

# Lecture 9: Transformer

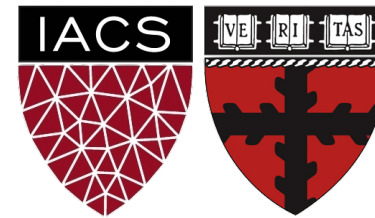
From Attention to Self-Attention

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**Harvard**

AC295/CS287r/CSCI E-115B

Chris Tanner





# Self [Attention]

-- Mac Miller (2018)



<https://wellness.huhs.harvard.edu/alcohol-substance-use>

[basics@huhs.harvard.edu](mailto:basics@huhs.harvard.edu)

# ANNOUNCEMENTS

- **Quizzes 3** have been graded and are logged on Canvas
- **HW1** is being graded. Solutions are posted on Canvas -> Files
- **HW2** is due next **Tues, Oct 5 @ 11:59pm!** Determine your mystery language.
- **Research Proposals** are due tonight, **Sept 30 @ 11:59pm.**
  - If submitting w/ others, please see the updated Canvas instructions

# RESEARCH PROJECTS

- Most research experiences/opportunities are “top-down”
- You’re all creative and fully capable.
- Allow yourselves to become comfortable with the unknown.
- It’s okay if your **Phase 1 Proposals** aren’t *perfect* ideas. The point is to gain practice with the inquisition and overall process of executing your ideas.
- We’ll help provide structure **after Phase 1** (e.g., filtering projects, feedback, helping you find the optimal project partners, TF support, etc)

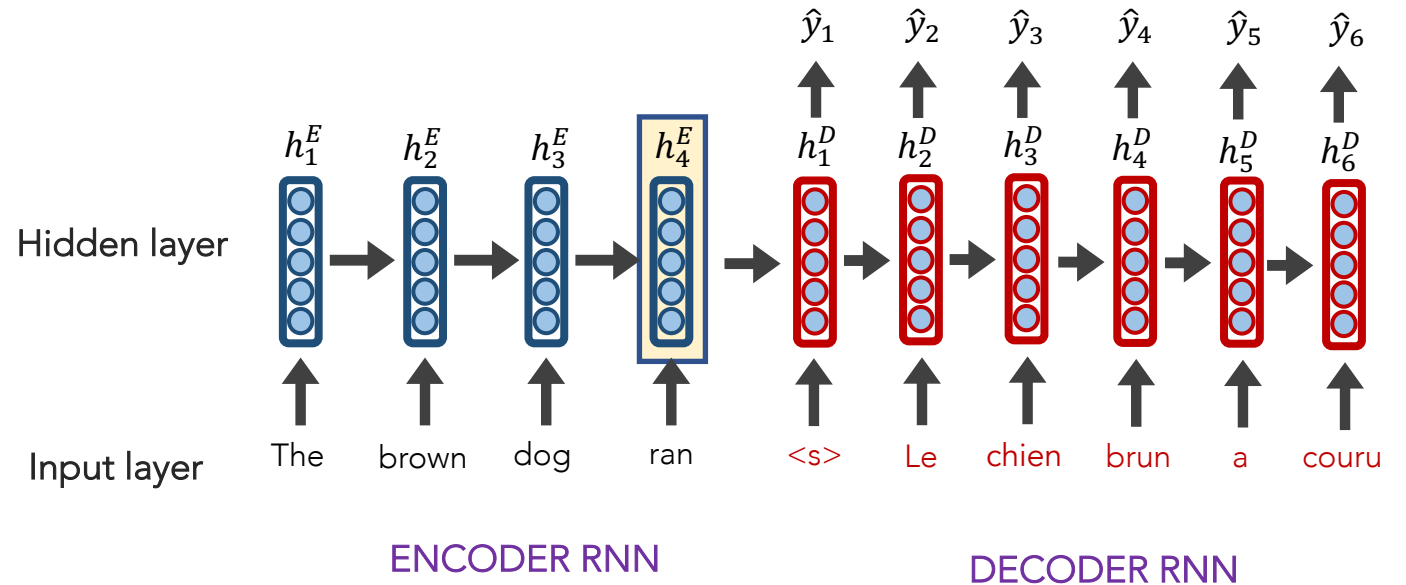
# RESEARCH PROJECTS

- I'll filter projects by rating them according to:
  - researchy vs application
  - how grounded/well-reasoned it is
  - technical difficulty (there's a sweet spot)
  - feasibility (e.g., required compute power, data availability, metrics)
  - interestingness / significance

# RECAP: L8

## seq2seq models

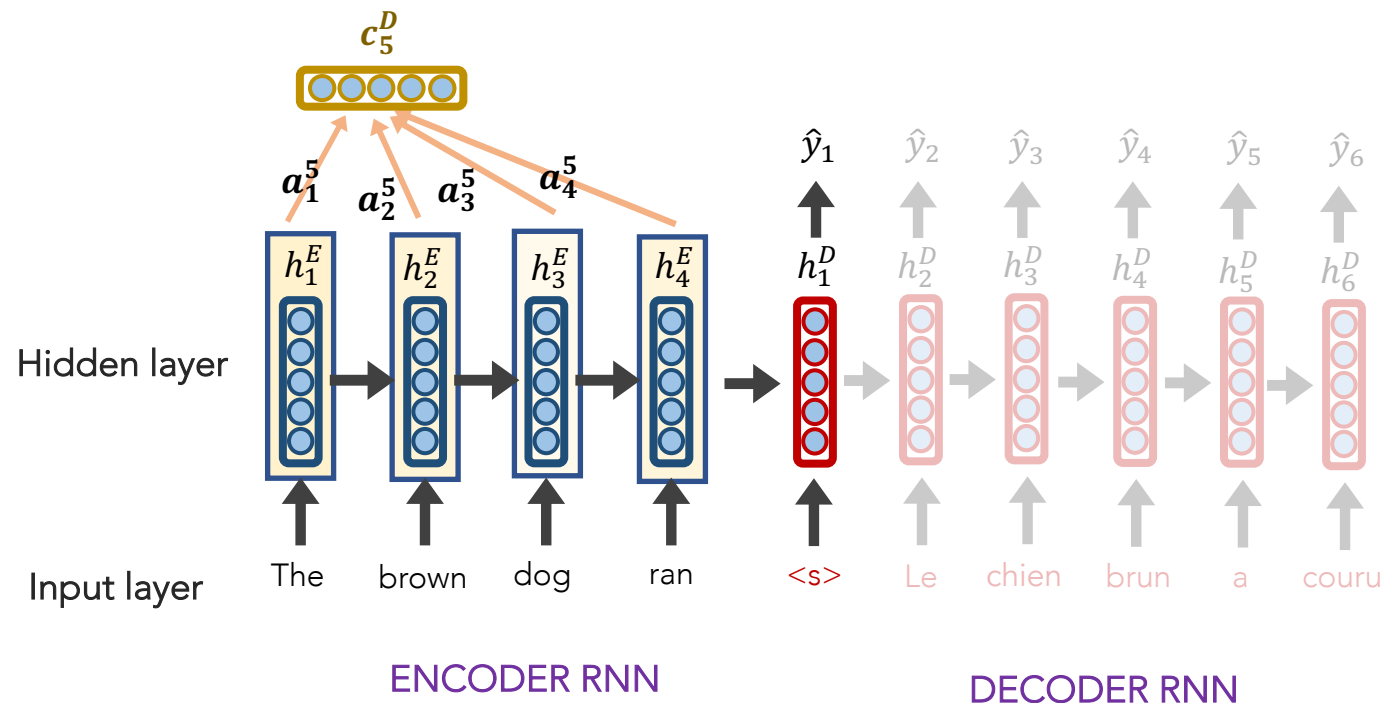
- are a general-purpose encoder-decoder architecture
- can be implemented with RNNs (or Transformers even)
- Allow for  $n \rightarrow m$  predictions
- Natural approach to Neural MT
- If implemented end-to-end can be good but slow



# RECAP: L8

## seq2seq models

- **Attention** allows a decoder, at each time step, to focus/use different amounts of the encoder's hidden states
- The resulting **context vector**  $c_i$  is used, with the **decoder's current hidden state**  $h_i$ , to predict  $\hat{y}_i$



# RECAP: L8

MT

$$\operatorname{argmax}_y P(\textcolor{red}{x} | \textcolor{blue}{y}) P(\textcolor{blue}{y})$$

- Converts text from a source language  $\textcolor{red}{x}$  to a target language  $\textcolor{blue}{y}$
- $\textcolor{red}{SMT}$  made huge progress but was brittle
- $\textcolor{red}{NMT}$  (starting w/ LSTM-based seq2seq models) blew  $\textcolor{red}{SMT}$  out of the water
- Attention greatly helps LSTM-based seq2seq models
- **Next:** Transformer-based seq2seq models w/ Self-Attention and Attention



# Outline

 seq2seq + Attention

 Self-Attention

# Outline

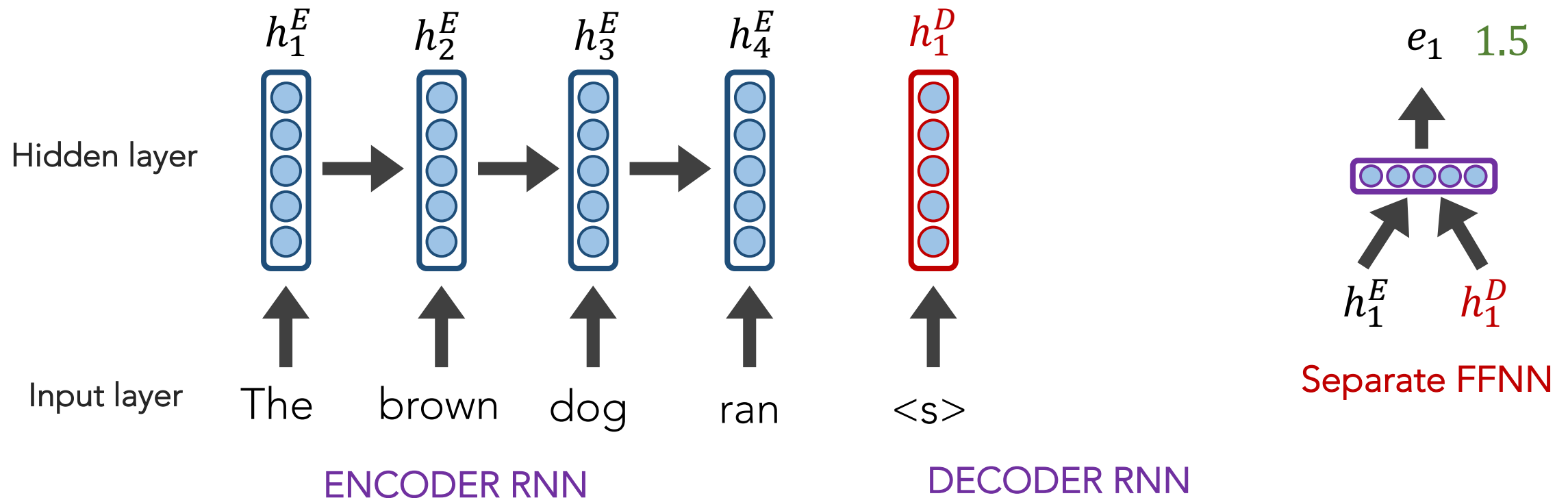
 seq2seq + Attention

 Self-Attention

# seq2seq + Attention

**Q:** How do we determine how much to pay attention to each of the encoder's hidden layers?

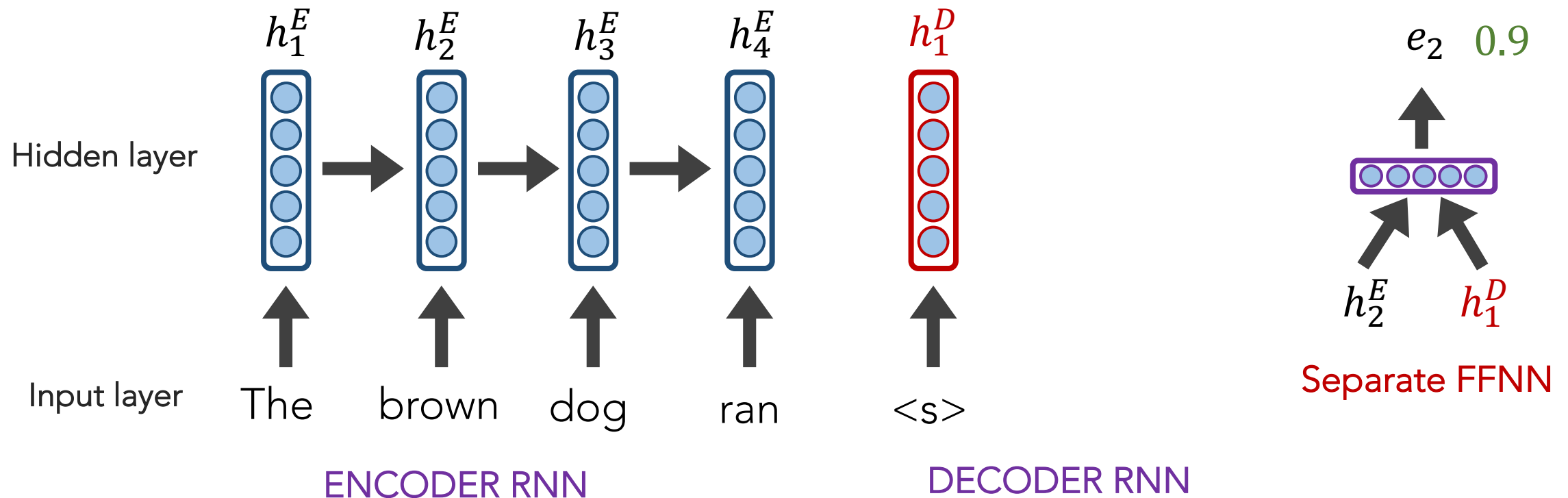
**A:** Let's base it on our decoder's current hidden state (our current representation of meaning) and all of the encoder's hidden layers!



# seq2seq + Attention

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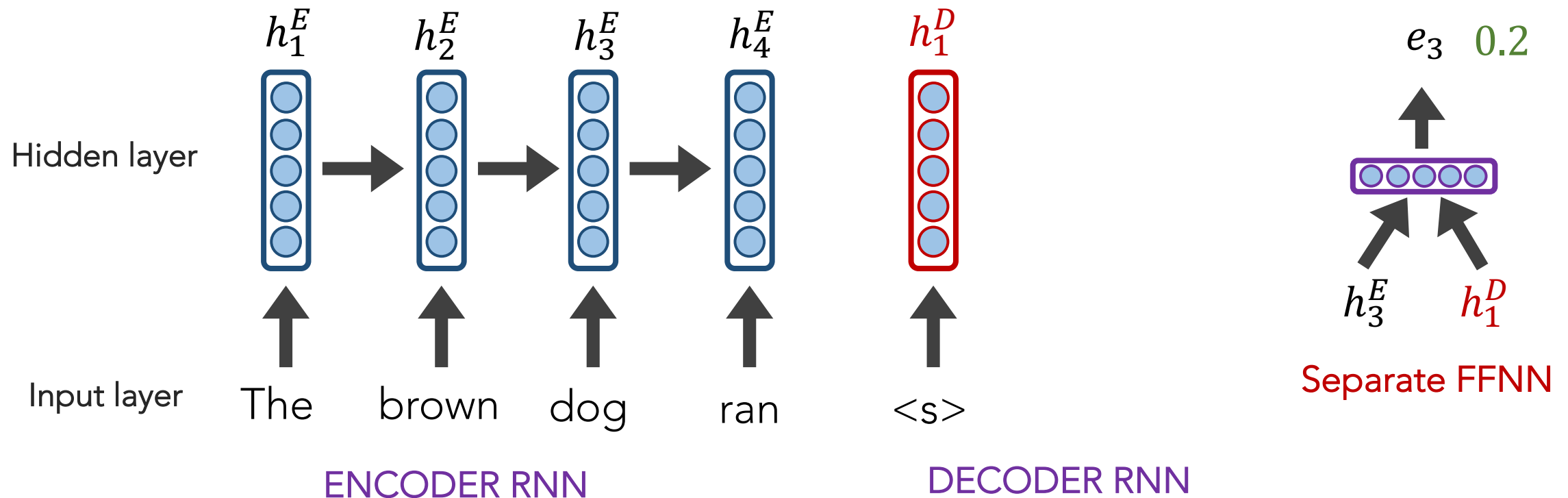
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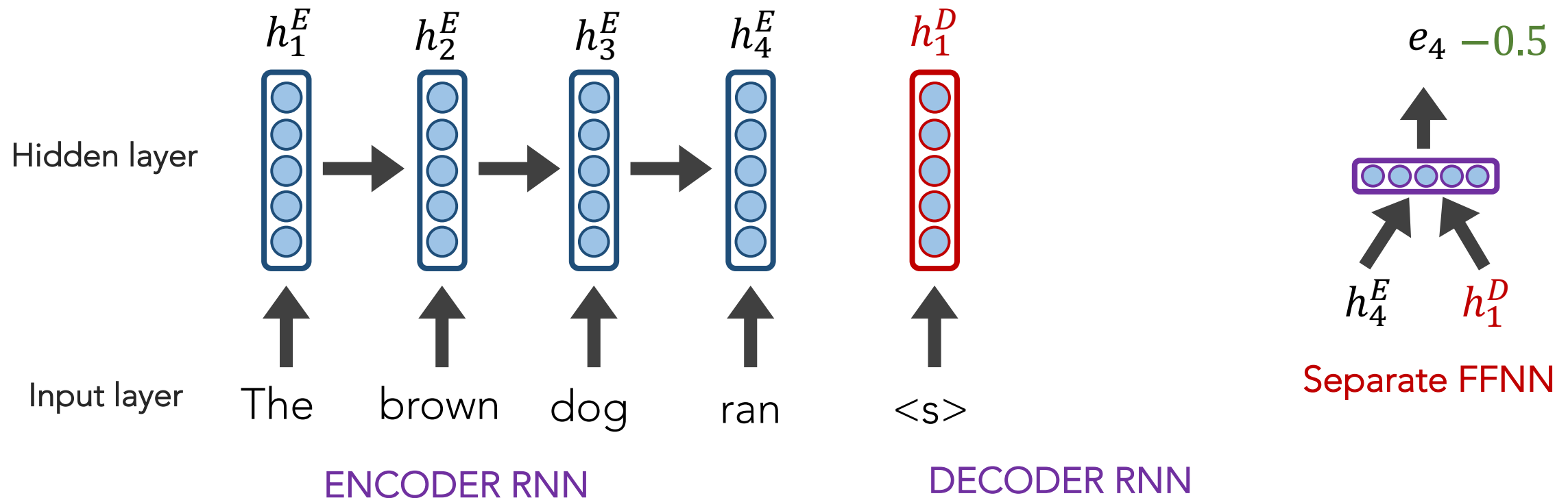
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# seq2seq + Attention

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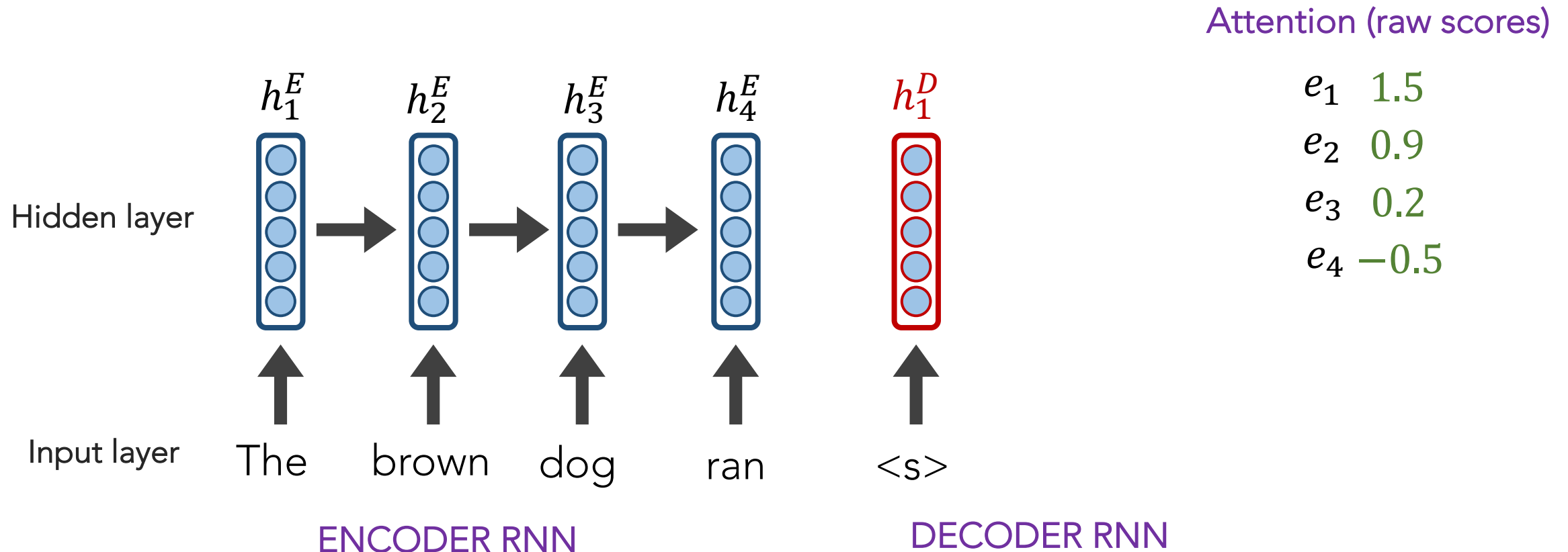
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# seq2seq + Attention

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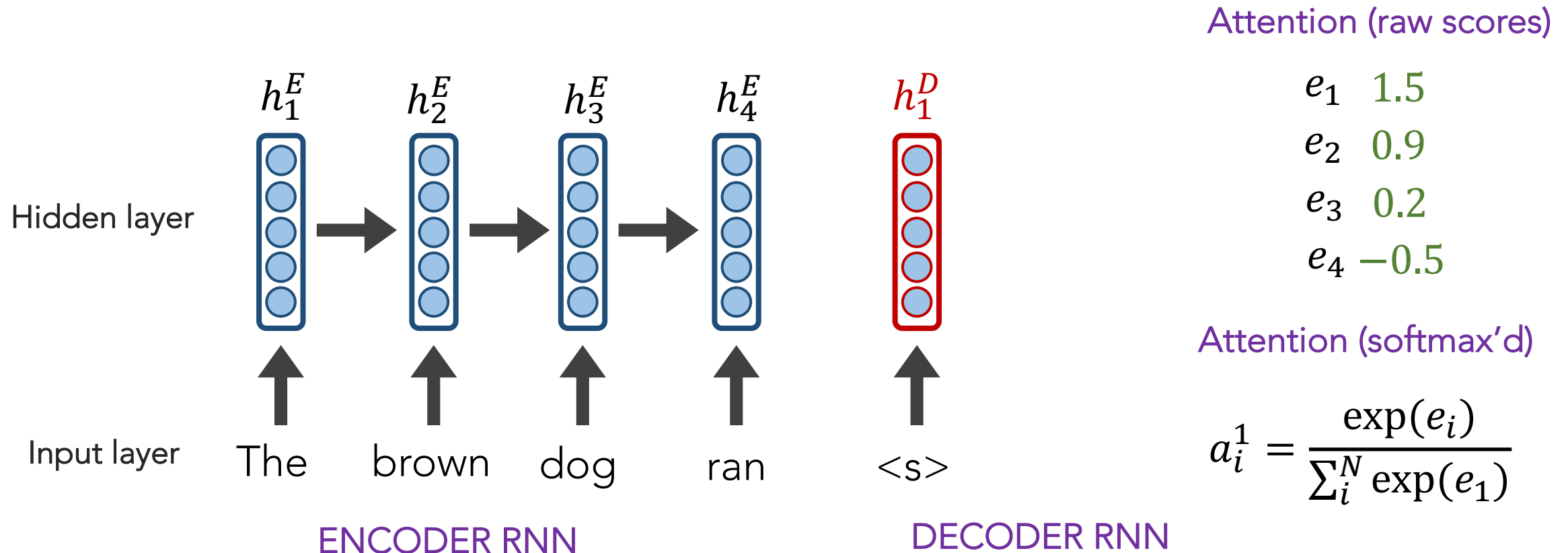
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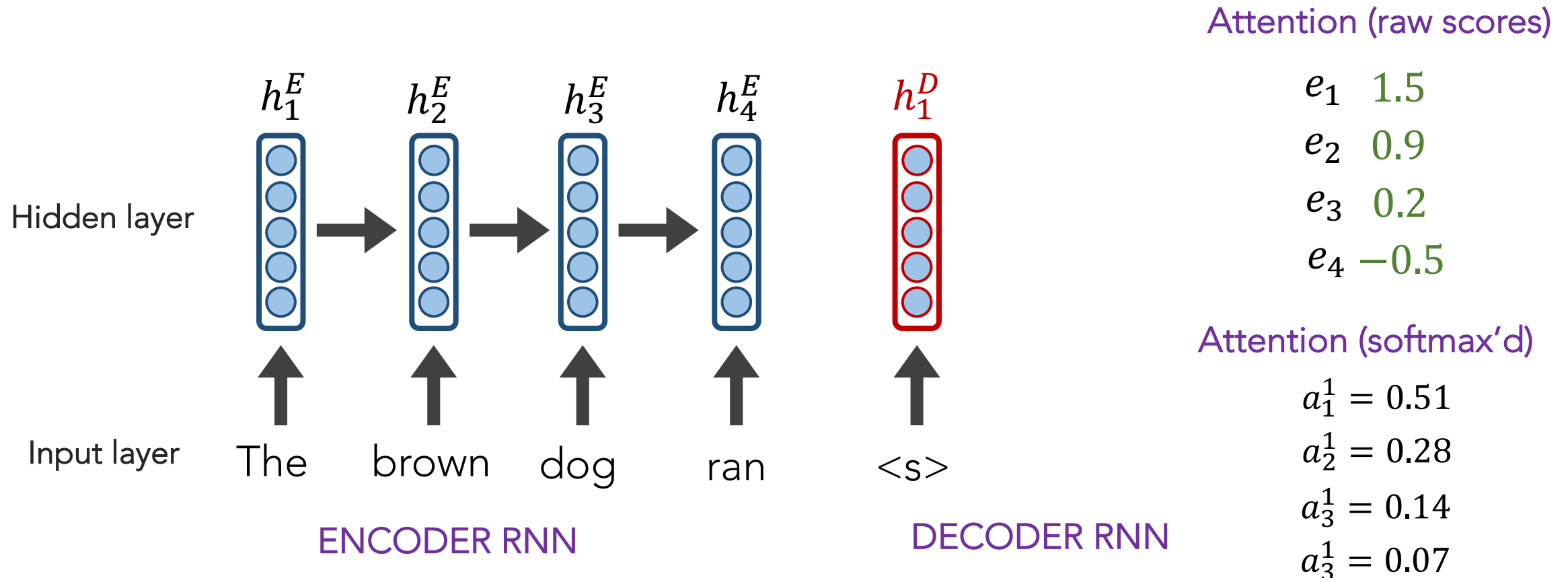




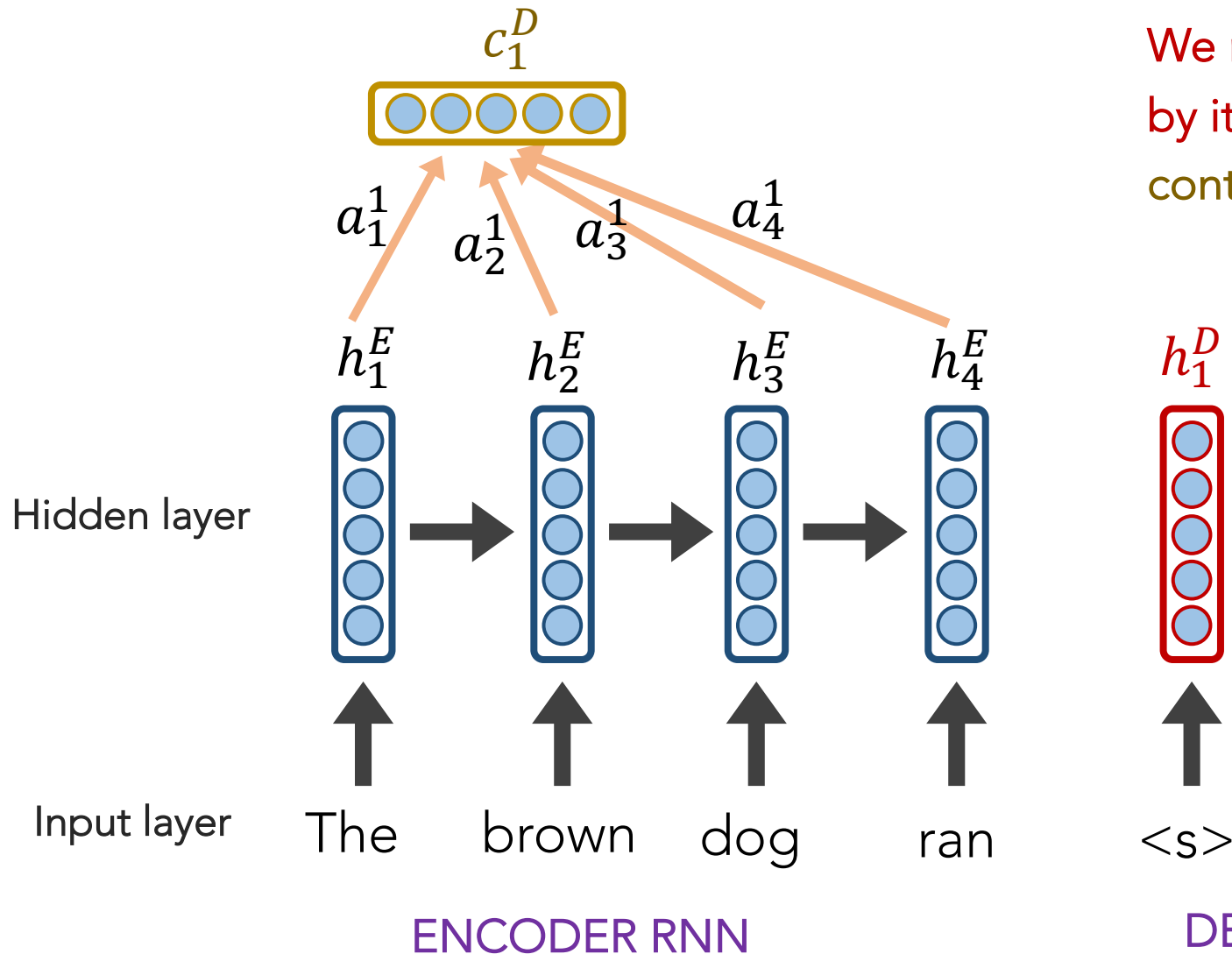
# seq2seq + Attention

**Q:** How do we determine how much to pay attention to each of the encoder's hidden layers?

**A:** Let's base it on our decoder's current hidden state (our current representation of meaning) and all of the encoder's hidden layers!



