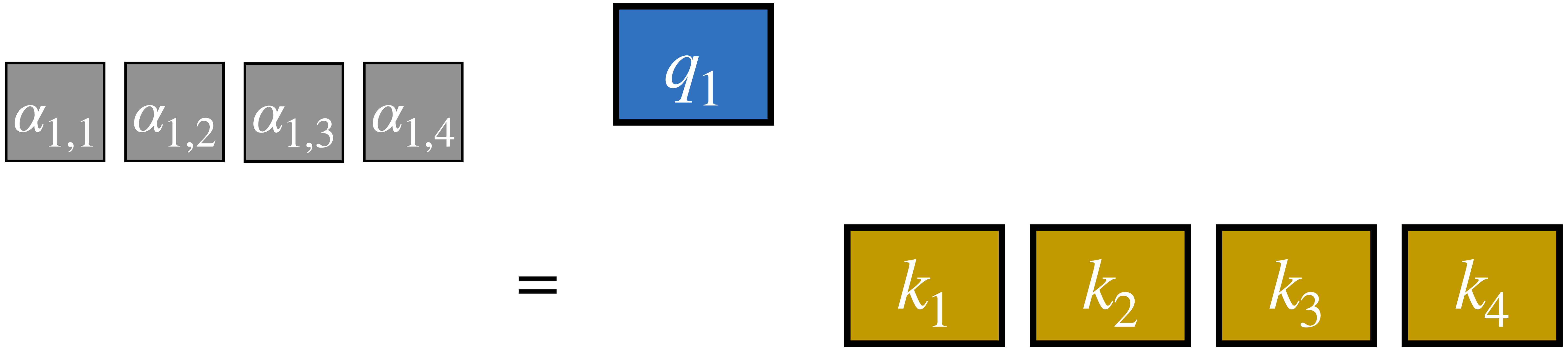


Parallelize the computation!
Attention Scores



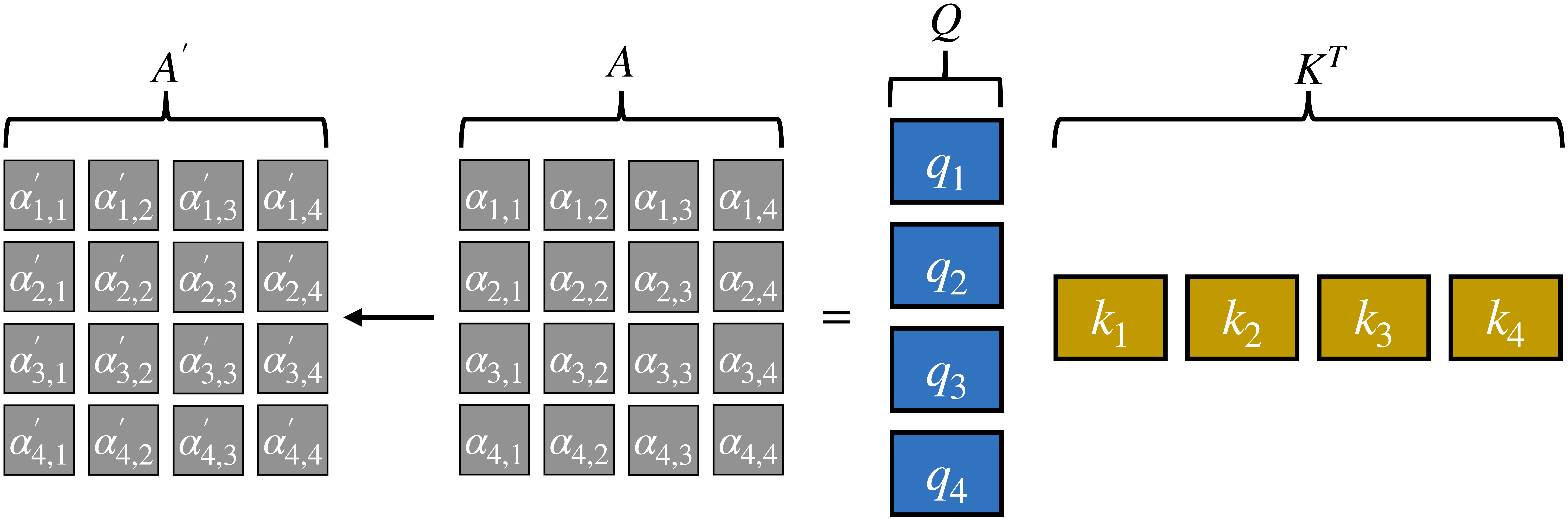
Parallelize the computation!

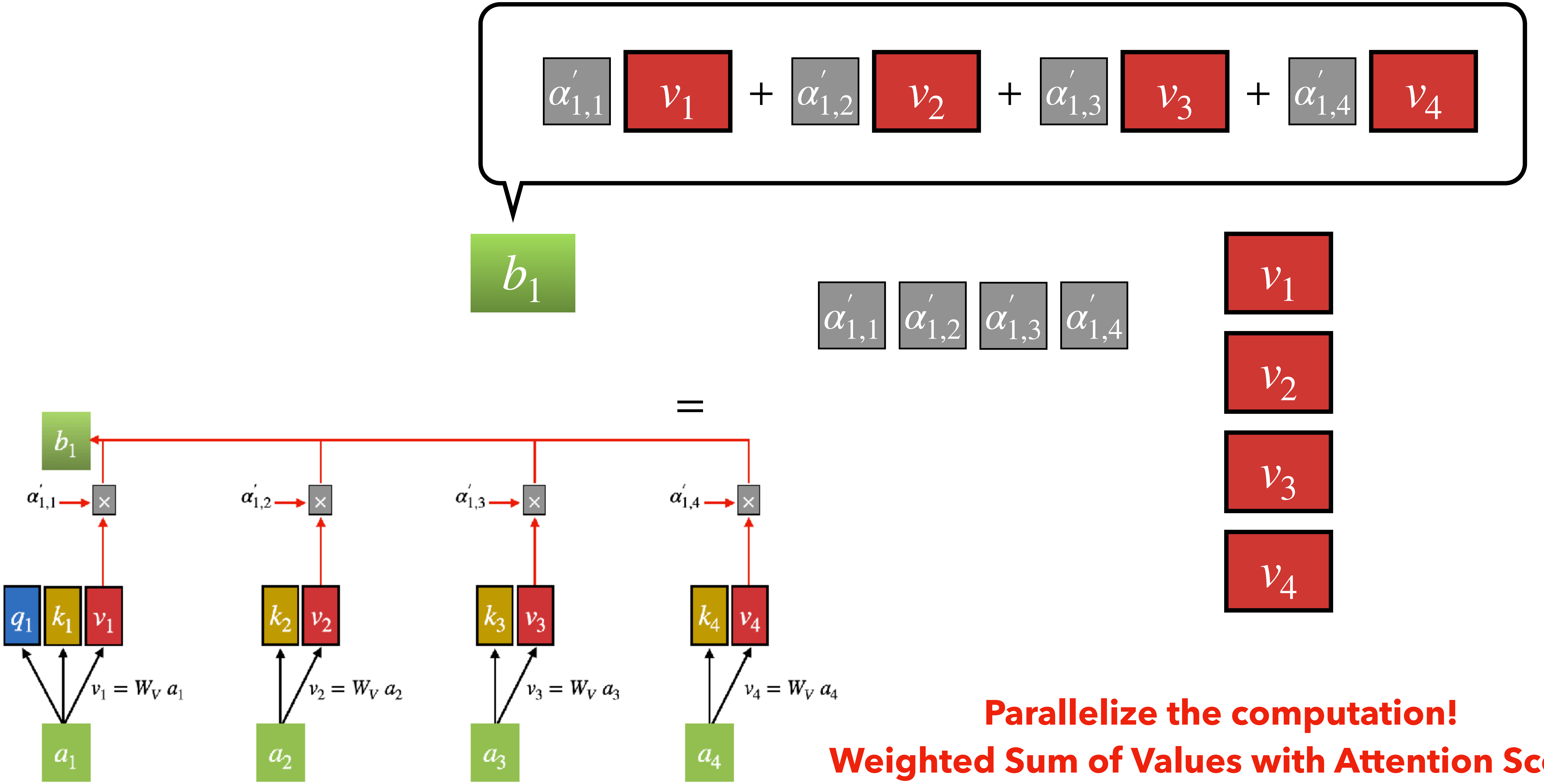
Attention Scores



Parallelize the computation!

Attention Scores





Parallelize the computation!

Weighted Sum of Values with Attention Scores

Parallelize the computation!

$$\overbrace{\begin{bmatrix} b_1 \\ b_2 \\ b_3 \\ b_4 \end{bmatrix}}^{O} = \overbrace{\begin{bmatrix} \alpha'_{1,1} & \alpha'_{1,2} & \alpha'_{1,3} & \alpha'_{1,4} \\ \alpha'_{2,1} & \alpha'_{2,2} & \alpha'_{2,3} & \alpha'_{2,4} \\ \alpha'_{3,1} & \alpha'_{3,2} & \alpha'_{3,3} & \alpha'_{3,4} \\ \alpha'_{4,1} & \alpha'_{4,2} & \alpha'_{4,3} & \alpha'_{4,4} \end{bmatrix}}^{A'} \overbrace{\begin{bmatrix} v_1 \\ v_2 \\ v_3 \\ v_4 \end{bmatrix}}^{V}$$

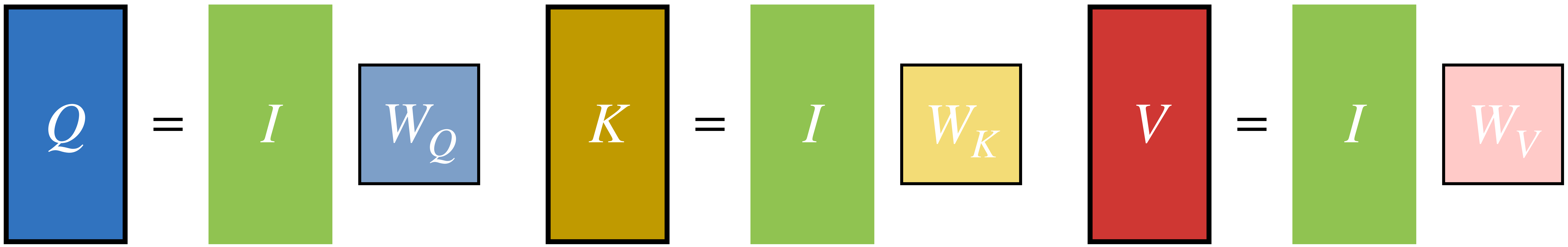
Parallelize the computation!

