Lecture 11: Transformers: Self-Attention Networks

Instructor: Swabha Swayamdipta
USC CSCI 544 Applied NLP
Oct 01, Fall 2024

Some slides adapted from Dan Jurafsky and Chris Manning

Announcements

- Thu: Quiz 3
  - Before that: **Install Lockdown Browser**
  - Cannot take Quiz 3 onwards otherwise
  - 36 students did not sign the acknowledgment for the lockdown browser, and may not be able to take the quiz in time… I won't be making exceptions for anyone
- Next Tue:
  - HW2 due - please follow naming format etc. (see Brightspace announcement)
  - Guest lecture by TA Sayan Ghosh on PyTorch for Transformers
- Next Thu: No class / Fall Break
- Tue 10/15: Midterm Exam
  - 1 hr - format similar to quizzes
- HW1 / Project Proposal grades will be available by the end of the week
- Sign up sheet now open for Paper Presentation and Final Project Presentation dates (see Brightspace announcement)

Lecture Outline

- Announcements
- Recap: Seq2Seq and Attention
- More on Attention
- Transformers: Self-Attention Networks
  - Multiheaded Attention
  - Positional Embeddings
  - Transformer Blocks
- Transformers as Encoders, Decoders and Encoder-Decoders

Recap: Sequence-to-Sequence and Attention

RNNLMs are Autoregressive Models

- Autoregressive models predict 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!

(Neural) Machine Translation

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- Sequence Generation Problem (as opposed to sequence classification)
  - $\mathbf{x}$ = Source sequence of length n
  - $\mathbf{y}$ = Target sequence of length m

Sequence-to-Sequence (Seq2seq)

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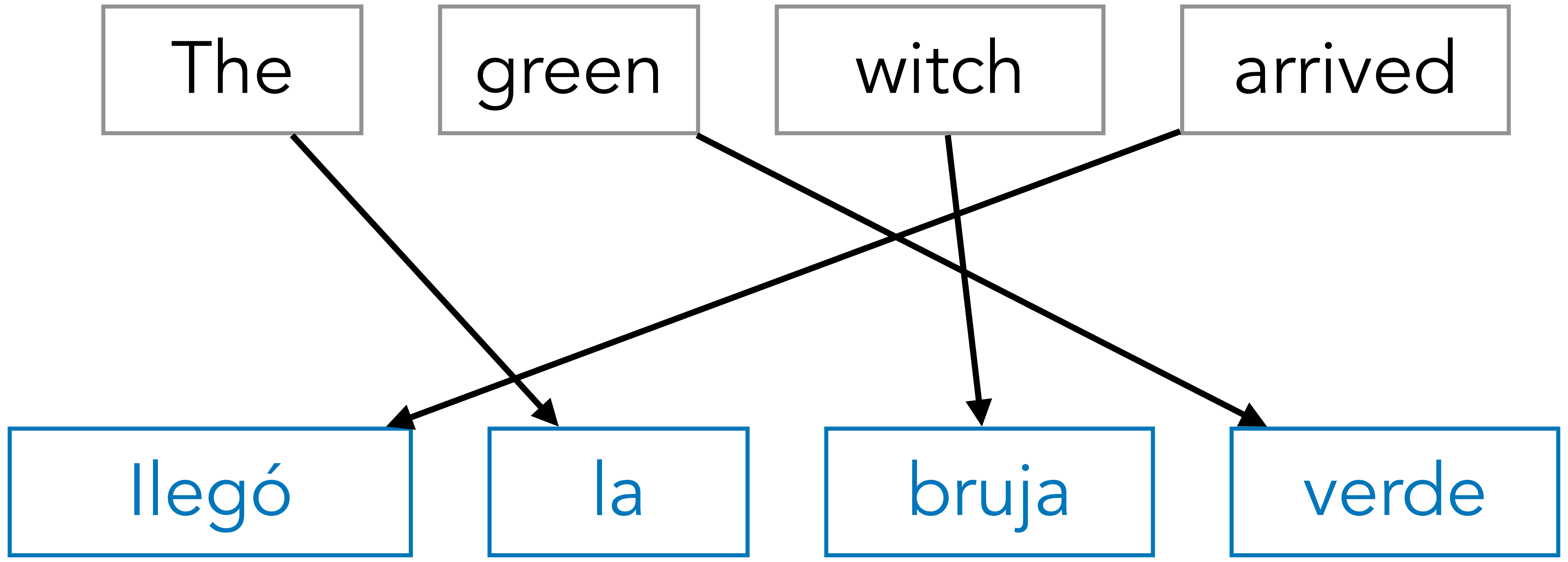
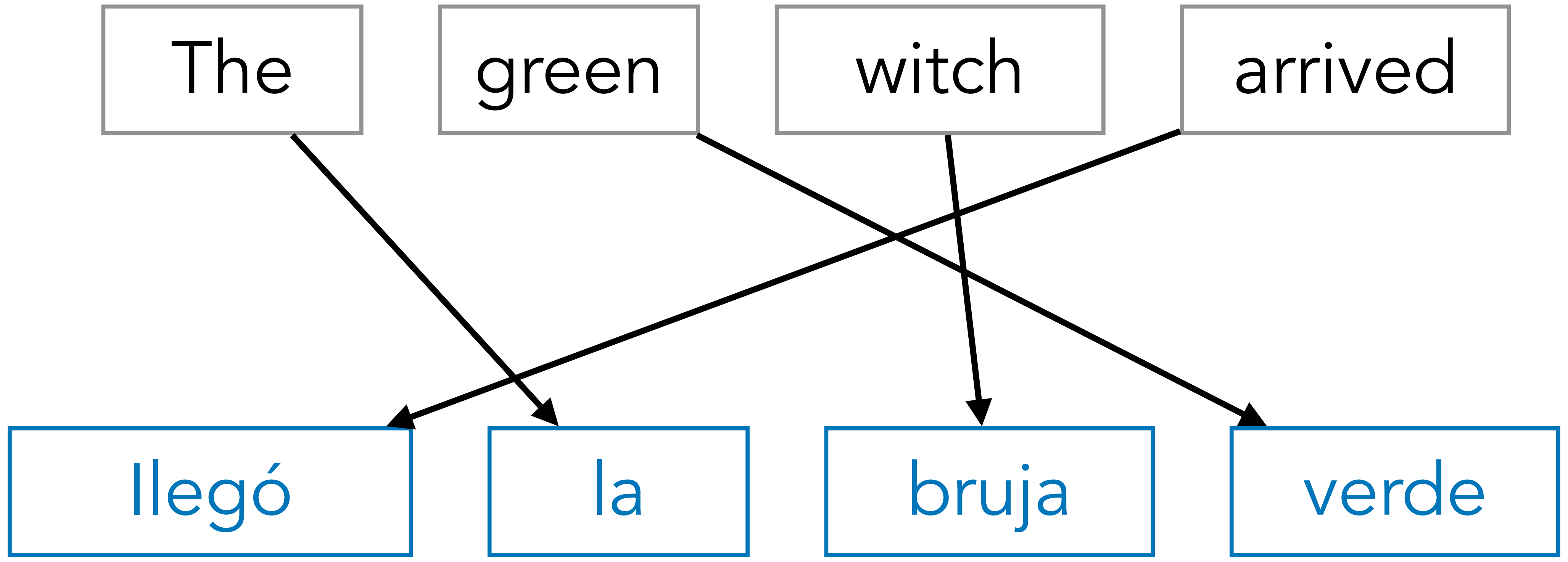


Sequence-to-Sequence (Seq2seq)

(Neural) Machine Translation

Provide rich task-appropriate context!

- Sequence Generation Problem (as opposed to sequence classification)
  - $\mathbf{x}$ = Source sequence of length n
  - $\mathbf{y}$ = Target sequence of length m
- Different from regular generation from an LM
  - Since we expect the target sequence to serve a specific utility (translate the source)



Sequence-to-Sequence (Seq2seq)

Sequence-to-Sequence Models

- Models capable of generating contextually appropriate, arbitrary length, output sequences given an input sequence.
- The key idea underlying these networks is the use of an **encoder network** that takes an input sequence and creates a contextualized representation of it, often called the context.
- This representation is then passed to a **decoder network** which generates a task- specific output sequence.

Encoder-Decoder Networks

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Encoder-decoder networks consist of three components:

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1. An **encoder** that accepts an input sequence, $\mathbf{x}_{1:n}$ and generates a corresponding sequence of contextualized representations, $\mathbf{h}_1^e \ldots \mathbf{h}_n^e$

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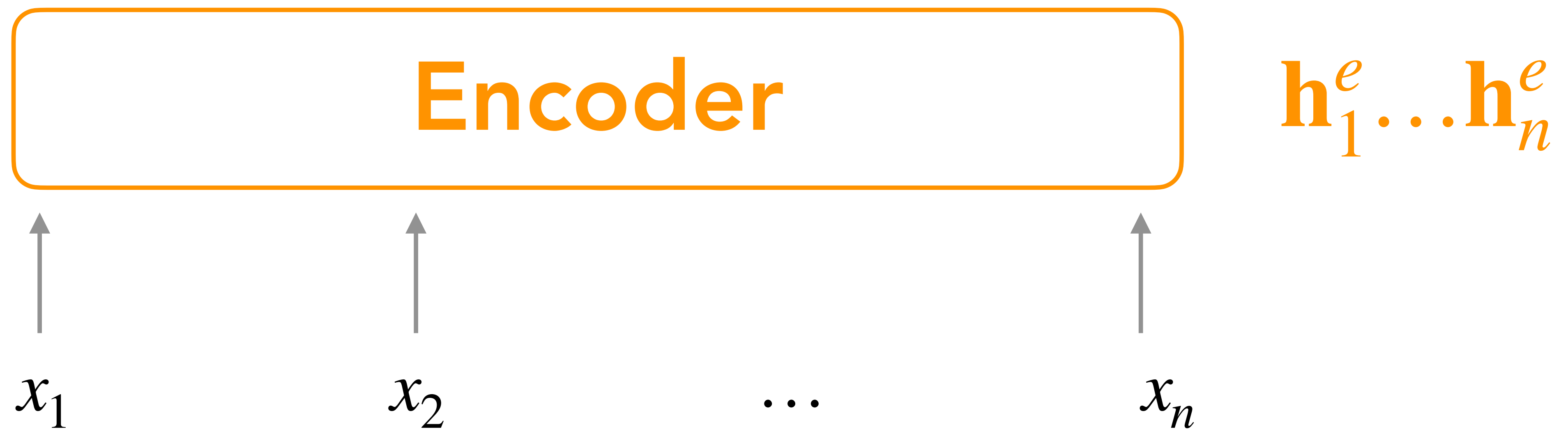

Encoder-Decoder Networks

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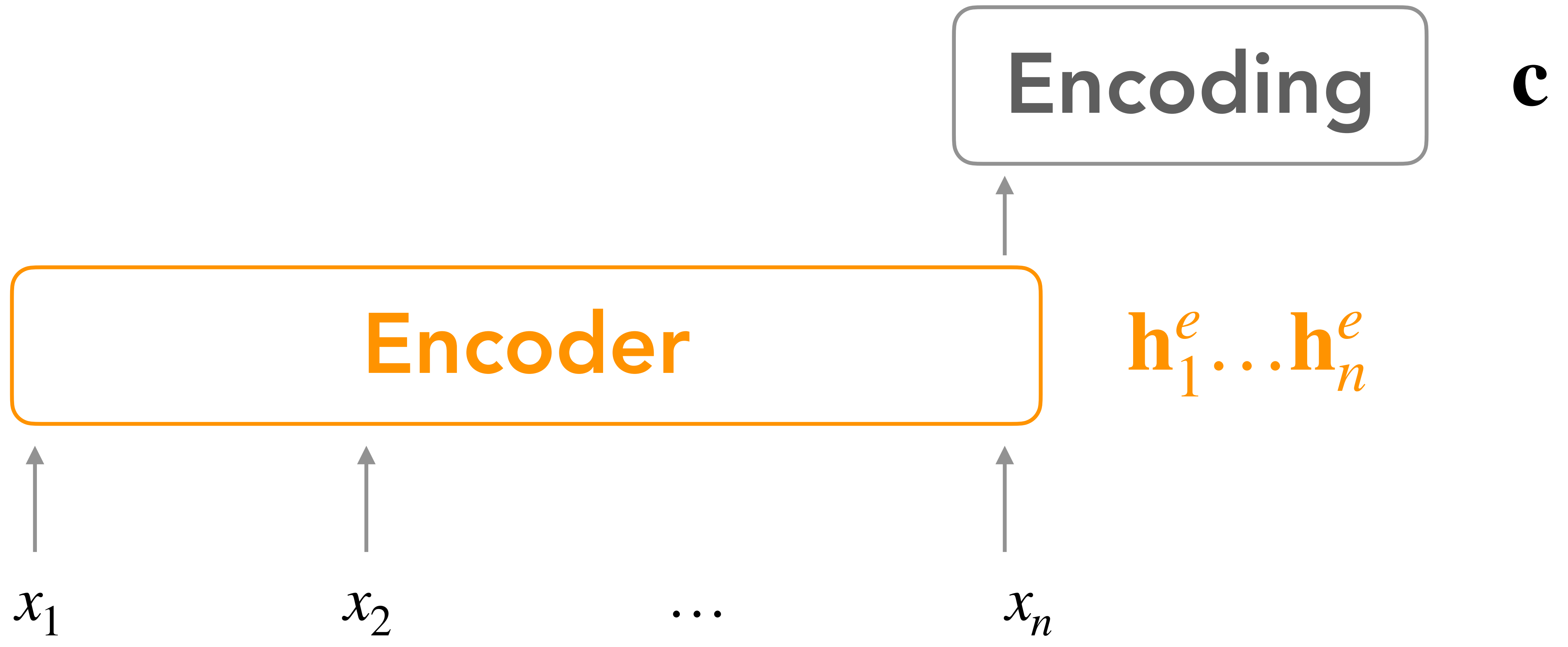
2. A **encoding** vector, $\mathbf{c}$ which is a function of $\mathbf{h}^e_1 \ldots \mathbf{h}^e_n$ and conveys the essence of the input to the decoder



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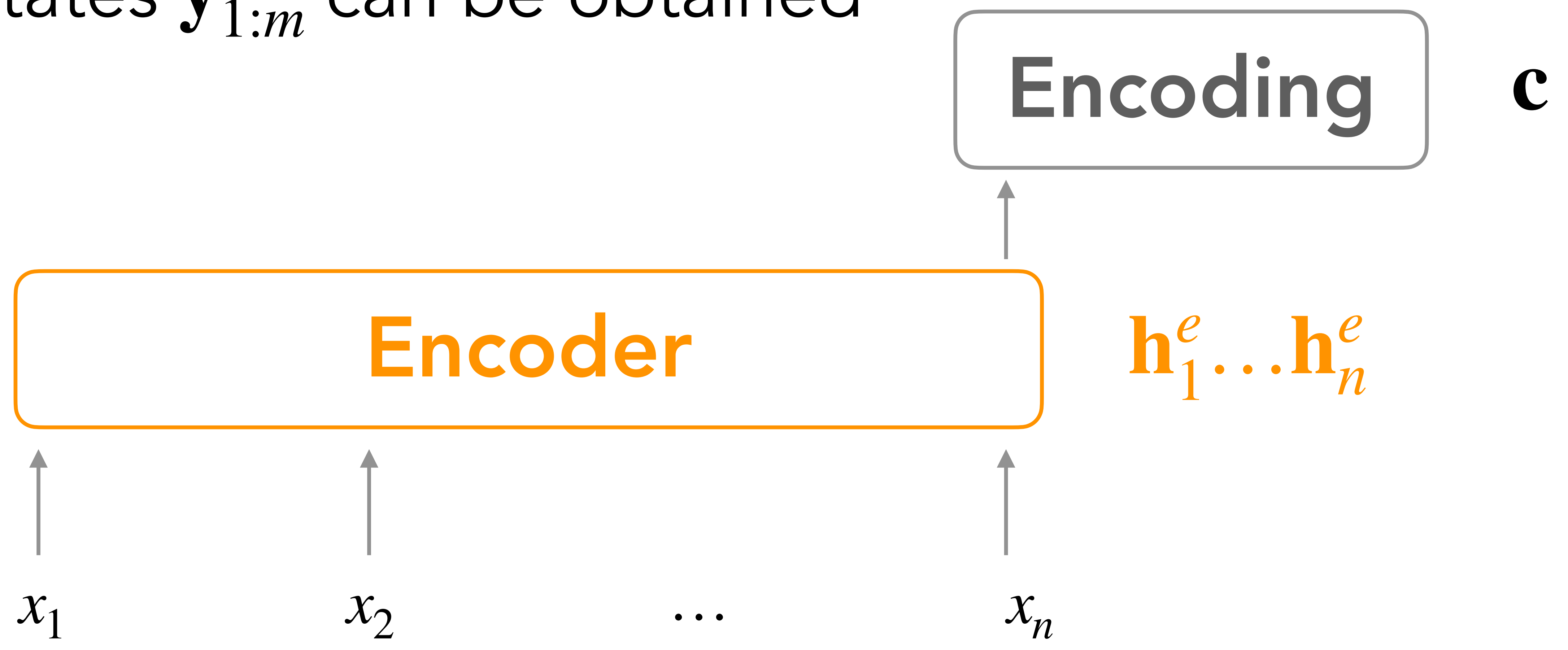
3. A **decoder** which accepts $\mathbf{c}$ as input and generates an arbitrary length sequence of hidden states $\mathbf{h}^d_1 \ldots \mathbf{h}^d_m$, from which a corresponding sequence of output states $\mathbf{y}_{1:m}$ can be obtained



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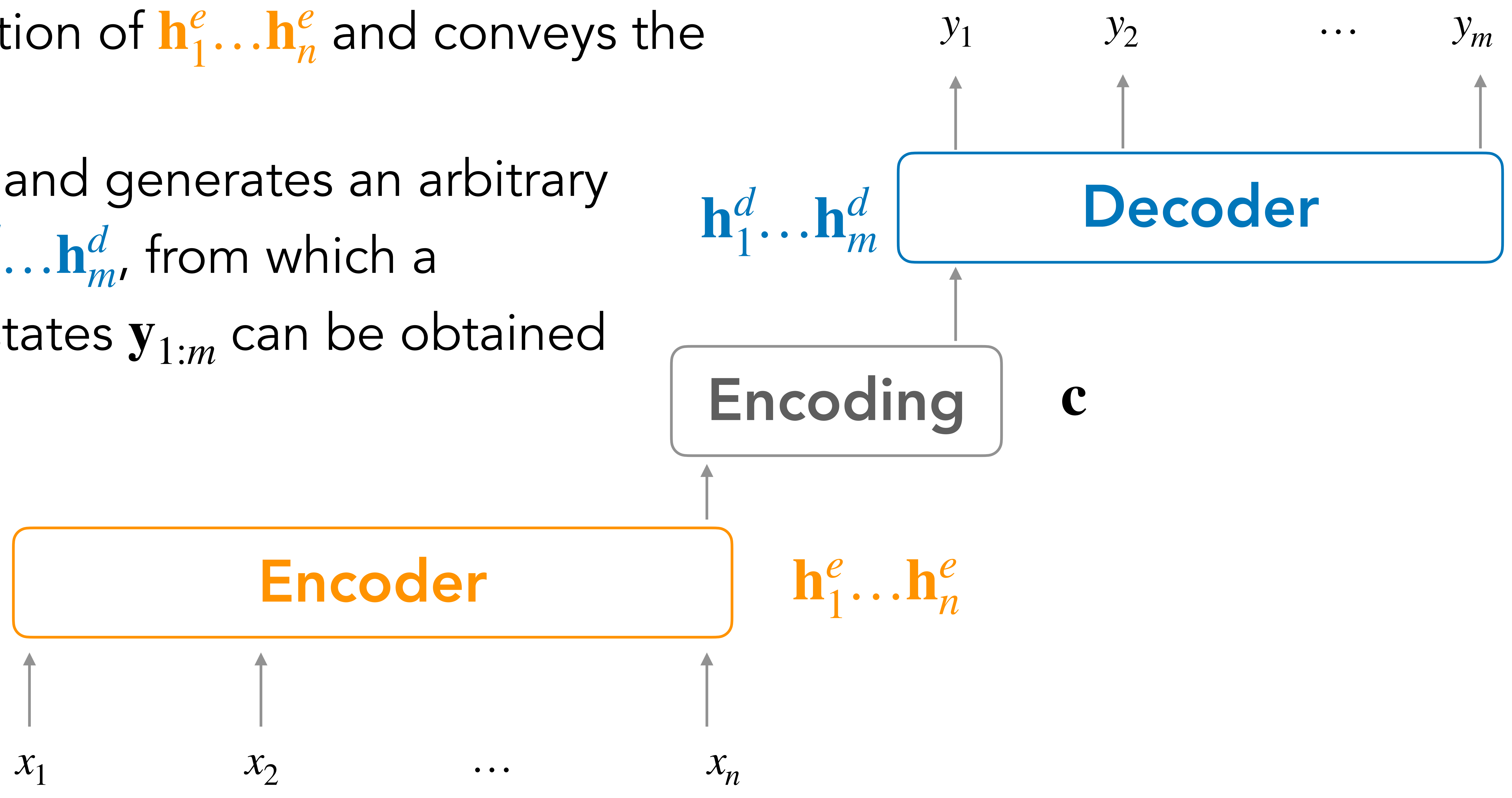

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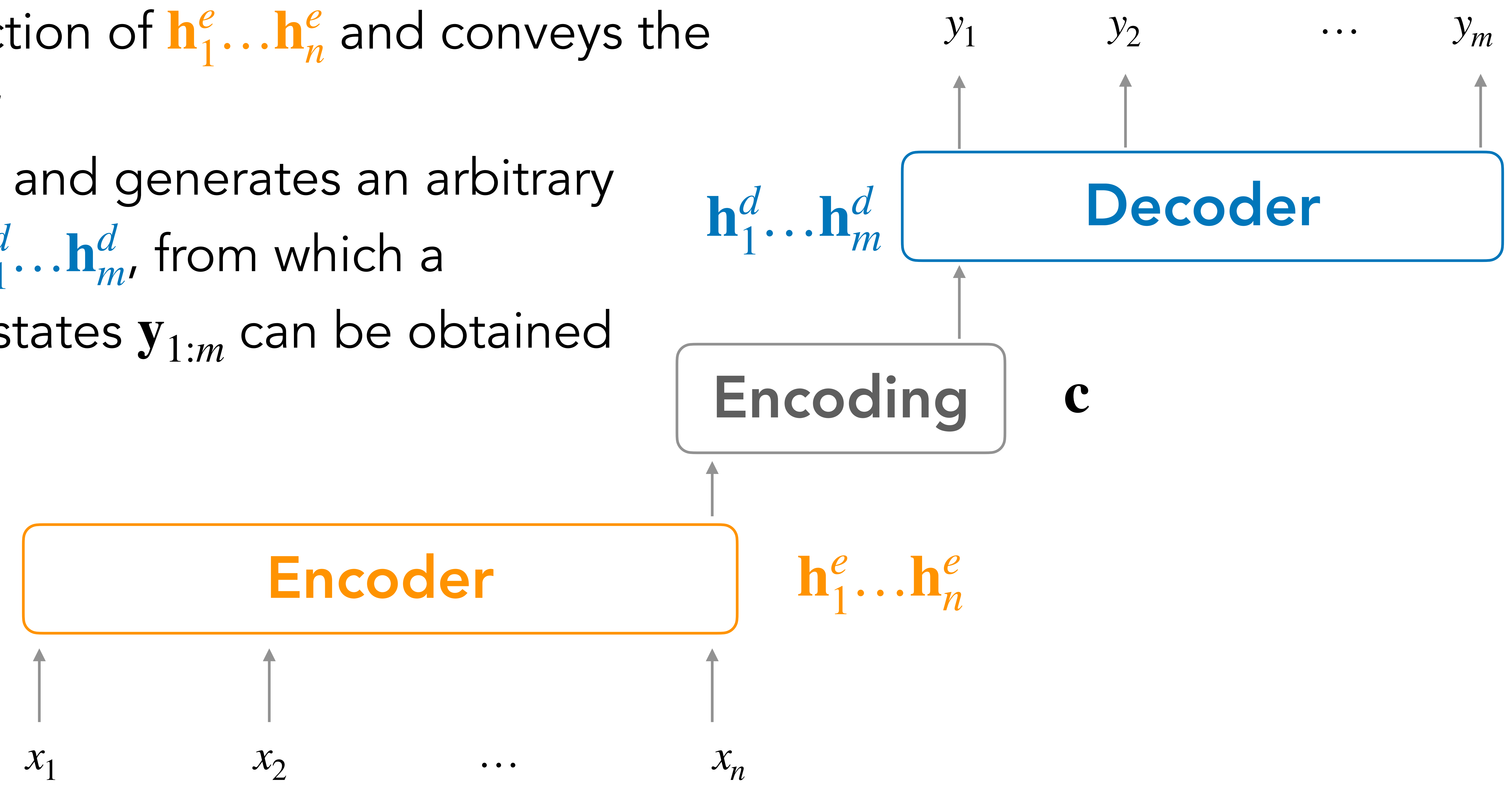

Encoders and decoders can be made of FFNNs, RNNs, or Transformers

The	green	witch	arrived

Source Sentence $\mathbf{x}$

Produces an encoding of the source sequence

Encoder RNN

The	green	witch	arrived

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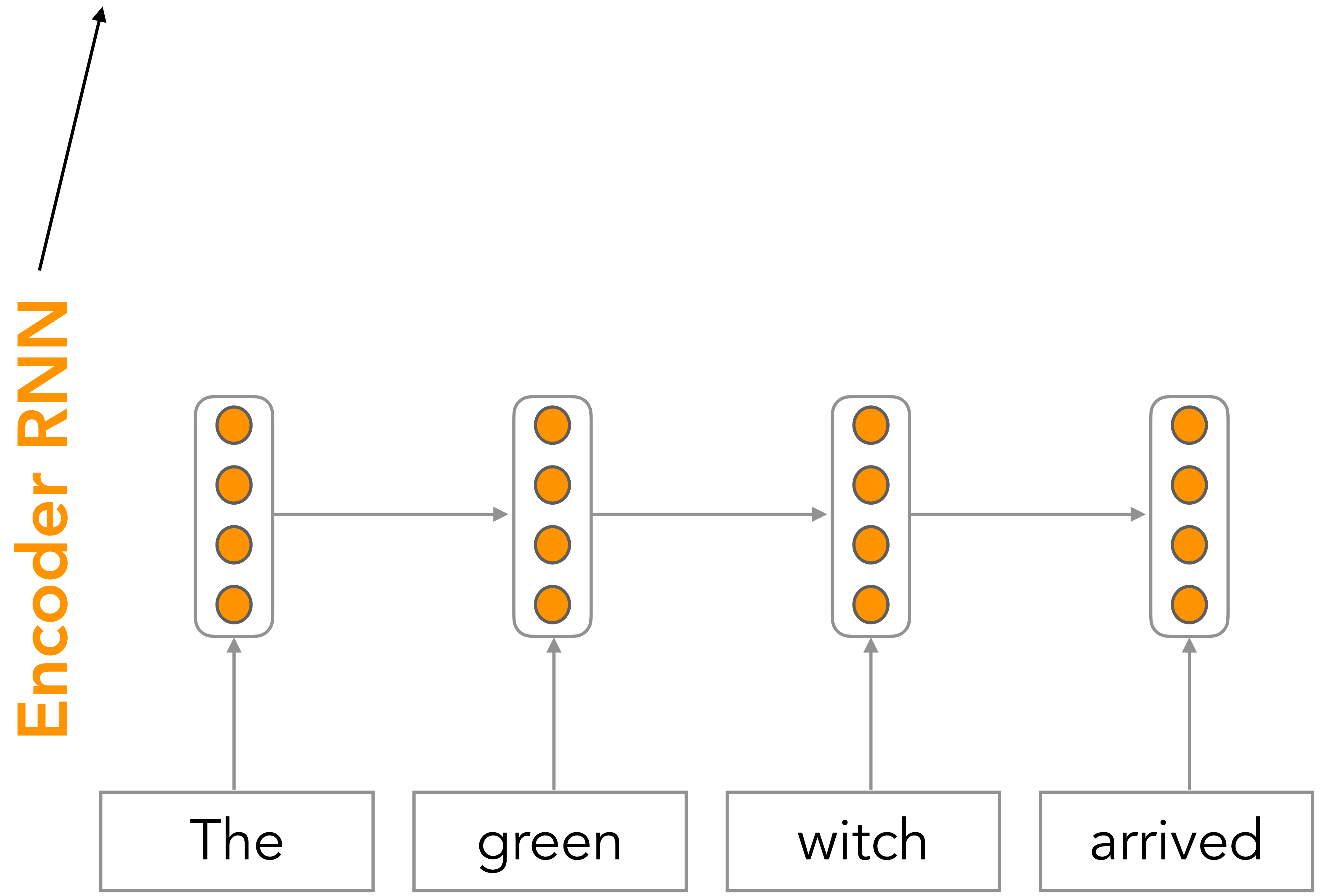
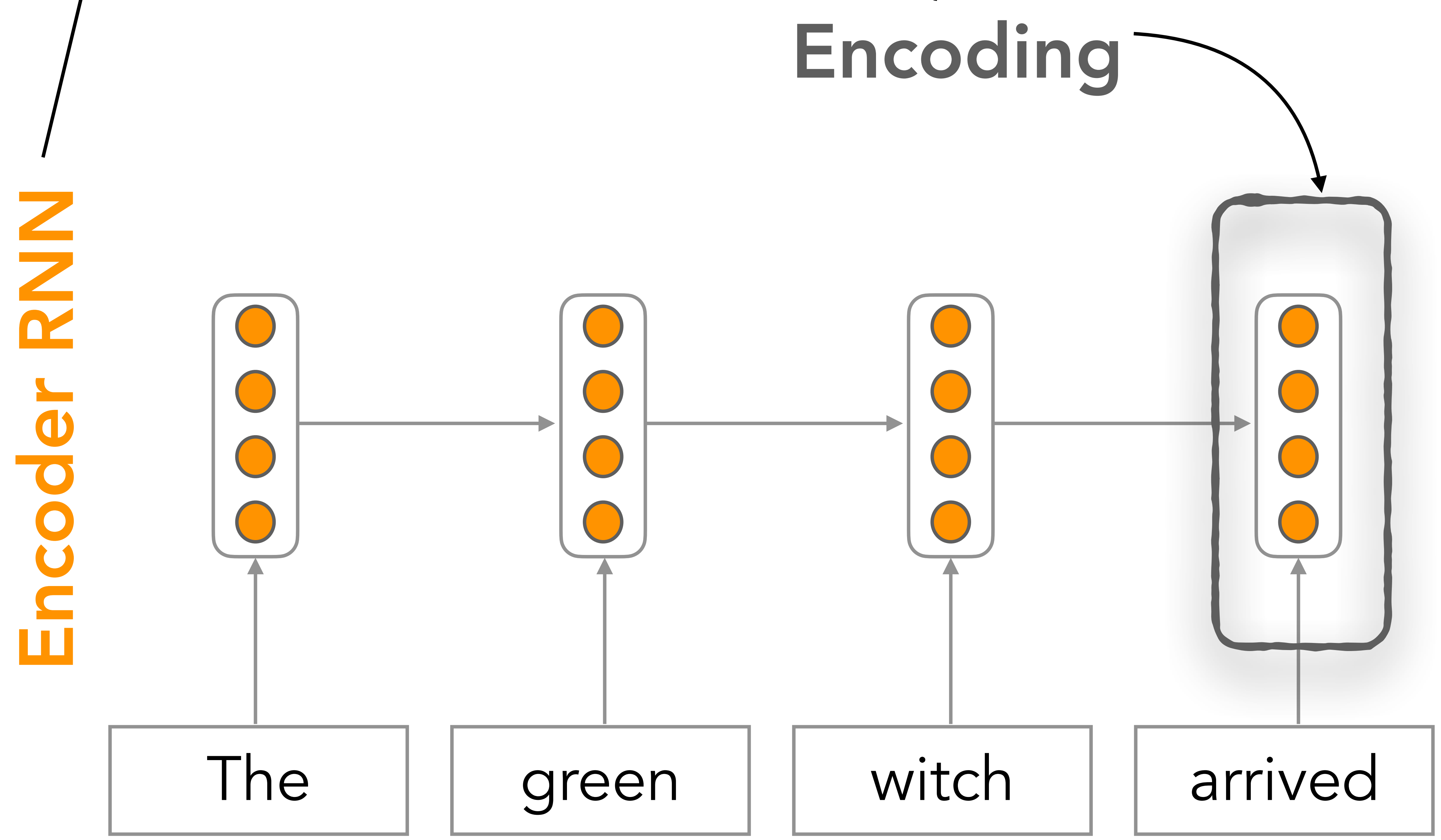
Produces an encoding of the source sequence



Source Sentence x

Produces an encoding of the source sequence

Represents input sequence. Provides initial hidden state for Decoder RNN



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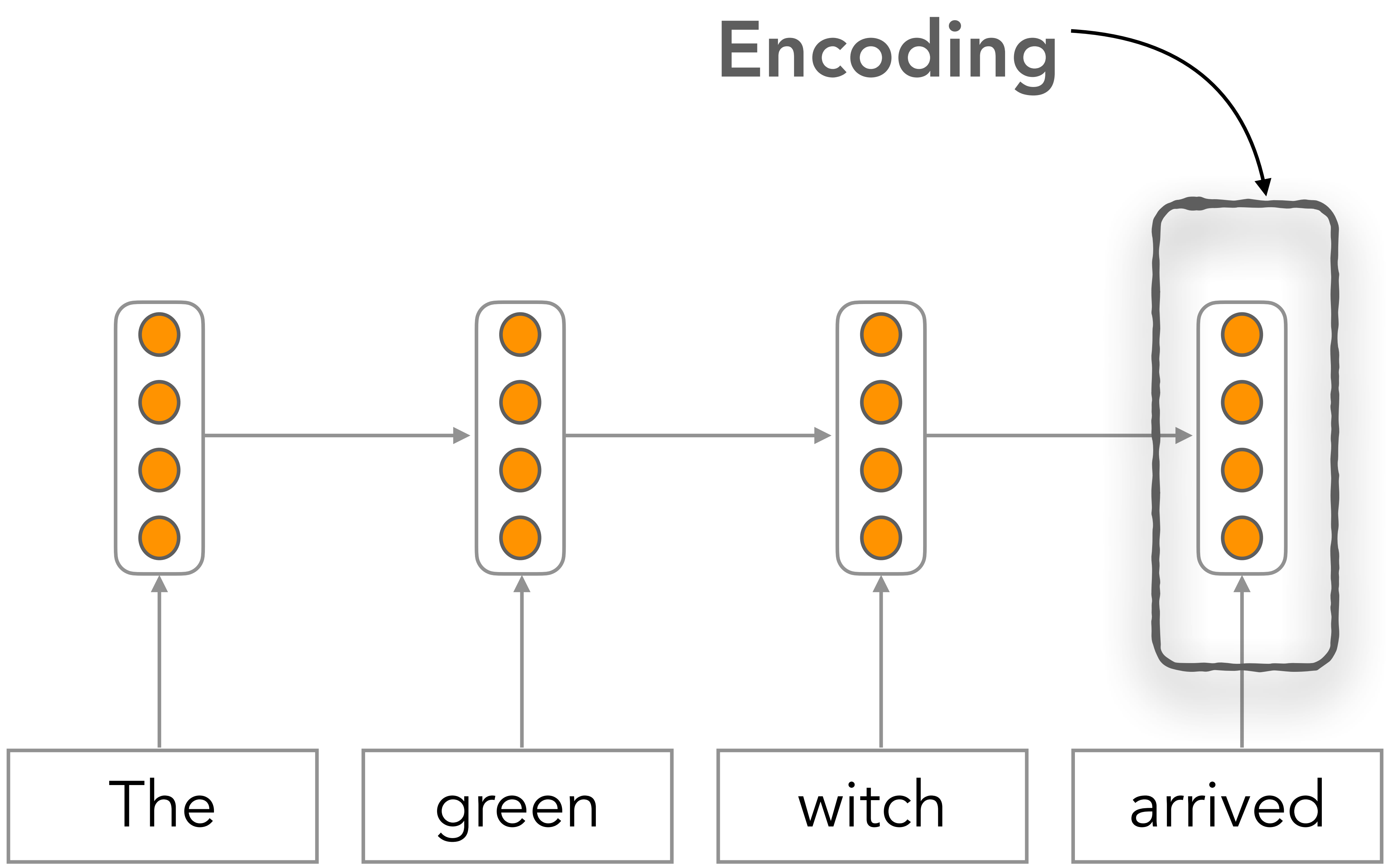


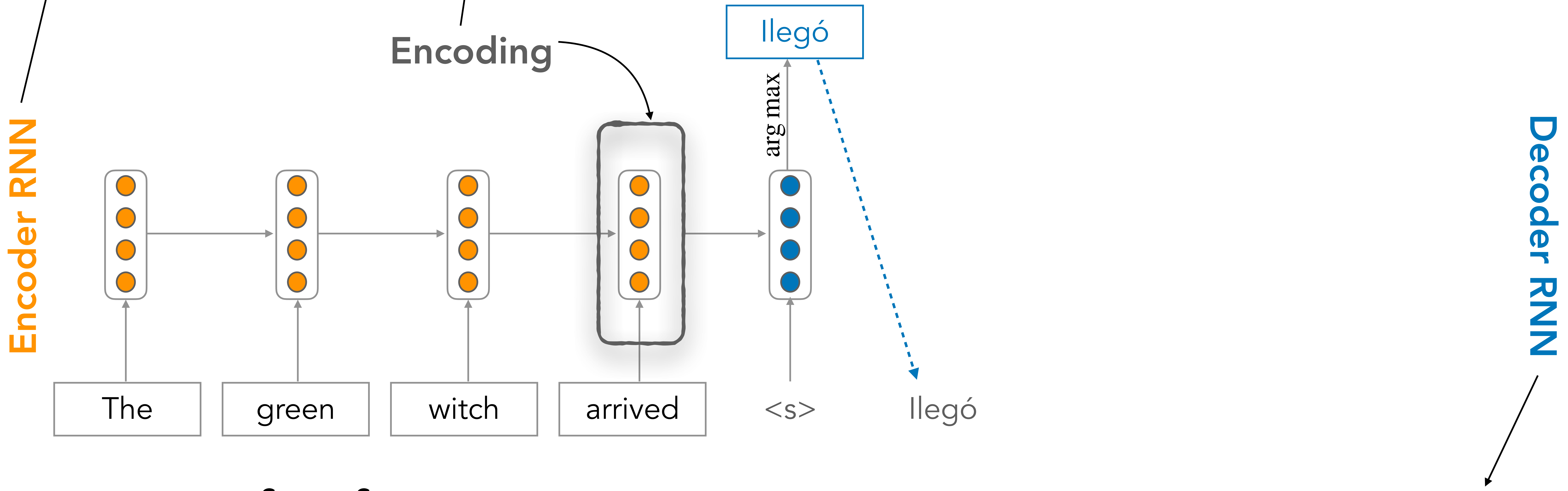
Source Sentence x

Decoder RNN

Language Model that produces the target sentence conditioned on the encoding

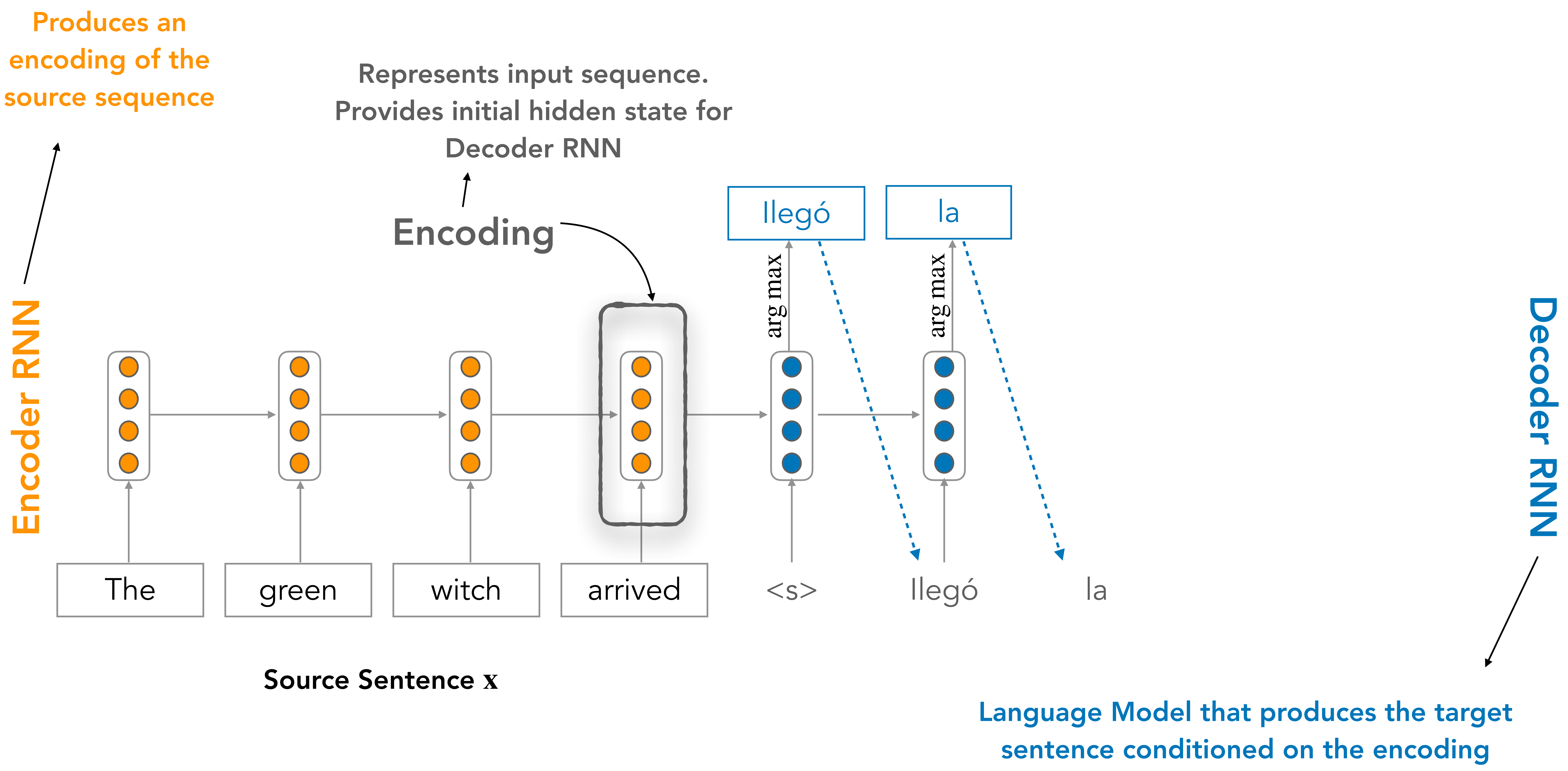
Produces an encoding of the source sequence

