

The Transformer

NLP Week 8

Thanks to Dan Jurafsky for most of the slides this week!

Plan for today

1. Review of notation and matrix multiplication
2. (Multi-head) self-attention
3. Residual stream
4. Position embeddings
5. Putting it all together —> The Transformer
6. GPT and BERT
7. *Group exercises*

This semester

We will build language models adding to each layer of their complexity:

1. **Bag of words models** (basic statistical models of language)
2. **N-gram models** (+ sequential dependencies)
3. **Hidden Markov models** (+ latent categories)
4. **Recurrent neural networks** (+ distributed representations)
5. **LSTM language models** (+ long distance dependencies)
6. **Transformer language models** (+ attention-based dependency learning)

= Today's language models!

A note on notation

Quick recap on our notation and matrix-matrix and matrix-vector multiplication

- Let \mathbf{A} denote an $p \times d$ matrix
- Let \mathbf{X} denote an $d \times n$ matrix
- Let \mathbf{x} denote a $d \times 1$ vector (column vector)
- \mathbf{x}^\top is a $1 \times d$ vector (row vector)
- Note that: $(\mathbf{AX})^\top = \mathbf{X}^\top \mathbf{A}^\top$

We need to understand:

- $\mathbf{y} = \mathbf{Ax}$
- $\mathbf{y}^\top = \mathbf{x}^\top \mathbf{A}^\top$
- $\mathbf{Y} = \mathbf{AX}$
- $\mathbf{Y}^\top = \mathbf{X}^\top \mathbf{A}^\top$

👉 will do this on the whiteboard ...

The paper that started it all

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

Attention Is All You Need

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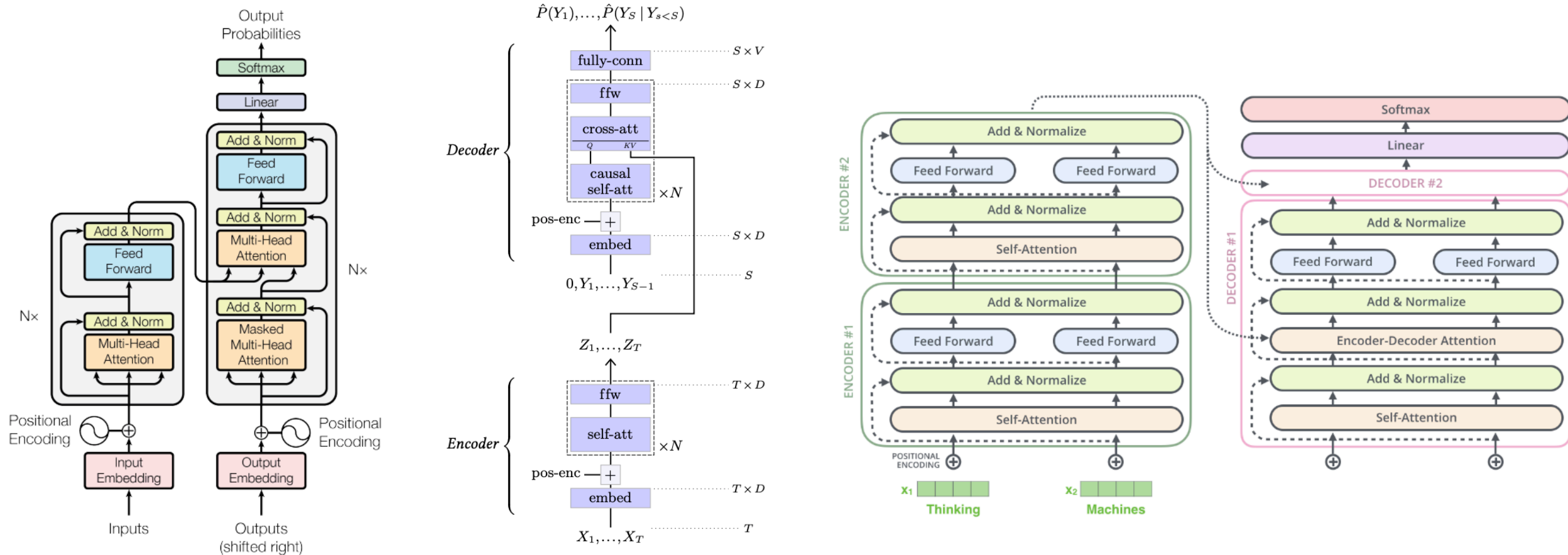
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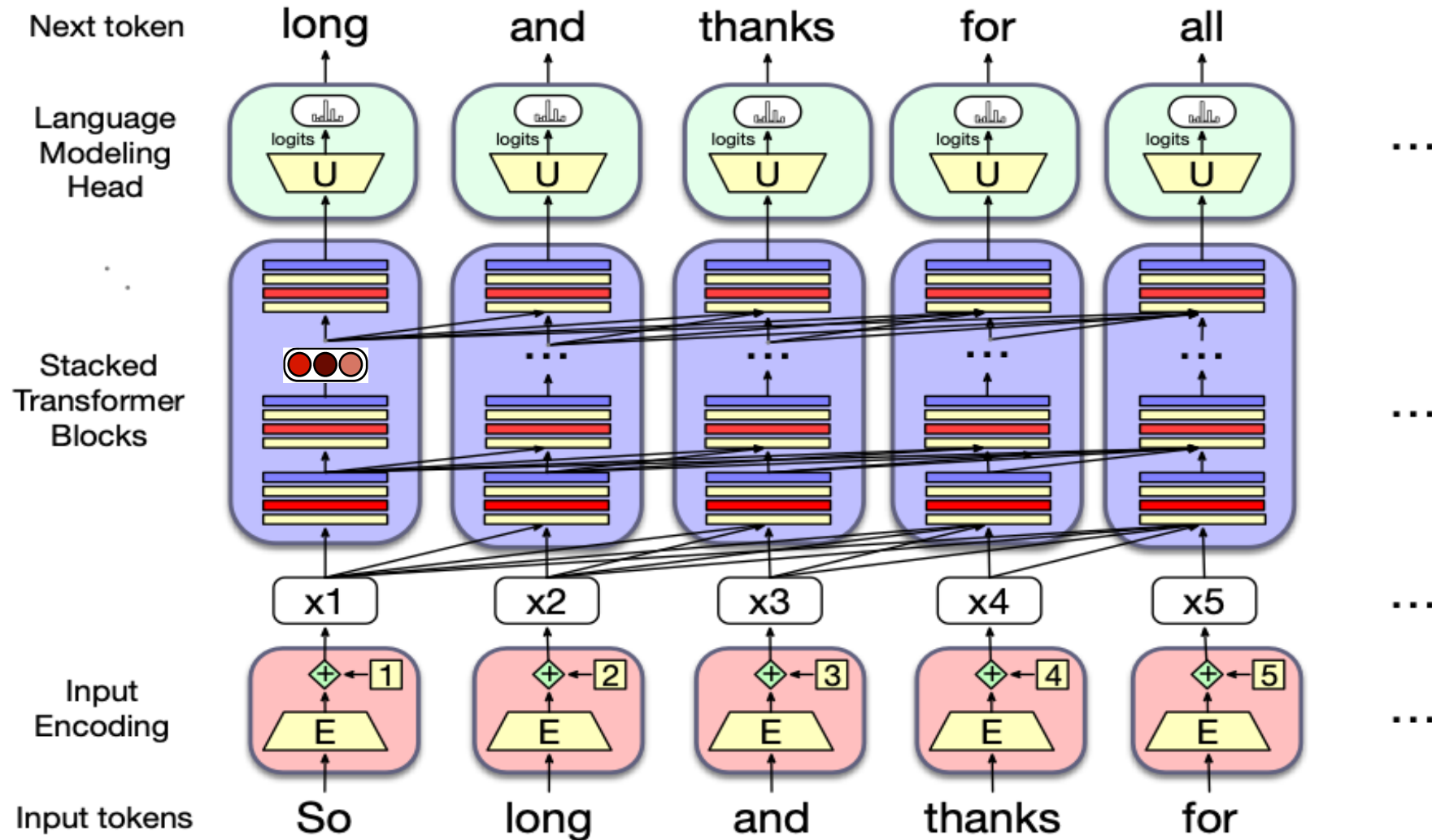
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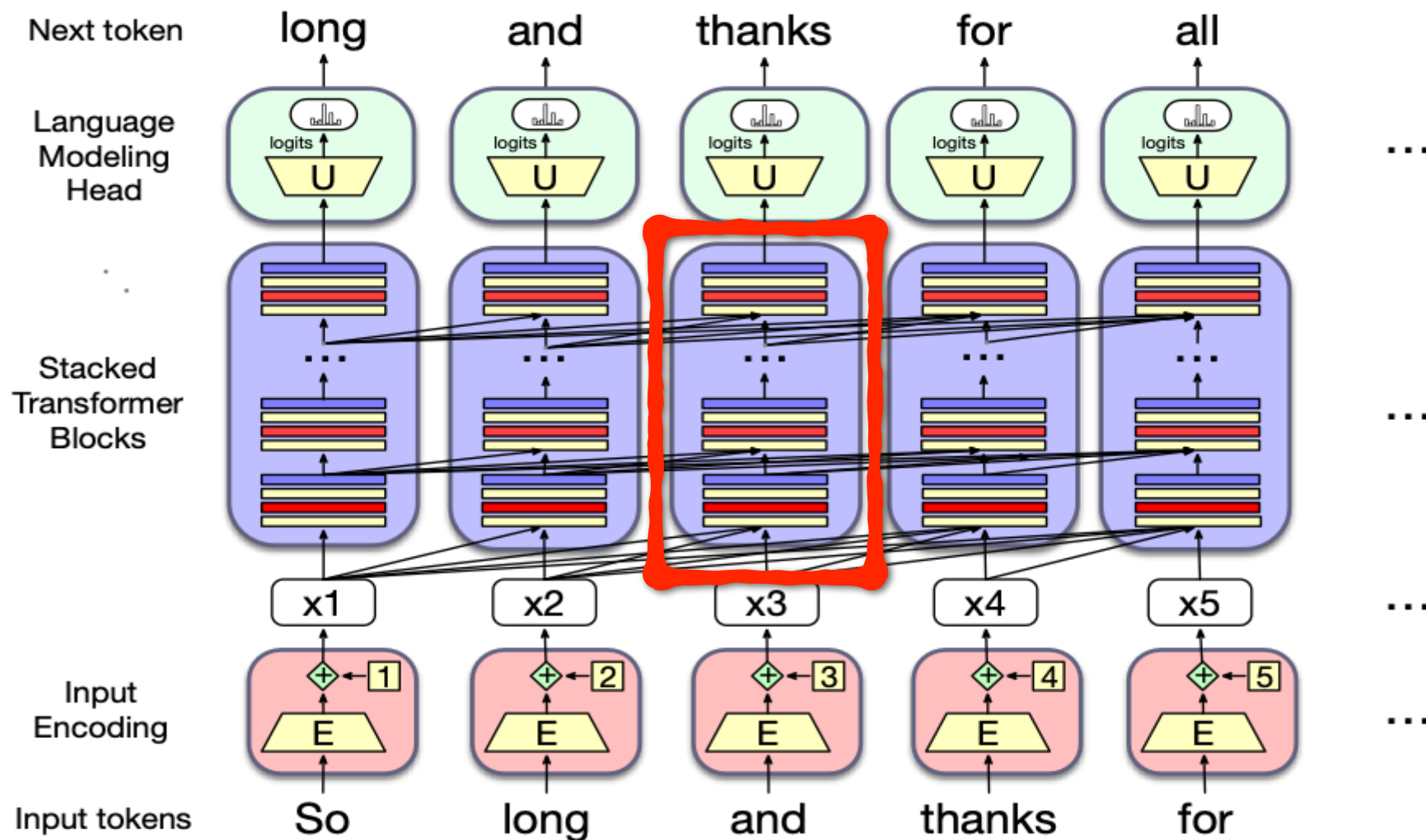
What is a Transformer?



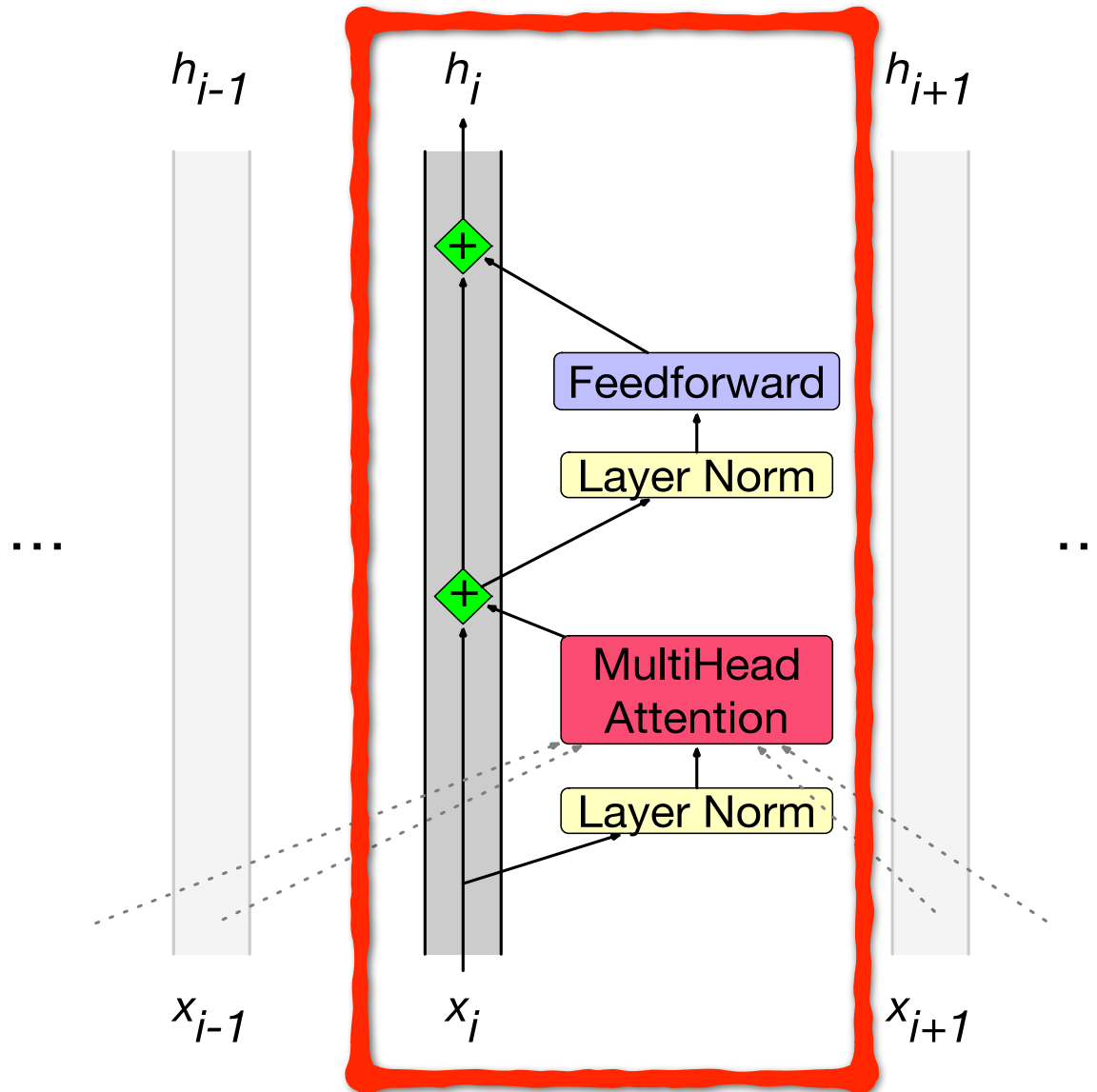
We will stick to the following illustration