Weighted Sum of Values with Attention Scores

$$Q = I\,W_Q$$

$$K = I\,W_K$$

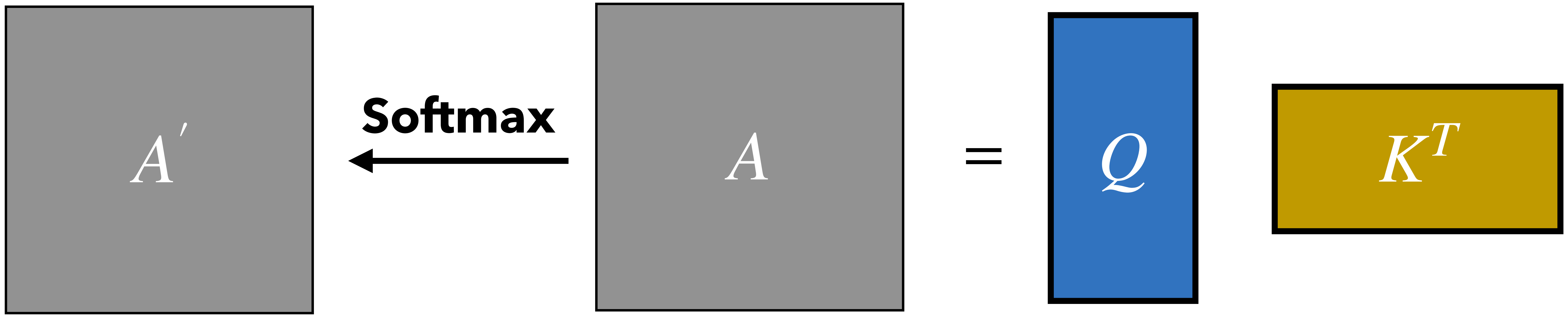
$$V = I\,W_V$$



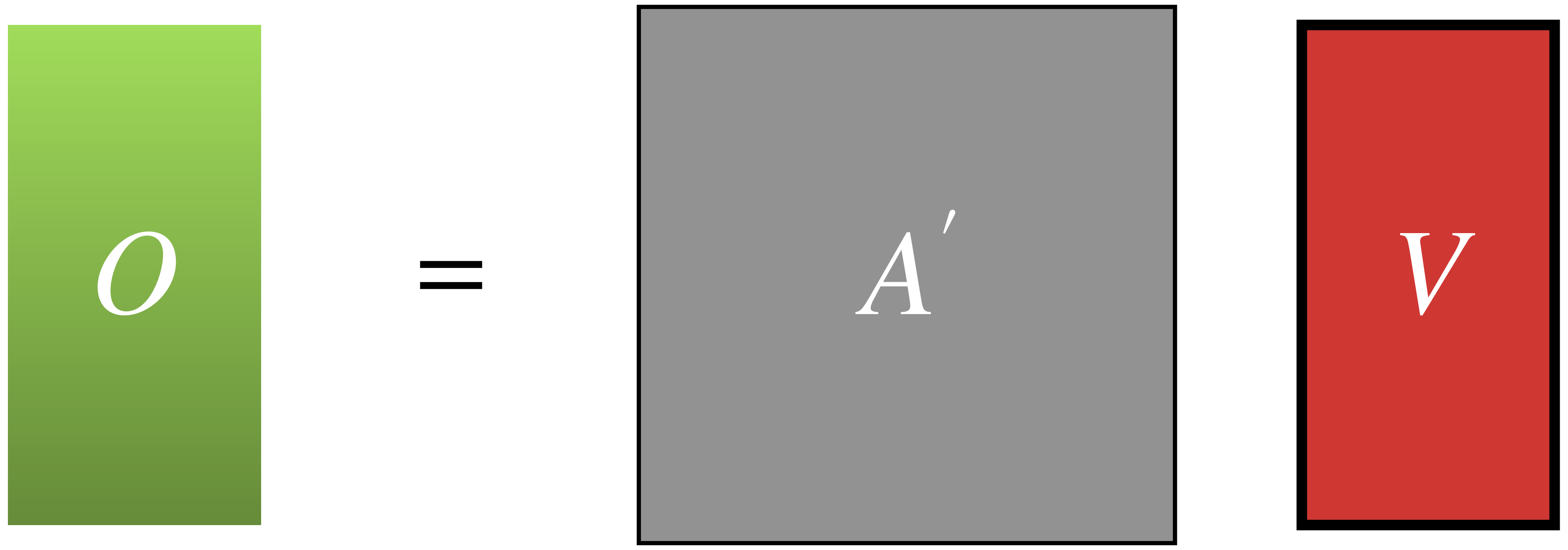
$$A = Q\,K^T$$

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

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



$$O = A'\,V$$



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 $a_i \in \mathbb{R}^d$

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

$Q, K, V \in \boxed{?}$

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

$A', A \in \boxed{?}$

Dimensions?

$$O = A'\,V$$

$O \in \boxed{?}$

The Matrices Form of Self-Attention

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

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

Dimensions?

$$O = A'\,V$$

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

Self-Attention: Summary

Let $w_{1:n}$ be a sequence of words in vocabulary V, like *Steve Jobs founded Apple*.

For each w_i, let $a_i = E w_i$, where $E \in \mathbb{R}^{d \times |V|}$ is an embedding matrix.

1. Transform each word embedding with weight matrices W_Q, W_K, W_V, each in $\mathbb{R}^{d \times d}$

$q_i = W_Q \, a_i$ **(queries)** $\quad k_i = W_K \, a_i$ **(keys)** $\quad v_i = W_V \, a_i$ **(values)**

2. Compute pairwise similarities between keys and queries; normalize with softmax

$$\alpha_{i,j} = k_j \, q_i \qquad \alpha'_{i,j} = \frac{e^{\alpha_{i,j}}}{\sum_j e^{\alpha_{i,j}}}$$

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

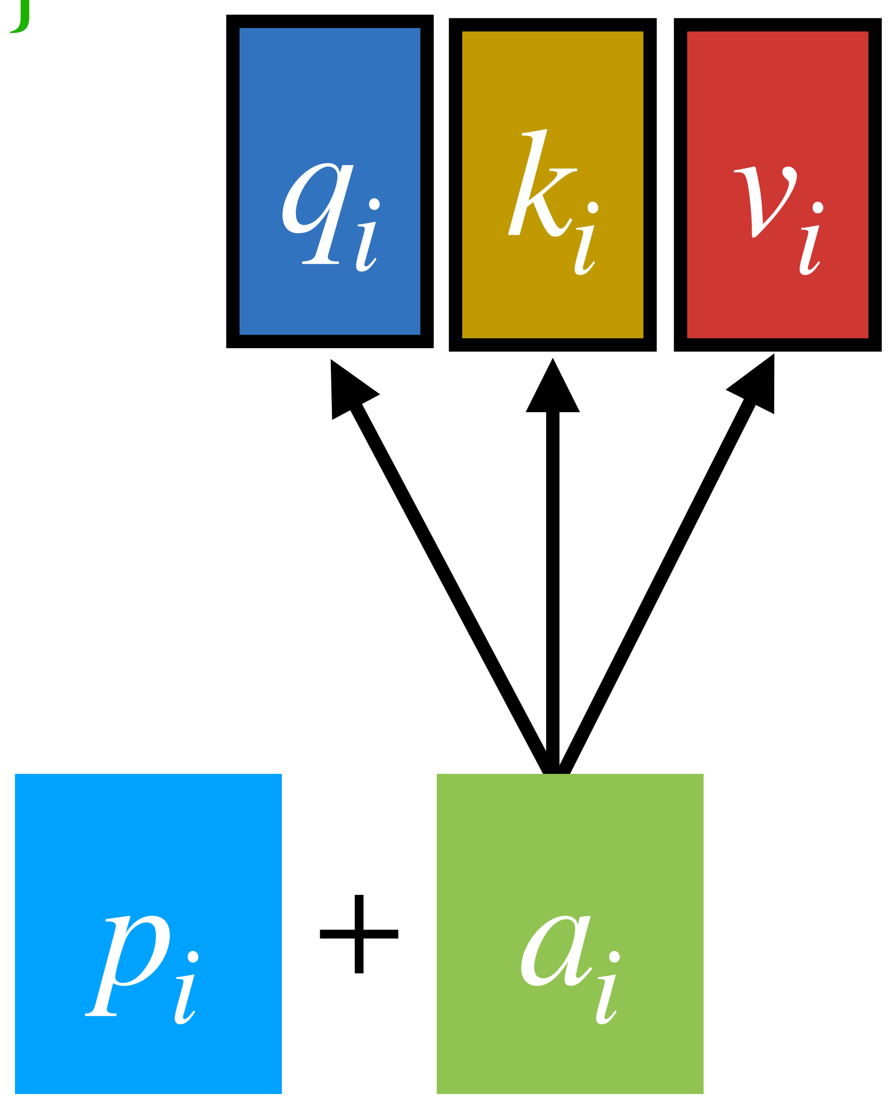
No Sequence Order →	Position Embedding
No Nonlinearities →	Adding Feed-forward Networks
Looking into the Future →	Masking

Limitations and Solutions of Self-Attention

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

No Sequence Order → Position Embedding

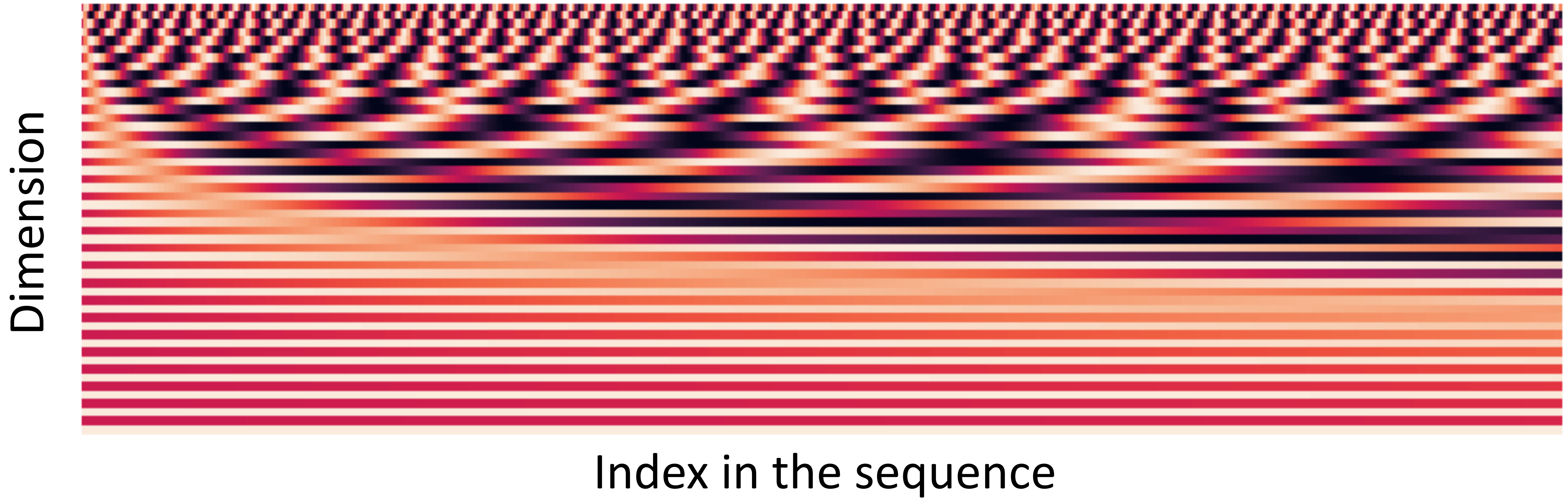
- All tokens in an input sequence are **simultaneously** fed into self-attention blocks. Thus, there's no difference between tokens at different positions.
  - **We lose the position info!**
- **How do we bring the position info back, just like in RNNs?**
  - **Representing each sequence index as a vector:** $p_i \in \mathbb{R}^d$, 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.



Position Representation Vectors via Sinusoids

Sinusoidal Position Representations (from the original Transformer paper): concatenate sinusoidal functions of varying periods.

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



https://timodenk.com/blog/linear-relationships-in-the-transformers-positional-encoding/

- Periodicity indicates that maybe "absolute position" isn't as important
- Maybe can extrapolate to longer sequences as periods restart!

- 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
- Most systems use this method.

- **Flexibility:** each position gets to be learned to fit the data
- Cannot extrapolate to indices outside $1, \ldots, n$.

