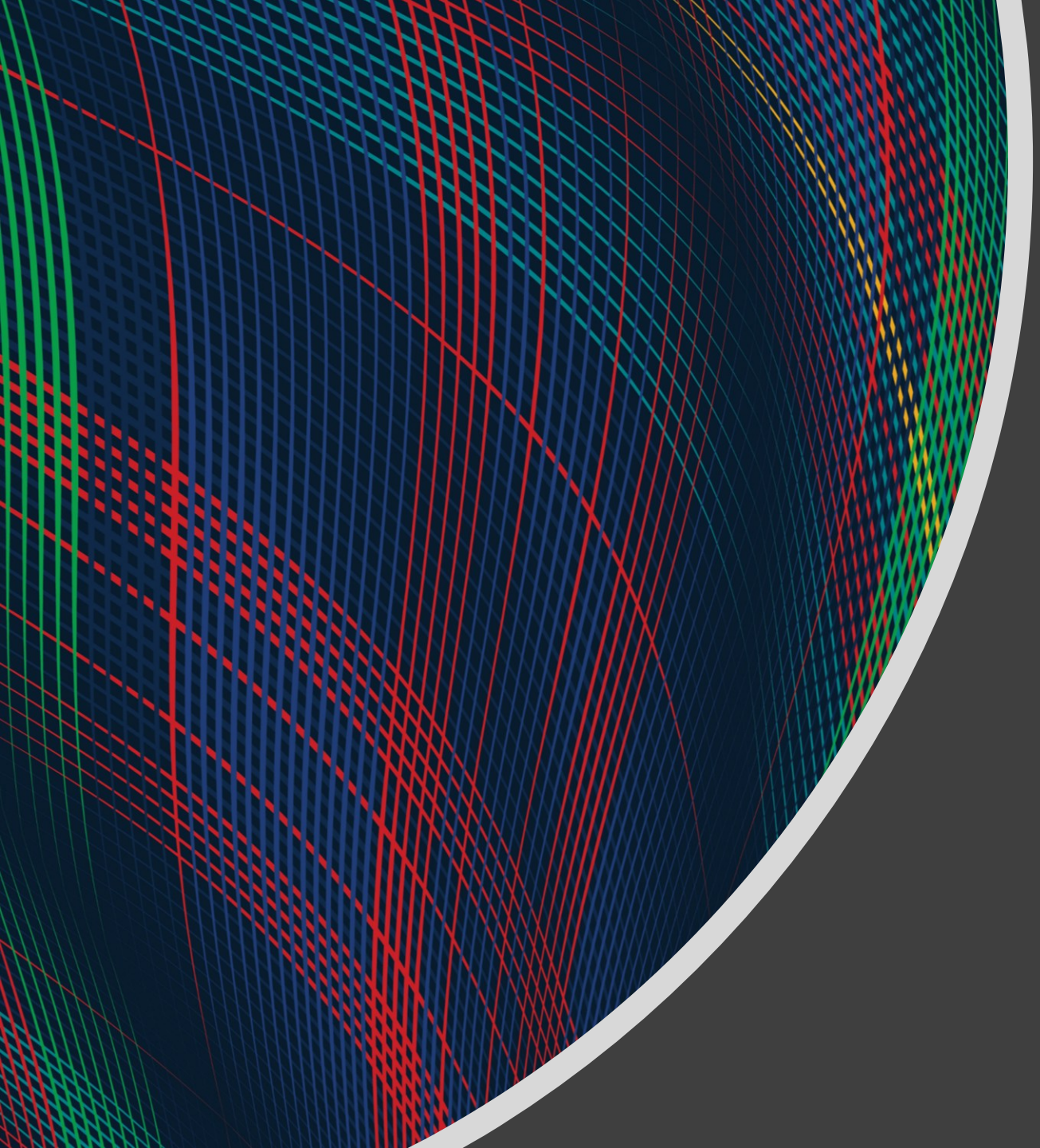


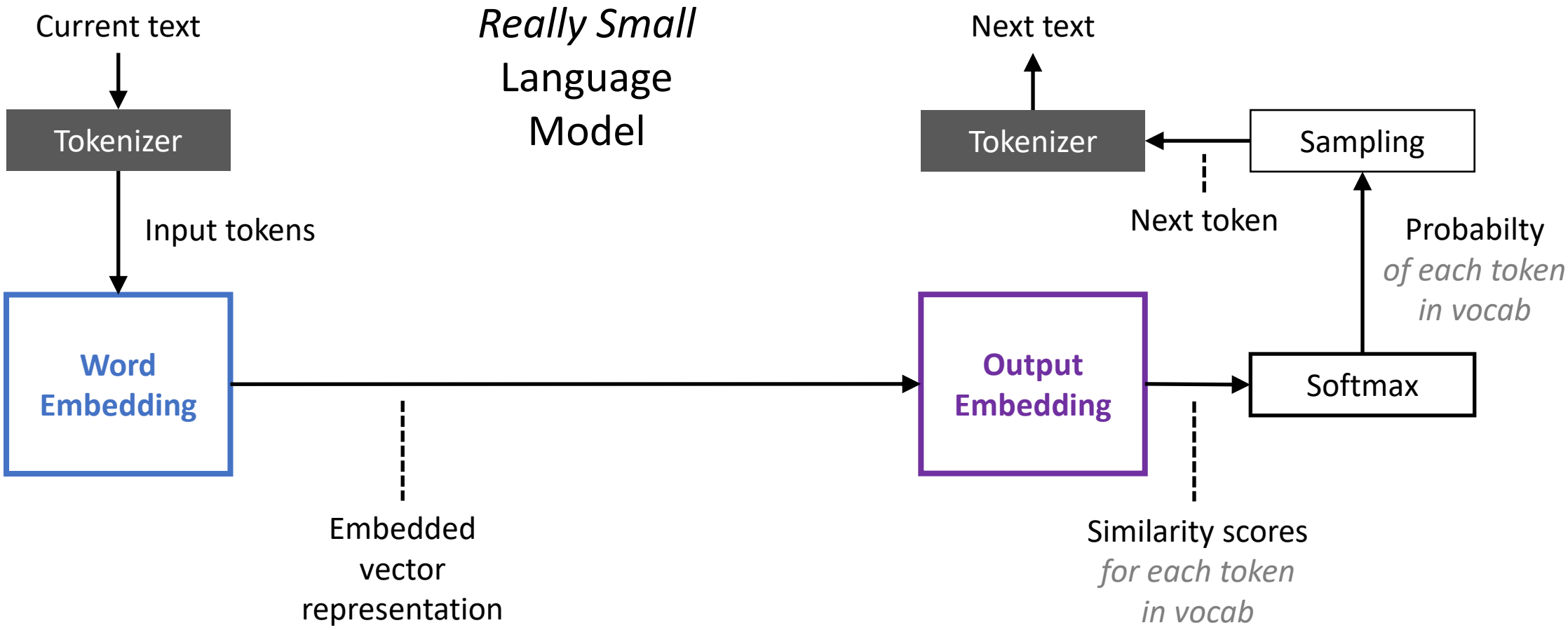
07-280
AI & ML I

Attention & Transformers

Instructors:
Pat Virtue & Nihar Shah

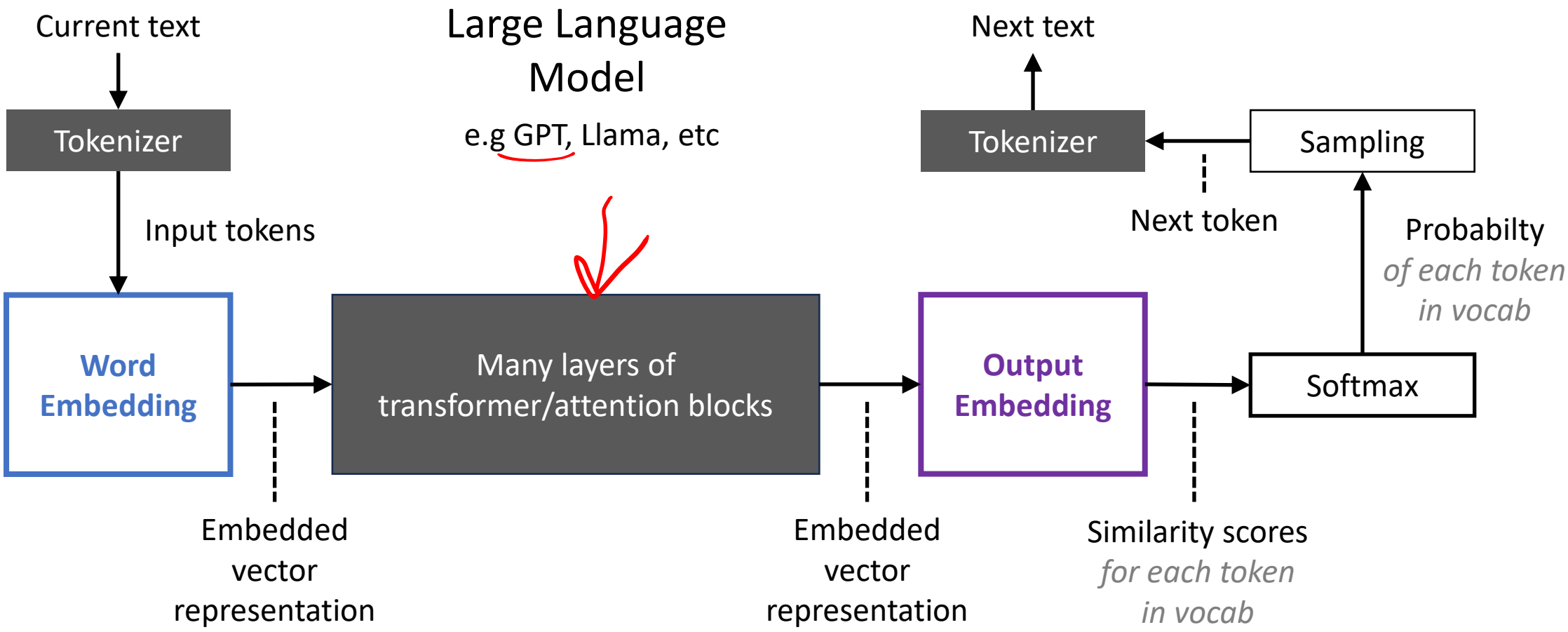
Simple Word Embedding LM

Building a language model with just word embedding layers ☺



Word (Token) Embeddings

The beginning and the end of LLM networks



Large Language Models!

Last time

Word Embeddings

Today

Increasing the conext size

- Positional Encoding
- Attention

Building GPT2!

- Multiheaded attention
- Transformers

Context size > 1

Transformer Language Models

Increasing context size

- Uniform average of context vectors
- Position encoding

Attention

- Weighted average of context vectors
- Query Keys Values
- Expressive power of linear transforms

Building GPT2!

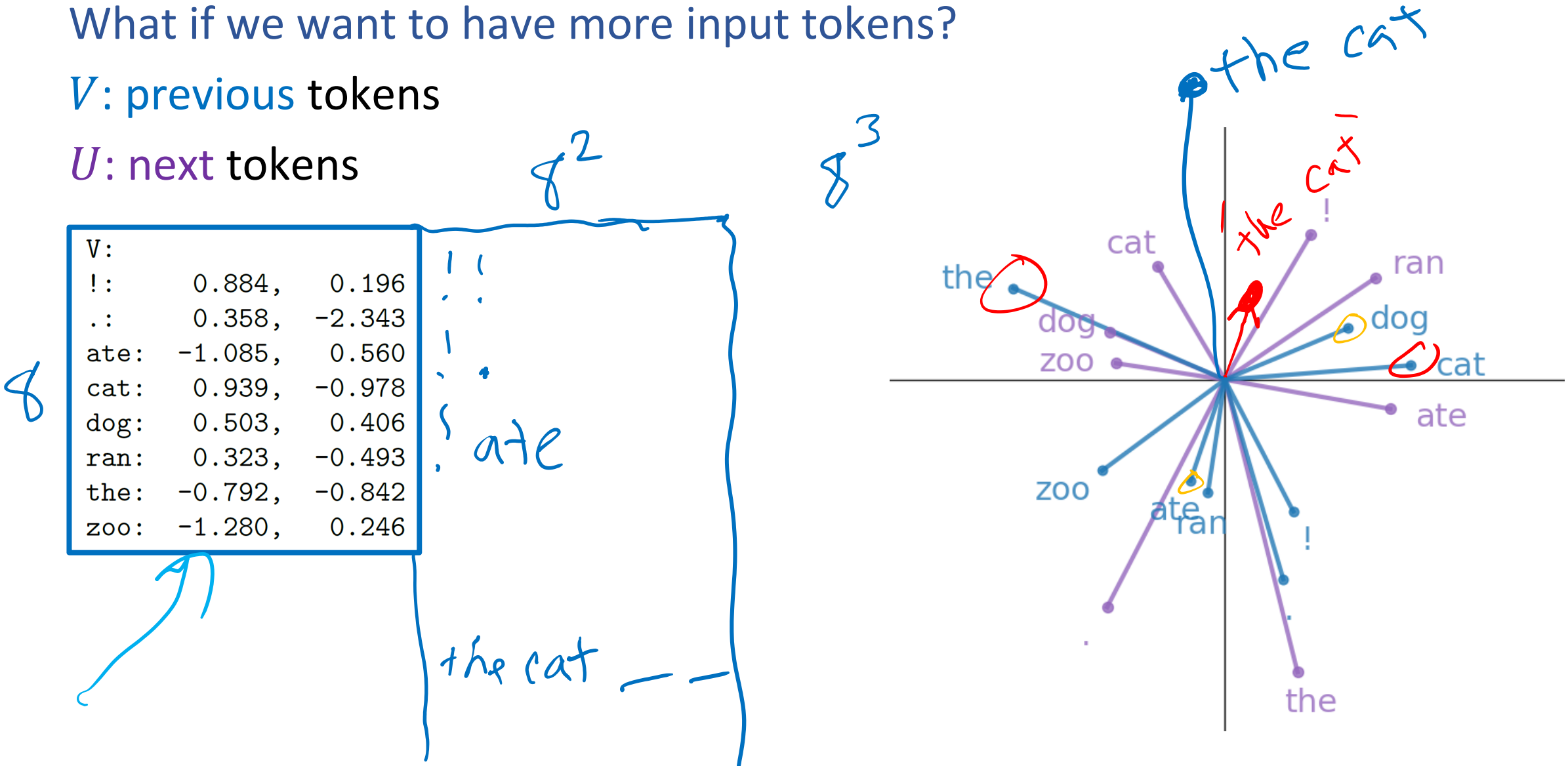
Increasing Context Size

What if we want to have more input tokens?

V: previous tokens

U: next tokens

V:		
!:	0.884,	0.196
.:	0.358,	-2.343
ate:	-1.085,	0.560
cat:	0.939,	-0.978
dog:	0.503,	0.406
ran:	0.323,	-0.493
the:	-0.792,	-0.842
zoo:	-1.280,	0.246

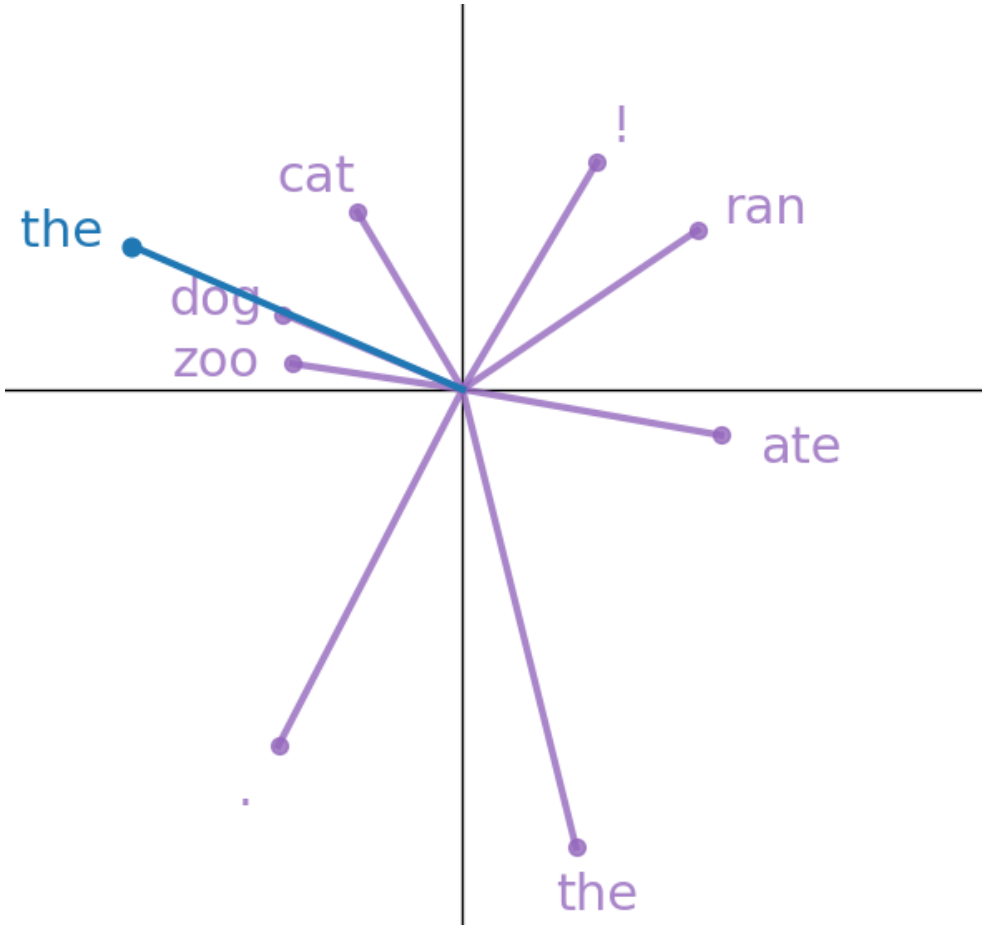


Increasing Context Size

What if we want to have more input tokens?

V: for context

U: for next token

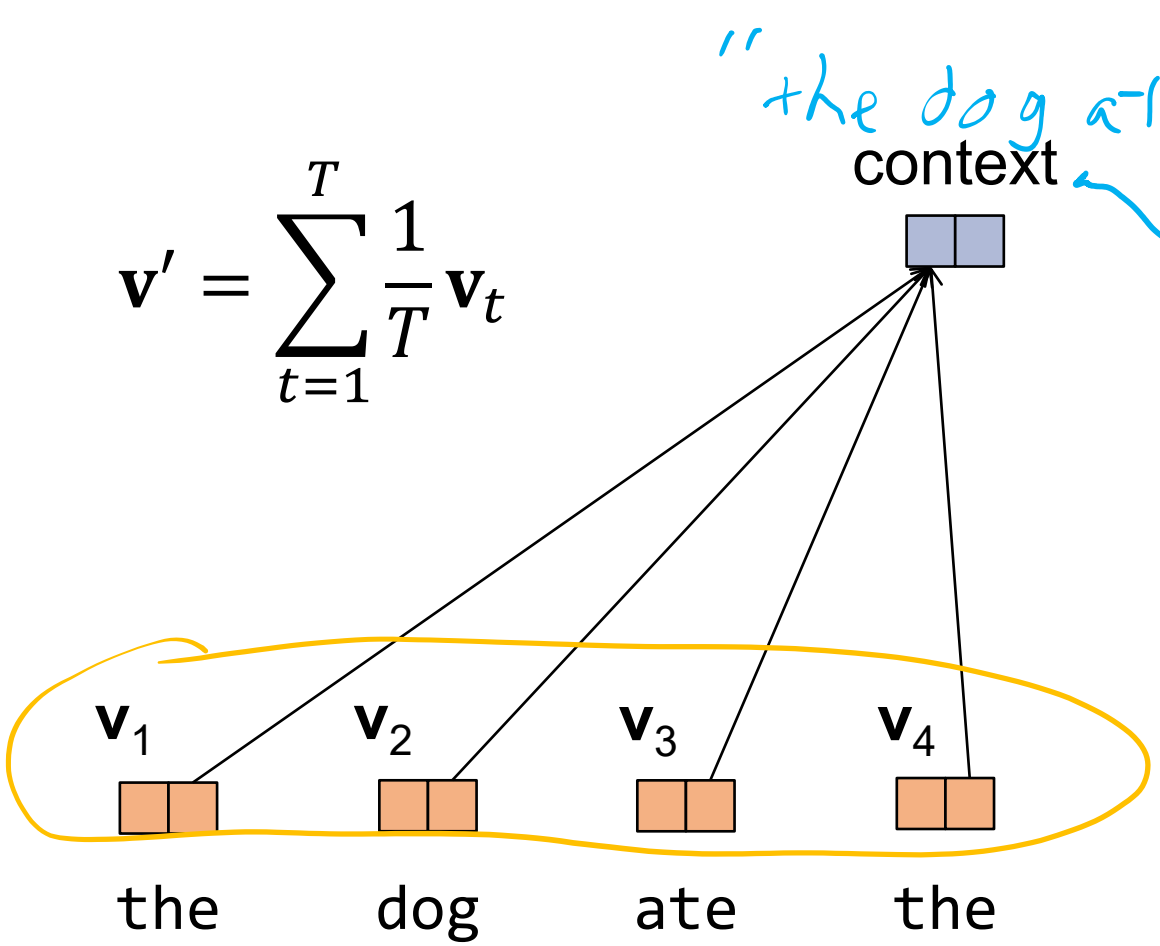


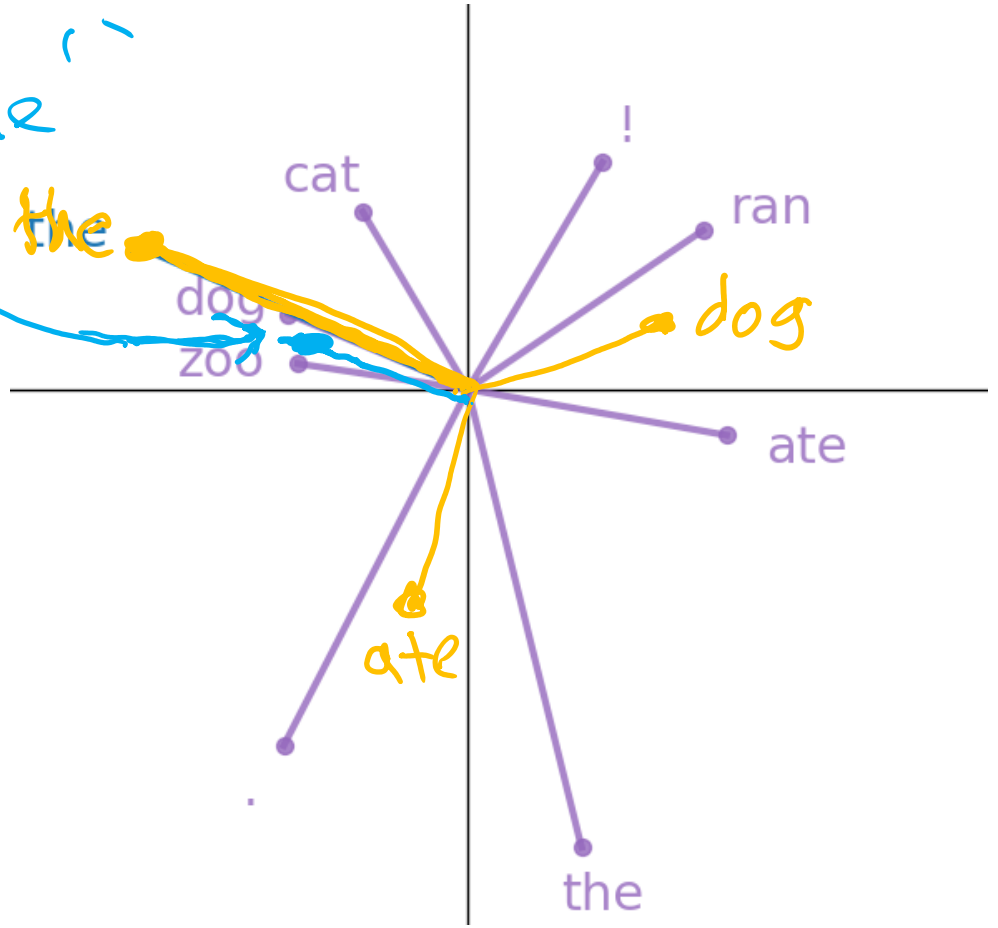
Increasing Context Size

What if we want to have more input tokens?

Uniform average over T input context tokens

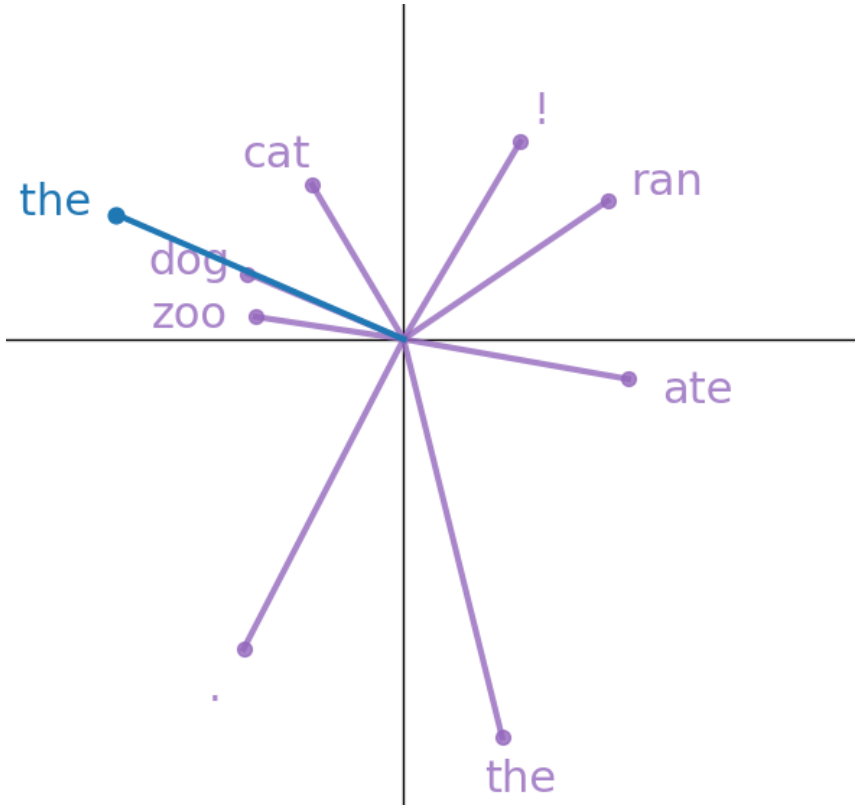
$$\mathbf{v}' = \sum_{t=1}^{T} \frac{1}{T} \mathbf{v}_t$$

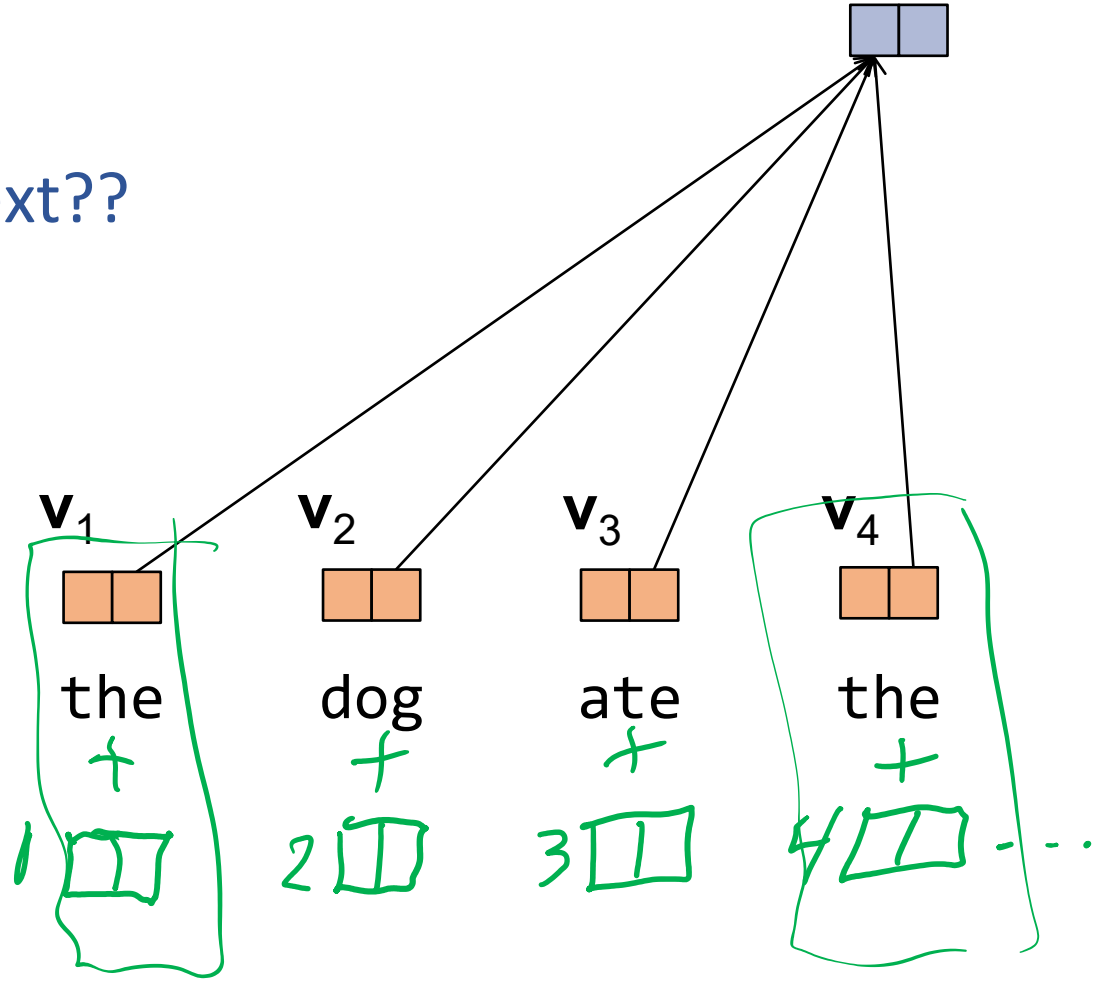




Positional Encoding

What about position within the input context??





Positional Encoding

2D example of positional encoding being added to token

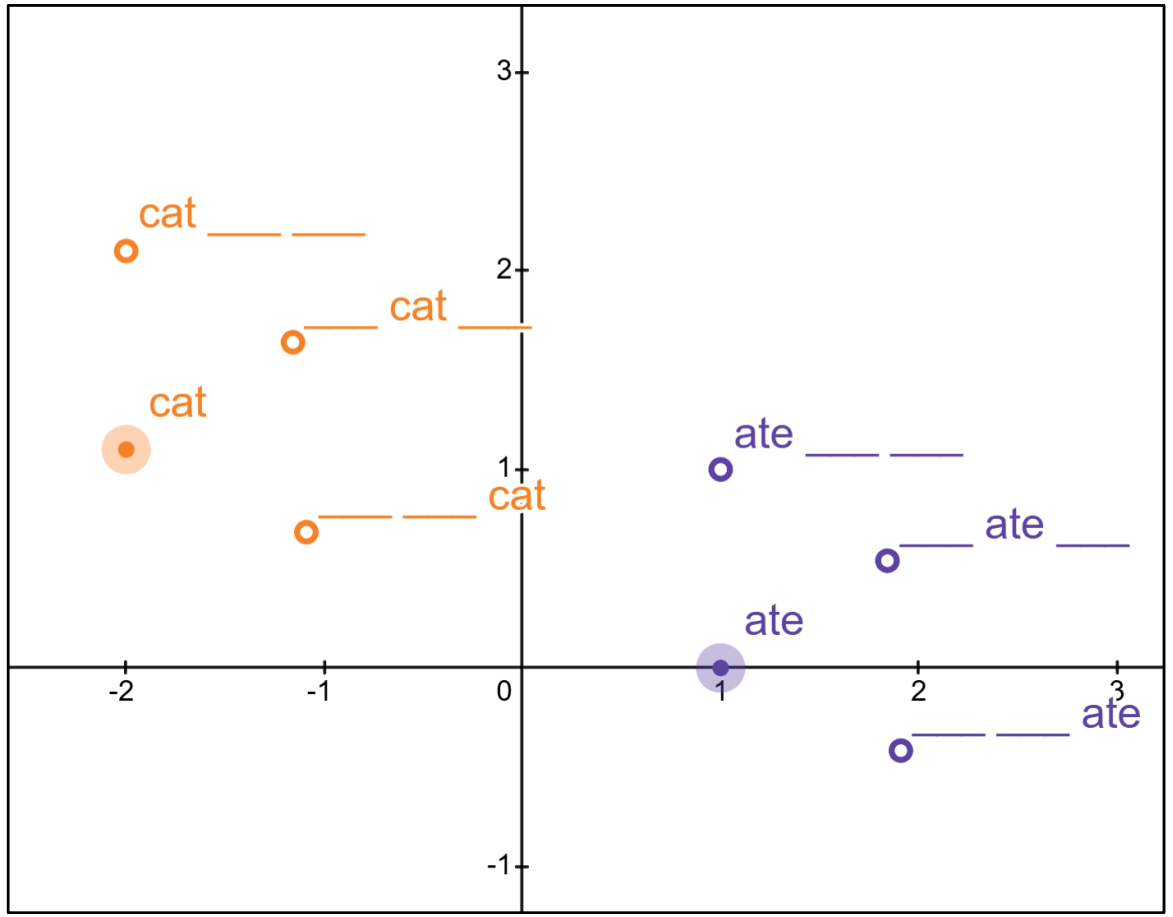
https://www.desmos.com/calculator/8e1fafb2fe

$$\mathbf{v}_{cat} + \begin{bmatrix} \sin(pos) \\ \cos(pos) \end{bmatrix}$$

$$\mathbf{v}'_{cat\ \_\_} = \mathbf{v}_{cat} + \begin{bmatrix} \sin(0) \\ \cos(0) \end{bmatrix}$$

$$\mathbf{v}'_{\_\ cat\ \_} = \mathbf{v}_{cat} + \begin{bmatrix} \sin(1) \\ \cos(1) \end{bmatrix}$$

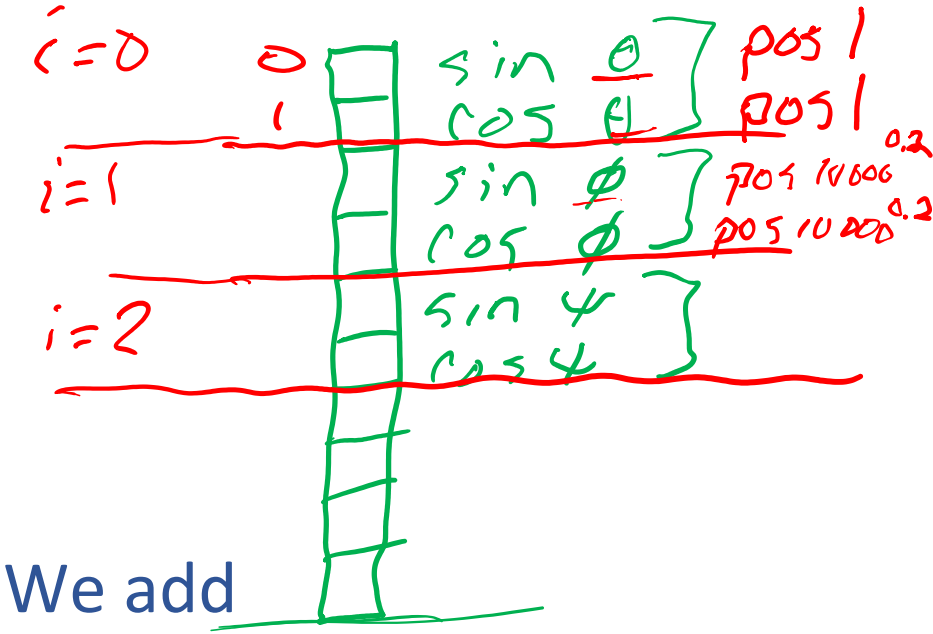
$$\mathbf{v}'_{\_\ \_cat} = \mathbf{v}_{cat} + \begin{bmatrix} \sin(2) \\ \cos(2) \end{bmatrix}$$



Positional Encoding

What about position within the input context??

