Lecture 8:
Sequence-to-Sequence Model (conts.) & Transformers

Instructor: Xiang Ren
USC CSCI 444 NLP
2026 Spring

Slides mostly adapted from Dan Jurafsky, some from Mohit Iyyer

Logistics / Announcements

- Project Proposal due today!
- HW1 graded by 2/18

Feb 11	Recurrent Neural Nets	J&M, Chap 13;	Project Proposal Due
Feb 16	Presidents Day		
Feb 18	Seq2Seq and Attention	J&M, Chap 8;	
Feb 23	Transformers - Building Blocks	J&M, Chap 8;	
Feb 25	PyTorch for Transformers		
Mar 2	Transformer Language Models	J&M Chap 8;	
Mar 4	Tokenization	J&M, Chap 2.5;	HW2 Due

Recap

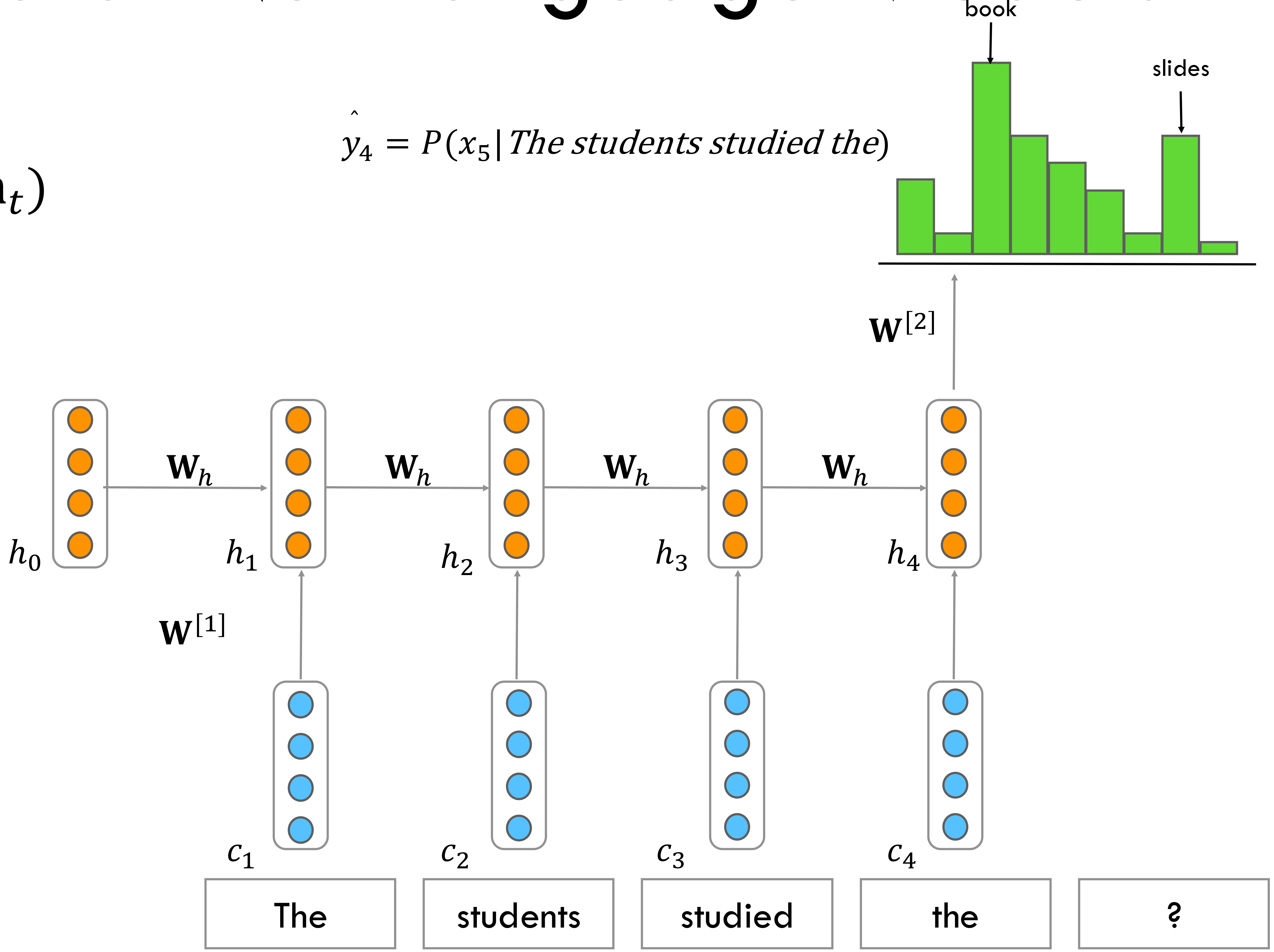
Recurrent Neural Net Language Models

Output layer: $\hat{\mathbf{y}}_t = softmax(\mathbf{W}^{[2]}\mathbf{h}_t)$

Hidden layer: $\mathbf{h}_t = g(\mathbf{W}_h\mathbf{h}_{t-1} + \mathbf{W}^{[1]}\mathbf{c}_t)$

Initial hidden state: $\mathbf{h}_0$

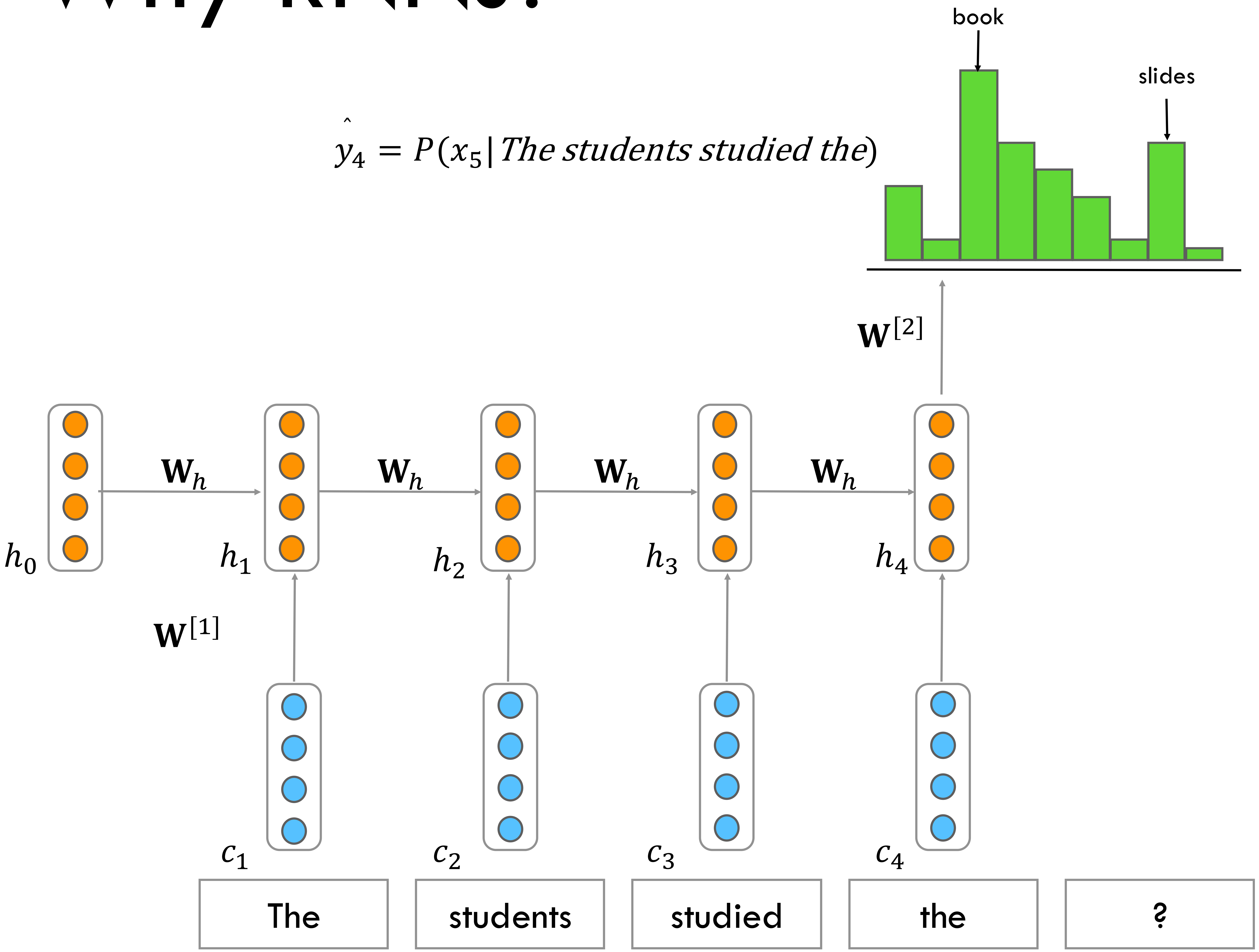
Word Embeddings, $\mathbf{c}_i$



Why RNNs?

RNN Advantages:

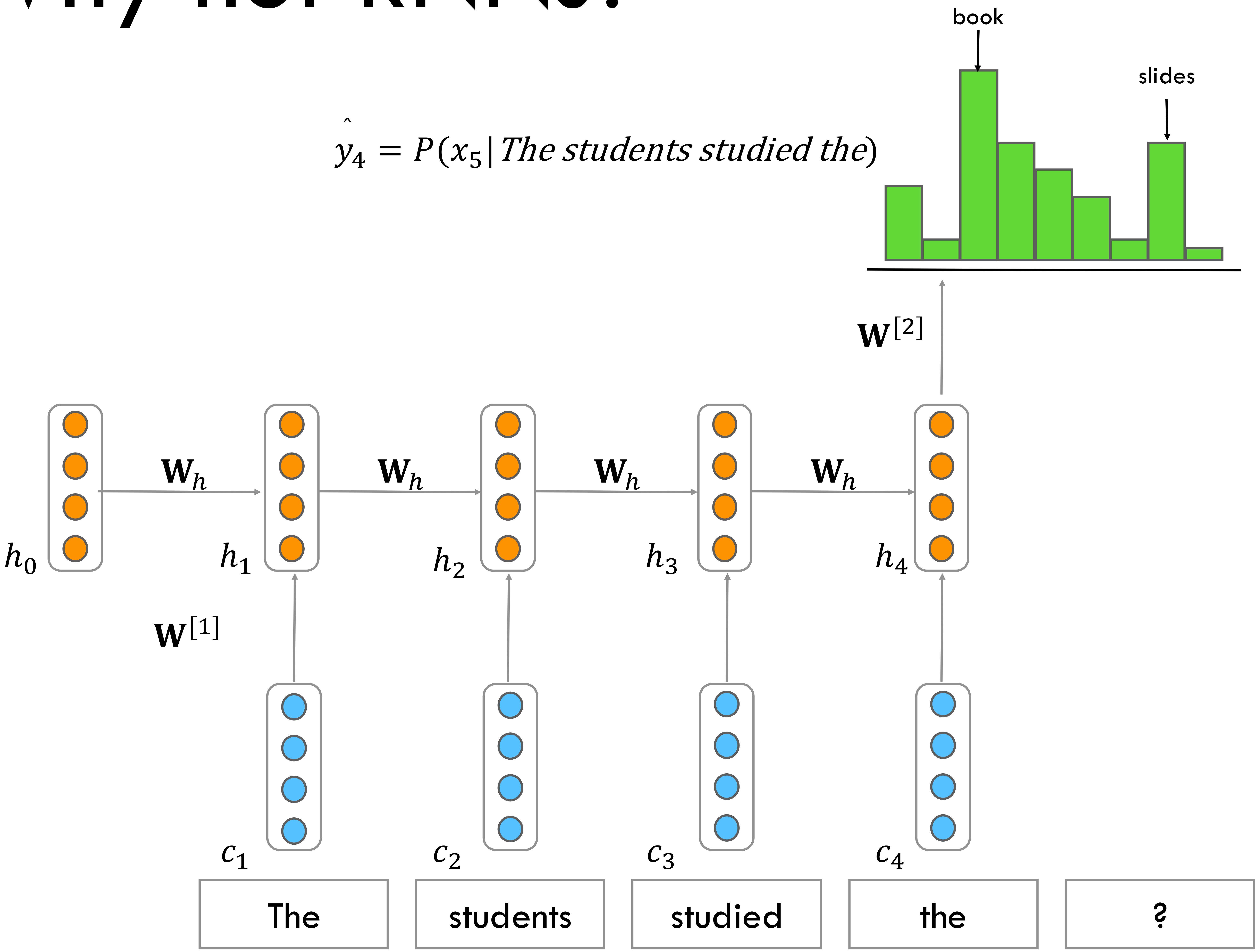
- Can process any length input
- Model size doesn't increase for longer input
- Computation for step t can (in theory) use information from many steps back
- Weights $\mathbf{W}^{[1]}$ are shared (tied) across timesteps $\rightarrow$ Condition the neural network on all previous words



Why not RNNs?

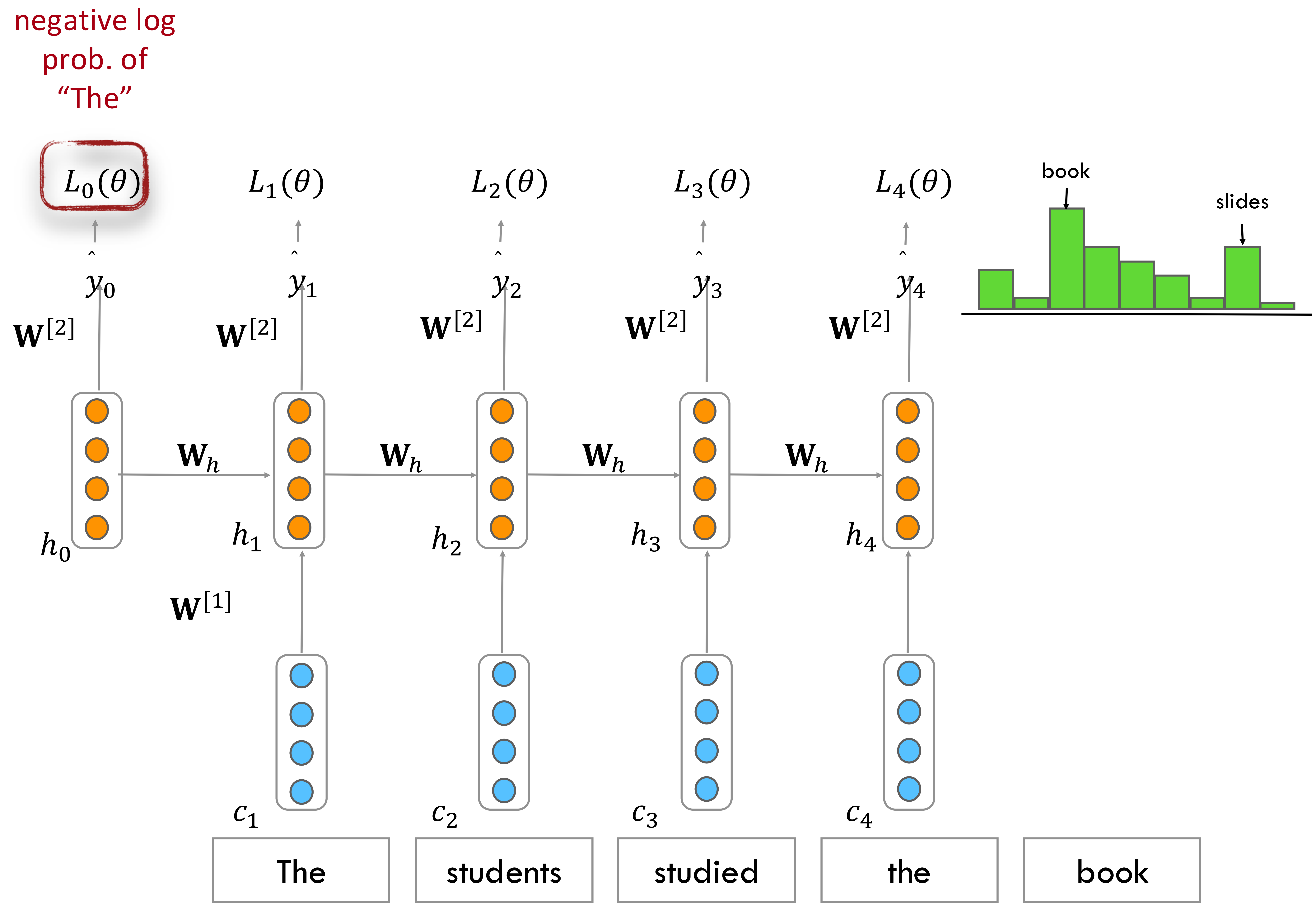
RNN Disadvantages:

- Recurrent computation is slow
- In practice, difficult to access information from many steps back