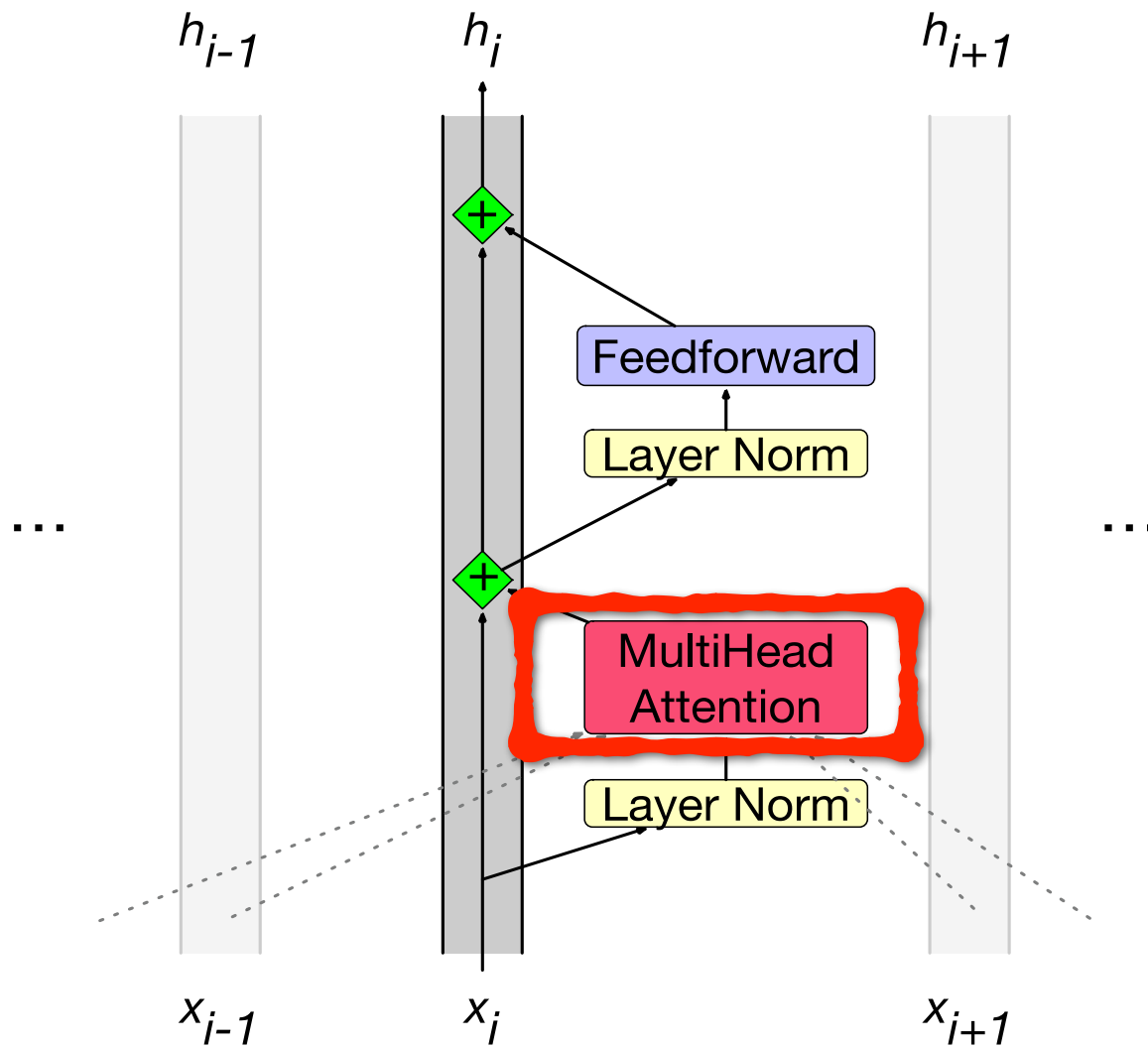
The Transformer



Zooming in



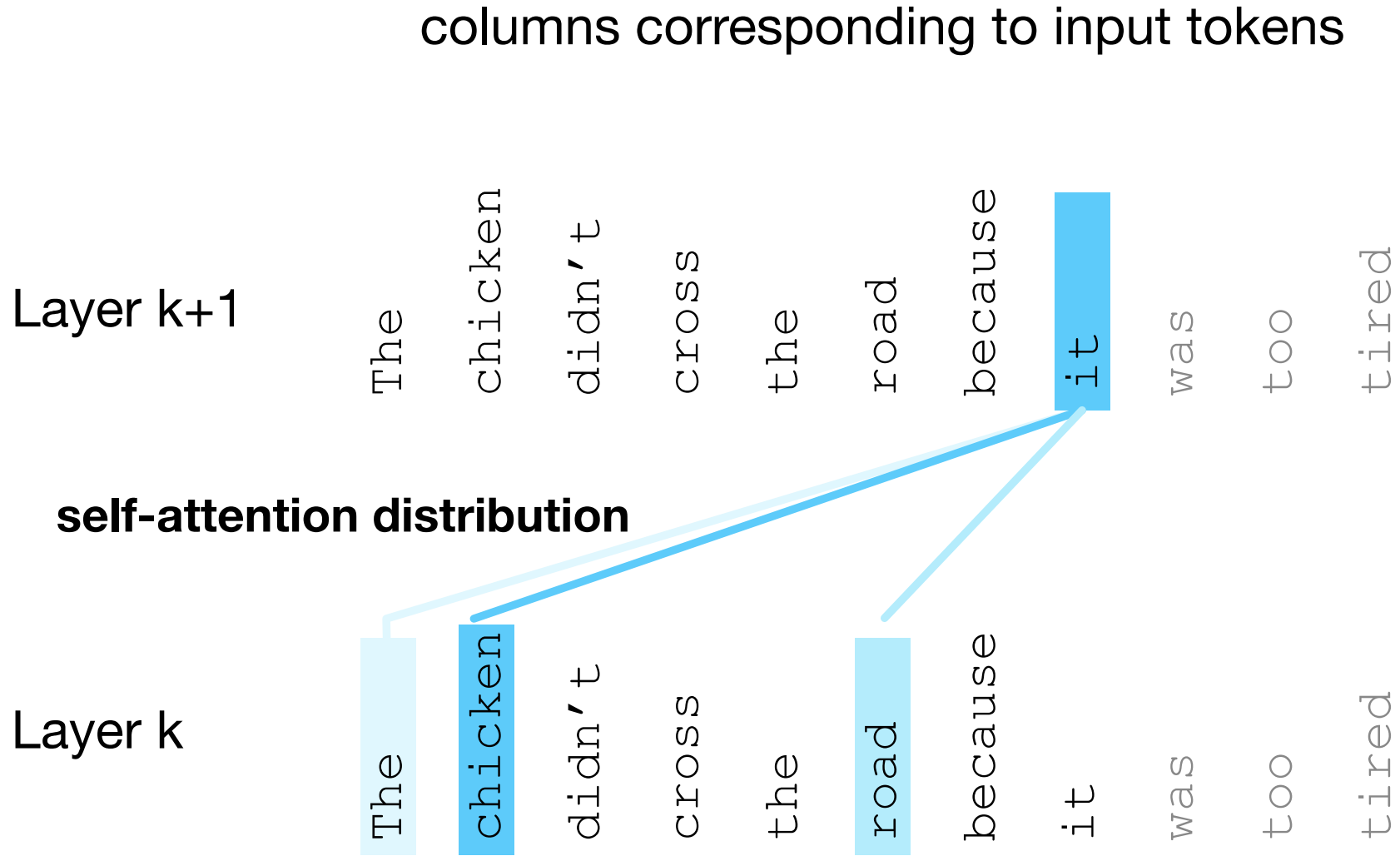
Zooming in



Intuition of attention

- Build up the representation of a word by selectively integrating information from all the neighbouring words
- We say that a word "attends to" some neighbouring words more than others

Intuition of attention



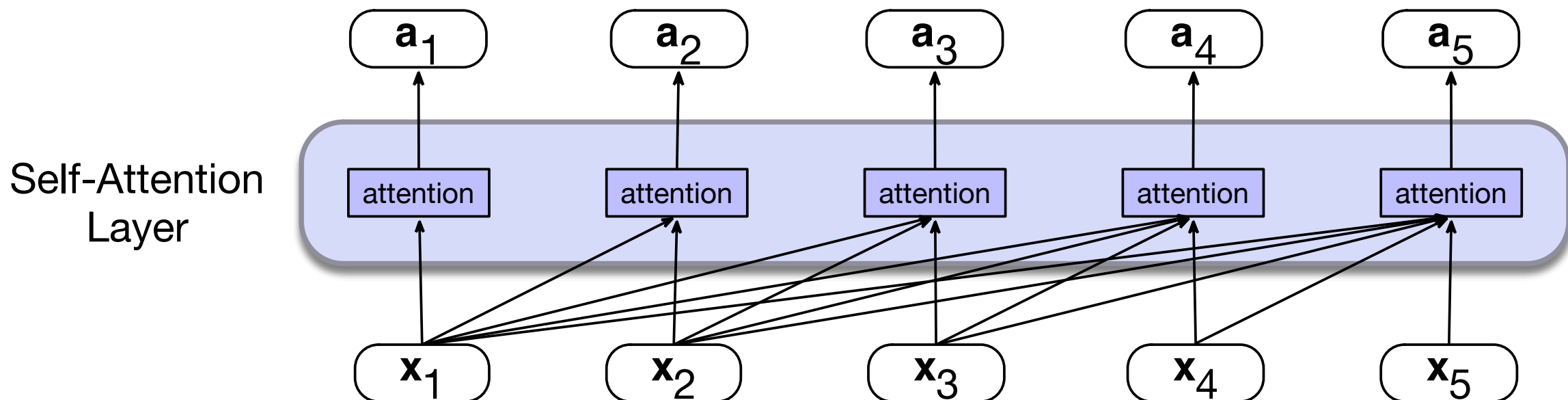
Attention definition

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.

$$\mathbf{v}^{k+1} = \sum_{i=1}^n \alpha_i \cdot \mathbf{v}_i^k$$

Attention can respect time (causal)



$$\mathbf{a}_j = \sum_{i=1}^n (\alpha_i \cdot \mathbb{M}(i, j)) \cdot \mathbf{x}_i \quad \mathbb{M} = \begin{cases} 1 & \text{if } i \leq j \\ 0 & \text{else} \end{cases}$$

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

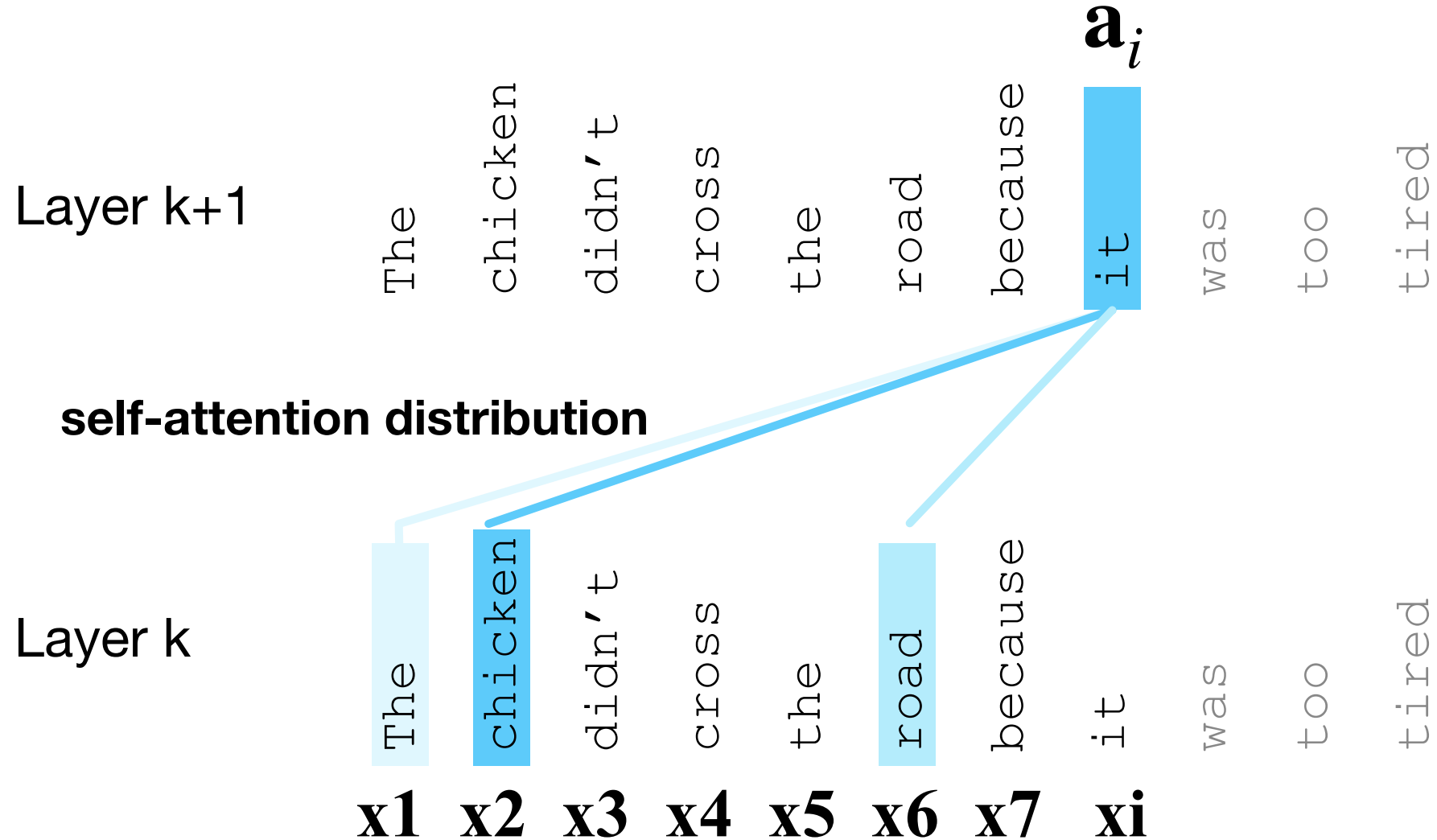
$$\mathbf{a}_i = \sum_{j \leq i} \alpha_j \cdot \mathbf{x}_j$$

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

$$\alpha = \text{softmax}([\text{score}(\mathbf{x}_i, \mathbf{x}_j) \text{ for } j \text{ in } 1 \dots 7, i]) \quad \mathbf{a}_i = \left(\sum_{j=1}^7 \alpha_j \cdot \mathbf{x}_j \right) + \alpha_i \cdot \mathbf{x}_i$$

