Lecture 9: Self-Attention

From Attention to Self-Attention

Harvard

AC295/CS287r/CSCI E-115B

Chris Tanner

Self [Attention]

-- Mac Miller (2018)

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basics@huhs.harvard.edu

ANNOUNCEMENTS

- HW1 is being graded double-blind. 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.
- After Phase 1 we will filter projects, give feedback, help you find the optimal project partners, offer TF support, etc

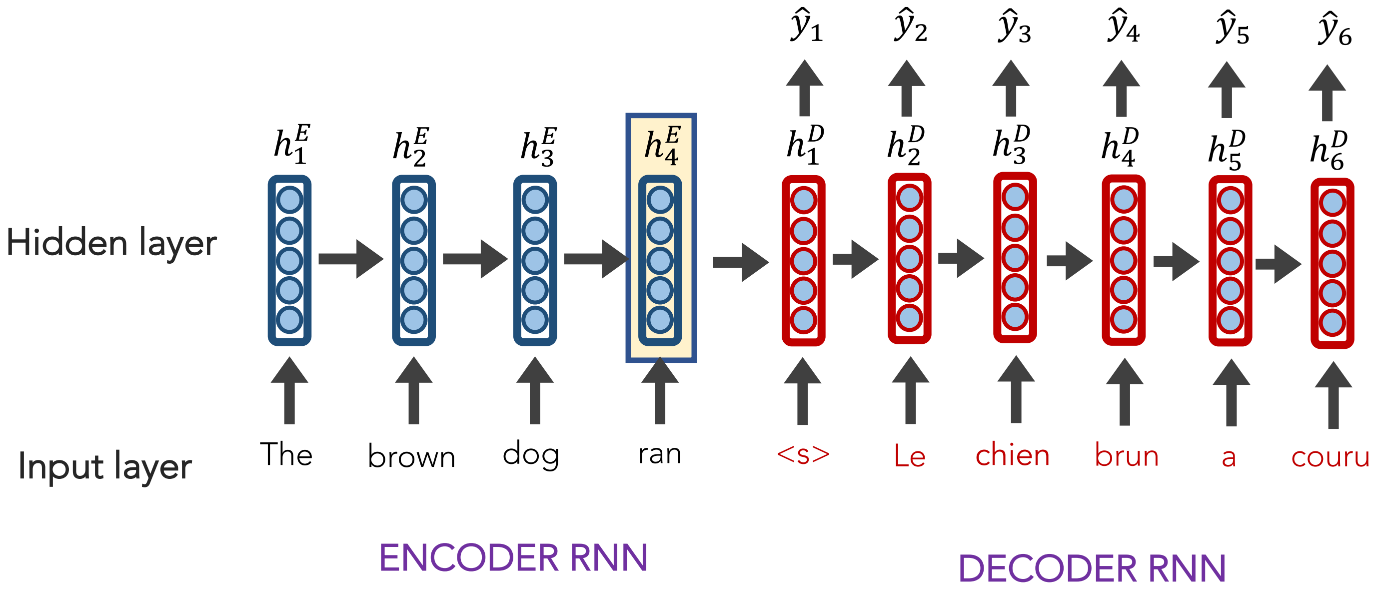
RESEARCH PROJECTS

- 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

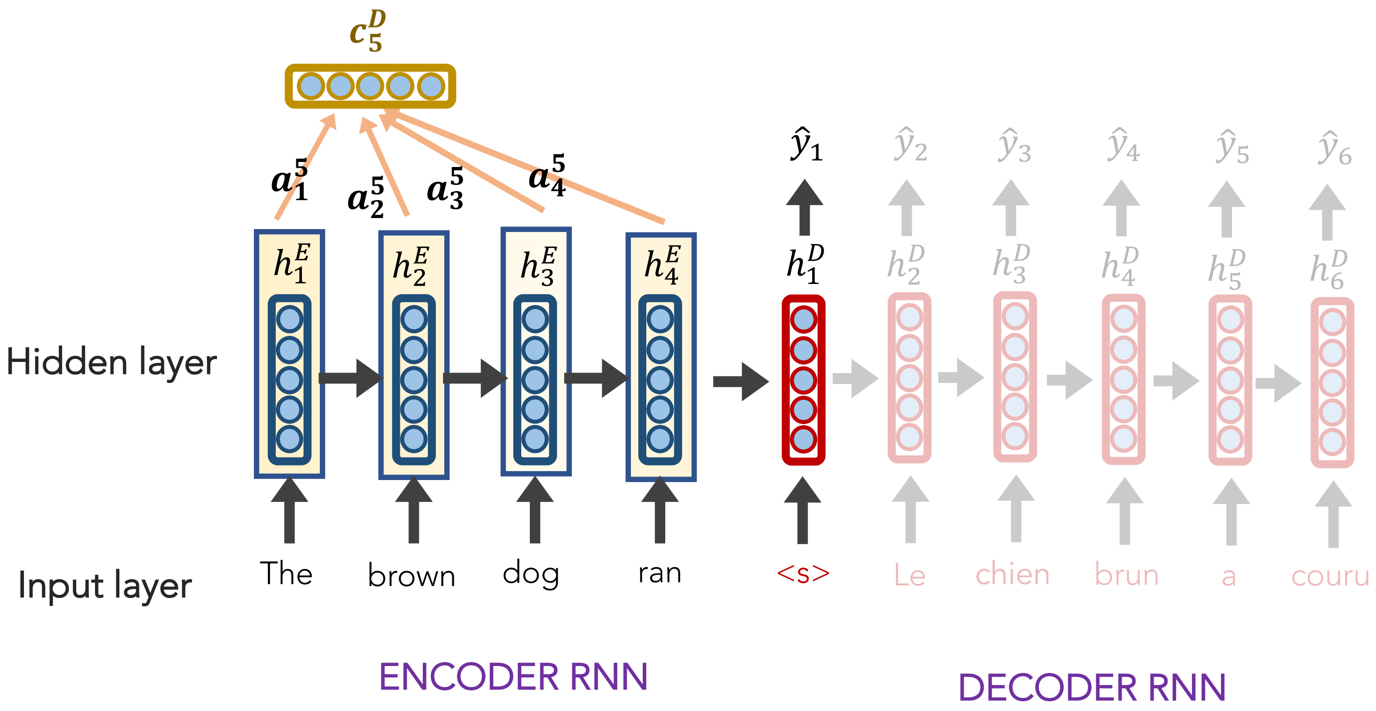
- are a general-purpose encoder-decoder architecture
- can be implemented with RNNs (or Transformers even)
- Allow for n → m predictions
- Natural approach to **Neural MT**
- If implemented end-to-end can be good but slow



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

$$\text{argmax}_{\mathrm{y}} P(x|y)P(y)$$

- Converts text from a source language x to a target language y
- SMT made huge progress but was brittle
- NMT (starting w/ **LSTM-based seq2seq models**) blew 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

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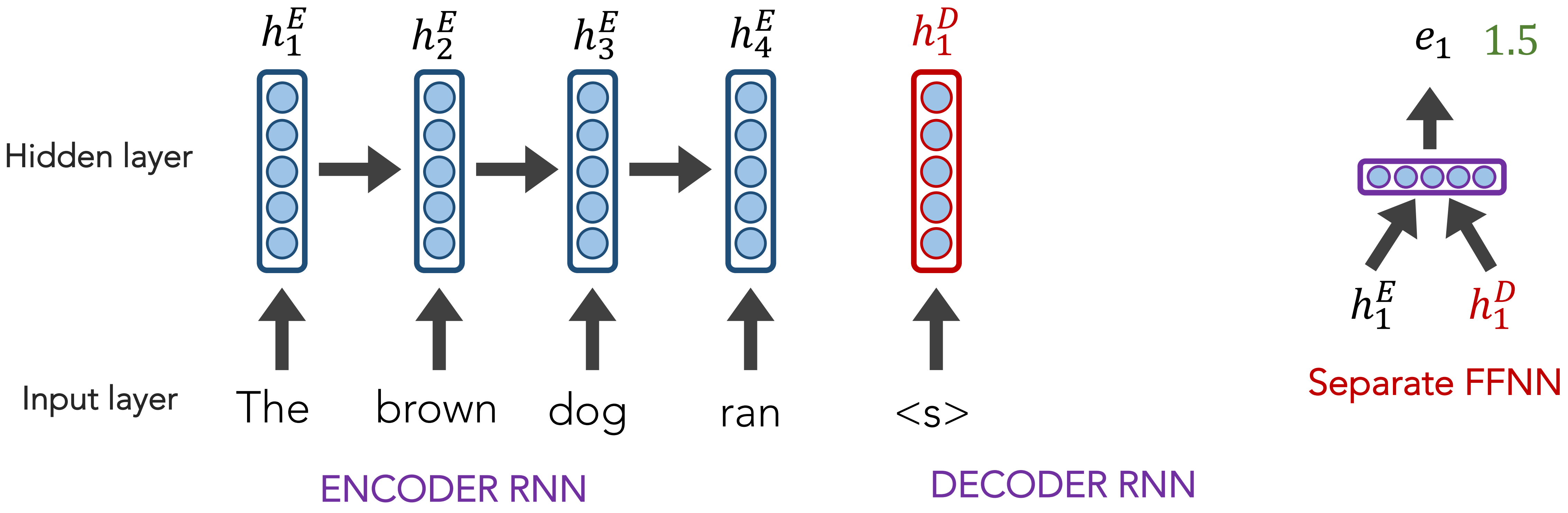
seq2seq + Attention

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

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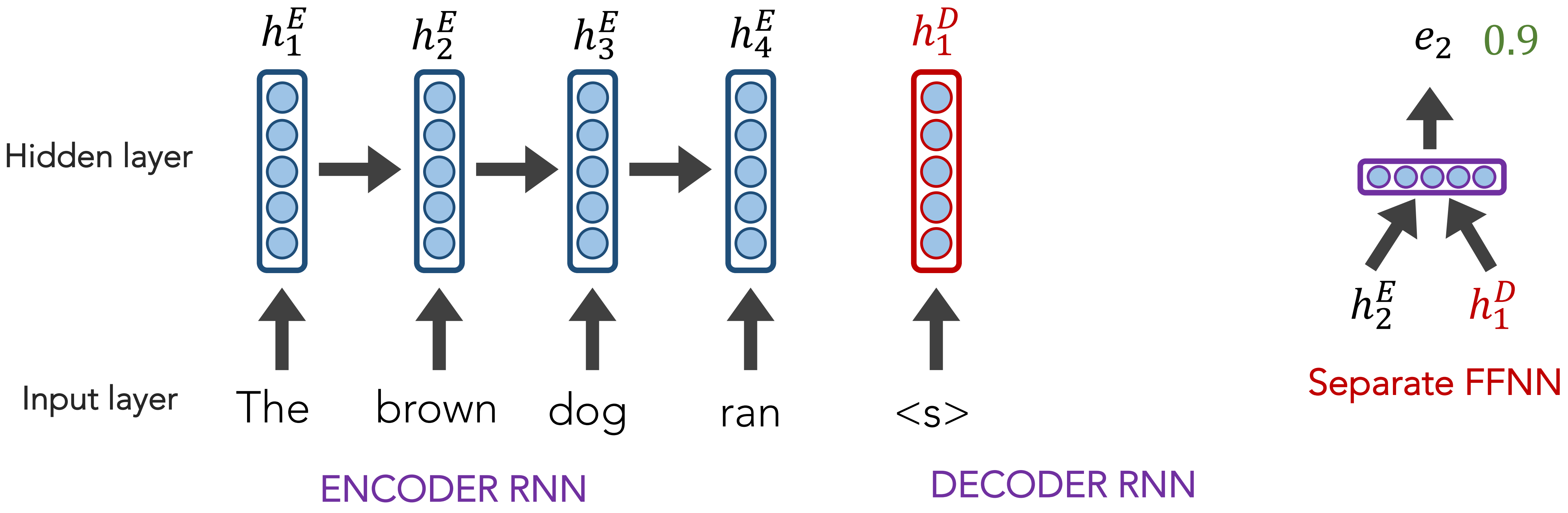

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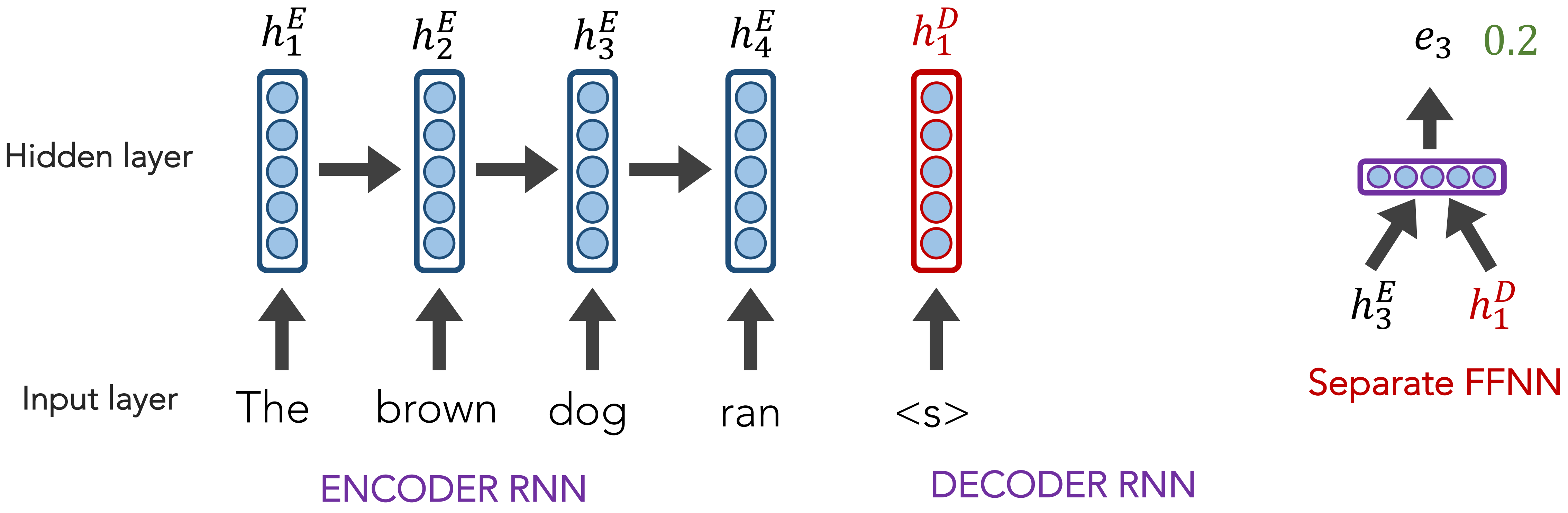