Sometimes people try more flexible representations of position:

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

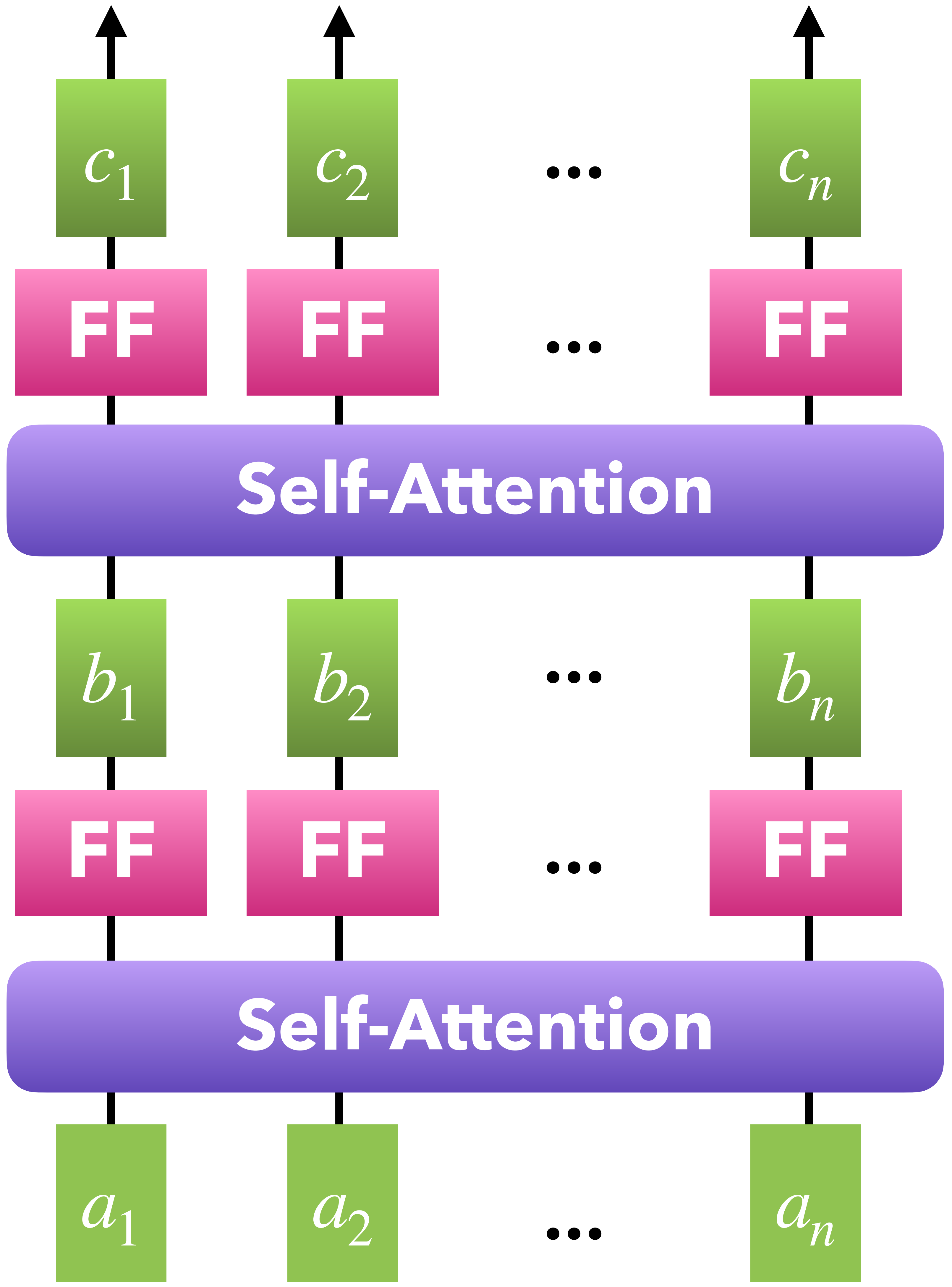
Limitations and Solutions of Self-Attention

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

No Nonlinearities → Add Feed-forward Networks

There are **no element-wise nonlinearities** in self-attention; stacking more self-attention layers just re-averages value vectors.

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



Limitations and Solutions of Self-Attention

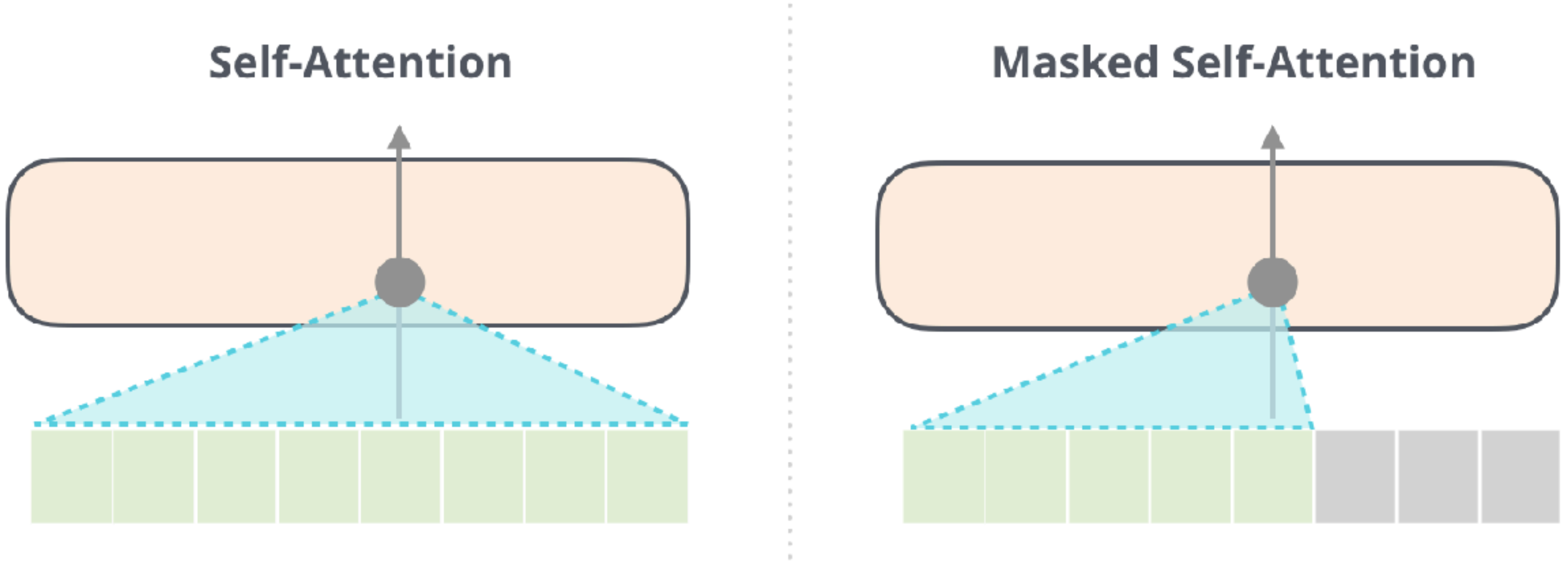
No Sequence Order → Position Embedding

No Nonlinearities → Adding Feed-forward Networks

Looking into the Future → Masking

Looking into the Future → Masking

- In **decoders** (language modeling, producing the next word given previous context), we need to ensure we **don't** peek at the future.



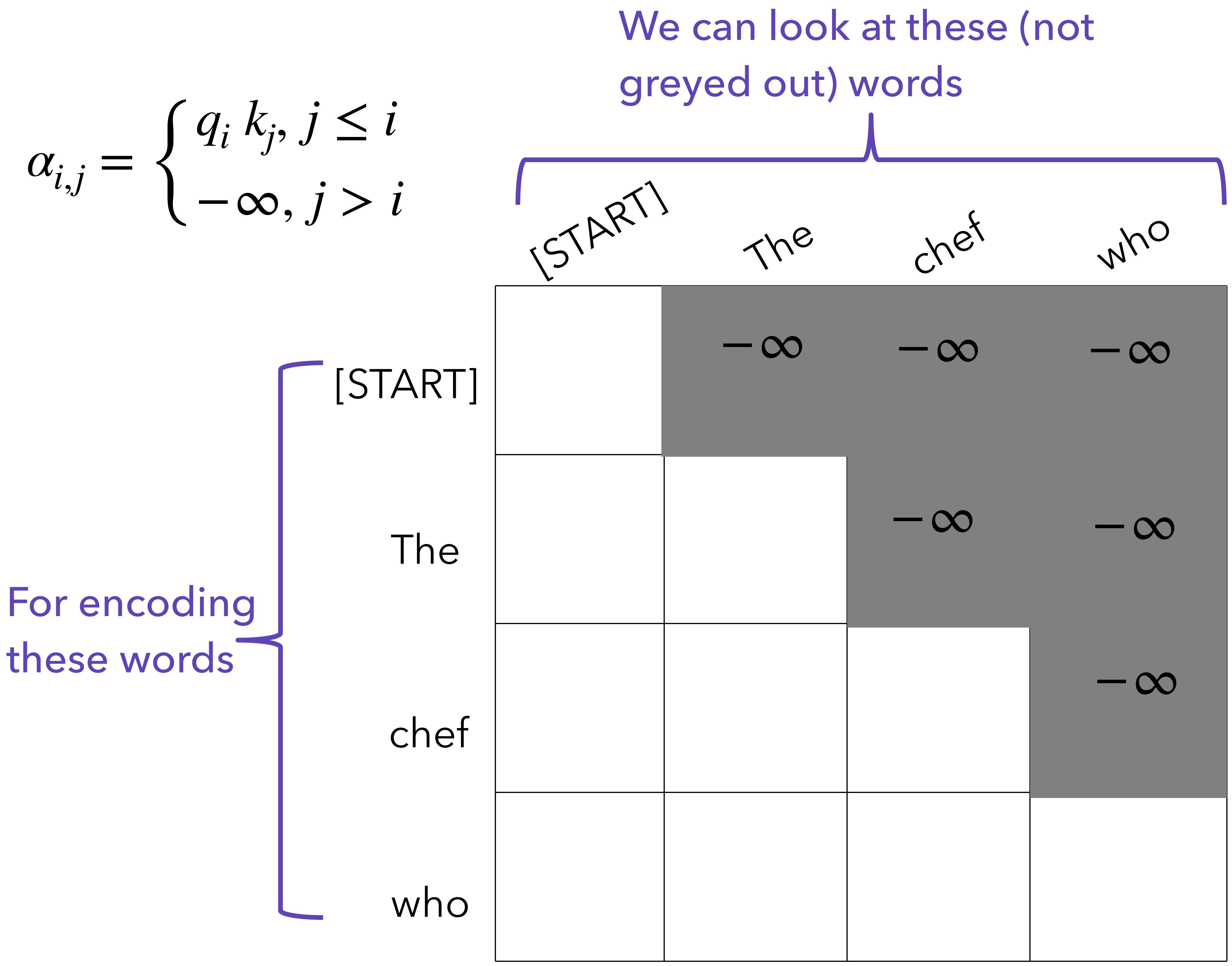
https://jalammar.github.io/illustrated-gpt2/

Looking into the Future → Masking

- In **decoders** (language modeling, producing the next word given previous context), we need to ensure we **don't** peek at the future.

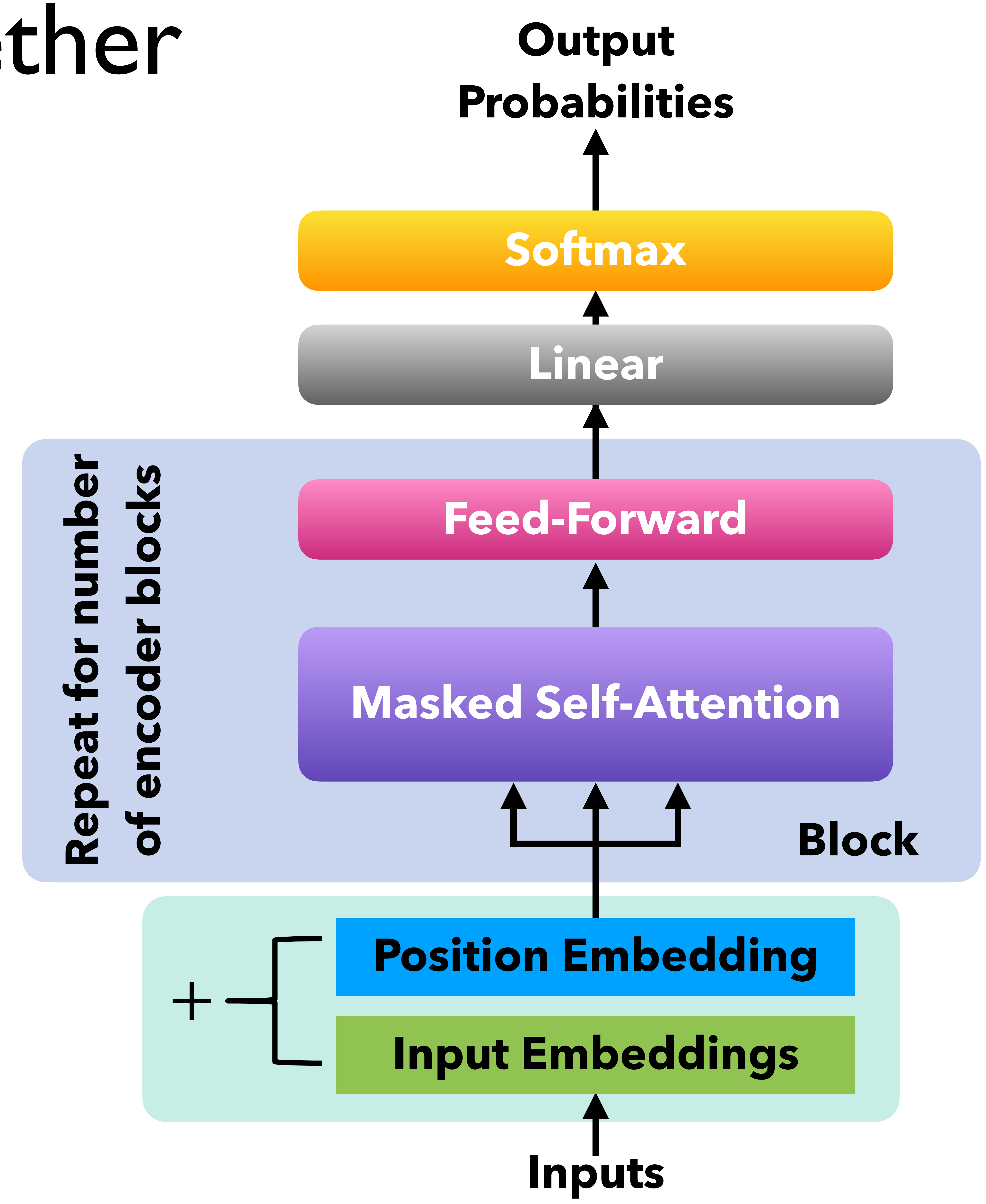
- To enable parallelization, we mask out attention to future words by setting attention scores to $-\infty$.