Training RNNLMs

Loss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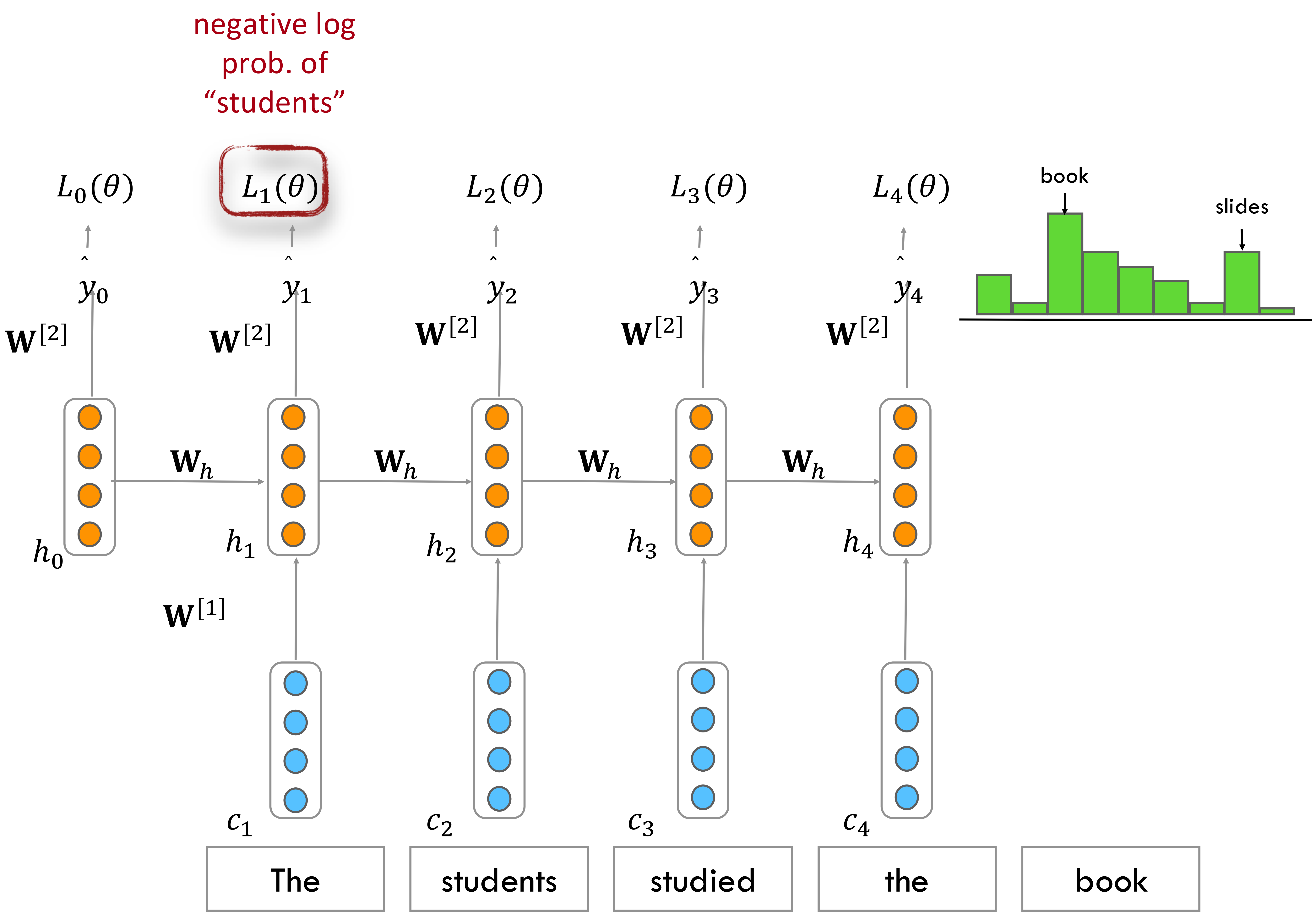
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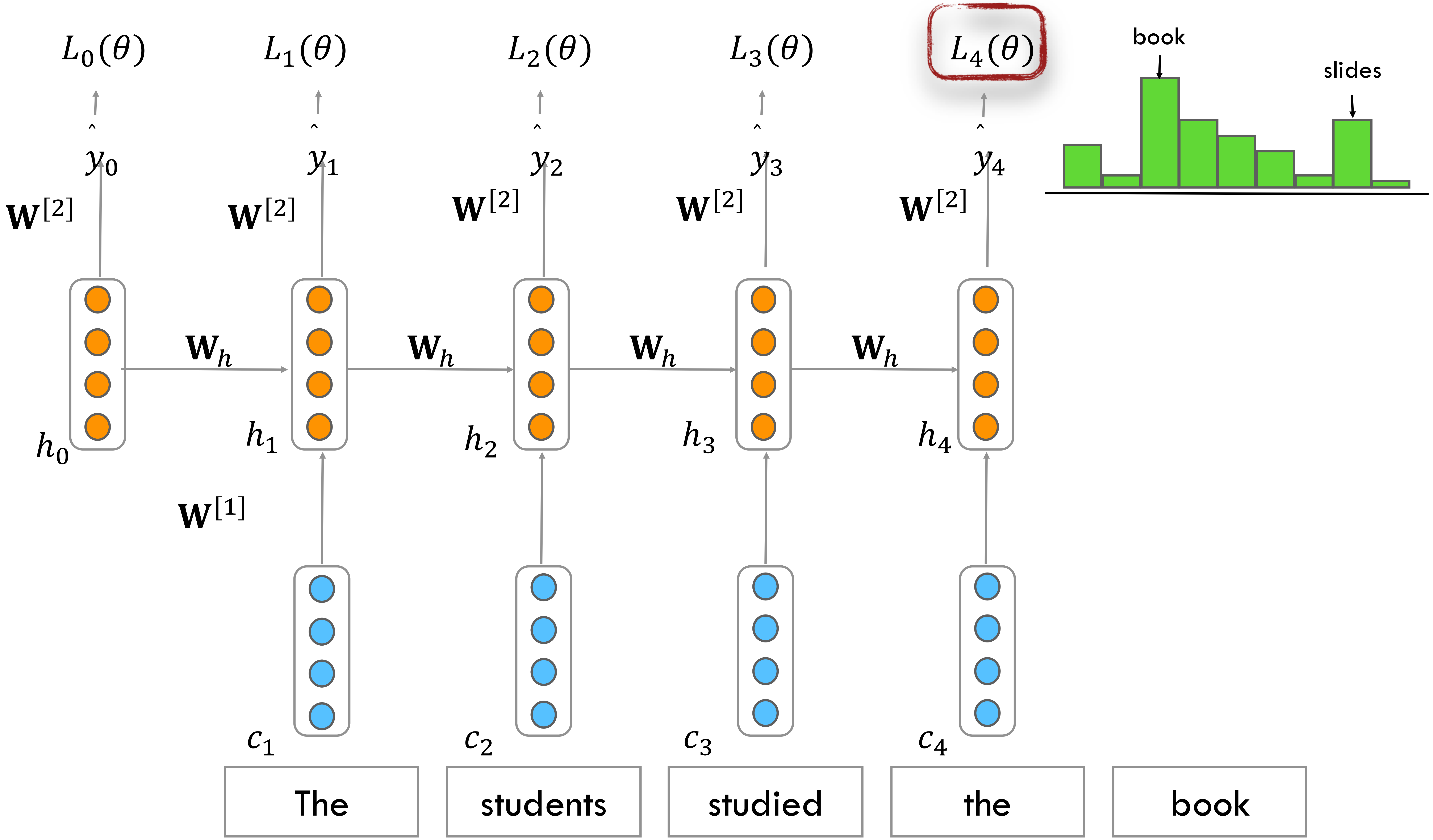
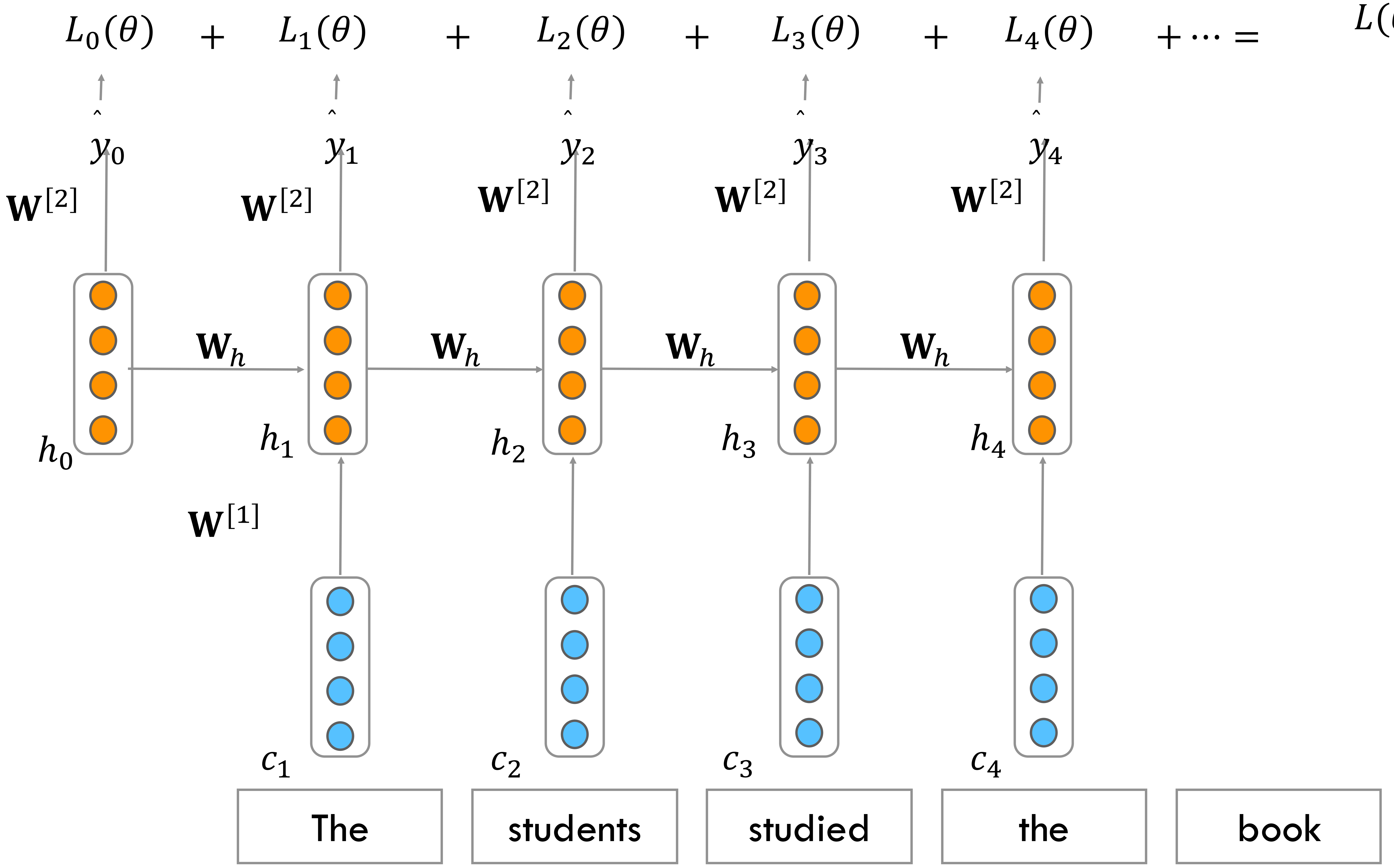


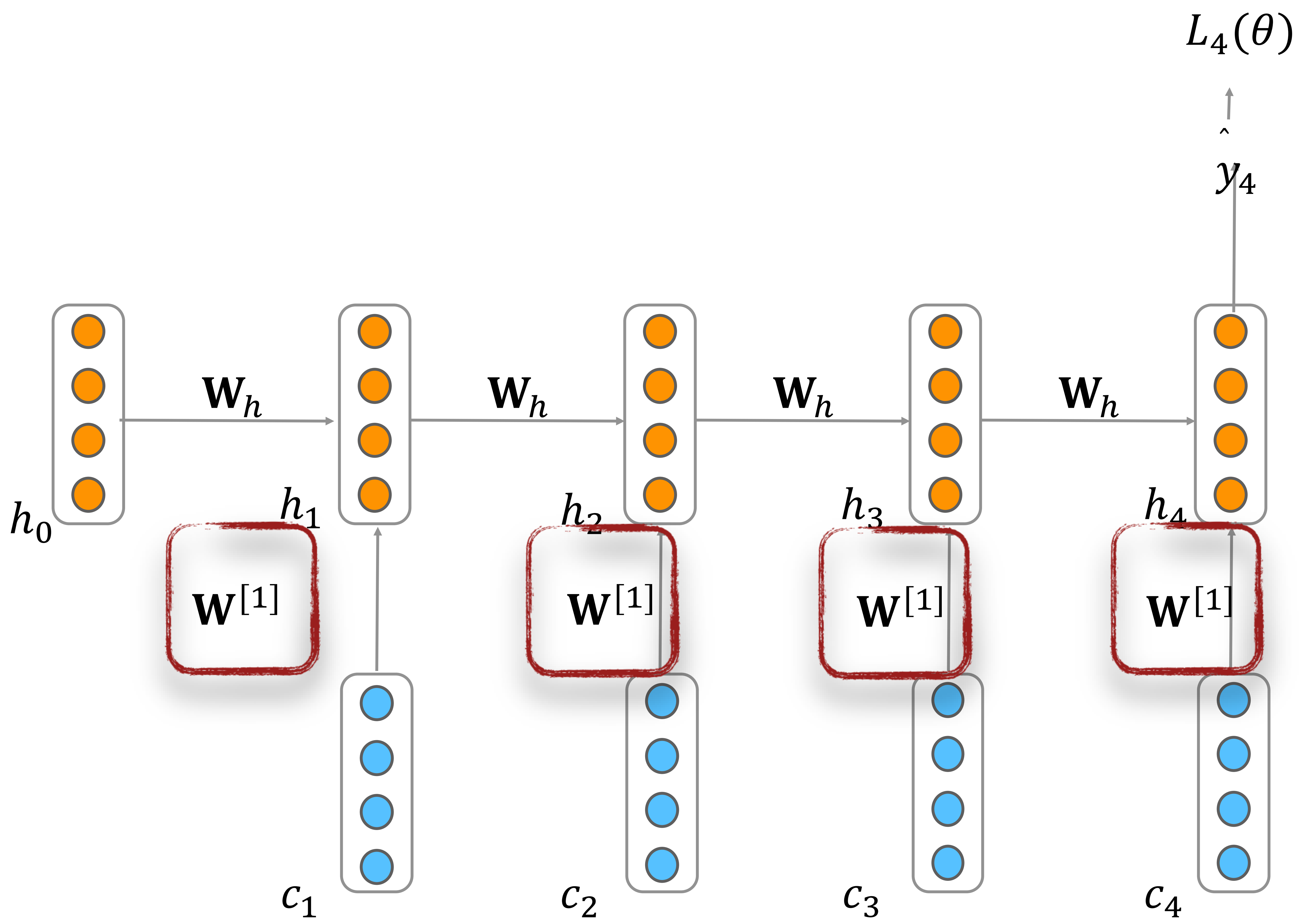
Loss

$$L(\theta) = \frac{1}{T}\sum_{t=1}^{T} L_t(\theta)$$



Training RNNs is hard

- Multiply the same matrix at each time step during forward propagation
- Ideally inputs from many time steps ago can modify output y
- This leads to something called the vanishing gradient problem

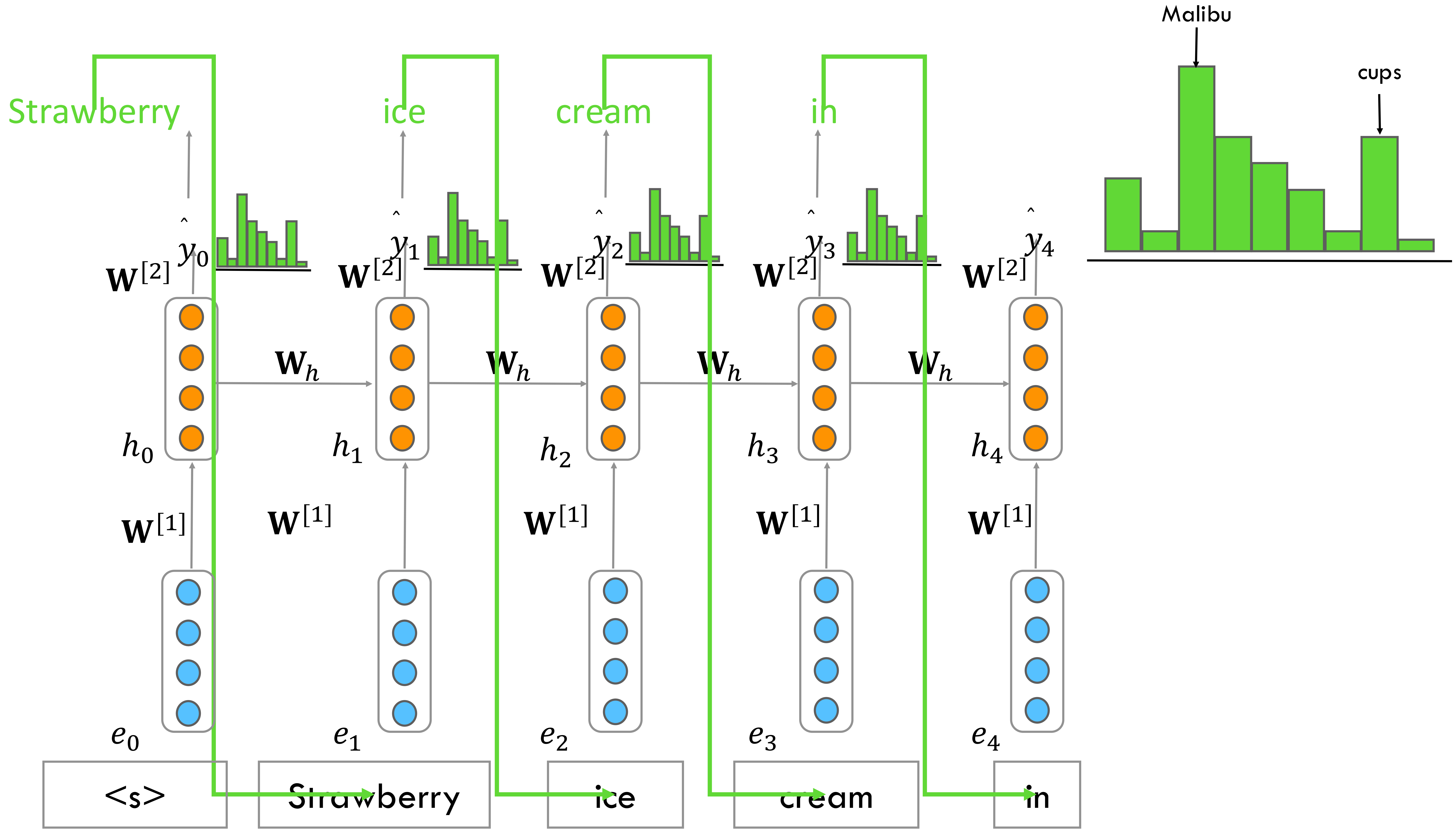


Generation with RNNLMs

$\hat{y}_4 = P(x_5 | Strawberry\ ice\ cream\ in)$

$argmax\hat{y}_i$

Initial hidden state: $\mathbf{h}_0$



RNNLMs are Autoregressive Models

- Model that predicts a value at time t based on a function of the previous values at times $t-1, t-2$, and so on
- Word generated at each time step is conditioned on the word selected by the network from the previous step
- State-of-the-art generation approaches are all autoregressive!
    - Machine translation, question answering, summarization
- Key technique: prime the generation with the most suitable context

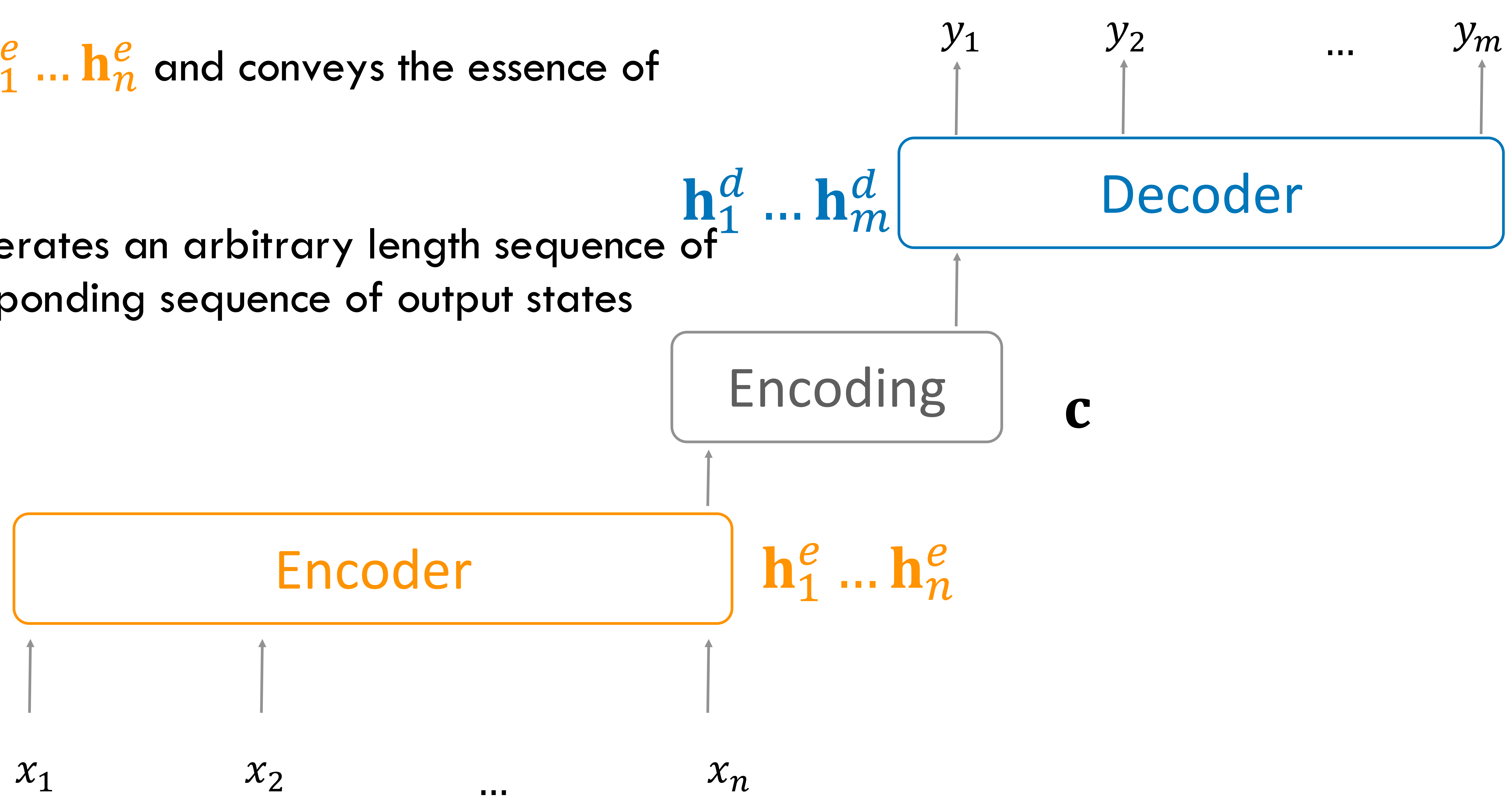
Can do better than <s>!

Provide rich task-appropriate context!