# seq2seq + Attention



We multiply each encoder's hidden layer by its  $a_i^1$  attention weights to create a context vector  $c_1^D$

Attention (softmax'd)

$$a_1^1 = 0.51$$

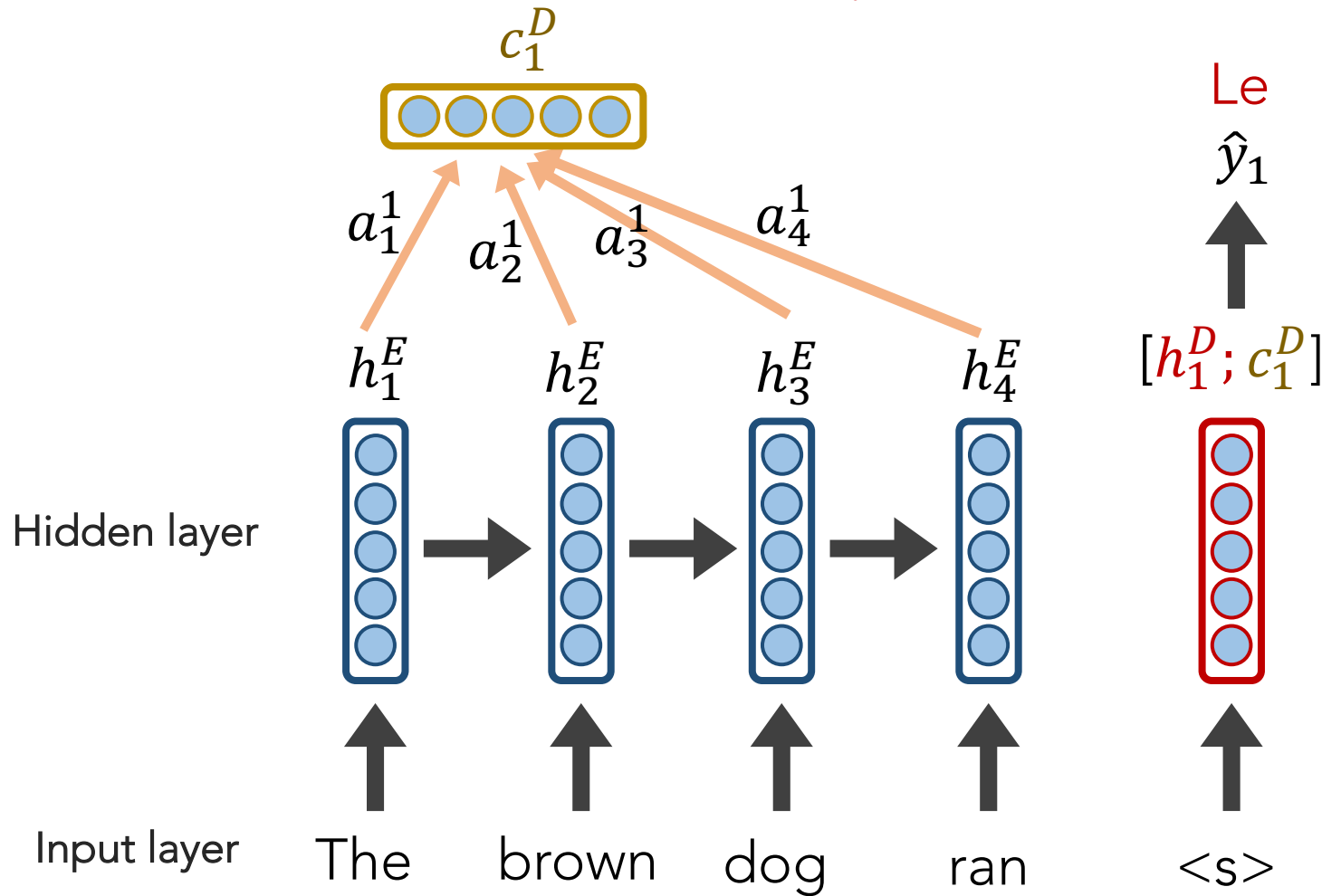
$$a_2^1 = 0.28$$

$$a_3^1 = 0.14$$

$$a_4^1 = 0.07$$

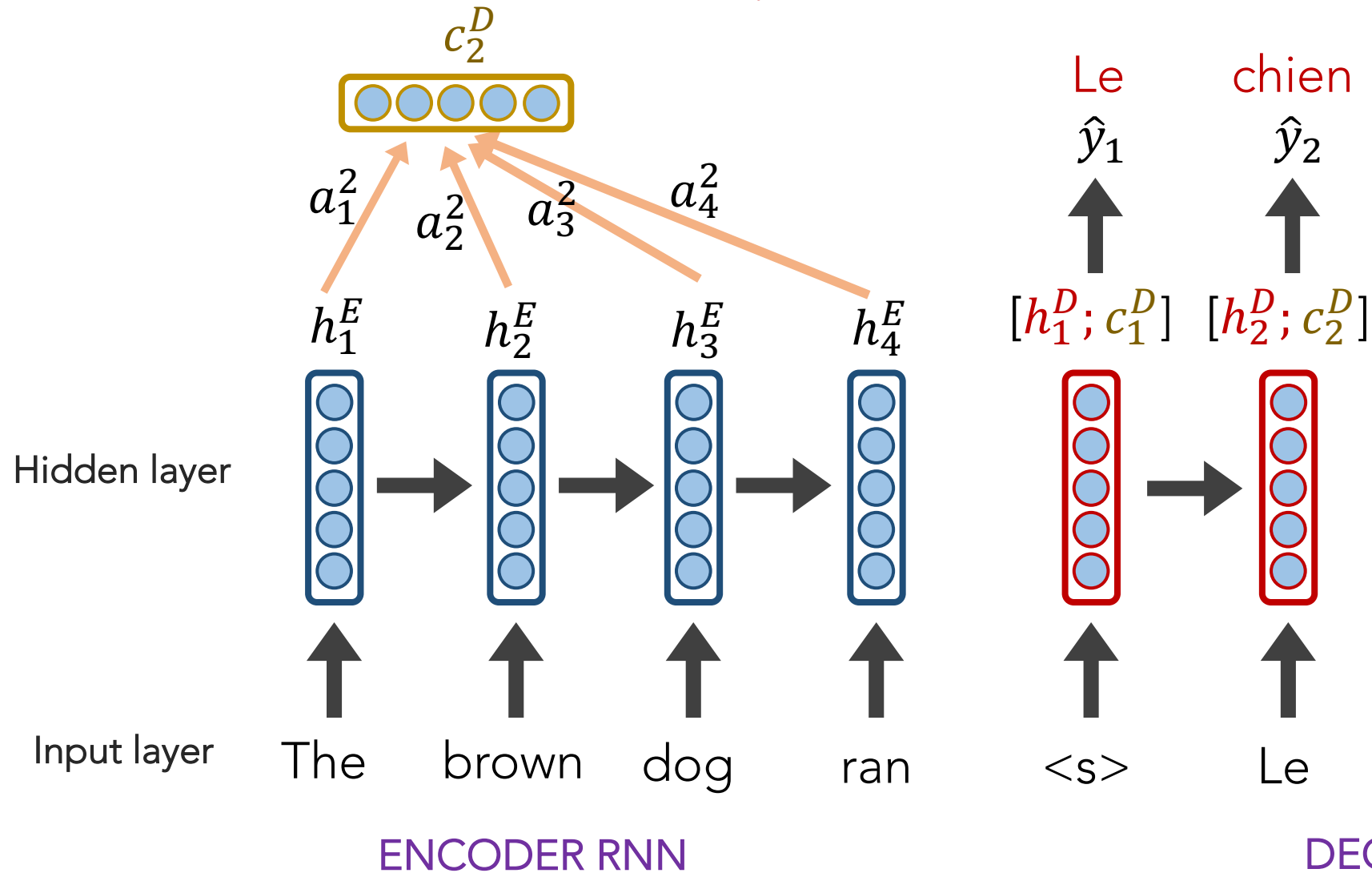
# seq2seq + Attention

**REMEMBER:** each attention weight  $a_i^j$  is based on the **decoder's** current hidden state, too.



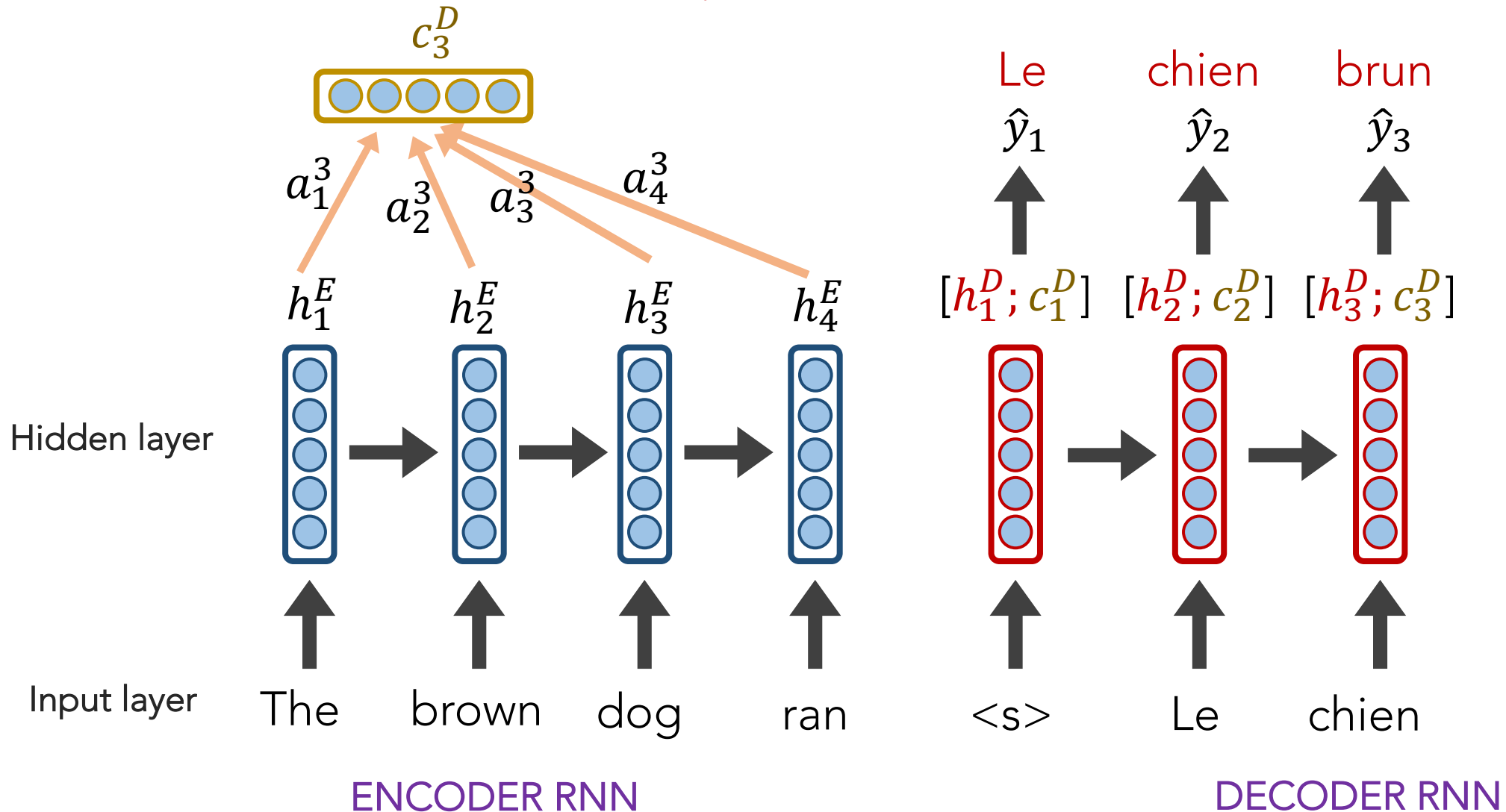
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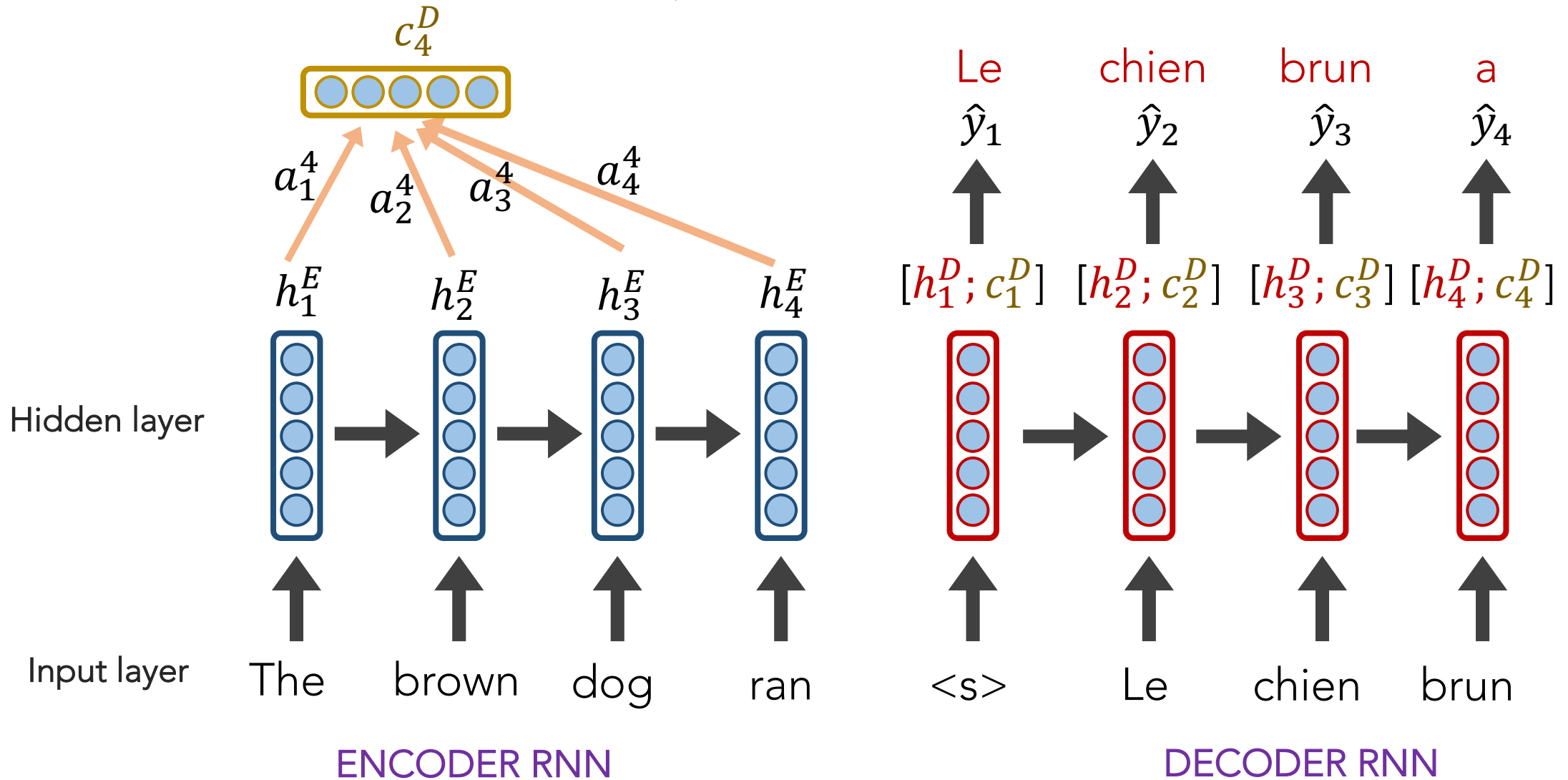
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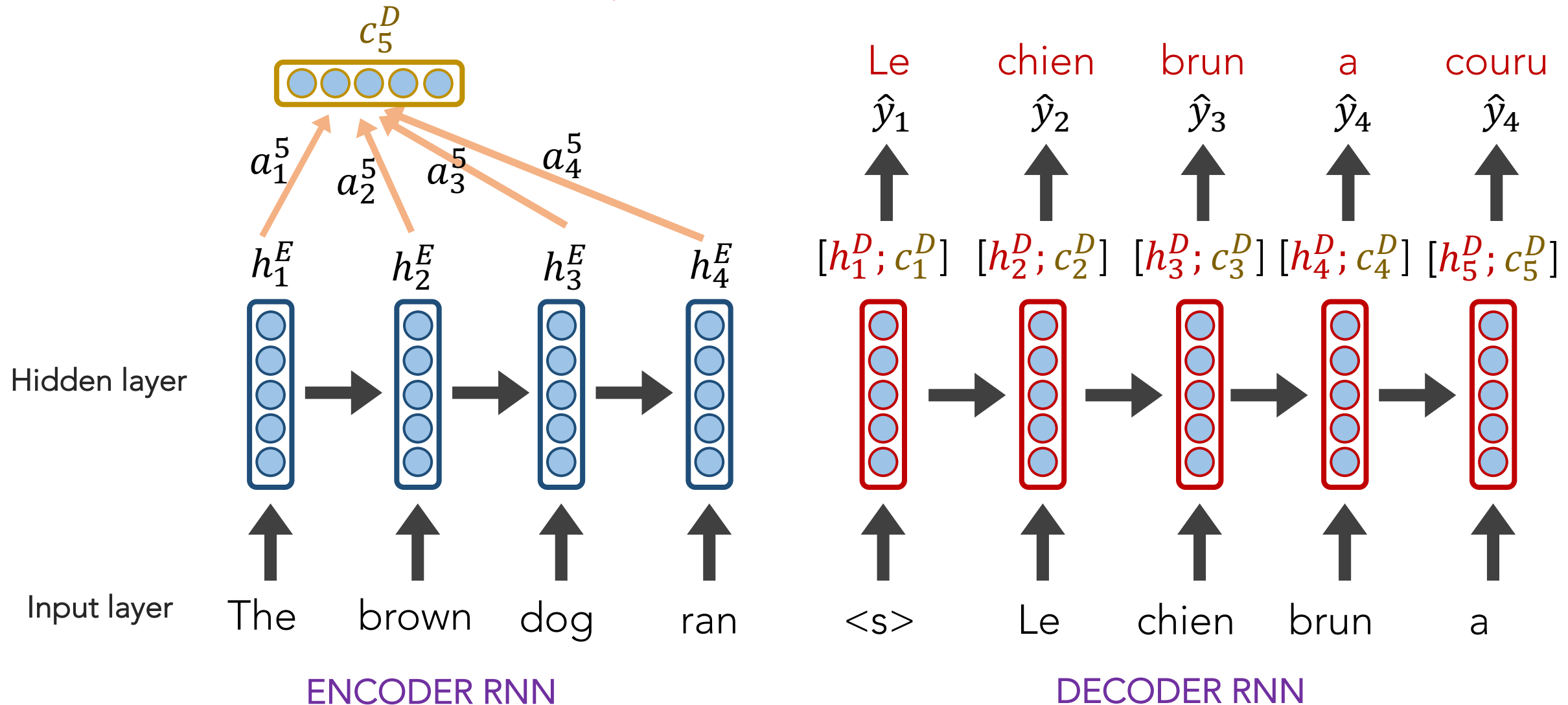
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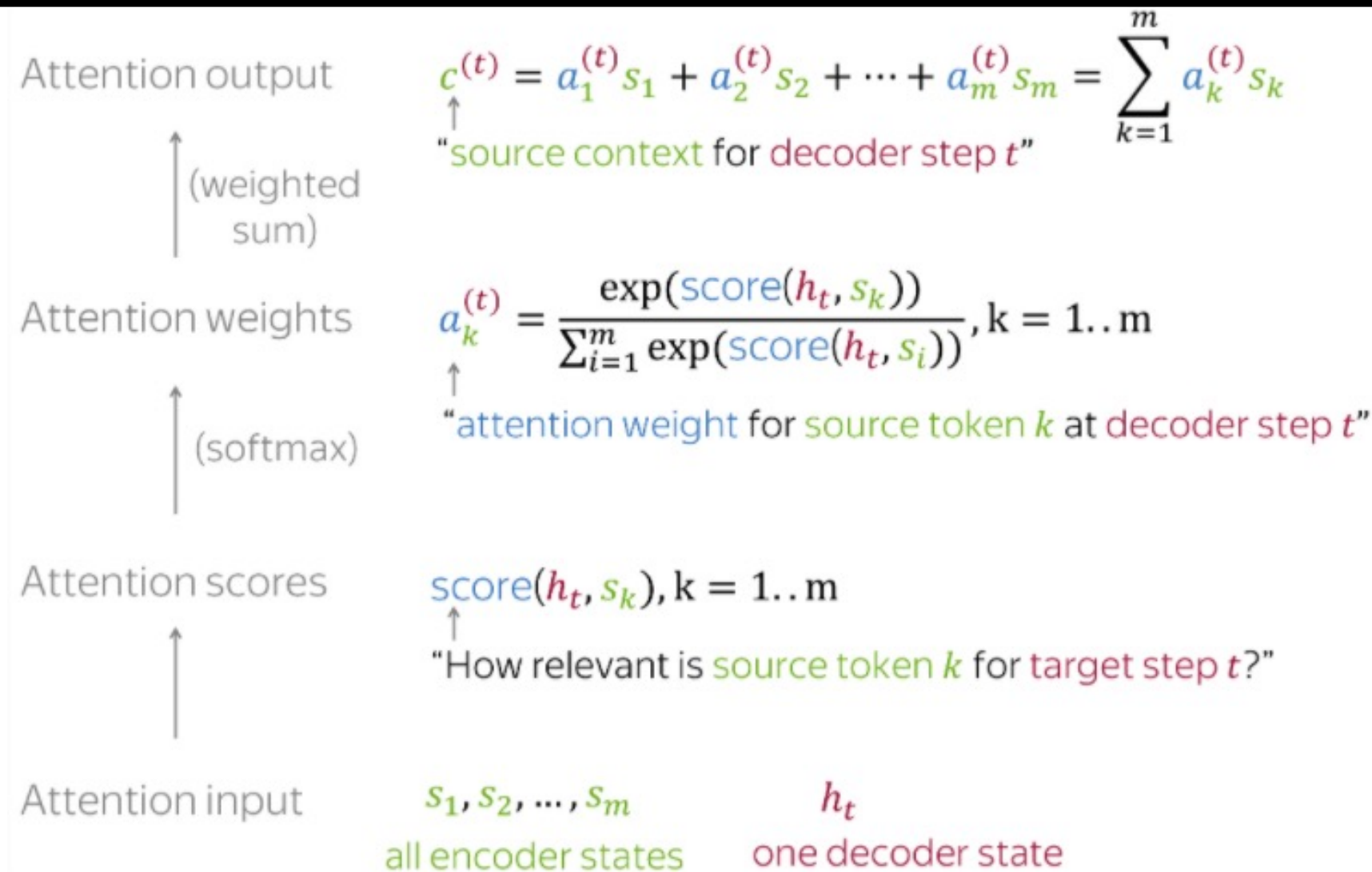


# seq2seq + Attention

**REMEMBER:** each attention weight  $a_i^j$  is based on the **decoder's** current hidden state, too.



For convenience, here's the Attention calculation summarized on 1 slide





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Attention output

$$c^{(t)} = a_1^{(t)} s_1 + a_2^{(t)} s_2 + \dots + a_m^{(t)} s_m = \sum_{k=1}^m a_k^{(t)} s_k$$

The **Attention mechanism** that produces scores doesn't have to be a **FFNN** like I illustrated. It can be any function you wish.

Attention scores

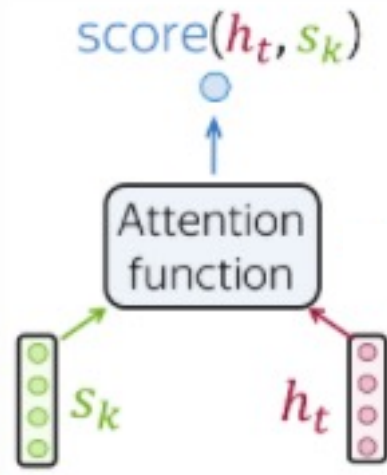
$$\text{score}(h_t, s_k), k = 1..m$$

"How relevant is source token  $k$  for target step  $t$ ?"

Attention input

$$s_1, s_2, \dots, s_m \quad h_t$$

all encoder states      one decoder state



## Popular Attention Scoring functions:

Dot-product

$$h_t^T \times s_k$$

$$\text{score}(h_t, s_k) = h_t^T s_k$$

Bilinear

$$h_t^T \times [W] \times s_k$$

$$\text{score}(h_t, s_k) = h_t^T W s_k$$

Multi-Layer Perceptron

$$w_2^T \times \tanh \left[ W_1 \times \begin{bmatrix} h_t \\ s_k \end{bmatrix} \right]$$

$$\text{score}(h_t, s_k) = w_2^T \cdot \tanh(W_1 [h_t, s_k])$$

# seq2seq + Attention

## Attention:

- greatly improves seq2seq results
- allows us to visualize the contribution each **encoding** word gave for each **decoder's** word

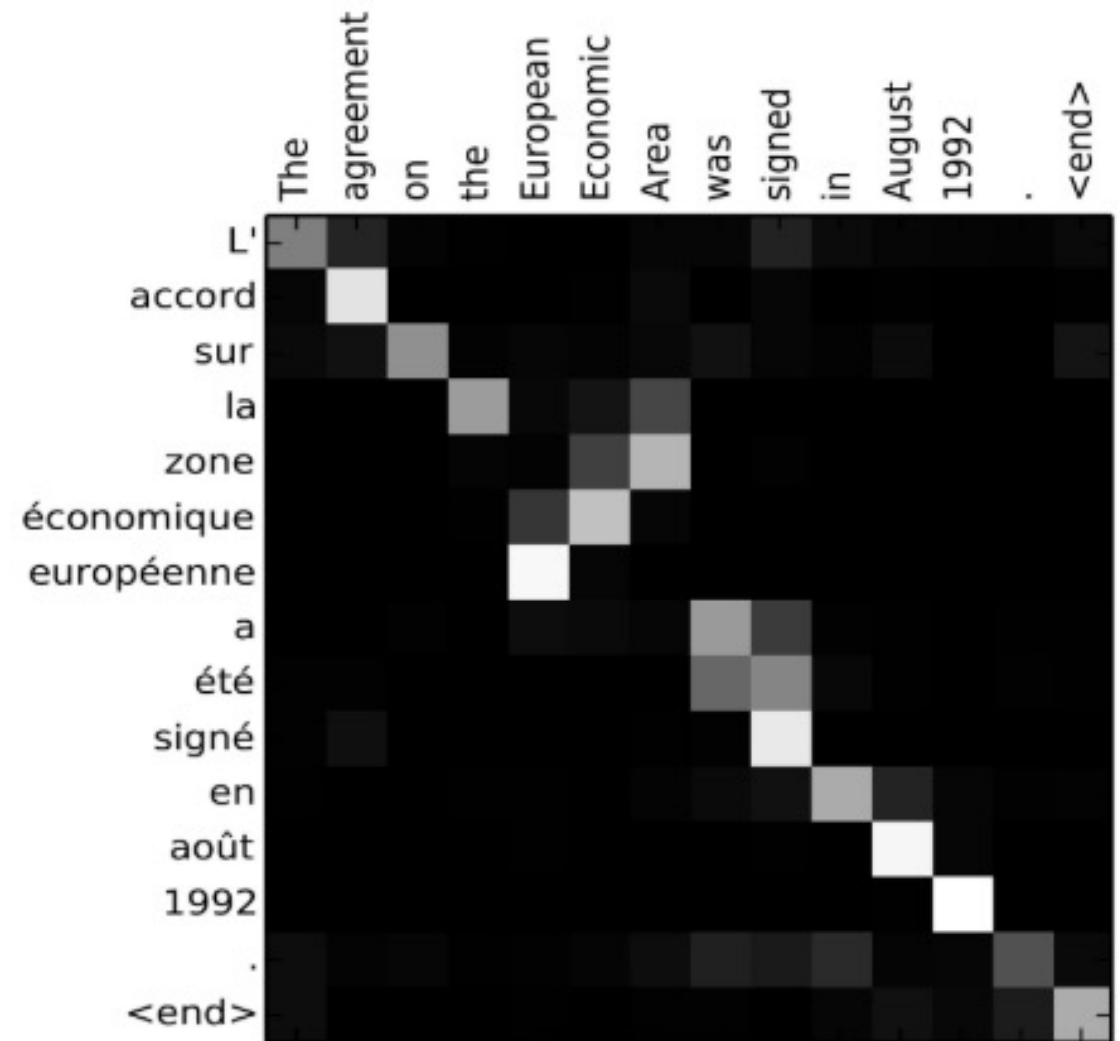


Image source: Fig 3 in [Bahdanau et al., 2015](#)

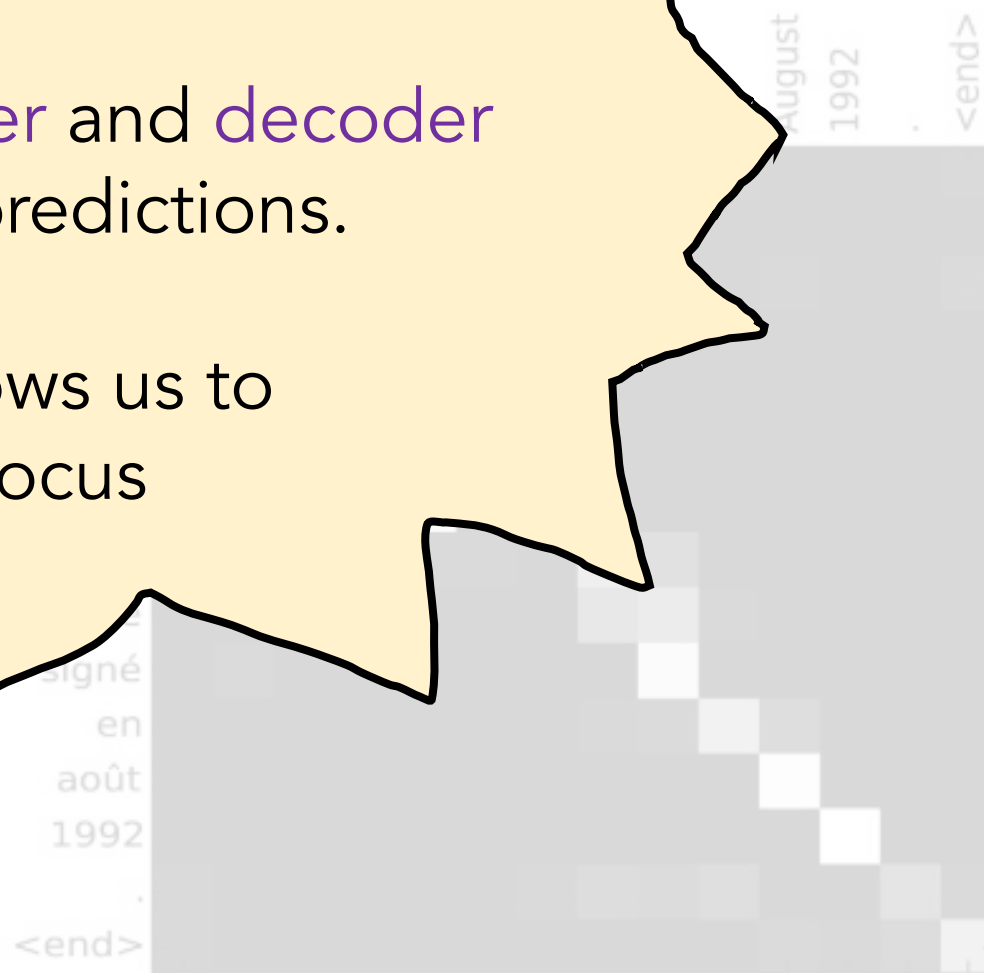
seq2seq + Attention

Attention

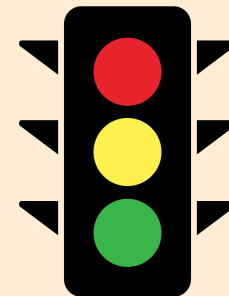
Takeaway:

Having a separate **encoder** and **decoder** allows for **n**  $\rightarrow$  **m** length predictions.