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



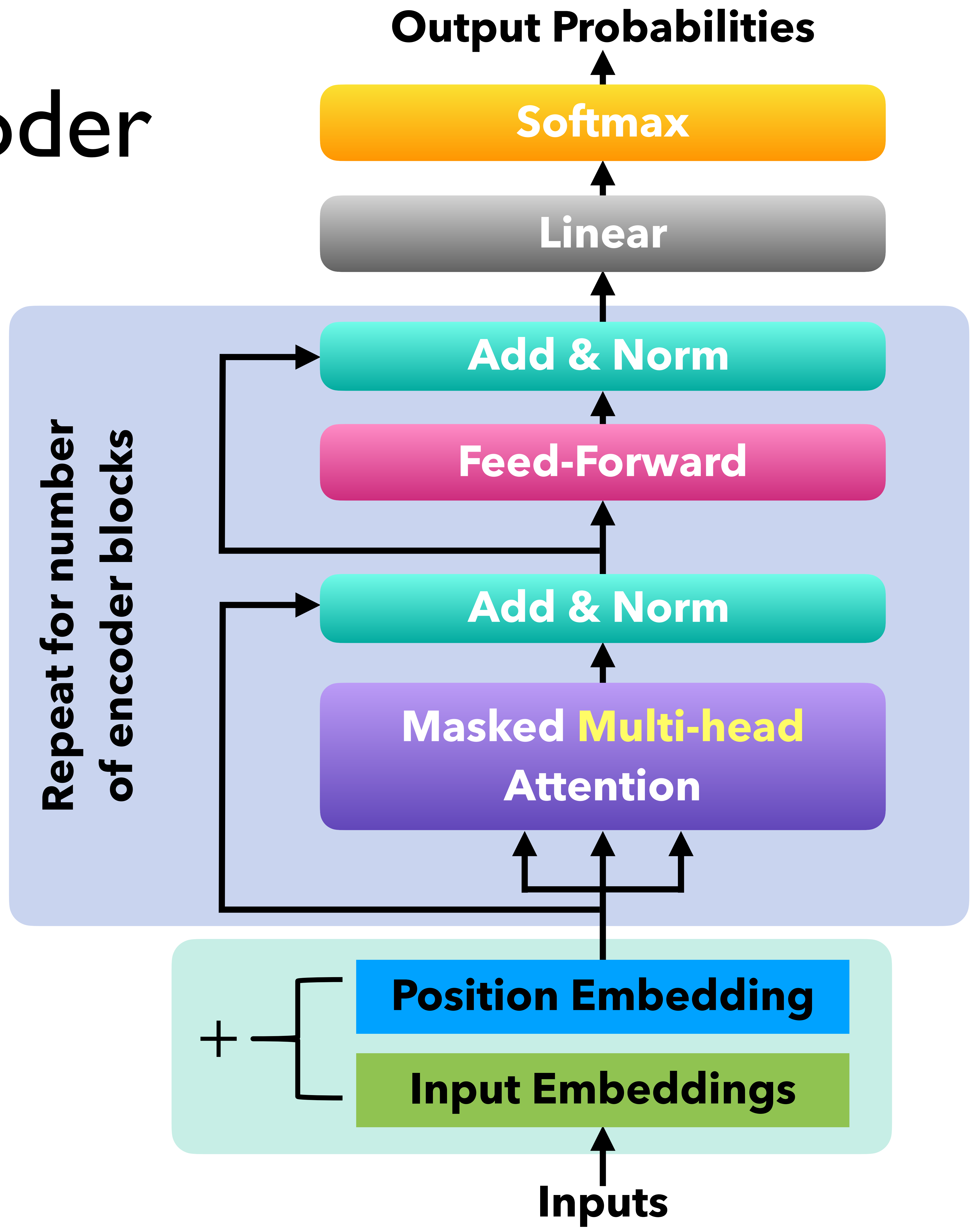
Now We Put Things Together

- **Self-attention**
  - The basic computation
- **Positional Encoding**
  - Specify the sequence order
- **Nonlinearities**
  - Adding a feed-forward network at the output of the self-attention block
- **Masking**
  - Parallelize operations (looking at all tokens) while not leaking info from the future



The Transformer Decoder

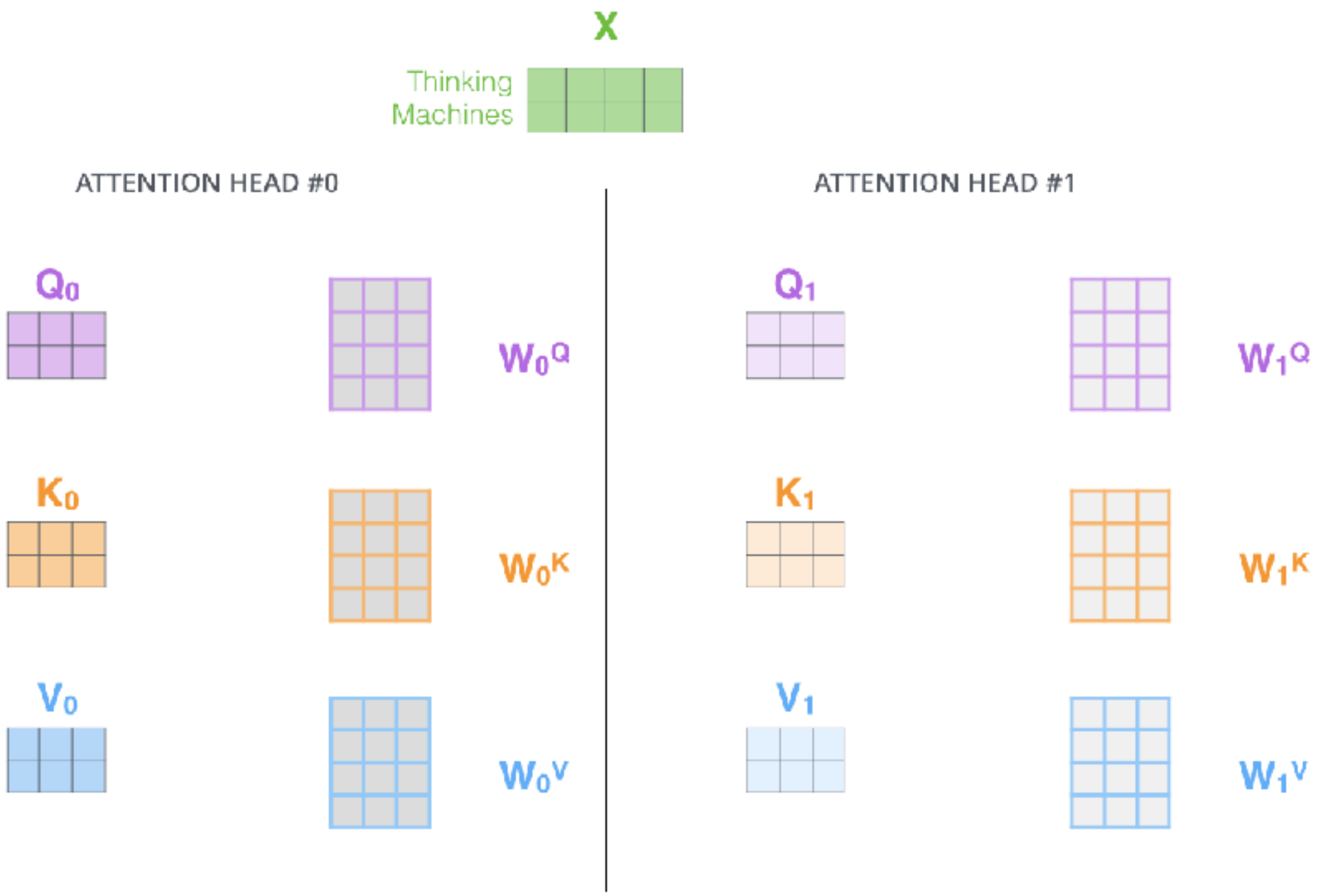
- A **Transformer decoder** is what we use to build systems like language models.
- It's a lot like our minimal self-attention architecture, but with a few more components.
  - ***Residual connection ("Add")***
  - ***Layer normalization ("Norm")***
- Replace self-attention with **multi-head self-attention**.

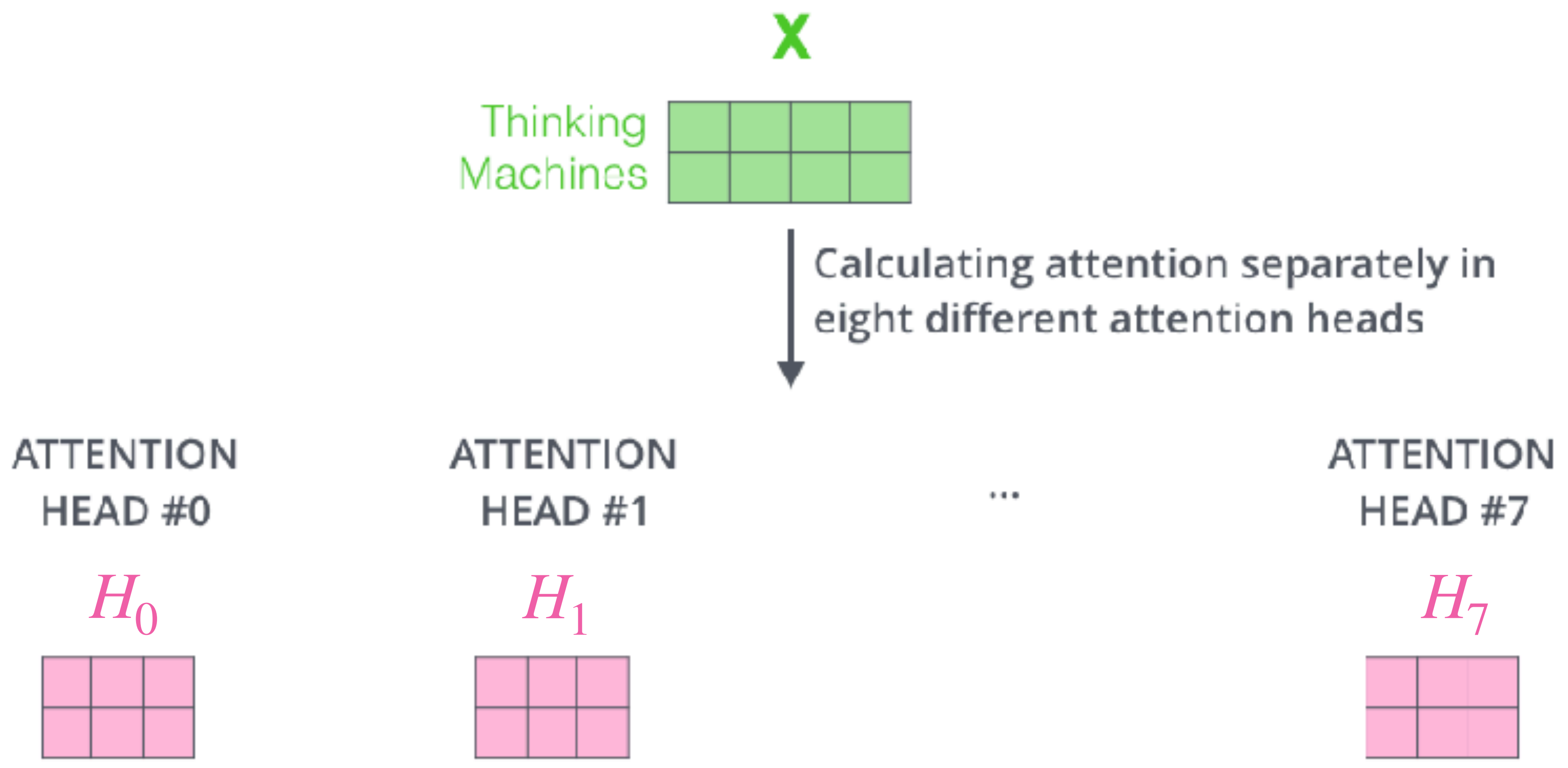


Multi-head Attention

"The Beast with Many Heads"