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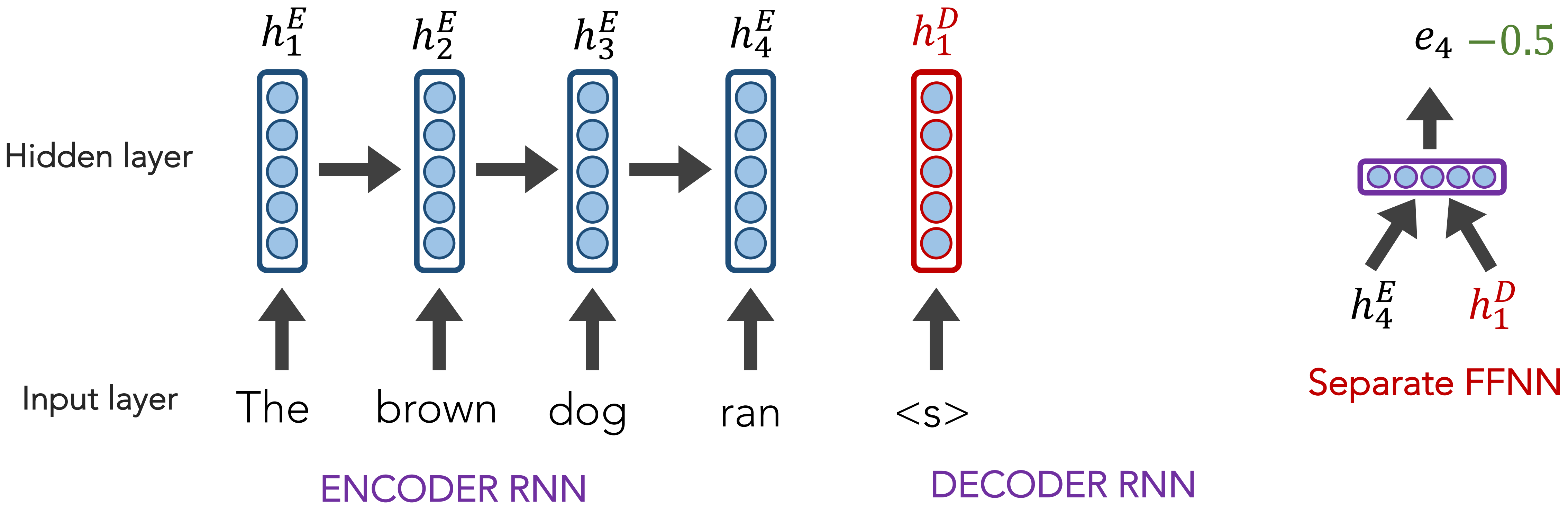

seq2seq + Attention

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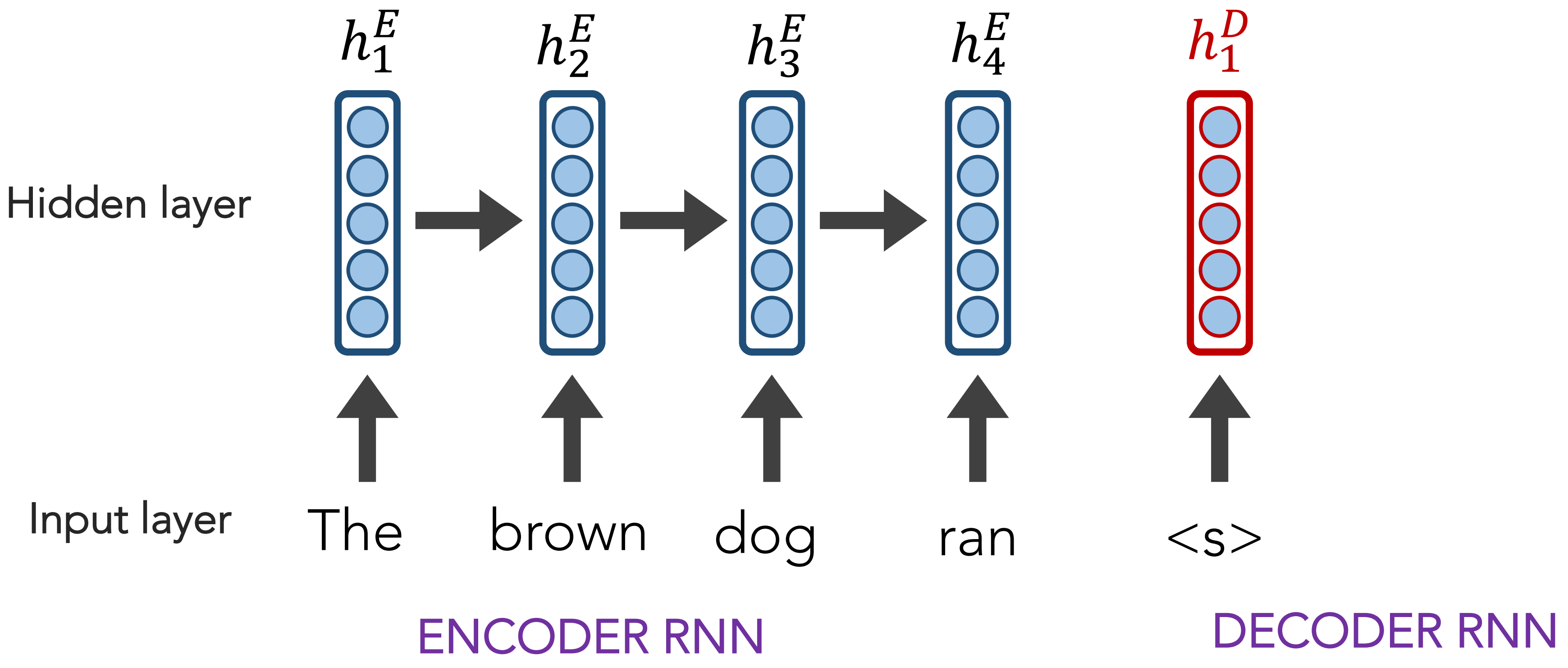

Attention (raw scores)

e_1 1.5
e_2 0.9
e_3 0.2
e_4 -0.5

seq2seq + Attention

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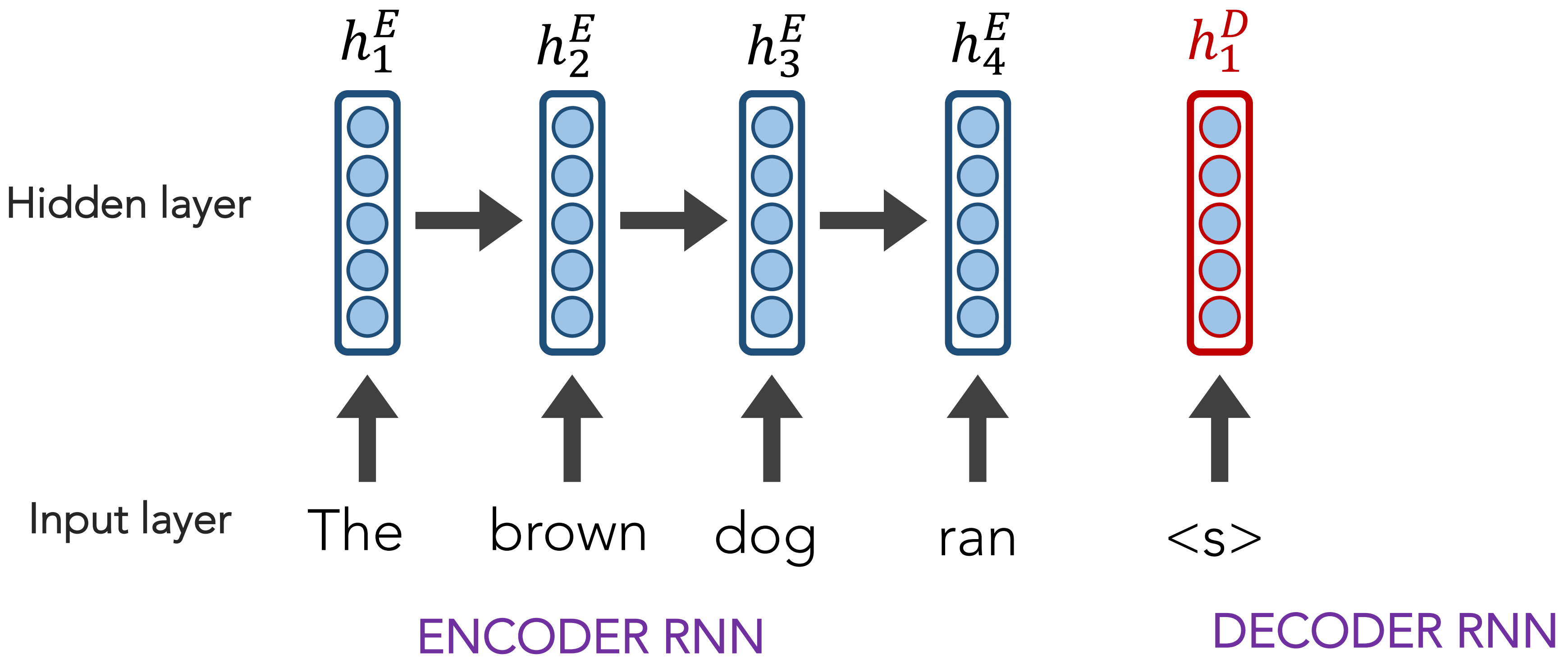

Attention (raw scores)

e_1 1.5
e_2 0.9
e_3 0.2
e_4 -0.5

Attention (softmax'd)

$$a_i^1 = \frac{\exp(e_i)}{\sum_i^N \exp(e_1)}$$

seq2seq + Attention

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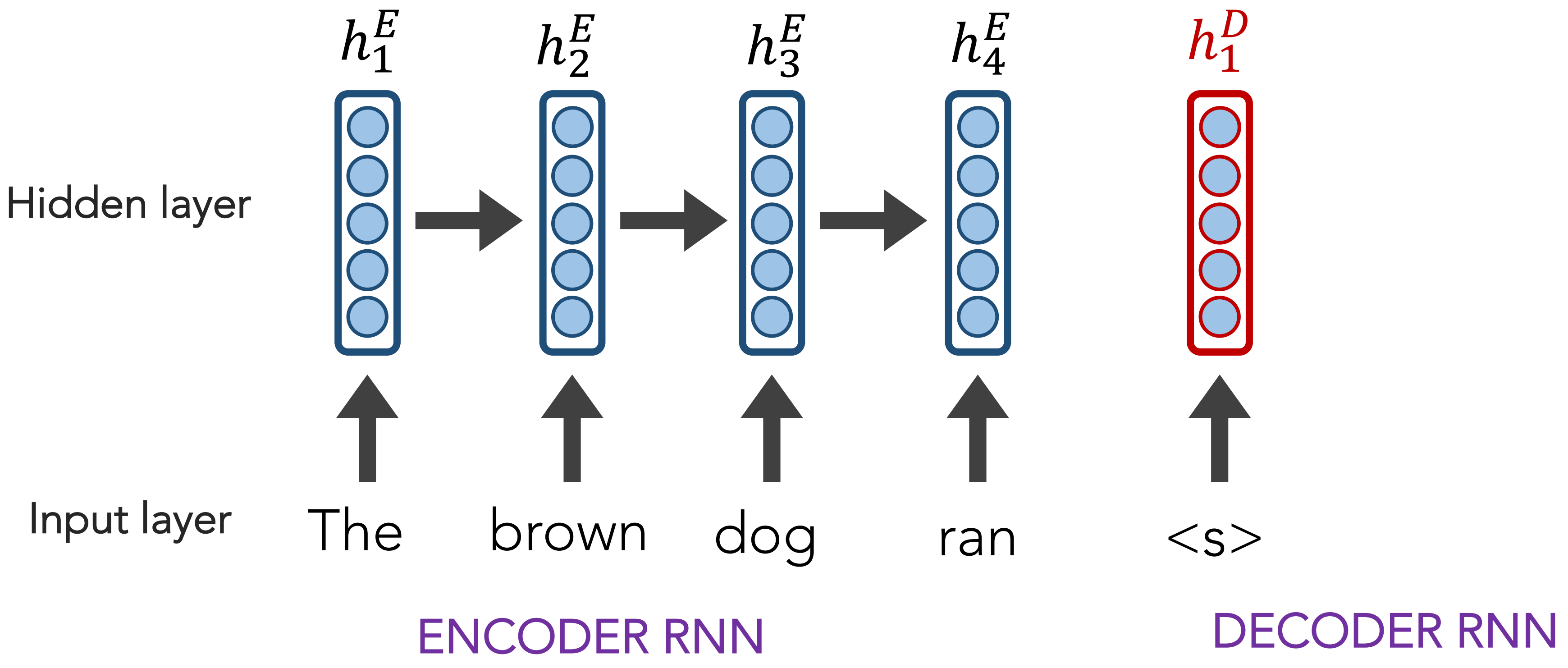


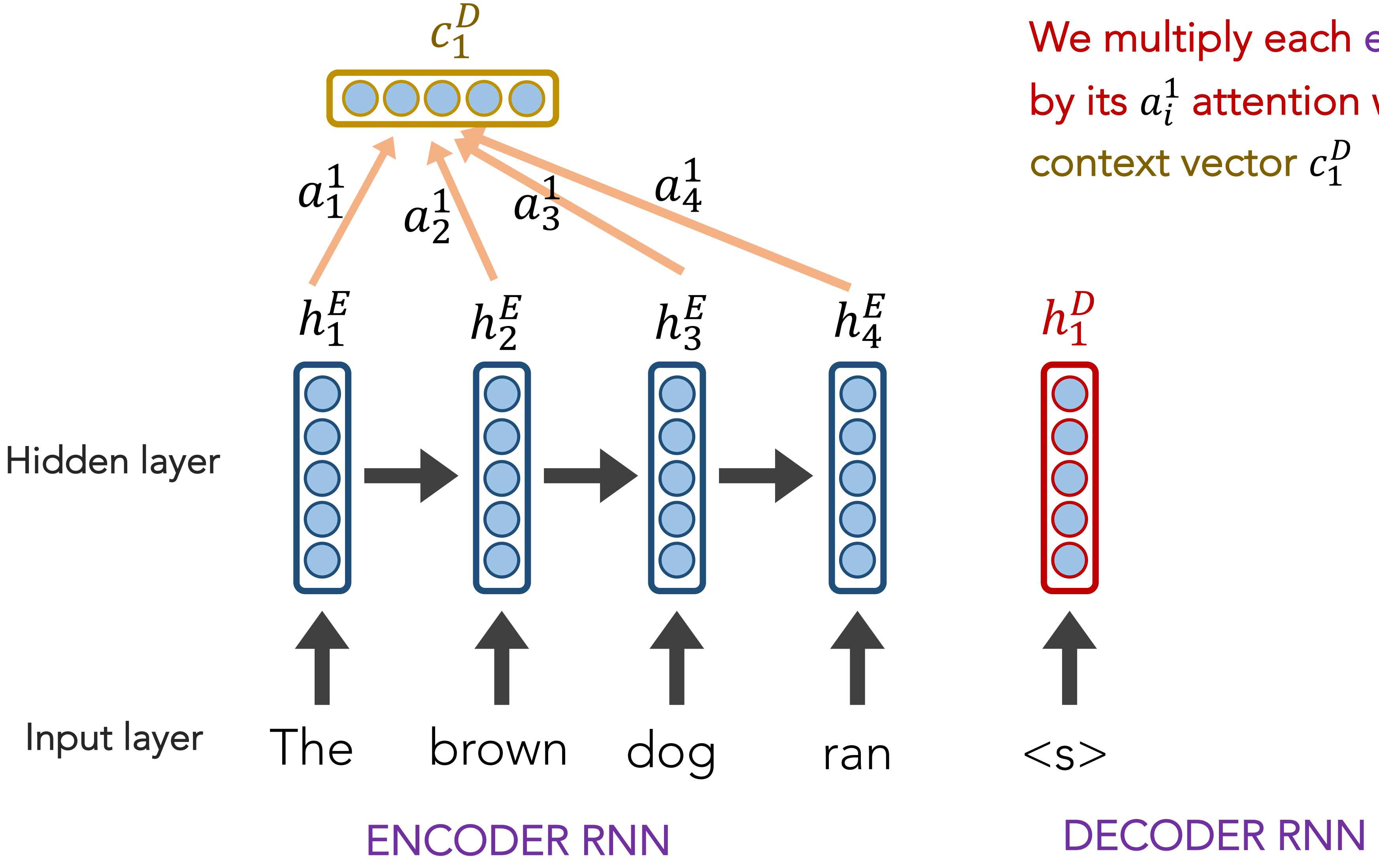
Attention (raw scores)

e_1 1.5
e_2 0.9
e_3 0.2
e_4 -0.5

Attention (softmax'd)

$a_1^1 = 0.51$
$a_2^1 = 0.28$
$a_3^1 = 0.14$
$a_3^1 = 0.07$

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)