Intuition of attention

columns corresponding to input tokens

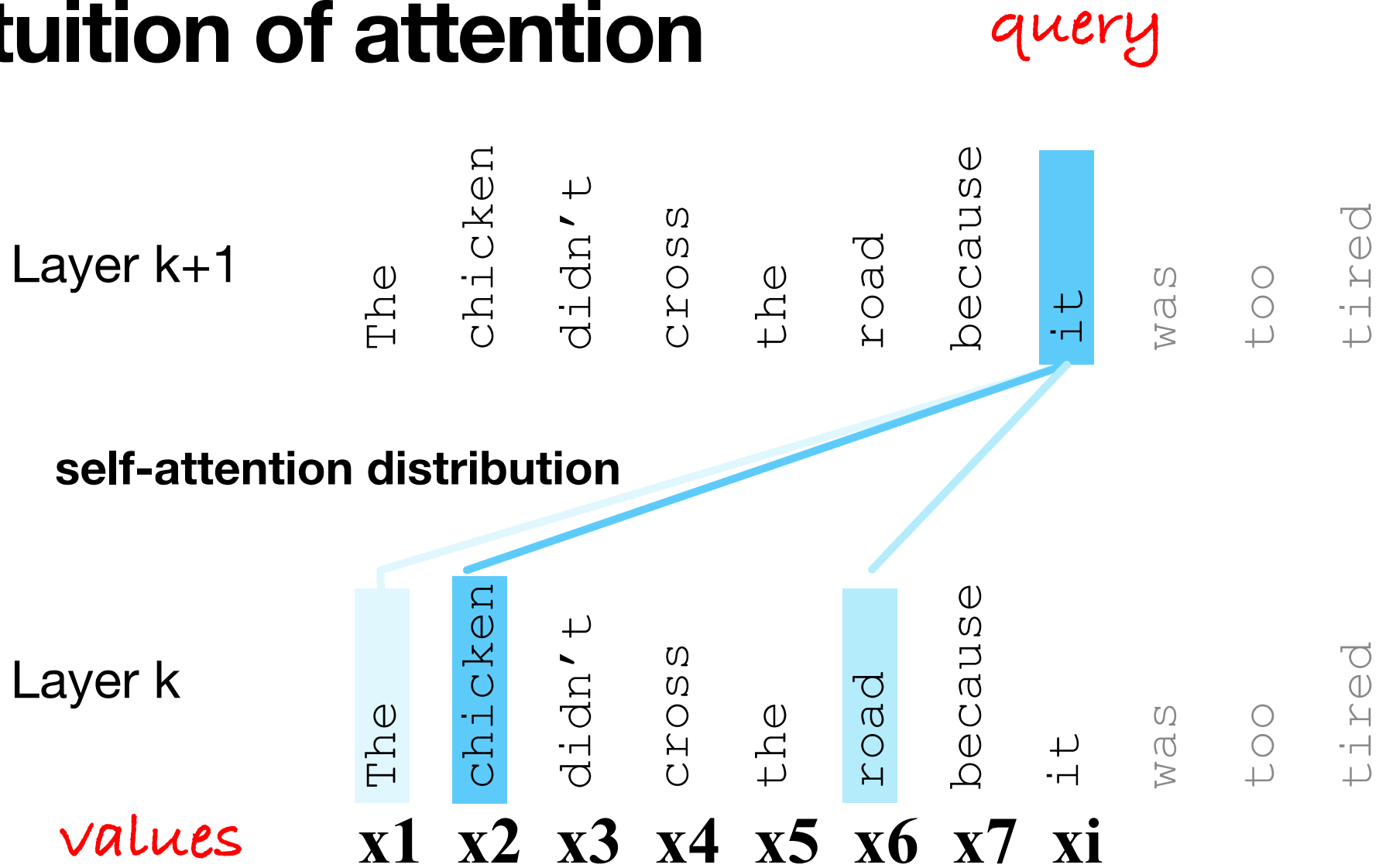


An Actual Attention Head is slightly more complicated

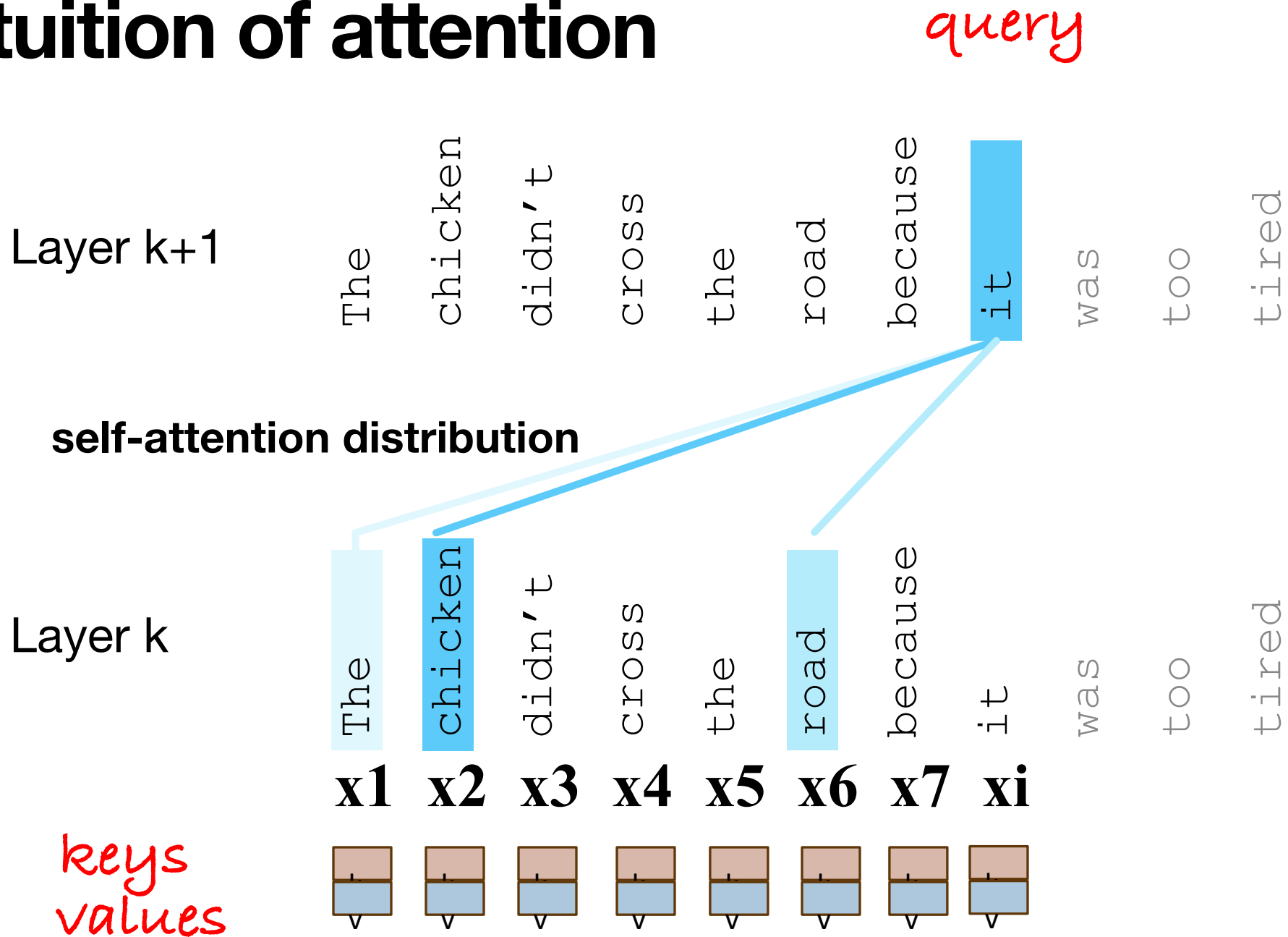
High-level idea: instead of using vectors (like x_i and x_4) directly, we'll represent 3 separate roles each vector x_i plays:

- **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

Intuition of attention



Intuition of attention



An Actual Attention Head is 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

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

Note: $\mathbf{x}_i, \mathbf{q}_i, \mathbf{k}_i, \mathbf{v}_i$ are row vectors here

An Actual Attention Head is 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

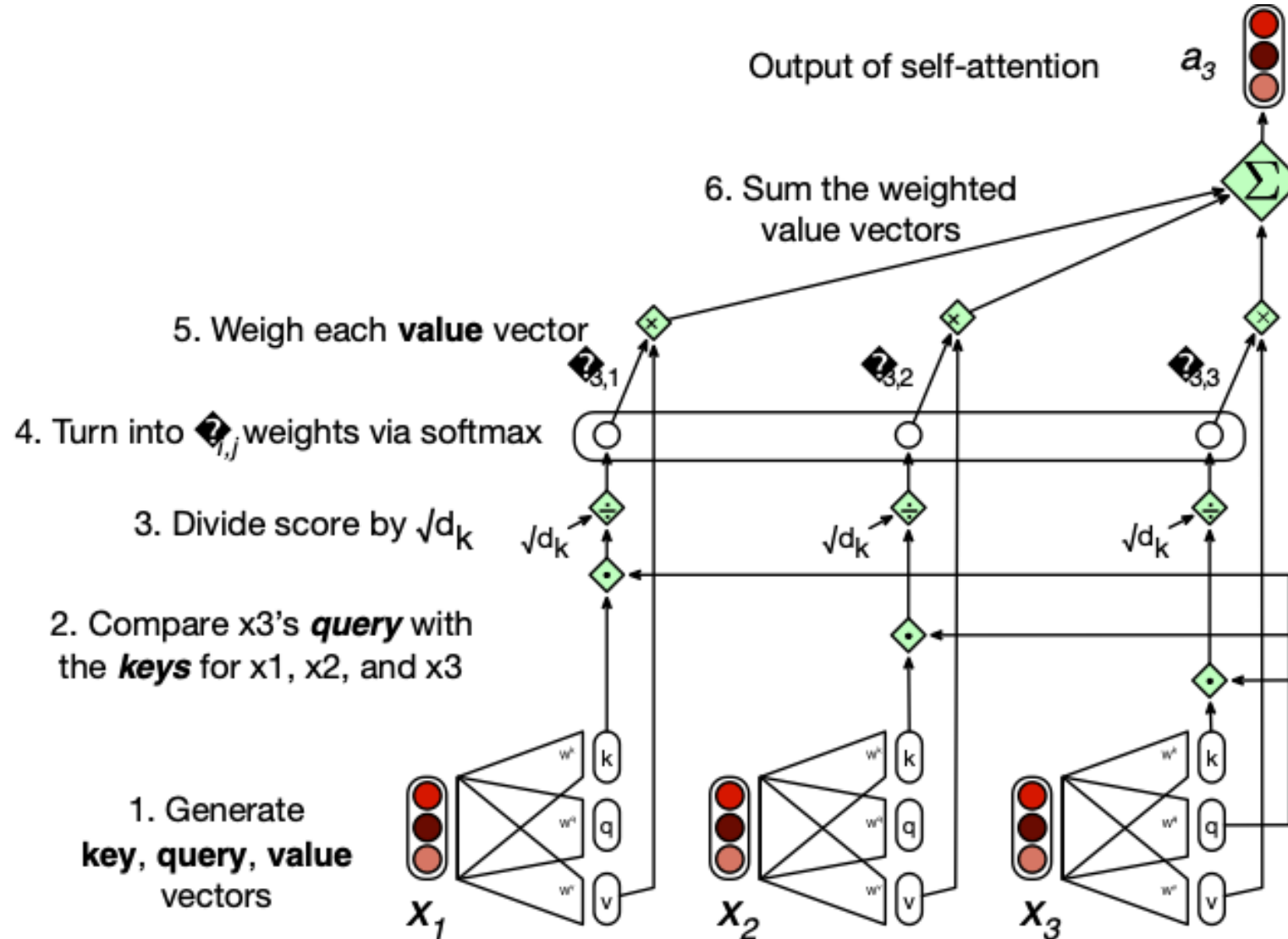
Final equations for one attention head

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

$$\text{score}(\mathbf{x}_i, \mathbf{x}_j) = \frac{\mathbf{q}_i \mathbf{k}_j^\top}{\sqrt{d^k}} \quad \alpha = \text{softmax}([\text{score}(\mathbf{x}_i, \mathbf{x}_j) \forall j \leq i])$$

$$\mathbf{a}_i = \sum_{j \leq i} \alpha_j \cdot \mathbf{v}_j$$

Example: calculating the value of a_3



An Actual Attention Head is 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
 - E.g., different linguistic relationships or patterns in the context

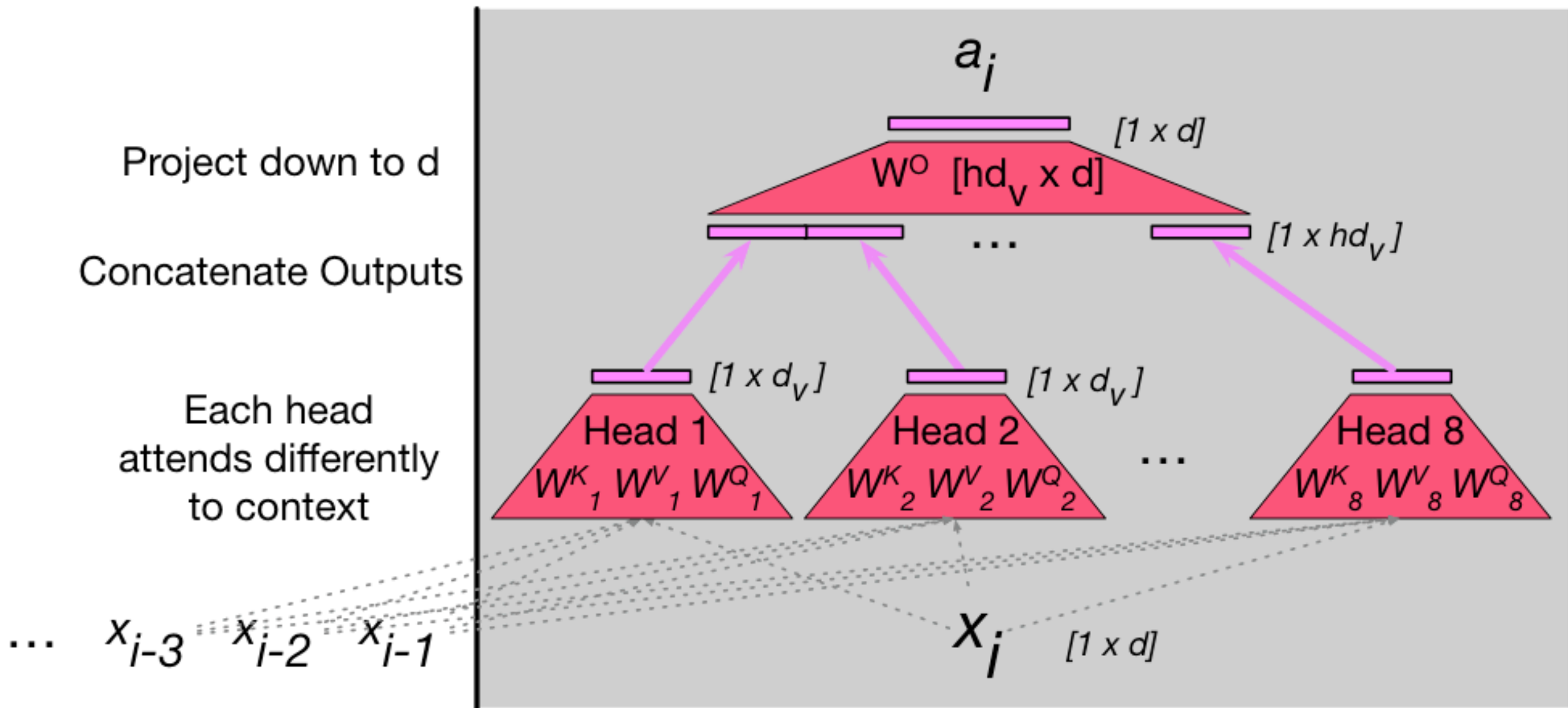
$$\mathbf{q}_i^c = \mathbf{x}_i \mathbf{W}^{Qc} \quad \mathbf{k}_i^c = \mathbf{x}_i \mathbf{W}^{Kc} \quad \mathbf{v}_i^c = \mathbf{x}_i \mathbf{W}^{Vc}$$

$$\text{score}^c(\mathbf{x}_i, \mathbf{x}_j) = \frac{\mathbf{q}_i^c \mathbf{k}_j^{c\top}}{\sqrt{d^k}} \quad \alpha_i^c = \text{softmax}([\text{score}^c(\mathbf{x}_i, \mathbf{x}_j) \forall j \leq i])$$

$$\text{head}_i^c = \sum_{j \leq i} \alpha_{i,j}^c \cdot \mathbf{v}_j^c \quad \mathbf{a}_i = (\text{head}^1 \oplus \text{head}^2 \dots \oplus \text{head}^h) \mathbf{W}^O$$