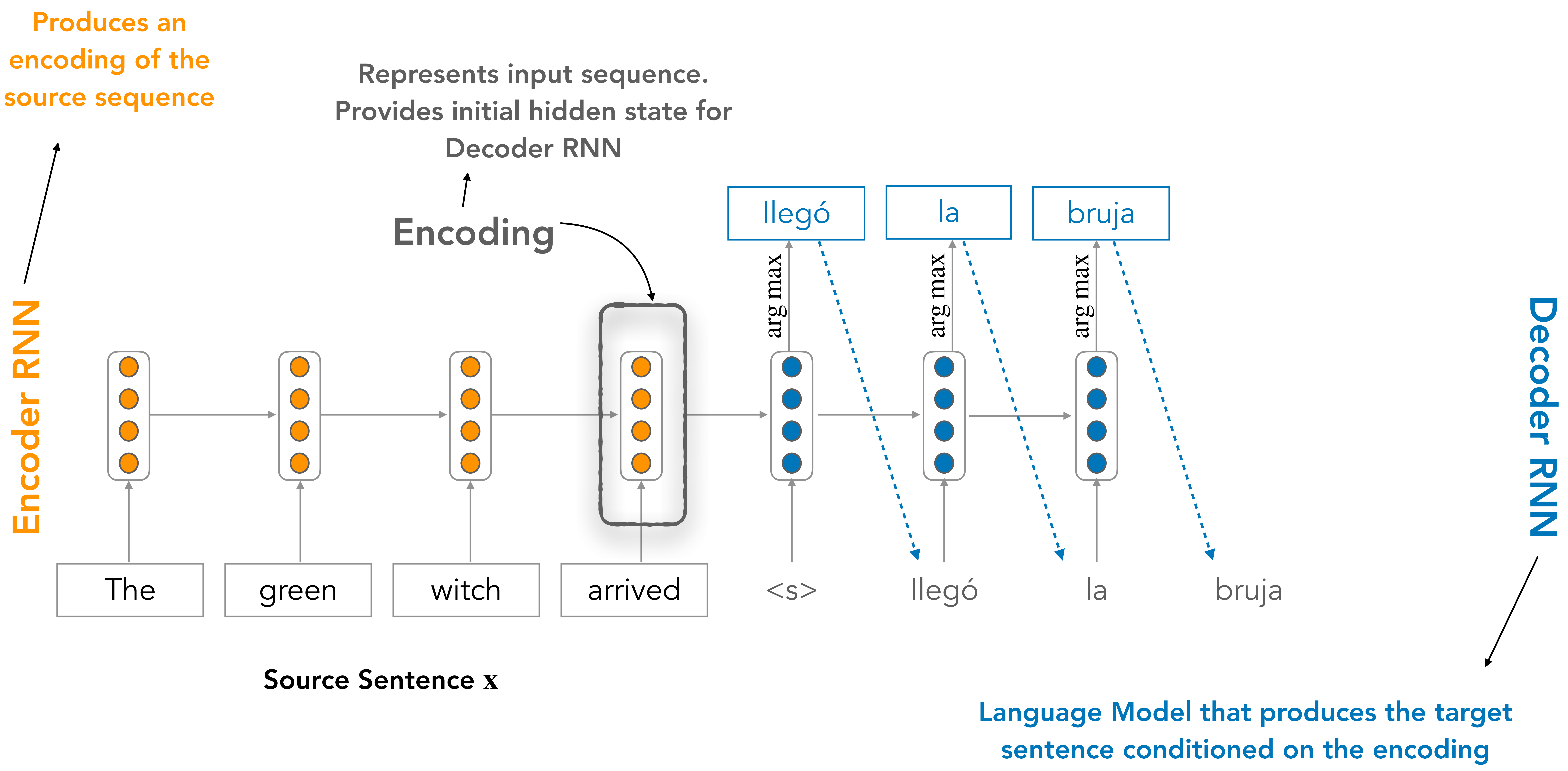
Represents input sequence. Provides initial hidden state for Decoder RNN



Source Sentence **x**

Language Model that produces the target sentence conditioned on the encoding


Produces an encoding of the source sequence
Represents input sequence. Provides initial hidden state for Decoder RNN
Encoding
Encoder RNN
Decoder RNN
llegó
la
arg max
arg max
The
green
witch
arrived
<s>
llegó
la
Source Sentence $\mathbf{x}$
Language Model that produces the target sentence conditioned on the encoding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llegó
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Decoder RNN
Source Sentence $\mathbf{x}$
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Produces an encoding of the source sequence

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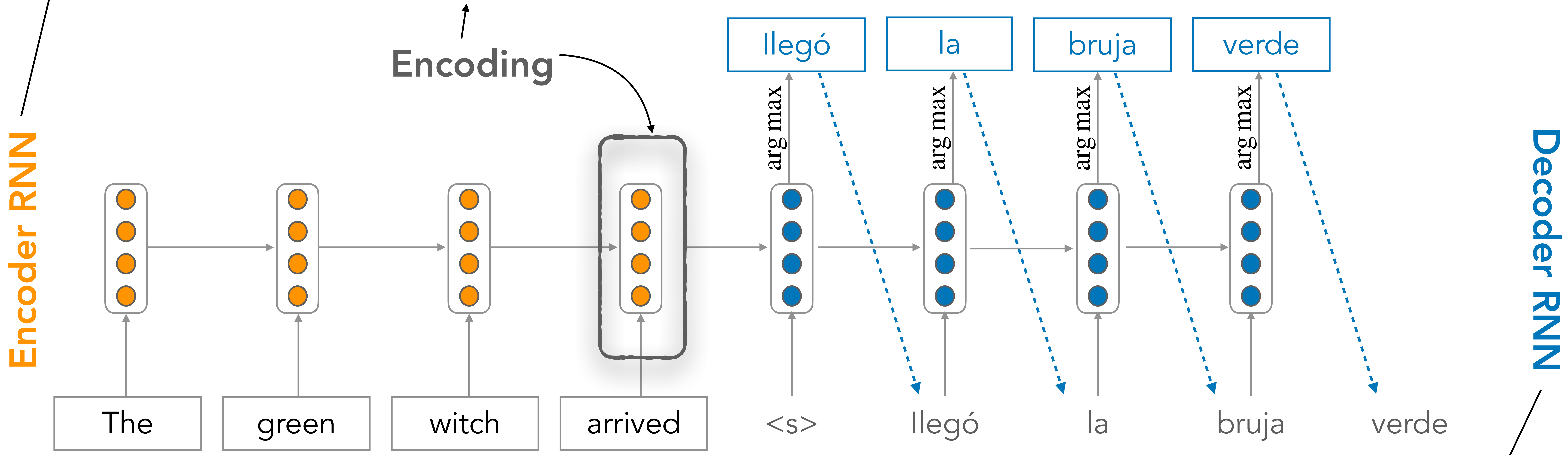
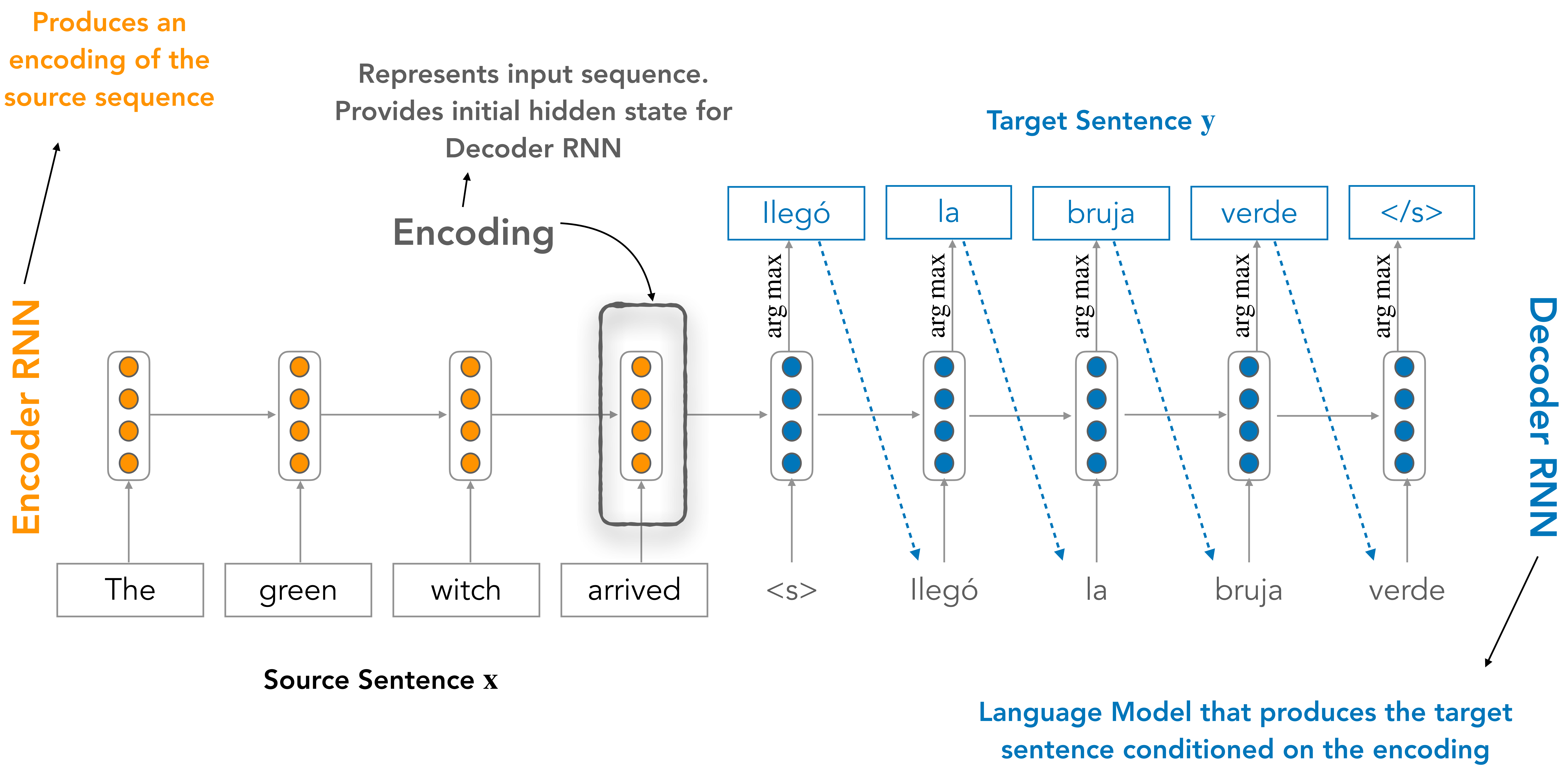


Source Sentence x

Language Model that produces the target sentence conditioned on the encoding


Produces an encoding of the source sequence
Represents input sequence. Provides initial hidden state for Decoder RNN
Target Sentence y
Encoding
llegó
la
bruja
verde
</s>
arg max
Encoder RNN
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The
green
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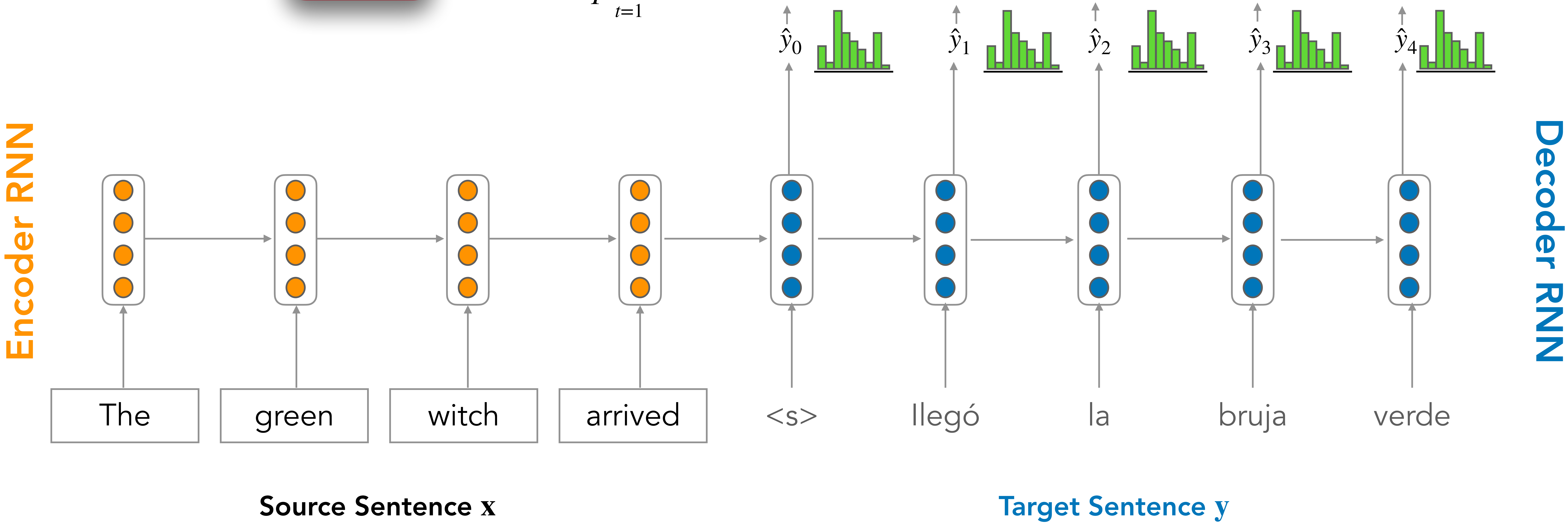
Language Model that produces the target sentence conditioned on the encoding

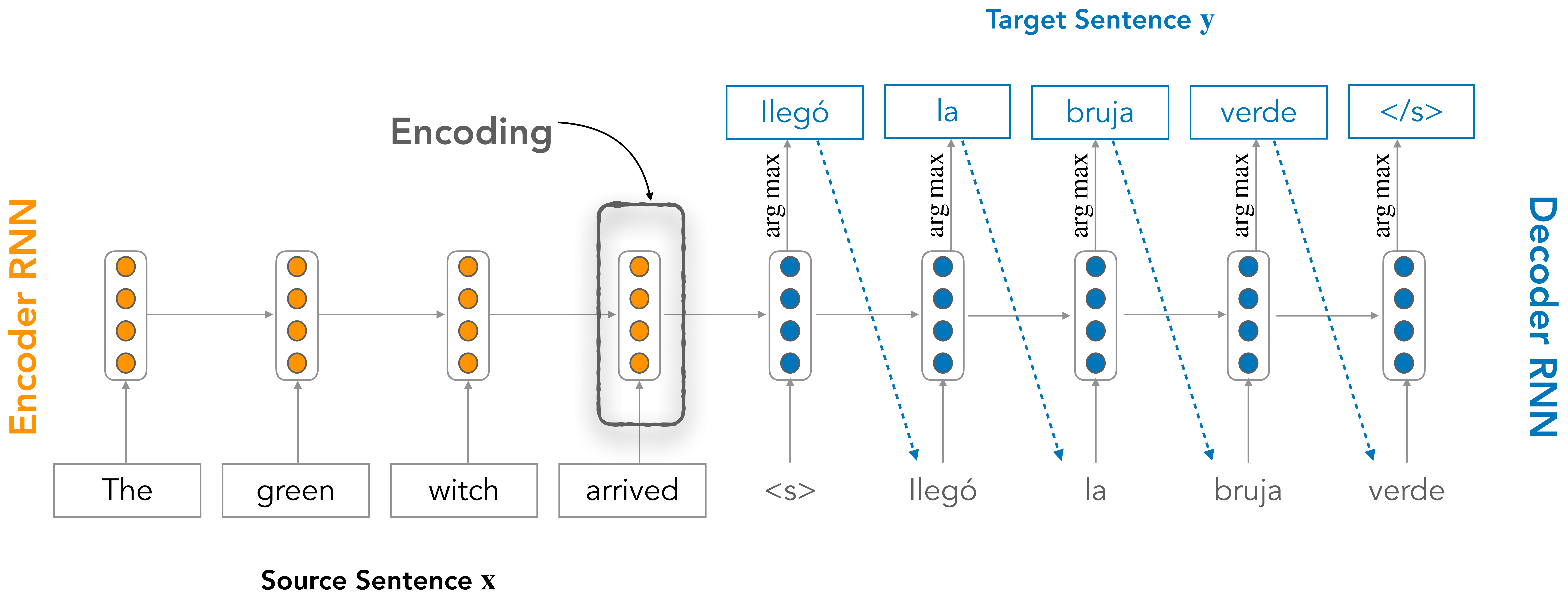
Loss

negative log prob. of "llegó"

negative log prob. of "</s>"

$$L(\theta) = \frac{1}{T}\sum_{t=1}^{T} L_t(\theta) = L_0(\theta) + L_1(\theta) + L_2(\theta) + L_3(\theta) + L_4(\theta)$$




Target Sentence y
llegó
la
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Encoding
Encoder RNN
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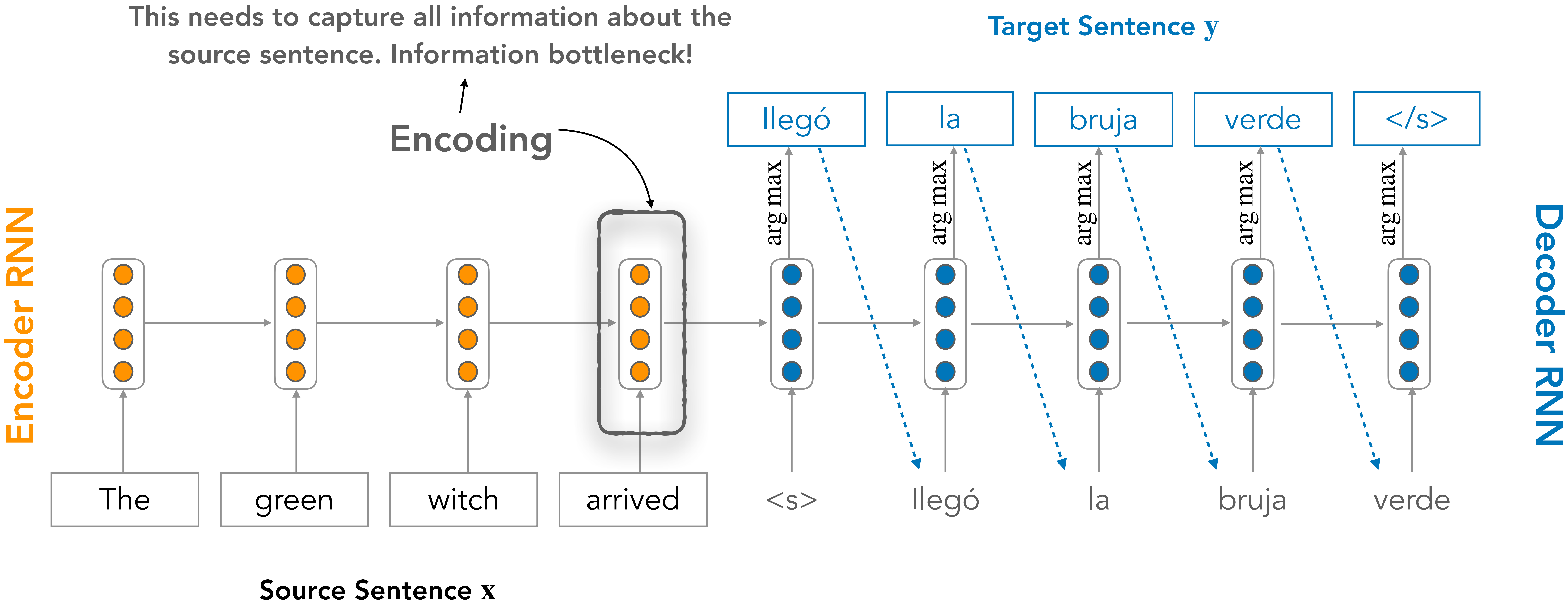
Source Sentence x


This needs to capture all information about the source sentence. Information bottleneck!
Target Sentence y
Encoding
llegó
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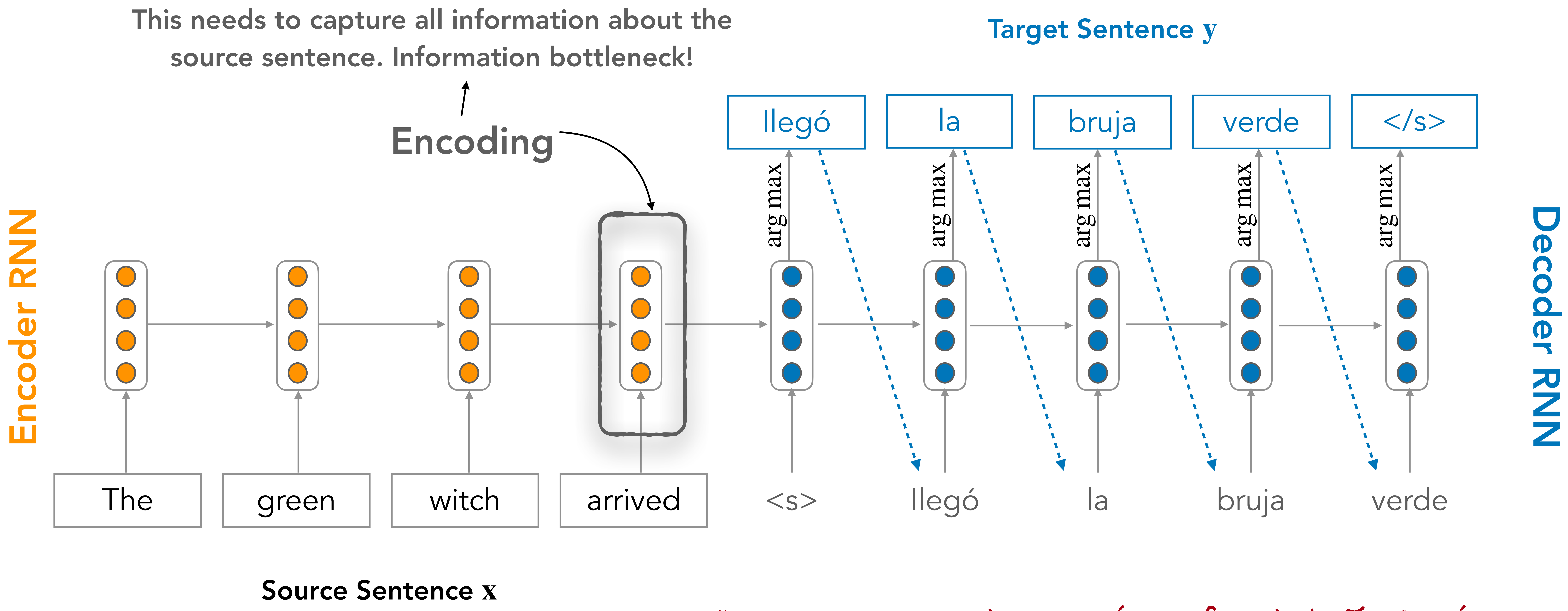
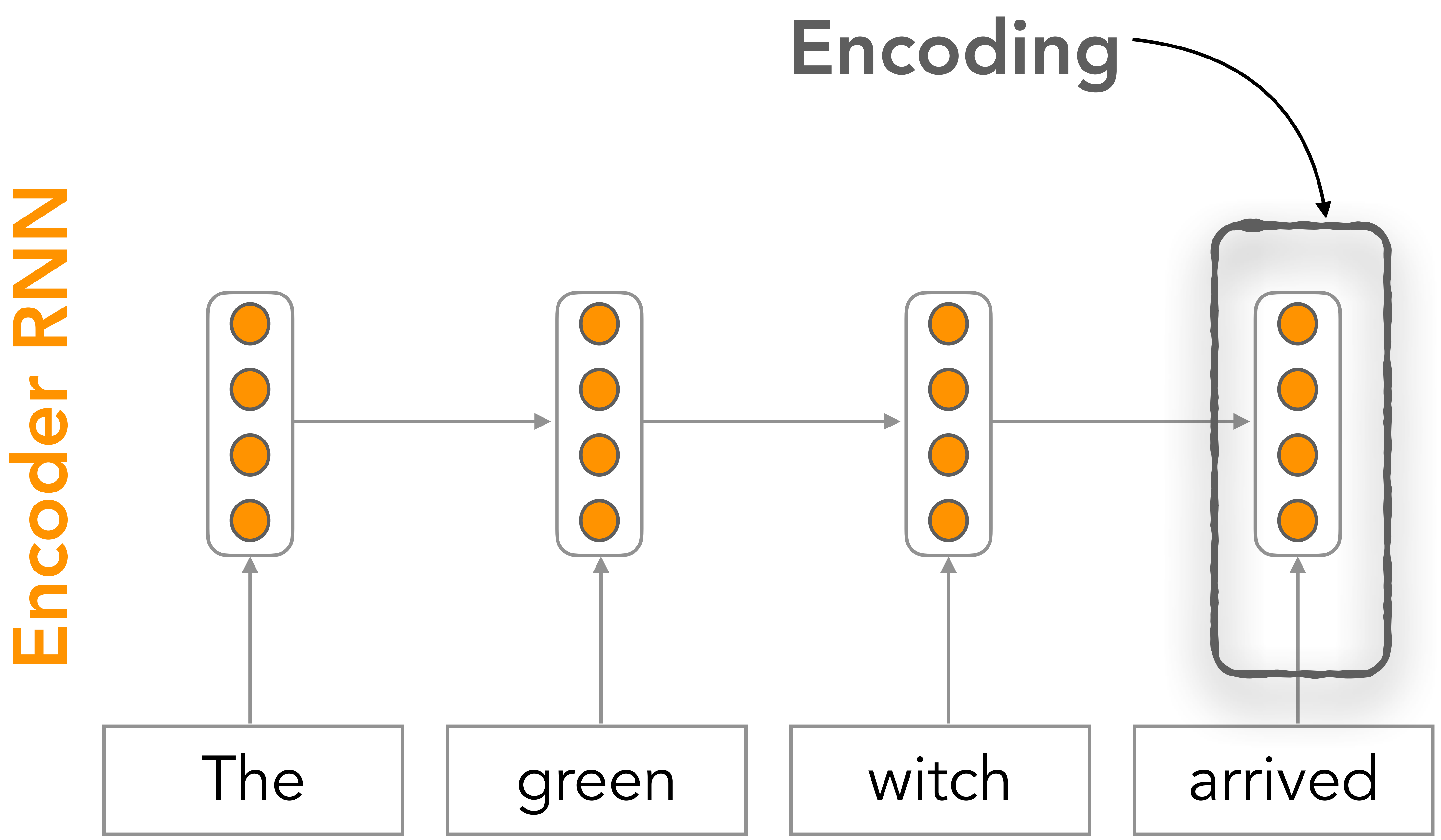


"you can't cram the meaning of a whole %&@#&ing sentence into a single $(&@ing vector!"*

– Ray Mooney, Professor of Computer Science, UT Austin

Information Bottleneck: One Solution



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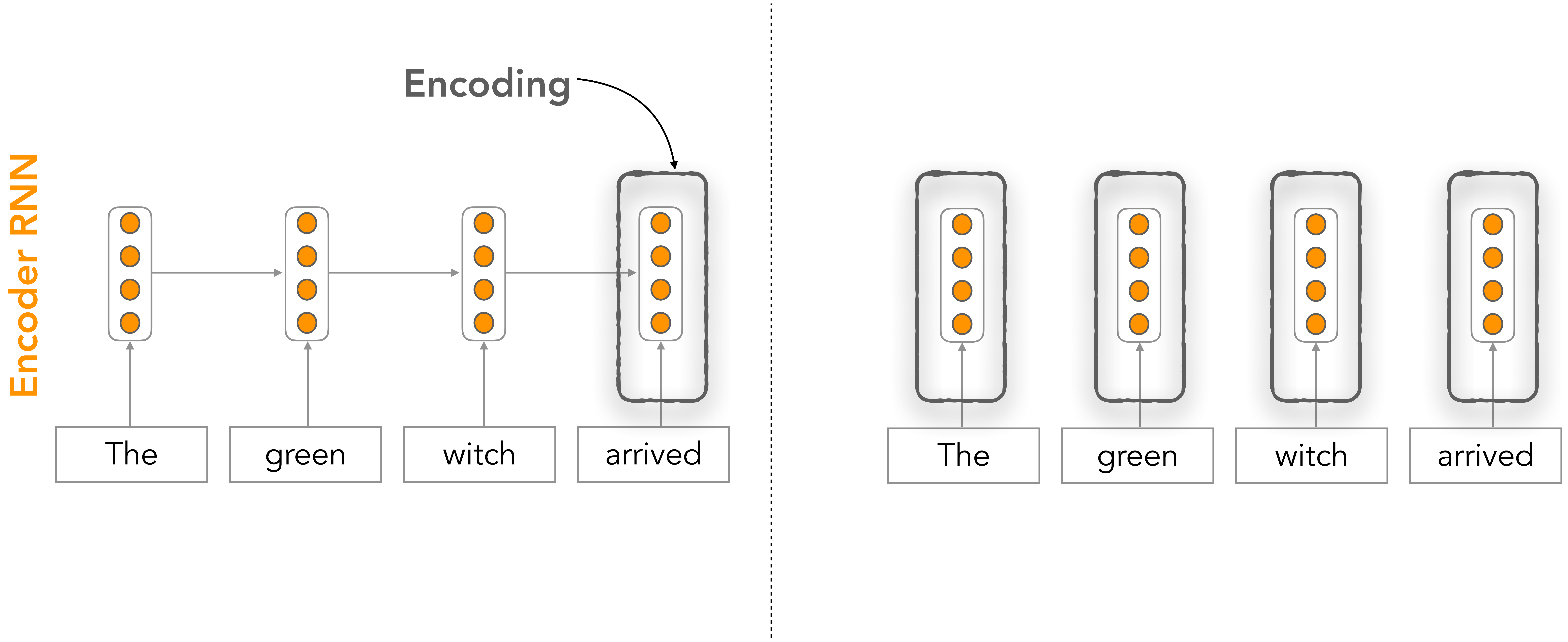

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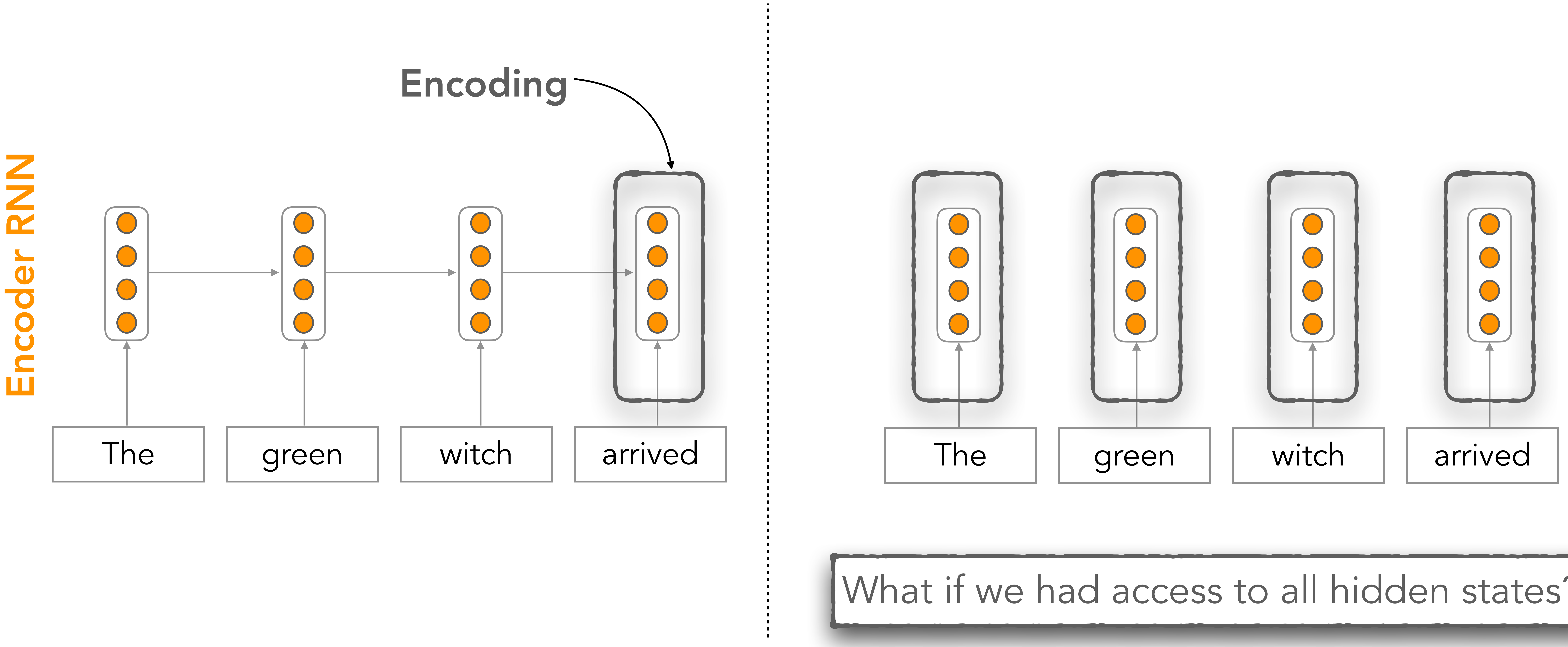

What if we had access to all hidden states?

USC Viterbi

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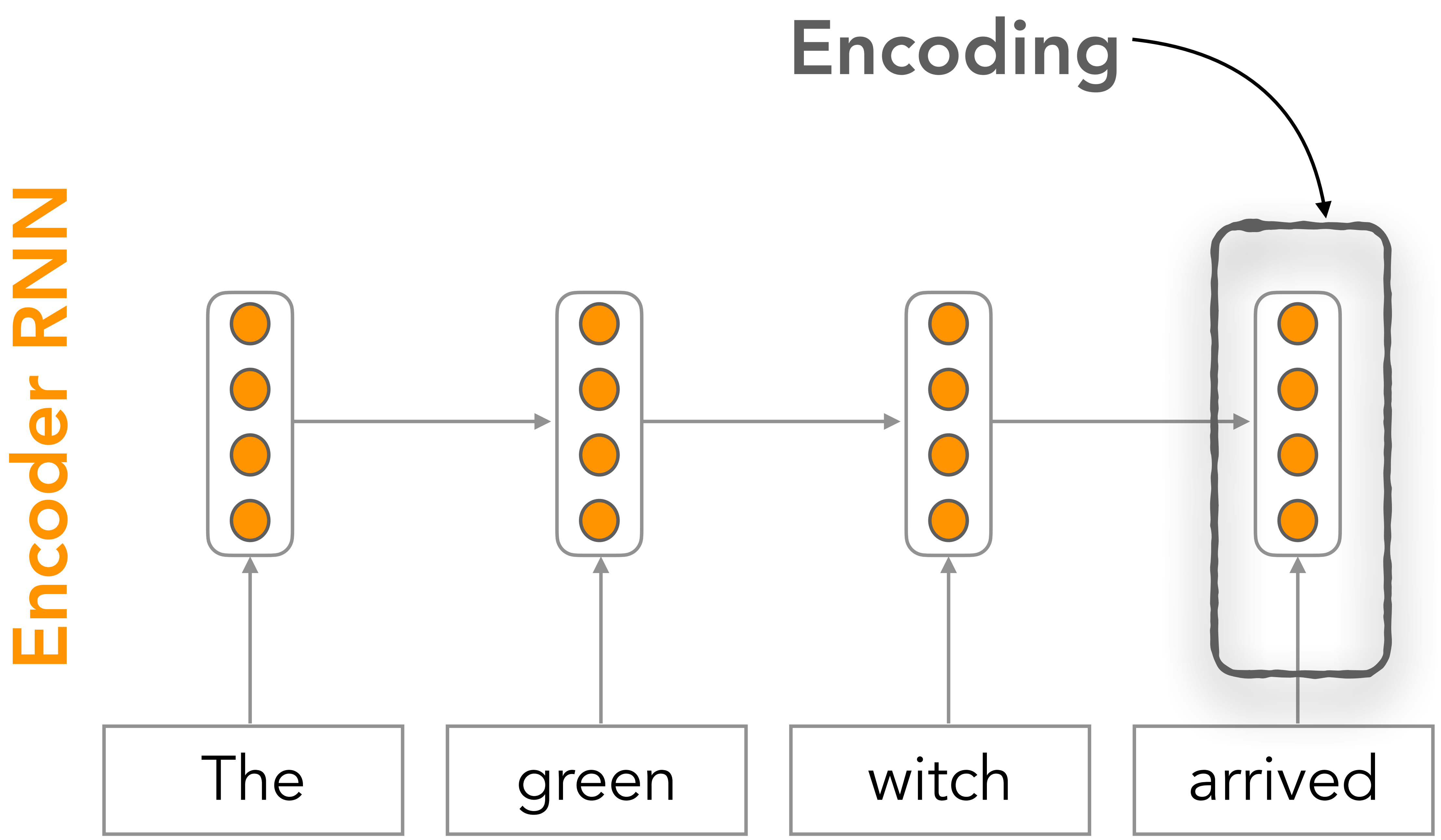
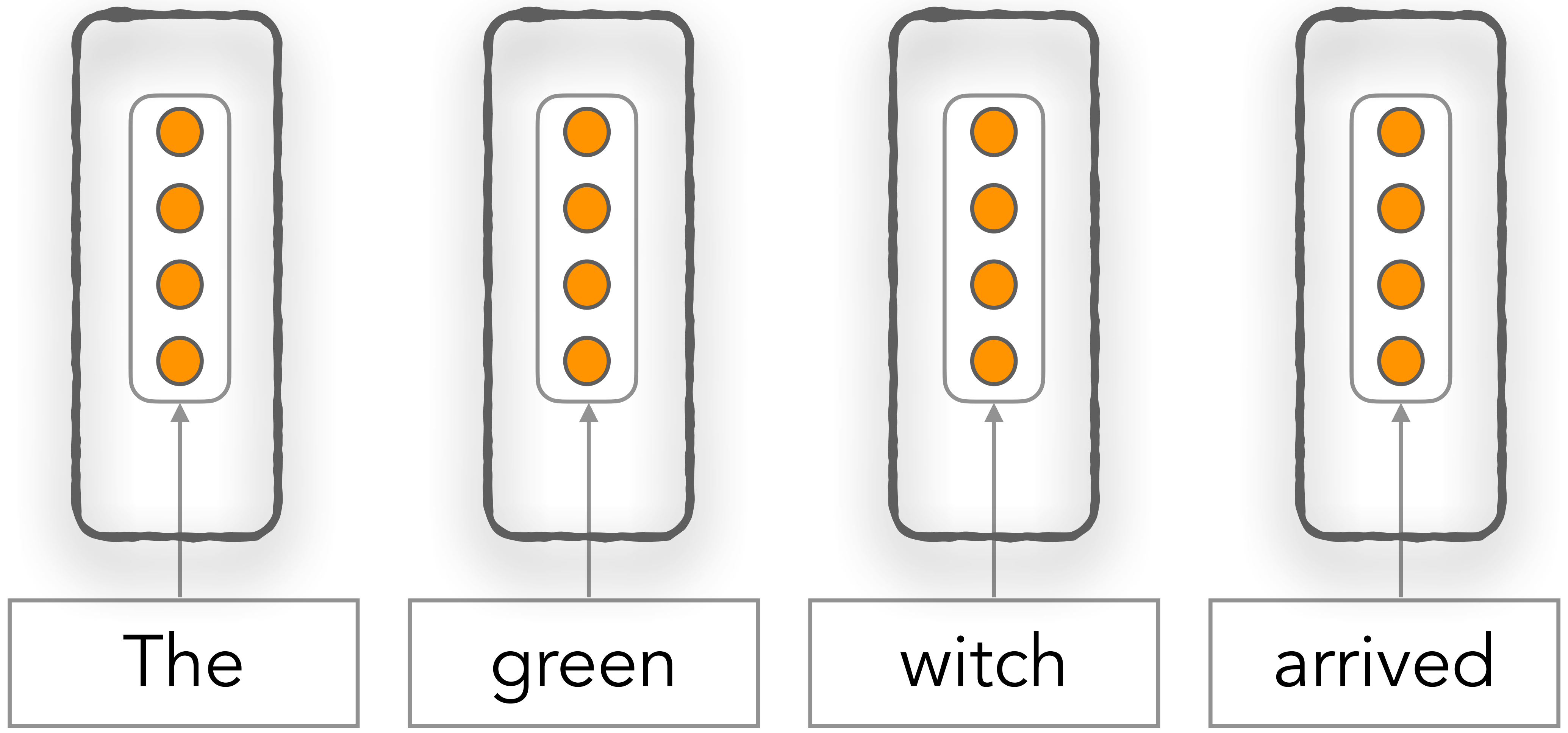


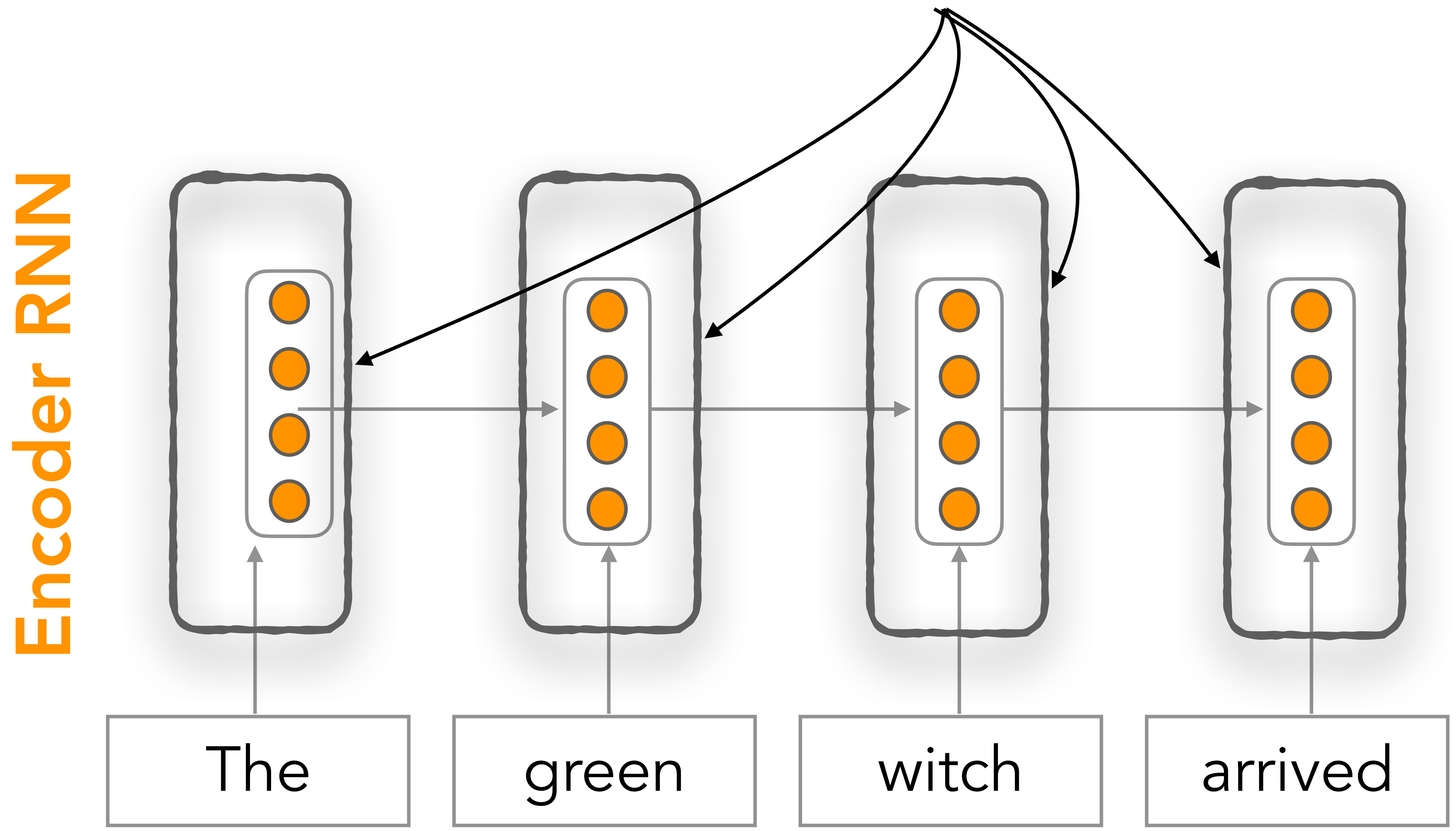


What if we had access to all hidden states?