Position Encoding Desmos Demo



Transformers have no built-in notion of position. We add **sinusoidal positional encodings** from Vaswani et al. 2017 so each position gets a unique pattern of sines and cosines:

$$PE_{2i} = \sin\left(pos \,/\, 10000^{\frac{2i}{d_{model}}}\right)$$

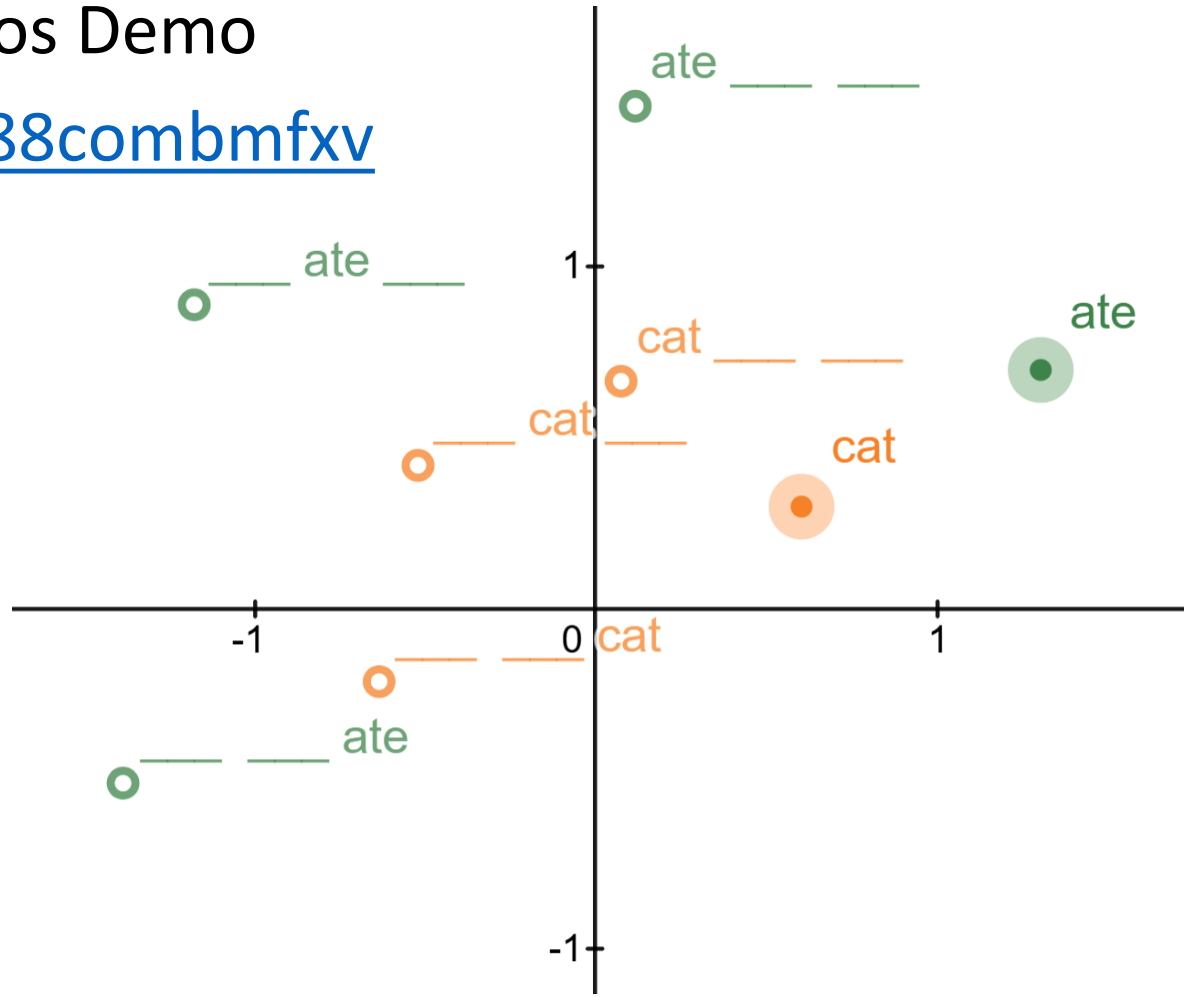
$$PE_{2i+1} = \cos\left(pos \,/\, 10000^{\frac{2i}{d_{model}}}\right)$$

Rotary Position Encoding

What about position within the input context??

Rotary Position Encoding (RoPE) Desmos Demo

https://www.desmos.com/calculator/88combmfxv



2D version:

Given a fixed base rotation angle θ_1,

an embedded vector $\mathbf{x}$ at integer position, i_{pos}, will be rotated by angle $\theta = i_{pos}\theta_1$:

$$\mathbf{x}' = \text{Rotate}(\mathbf{x}, \theta) = \begin{bmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{bmatrix} \mathbf{x}$$

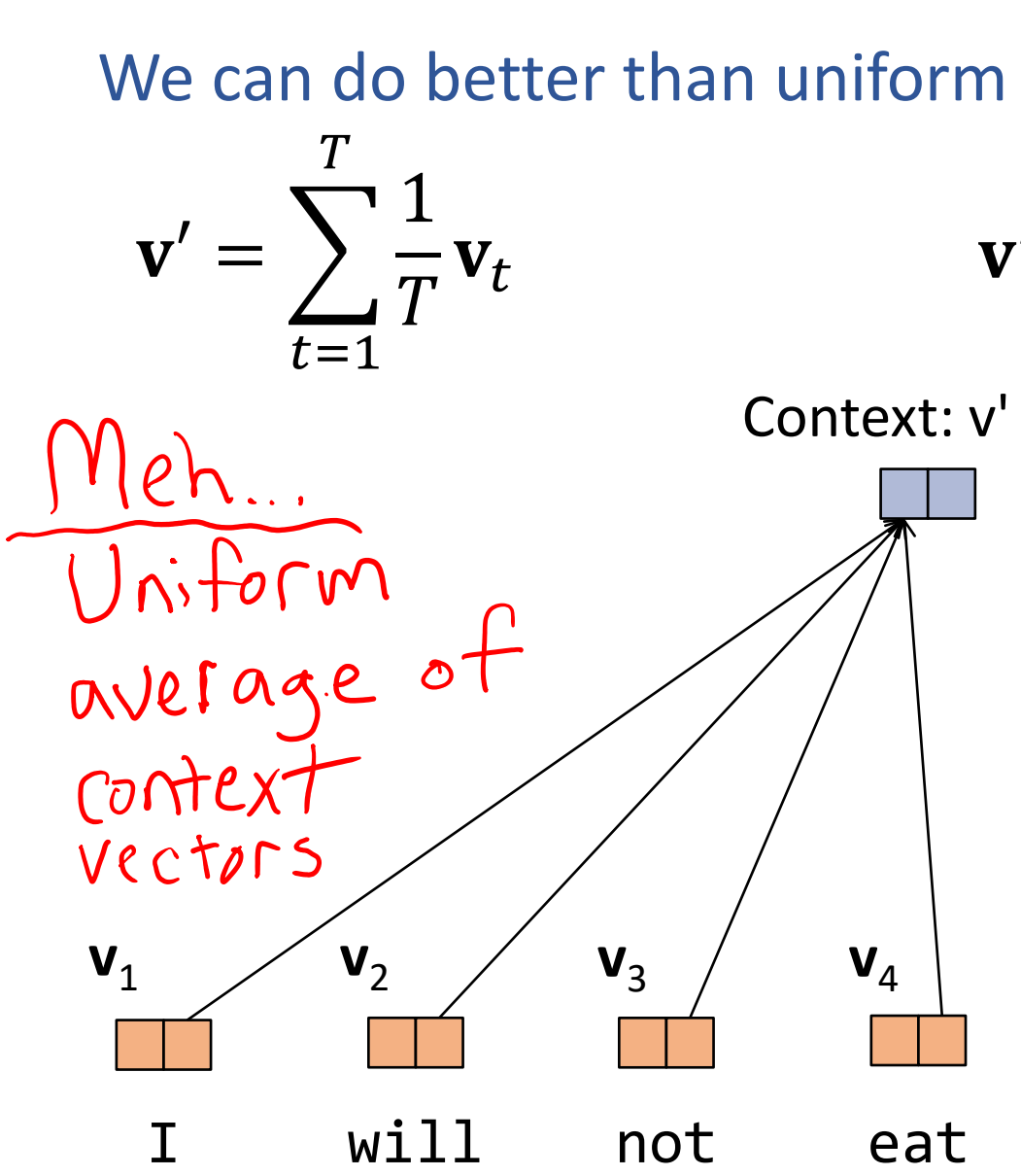
Attention

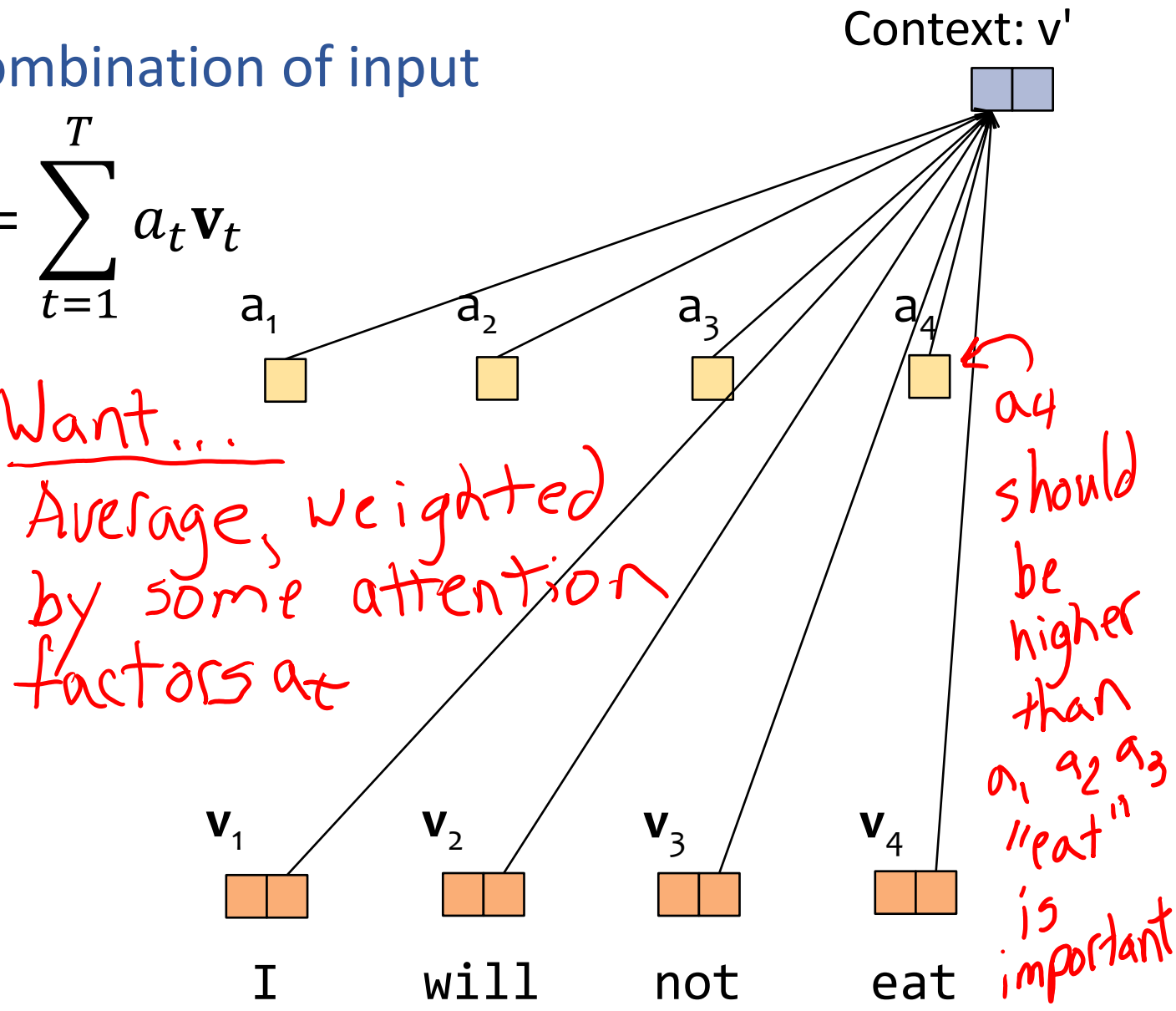
Learn to pay attention!

We can do better than uniform combination of input

$$\mathbf{v}' = \sum_{t=1}^{T} \frac{1}{T} \mathbf{v}_t$$

$$\mathbf{v}' = \sum_{t=1}^{T} a_t \mathbf{v}_t$$



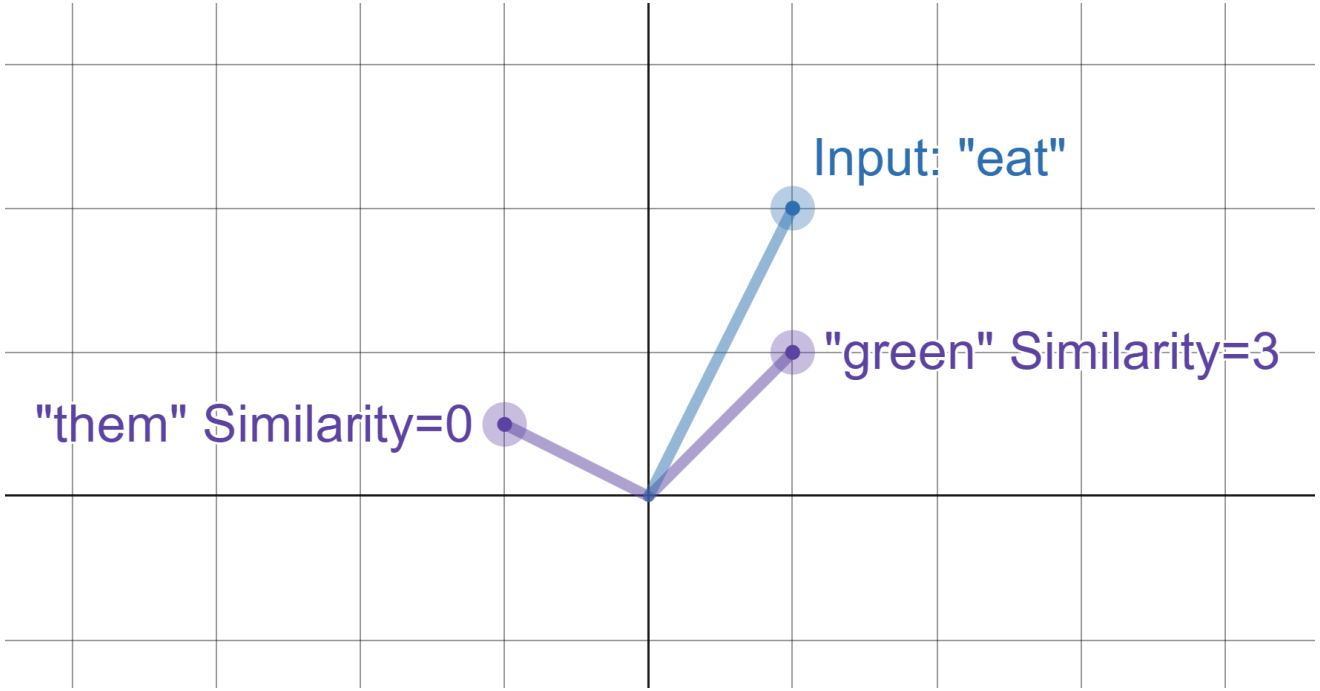


Reminder: Poll 1

Take 1: Collecting vector data (about you!)

Take 2: Compute similarity score with yourself and your neighbor

$$f(\mathbf{u}, \mathbf{v}) = \mathbf{u}^T \mathbf{v}$$

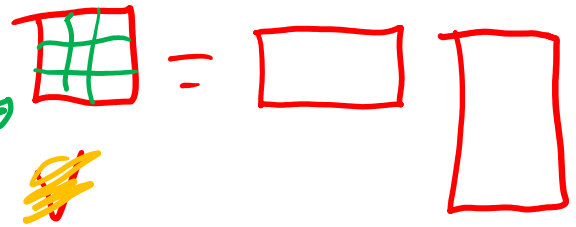


Reminder: Similarity Matrix

Let each row of matrix V be vector $\mathbf{v}_j^T$ representing student j in a group.

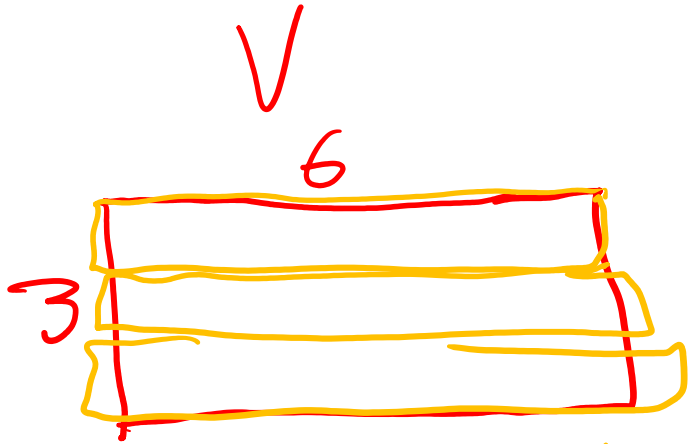
We can compare all pairs of vectors by doing matrix multiplication of V with itself.

$$f(\boldsymbol{V}) = V\,V^T$$



$S = V\,V^T$

3 × 3



$d_{model} = 6$

$T = 3$

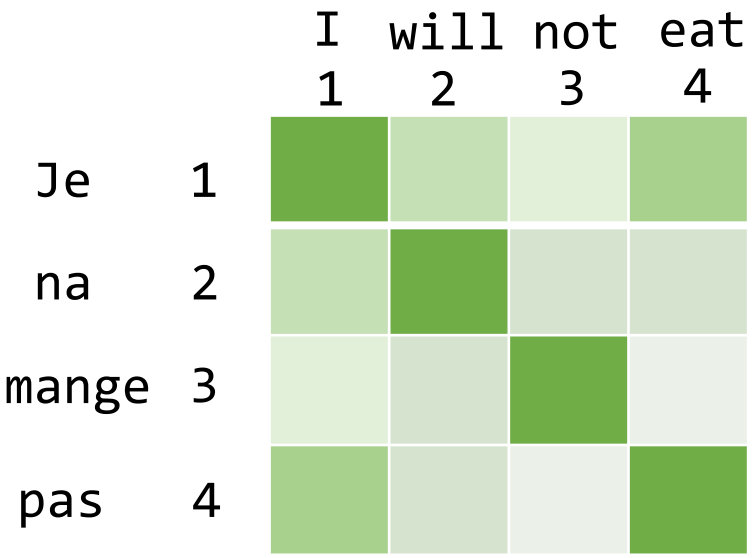
Learn to pay attention!

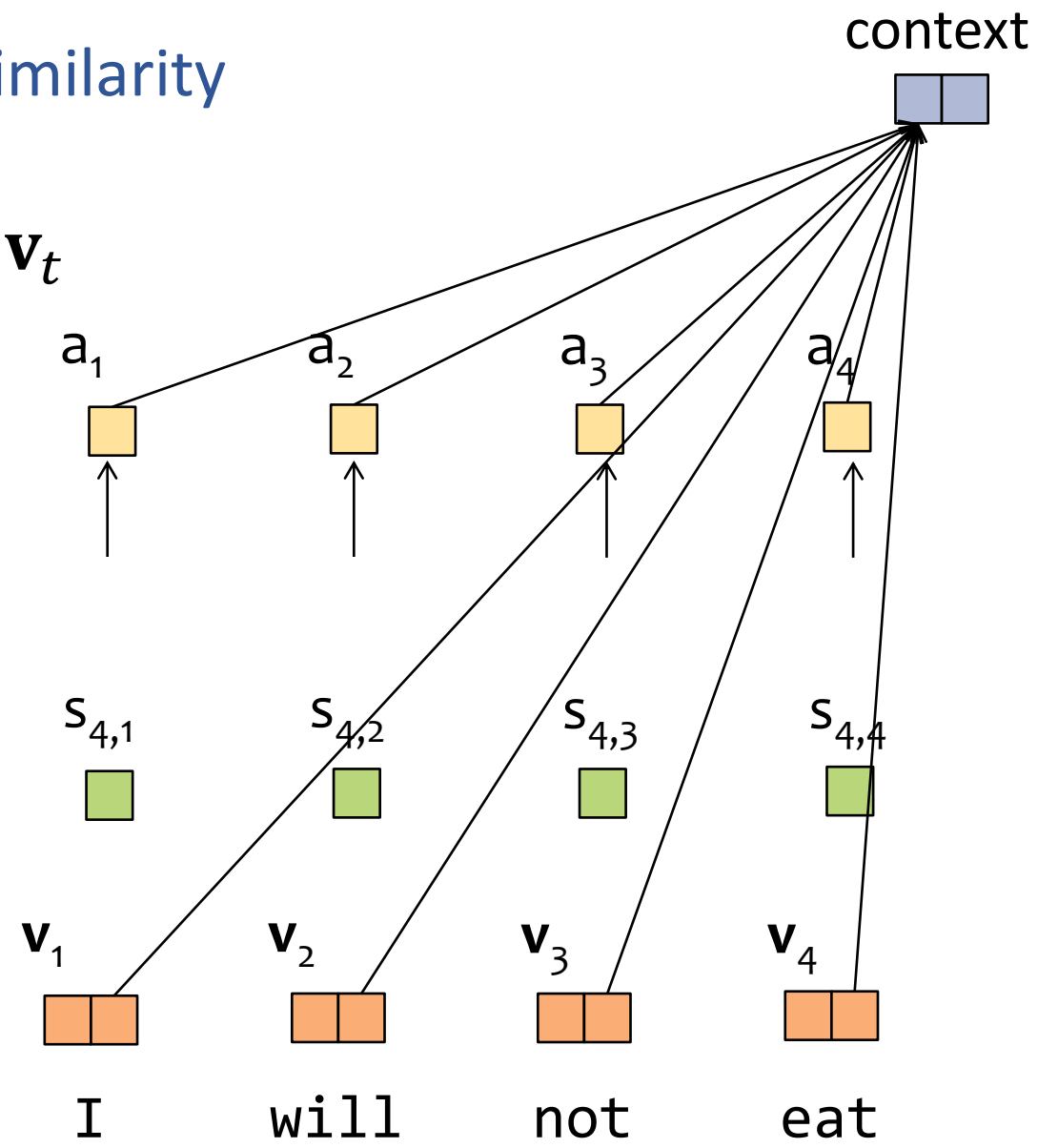
If only we had a way to measure vector similarity

$$\mathbf{v}' = \sum_{t=1}^{T} a_t \mathbf{v}_t$$

Cosine similarity matrix!

$$S = VV^T$$





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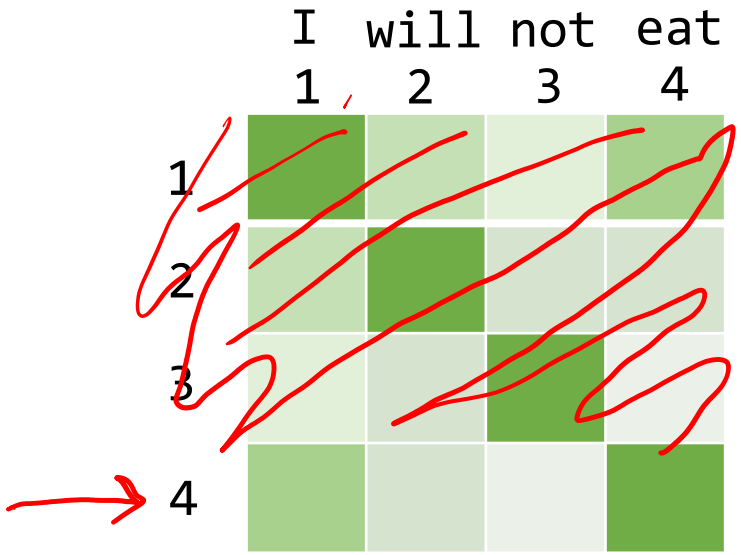

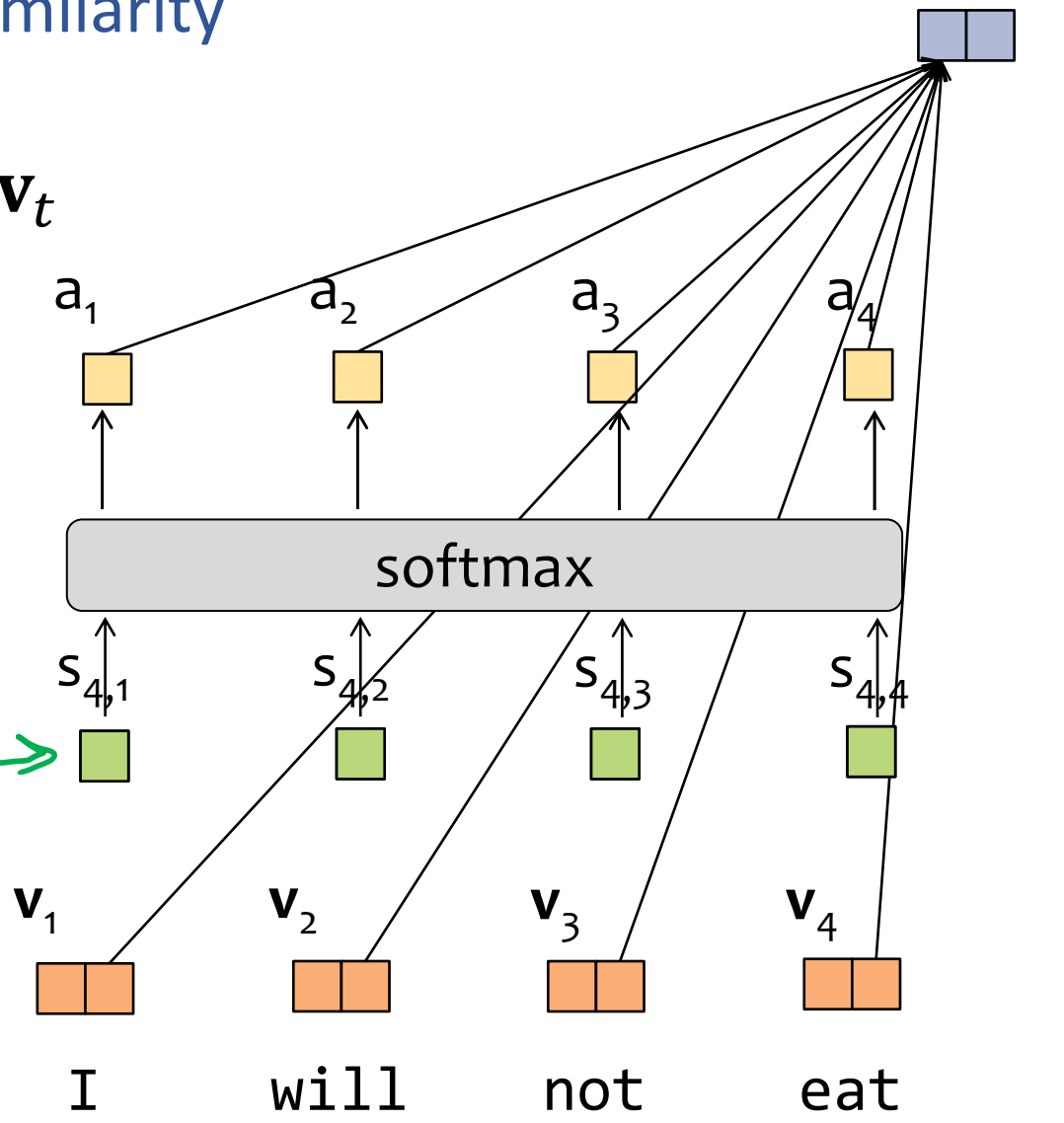

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$$\mathbf{v} = \sum_{t=1}^{T} \frac{1}{T} \mathbf{v}_t$$

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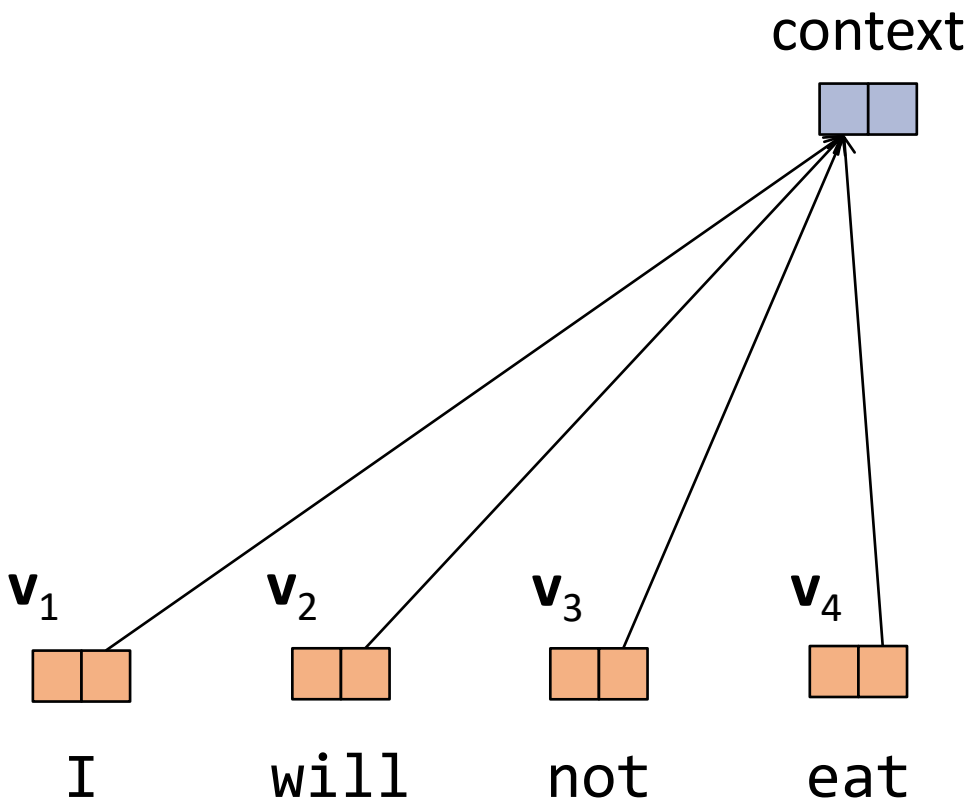
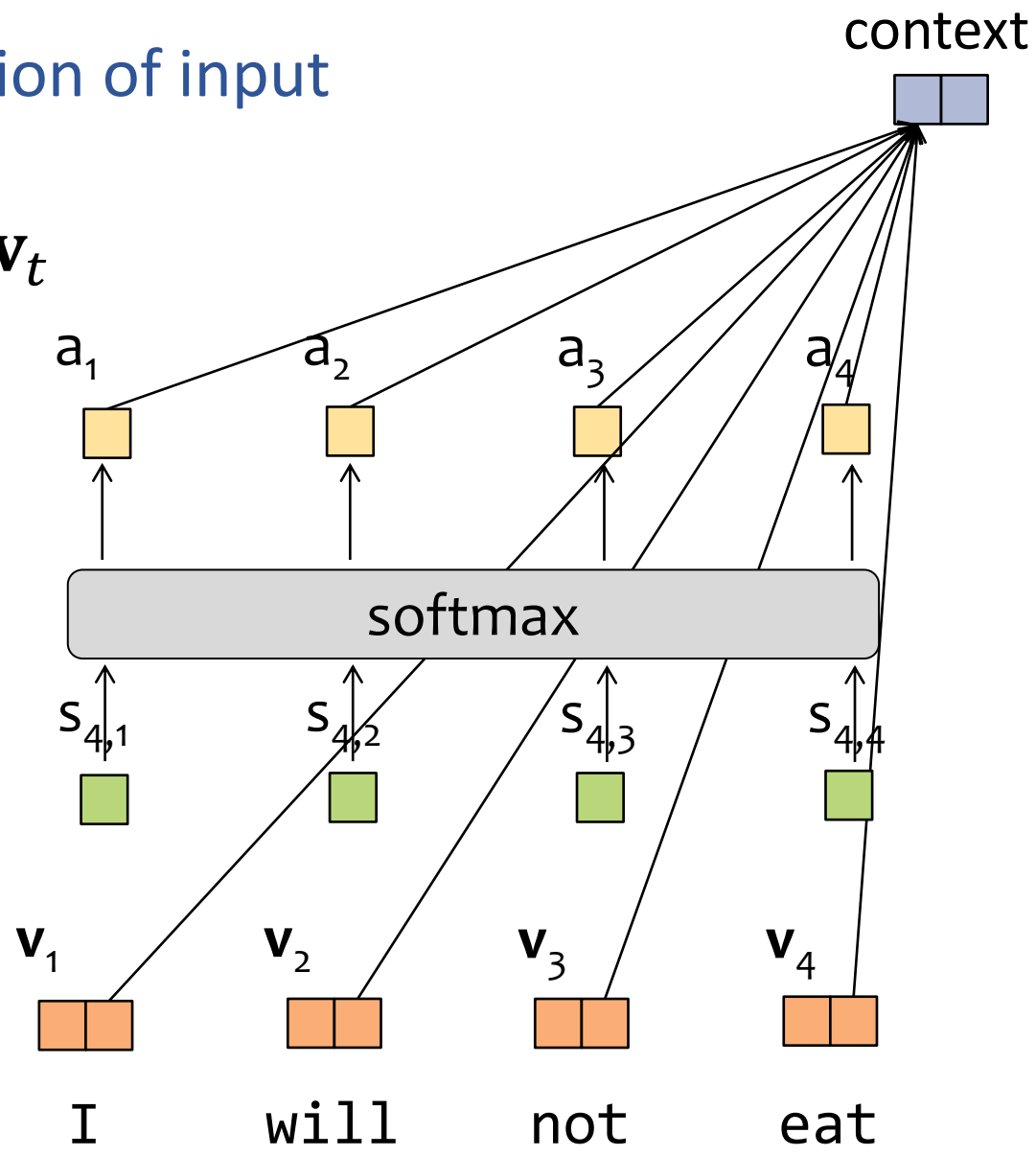




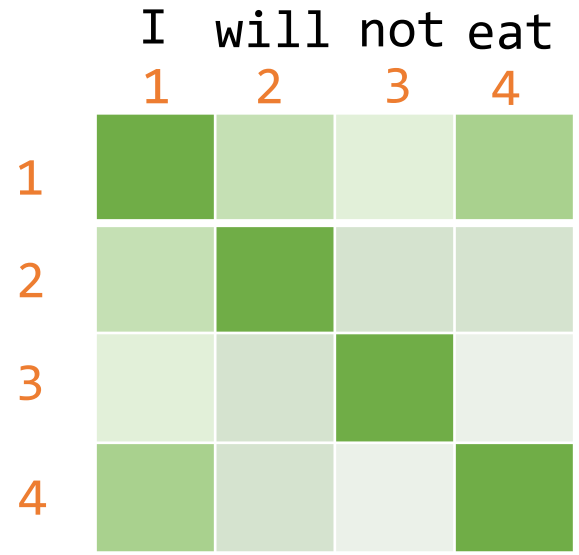
Learn to pay attention!

