CS60010: Deep Learning
Spring 2023

Sudeshna Sarkar

Transformer- Part 1

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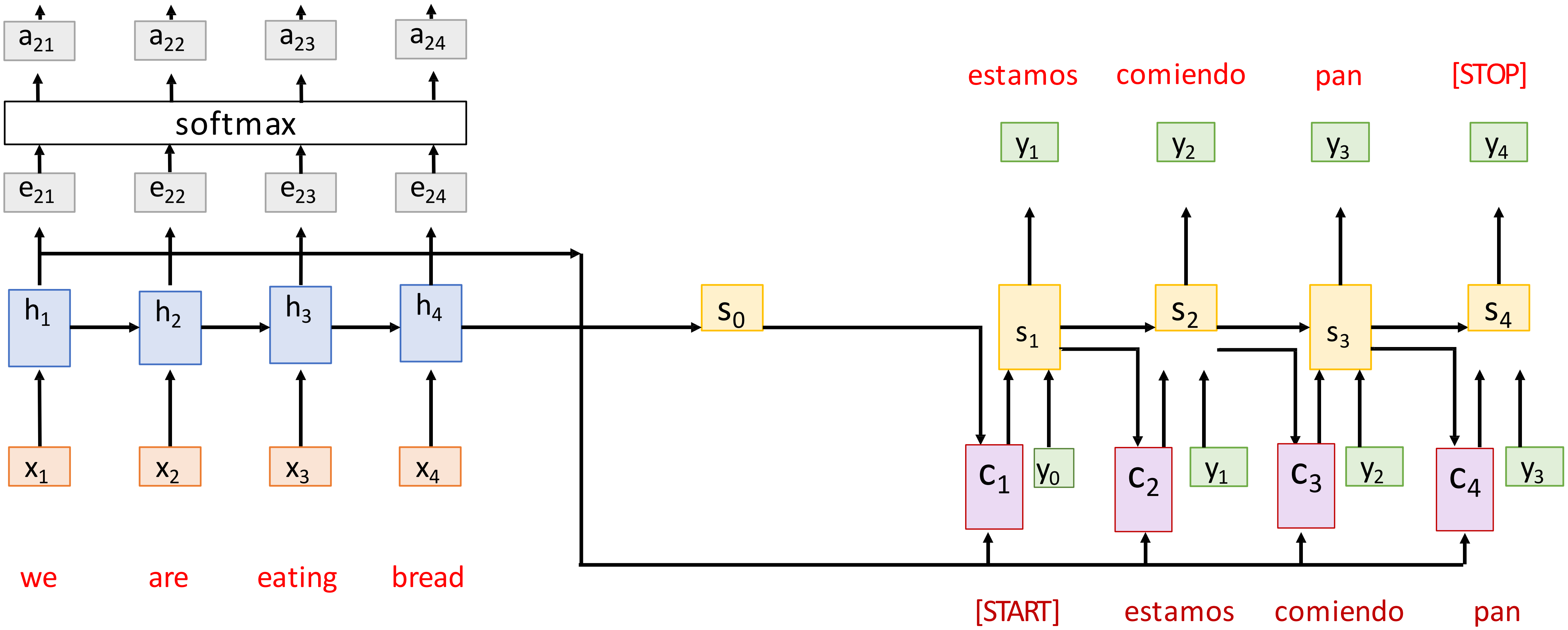
10 Mar 2023

Encoder Decoder Attention



Attention-only Translation Models

- Problems with recurrent networks:
- Sequential training and inference: Time grows in proportion to sentence length. Hard to parallelize.
- Long-range dependencies have to be remembered across many single time steps.
- Tricky to learn hierarchical structures (“car”, “blue car”, “into the blue car”…)

- Alternative:
- Convolution – but has other limitations.

Self-Attention

- Consider an input (or intermediate) sequence
- Construct the next level representation:
  which can choose “where to look”, by assigning a weight to each input position.
- Create a weighted sum.

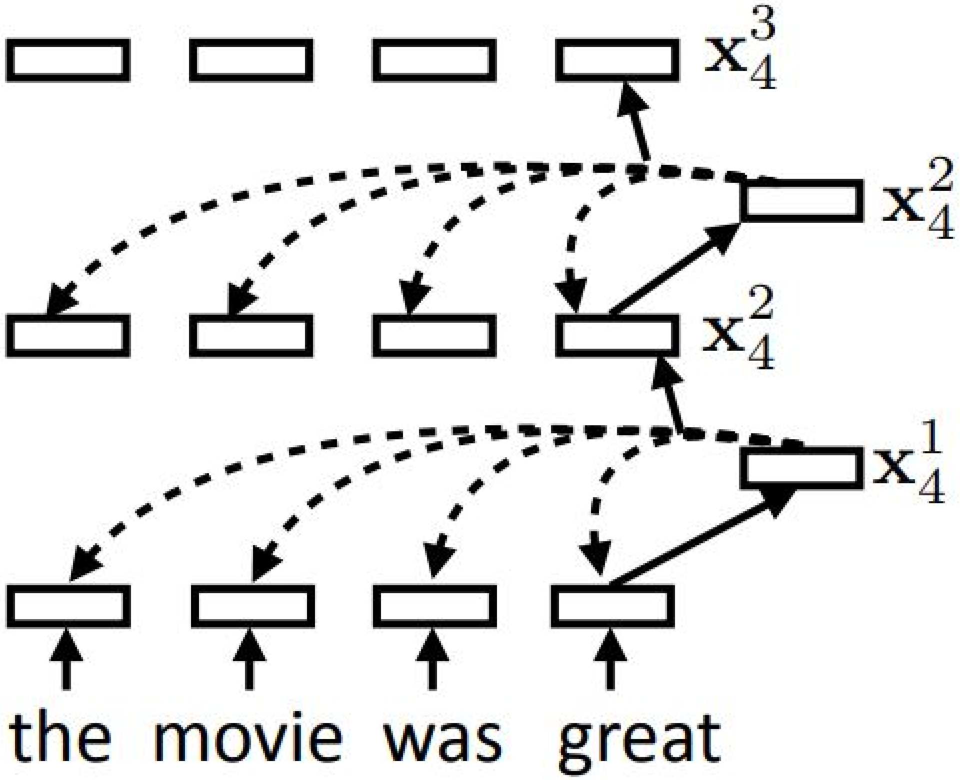
Level k+1

Softmax over lower locations conditioned on context at lower and higher locations

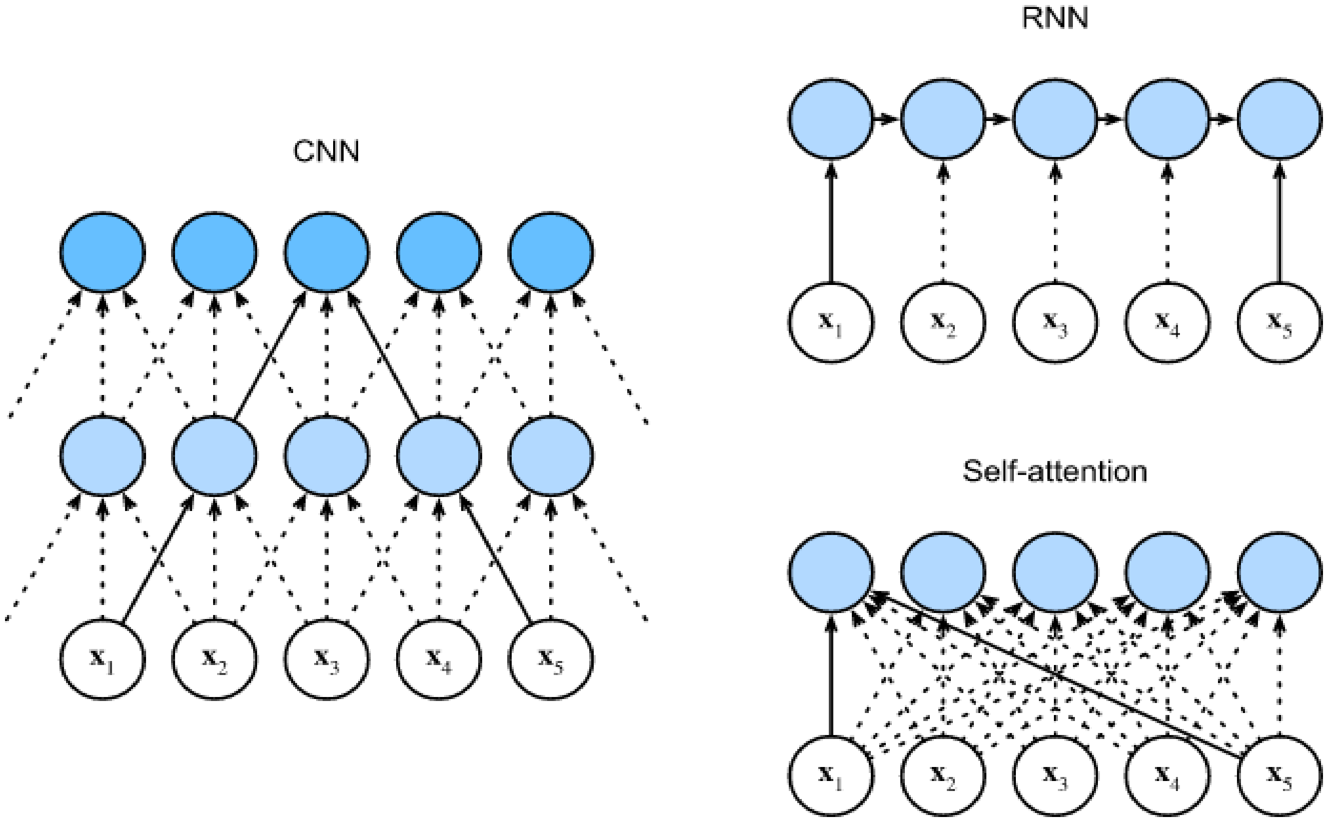
Level k

Self-attention

- Each word is a query to form attention over all tokens
- This generates a context-dependent representation of each token: a weighted sum of all tokens
- The attention weights dynamically mix how much is taken from each token



Comparing CNNs, RNNs, and Self-Attention



Self-Attention "Transformers"

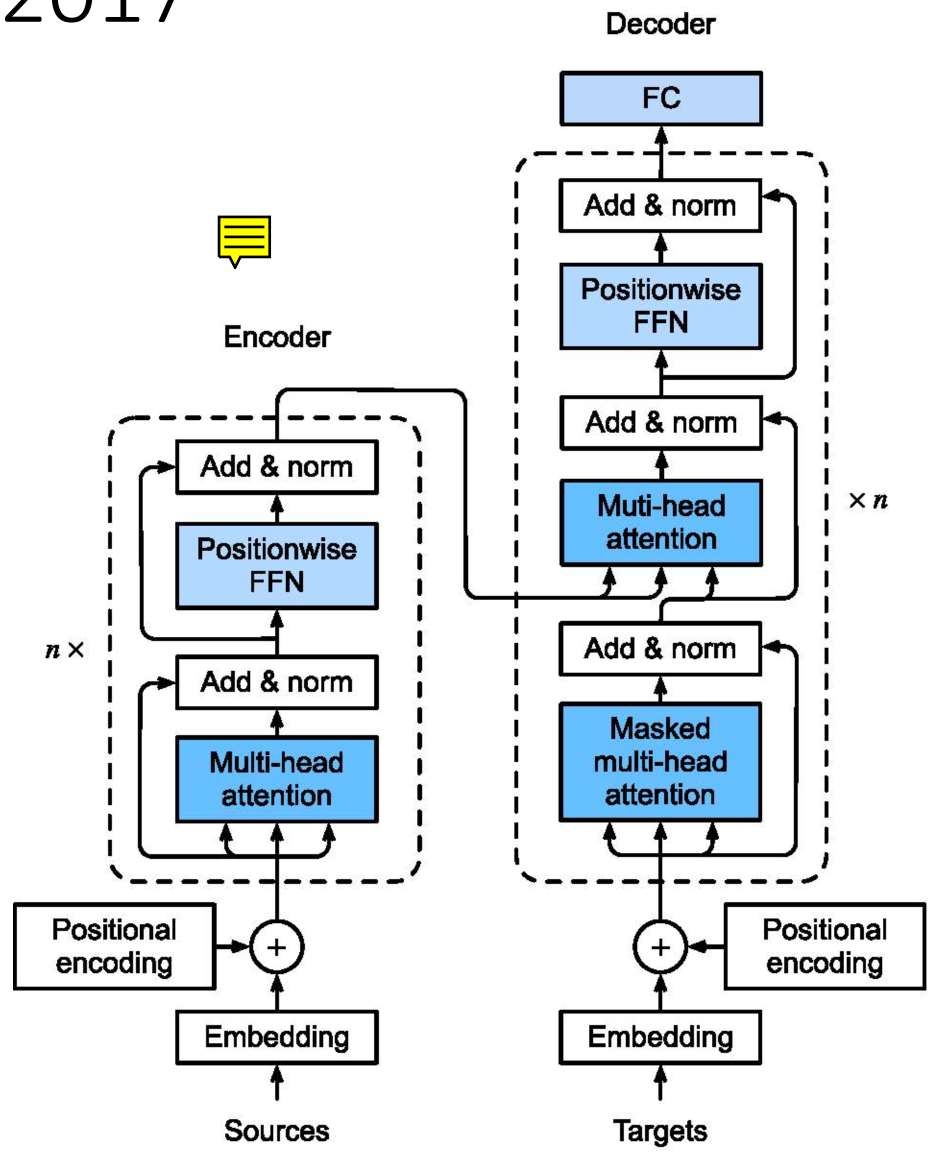
- Constant path length between any two positions.
- Variable receptive field (or the whole input sequence).
- Supports hierarchical information flow by stacking self-attention layers.
- Trivial to parallelize.
- Attention weighting controls information propagation.
- If we have attention, do we even need recurrent connections?
- Can we transform our RNN into a purely attention-based model?

Vaswani et al. "Attention is all you need", arXiv 2017

https://arxiv.org/abs/1706.03762

Transformer Model Vaswani et al. 2017

- Transformers map sequences of input vectors $(x_1, x_2, \ldots, x_n)$ to sequences of output vectors $(y_1, y_2, \ldots, y_m)$.
- Made up of stacks of Transformer blocks.
  - combine linear layers, feedforward networks, and self-attention layers.
- **Self-attention** allows a network to directly extract and use information from arbitrarily large contexts



Transformer Model

Queries, Keys, and Values

- For each element in the sequence S (length m) define key, value and query

$$Attention(q, S) \stackrel{def}{=} \sum_{i=1}^{m} \alpha(q, k_i)\, v_i$$

- Normalize attention weights to sum to 1 and be non-negative.

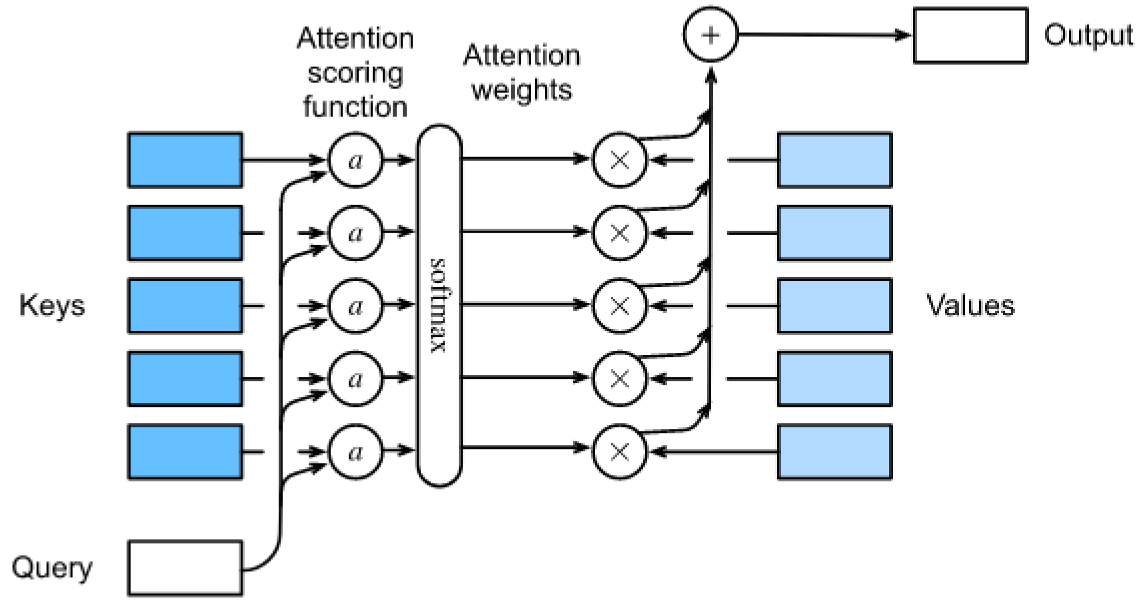
$$\alpha(q, k_i) = \frac{\exp(\alpha(q, k_i))}{\sum_j \exp\left(\alpha(q, k_j)\right)}$$

Dot Product Attention

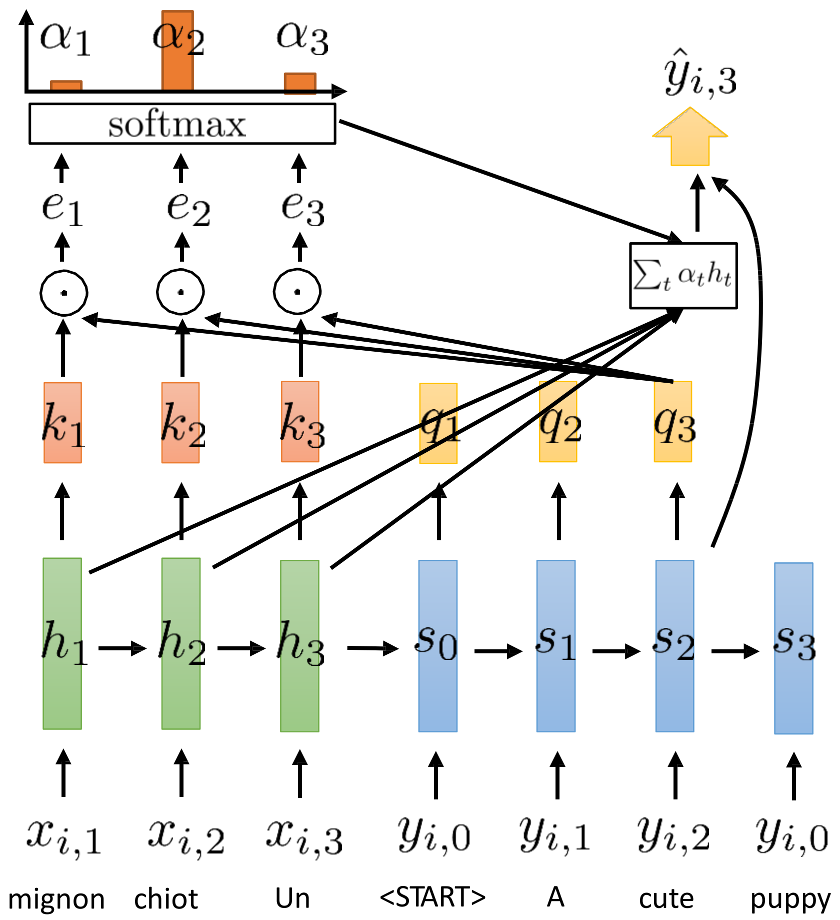
$$\alpha(q, k_i) = \frac{q^T k_i}{\sqrt{d}}$$

$$\alpha(q, k_i) = \mathrm{softmax}(\alpha(q, k_i))$$

$$= \frac{\exp(q^T k_i / \sqrt{d})}{\sum_j \exp(q^T k_j / \sqrt{d})}$$



Is Attention all we need?