Encoder-Decoder Networks

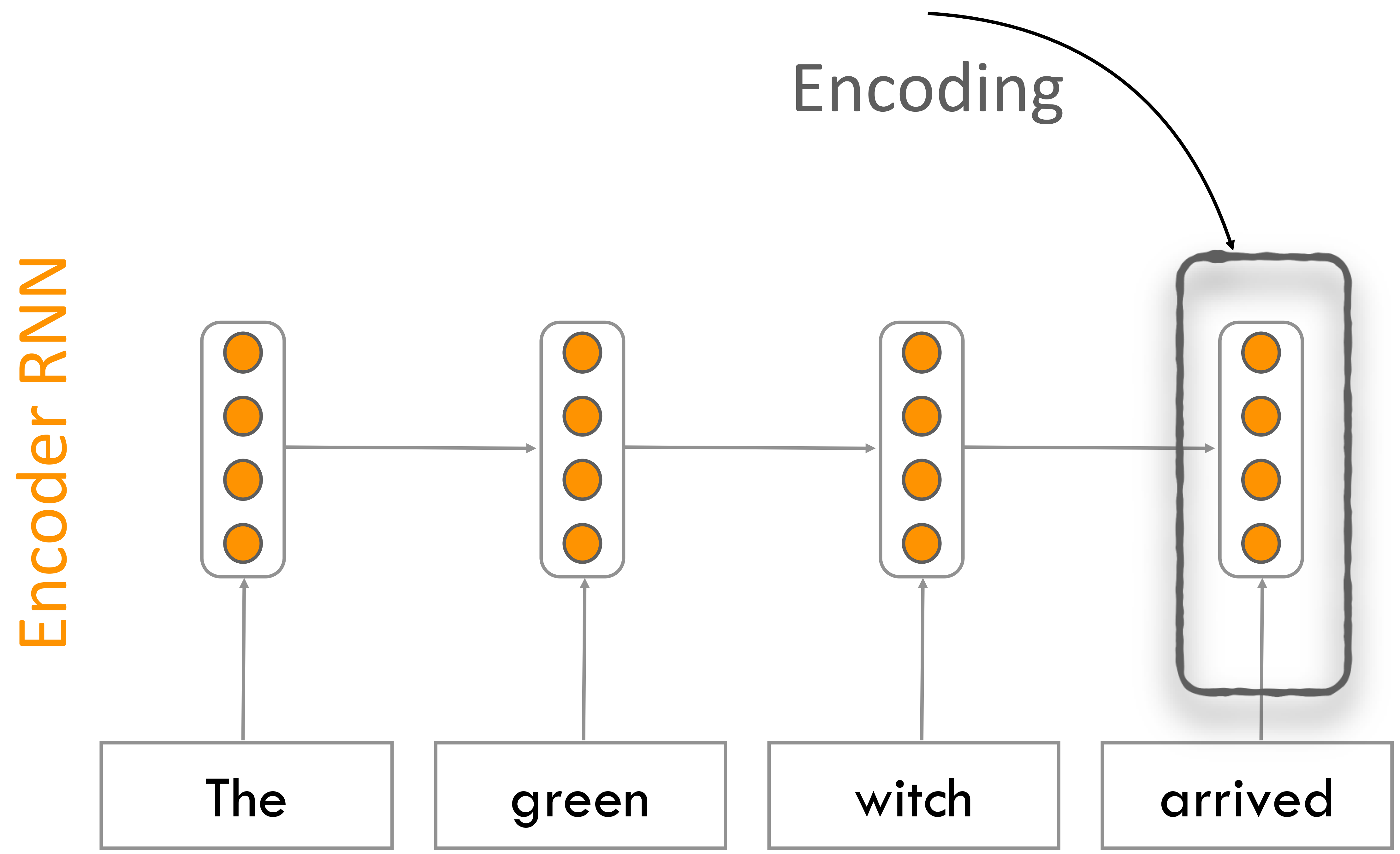
Encoder-decoder networks consist of three components:

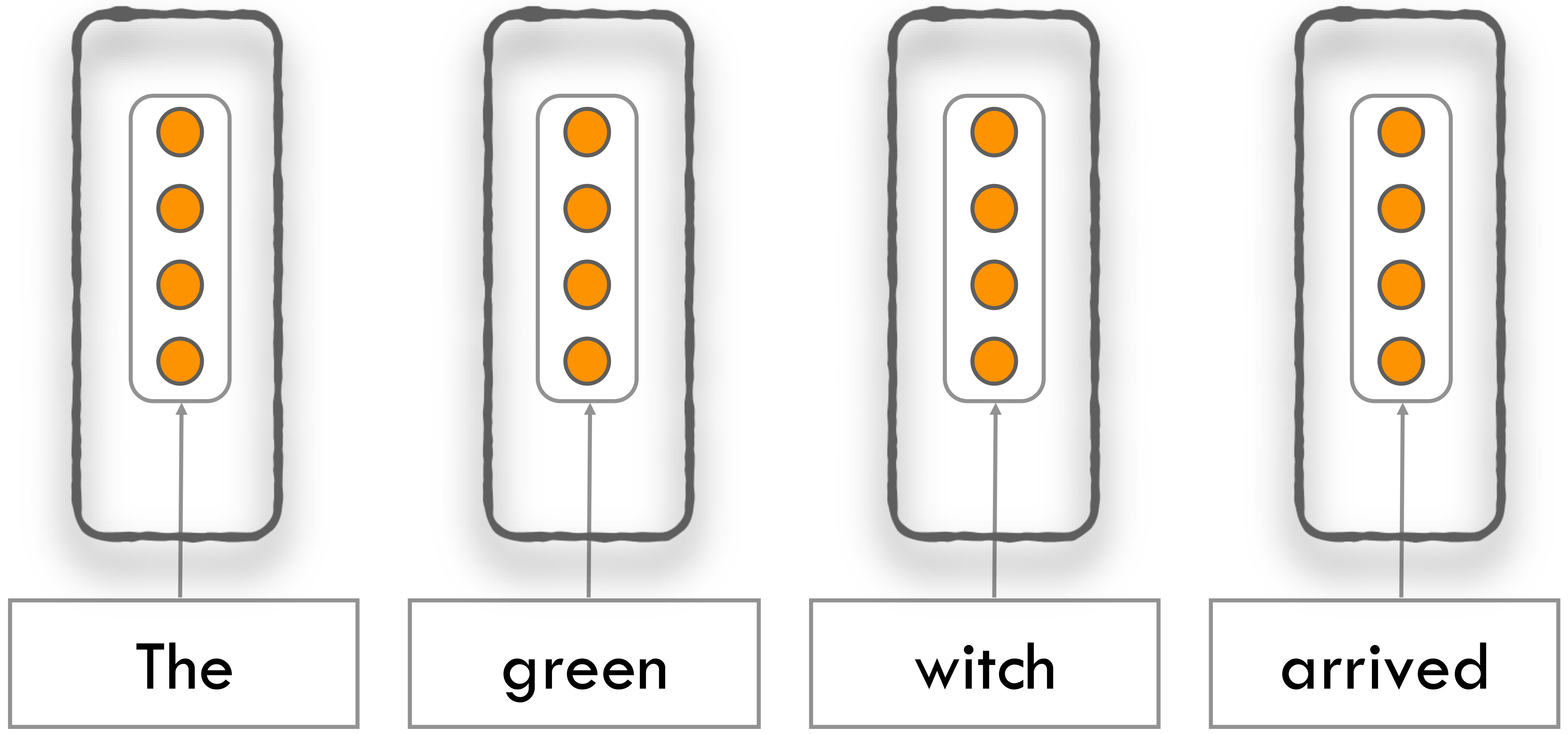
1. An encoder that accepts an input sequence, $\mathbf{x}_{1:n}$ and generates a corresponding sequence of contextualized representations, $\mathbf{h}_1^e \ldots \mathbf{h}_n^e$
2. A encoding vector, $\mathbf{c}$ which is a function of $\mathbf{h}_1^e \ldots \mathbf{h}_n^e$ and conveys the essence of the input to the decoder
3. A decoder which accepts $\mathbf{c}$ as input and generates an arbitrary length sequence of hidden states $\mathbf{h}_1^d \ldots \mathbf{h}_m^d$, from which a corresponding sequence of output states $\mathbf{y}_{1:m}$ can be obtained



Encoders and decoders can be made of FFNNs, RNNs, or Transformers

Information Bottleneck: One Solution

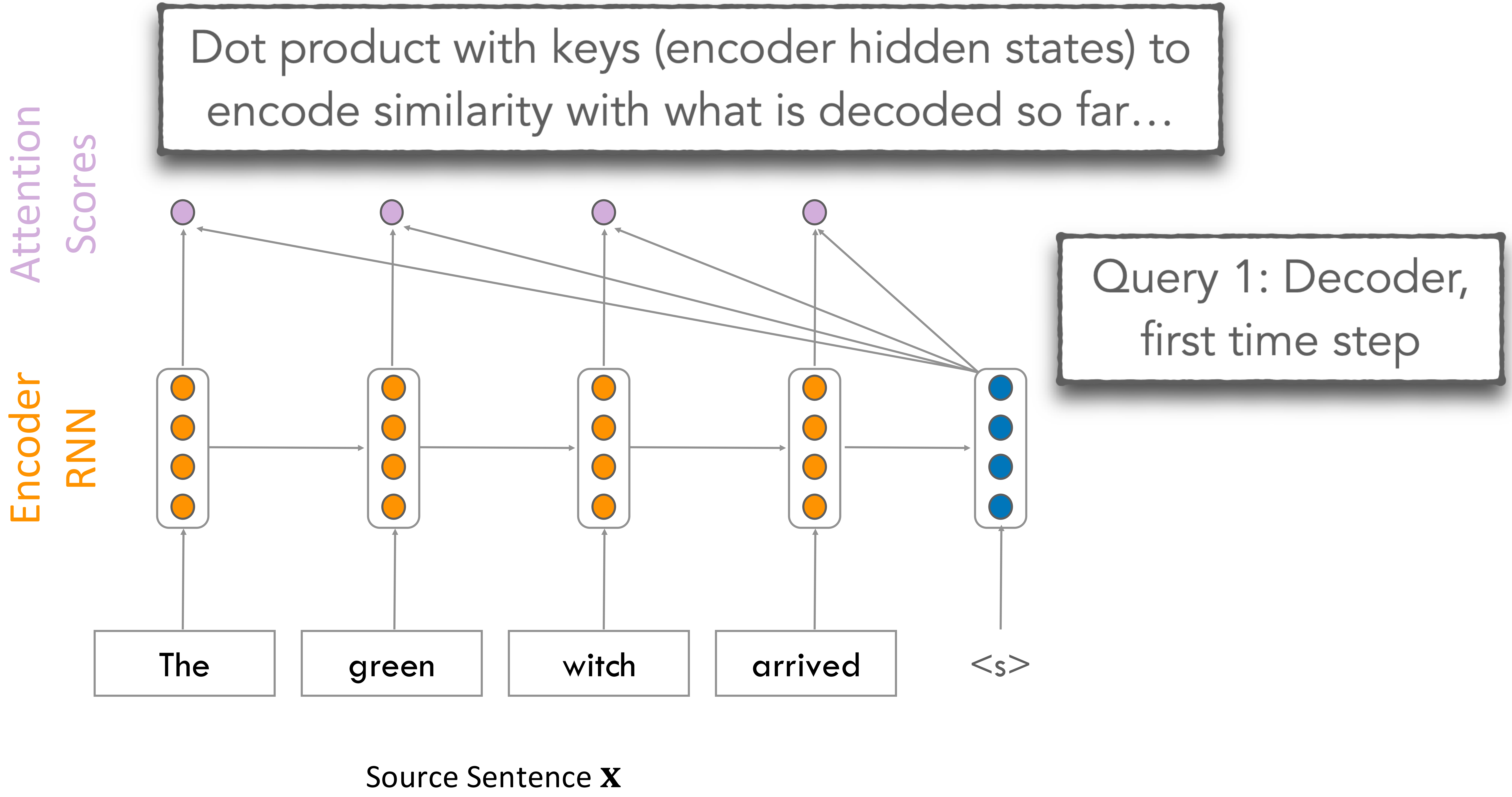


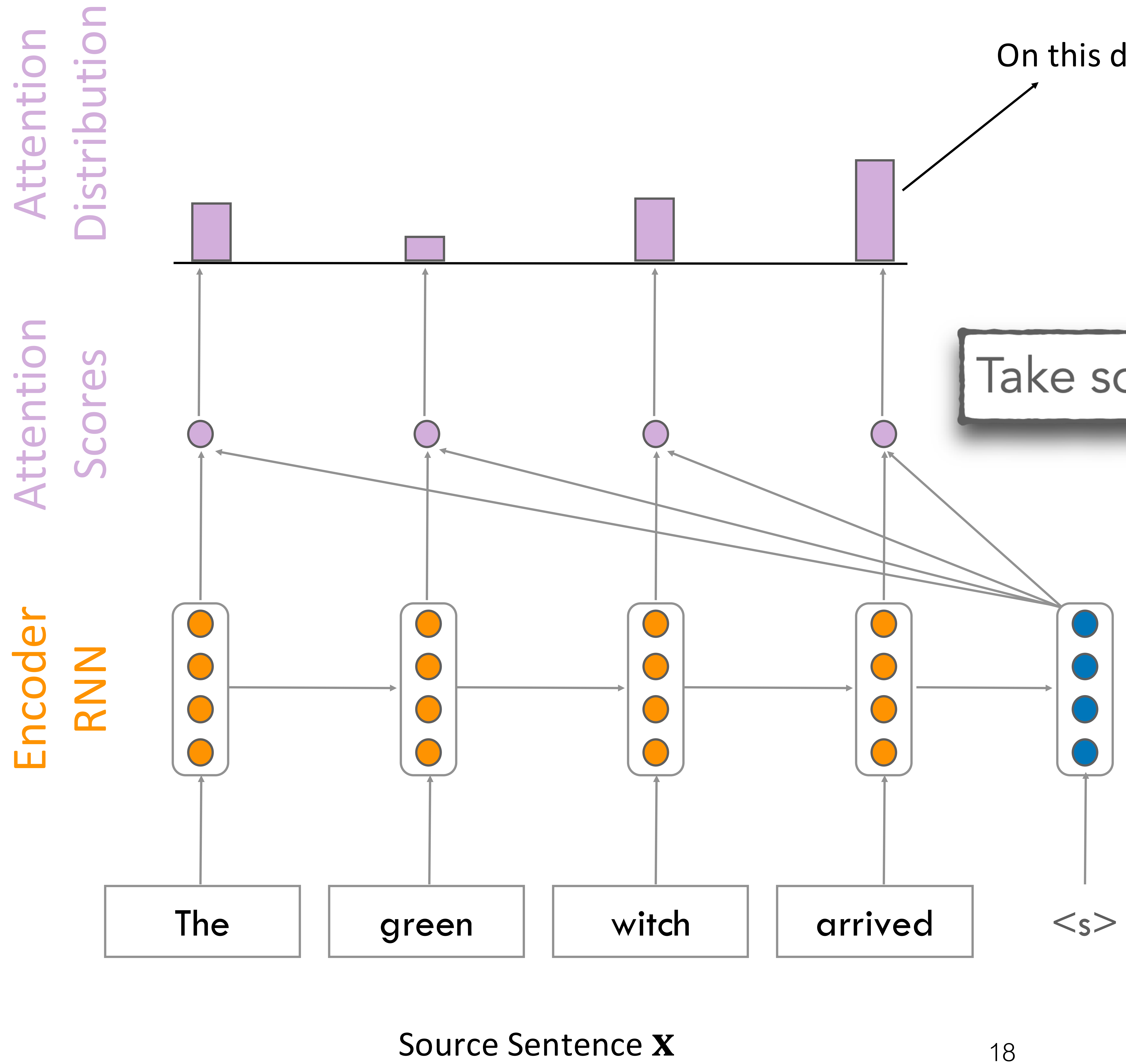


What if we had access to all hidden states?

How to create this?

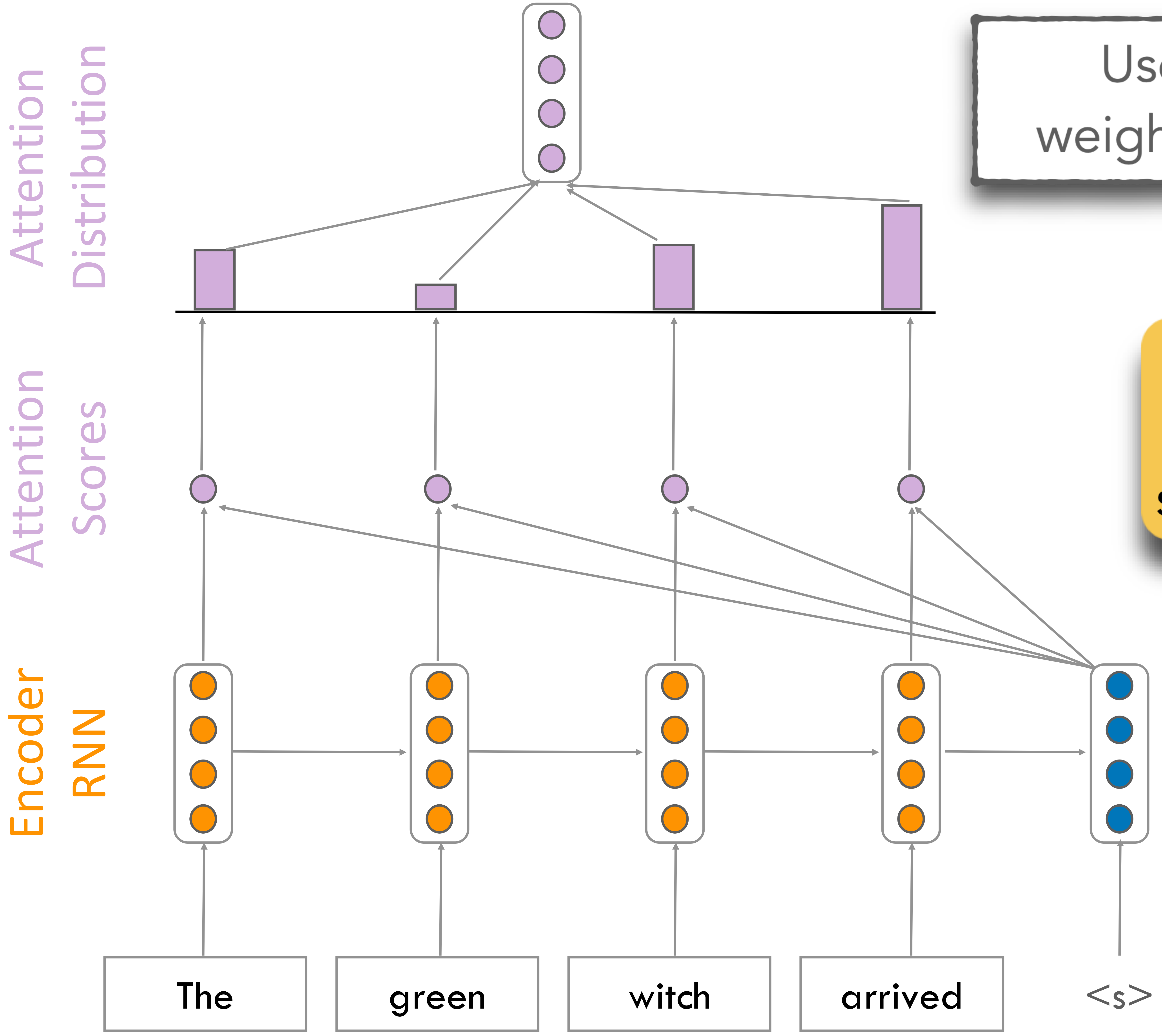
Seq2Seq with Attention





On this decoder tilmestep we are mostly focusing on the source token "arrived"

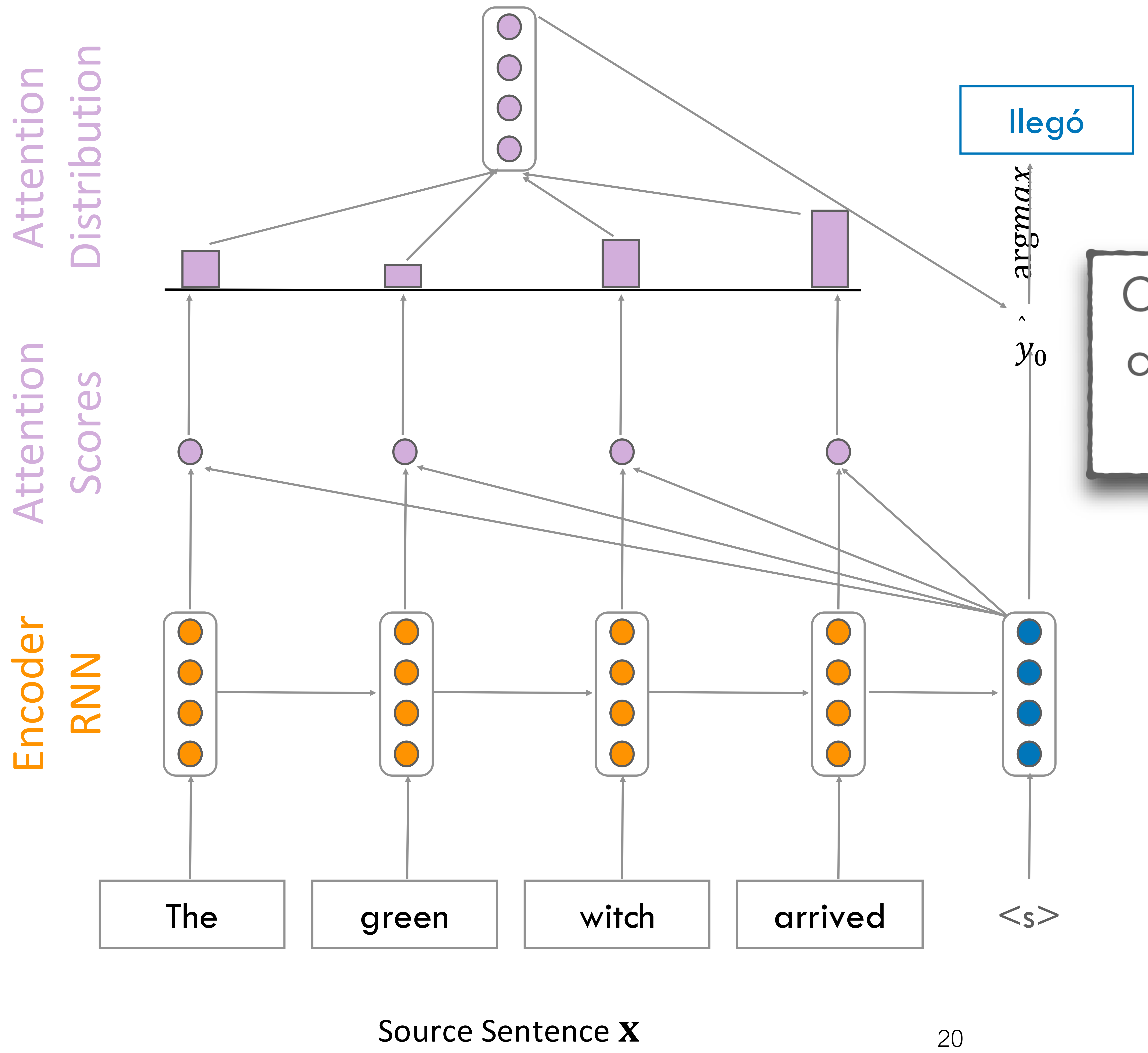
Take softmax to turn into probability distribution



Use the attention distribution to take a weighted sum of the encoder hidden states.