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

Multi-head attention



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**)

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

QK^T

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

$$\text{score}(\mathbf{x}_i, \mathbf{x}_j) = \frac{\mathbf{q}_i \mathbf{k}_j^T}{\sqrt{d^k}}$$

$$\mathbf{S} = \frac{\mathbf{QK}^T}{\sqrt{d^k}}$$

N

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

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

$$\mathbf{A} = \text{softmax} \left(\mathbb{M} \left(\frac{\mathbf{Q}\mathbf{K}^\top}{\sqrt{d^k}} \right) \right) \mathbf{V}$$

Masking out the future

- What is this mask function?
 \mathbf{QK}^\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!

$$\mathbf{A} = \text{softmax} \left(\mathbb{M} \left(\frac{\mathbf{QK}^\top}{\sqrt{d^k}} \right) \right) \mathbf{V}$$

Masking out the future

Add $-\infty$ to cells in upper triangle

The softmax will turn it to 0

$$\mathbf{A} = \text{softmax} \left(\mathbb{M} \left(\frac{\mathbf{QK}^T}{\sqrt{d^k}} \right) \right) \mathbf{V} \quad \mathbf{N}$$

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

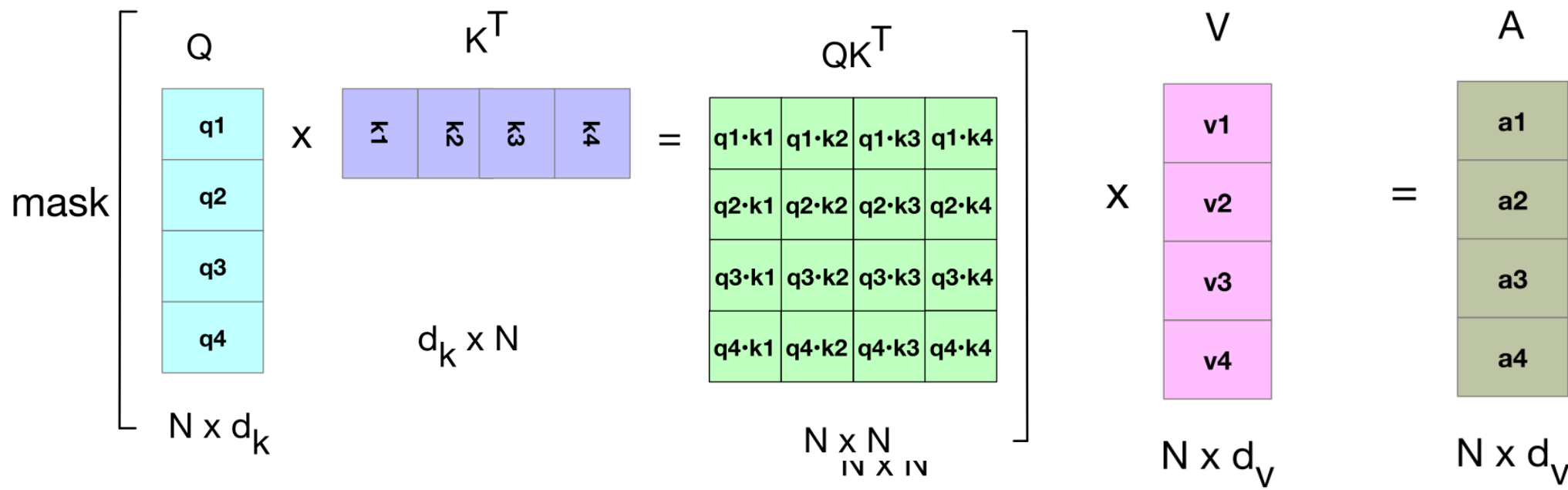
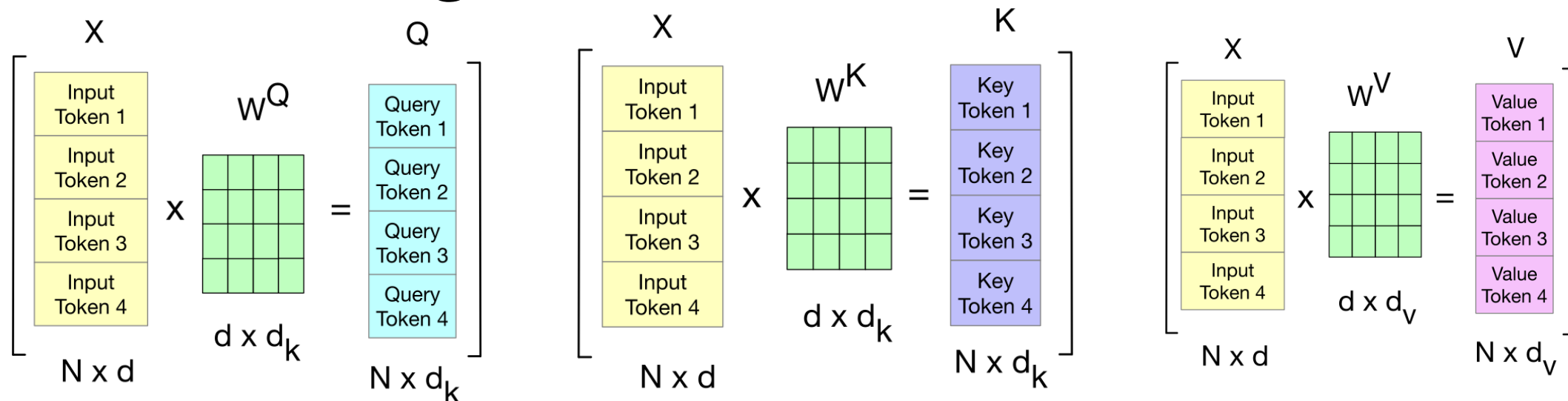
$$\mathbf{A} = \text{softmax} \left(\mathbb{M} \left(\frac{\mathbf{Q}\mathbf{K}^\top}{\sqrt{d^k}} \right) \right) \mathbf{V}$$

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

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

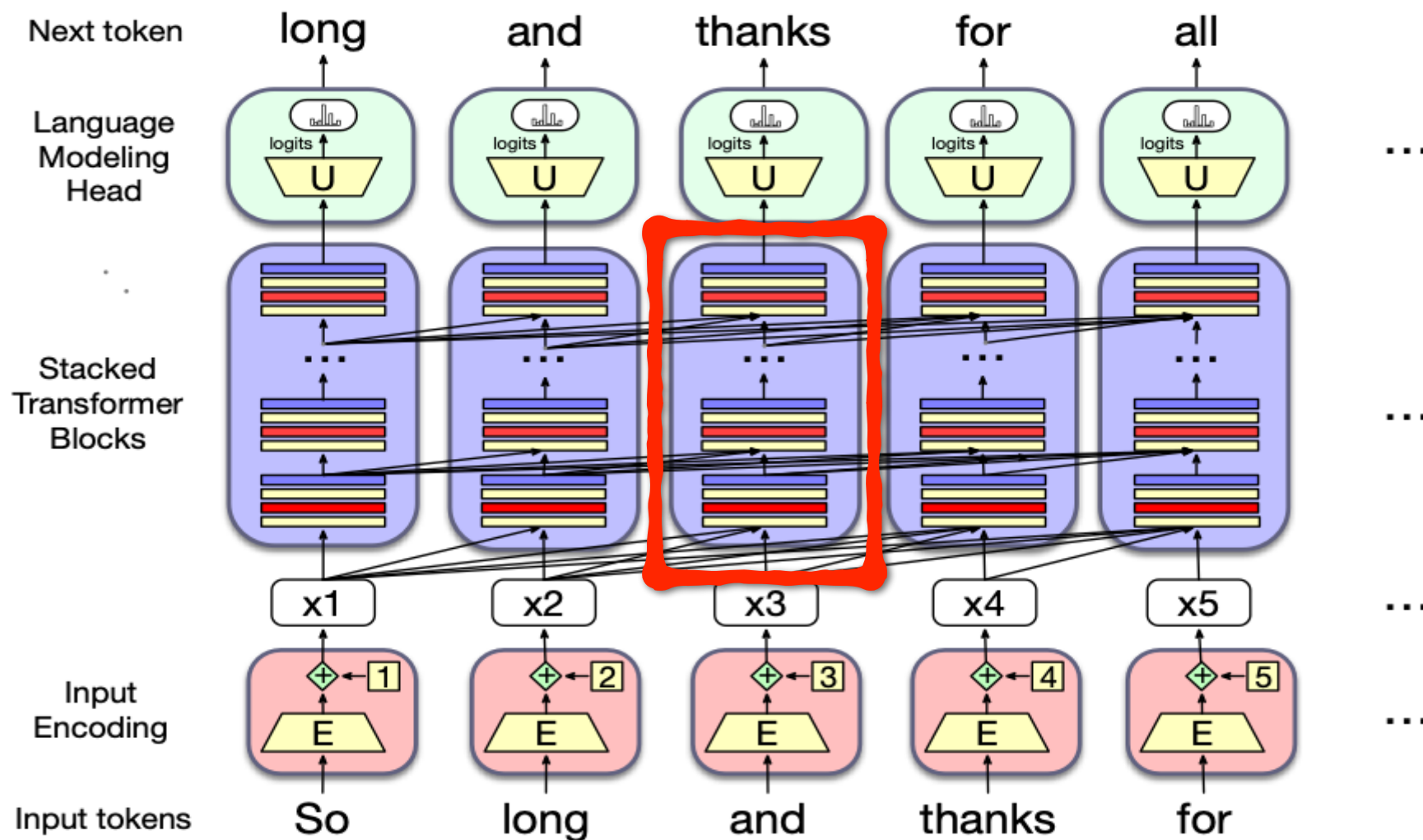
$$\mathbf{head}_i = \text{SelfAttention}(\mathbf{Q}^i, \mathbf{K}^i, \mathbf{V}^i) = \text{softmax}\left(\frac{\mathbf{Q}^i \mathbf{K}^{i\top}}{\sqrt{d_k}}\right) \mathbf{V}^i$$

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

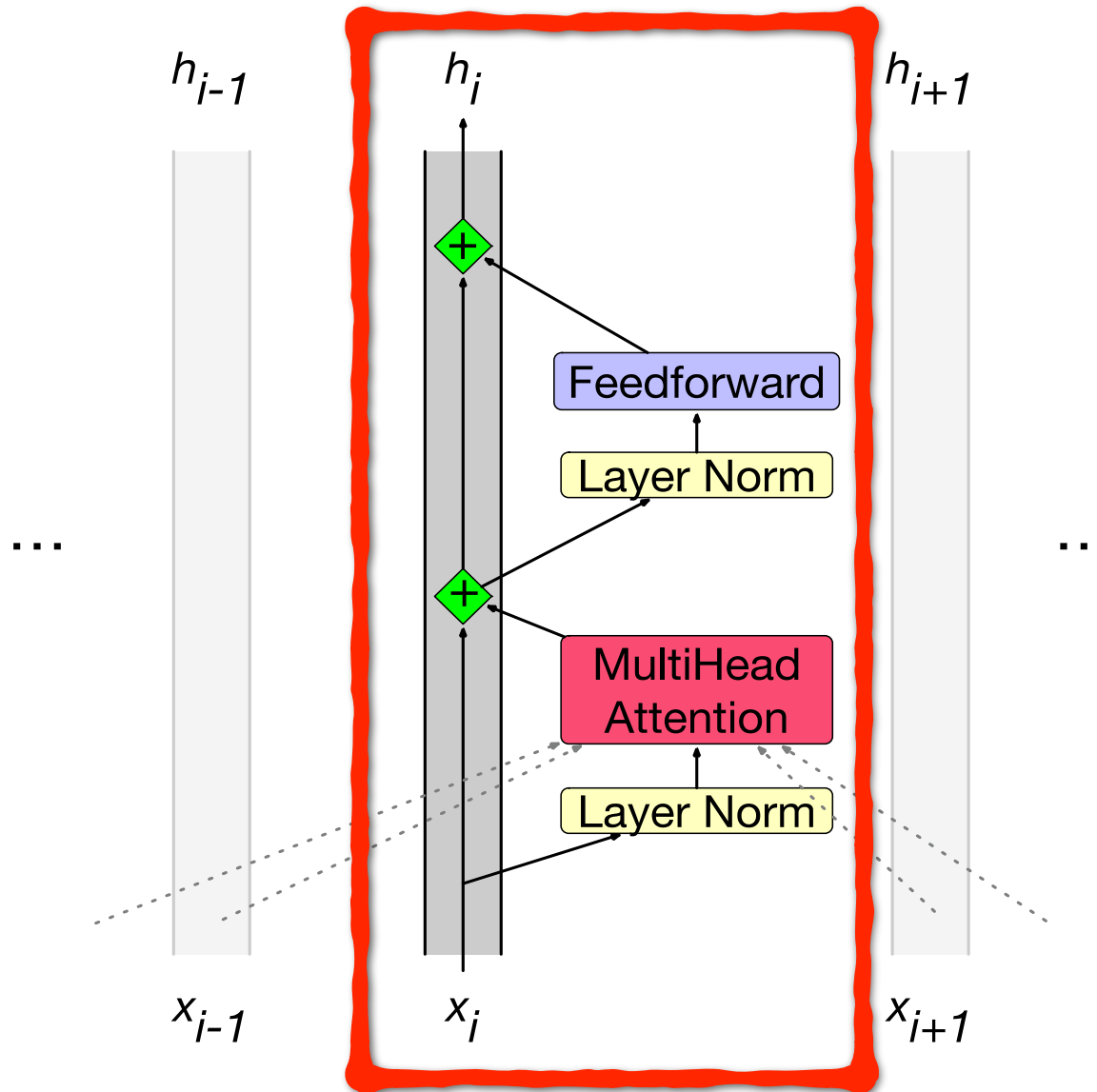


This is equivalent to running the attention heads in parallel and adding their results back to the residual stream
(Whiteboard)