$a_1^1 = 0.51$

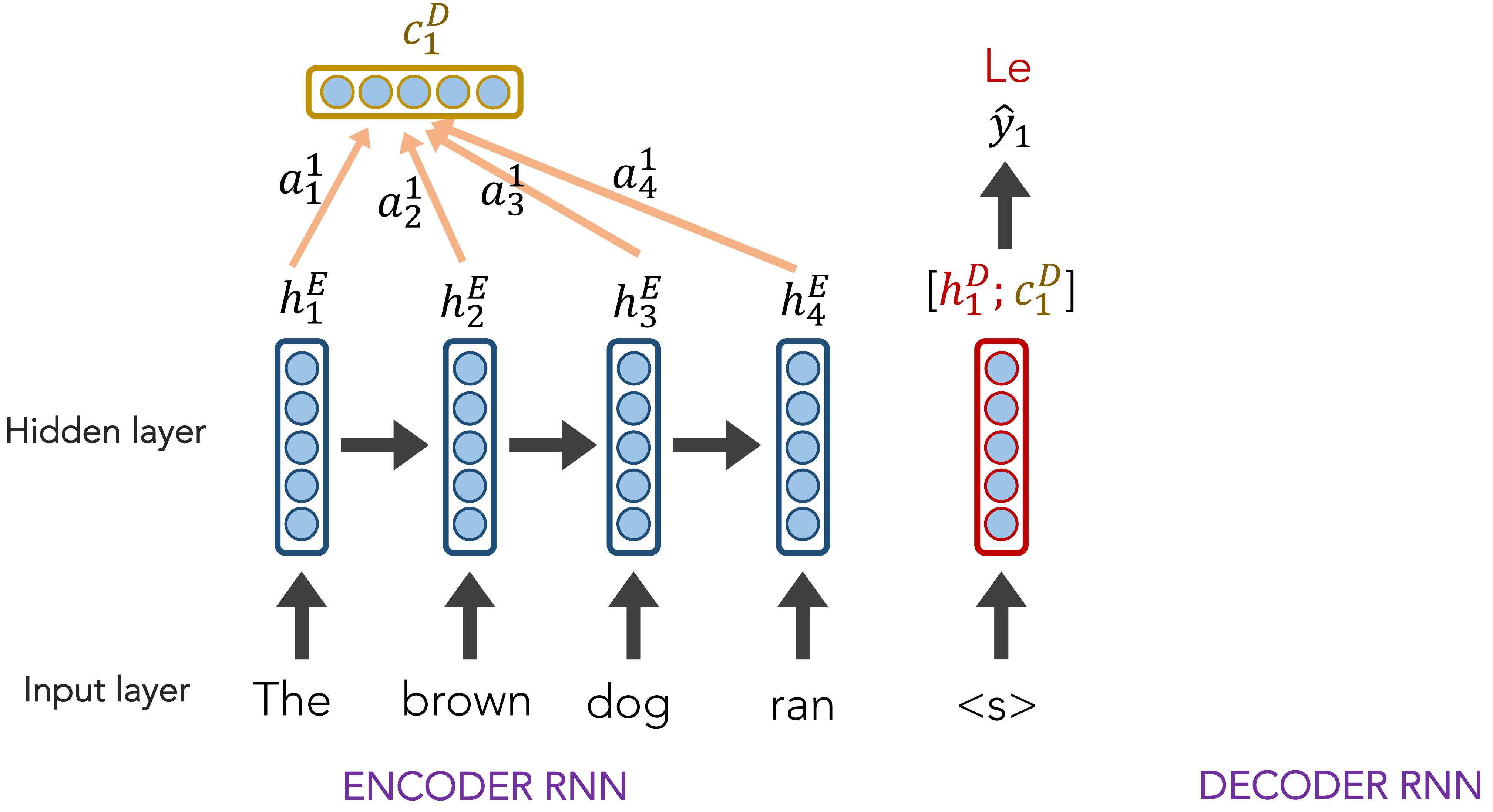
$a_2^1 = 0.28$

$a_3^1 = 0.14$

$a_3^1 = 0.07$

seq2seq + Attention

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



seq2seq + Attention

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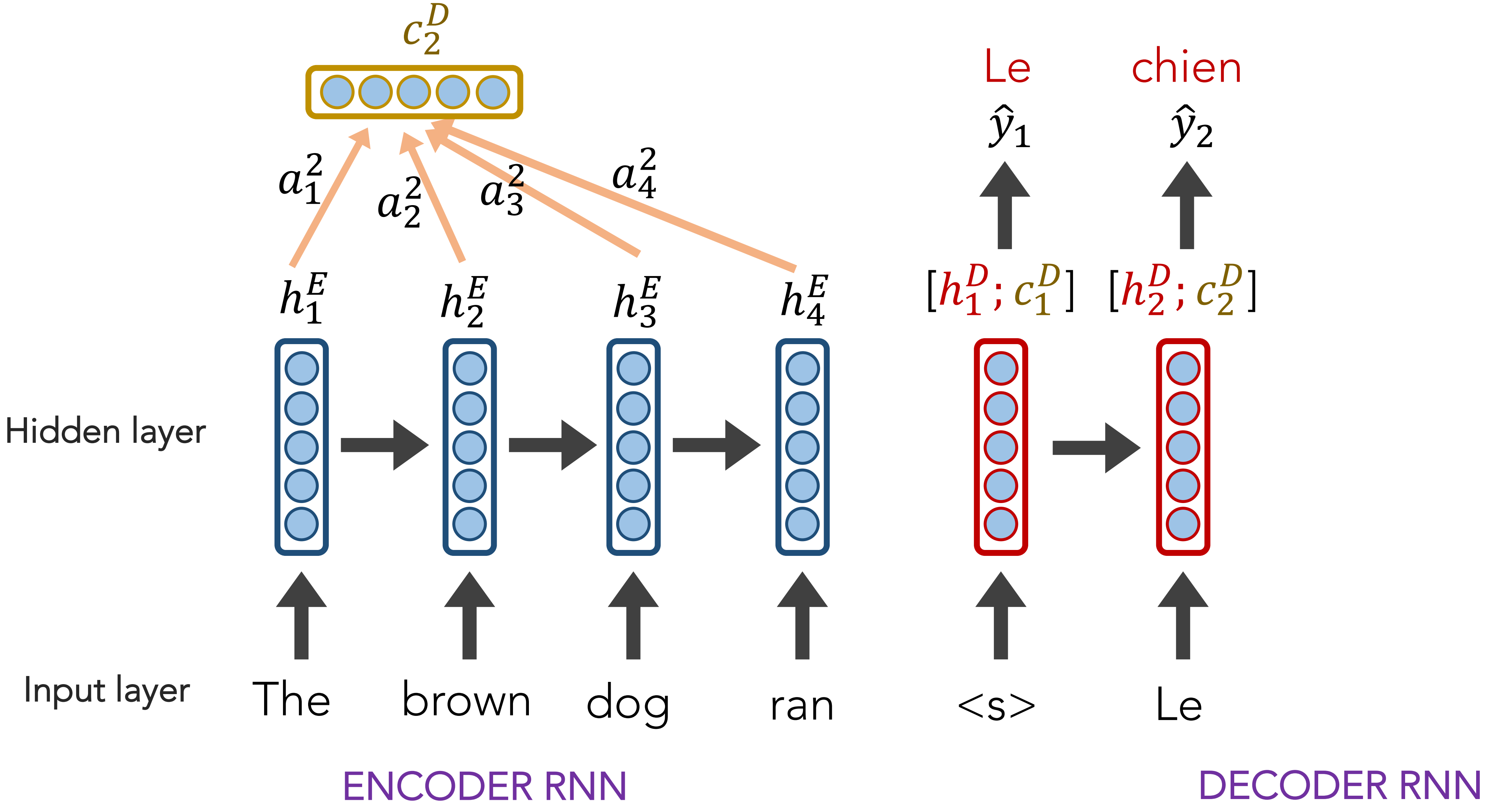

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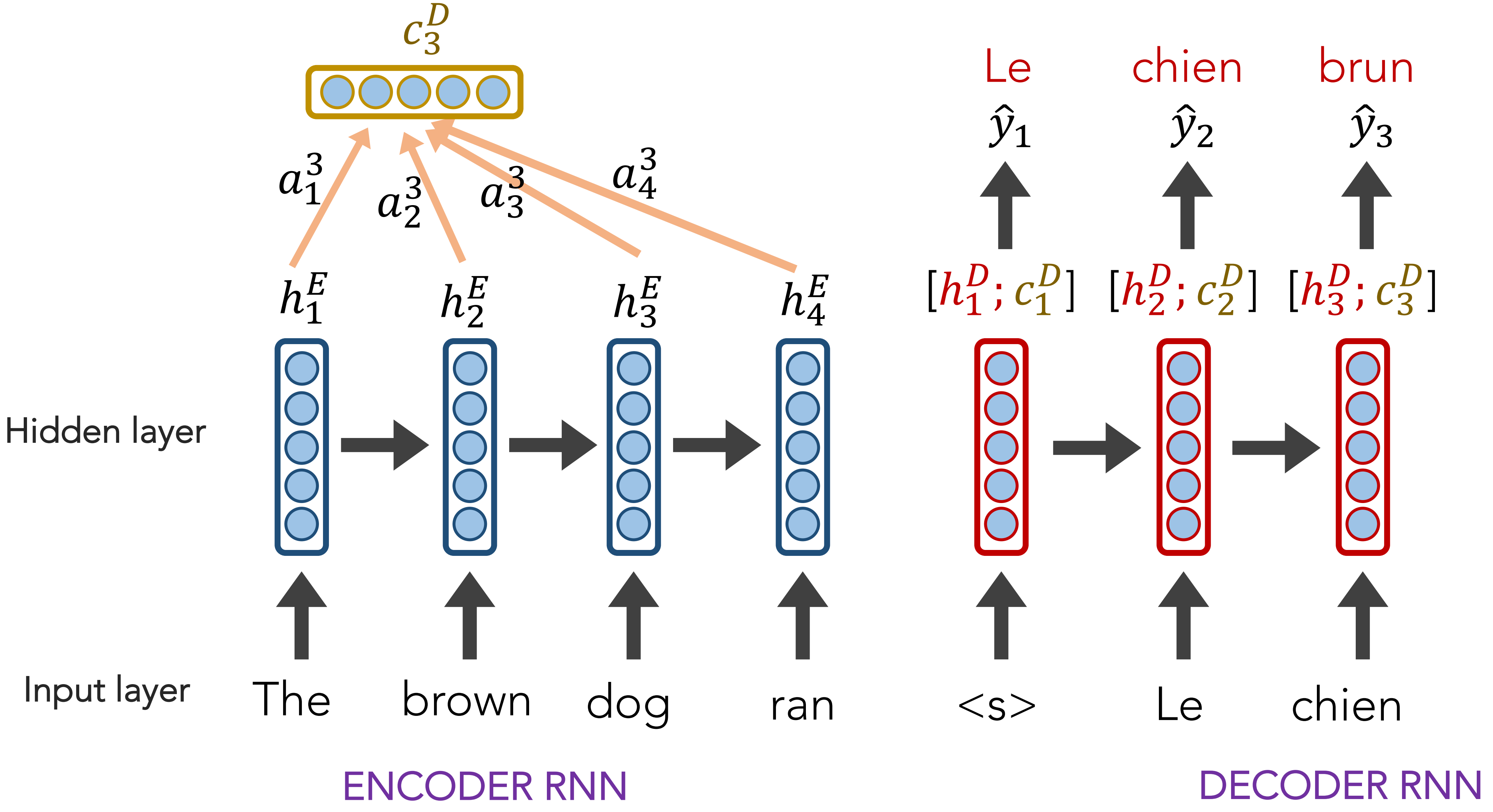

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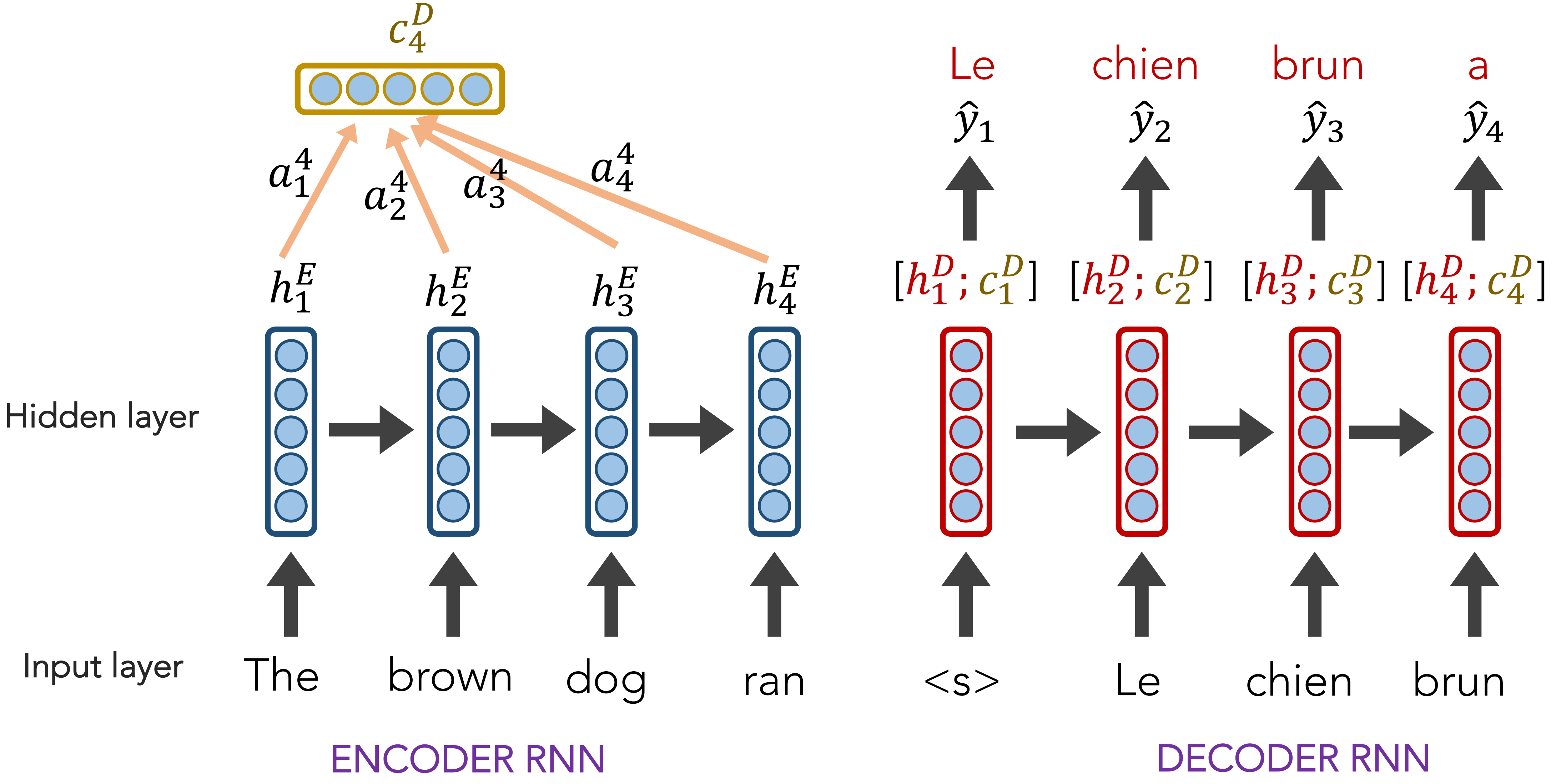