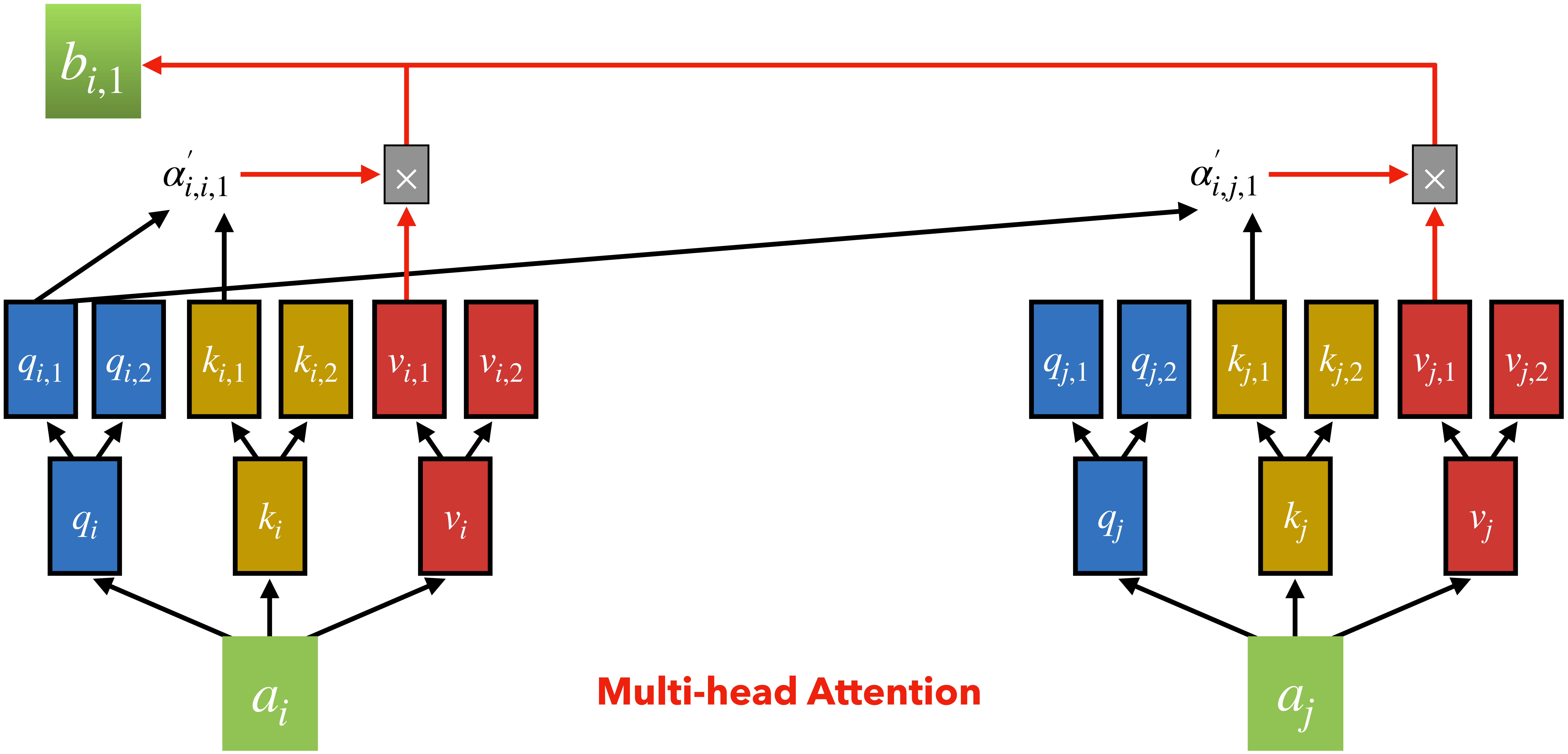
- It is better to use multiple attention functions instead of one!
  - Each attention function ("head") can focus on different positions.



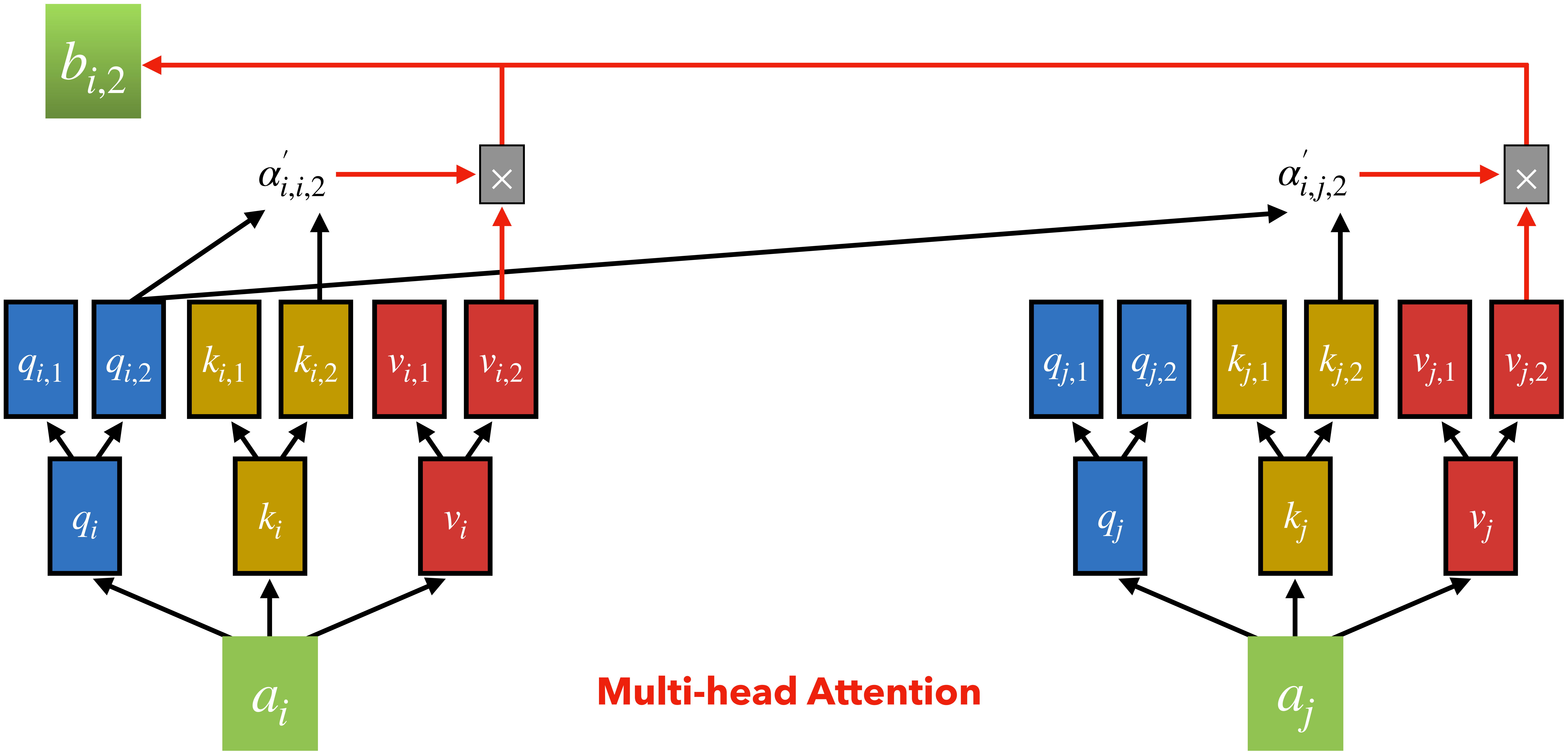


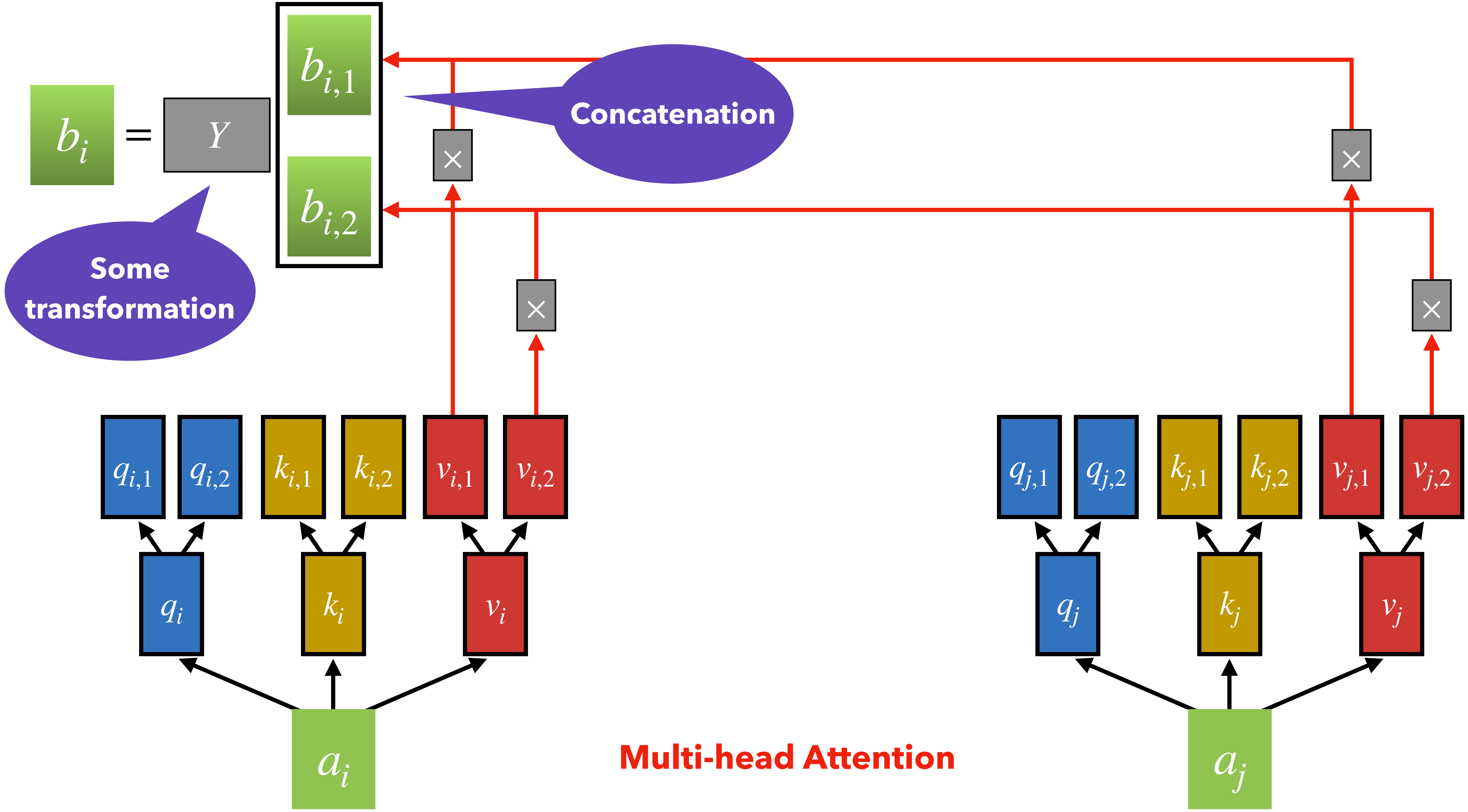
https://jalammar.github.io/illustrated-transformer/

Multi-Head Attention: Walk-through



Multi-Head Attention: Walk-through




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

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:
  - $O^l = \text{softmax}(I\ W_Q^l\ {W_K^l}^T\ I^T)\ I\ W_V^l$
- 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 $a_i \in \mathbb{R}^d$

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

$Q^l, K^l, V^l \in$?