**Attention** is powerful; allows us to conditionally weight our focus



# CHECKPOINT



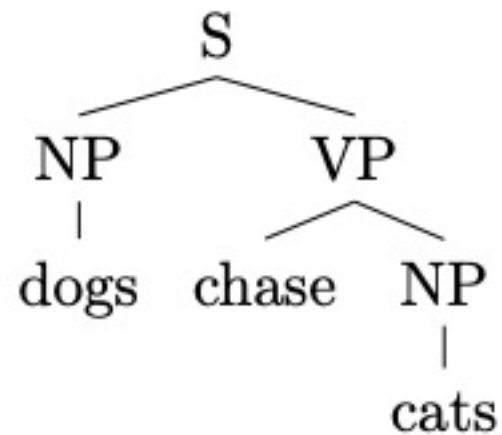
- seq2seq doesn't have to use RNNs/LSTMs
- seq2seq doesn't have to be used exclusively for NMT
- NMT doesn't have to use seq2seq  
(but it's natural and the best we have for now)

# Constituency Parsing

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**Input:** dogs chase cats

**Output:**



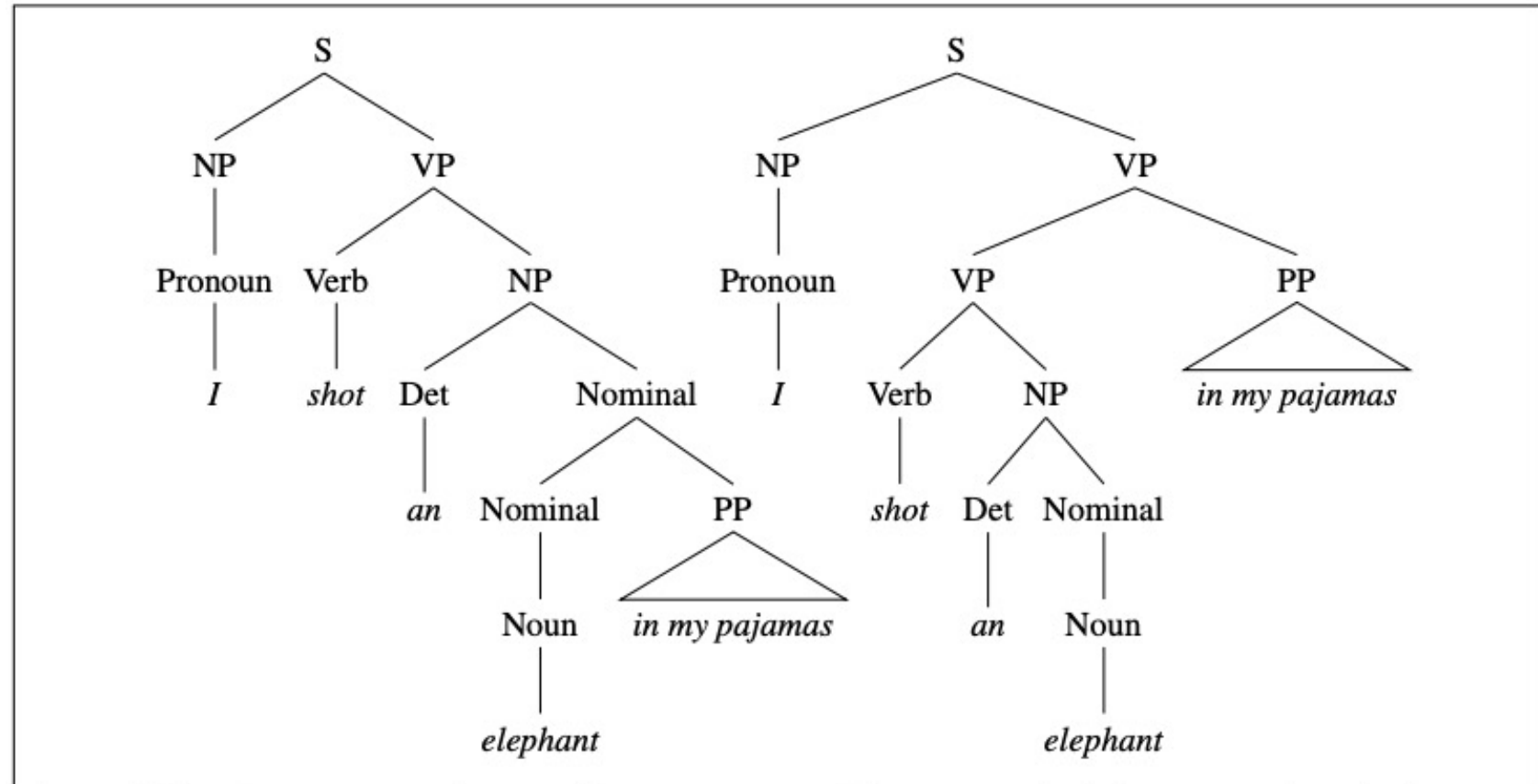
or a flattened representation

(S (NP dogs )<sub>NP</sub> (VP chase (NP cats )<sub>NP</sub> )<sub>VP</sub> )<sub>S</sub>

# Constituency Parsing

**Input:** I shot an elephant in my pajamas

**Output:**



**Figure 13.2** Two parse trees for an ambiguous sentence. The parse on the left corresponds to the humorous reading in which the elephant is in the pajamas, the parse on the right corresponds to the reading in which Captain Spaulding did the shooting in his pajamas.

## Results

Model	English			Chinese		
	LR	LP	F1	LR	LP	F1
Shen et al. (2018)	92.0	91.7	91.8	86.6	86.4	86.5
Fried and Klein (2018)	-	-	92.2	-	-	87.0
Teng and Zhang (2018)	92.2	92.5	92.4	86.6	88.0	87.3
Vaswani et al. (2017)	-	-	92.7	-	-	-
Dyer et al. (2016)	-	-	93.3	-	-	84.6
Kuncoro et al. (2017)	-	-	93.6	-	-	-
Charniak et al. (2016)	-	-	93.8	-	-	-
Liu and Zhang (2017b)	91.3	92.1	91.7	85.9	85.2	85.5
Liu and Zhang (2017a)	-	-	94.2	-	-	86.1
Suzuki et al. (2018)	-	-	94.32	-	-	-
Takase et al. (2018)	-	-	94.47	-	-	-
Fried et al. (2017)	-	-	94.66	-	-	-
Kitaev and Klein (2018)	94.85	95.40	95.13	-	-	-
Kitaev et al. (2018)	95.51	96.03	95.77	91.55	91.96	91.75
Zhou and Zhao (2019)	95.70	95.98	95.84	<b>92.03</b>	92.33	92.18
(BERT)						
Zhou and Zhao (2019)	96.21	96.46	96.33	-	-	-
(XLNet)						
Our work	<b>96.24</b>	<b>96.53</b>	<b>96.38</b>	91.85	<b>93.45</b>	<b>92.64</b>

Table 3: Constituency Parsing on PTB & CTB test sets.



# Image Captioning

**Input:** image

**Output:** generated text



A woman is throwing a frisbee in a park.



A dog is standing on a hardwood floor.

Figure 3. Examples of attending to the correct object (*white* indicates the attended regions, *underlines* indicated the corresponding word)

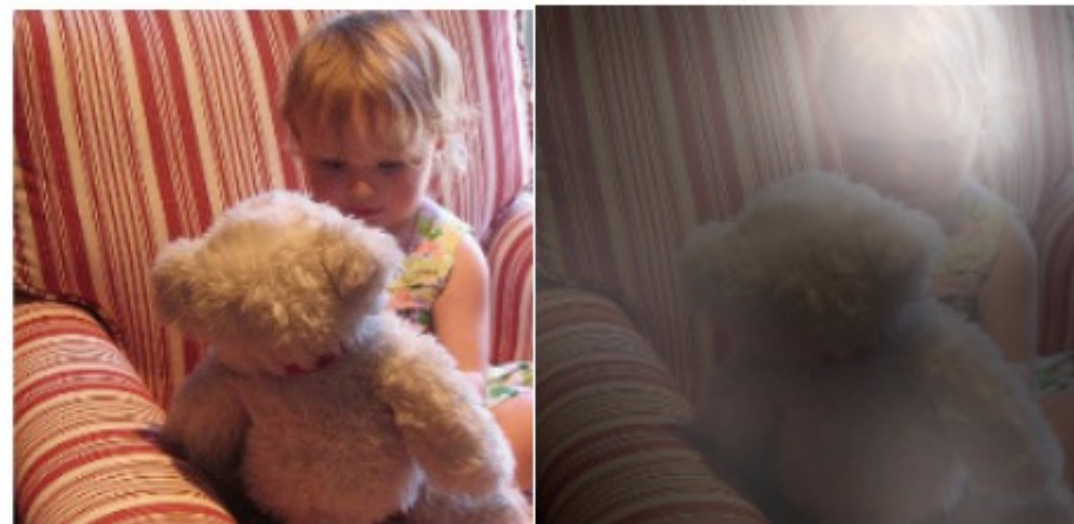
# Image Captioning

**Input:** image

**Output:** generated text



A stop sign is on a road with a mountain in the background.



A little girl sitting on a bed with a teddy bear.

Figure 3. Examples of attending to the correct object (*white* indicates the attended regions, *underlines* indicated the corresponding word)

# Image Captioning



A large white bird standing in a forest.



A woman holding a clock in her hand.

*Figure 5.* Examples of mistakes where we can use attention to gain intuition into what the model saw.



# Image Captioning



A woman is sitting at a table with a large pizza.



A person is standing on a beach with a surfboard.

*Figure 5. Examples of mistakes where we can use attention to gain intuition into what the model saw.*

# SUMMARY

- **LSTMs** yielded state-of-the-art results on most NLP tasks (2014-2018)
- **seq2seq+Attention** was an even more revolutionary idea (Google Translate used it)
- **Attention** allows us to place appropriate weight to the encoder's hidden states
- But:

# SUMMARY

- LSTMs are sequential in nature (prohibits parallelization). *Very wasteful.*
- No explicit modelling of long- and short- range dependencies
- Language is naturally hierarchical  
(can we do better than Stacked LSTMs?)
- Can we apply the concept of Attention to improve our **representations**?  
(i.e., *contextualized representations*)

# Outline

 seq2seq + Attention

 Self-Attention

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 seq2seq + Attention

 Self-Attention

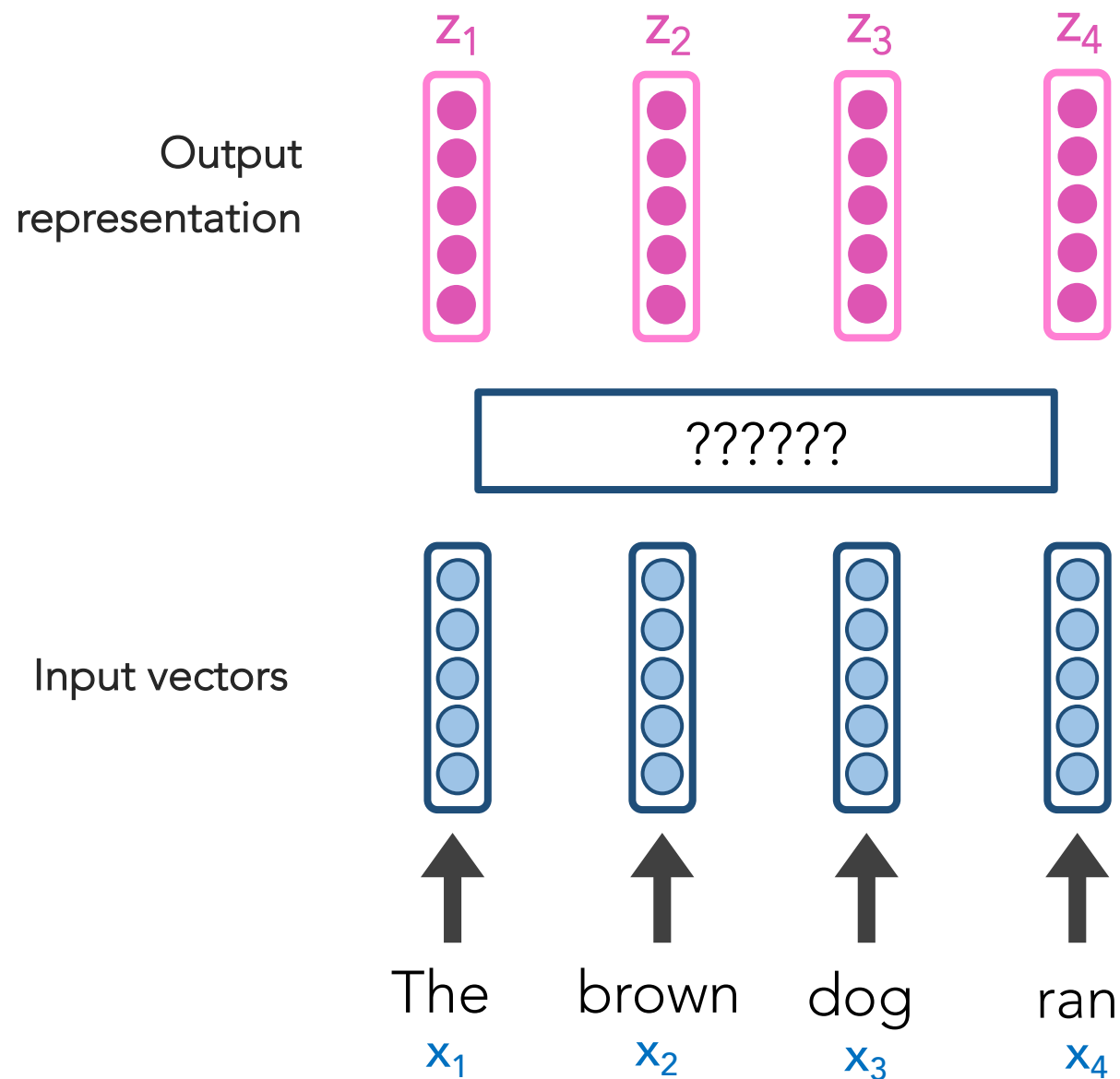


# Goals

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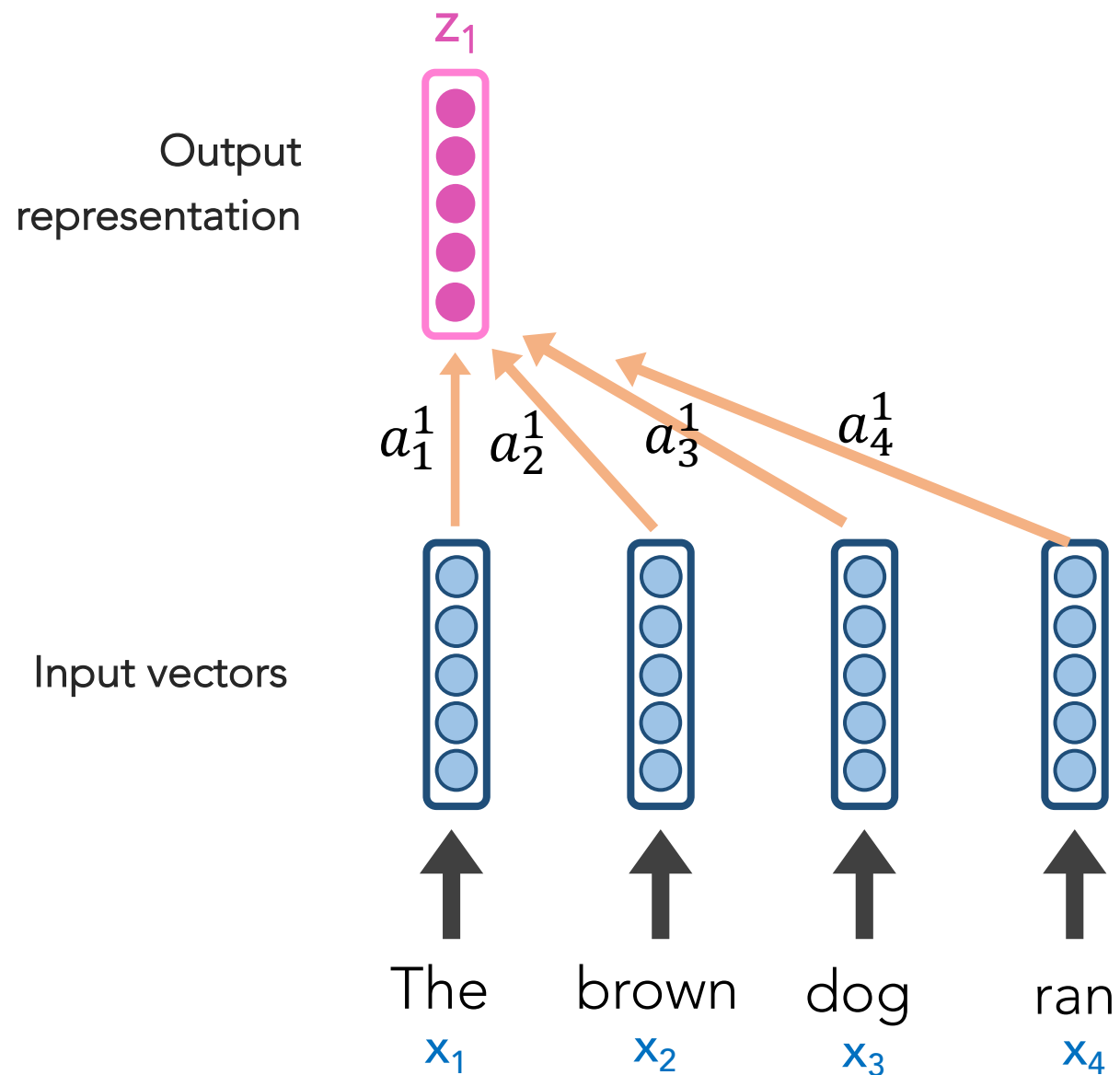
- Each word in a sequence to be transformed into a rich, abstract **representation** (context embedding) based on the weighted sums of the other words in the same sequence (akin to deep CNN layers)
- Inspired by Attention, we want each word to determine, “how much should I be influenced by each of my neighbors”
- Want positionality

# Self-Attention



Self-Attention's goal is to create great representations,  $z_i$ , of the input

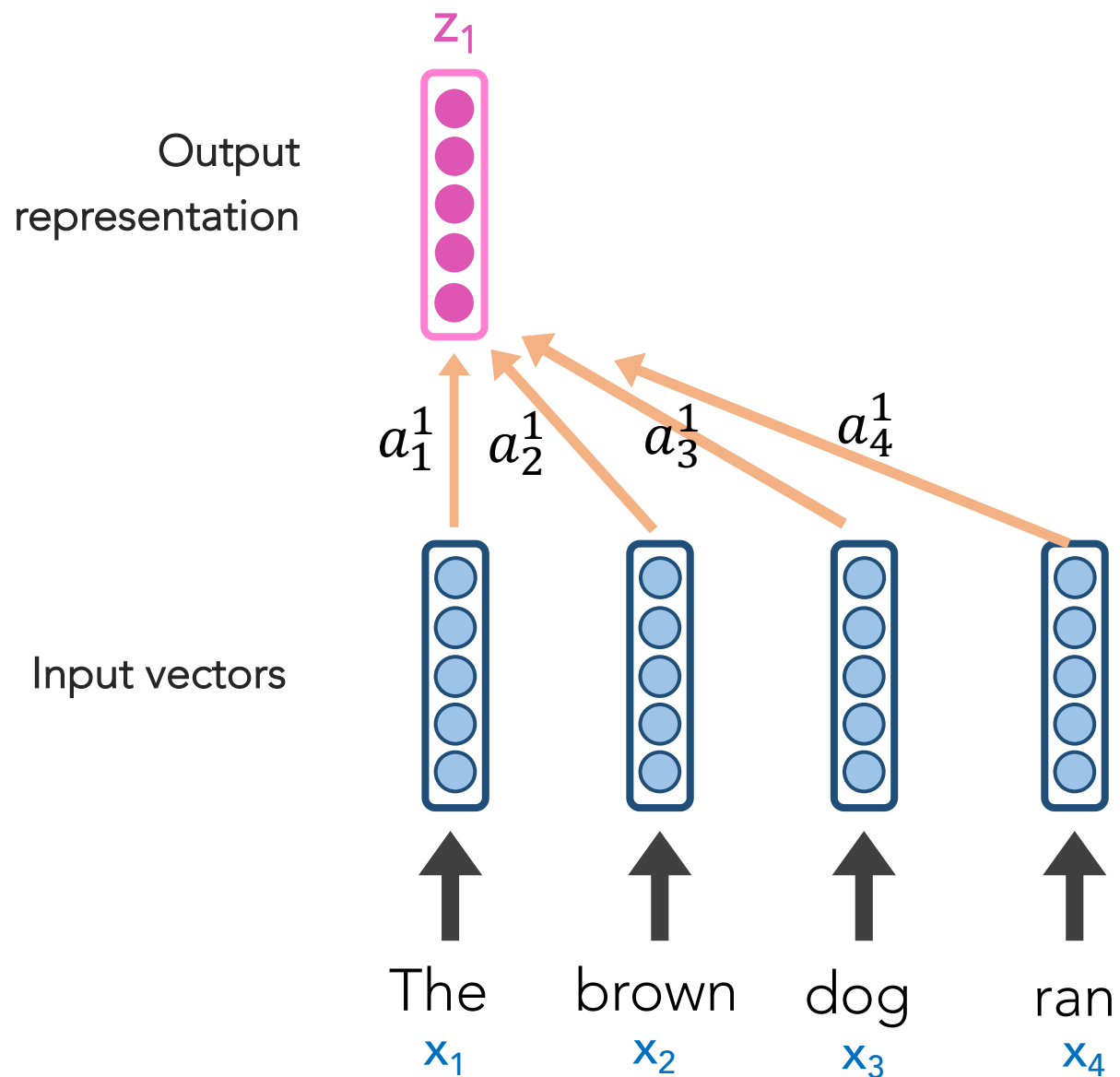
# Self-Attention



Self-Attention's goal is to create great representations,  $z_i$ , of the input

$z_1$  will be based on a weighted contribution of  $x_1, x_2, x_3, x_4$

# Self-Attention

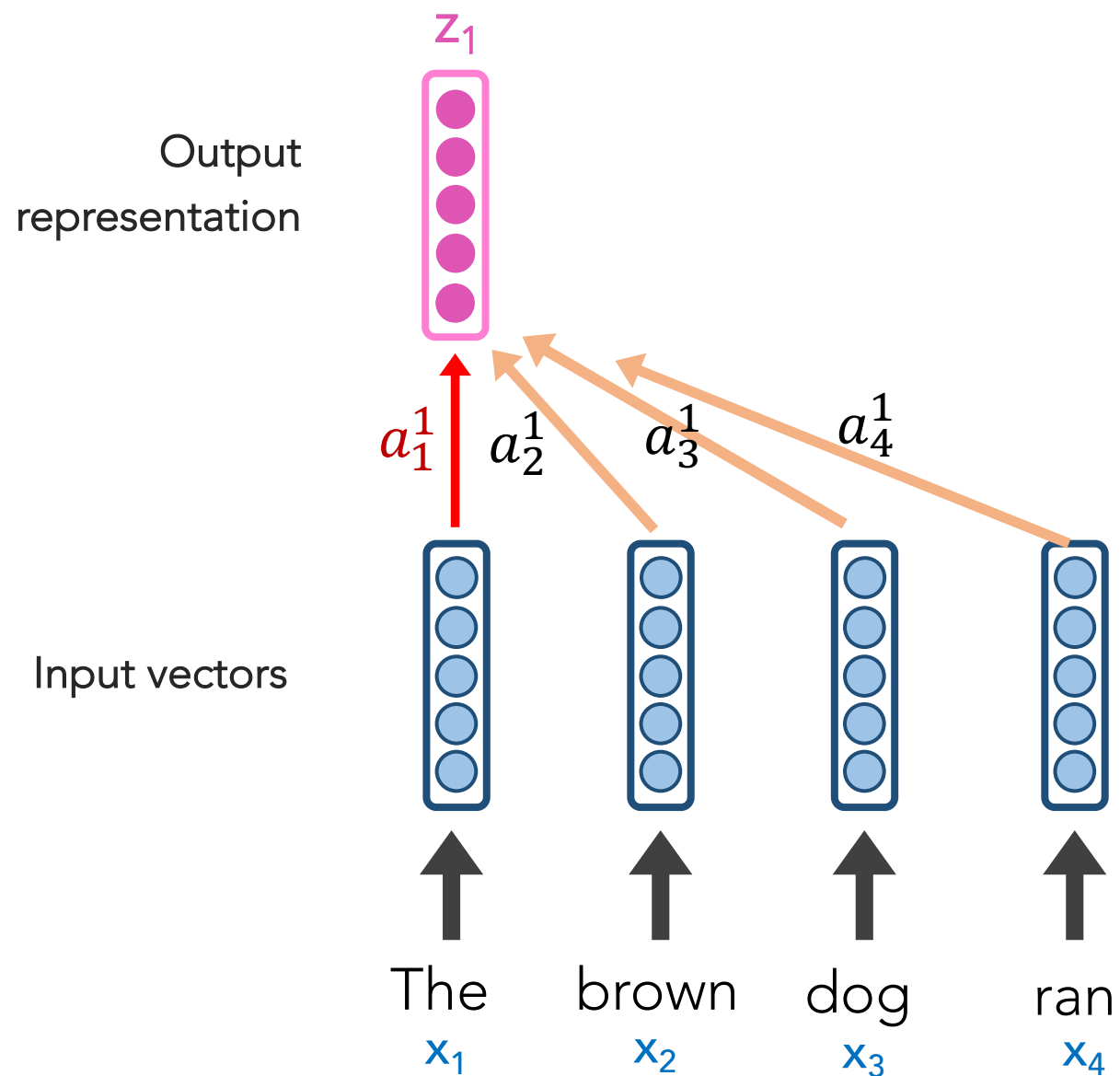


Self-Attention's goal is to create great representations,  $z_i$ , of the input

$z_1$  will be based on a weighted contribution of  $x_1, x_2, x_3, x_4$

$a_i^1$  is "just" a weight. More is happening under the hood, but it's effectively weighting versions of  $x_1, x_2, x_3, x_4$

# Self-Attention



Under the hood, each  $x_i$  has 3 small, associated vectors.