How to create this?

Attention Mechanism

Encoding $\mathbf{c}_t^{att} = f(\mathbf{h}_1^e, \ldots, \mathbf{h}_N^e, \mathbf{h}_t^d)$



Source Sentence $\mathbf{x}$

Note: Notation different from J&M

Bahdanau et al., 2015

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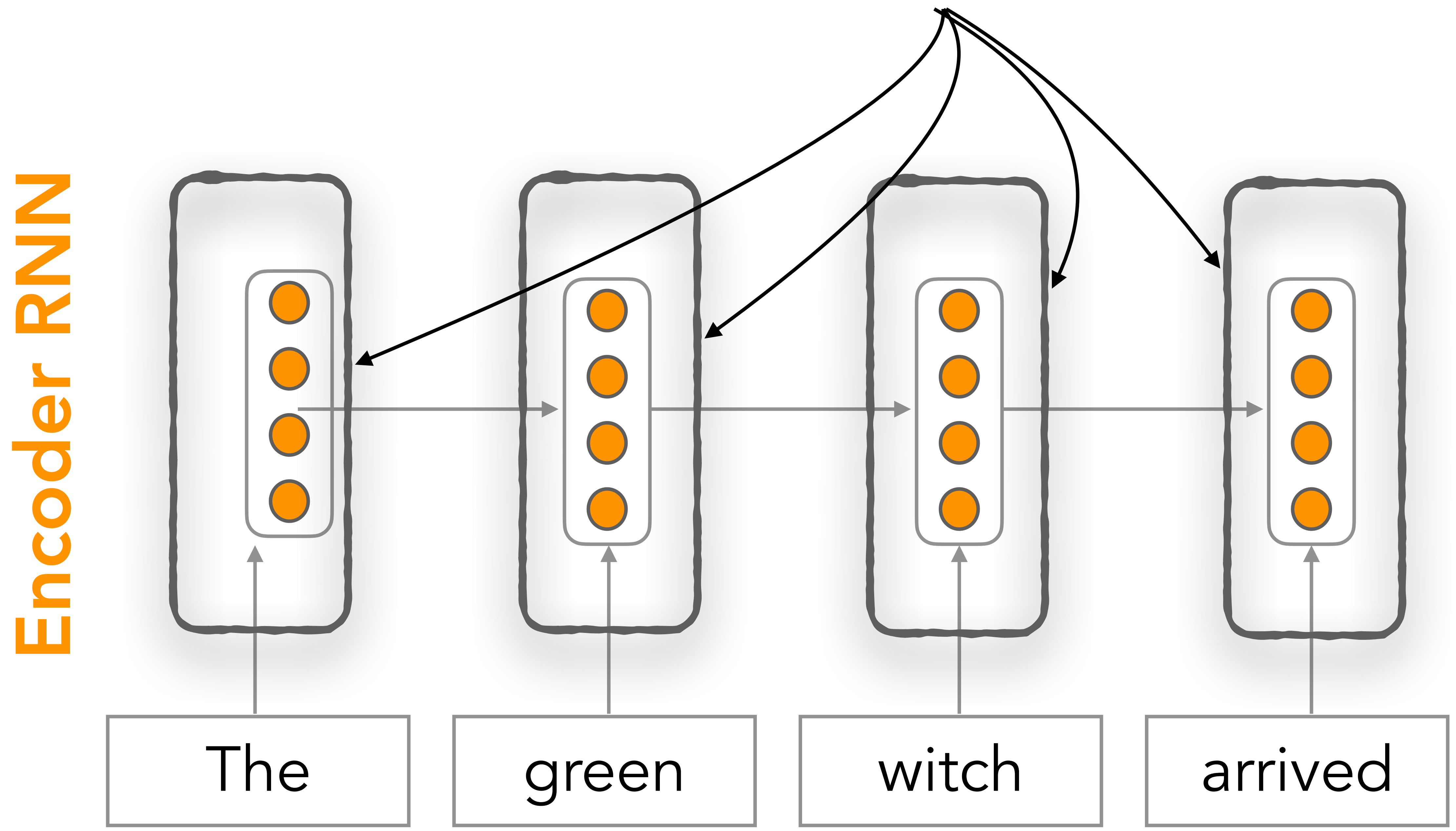

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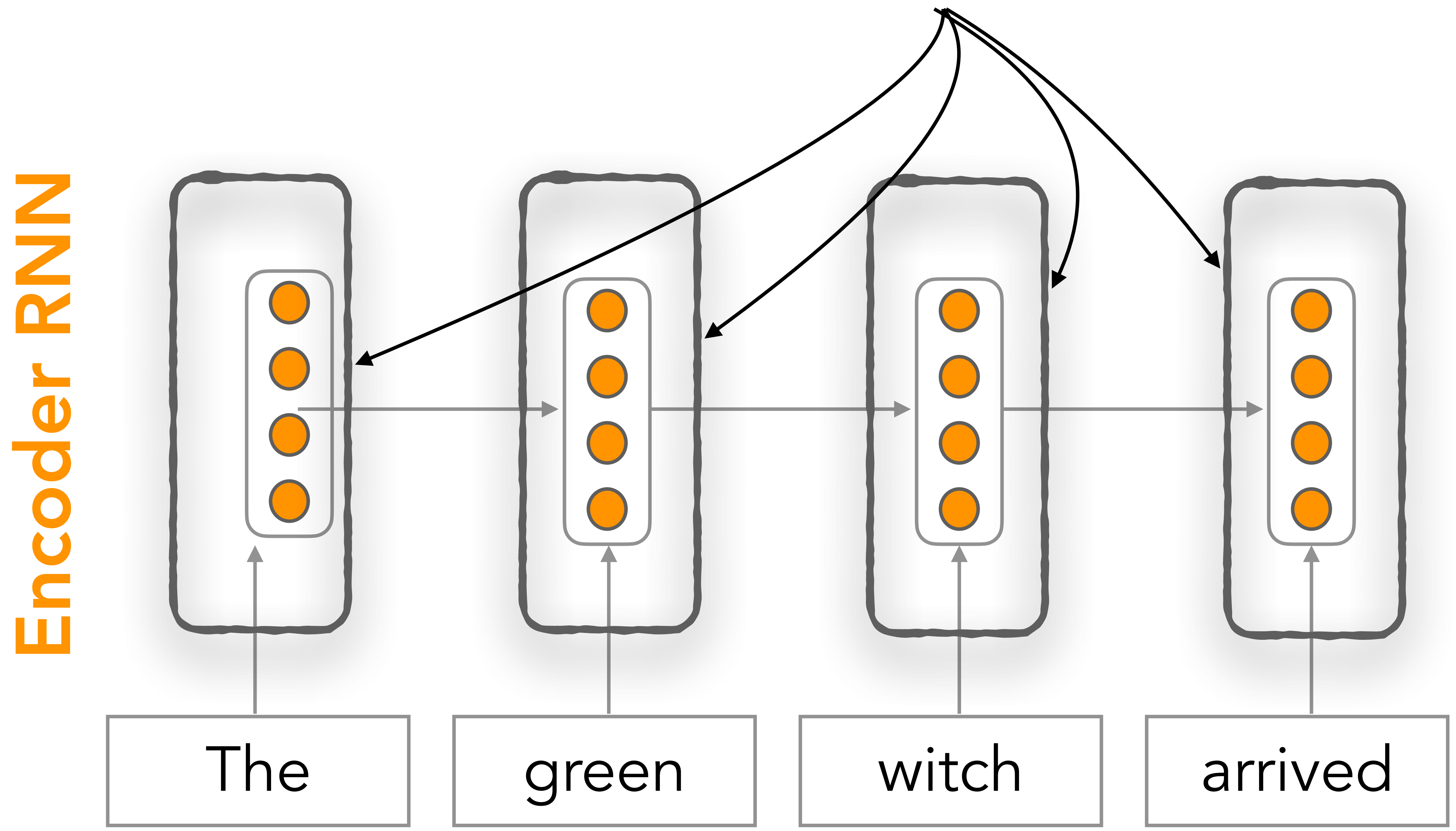

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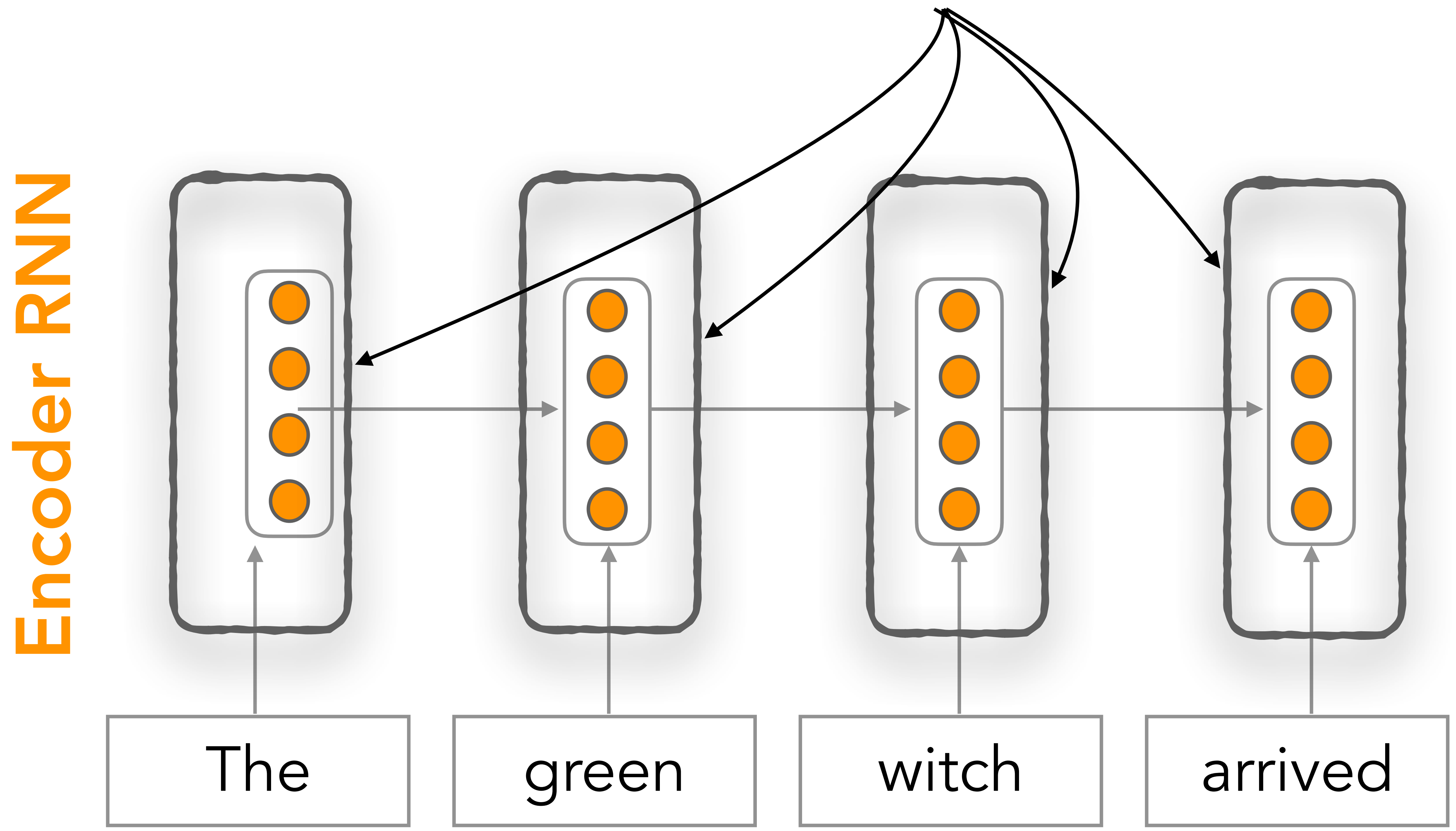

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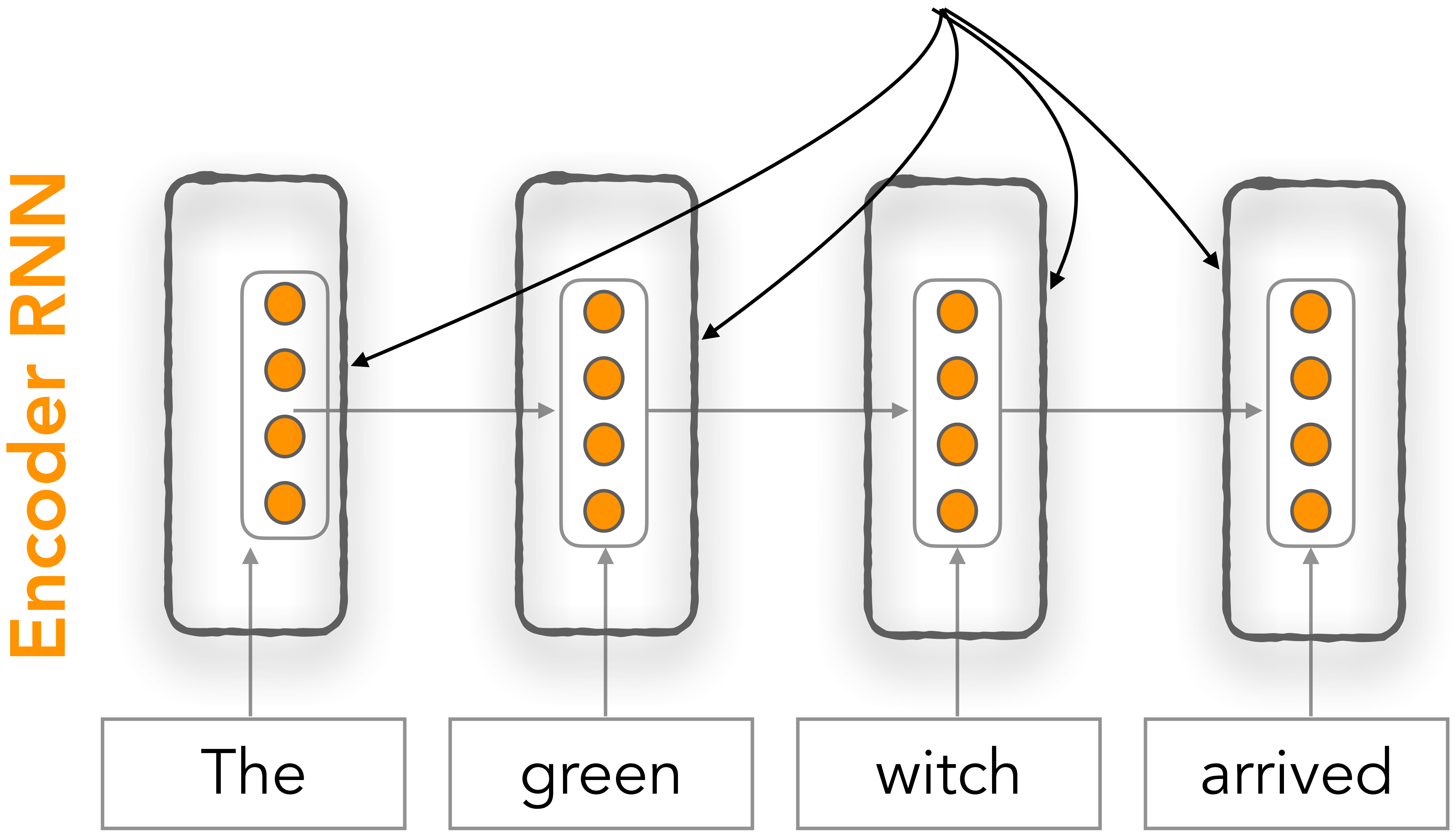

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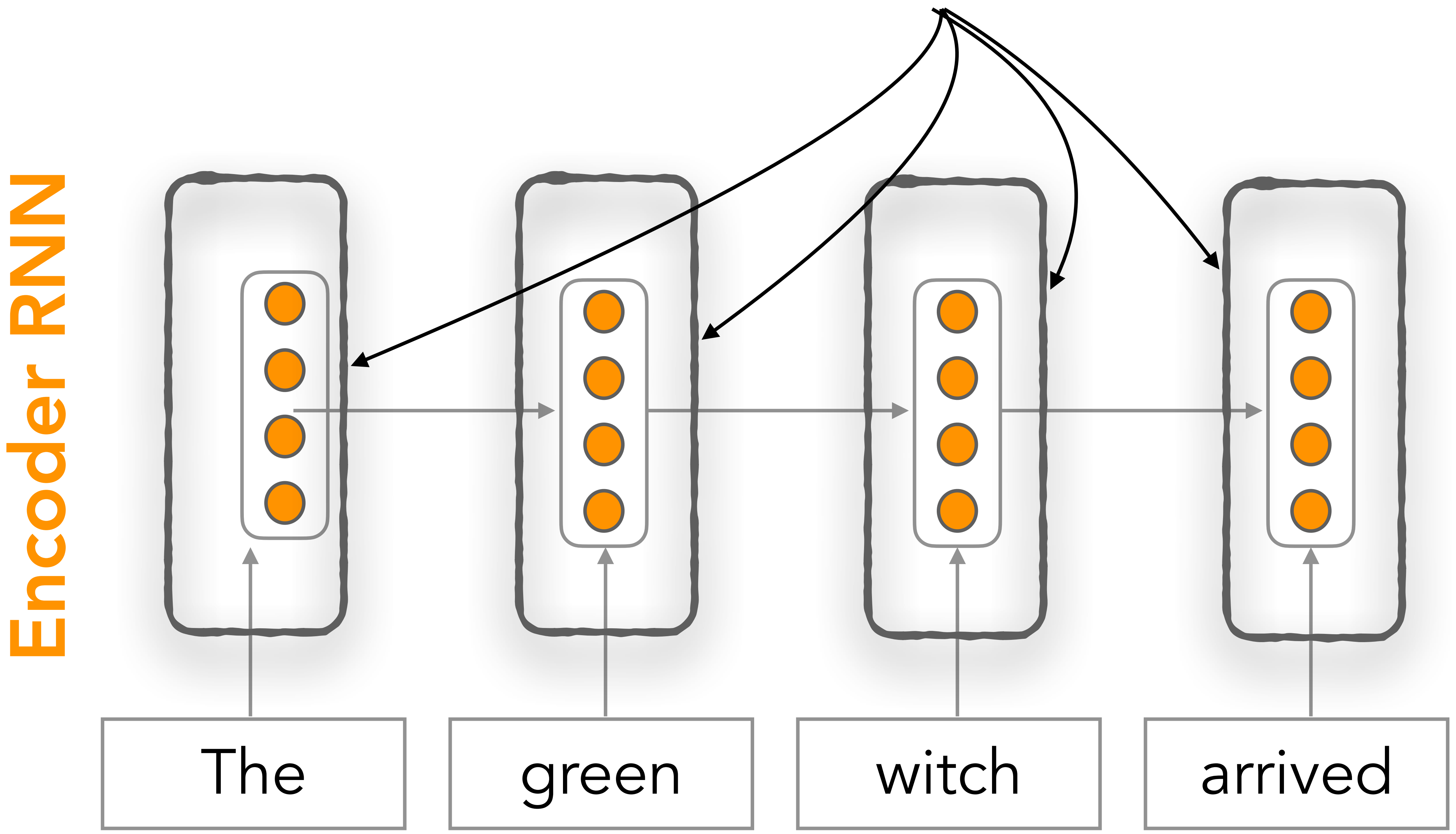

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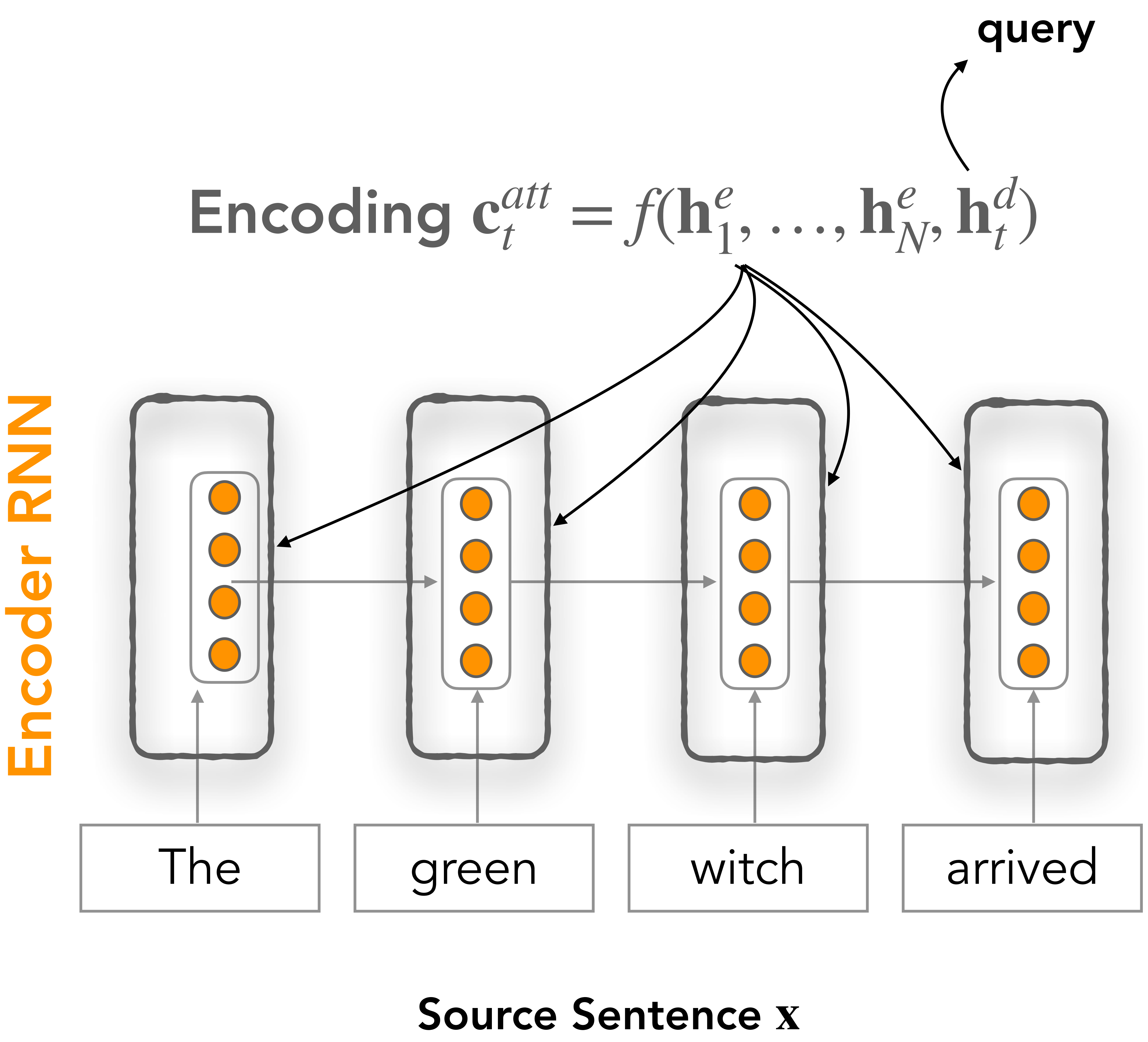

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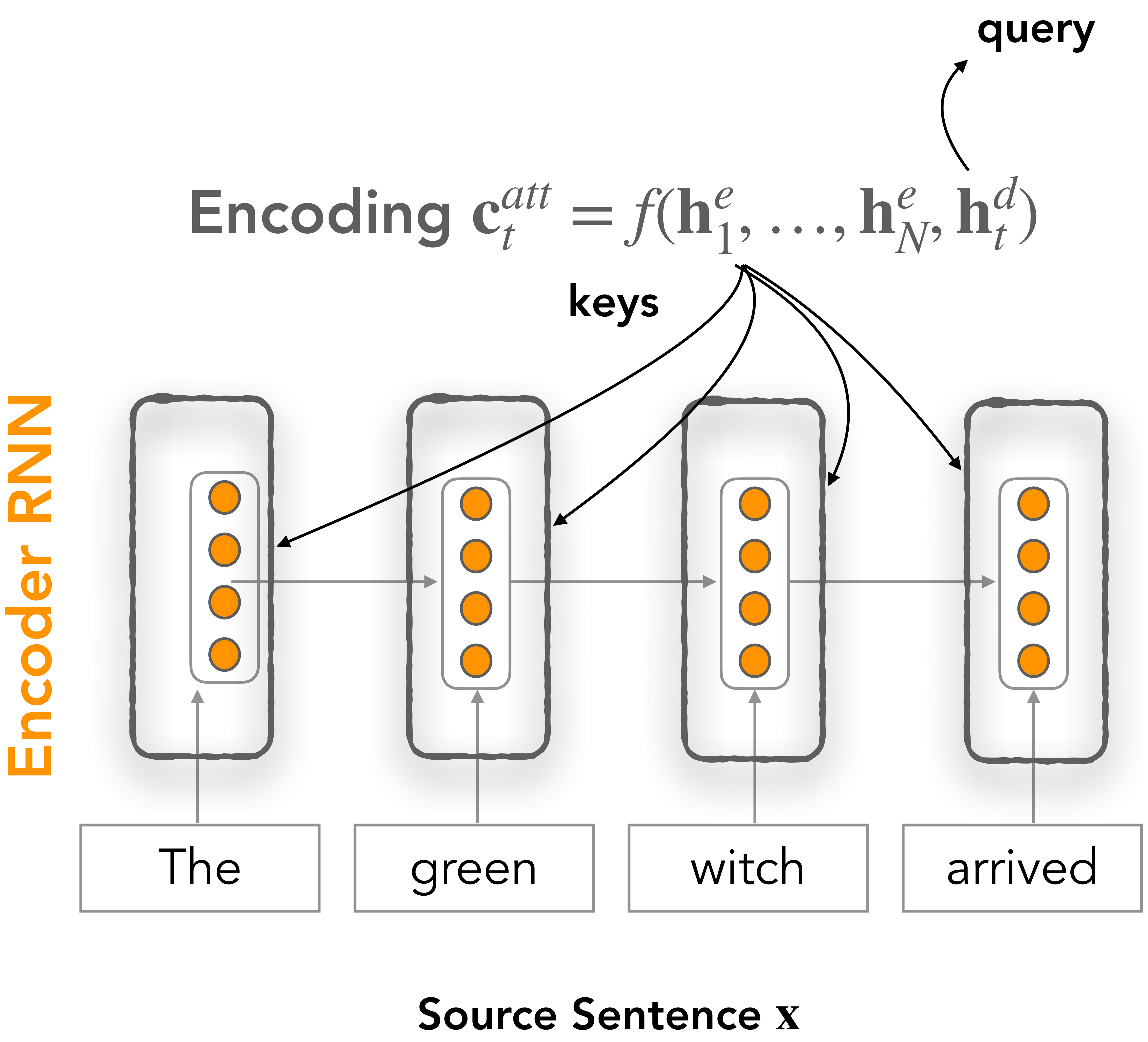
- In general, we have a single **query** vector and multiple **key** vectors.
  - We want to score each query-key pair



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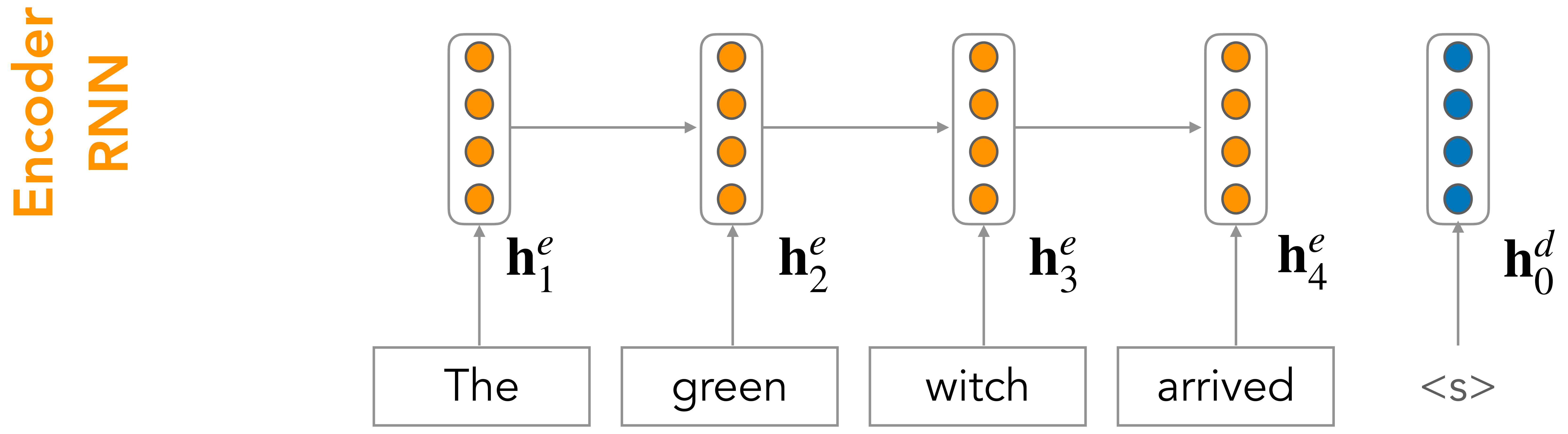
Seq2Seq with Attention



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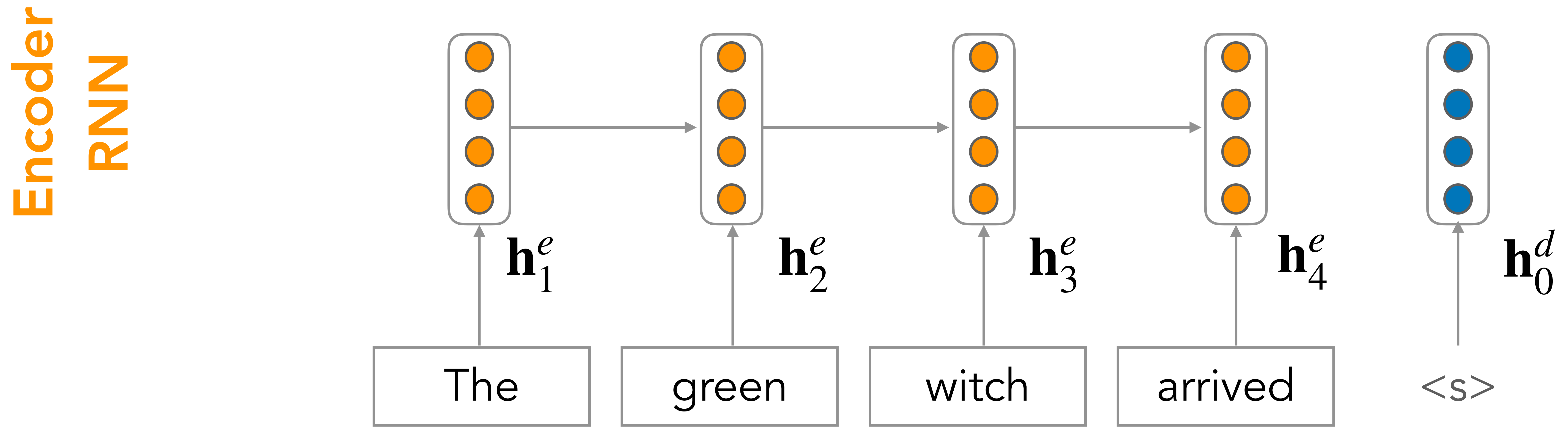
Seq2Seq with Attention

Query 1: Decoder, first time step



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Seq2Seq with Attention

Dot product with keys (encoder hidden states) to encode similarity with what is decoded so far…

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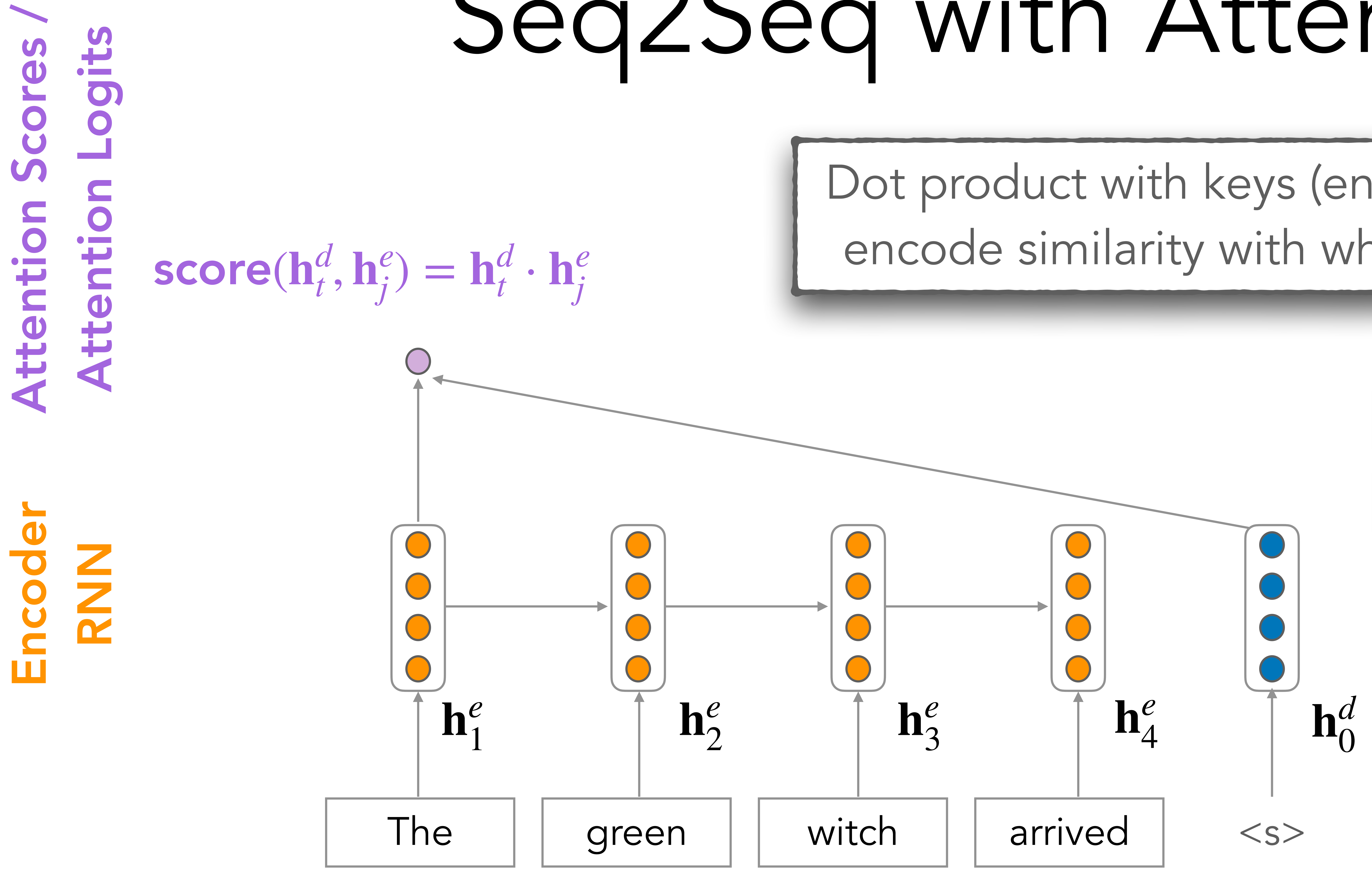

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Seq2Seq with Attention

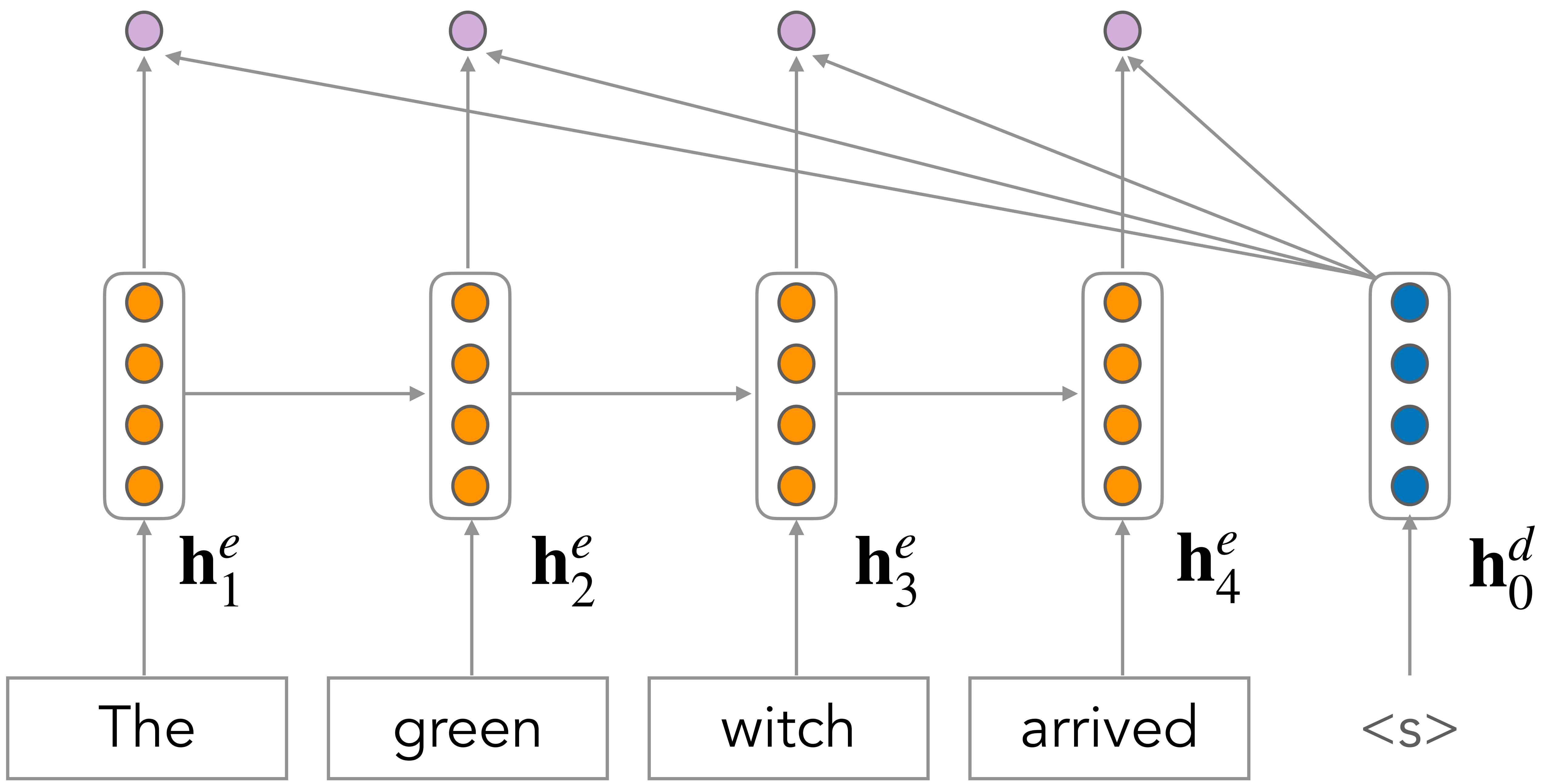
Attention Scores / Attention Logits

$$\text{score}(\mathbf{h}_t^d, \mathbf{h}_j^e) = \mathbf{h}_t^d \cdot \mathbf{h}_j^e$$