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

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

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

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

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

Dimensions?

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

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

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

$O \in \mathbb{R}$?

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 $a_i \in \mathbb{R}^d$

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

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

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

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

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

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

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

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

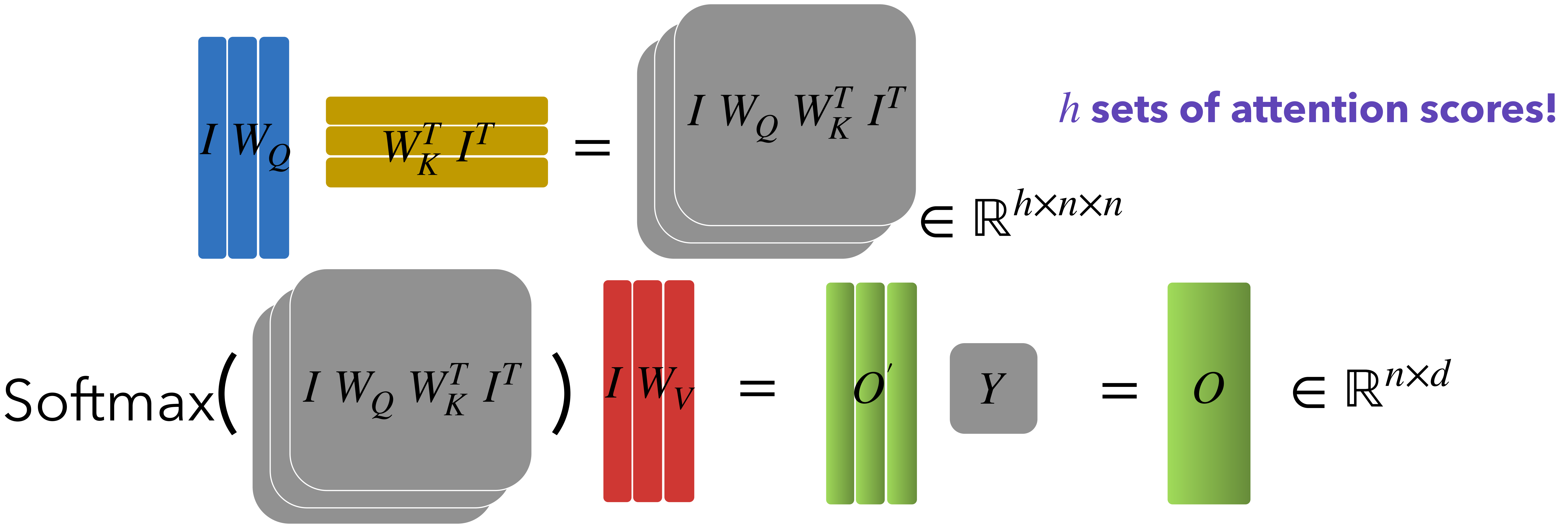
$[O^1; \ldots; O^h] \in \mathbb{R}^{n \times d}$

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

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!



Scaled Dot Product

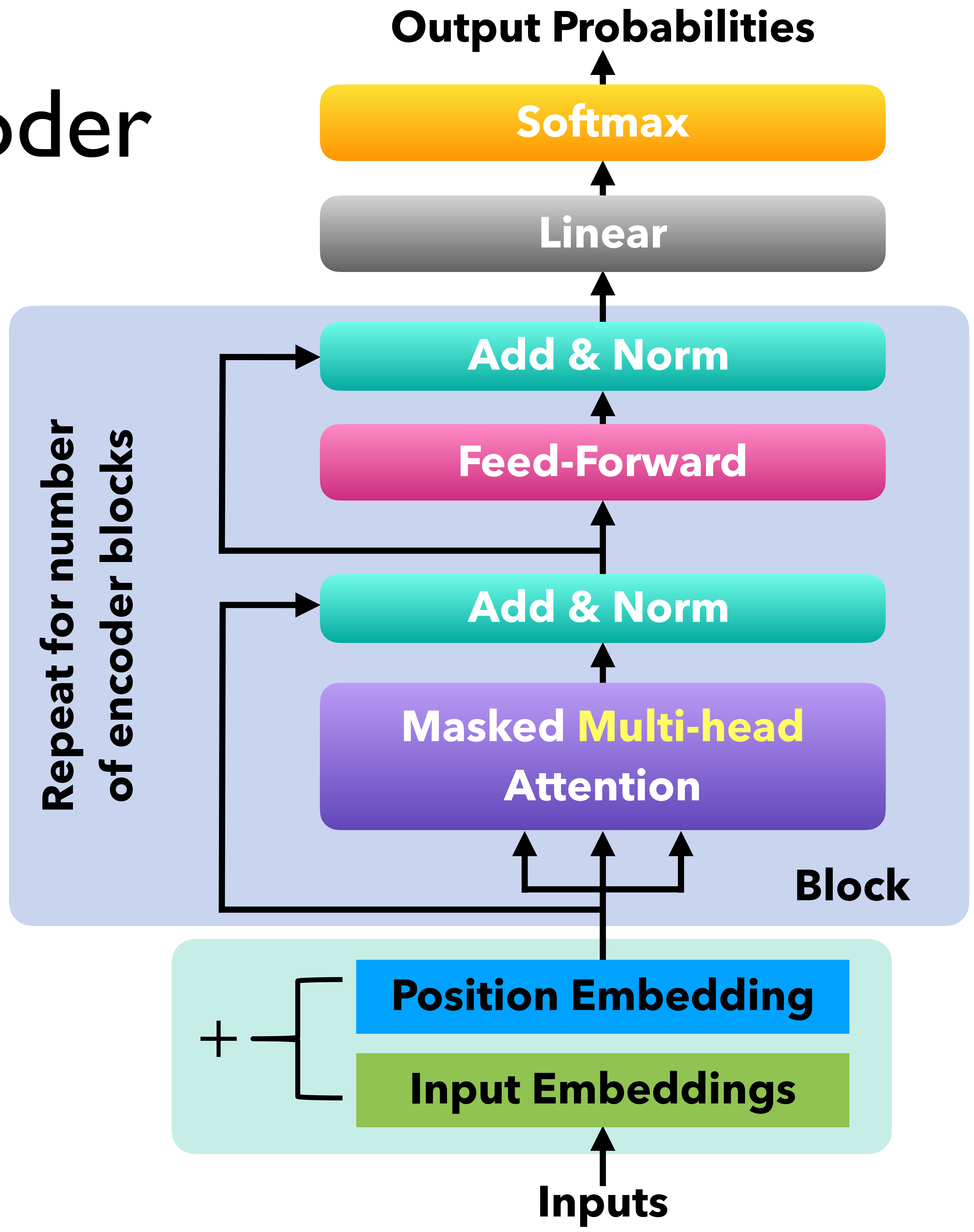
- **"Scaled Dot Product"** attention aids in training.
- When dimensionality d becomes large, dot products between vectors tend to become large.
    - Because of this, inputs to the softmax function can be large, making the gradients small.

- 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).

$$O^l = \textbf{softmax}\left(\frac{I\, W_Q^l\, {W_K^l}^T\, I^T}{\sqrt{d/h}}\right) I\, W_V^l$$

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")***

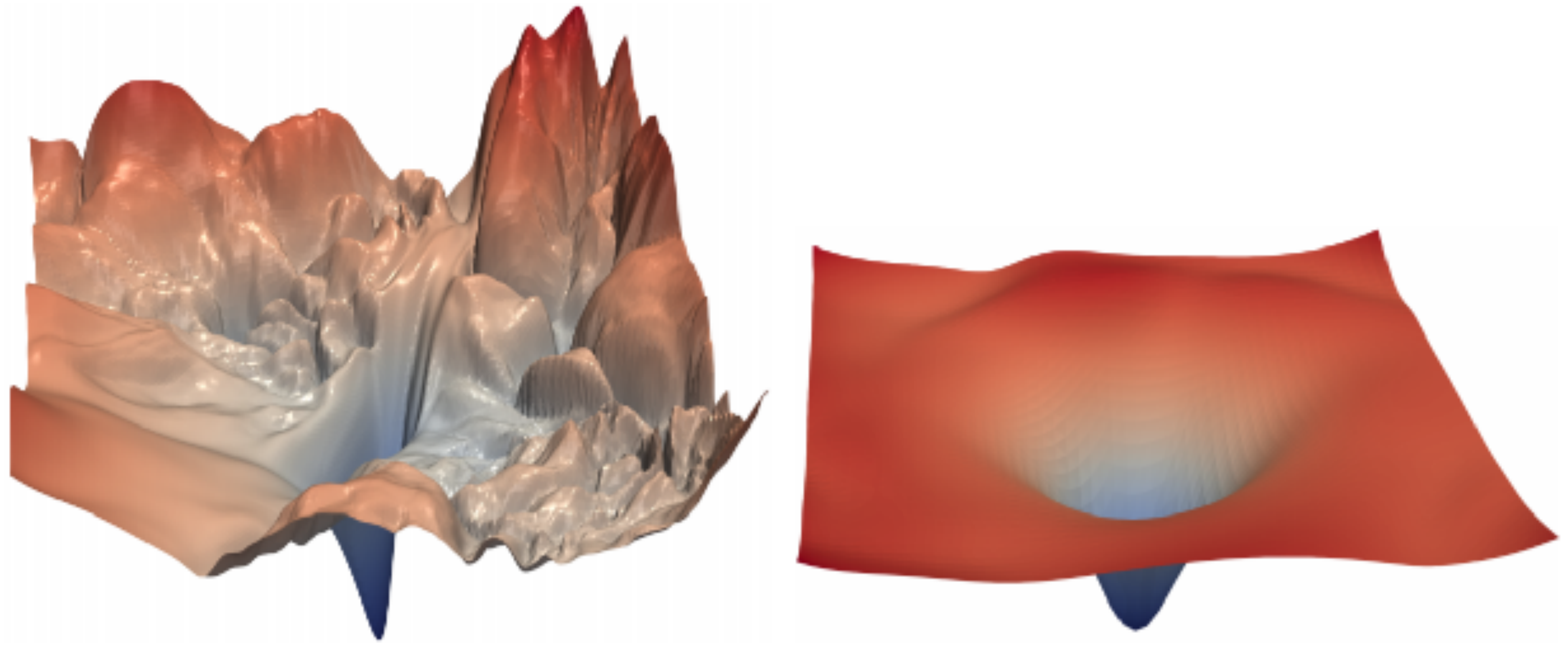


Residual Connections

- Residual connections are a trick to help models train better.
  - Instead of $X^{(i)} = \text{Layer}(X^{(i-1)})$ (where i represents the layer)

  - We let $X^{(i)} = X^{(i-1)} + \text{Layer}(X^{(i-1)})$ (so we only have to learn "the residual" from the previous layer)

  - Gradient is great through the residual connection; it's 1!
  - Bias towards the identity function!