For example,  $x_1$  has:

- Query  $q_i$
- Key  $k_i$
- Value  $v_i$

# Self-Attention

**Step 1:** Our Self-Attention Head has just 3 weight matrices  $W_q$ ,  $W_k$ ,  $W_v$  in total. **These same 3 weight matrices** are multiplied by each  $x_i$  to create all vectors:

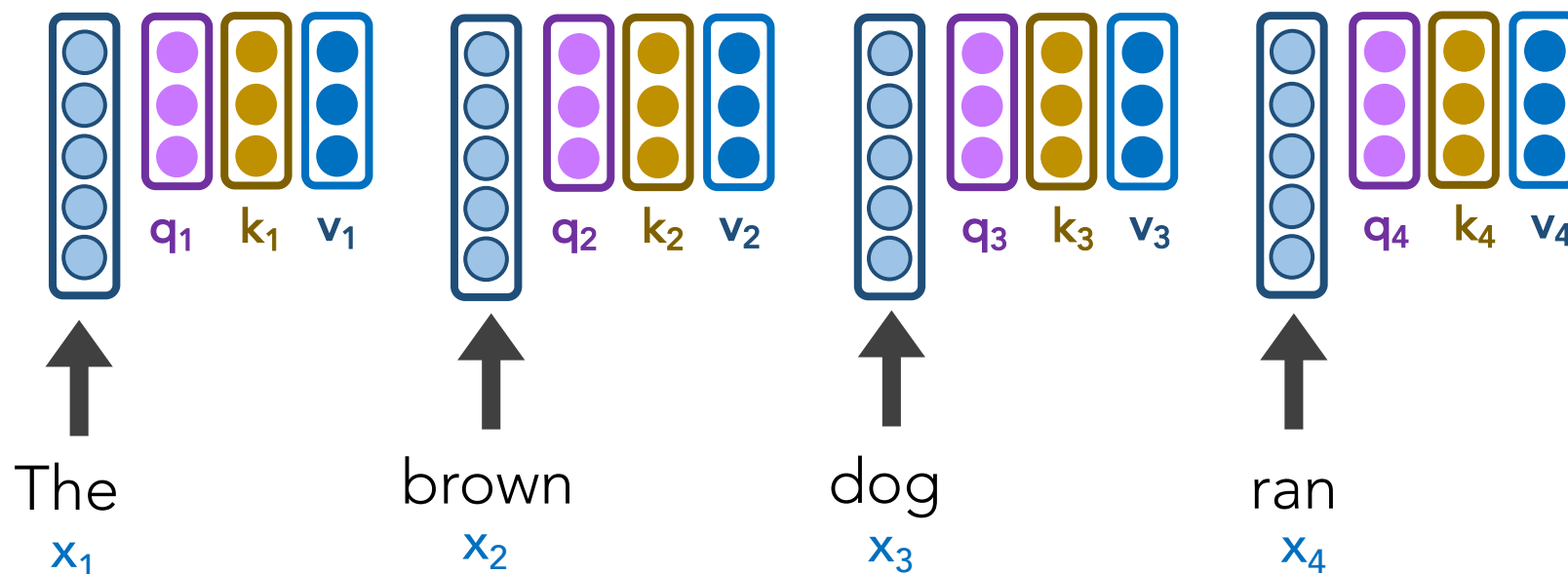
$$q_i = W_q x_i$$

$$k_i = W_k x_i$$

$$v_i = W_v x_i$$

Under the hood, each  $x_i$  has 3 small, associated vectors. For example,  $x_1$  has:

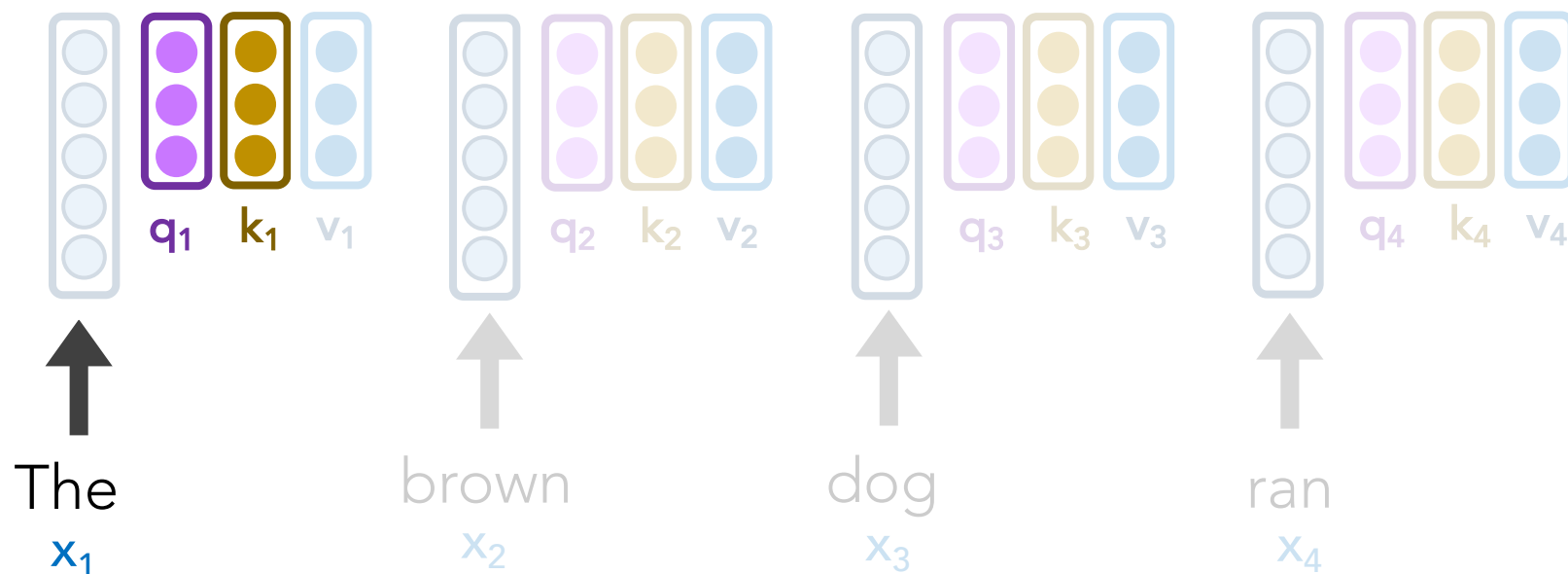
- Query  $q_1$
- Key  $k_1$
- Value  $v_1$



# Self-Attention

**Step 2:** For word  $x_1$ , let's calculate the scores  $s_1, s_2, s_3, s_4$ , which represent how much attention to pay to each respective "word"  $v_i$

$$s_1 = q_1 \cdot k_1 = 112$$

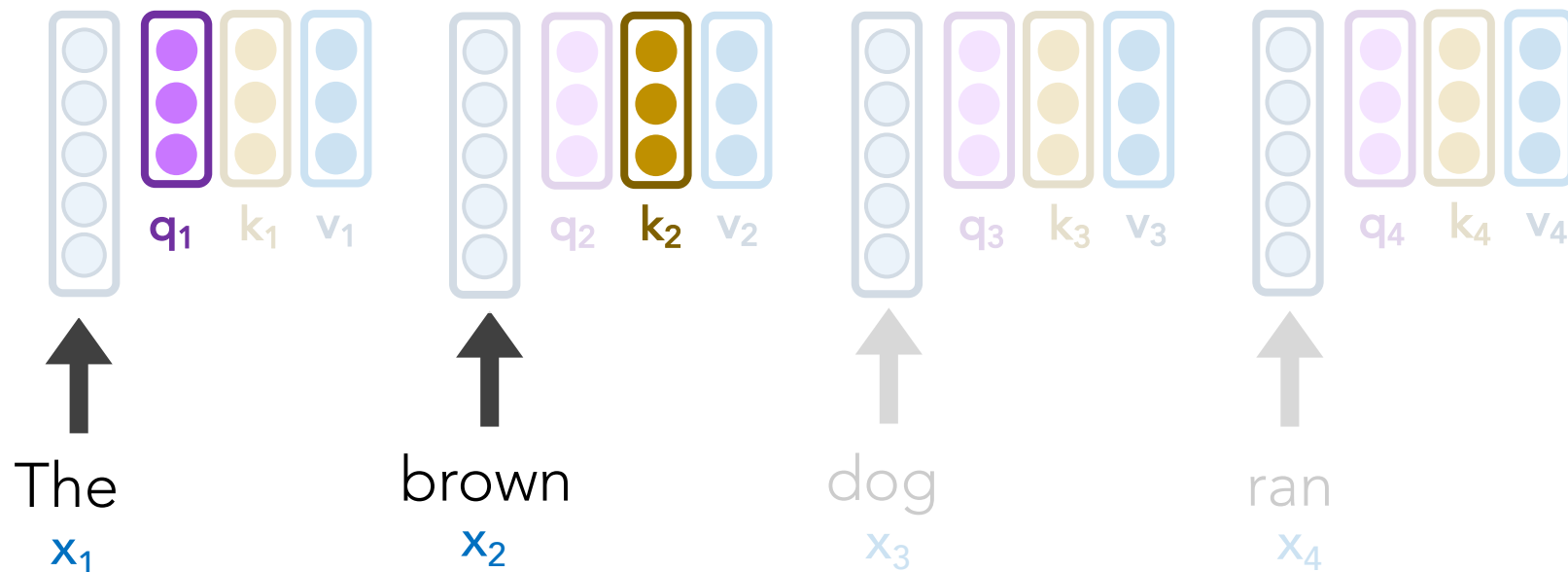


# Self-Attention

**Step 2:** For word  $x_1$ , let's calculate the scores  $s_1, s_2, s_3, s_4$ , which represent how much attention to pay to each respective "word"  $v_i$

$$s_2 = q_1 \cdot k_2 = 96$$

$$s_1 = q_1 \cdot k_1 = 112$$





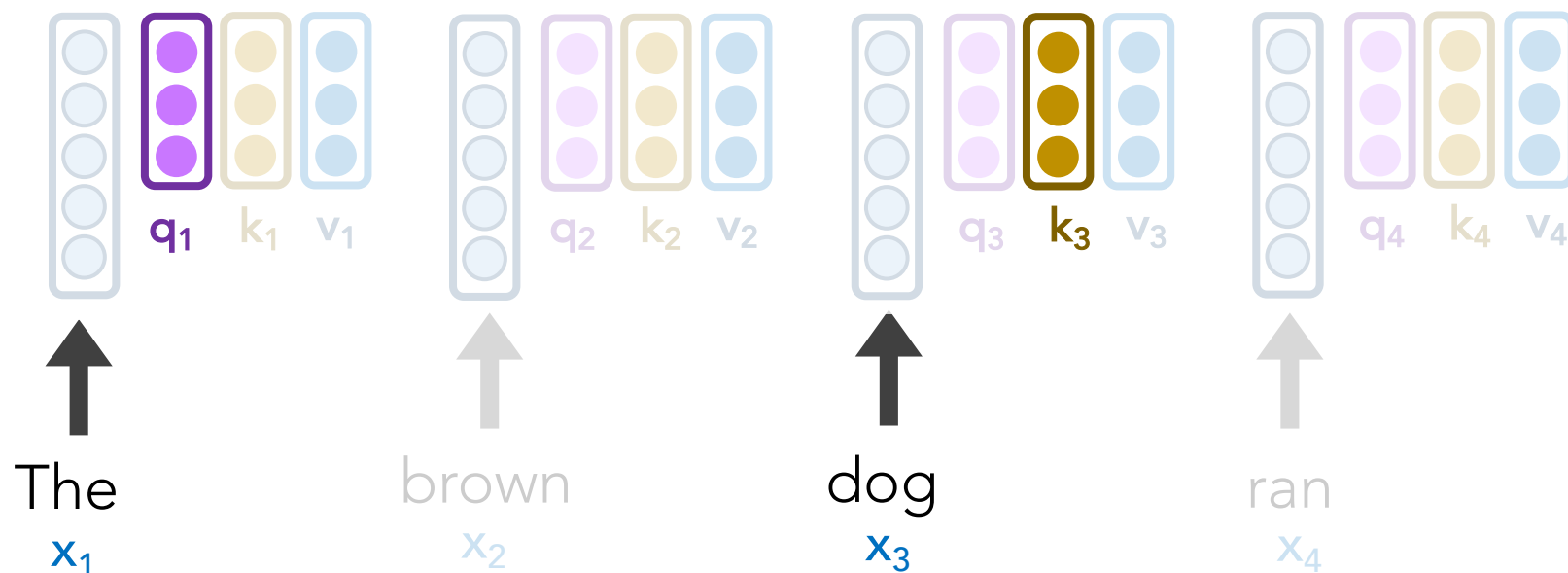
# Self-Attention

**Step 2:** For word  $x_1$ , let's calculate the scores  $s_1, s_2, s_3, s_4$ , which represent how much attention to pay to each respective "word"  $v_i$

$$s_3 = q_1 \cdot k_3 = 16$$

$$s_2 = q_1 \cdot k_2 = 96$$

$$s_1 = q_1 \cdot k_1 = 112$$



# Self-Attention

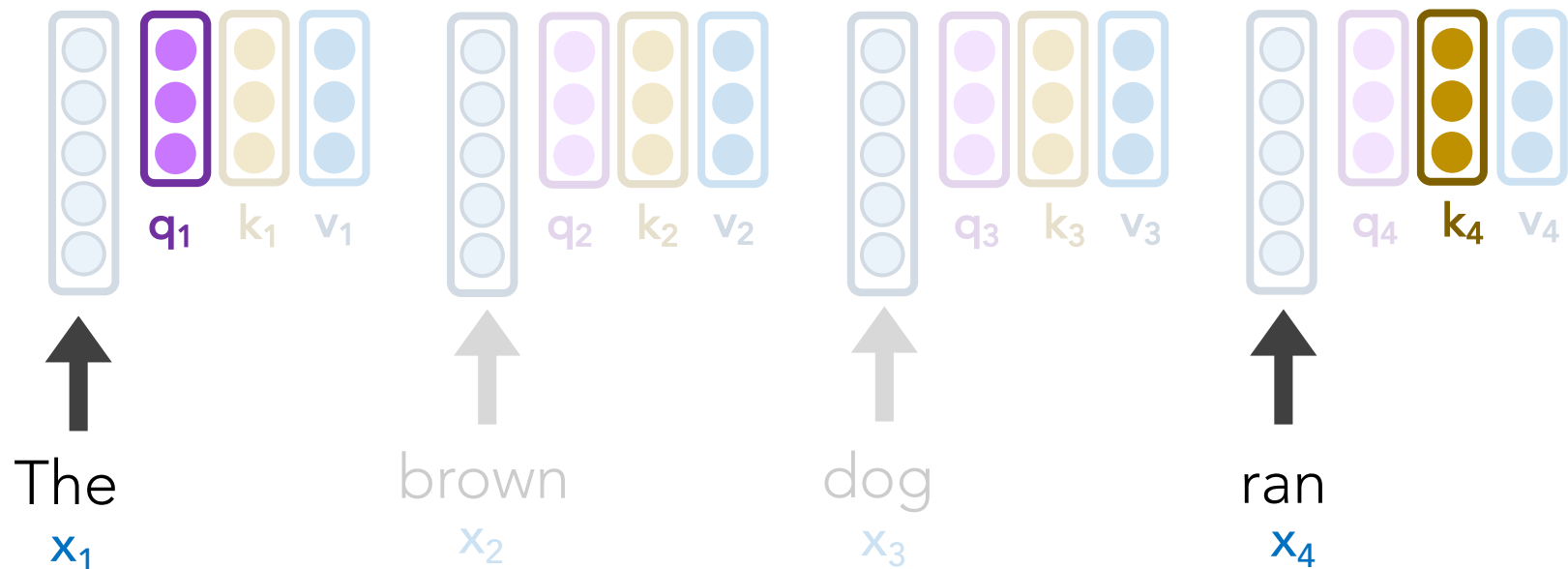
**Step 2:** For word  $x_1$ , let's calculate the scores  $s_1, s_2, s_3, s_4$ , which represent how much attention to pay to each respective "word"  $v_i$

$$s_4 = q_1 \cdot k_4 = 8$$

$$s_3 = q_1 \cdot k_3 = 16$$

$$s_2 = q_1 \cdot k_2 = 96$$

$$s_1 = q_1 \cdot k_1 = 112$$



# Self-Attention

**Step 3:** Our scores  $s_1, s_2, s_3, s_4$  don't sum to 1. Let's divide by  $\sqrt{\text{len}(k_i)}$  and **softmax** it

$$s_4 = q_1 \cdot k_4 = 8$$

$$a_4 = \sigma(s_4/8) = 0$$

$$s_3 = q_1 \cdot k_3 = 16$$

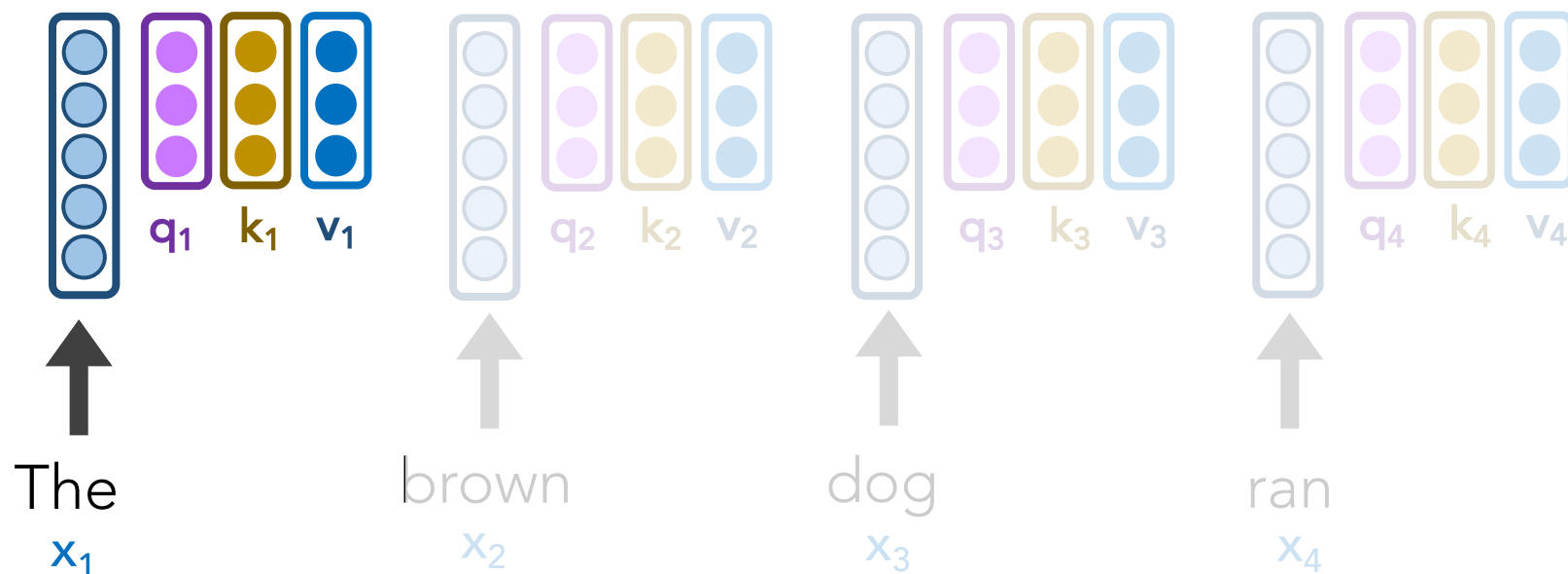
$$a_3 = \sigma(s_3/8) = .01$$

$$s_2 = q_1 \cdot k_2 = 96$$

$$a_2 = \sigma(s_2/8) = .12$$

$$s_1 = q_1 \cdot k_1 = 112$$

$$a_1 = \sigma(s_1/8) = .87$$



# Self-Attention

**Step 3:** Our scores  $s_1, s_2, s_3, s_4$  don't sum to 1. Let's divide by  $\sqrt{\text{len}(k_i)}$  and **softmax** it

$$s_4 = q_1 \cdot k_4 = 8$$

$$a_4 = \sigma(s_4/8) = 0$$

$$s_3 = q_1 \cdot k_3 = 16$$

$$a_3 = \sigma(s_3/8) = .01$$

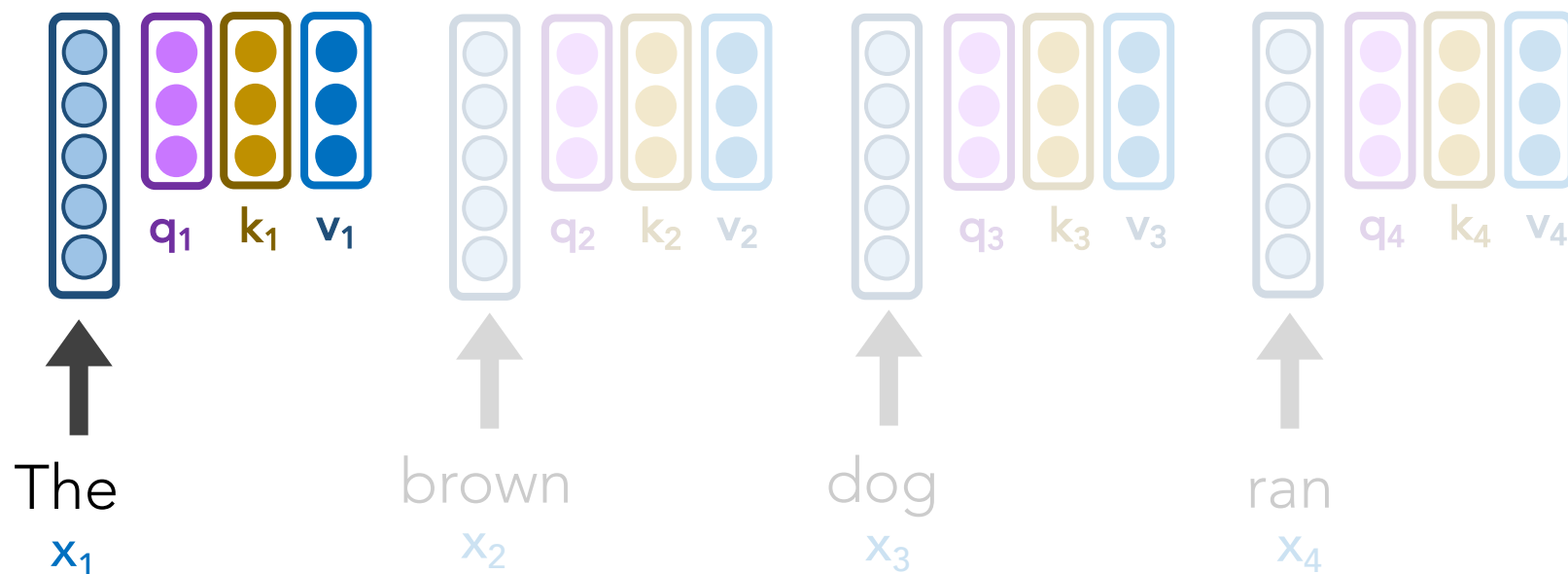
$$s_2 = q_1 \cdot k_2 = 96$$

$$a_2 = \sigma(s_2/8) = .12$$

$$s_1 = q_1 \cdot k_1 = 112$$

$$a_1 = \sigma(s_1/8) = .87$$


Instead of these  $a_i$  values directly weighting our original  $x_i$  word vectors, they directly weight our  $v_i$  vectors.

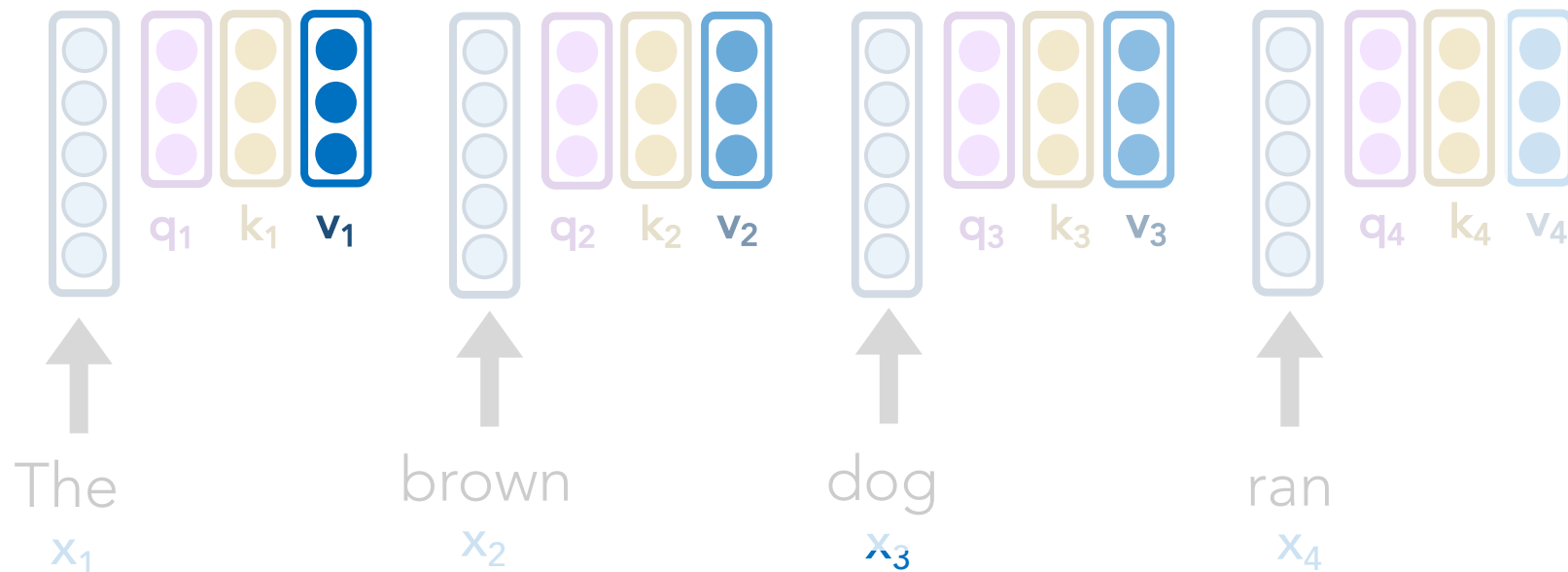


# Self-Attention

**Step 4:** Let's weight our  $\mathbf{v}_i$  vectors and simply sum them up!

$z_1$


$$\begin{aligned} z_1 &= \mathbf{a}_1 \cdot \mathbf{v}_1 + \mathbf{a}_2 \cdot \mathbf{v}_2 + \mathbf{a}_3 \cdot \mathbf{v}_3 + \mathbf{a}_4 \cdot \mathbf{v}_4 \\ &= 0.87 \cdot \mathbf{v}_1 + 0.12 \cdot \mathbf{v}_2 + 0.01 \cdot \mathbf{v}_3 + 0 \cdot \mathbf{v}_4 \end{aligned}$$

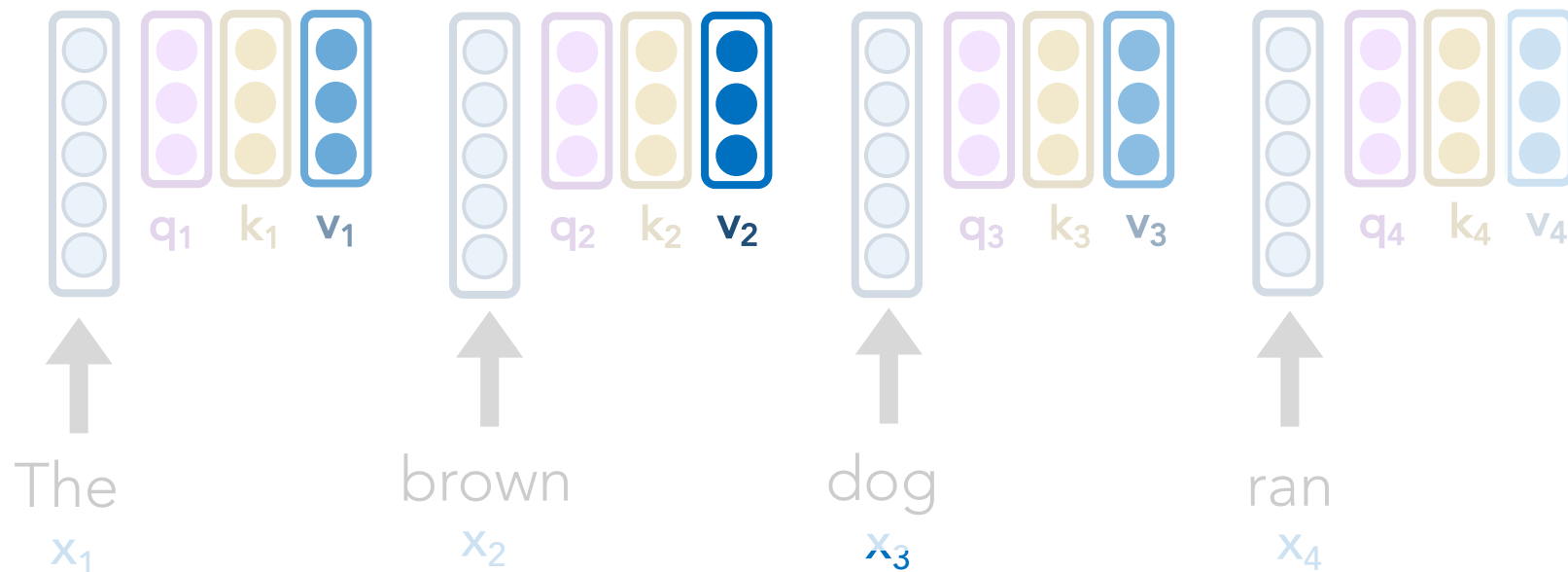


# Self-Attention

**Step 5:** We repeat this for all other words, yielding us with great, new  $z_i$  representations!



$$z_2 = a_1 \cdot v_1 + a_2 \cdot v_2 + a_3 \cdot v_3 + a_4 \cdot v_4$$

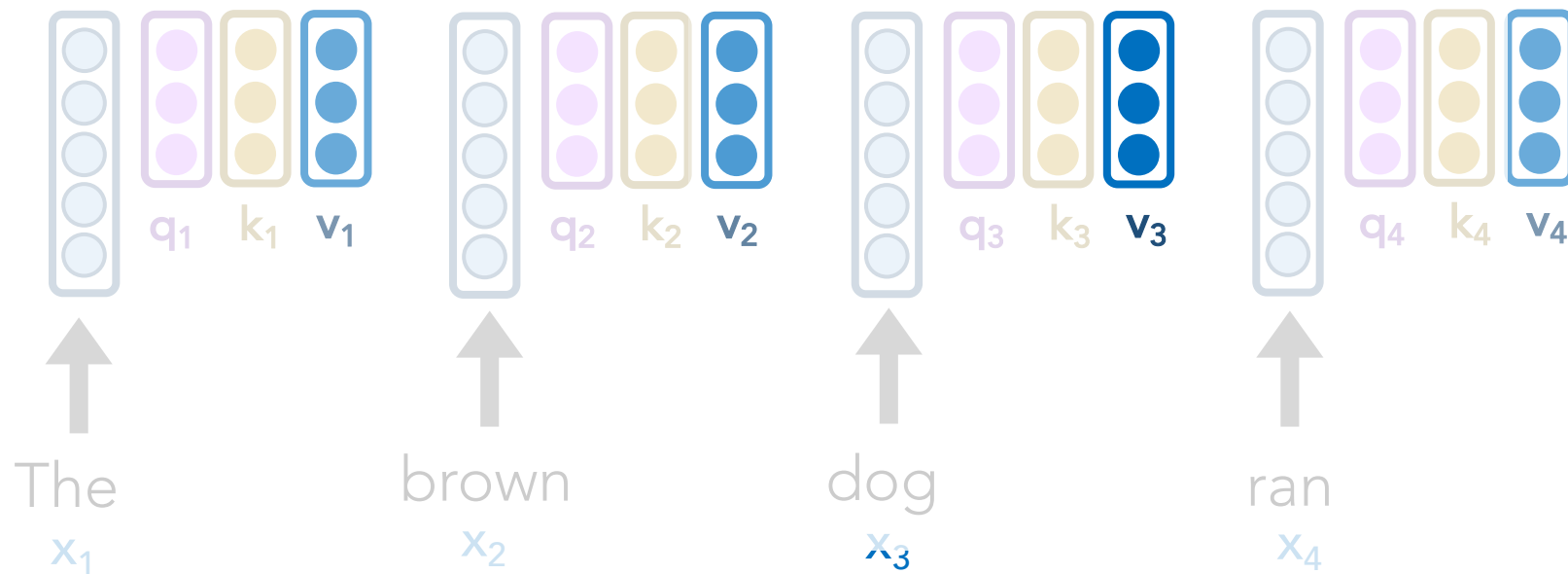


# Self-Attention

**Step 5:** We repeat this for all other words, yielding us with great, new  $z_i$  representations!



$$z_3 = a_1 \cdot v_1 + a_2 \cdot v_2 + a_3 \cdot v_3 + a_4 \cdot v_4$$



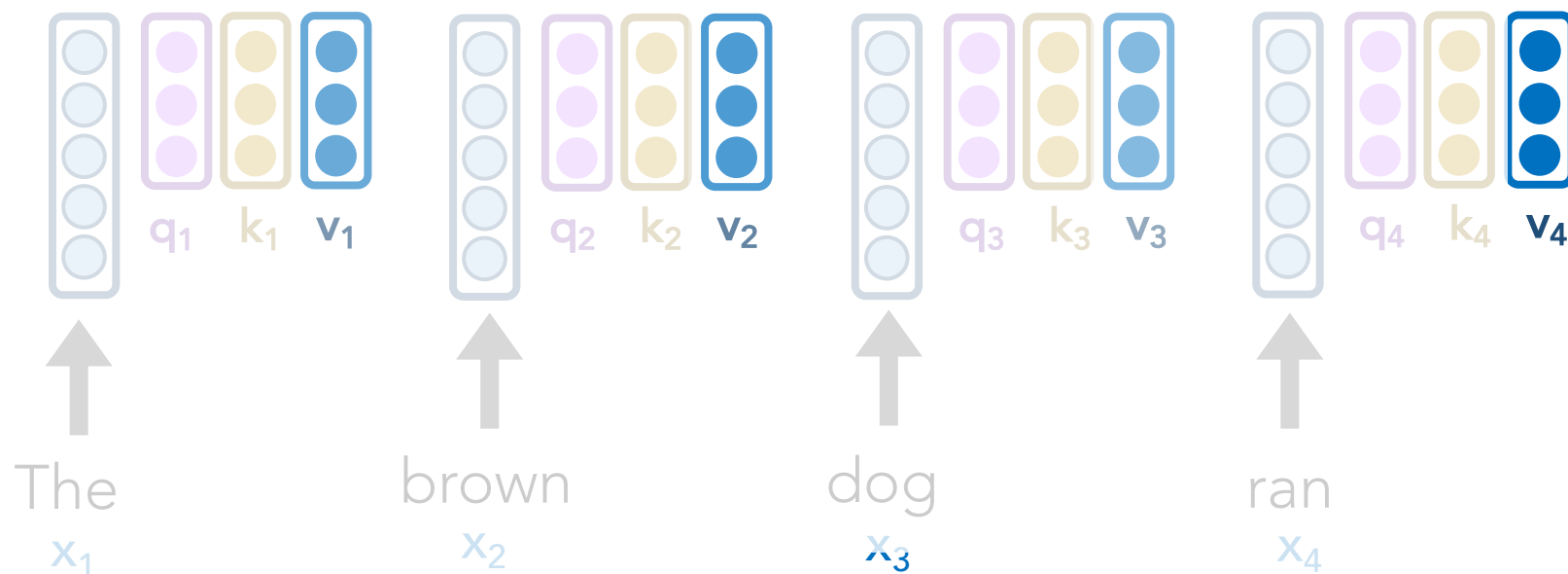
# Self-Attention

**Step 5:** We repeat this for all other words, yielding us with great, new  $z_i$  representations!

$z_4$



$$z_4 = a_1 \cdot v_1 + a_2 \cdot v_2 + a_3 \cdot v_3 + a_4 \cdot v_4$$





Let's illustrate another example:



$$z_2 = a_1 \cdot v_1 + a_2 \cdot v_2 + a_3 \cdot v_3 + a_4 \cdot v_4$$

Remember, we use the same 3 weight matrices

$W_q$ ,  $W_k$ ,  $W_v$  as we did for computing  $z_1$ .