Dot product with keys (encoder hidden states) to encode similarity with what is decoded so far…

Query 1: Decoder, first time step

Encoder RNN



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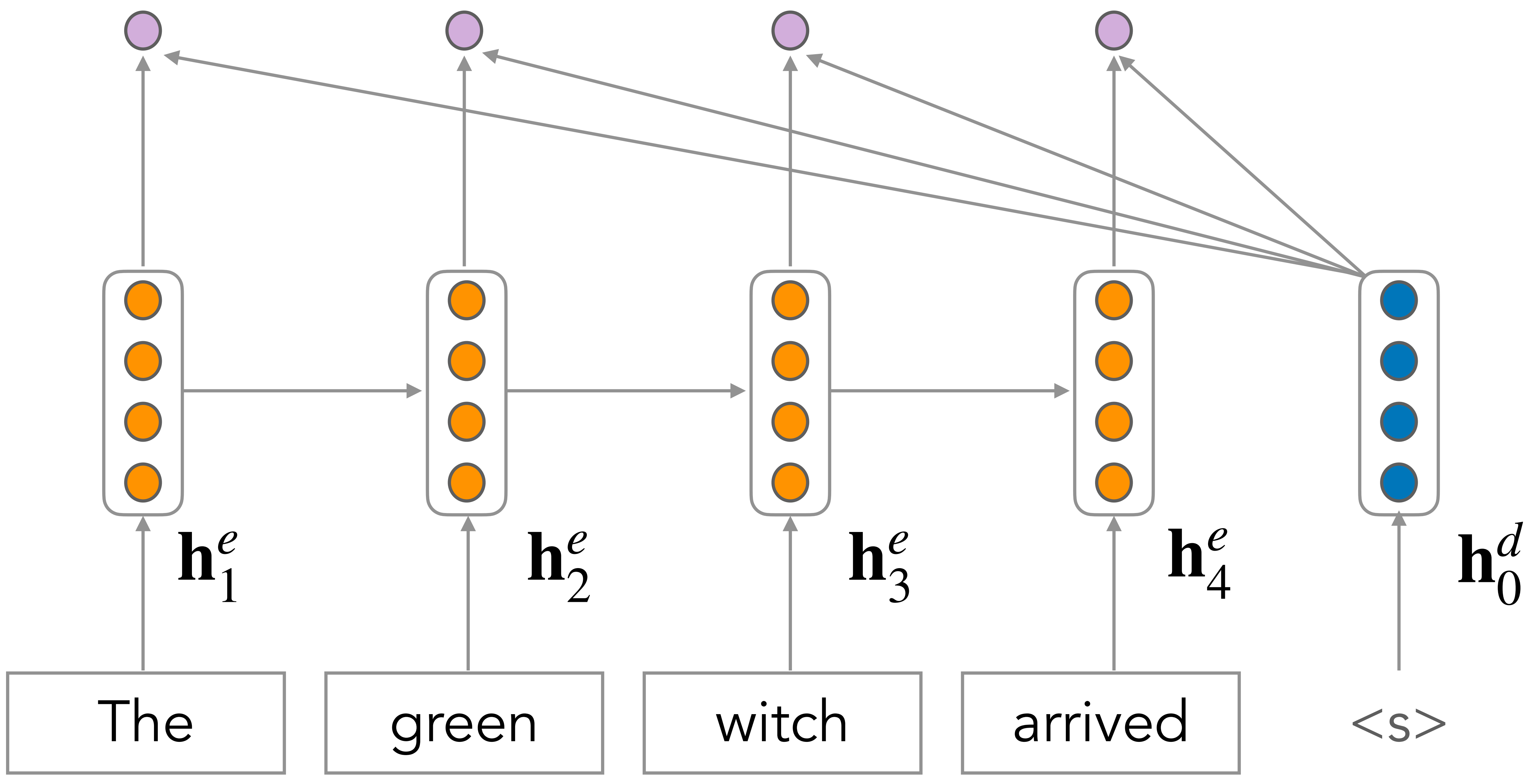

Query 1: Decoder, first time step

Source Sentence x

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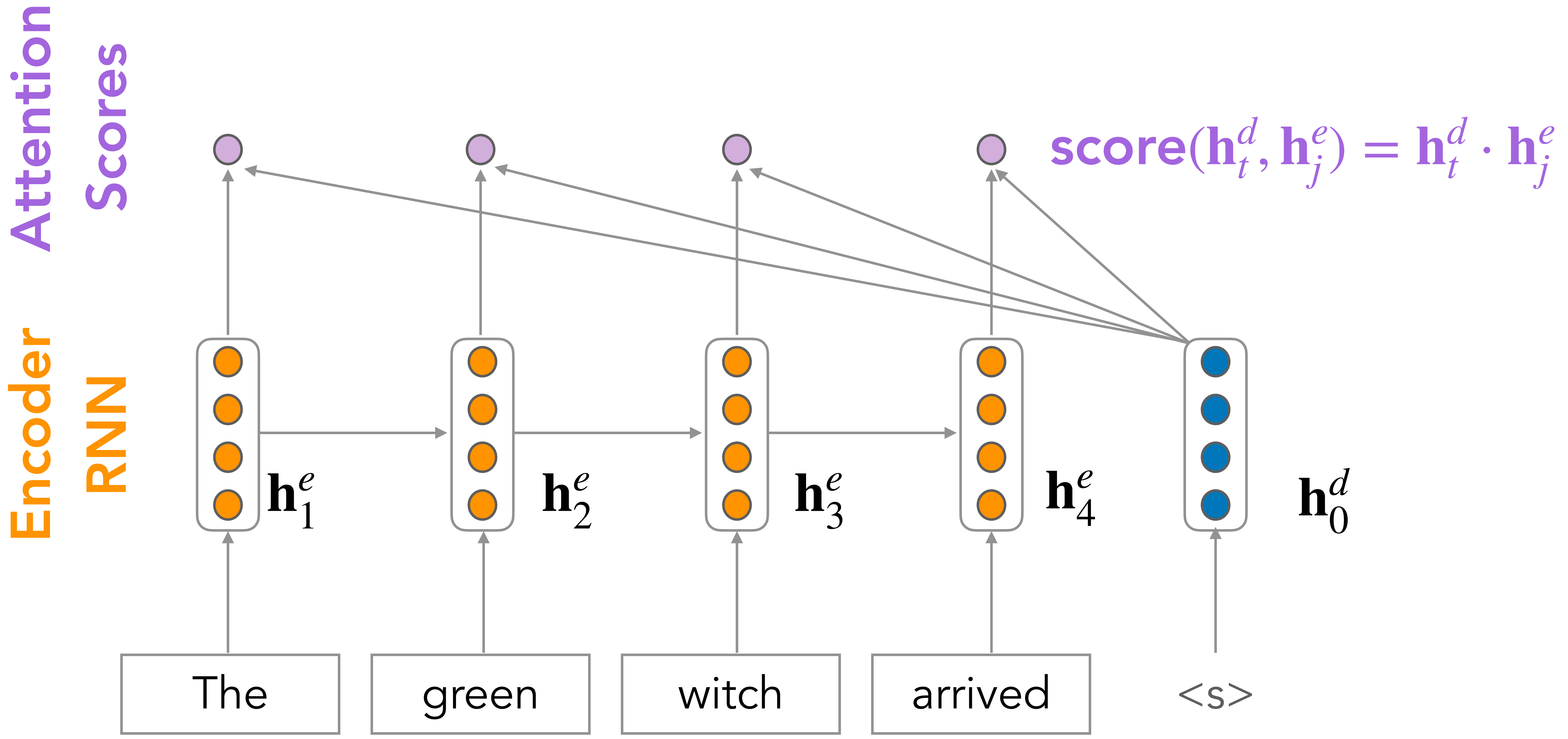
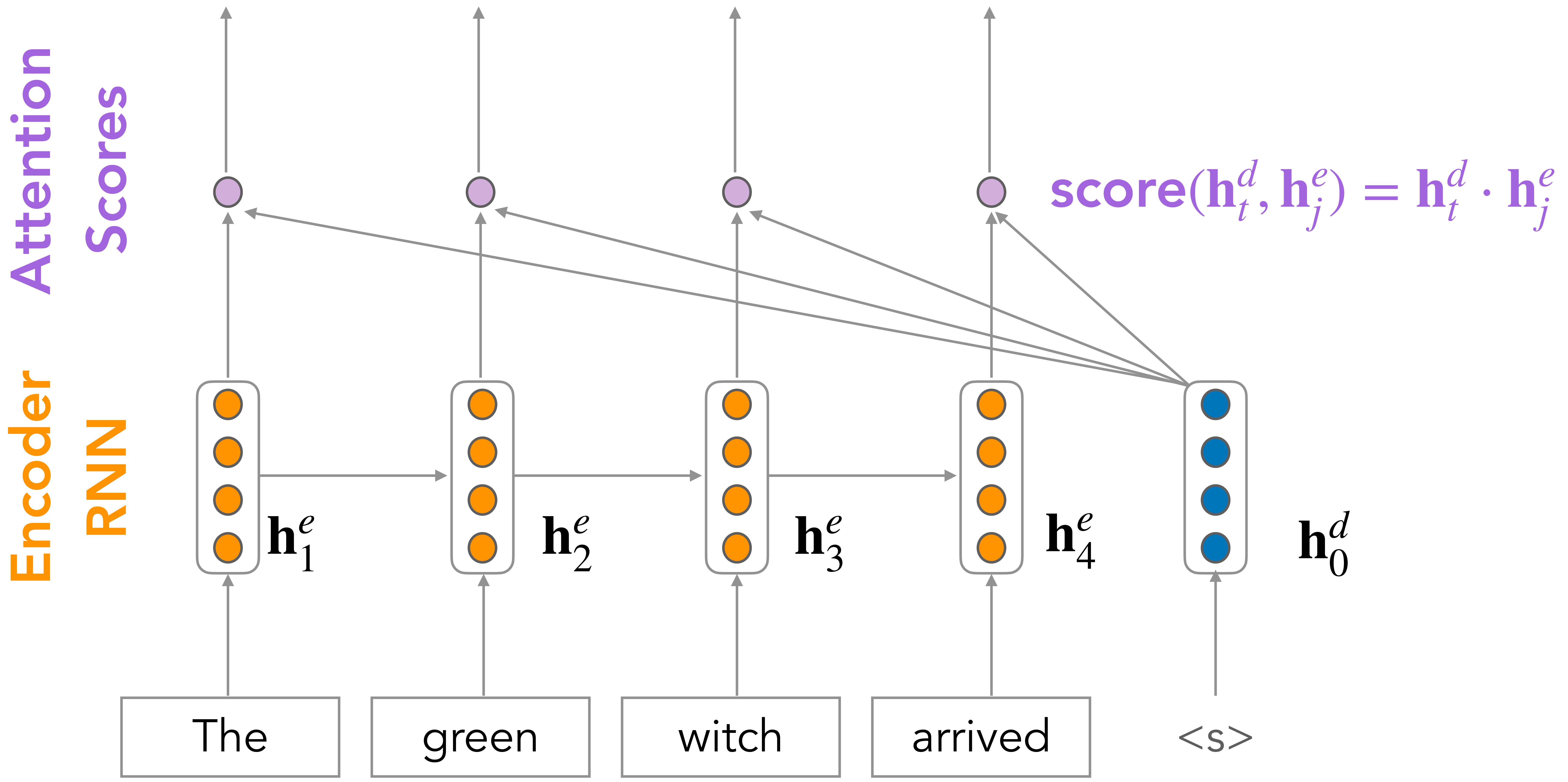
Dot product attention



Source Sentence $\mathbf{x}$

Note: Notation different from J&M



Source Sentence x

Take softmax to turn into probability distribution

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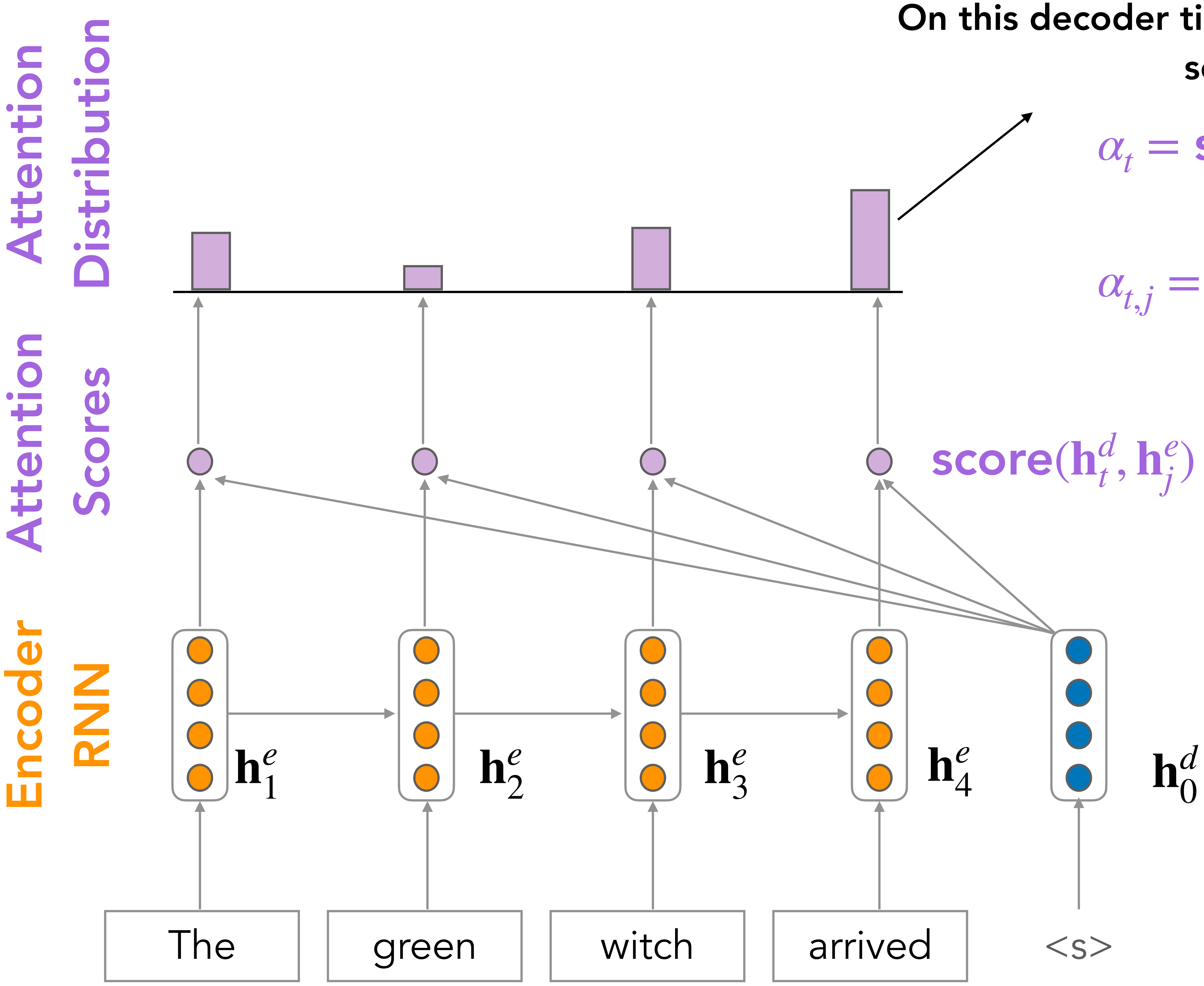

Source Sentence $\mathbf{x}$

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

$$\alpha_t = \textbf{softmax}(\textbf{score}(\mathbf{h}_t^d, \mathbf{h}_j^e)) \in \Delta^N$$

$$\alpha_{t,j} = \frac{\exp \mathbf{h}_t^d \cdot \mathbf{h}_j^e}{\sum_{n=1}^N \exp \mathbf{h}_t^d \cdot \mathbf{h}_n^e}$$

$$\textbf{score}(\mathbf{h}_t^d, \mathbf{h}_j^e) = \mathbf{h}_t^d \cdot \mathbf{h}_j^e$$

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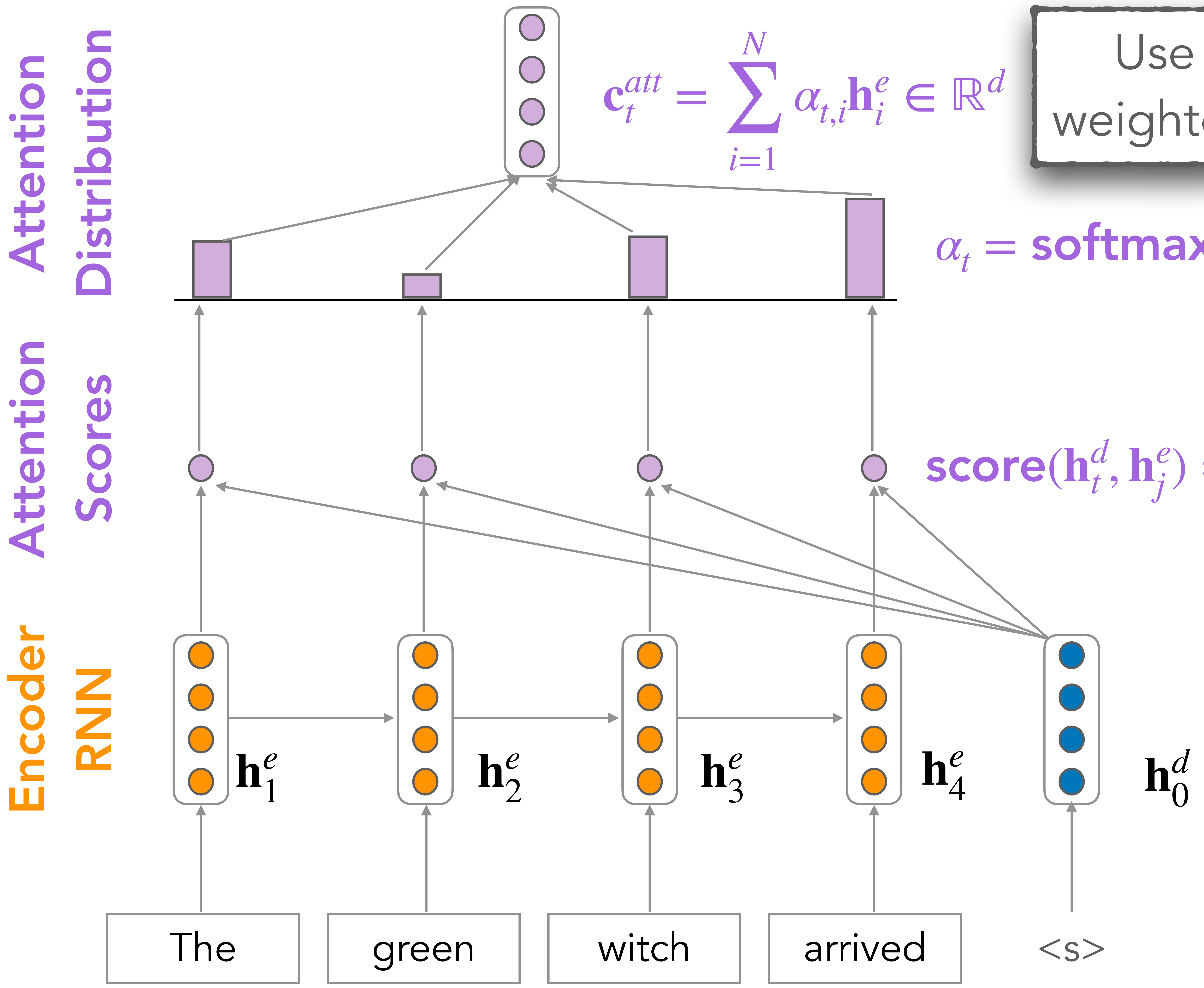

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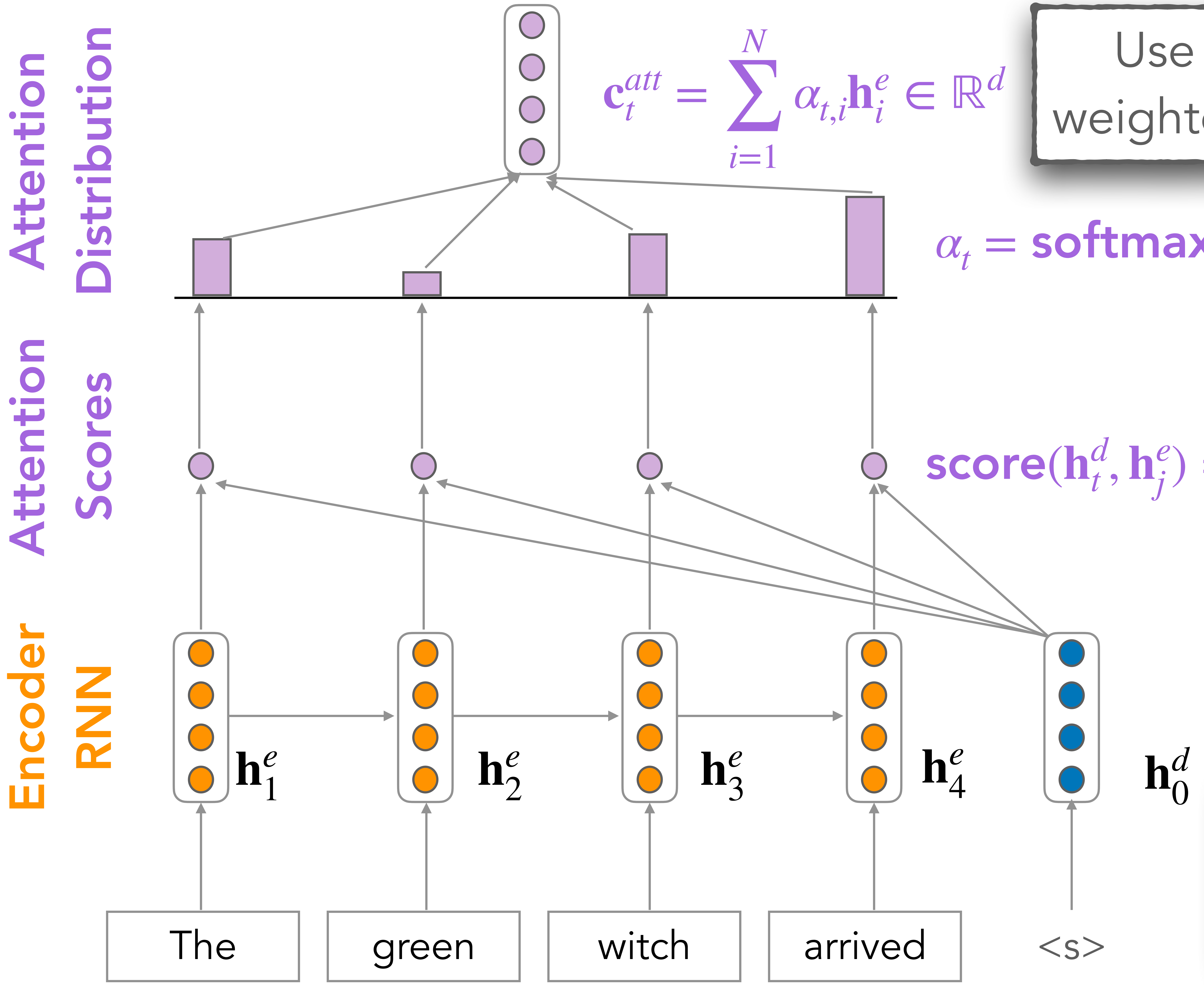

$$\mathbf{c}_t^{att} = \sum_{i=1}^{N} \alpha_{t,i}\mathbf{h}_i^e \in \mathbb{R}^d$$

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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.

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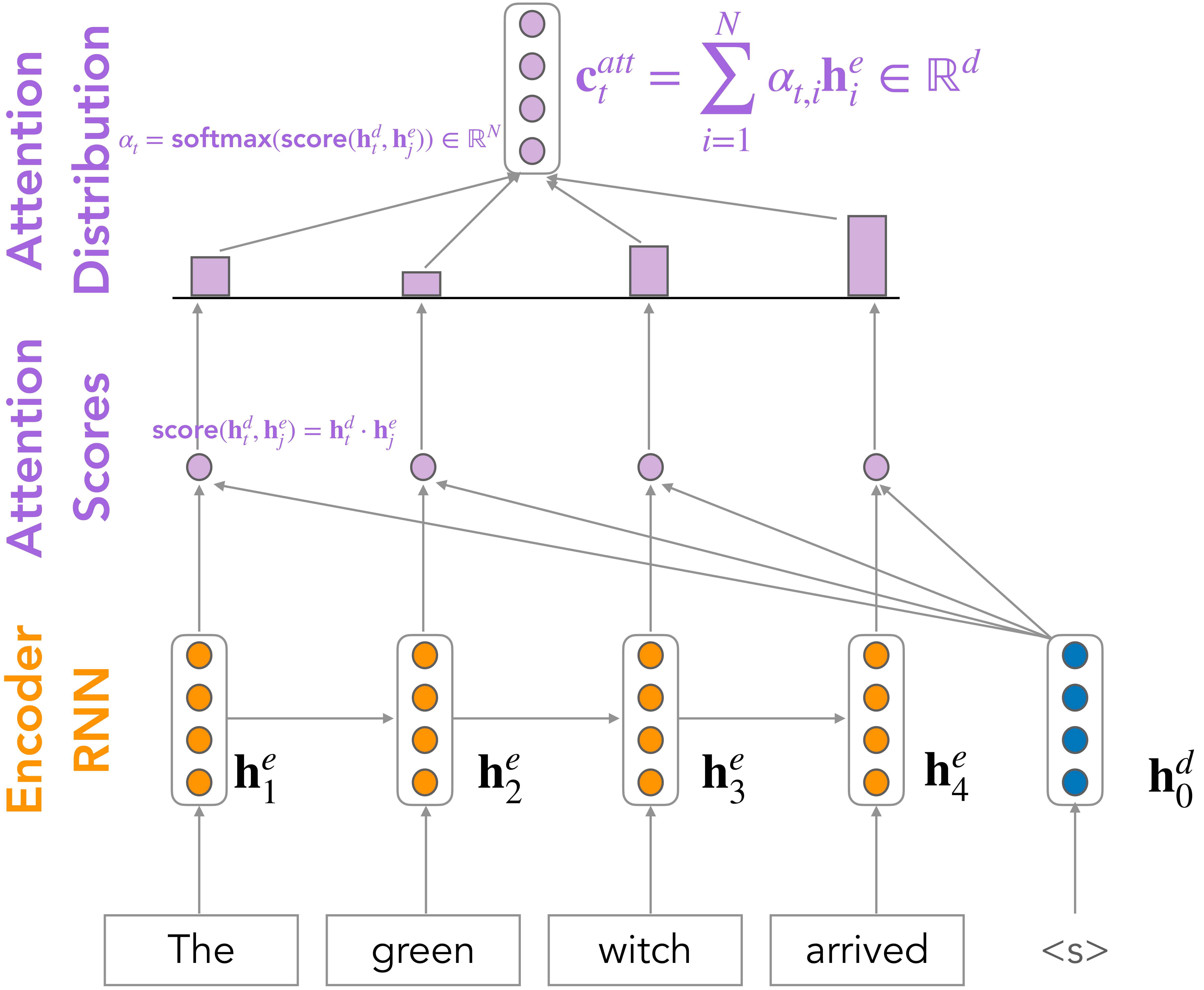

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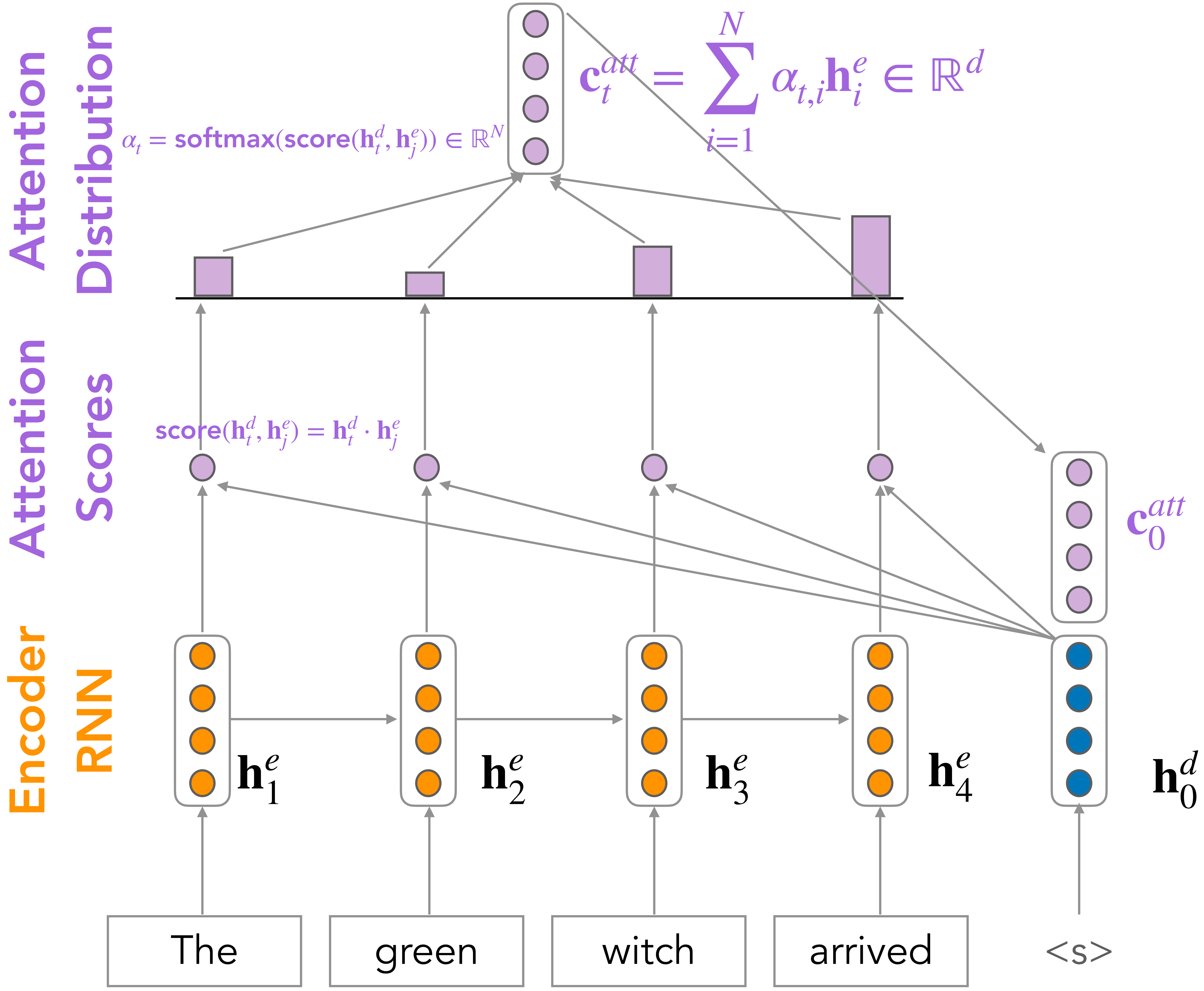

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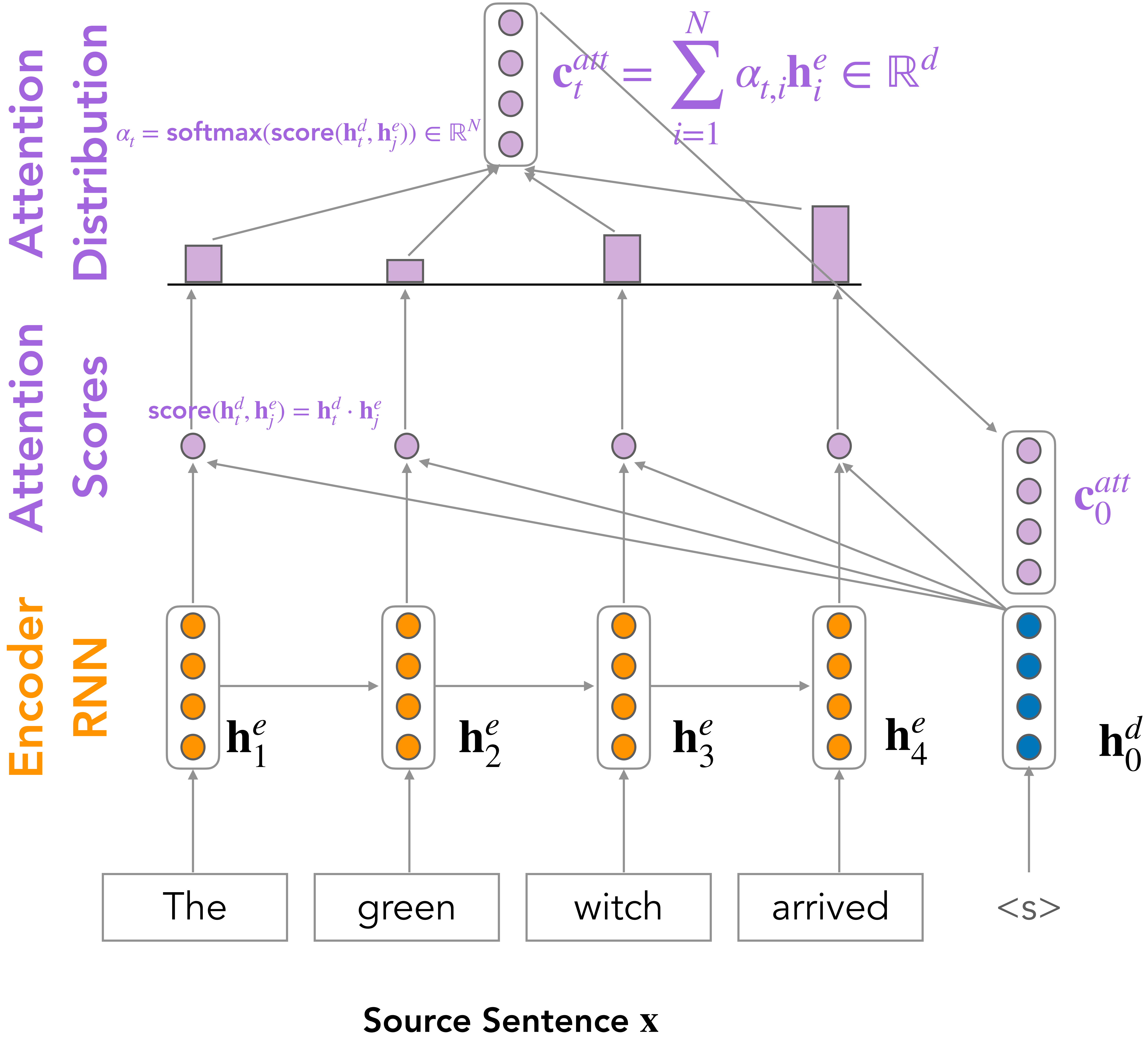

Concatenate attention output with decoder hidden state, then use to compute $\hat{y}_0$ as before

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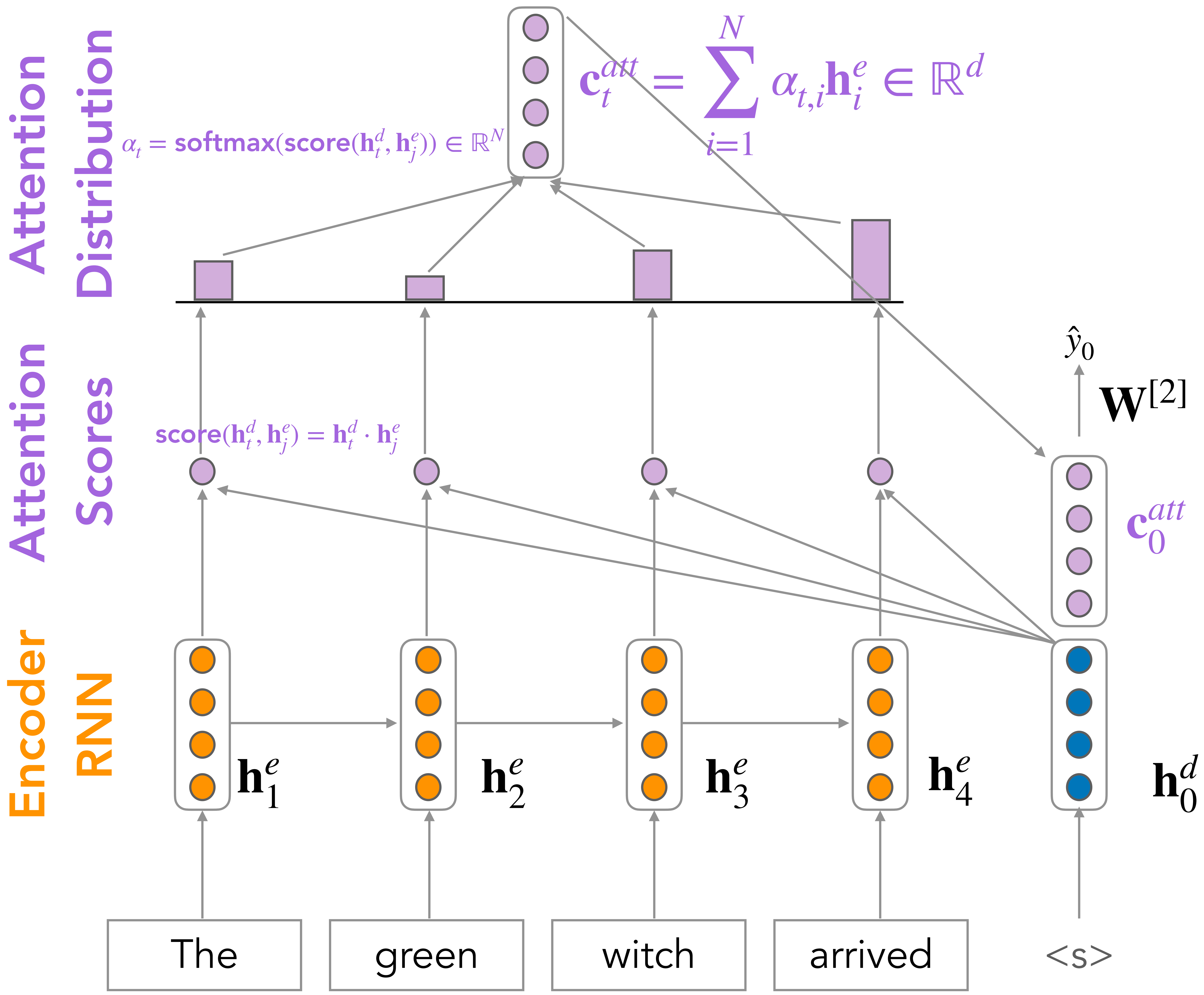

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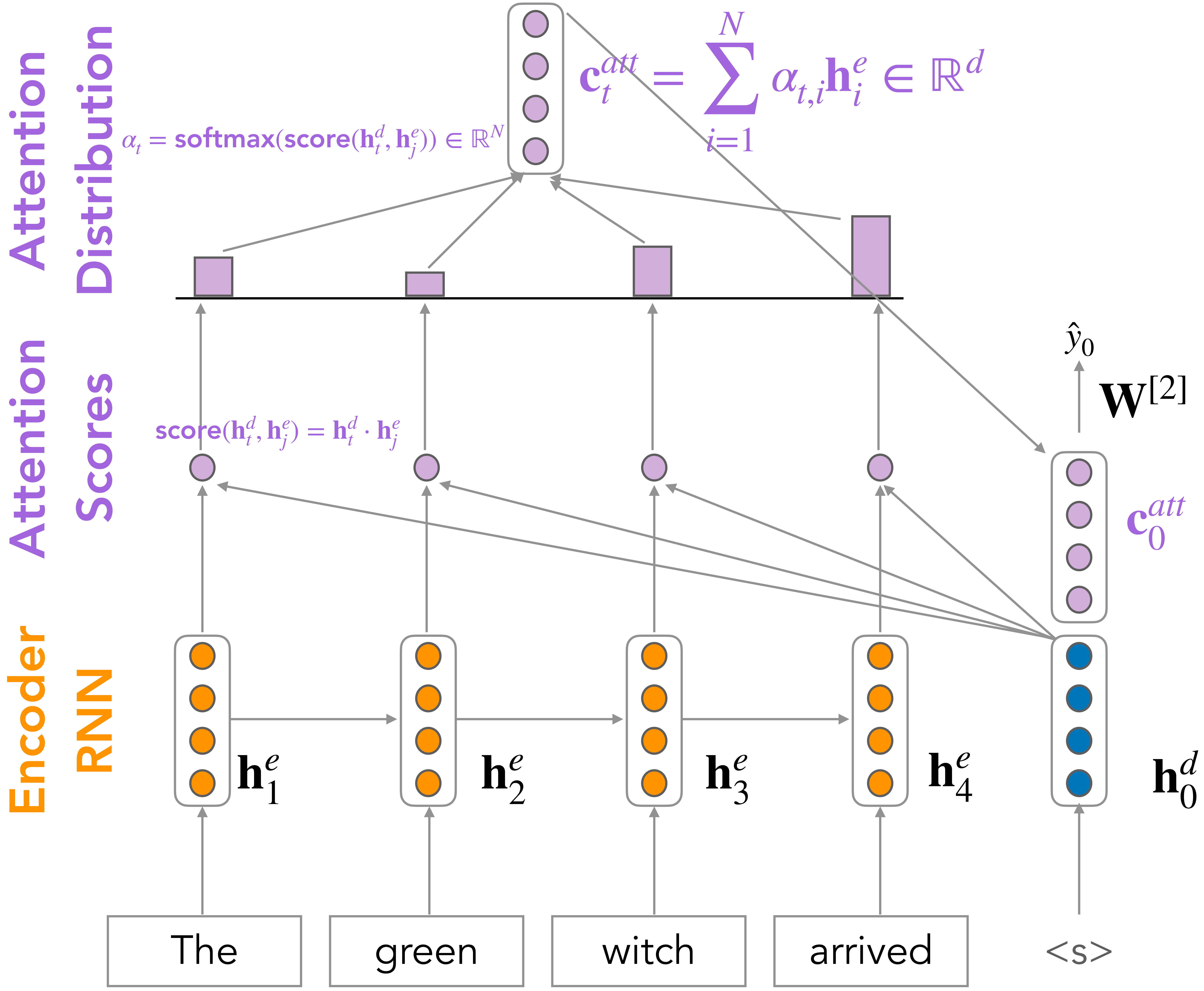

$$\hat{y}_t = \text{softmax}(\mathbf{W}^{[2]}[\mathbf{h}_t^d; \mathbf{c}_t^{att}])$$