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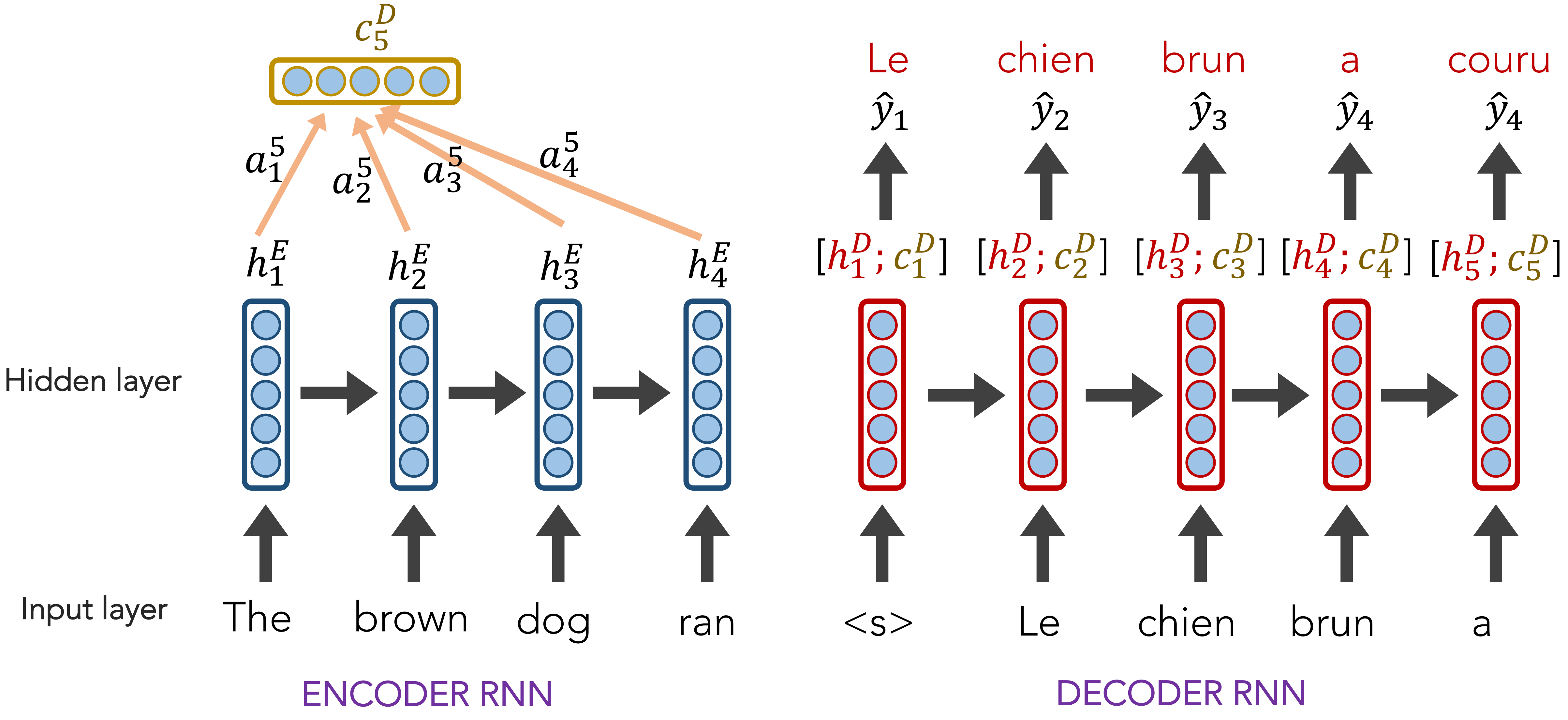


For convenience, here's the Attention calculation summarized on 1 slide

Attention output

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

"source context for decoder step t"

(weighted sum)

Attention weights

$$a_k^{(t)} = \frac{\exp(\text{score}(h_t, s_k))}{\sum_{i=1}^{m} \exp(\text{score}(h_t, s_i))}, \mathrm{k} = 1..\mathrm{m}$$

"attention weight for source token k at decoder step t"

(softmax)

Attention scores

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

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

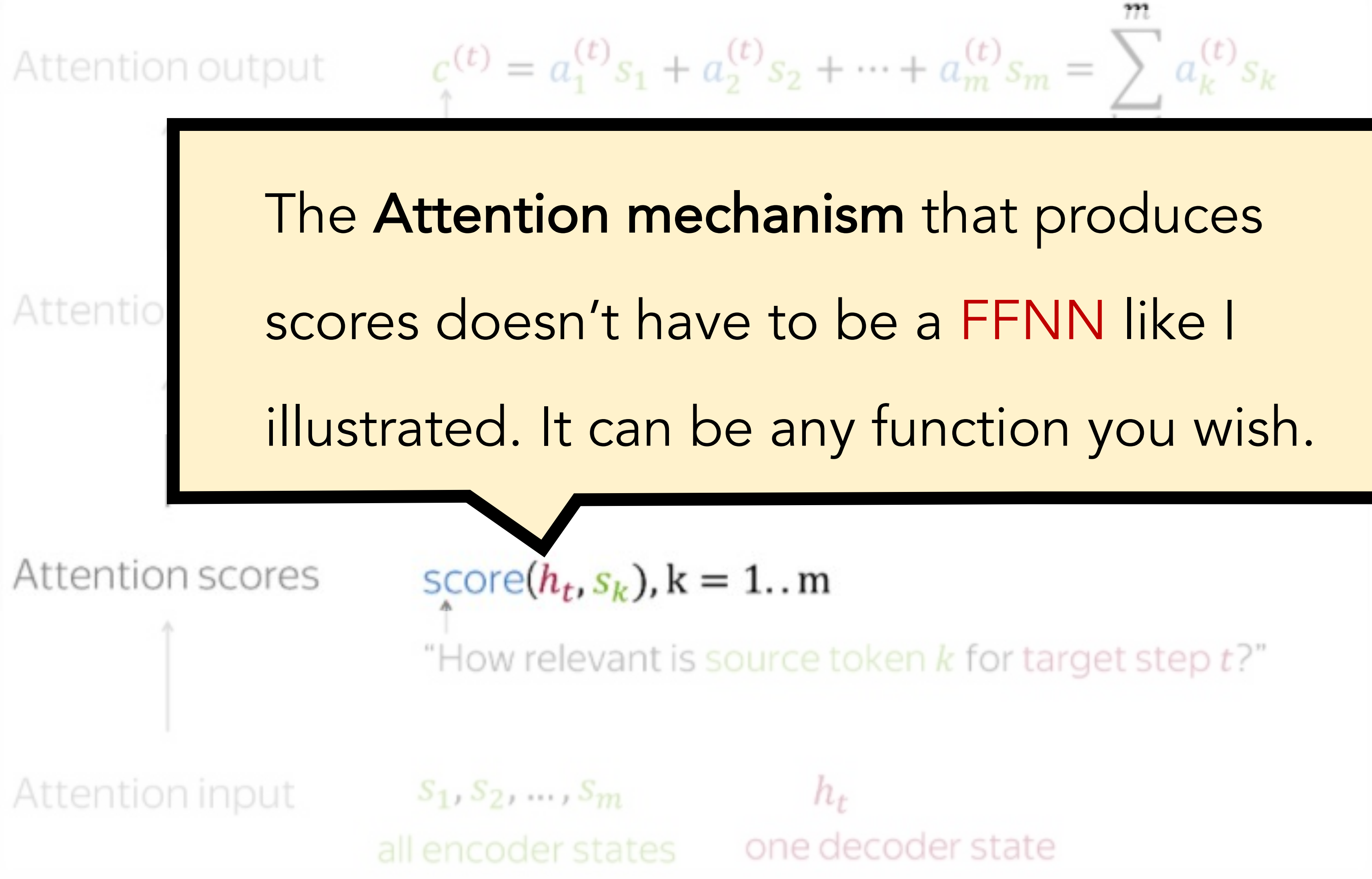
Attention input

$s_1, s_2, \dots, s_m$ — all encoder states

h_t — one decoder state

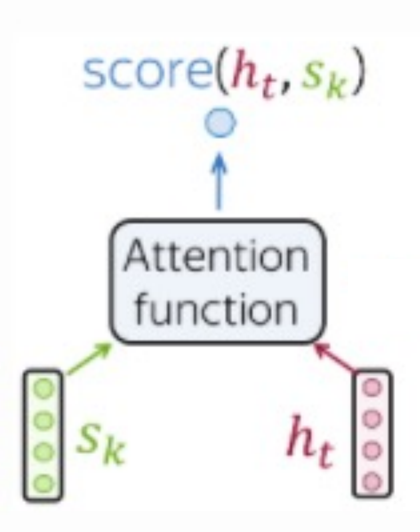
Photo credit: https://lena-voita.github.io/nlp_course/seq2seq_and_attention.html

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



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

Photo credit: https://lena-voita.github.io/nlp_course/seq2seq_and_attention.html



Popular Attention Scoring functions:

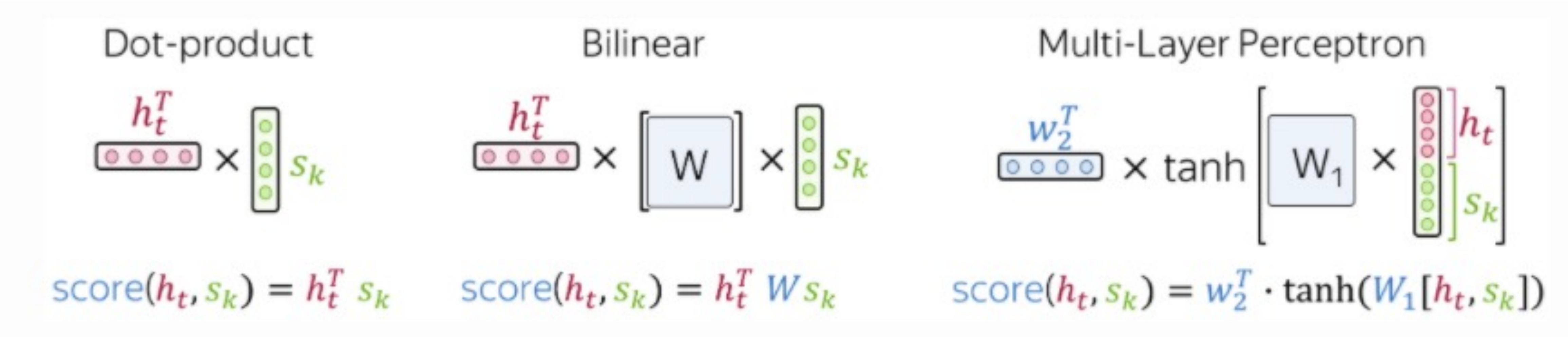


Photo credit: https://lena-voita.github.io/nlp_course/seq2seq_and_attention.html

seq2seq + Attention

Attention:

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

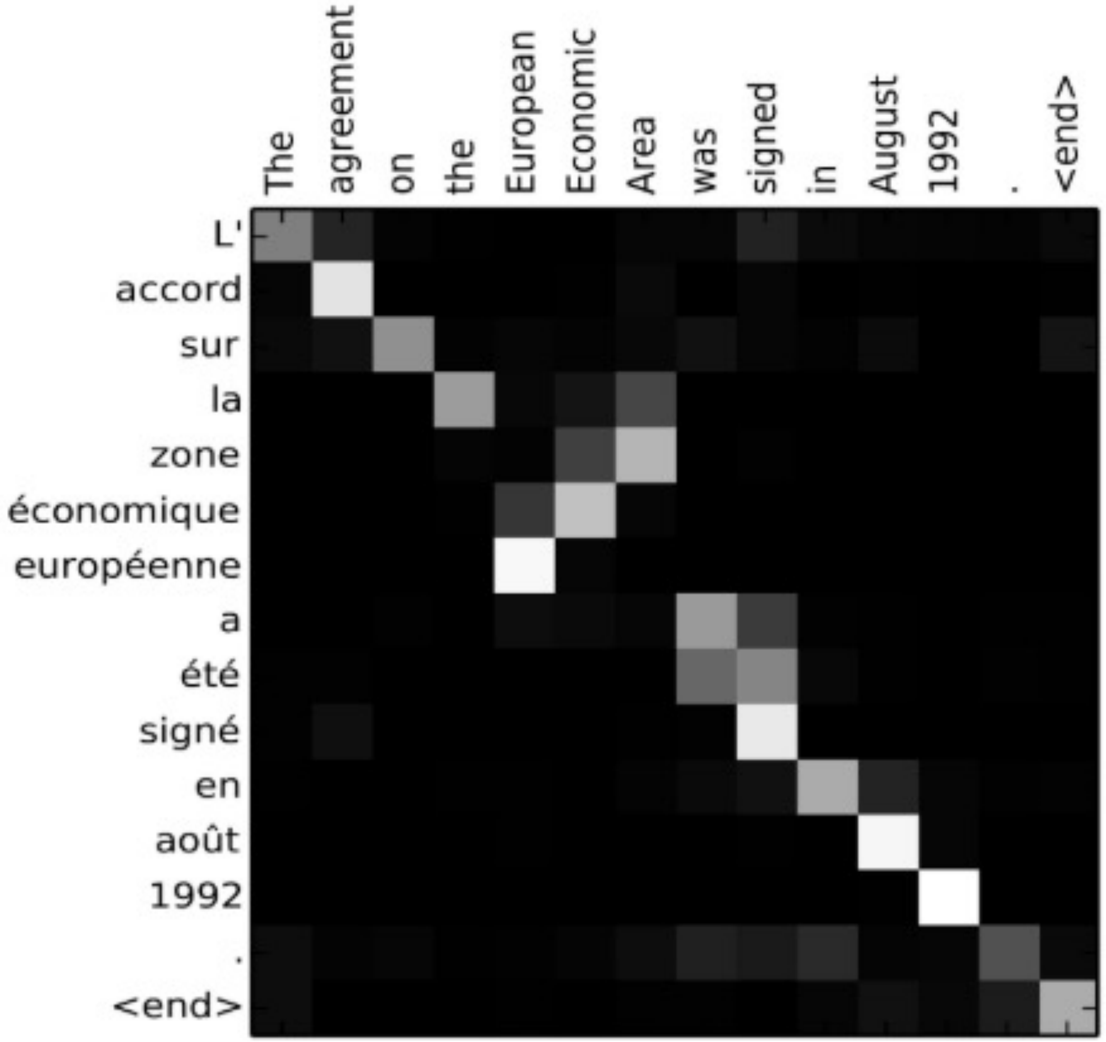


Image source: Fig 3 in [Bahdanau et al., 2015]

Takeaway:

Having a separate encoder and decoder allows for n → m length predictions.

Attention is powerful; allows us to conditionally weight our focus

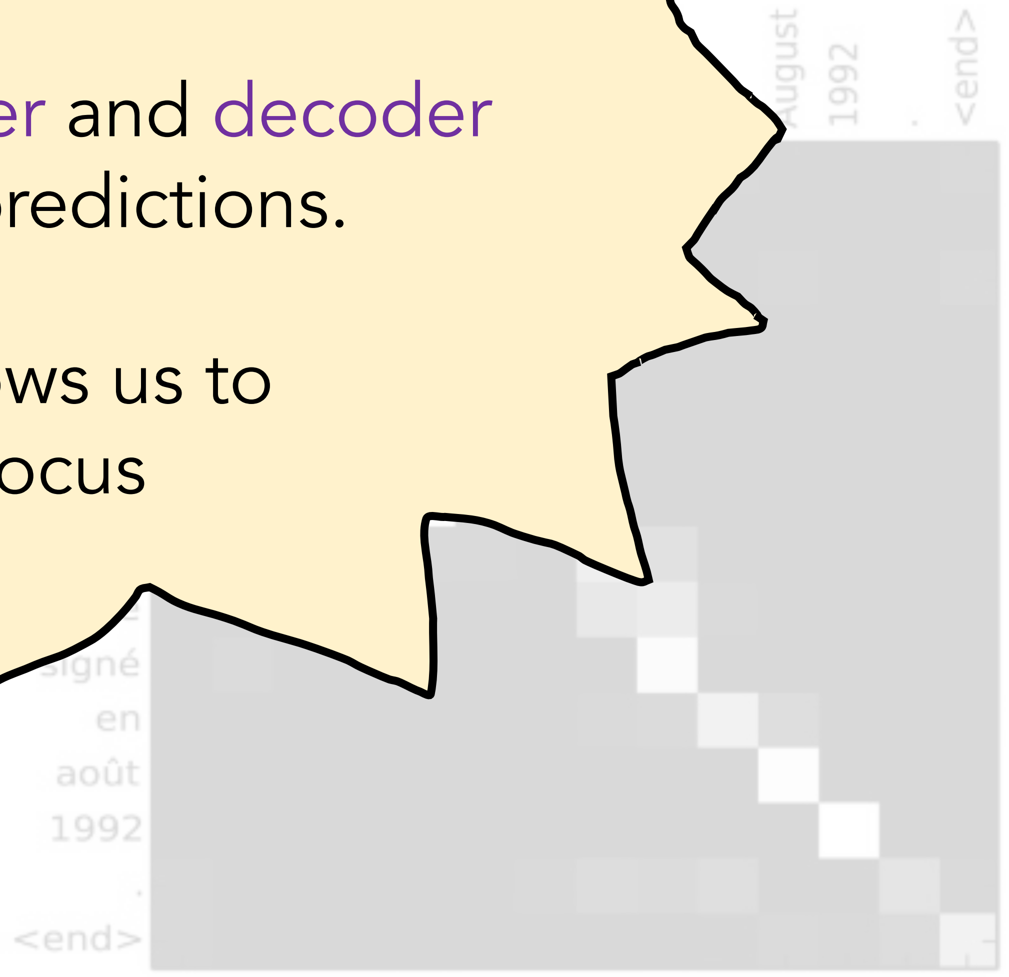
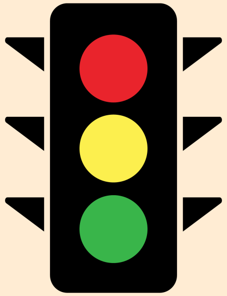