This gives us  $q_2$ ,  $k_2$ ,  $v_2$

# Self-Attention

**Step 1:** Our Self-Attention Head I has just 3 weight matrices  $W_q$ ,  $W_k$ ,  $W_v$  in total. **These same 3 weight matrices** are multiplied by each  $x_i$  to create all vectors:

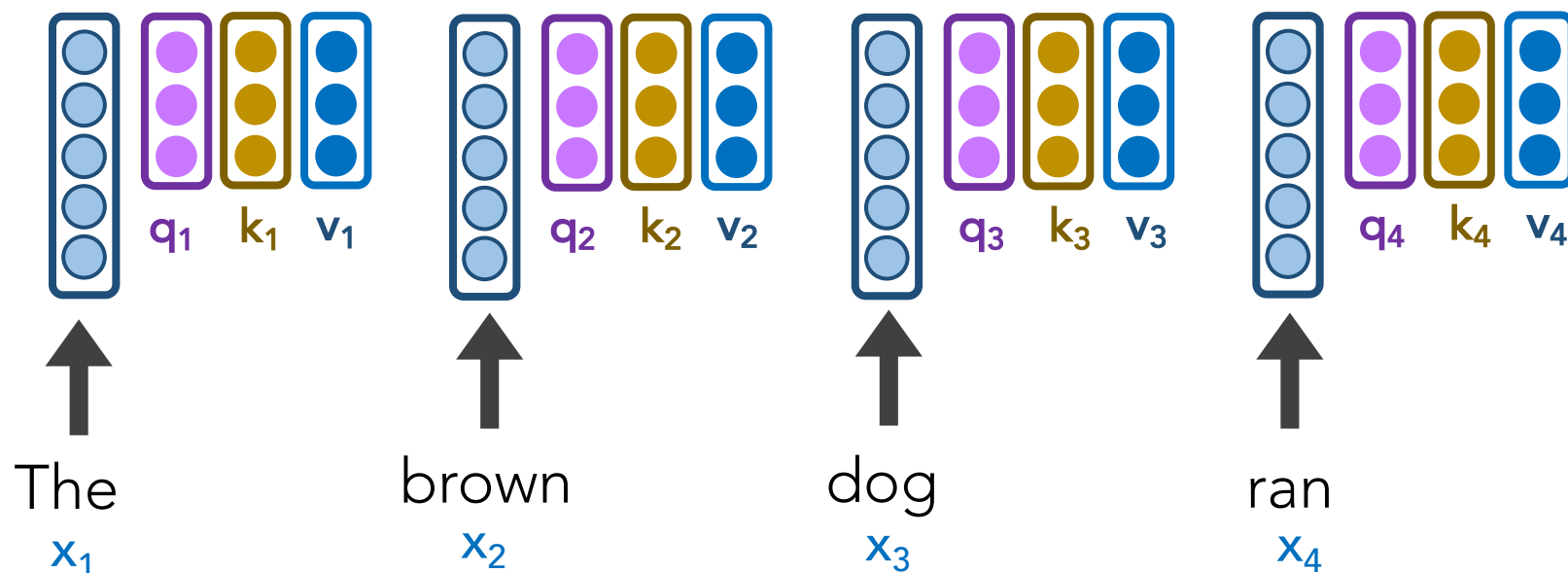
$$q_i = W_q x_i$$

$$k_i = W_k x_i$$

$$v_i = W_v x_i$$

Under the hood, each  $x_i$  has 3 small, associated vectors. For example,  $x_1$  has:

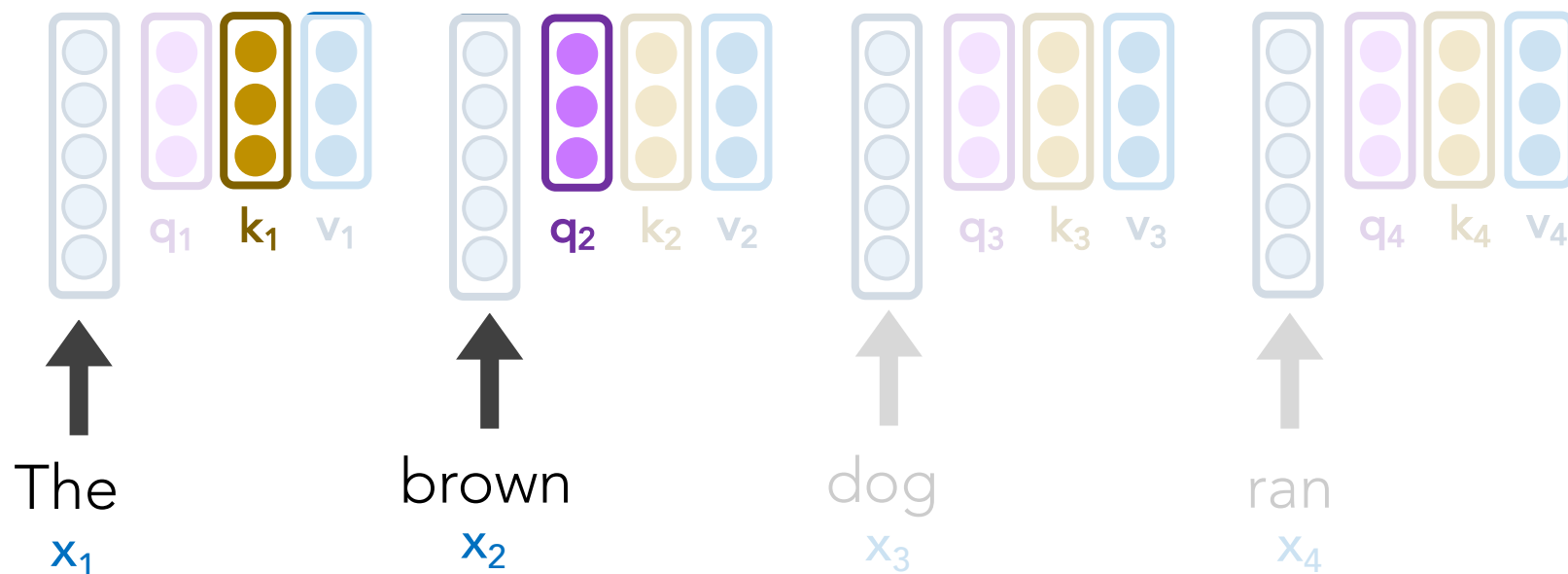
- Query  $q_1$
- Key  $k_1$
- Value  $v_1$



# Self-Attention

**Step 2:** For word  $x_2$ , let's calculate the scores  $s_1, s_2, s_3, s_4$ , which represent how much attention to pay to each respective "word"  $v_i$

$$s_1 = q_2 \cdot k_1 = 92$$

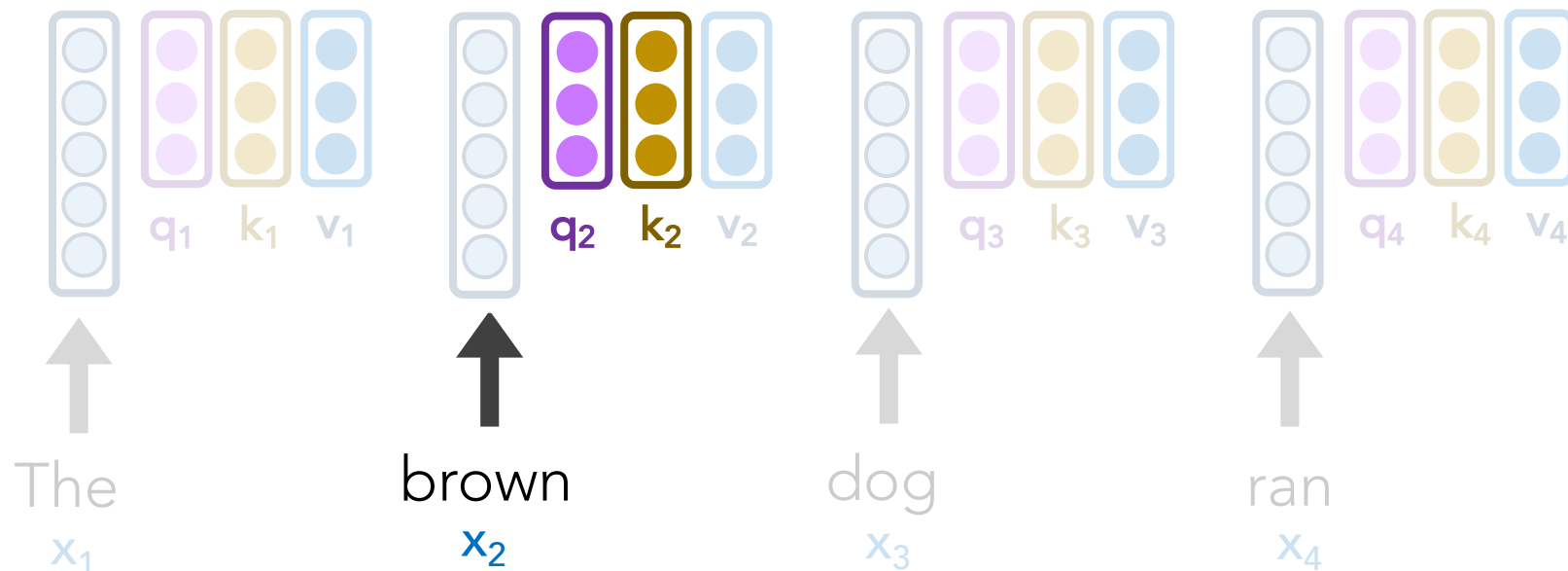


# Self-Attention

**Step 2:** For word  $x_2$ , let's calculate the scores  $s_1, s_2, s_3, s_4$ , which represent how much attention to pay to each respective "word"  $v_i$

$$s_2 = q_2 \cdot k_2 = 124$$

$$s_1 = q_2 \cdot k_1 = 92$$



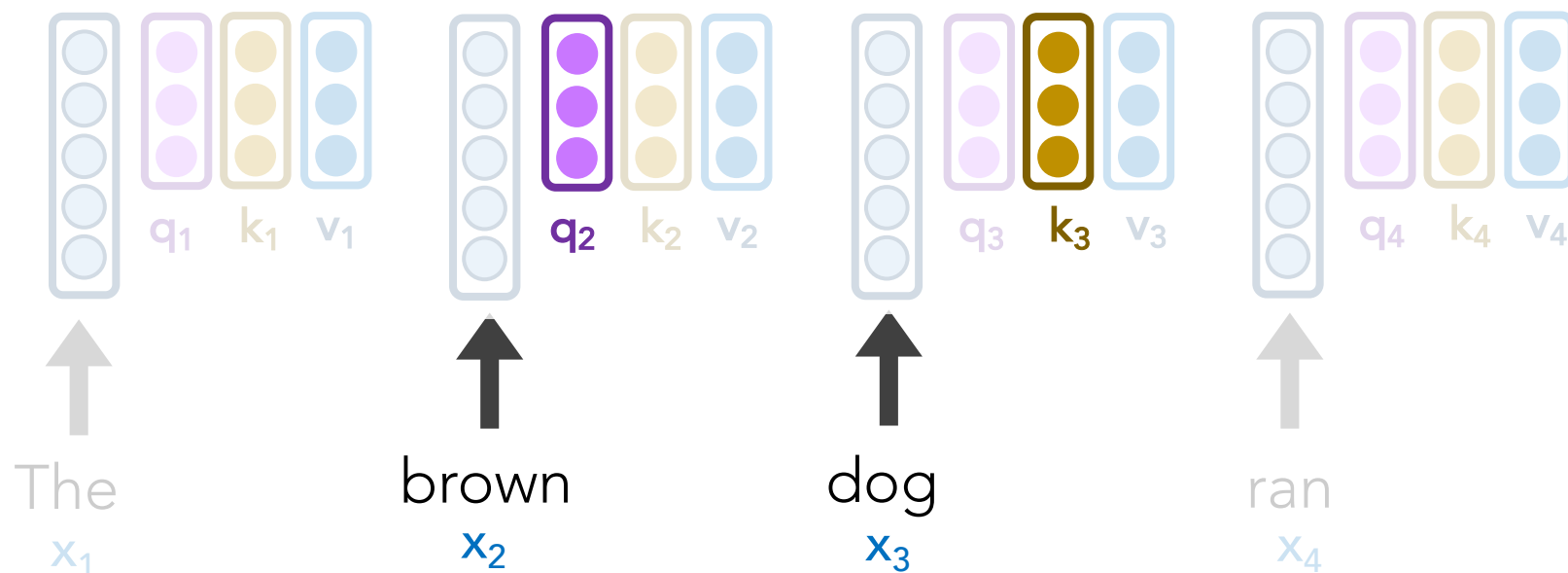
# Self-Attention

**Step 2:** For word  $x_2$ , let's calculate the scores  $s_1, s_2, s_3, s_4$ , which represent how much attention to pay to each respective "word"  $v_i$

$$s_3 = q_2 \cdot k_3 = 22$$

$$s_2 = q_2 \cdot k_2 = 124$$

$$s_1 = q_2 \cdot k_1 = 92$$



# Self-Attention

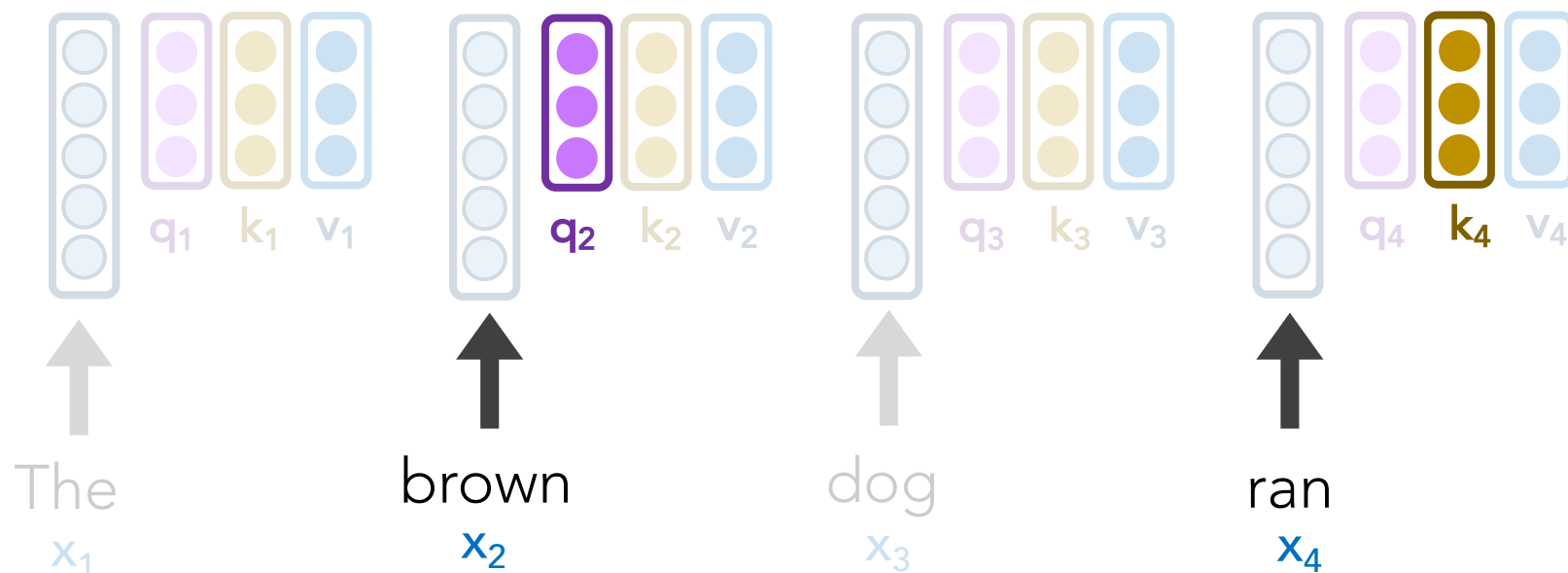
**Step 2:** For word  $x_2$ , let's calculate the scores  $s_1, s_2, s_3, s_4$ , which represent how much attention to pay to each respective "word"  $v_i$

$$s_4 = q_2 \cdot k_4 = 8$$

$$s_3 = q_2 \cdot k_3 = 22$$

$$s_2 = q_2 \cdot k_2 = 124$$

$$s_1 = q_2 \cdot k_1 = 92$$



# Self-Attention

**Step 3:** Our scores  $s_1, s_2, s_3, s_4$  don't sum to 1. Let's divide by  $\sqrt{\text{len}(k_i)}$  and **softmax** it

$$s_4 = q_2 \cdot k_4 = 8$$

$$a_4 = \sigma(s_4/8) = 0$$

$$s_3 = q_2 \cdot k_3 = 22$$

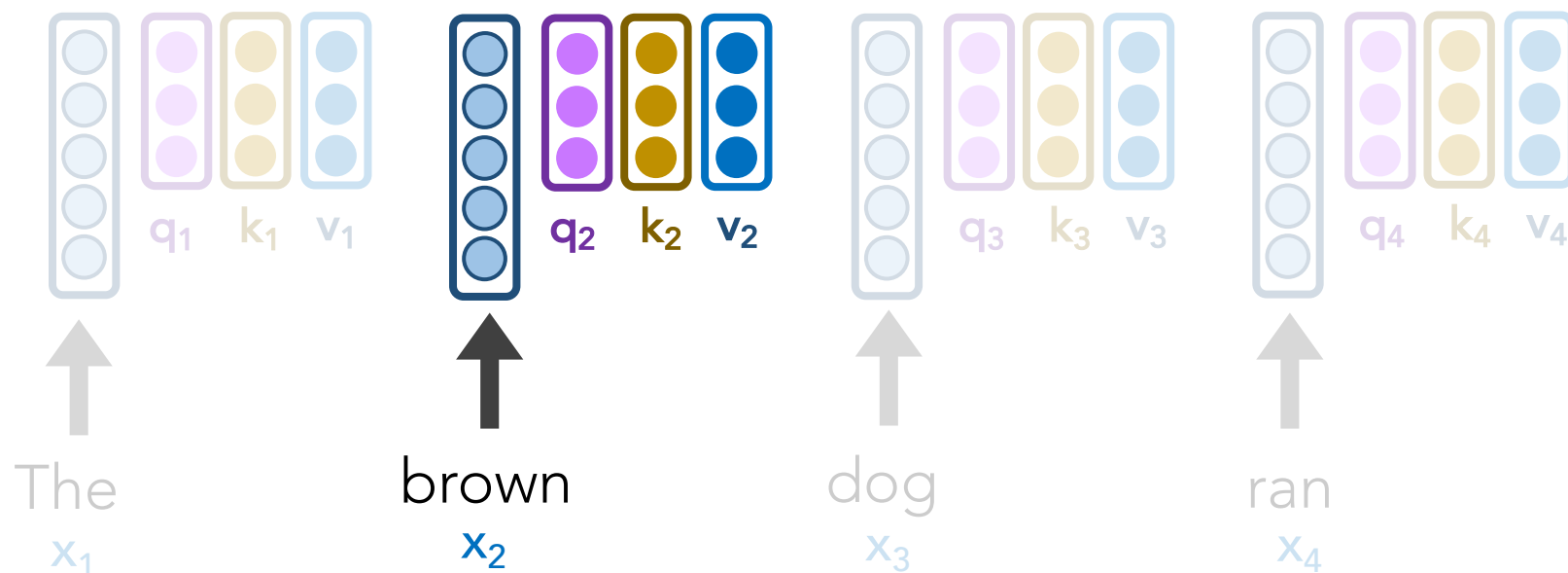
$$a_3 = \sigma(s_3/8) = .01$$

$$s_2 = q_2 \cdot k_2 = 124$$

$$a_2 = \sigma(s_2/8) = .91$$

$$s_1 = q_2 \cdot k_1 = 92$$

$$a_1 = \sigma(s_1/8) = .08$$



# Self-Attention

**Step 3:** Our scores  $s_1, s_2, s_3, s_4$  don't sum to 1. Let's divide by  $\sqrt{\text{len}(k_i)}$  and **softmax** it

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$$a_3 = \sigma(s_3/8) = .01$$

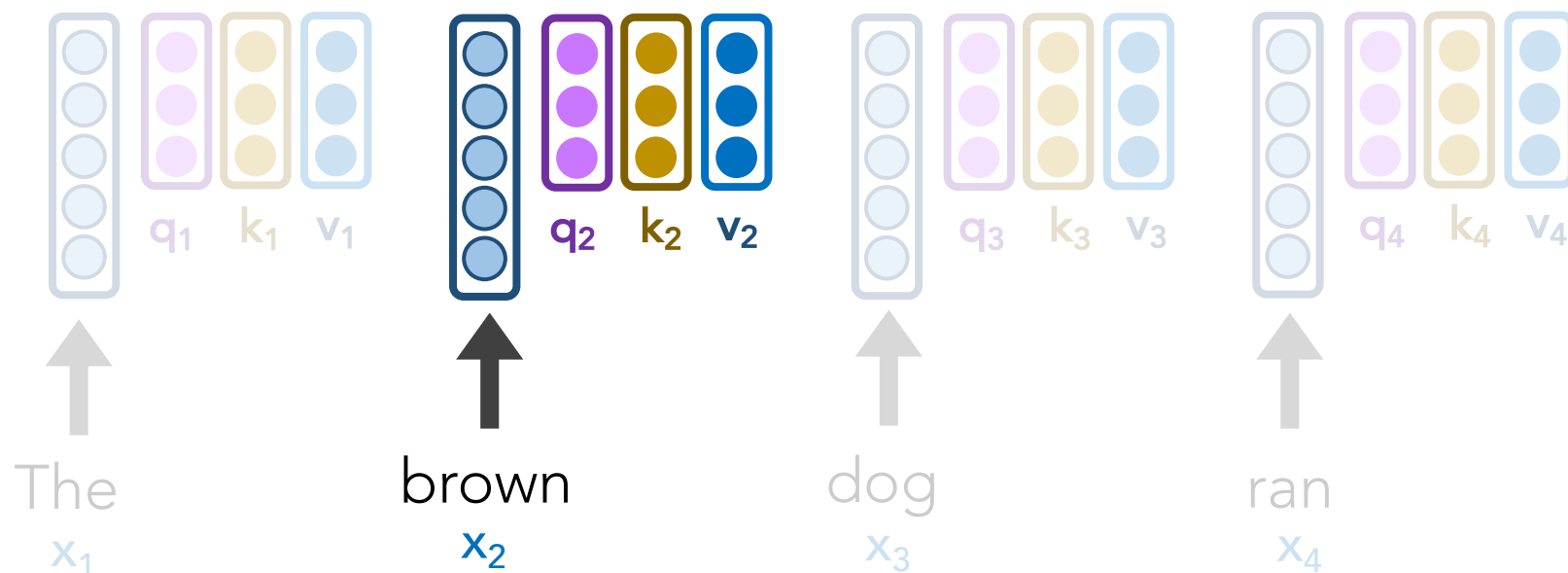
$$s_2 = q_2 \cdot k_2 = 124$$

$$a_2 = \sigma(s_2/8) = .91$$

$$s_1 = q_2 \cdot k_1 = 92$$

$$a_1 = \sigma(s_1/8) = .08$$

Instead of these  $a_i$  values directly weighting our original  $x_i$  word vectors, they directly weight our  $v_i$  vectors.