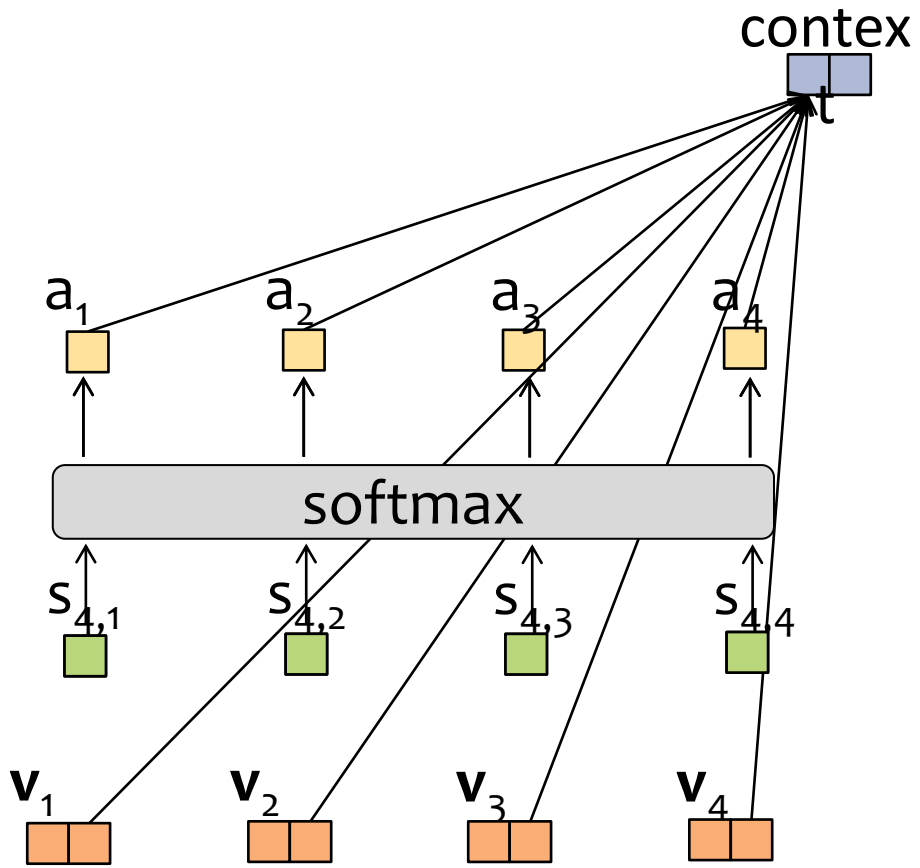
But...there is an issue with just doing VV^T ☹

We're really just comparing input to input

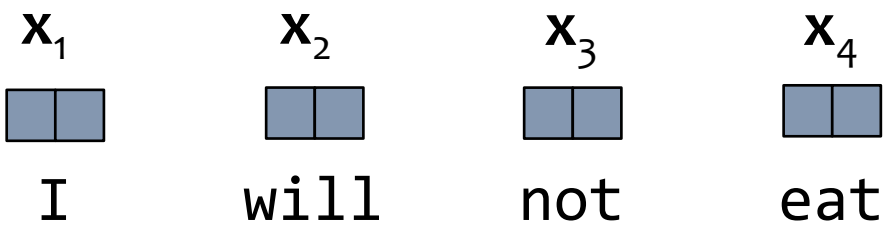
→ Symmetric with strong diagonal ☹

$$S = VV^T$$





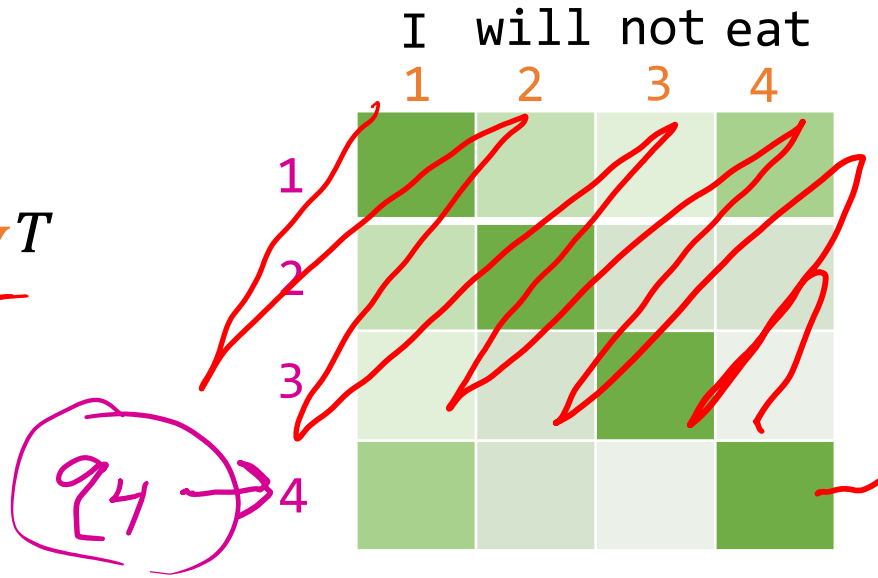
$$V = XW_V$$

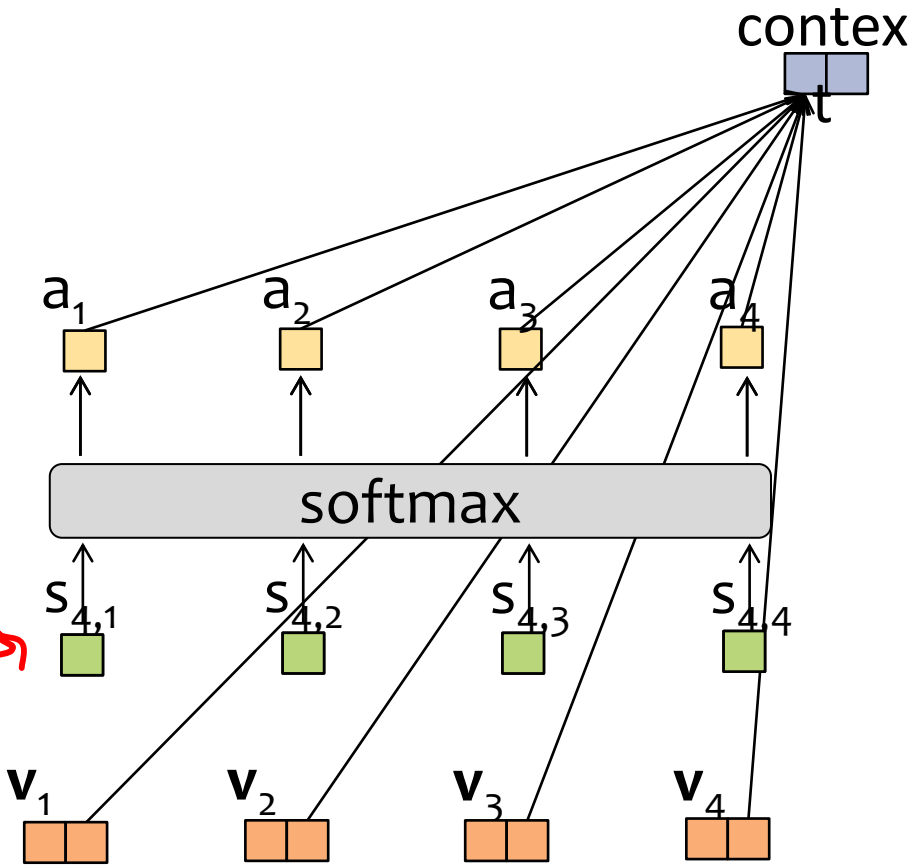


Learn to pay attention!

Instead learn a query vectors $\mathbf{q}_t$ to represent the output

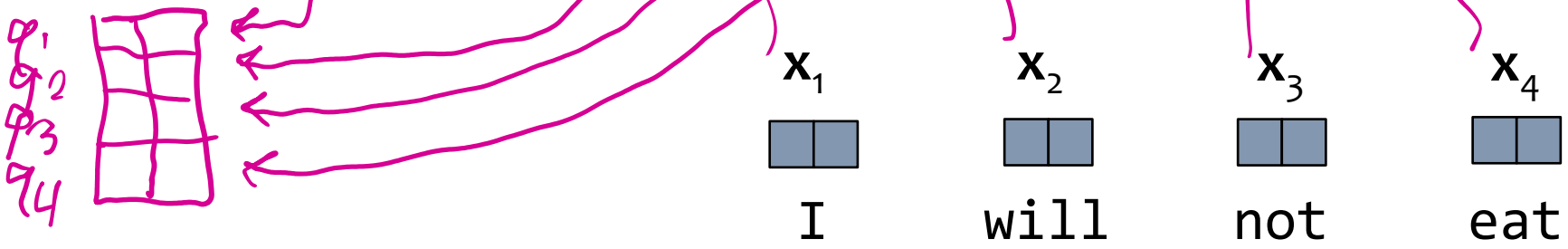
$$S = QV^T$$





$$Q = XW_Q$$

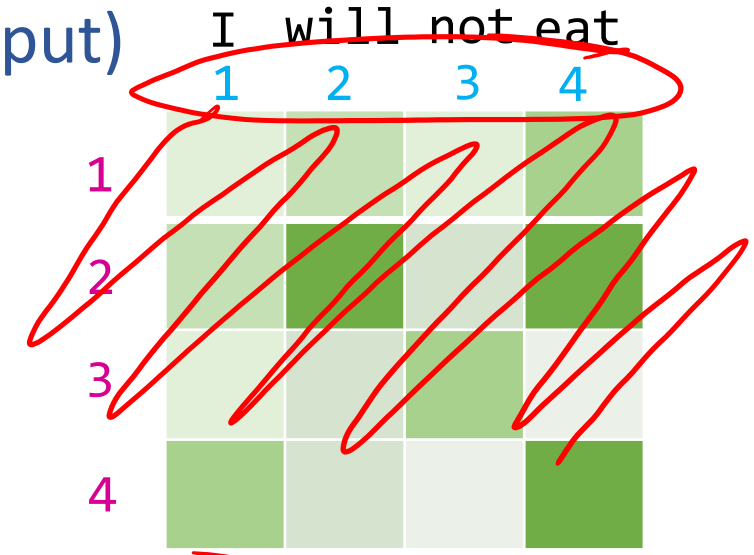
$$V = XW_V$$

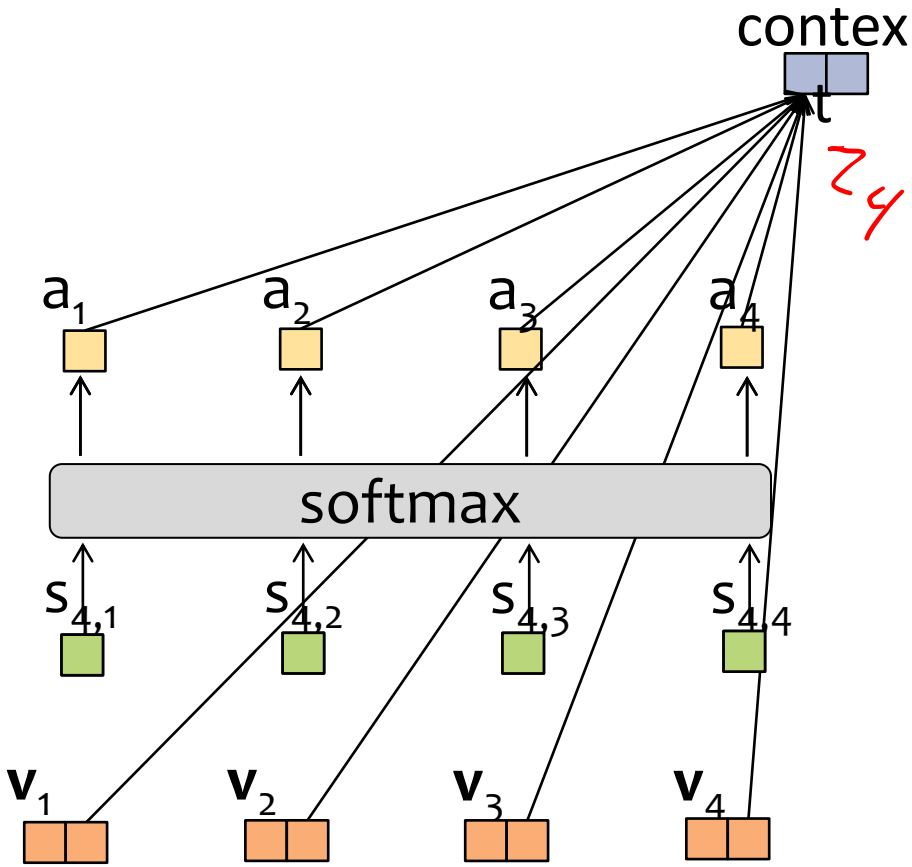


Learn to pay attention!

Instead learn a query vectors $\mathbf{q}_t$ to represent the output

(And also $\mathbf{k}_t$ for the input)



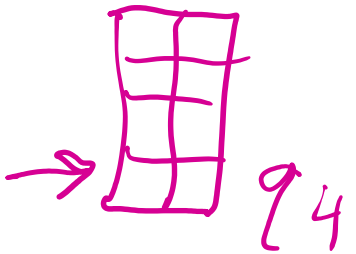


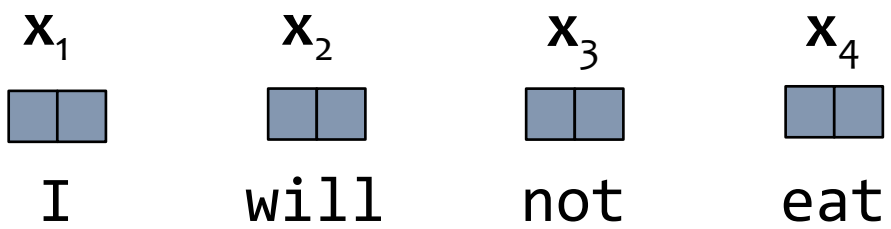
$$S = QK^T/\sqrt{d_k}$$

$$Q = XW_Q$$

$$K = XW_K$$

$$V = XW_V$$





Attention

Vector representation

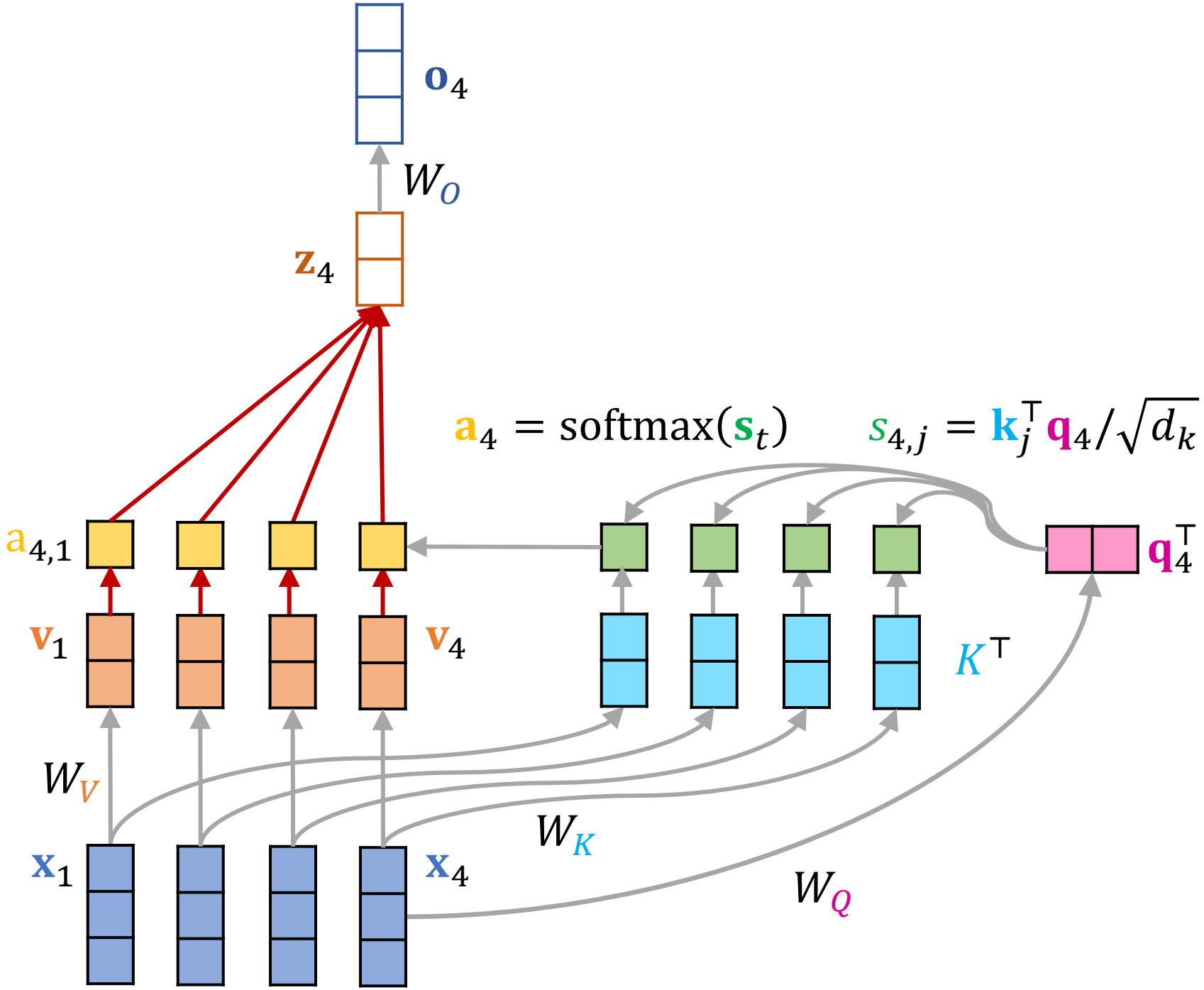
$$\mathbf{o}_t = W_O^\top \mathbf{z}_t$$

$$\mathbf{z}_t = V^\top \mathbf{a}_t$$

$$\mathbf{a}_t = \text{softmax}(\mathbf{s}_t)$$

$$\mathbf{s}_t = K\mathbf{q}_t/\sqrt{d_k}$$

$$\mathbf{q}_t = W_Q^\top \mathbf{x}_t$$
$$\mathbf{k}_t = W_K^\top \mathbf{x}_t$$
$$\mathbf{v}_t = W_V^\top \mathbf{x}_t$$



(Full) Attention

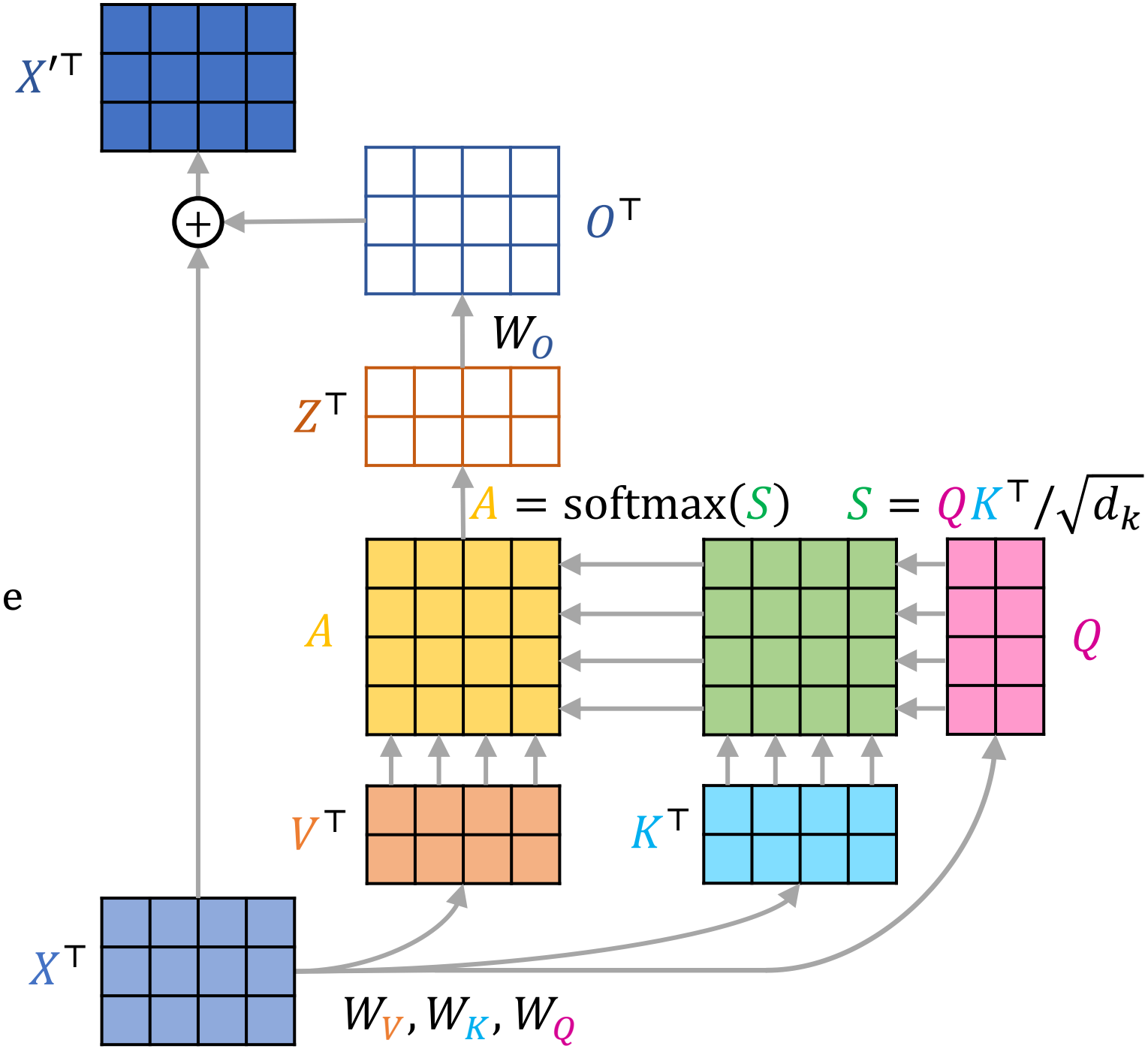
Matrix representation

$$X' = X \oplus O$$
$$O = ZW_O$$

$$Z = AV$$

$$A = \text{softmax}(S)_{\text{row-wise}}$$
$$S = QK^\top/\sqrt{d_k}$$

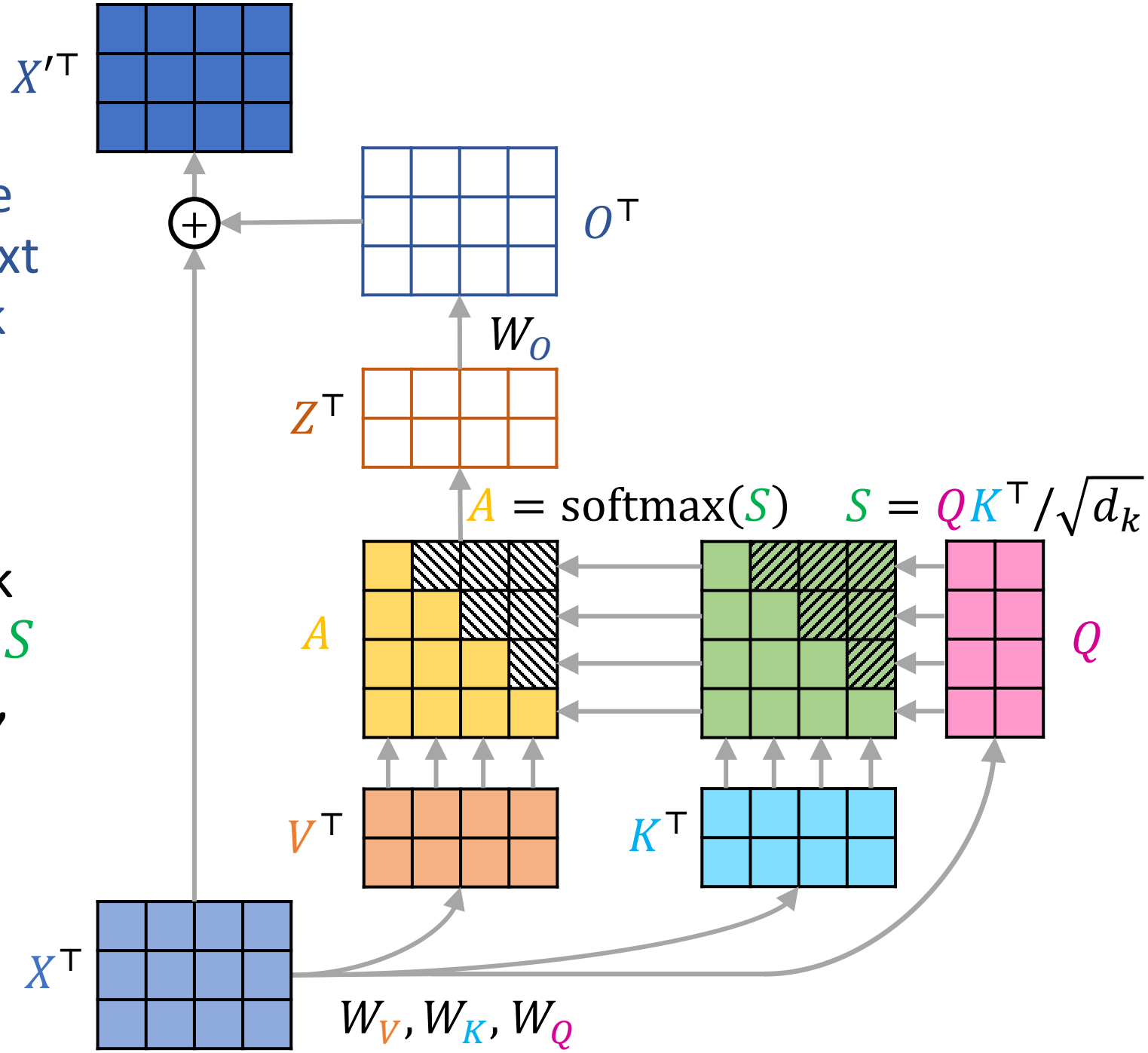
$$Q = XW_Q$$
$$K = XW_K$$
$$V = XW_V$$



Causal Attention

When learning to generate the next token from context $1{:}\,t$, we don't want to look ahead and use any information from $t+1$ or greater

- We apply a causal mask to the attention scores S (filled with $-\infty$ values), which zeros out the appropriate attention weights in A



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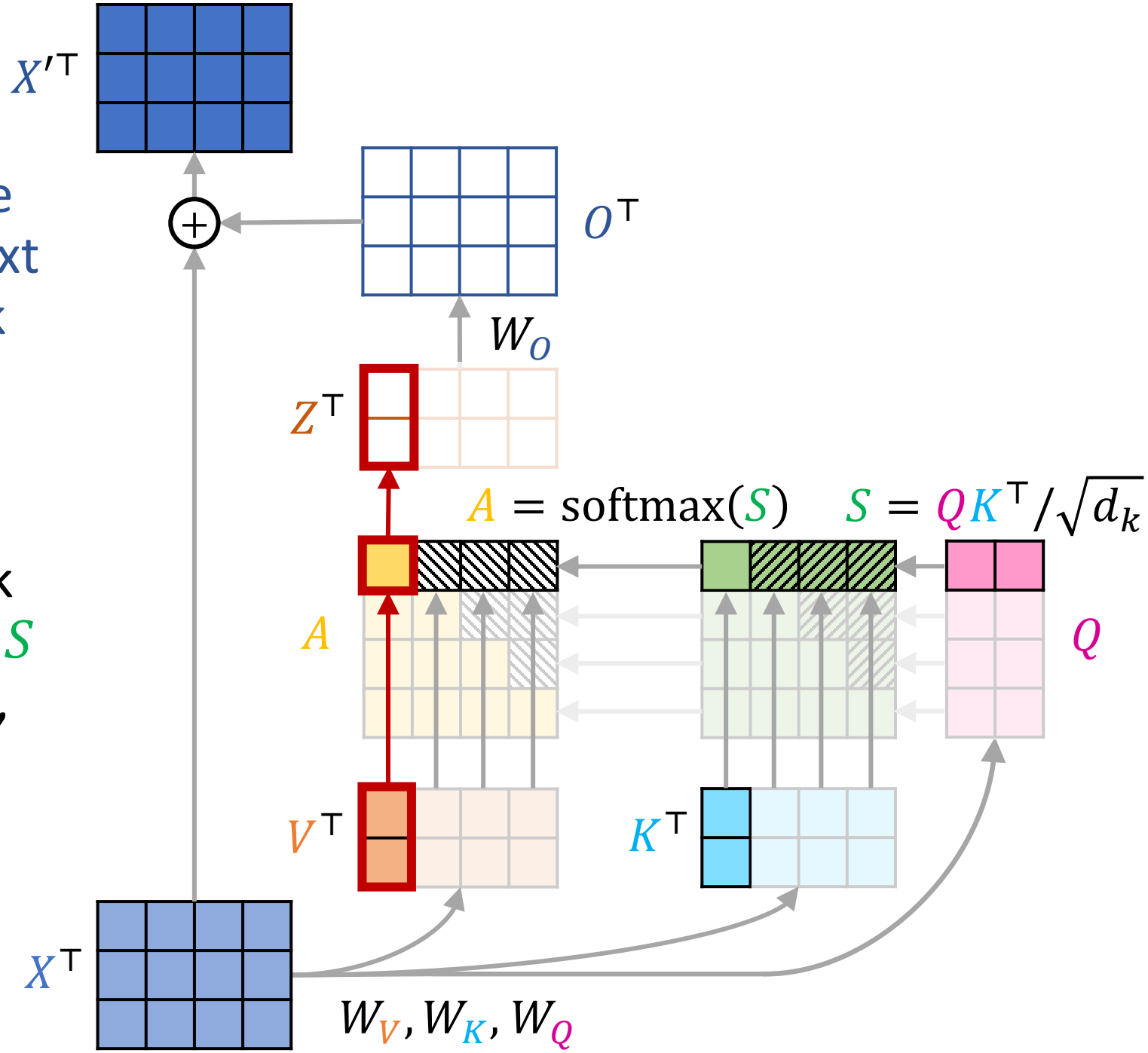

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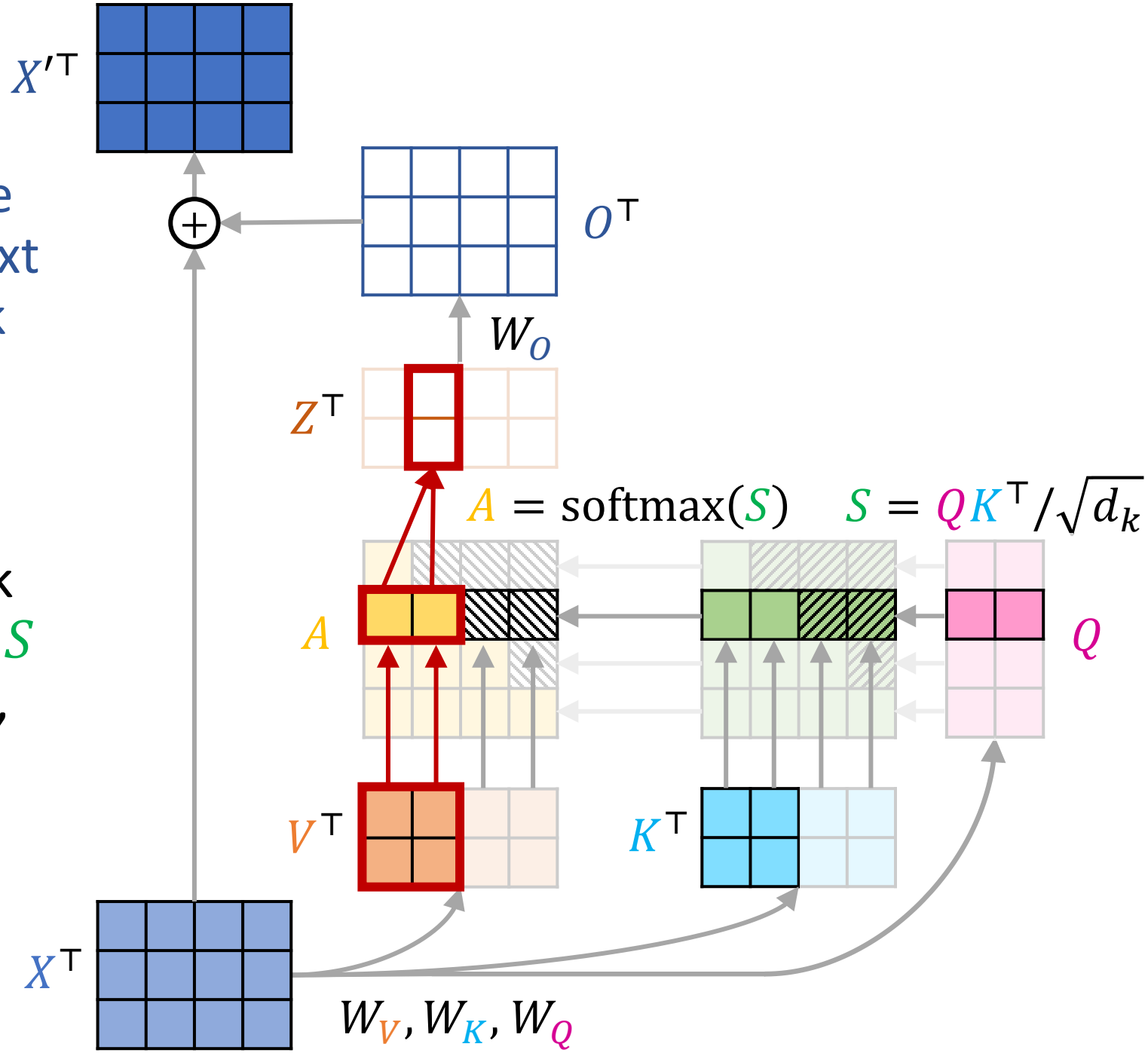