The attention output mostly contains information the hidden states that received high attention.

Source Sentence $\mathbf{x}$



Concatenate attention output with decoder hidden state, then use to compute $\hat{y}_0$ as before

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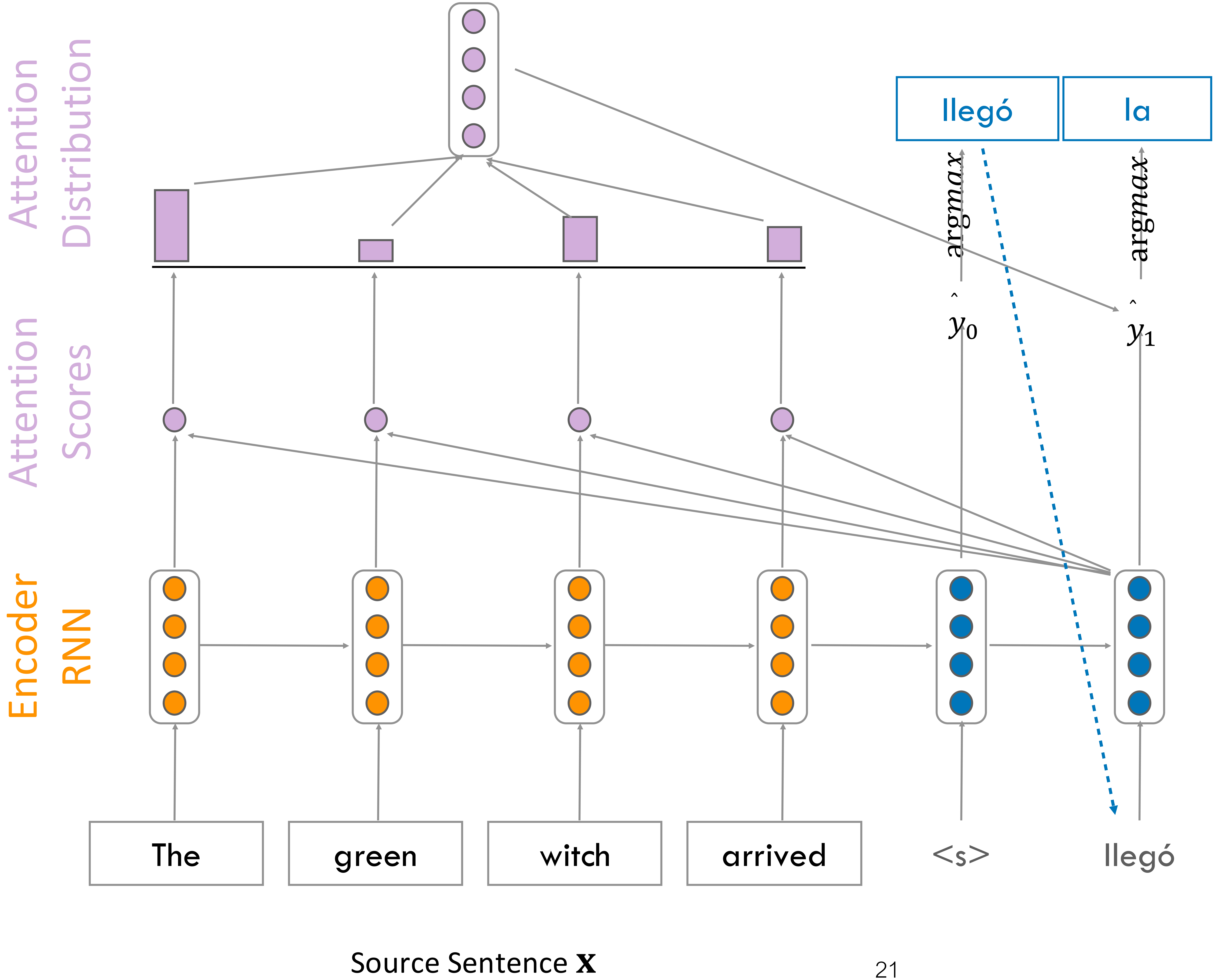

Query 2: Decoder, second time step

More on Attention

Attention Variants

- In general, we have some values $\mathbf{h}_1 \ldots \mathbf{h}_N \in \mathbb{R}^{d_1}$ and a query $\mathbf{q} \in \mathbb{R}^{d_2}$
- Attention always involves
  1. Computing the attention scores, $e(\mathbf{q}, \mathbf{h}_{1:N}) \in \mathbb{R}^N$

     Can be done in multiple ways!
  2. Taking softmax to get attention distribution $\alpha_t = softmax(e(\mathbf{q}, \mathbf{h}_{1:N})) \in [0,1]^N$
  3. Using attention distribution to take weighted sum of values:

$$\mathbf{c}_t^{att} = \sum_{i=1}^{N} \alpha_{t,i} \mathbf{h}_i \in \mathbb{R}^{d_1}$$

thus obtaining the attention output $\mathbf{c}_t^{att}$ (sometimes called the context vector)

Attention Variants

- There are several ways you can compute $e(\mathbf{q}, \mathbf{h}_{1:N}) \in \mathbb{R}^N$ from $\mathbf{h}_1 \ldots \mathbf{h}_N \in \mathbb{R}^{d_1}$ and $\mathbf{q} \in \mathbb{R}^{d_2}$
- Basic dot-product attention: $e(\mathbf{q}, \mathbf{h}_{1:N}) = [\mathbf{q} \cdot \mathbf{h}_j]_{j=1:N}$
  - This assumes $d_1 = d_2$
  - We applied this in encoder-decoder RNNs
- Multiplicative attention: $e(\mathbf{q}, \mathbf{h}_{1:N}) = [\mathbf{q}^T \mathbf{W} \mathbf{h}_j]_{j=1:N}$
  - Where $\mathbf{W} \in \mathbb{R}^{d_1 \times d_2}$ is a learned weight matrix.
  - Also called “bilinear attention”

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More on Attention

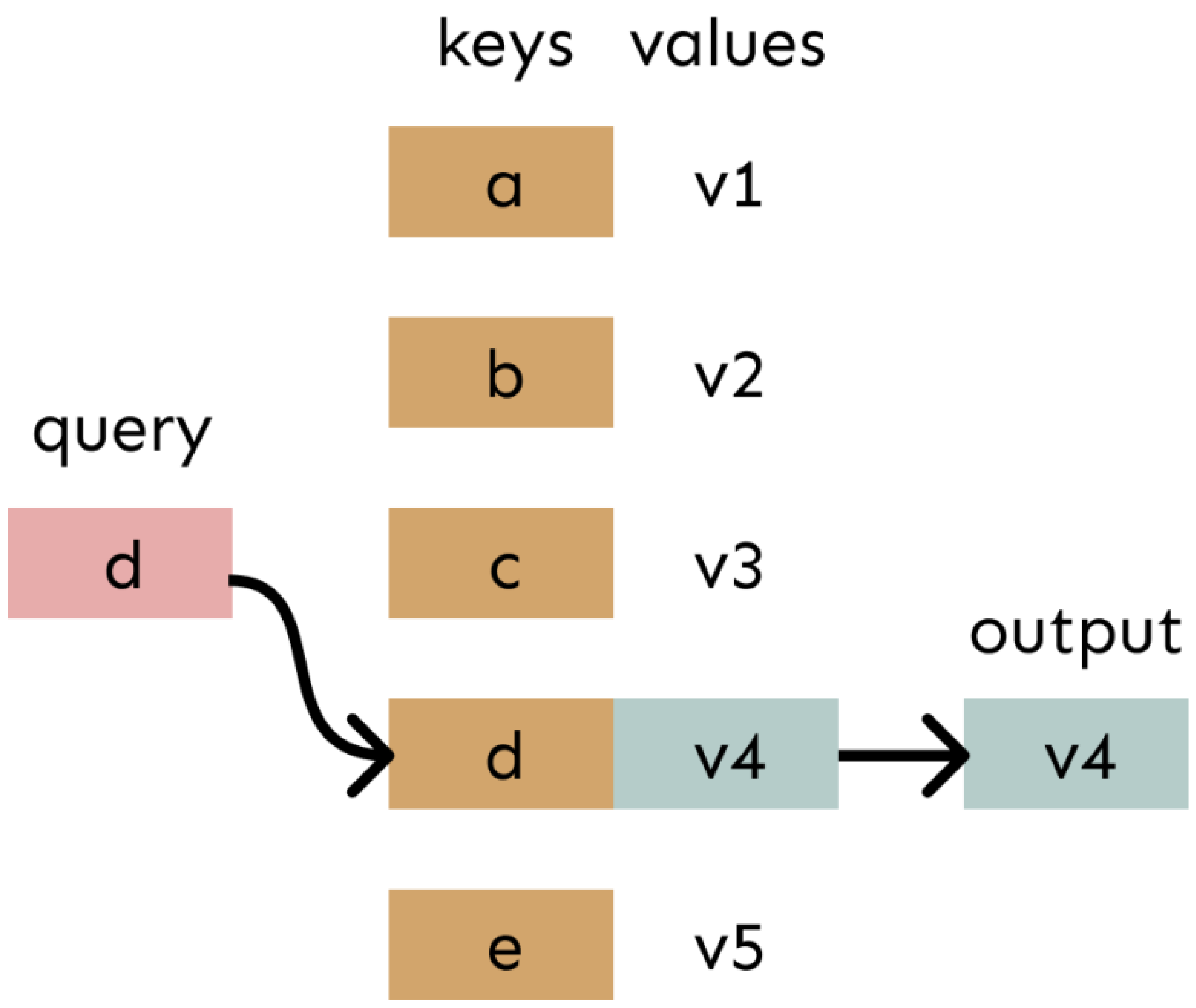
Given a set of vector values, and a vector query, attention is a technique to compute a weighted sum of the values, dependent on the query

- We sometimes say that the query attends to the values.
  - For example, in the seq2seq + attention model, each decoder hidden state (query) attends to all the encoder hidden states (values)
  - Here, keys and values are the same!
- The weighted sum is a selective summary of the information contained in the values, where the query determines which values to focus on.
- Attention is a way to obtain a fixed-size representation of an arbitrary set of representations (the values), dependent on some other representation (the query).
- Attention is a powerful, flexible, general deep learning technique in all deep learning models.
  - A new idea from after 2010! Originated in NMT

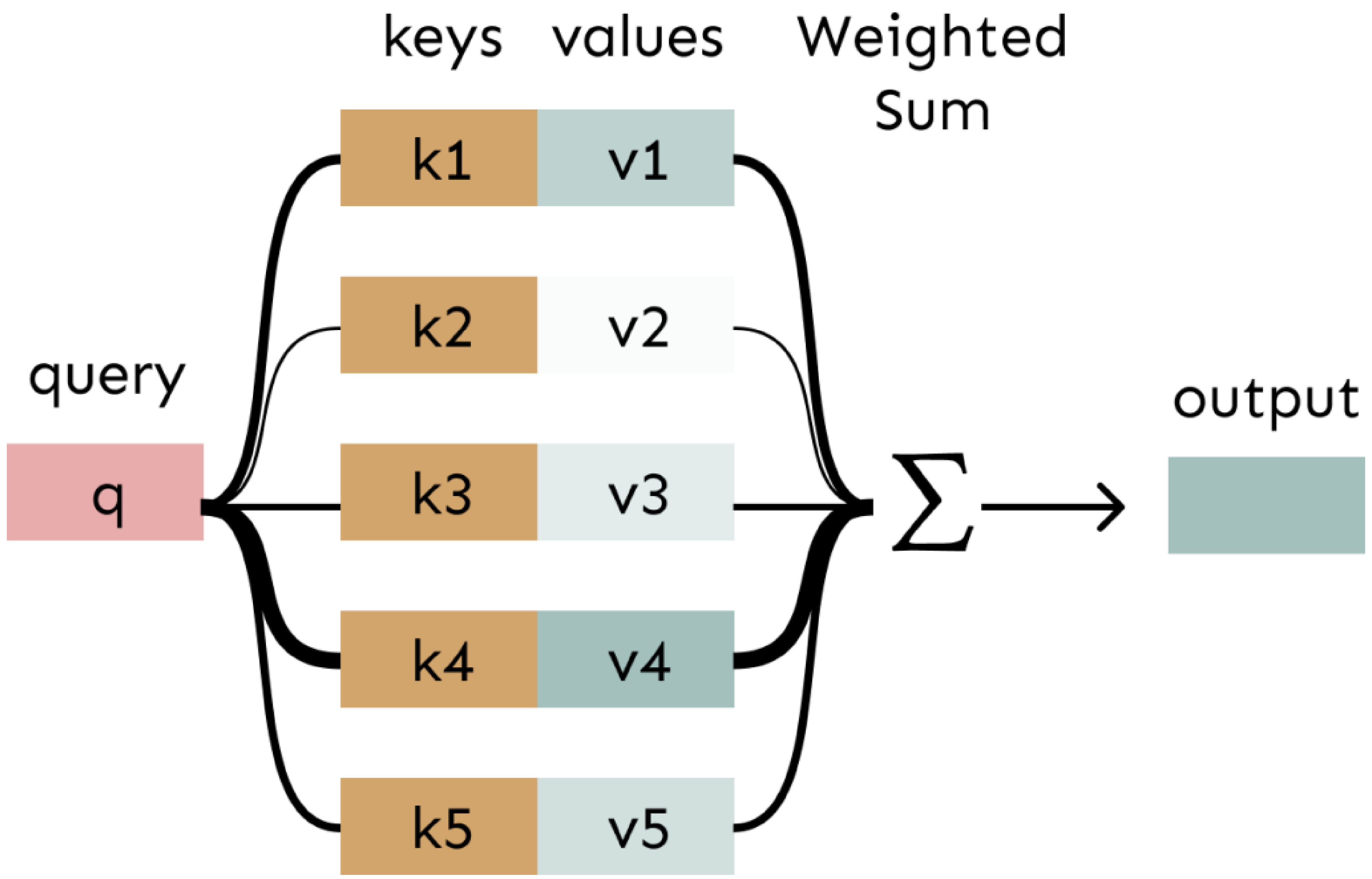
Attention and lookup tables

Attention performs fuzzy lookup in a key-value store

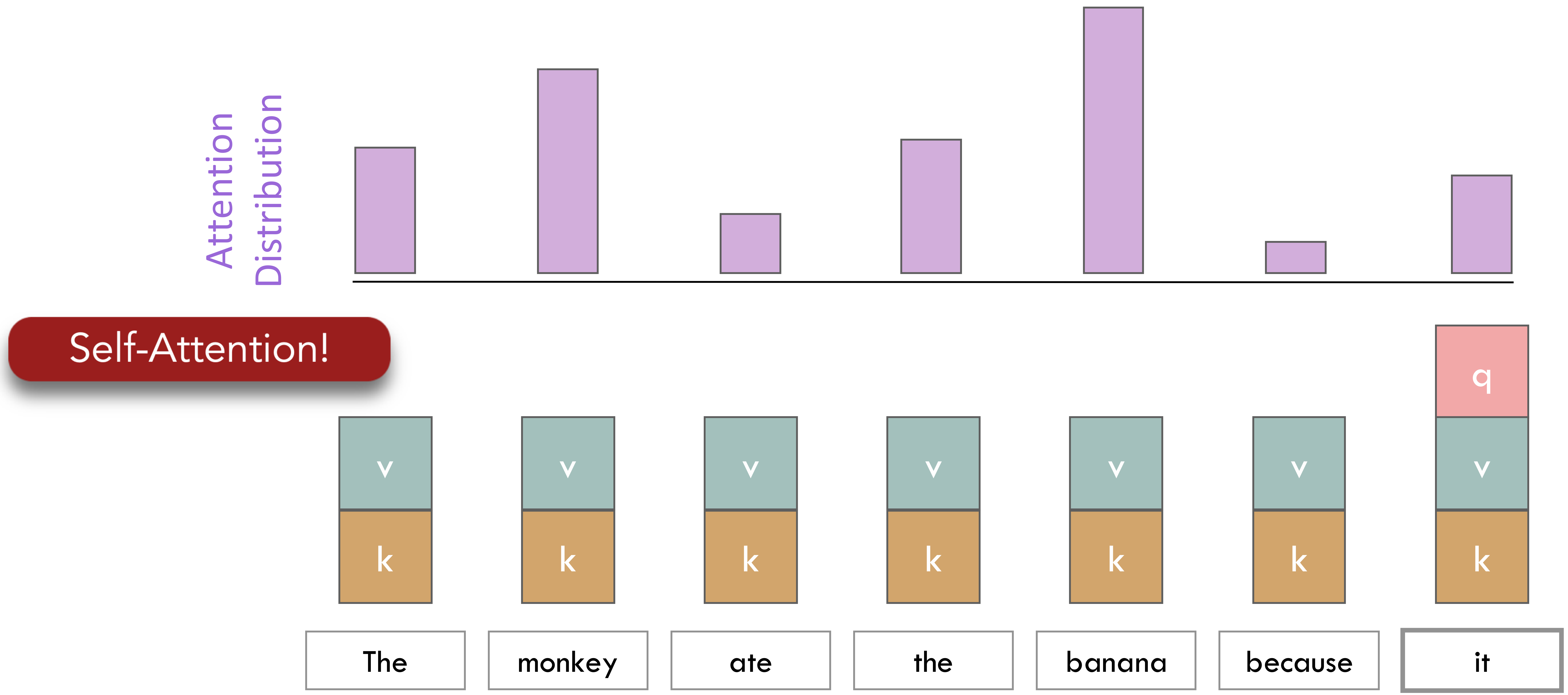
In a lookup table, we have a table of keys that map to values. The query matches one of the keys, returning its value.