Attention can in principle do **everything** that recurrence can, and more!

This has a few issues we must overcome:

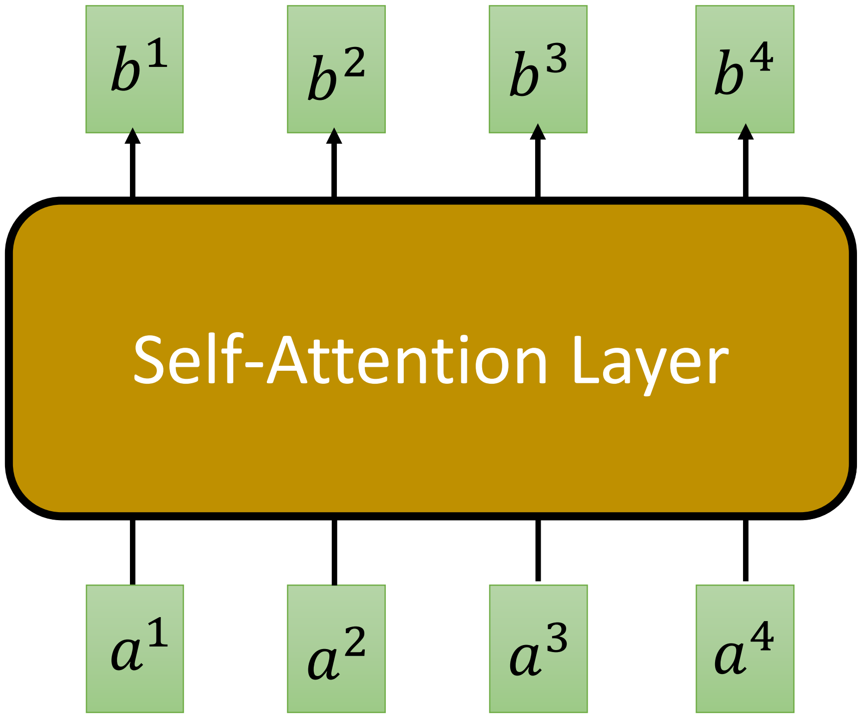
1. The encoder has no temporal dependencies.

From Self-Attention to Transformers

1. Positional encoding — addresses lack of sequence information
2. Multi-headed attention — allows querying multiple positions at each layer
3. Adding nonlinearities
4. Masked decoding — how to prevent attention lookups into the future?

Self-Attention explained

Self-Attention



b^i is obtained based on the whole input sequence.
b^1, b^2, b^3, b^4 can be computed in parallel.

q: query (to match others)

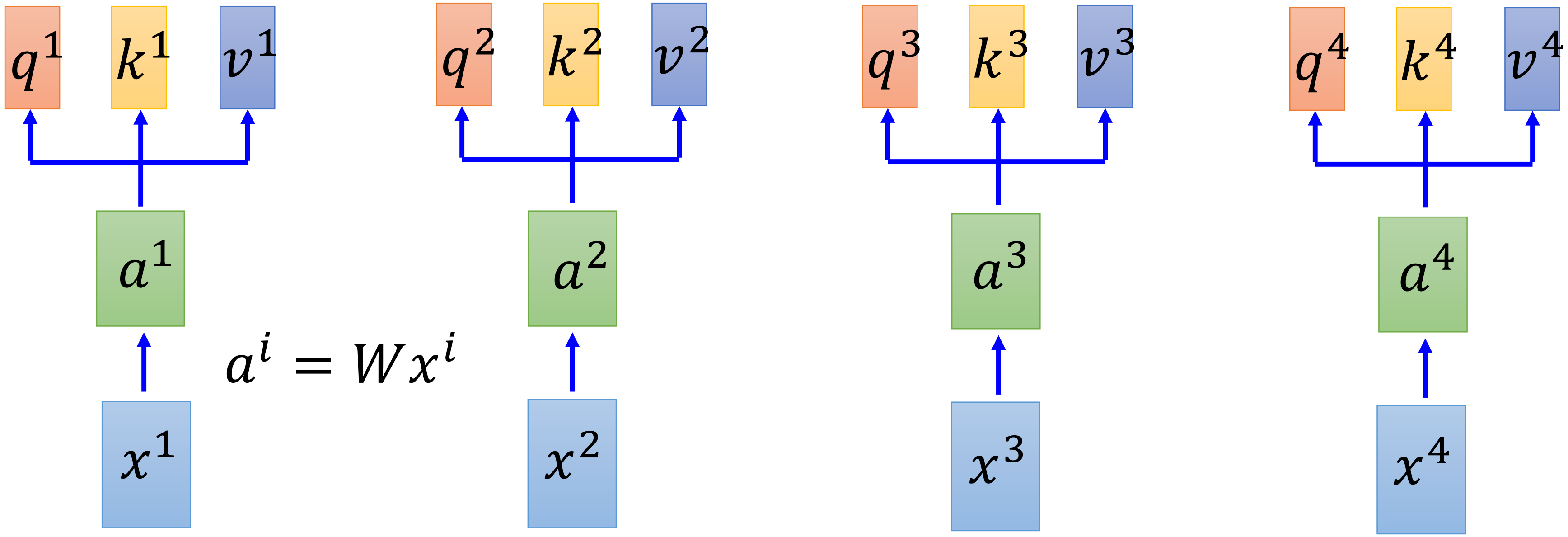
$$q^i = W^q a^i$$

k: key (to be matched)

$$k^i = W^k a^i$$

v: information to be extracted

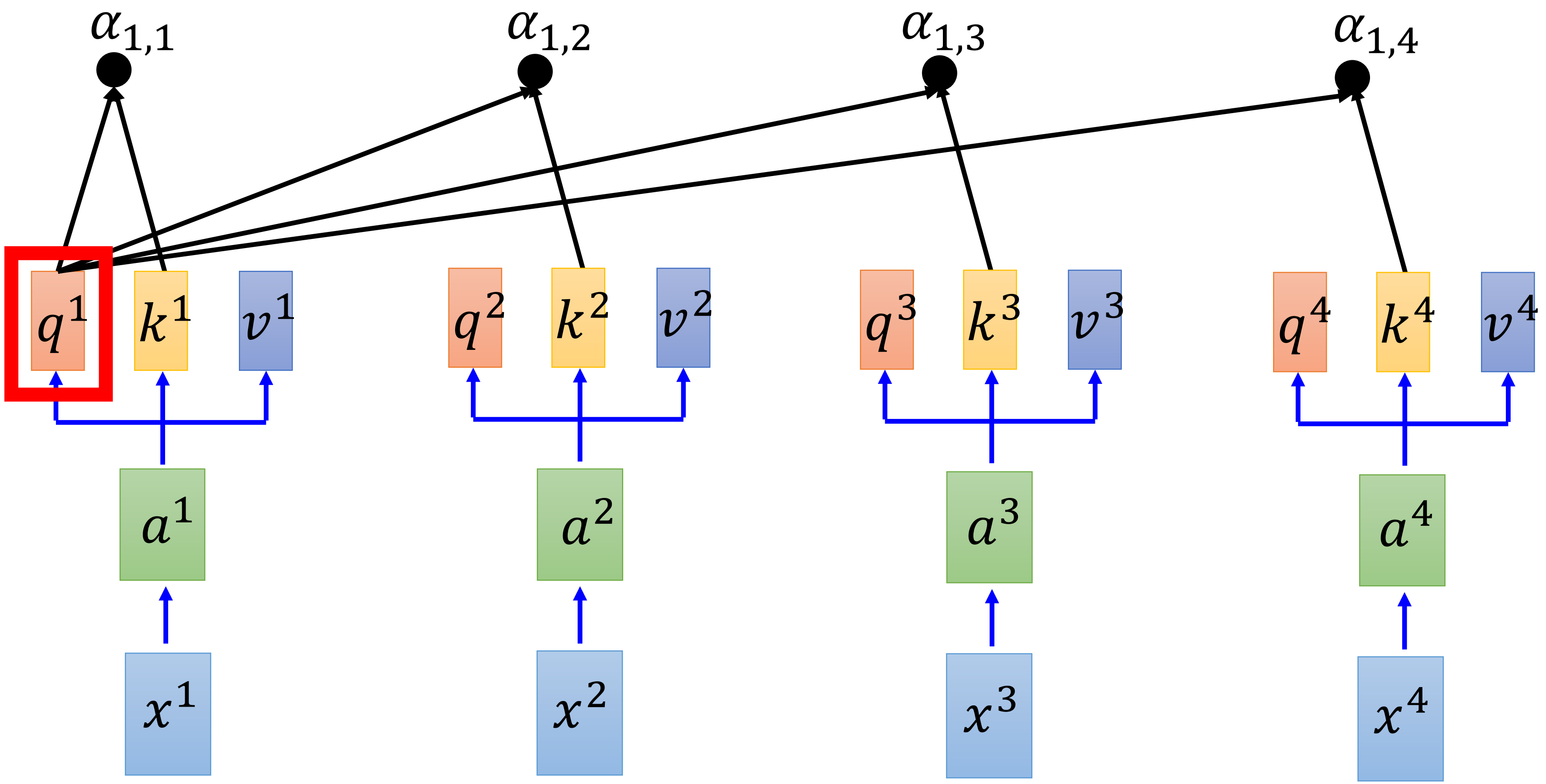
$$v^i = W^v a^i$$



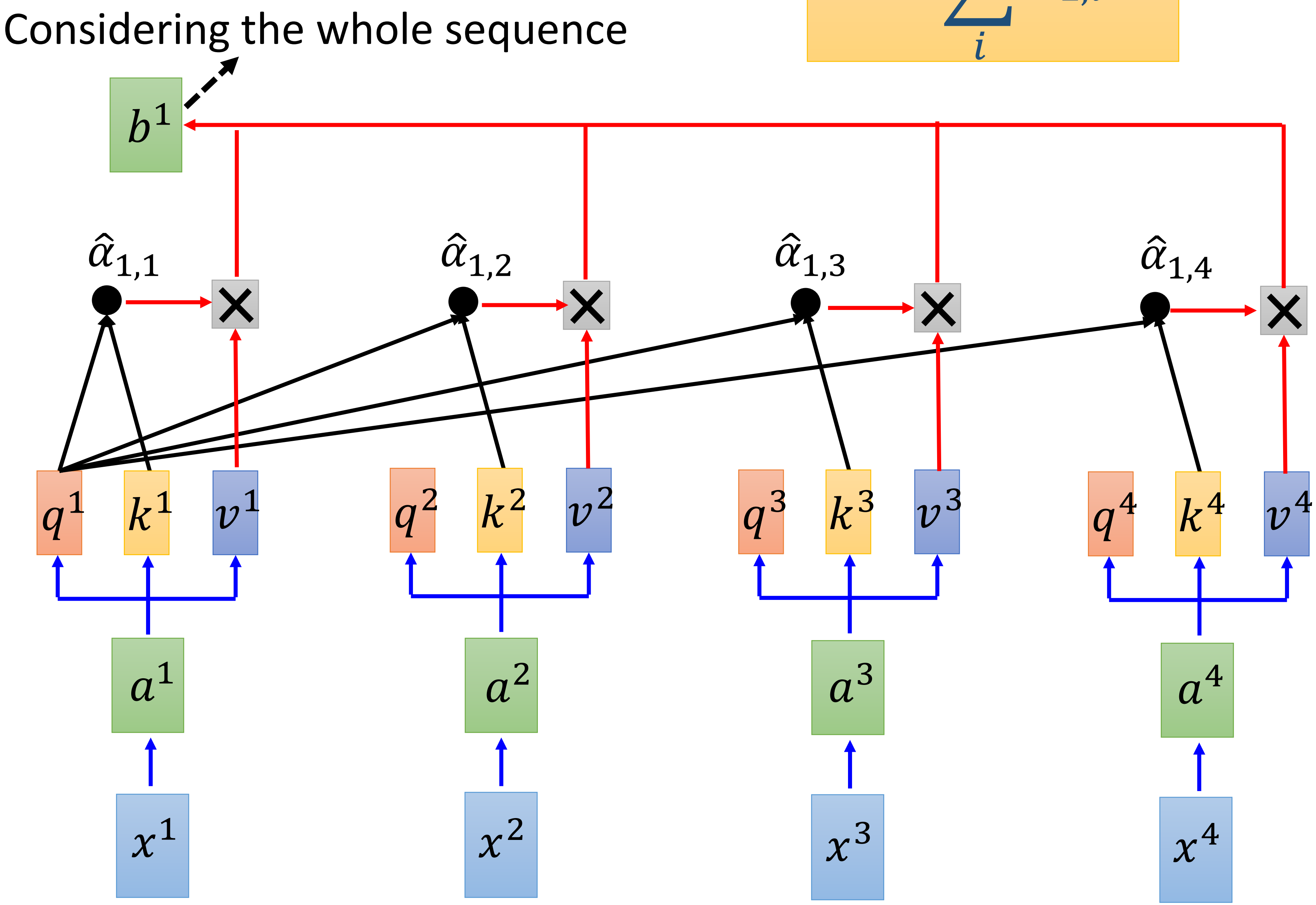
Scaled Dot-Product Attention

d is the dim of q and k

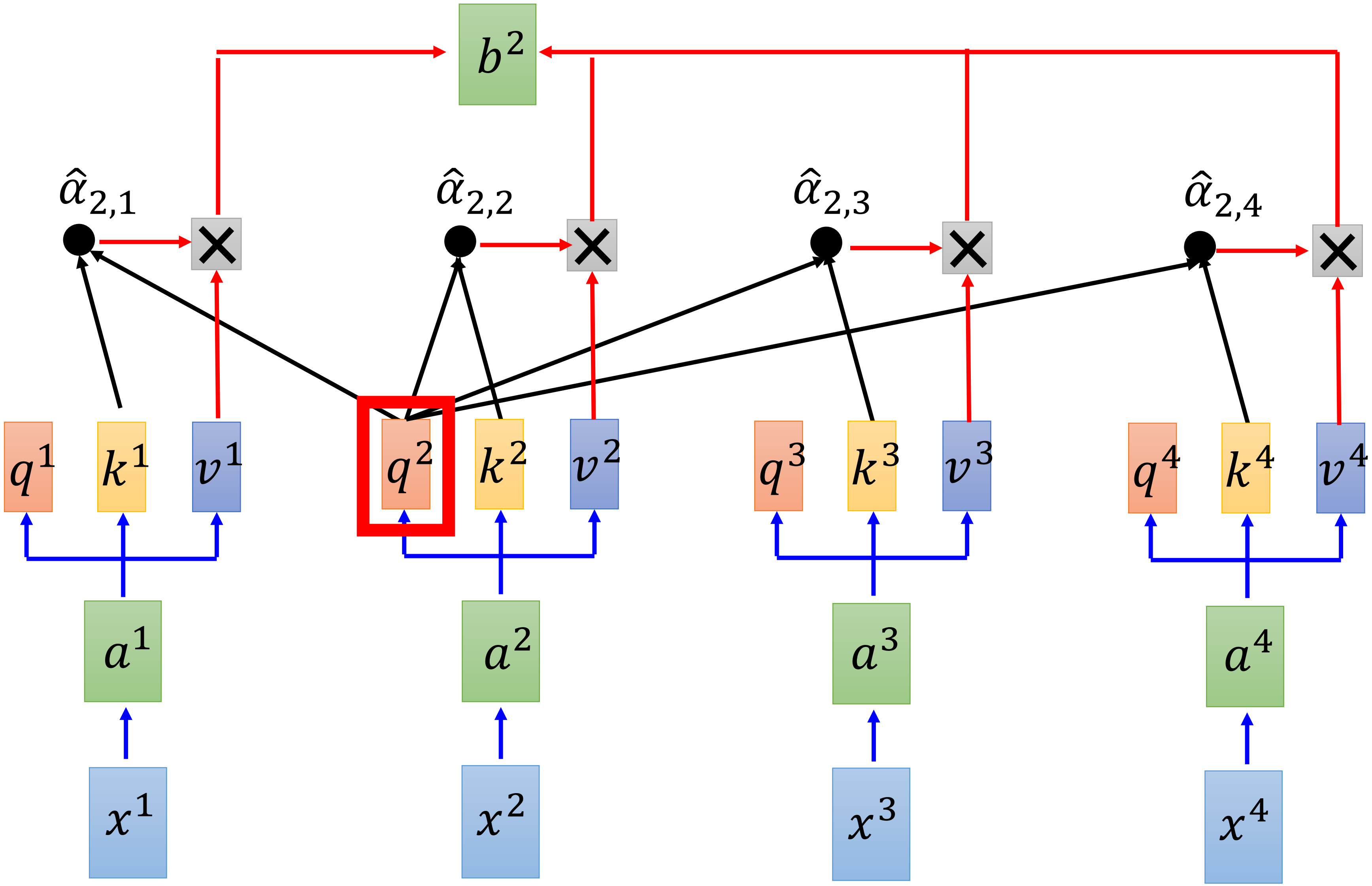
$$\alpha_{1,i} = \underbrace{q^1 \cdot k^i}_{\text{dot product}} / \sqrt{d}$$



