

# Transformers

## Introduction to Transformers

From: Dan Jurafsky and James  
H. Martin, Chapter 9, Aug 2024

Adapted by Diana Inkpen for CSI  
5386, Jan 2025

# LLMs are built out of transformers

Transformer: a specific kind of network architecture, like a fancier feedforward network, but based on attention

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## Attention Is All You Need

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**Ashish Vaswani\***  
Google Brain  
avaswani@google.com

**Noam Shazeer\***  
Google Brain  
noam@google.com

**Niki Parmar\***  
Google Research  
nikip@google.com

**Jakob Uszkoreit\***  
Google Research  
usz@google.com

**Llion Jones\***  
Google Research  
llion@google.com

**Aidan N. Gomez\* †**  
University of Toronto  
aidan@cs.toronto.edu

**Łukasz Kaiser\***  
Google Brain  
lukaszkaizer@google.com

**Illia Polosukhin\* ‡**  
illia.polosukhin@gmail.com

# A very approximate timeline

1990 Static Word Embeddings

2003 Neural Language Model

2008 Multi-Task Learning

2015 Attention

2017 Transformer

2018 Contextual Word Embeddings and Pretraining

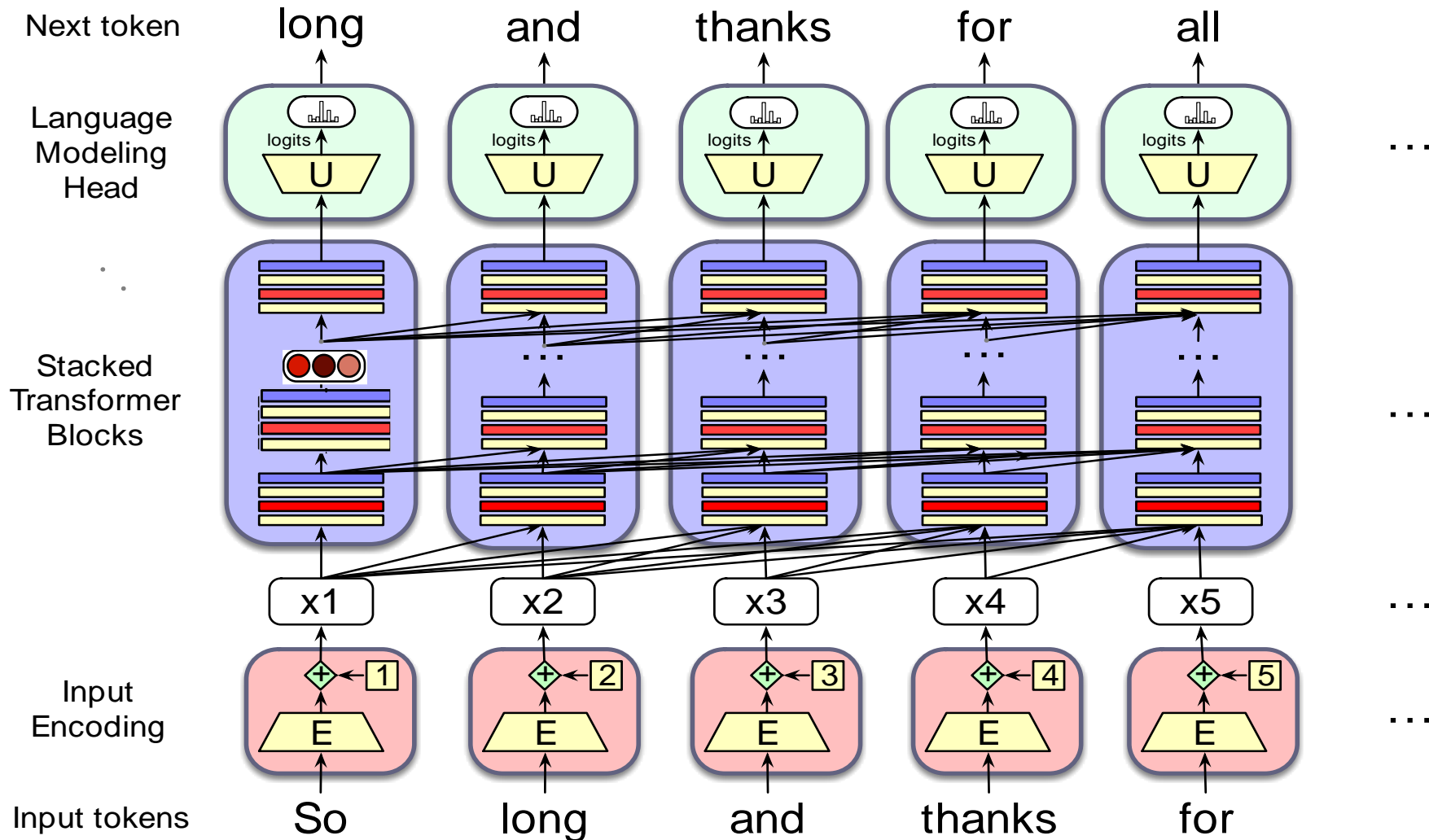
2019 Prompting

Attention

Transformers

# Instead of starting with the big picture

Let's consider the embeddings for an individual word from a particular layer



# Problem with static embeddings (word2vec)

They are static! The embedding for a word doesn't reflect how its meaning changes in context.

The chicken didn't cross the road because  it was too tired

What is the meaning represented in the static embedding for "it"?

# Contextual Embeddings

- Intuition: a representation of meaning of a word should be different in different contexts!
- **Contextual Embedding:** each word has a different vector that expresses different meanings depending on the surrounding words
- How to compute contextual embeddings?
  - **Attention**

# Contextual Embeddings

The chicken didn't cross the road because it

What should be the properties of "it"?

The chicken didn't cross the road because it was too **tired**

The chicken didn't cross the road because it was too **wide**

At this point in the sentence, it's probably referring to either the chicken or the street

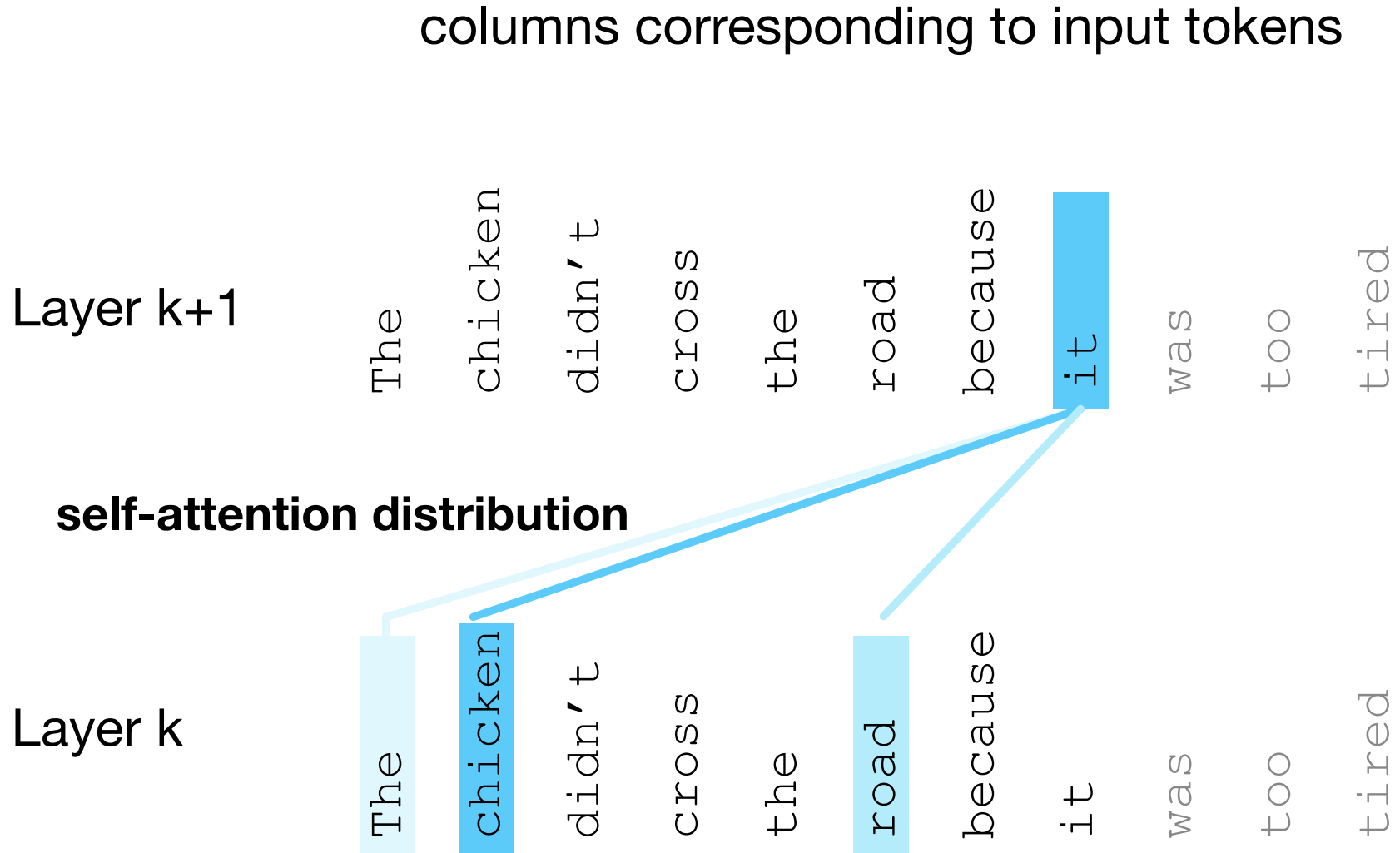


# Intuition of attention

Build up the contextual embedding from a word by selectively integrating information from all the neighboring words

We say that a word "attends to" some neighboring words more than others

# Intuition of attention:

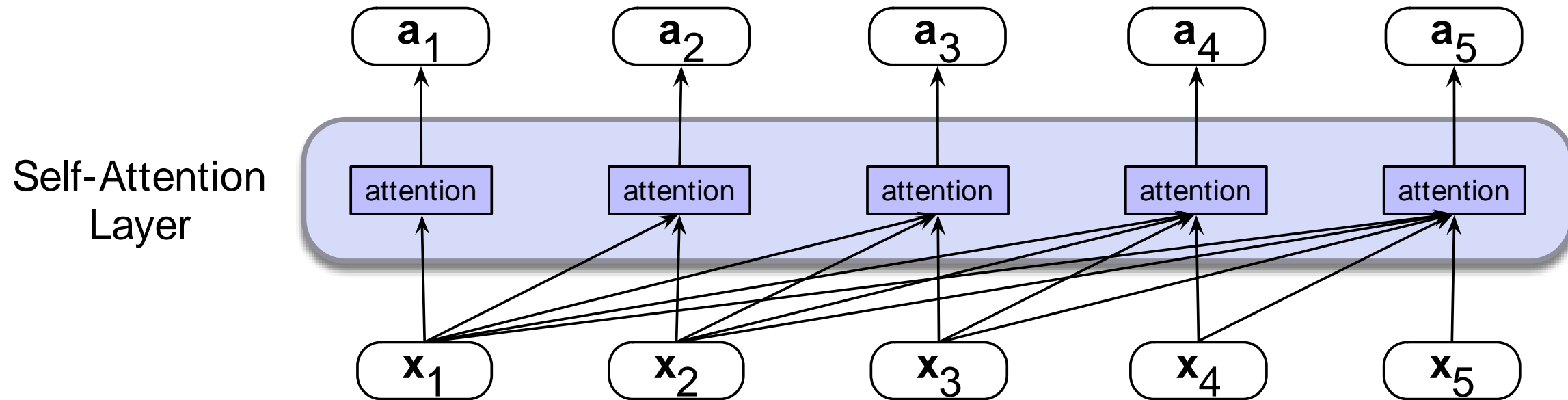


# Attention definition

A mechanism for helping compute the embedding for a token by selectively attending to and integrating information from surrounding tokens (at the previous layer).