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



Attention in the decoder



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Transformers: Self-Attention

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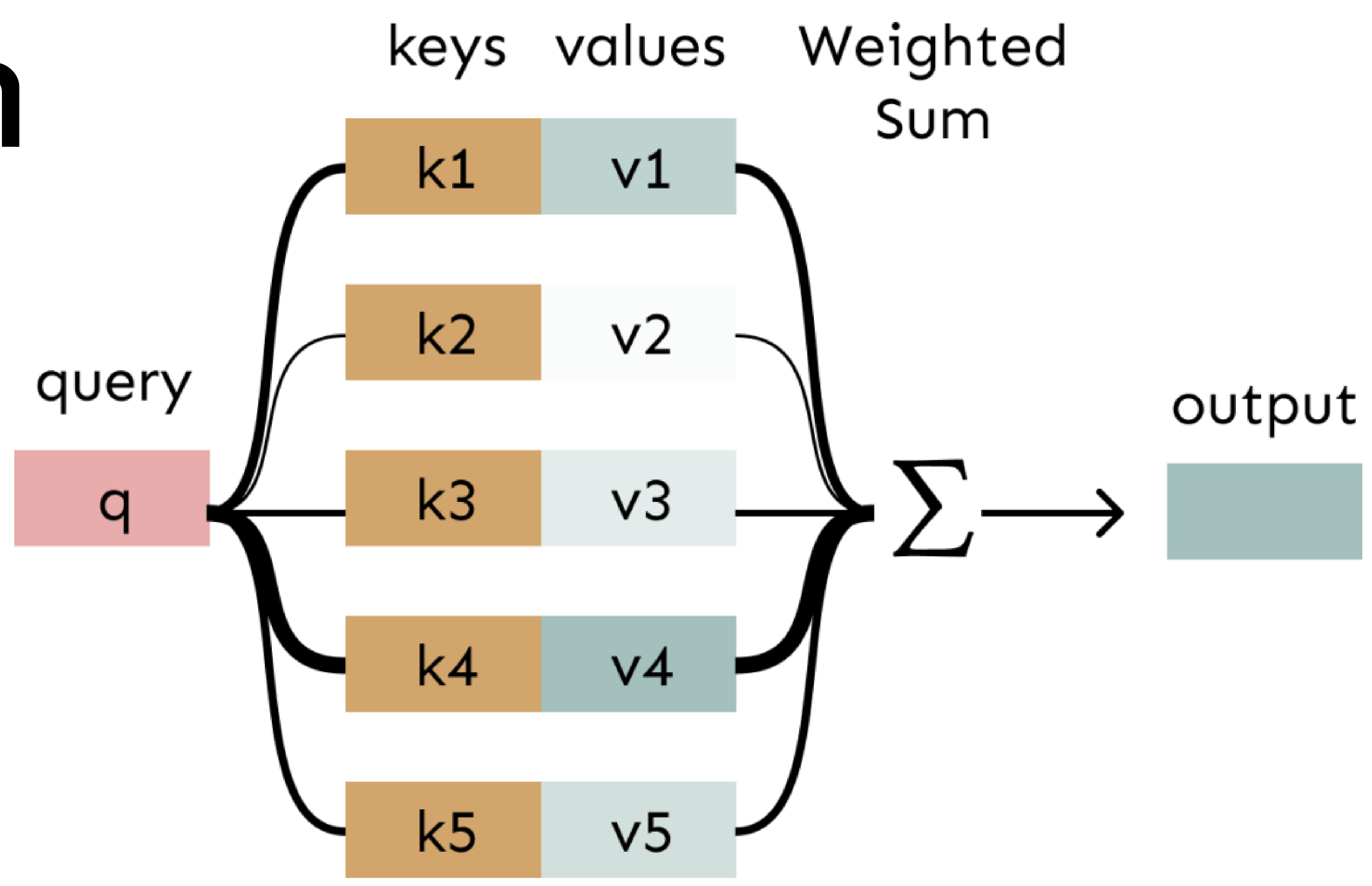
Self-Attention



Keys, Queries, Values from the same sequence

Let $\mathbf{w}_{1:N}$ be a sequence of words in vocabulary V

For each $\mathbf{w}_i$, let $\mathbf{x}_i = \mathbf{E}_{w_i}$, where $\mathbf{E} \in \mathbb{R}^{d \times V}$ is an embedding matrix.

1. Transform each word embedding with weight matrices $\mathbf{Q}, \mathbf{K}, \mathbf{V}$, each in $\mathbb{R}^{d \times d}$

$q_i = Q\boldsymbol{x_i}$ (queries) $\quad k_i = K\boldsymbol{x_i}$ (keys) $\quad v_i = V\boldsymbol{x_i}$ (values)

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

$$\boldsymbol{e}_{ij} = \boldsymbol{q}_i^\top \boldsymbol{k_j} \qquad \boldsymbol{\alpha}_{ij} = \frac{\exp(\boldsymbol{e}_{ij})}{\sum_{j'} \exp(\boldsymbol{e}_{ij'})}$$

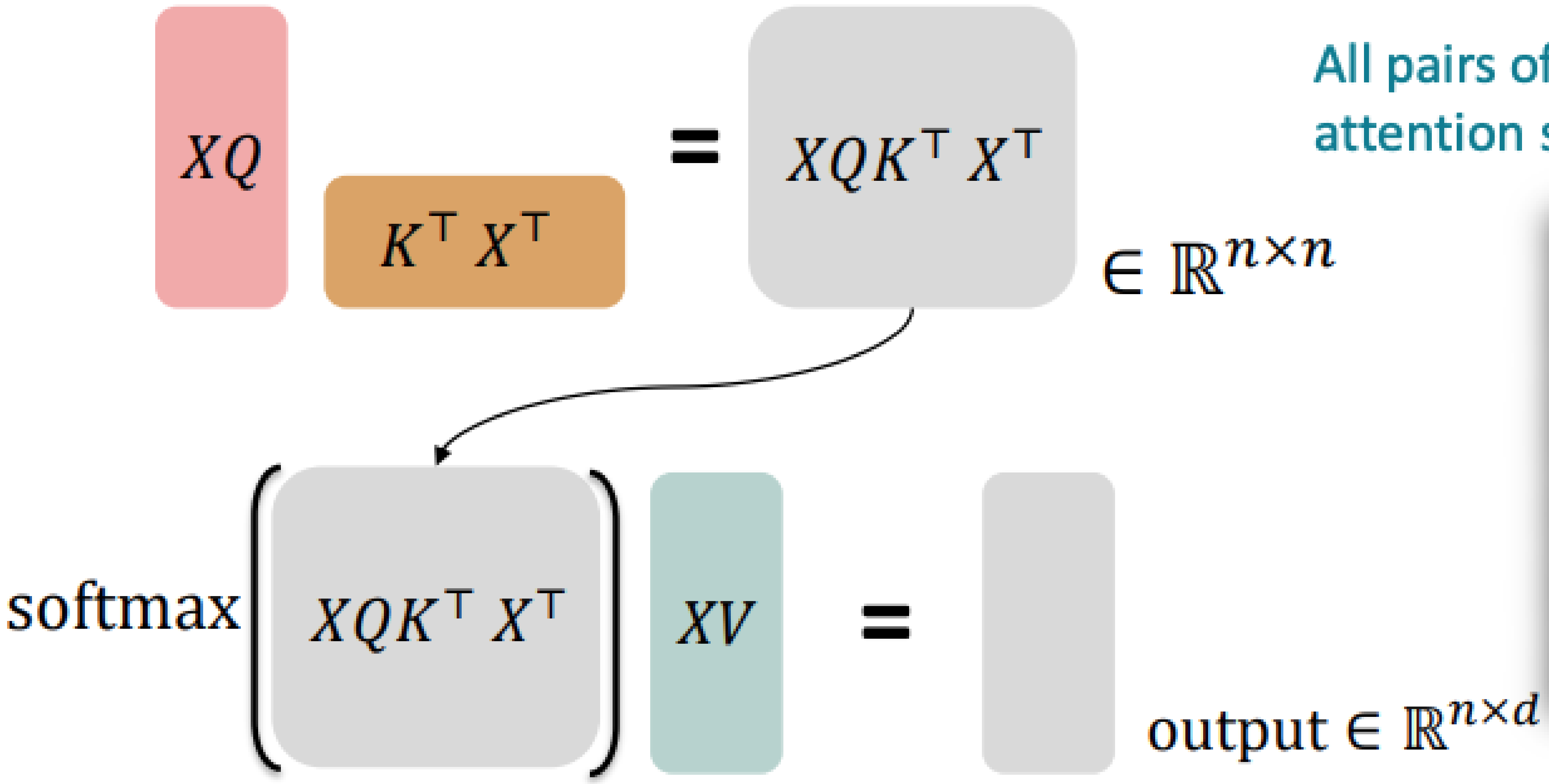
3. Compute output for each word as weighted sum of values

$$\boldsymbol{o}_i = \sum_j \boldsymbol{\alpha}_{ij}\, v_i$$

Self-Attention as Matrix Multiplications

- Key-query-value attention is typically computed as matrices.
  - Let $\mathbf{X} = [\mathbf{x}_1; \ldots; \mathbf{x}_n] \in \mathbb{R}^{n \times d}$ be the concatenation of input vectors
  - First, note that $\mathbf{XK} \in \mathbb{R}^{n \times d}$, $\mathbf{XQ} \in \mathbb{R}^{n \times d}$, and $\mathbf{XV} \in \mathbb{R}^{n \times d}$
  - The output is defined as $softmax(\mathbf{XQ}(\mathbf{XK})^T)\mathbf{XV} \in \mathbb{R}^{n \times d}$

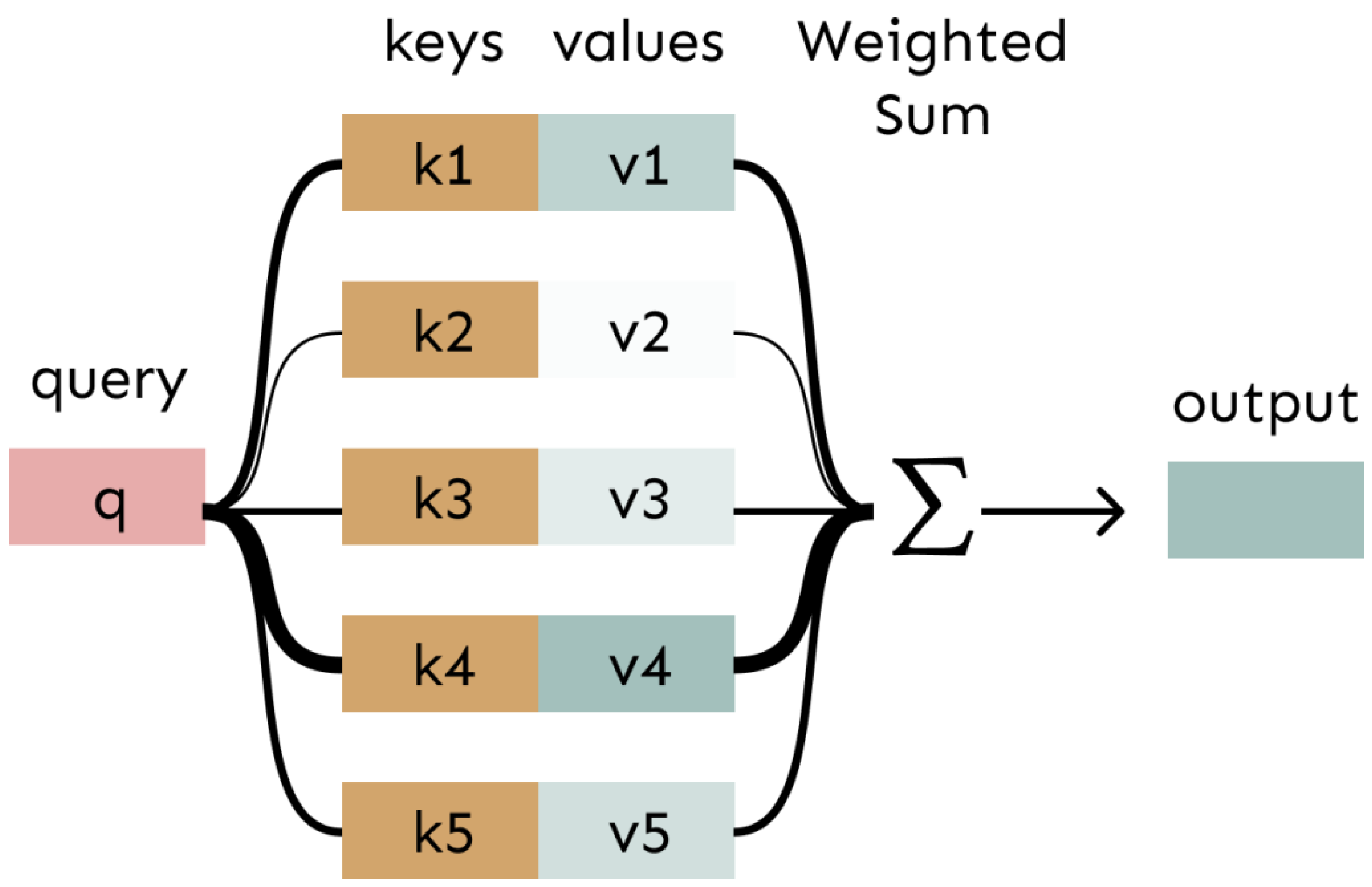
First, take the query-key dot products in one matrix multiplication: $\mathbf{XQ}(\mathbf{XK})^T$



All pairs of attention scores!

Next, softmax, and compute the weighted average with another matrix multiplication.

Why Self-Attention?



- Self-attention allows a network to directly extract and use information from arbitrarily large contexts without the need to pass it through intermediate recurrent connections as in RNNs
- Used often with feedforward networks!

Transformers are Self-Attention Networks

- Self-Attention is the key innovation behind Transformers!
- Transformers map sequences of input vectors $(x_1, \dots, x_n)$ to sequences of output vectors $(y_1, \dots, y_n)$ of the same length.
- Made up of stacks of Transformer blocks
  - each of which is a multilayer network made by combining
    - simple linear layers,
    - feedforward networks, and
    - self-attention layers

Attention Is All You Need

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

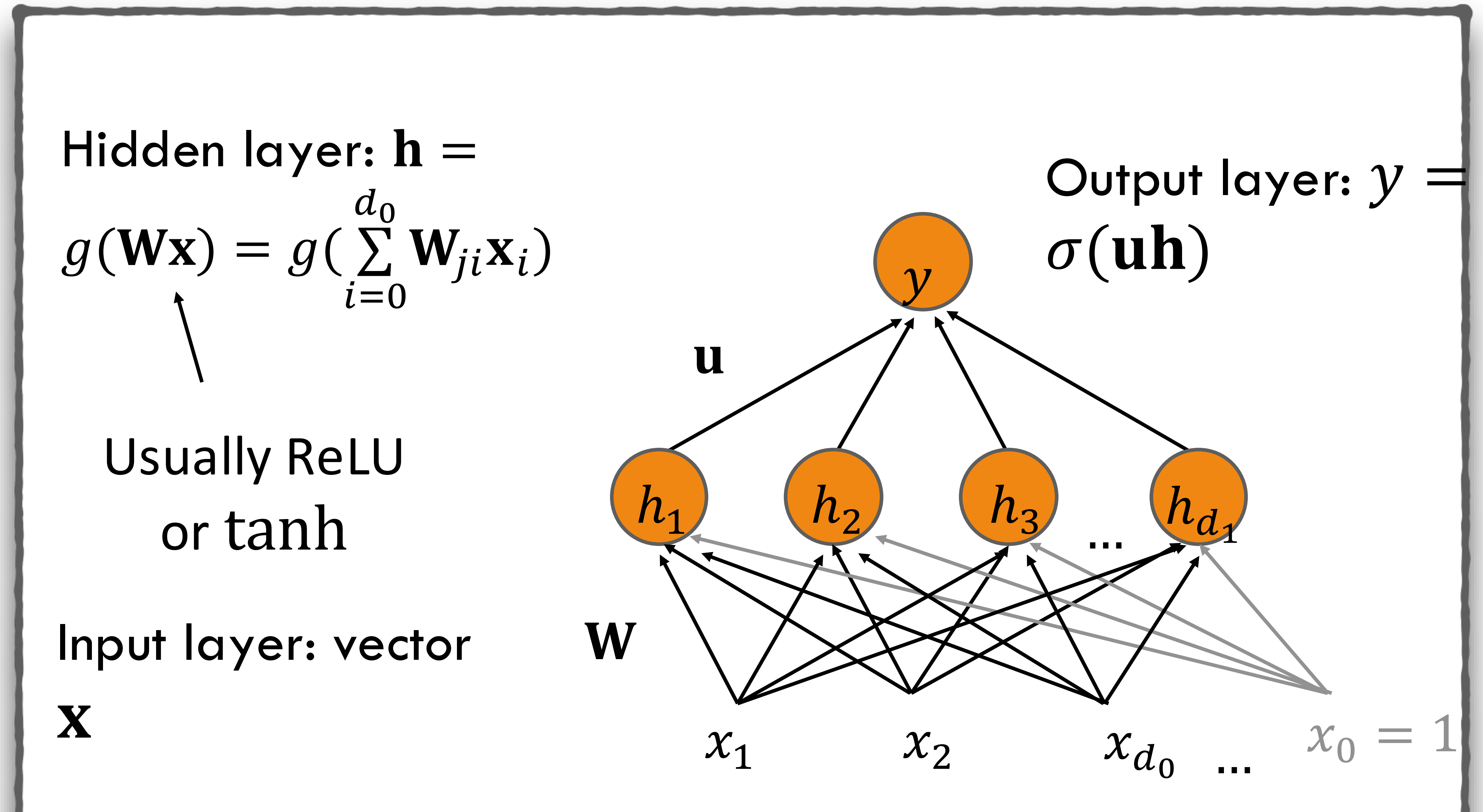
Łukasz Kaiser* Google Brain lukaszkaiser@google.com

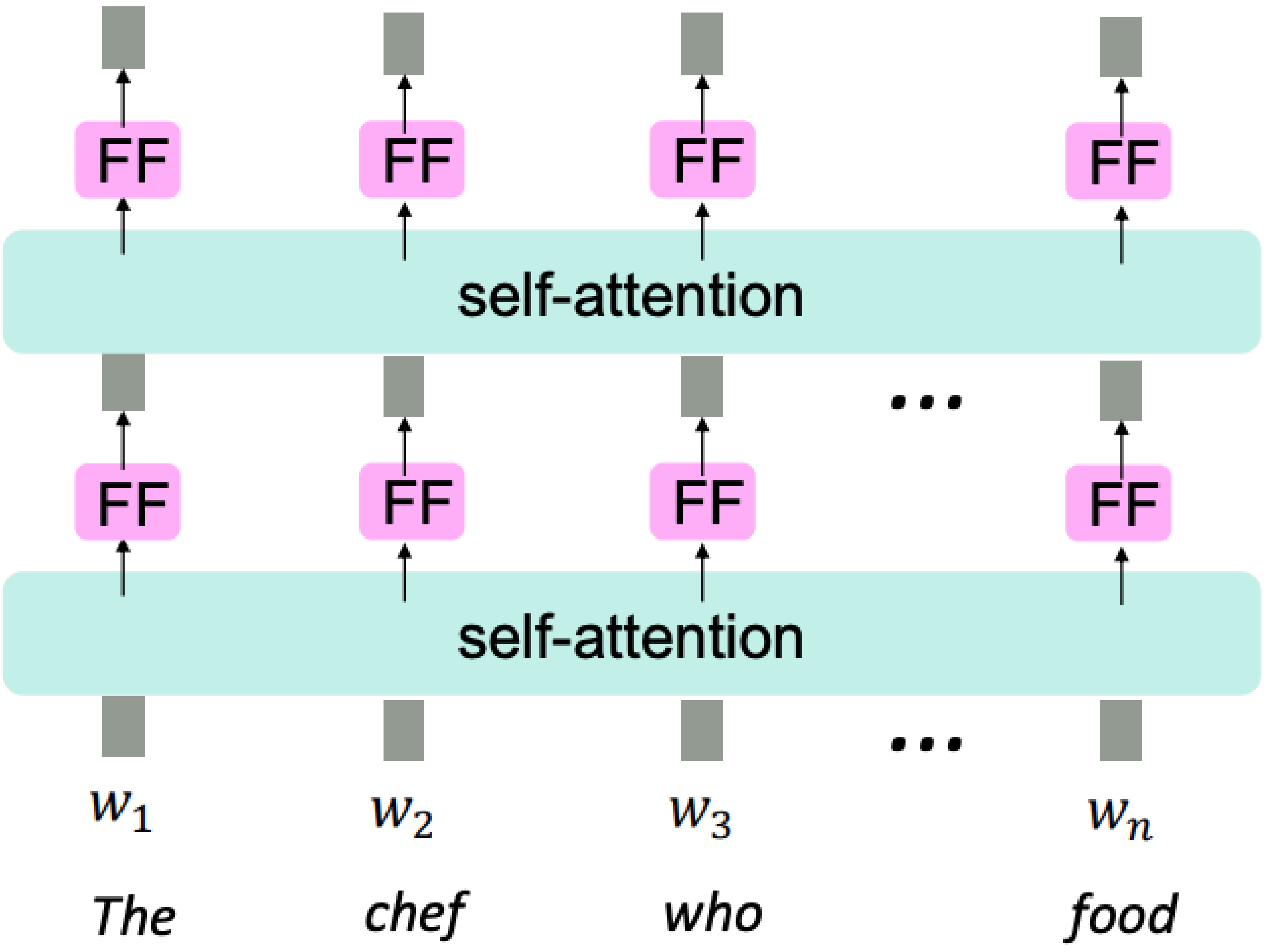
Illia Polosukhin* ‡ illia.polosukhin@gmail.com