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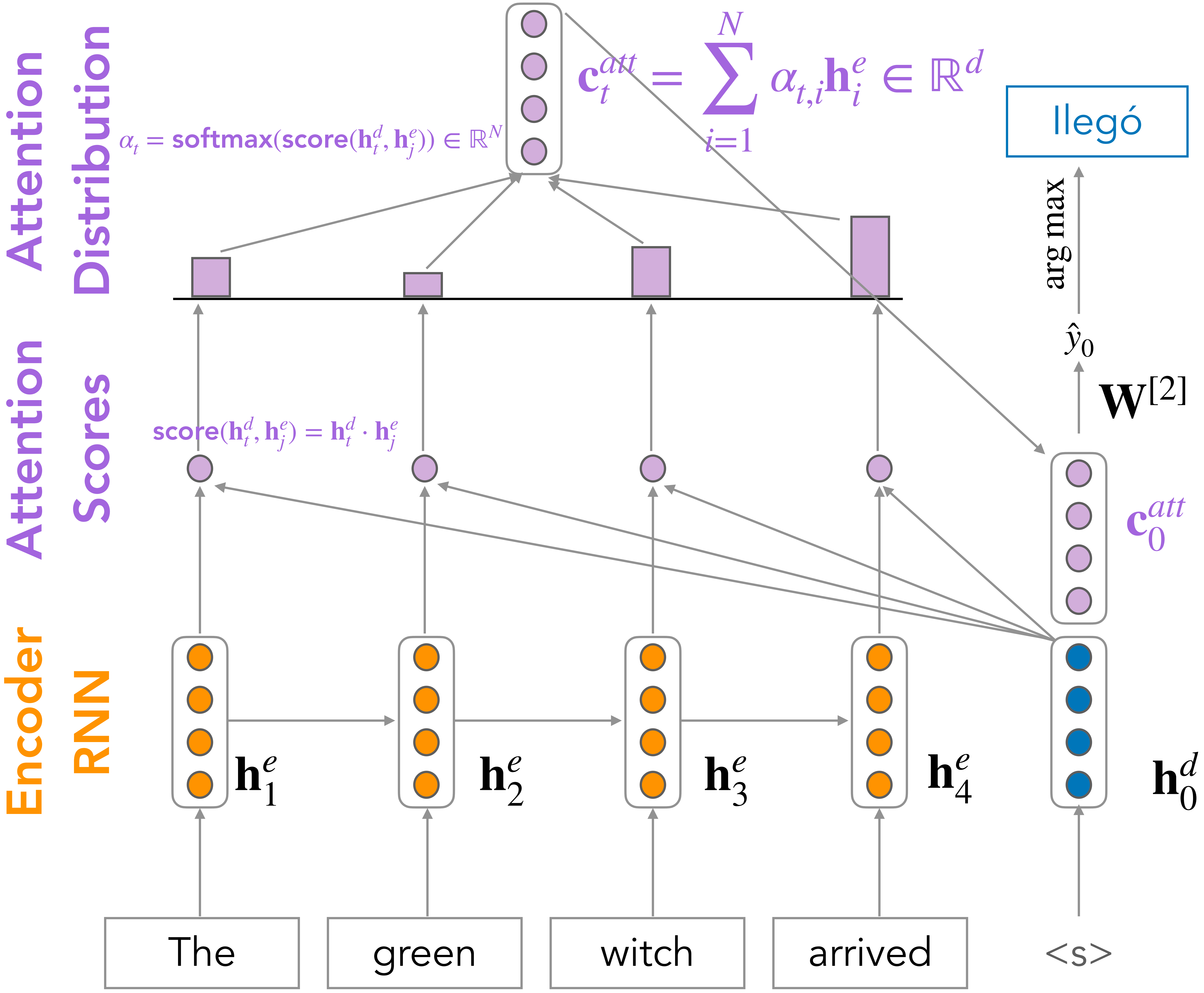

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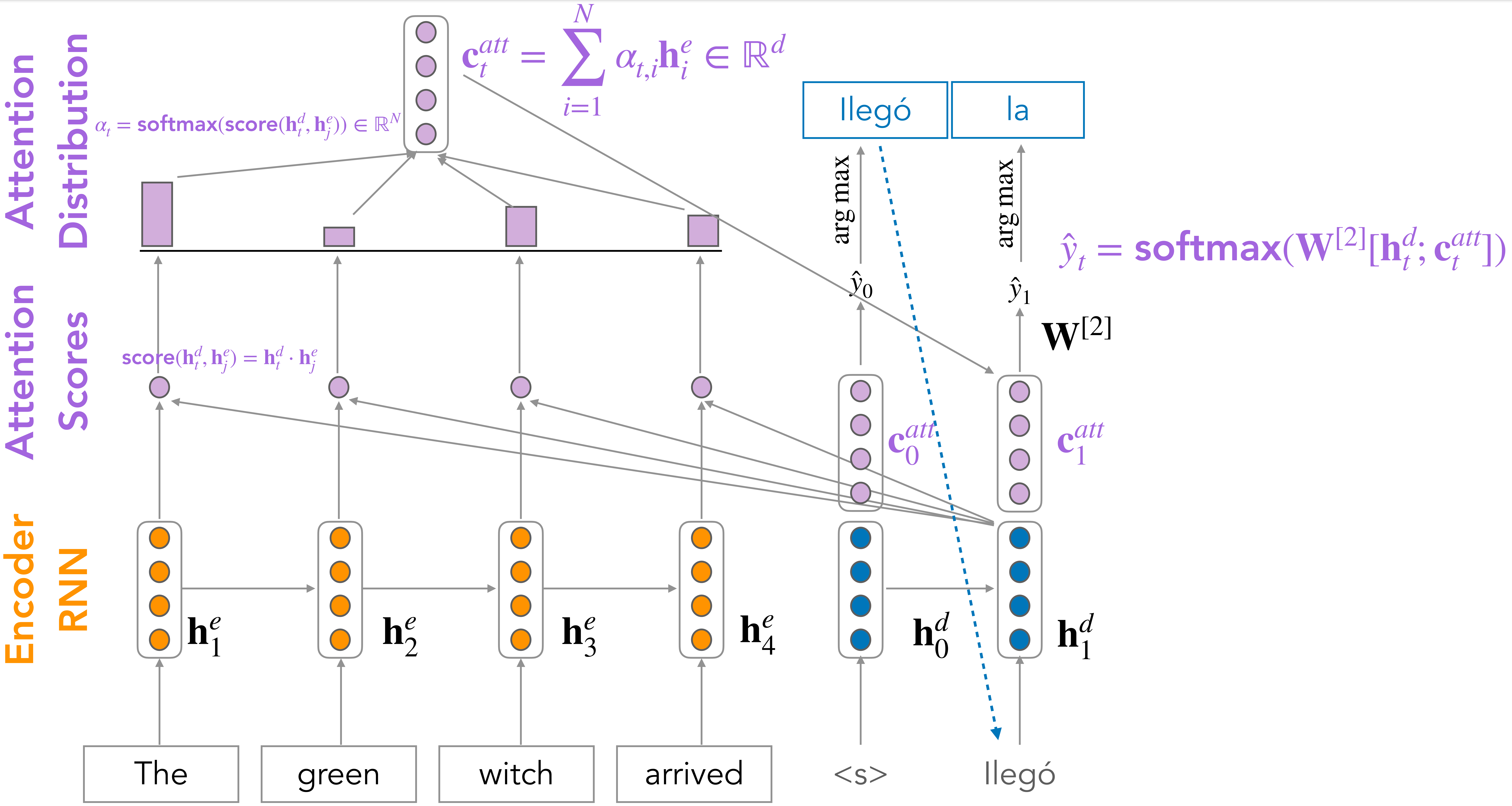

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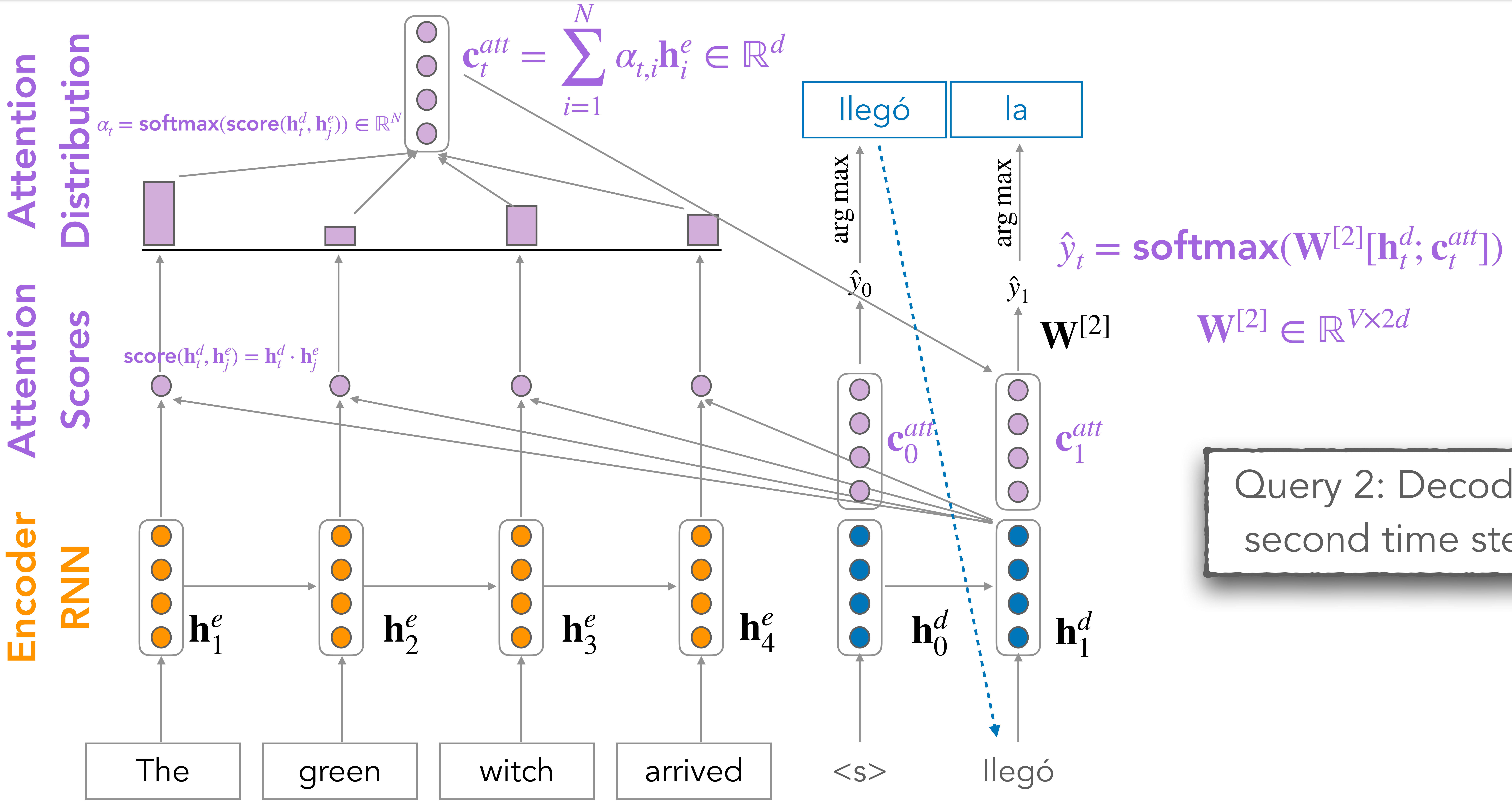

Query 2: Decoder, second time step

Source Sentence x

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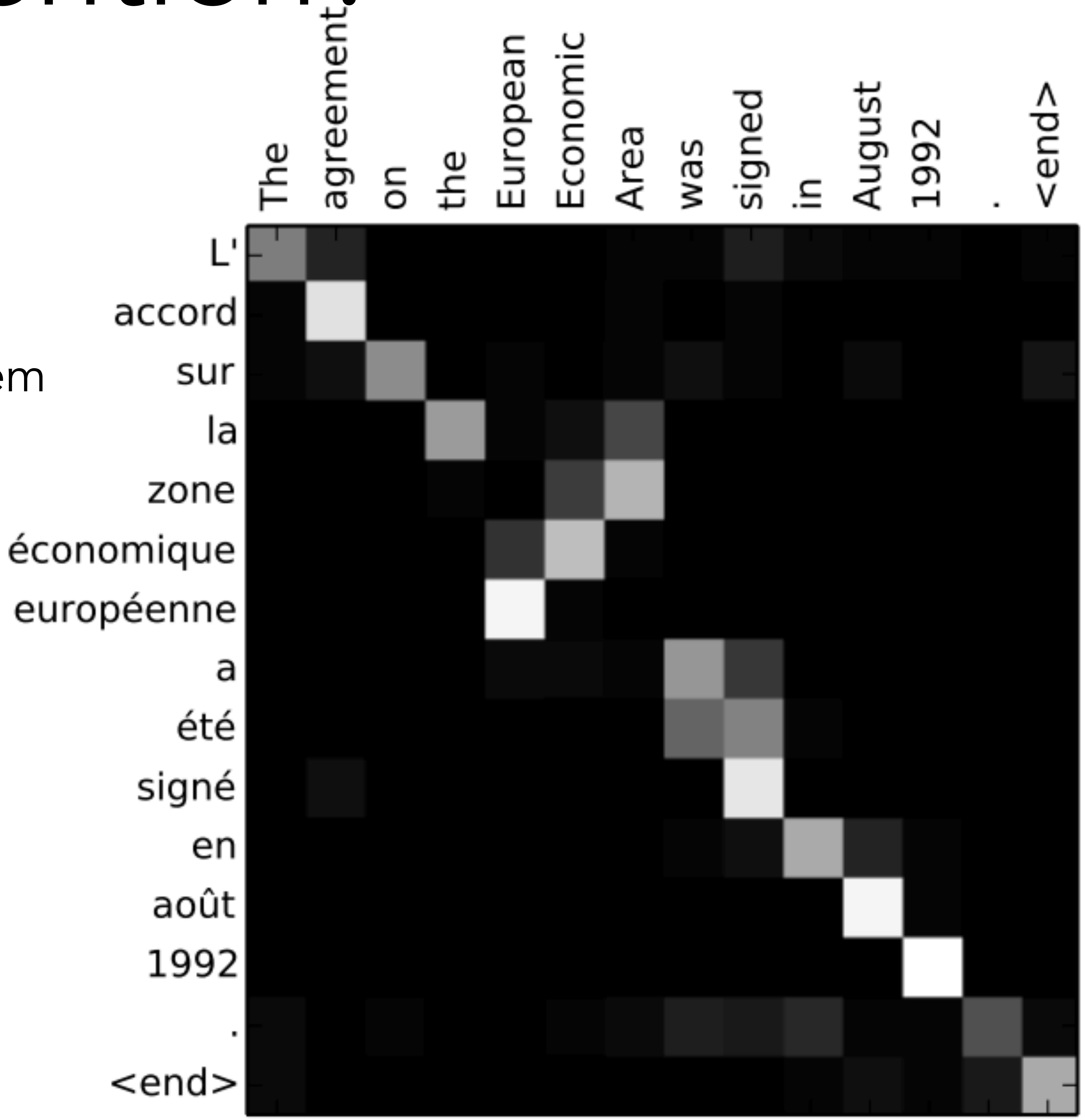
Why Attention?

- Attention significantly **improves** neural machine translation **performance**
  - Very useful to allow decoder to focus on certain parts of the source
- Attention **solves the information bottleneck** problem
  - Attention allows decoder to look directly at source; bypass bottleneck
- Attention **helps with vanishing gradient problem**
  - Provides shortcut to faraway states
- Attention provides some **interpretability**
  - By inspecting attention distribution, we can see what the decoder was focusing on →
  - We get alignment for free! We never explicitly trained an alignment system! The network just learned alignment by itself



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- Announcements
- Recap: Seq2Seq and Attention
- More on Attention
- Transformers: Self-Attention Networks
    - Multiheaded Attention
    - Positional Embeddings
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More on Attention

Attention Variants

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

This leads to the attention output $\mathbf{c}_t^{att}$ (sometimes called the attention context vector)

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- Linear attention: No non-linearity, i.e. no step (2).
  - Unsurprisingly, does not work too well…

More on Attention

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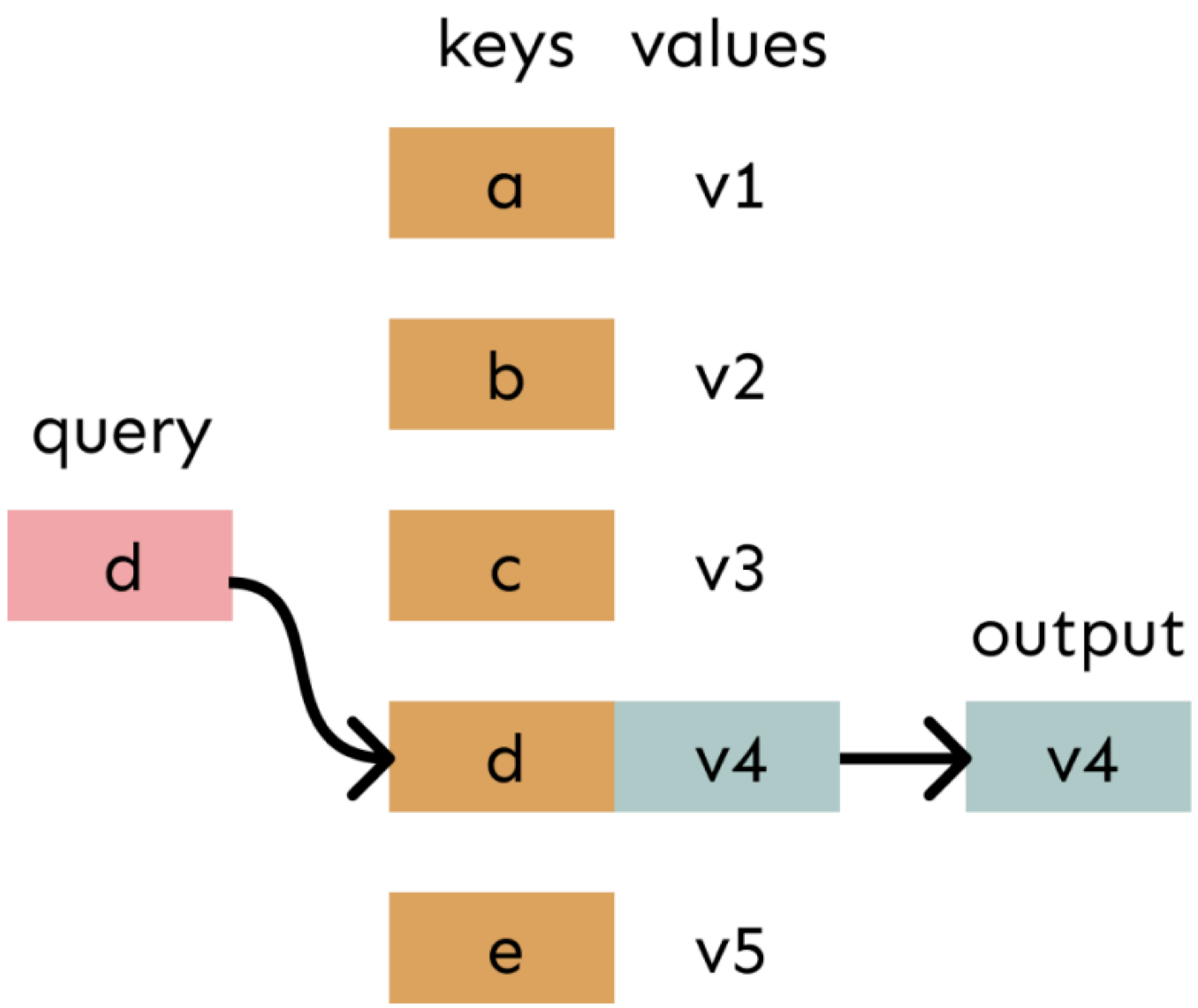
- Attention is a powerful, flexible, general deep learning technique in all deep learning models.
  - A new idea from after 2010! Originated in NMT

Attention and lookup tables

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



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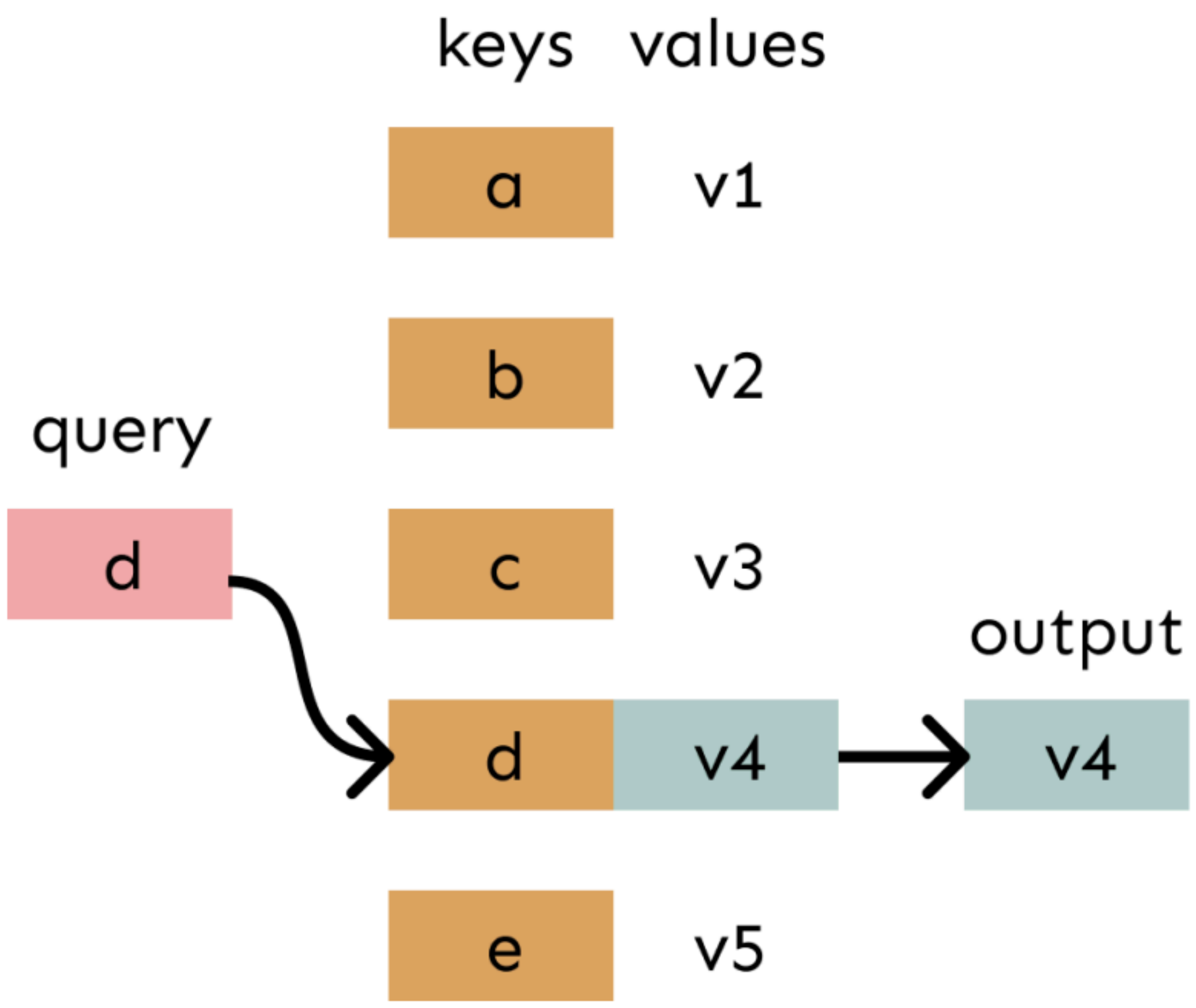

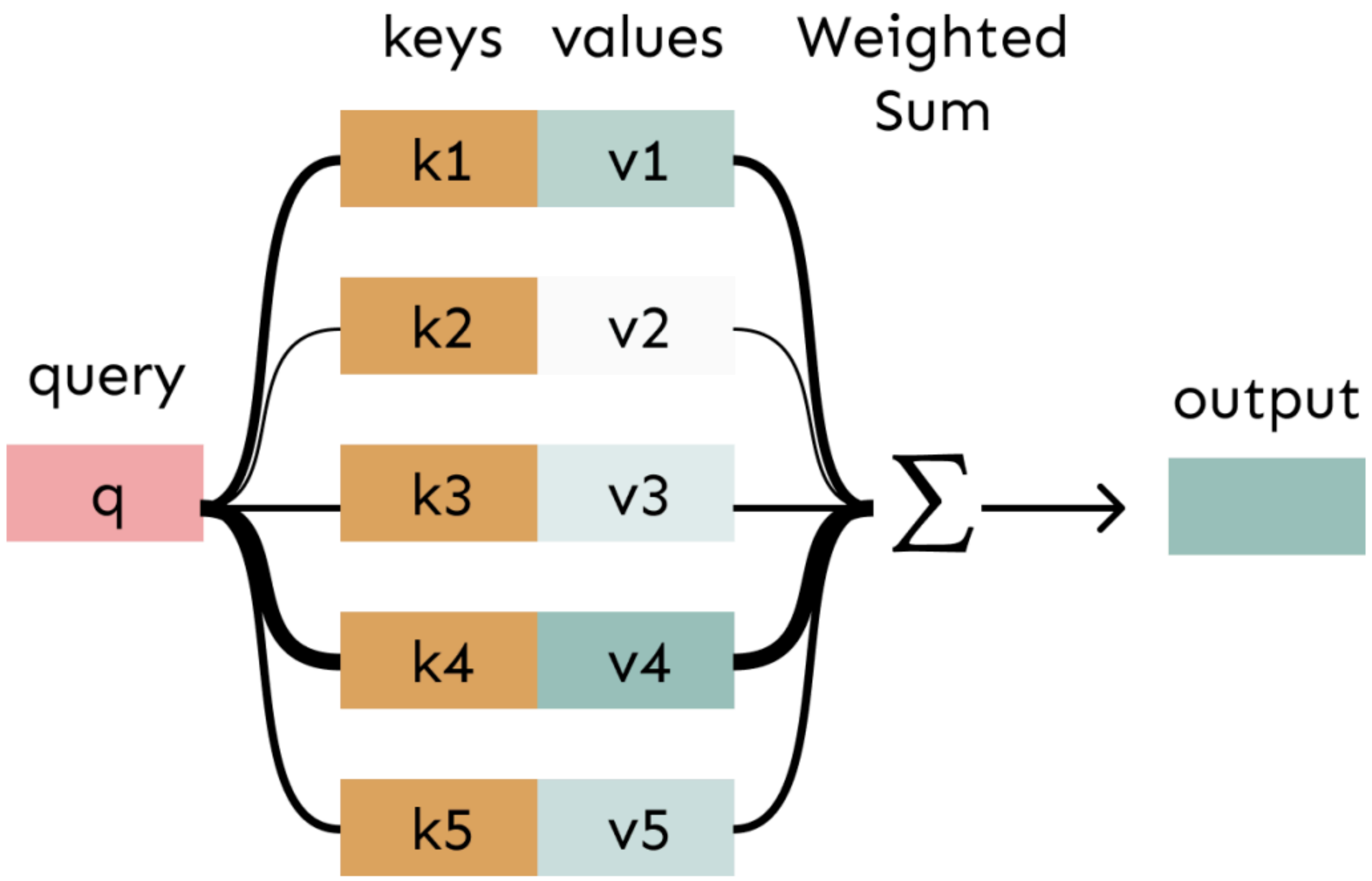

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Attention performs fuzzy lookup in a key-value store

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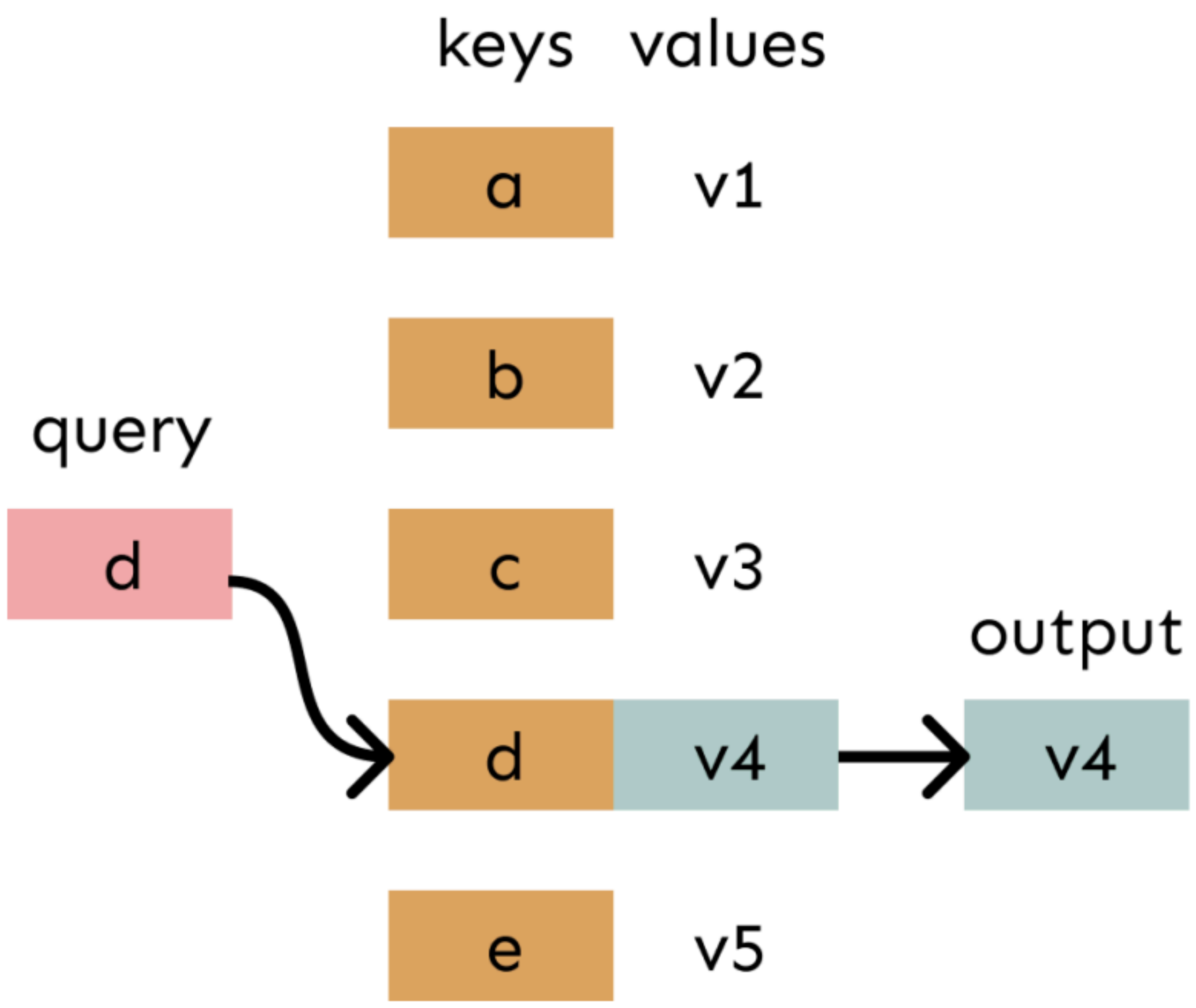

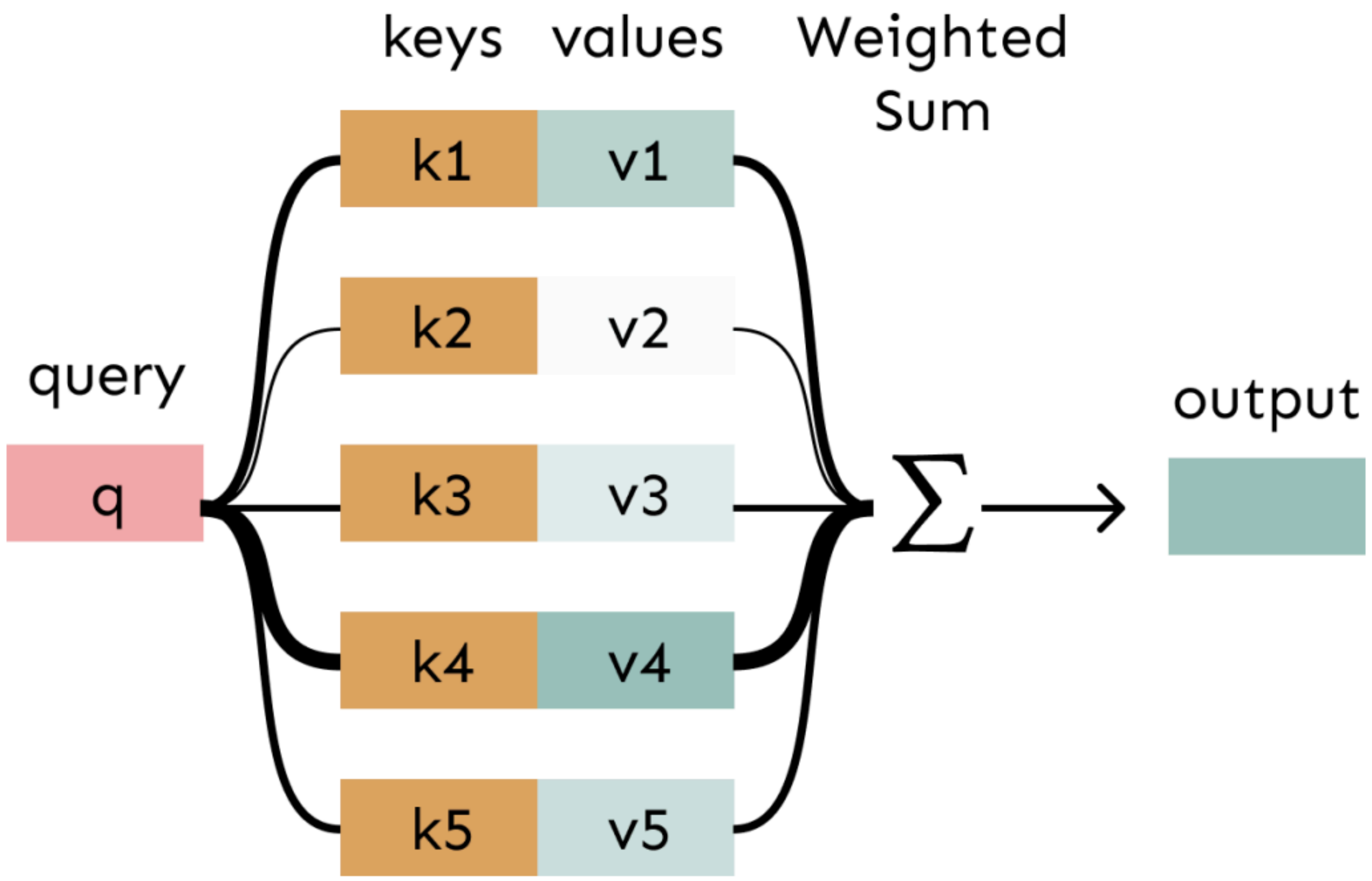

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q

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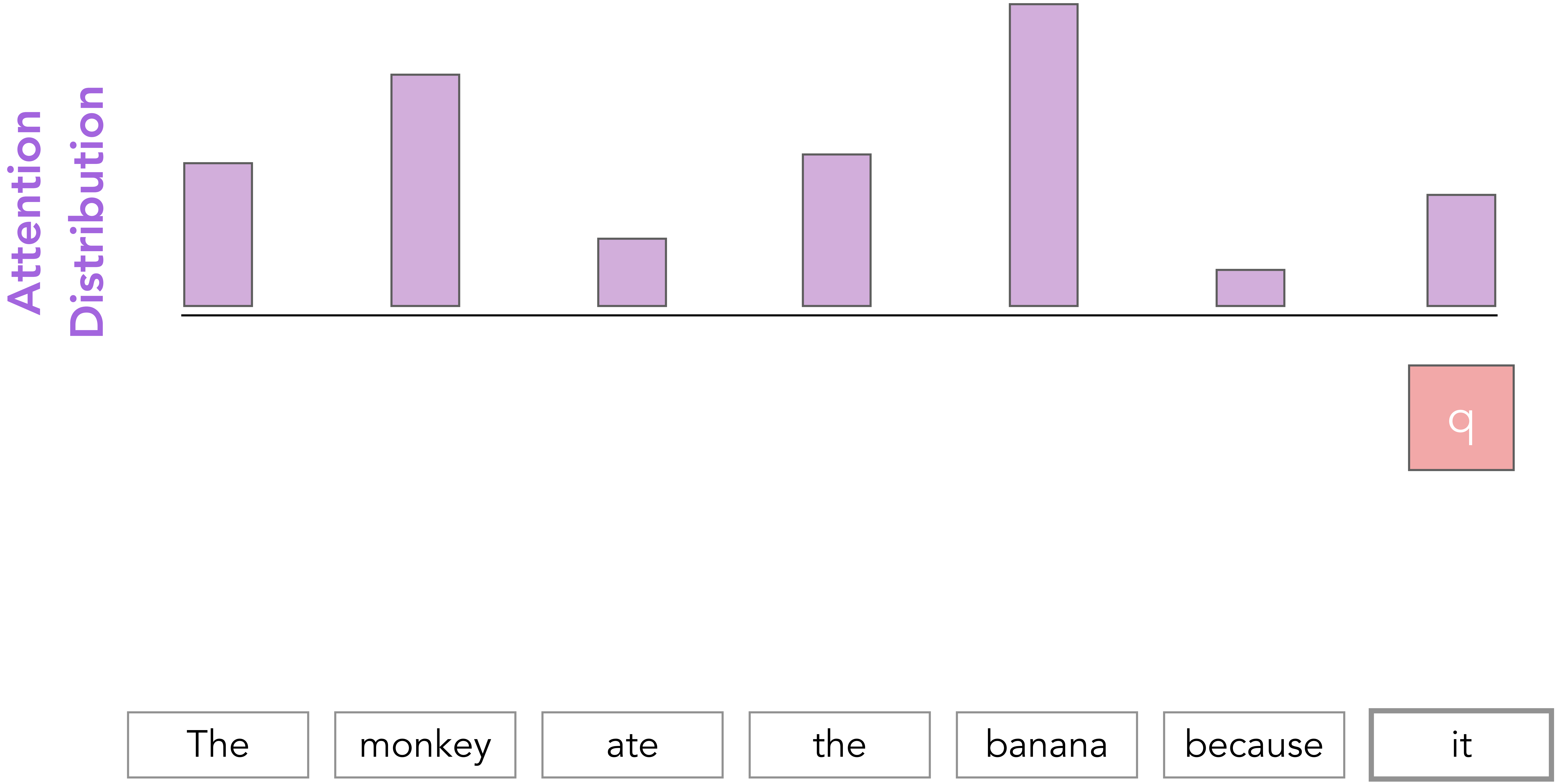
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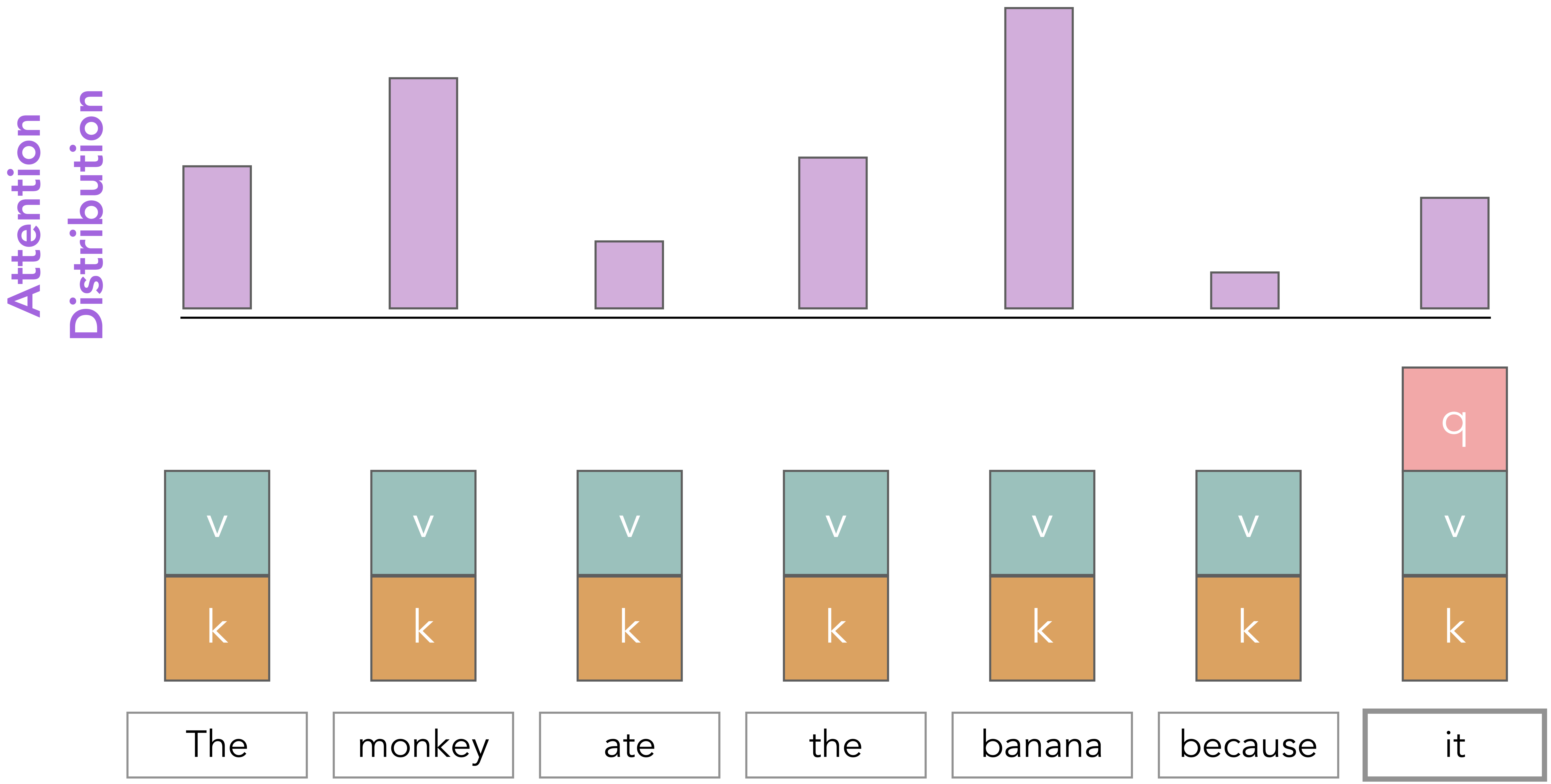
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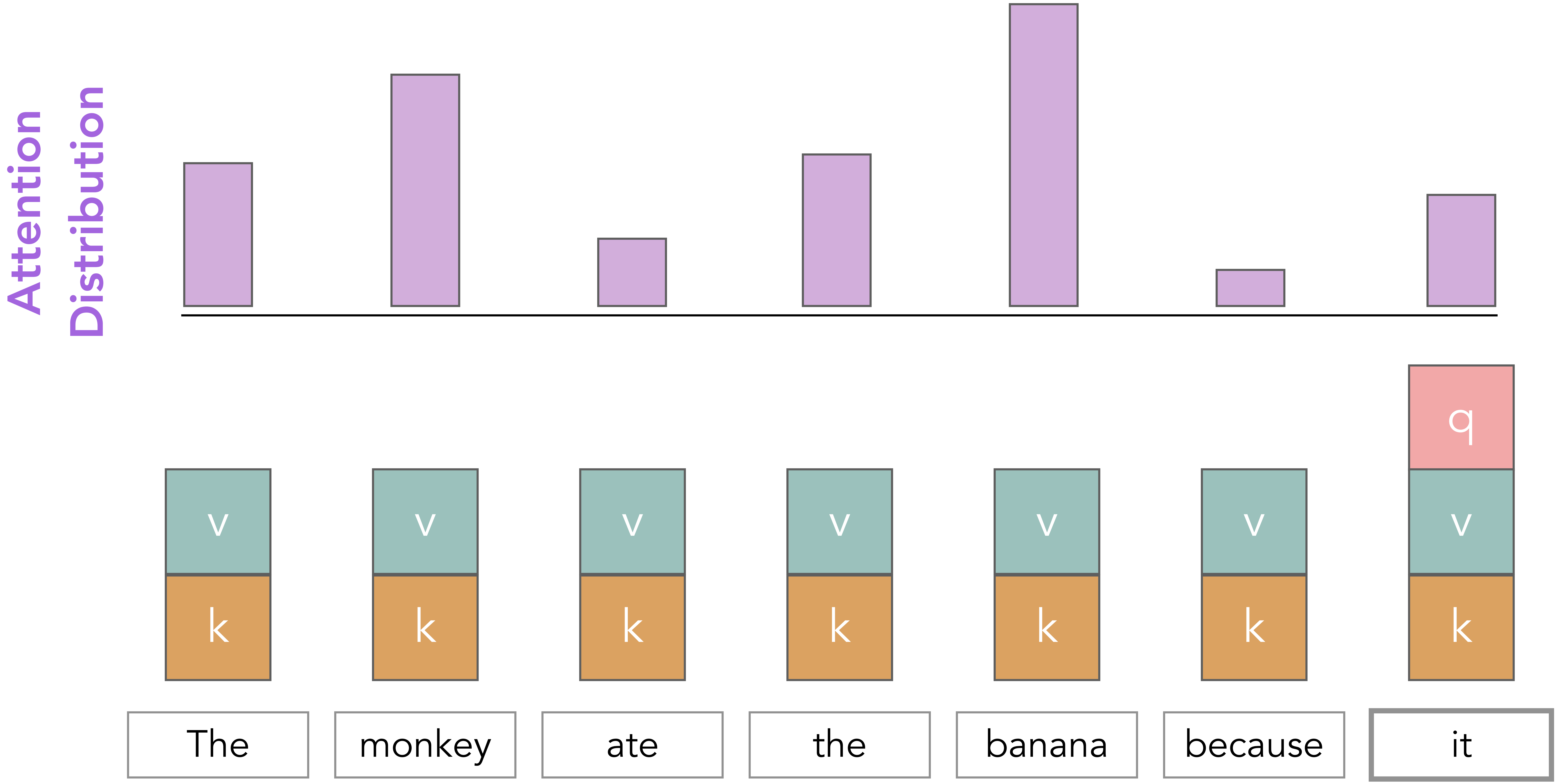
Attention in the decoder