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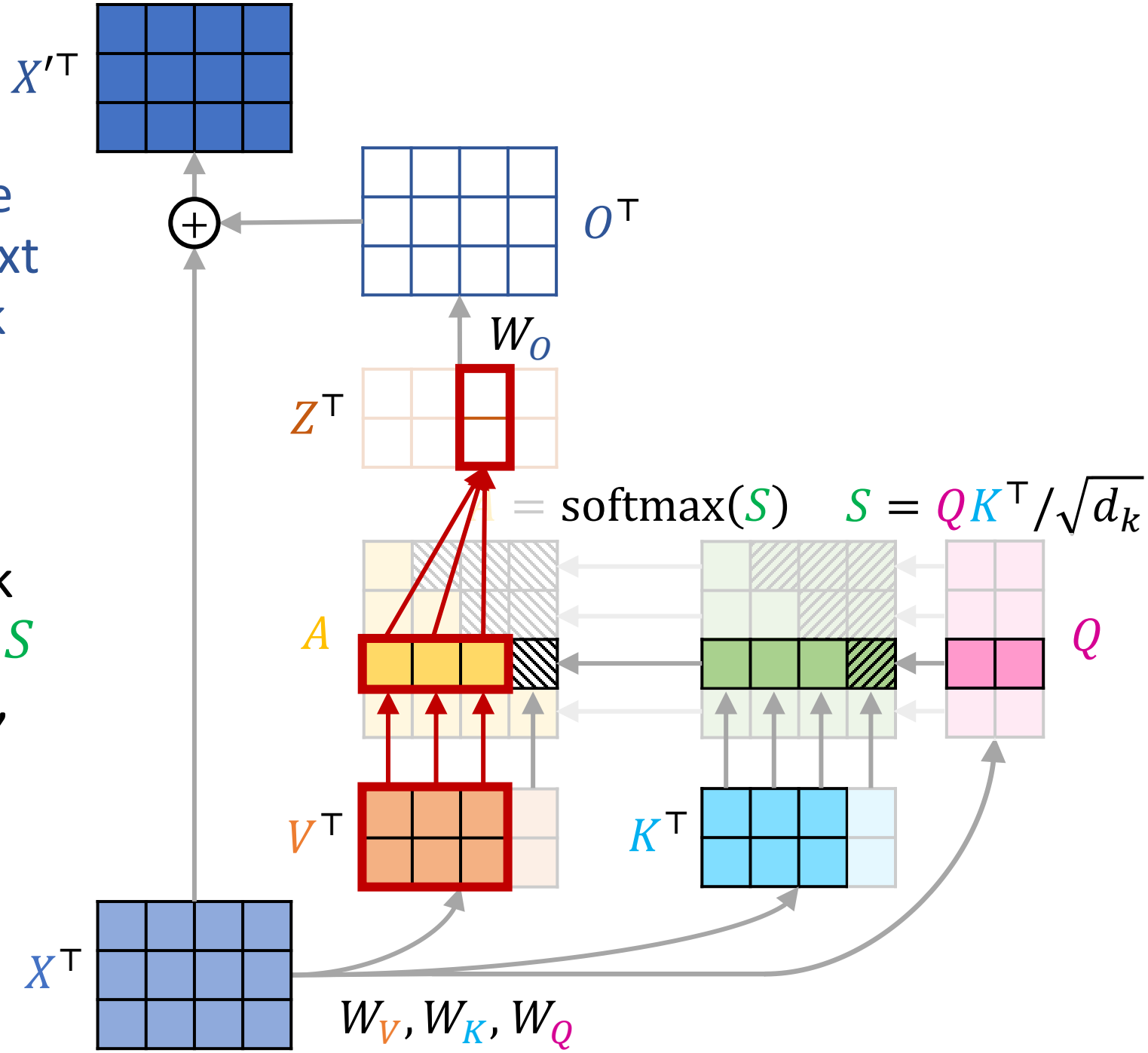

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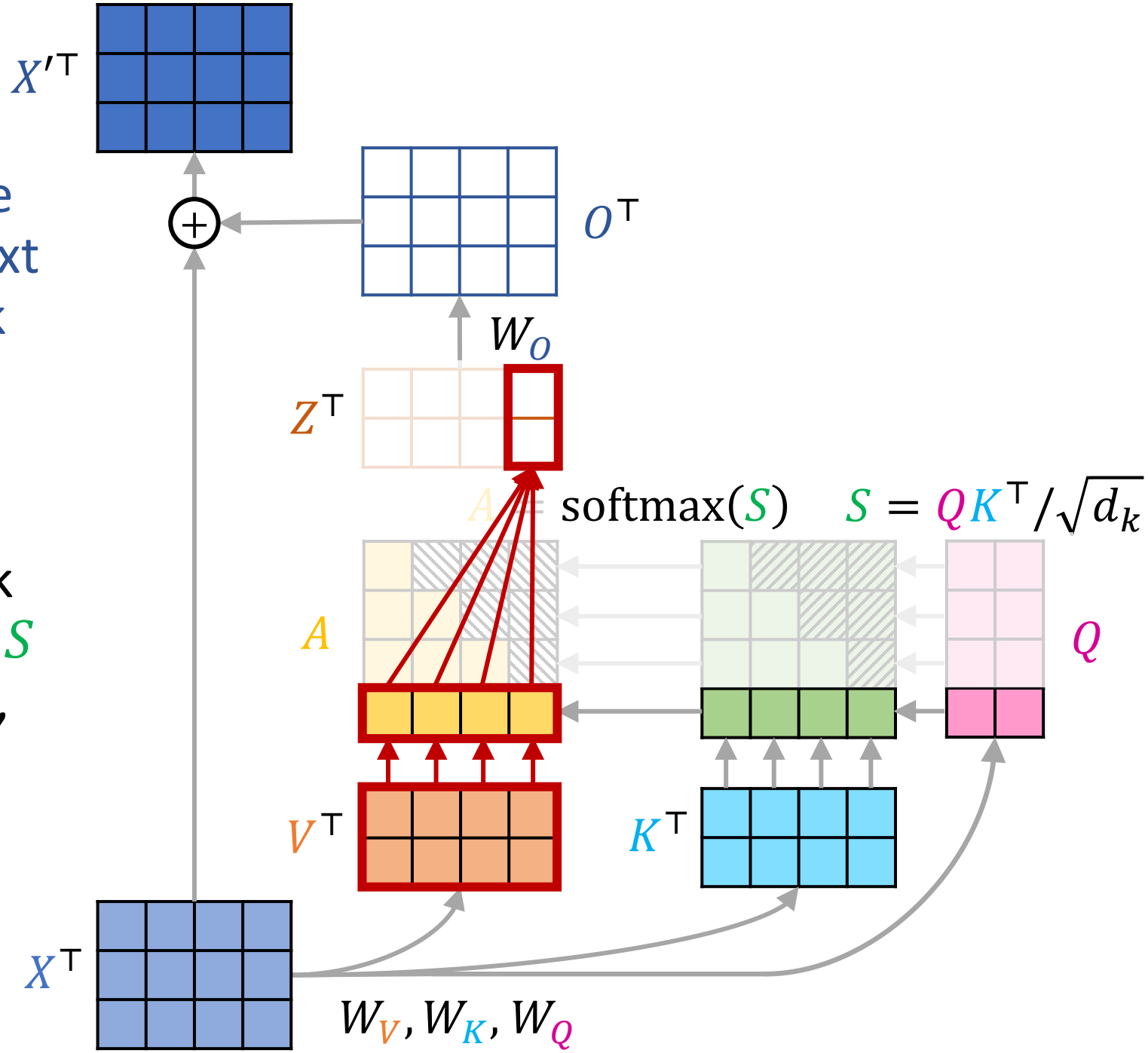
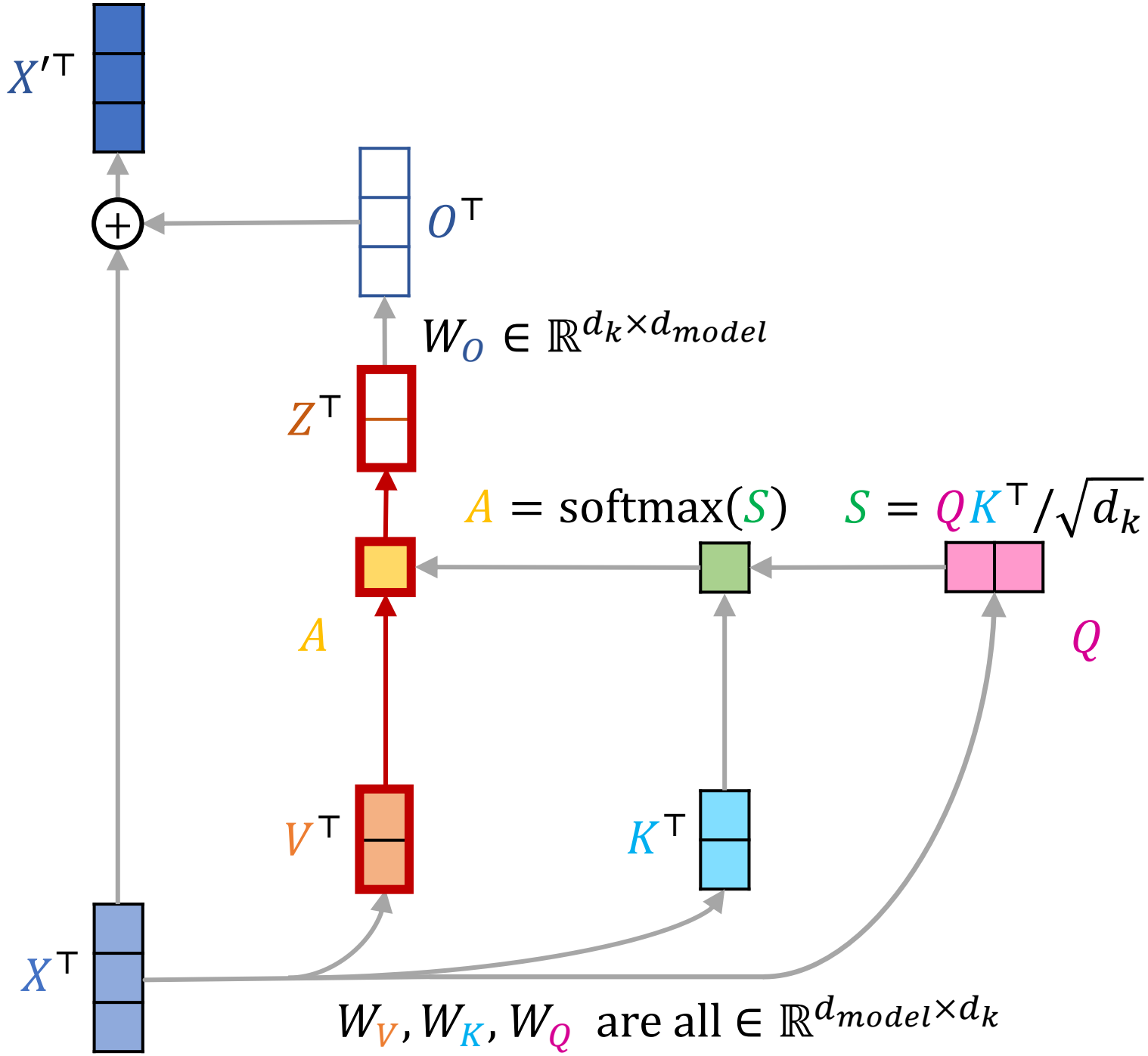


Causal Attention

Inference time

- Done training. Watch this attention block as the context size increases as we generate more and more tokens
- Note how different components build up as the context grows
- But the size of the parameters don't change!



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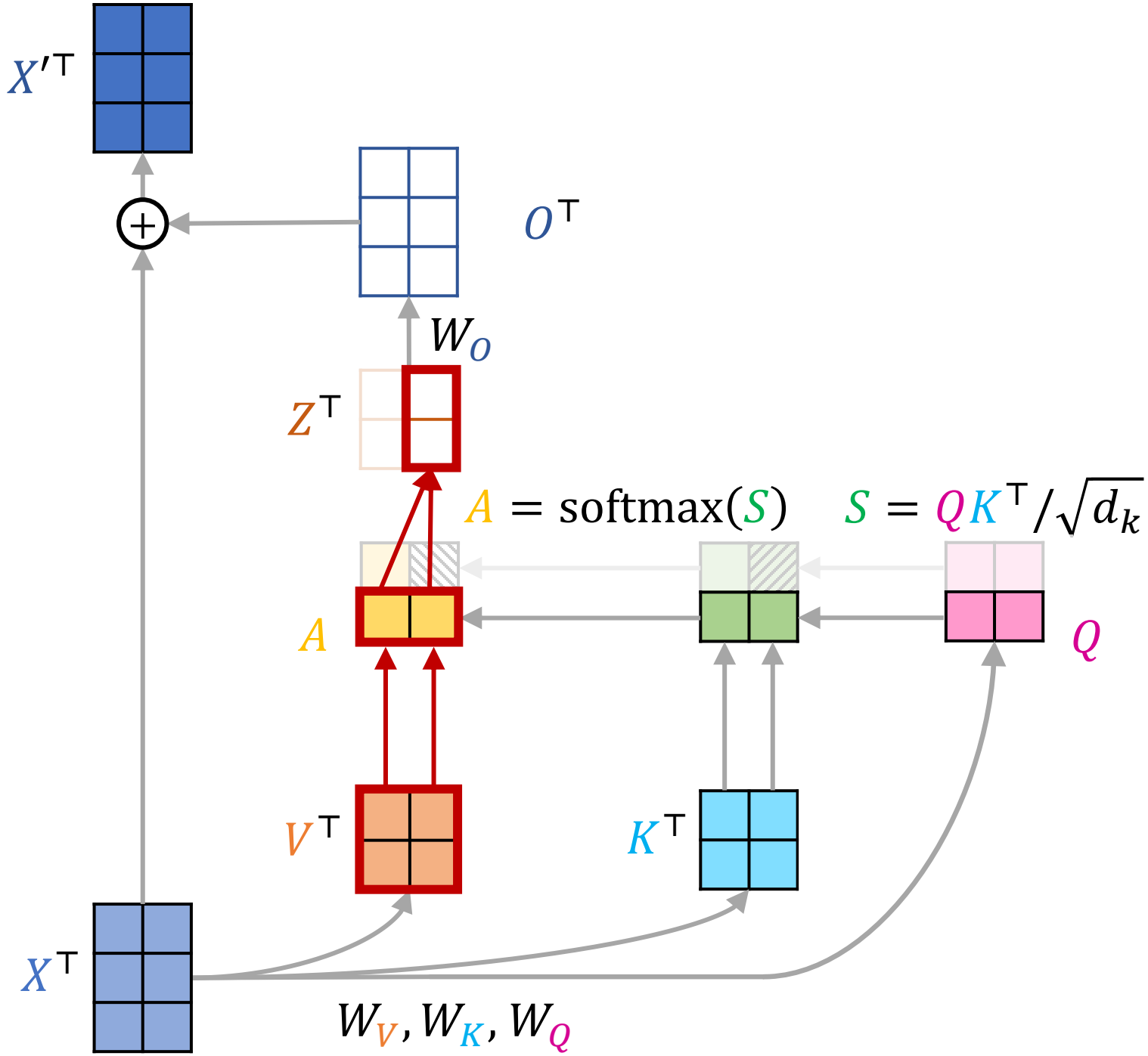

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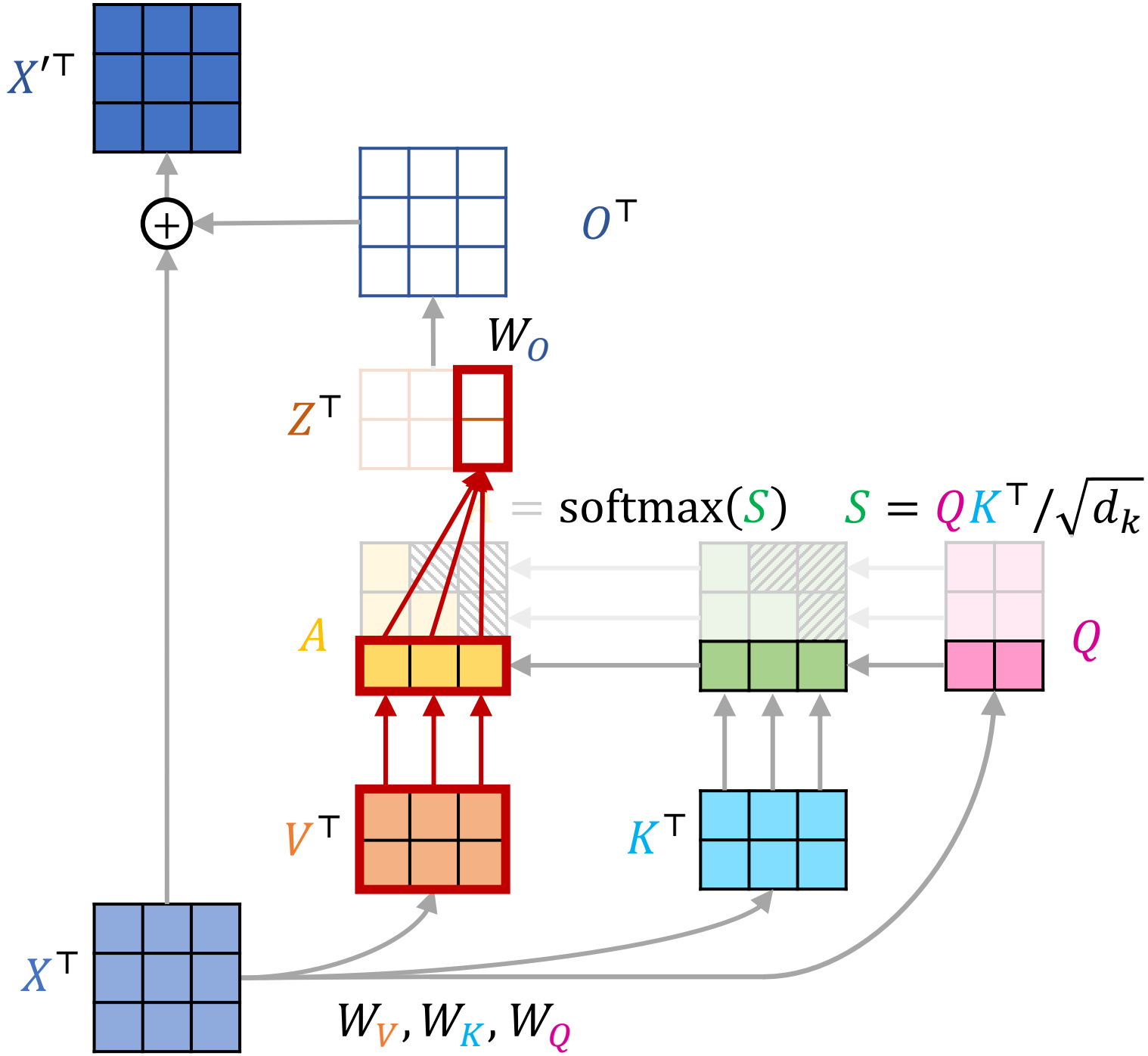

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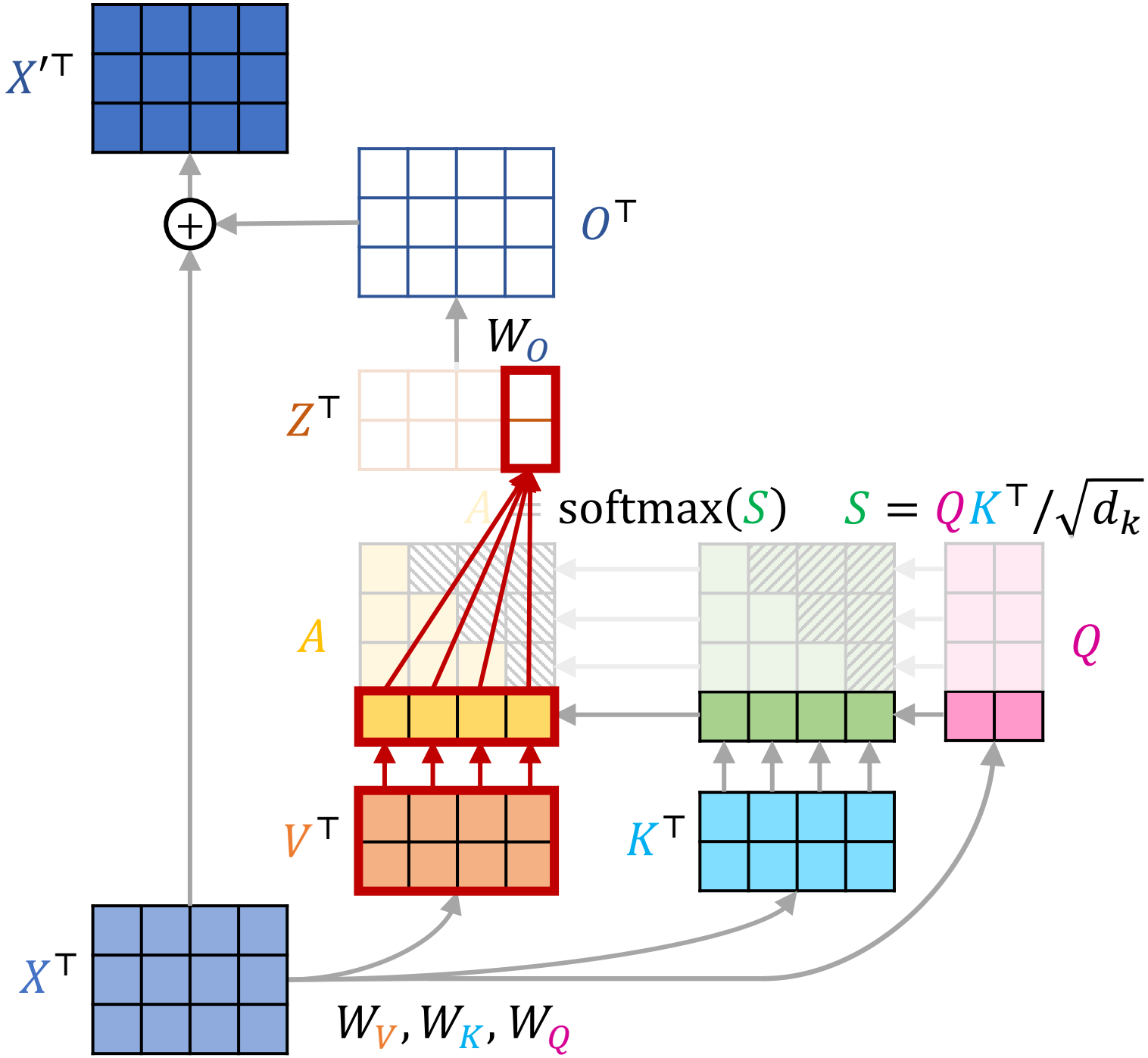
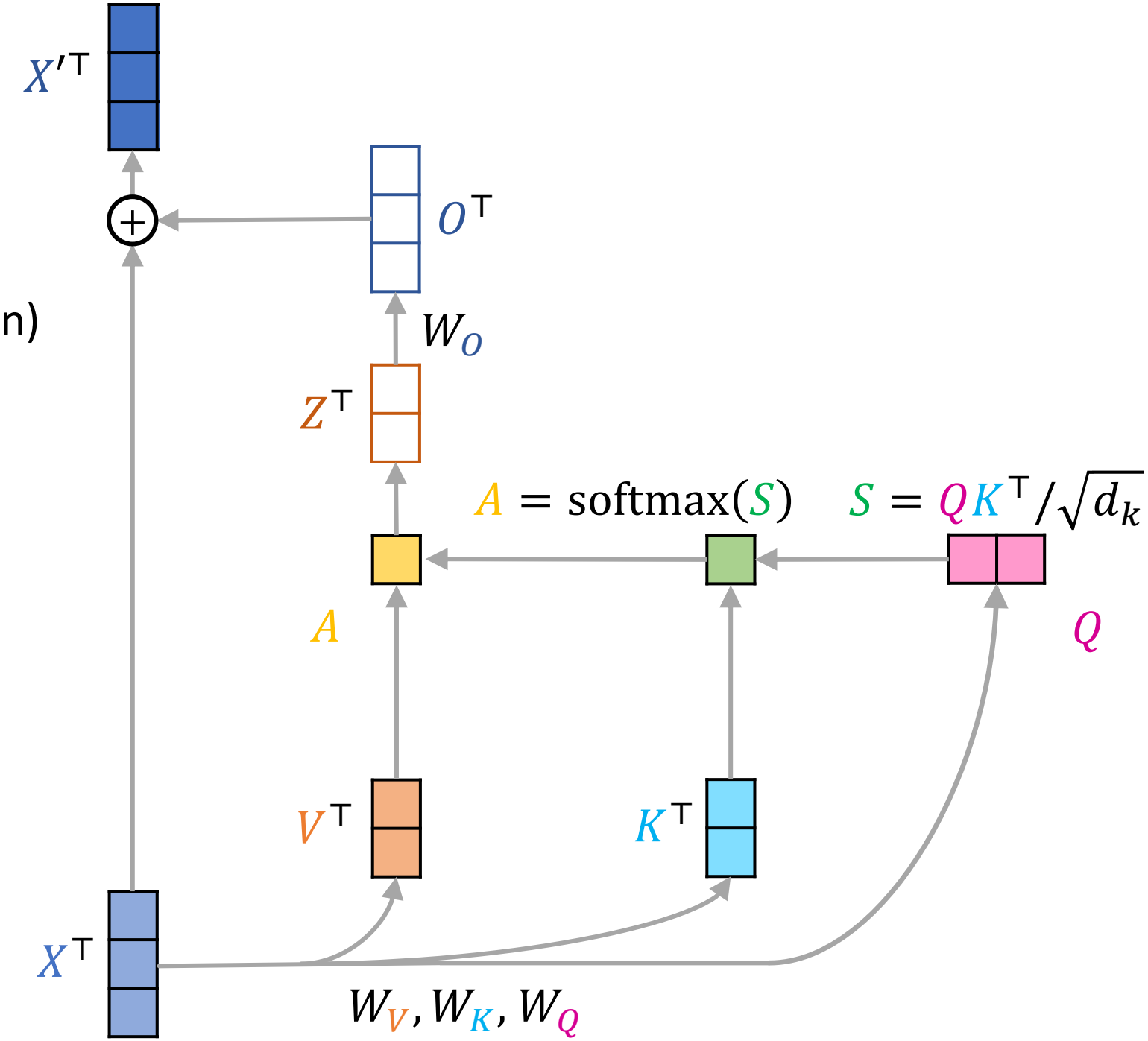


Causal Attention

Inference time

(Repeated without red arrows showing attention combination)



Causal Attention

Inference time

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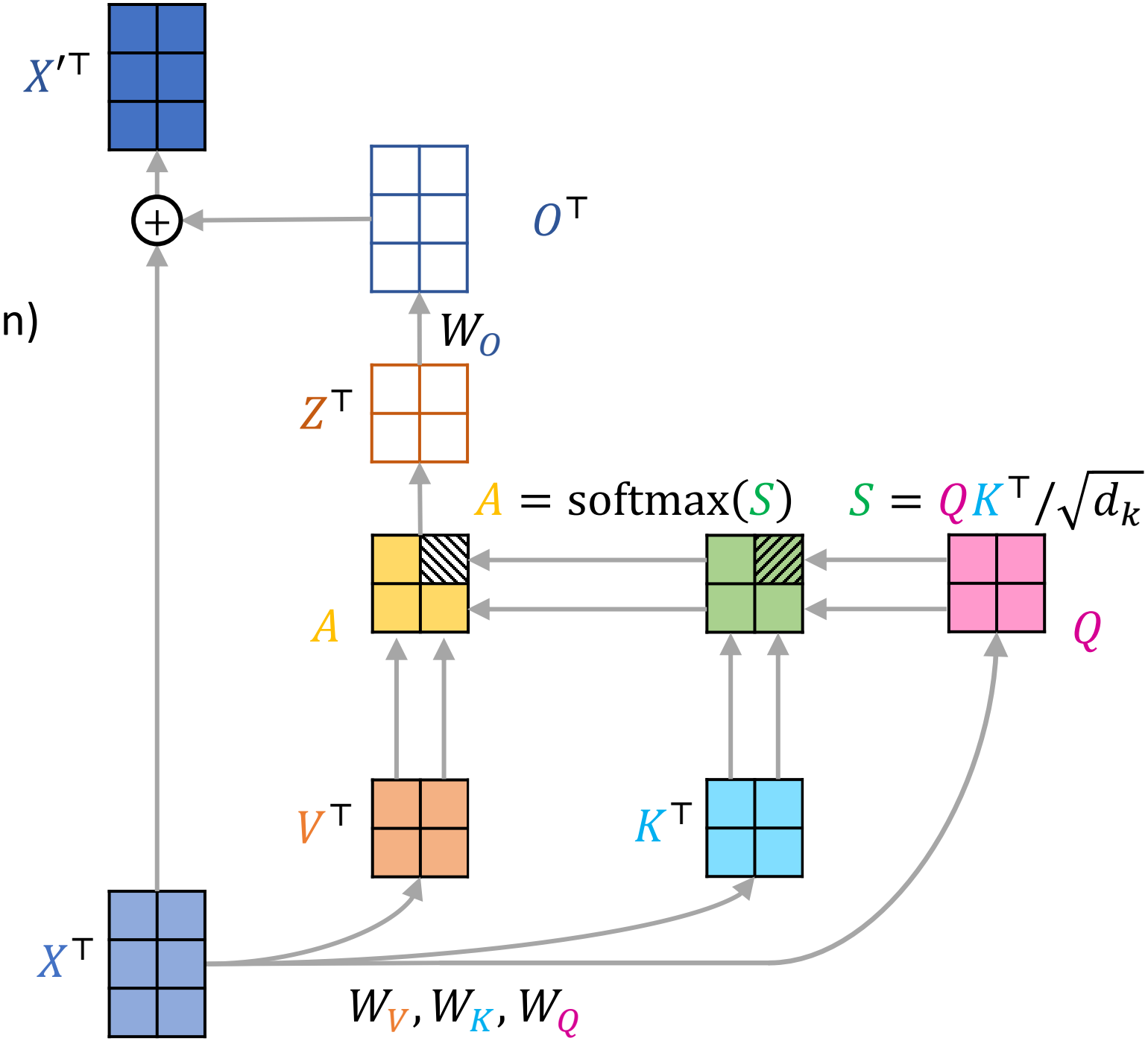

Causal Attention

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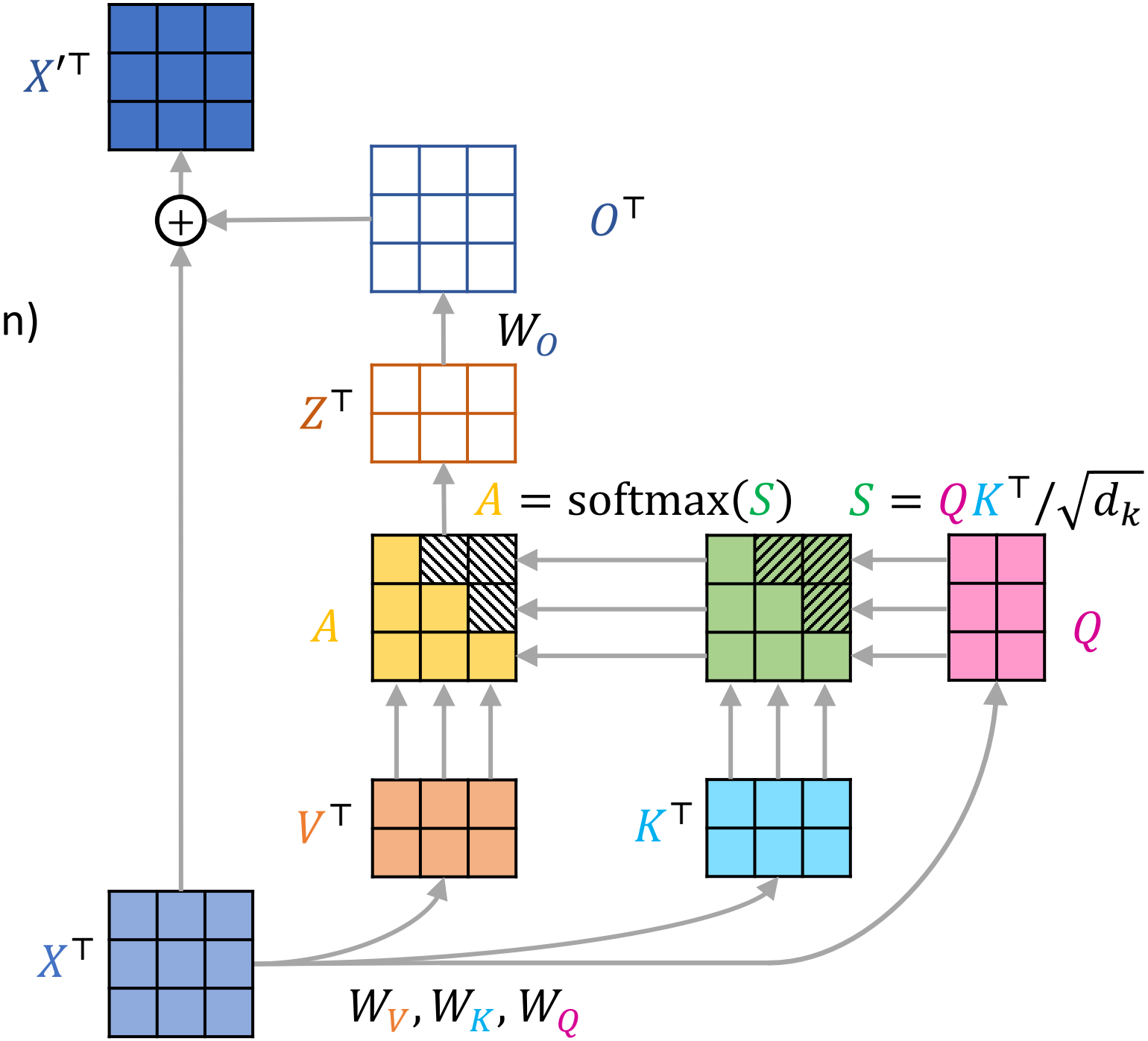