Reminder: transformer architecture

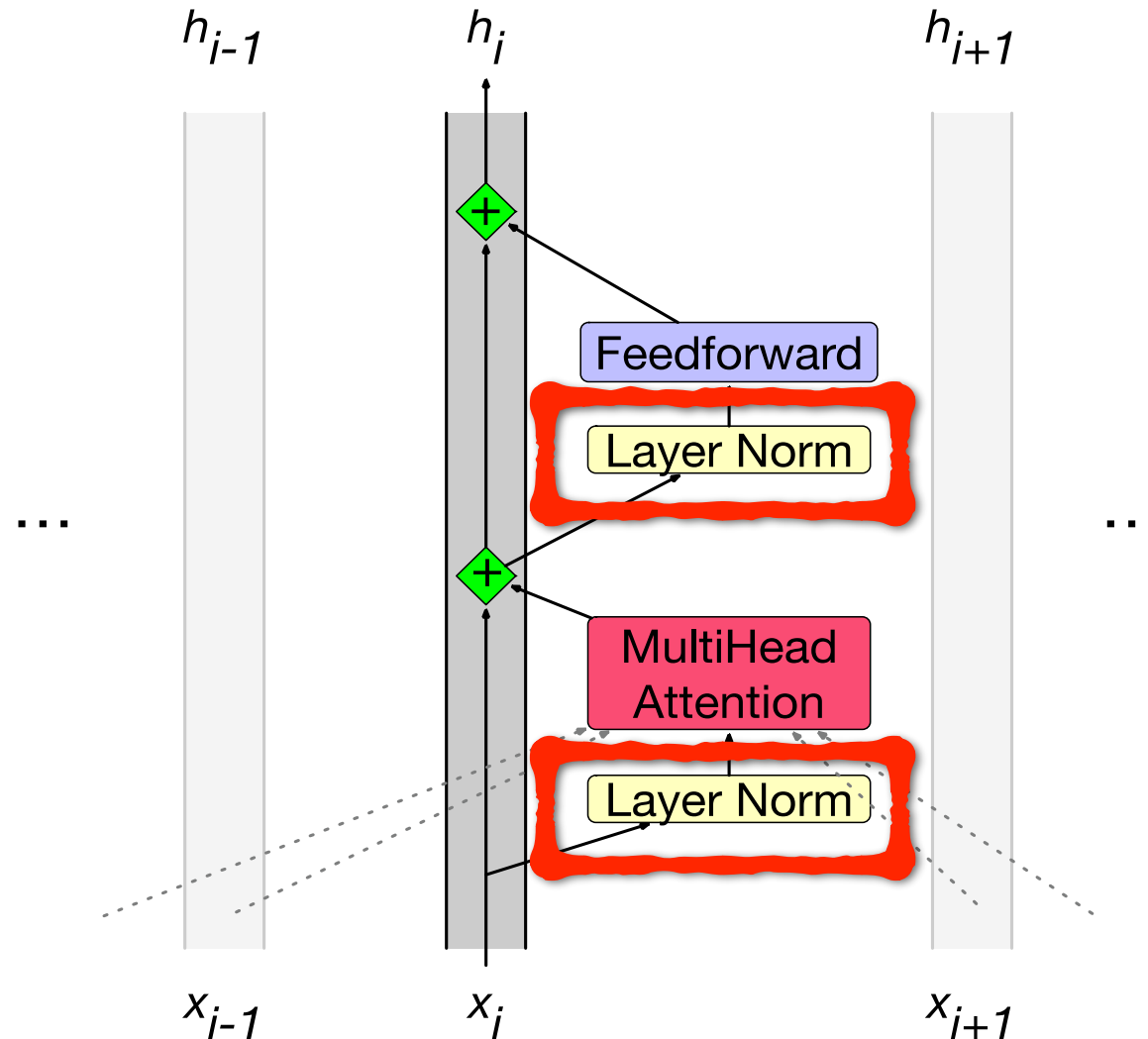


A single transformer block



Sublayers of the transformer block: Layer Norm

$$\text{LayerNorm}(\mathbf{x}_i) = \dots$$



Layer Norm

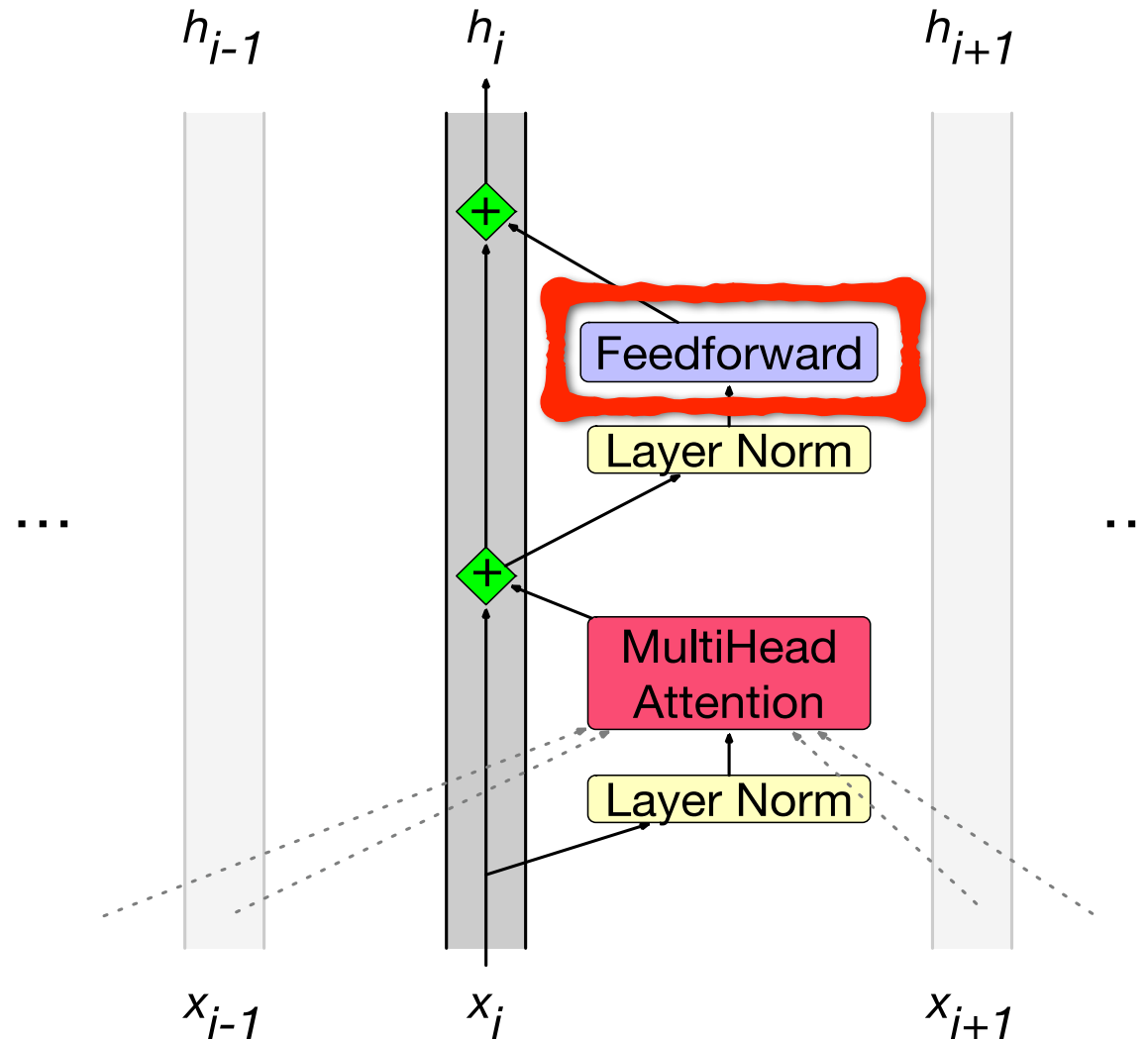
Layer norm is a variation of the z-score from statistics, applied to a single vector in a hidden layer

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

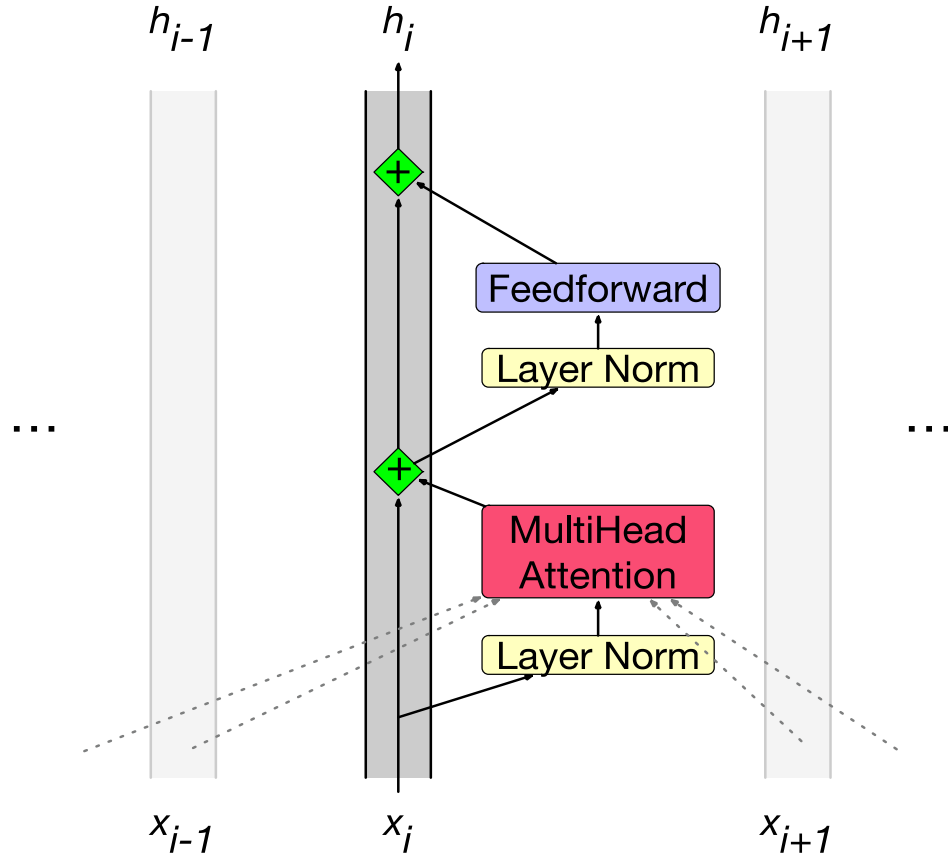
$$\text{LayerNorm}(\mathbf{x}) = \gamma \frac{(\mathbf{x} - \mu)}{\sigma} + \beta$$

Sublayers of the transformer block: FFN

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



Putting together a single transformer block



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

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

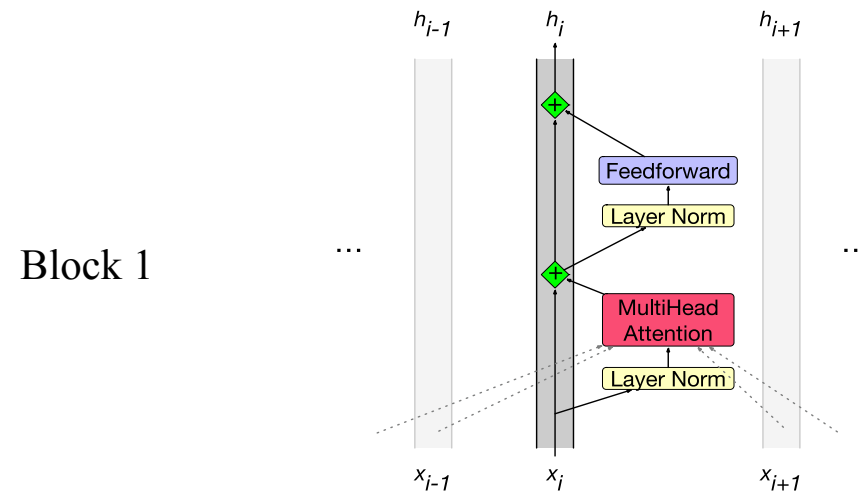
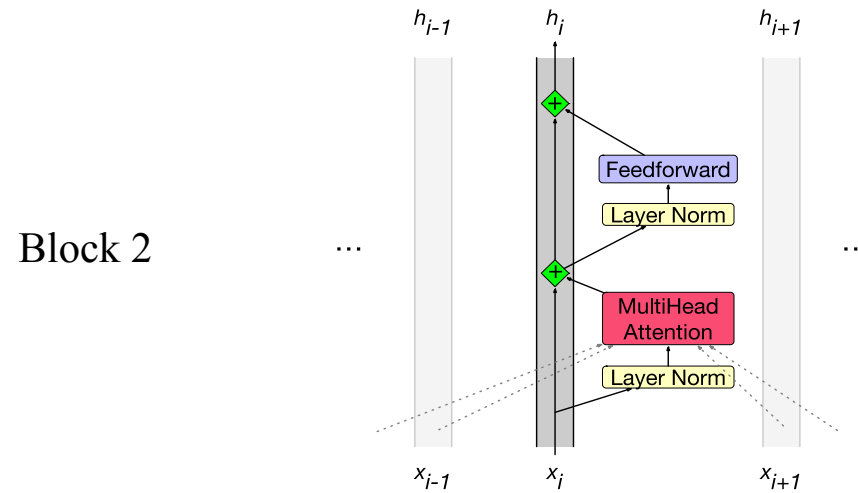
$$\mathbf{t}_i^3 = \mathbf{t}_i^2 + \mathbf{x}_i$$

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

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

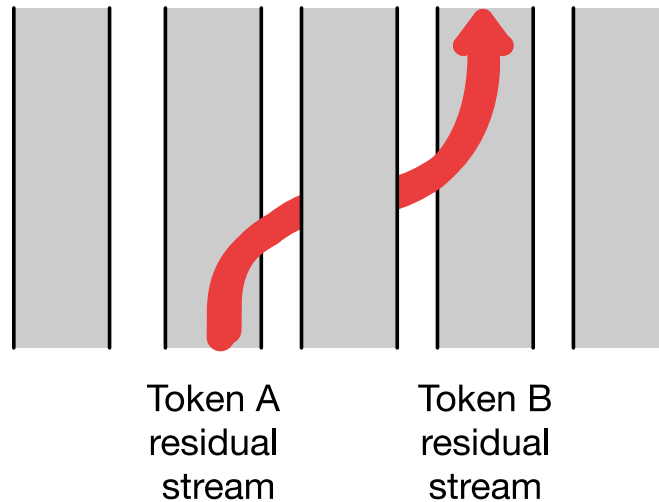
$$\mathbf{h}_i = \mathbf{t}_i^5 + \mathbf{t}_i^3$$