Self-Attention and Weighted Averages

- Problem: there are no element-wise nonlinearities in self-attention; stacking more self-attention layers just re-averages value vectors

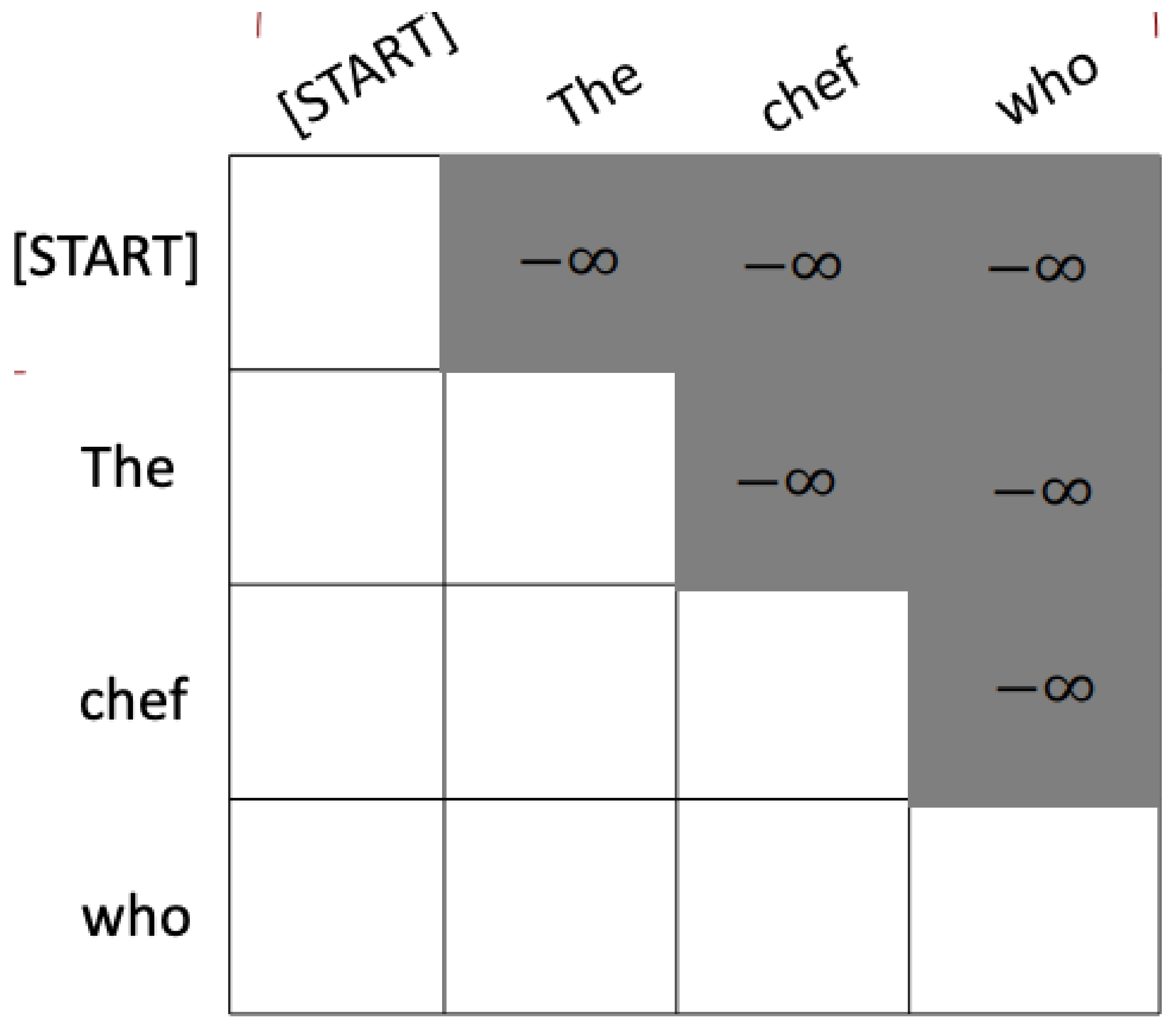
- Solution: add a feed-forward network to post-process each output vector.





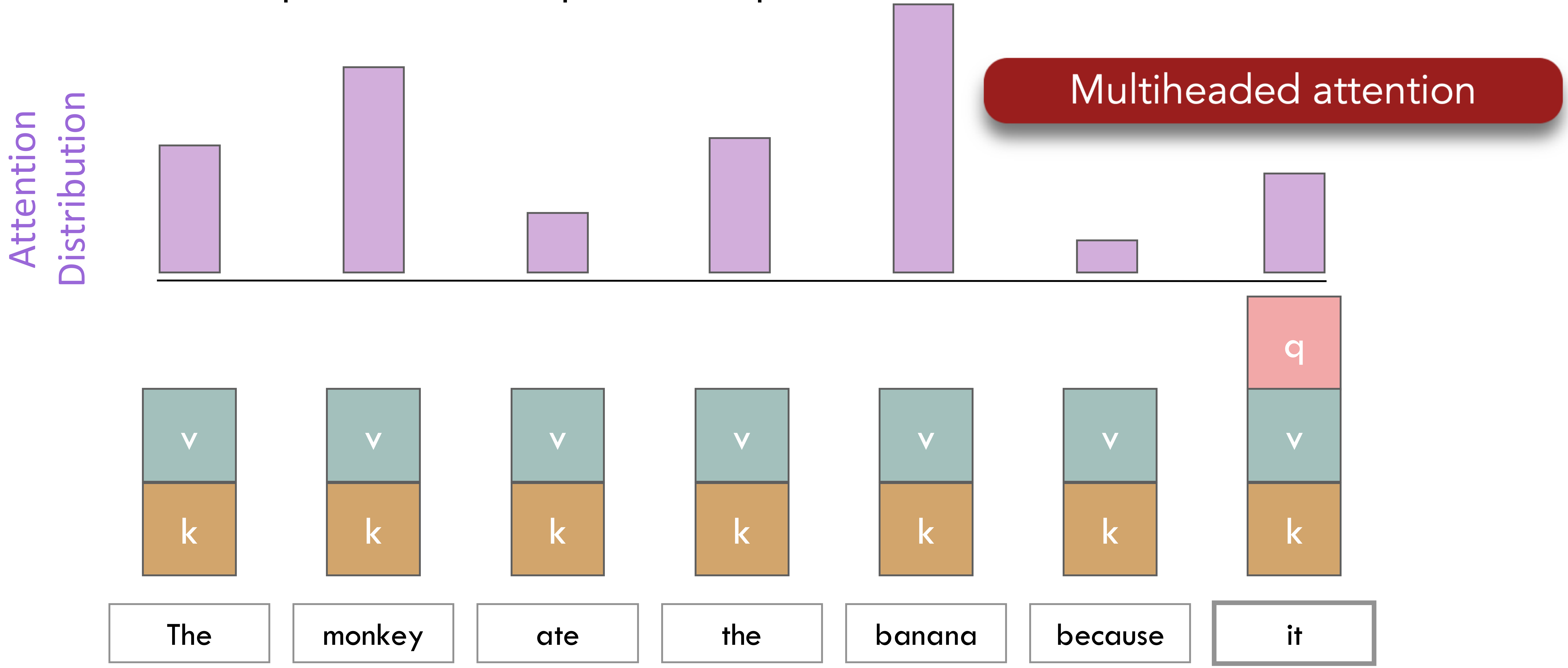
Self Attention and Future Information

- Problem: Need to ensure we don't "look at the future" when predicting a sequence
  - e.g. Target sentence in machine translation or generated sentence in language modeling
  - To use self-attention in decoders, we need to ensure we can't peek at the future.
- Solution (Naïve): At every time step, we could change the set of keys and queries to include only past words.
  - (Inefficient!)
- Solution: To enable parallelization, we mask out attention to future words by setting attention scores to $-\infty$



Self-Attention and Heads

- What if we needed to pay attention to multiple different kinds of things e.g. entities, syntax
- Solution: Consider multiple attention computations in parallel



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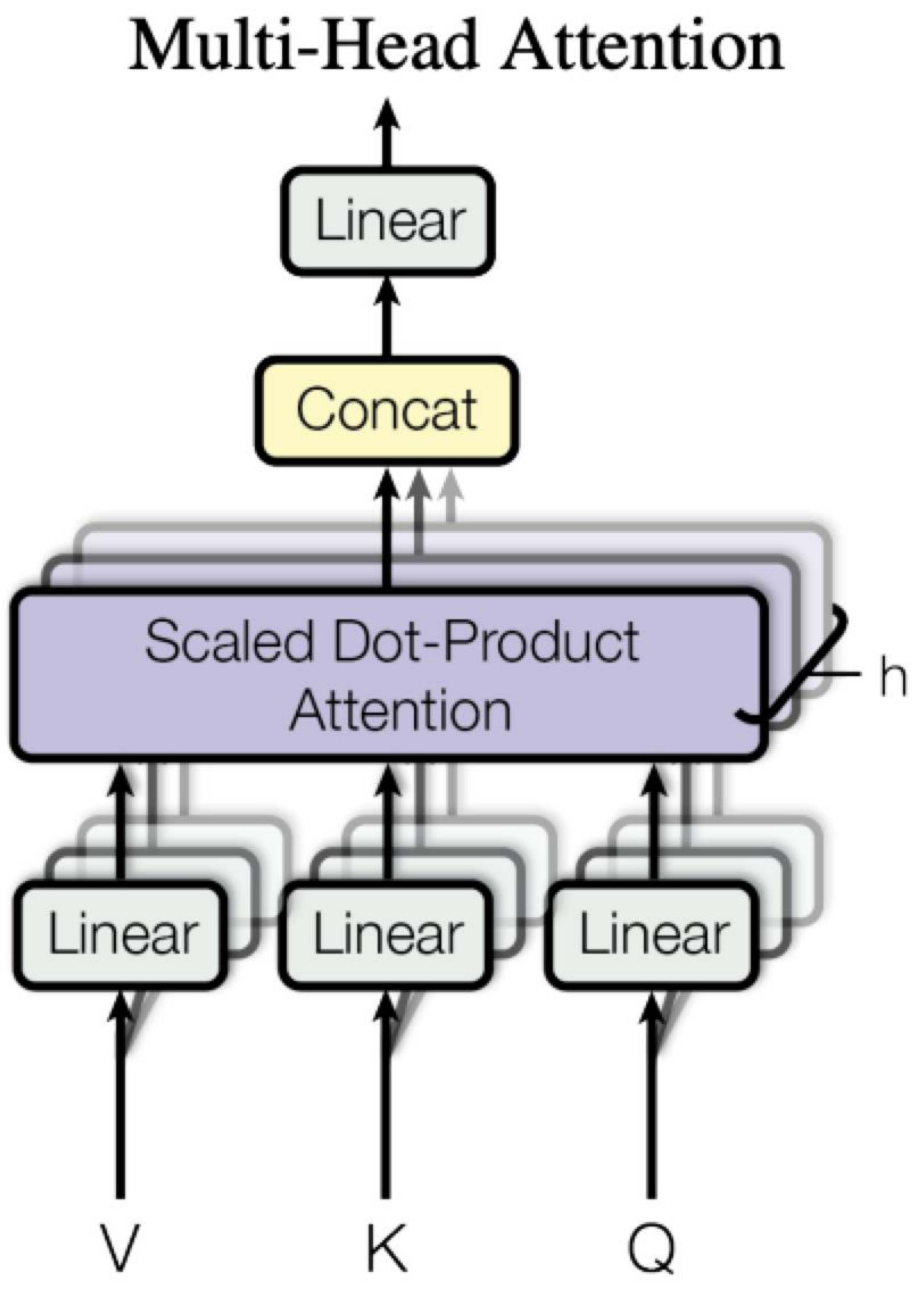
Transformers: Multiheaded Attention

Multi-headed attention

- What if we want to look in multiple places in the sentence at once?
  - For word i, self-attention "looks" where $\mathbf{x}_i^T \mathbf{Q}^T (\mathbf{K}\mathbf{x}_j)$ is high, but maybe we want to focus on different j for different reasons?
- We'll define multiple attention "heads" through multiple $\mathbf{Q}, \mathbf{K}, \mathbf{V}$ matrices
- Let $\mathbf{Q}_l, \mathbf{K}_l, \mathbf{V}_l$, each in $\mathbb{R}^{d \times \frac{d}{h}}$, where h is the number of attention heads, and $1 \leq l \leq h$.
- Each attention head performs attention independently:
- Then the outputs of all the heads are combined!



Each head gets to "look" at different things, and construct value vectors differently

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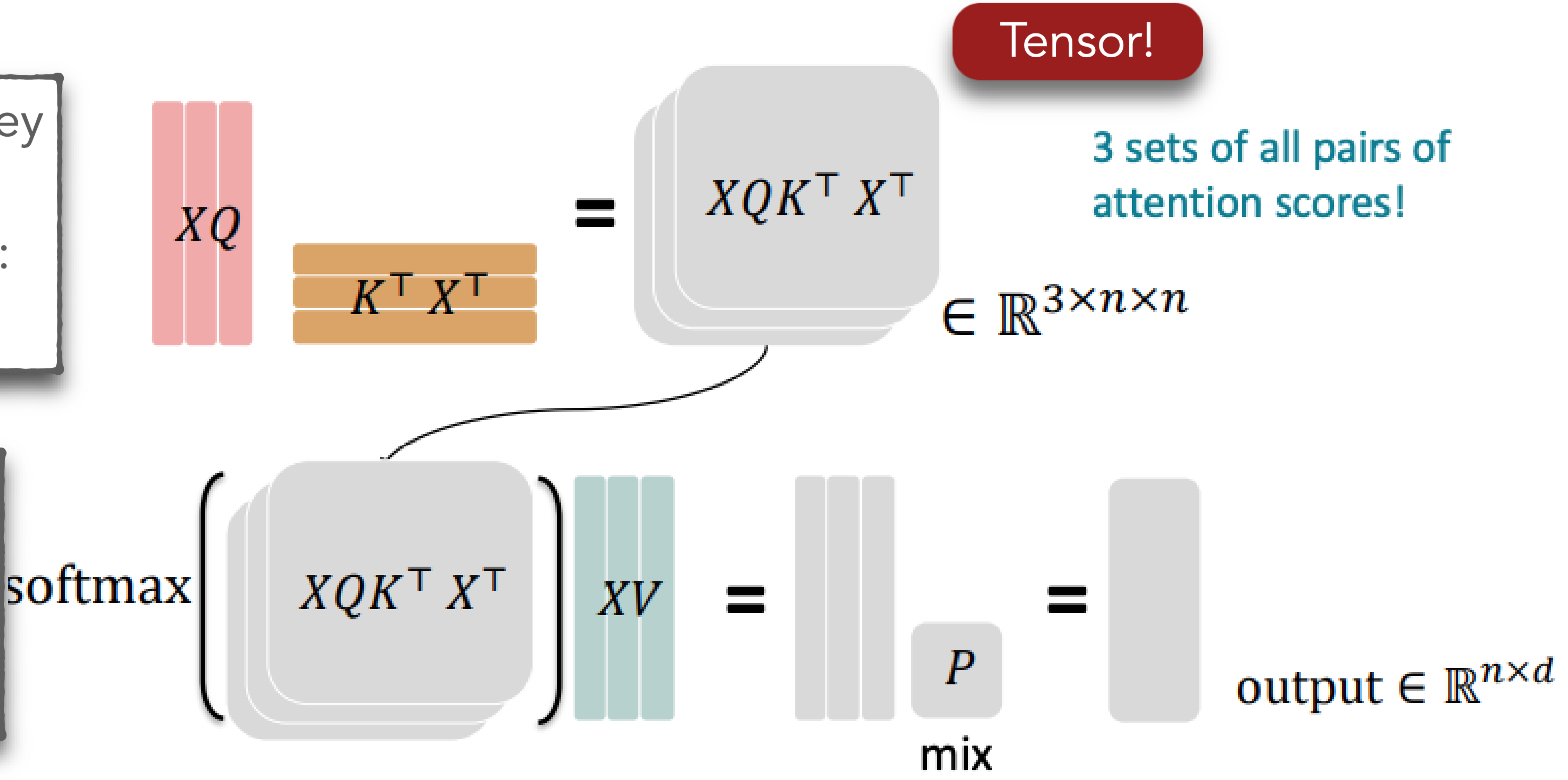
Multiheaded Attention: Visualization

Still efficient, can be parallelized!

First, take the query-key dot products in one matrix multiplication: $\mathbf{XQ}_l(\mathbf{XK}_l)^T$



Next, softmax, and compute the weighted average with another matrix multiplication.

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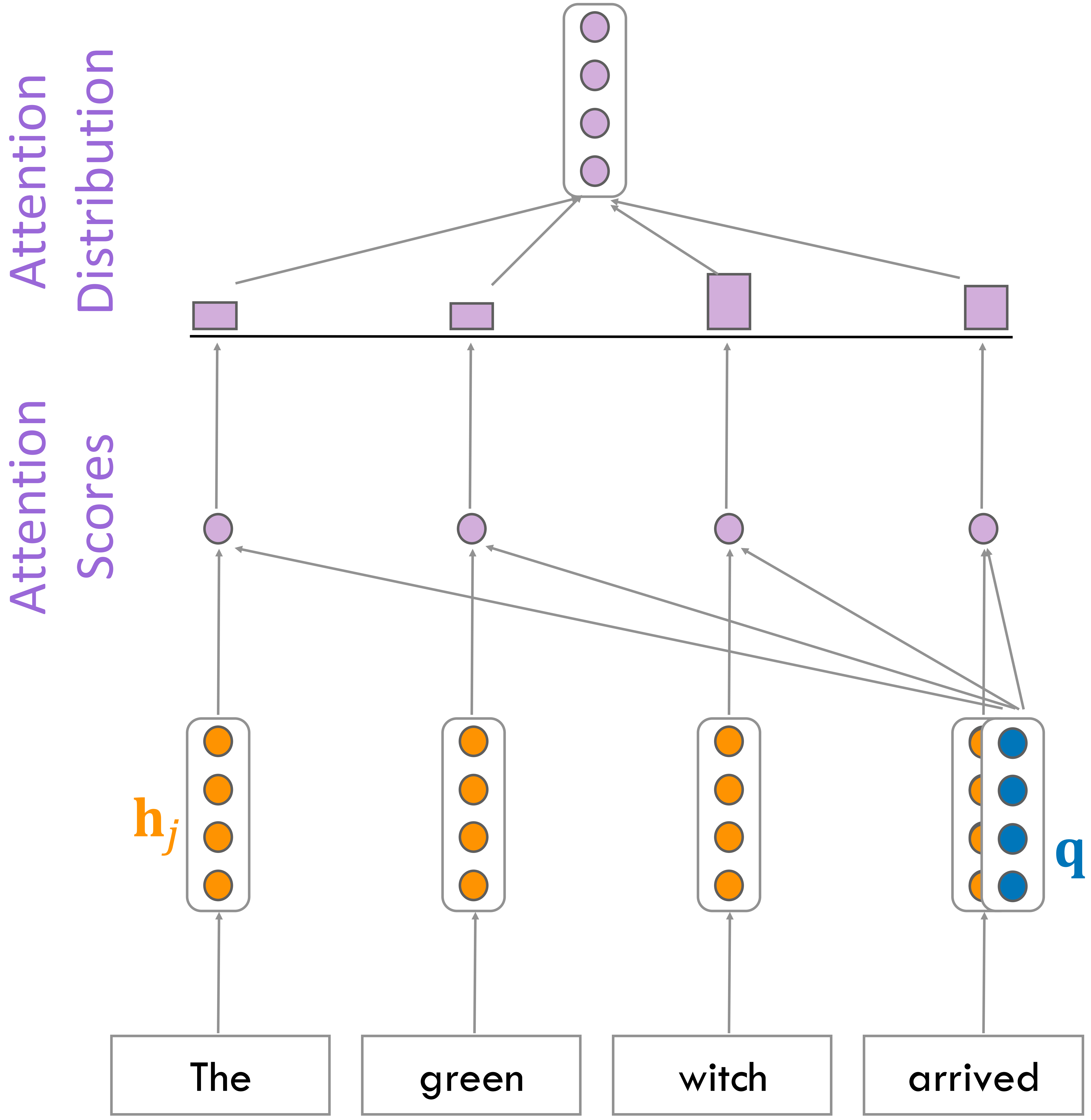
Self-Attention: Order Information?