More formally: a method for doing a weighted sum of vectors.

# Attention is left-to-right



Simplified version of attention: a sum of prior words weighted by their similarity with the current word

Given a sequence of token embeddings:

$$\mathbf{x}_1 \quad \mathbf{x}_2 \quad \mathbf{x}_3 \quad \mathbf{x}_4 \quad \mathbf{x}_5 \quad \mathbf{x}_6 \quad \mathbf{x}_7 \quad \mathbf{x}_i$$

Produce:  $\mathbf{a}_i$  = a weighted sum of  $\mathbf{x}_1$  through  $\mathbf{x}_7$  (and  $\mathbf{x}_i$ )  
Weighted by their similarity to  $\mathbf{x}_i$

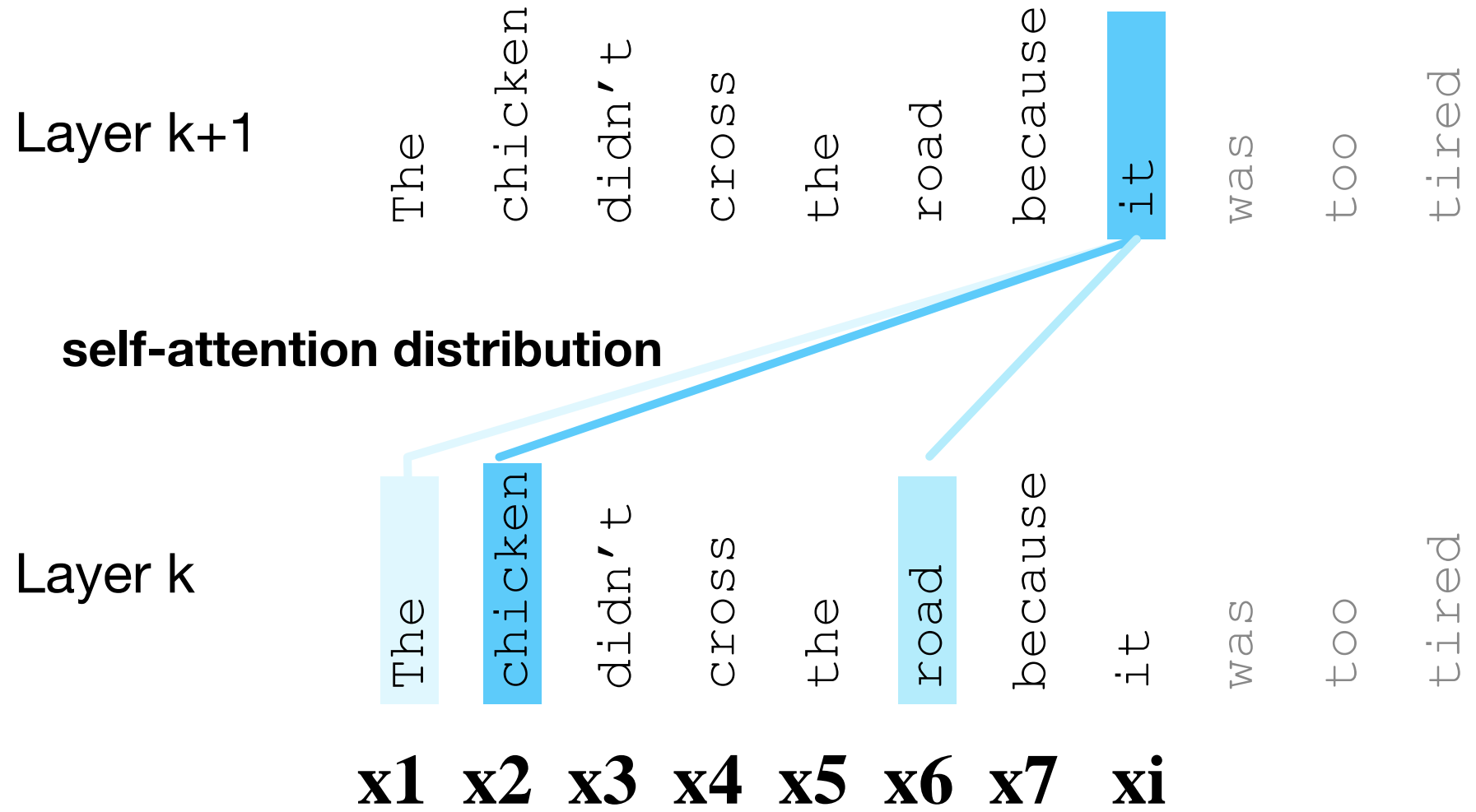
$$\text{score}(\mathbf{x}_i, \mathbf{x}_j) = \mathbf{x}_i \cdot \mathbf{x}_j$$

$$a_{ij} = \text{softmax}(\text{score}(\mathbf{x}_i, \mathbf{x}_j)) \quad \forall j \leq i$$

$$\mathbf{a}_i = \sum_{j \leq i} \alpha_{ij} \mathbf{x}_j$$

# Intuition of attention:

columns corresponding to input tokens

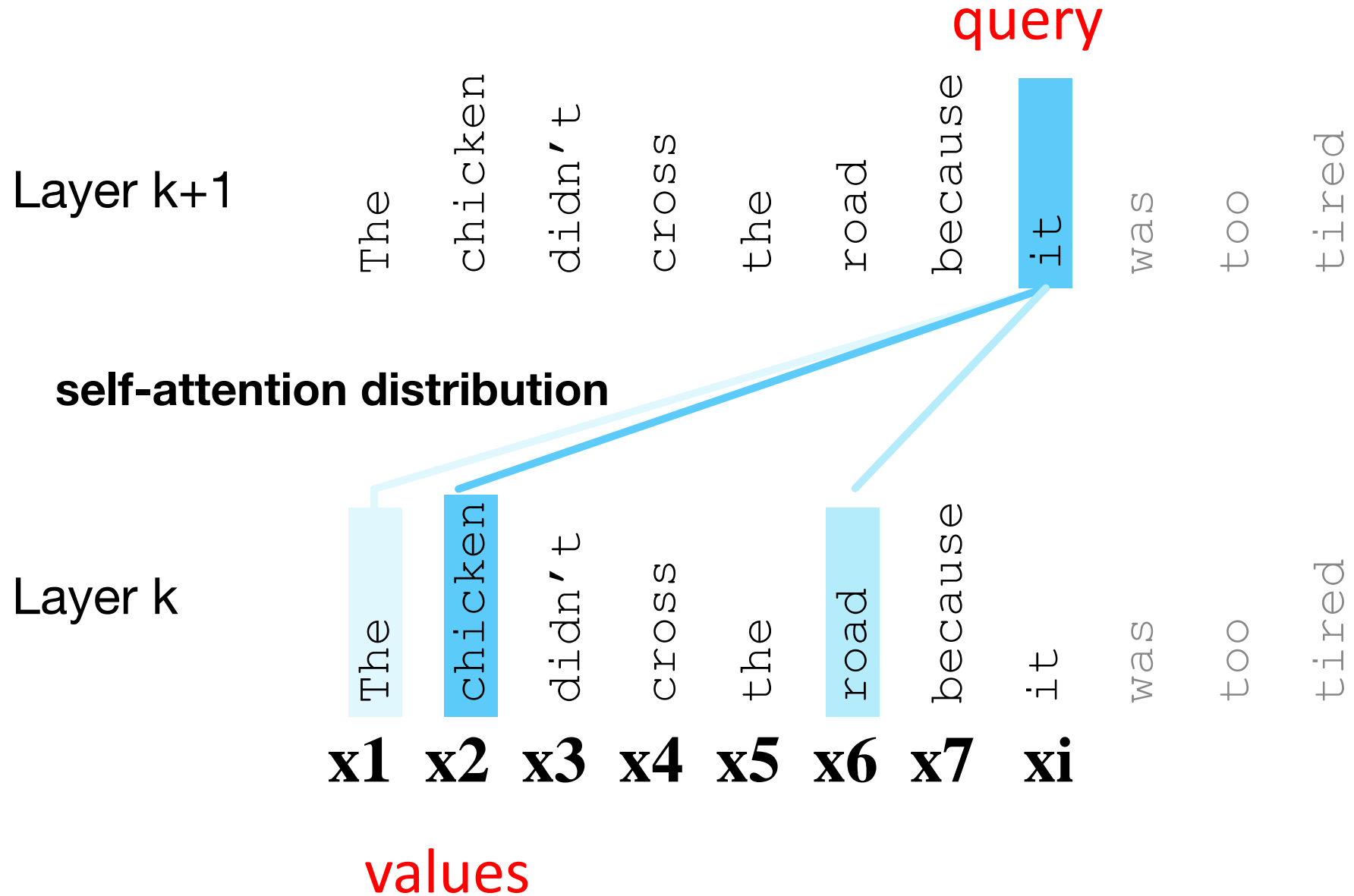


## An Actual Attention Head: slightly more complicated

High-level idea: instead of using vectors (like  $x_i$  and  $x_4$ ) directly, we'll represent 3 separate roles each vector  $x_i$  plays:

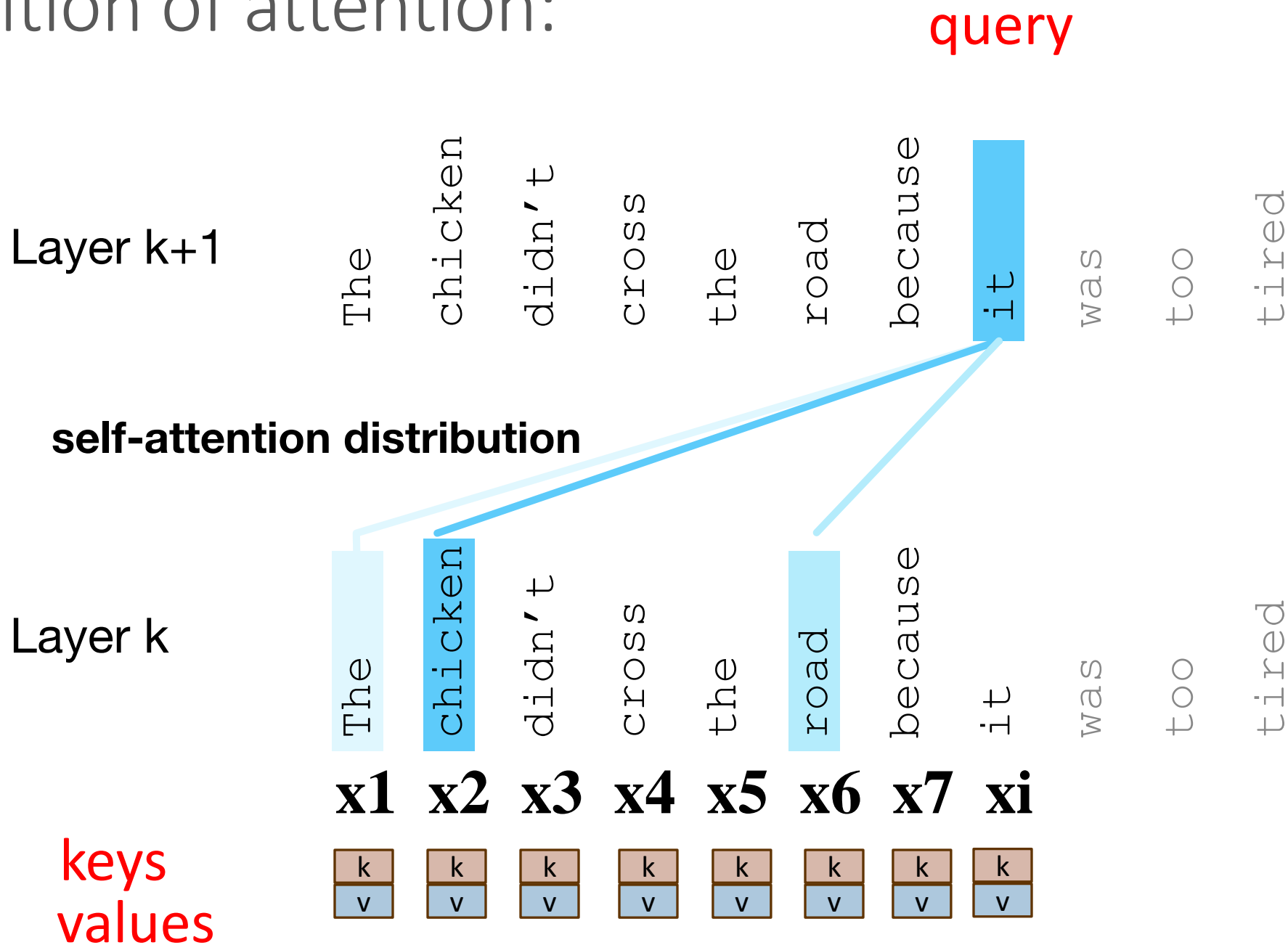
- **query**: *As the current element* being compared to the preceding inputs.
- **key**: *as a preceding input* that is being compared to the current element to determine a similarity
- **value**: a value of a preceding element that gets weighted and summed

# Attention intuition





## Intuition of attention:



## An Actual Attention Head: slightly more complicated

We'll use matrices to project each vector  $\mathbf{x}_i$  into a representation of its role as query, key, value:

- **query:  $\mathbf{W}^Q$**
- **key:  $\mathbf{W}^K$**
- **value:  $\mathbf{W}^V$**

$$\mathbf{q}_i = \mathbf{x}_i \mathbf{W}^Q; \quad \mathbf{k}_i = \mathbf{x}_i \mathbf{W}^K; \quad \mathbf{v}_i = \mathbf{x}_i \mathbf{W}^V$$

An Actual Attention Head: slightly more complicated

Given these 3 representation of  $\mathbf{x}_i$

$$\mathbf{q}_i = \mathbf{x}_i \mathbf{W}^Q; \quad \mathbf{k}_i = \mathbf{x}_i \mathbf{W}^K; \quad \mathbf{v}_i = \mathbf{x}_i \mathbf{W}^V$$

To compute similarity of current element  $\mathbf{x}_i$  with some prior element  $\mathbf{x}_j$

We'll use dot product between  $\mathbf{q}_i$  and  $\mathbf{k}_j$ .

And instead of summing up  $\mathbf{x}_j$ , we'll sum up  $\mathbf{v}_j$

Final equations for one attention head

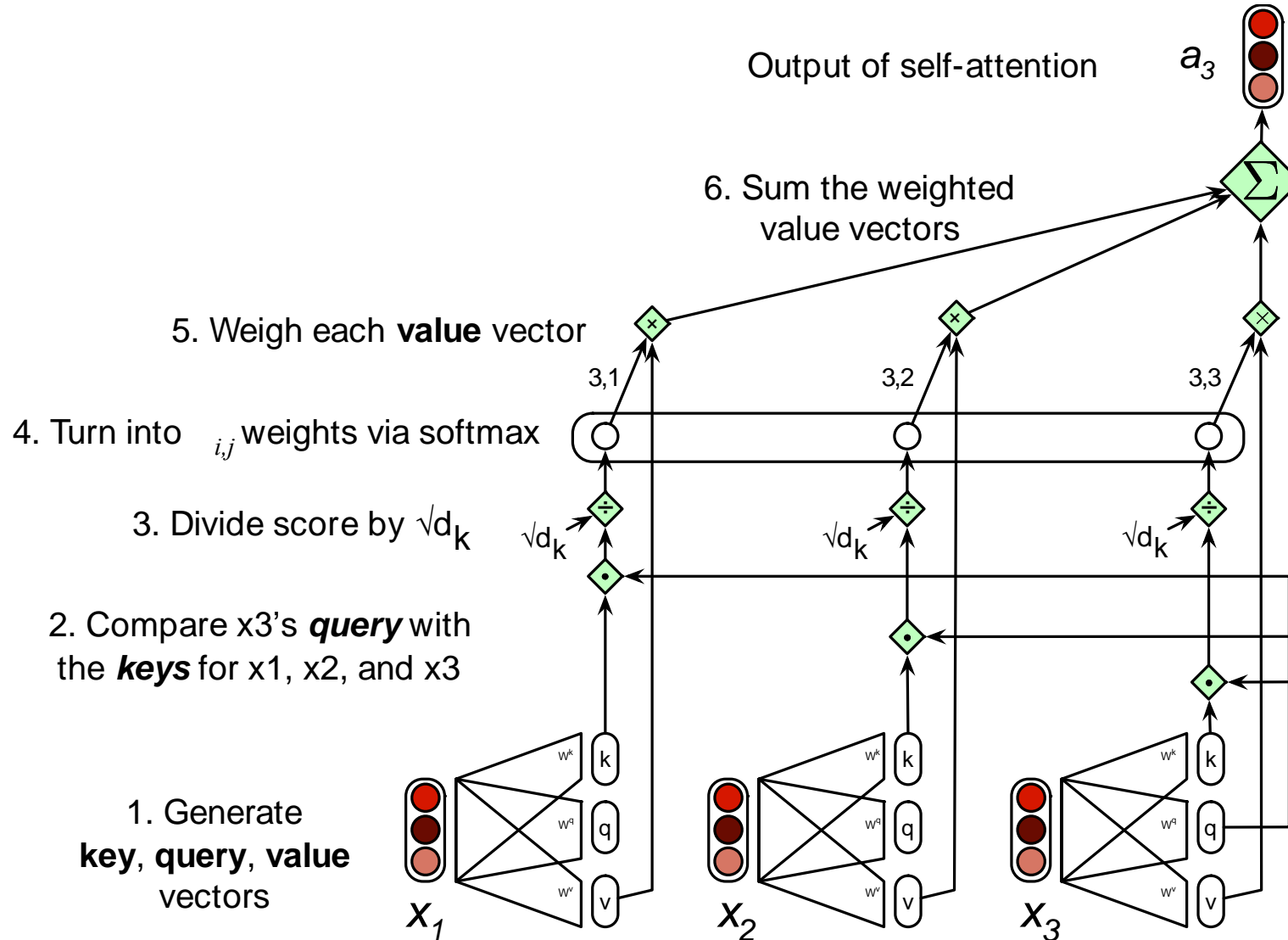
$$\mathbf{q}_i = \mathbf{x}_i \mathbf{W}^Q; \quad \mathbf{k}_j = \mathbf{x}_j \mathbf{W}^K; \quad \mathbf{v}_j = \mathbf{x}_j \mathbf{W}^V$$

$$\text{score}(\mathbf{x}_i, \mathbf{x}_j) = \frac{\mathbf{q}_i \cdot \mathbf{k}_j}{\sqrt{d_k}}$$

$$\alpha_{ij} = \text{softmax}(\text{score}(\mathbf{x}_i, \mathbf{x}_j)) \quad \forall j \leq i$$

$$\mathbf{a}_i = \sum_{j \leq i} \alpha_{ij} \mathbf{v}_j$$

# Calculating the value of $a_3$



# Actual Attention: slightly more complicated

- Instead of one attention head, we'll have lots of them!
- Intuition: each head might be attending to the context for different purposes
  - Different linguistic relationships or patterns in the context

$$\mathbf{q}_i^c = \mathbf{x}_i \mathbf{W}^{\mathbf{Q}^c}; \quad \mathbf{k}_j^c = \mathbf{x}_j \mathbf{W}^{\mathbf{K}^c}; \quad \mathbf{v}_j^c = \mathbf{x}_j \mathbf{W}^{\mathbf{V}^c}; \quad \forall c \quad 1 \leq c \leq h$$

$$\text{score}^c(\mathbf{x}_i, \mathbf{x}_j) = \frac{\mathbf{q}_i^c \cdot \mathbf{k}_j^c}{\sqrt{d_k}}$$