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

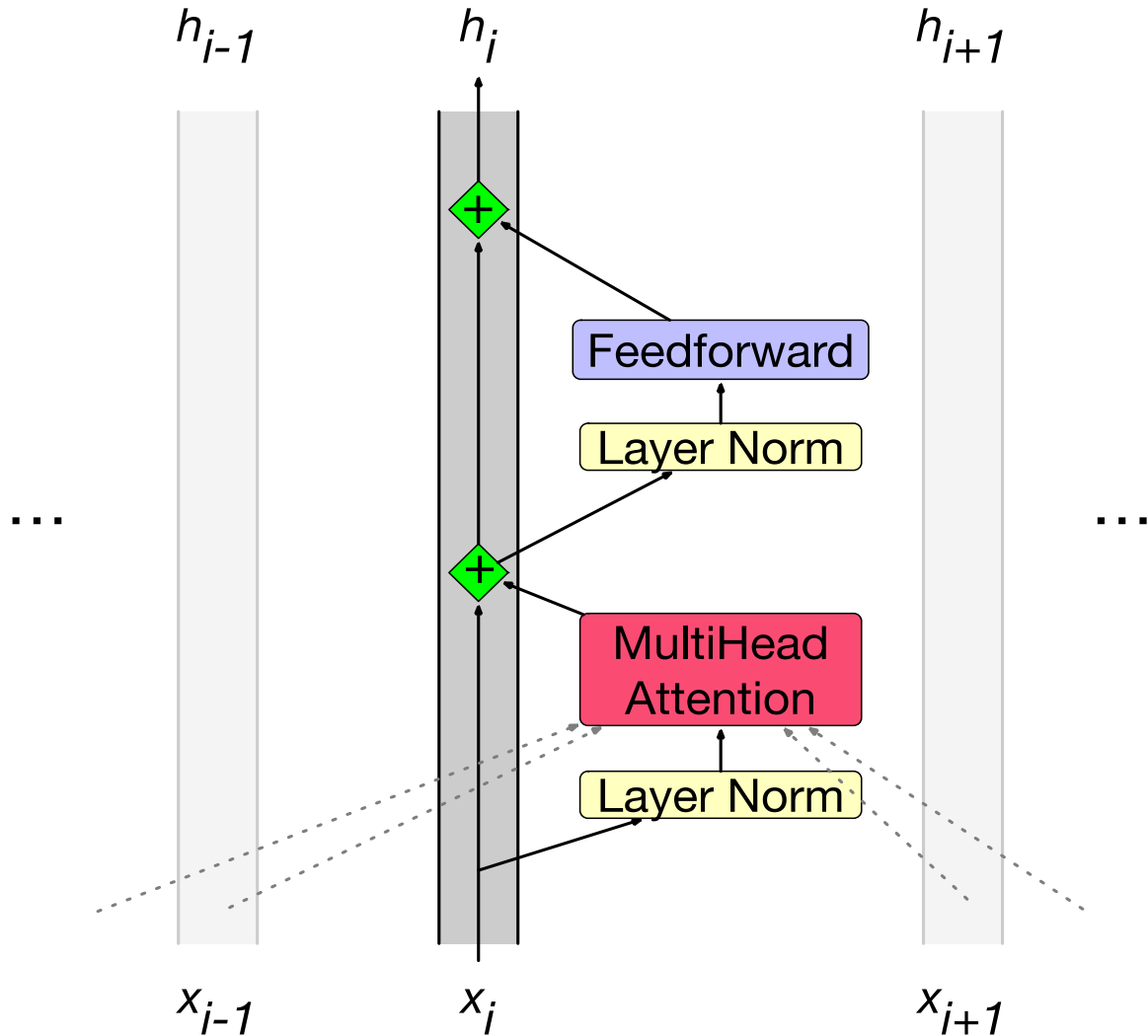


Residual streams and attention

- Notice that all parts of the transformer block apply to 1 residual stream 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



Residual stream view



- FFN and attention layers **read** from and **write** to the residual stream
- FFN layers have access to “one lane” only. Same computation applied on every “lane”
- Attention layers can read from from other “lanes” too
- \mathbf{x}_i is transformed into \mathbf{h}_i^L through a sequence of non-linear transformations

Putting together a single transformer block

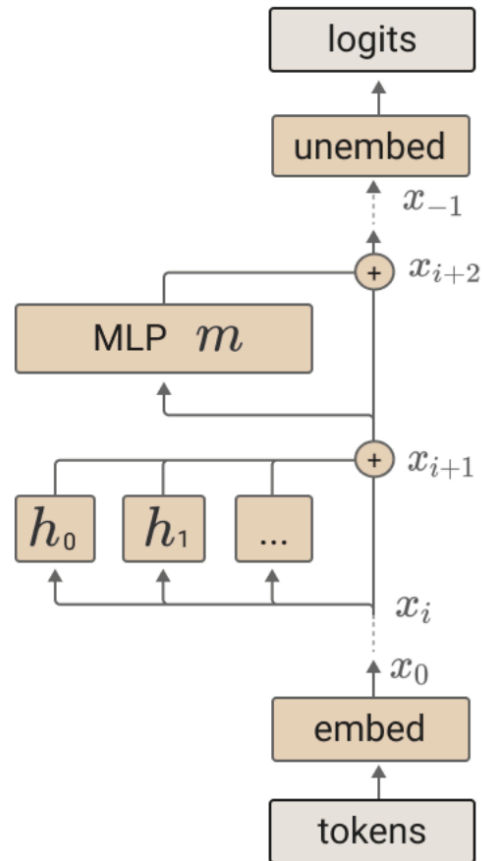
Single vector:

$$\begin{aligned}\mathbf{t}_i^1 &= \text{LayerNorm}(\mathbf{x}_i) \\ \mathbf{t}_i^2 &= \text{MultiHeadAttention}(\mathbf{t}_i^1, [\mathbf{t}_1^1, \dots, \mathbf{t}_N^1]) \\ \mathbf{t}_i^3 &= \mathbf{t}_i^2 + \mathbf{x}_i \\ \mathbf{t}_i^4 &= \text{LayerNorm}(\mathbf{t}_i^3) \\ \mathbf{t}_i^5 &= \text{FFN}(\mathbf{t}_i^4) \\ \mathbf{h}_i &= \mathbf{t}_i^5 + \mathbf{t}_i^3\end{aligned}$$

Matrix of inputs:

$$\begin{aligned}\mathbf{T}^1 &= \text{LayerNorm}(\mathbf{X}) \\ \mathbf{T}^2 &= \text{MultiHeadAttention}(\mathbf{T}^1) \\ \mathbf{T}^3 &= \mathbf{T}^2 + \mathbf{X} \\ \mathbf{T}^4 &= \text{LayerNorm}(\mathbf{T}^3) \\ \mathbf{T}^5 &= \text{FFN}(\mathbf{T}^4) \\ \mathbf{H} &= \mathbf{T}^5 + \mathbf{T}^3\end{aligned}$$

Residual stream view



The final logits are produced by applying the unembedding.

$$T(t) = W_U x_{-1}$$

An MLP layer, m , is run and added to the residual stream.

$$x_{i+2} = x_{i+1} + m(x_{i+1})$$

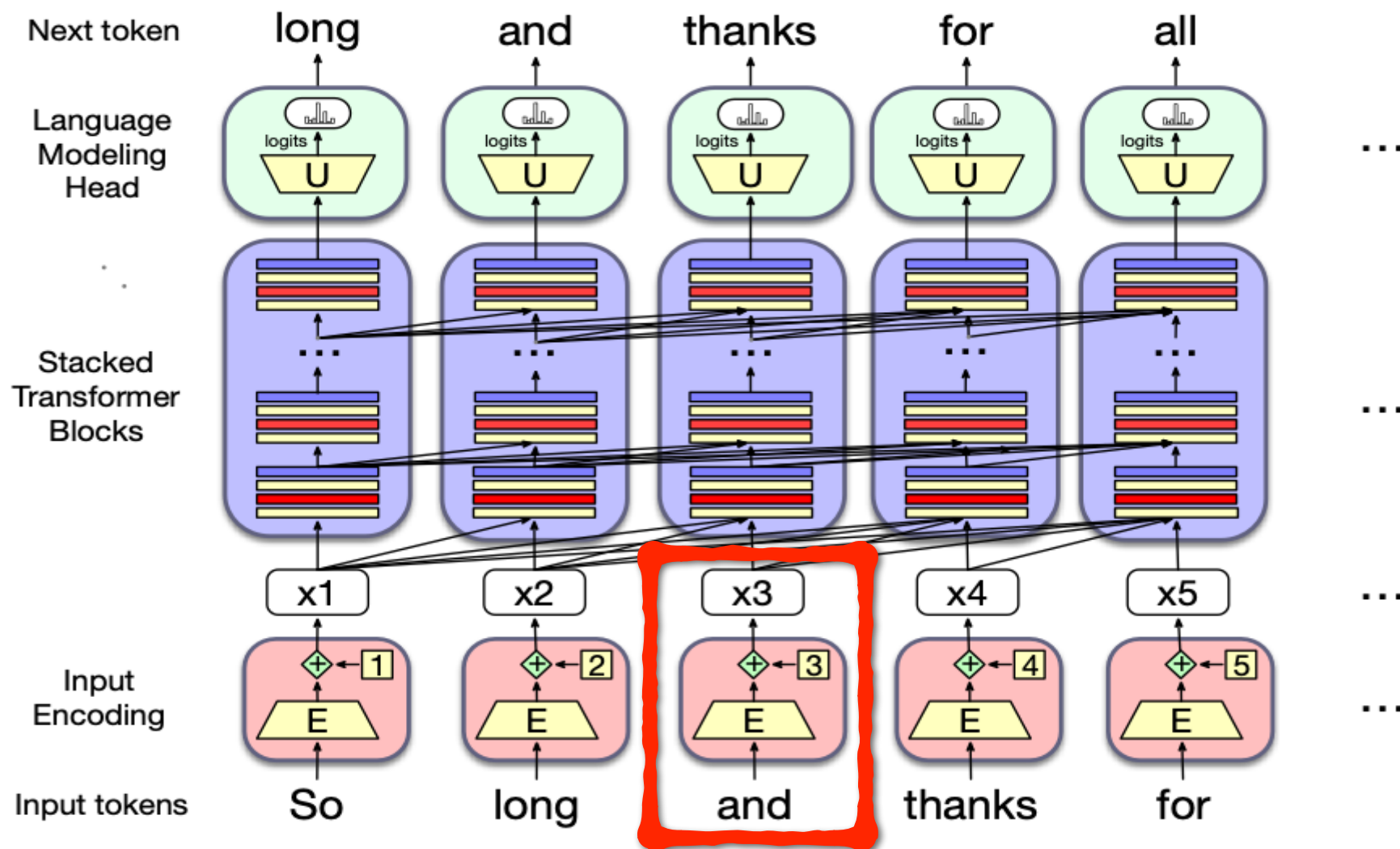
Each attention head, h , is run and added to the residual stream.

$$x_{i+1} = x_i + \sum_{h \in H_i} h(x_i)$$

Token embedding.

$$x_0 = W_E t$$

Reminder: transformer architecture

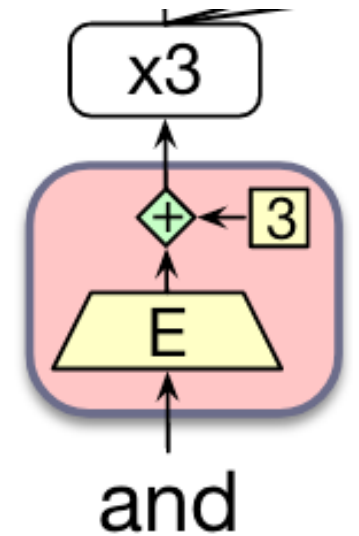


Token and Position Embeddings

The matrix \mathbf{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 \mathbf{E} has shape $|\mathcal{V}| \times d$.

- One row for each of the $|\mathcal{V}|$ 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

input_ids = [5, 4000, 10532, 2224]

2. Select the corresponding rows from \mathbf{E} , each row an embedding
- (row 5, row 4000, row 10532, row 2224).

Position Embeddings

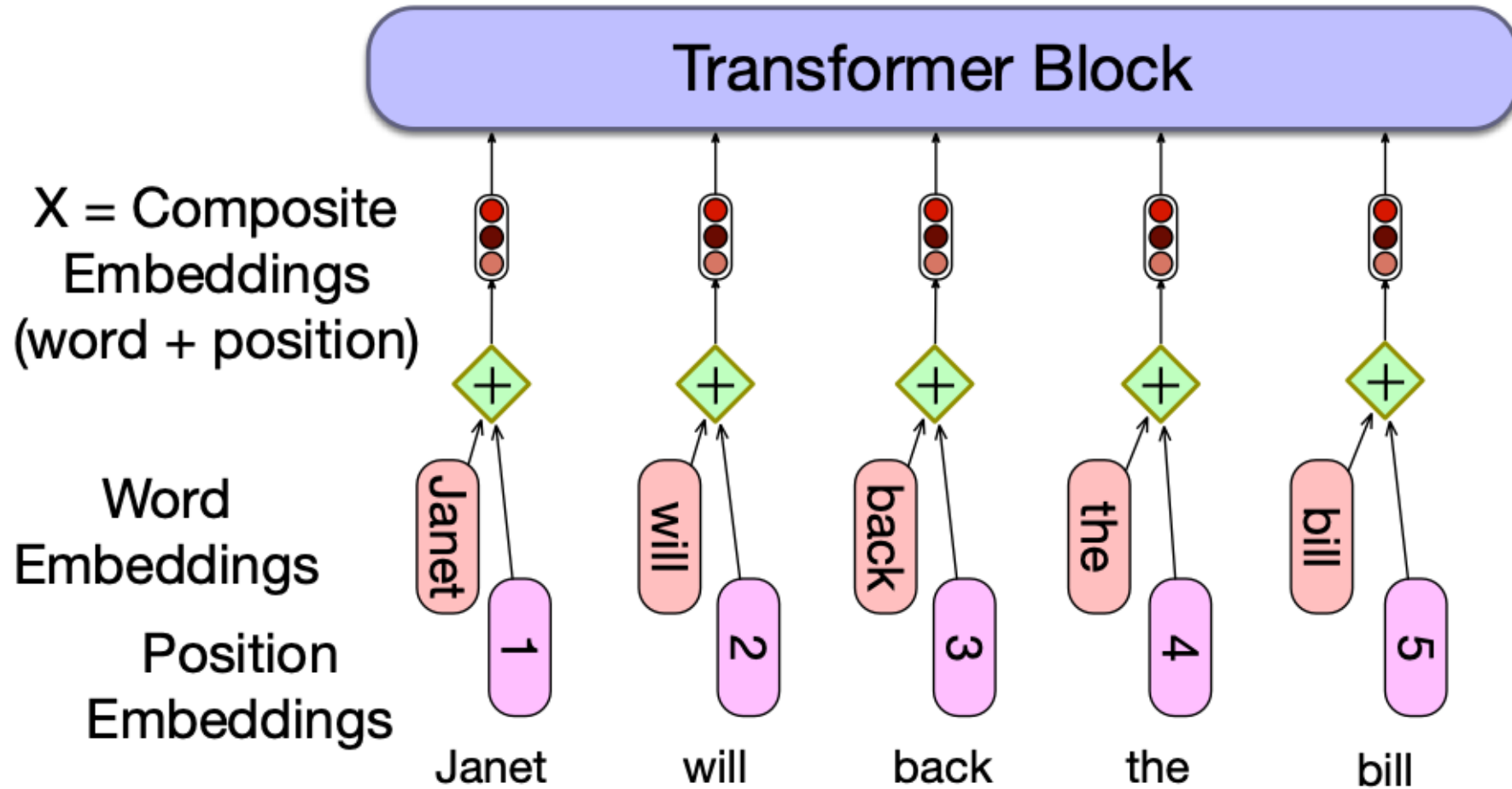
There are many methods, but we'll just describe the simplest: absolute position.

Goal: learn a position embedding matrix \mathbf{E}_{pos} of shape $N \times d$.