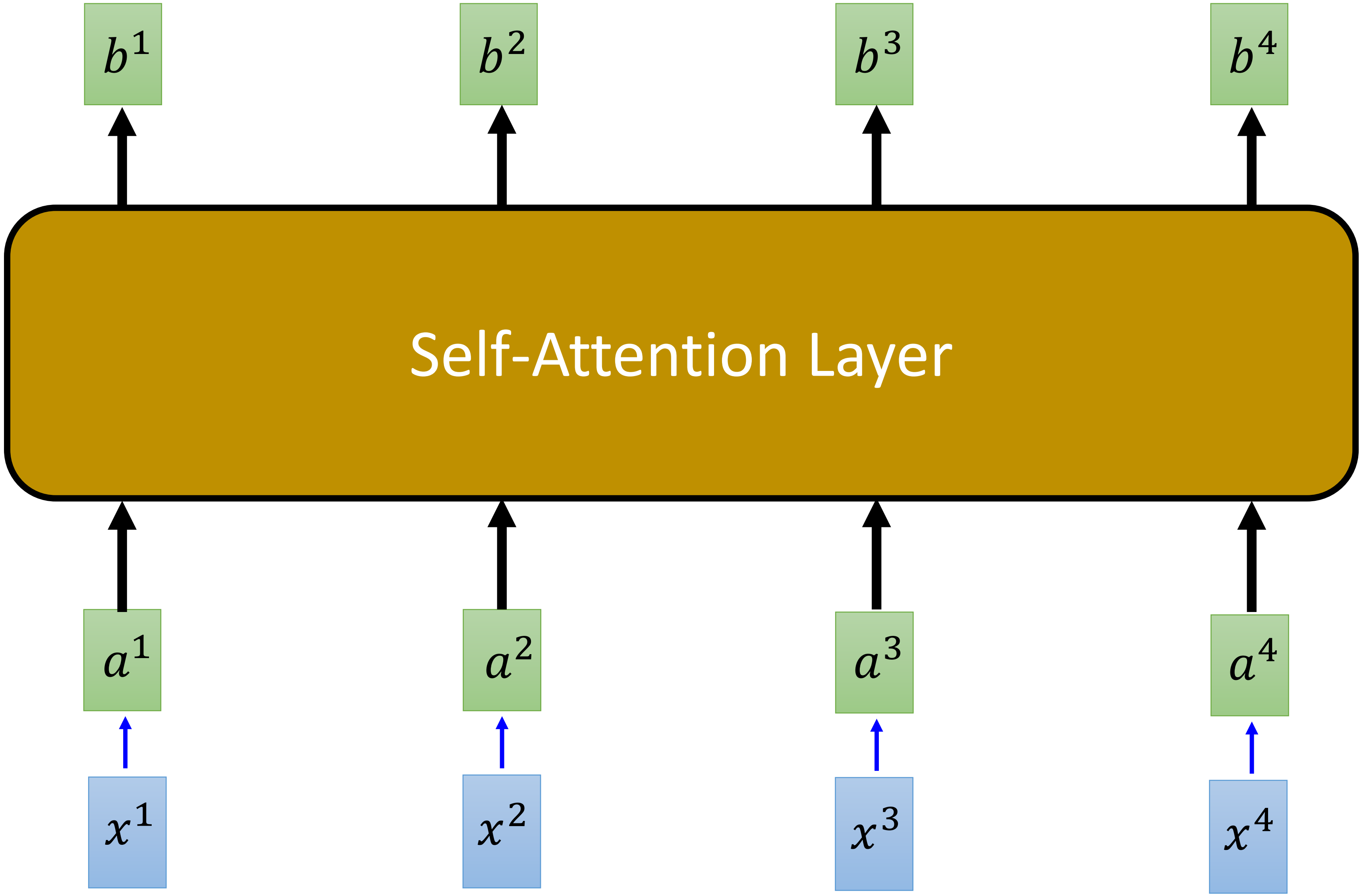
$$b^1 = \sum_i \hat{\alpha}_{1,i} v^i$$



$$b^2 = \sum_i \hat{\alpha}_{2,i} v^i$$



b^1, b^2, b^3, b^4 can be computed in parallel.



$$q^i = W^q a^i$$

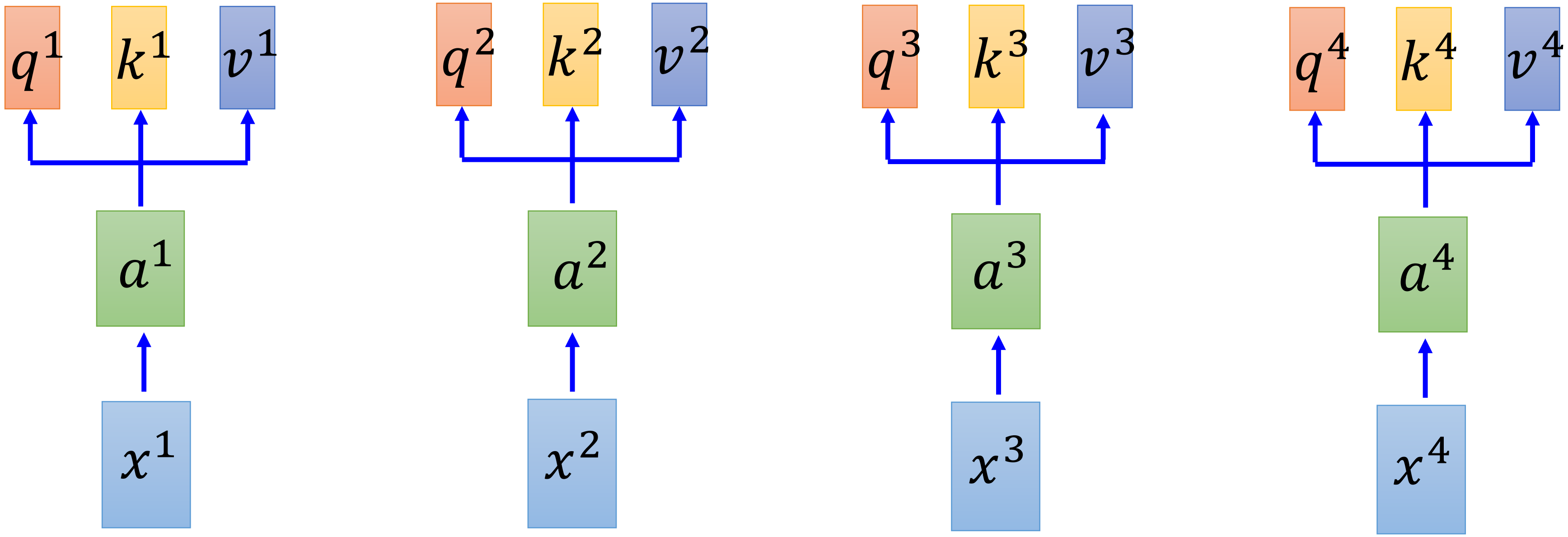
$$k^i = W^k a^i$$

$$v^i = W^v a^i$$

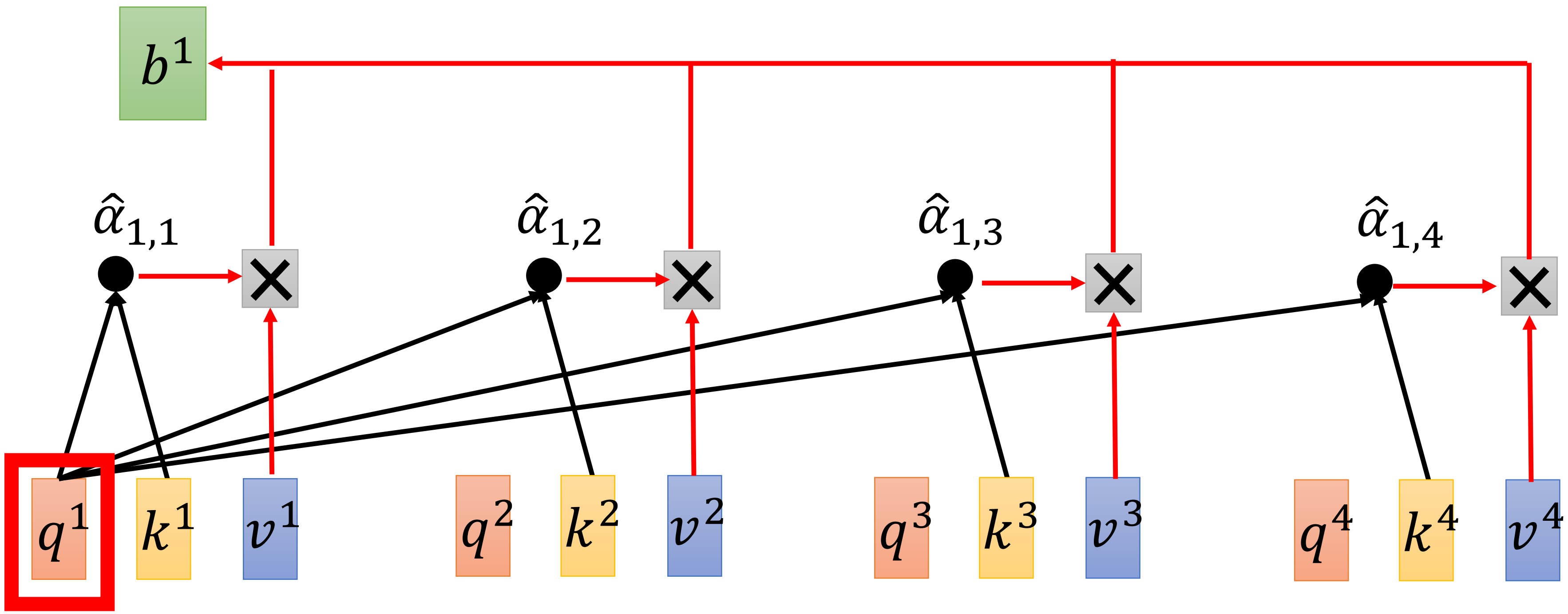
$$\underset{Q}{\begin{bmatrix} q^1 & q^2 & q^3 & q^4 \end{bmatrix}} = W^q \underset{I}{\begin{bmatrix} a^1 & a^2 & a^3 & a^4 \end{bmatrix}}$$

$$\underset{K}{\begin{bmatrix} k^1 & k^2 & k^3 & k^4 \end{bmatrix}} = W^k \underset{I}{\begin{bmatrix} a^1 & a^2 & a^3 & a^4 \end{bmatrix}}$$

$$\underset{V}{\begin{bmatrix} v^1 & v^2 & v^3 & v^4 \end{bmatrix}} = W^v \underset{I}{\begin{bmatrix} a^1 & a^2 & a^3 & a^4 \end{bmatrix}}$$



Self-attention



$\alpha_{1,1} = k^1 \; q^1$ $\quad \alpha_{1,2} = k^2 \; q^1$

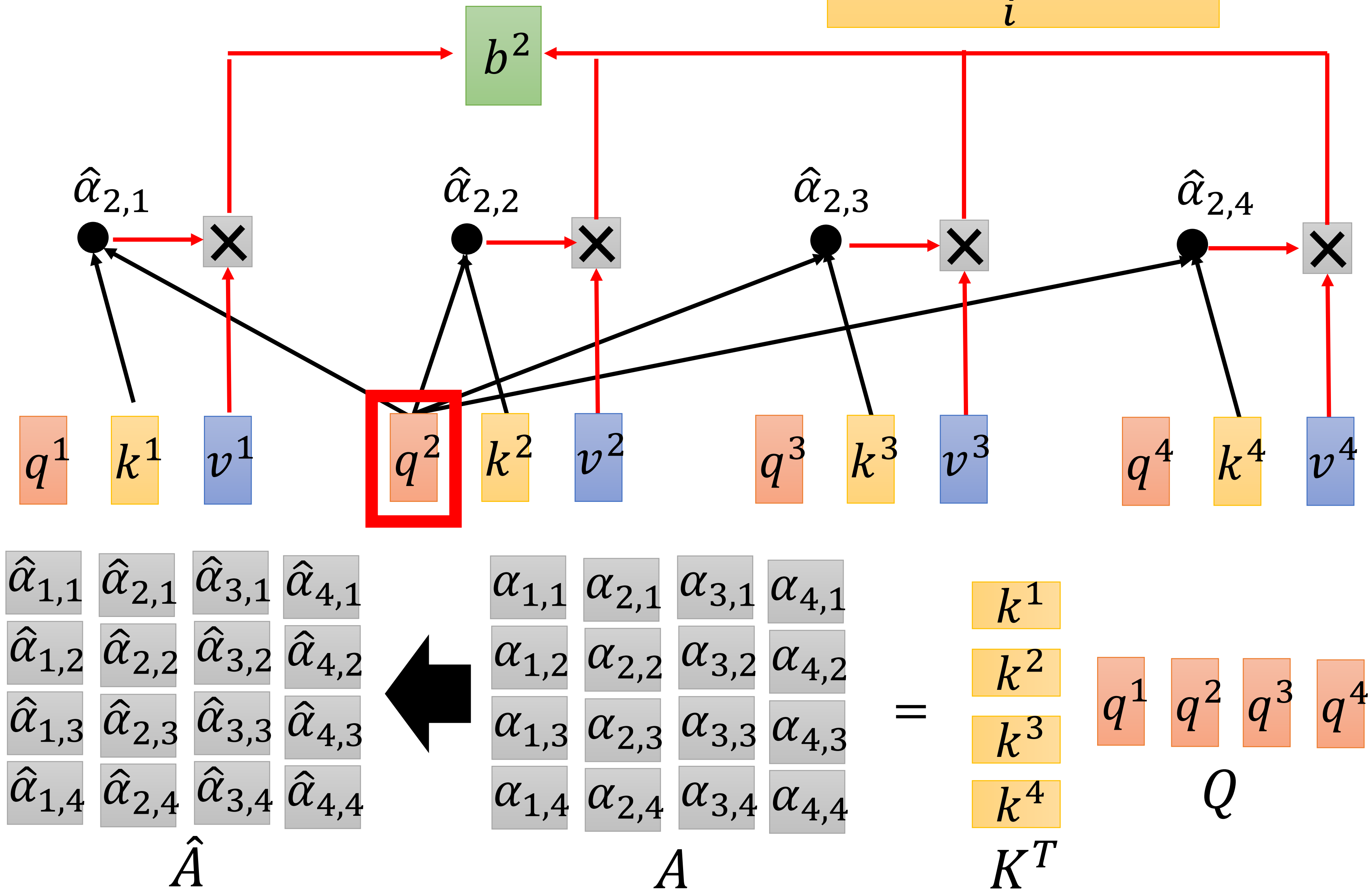
$\alpha_{1,3} = k^3 \; q^1$ $\quad \alpha_{1,4} = k^4 \; q^1$

$$\begin{bmatrix} \alpha_{1,1} \\ \alpha_{1,2} \\ \alpha_{1,3} \\ \alpha_{1,4} \end{bmatrix} = \begin{bmatrix} k^1 \\ k^2 \\ k^3 \\ k^4 \end{bmatrix} q^1$$

(ignore $\sqrt{d}$ for simplicity)