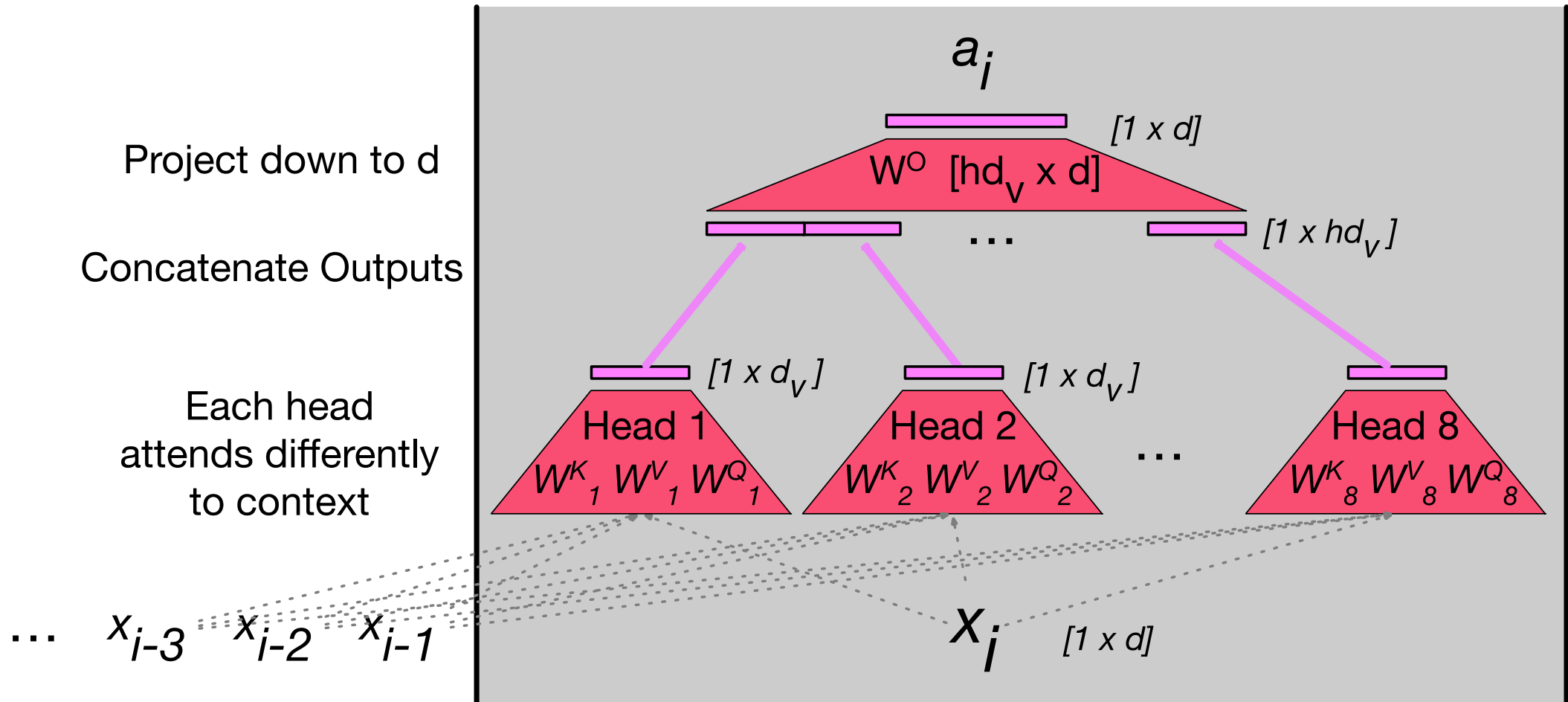
$$\alpha_{ij}^c = \text{softmax}(\text{score}^c(\mathbf{x}_i, \mathbf{x}_j)) \quad \forall j \leq i$$

$$\text{head}_i^c = \sum_{j \leq i} \alpha_{ij}^c \mathbf{v}_j^c$$

$$\mathbf{a}_i = (\text{head}^1 \oplus \text{head}^2 \dots \oplus \text{head}^h) \mathbf{W}^O$$

$$\text{MultiHeadAttention}(\mathbf{x}_i, [\mathbf{x}_1, \dots, \mathbf{x}_N]) = \mathbf{a}_i$$

# Multi-head attention



# Summary

Attention is a method for enriching the representation of a token by incorporating contextual information

The result: the embedding for each word will be different in different contexts!

Contextual embeddings: a representation of word meaning in its context.

We'll see in the next lecture that attention can also be viewed as a way to move information from one token to another.