Image source: Fig 3 in Bahdanau et al., 2015

CHECKPOINT



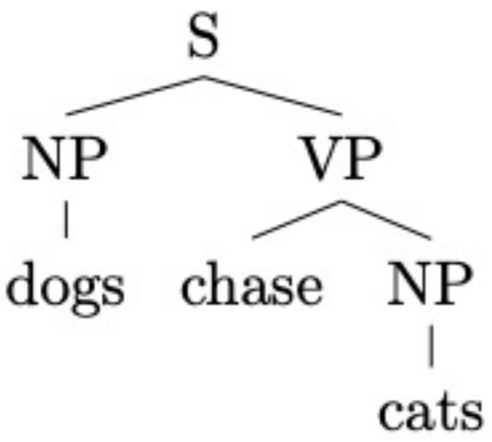
- seq2seq doesn't have to use RNNs/LSTMs
- seq2seq doesn't have to be used exclusively for NMT
- NMT doesn't have to use seq2seq

  (but it's natural and the best we have for now)

Constituency Parsing

Input: dogs chase cats

Output:



or a flattened representation

$$(\text{S}\ (\text{NP dogs }){}_{\text{NP}}\ (\text{VP chase }(\text{NP cats }){}_{\text{NP}}\ ){}_{\text{VP}}\ ){}_{\text{S}}$$

Constituency Parsing

Input: I shot an elephant in my pajamas

Output:

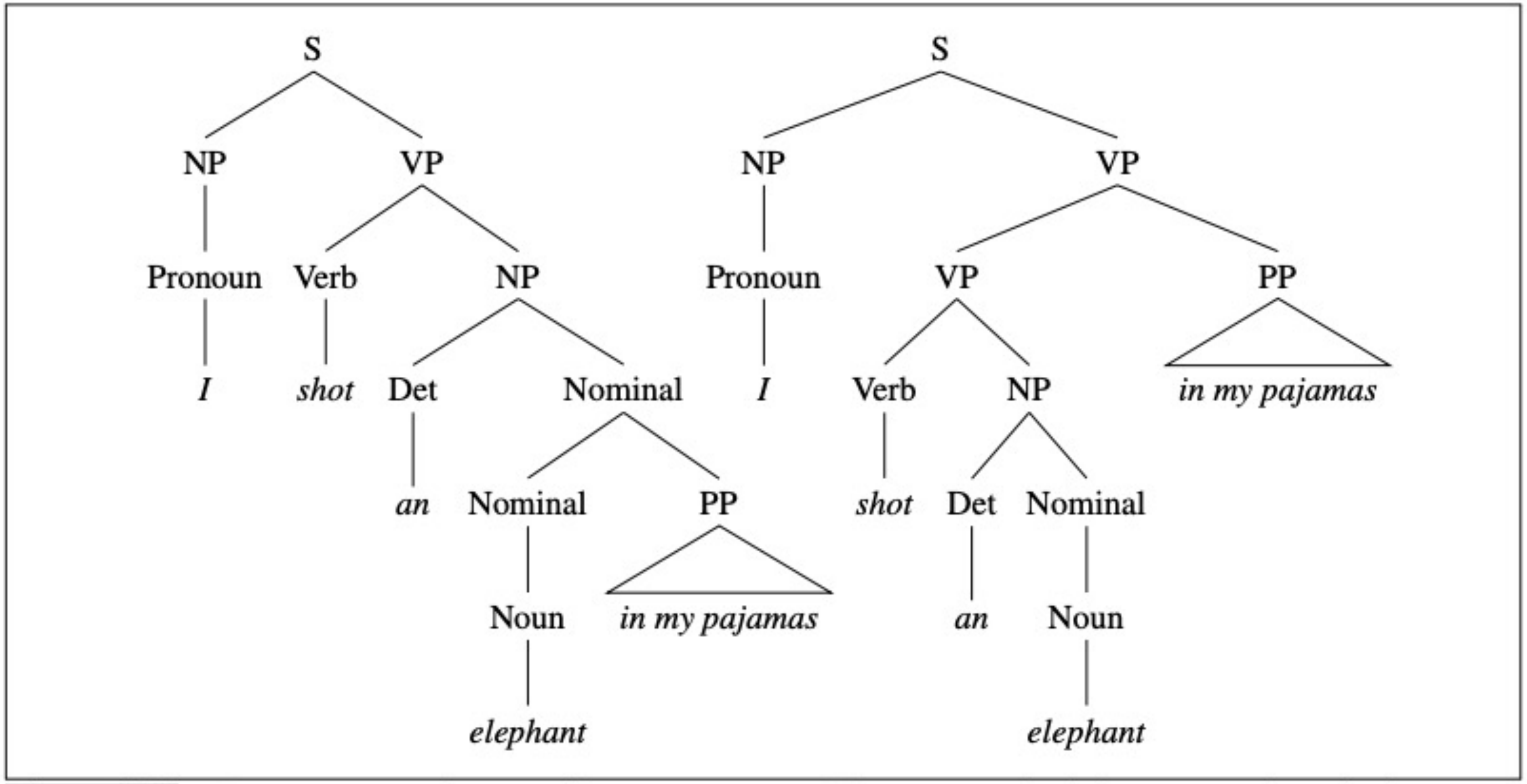


Figure 13.2 Two parse trees for an ambiguous sentence. The parse on the left corresponds to the humorous reading in which the elephant is in the pajamas, the parse on the right corresponds to the reading in which Captain Spaulding did the shooting in his pajamas.

https://web.stanford.edu/~jurafsky/slp3/13.pdf

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) (BERT)	95.70	95.98	95.84	**92.03**	92.33	92.18
Zhou and Zhao (2019) (XLNet)	96.21	96.46	96.33	-	-	-
Our work	**96.24**	**96.53**	**96.38**	91.85	**93.45**	**92.64**

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

https://aclanthology.org/2020.findings-emnlp.65.pdf

Image Captioning

Input: image

Output: generated text

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

Show, Attend and Tell: Neural Image Caption Generation with Visual Attention. Xu et al. CVPR (2016)

Image Captioning

Input: image

Output: generated text

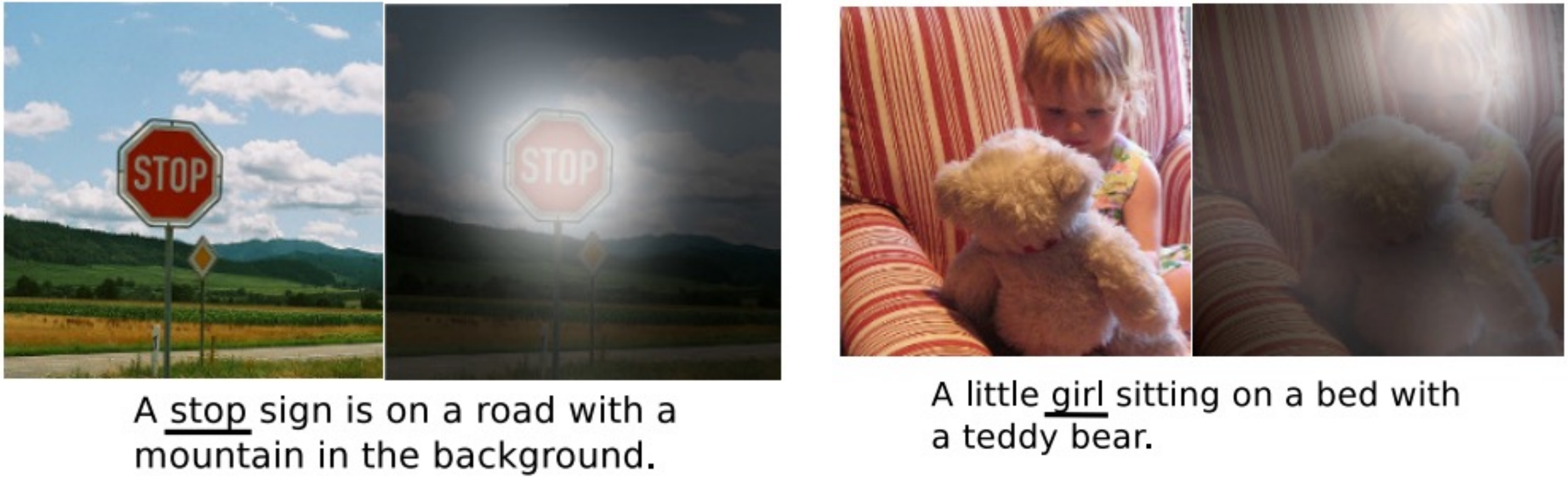


Figure 3. Examples of attending to the correct object (*white* indicates the attended regions, *underlines* indicated the corresponding word)

Show, Attend and Tell: Neural Image Caption Generation with Visual Attention. Xu et al. CVPR (2016)

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.

Show, Attend and Tell: Neural Image Caption Generation with Visual Attention. Xu et al. CVPR (2016)

Image Captioning

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

Show, Attend and Tell: Neural Image Caption Generation with Visual Attention. Xu et al. CVPR (2016)

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 <u>explicit</u> 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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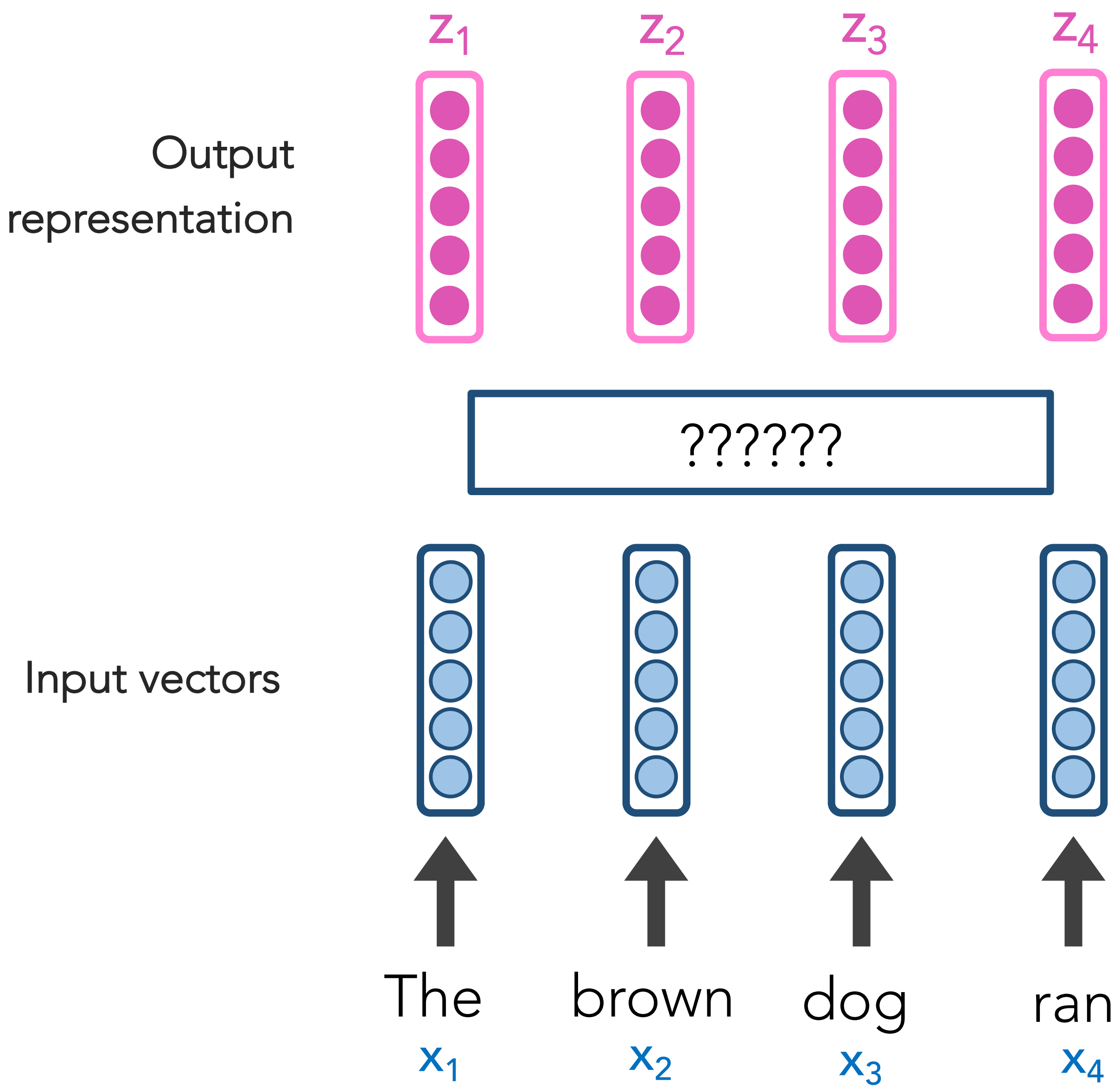
Goals

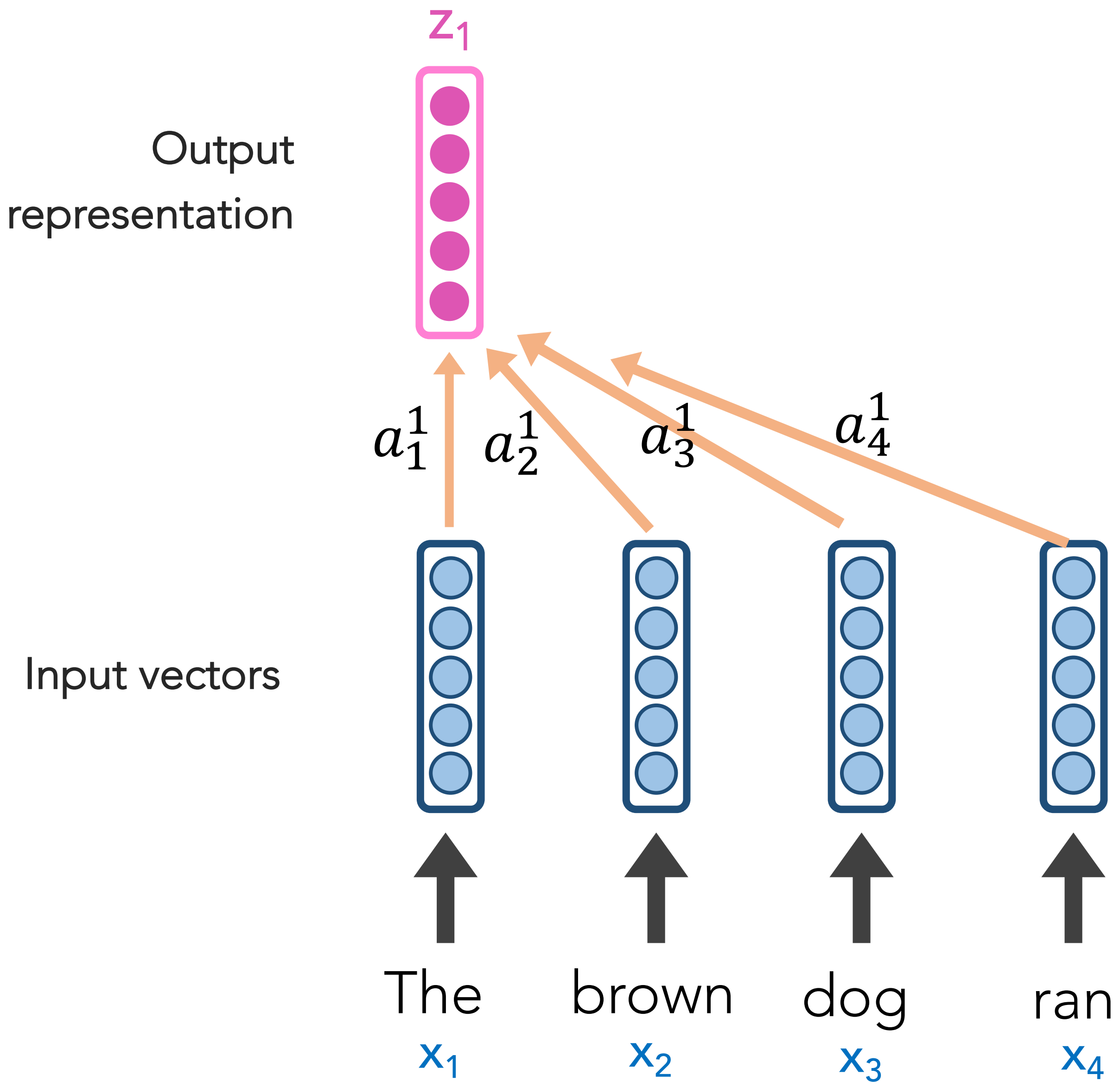
- Each word in a sequence to be transformed into a rich, abstract **representation** (context embedding) based on the weighted sums of the other words in the same sequence (akin to deep CNN layers)
- Inspired by Attention, we want each word to determine, "how much should I be influenced by each of my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