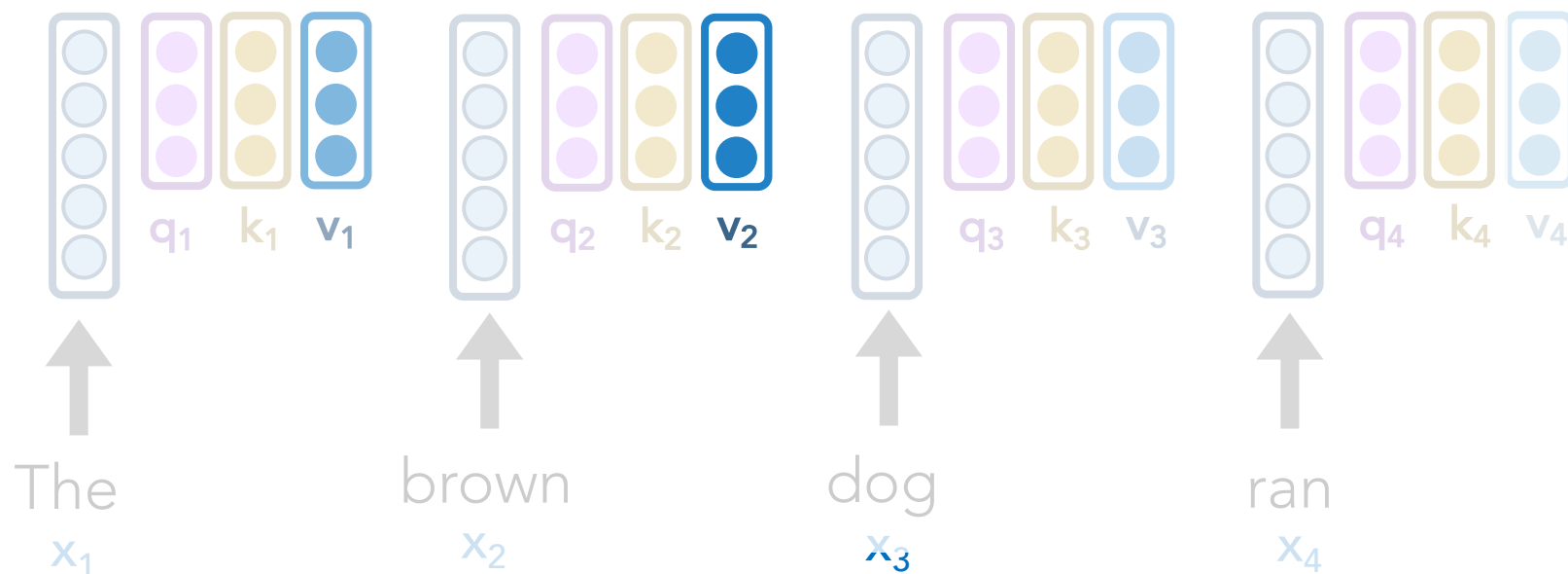


# Self-Attention

**Step 4:** Let's weight our  $\mathbf{v}_i$  vectors and simply sum them up!

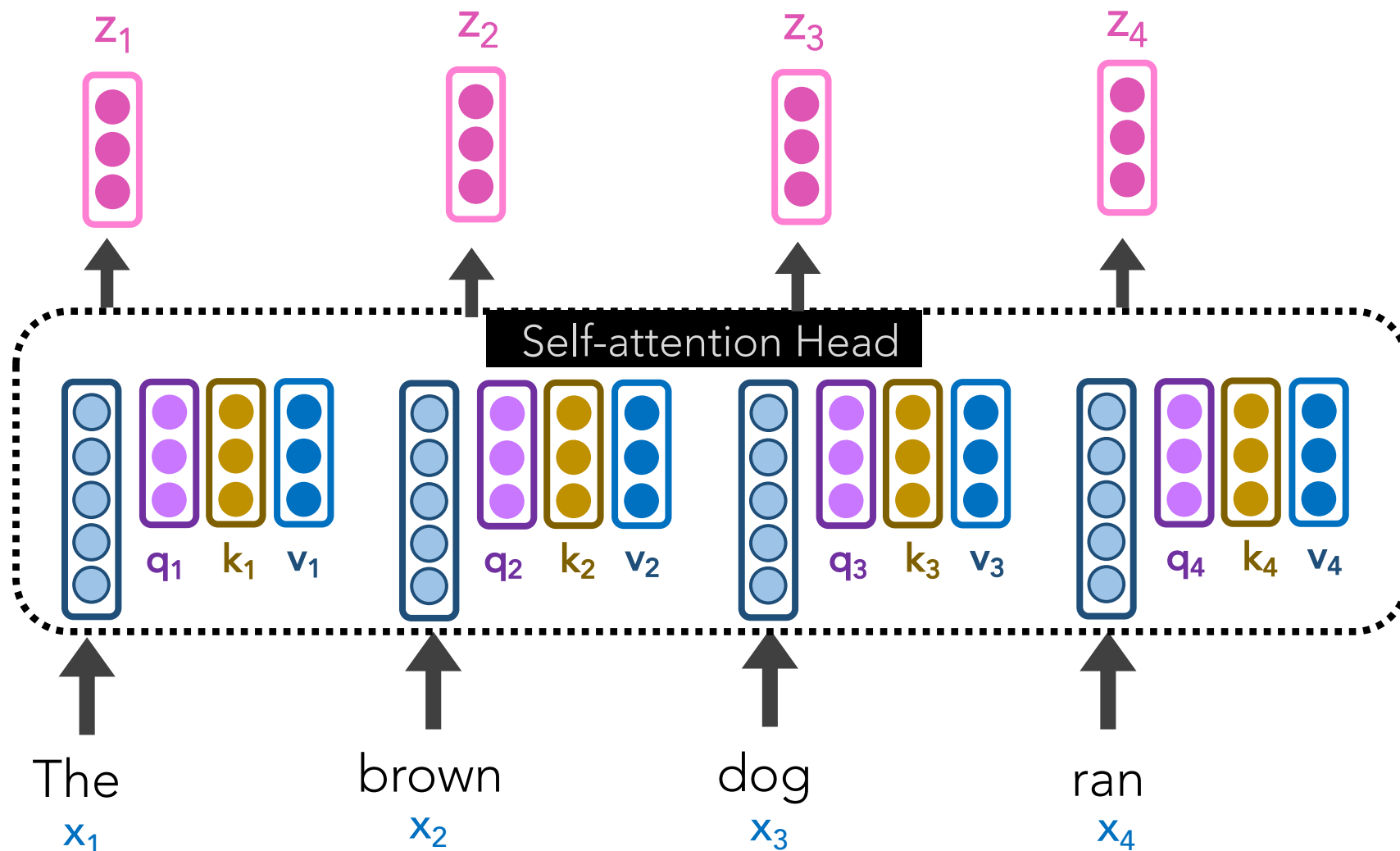


$$\begin{aligned}\mathbf{z}_2 &= \mathbf{a}_1 \cdot \mathbf{v}_1 + \mathbf{a}_2 \cdot \mathbf{v}_2 + \mathbf{a}_3 \cdot \mathbf{v}_3 + \mathbf{a}_4 \cdot \mathbf{v}_4 \\ &= 0.08 \cdot \mathbf{v}_1 + 0.91 \cdot \mathbf{v}_2 + 0.01 \cdot \mathbf{v}_3 + 0 \cdot \mathbf{v}_4\end{aligned}$$



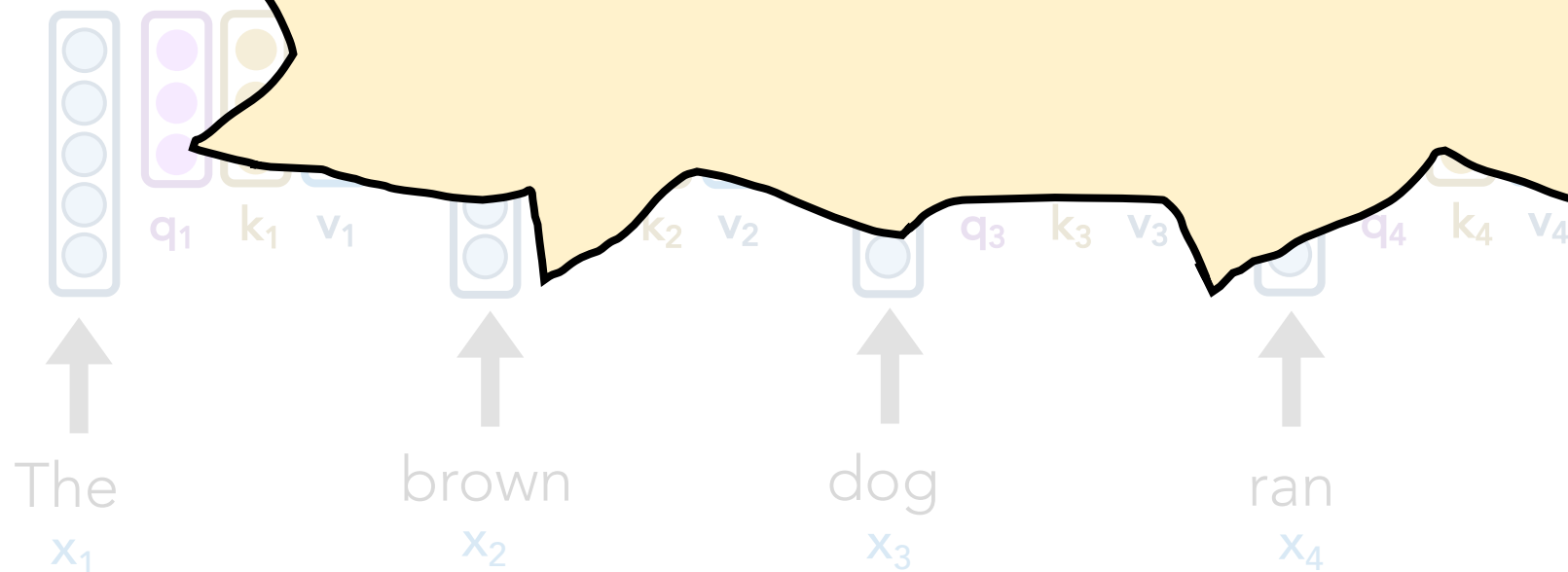
# Self-Attention

Tada! Now we have great, new representations  $z_i$  via a self-attention head



Takeaway:

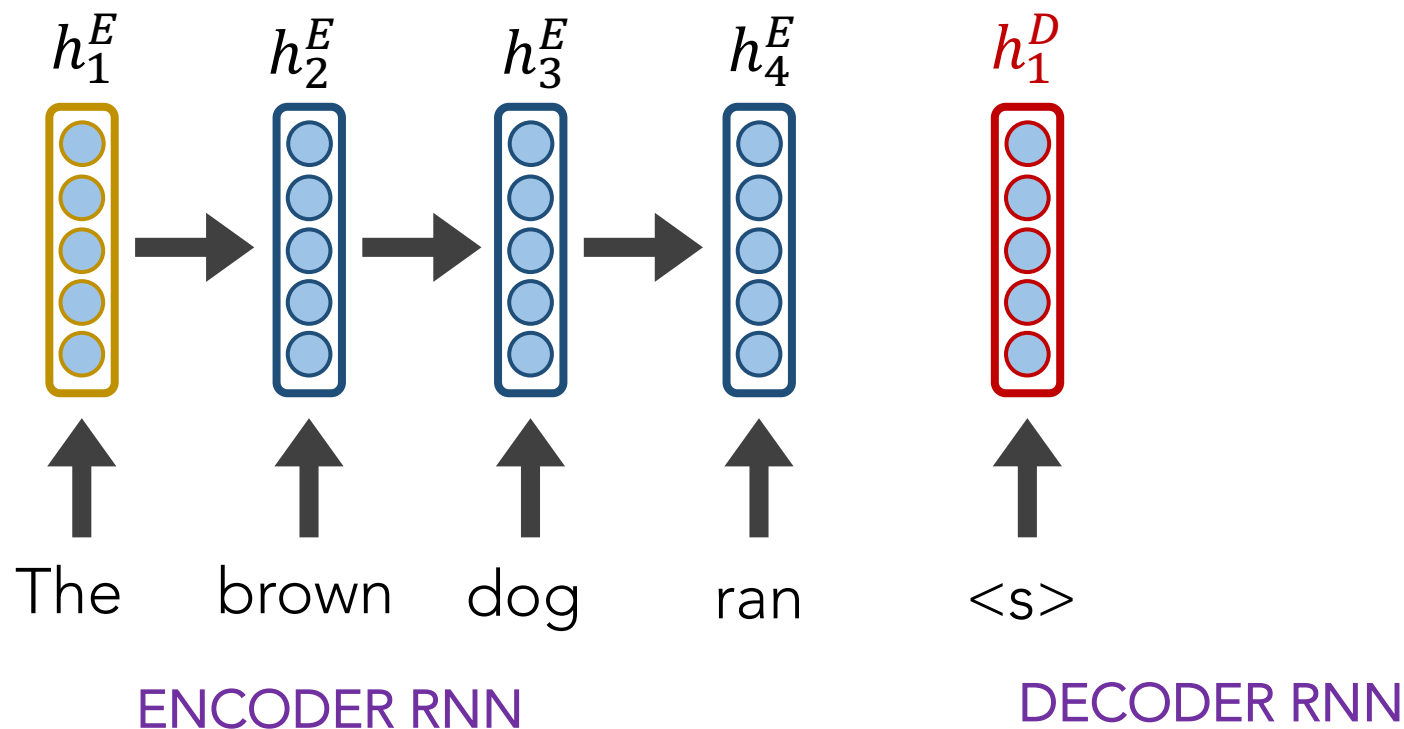
**Self-Attention** is powerful; allows us to create great, context-aware representations



Self-Attention may seem strikingly  
like **Attention** in **seq2seq** models

$$\begin{aligned} \mathbf{s}_4 &= \mathbf{h}_1^D * \mathbf{h}_4^E & \mathbf{a}_4 &= \sigma(\mathbf{s}_4) \\ \mathbf{s}_3 &= \mathbf{h}_1^D * \mathbf{h}_3^E & \mathbf{a}_3 &= \sigma(\mathbf{s}_3) \\ \mathbf{s}_2 &= \mathbf{h}_1^D * \mathbf{h}_2^E & \mathbf{a}_2 &= \sigma(\mathbf{s}_2) \\ \mathbf{s}_1 &= \mathbf{h}_1^D * \mathbf{h}_1^E & \mathbf{a}_1 &= \sigma(\mathbf{s}_1) \end{aligned}$$

# Attention



$$\mathbf{s}_4 = \mathbf{h}_1^D * \mathbf{h}_4^E \quad \mathbf{a}_4 = \sigma(\mathbf{s}_4)$$

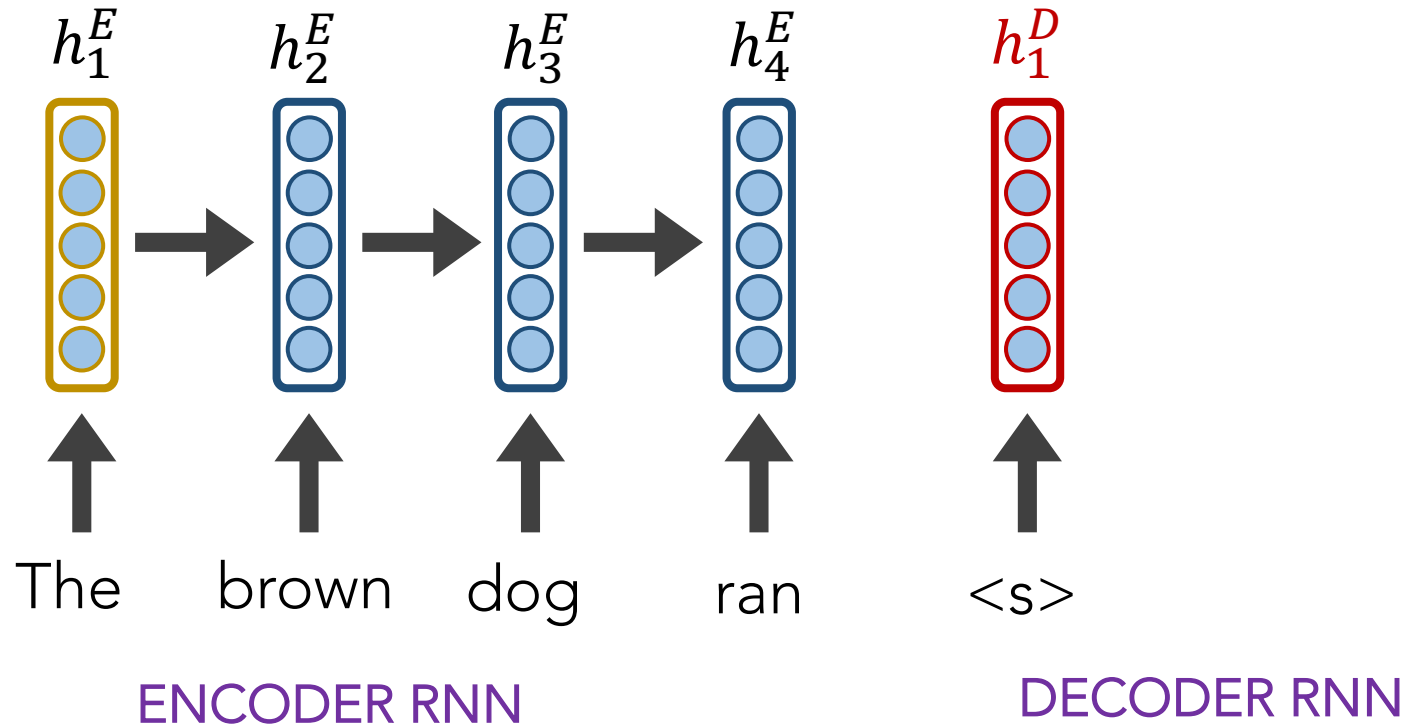
$$\mathbf{s}_3 = \mathbf{h}_1^D * \mathbf{h}_3^E \quad \mathbf{a}_3 = \sigma(\mathbf{s}_3)$$

$$\mathbf{s}_2 = \mathbf{h}_1^D * \mathbf{h}_2^E \quad \mathbf{a}_2 = \sigma(\mathbf{s}_2)$$

$$\mathbf{s}_1 = \mathbf{h}_1^D * \mathbf{h}_1^E \quad \mathbf{a}_1 = \sigma(\mathbf{s}_1)$$

We multiply each encoder's hidden layer by its  $\mathbf{a}_i^1$  attention weights to create a context vector  $\mathbf{c}_1^D$

# Attention



$$\mathbf{s}_4 = \mathbf{h}_1^D * \mathbf{h}_4^E \quad \mathbf{a}_4 = \sigma(\mathbf{s}_4)$$

$$\mathbf{s}_3 = \mathbf{h}_1^D * \mathbf{h}_3^E \quad \mathbf{a}_3 = \sigma(\mathbf{s}_3)$$

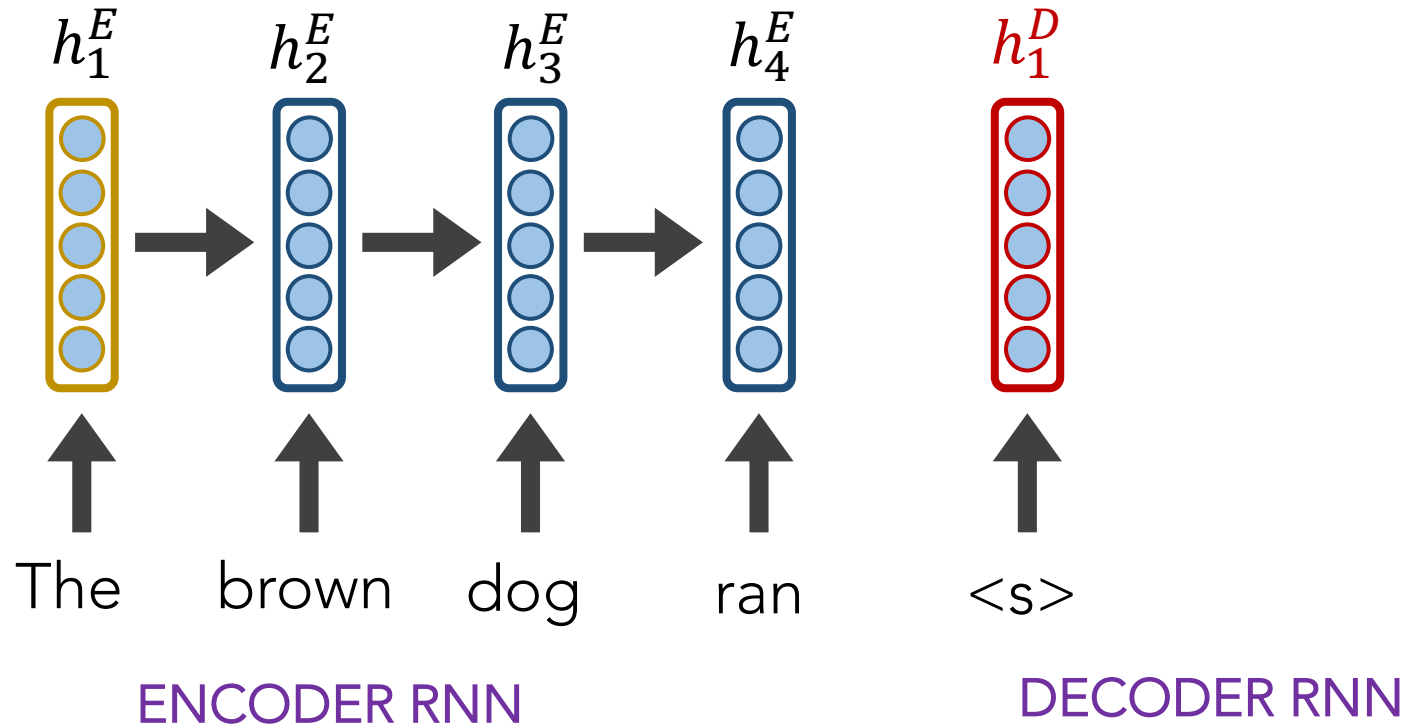
$$\mathbf{s}_2 = \mathbf{h}_1^D * \mathbf{h}_2^E \quad \mathbf{a}_2 = \sigma(\mathbf{s}_2)$$

$$\mathbf{s}_1 = \mathbf{h}_1^D * \mathbf{h}_1^E \quad \mathbf{a}_1 = \sigma(\mathbf{s}_1)$$

We multiply each encoder's hidden layer by its  $a_i^1$  attention weights to create a context vector  $c_1^D$

$$\mathbf{c}_1^D = \mathbf{a}_1 \cdot \mathbf{h}_1^E + \mathbf{a}_2 \cdot \mathbf{h}_2^E + \mathbf{a}_3 \cdot \mathbf{h}_3^E + \mathbf{a}_4 \cdot \mathbf{h}_4^E$$

# Attention



$$s_4 = q_2 \cdot k_4$$

$$a_4 = \sigma(s_4/8)$$

$$s_3 = q_2 \cdot k_3$$

$$a_3 = \sigma(s_3/8)$$

$$s_2 = q_2 \cdot k_2$$

$$a_2 = \sigma(s_2/8)$$

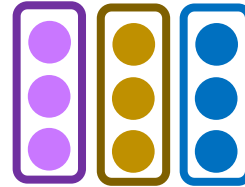
$$s_1 = q_2 \cdot k_1$$

$$a_1 = \sigma(s_1/8)$$

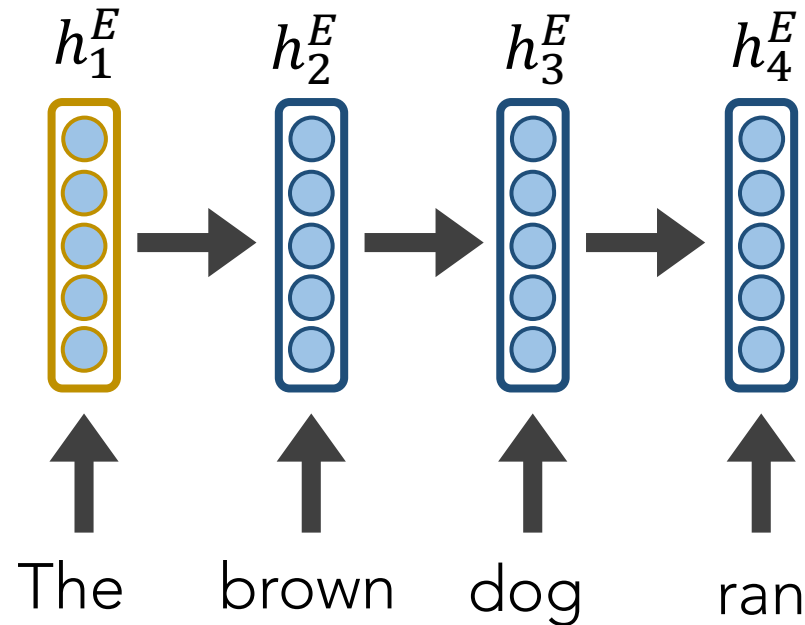
We multiply each word's value vector by its  $a_i^1$  attention weights to create a better vector  $z_1$

$$z_1 = a_1 \cdot v_1^E + a_2 \cdot v_2^E + a_3 \cdot v_3^E + a_4 \cdot v_4^E$$

# Self-Attention



$q_1$   $k_1$   $v_1$



ENCODER RNN

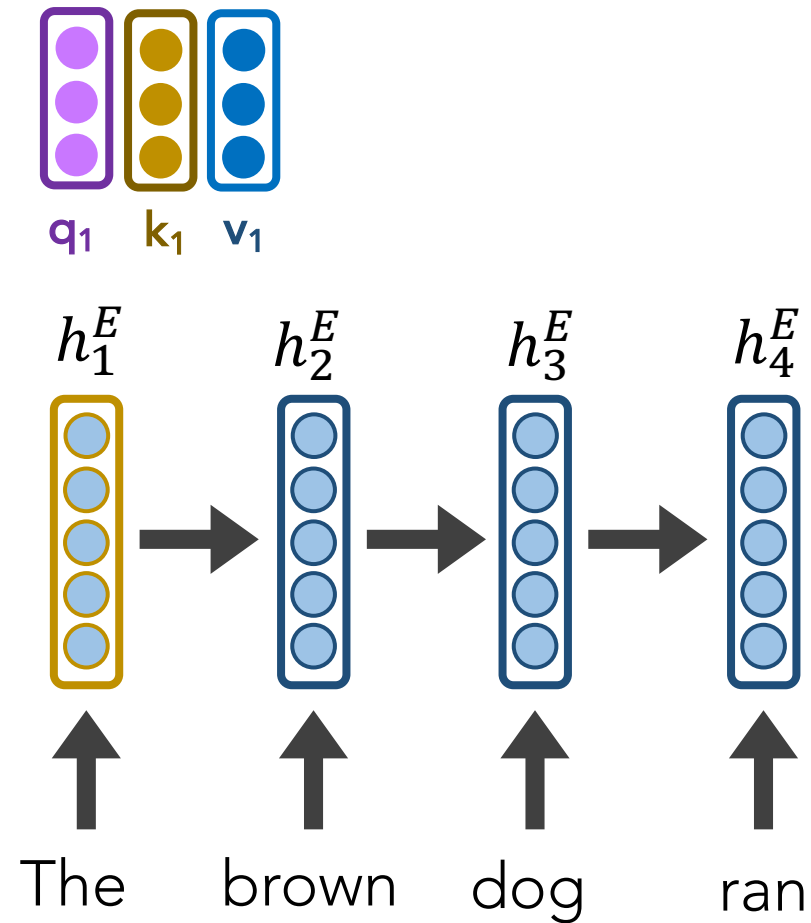


# Self-Attention

Self-Attention	Attention	Description
$q_i$	$h_i^D$	the probe
$k_i$	$h_i^E$	item being compared
$v_i$	$h_i^E$	item being weighted

vector by its  $a_i^1$  attention weights to create a better vector  $z_1$

$$z_1 = a_1 \cdot v_1^E + a_2 \cdot v_2^E + a_3 \cdot v_3^E + a_4 \cdot v_4^E$$



ENCODER RNN

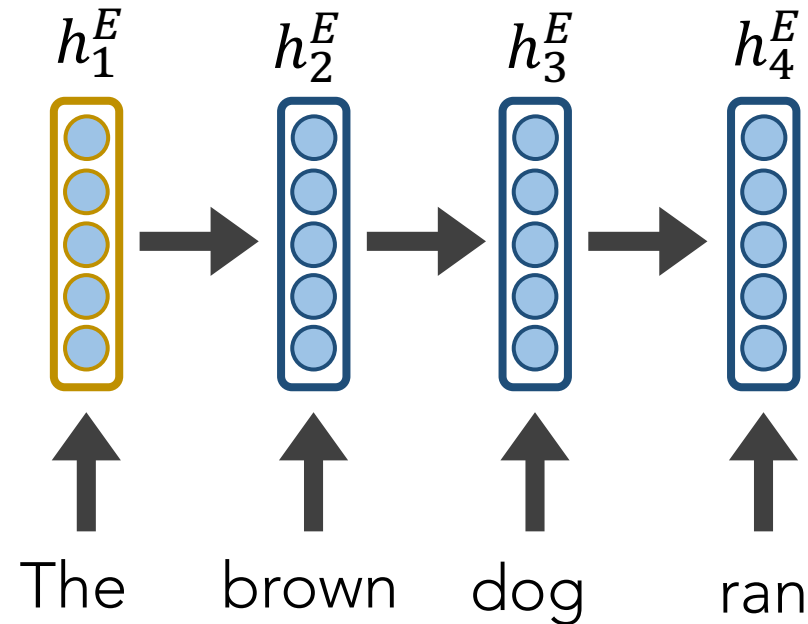
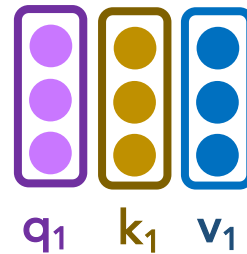
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$q_i$	$h_i^D$	the probe
$k_i$	$h_i^E$	item being compared
$v_i$	$h_i^E$	item being weighted

↑ All of these are like  
surrogates/proxies/abstractions.

This provides **flexibility and fewer constraints**.

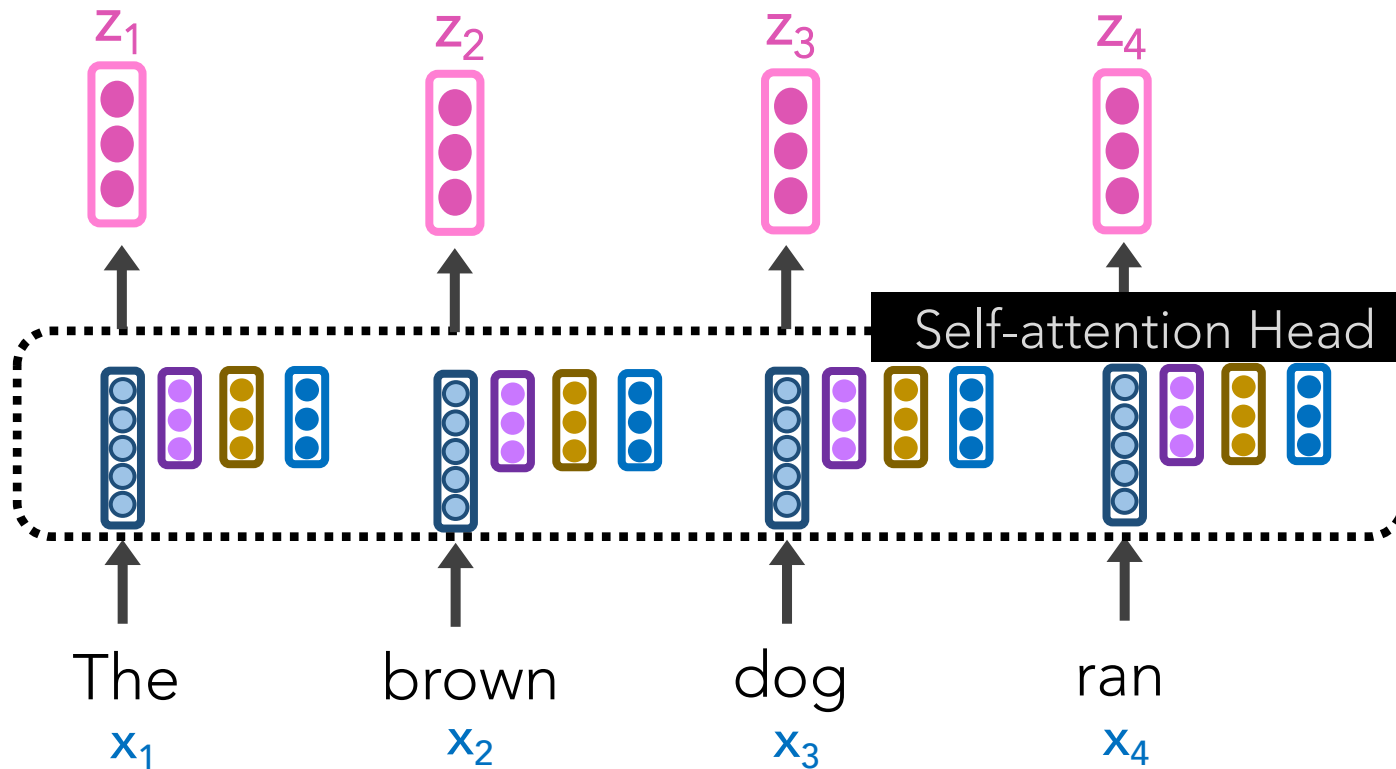
More room for rich **abstractions**.