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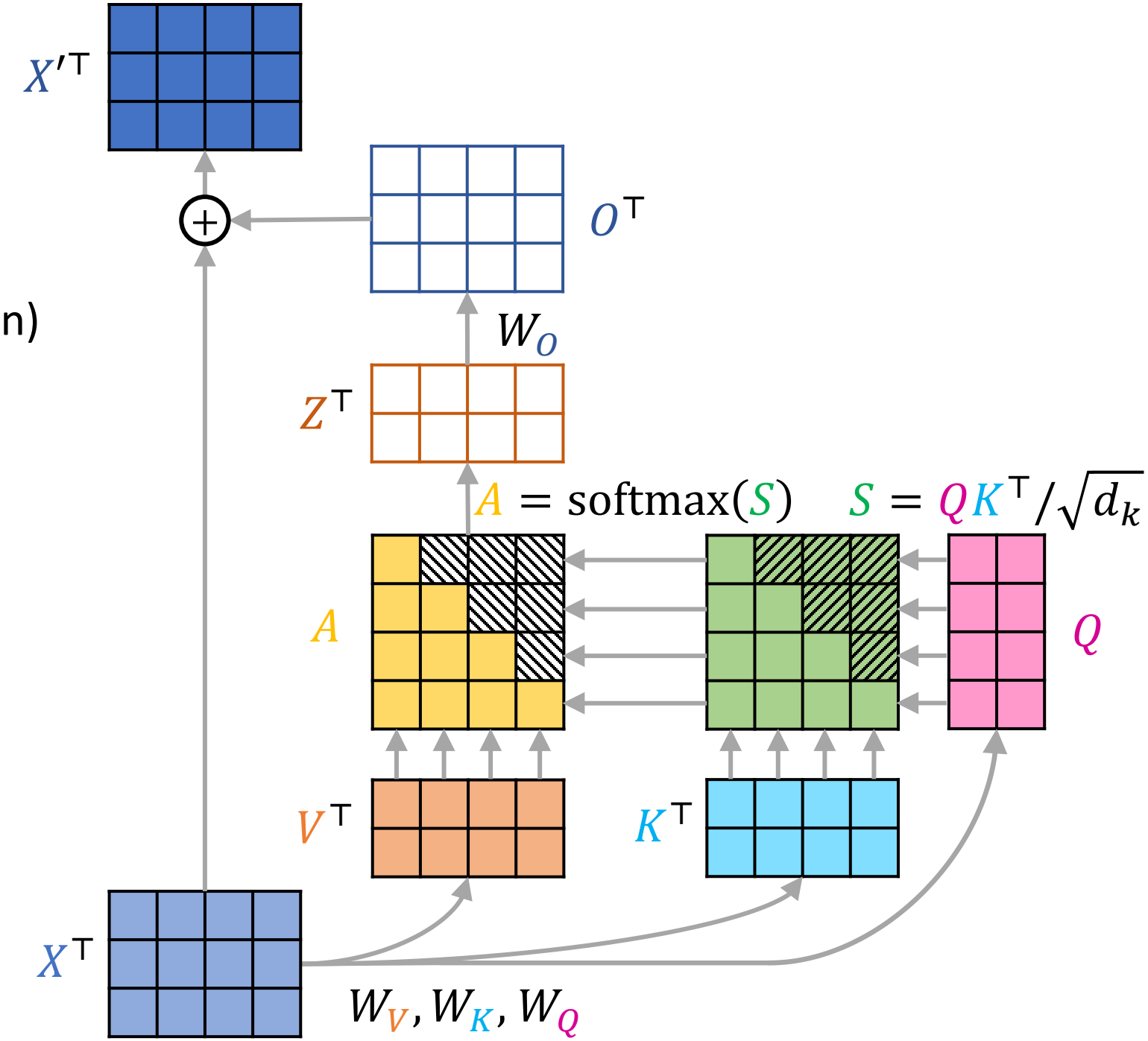
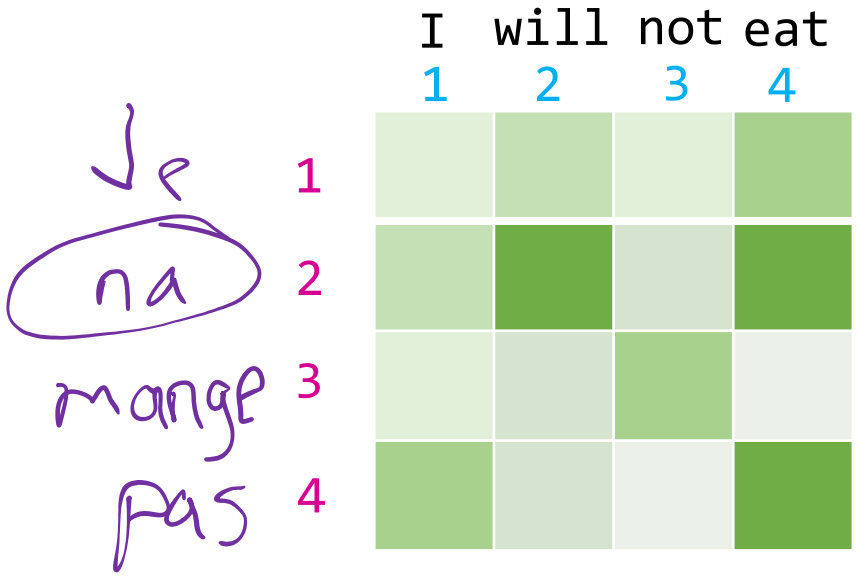
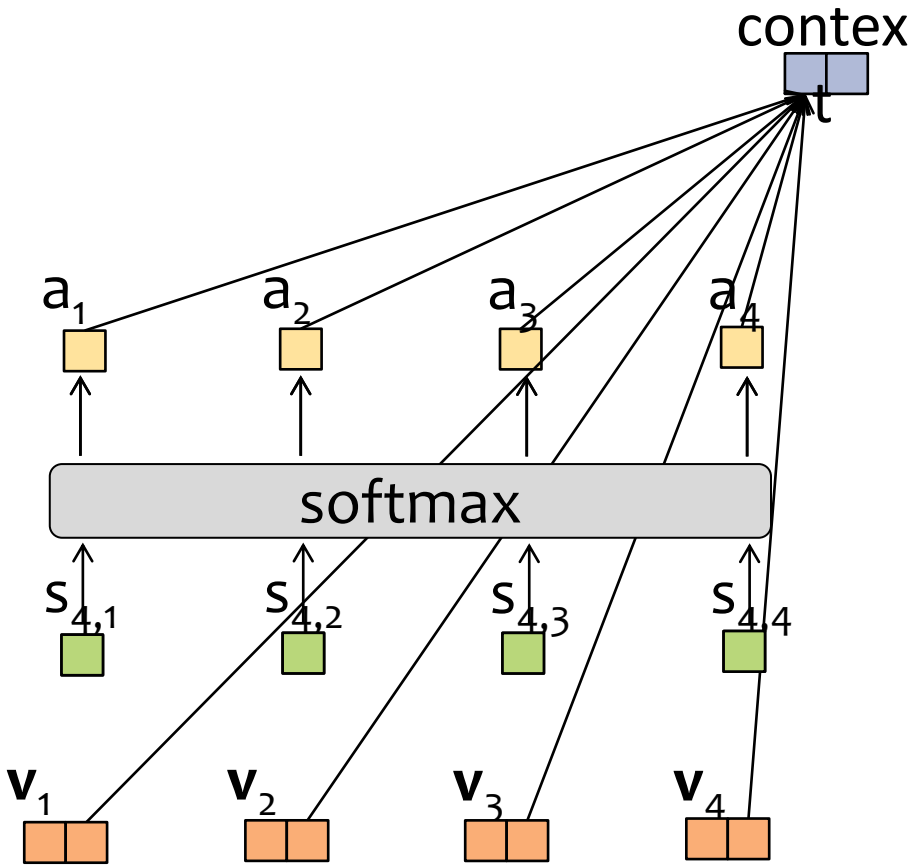


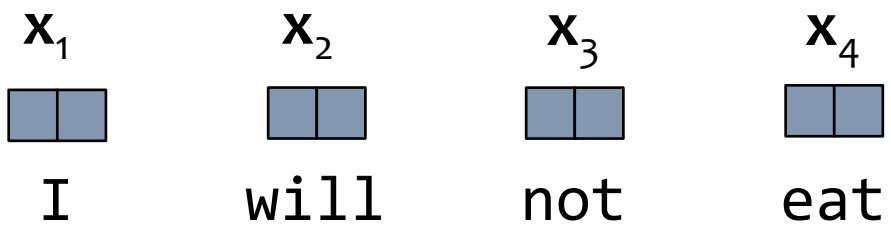
Full Attention

What if we want to translate an input context to another language?





$$S = QK^T/\sqrt{d_k} \qquad Q = XW_Q \qquad K = XW_K \qquad V = XW_V$$



(Full) Attention

Matrix representation

$$X' = X \oplus O$$
$$O = ZW_O$$

$$Z = AV$$

$$A = \text{softmax}(S)_{\text{row-wise}}$$
$$S = QK^\top/\sqrt{d_k}$$

$$Q = XW_Q$$
$$K = XW_K$$
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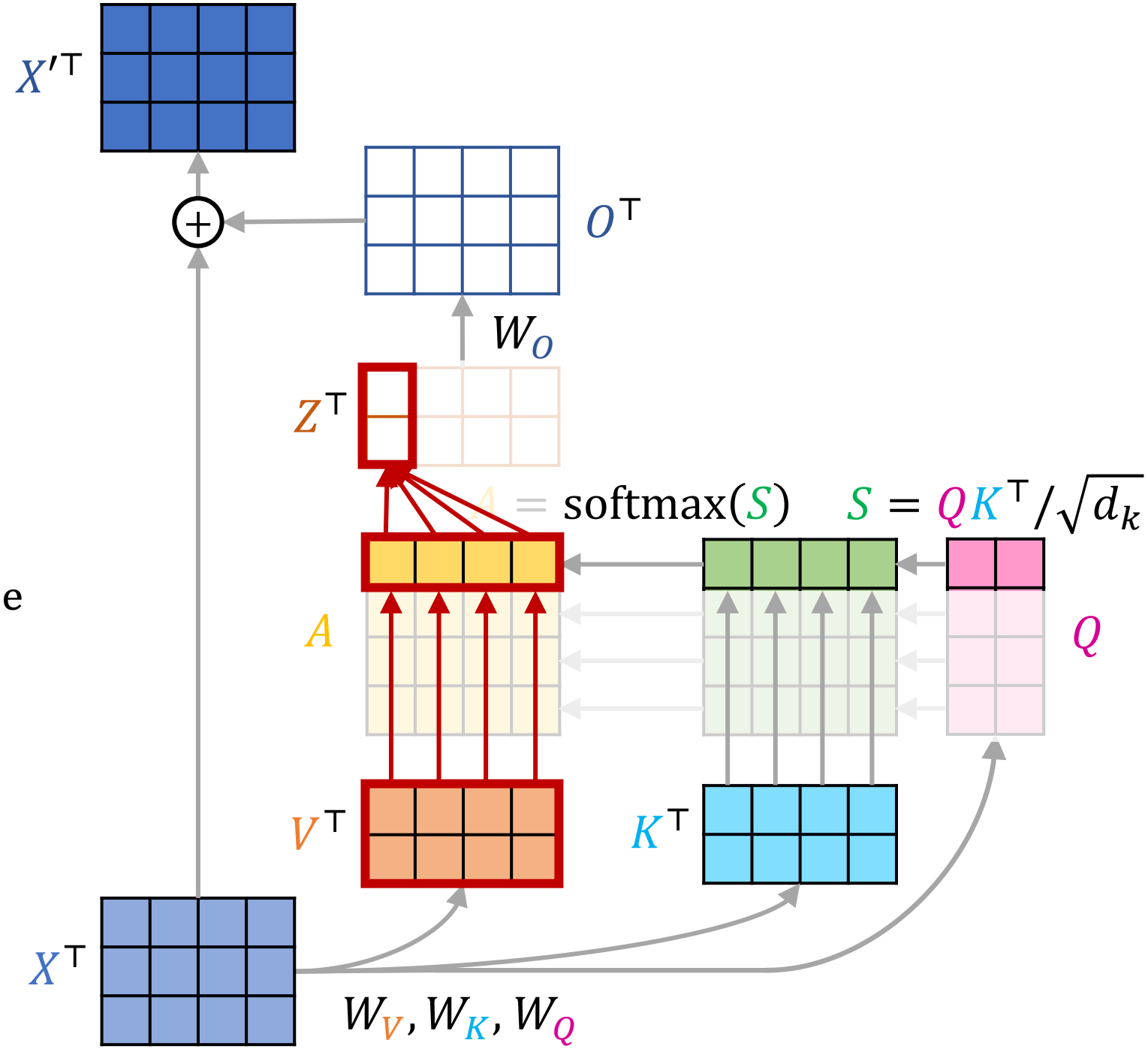

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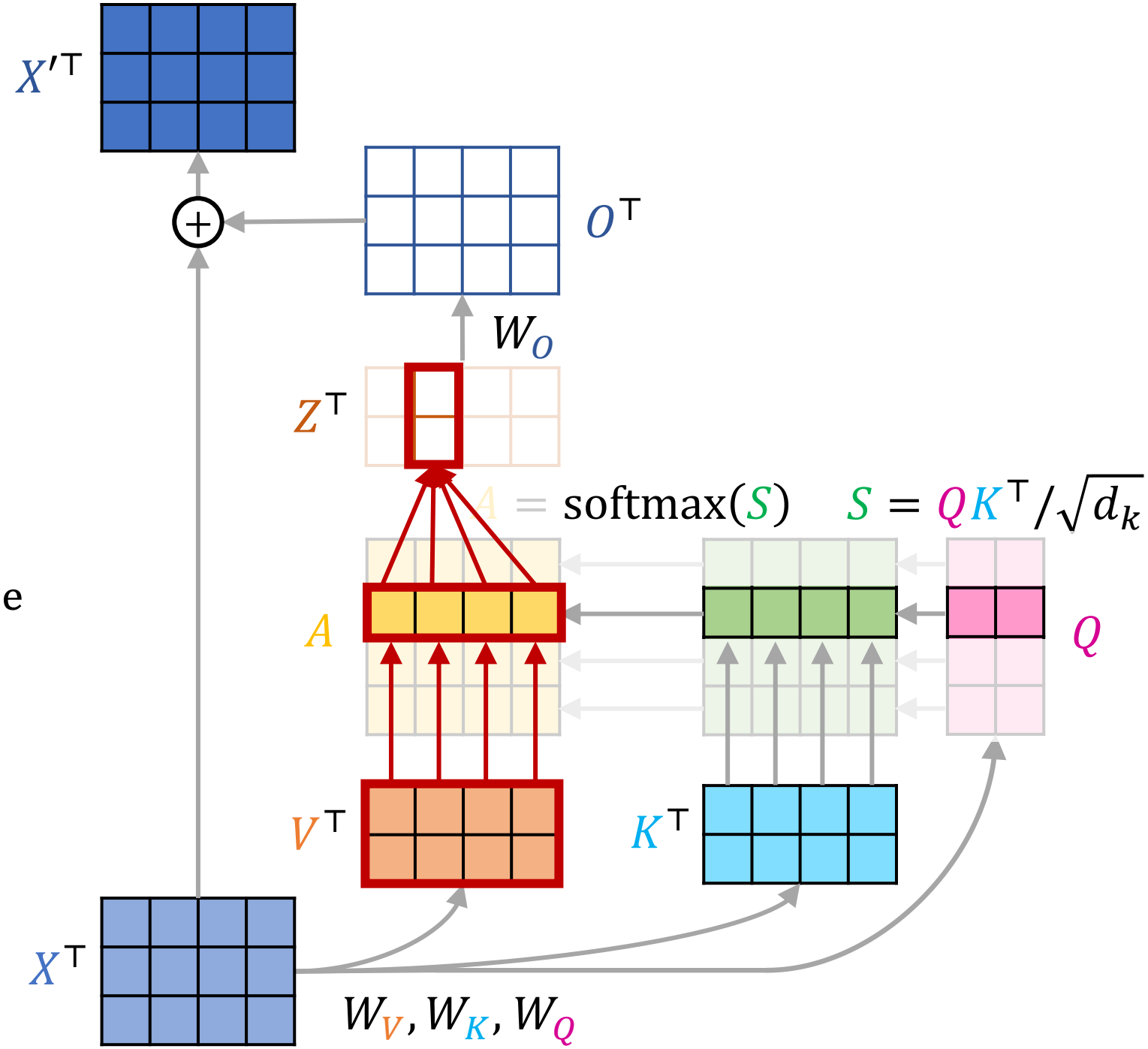

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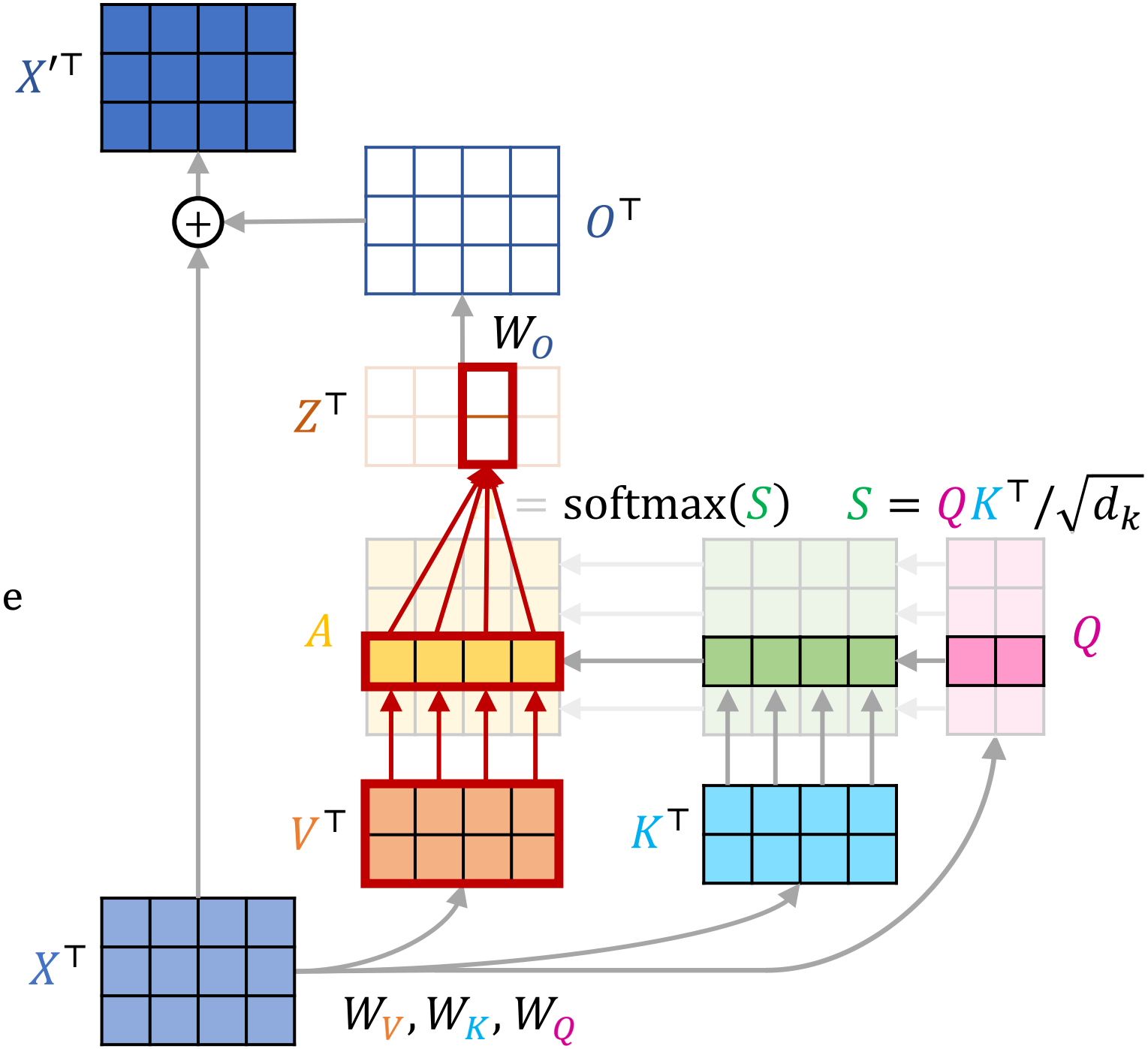

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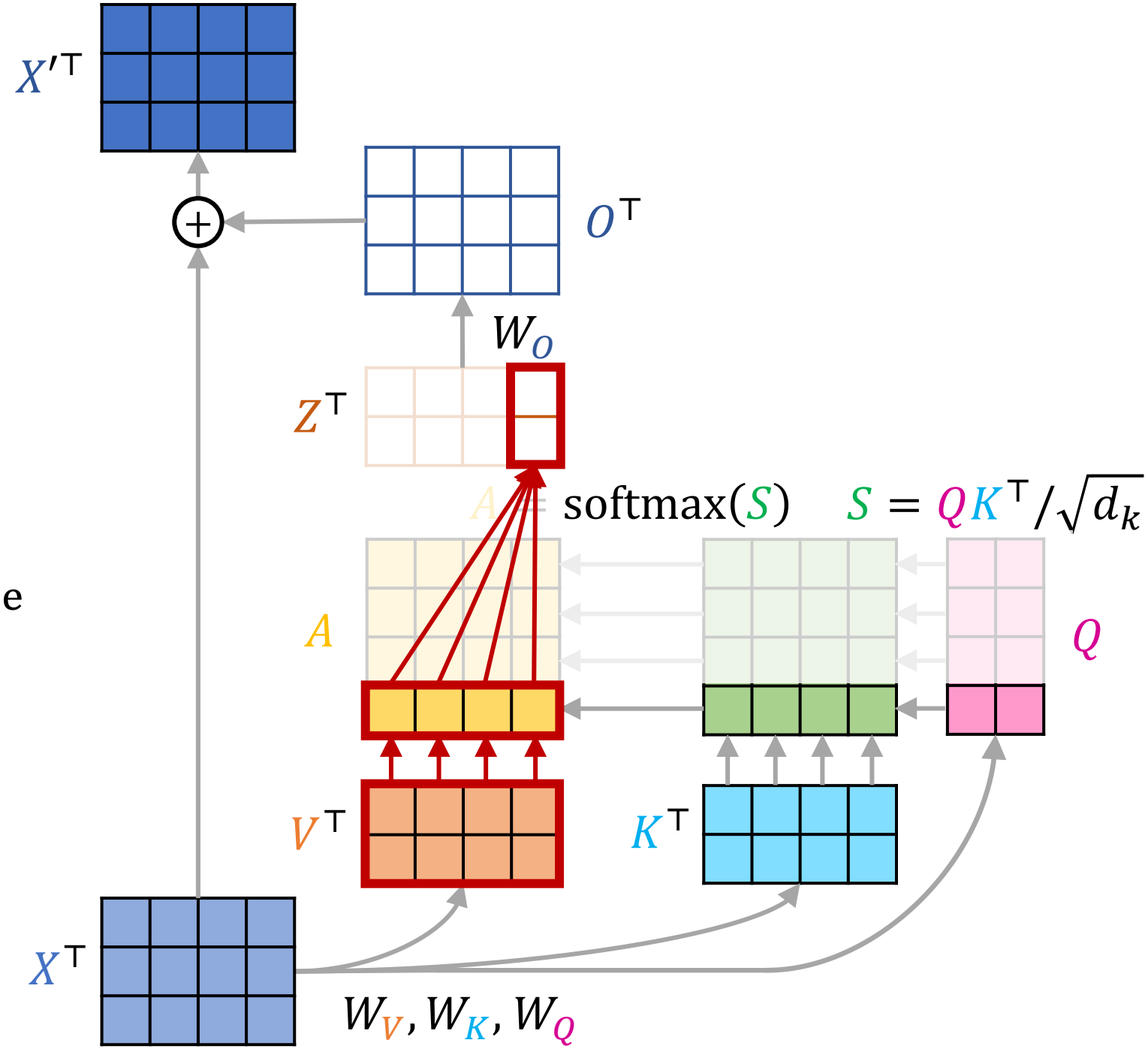

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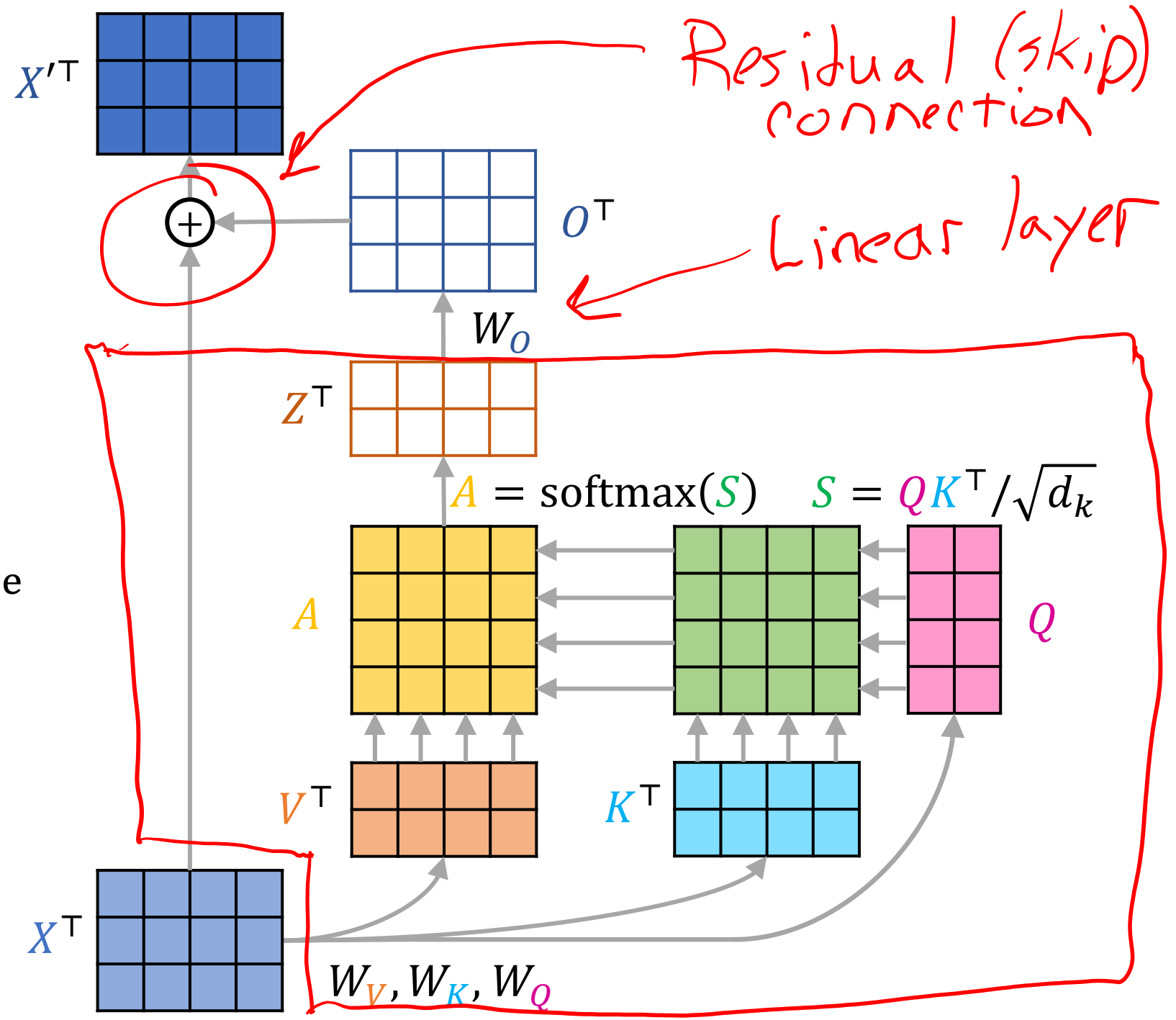


Attention Takeaways

Size of weights doesn't change when the context size changes!

- Weights have to learn a good way to convert input tokens to q, k, v regardless of context length
- Better than having different copies of weights for every context size

Similarity matrix in attention is calcuated (not a parameter matrix)!

- S does change side based on context but it is generated from two generated matrices Q and K
- Attention is learned from Q and K via W_Q and W_K

Linear operations!

- GPUs already do this fast

Transformer Language Models

Increasing context size

- Uniform average of context vectors
- Position encoding

Attention

- Weighted average of context vectors
- Query Keys Values
- **Expressive power of linear transforms**

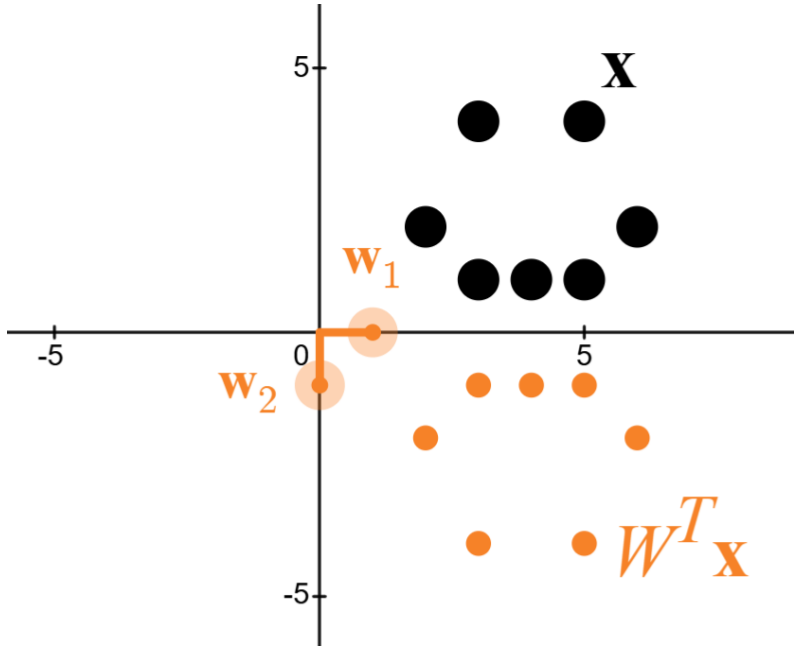
Building GPT2!