[no residuals] **[residuals]**

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

Layer Normalization

- Layer normalization is a trick to help models train faster.
- **Idea:** cut down on uninformative variation in hidden vector values by normalizing to unit mean and standard deviation within each layer.
  - LayerNorm's success may be due to its normalizing gradients [Xu et al., 2019]
- Let $x \in \mathbb{R}^d$ be an individual (word) vector in the model.
- Let $\mu = \sum_{j=1}^{d} x_j$; this is the mean; $\mu \in \mathbb{R}$.
- Let $\sigma = \sqrt{\frac{1}{d} \sum_{j=1}^{d} \left(x_j - \mu\right)^2}$; this is the standard deviation; $\sigma \in \mathbb{R}$.
- Let $\gamma \in \mathbb{R}^d$ and $\beta \in \mathbb{R}^d$ be learned "gain" and "bias" parameters. (Can omit!)
- Then layer normalization computes:

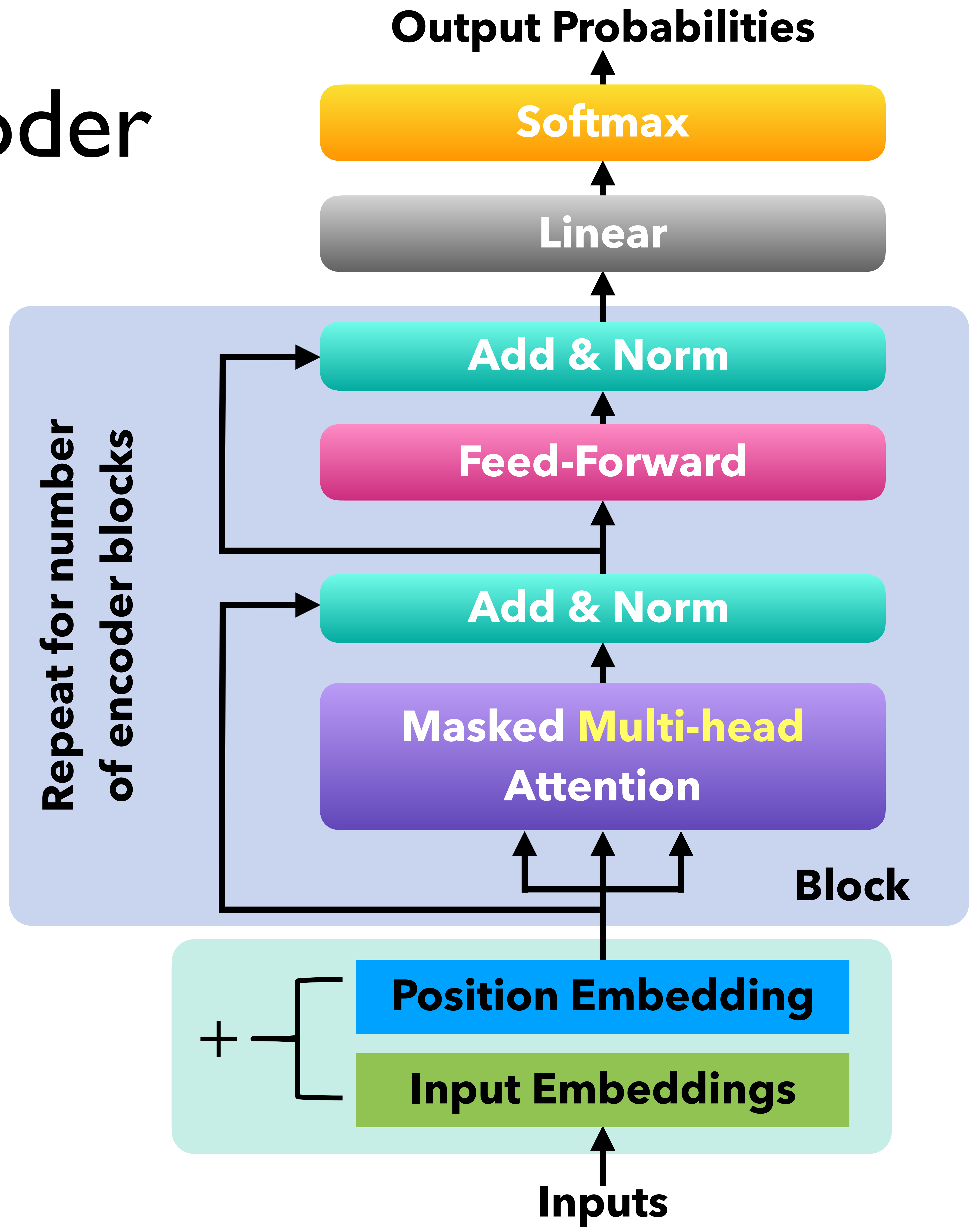
Normalize by scalar mean and variance

- $$\text{output} = \frac{x - \mu}{\sqrt{\sigma} + \epsilon} * \gamma + \beta$$

Modulate by learned element-wise gain and bias

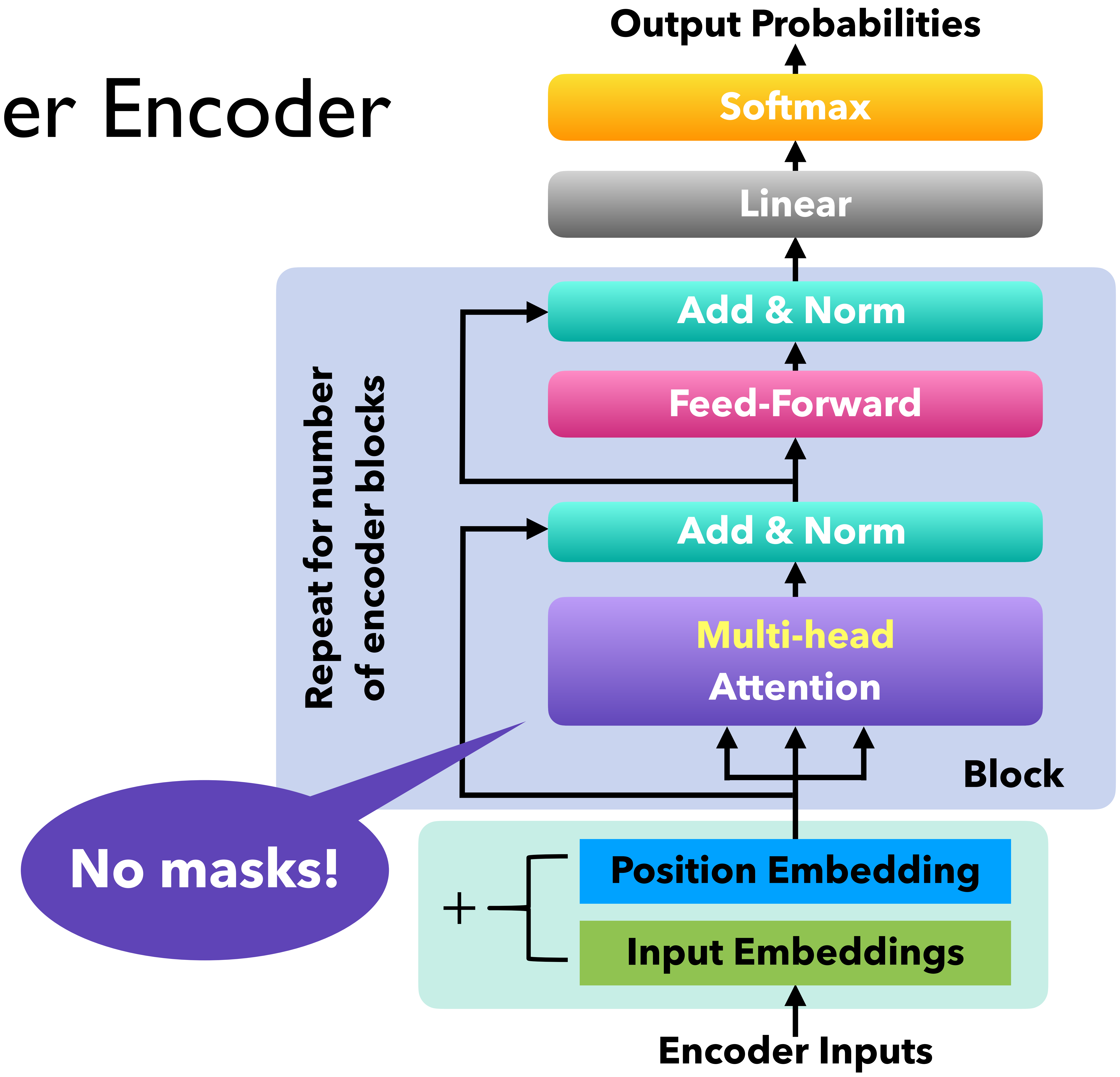
The Transformer Decoder

- 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



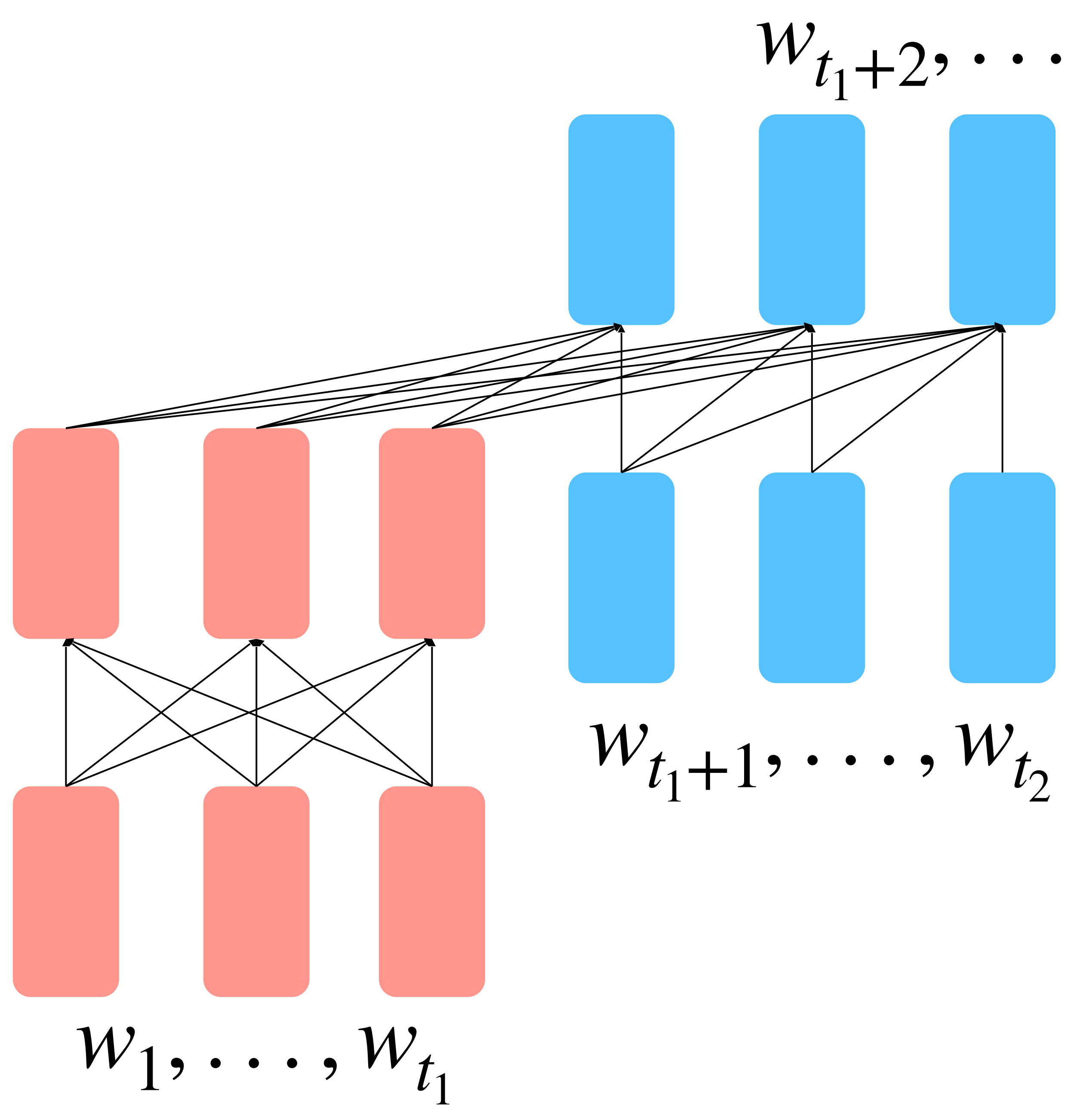
The Transformer Encoder

- The Transformer **Decoder** constrains to **unidirectional** context, as for language models.
- What if we want **bidirectional** context, like in a bidirectional RNN?
- We use **Transformer Encoder** – the ONLY difference is that we **remove the masking** in self-attention.