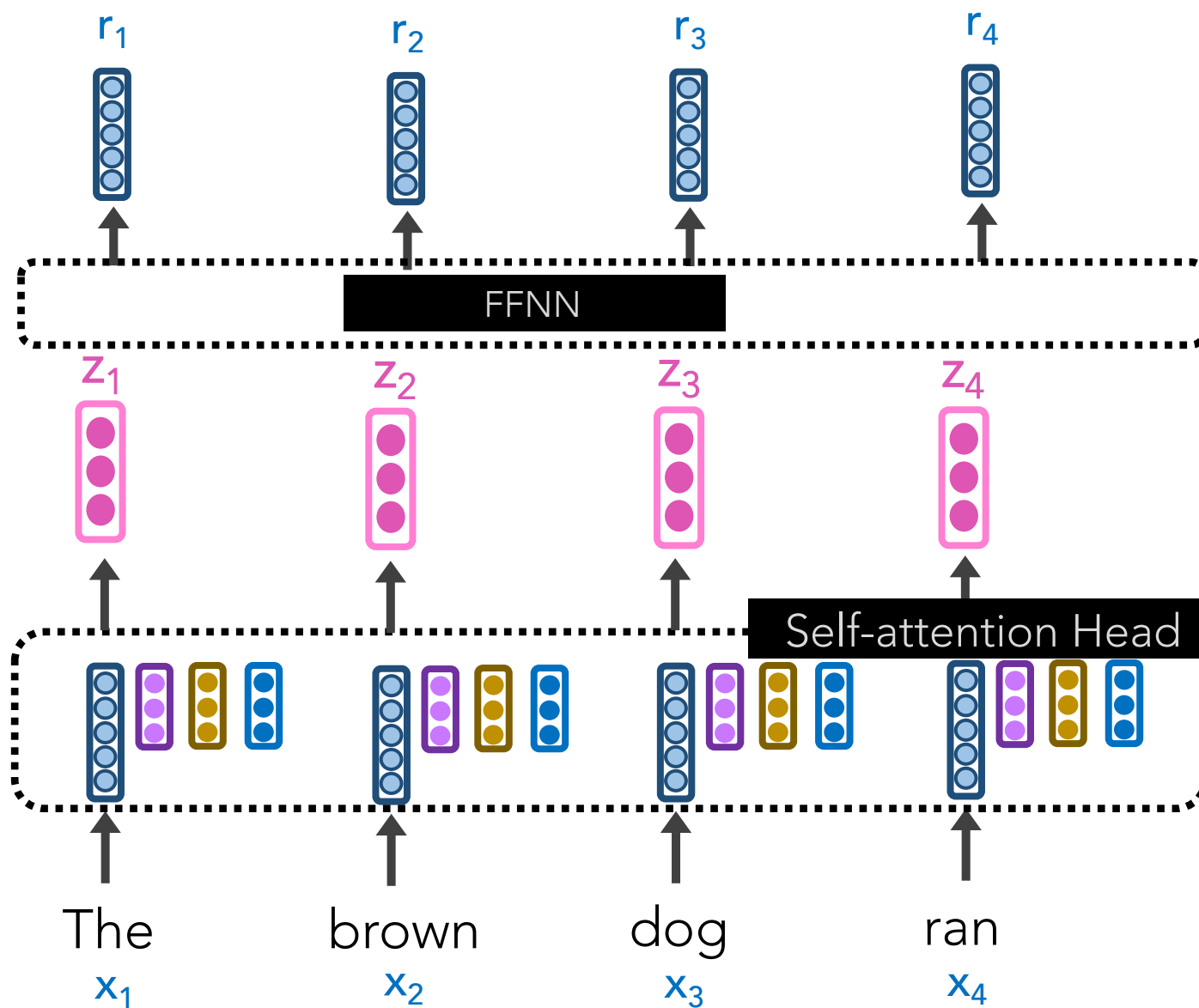
ENCODER RNN

# Self-Attention

Let's further pass each  $z_i$  through a FFNN

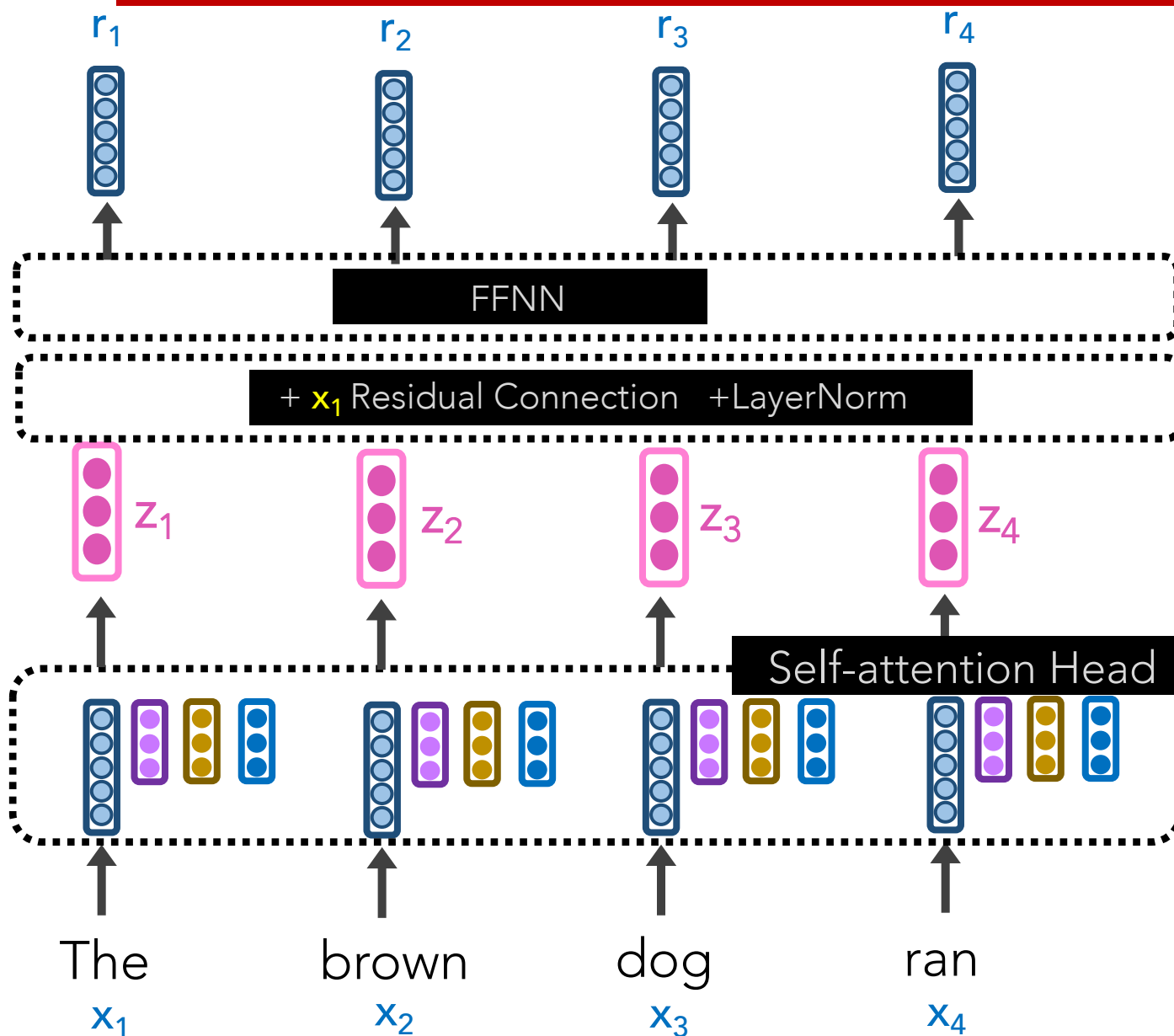


# Self-Attention + FFNN



Let's further pass each  $z_i$  through a FFNN

# Self-Attention + FFNN

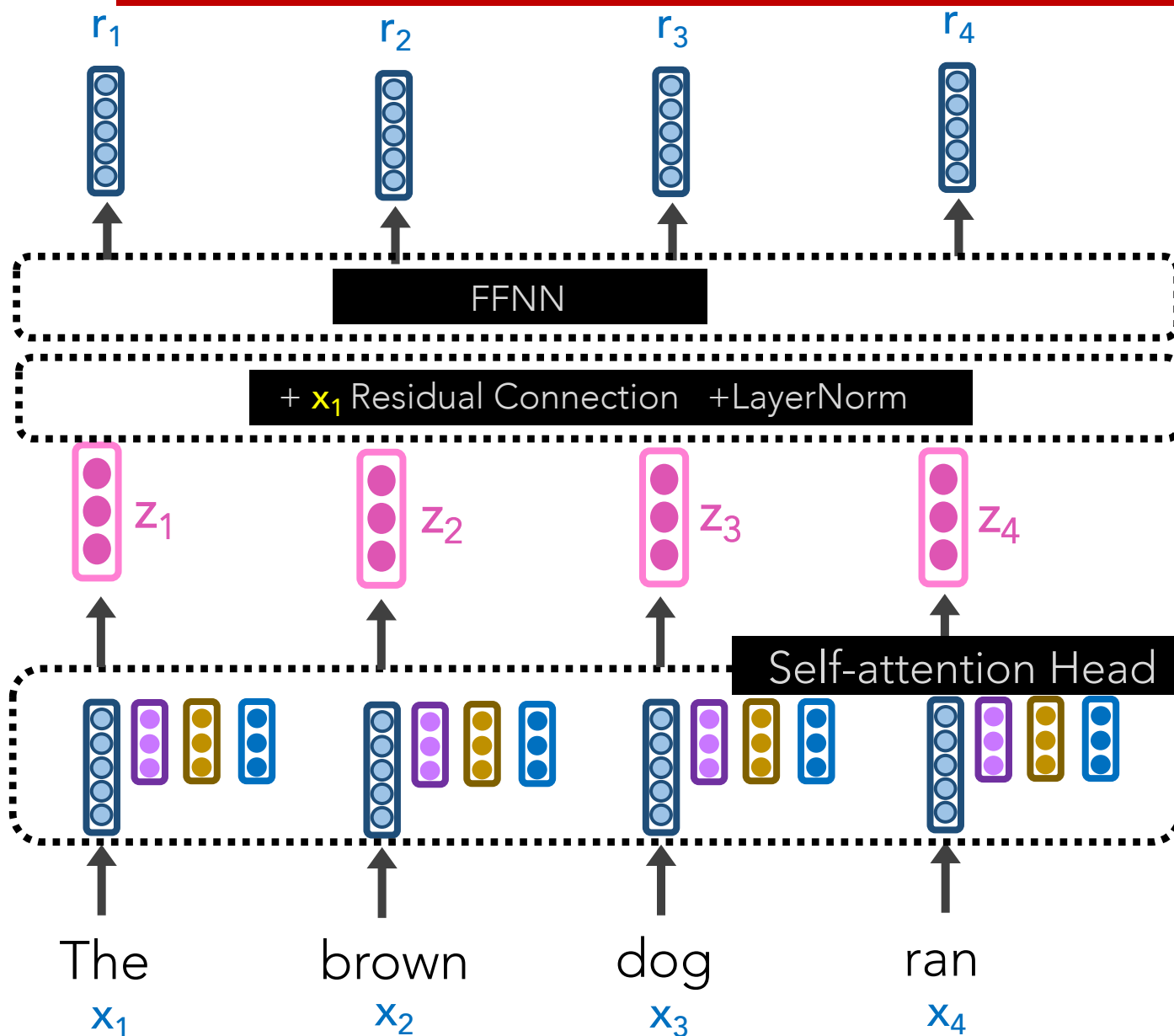


Let's further pass each  $z_i$  through a FFNN

We concat w/ a **residual connection** to help ensure relevant info is getting forward passed.

We perform **LayerNorm** to stabilize the network and allow for proper gradient flow.

# Self-Attention + FFNN



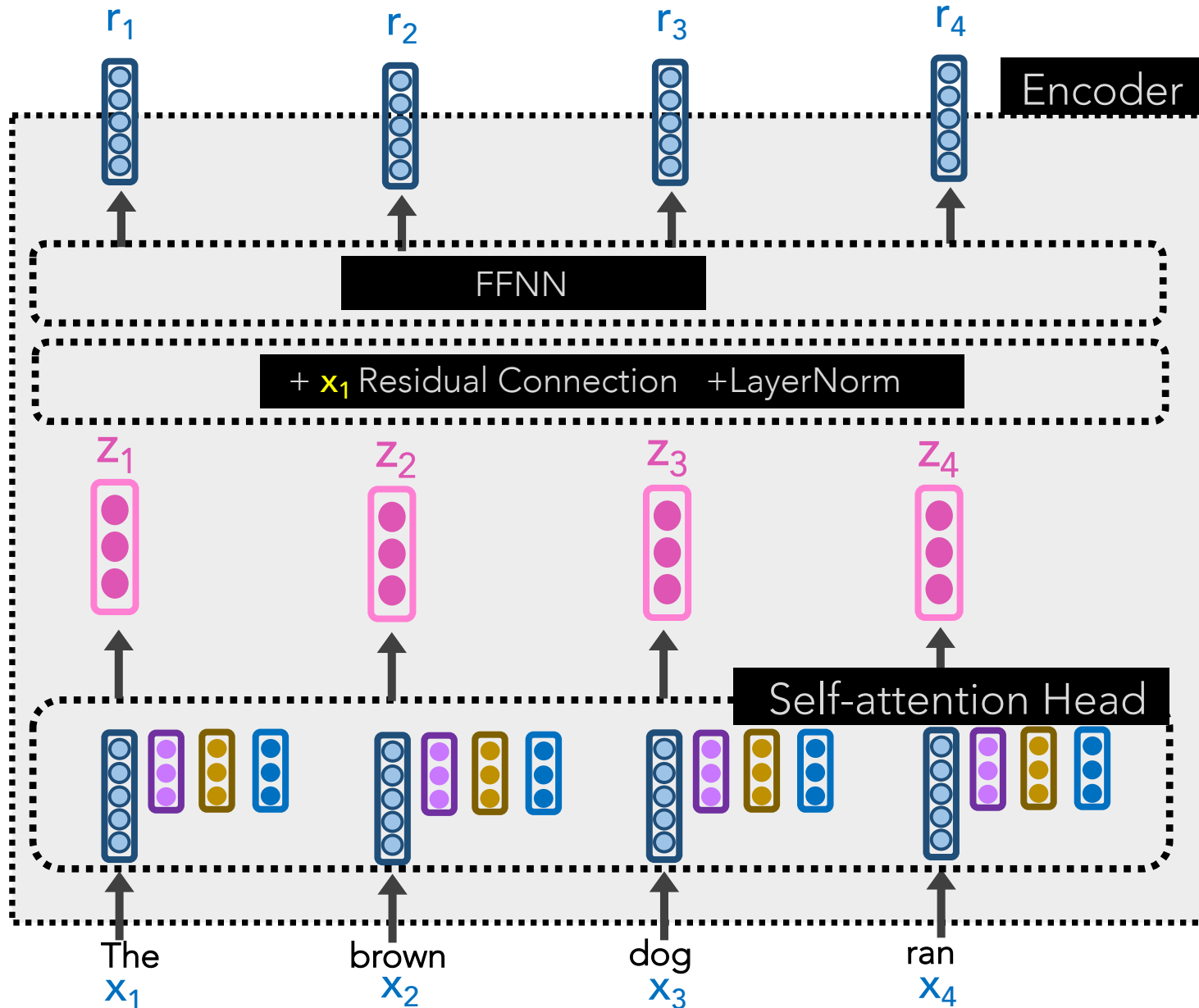
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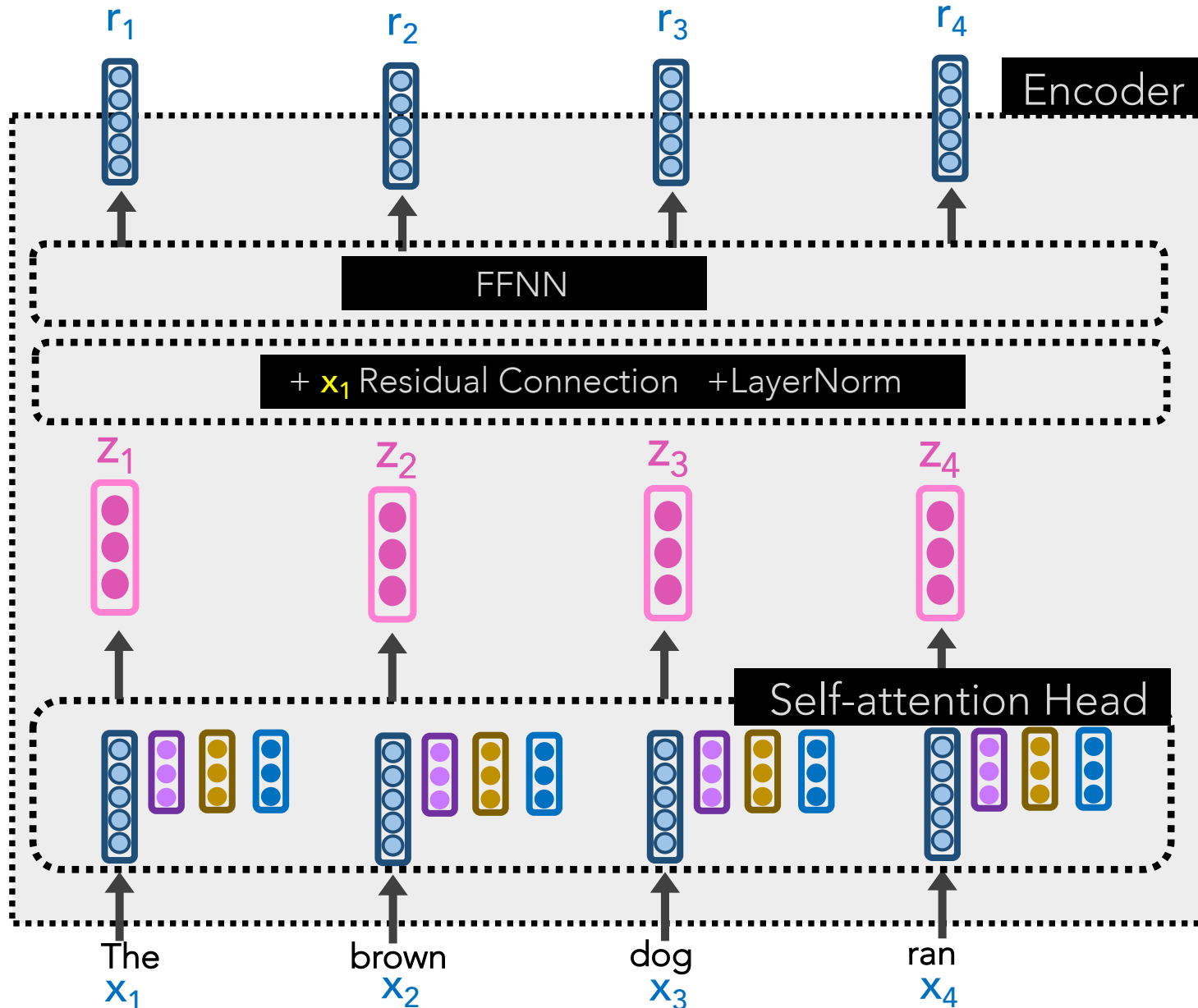
Each  $z_i$  can be computed in **parallel**, unlike LSTMs!

# Transformer Encoder



Yay! Our  $r_i$  vectors are our new representations, and this entire process is called a **Transformer Encoder**

# Transformer Encoder

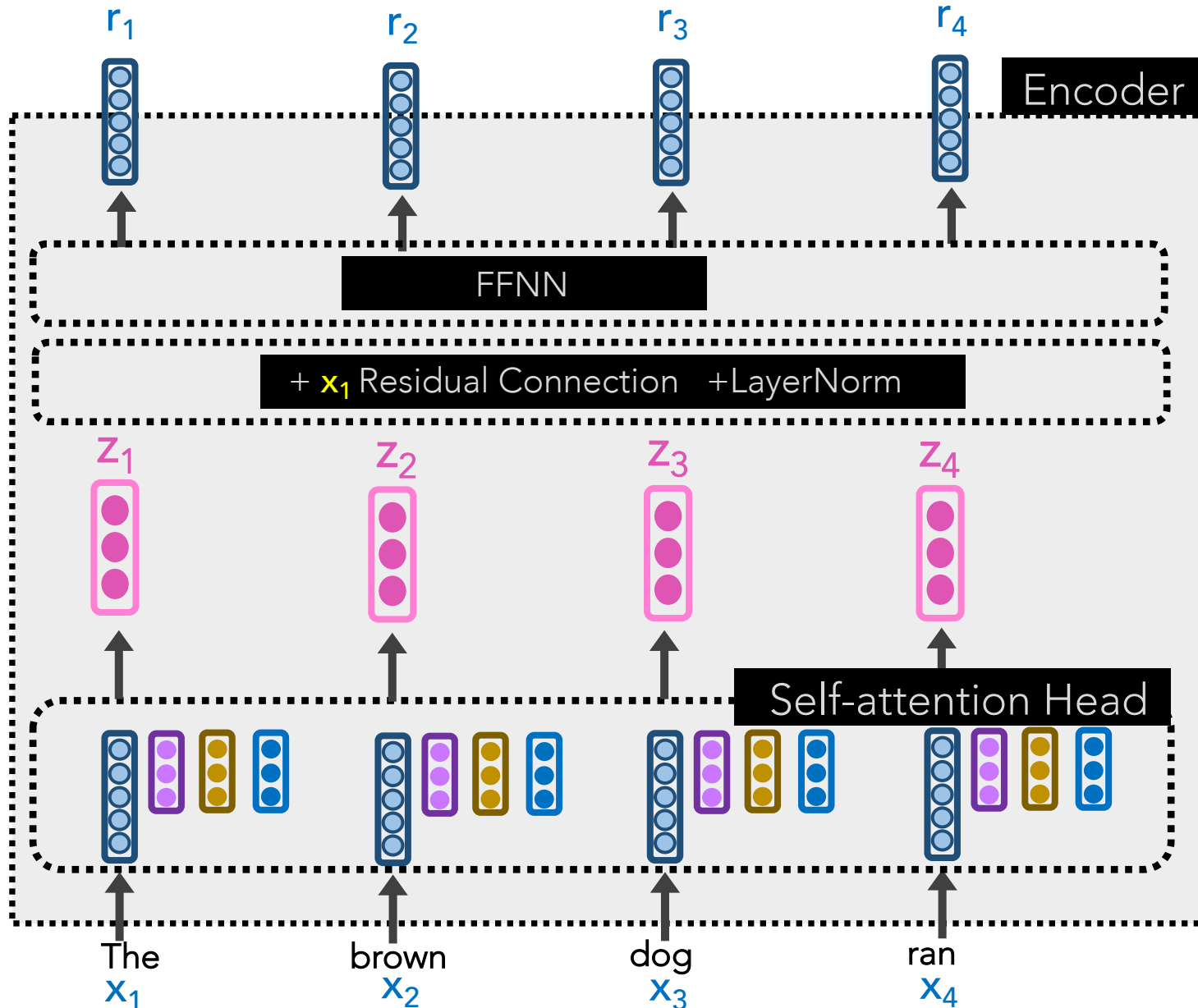


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**Problem:** there is no concept of positionality. Words are weighted as if a "bag of words"



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**Problem:** there is no concept of positionality. Words are weighted as if a "bag of words"

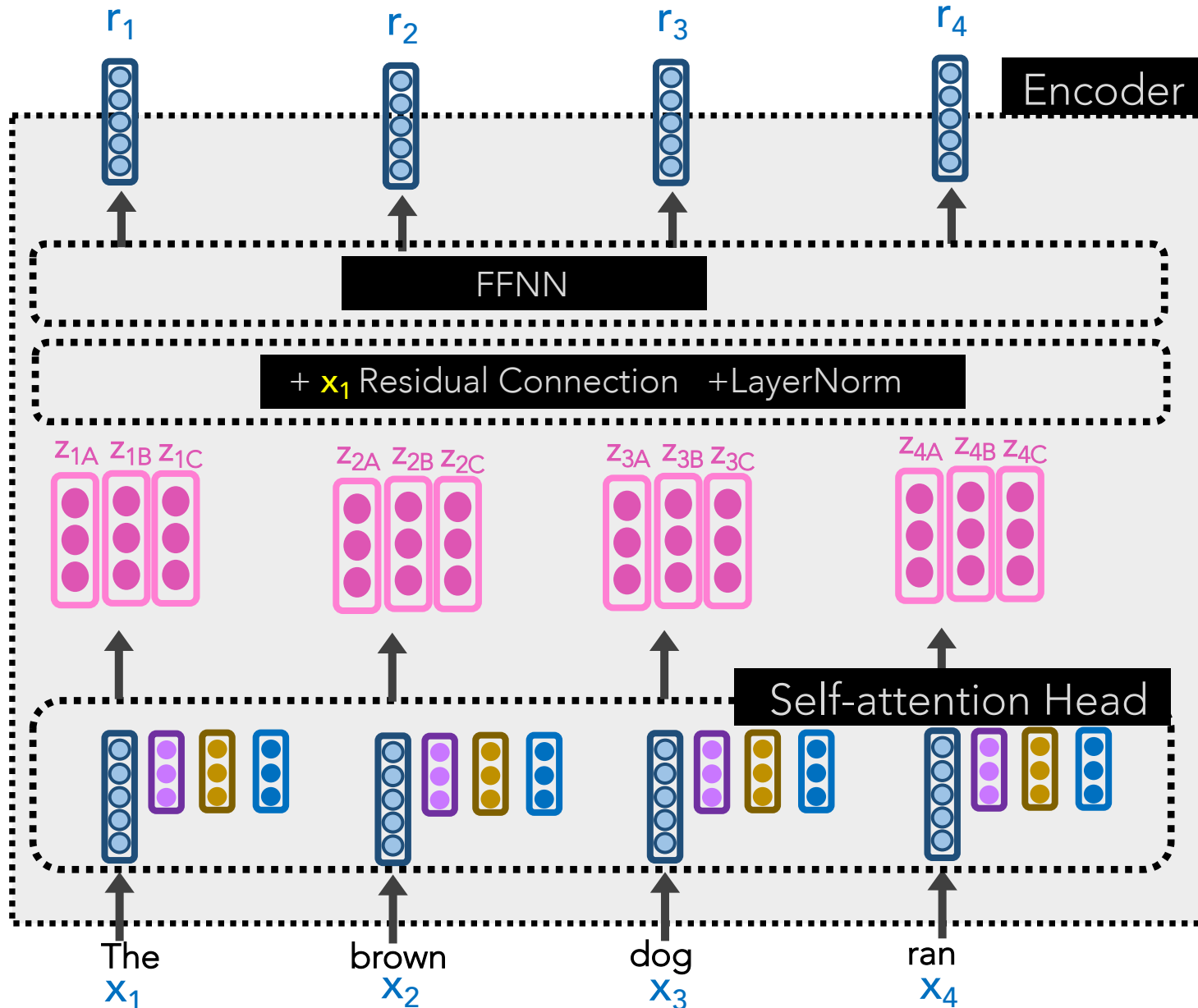
**Solution:** append each input word  $x_i$  with a **positional encoding**:  $\sin(i) \cos(i)$

A **Self-Attention Head** has just one set of **query/key/value** weight matrices  $w_q, w_k, w_v$

Words can relate in many ways, so it's restrictive to rely on just one Self-Attention Head in the system.

Let's create Multi-headed Self-Attention

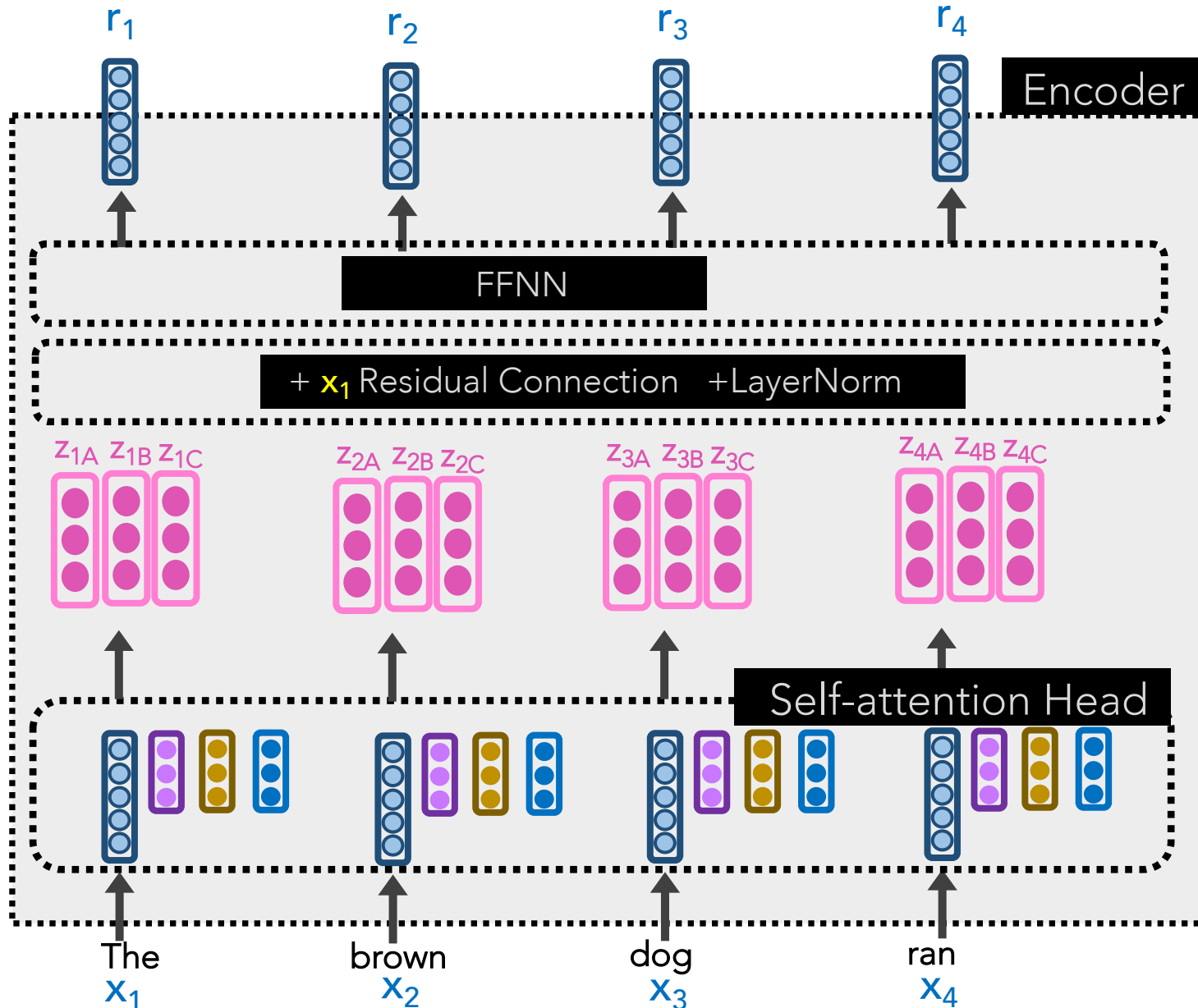
# Transformer Encoder



Each **Self-Attention Head** produces a  $z_i$  vector.

We can, in parallel, use **multiple heads** and concat the  $z_i$ 's.