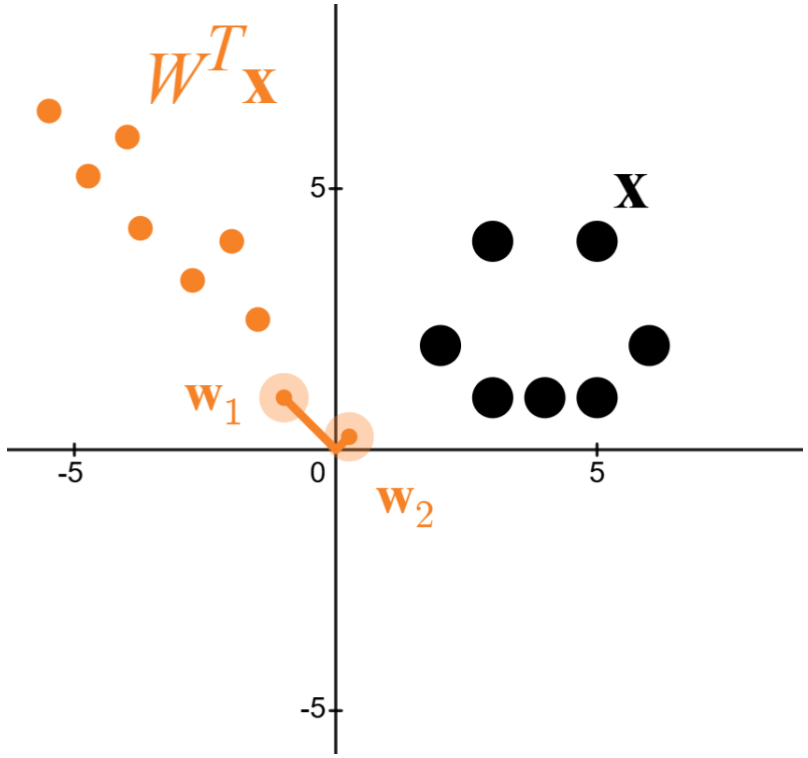
Linear Transforms: Graphical Intuition

In Transformer models, we see quite a few linear transforms

A simple $\mathbf{z} = W^{\top}\mathbf{x}$ can move points quite a bit

Desmos example for $\boldsymbol{x}$ and $\mathbf{z}$ in $\mathbb{R}^2$
https://www.desmos.com/calculator/gl5ljvorcy

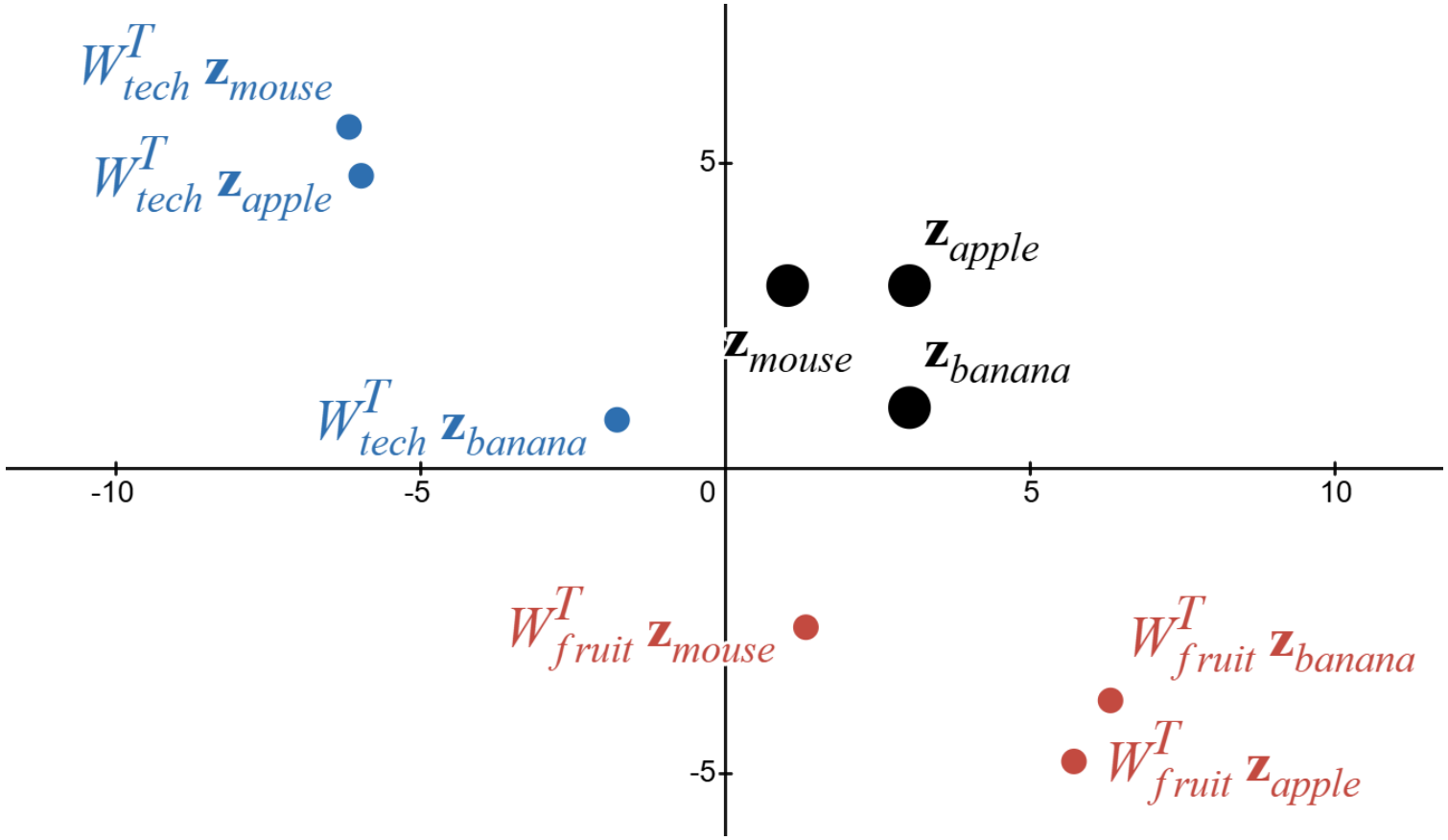




Linear Transforms: Graphical Intuition

Two different transforms $W_{tech}^{\top}\mathbf{z}$ and $W_{fruit}^{\top}\mathbf{z}$ can create two different meaningful embeddings for the input vectors $\mathbf{z}$

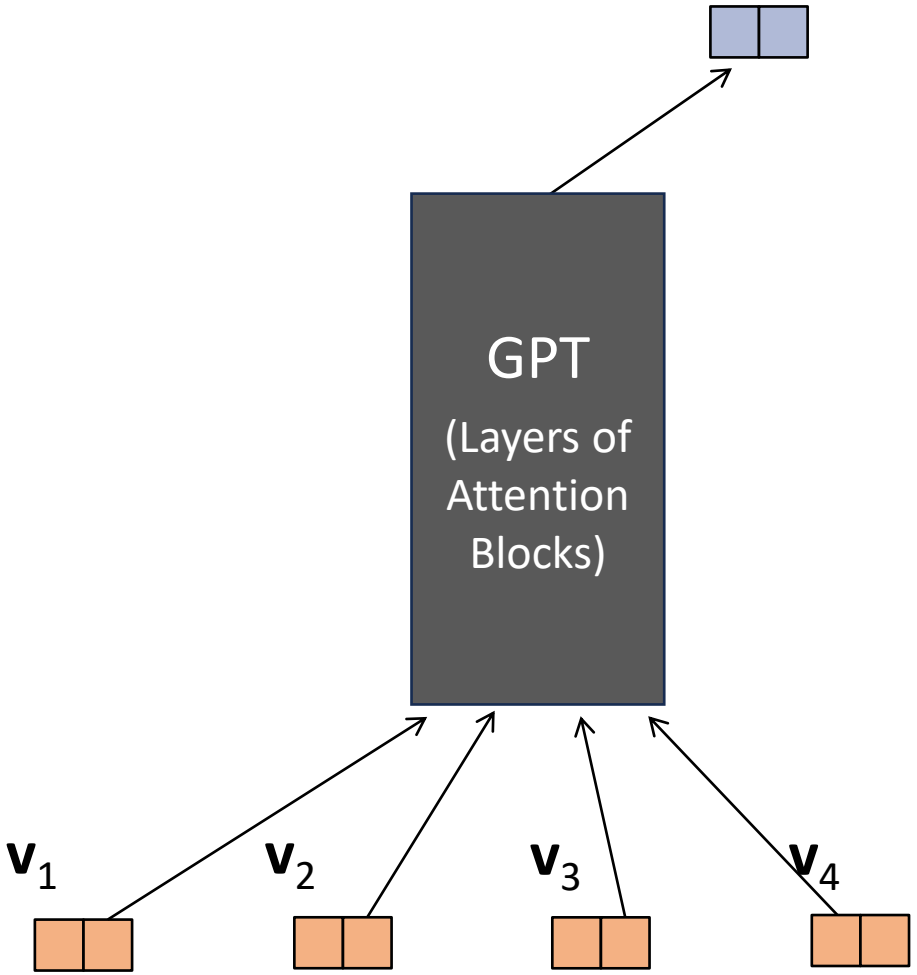
Desmos example for W in $\mathbb{R}^{2\times 2}$ https://www.desmos.com/calculator/tbeclbo83h



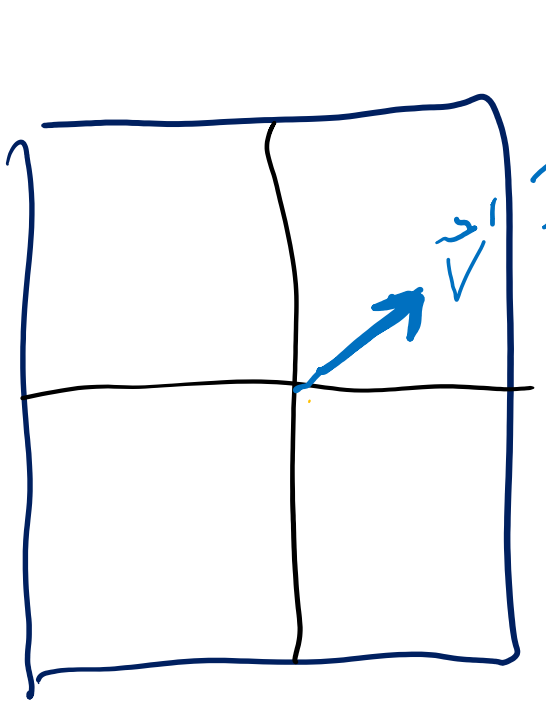
Building GPT2!

GPT Skeleton

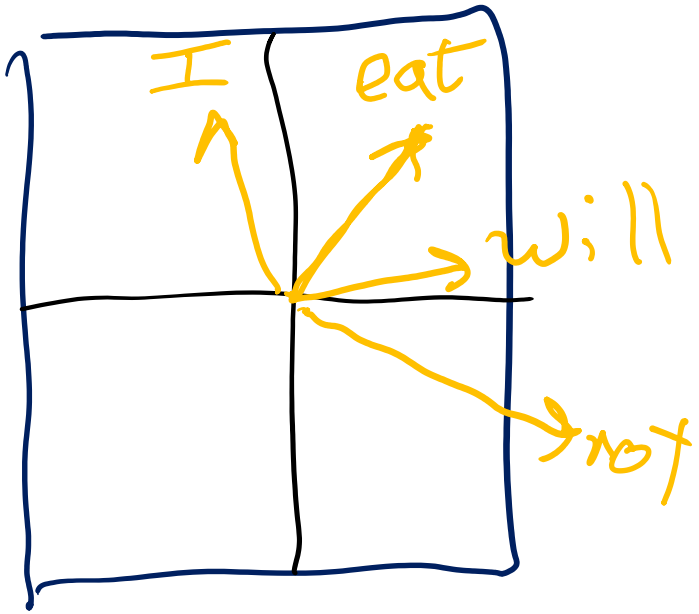
2 M



Embedded context tokens

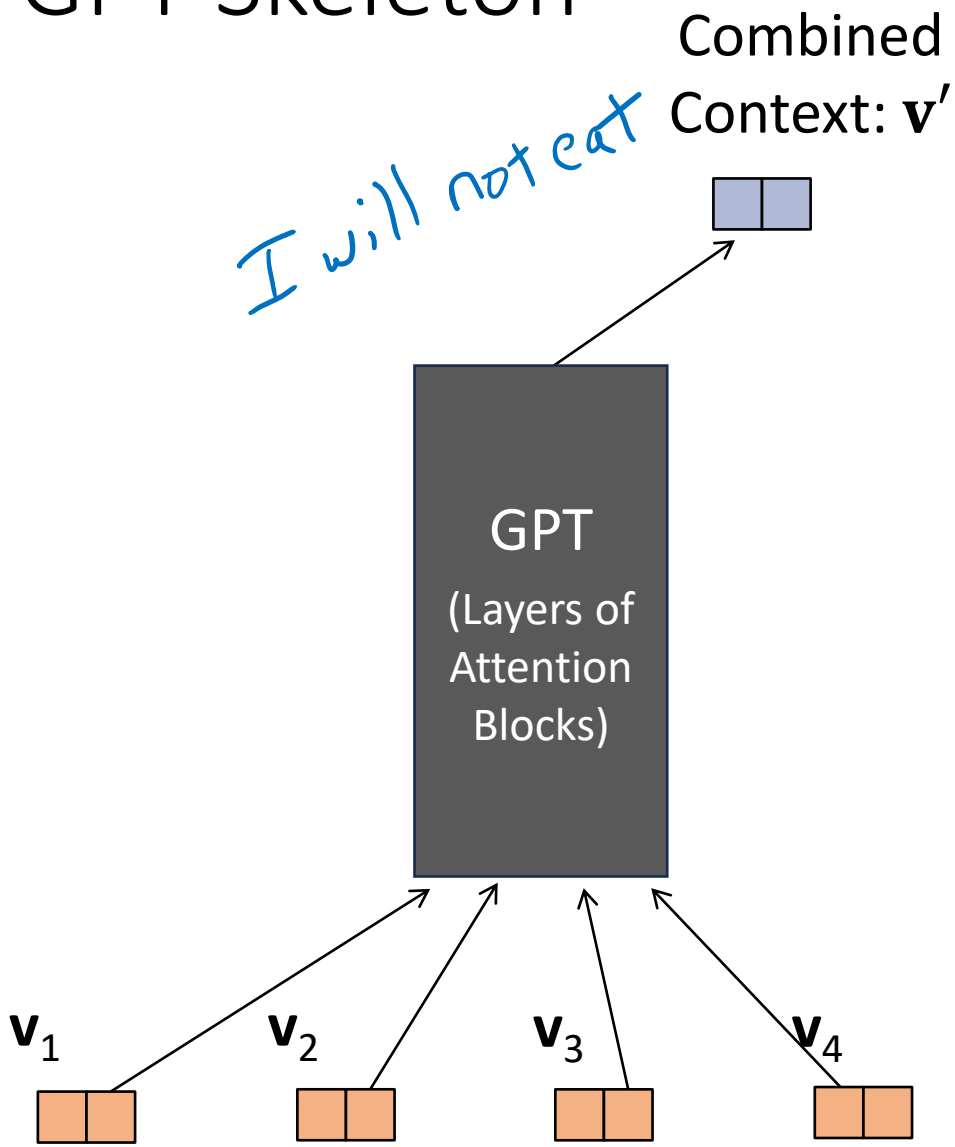


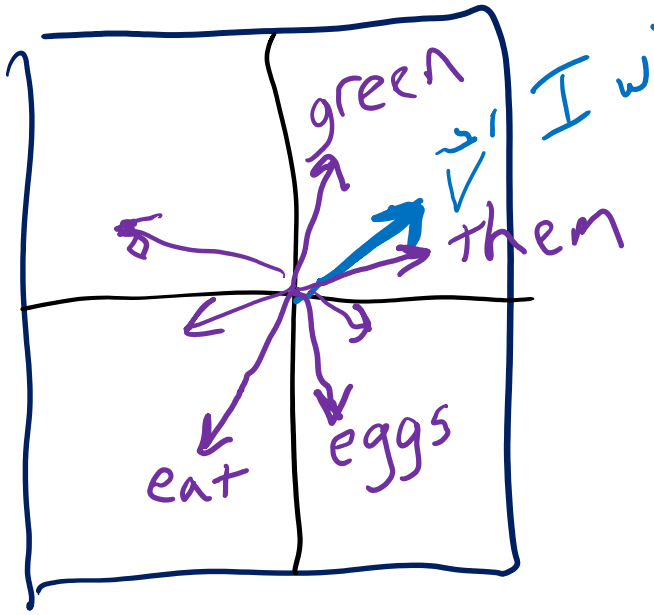
Final GPT Embedded Space (single head)



Token Embedded Space

GPT Skeleton





Final GPT linear layer

$$\hat{\mathbf{y}} = g_{softmax}(U\mathbf{v}')$$

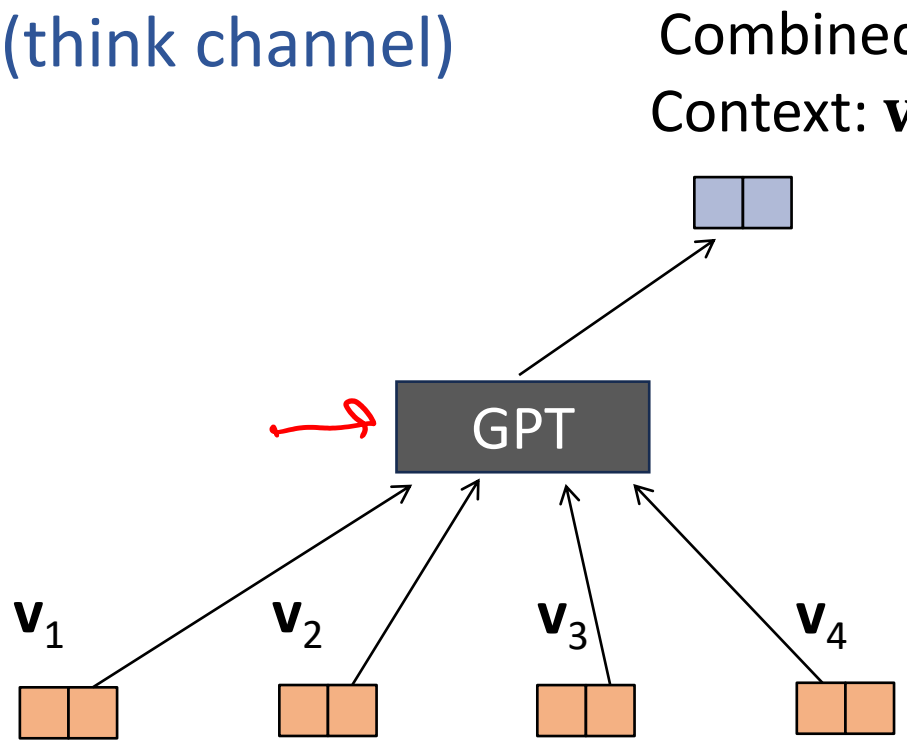
$$next\_idx = \underset{j}{\text{argmax}}\, \hat{\mathbf{y}}$$

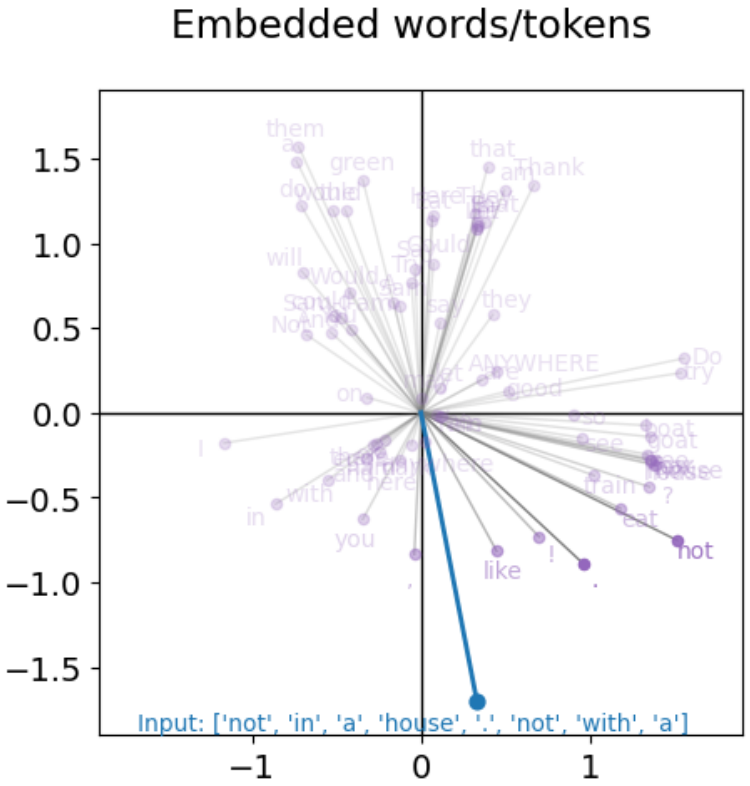
MinGPT Femto

2-D embedded space

1 attention layer

1 attention head (think channel)





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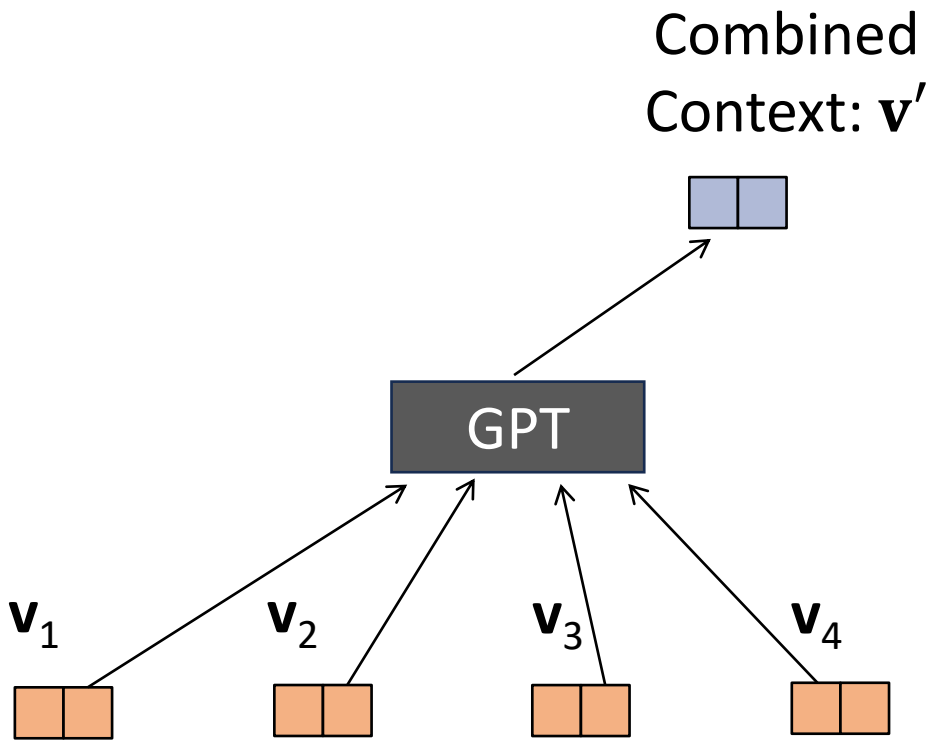
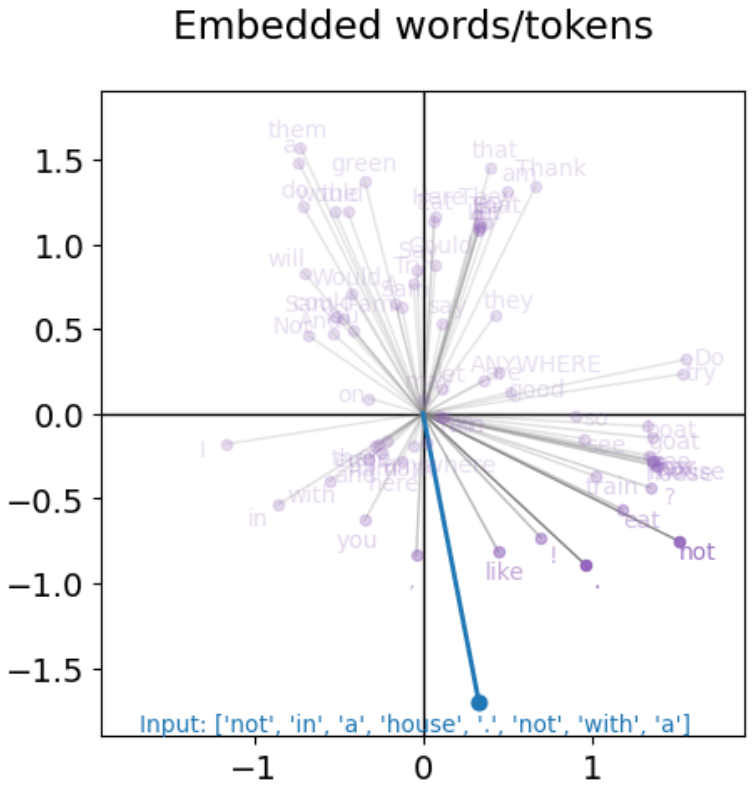
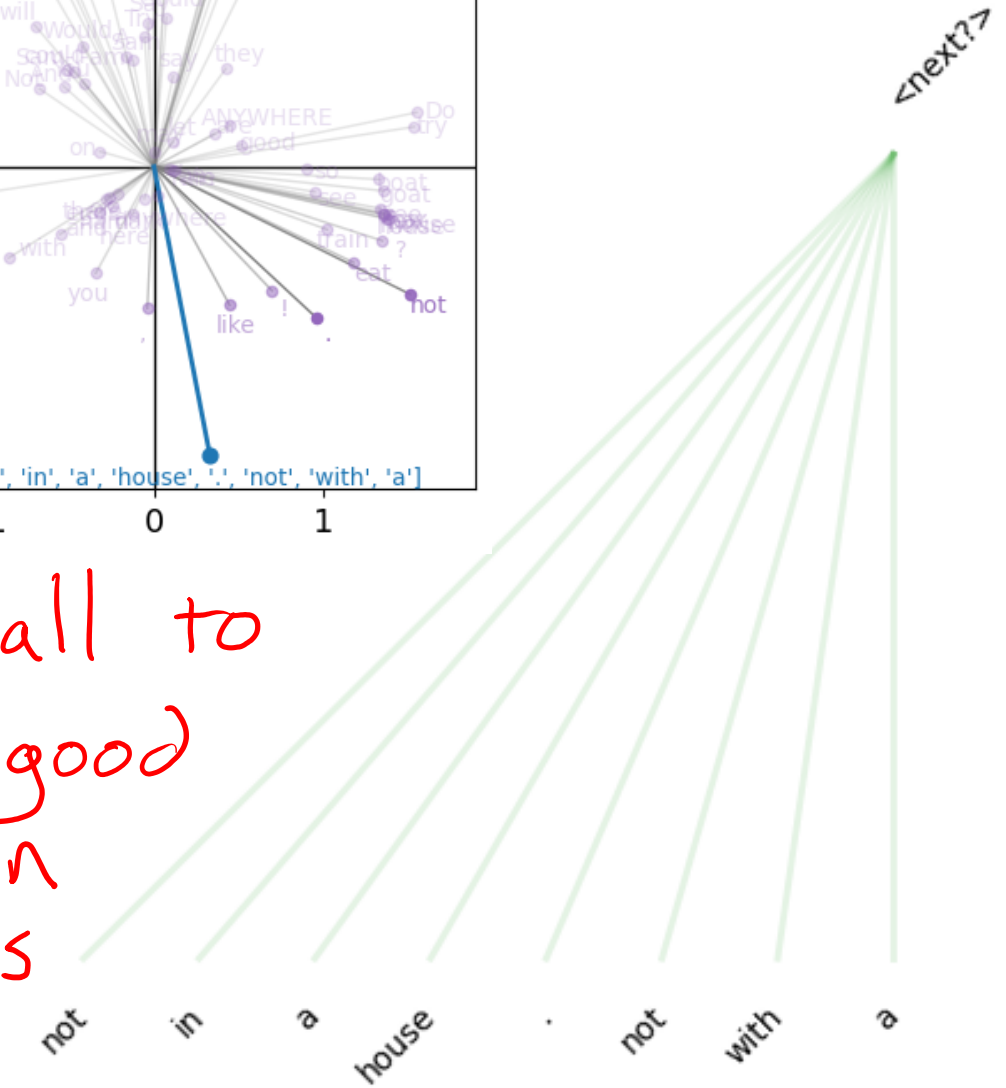




Too small to learn good attention weights

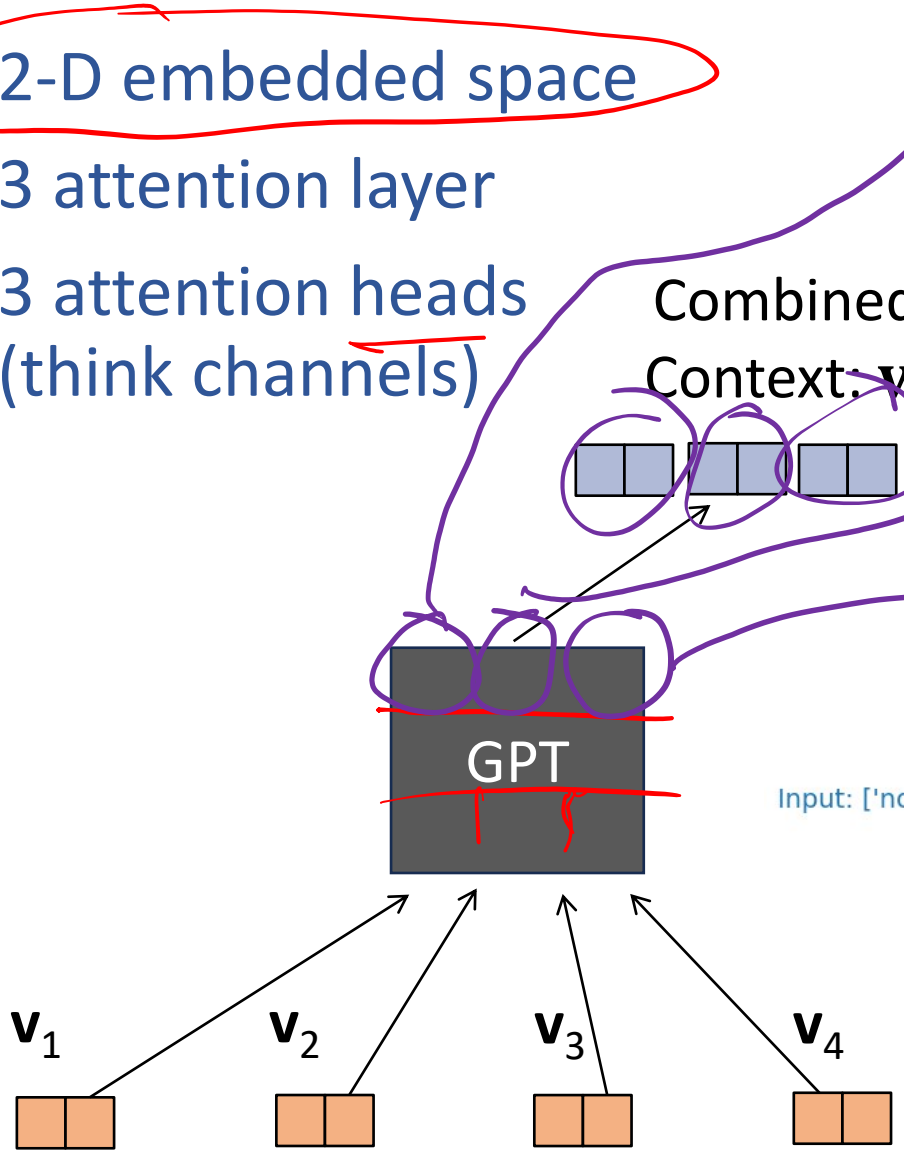


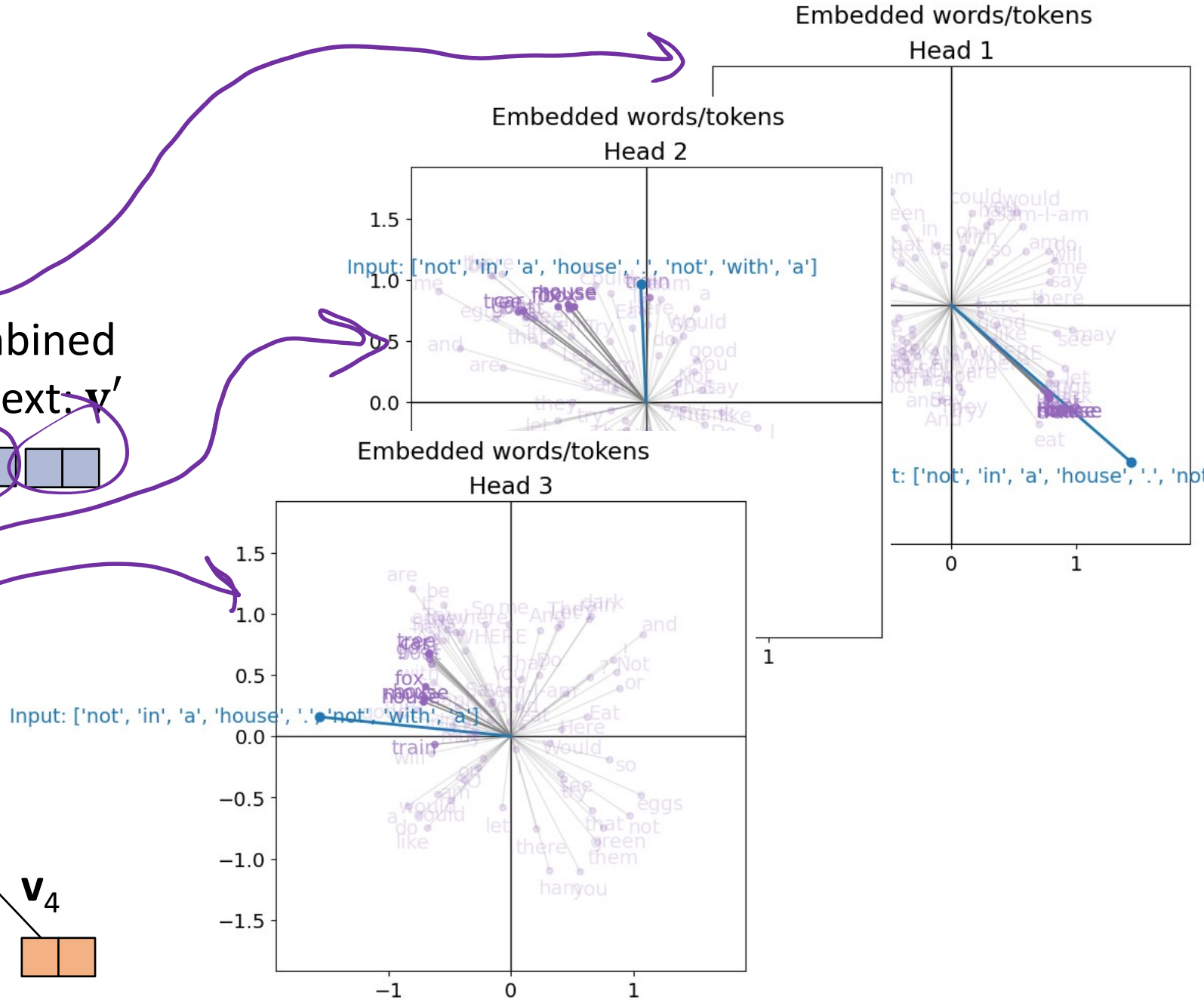
MinGPT Pico

2-D embedded space

3 attention layer

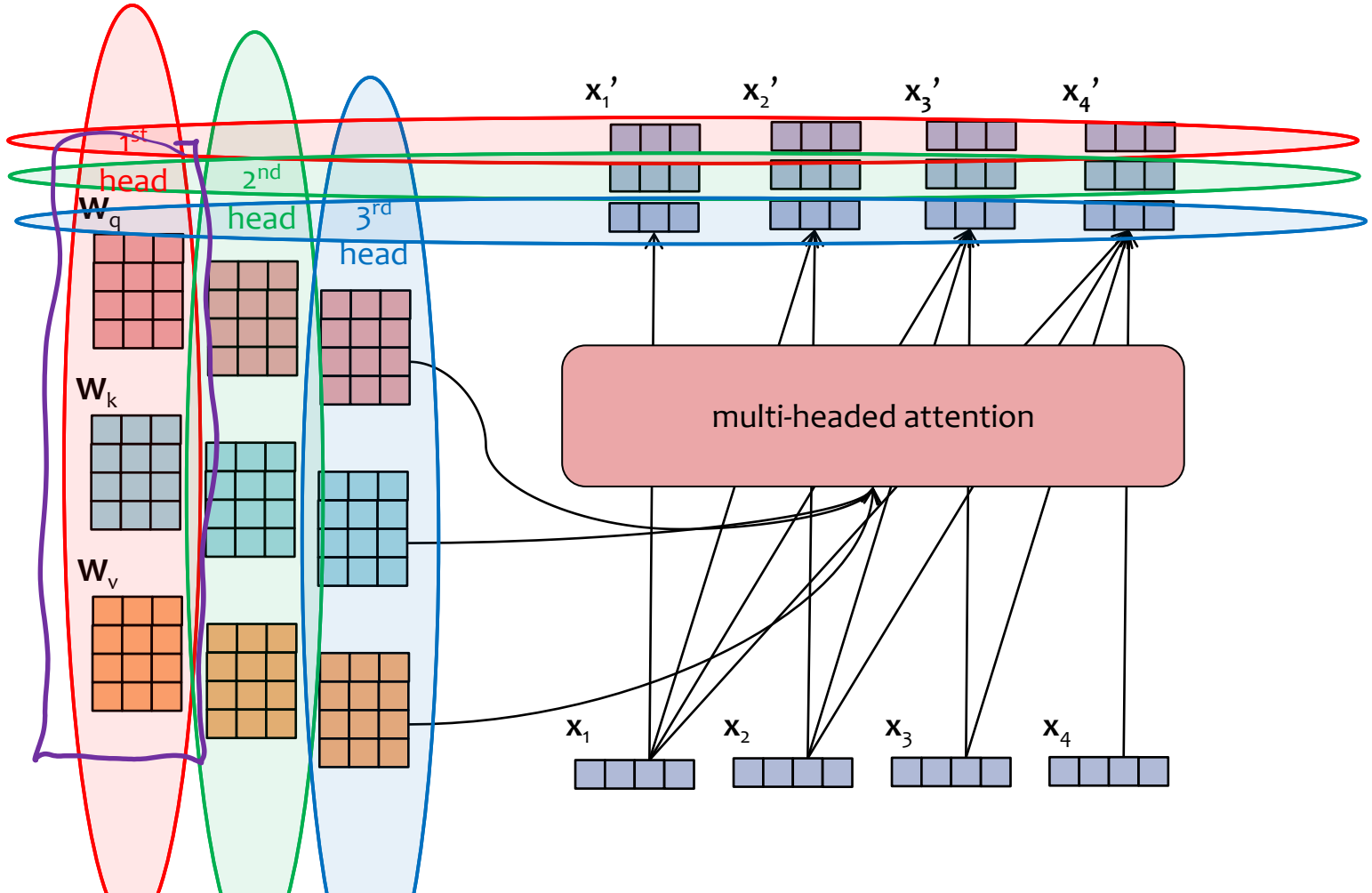
3 attention heads (think channels)