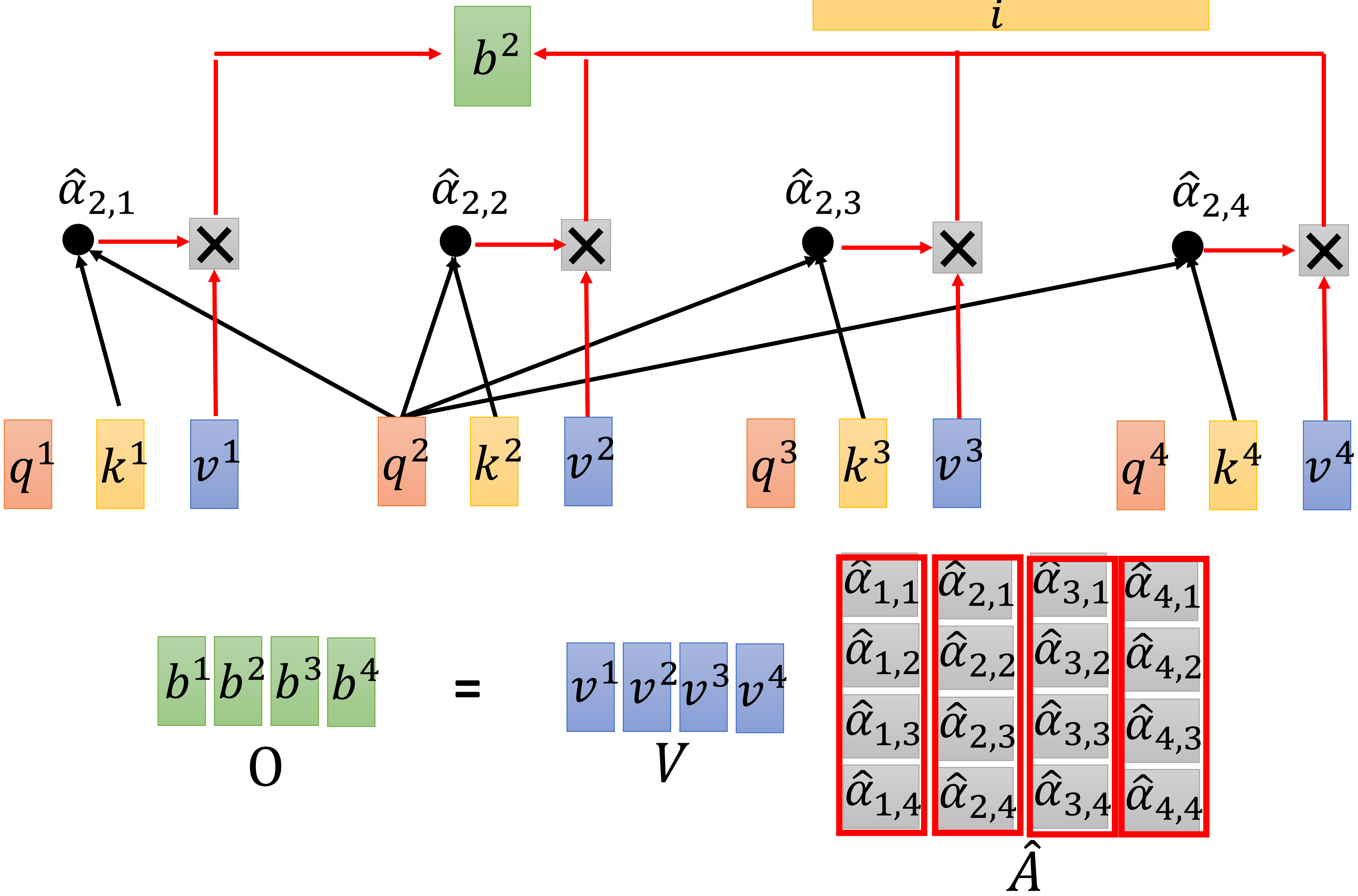
Self-attention

$$b^2 = \sum_i \hat{\alpha}_{2,i} v^i$$

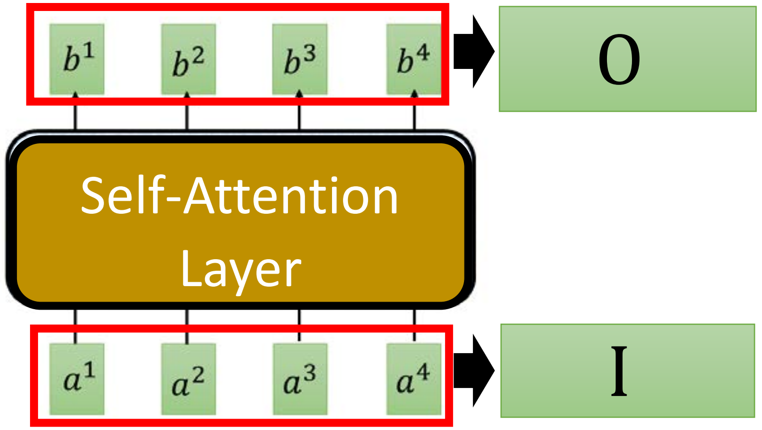


Self-attention

$$b^2 = \sum_i \hat{\alpha}_{2,i} v^i$$



Self-attention



$$Q = W^q I$$

$$K = W^k I$$

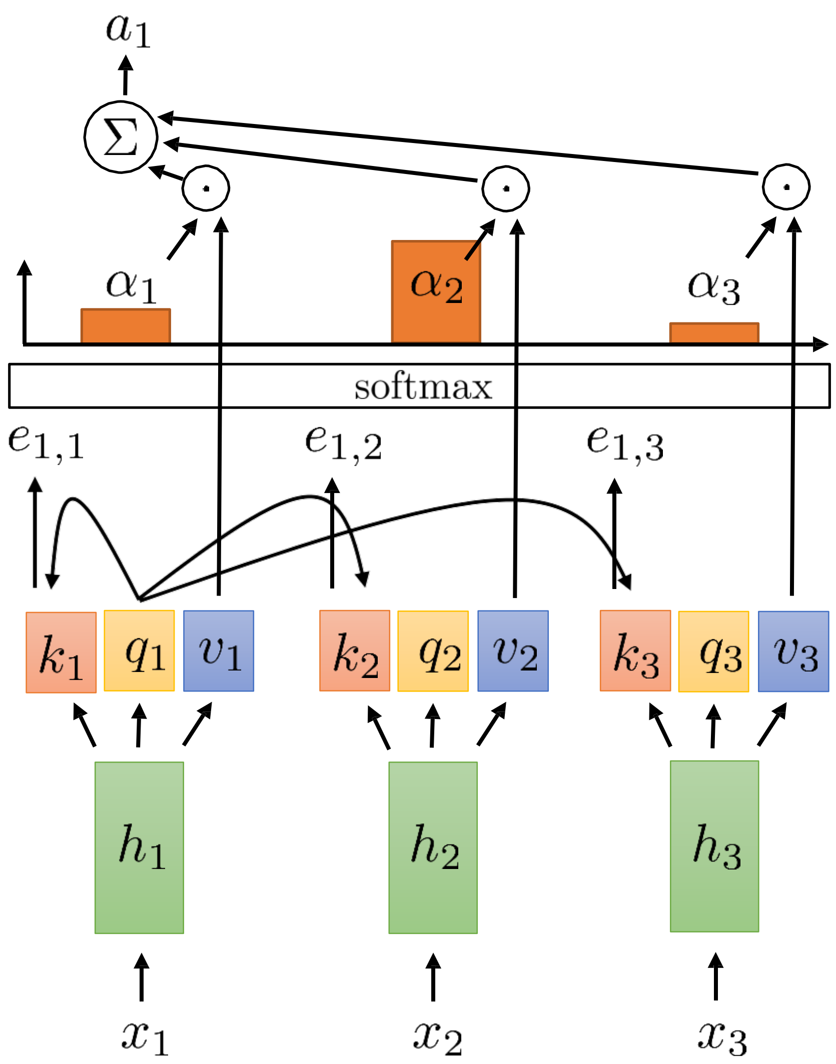
$$V = W^v I$$

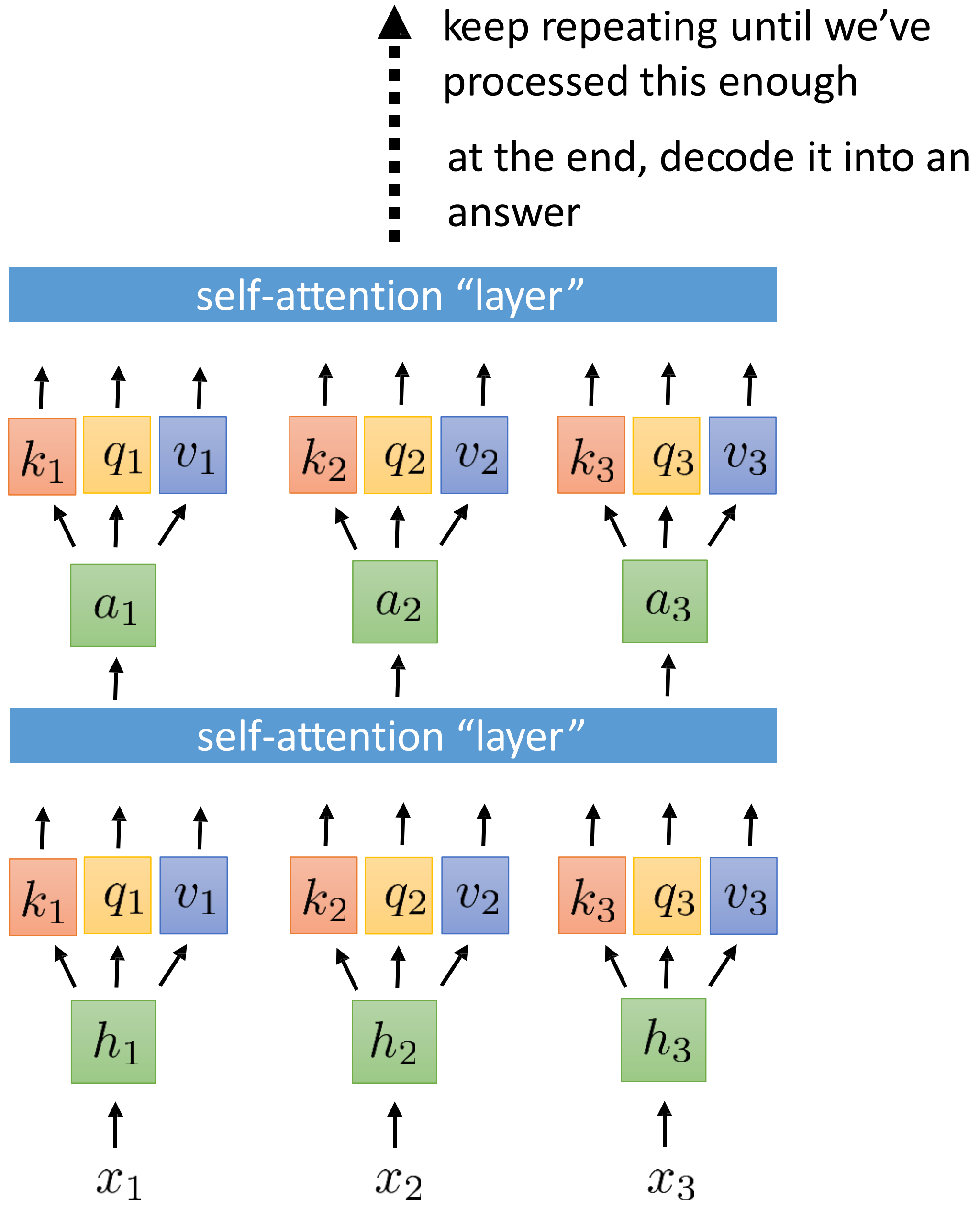
$$A = K^T Q$$

$$\hat{A} \Leftarrow A$$

$$O = V \hat{A}$$

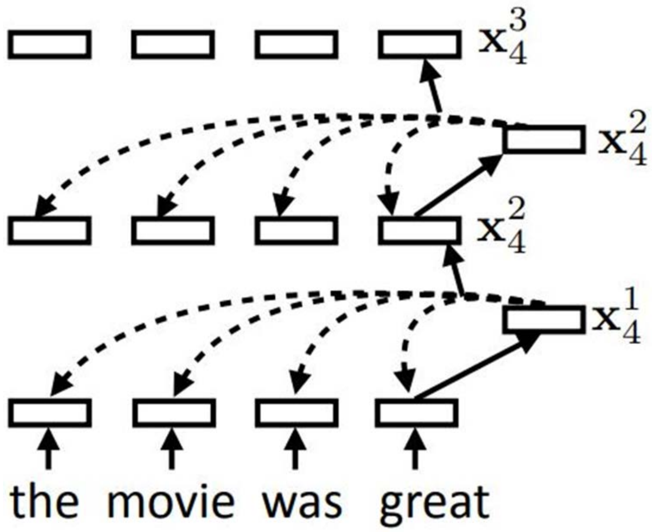
Self-Attention





Multiple Attention Heads

- Multiple attention heads can learn to attend in different ways
- Requires additional parameters to compute different attention values and transform vectors



k : level number

L: number of heads

$X = \mathbf{x}_1, \ldots, \mathbf{x}_n$

$\mathbf{x}_i^1 = \mathbf{x}_i$

$$\bar{\alpha}_{i,j}^{k,l} = \mathbf{x}_i^{k-1} \mathbf{W}^{k,l}\, \mathbf{x}_j^{k-1}$$

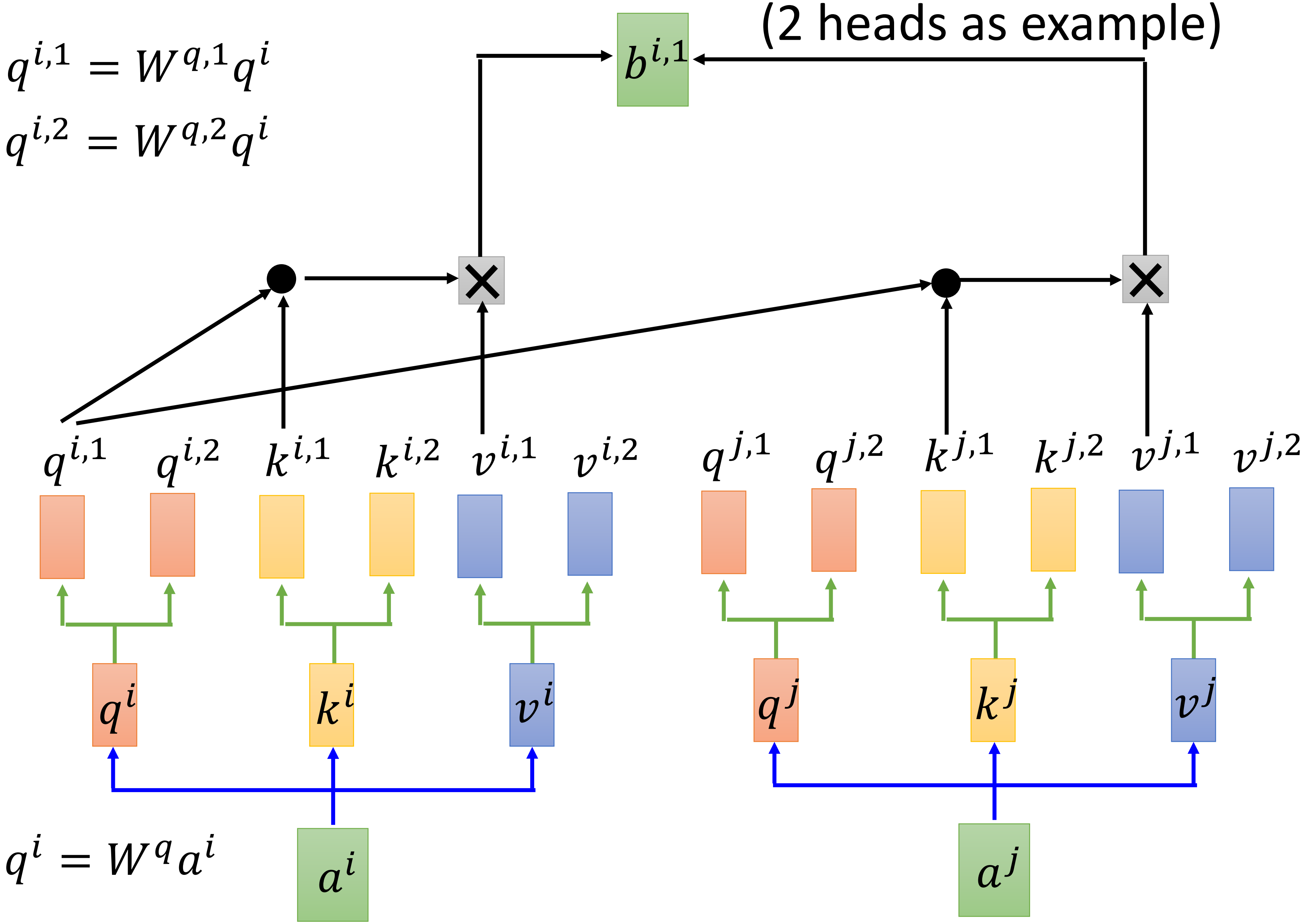
$$\alpha_i^{k,l} = \mathrm{softmax}(\bar{\alpha}_{i,1}^{k,l}, \ldots, \bar{\alpha}_{i,n}^{k,l})$$

$$x_i^{k,l} = \sum_{i=1}^{n} \alpha_{i,j}^{k,l} \mathbf{x}_j^{k-1}$$

$$\mathbf{x}_i^k = V^k[\mathbf{x}_i^{k,1}; \ldots ; \mathbf{x}_i^{k,L}]$$

Multi-head Self-attention

(2 heads as example)