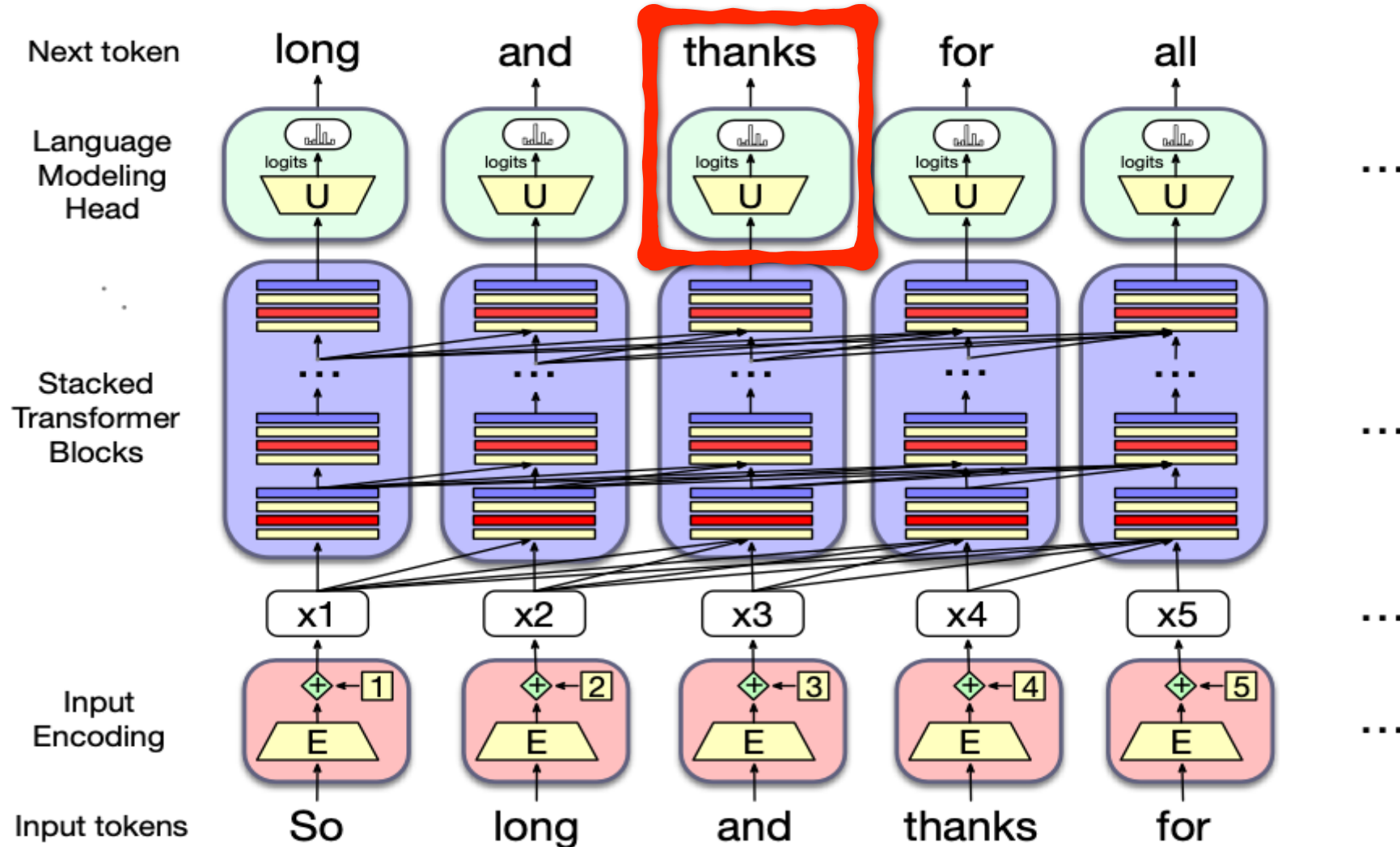
Start with randomly initialized embeddings

- 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_i is just the sum of word and position embeddings



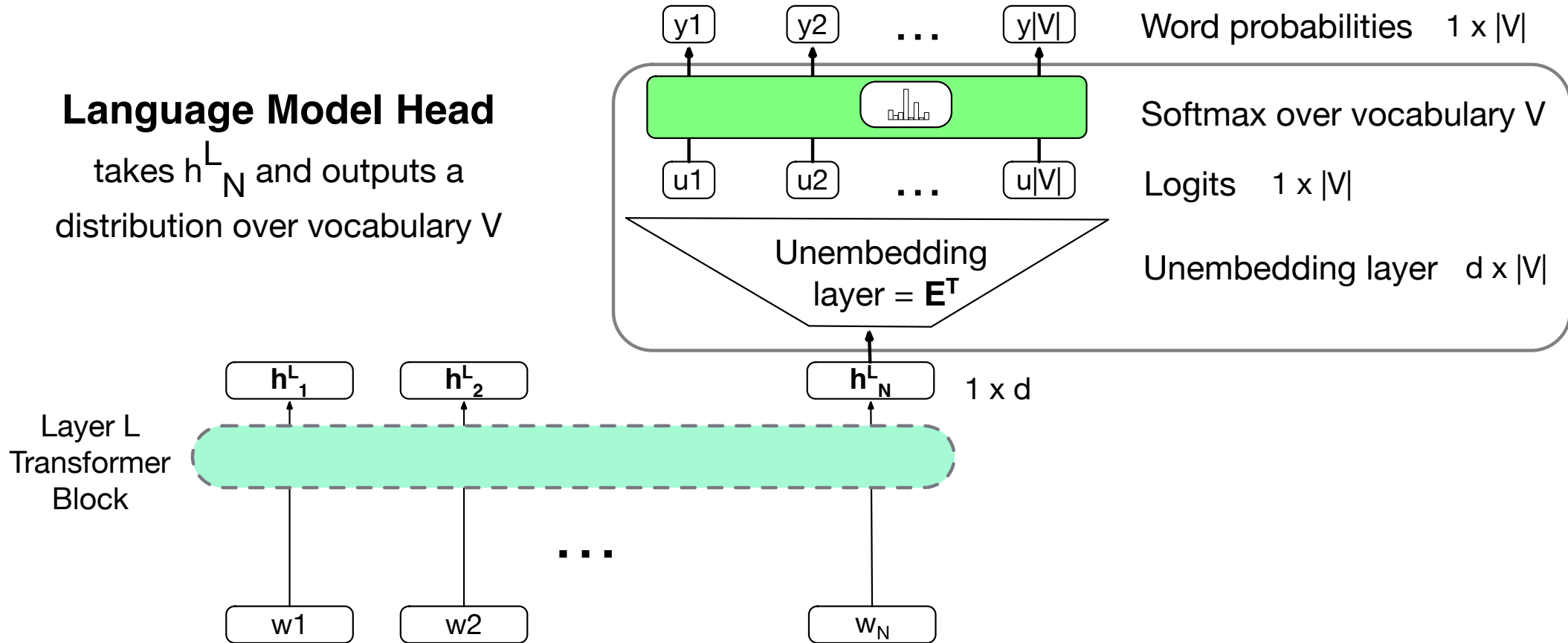
Reminder: transformer architecture



Language modeling head

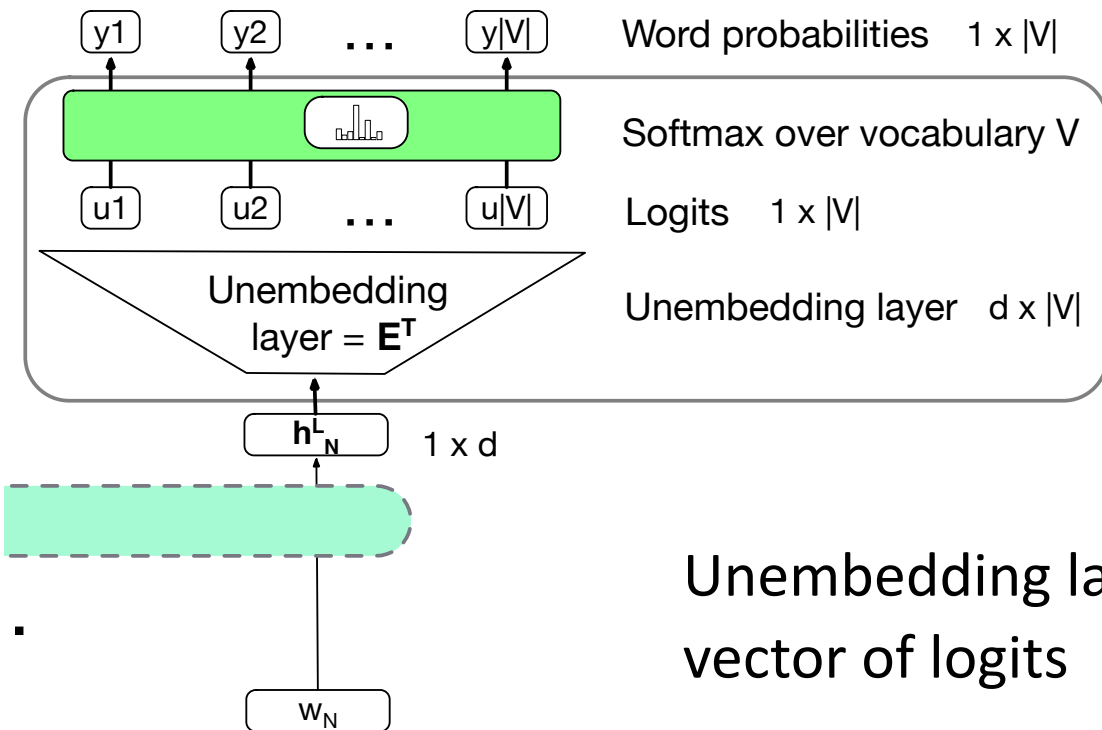
Language Model Head

takes h_N^L and outputs a distribution over vocabulary V



Language modeling head

Unembedding layer: linear layer projects from \mathbf{h}_N^L (shape $1 \times d$) to logit vector



Why "unembedding"? **Tied** to \mathbf{E}^T

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

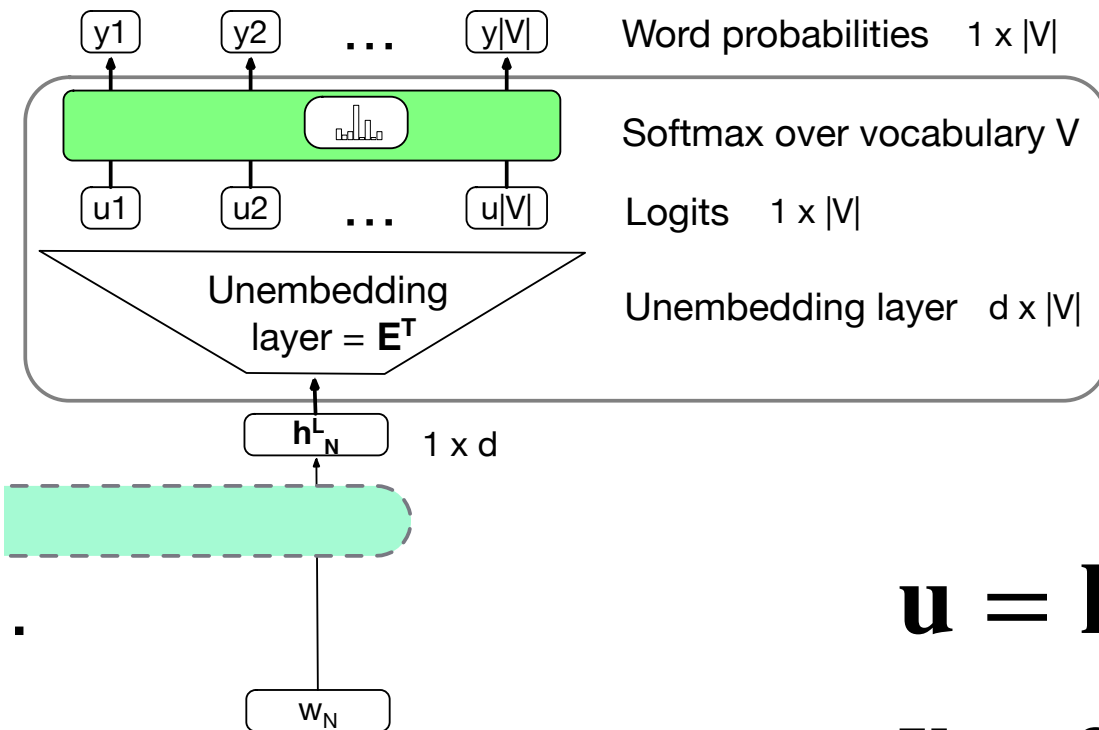
Unembedding layer maps from an embedding to a $1 \times |\mathcal{V}|$ vector of logits

Language modeling head

Logits, the score vector \mathbf{u}

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

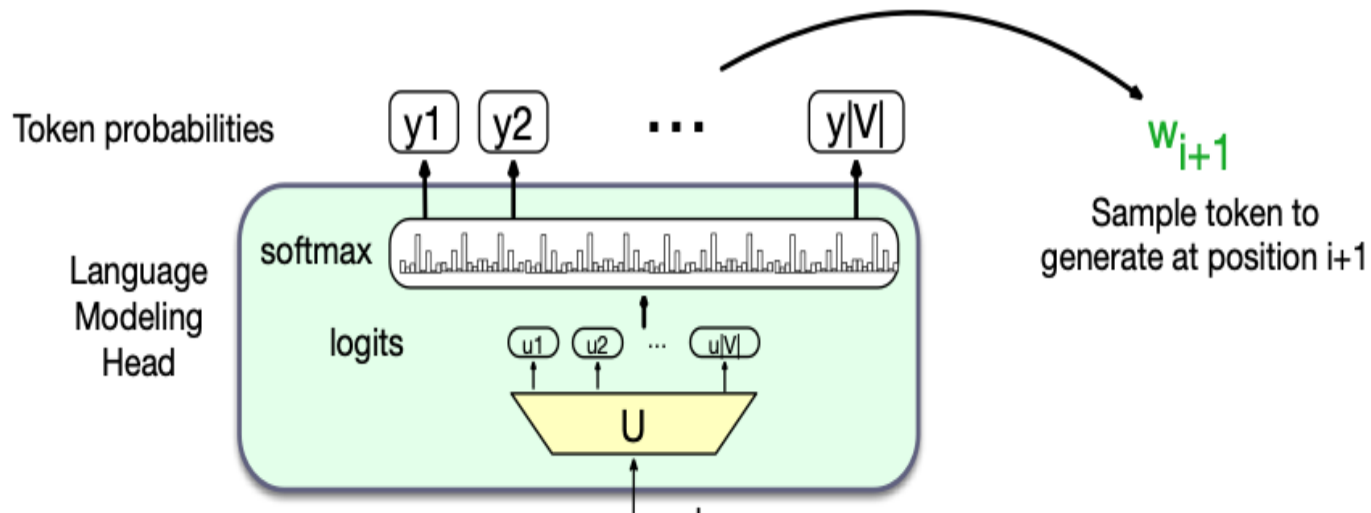
Softmax turns the logits into probabilities over vocabulary. Shape $1 \times |\mathcal{V}|$.