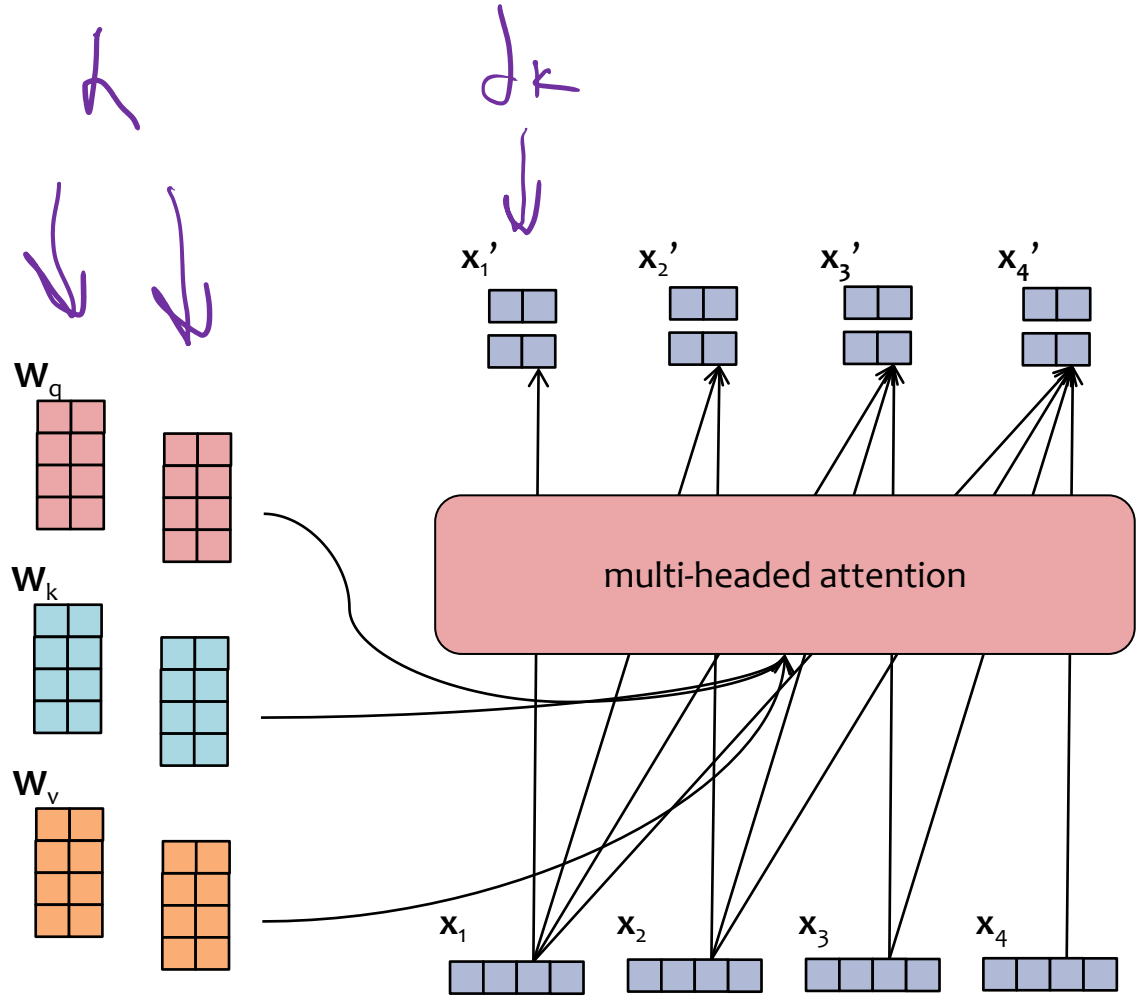
Multi-headed Attention

Multi-headed Attention



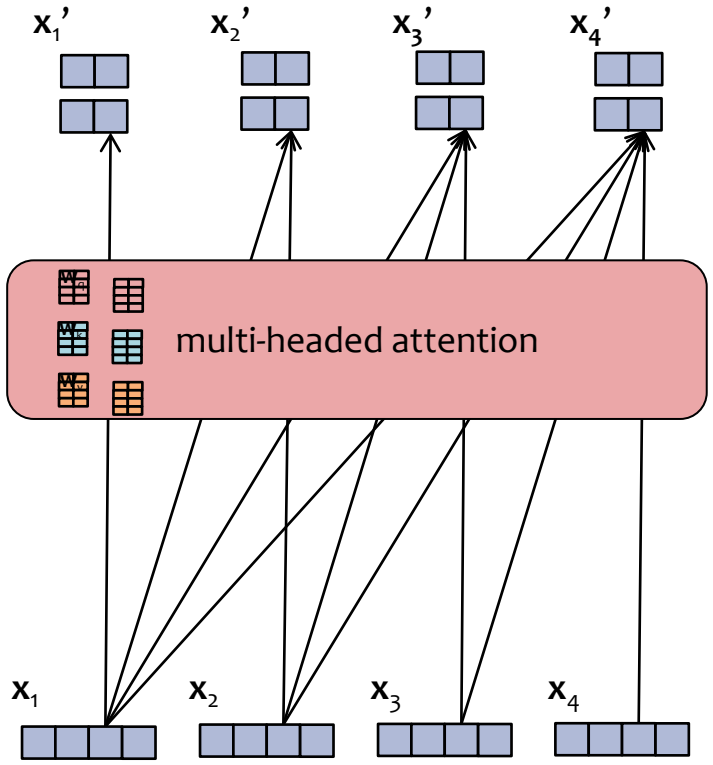
- Just as we can have **multiple channels** in a **convolution** layer, we can use **multiple heads** in an **attention** layer
- Each head gets **its own parameters**
- We can **concatenate** all the outputs to get a single vector for each time step

Multi-headed Attention



- To ensure the dimension of the **input** embedding $\mathbf{x}_t$ is the same as the **output** embedding $\mathbf{x}_t'$, Transformers usually choose the embedding sizes and number of heads appropriately:
  - d_{model} = dim. of inputs
  - d_k = dim. of each output
  - h = # of heads
  - Choose $d_k = d_{model} / h$
- Then concatenate the outputs

Multi-headed Attention



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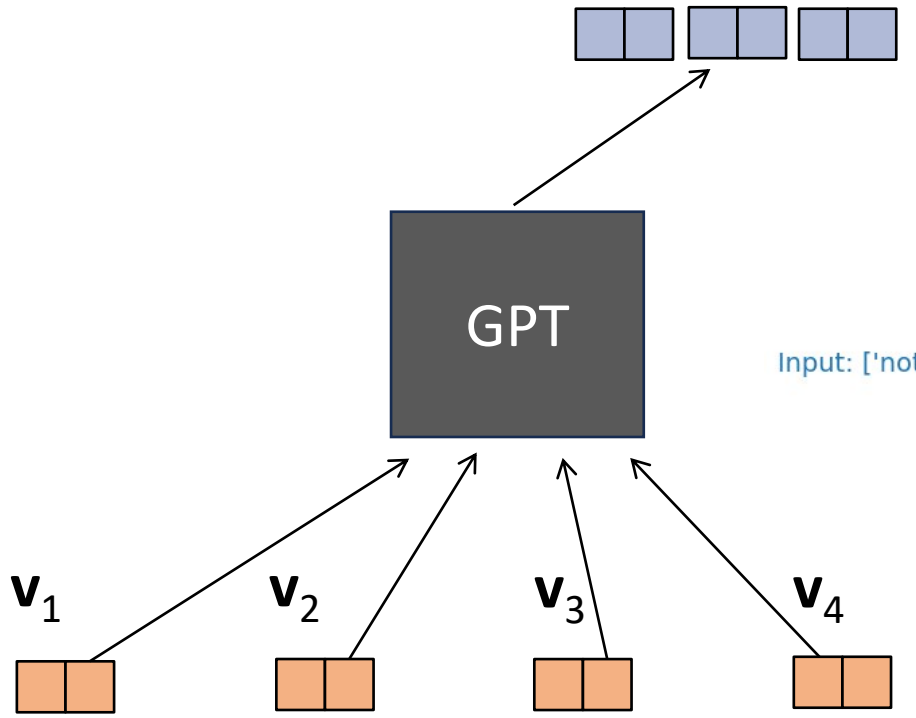
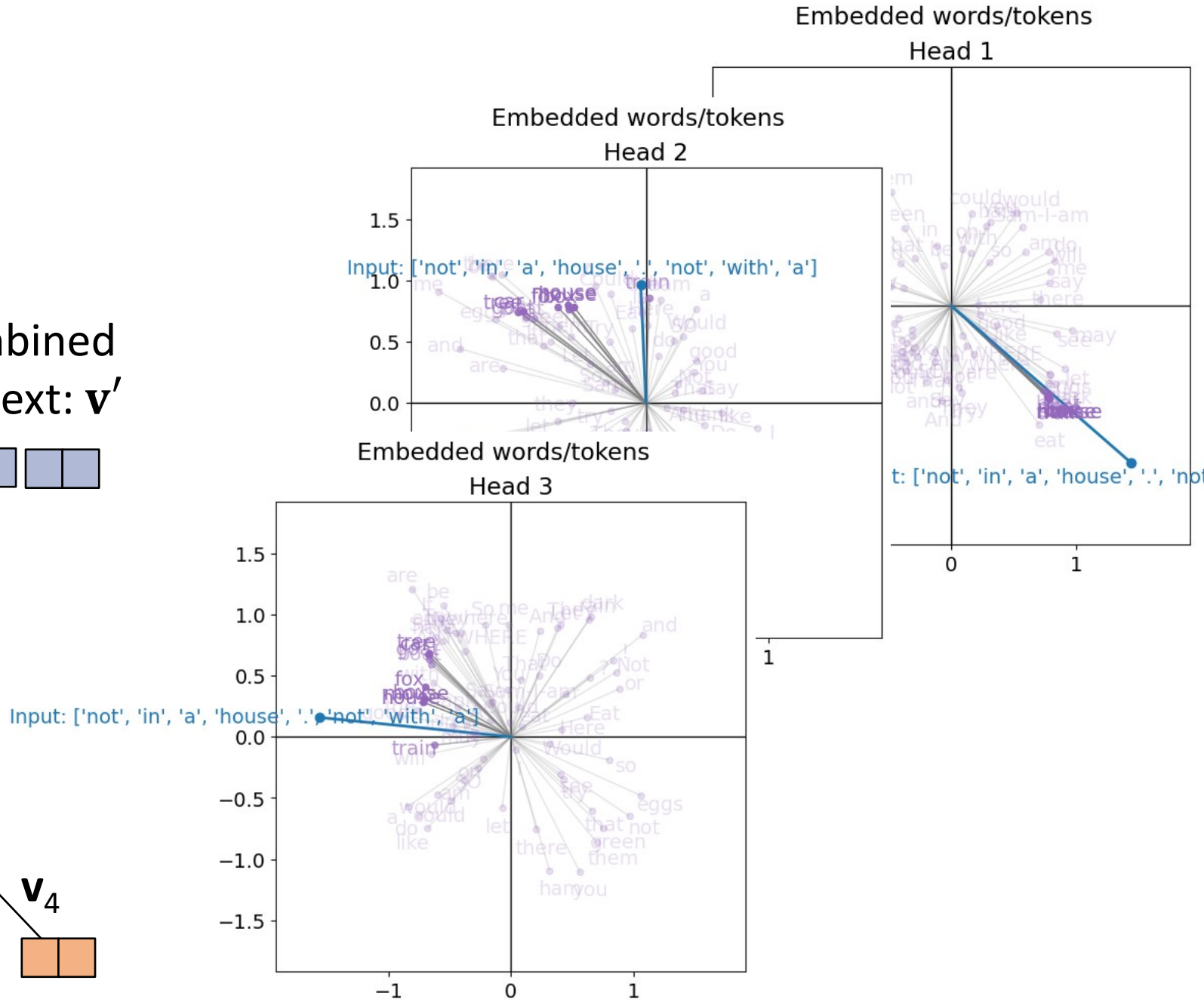
MinGPT Pico

2-D embedded space

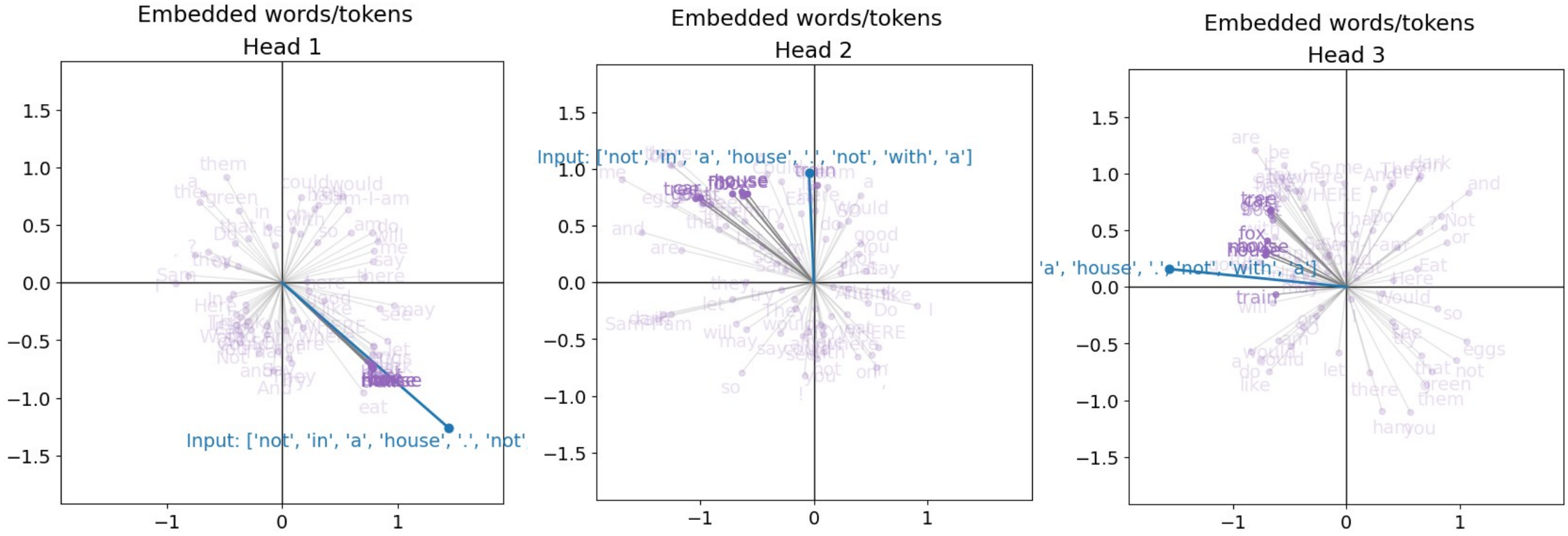
3 attention layer

3 attention heads (think channels)



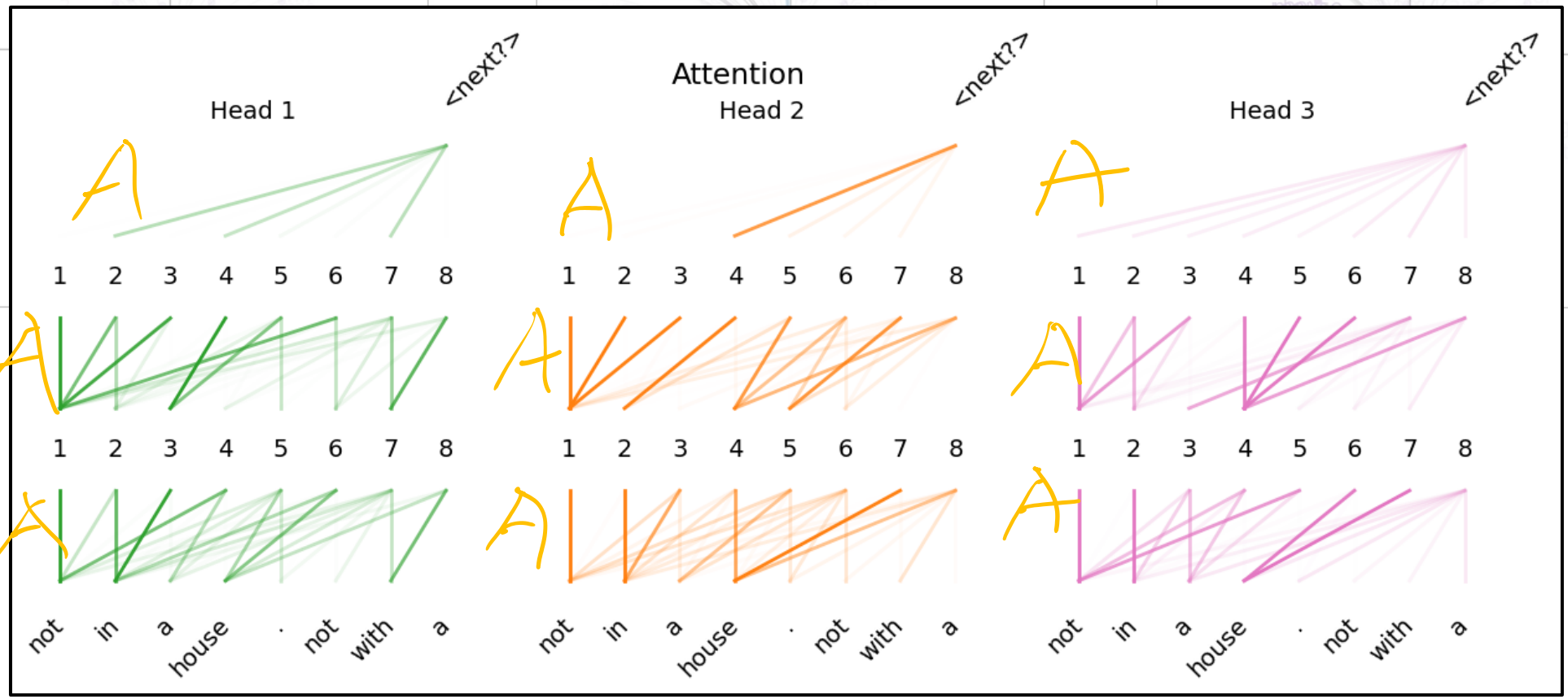


MinGPT Pico: Output embedded space - 3 heads



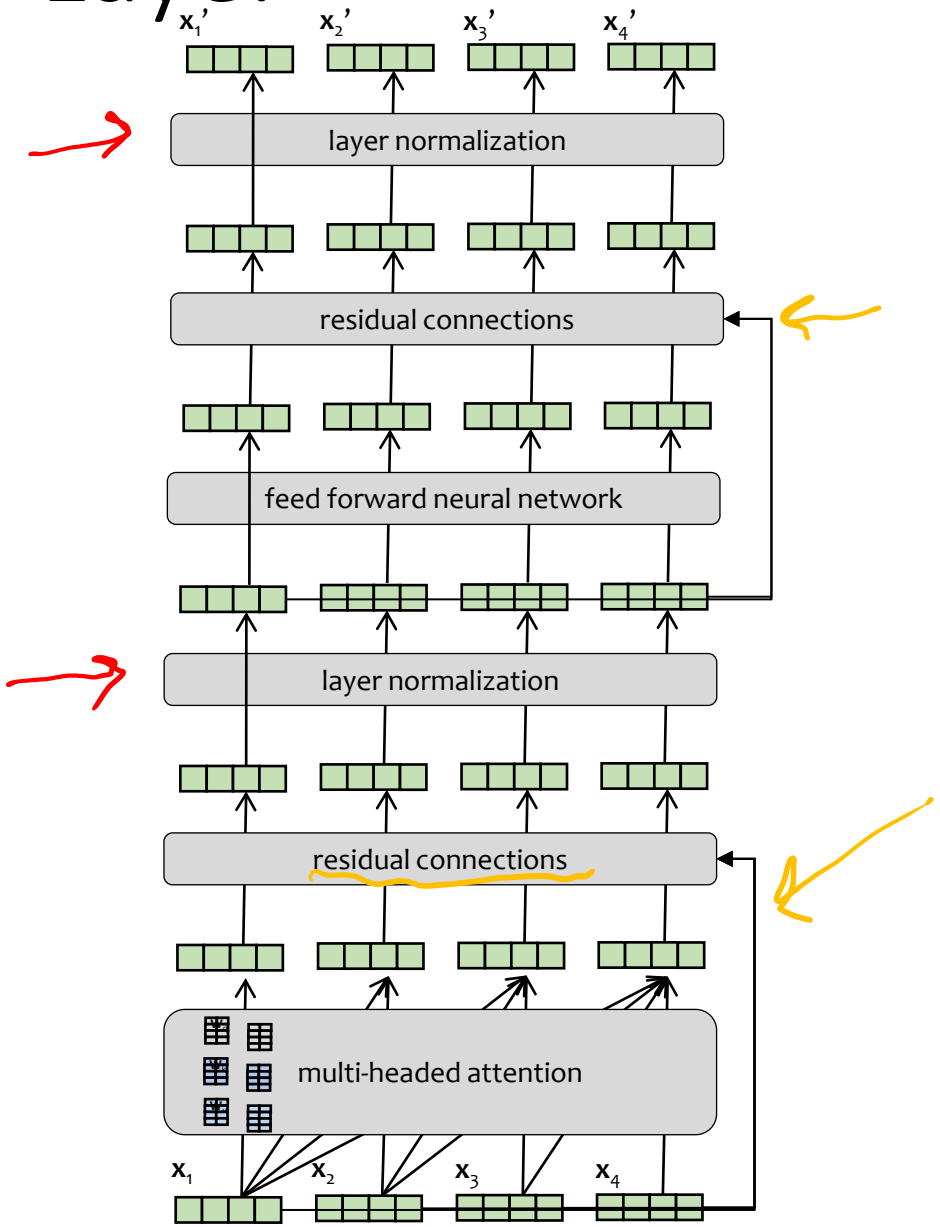
Three heads allows more room to learn diffent feature representations

MinGPT Pico: Attention Weights – 3 layers, 3 heads



Transformer Layer

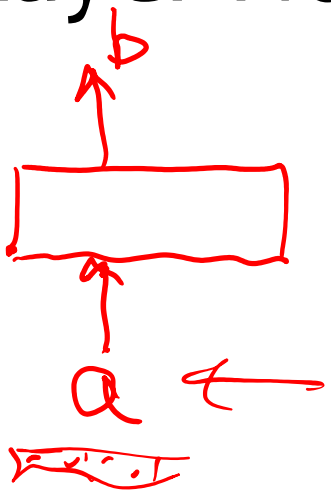
Transformer Layer



Each layer of a Transformer LM consists of several **sublayers:**

1. attention
2. feed-forward neural network
3. layer normalization
4. residual connections

Layer Normalization



The Problem: **internal covariate shift** occurs during training of a deep network when a small change in the low layers amplifies into a large change in the high layers

One Solution: **Layer normalization** normalizes each layer and learns elementwise gain/bias

- Such normalization allows for higher learning rates (for **faster convergence**) without issues of diverging gradients

Figure from https://arxiv.org/pdf/1607.06450.pdf

Layer Normalization

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Given input $\mathbf{a} \in \mathbb{R}^K$, LayerNorm computes output $\mathbf{b} \in \mathbb{R}^K$:

$$\mathbf{b} = \boldsymbol{\gamma} \odot \frac{\mathbf{a} - \mu}{\sigma} \oplus \boldsymbol{\beta}$$

where we have mean $\mu = \frac{1}{K}\sum_{k=1}^{K} a_k$,
standard deviation $\sigma = \sqrt{\frac{1}{K}\sum_{k=1}^{K}(a_k - \mu)^2}$,
and parameters $\boldsymbol{\gamma} \in \mathbb{R}^K$, $\boldsymbol{\beta} \in \mathbb{R}^K$.
$\odot$ and $\oplus$ denote elementwise multiplication and addition.

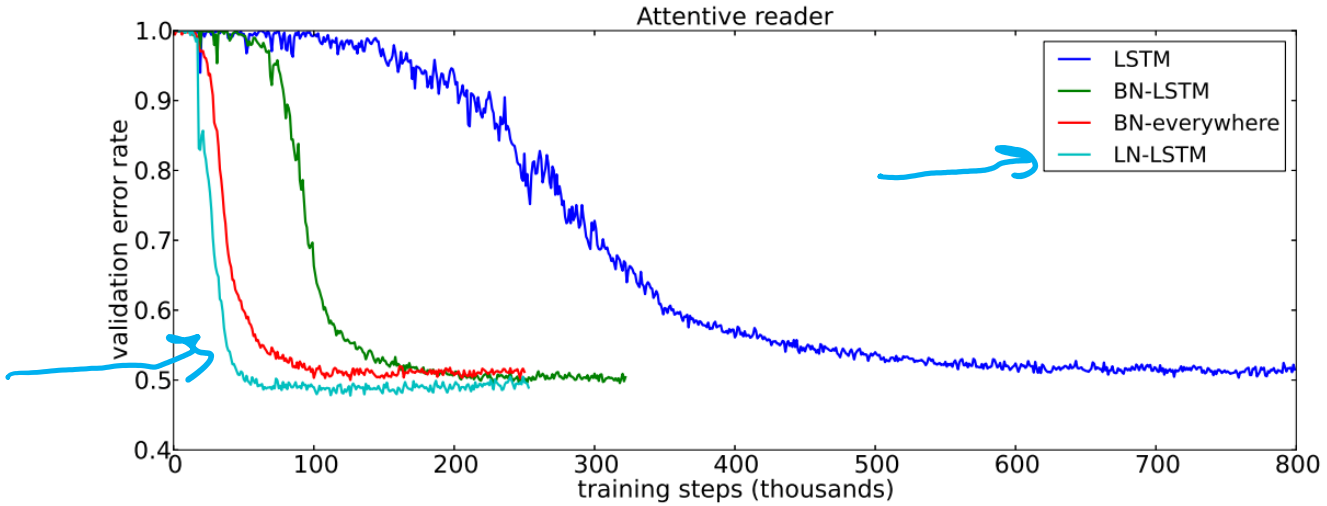


Figure from https://arxiv.org/pdf/1607.06450.pdf

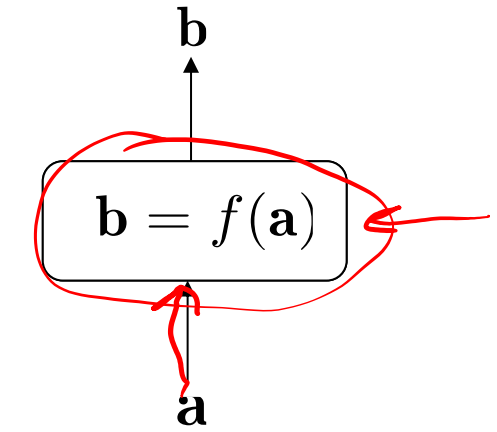
Residual Connections

The Problem: as network depth grows very large, a **performance degradation** occurs that is not explained by overfitting (i.e. train / test error both worsen)

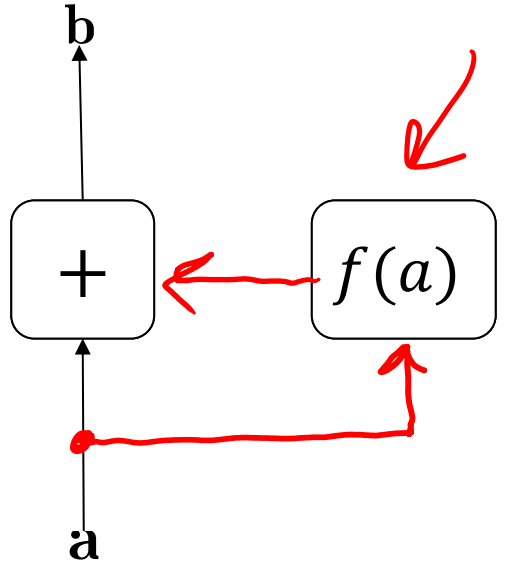
One Solution: **Residual connections** pass a copy of the input alongside another function so that information can flow more directly

- These residual connections allow for **effective training of very deep networks** that perform better than their shallower (though still deep) counterparts

Plain Connection



Residual Connection



Why are residual connections helpful?

Instead of f(a) having to learn a full transformation of a, f(a) only needs to learn an additive modification of a (i.e. the residual).

Figure from https://arxiv.org/pdf/1512.03385.pdf

Residual Connections

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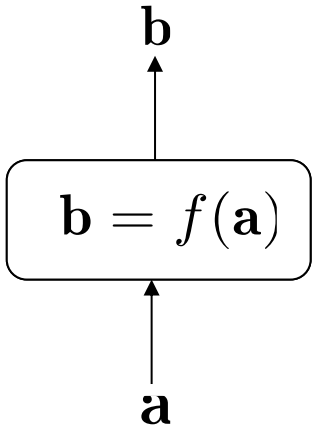
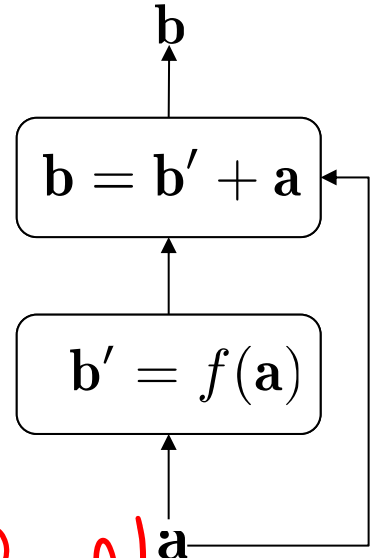
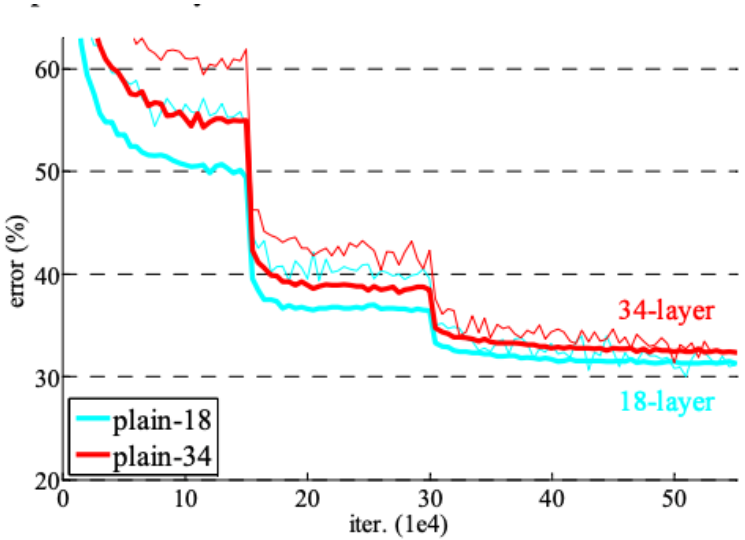


Residual Connection



ResNet



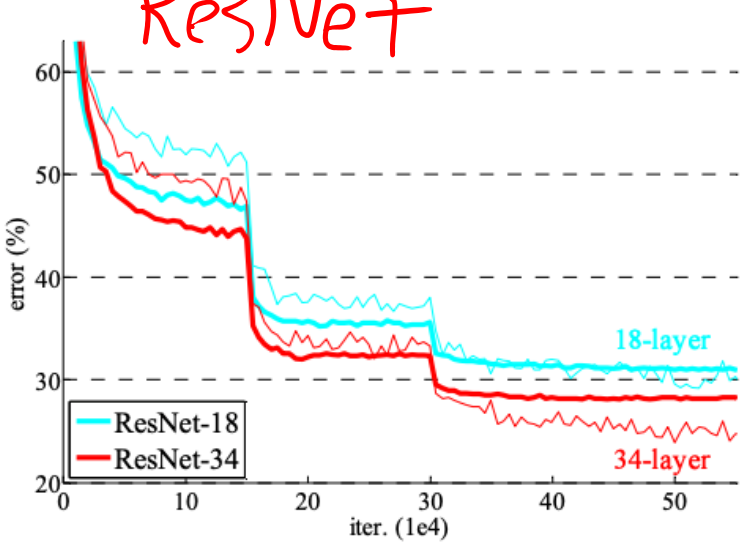
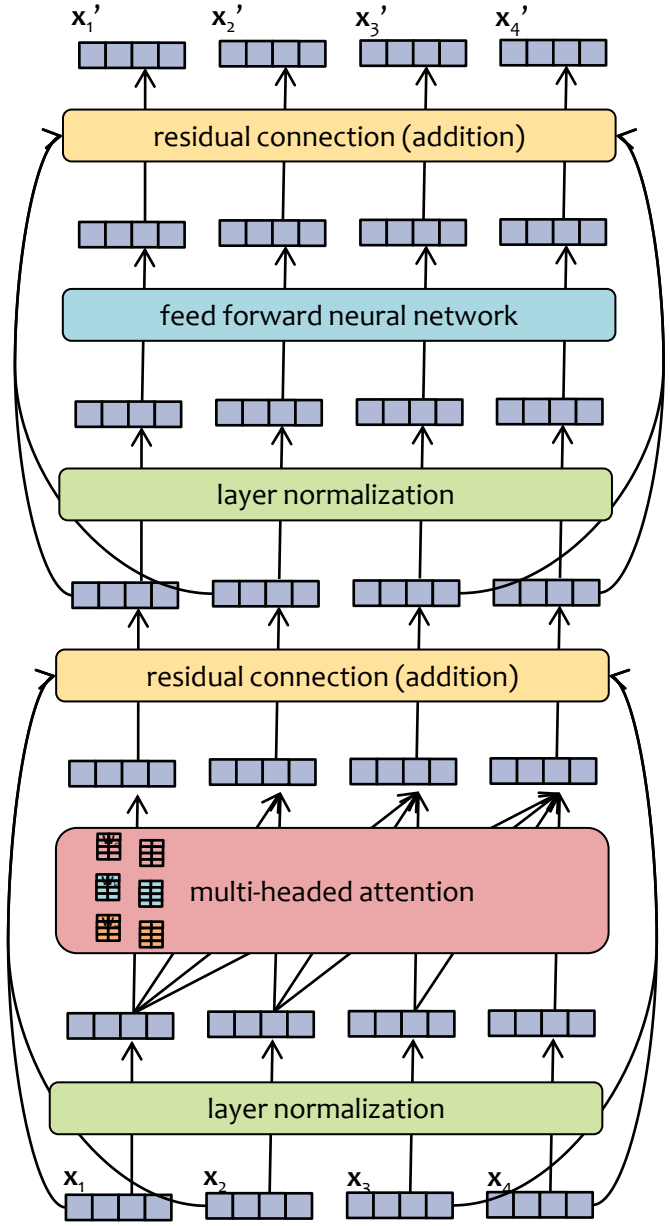


Figure from https://arxiv.org/pdf/1512.03385.pdf

Transformer Layer

Pre-LN Version:

However, subsequent work found that reordering such that the LayerNorm's came at the beginning of each set of 3 layers, the multi-headed attention and feed-forward NN layers tend to be better behaved (i.e. tricks like warm-up are less important).