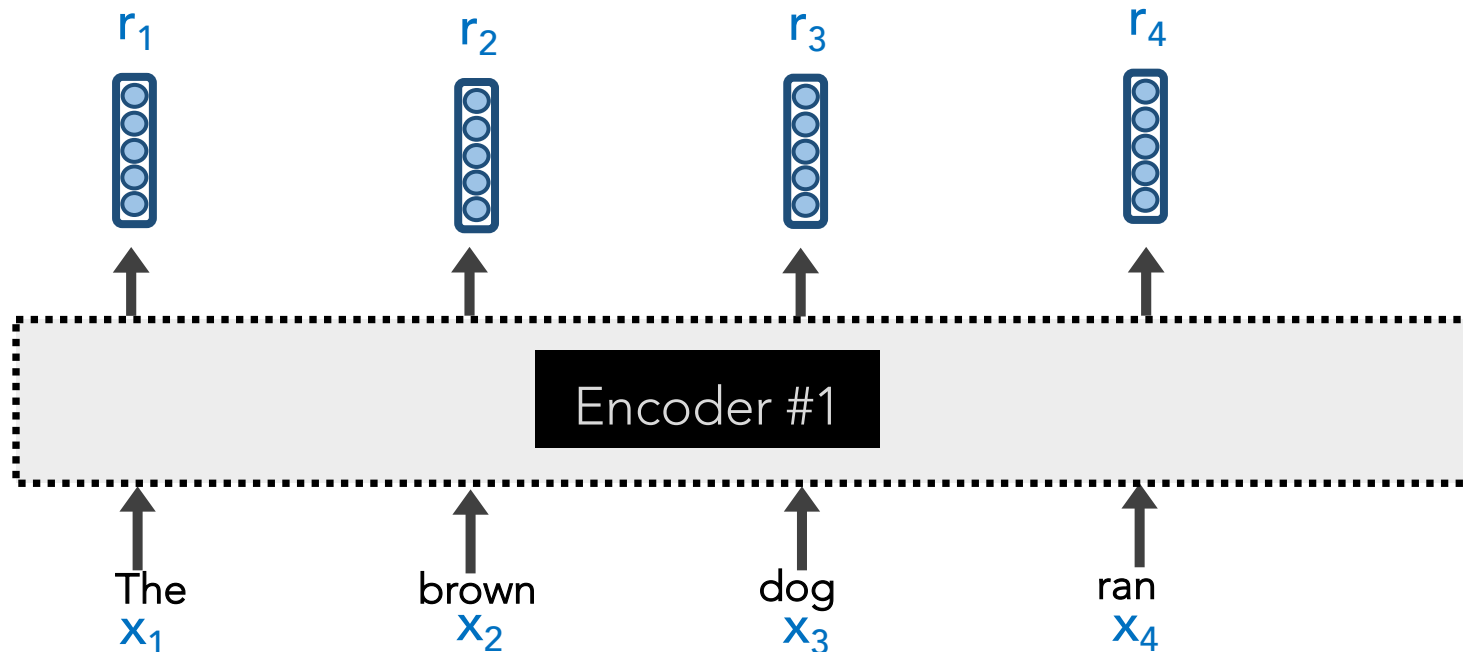
# Transformer Encoder



To recap: all of this looks fancy, but ultimately it's just producing a very good **contextualized embedding**  $r_i$  of each word  $x_i$

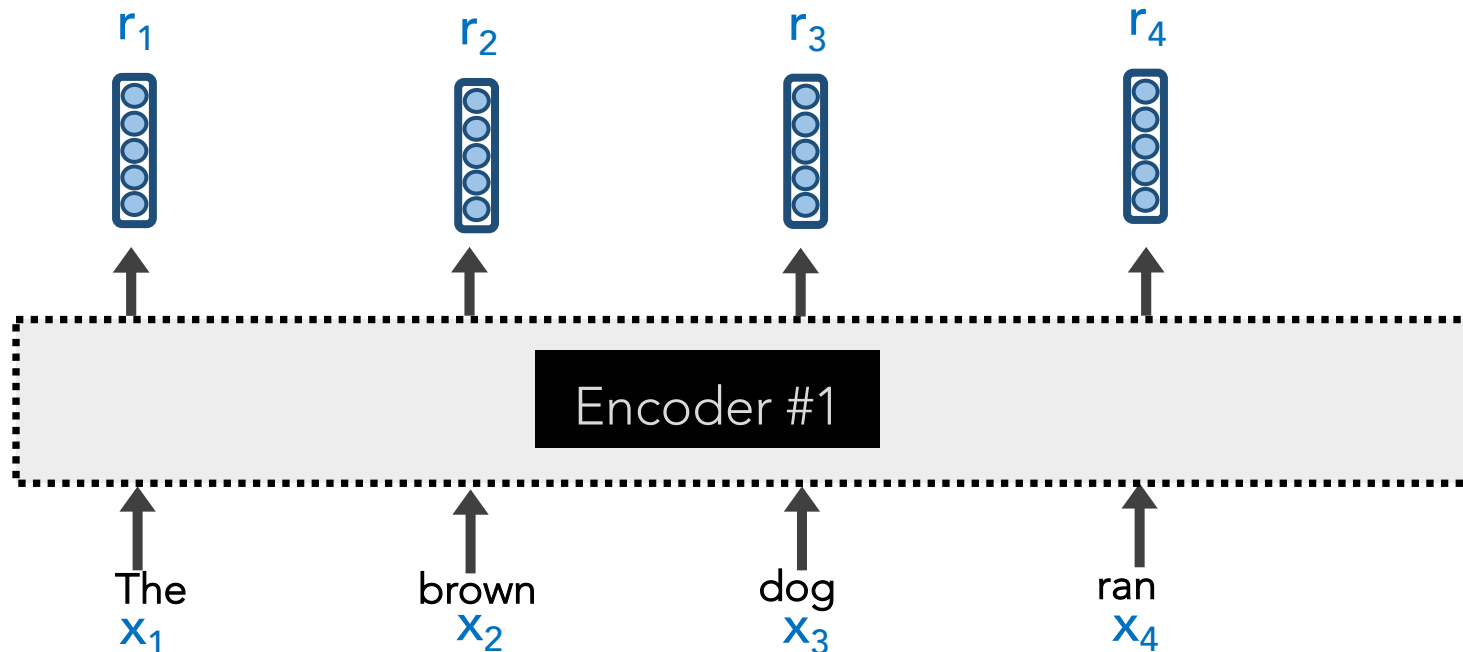
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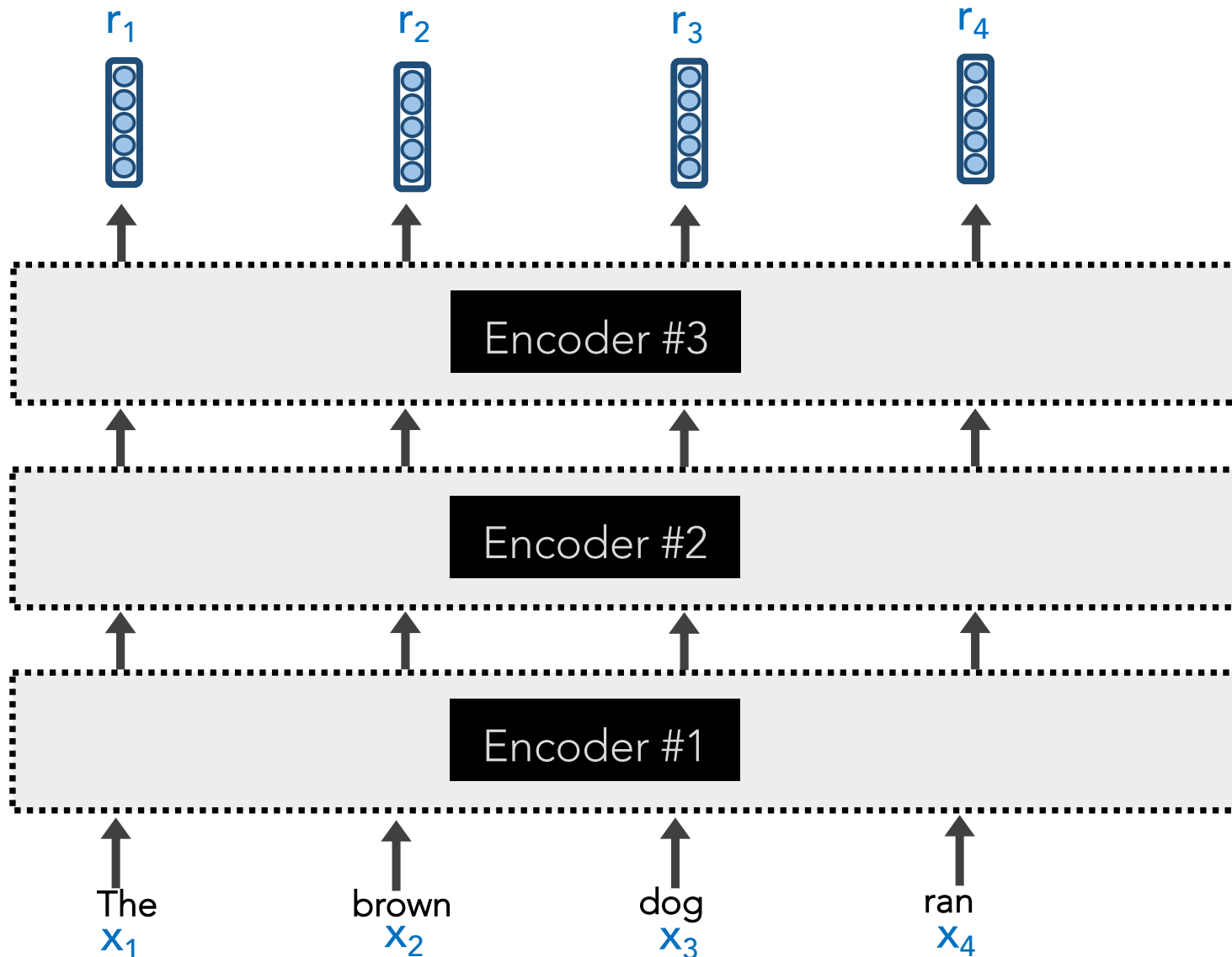
# Transformer Encoder

To recap: all of this looks fancy, but ultimately it's just producing a very good **contextualized embedding**  $r_i$  of each word  $x_i$



Why stop with just 1  
**Transformer Encoder**?  
We could stack several!

# Transformer Encoder



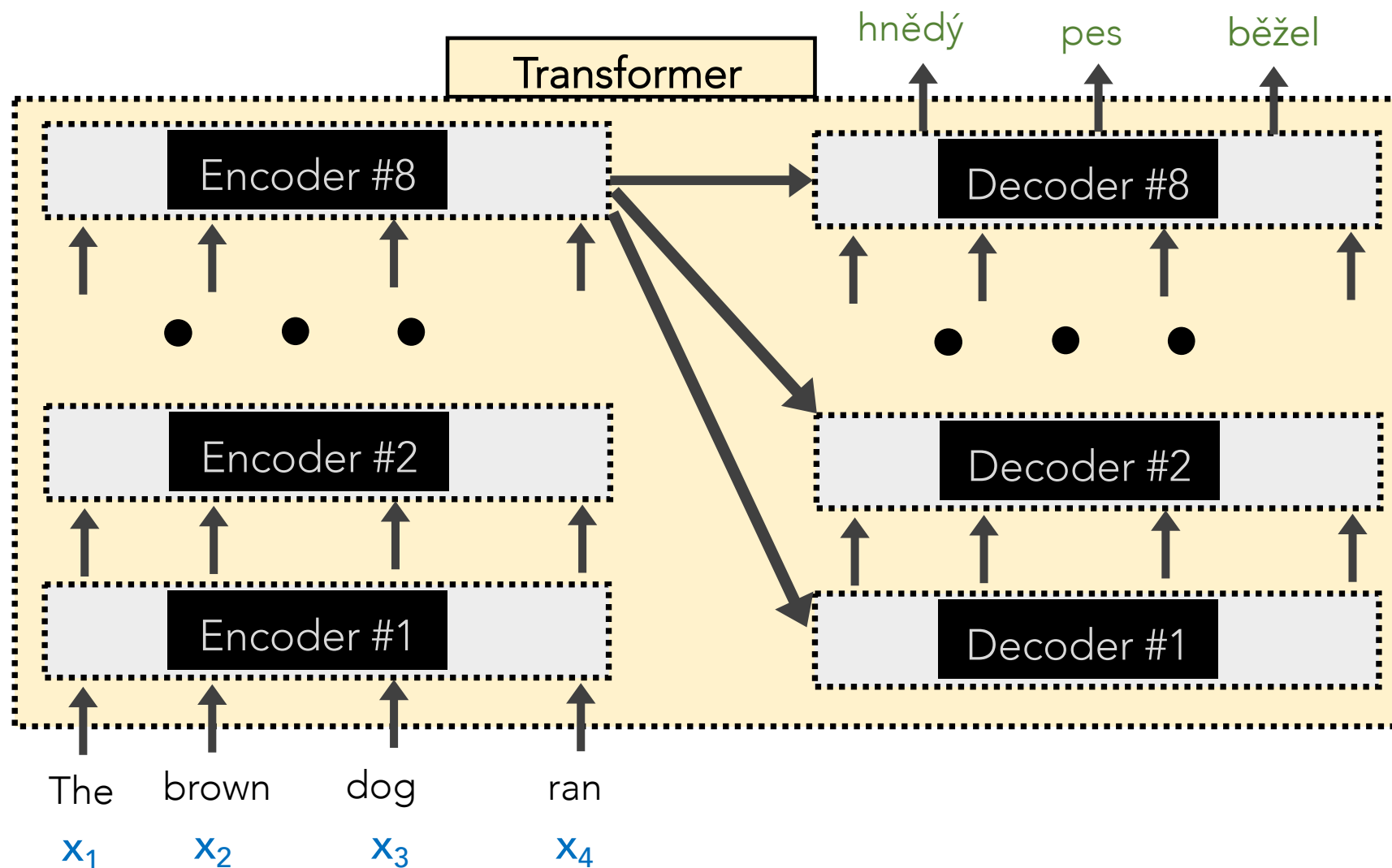
To recap: all of this looks fancy, but ultimately it's just producing a very good **contextualized embedding**  $r_i$  of each word  $x_i$

Why stop with just 1 **Transformer Encoder**?  
We could stack several!

The original Transformer model was intended for Machine Translation, so it had **Decoders**, too



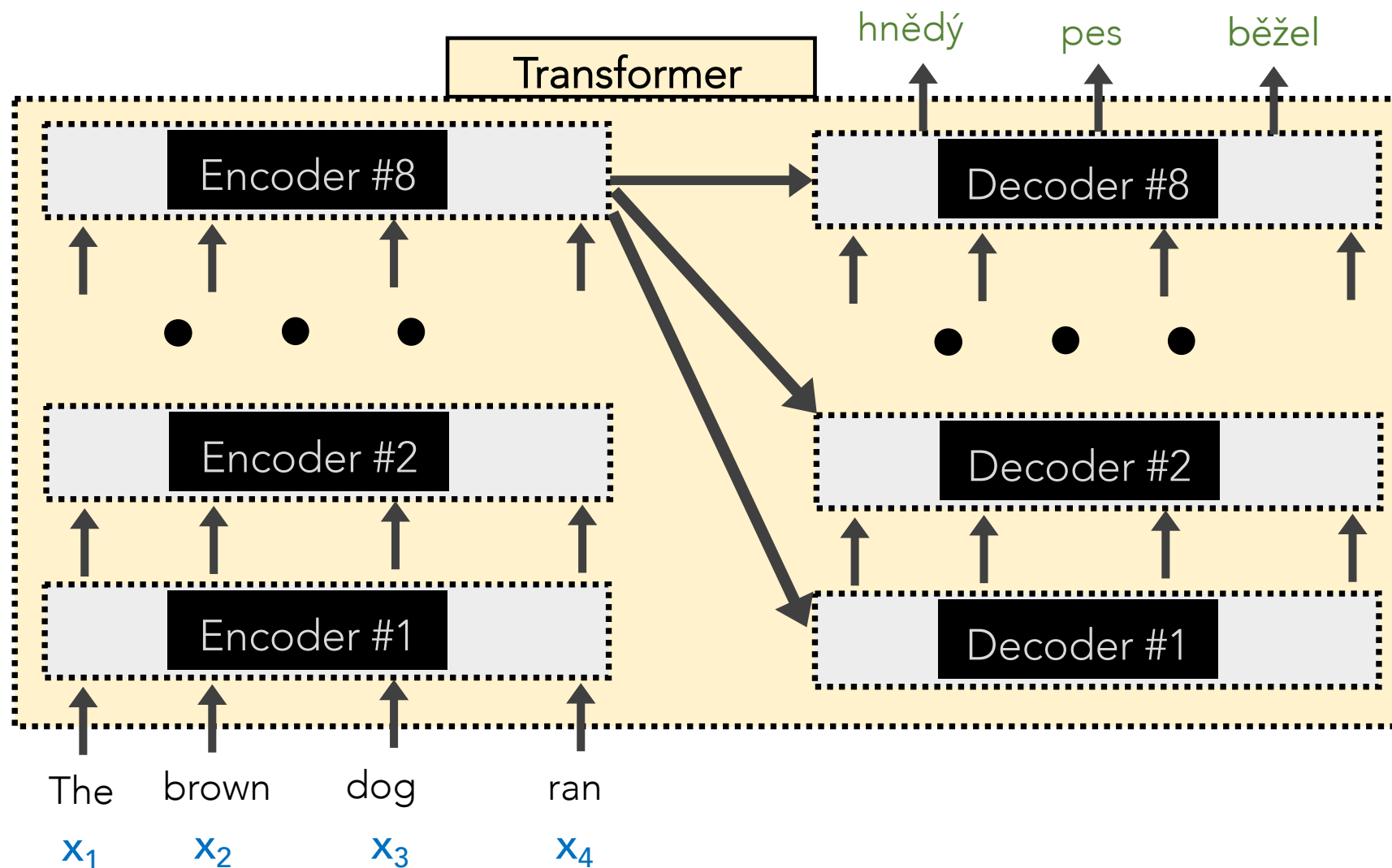
# Transformer Encoders and Decoders



Transformer Encoders produce **contextualized embeddings** of each word

Transformer Decoders generate new sequences of text

# Transformer Encoders and Decoders

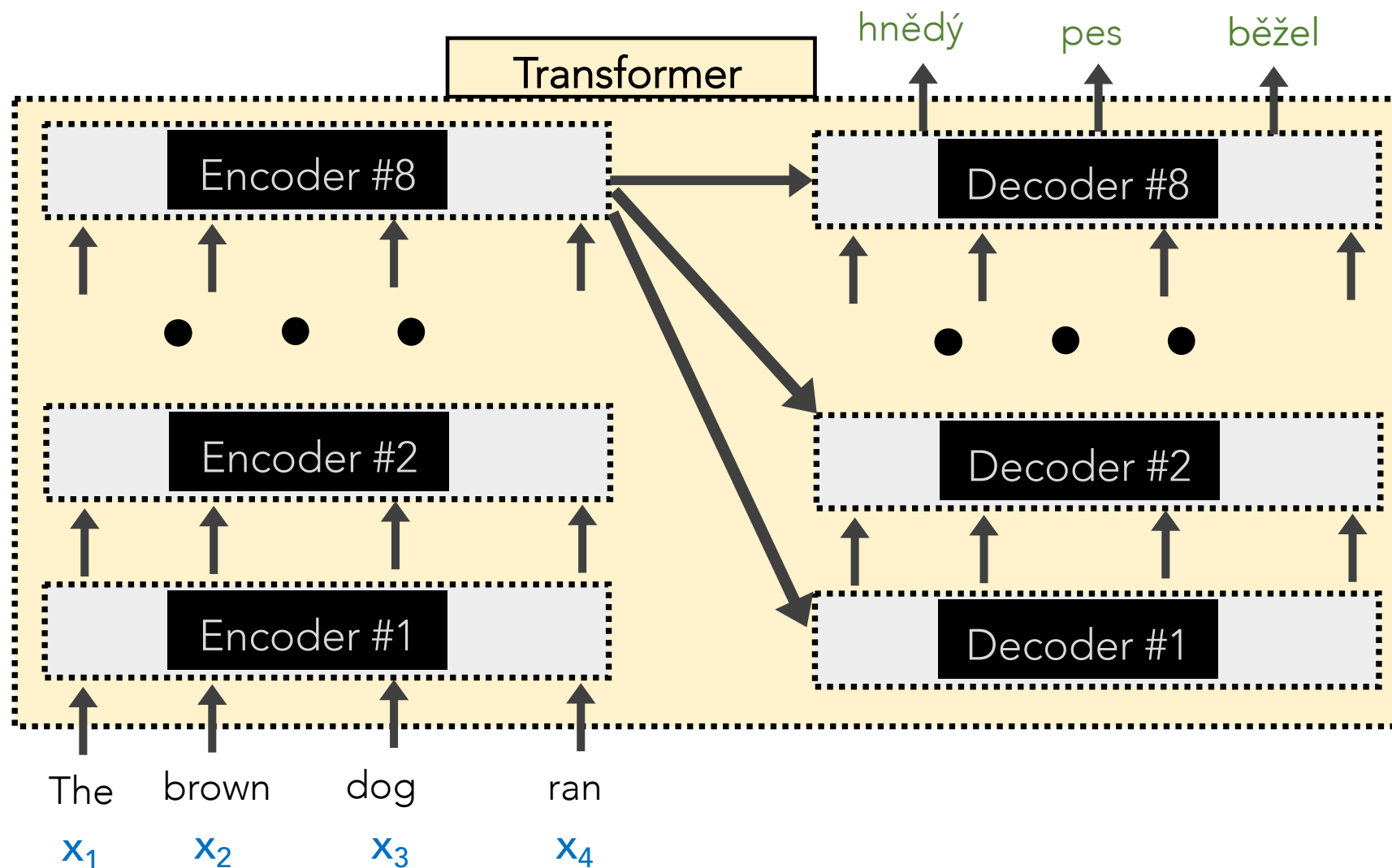


## NOTE

Transformer Decoders are identical to the Encoders, except they have an additional **Attention Head** in between the Self-Attention and FFNN layers.

This additional **Attention Head** focuses on parts of the encoder's representations.

# Transformer Encoders and Decoders

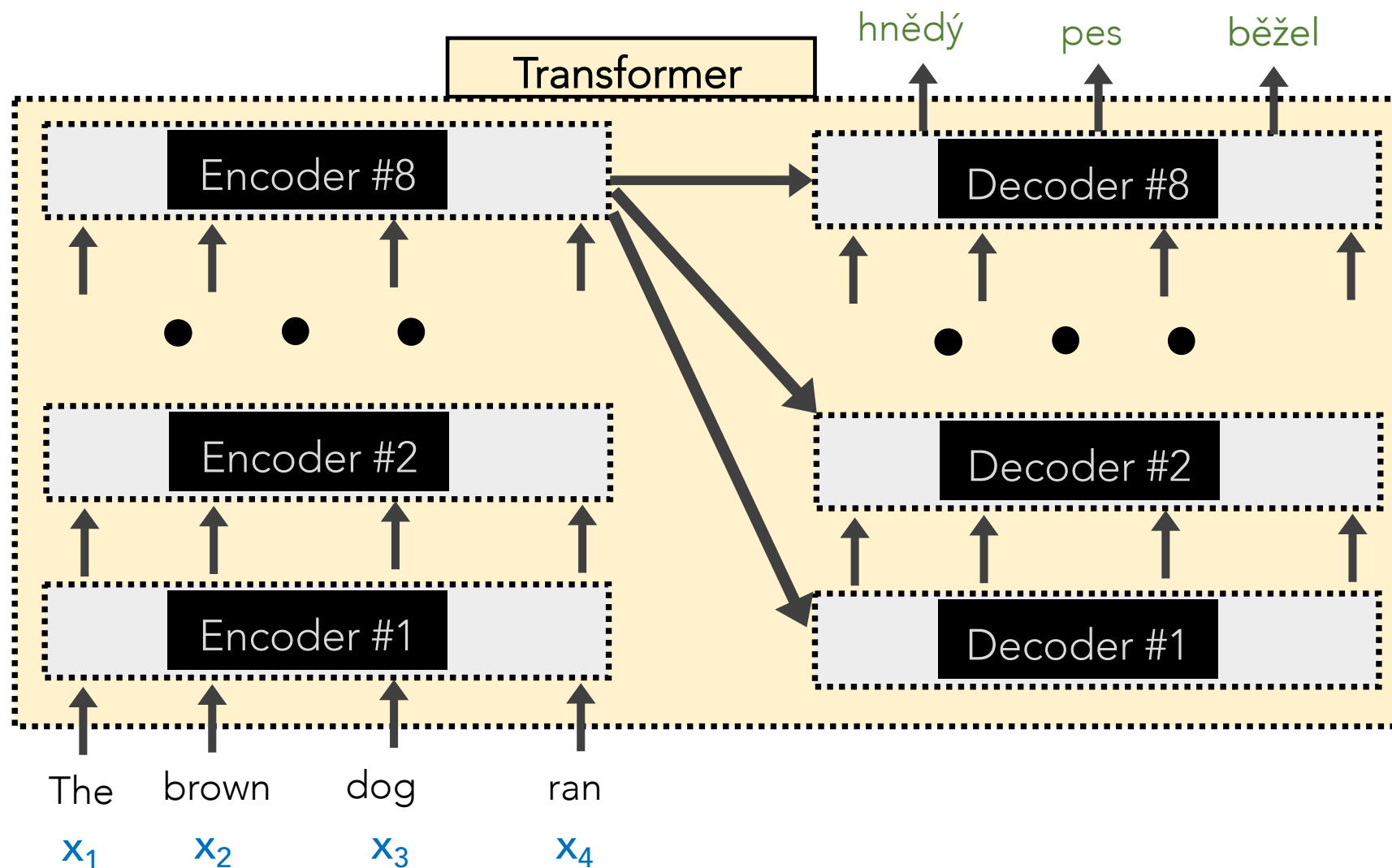


## NOTE

The **query** vector for a Transformer **Decoder's Attention Head** (not Self-Attention Head) is from the output of the previous decoder layer.

However, the **key** and **value** vectors are from the **Transformer Encoders'** outputs.

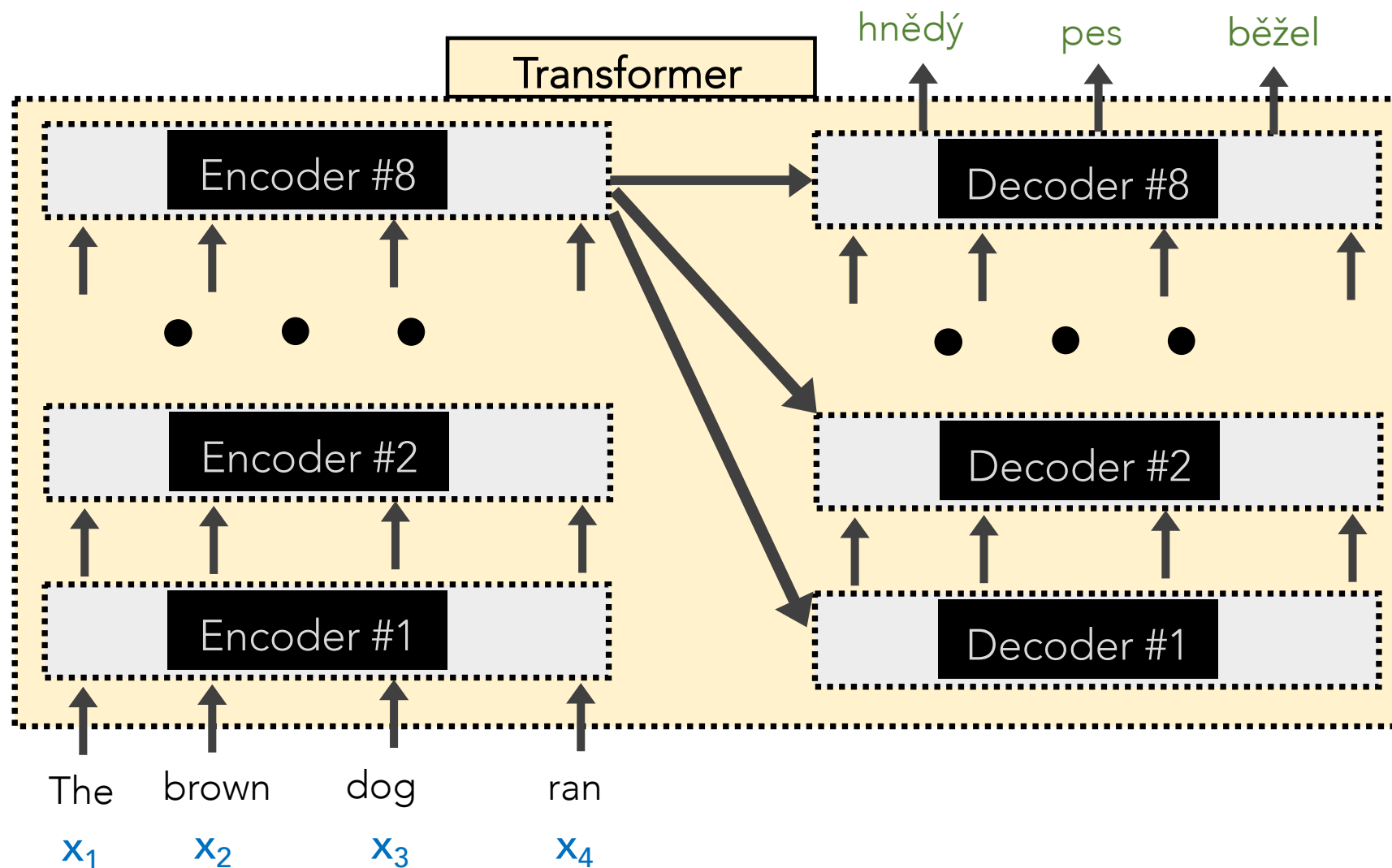
# Transformer Encoders and Decoders



## NOTE

The **query**, **key**, and **value** vectors for a Transformer **Decoder's Self-Attention Head** (not Attention Head) are all from the output of the previous decoder layer.

# Transformer Encoders and Decoders



## IMPORTANT

The Transformer **Decoders** have **positional embeddings**, too, just like the **Encoders**.

Critically, each position is **only allowed to attend to the previous indices**. This *masked Attention* preserves it as being an auto-regressive LM.

**Loss Function:** cross-entropy (predicting translated word)

**Training Time:** ~4 days on (8) GPUs

Layer Type	Complexity per Layer	Sequential Operations	Maximum Path Length
Self-Attention	$O(n^2 \cdot d)$	$O(1)$	$O(1)$
Recurrent	$O(n \cdot d^2)$	$O(n)$	$O(n)$
Convolutional	$O(k \cdot n \cdot d^2)$	$O(1)$	$O(\log_k(n))$
Self-Attention (restricted)	$O(r \cdot n \cdot d)$	$O(1)$	$O(n/r)$

## Machine Translation results: state-of-the-art (at the time)

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	<b>41.29</b>	$7.7 \cdot 10^{19}$	$1.2 \cdot 10^{21}$
Transformer (base model)	27.3	38.1	<b><math>3.3 \cdot 10^{18}</math></b>	
Transformer (big)	<b>28.4</b>	<b>41.8</b>	$2.3 \cdot 10^{19}$	

**Machine Translation results:** state-of-the-art (at the time)

You can train to translate from Language A to Language B.

Then train it to translate from Language B. to Language C.

Then, without training, it can translate from Language A to Language C



- What if we don't want to decode/translate?
- Just want to perform a particular task (e.g., classification)
- Want even more robust, flexible, rich representation!
- Want **positionality** to play a more explicit role, while not being restricted to a particular form (e.g., CNNs)