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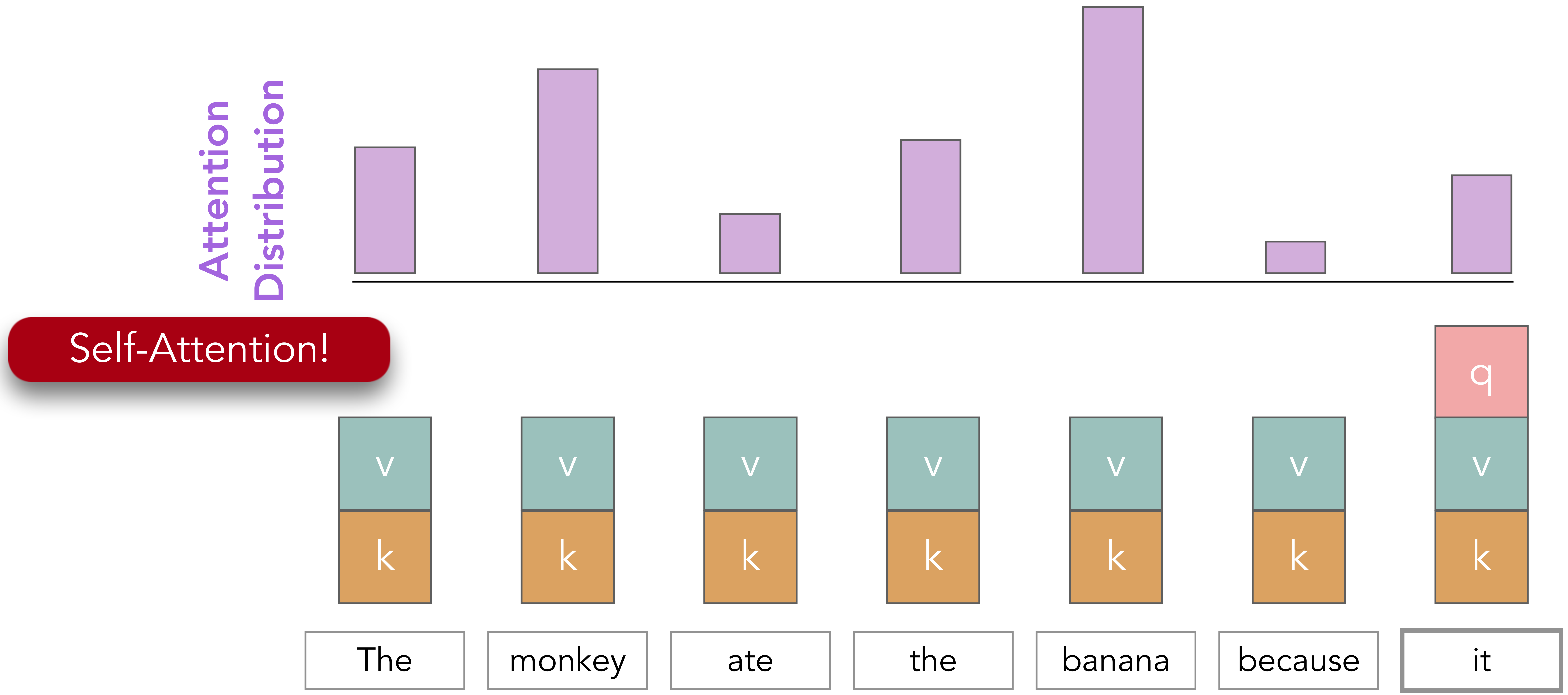

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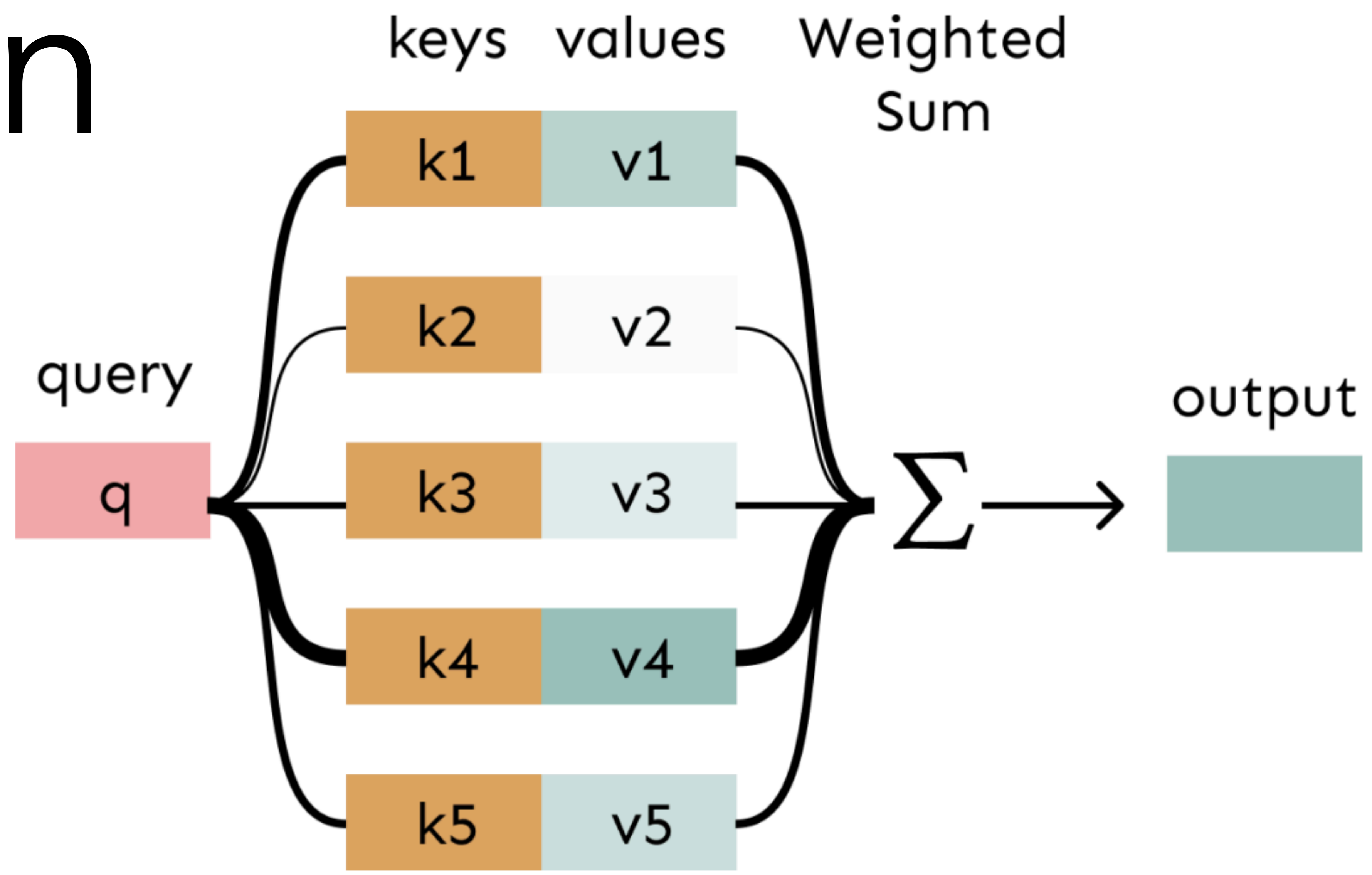
Transformers:
Self-Attention Networks

Self-Attention

Keys, Queries, Values from the same sequence



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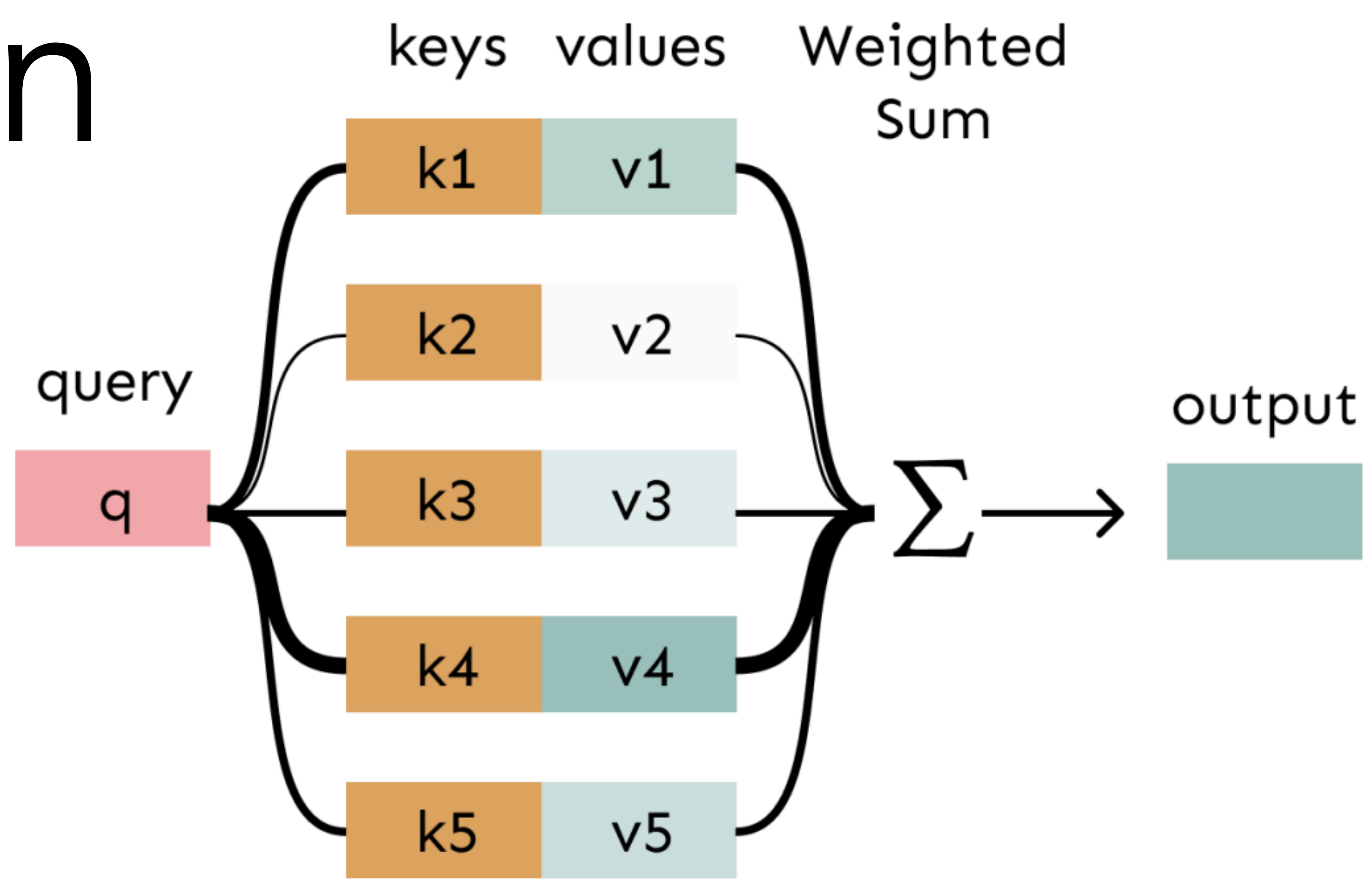

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Let $w_{1:N}$ be a sequence of words in vocabulary V

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

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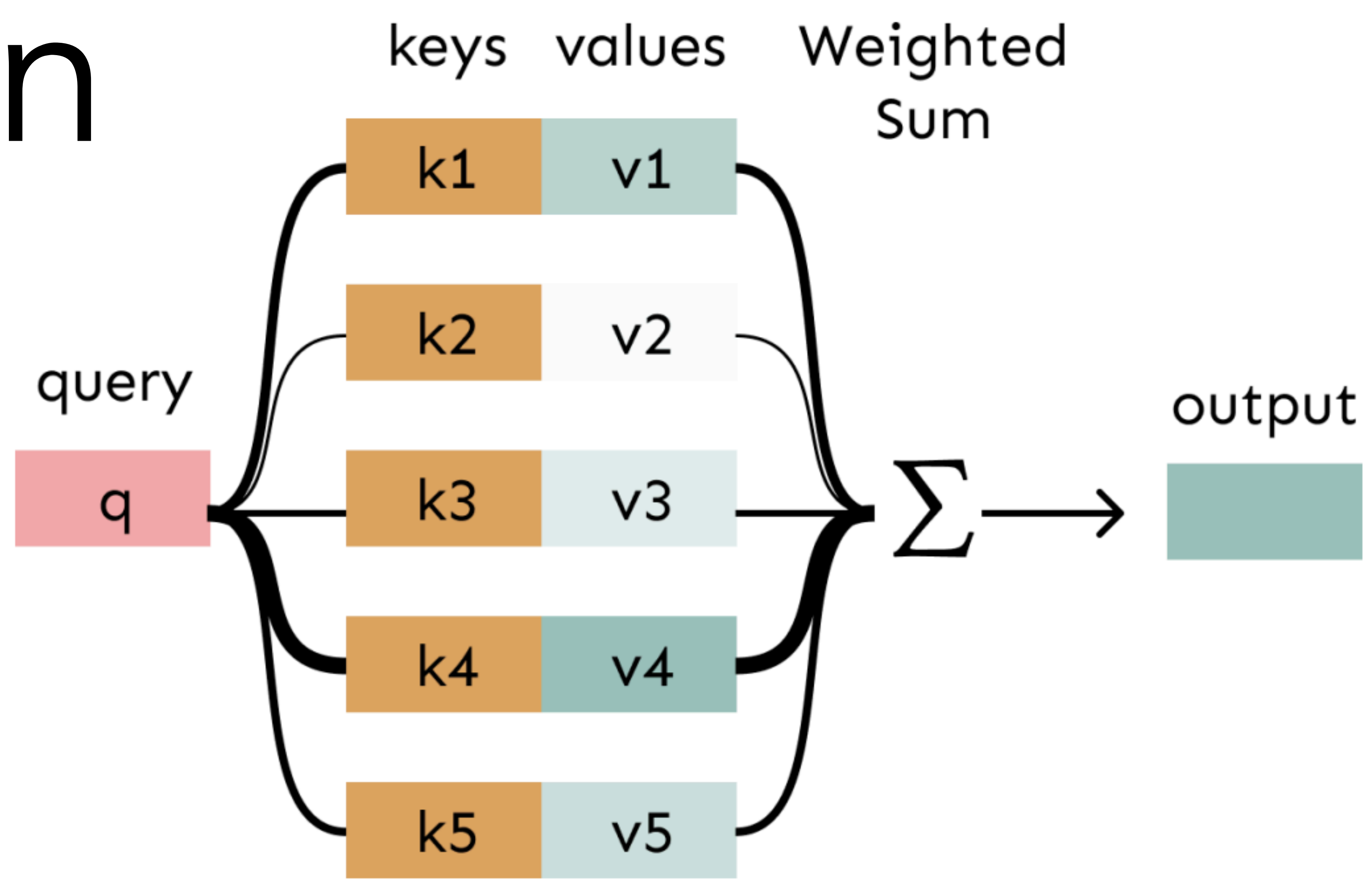

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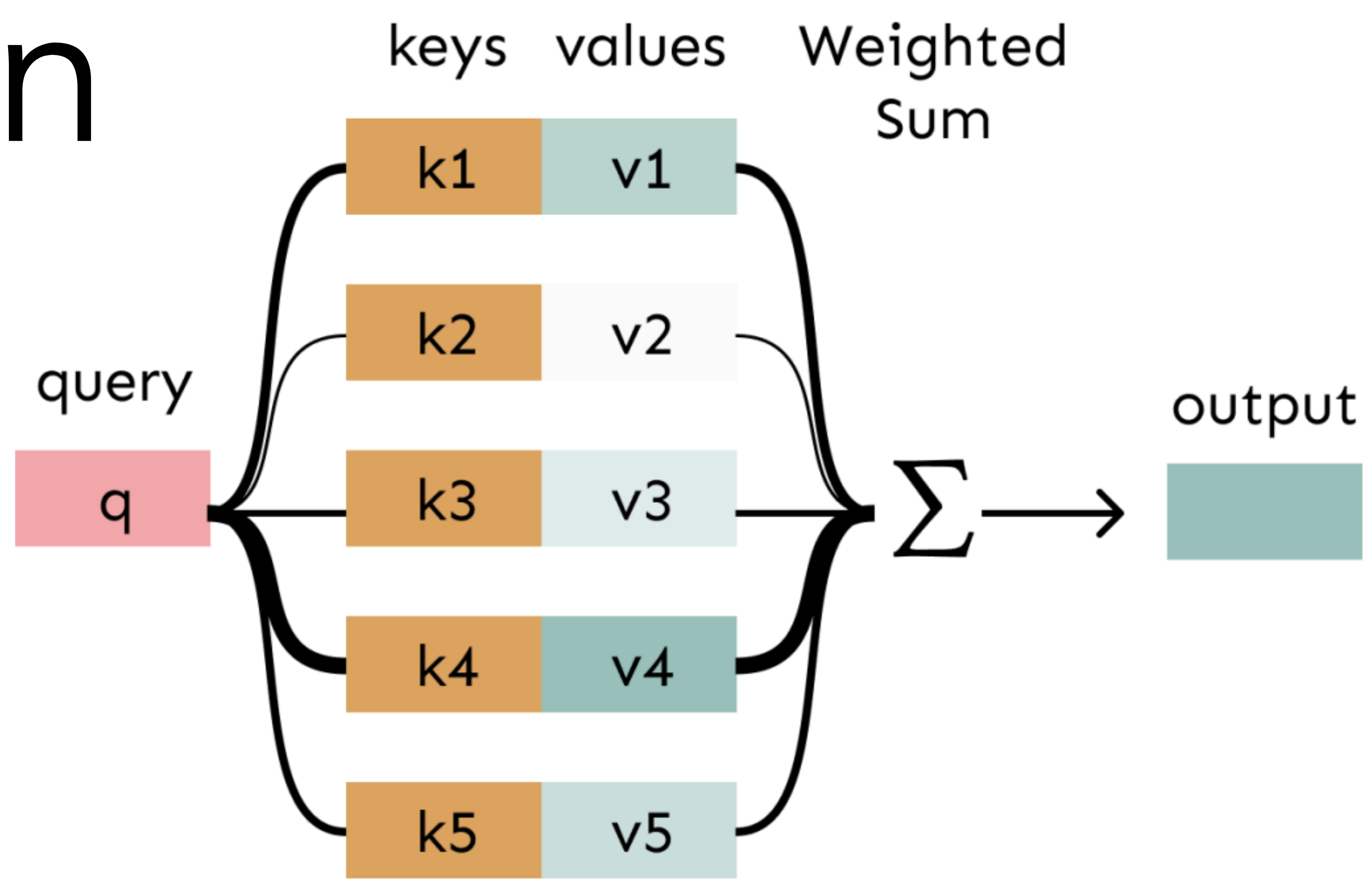
$q_i = Q\boldsymbol{x_i}$ (queries) $k_i = K\boldsymbol{x_i}$ (keys) $v_i = V\boldsymbol{x_i}$ (values)

Self-Attention



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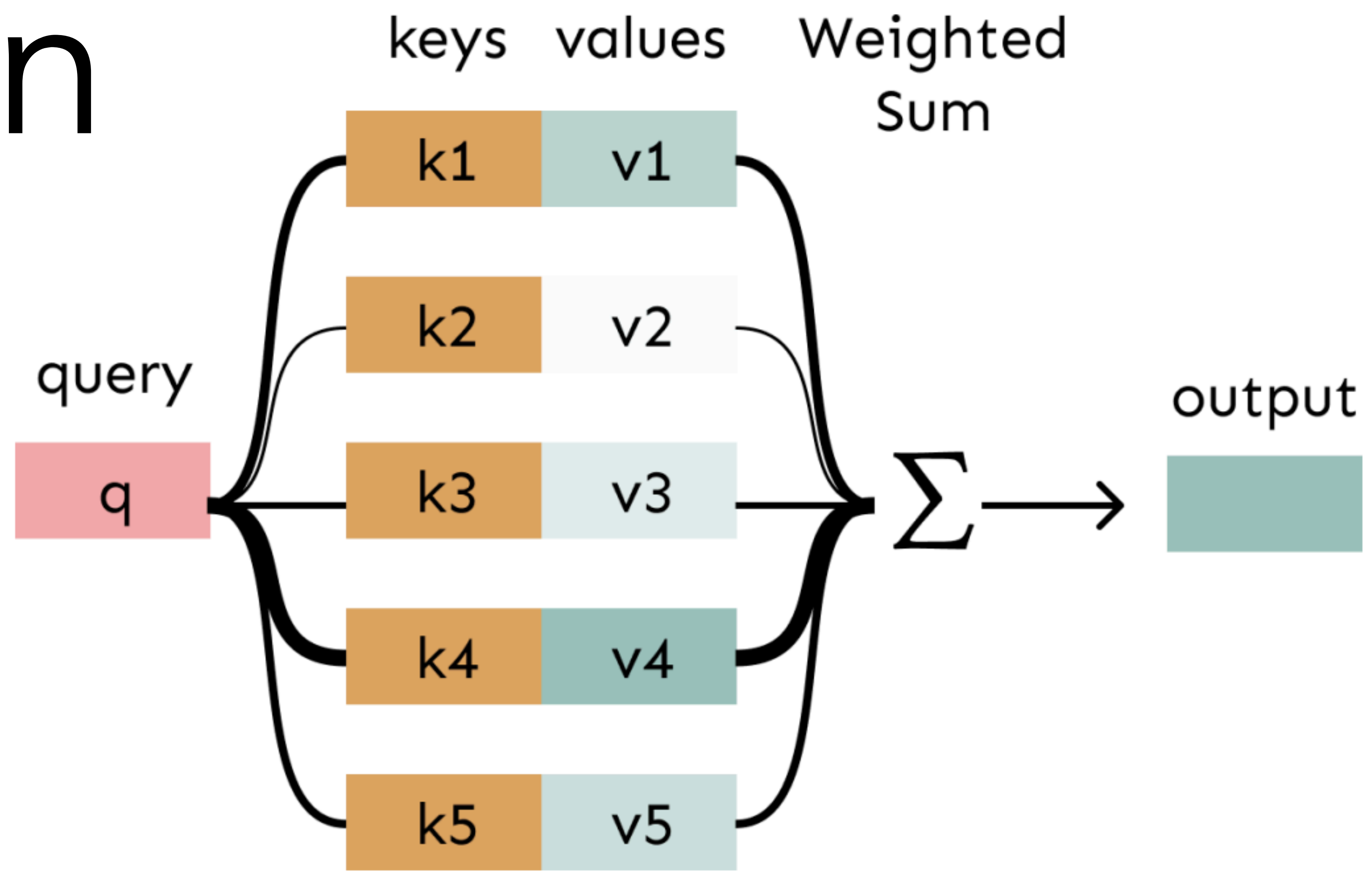
$q_i = Q\boldsymbol{x_i}$ (queries) $\quad$ $k_i = K\boldsymbol{x_i}$ (keys) $\quad$ $v_i = V\boldsymbol{x_i}$ (values)

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

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

Self-Attention



Keys, Queries, Values from the same sequence

Let $w_{1:N}$ be a sequence of words in vocabulary V

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

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

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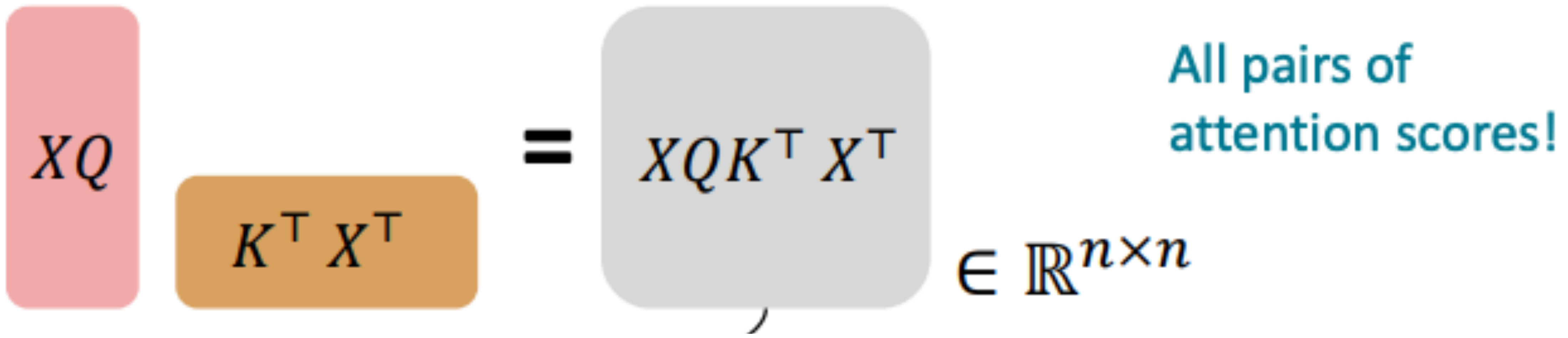

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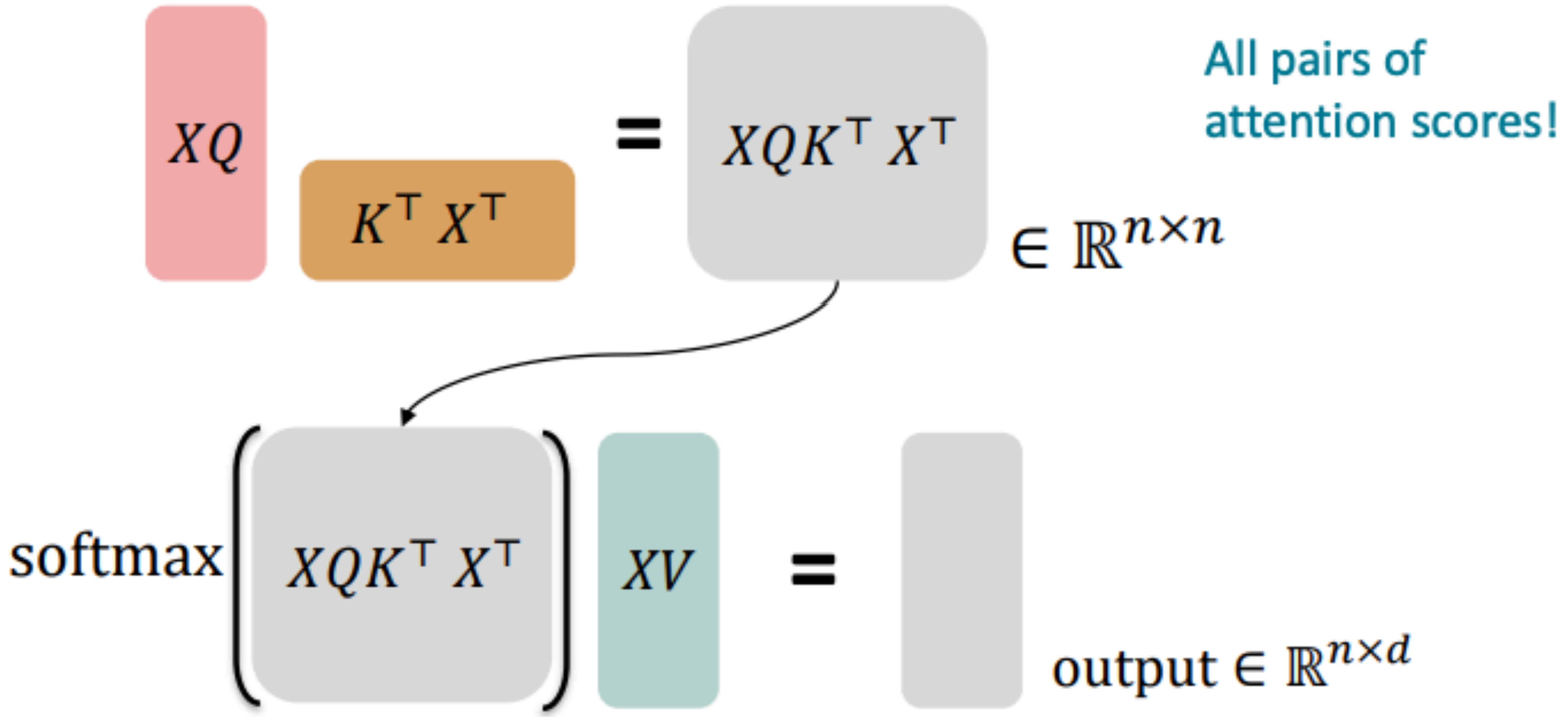
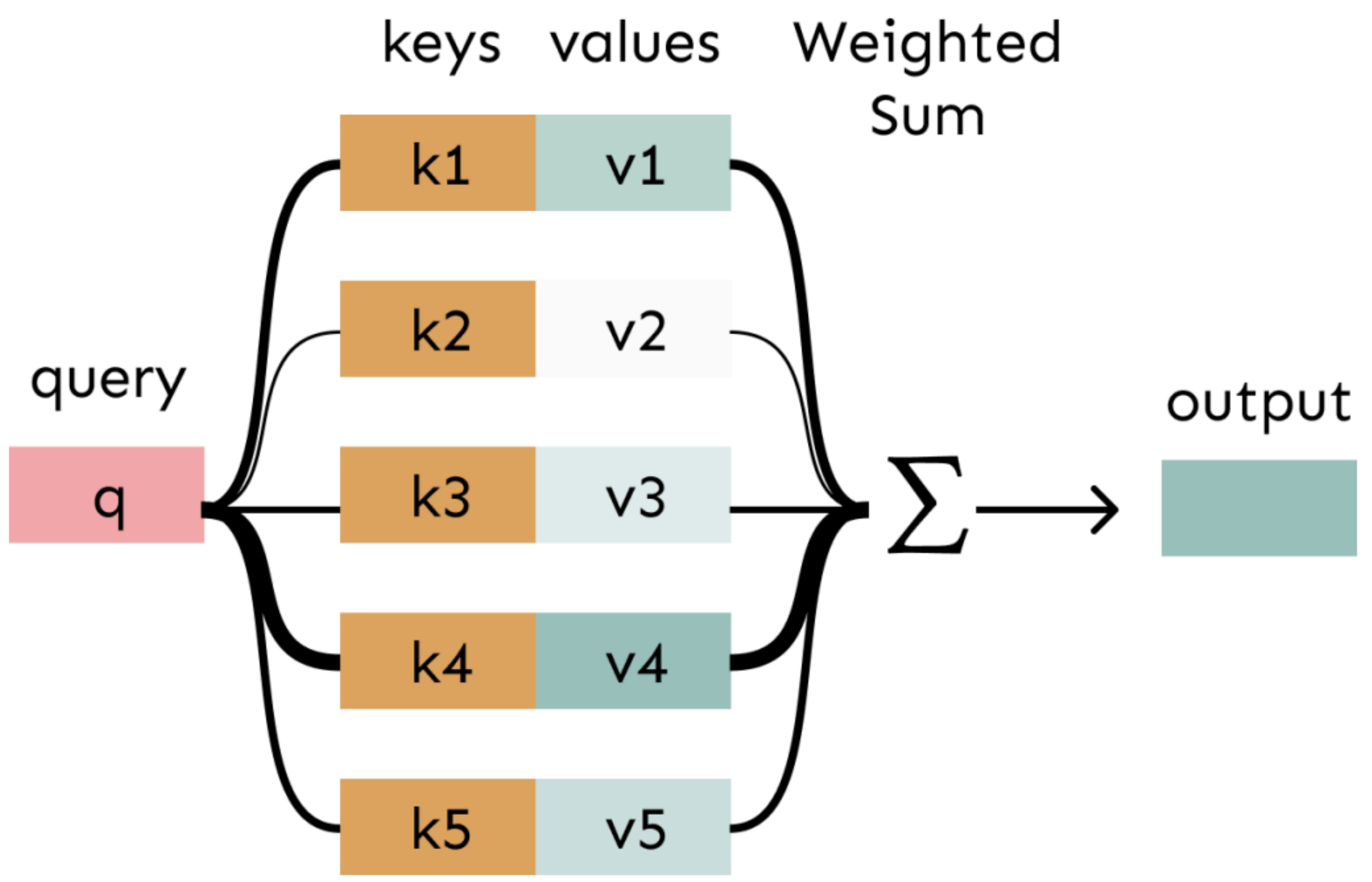


Next, softmax, and compute the weighted average with another matrix multiplication.

Why Self-Attention?