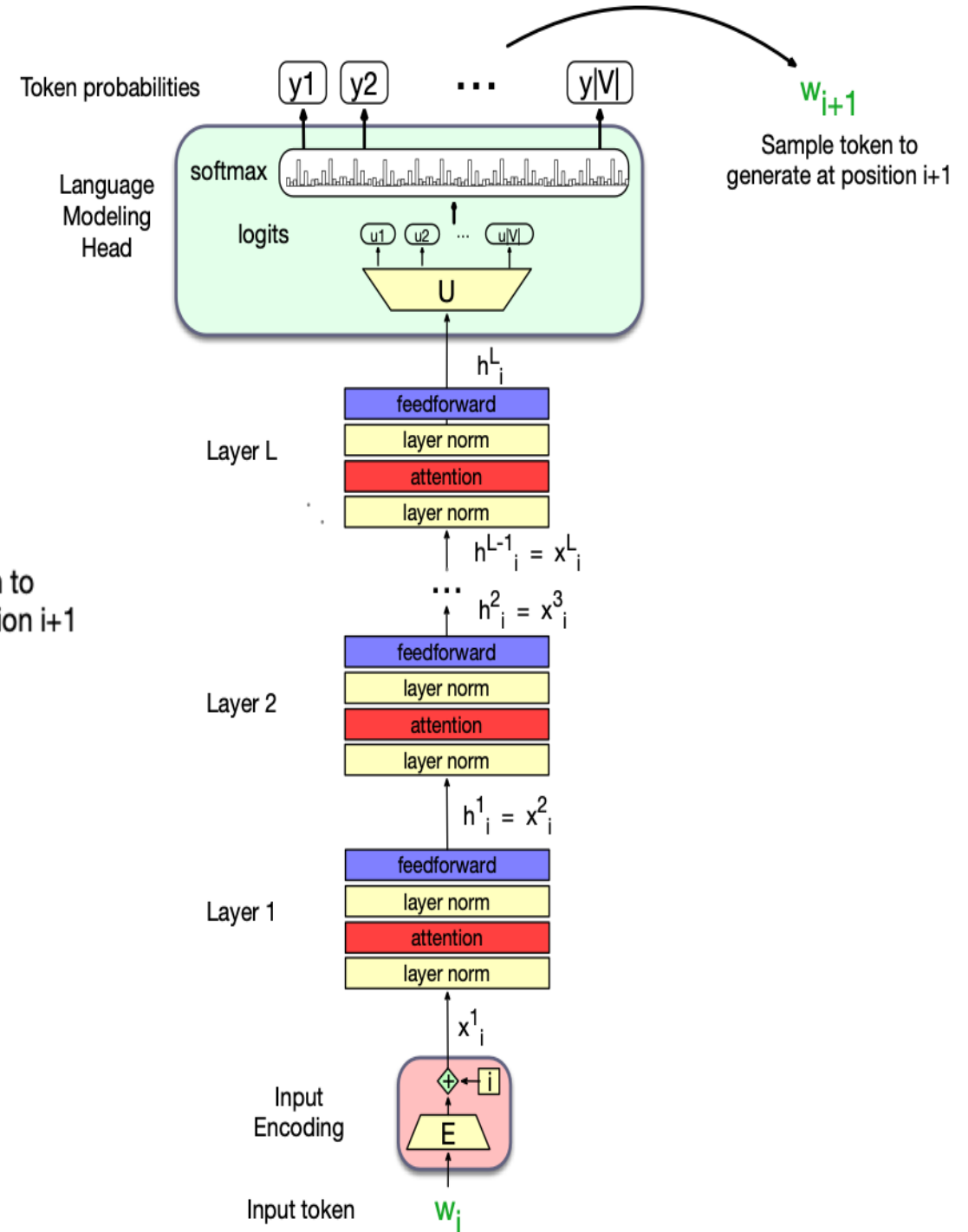
$$\mathbf{u} = \mathbf{h}_N^L \mathbf{E}^T$$

$$\mathbf{y} = \text{softmax}(\mathbf{u})$$

The final transformer model



~ GPT



LM loss

The LM head takes output of final transformer layer L , multiplies it by unembedding layer and turns into probabilities:

$$\mathbf{u}_i = E\mathbf{h}_i^L \quad \mathbf{y}_i = \text{softmax}(\mathbf{u}_i)$$

The loss is the probability of the next word, given output \mathbf{h}_i^L :

$$\mathcal{L}_{LM}(x_i) = -\log P(x_{i+1} \mid \mathbf{h}_i^L) = -\log \hat{\mathbf{y}}[\mathbf{x}_{i+1}]$$

We get the gradients by taking the average of this loss over the batch

$$\mathcal{L}_{LM} = -\frac{1}{|\mathcal{B}|} \sum_{s \in \mathcal{B}} \frac{1}{|s|} \sum_{i \in s} \log P(x_{i+1} \mid \mathbf{h}_i^L)$$

Language Models are Unsupervised Multitask Learners

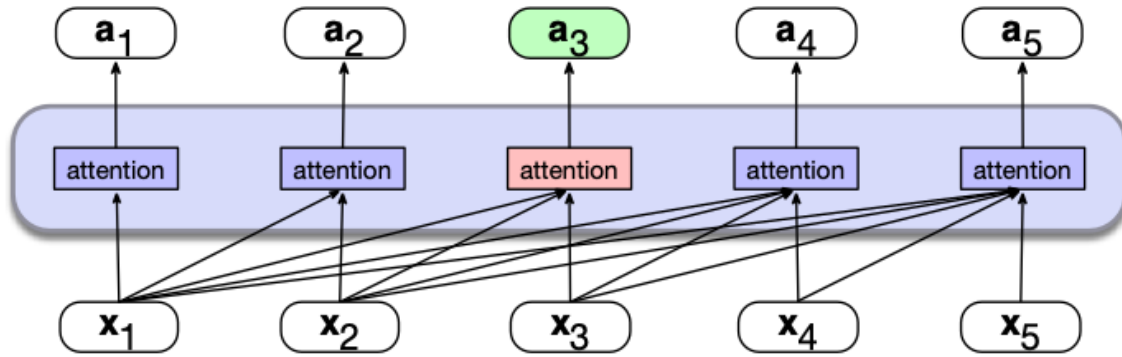
GPT-2 ([Radford et al., 2019](#))

- Trained on ~40GB of text crawled from the internet
- Input context window $N=1024$ tokens, and model dimensionality $\{d=768, d=1024, d=1280, d=1600\}$
- $\{L=12, L=24, L=36, L=48\}$ layers of transformer blocks
- *The resulting models have around $\{117M, 335M, 762M, 1542M\}$ parameters*

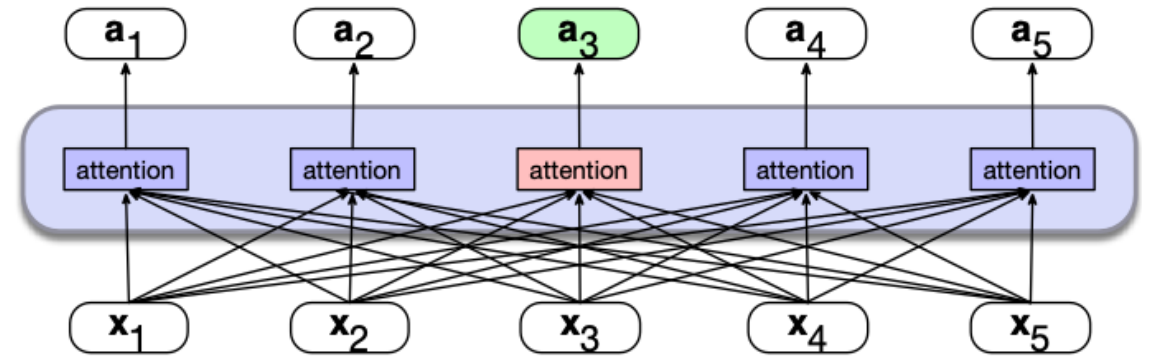
Masked Language Modeling

- We've seen autoregressive (causal, left-to-right) LMs.
- But what about tasks for which we want to peak at future tokens?
 - Especially true for tasks where we map each input token to an output token
- **Bidirectional encoders** use **unmasked self-attention** to
 - map sequences of input embeddings $\mathbf{x}_1, \dots, \mathbf{x}_n$
 - to sequences of output embeddings of the same length $\mathbf{h}_1, \dots, \mathbf{h}_n$
 - where the output vectors have been contextualized using information from the entire input sequence.

Bidirectional Self-Attention



a) A causal self-attention layer



b) A bidirectional self-attention layer

We just remove the mask

Casual self-attention

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

$$\mathbf{A} = \text{softmax} \left(\mathbb{M} \left(\frac{\mathbf{QK}^T}{\sqrt{d^k}} \right) \right)$$

Bidirectional self-attention

N	$q1 \cdot k1$	$q1 \cdot k2$	$q1 \cdot k3$	$q1 \cdot k4$
	$q2 \cdot k1$	$q2 \cdot k2$	$q2 \cdot k3$	$q2 \cdot k4$
	$q3 \cdot k1$	$q3 \cdot k2$	$q3 \cdot k3$	$q3 \cdot k4$
	$q4 \cdot k1$	$q4 \cdot k2$	$q4 \cdot k3$	$q4 \cdot k4$
N				

$$\mathbf{A} = \text{softmax} \left(\frac{\mathbf{QK}^T}{\sqrt{d^k}} \right)$$

Masked training intuition

- For **left-to-right (causal; decoder-only) LMs**, the model tries to predict the last word from prior words:

The water of Walden Pond is so beautifully _____

- And we train it to improve its predictions.

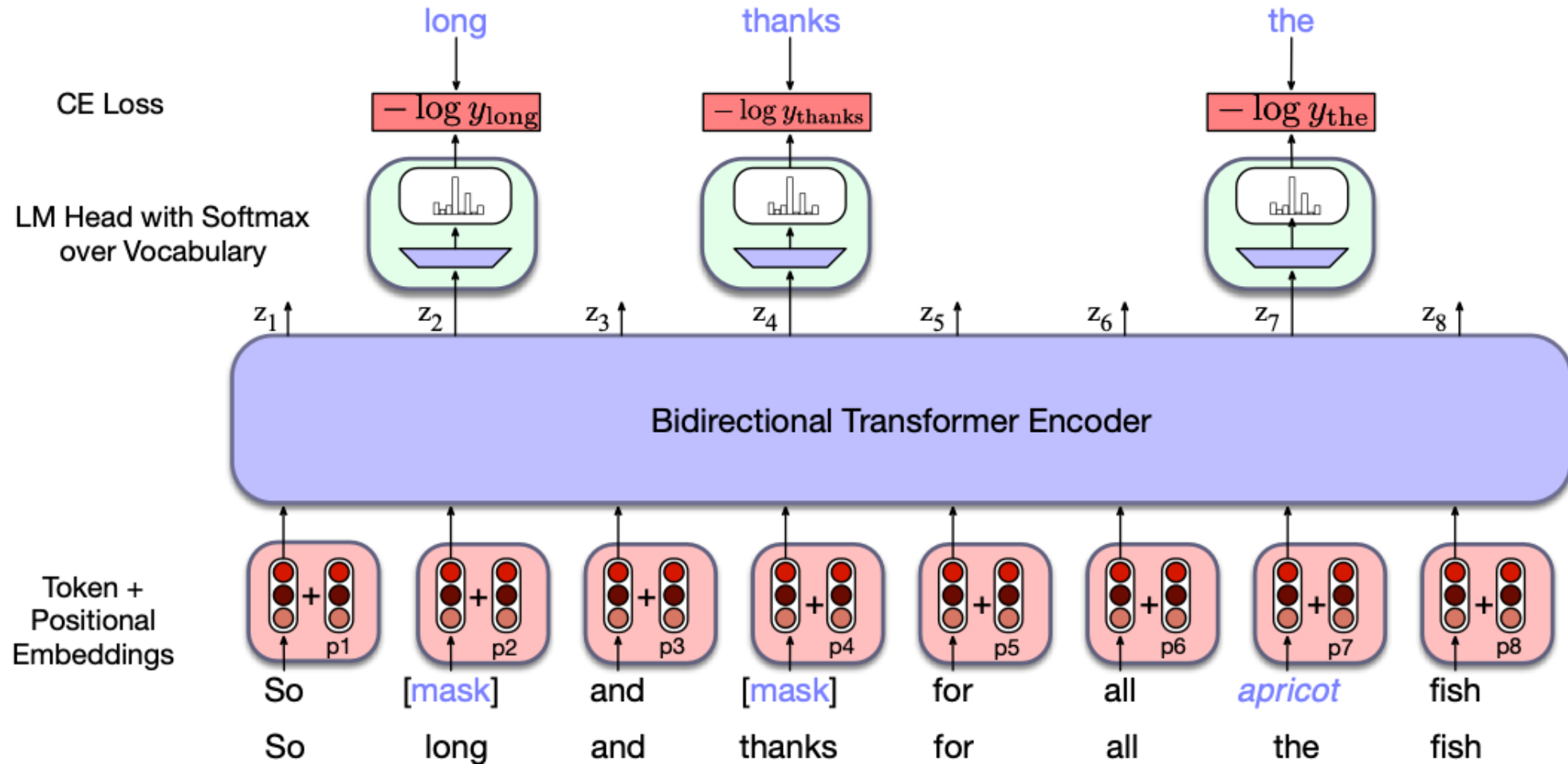
- For **bidirectional masked LMs**, the model tries to predict one or more missing words from all the rest of the words:

blue The _____ of Walden Pond _____ so beautifully

- The model generates a probability distribution over the vocabulary for each missing token
- We use the cross-entropy loss from each of the model's predictions to drive the learning process.

Bidirectional Transformer

~ BERT



MLM training in BERT

15% of the tokens are randomly chosen to be part of the masking

Example: "Lunch was **delicious**", if delicious was randomly chosen:

Three possibilities:

1. 80%: Token is replaced with special token [MASK]

Lunch was **delicious** -> Lunch was **[MASK]**

2. 10%: Token is replaced with a random token (sampled from unigram prob)

Lunch was **delicious** -> Lunch was **gasp**

3. 10%: Token is unchanged

Lunch was **delicious** -> Lunch was **delicious**

MLM loss

The LM head takes output of final transformer layer L , multiplies it by unembedding layer and turns into probabilities:

$$\mathbf{u}_i = E\mathbf{h}_i^L \qquad \mathbf{y}_i = \text{softmax}(\mathbf{u}_i)$$

E.g., for the x_i corresponding to "long", the loss is the probability of the correct word *long*, given output \mathbf{h}_i^L):

$$\mathcal{L}_{\text{MLM}}(x_i) = -\log P(x_i \mid \mathbf{h}_i^L)$$

We get the gradients by taking the average of this loss over the batch

$$\mathcal{L}_{\text{MLM}} = -\frac{1}{|\mathcal{B}|} \sum_{s \in \mathcal{B}} \frac{1}{|\mathcal{M}_s|} \sum_{i \in \mathcal{M}_s} \log P(x_i \mid \mathbf{h}_i^L)$$

Bidirectional Encoder Representations from Transformers

BERT (Devlin et al., 2019)

- 30,000 English-only tokens (WordPiece tokenizer)
- Input context window $N=512$ tokens, and model dimensionality $d=768$
- $L=12$ layers of transformer blocks, each with $A=12$ (bidirectional) multihead-attention layers.
- The resulting model has about 100M parameters.

XLM-RoBERTa (Conneau et al., 2020)

- 250,000 multilingual tokens (SentencePiece Unigram LM tokenizer)
- Input context window $N=512$ tokens, model dimensionality $d=1024$
- $L=24$ layers of transformer blocks, with $A=16$ multihead attention layers each
- The resulting model has about 550M parameters.

[15 minute break]

Implementing the Transformer!

Team up!

Open exercises/week 8 in your course folder and start writing/running code!