Self-Attention



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

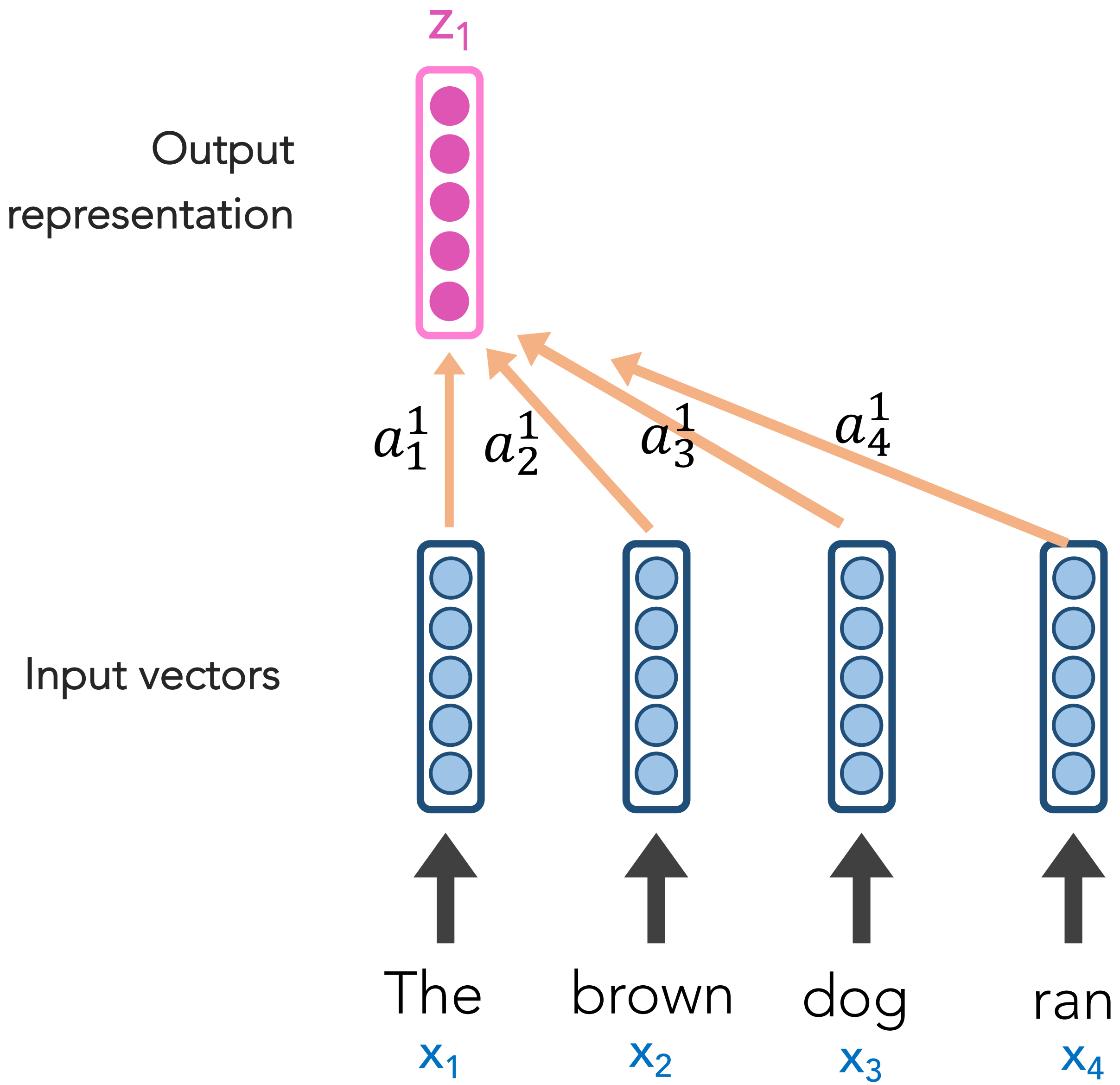
Self-Attention



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

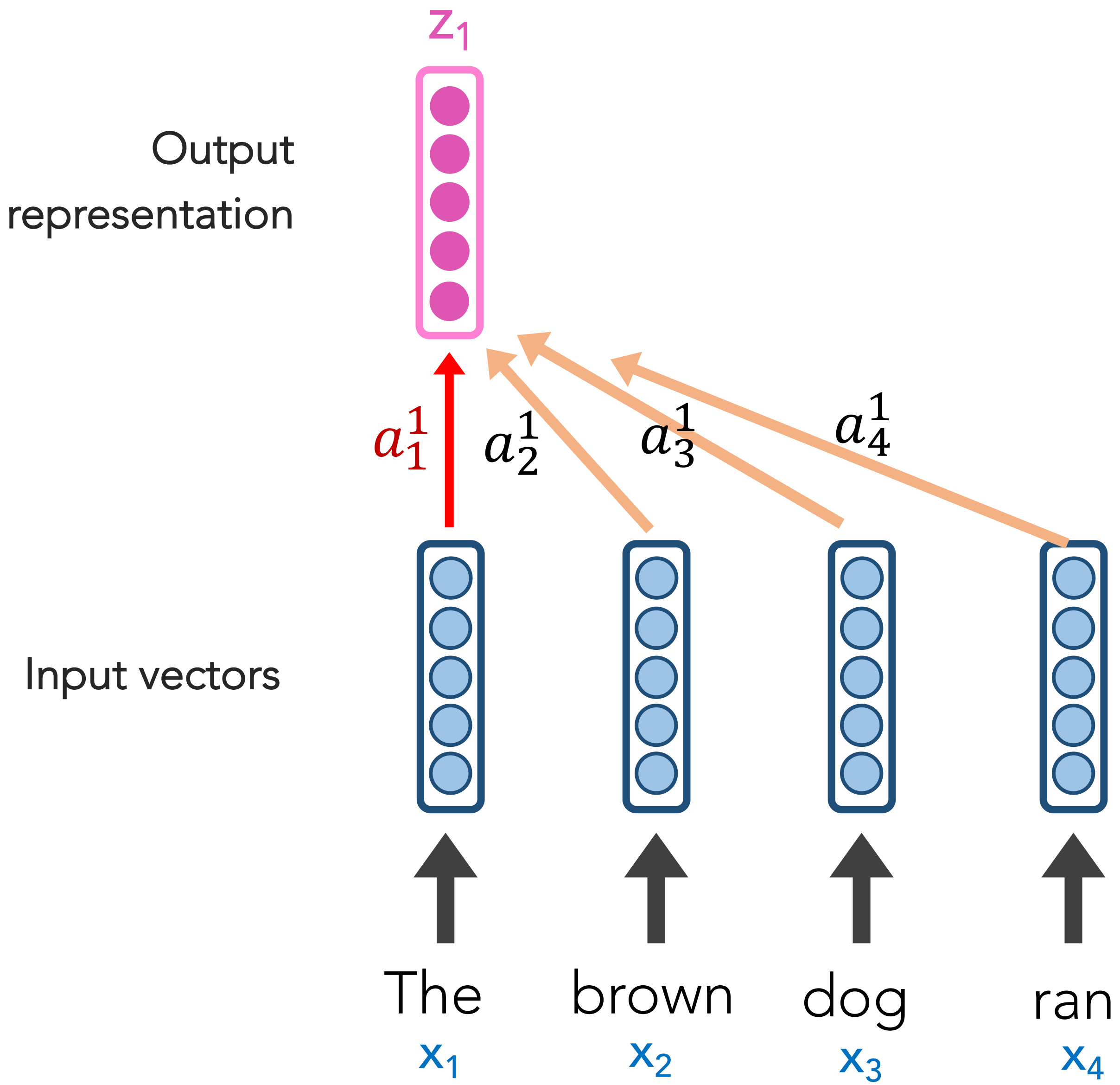


Self-Attention's goal is to create great representations, z_i, of the input

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 $\mathbf{q}_i$
- Key $\mathbf{k}_i$
- Value $\mathbf{v}_i$

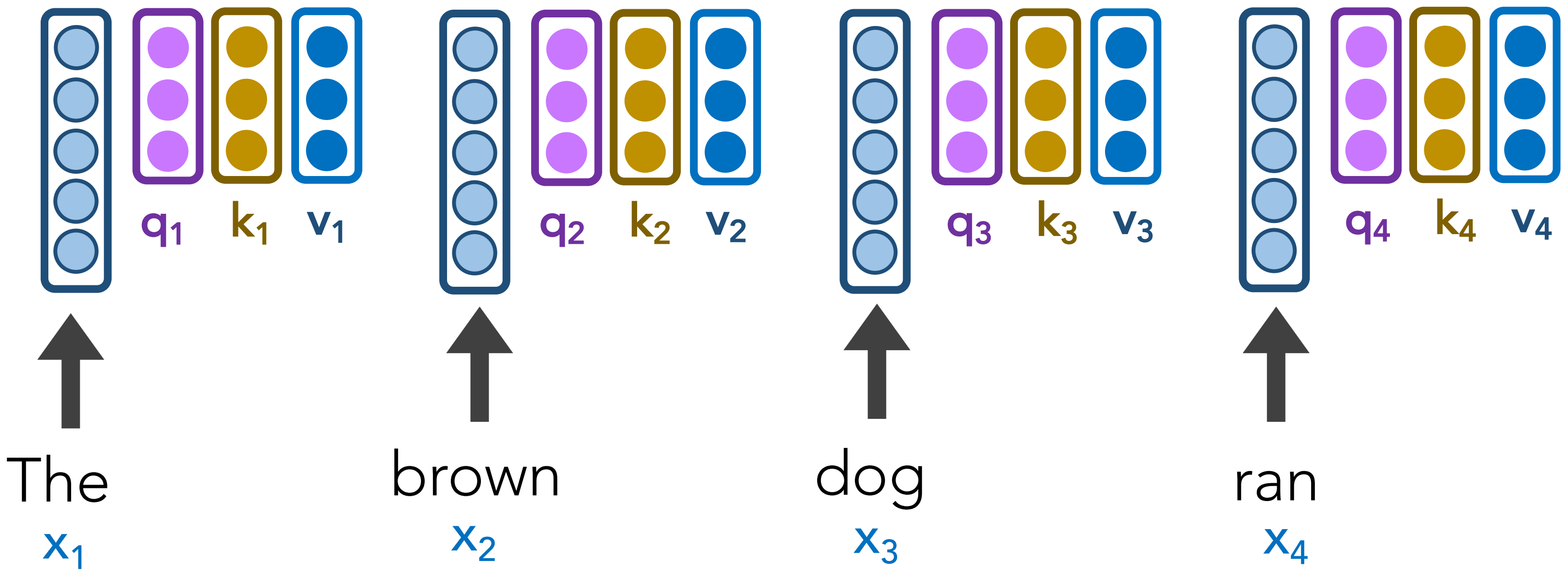
Self-Attention

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:

$$q_i = w_q x_i$$

$$k_i = w_k x_i$$

$$v_i = w_v x_i$$



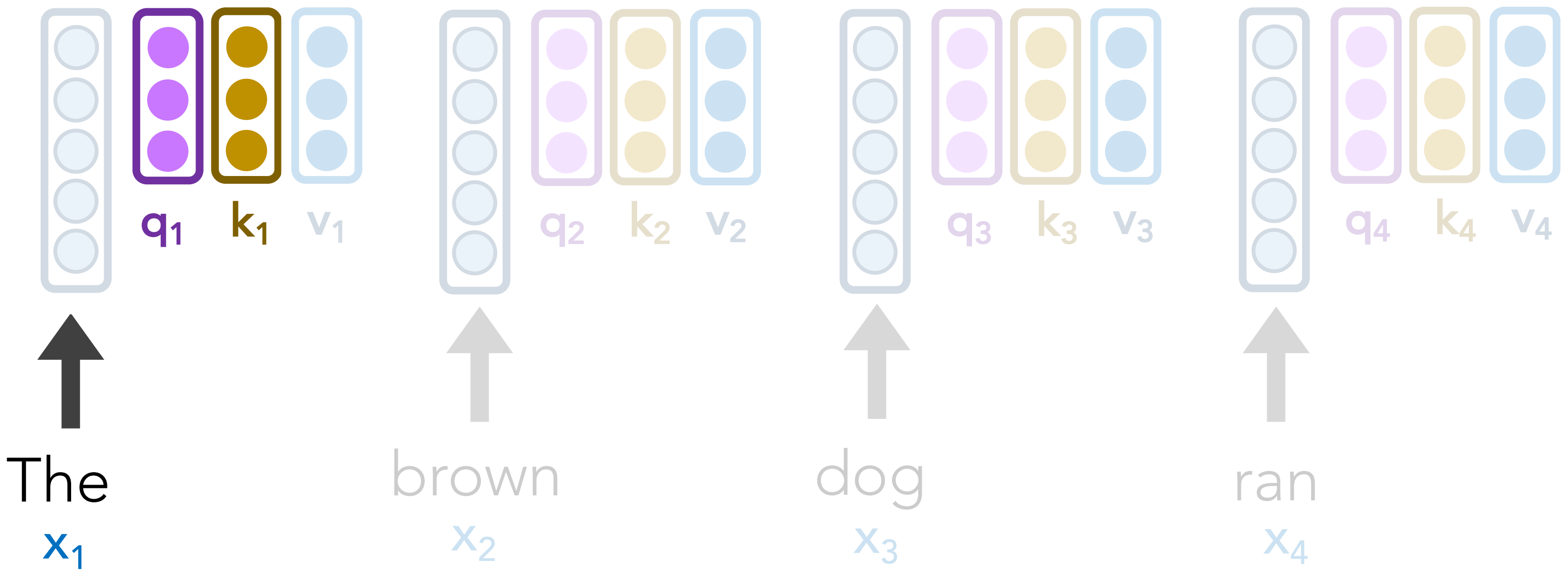
Under the hood, each x_i has 3 small, associated vectors. For example, x_1 has:

- Query $\mathbf{q_1}$
- Key $\mathbf{k_1}$
- Value $\mathbf{v_1}$

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

$s_1 = q_1 \cdot k_1 = 112$

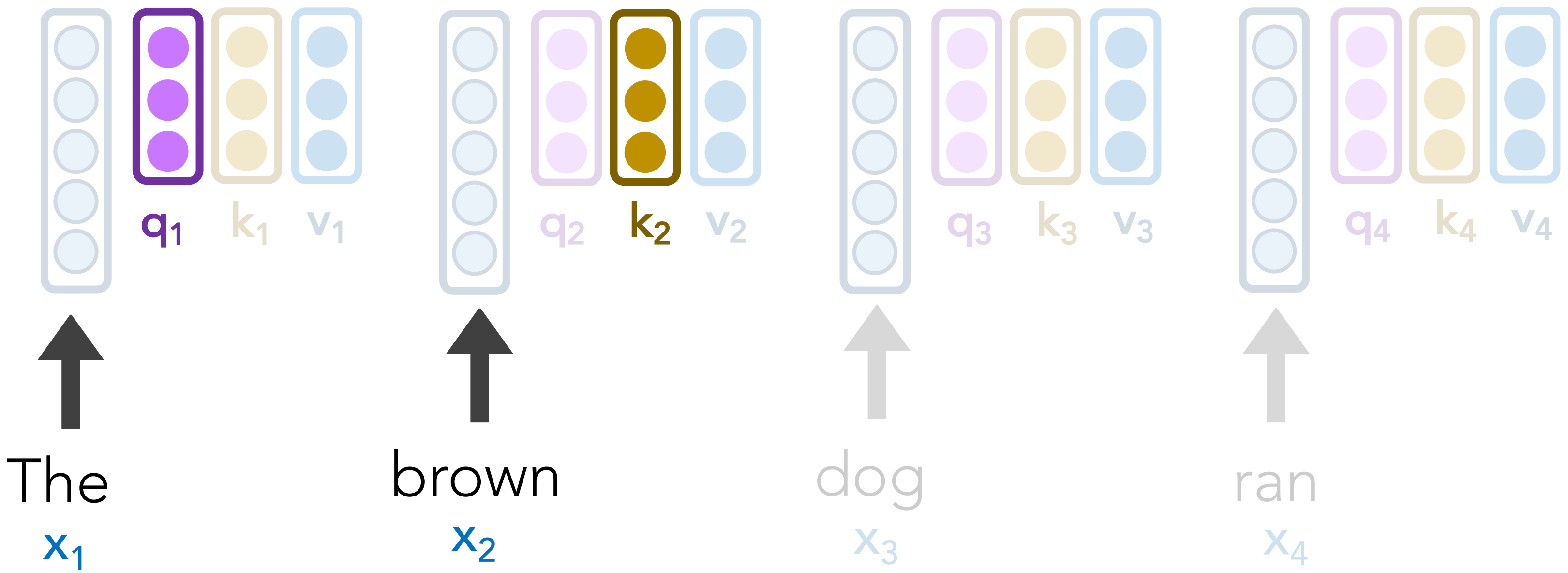


Self-Attention

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

$s_2 = q_1 \cdot k_2 = 96$

$s_1 = q_1 \cdot k_1 = 112$



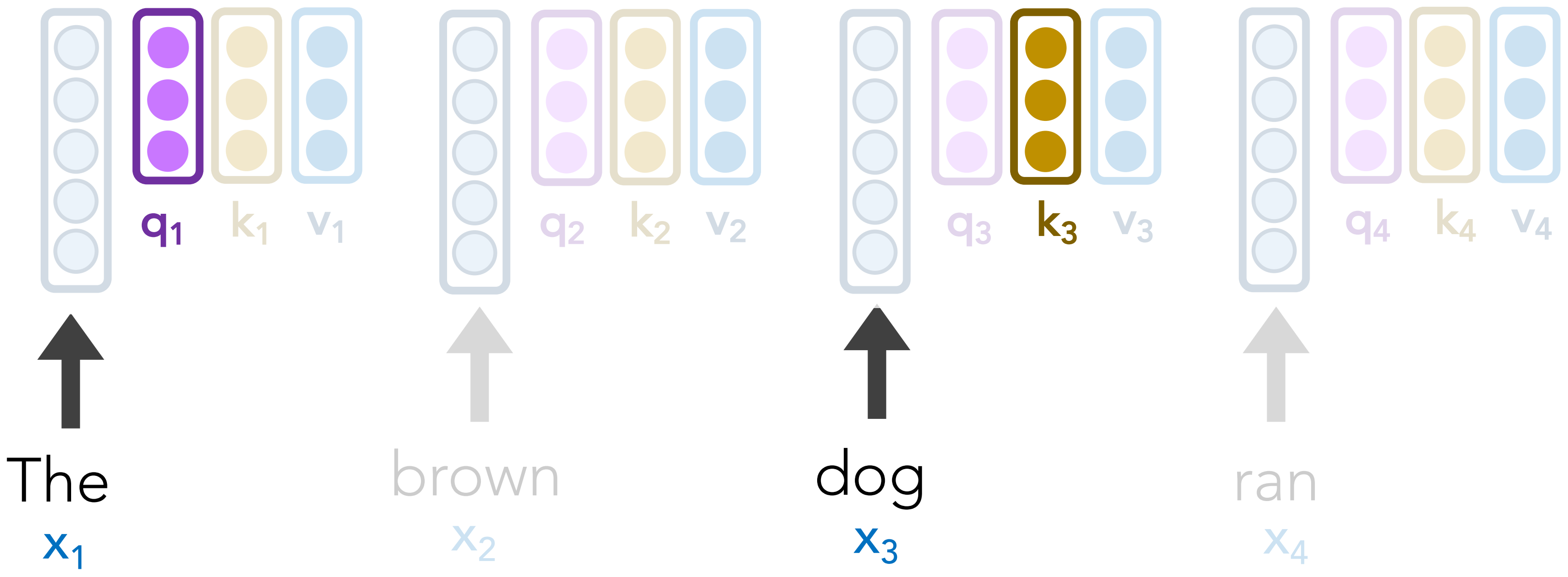
Self-Attention

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

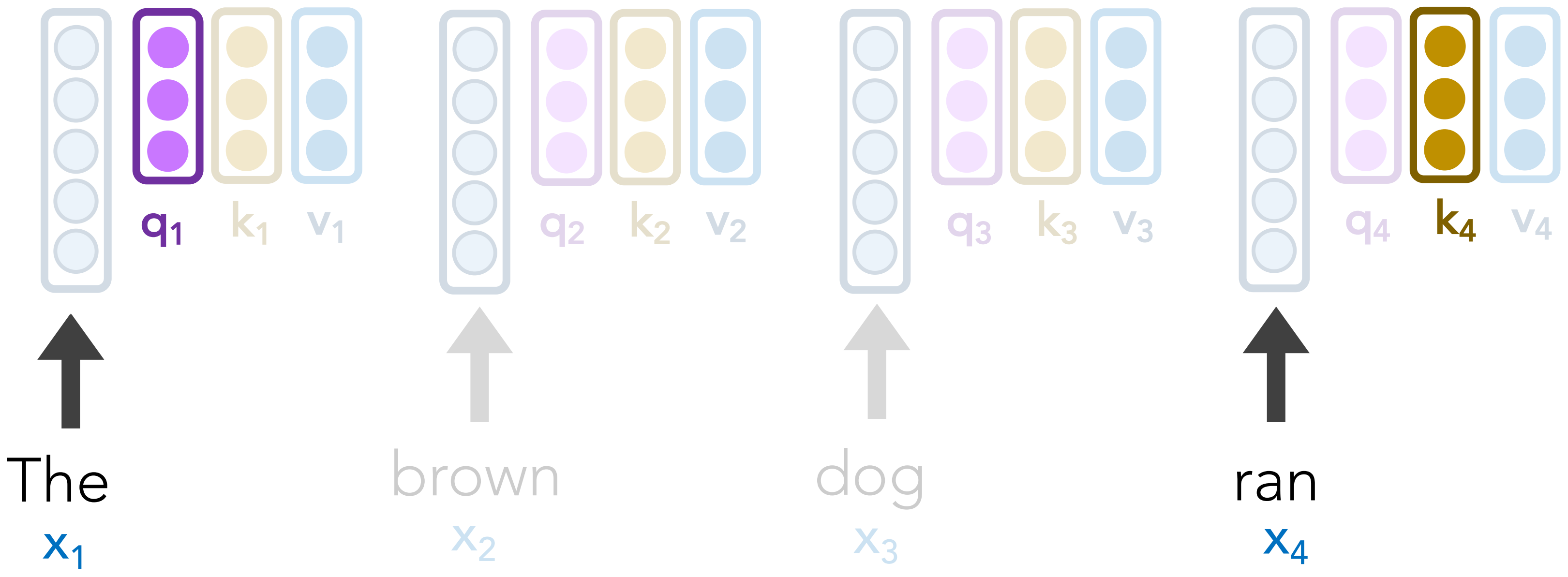
Step 2: For word x_1, let's calculate the scores s_1, s_2, s_3, s_4, which represent how much attention to pay to each respective "word" v_i

$s_4 = q_1 \cdot k_4 = 8$

$s_3 = q_1 \cdot k_3 = 16$

$s_2 = q_1 \cdot k_2 = 96$

$s_1 = q_1 \cdot k_1 = 112$



Self-Attention

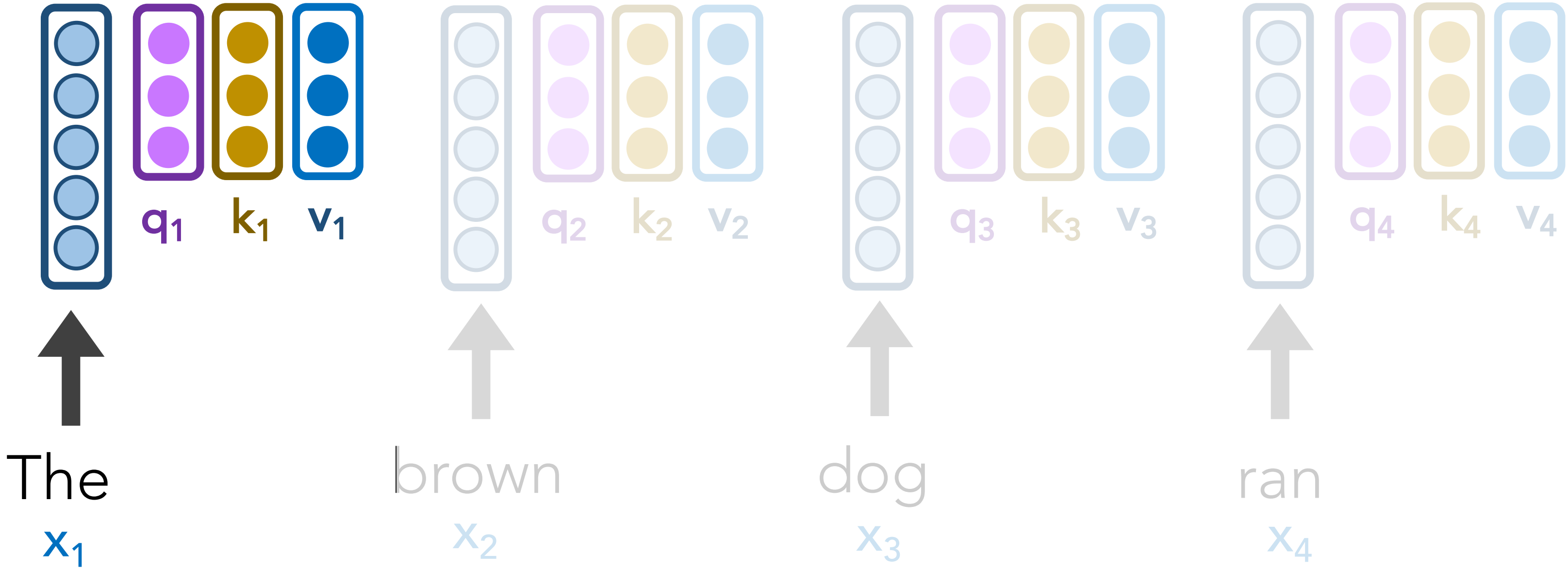
Step 3: Our scores s_1, s_2, s_3, s_4 don't sum to 1. Let's divide by $\sqrt{len(k_i)}$ and softmax it

$s_4 = q_1 \cdot k_4 = 8$ $\quad a_4 = \sigma(s_4/8) = 0$

$s_3 = q_1 \cdot k_3 = 16$ $\quad a_3 = \sigma(s_3/8) = .01$

$s_2 = q_1 \cdot k_2 = 96$ $\quad a_2 = \sigma(s_2/8) = .12$

$s_1 = q_1 \cdot k_1 = 112$ $\quad a_1 = \sigma(s_1/8) = .87$



Self-Attention

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

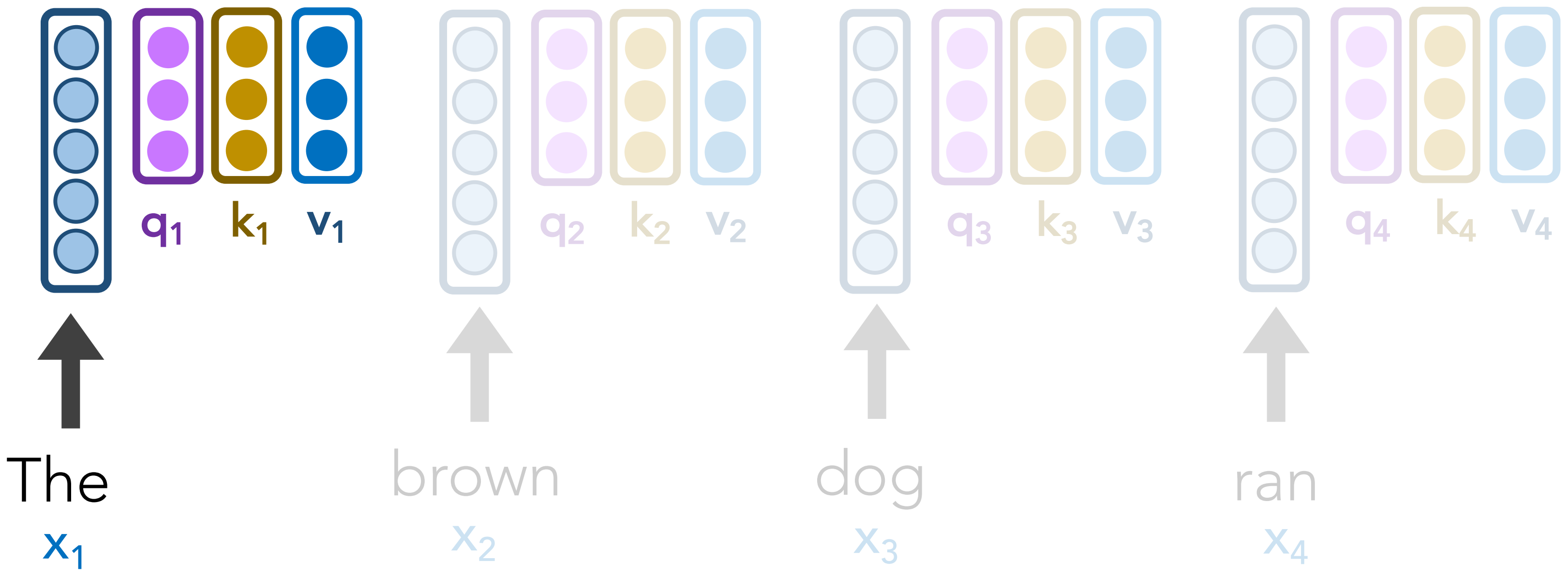
$s_4 = q_1 \cdot k_4 = 8$ $a_4 = \sigma(s_4/8) = 0$