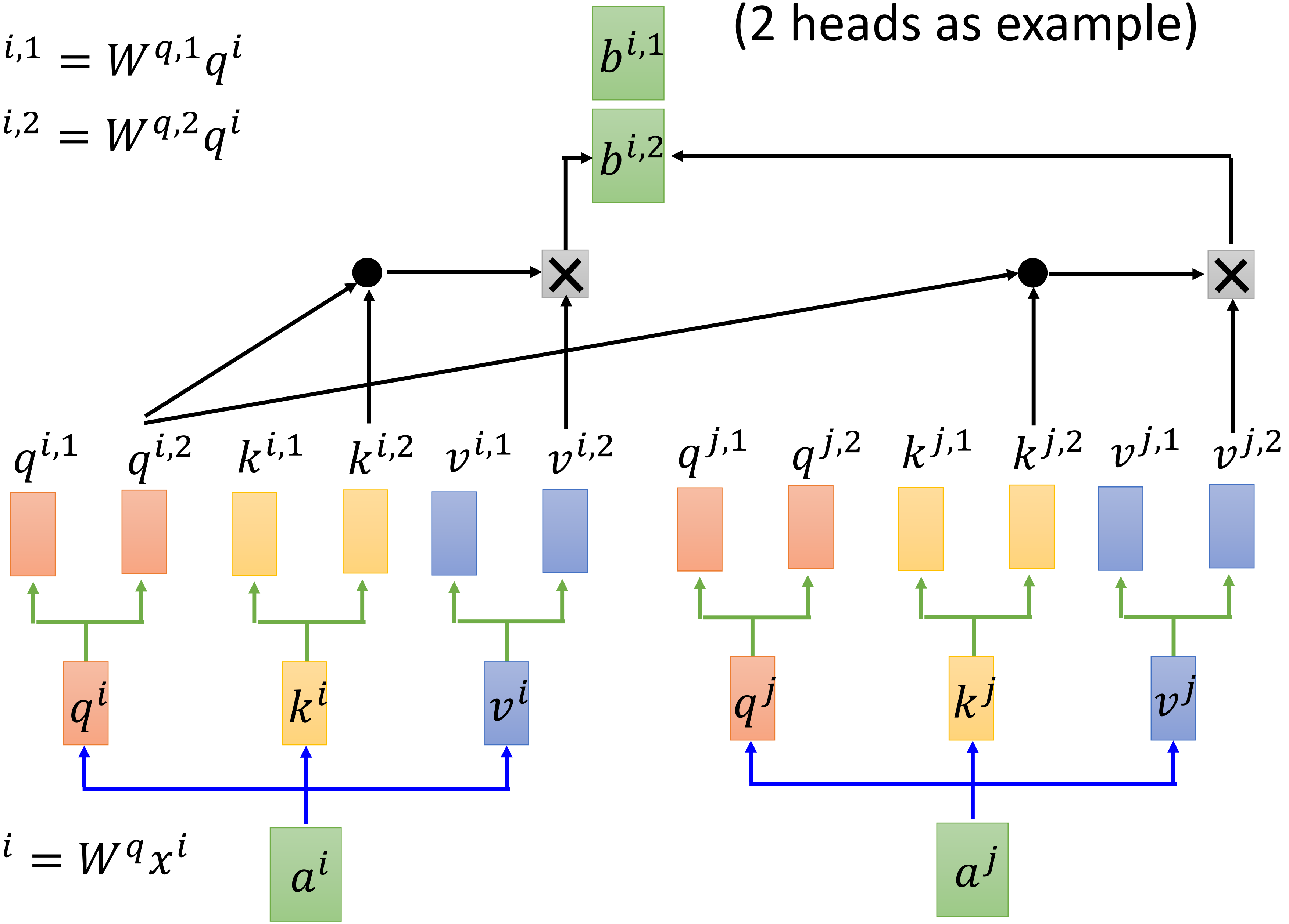


Multi-head Self-attention

(2 heads as example)

$$q^{i,1} = W^{q,1} q^i$$

$$q^{i,2} = W^{q,2} q^i$$

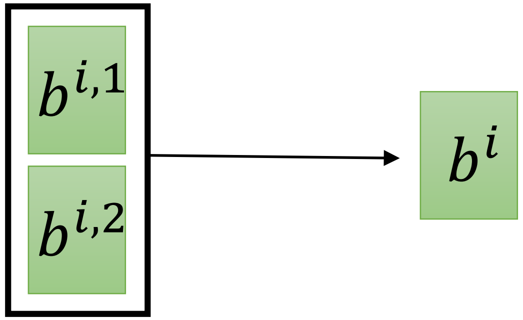


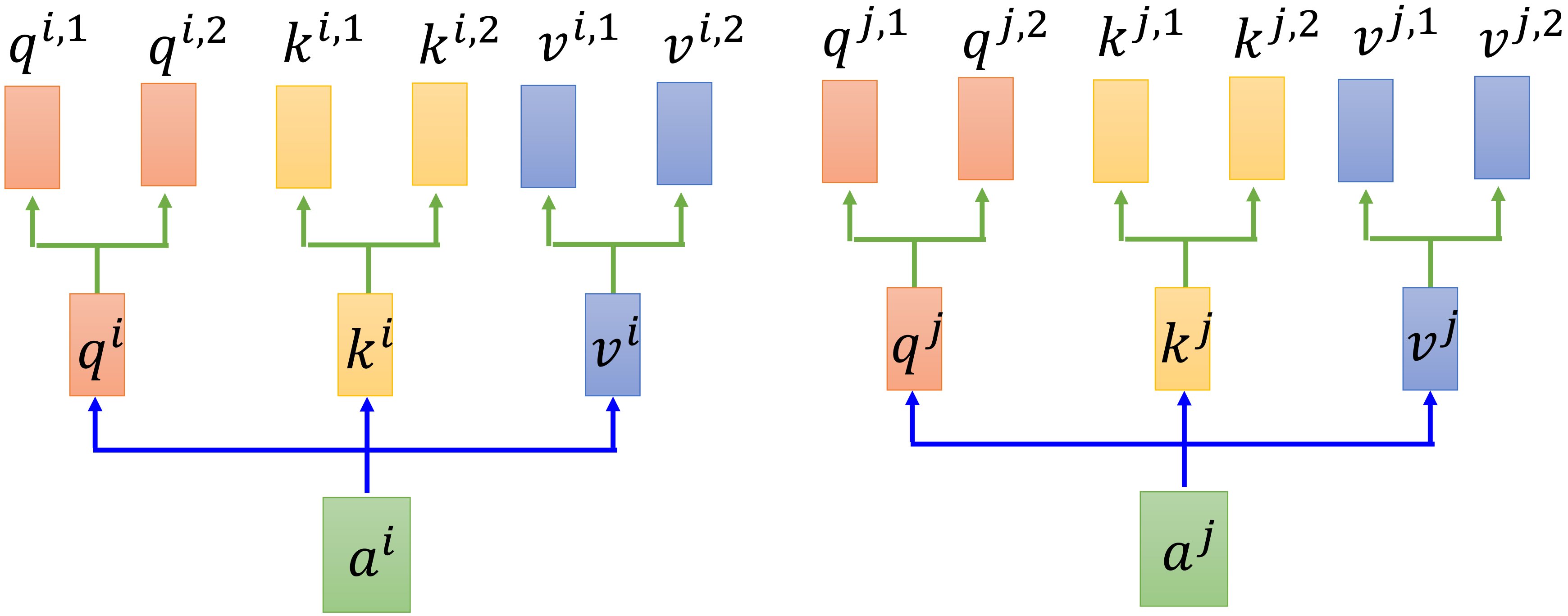
$$q^i = W^q x^i$$

Multi-head Self-attention

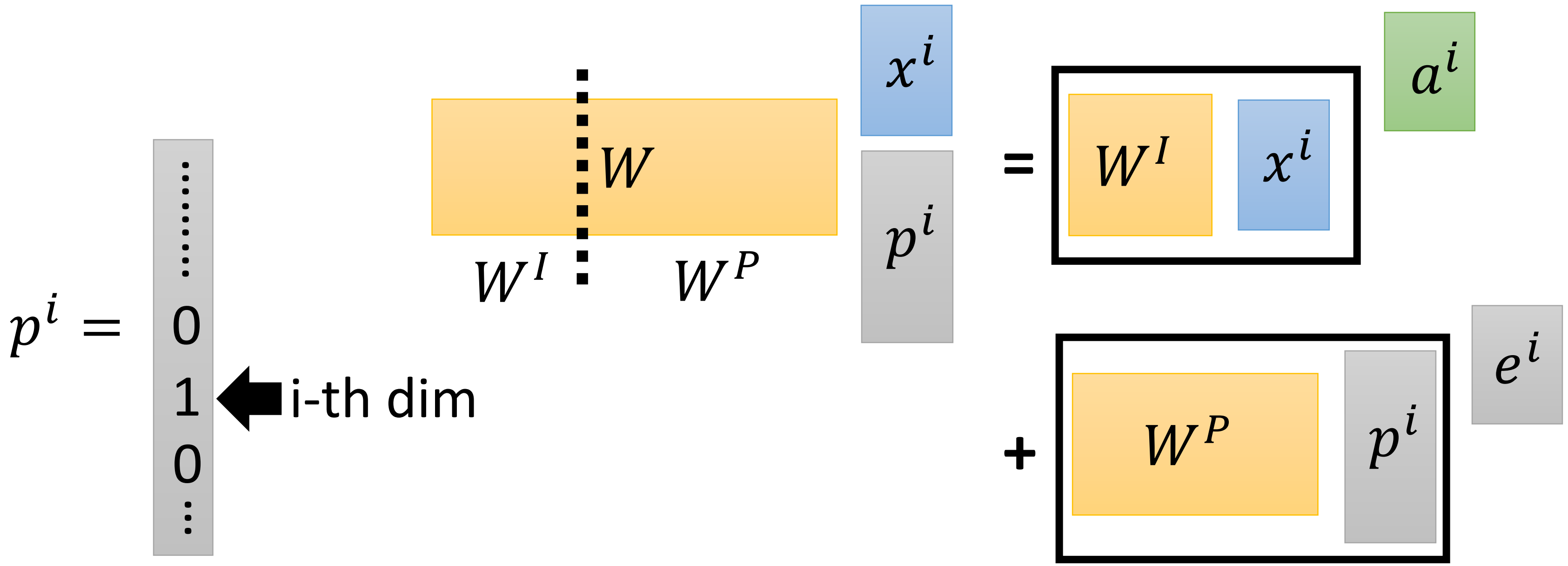
(2 heads as example)

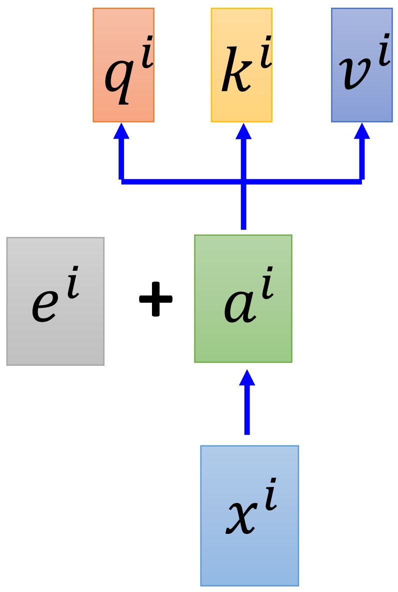
$$b^i = W^O \begin{bmatrix} b^{i,1} \\ b^{i,2} \end{bmatrix}$$





Positional Encoding

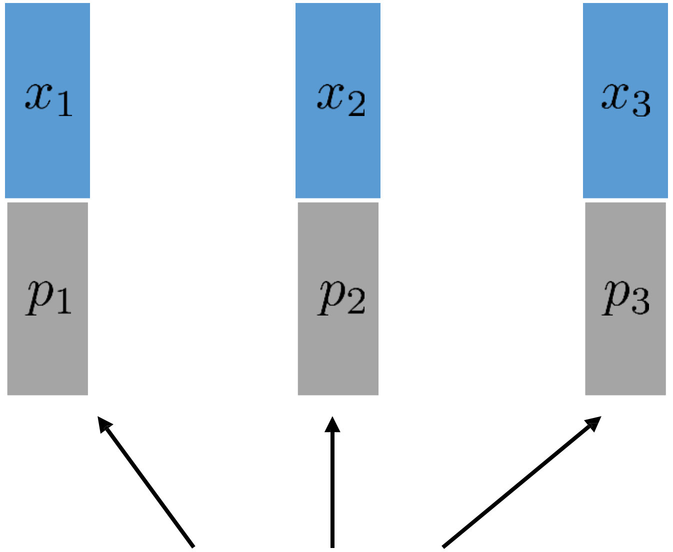




- Each position has a unique positional vector e^i (not learned from data)
- each x^i appends a one-hot vector p^i orr add them

Positional encoding: learned

Another idea: just learn a positional encoding



Different for every input sequence

The same learned values for every sequence

but different for different time steps

dimensionality

max sequence length

How many values do we need to learn?

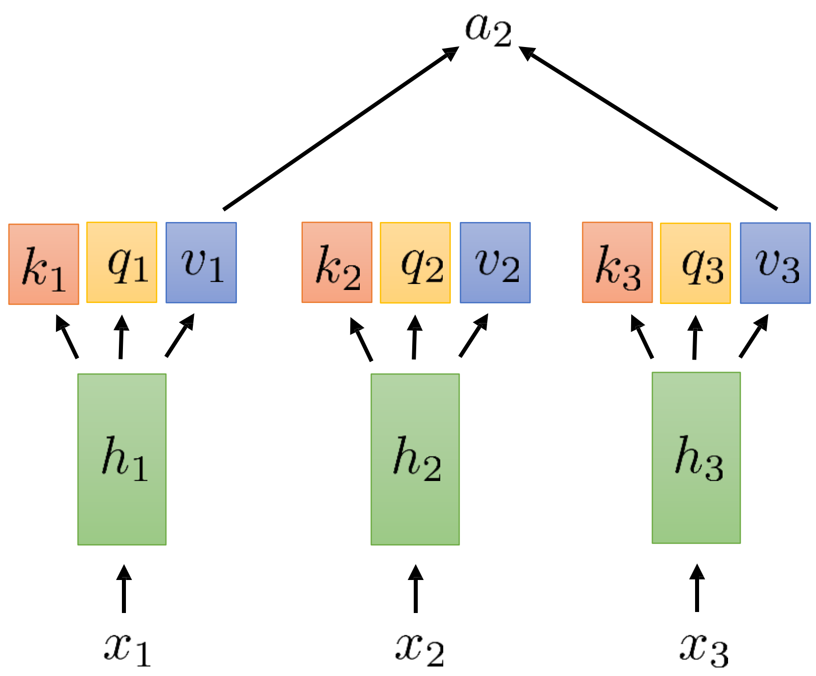
$$P = [p_1, p_2, \ldots, p_T] \in R^{d \times T}$$

+ more flexible (and perhaps more optimal) than sin/cos encoding

+ a bit more complex, need to pick a max sequence length (and can't generalize beyond it)

Multi-head attention

Since we are relying **entirely** on attention now, we might want to incorporate **more than one** time step



$$a_l = \sum_t \alpha_{l,t} v_t$$

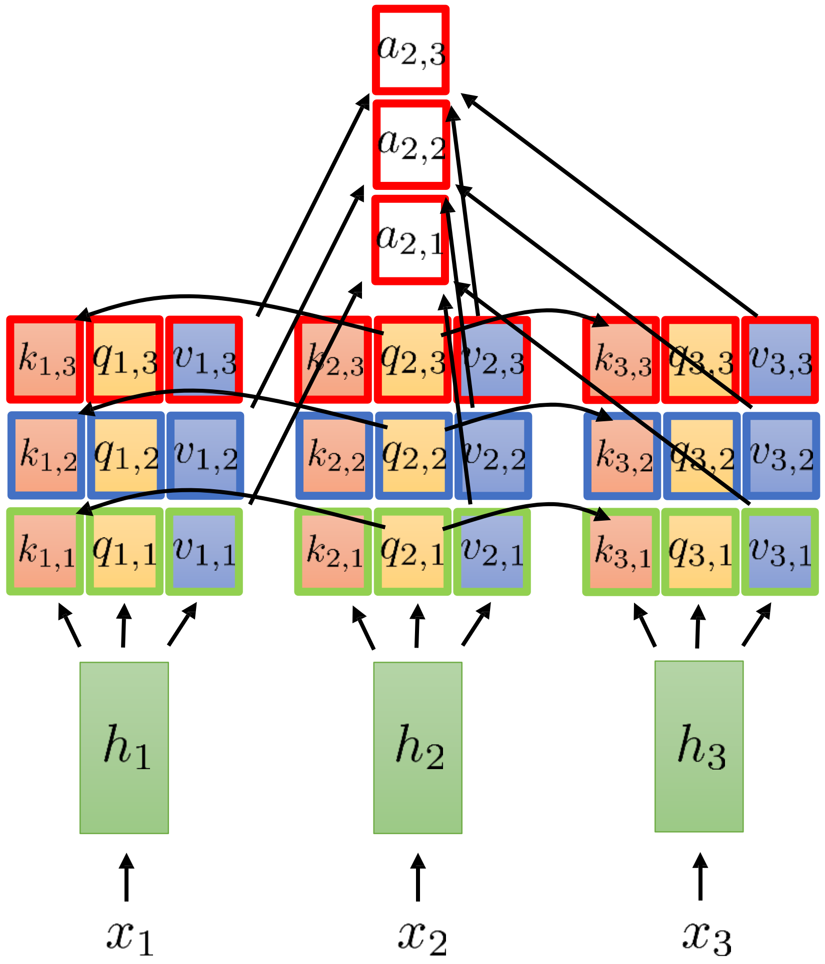
because of softmax, this will be dominated by one value

$$e_{l,t} = q_l \cdot k_t$$

hard to specify that you want two different things (e.g., the subject and the object in a sentence)