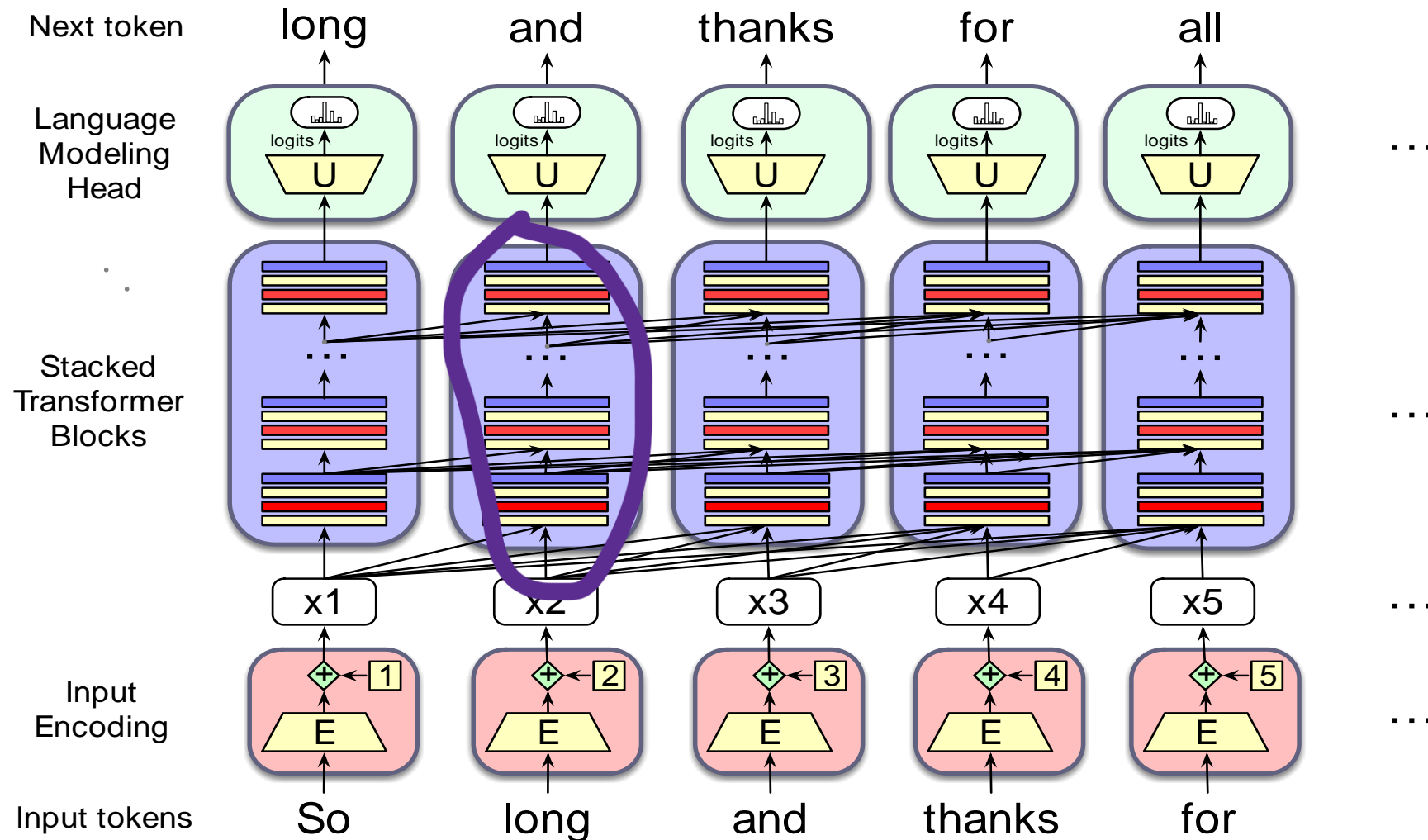
Attention

Transformers

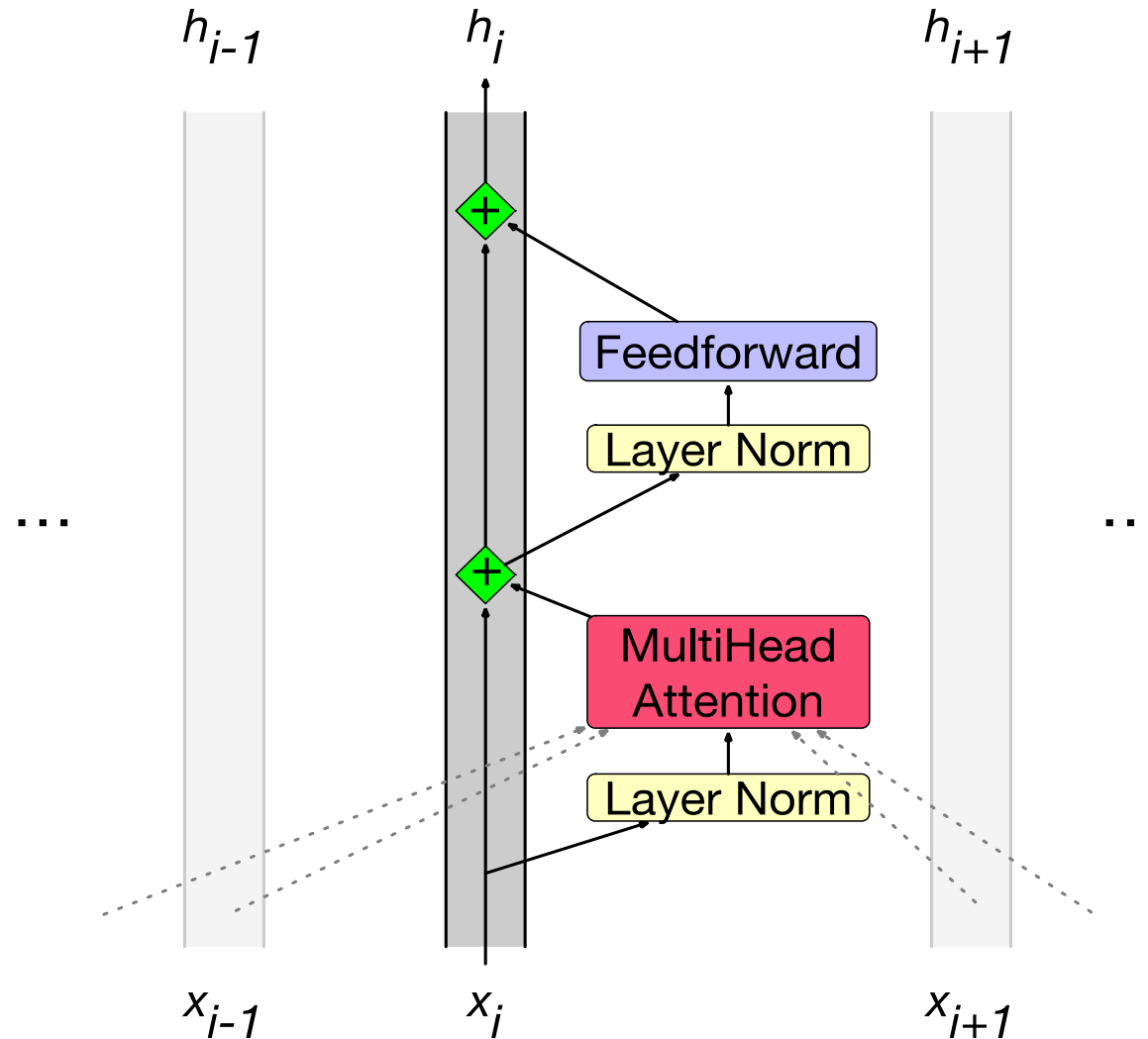
Transformers

## The Transformer Block

# Reminder: transformer language model

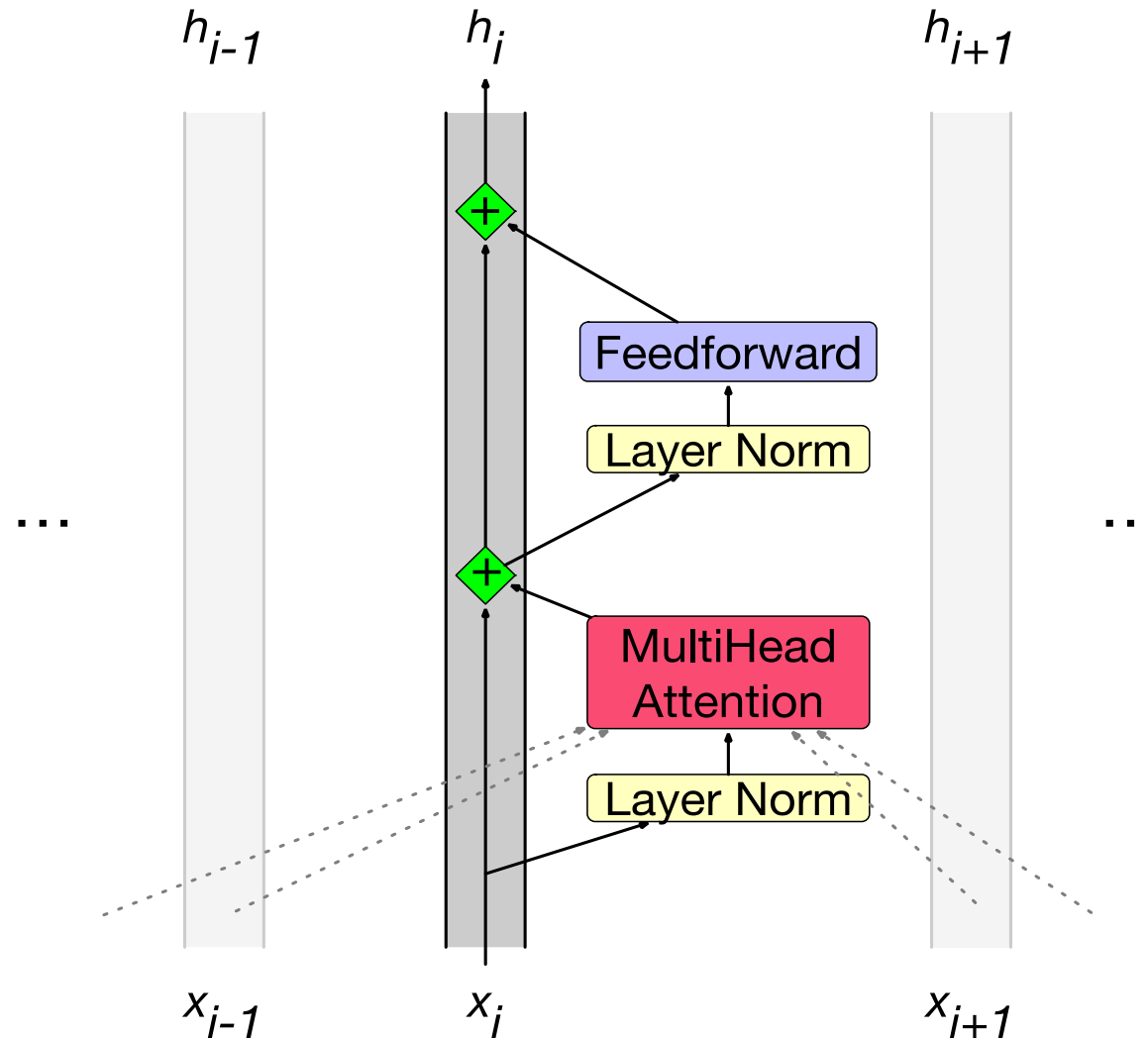


The residual stream: each token gets passed up and modified

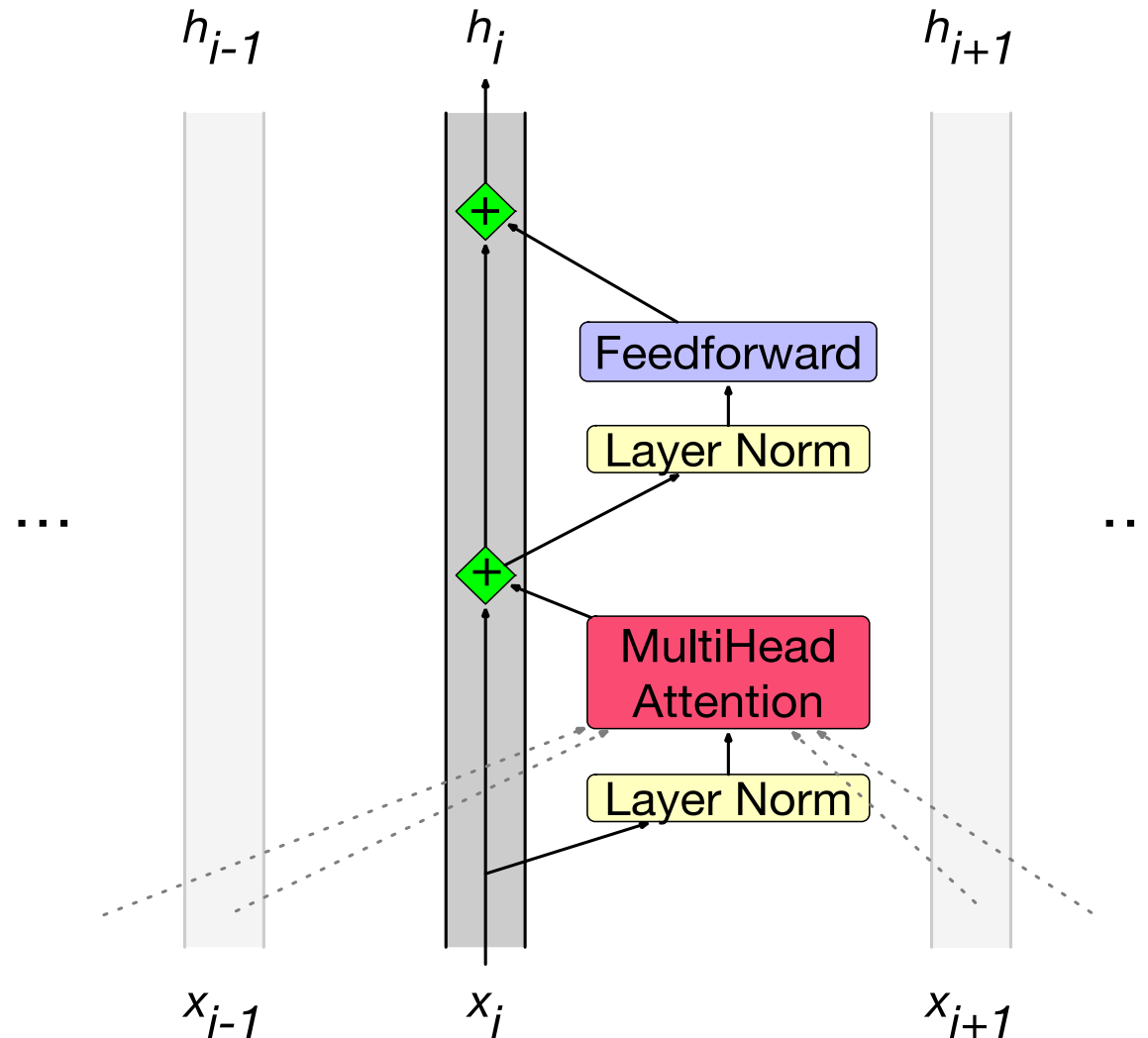


We'll need nonlinearities, so a feedforward layer

$$\text{FFN}(\mathbf{x}_i) = \text{ReLU}(\mathbf{x}_i \mathbf{W}_1 + b_1) \mathbf{W}_2 + b_2$$



Layer norm: the vector  $x_i$  is normalized twice



# Layer Norm

Layer norm is a variation of the z-score from statistics, applied to a single vector in a hidden layer

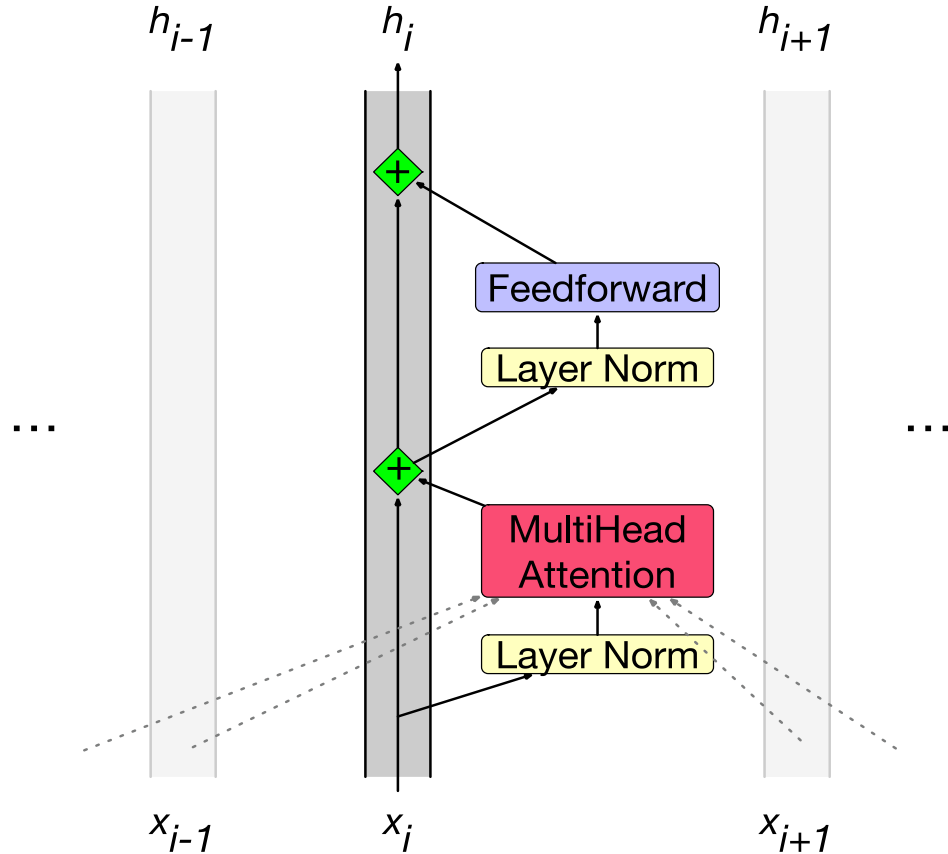
$$\mu = \frac{1}{d} \sum_{i=1}^d x_i$$

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

$$\hat{\mathbf{x}} = \frac{(\mathbf{x} - \mu)}{\sigma}$$

$$\text{LayerNorm}(\mathbf{x}) = \gamma \frac{(\mathbf{x} - \mu)}{\sigma} + \beta$$