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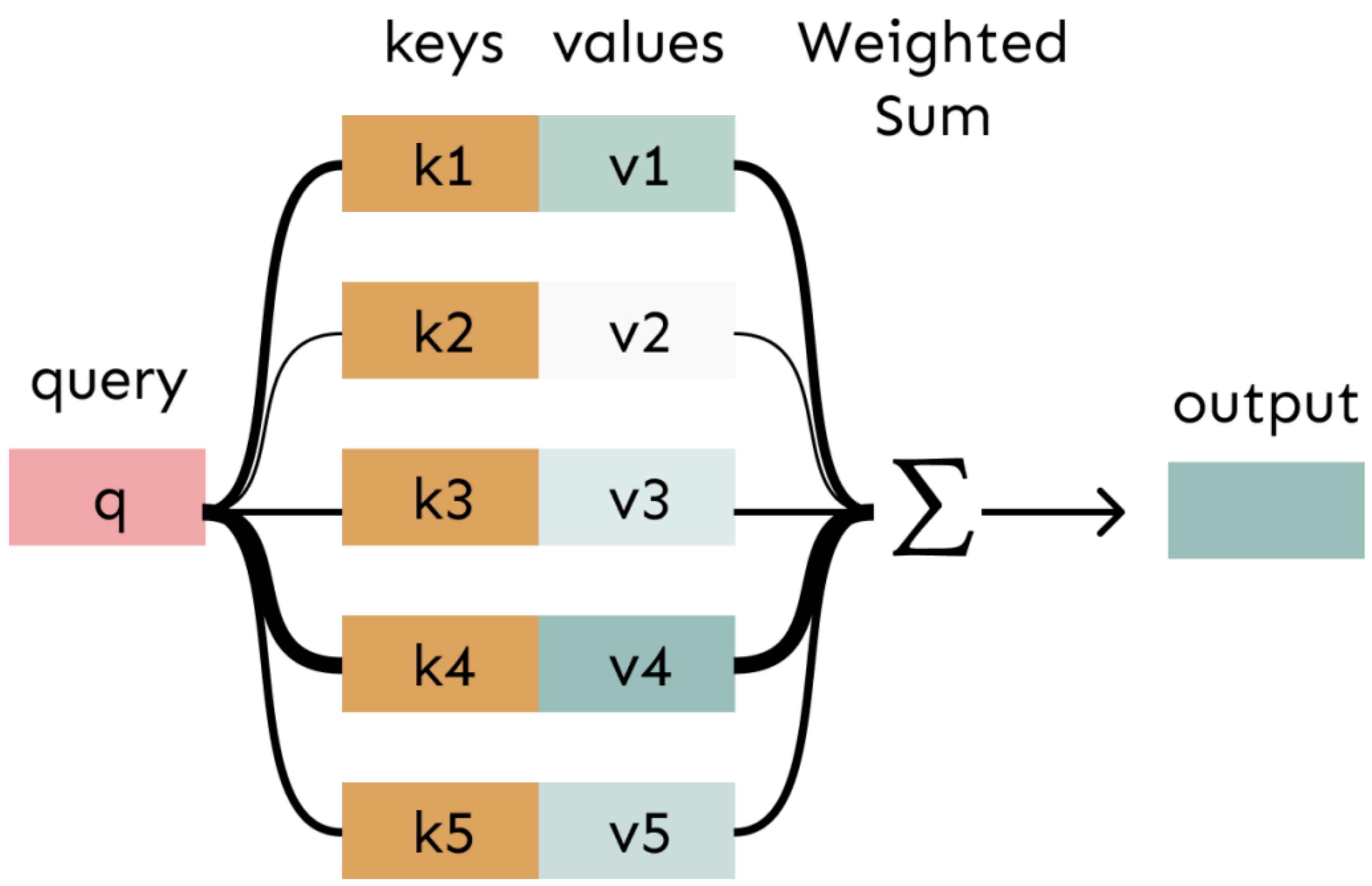

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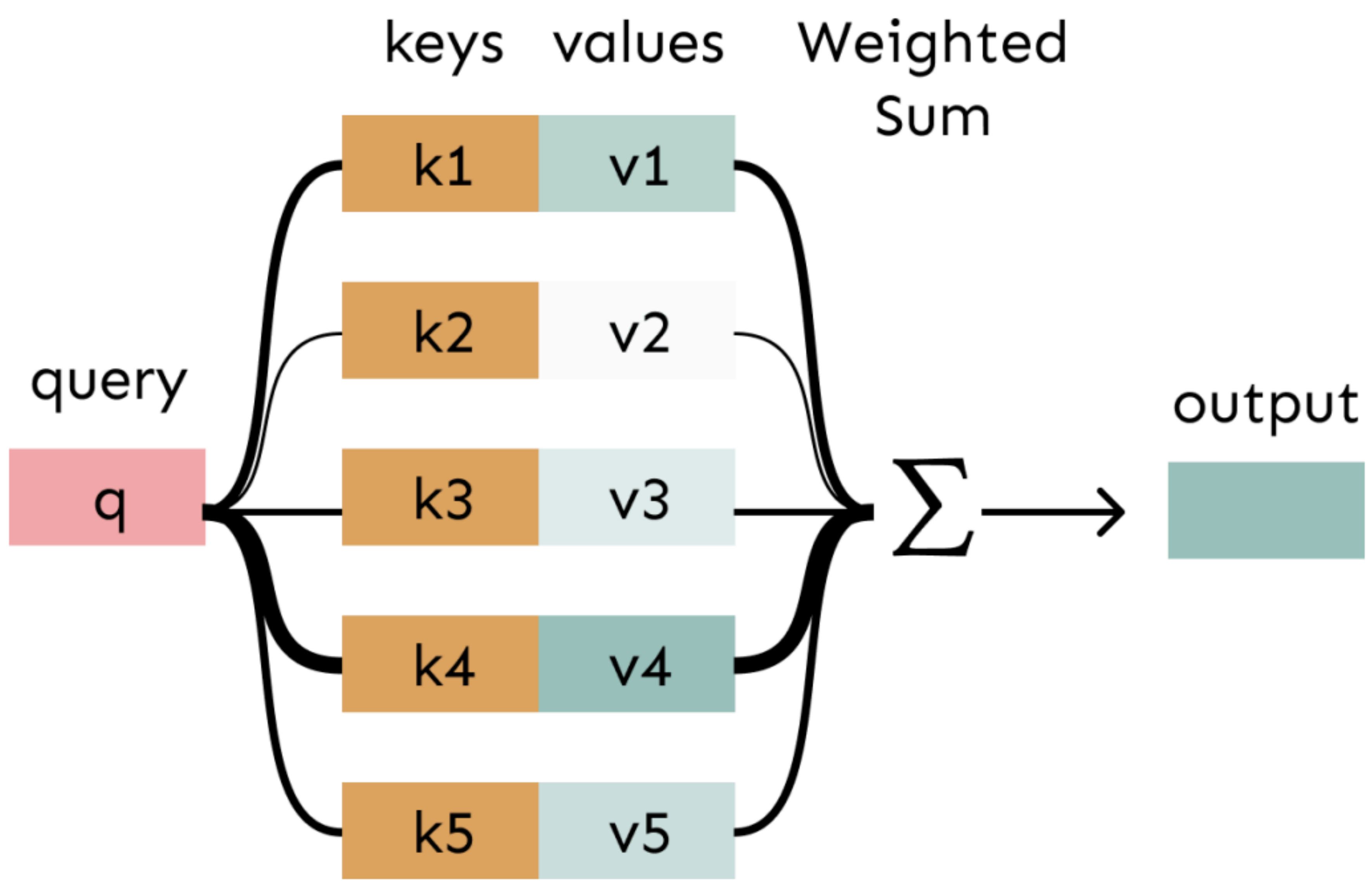

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- Used often with feedforward networks!

Transformers are Self-Attention Networks

Attention Is All You Need

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- 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
  - No more recurrent connections!

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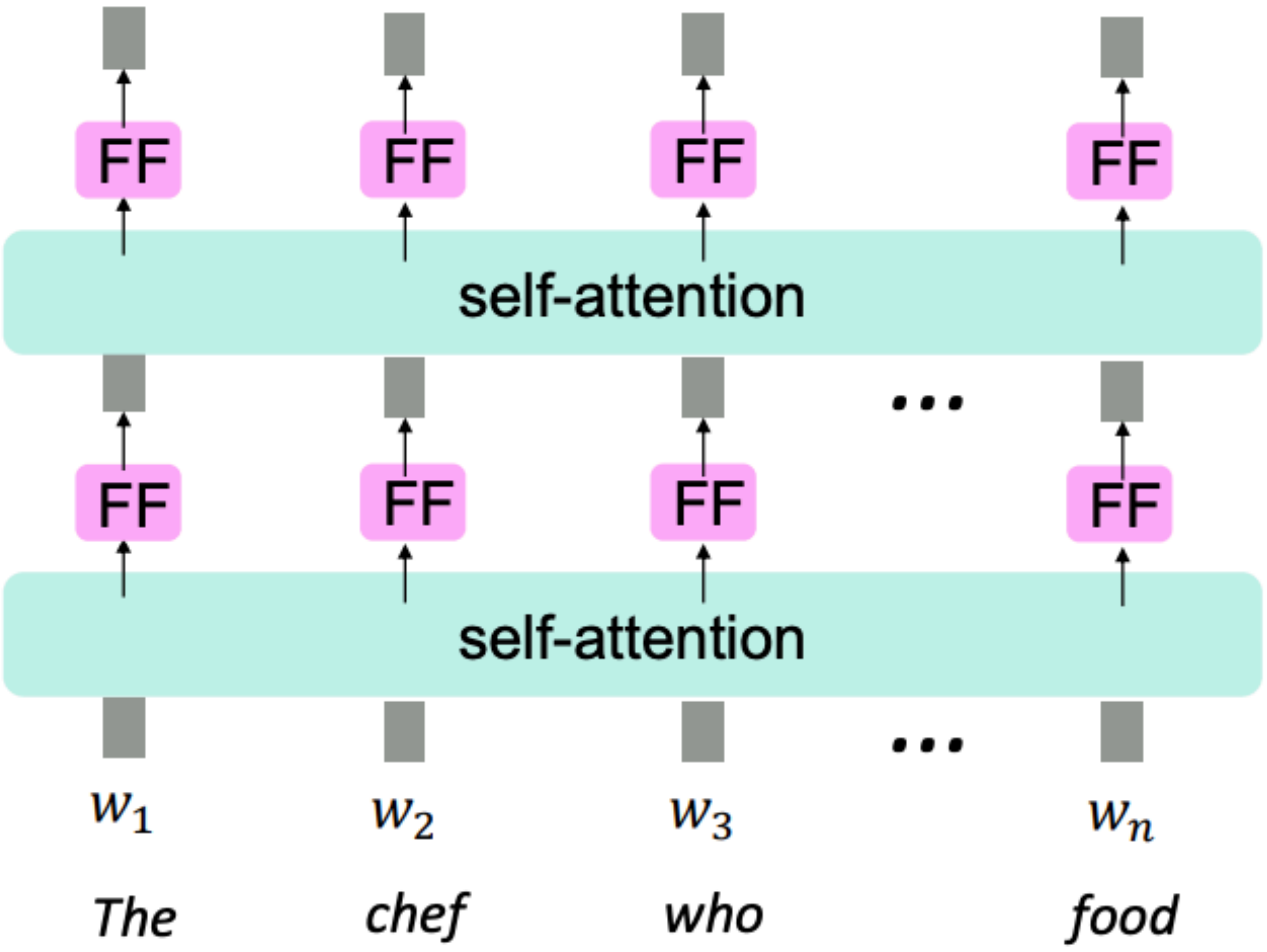

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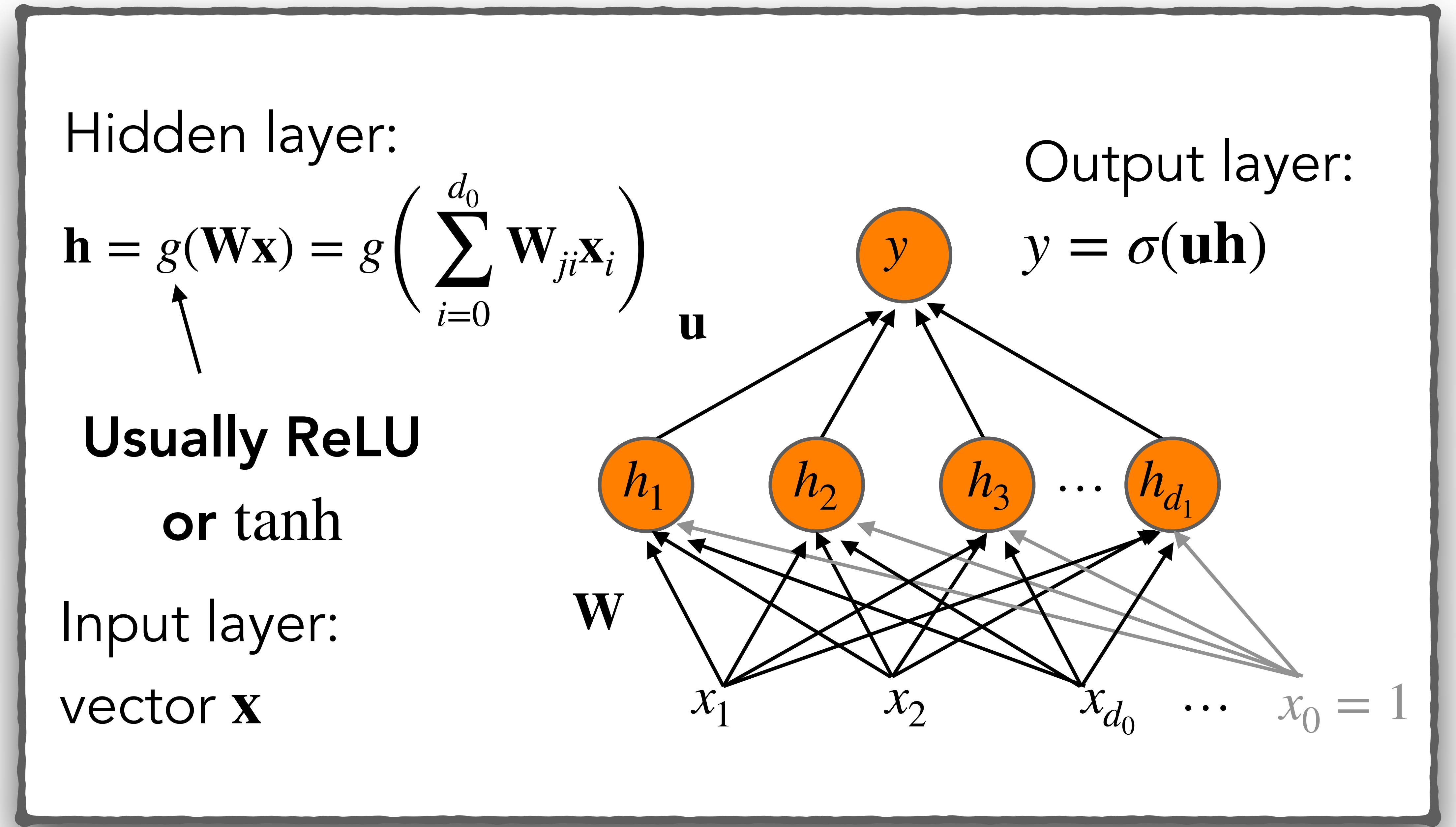

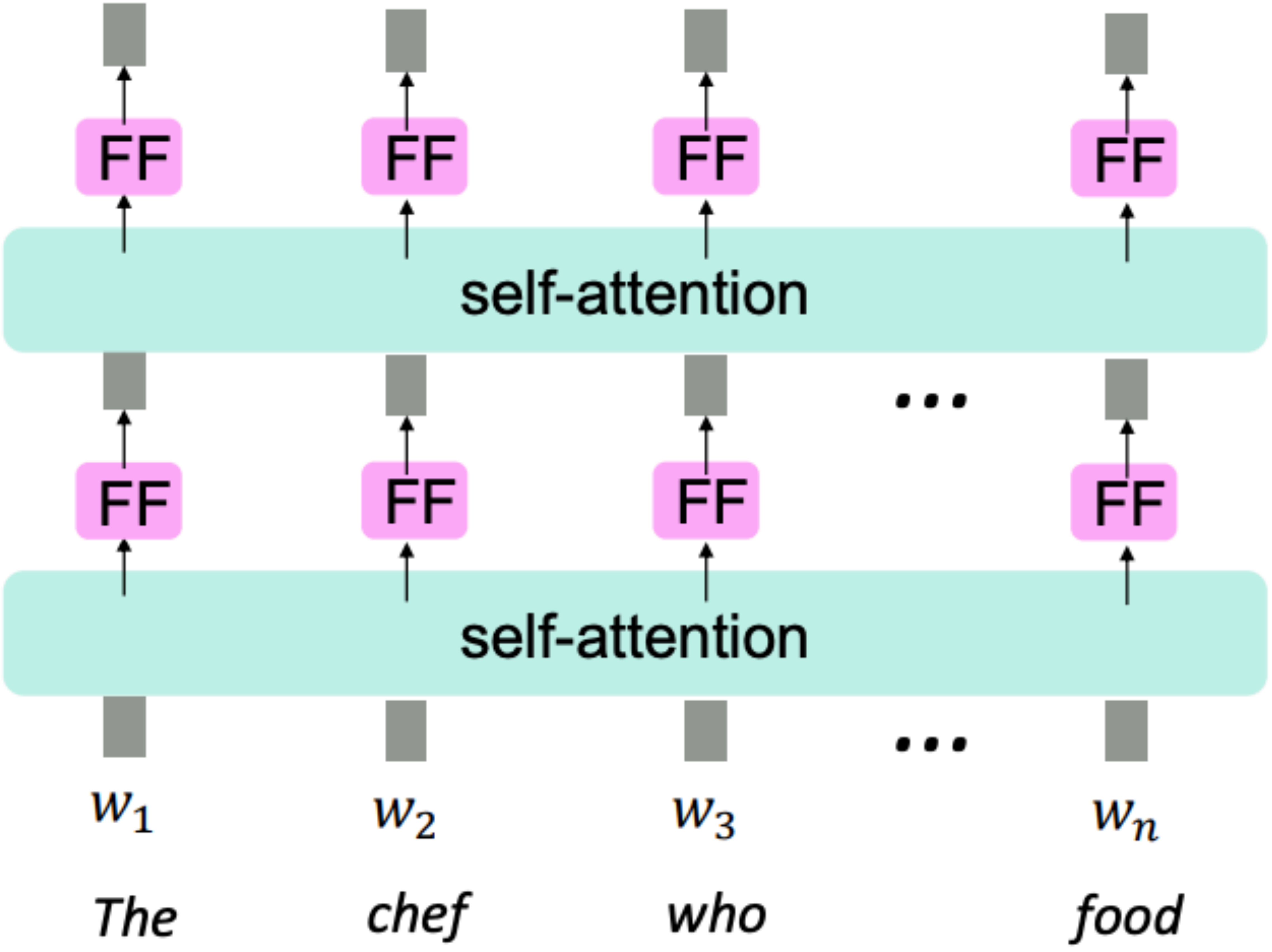

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	[START]	The	chef	who
[START]		$-\infty$	$-\infty$	$-\infty$
The			$-\infty$	$-\infty$
chef				$-\infty$
who				

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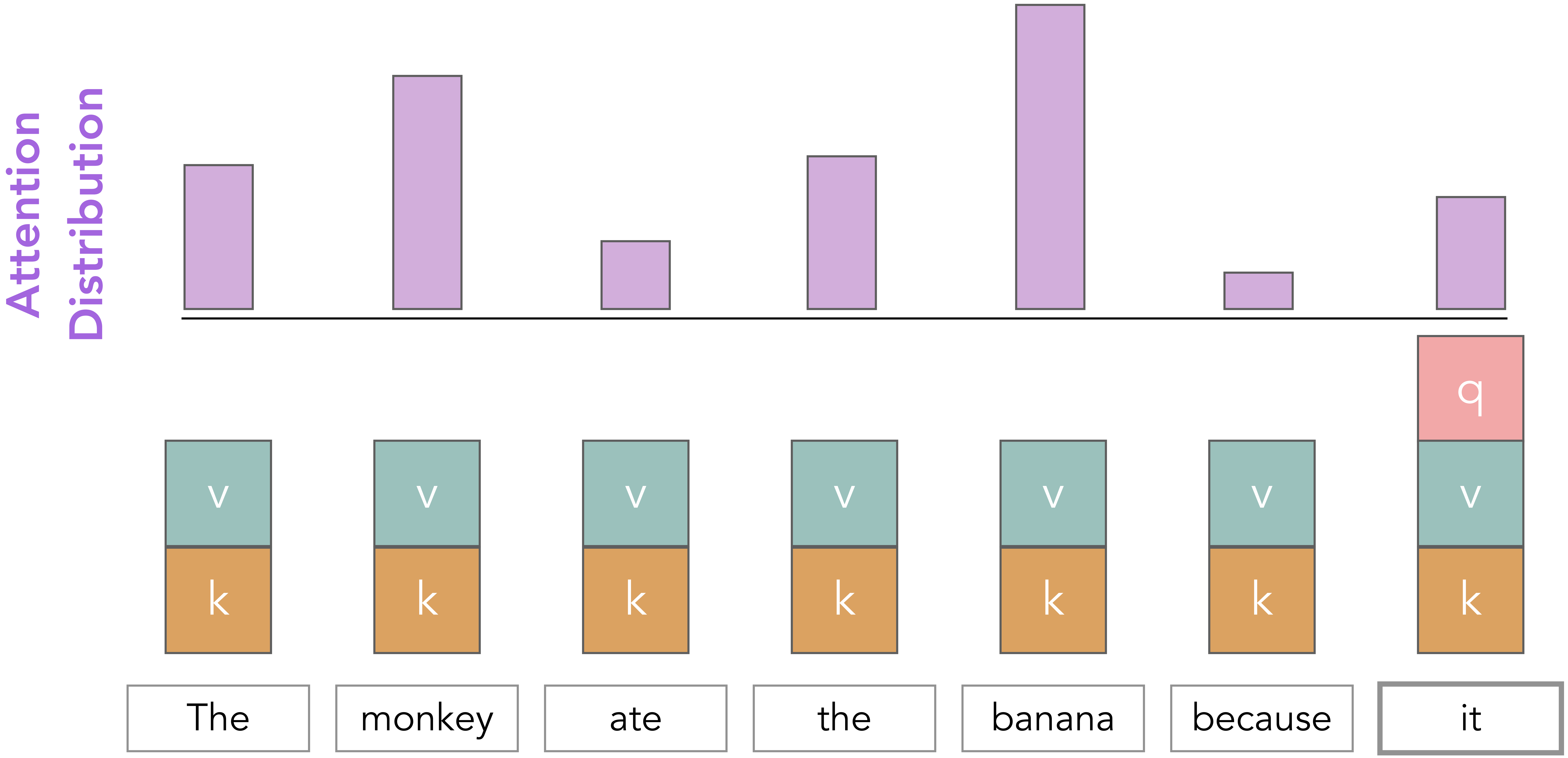

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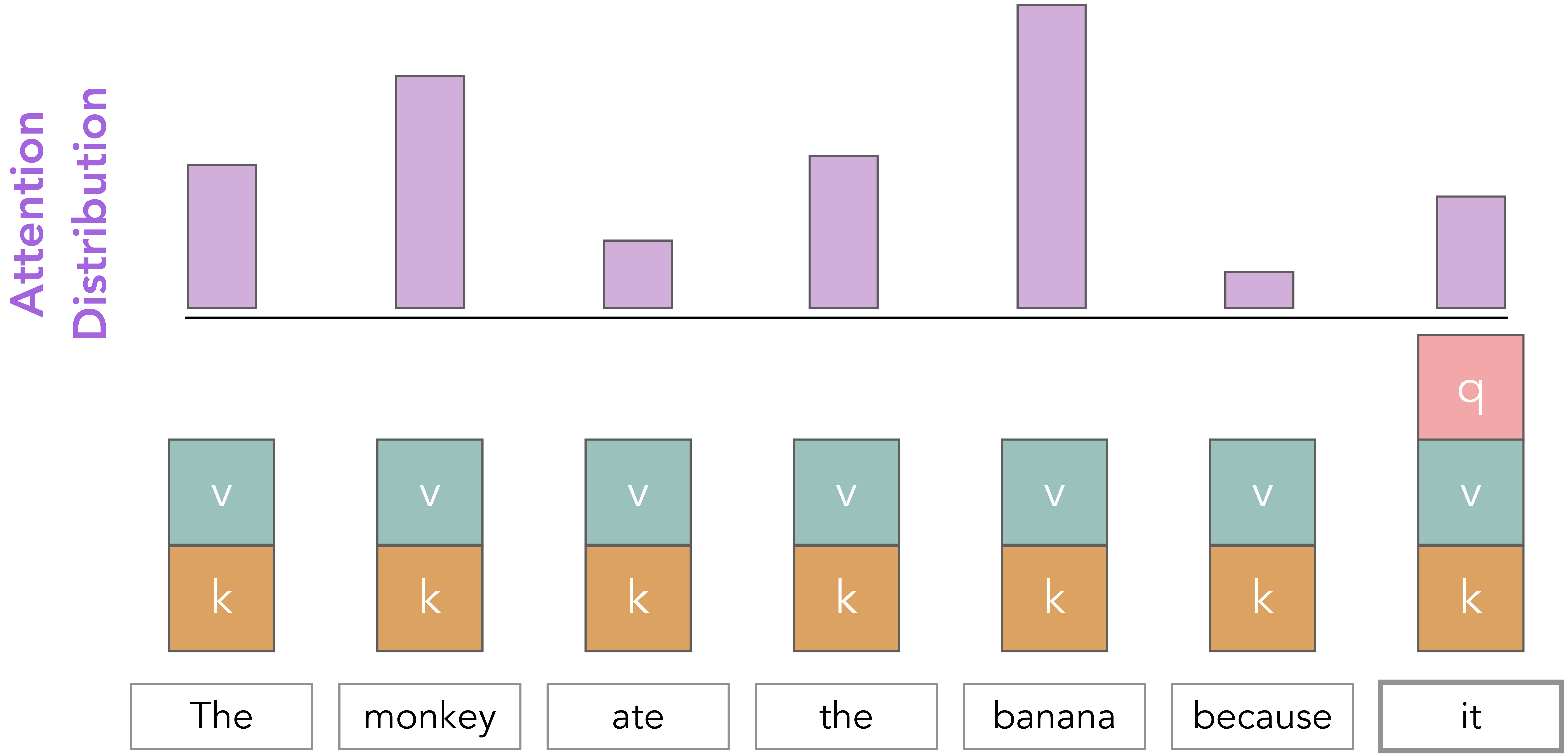

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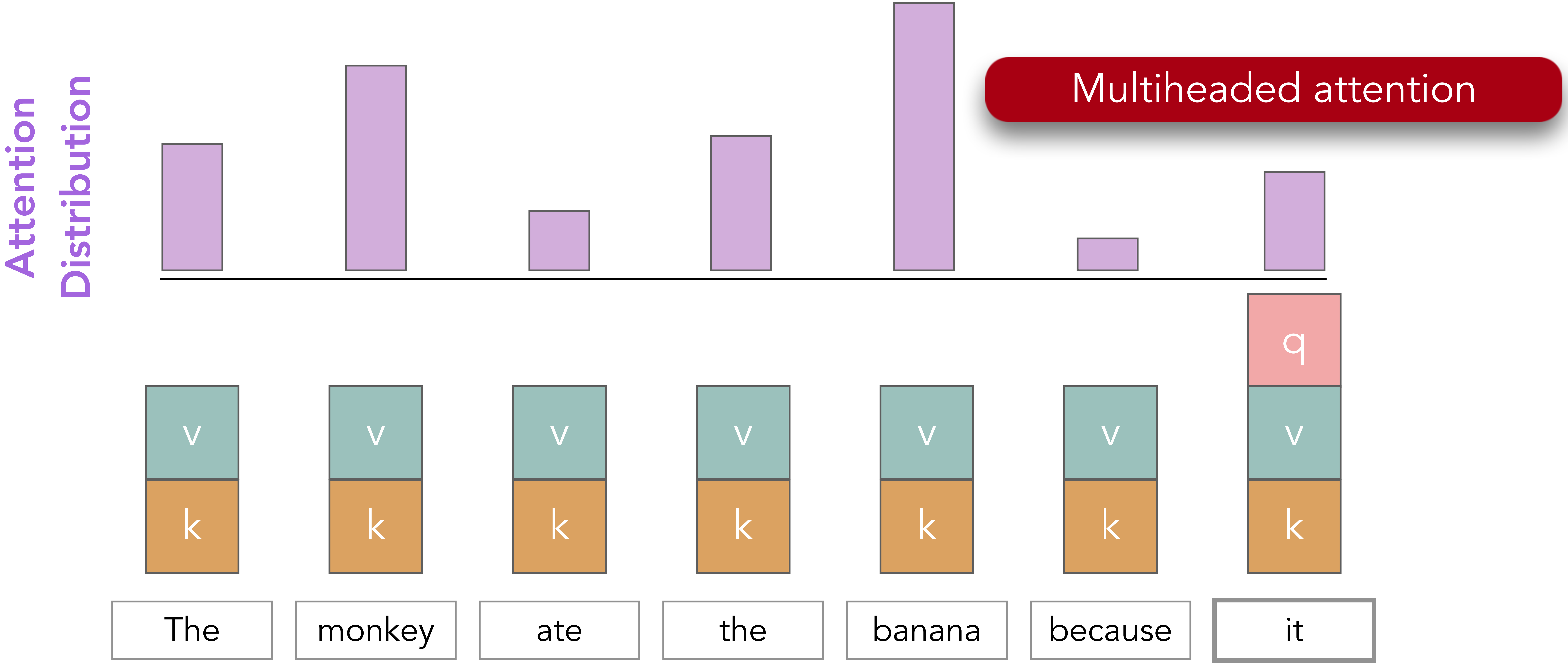
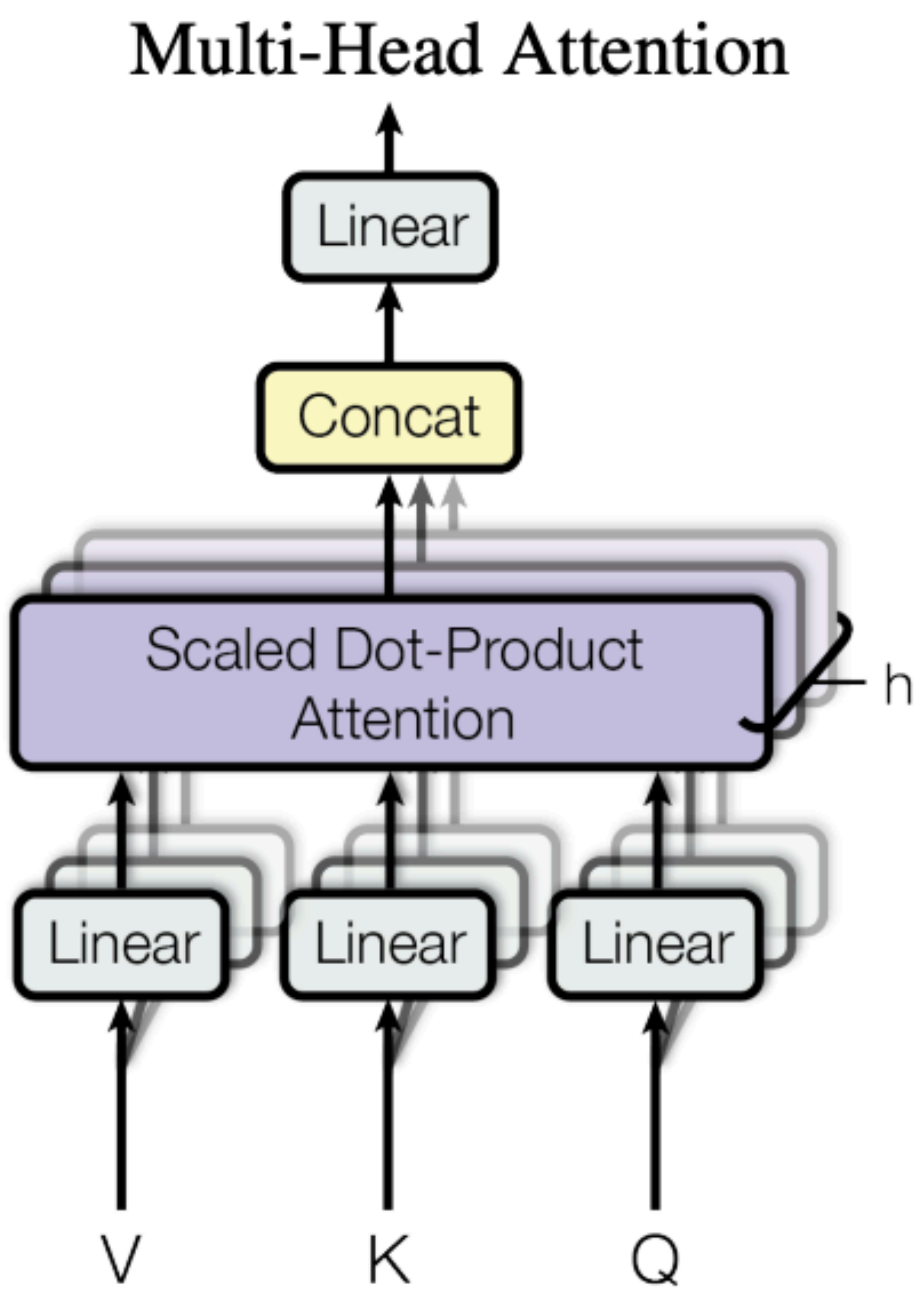


Transformers: Multiheaded Attention

Multi-headed attention



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- What if we want to look in multiple places in the sentence at once?
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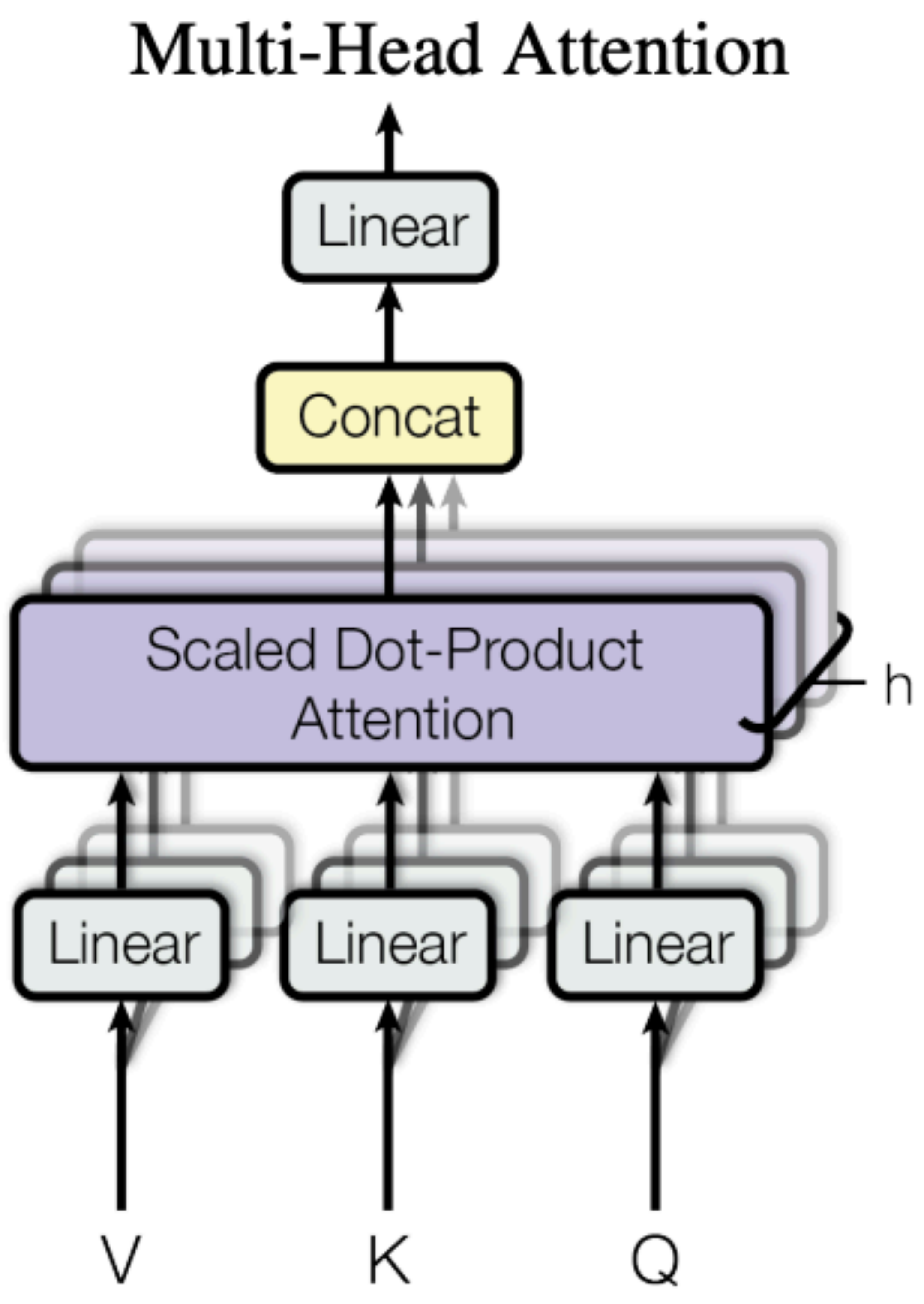

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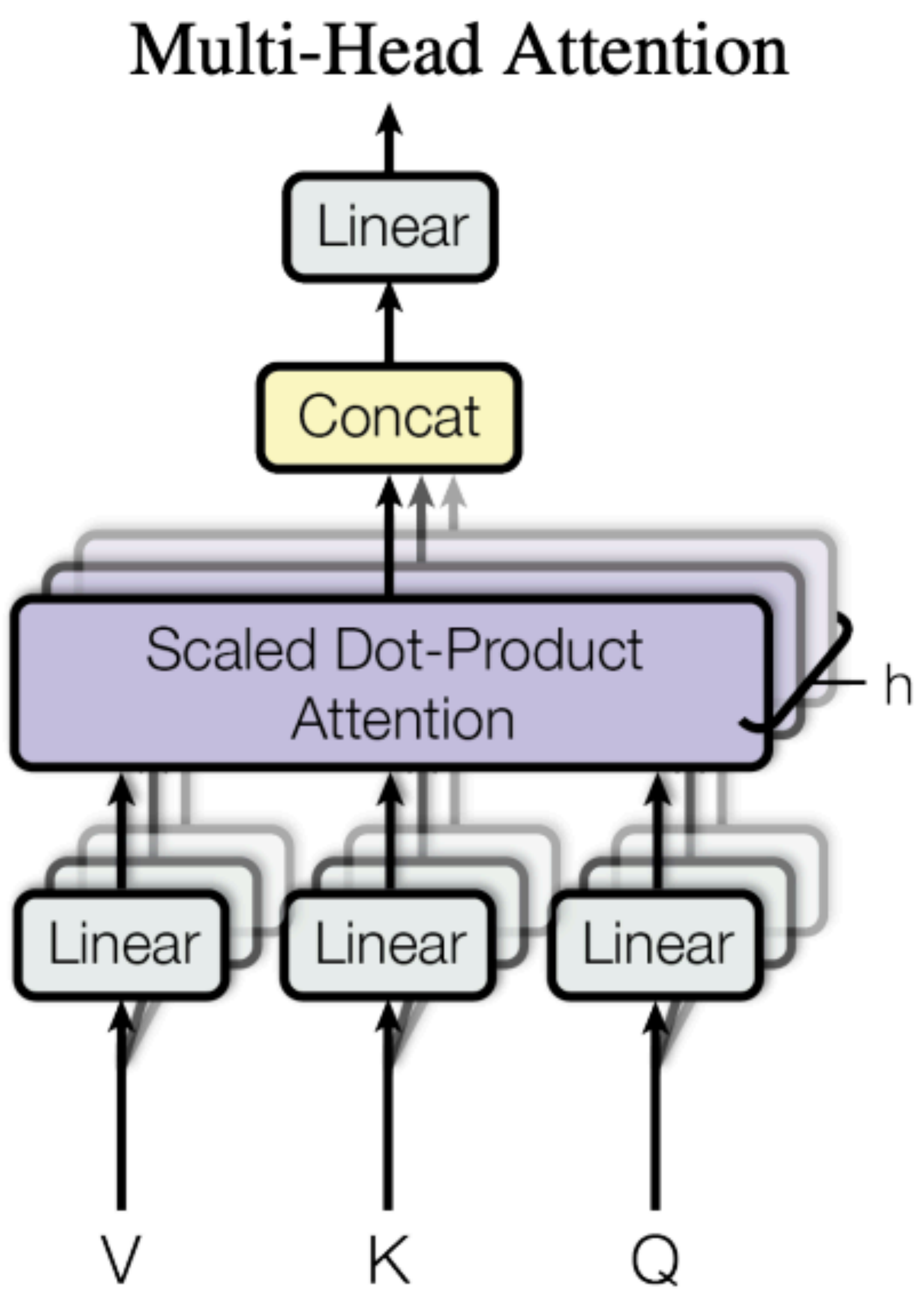

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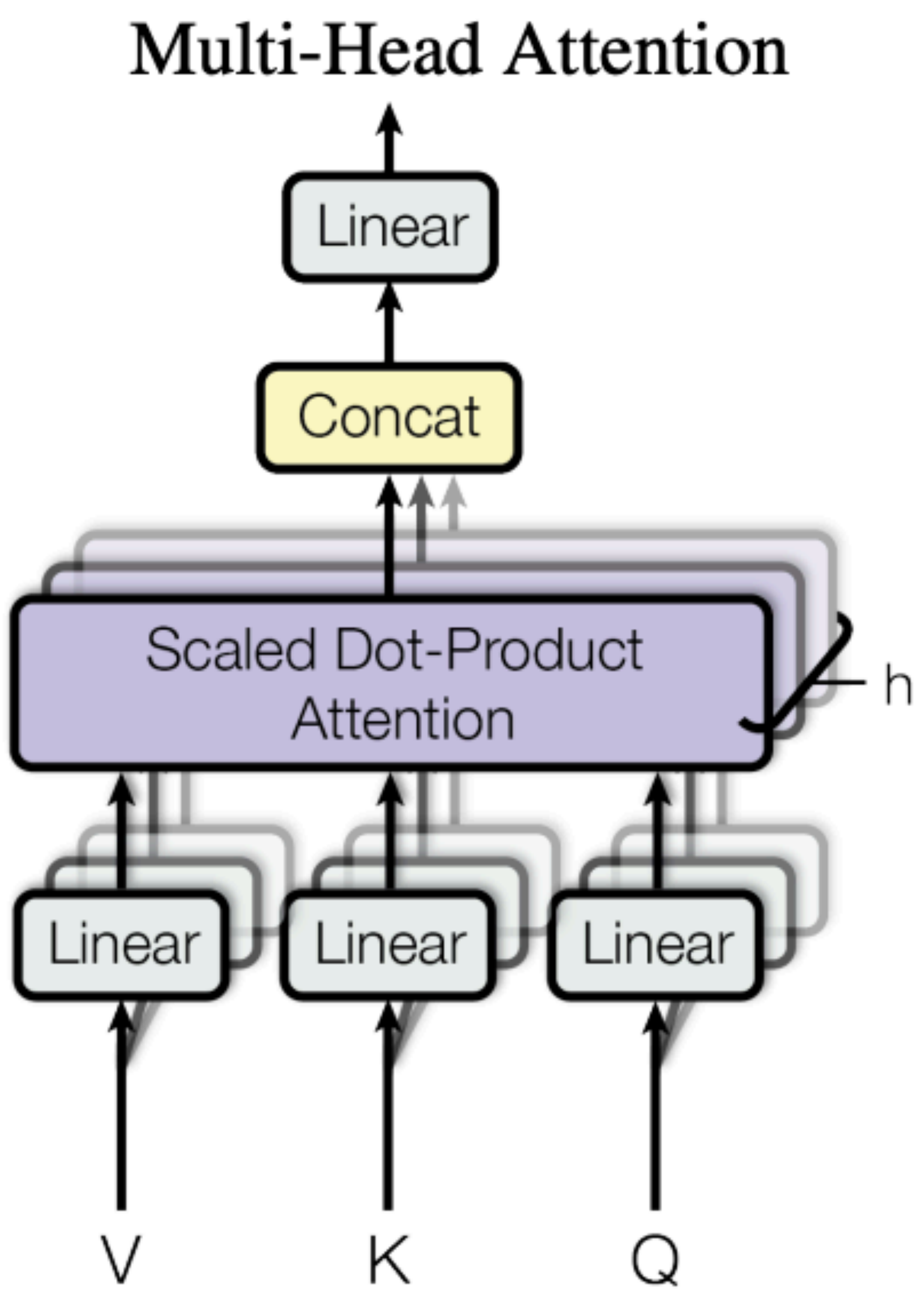