Multi-head attention

Idea: have multiple keys, queries, and values for every time step!



full attention vector formed by concatenation:

$$a_2 = \begin{bmatrix} a_{2,1} \\ a_{2,2} \\ a_{2,3} \end{bmatrix}$$

compute weights **independently** for each head

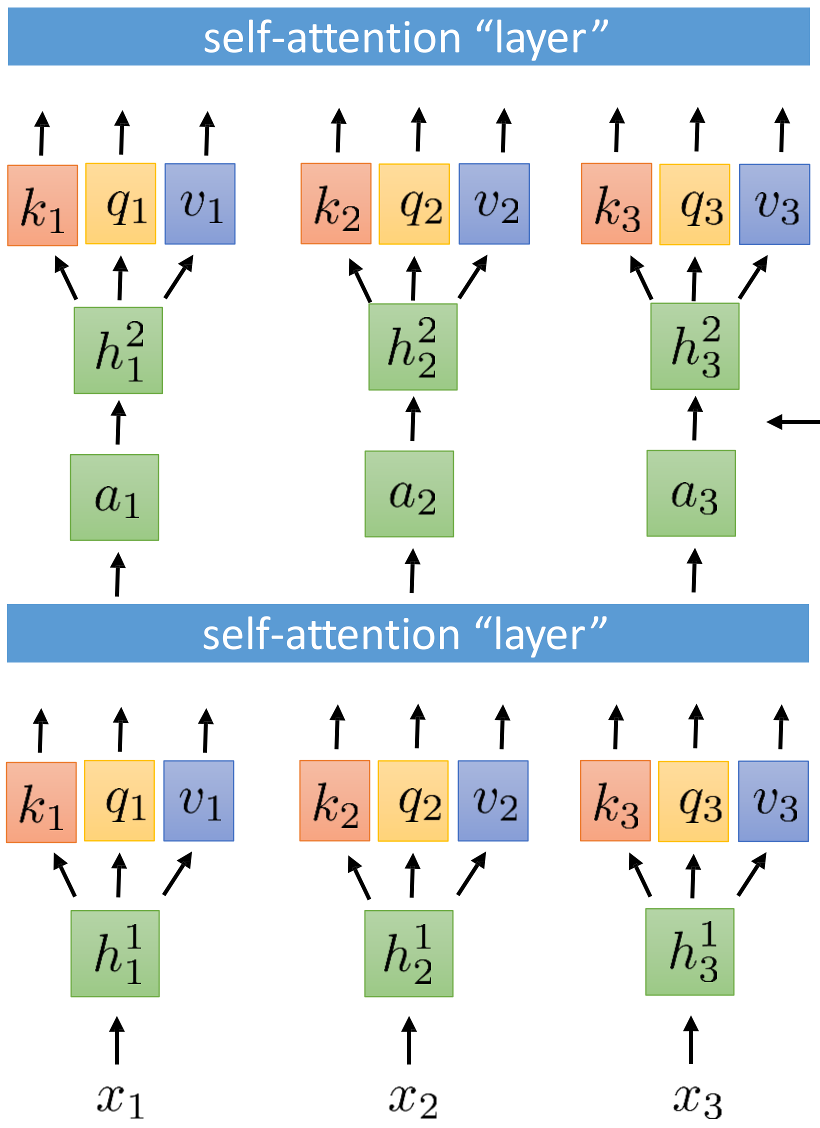
$$e_{l,t,i} = q_{l,i} \cdot k_{l,i}$$

$$\alpha_{l,t,i} = \exp(e_{l,t,i}) / \sum_{t'} \exp(e_{l,t',i})$$

$$a_{l,i} = \sum_t \alpha_{l,t,i} v_{t,i}$$

around **8** heads seems to work pretty well for big models

Alternating self-attention & nonlinearity



some non-linear (learned) function
e.g., $h_t^\ell = \sigma(W^\ell a_t^\ell + b^\ell)$

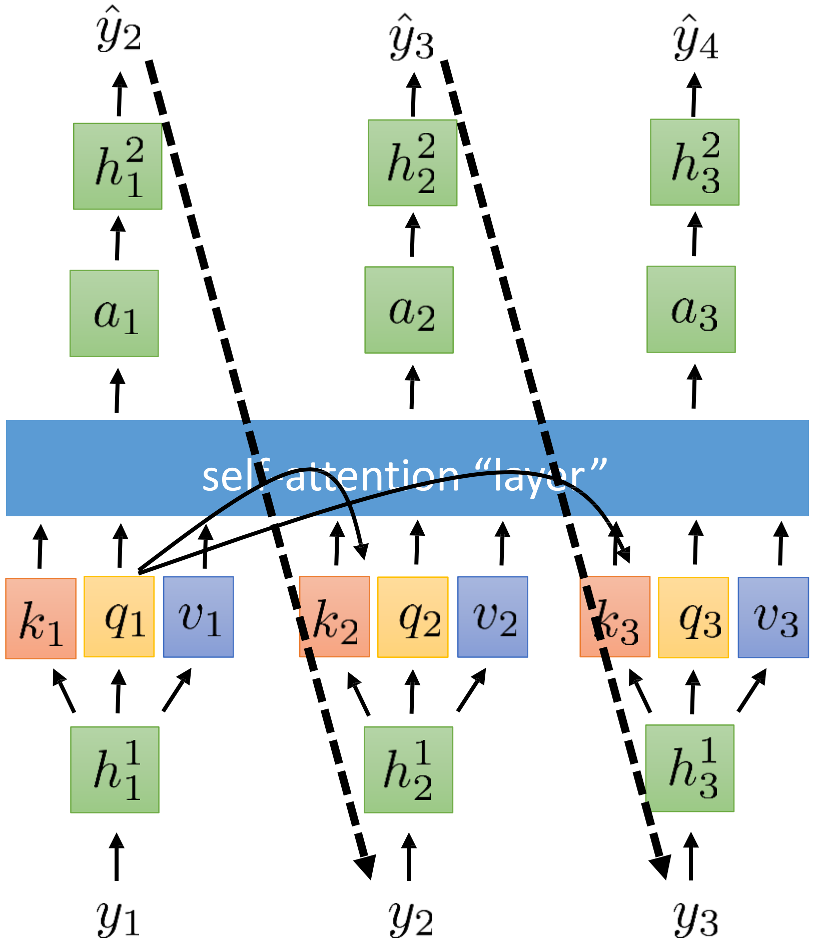
just a neural net applied at every position after every self-attention layer!

Sometimes referred to as "position-wise feedforward network"

We'll describe some specific commonly used choices shortly

Self-attention can see the future!

A **crude** self-attention "language model":



(in reality, we would have many alternating self-attention layers and position-wise feedforward networks, not just one)

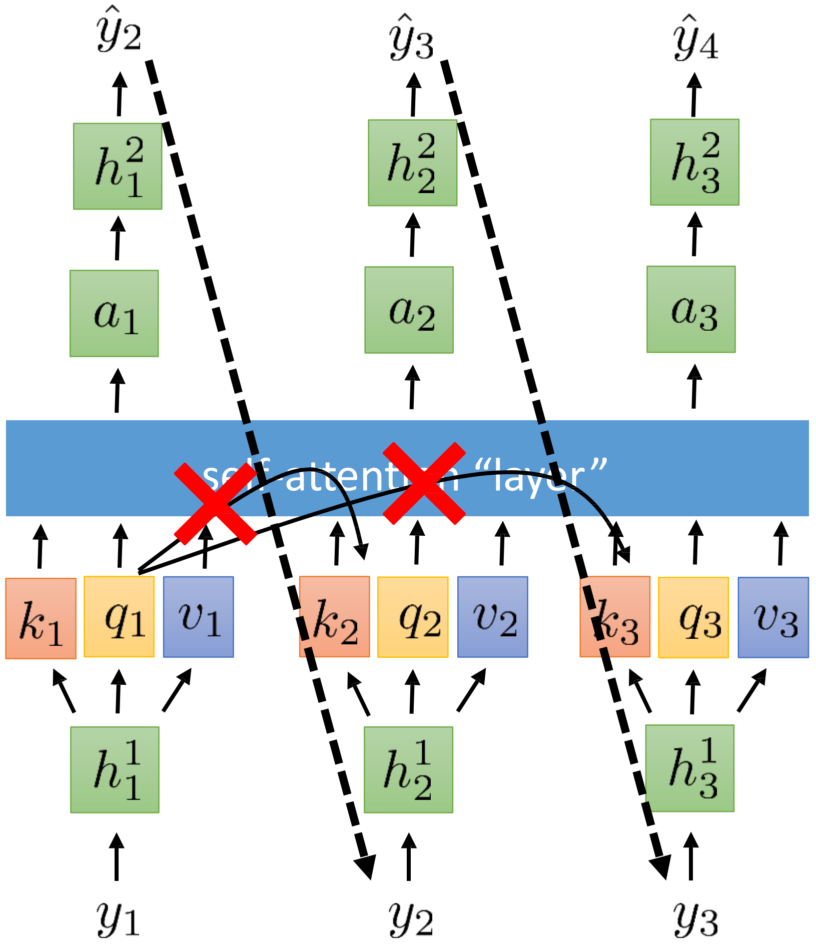
Big problem: self-attention at step 1 can look at the value at steps 2 & 3, which is based on the **inputs** at steps 2 & 3

At test time (when decoding), the **inputs** at steps 2 & 3 will be based on the output at step 1…

…which requires knowing the **input** at steps 2 & 3

Masked attention

A **crude** self-attention "language model":



At test time (when decoding), the **inputs** at steps 2 & 3 will be based on the output at step 1…

…which requires knowing the **input** at steps 2 & 3

Must allow self-attention into the **past**…

…but not into the **future**

Easy solution:

$$\cancel{e_{l,t} = q_l \cdot k_t}$$

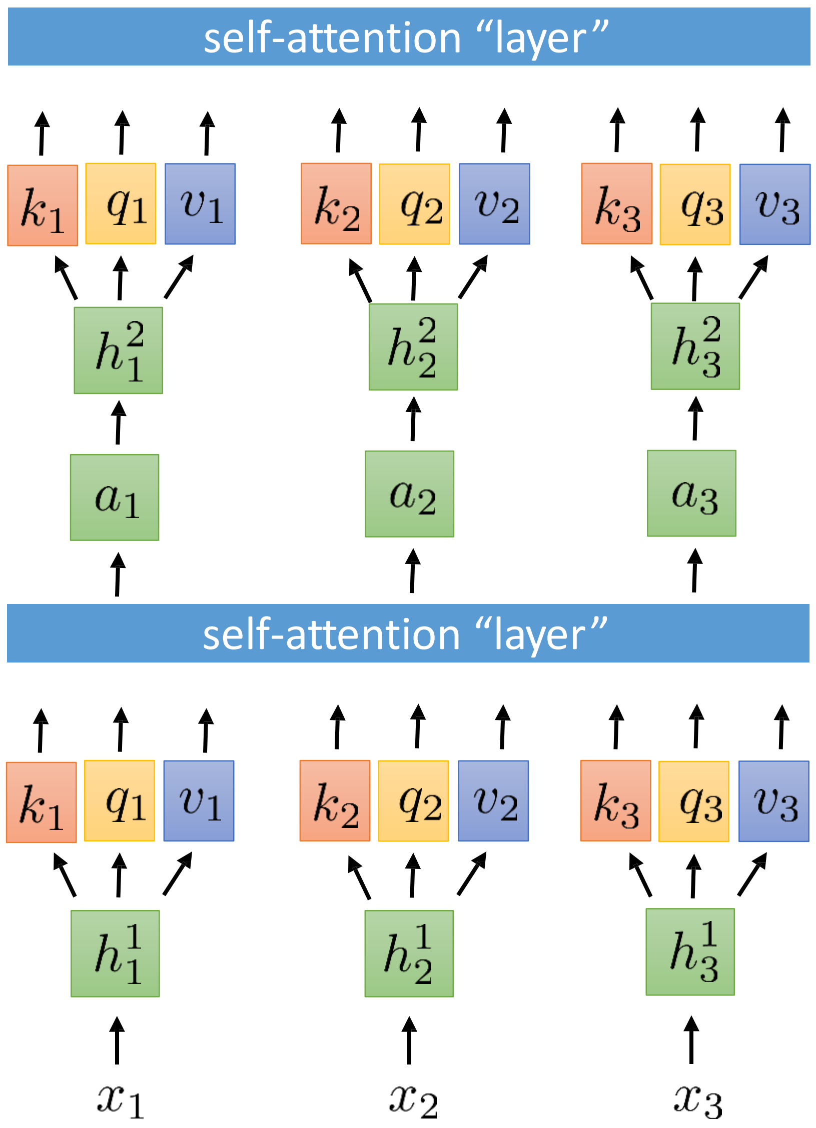
$$e_{l,t} = \begin{cases} q_l \cdot k_t & \text{if } l \geq t \\ -\infty & \text{otherwise} \end{cases}$$

in practice:

just replace $\exp(e_{l,t})$ with 0 if $l < t$

inside the softmax

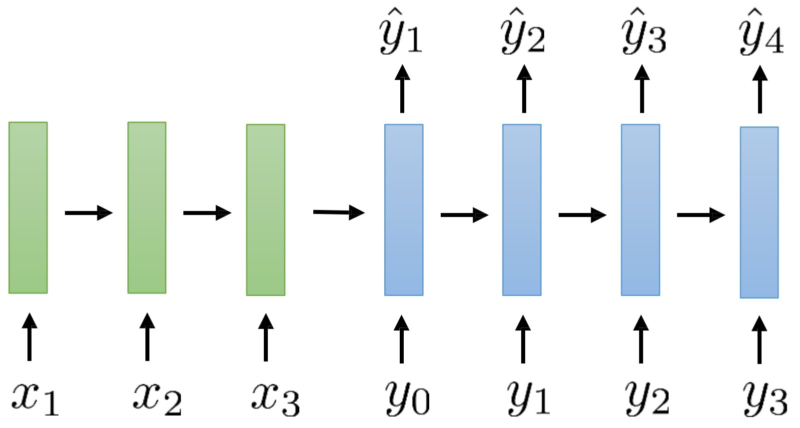
Transformer summary

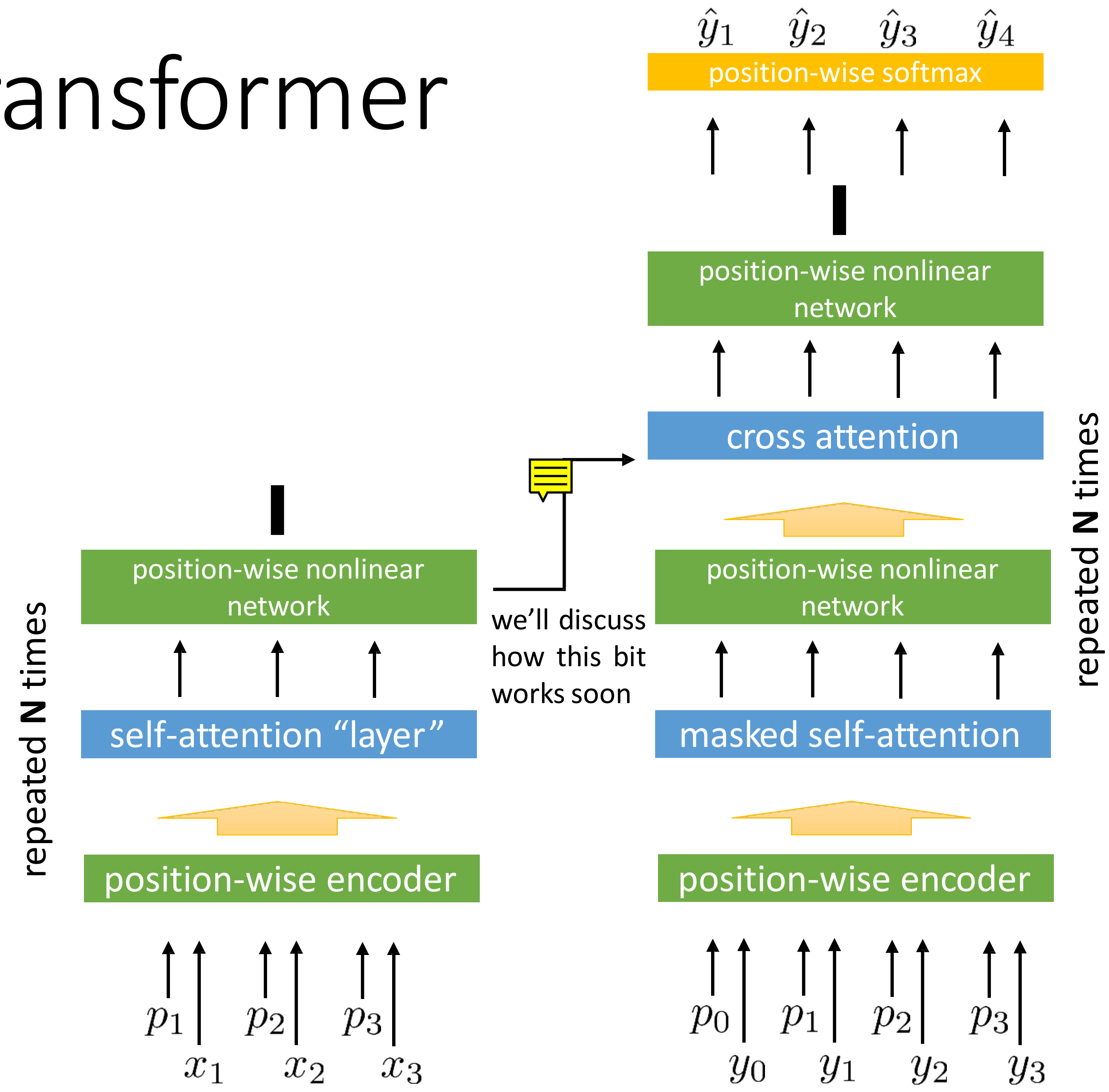


- These are generally called "Transformers" because they transform one sequence into another at each layer.
- Alternate self-attention "layers" with nonlinear position-wise feedforward networks (to get nonlinear transformations)
- Use positional encoding (on the input or input embedding) to make the model aware of relative positions of tokens
- Use multi-head attention
- Use masked attention if you want to use the model for decoding.