# Putting together a single transformer block



$$\mathbf{t}_i^1 = \text{LayerNorm}(\mathbf{x}_i)$$

$$\mathbf{t}_i^2 = \text{MultiHeadAttention}(\mathbf{t}_i^1, [\mathbf{x}_1^1, \dots, \mathbf{x}_N^1])$$

$$\mathbf{t}_i^3 = \mathbf{t}_i^2 + \mathbf{x}_i$$

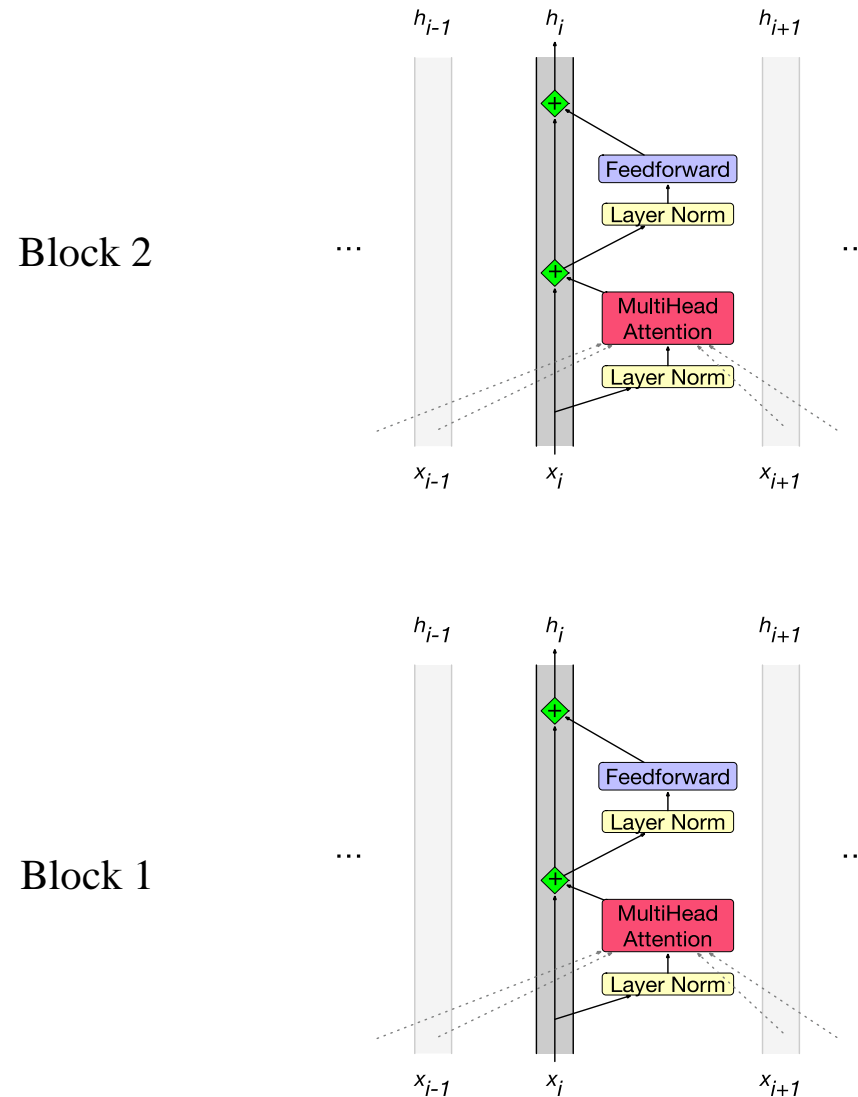
$$\mathbf{t}_i^4 = \text{LayerNorm}(\mathbf{t}_i^3)$$

$$\mathbf{t}_i^5 = \text{FFN}(\mathbf{t}_i^4)$$

$$\mathbf{h}_i = \mathbf{t}_i^5 + \mathbf{t}_i^3$$



A transformer is a stack of these blocks  
so all the vectors are of the same dimensionality  $d$

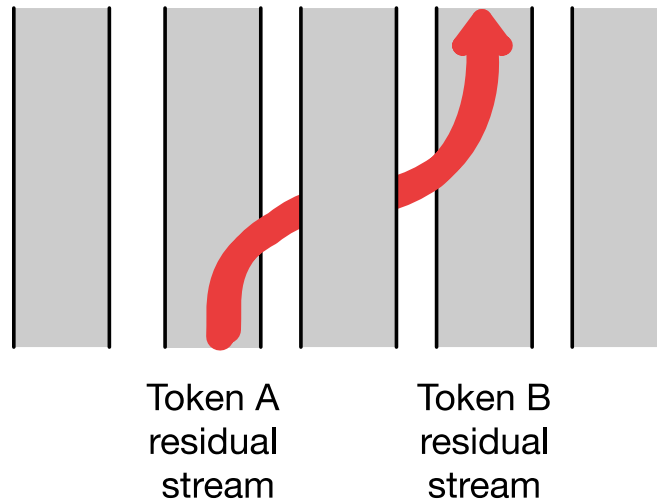


# Residual streams and attention

Notice that all parts of the transformer block apply to 1 residual stream (1 token).

Except attention, which takes information from other tokens

[Elhage et al. \(2021\)](#) show that we can view attention heads as literally moving information from the residual stream of a neighboring token into the current stream .



Transformers

## The Transformer Block

Transformers

# Parallelizing Attention Computation

# Parallelizing computation using $\mathbf{X}$

For attention/transformer block we've been computing a **single** output at a **single** time step  $i$  in a **single** residual stream.

But we can pack the  $N$  tokens of the input sequence into a single matrix  $\mathbf{X}$  of size  $[N \times d]$ .

Each row of  $\mathbf{X}$  is the embedding of one token of the input.

$\mathbf{X}$  can have 1K-32K rows, each of the dimensionality of the embedding  $d$  (the **model dimension**)

$$\mathbf{Q} = \mathbf{XW}^{\mathbf{Q}}; \quad \mathbf{K} = \mathbf{XW}^{\mathbf{K}}; \quad \mathbf{V} = \mathbf{XW}^{\mathbf{V}}$$

$$QK^T$$

Now can do a single matrix multiply to combine Q and  $K^T$

N	<b>q1•k1</b>	<b>q1•k2</b>	<b>q1•k3</b>	<b>q1•k4</b>
	<b>q2•k1</b>	<b>q2•k2</b>	<b>q2•k3</b>	<b>q2•k4</b>
	<b>q3•k1</b>	<b>q3•k2</b>	<b>q3•k3</b>	<b>q3•k4</b>
	<b>q4•k1</b>	<b>q4•k2</b>	<b>q4•k3</b>	<b>q4•k4</b>
	N			

# Parallelizing attention

- Scale the scores, take the softmax, and then multiply the result by  $V$  resulting in a matrix of shape  $N \times d$ 
  - An attention vector for each input token

$$\mathbf{A} = \text{softmax} \left( \text{mask} \left( \frac{\mathbf{Q}\mathbf{K}^\top}{\sqrt{d_k}} \right) \right) \mathbf{V}$$

# Masking out the future

$$\mathbf{A} = \text{softmax} \left( \text{mask} \left( \frac{\mathbf{Q}\mathbf{K}^\top}{\sqrt{d_k}} \right) \right) \mathbf{V}$$

- What is this mask function?  
 $\mathbf{Q}\mathbf{K}^\top$  has a score for each query dot every key, *including those that follow the query.*
- Guessing the next word is pretty simple if you already know it!



# Masking out the future

$$\mathbf{A} = \text{softmax} \left( \text{mask} \left( \frac{\mathbf{QK}^\top}{\sqrt{d_k}} \right) \right) \mathbf{V}$$

Add  $-\infty$  to cells in upper triangle  
The softmax will turn it to 0

N

q1•k1	$-\infty$	$-\infty$	$-\infty$
q2•k1	q2•k2	$-\infty$	$-\infty$
q3•k1	q3•k2	q3•k3	$-\infty$
q4•k1	q4•k2	q4•k3	q4•k4

N

Another point: Attention is quadratic in length

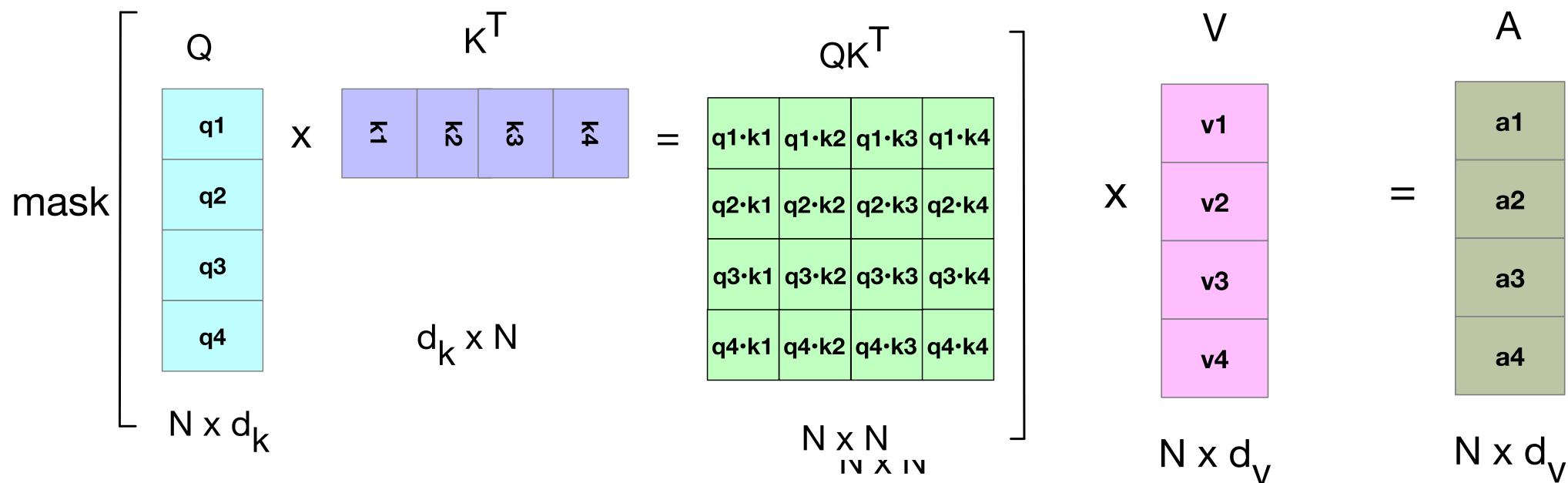
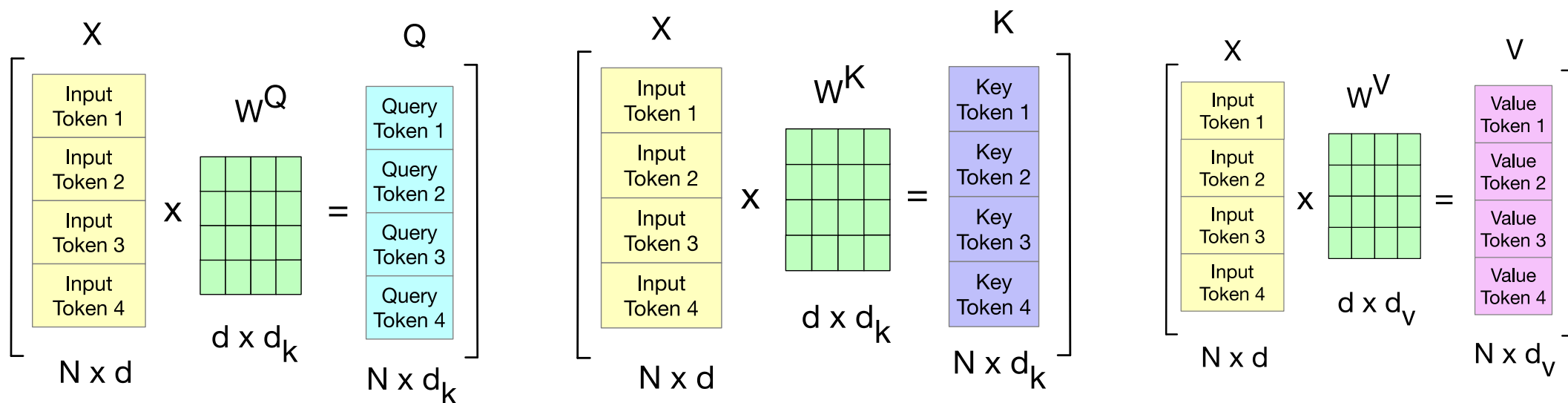
$$\mathbf{A} = \text{softmax} \left( \text{mask} \left( \frac{\mathbf{Q}\mathbf{K}^\top}{\sqrt{d_k}} \right) \right) \mathbf{V}$$