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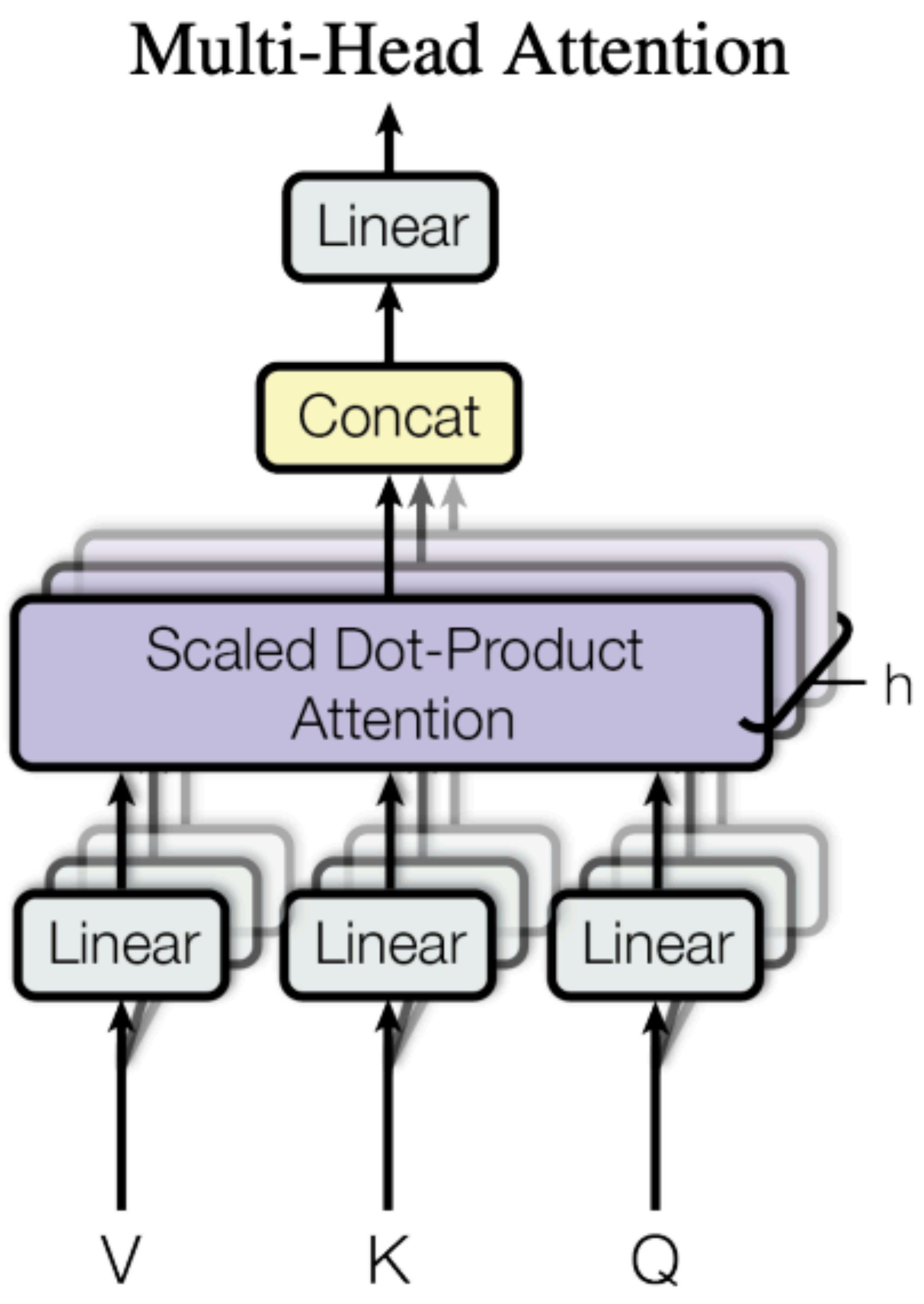

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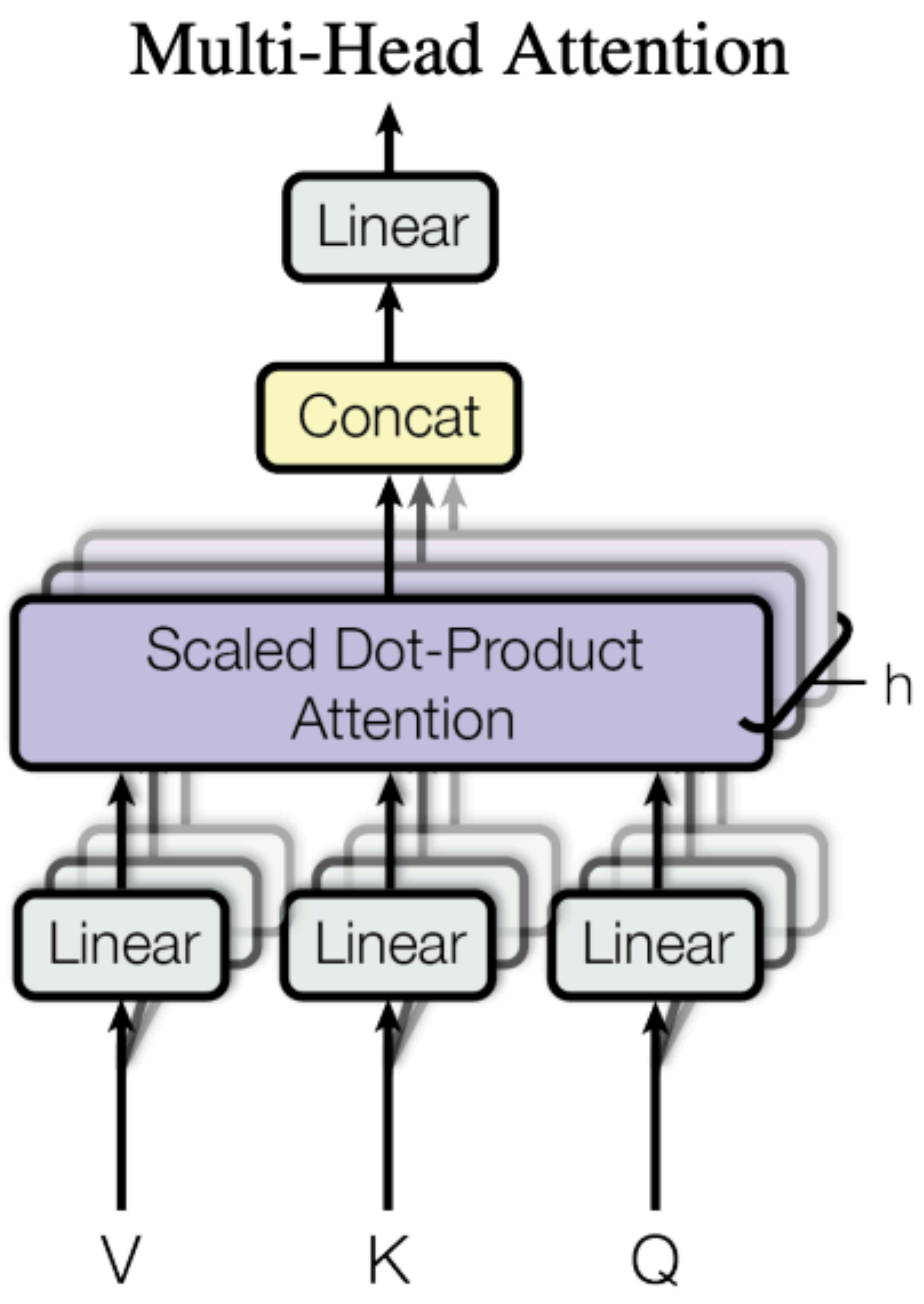

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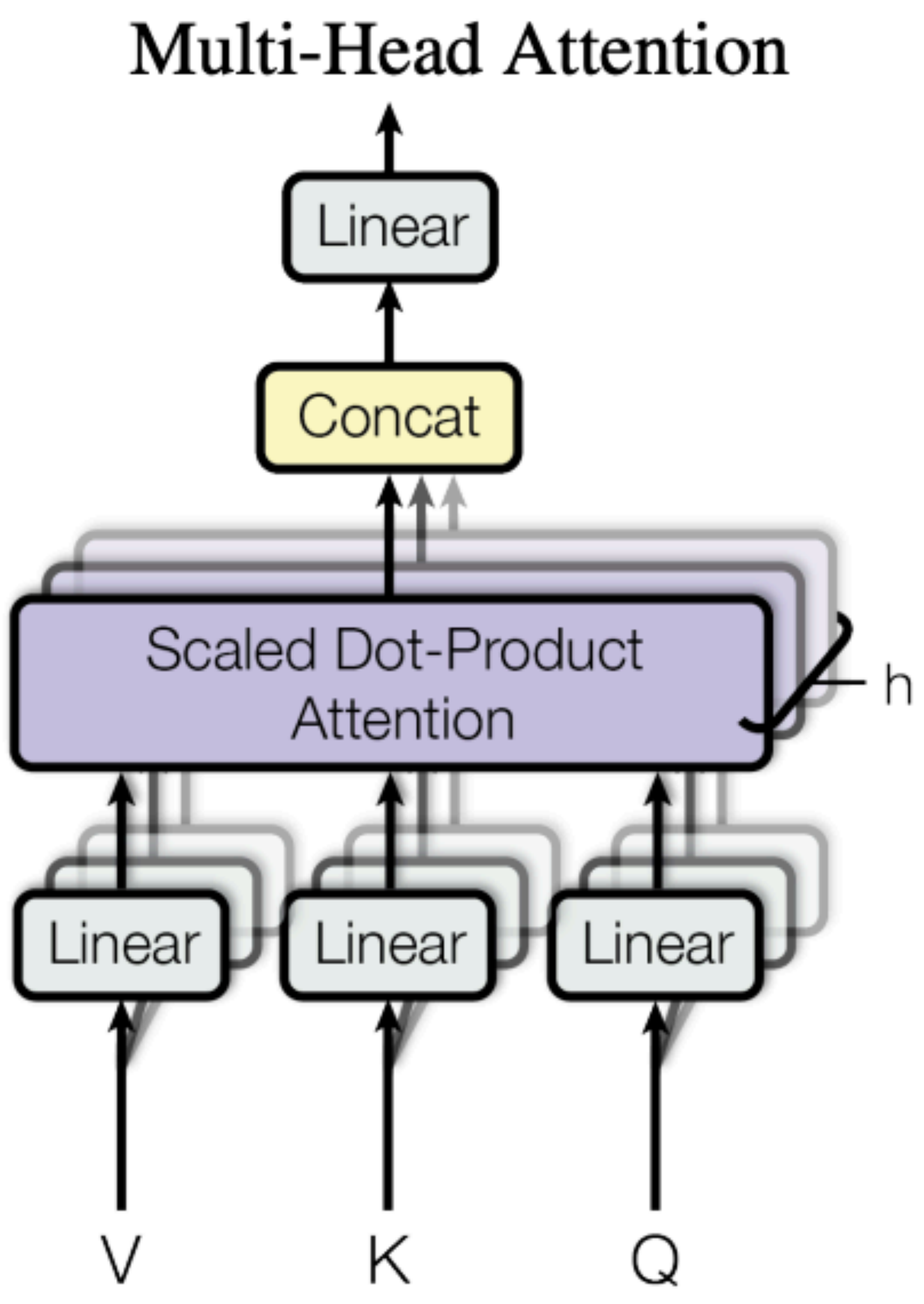

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Each head gets to "look" at different things, and construct value vectors differently

Multiheaded Attention: Visualization

Still efficient, can be parallelized!

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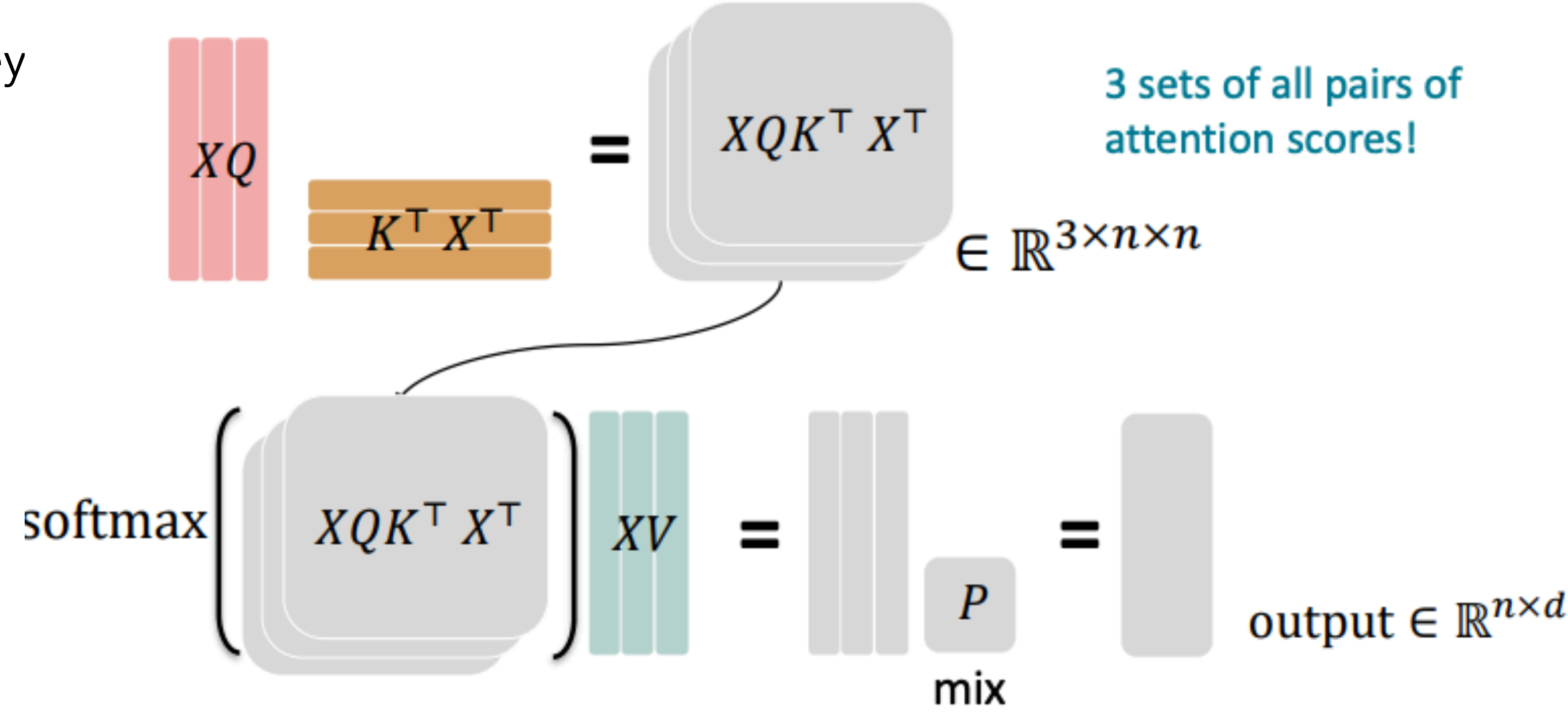

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Tensor!

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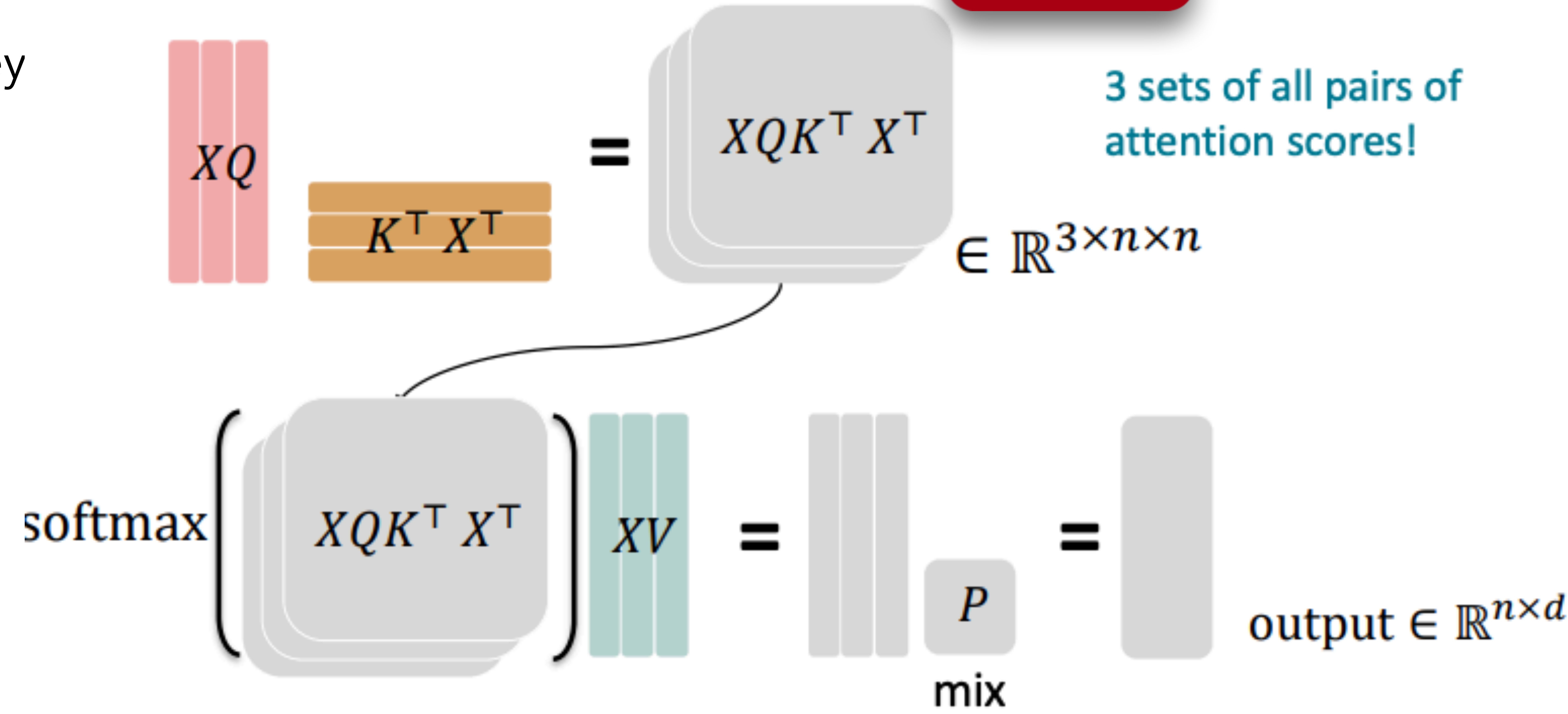

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Scaled Dot Product Attention

$$\textbf{output}_\ell = \textbf{softmax}(XQ_\ell K_\ell^T X^T) * XV_\ell$$

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

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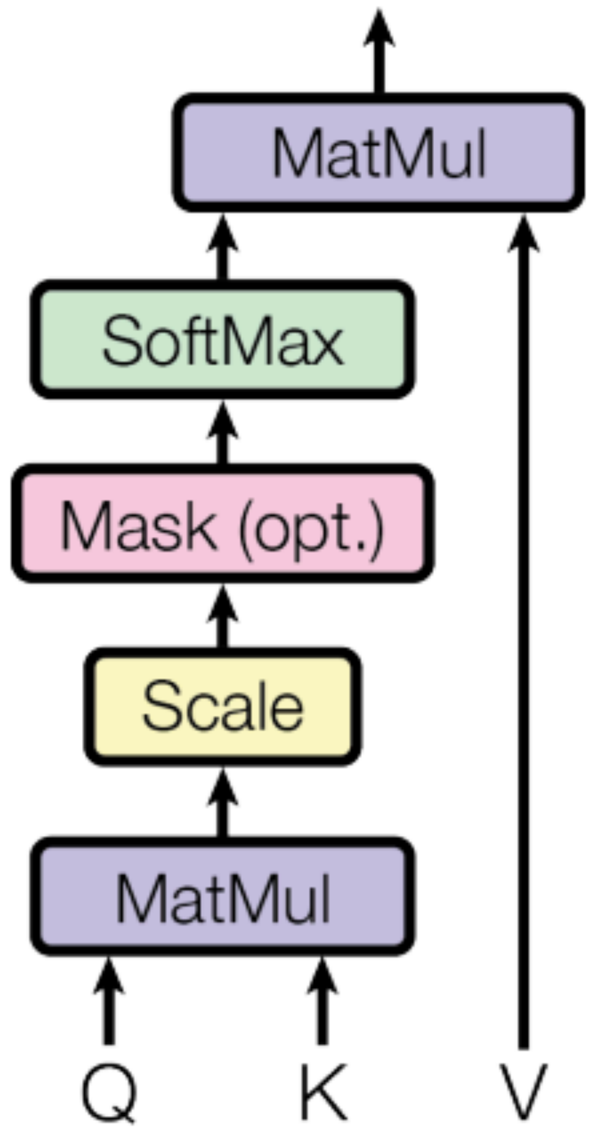

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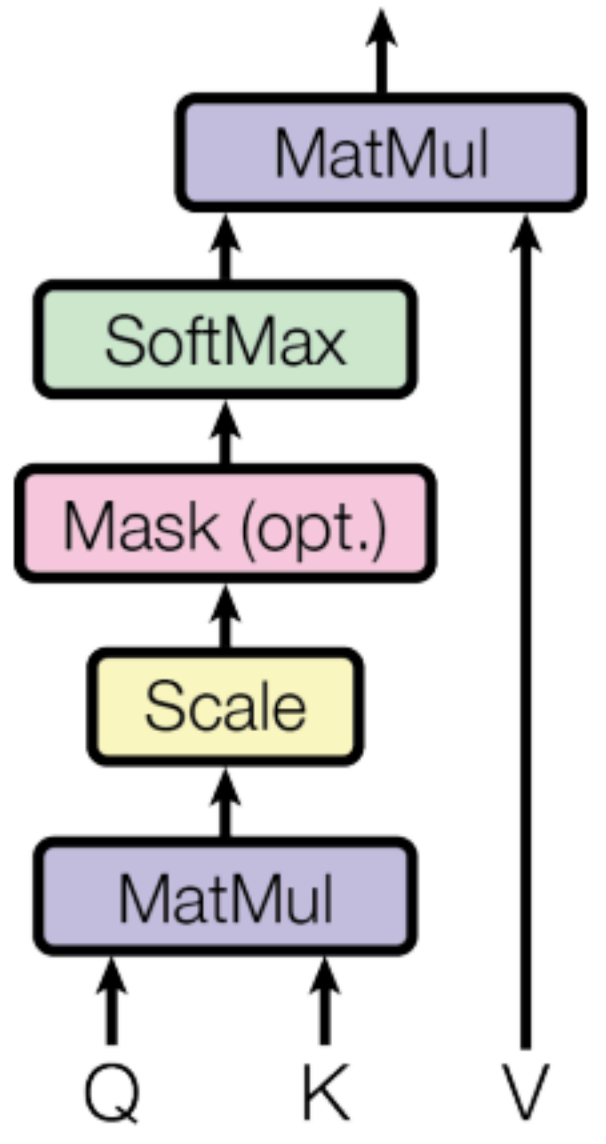

- We divide the attention scores by $\sqrt{d/h}$, to stop the scores from becoming large just as a function of d/h, where h is the number of heads

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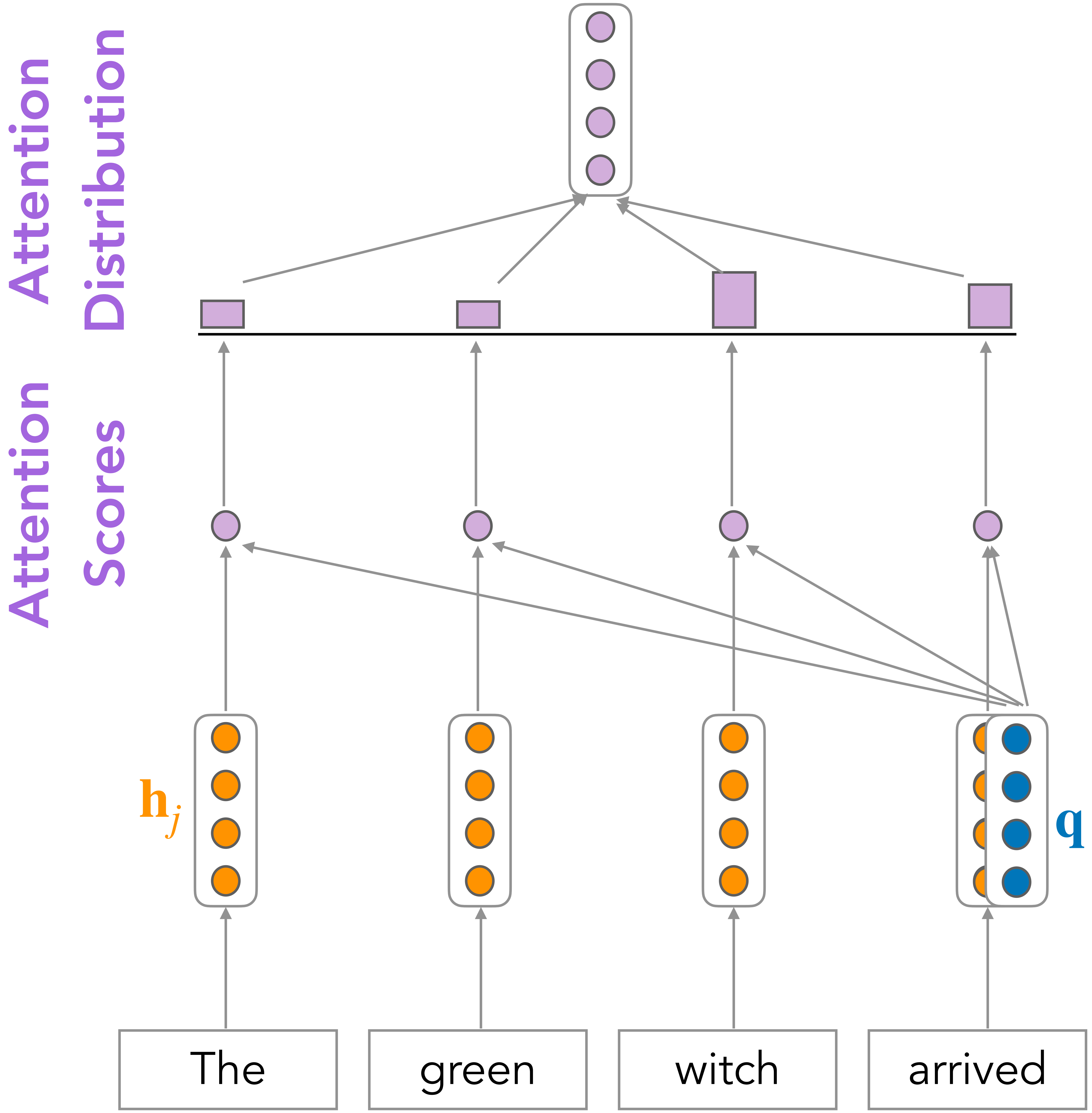
Self-Attention: Order Information?



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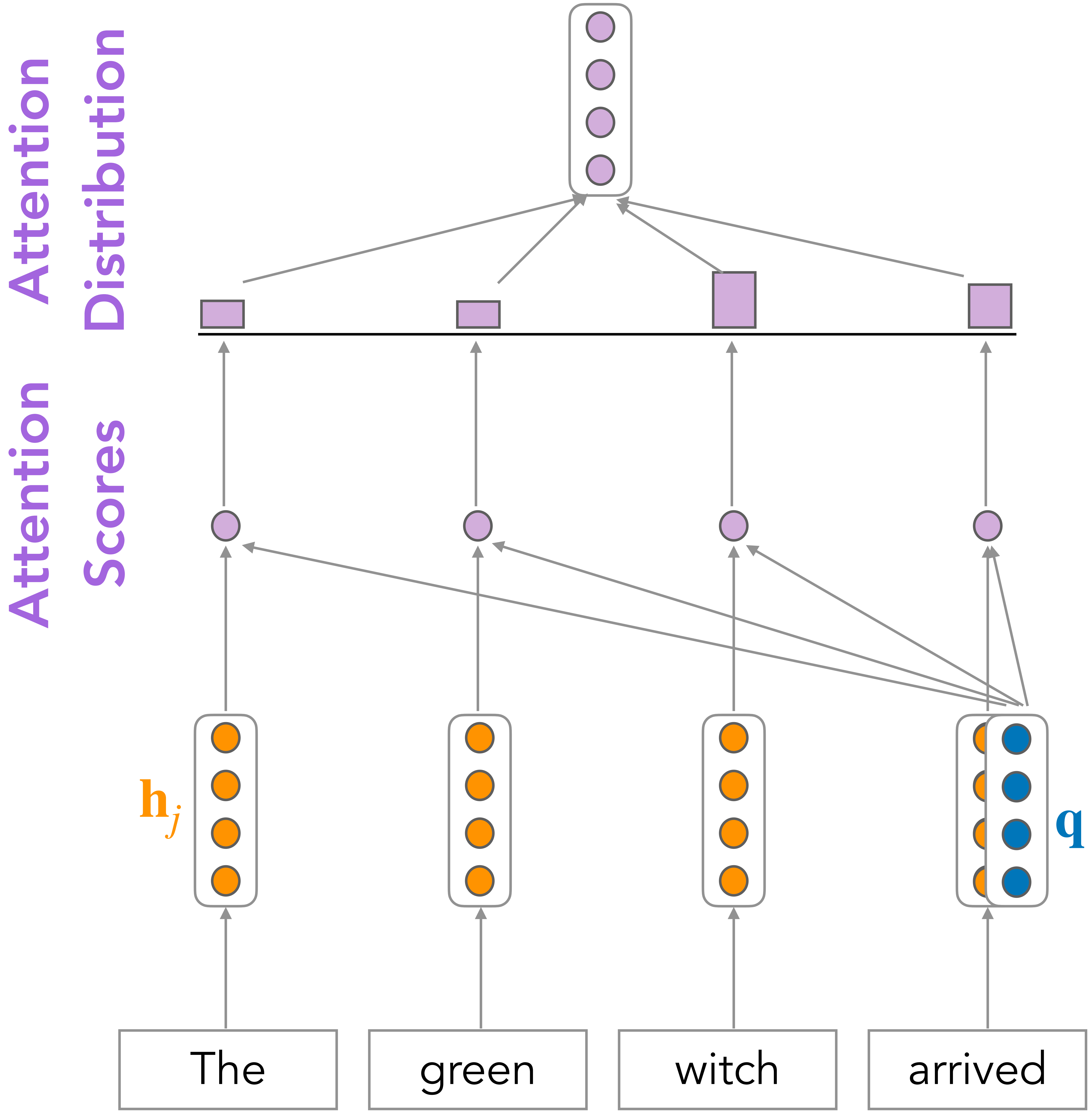

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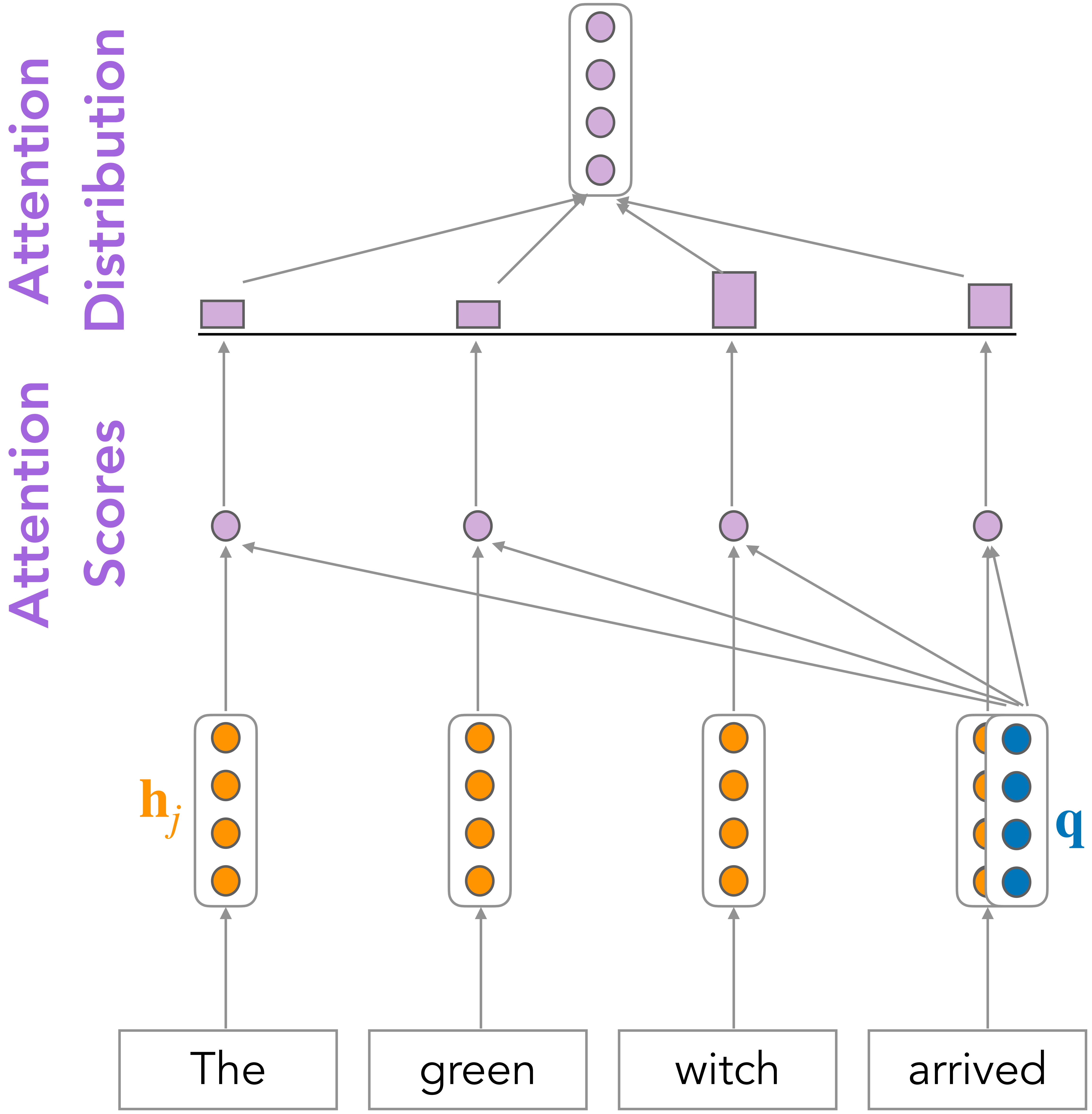

USC Viterbi

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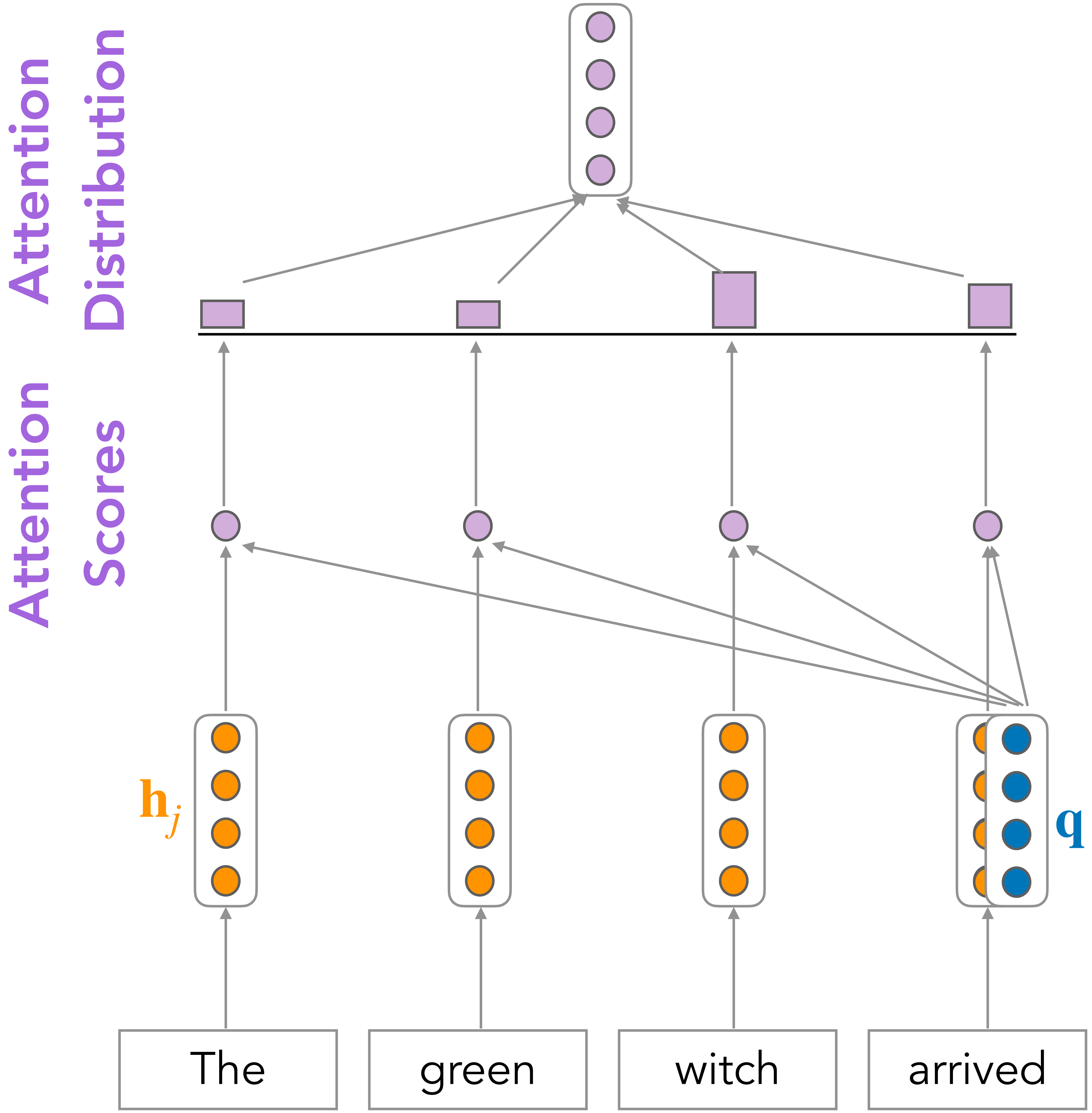
  - No more order information!
- Since self-attention doesn't build in order information, we need to encode the order of the sentence in our keys, queries, and values.



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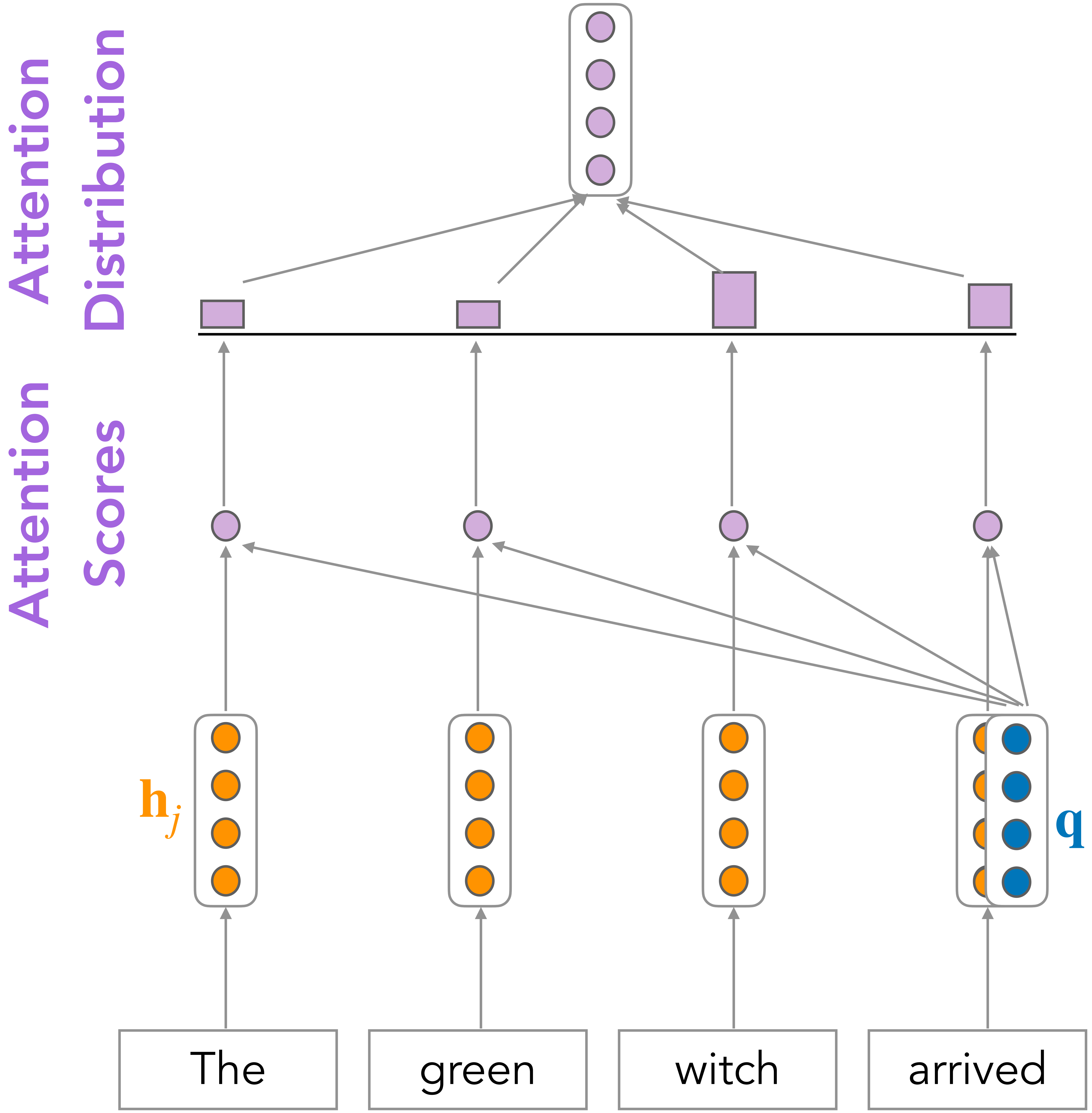
Do feedforward nets contain order information?



Transformers: Positional Embeddings

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

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- Pros:
    - Flexibility: each position gets to be learned to fit the data
- Cons:
    - Definitely can't extrapolate to indices outside $1, \ldots, n$, where n is the maximum length of the sequence allowed under the architecture
    - 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.