The “classic” transformer

As compared to a sequence
to sequence RNN model





The Final Linear and Softmax Layer

- A Softmax Layer to output word

- Let’s assume that our model knows 10,000 unique English words (our model’s “output vocabulary”) that it’s learned from its training dataset.

- The softmax layer then turns those scores into probabilities (all positive, all add up to 1.0). The cell with the highest probability is chosen, and the word associated with it is produced as the output for this time step.

Combining encoder and decoder values

"Cross-attention"

Much more like the **standard** attention from the previous lecture

$$\text{query:}\ \ q_l^\ell = W_q^\ell s_l^\ell$$

output of position-wise nonlinear network at (decoder) layer ℓ, step l

$$\text{key:}\ \ k_t^\ell = W_k^\ell h_t^\ell$$

output of position-wise nonlinear network at (encoder) layer ℓ, step t

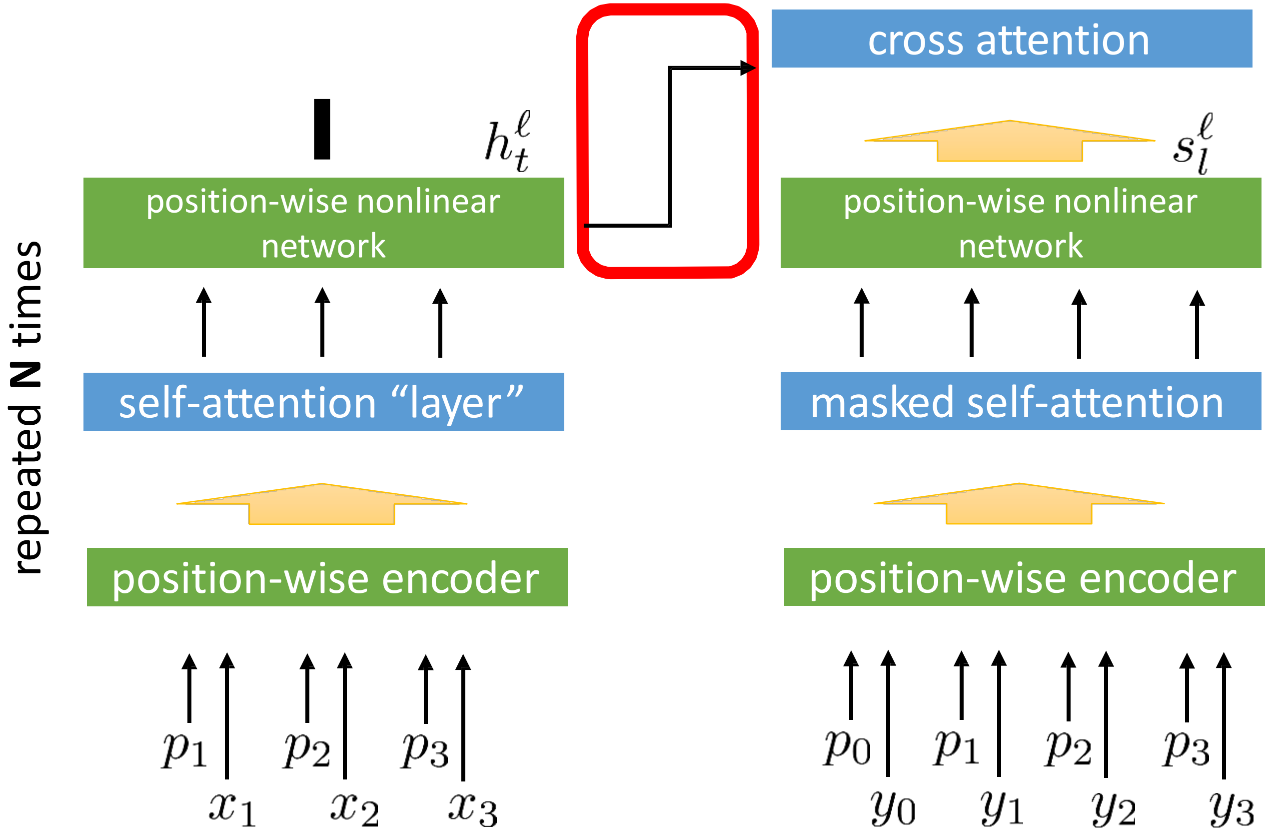
$$\text{value:}\ \ v_t^\ell = W_k^\ell h_t^\ell$$

$$e_{l,t}^\ell = q_l^\ell \cdot k_t^\ell$$

$$\alpha_{l,t}^\ell = \frac{\exp(e_{l,t}^\ell)}{\sum_{t'} \exp(e_{l,t'}^\ell)}$$

$$c_l^\ell = \sum_t \alpha_{l,t}^\ell v_t^\ell$$

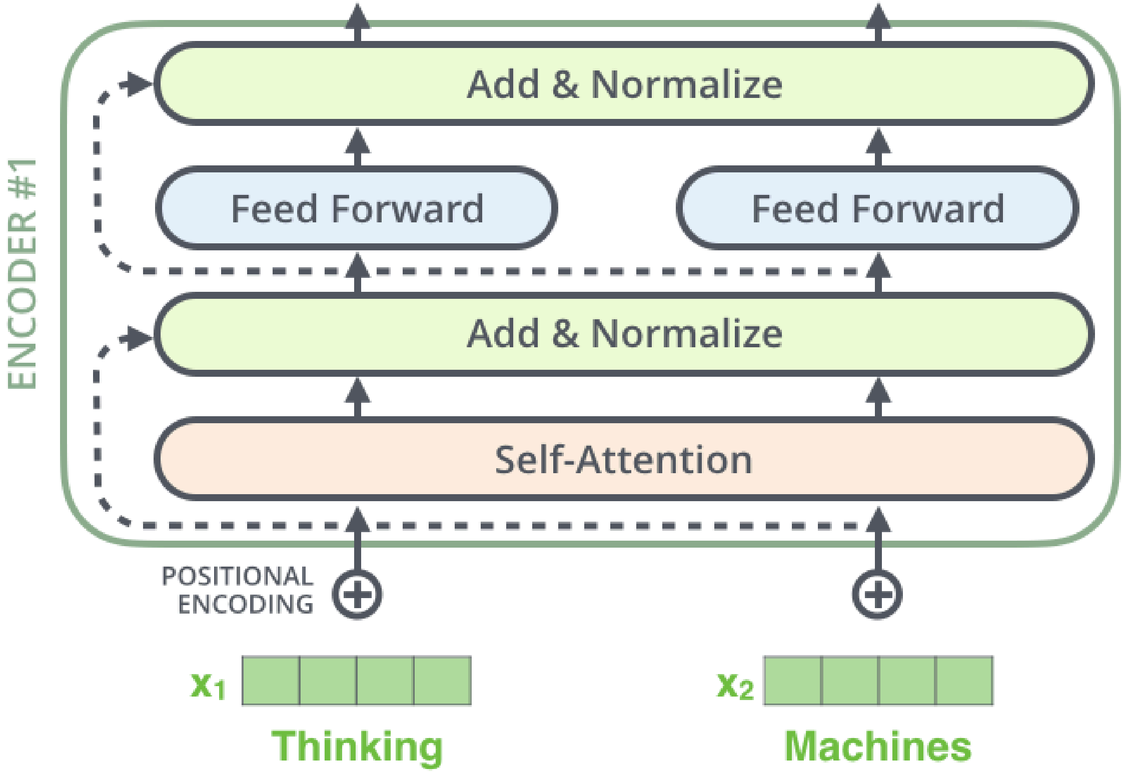
cross attention output

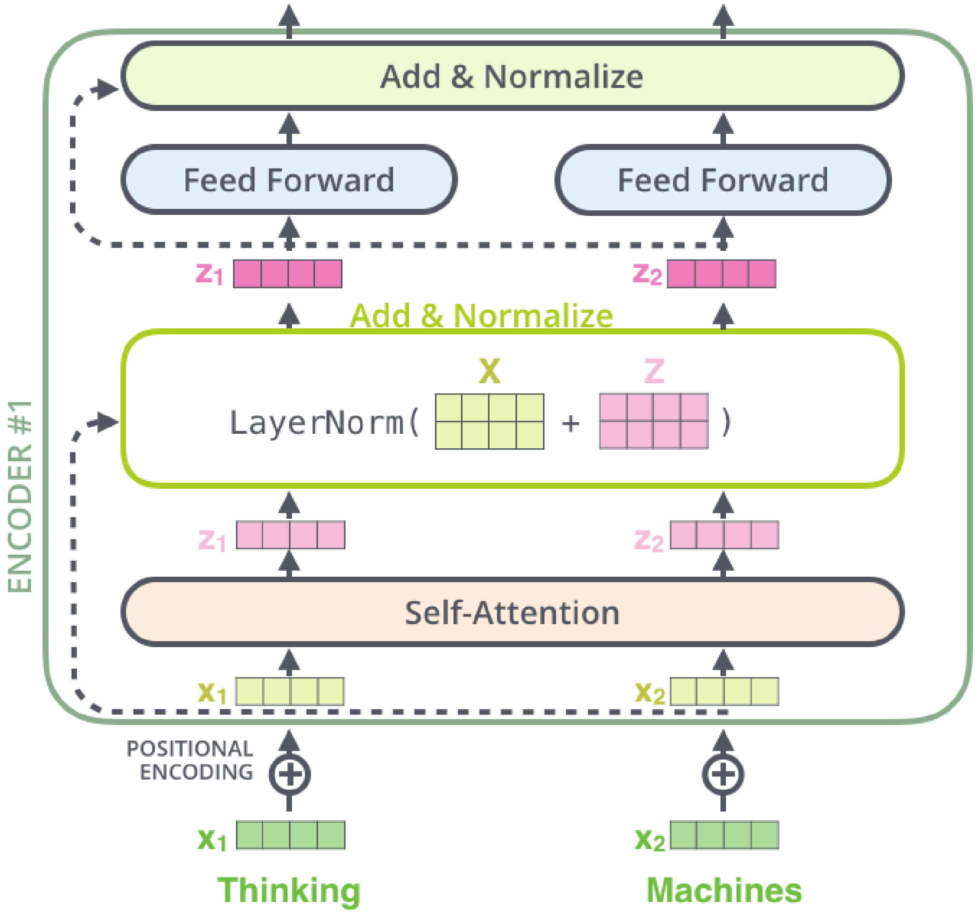


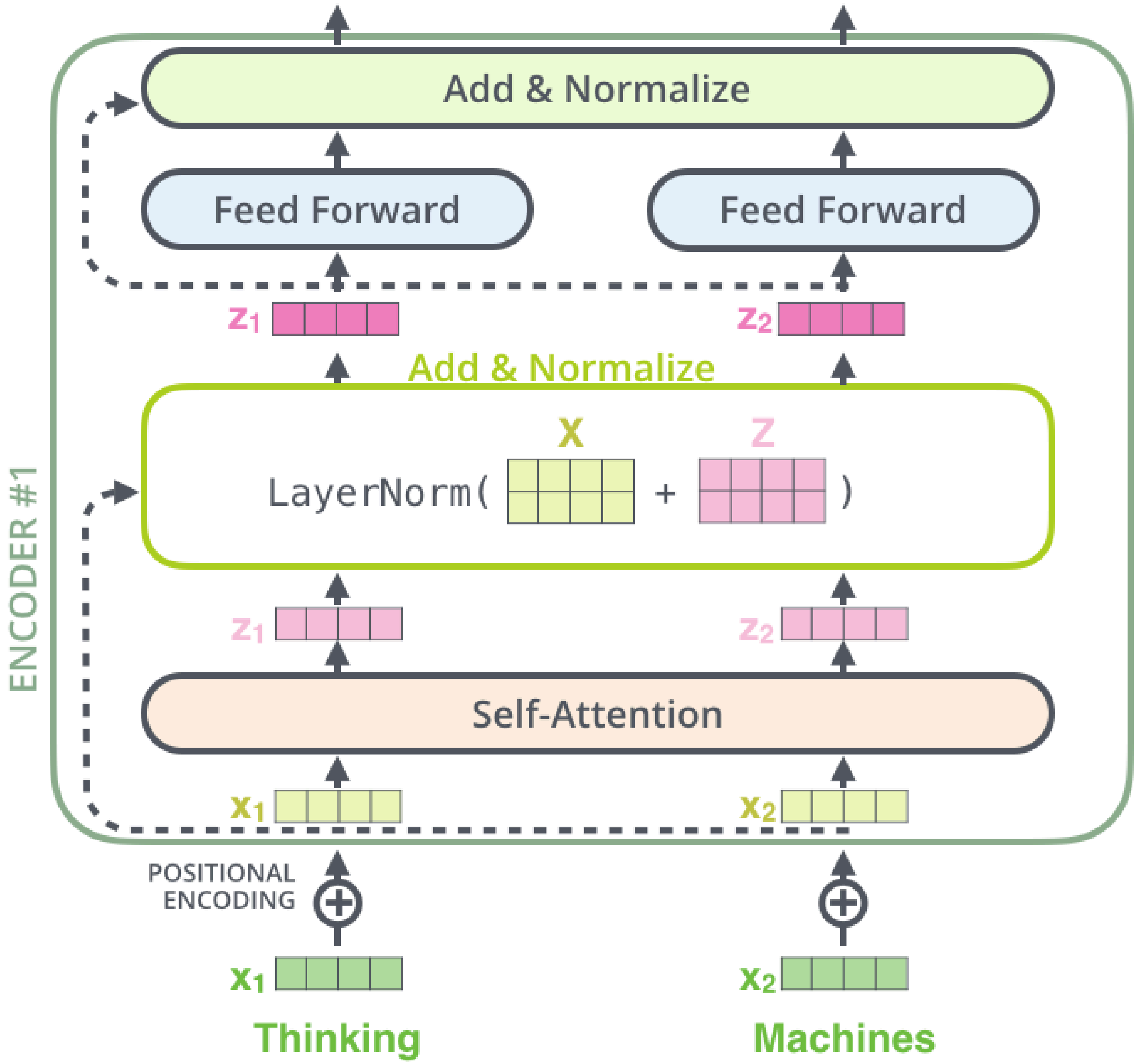
in reality, cross-attention is **also** multi-headed!

The Residuals

each sub-layer (self-attention, ffnn) in each encoder has a residual connection around it, and is followed by a layer-normalization step.