- Not necessarily (and not typically) based on Recurrent Neural Nets
- No more order information!
- Since self-attention doesn't build in order information, we need to encode the order of the sentence in our keys, queries, and values.

Do feedforward nets contain order information?



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Transformers: Positional Embeddings

Missing: Order Information

- Consider representing each sequence index as a vector
  - $\mathbf{p}_i \in \mathbb{R}^d$, for $i \in \{1,2,\dots,n\}$ are position vectors
- Don't worry about what the $\mathbf{p}_i$ are made of yet!
- Easy to incorporate this info: just add the $\mathbf{p}_i$ to our inputs!
- Recall that $\mathbf{x}_i$ is the embedding of the word at index i. The positioned embedding is:

In deep self-attention networks, we do this at the first layer! You could concatenate them as well, but people mostly just add…

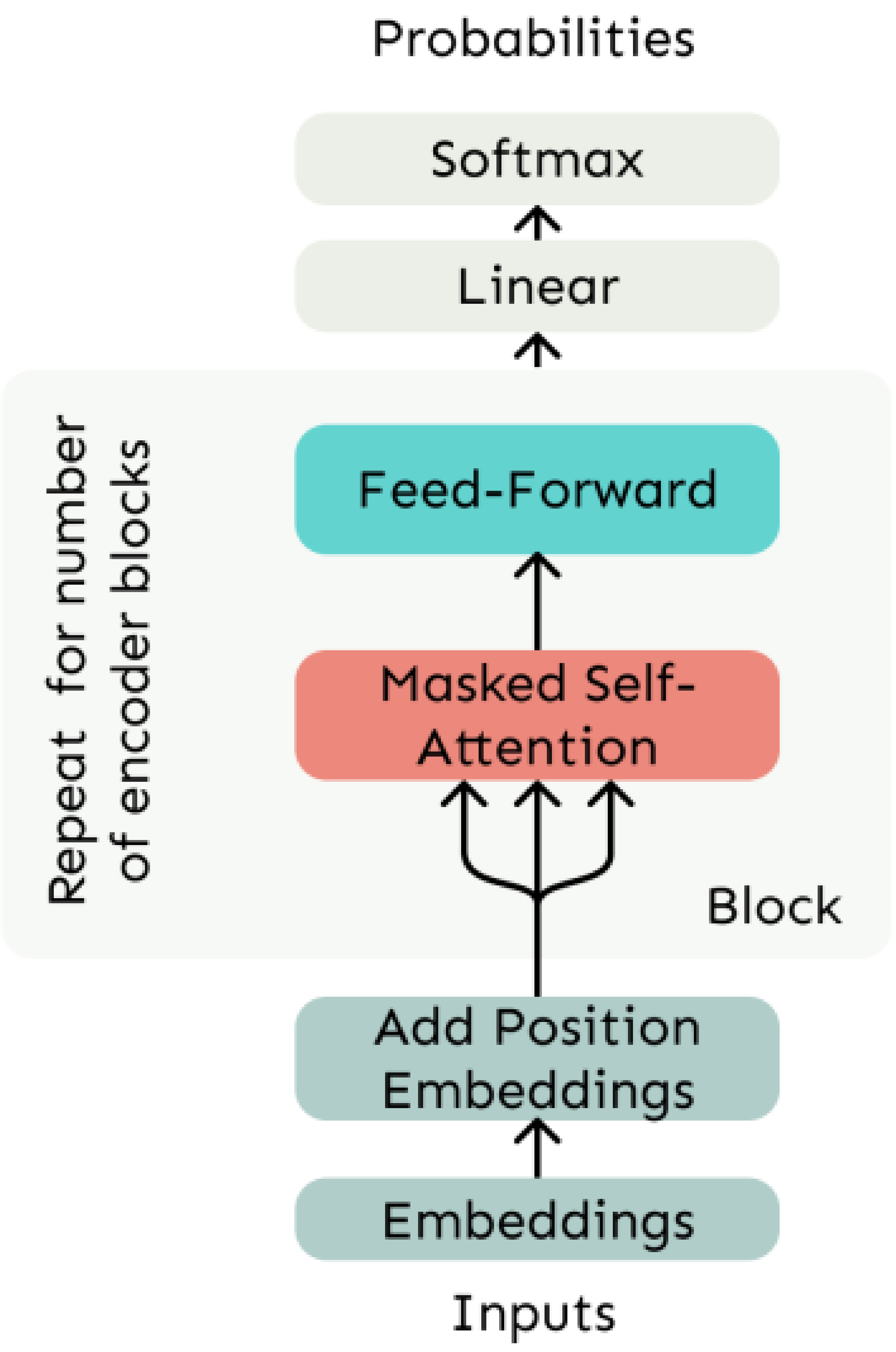
Positional Embeddings

- Maps integer inputs (for positions) to real-valued vectors
    - one per position in the entire context
- Can be randomly initialized and can let all $\mathbf{p}_i$ be learnable parameters (most common)
- Pros:
    - Flexibility: each position gets to be learned to fit the data
- Cons:
    - Definitely can't extrapolate to indices outside $1, \ldots, n$.
    - There will be plenty of training examples for the initial positions in our inputs and correspondingly fewer at the outer length limits

Putting it all together: Transformer Blocks

Self-Attention Transformer Building Block

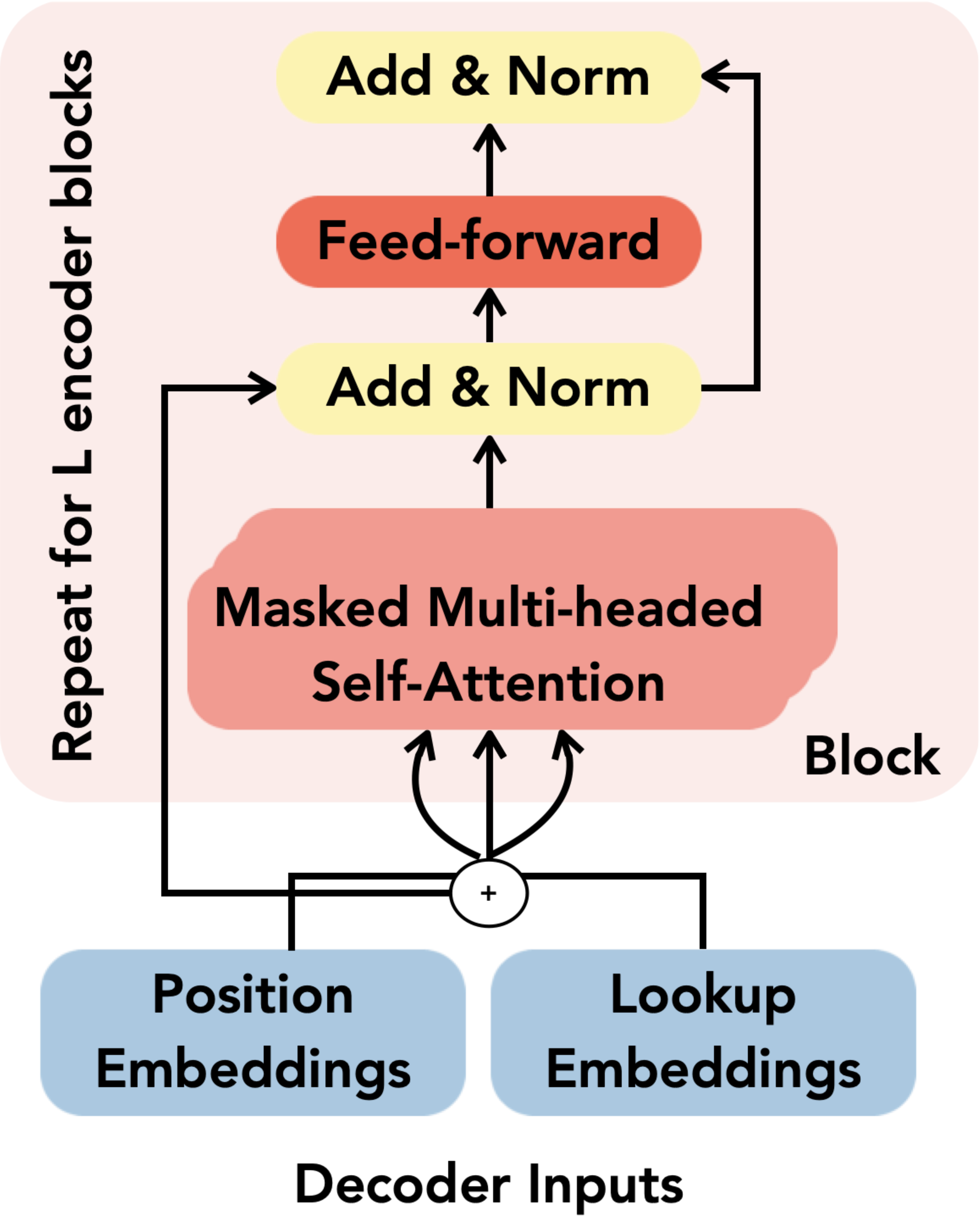
- Self-attention:
  - the basis of the method; with multiple heads
- Position representations:
  - Specify the sequence order, since self-attention is an unordered function of its inputs.
- Nonlinearities:
  - At the output of the self-attention block
  - Frequently implemented as a simple feedforward network.
- Masking:
  - In order to parallelize operations while not looking at the future.
  - Keeps information about the future from “leaking” to the past.



Transformers as Language Models

The Transformer Model

- Transformers are made up of stacks of transformer blocks, each of which is a multilayer network made by combining feedforward networks and self-attention layers, the key innovation of self-attention transformers
- The Transformer Decoder-only model corresponds to
  - a Transformer language model
- Lookup embeddings can be randomly initialized (more common) or taken from existing resources such as word2vec
  - We will look at tokenization (next class)



Transformer Decoder

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Scaled Dot Product Attention

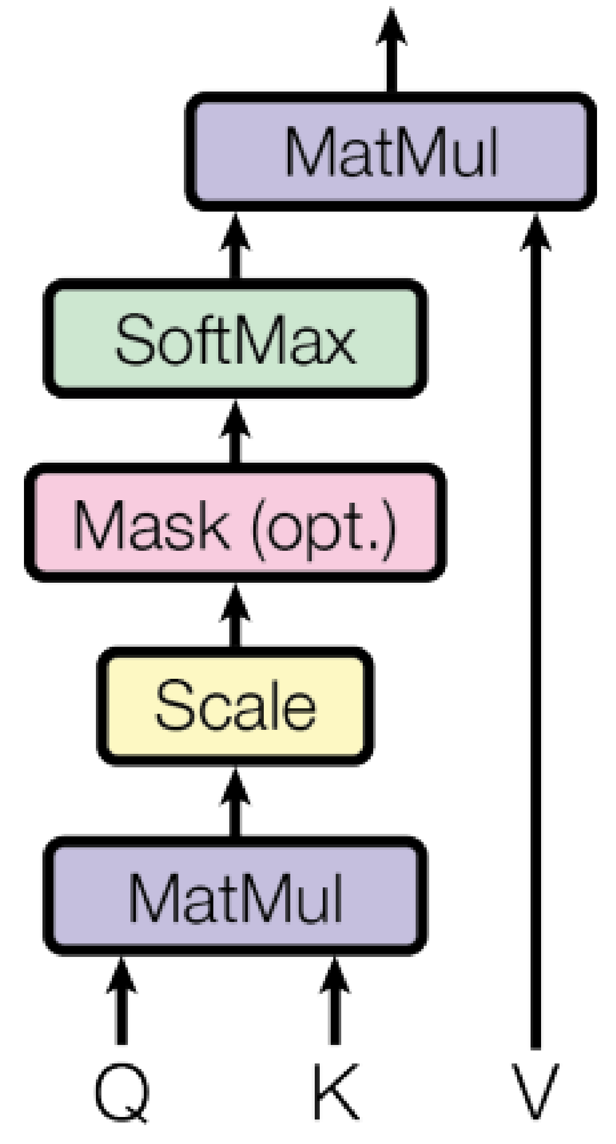
$$output_\ell = softmax(XQ_\ell K_\ell^T X^T) * XV_\ell$$

- So far: Dot product self-attention
- When dimensionality d becomes large, dot products between vectors tend to become large
- Because of this, inputs to the softmax function can be large, making the gradients small
- Now: Scaled Dot product self-attention to aid in training

$$output_\ell = softmax(\frac{XQ_\ell K_\ell^T X^T}{\sqrt{d/h}}) * XV_\ell$$

- We divide the attention scores by d/h, to stop the scores from becoming large just as a function of d/h, where h is the number of heads

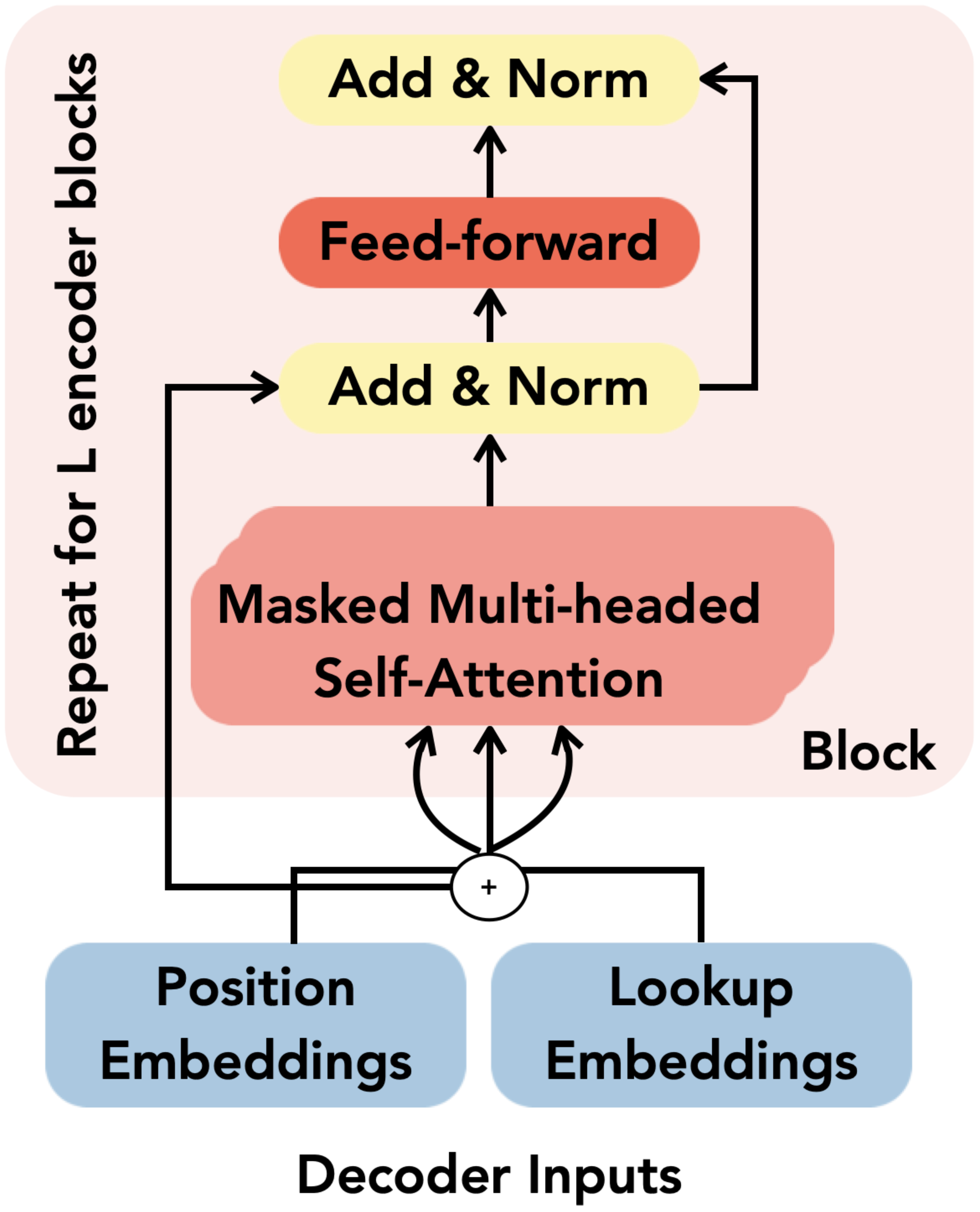
Scaled Dot-Product Attention



Attention is all you need (Vaswani et al., 2017)

The Transformer Decoder

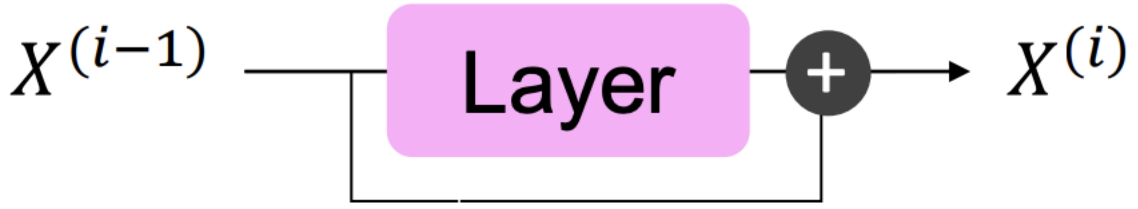
- Two optimization tricks that help training:
  - Residual Connections
  - Layer Normalization
- In most Transformer diagrams, these are often written together as "Add & Norm"
  - Add: Residual Connections
  - Norm: Layer Normalization



Transformer Decoder

Residual Connections

- Original Connections: $X^{(i)} = Layer(X^{(i-1)})$ where i represents the layer
- Residual Connections : trick to help models train better.
    - We let $X^{(i)} = X^{(i-1)} + Layer(X^{(i-1)})$
        - so we only have to learn "the residual" from the previous layer



Allowing information to skip a layer improves learning and gives higher level layers direct access to information from lower layers (He et al., 2016).