N

q1•k1	−∞	−∞	−∞
q2•k1	q2•k2	−∞	−∞
q3•k1	q3•k2	q3•k3	−∞
q4•k1	q4•k2	q4•k3	q4•k4

N

# Attention again



# Parallelizing Multi-head Attention

$$\mathbf{Q}^i = \mathbf{XW}^{\mathbf{Q}^i}; \quad \mathbf{K}^i = \mathbf{XW}^{\mathbf{K}^i}; \quad \mathbf{V}^i = \mathbf{XW}^{\mathbf{V}^i}$$

$$\mathbf{head}_i = \text{SelfAttention}(\mathbf{Q}^i, \mathbf{K}^i, \mathbf{V}^i) = \text{softmax} \left( \frac{\mathbf{Q}^i \mathbf{K}^{i\top}}{\sqrt{d_k}} \right) \mathbf{V}^i$$

$$\text{MultiHeadAttention}(\mathbf{X}) = (\mathbf{head}_1 \oplus \mathbf{head}_2 \dots \oplus \mathbf{head}_h) \mathbf{W}^0$$

# Parallelizing Multi-head Attention

$$\mathbf{O} = \text{LayerNorm}(\mathbf{X} + \text{MultiHeadAttention}(\mathbf{X}))$$

$$\mathbf{H} = \text{LayerNorm}(\mathbf{O} + \text{FFN}(\mathbf{O}))$$

or

$$\mathbf{T}^1 = \text{MultiHeadAttention}(\mathbf{X})$$

$$\mathbf{T}^2 = \mathbf{X} + \mathbf{T}^1$$

$$\mathbf{T}^3 = \text{LayerNorm}(\mathbf{T}^2)$$

$$\mathbf{T}^4 = \text{FFN}(\mathbf{T}^3)$$

$$\mathbf{T}^5 = \mathbf{T}^4 + \mathbf{T}^3$$

$$\mathbf{H} = \text{LayerNorm}(\mathbf{T}^5)$$

Transformers

# Parallelizing Attention Computation

# Transformers

Input and output: Position  
embeddings and the Language  
Model Head

# Token and Position Embeddings

The matrix  $X$  (of shape  $[N \times d]$ ) has an embedding for each word in the context.

This embedding is created by adding two distinct embeddings for each input

- token embedding
- positional embedding



# Token Embeddings

Embedding matrix  $E$  has shape  $[|V| \times d]$ .

- One row for each of the  $|V|$  tokens in the vocabulary.
- Each word is a row vector of  $d$  dimensions

Given: string "*Thanks for all the*"

1. Tokenize with BPE and convert into vocab indices

$w = [5, 4000, 10532, 2224]$

2. Select the corresponding rows from  $E$ , each row an embedding

- (row 5, row 4000, row 10532, row 2224).

# Position Embeddings

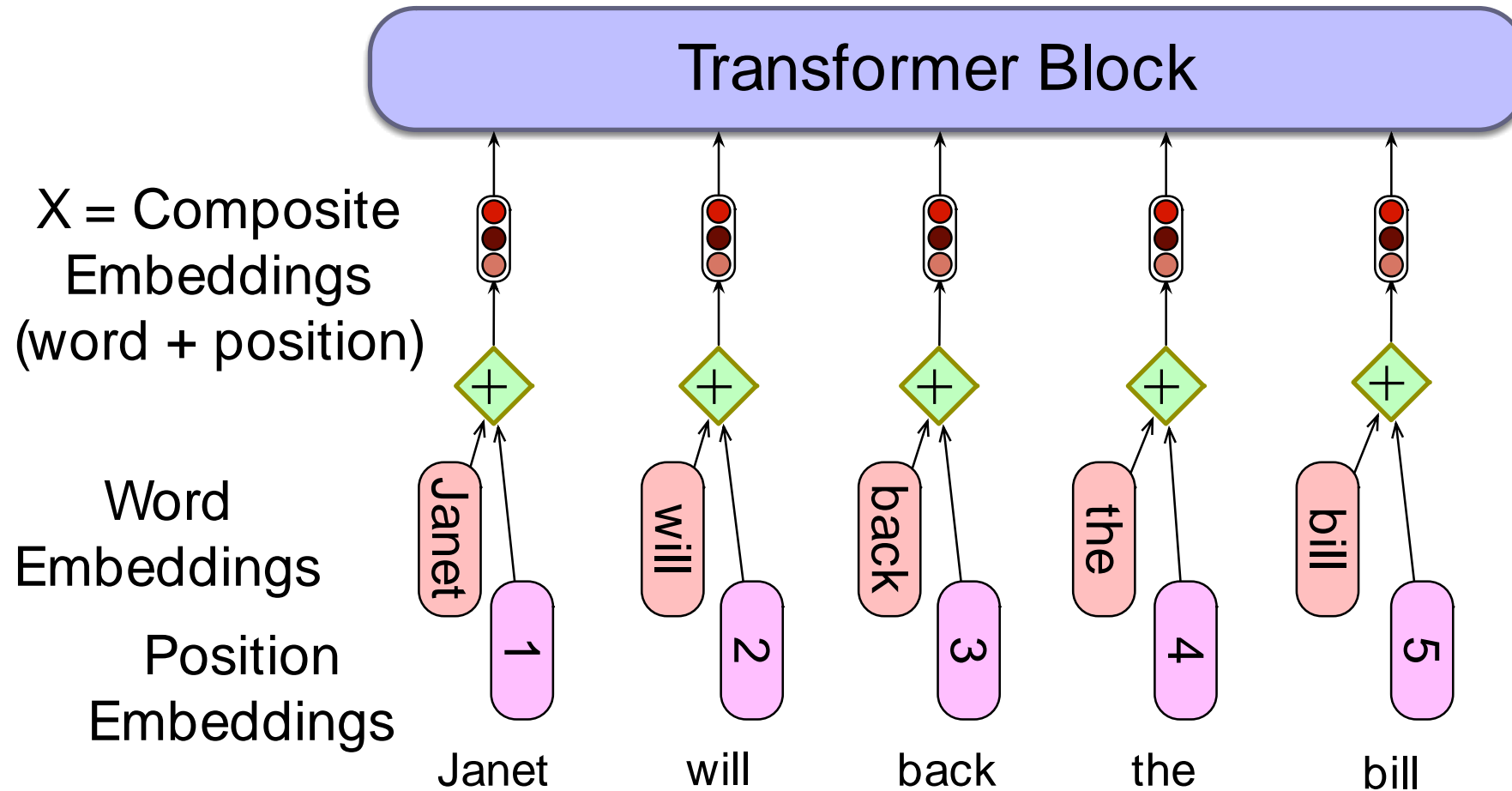
There are many methods, but we'll just describe the simplest: absolute position.

Goal: learn a position embedding matrix  $E_{pos}$  of shape  $[1 \times N]$ .

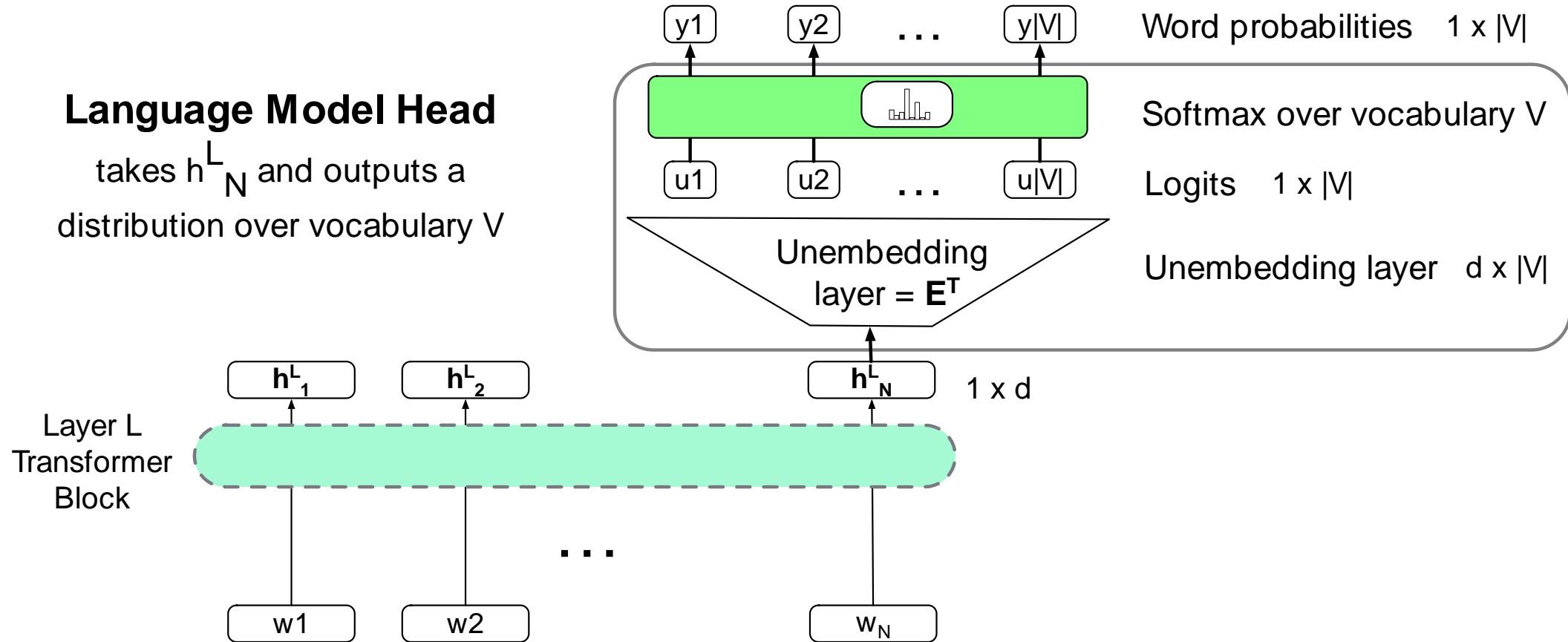
Start with randomly initialized embeddings

- one for each integer up to some maximum length.
- i.e., just as we have an embedding for token *fish*, we'll have an embedding for position 3 and position 17.
- As with word embeddings, these position embeddings are learned along with other parameters during training.