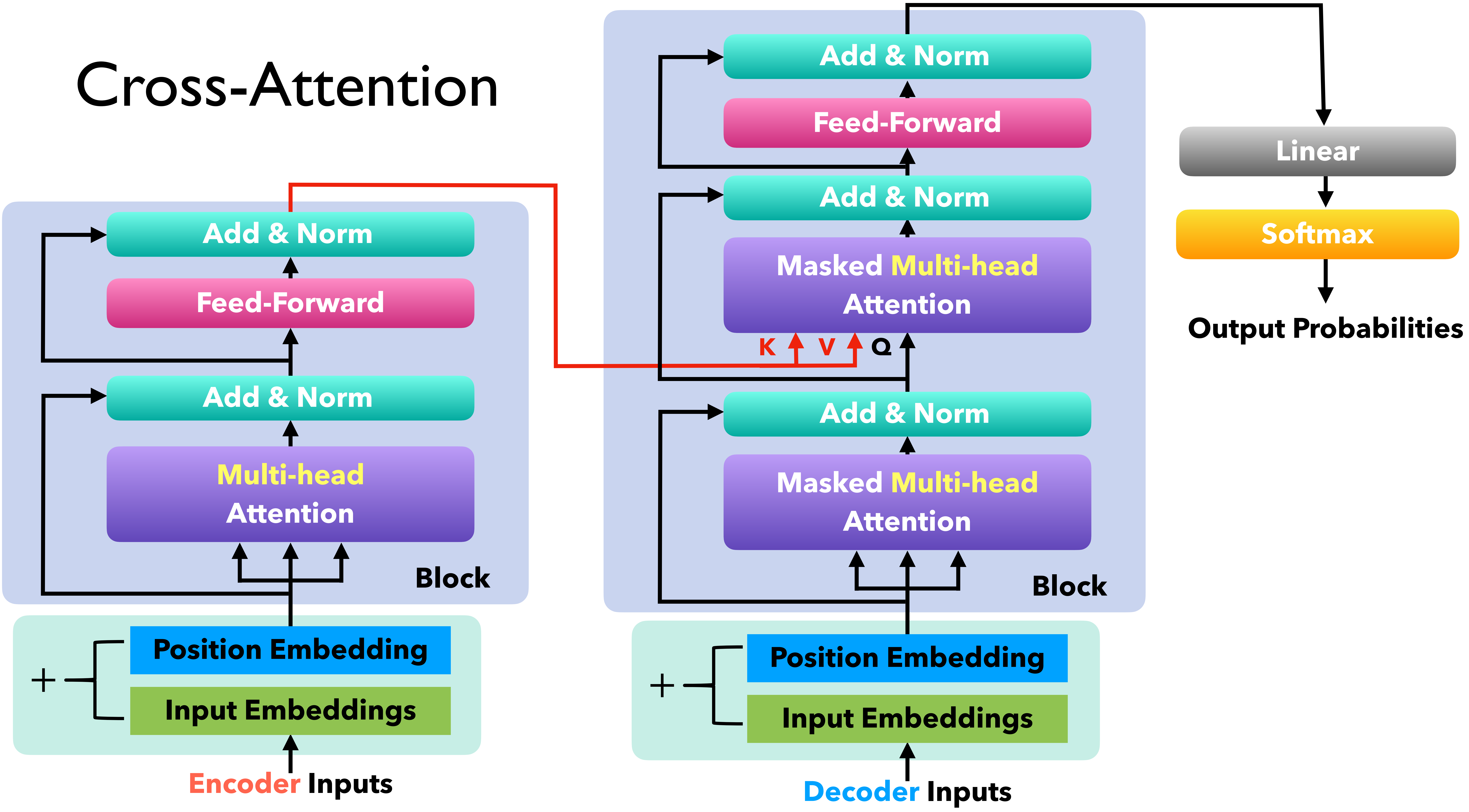


The Transformer Encoder-Decoder

- More on Encoder-Decoder models will be introduced in the next lecture!
- 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

- **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**:
  - $q_i = W_Q z_i$

Transformers: pros and cons

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

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

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

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

Otherwise self-attention is an unordered function of its input

- **Quadratic computation in self-attention**

Can become very slow when the sequence length is large

Quadratic computation as a function of sequence length

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

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

$n \times d_q$ $\quad$ $d_k \times n$ $\quad$ $n \times d_v$

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

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

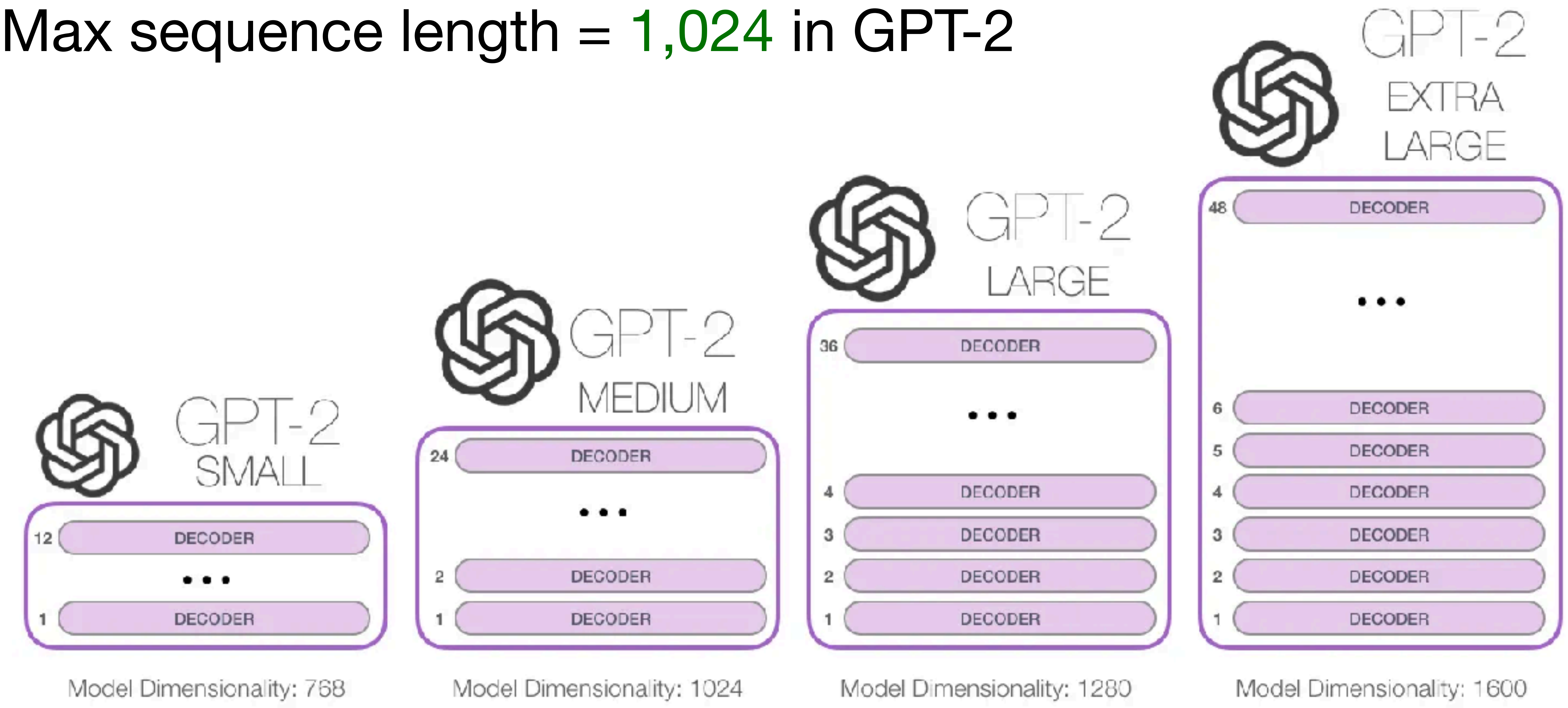
$$\mathbf{h}_t = g(\mathbf{W}\mathbf{h}_{t-1} + \mathbf{U}\mathbf{x}_t + \mathbf{b})$$

(assuming input dimension = hidden dimension = d)

Quadratic computation as a function of sequence length

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

Max sequence length = 1,024 in GPT-2

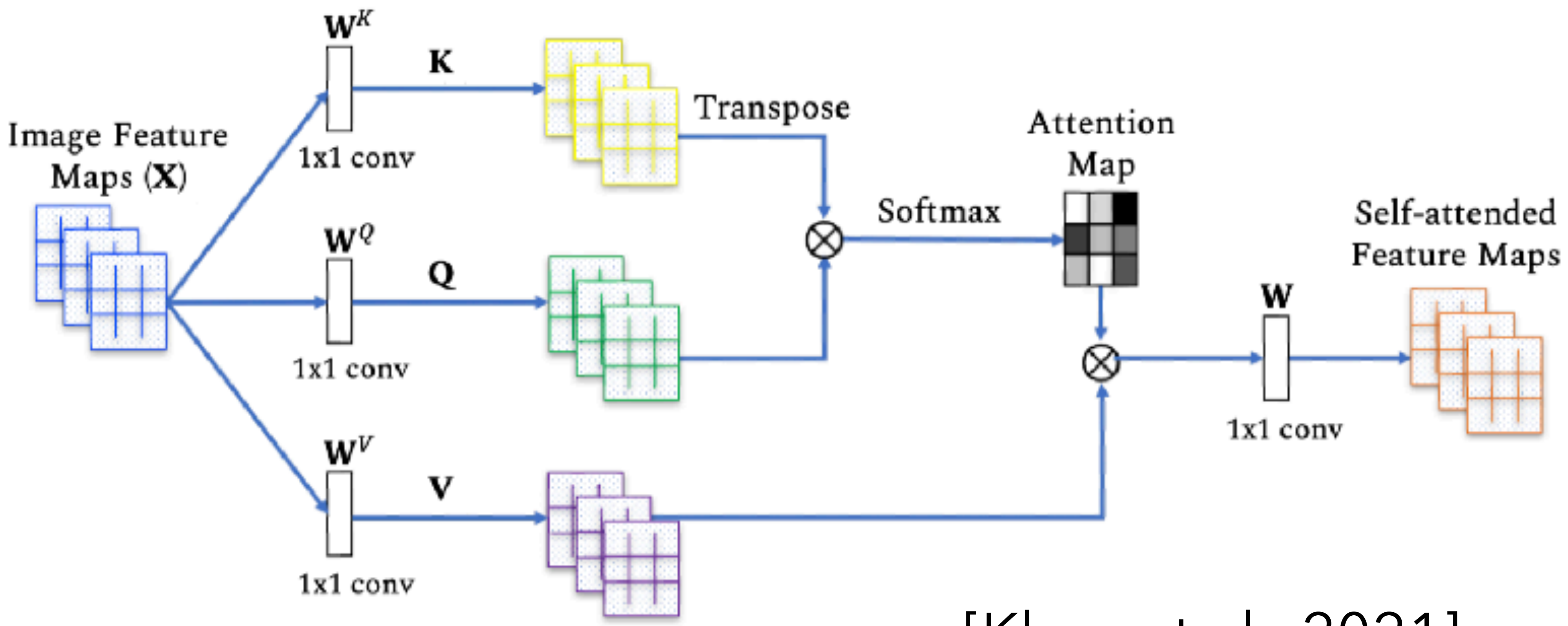


What if we want to scale $n \geq 50{,}000$? For example, to work on long documents?

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.

- Since Transformer has been popularized in language applications, computer vision also adapted Transformers, e.g., **Vision Transformers**.



[Khan et al., 2021]

What's next after Transformers?