Layer Normalization

- Layer normalization is another trick to help models train faster
- Idea: cut down on uninformative variation in hidden vector values by normalizing to unit mean and standard deviation within each layer
- Let $x \in \mathbb{R}^d$ be an individual (word) vector in the model.

$$\mu = \frac{1}{d}\sum_{j=1}^{d} x_j; \mu \in \mathbb{R} \qquad \sigma = \sqrt{\frac{1}{d}\sum_{j=1}^{d}(x_j - \mu)^2}; \sigma \in \mathbb{R}$$

Result: New vector with zero mean and a standard deviation of one

$$\hat{x} = \frac{x - \mu}{\sigma}$$

Component-wise subtraction

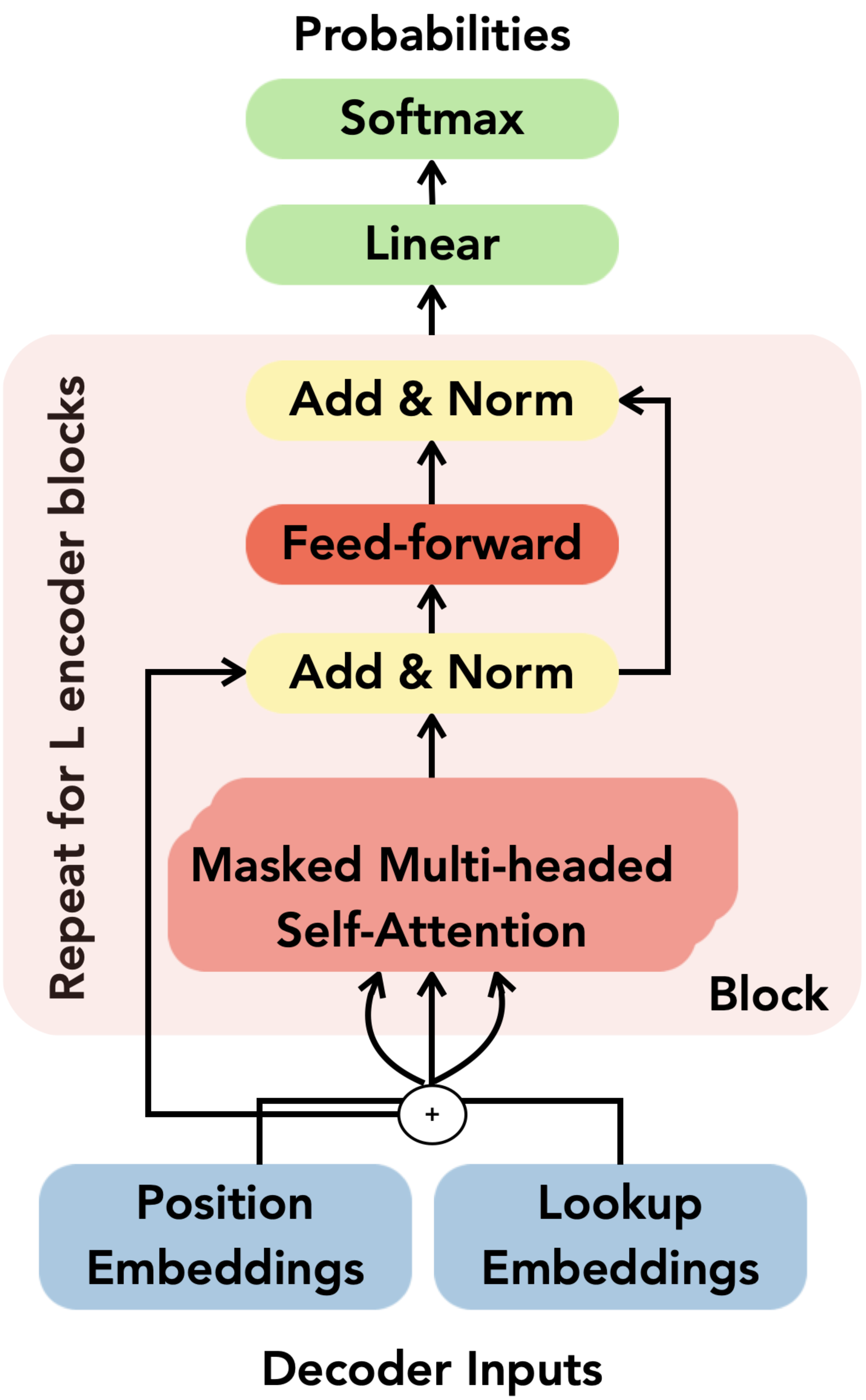
- Let $\gamma \in \mathbb{R}$ and $\beta \in \mathbb{R}^d$ be learned "gain" and "bias" parameters. (Can omit!)

$$LayerNorm = \gamma \hat{x} + \beta$$

Xu et al., 2019

The Transformer Decoder

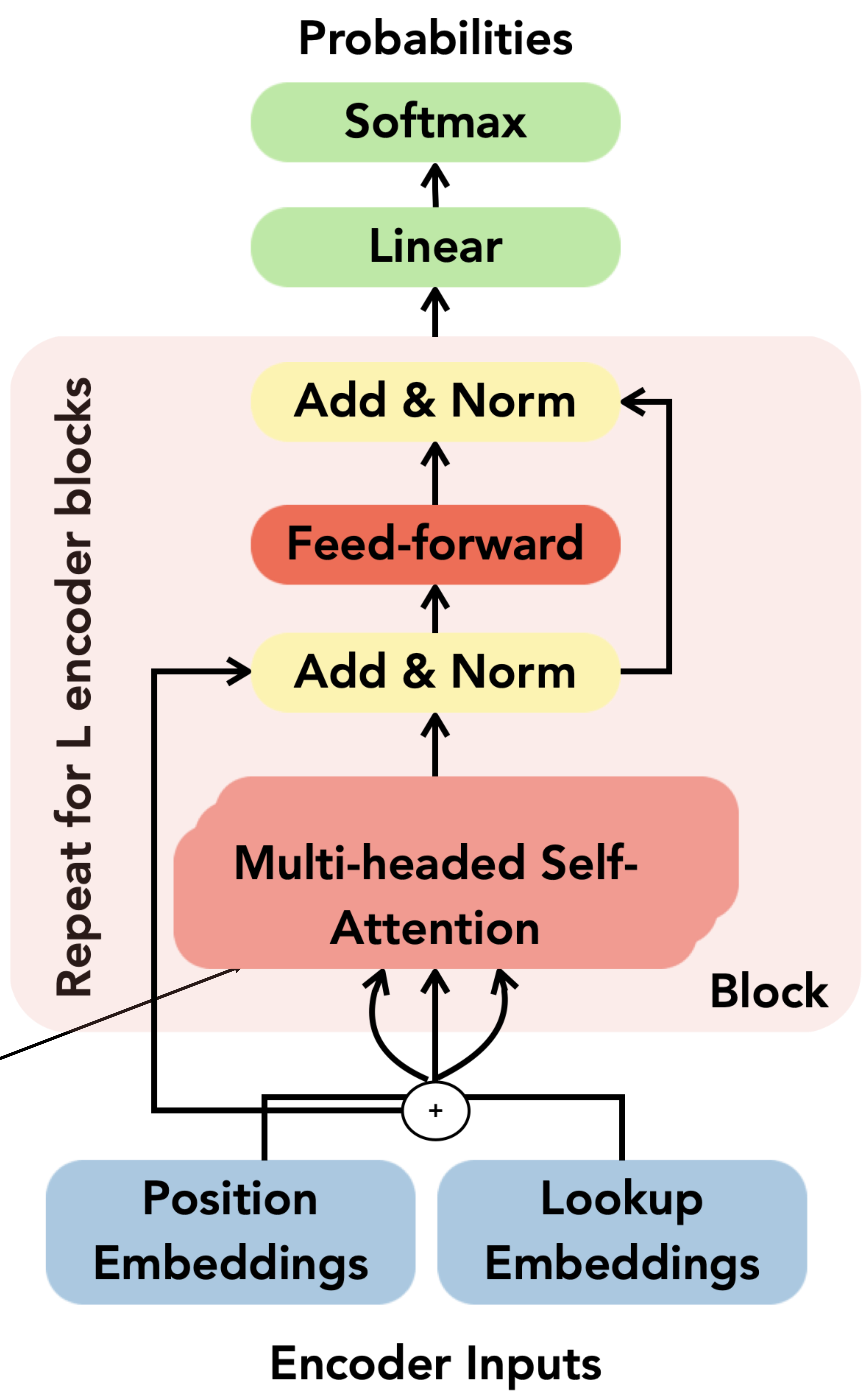
- The Transformer Decoder is a stack of Transformer Decoder Blocks.
- Each Block consists of:
  - Self-attention
  - Add & Norm
  - Feed-Forward
  - Add & Norm
- Output layer is as always a softmax layer



The Transformer Encoder

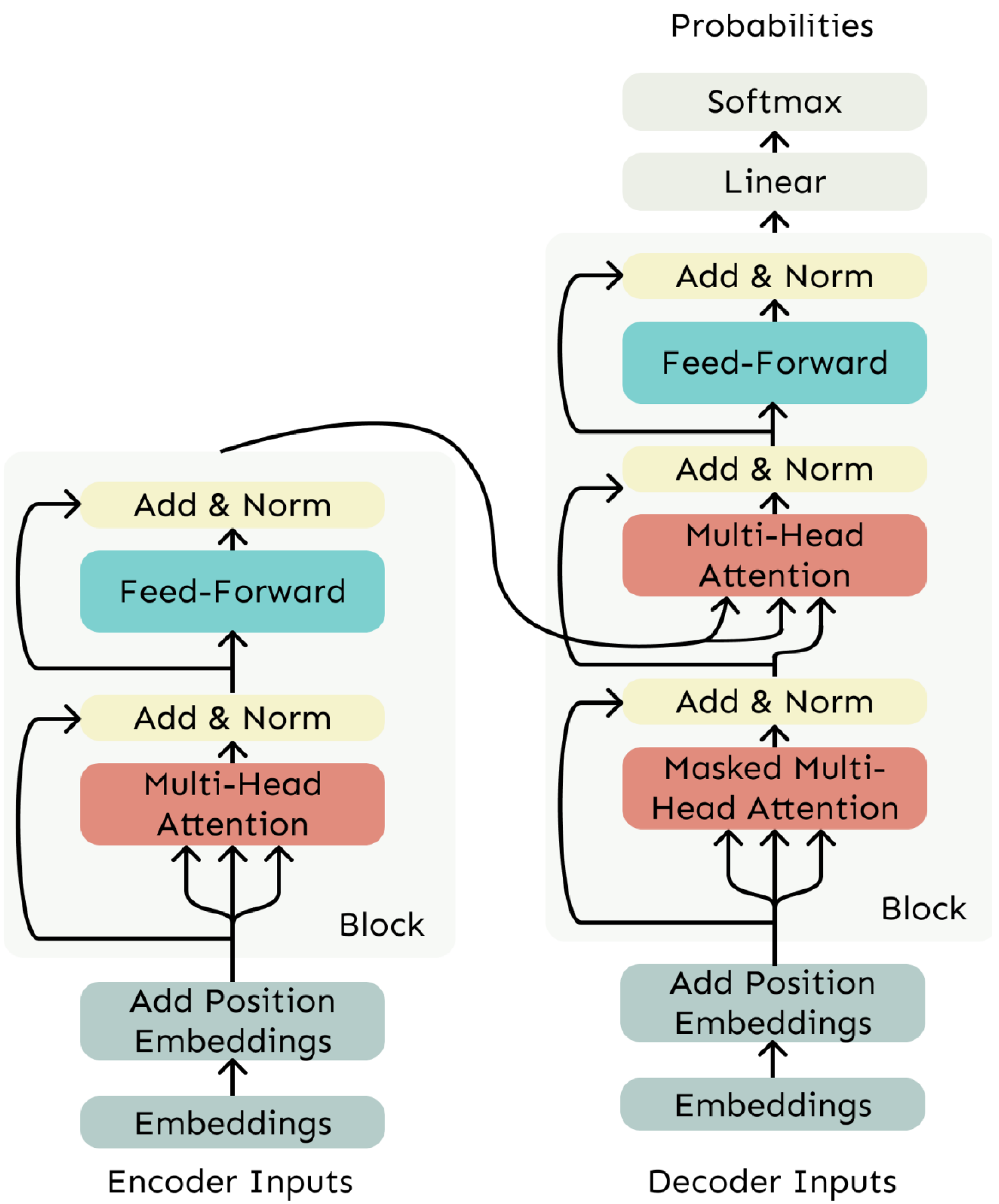
- The Transformer Decoder constrains to unidirectional context, as for language models.
- What if we want bidirectional context, i.e. both left to right as well as right to left?
- The only difference is that we remove the masking in the self-attention.
- Commonly used in sequence prediction tasks such as POS tagging
  - One output token y per input token x

No Masking!



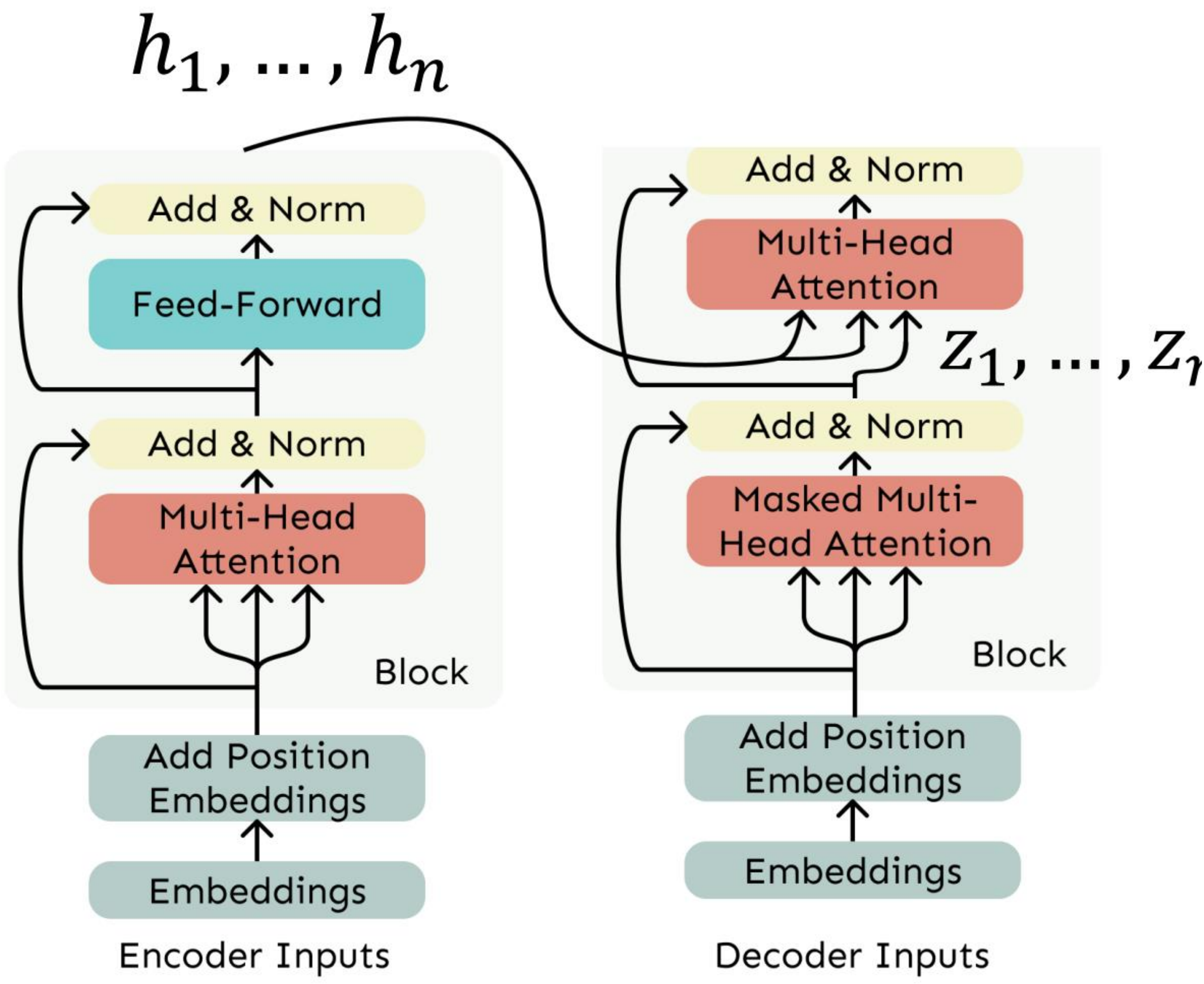
The Transformer Encoder-Decoder

- Recall that in machine translation, we processed the source sentence with a bidirectional model and generated the target with a unidirectional model.
- For this kind of seq2seq format, we often use a Transformer Encoder-Decoder.
- We use a normal Transformer Encoder.
- Our Transformer Decoder is modified to perform cross-attention to the output of the Encoder.

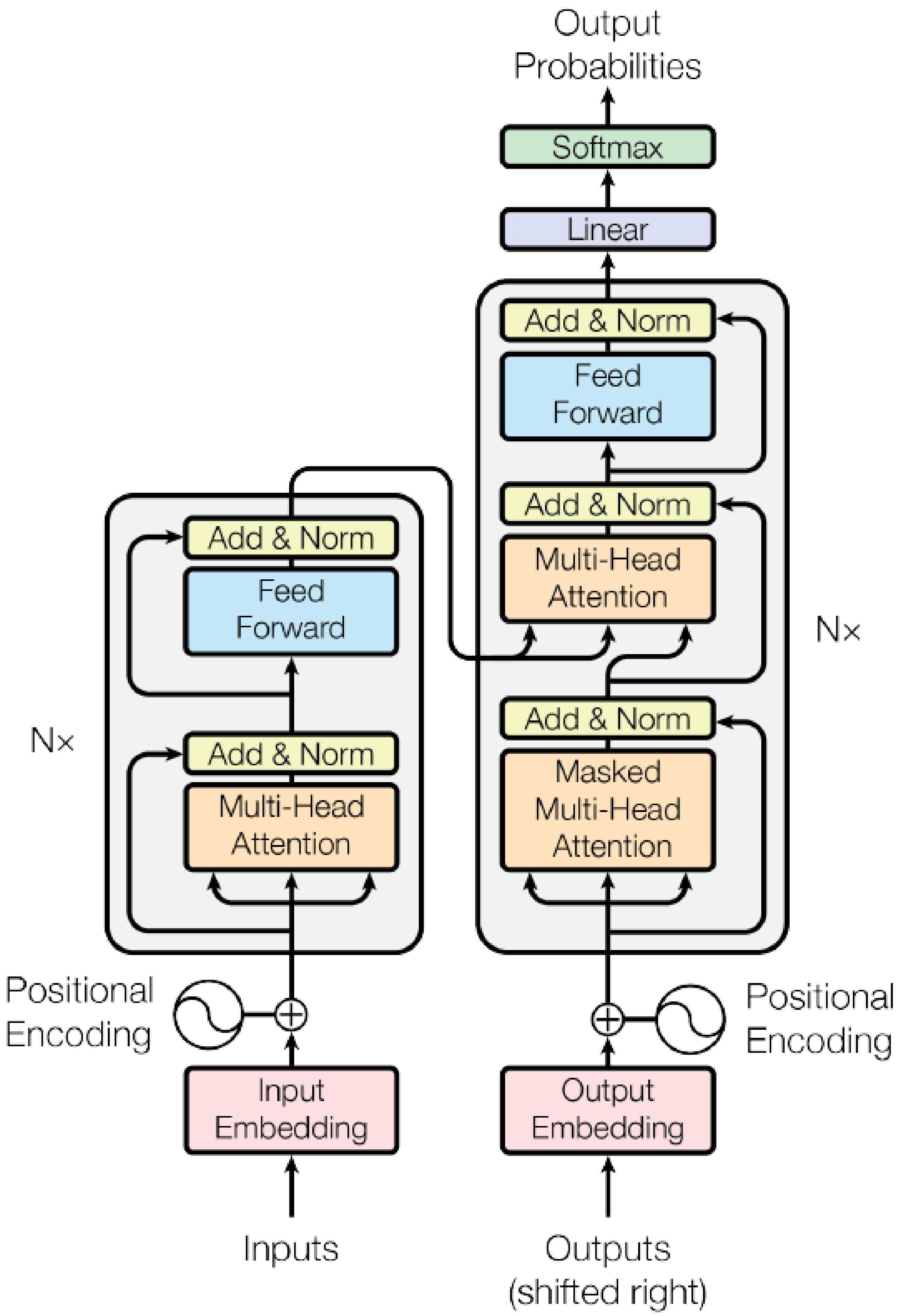


Cross Attention

- We saw that self -attention is when keys, queries, and values come from the same source.
- In the decoder, we have attention that looks more like what we saw last week.
- Let $\mathbf{h}_1, \ldots, \mathbf{h}_n$ be output vectors from the Transformer encoder; $\mathbf{h}_i \in \mathbb{R}^d$
- Let $\mathbf{z}_1, \ldots, \mathbf{z}_n$ be input vectors from the Transformer decoder, $\mathbf{z}_i \in \mathbb{R}^d$
- Then keys and values are drawn from the encoder (like a memory):
  - $\mathbf{k}_i = \mathbf{K}\mathbf{h}_i, \mathbf{v}_i = \mathbf{V}\mathbf{h}_i$
- And the queries are drawn from the decoder, $\mathbf{q}_i = \mathbf{Q}\mathbf{z}_i$



Transformer Diagram



Attention is all you need (Vaswani et al., 2017)

Transformers: Performance

Machine Translation

Language Modeling

Table 2: The Transformer achieves better BLEU scores than previous state-of-the-art models on the English-to-German and English-to-French newstest2014 tests at a fraction of the training cost.

Model	BLEU		Training Cost (FLOPs)	
	EN-DE	EN-FR	EN-DE	EN-FR
ByteNet [18]	23.75			
Deep-Att + PosUnk [39]		39.2		$1.0 \cdot 10^{20}$
GNMT + RL [38]	24.6	39.92	$2.3 \cdot 10^{19}$	$1.4 \cdot 10^{20}$
ConvS2S [9]	25.16	40.46	$9.6 \cdot 10^{18}$	$1.5 \cdot 10^{20}$
MoE [32]	26.03	40.56	$2.0 \cdot 10^{19}$	$1.2 \cdot 10^{20}$
Deep-Att + PosUnk Ensemble [39]		40.4		$8.0 \cdot 10^{20}$
GNMT + RL Ensemble [38]	26.30	41.16	$1.8 \cdot 10^{20}$	$1.1 \cdot 10^{21}$
ConvS2S Ensemble [9]	26.36	**41.29**	$7.7 \cdot 10^{19}$	$1.2 \cdot 10^{21}$
Transformer (base model)	27.3	38.1	$\mathbf{3.3 \cdot 10^{18}}$	
Transformer (big)	**28.4**	**41.8**	$2.3 \cdot 10^{19}$	

Model	**Test perplexity**	**ROUGE-L**
seq2seq-attention, $L = 500$	5.04952	12.7
Transformer-ED, $L = 500$	2.46645	34.2
Transformer-D, $L = 4000$	2.22216	33.6
Transformer-DMCA, no MoE-layer, $L = 11000$	2.05159	36.2
Transformer-DMCA, MoE-128, $L = 11000$	1.92871	37.9
Transformer-DMCA, MoE-256, $L = 7500$	1.90325	38.8

The real power of Transformers comes from pretraining language models which are then adapted for different tasks

Next Class!