Each  $x$  is just the sum of word and position embeddings

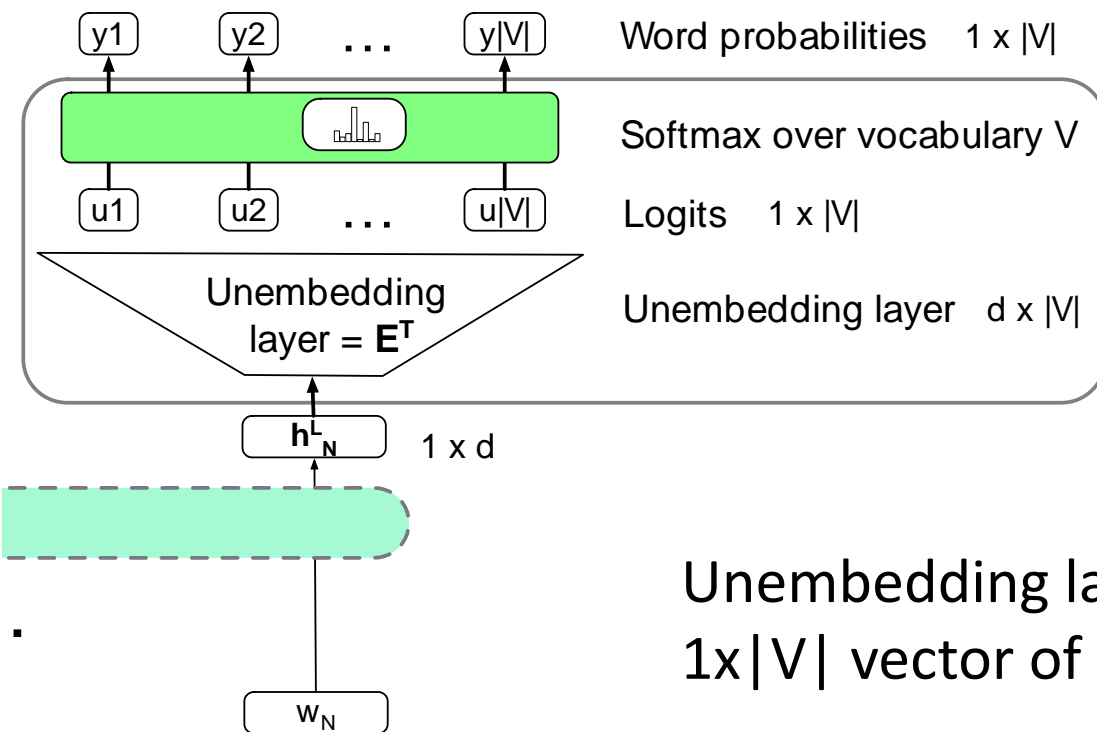


# Language modeling head



# Language modeling head

**Unembedding layer:** linear layer projects from  $h_N^L$  (shape  $[1 \times d]$ ) to logit vector



Why "unembedding"? **Tied** to  $E^T$

**Weight tying**, we use the same weights for two different matrices

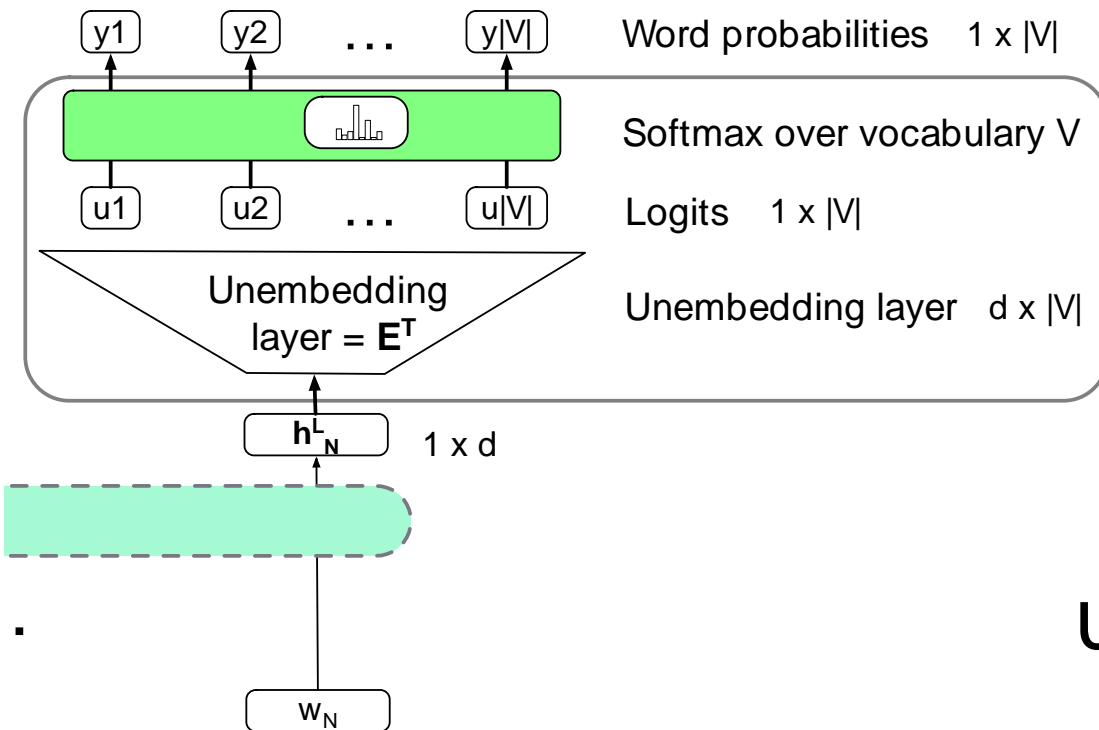
Unembedding layer maps from an embedding to a  $1 \times |V|$  vector of logits

# Language modeling head

**Logits**, the score vector  $u$

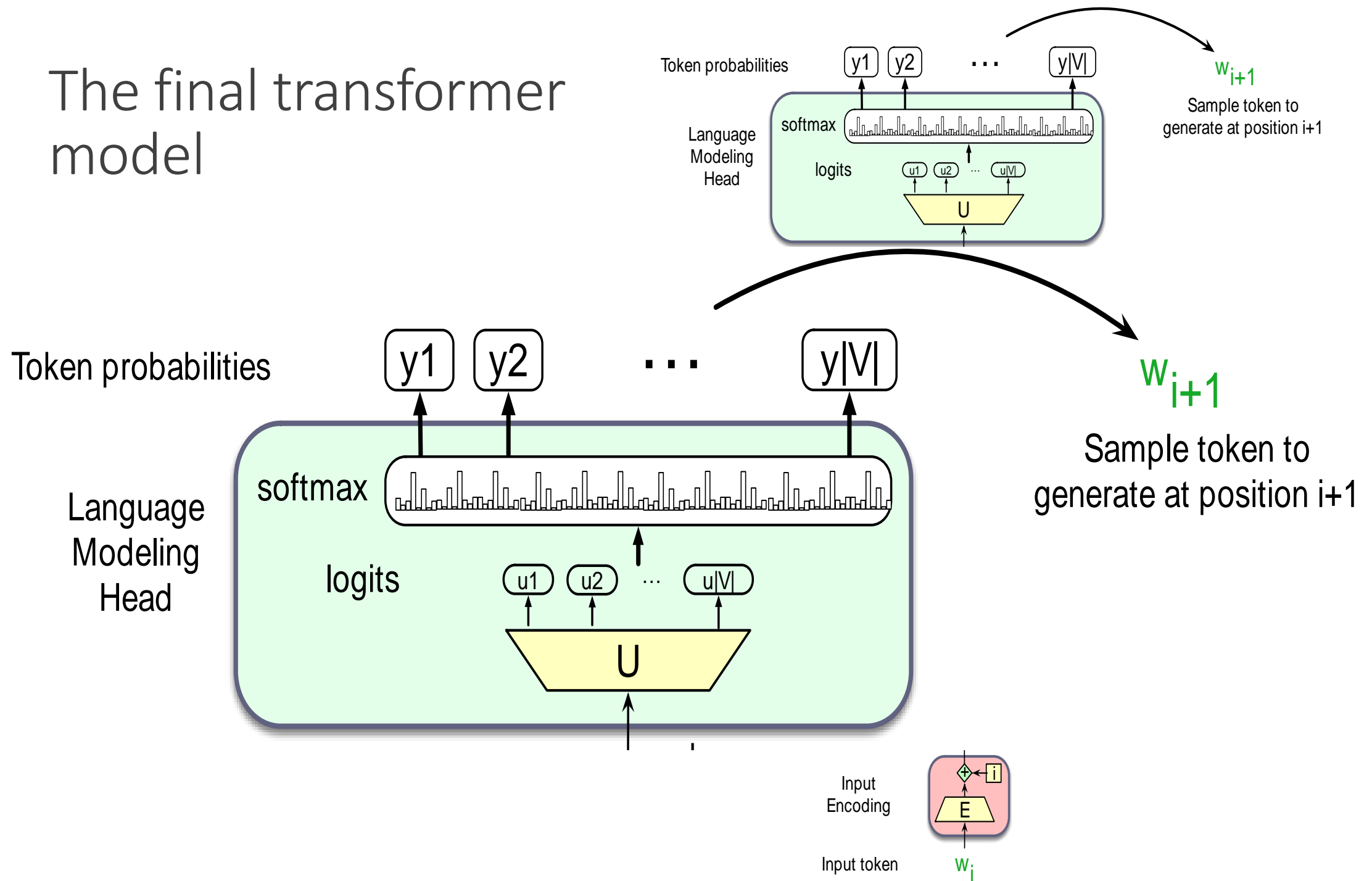
One score for each of the  $|V|$  possible words in the vocabulary  $V$ .  
Shape  $1 \times |V|$ .

**Softmax** turns the logits into probabilities over vocabulary.  
Shape  $1 \times |V|$ .



$$u = h_N^L E^T$$
$$y = \text{softmax}(u)$$

# The final transformer model



# Transformers

Input and output: Position  
embeddings and the Language  
Model Head