Add & Normalize
Feed Forward
Feed Forward
z_1
z_2
Add & Normalize
X
Z
LayerNorm(+)
ENCODER #1
z_1
z_2
Self-Attention
x_1
x_2
POSITIONAL ENCODING
x_1
x_2
Thinking
Machines

Layer normalization

Main idea: batch normalization is very helpful, but hard to use with sequence models Sequences are different lengths, makes normalizing across the batch hard Sequences can be very long, so we sometimes have small batches

Simple solution: "layer normalization" – like batch norm, but not across the batch

Batch norm

d-dimensional vectors for each sample in batch

$$a_1, a_2, \ldots, a_B$$

d-dim

$$\mu = \frac{1}{B}\sum_{i=1}^{B} a_i \qquad \sigma = \sqrt{\frac{1}{B}\sum_{i=1}^{B}(a_i - \mu)^2}$$

$$\bar{a}_i = \frac{a_i - \mu}{\sigma}\gamma + \beta$$

Layer norm

Different dimensions of a

$$a$$

$$\boxed{\mu = \frac{1}{d}\sum_{i=1}^{d} a_j} \qquad \boxed{\sigma = \sqrt{\frac{1}{d}\sum_{i=1}^{d}(a_j - \mu)^2}}$$

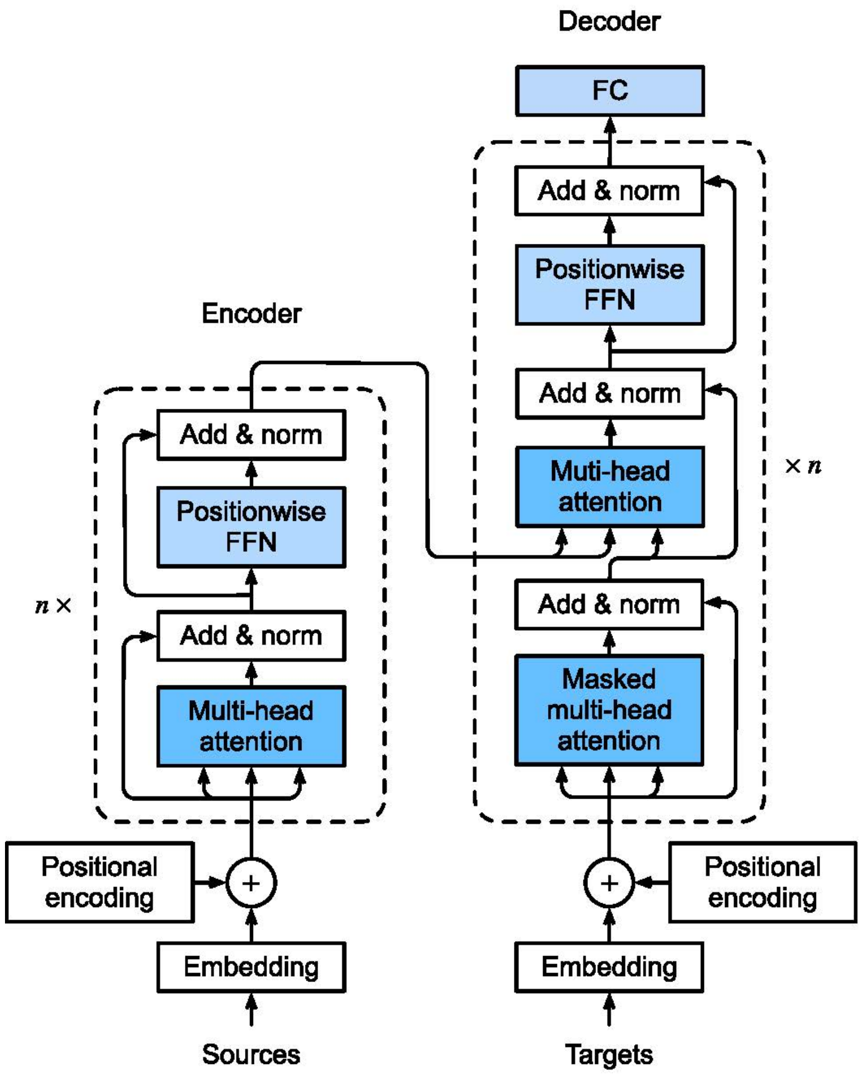
1-dim

$$\boxed{\bar{a} = \frac{a - \mu}{\sigma}\gamma + \beta}$$

The Transformer Architecture

Composed of an encoder and a decoder.

- Encoder:
  - a stack of multiple identical blocks
  - each block has two sublayers
  1. a multi-head self-attention pooling (queries, keys, and values are all from the outputs of the previous encoder layer)
  2. a positionwise feed-forward network
  3. A residual connection is employed around both sublayers followed by layer normalization



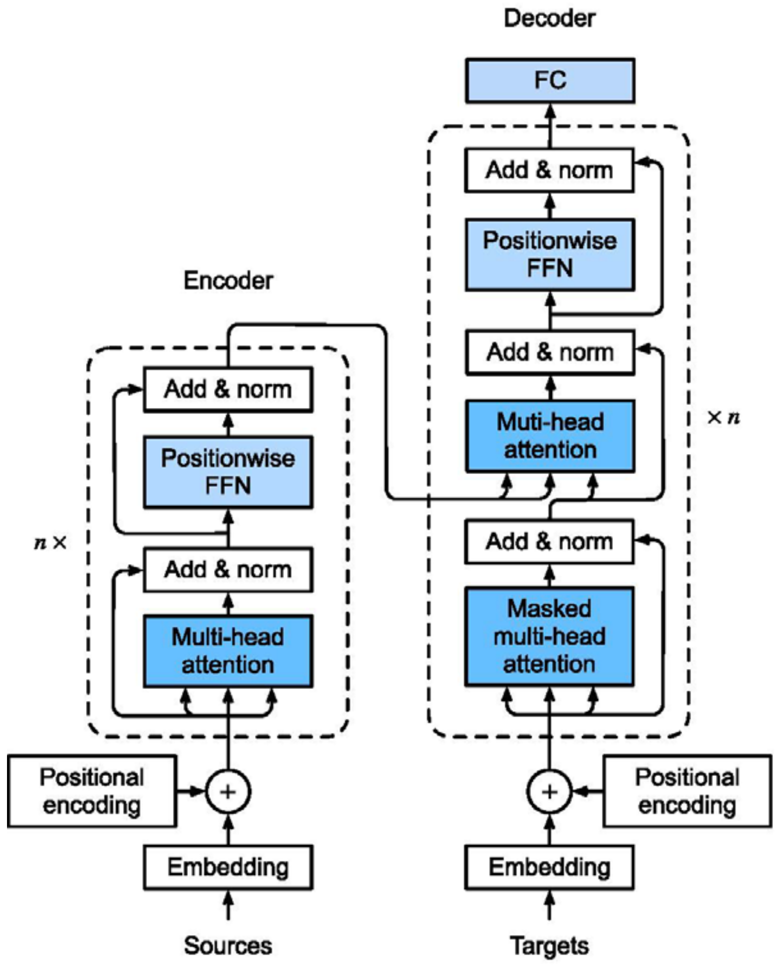
The Transformer Architecture

Decoder:

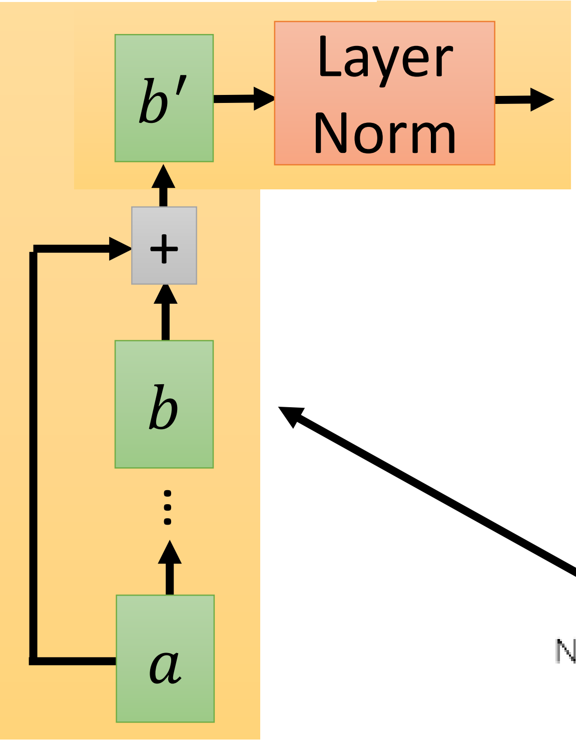
- a stack of multiple identical blocks
- each block has three sublayers.

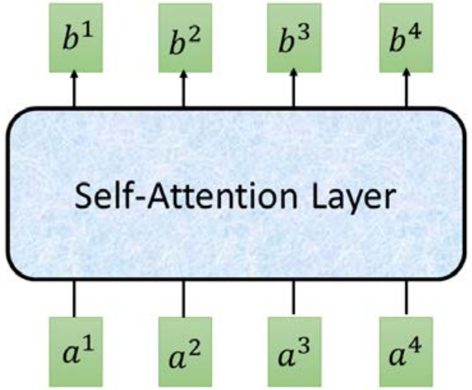
1. a multi-head self-attention pooling -- each position in the decoder is allowed to only attend to all positions in the decoder up to that position
2. Encoder-decoder attention: queries are from the outputs of the previous decoder layer, and the keys and values are from the Transformer encoder outputs
3. A positionwise feed-forward network

- A residual connection is employed around both sublayers followed by layer normalization



Transformer



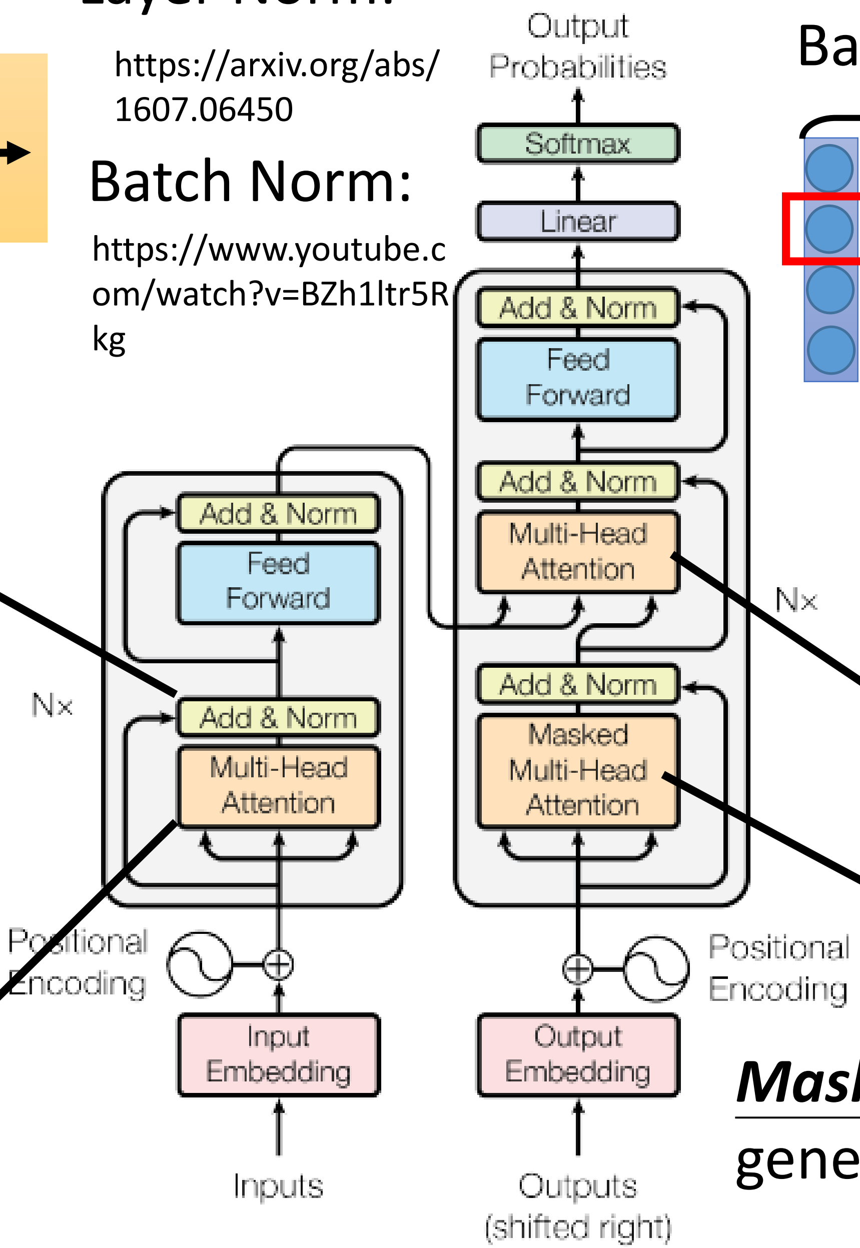


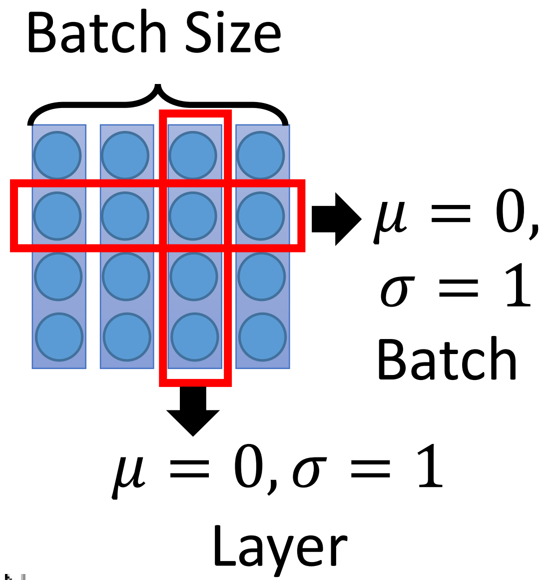
Layer Norm:

https://arxiv.org/abs/1607.06450

Batch Norm:

https://www.youtube.com/watch?v=BZh1ltr5Rkg





attend on the input sequence

Masked: attend on the generated sequence

Putting it all together

Decoder decodes one position at a time with masked attention

The Transformer

6 layers, each with d = 512

multi-head attention keys and values $k_{t,1}^\ell, \dots, k_{t,m}^\ell$ and $v_{t,1}^\ell, \dots, v_{t,m}^\ell$

$$\bar{h}_t^\ell = \mathrm{LayerNorm}(\bar{a}_t^\ell + h_t^\ell)$$

passed to next layer $\ell + 1$

$$h_t^\ell = W_2^\ell \mathrm{ReLU}(W_1^\ell \bar{a}_t^\ell + b_1^\ell) + b_2^\ell$$

2-layer neural net at each position

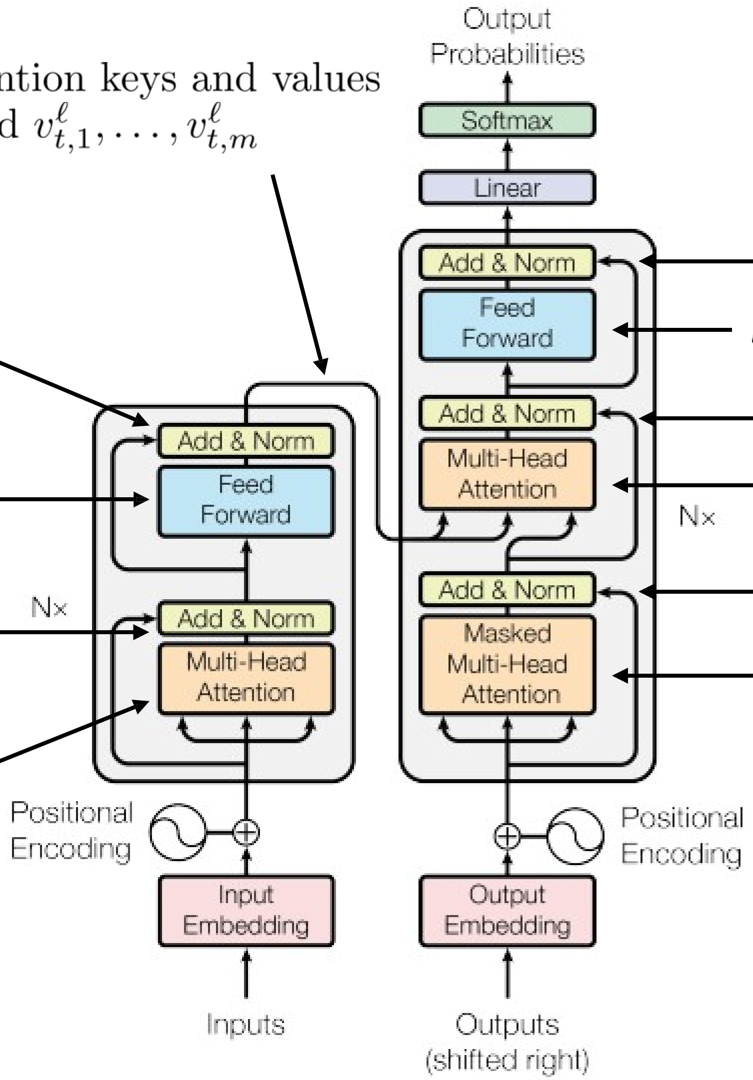
$$\bar{a}_t^\ell = \mathrm{LayerNorm}(\bar{h}_t^{\ell-1} + a_t^\ell)$$

essentially a residual connection with LN

input: $\bar{h}_t^{\ell-1}$

output: a_t^ℓ

concatenates attention from all heads



residual connection with LN

$$h_t^\ell = W_2^\ell \mathrm{ReLU}(W_1^\ell \bar{a}_t^\ell + b_1^\ell) + b_2^\ell$$

residual connection with LN

multi-head cross attention

residual connection with LN

same as encoder only **masked**

Vaswani et al. **Attention Is All You Need.** 2017.

Why transformers?

Downsides:

- **Attention computations are technically $O(n^2)$**
- **Somewhat more complex to implement (positional encodings, etc.)**

Benefits:

+ Much better long-range connections

+ Much easier to parallelize

+ In practice, can make it much deeper (more layers) than RNN

The benefits seem to **vastly** outweigh the downsides, and transformers work **much** better than RNNs (and LSTMs) in many cases

Arguably one of the most important sequence modeling improvements of the past decade