Each layer of a Transformer LM consists of several **sublayers:**

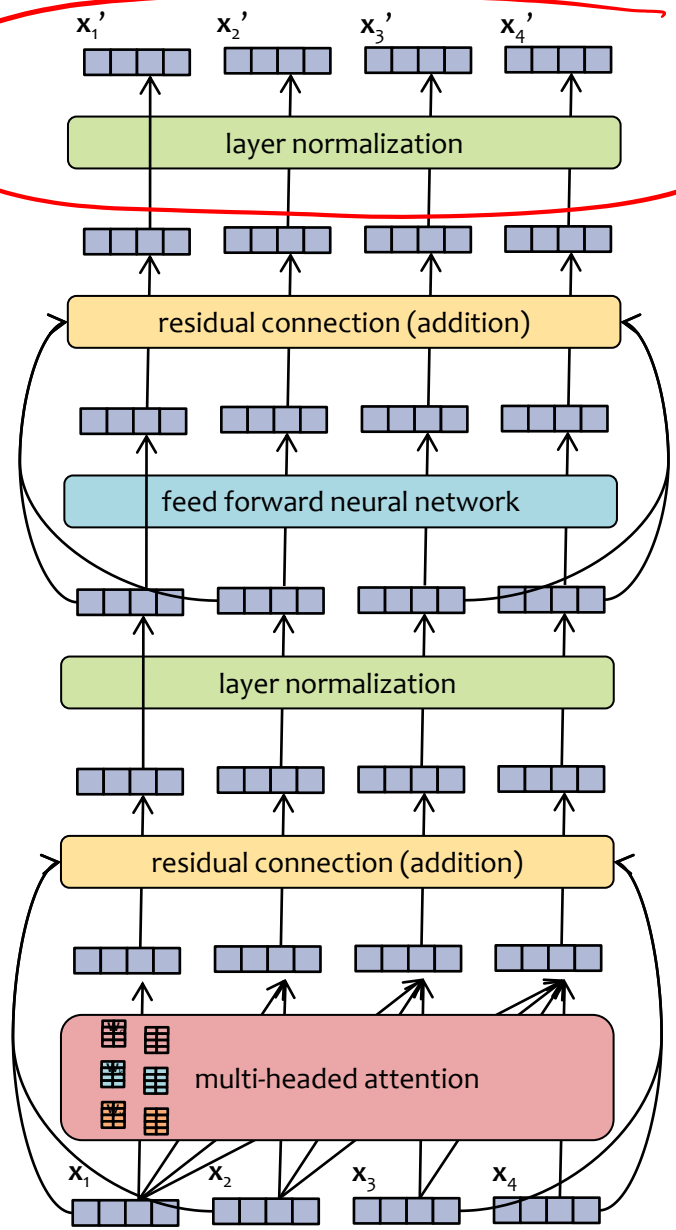
1. attention
2. feed-forward neural network
3. layer normalization
4. residual connections

Transformer Layer

Post-LN Version:

This is the version of the Transformer Layer that was introduced in the original paper in 2017.

The LayerNorm modules occur at the end of each set of 3 layers.



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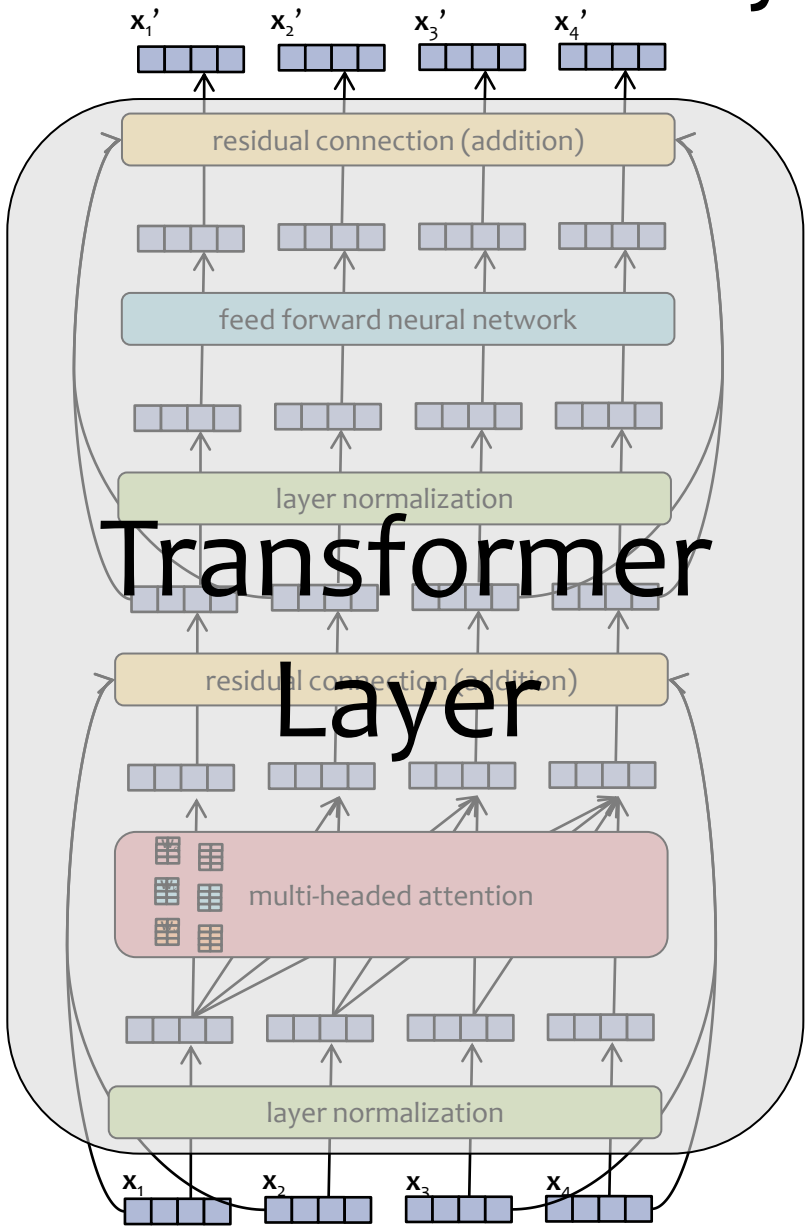

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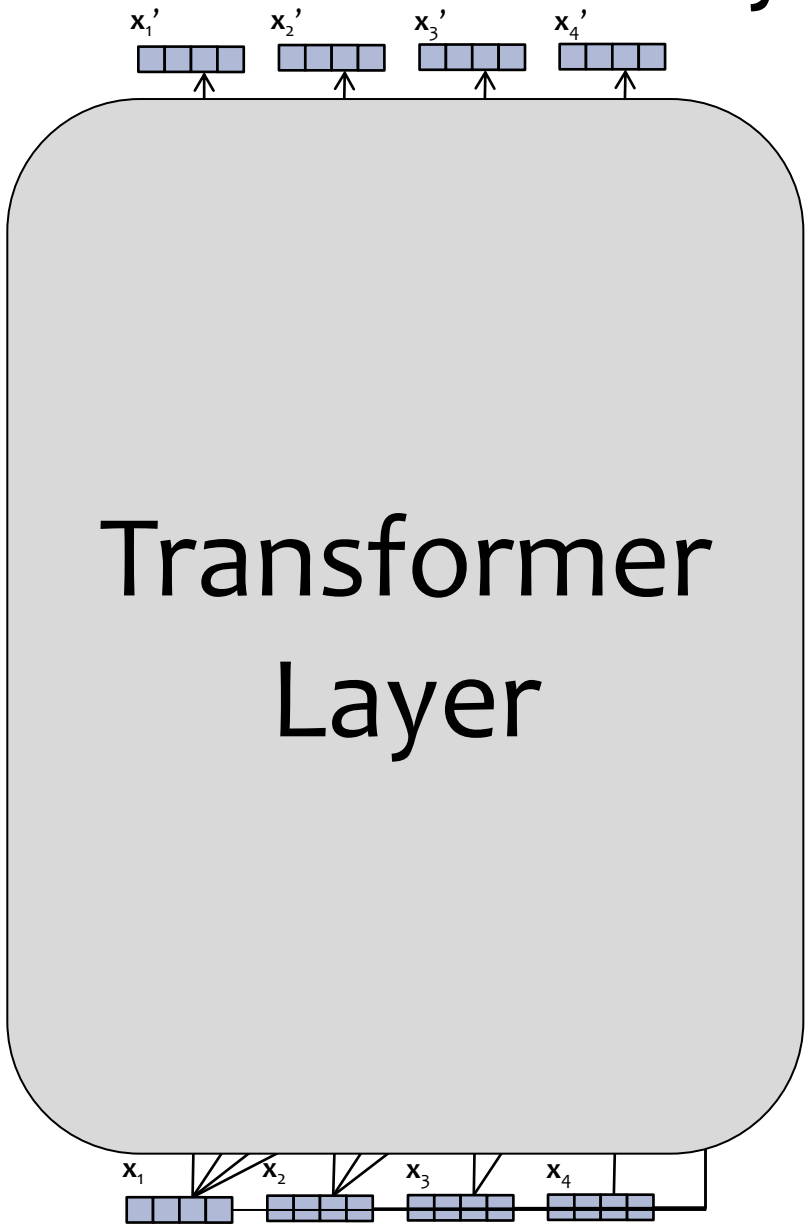

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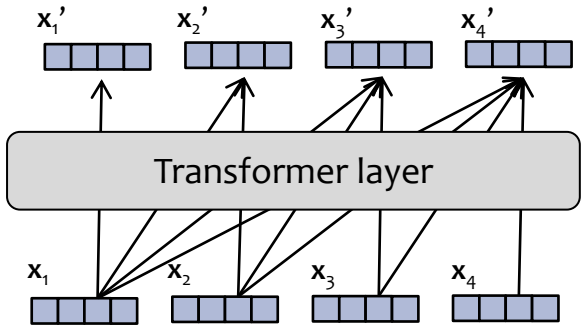
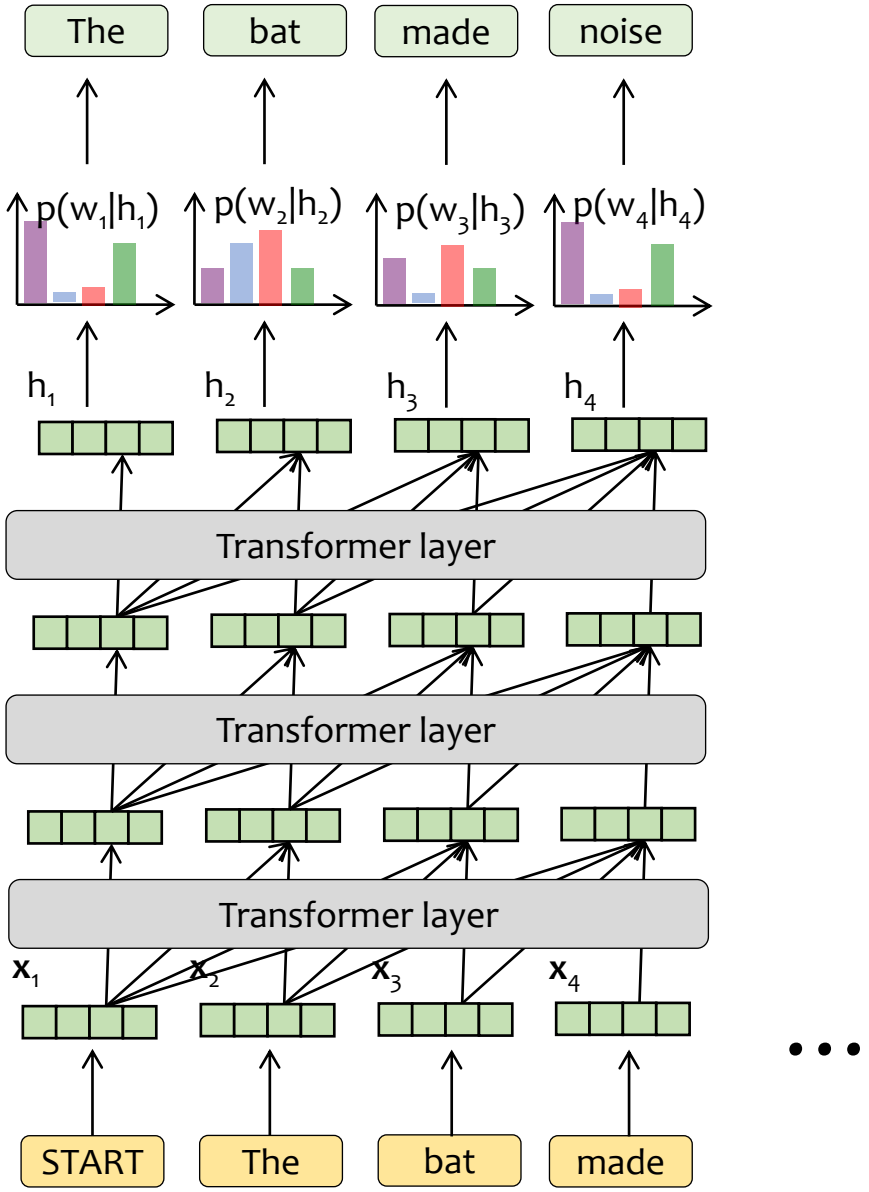


Transformer Language Model



...

Each layer of a Transformer LM consists of several **sublayers:**

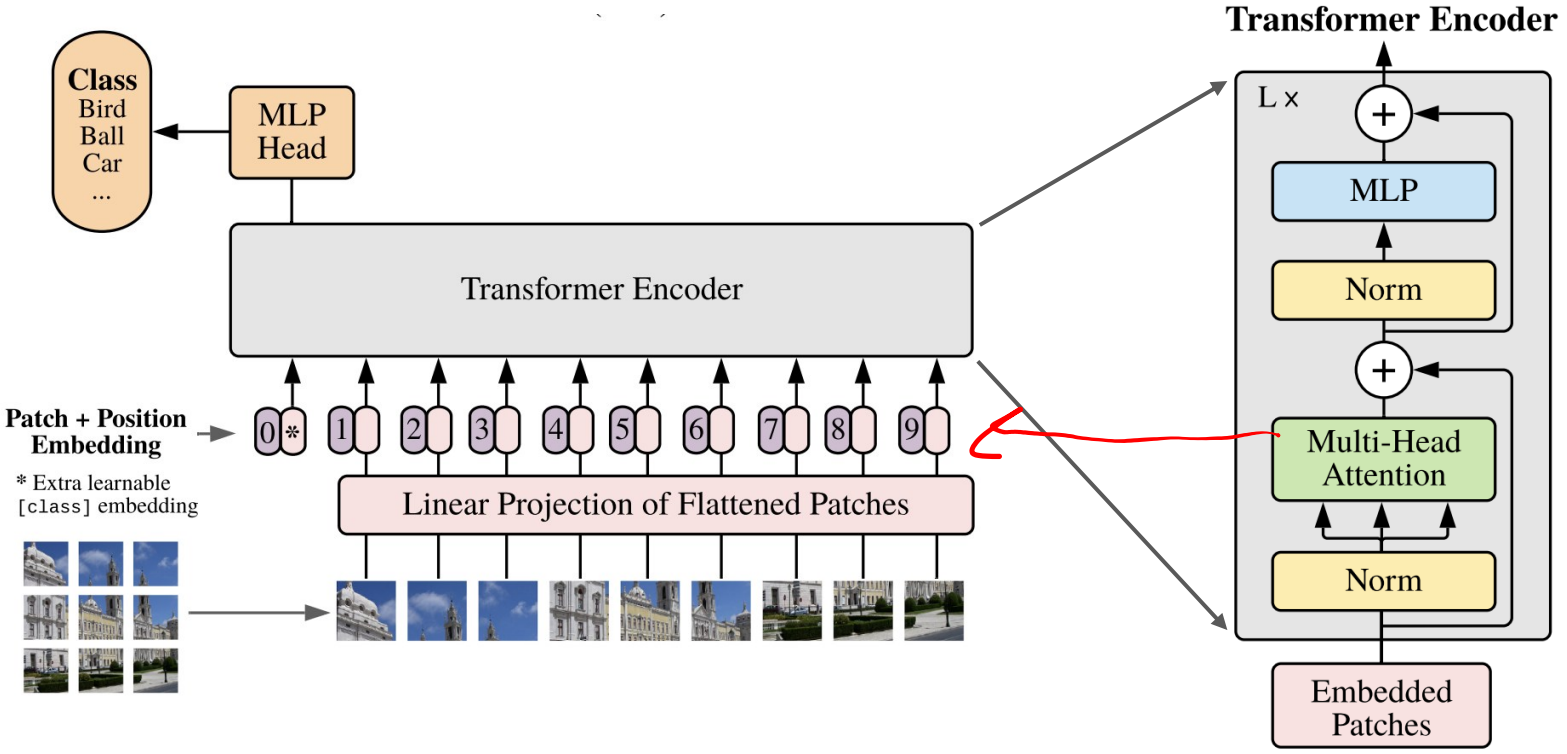
1. attention
2. feed-forward neural network
3. layer normalization
4. residual connections

Each hidden vector looks back at the hidden vectors of the **current and previous timesteps in the previous layer.**

The language model part is just like an RNN-LM!

Vision Transformers

Vision Transf



- Instead of words as input, the inputs are $P \times P$ pixel *patches*
- Each patch is embedded linearly into a vector of size 1024
- Uses 1D positional embeddings
- Pre-trained on a large, supervised dataset (e.g., ImageNet 21K, JFT-300M)

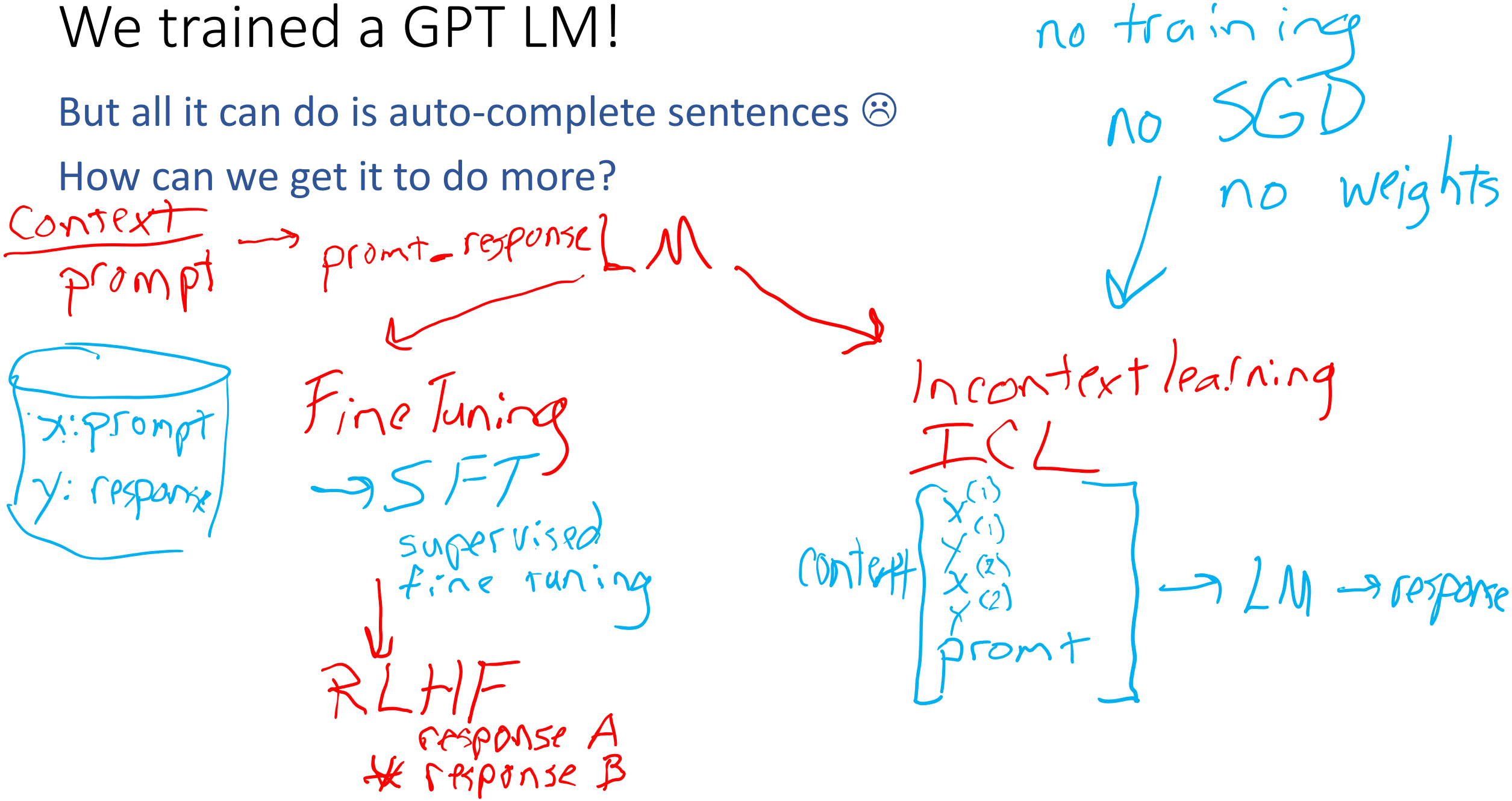
Source: https://arxiv.org/pdf/2010.11929

From LM to Chat

We trained a GPT LM!

But all it can do is auto-complete sentences ☹

How can we get it to do more?



In-Context Learning

Few-shot Learning

Definition: in **few-shot learning** we assume that training data contains a handful (maybe two, three, or four) examples of each label

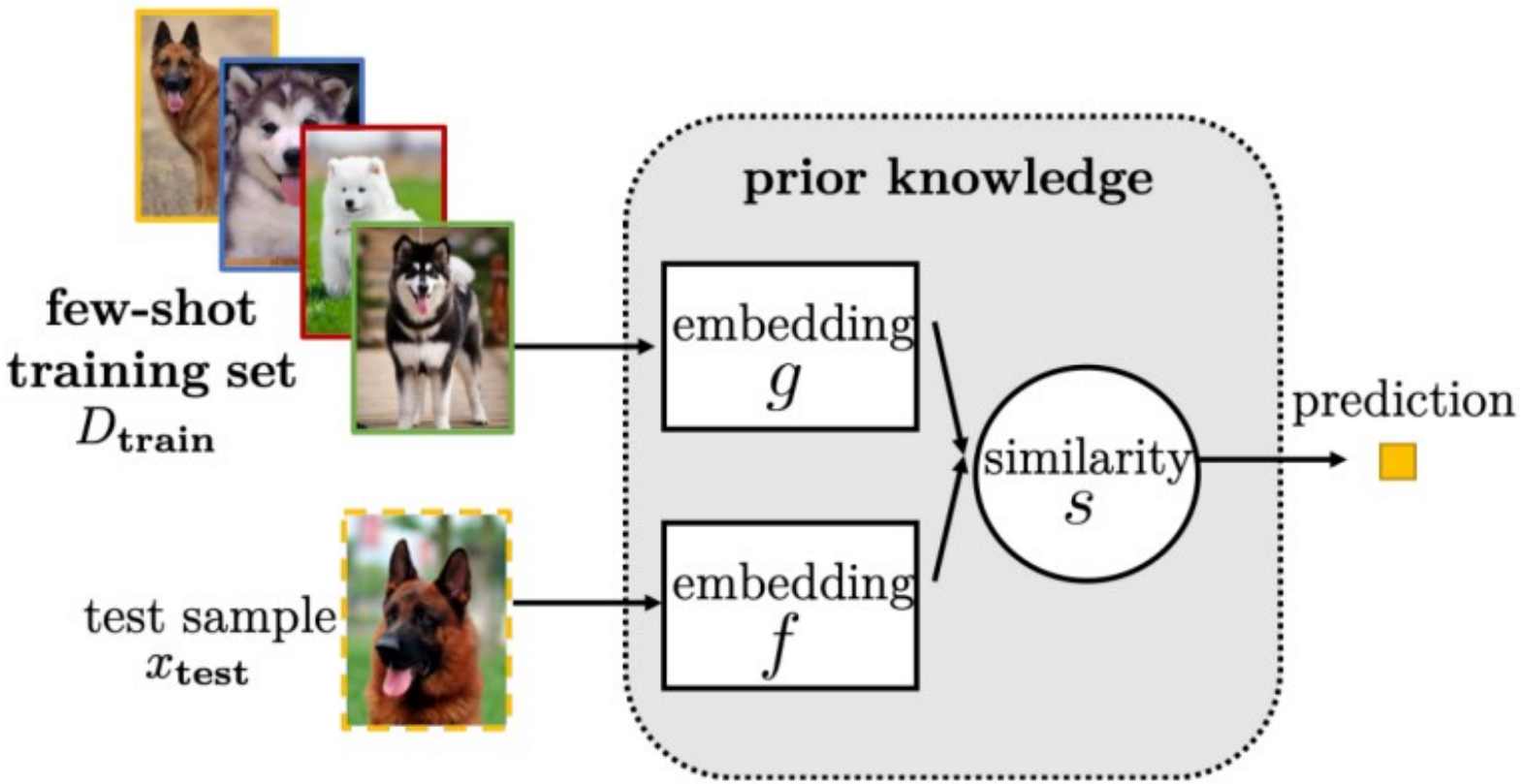


Figure from https://dl.acm.org/doi/10.1145/3386252

Few-shot Learning with LLMs

Suppose you have…

- a dataset $D = \{(x_i, y_i)\}_{i=1}^{N}$ and N is rather small (i.e. few-shot setting)
- a very large (billions of parameters) pre-trained language model

There are two ways to "learn"

This section!

Option A: Supervised fine-tuning

- **Definition**: fine-tune the LLM on the training data using…
  - a standard supervised objective
  - backpropagation to compute gradients
  - your favorite optimizer (e.g. Adam)
- **Pro**: fits into the standard ML recipe
- **Pro:** still works if N is large
- **Con**: backpropagation requires ~3x the memory and computation time as the forward computation
- **Con**: you might not have access to the model weights at all (e.g. because the model is proprietary)

Option B: In-context learning

- **Definition**:
  1. feed training examples to the LLM as a prompt
  2. allow the LLM to infer patterns in the training examples during inference (i.e. decoding)
  3. take the output of the LLM following the prompt as its prediction
- **Con**: the prompt may be very long and Transformer LMs require $O(N^2)$ time/space where N = length of context
- **Pro**: no backpropagation required and only one pass through the training data
- **Pro**: does not require model weights, only API access

Few-shot In-context Learning

Few-shot learning can be done via in-context learning

Typically, a task description is presented first

Then a sequence of input/output pairs from a training dataset are presented in sequence

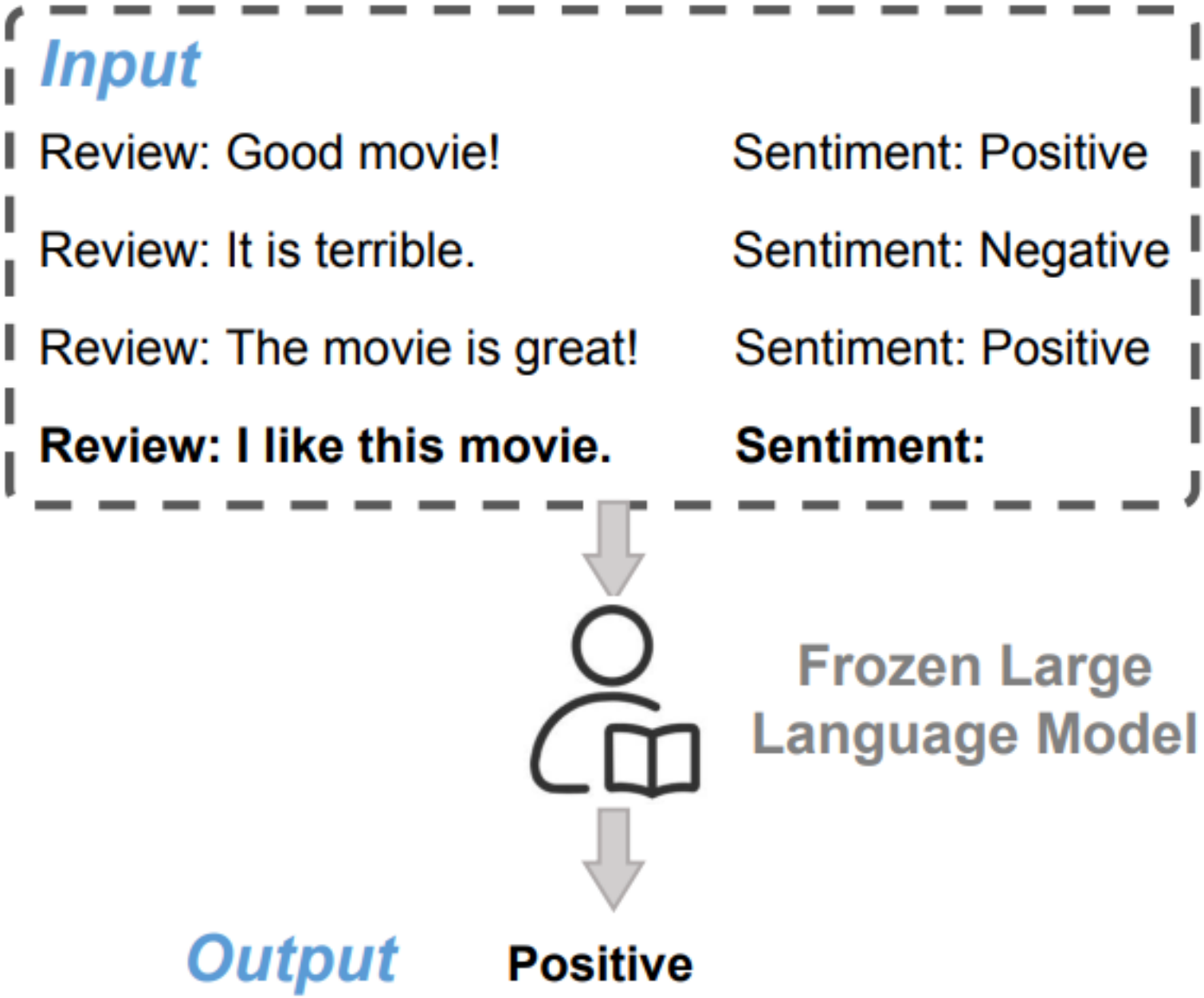


Figure from https://arxiv.org/pdf/2310.09881.pdf

Few-shot In-context Learning

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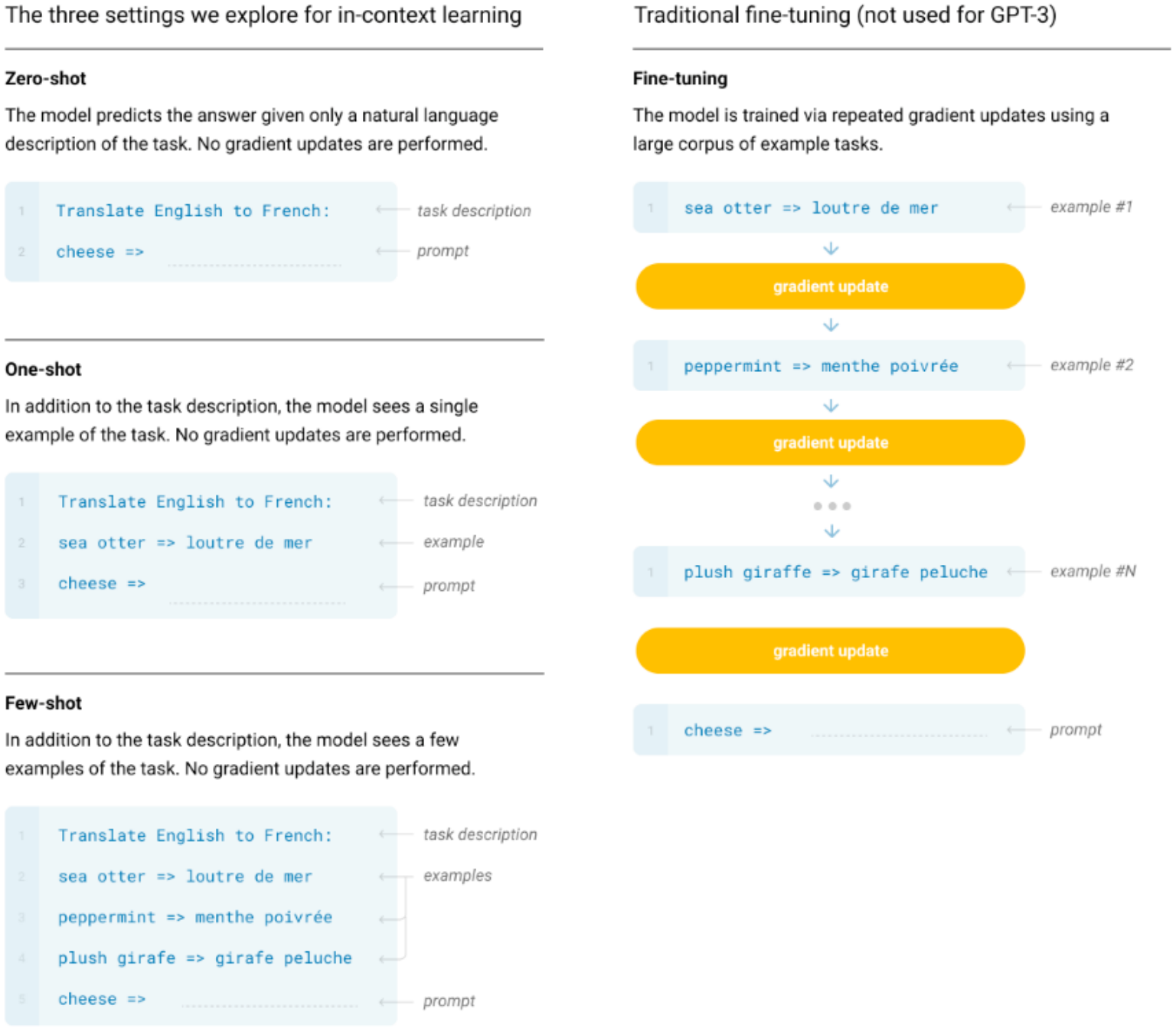

Figure from http://arxiv.org/abs/2005.14165