$s_3 = q_1 \cdot k_3 = 16$ $a_3 = \sigma(s_3/8) = .01$

$s_2 = q_1 \cdot k_2 = 96$ $a_2 = \sigma(s_2/8) = .12$

$s_1 = q_1 \cdot k_1 = 112$ $a_1 = \sigma(s_1/8) = .87$

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



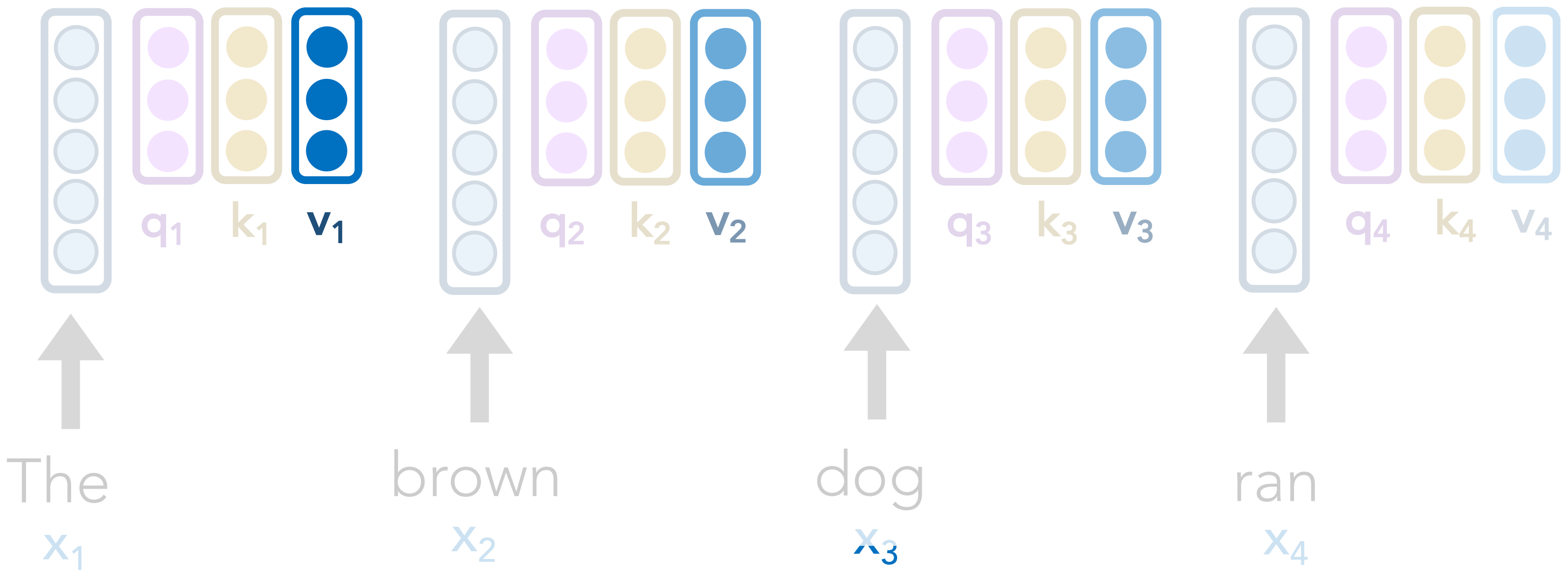
Self-Attention

Step 4: Let's weight our v_i vectors and simply sum them up!

z_1

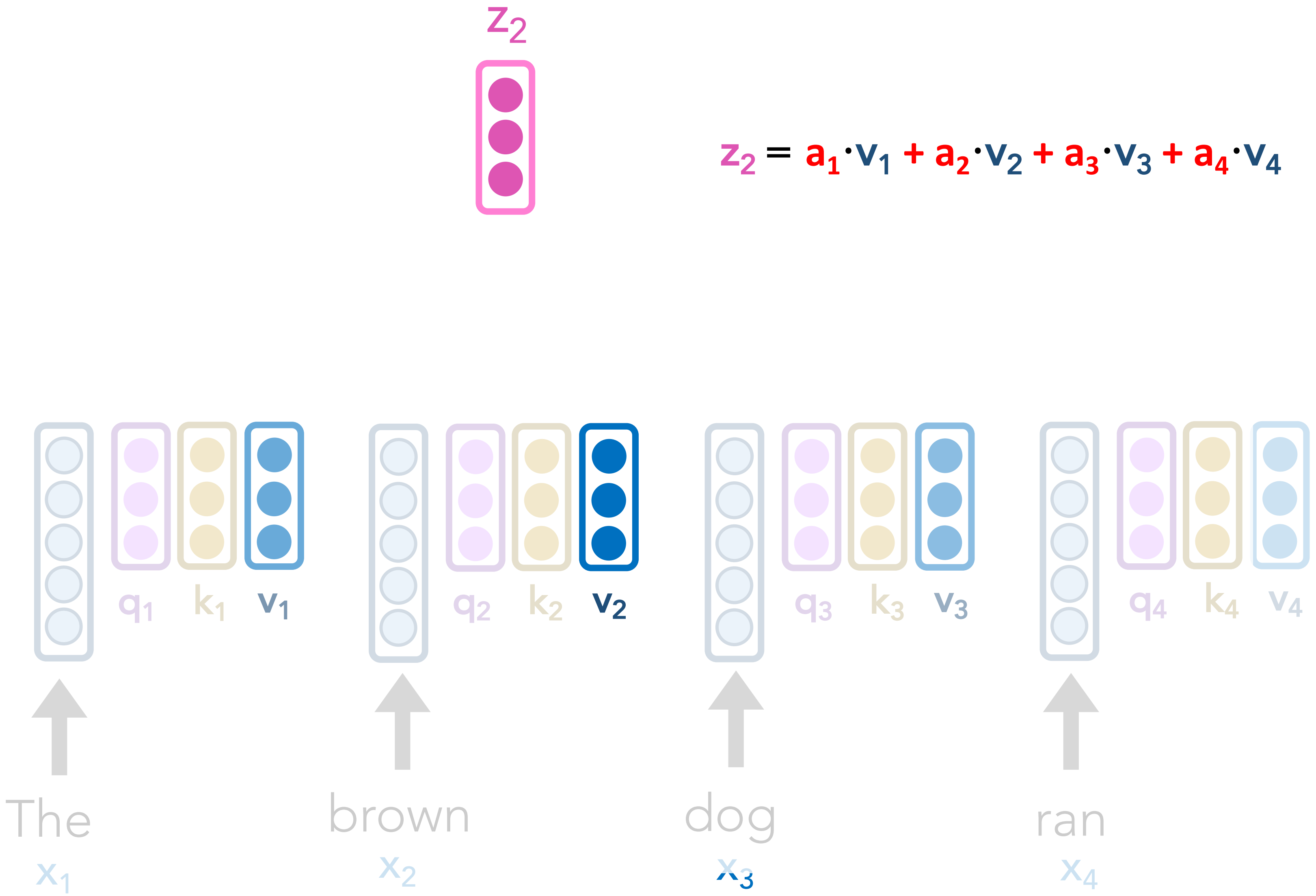
$$z_1 = a_1 \cdot v_1 + a_2 \cdot v_2 + a_3 \cdot v_3 + a_4 \cdot v_4$$

$$= 0.87 \cdot v_1 + 0.12 \cdot v_2 + 0.01 \cdot v_3 + 0 \cdot v_4$$



Self-Attention

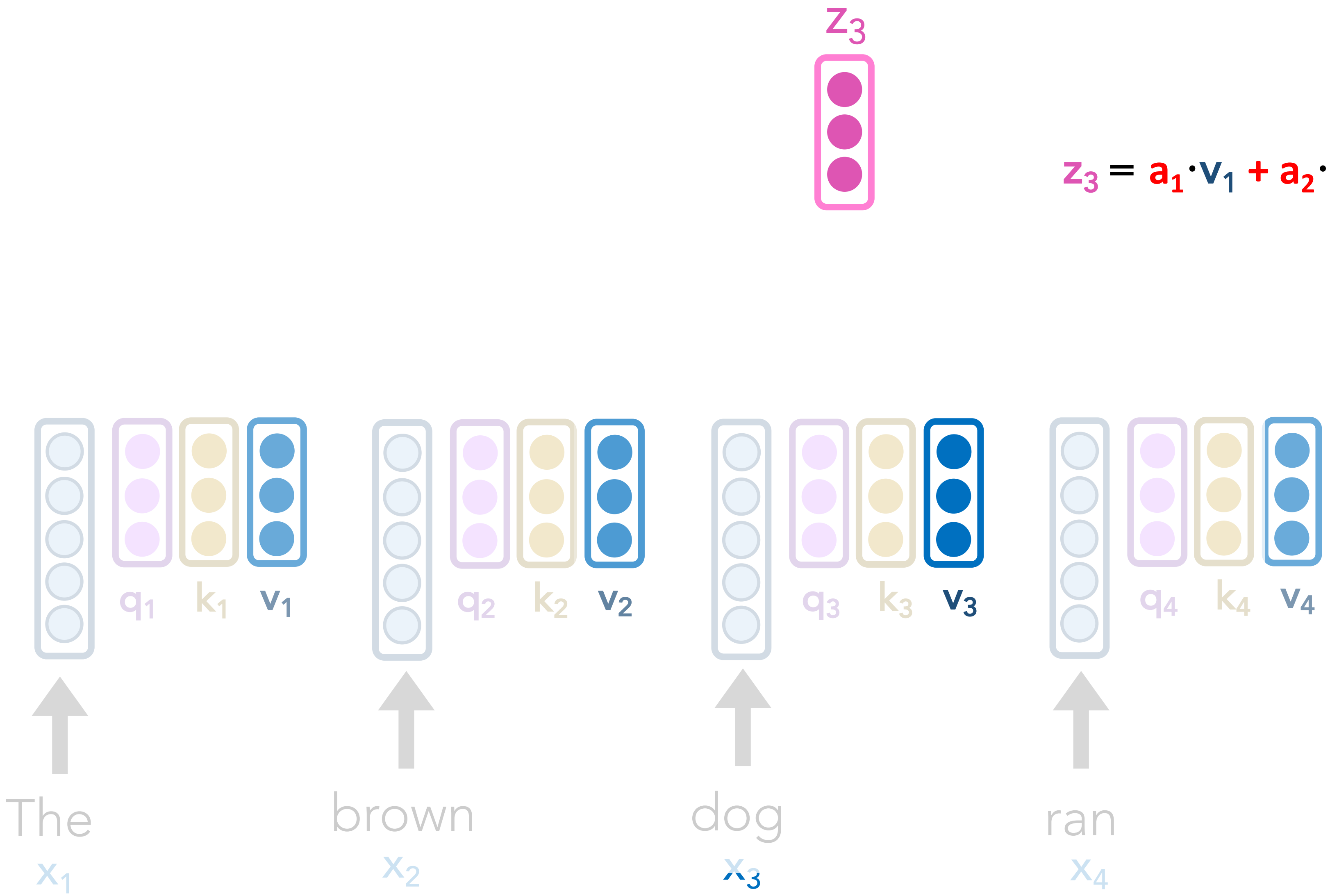
Step 5: We repeat this for all other words, yielding us with great, new z_i representations!



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

Self-Attention

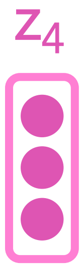
Step 5: We repeat this for all other words, yielding us with great, new z_i representations!



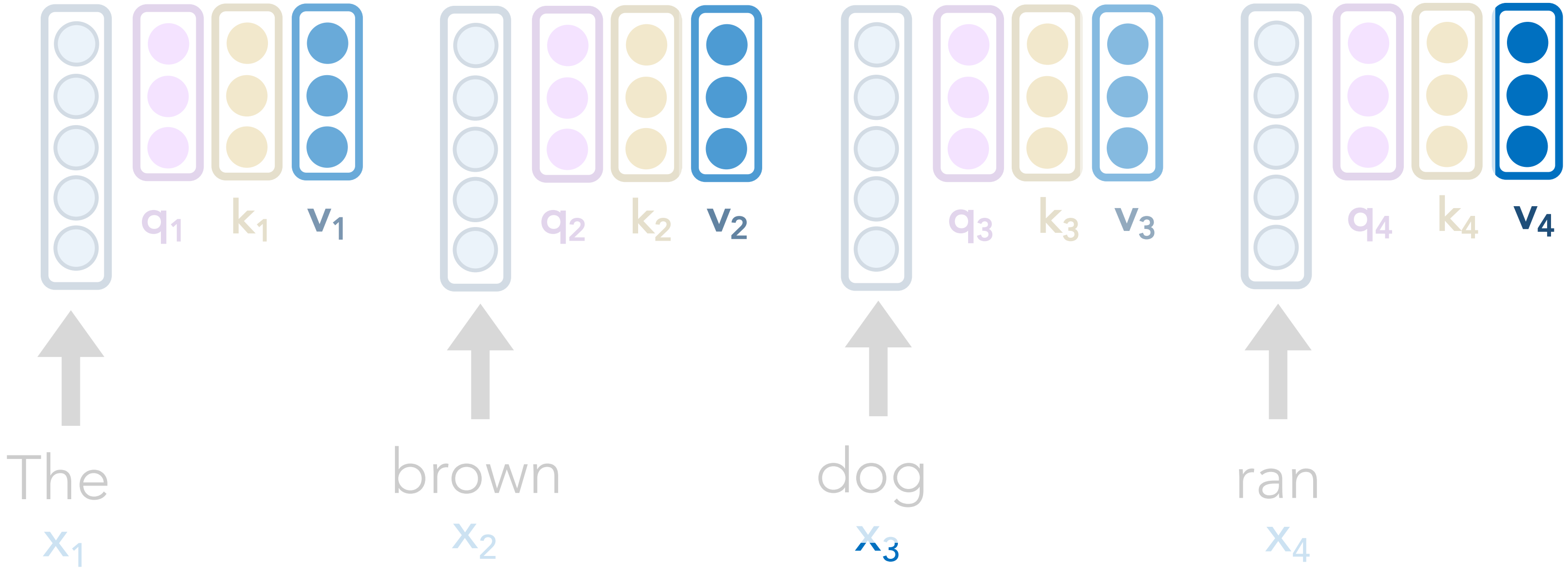
$$z_3 = a_1 \cdot v_1 + a_2 \cdot v_2 + a_3 \cdot v_3 + a_4 \cdot v_4$$

Self-Attention

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

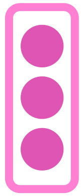


$$z_4 = a_1 \cdot v_1 + a_2 \cdot v_2 + a_3 \cdot v_3 + a_4 \cdot v_4$$



Let's illustrate another example:

z_2



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

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

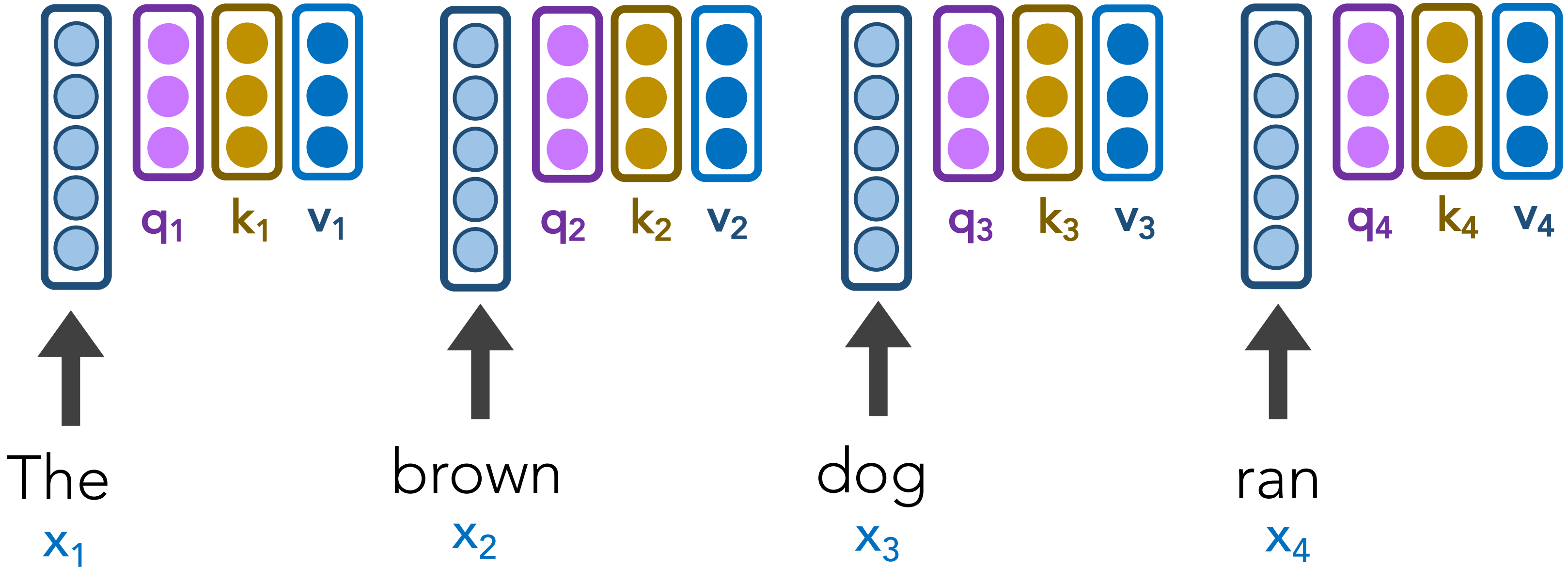
Self-Attention

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:

$$q_i = w_q x_i$$

$$k_i = w_k x_i$$

$$v_i = w_v x_i$$



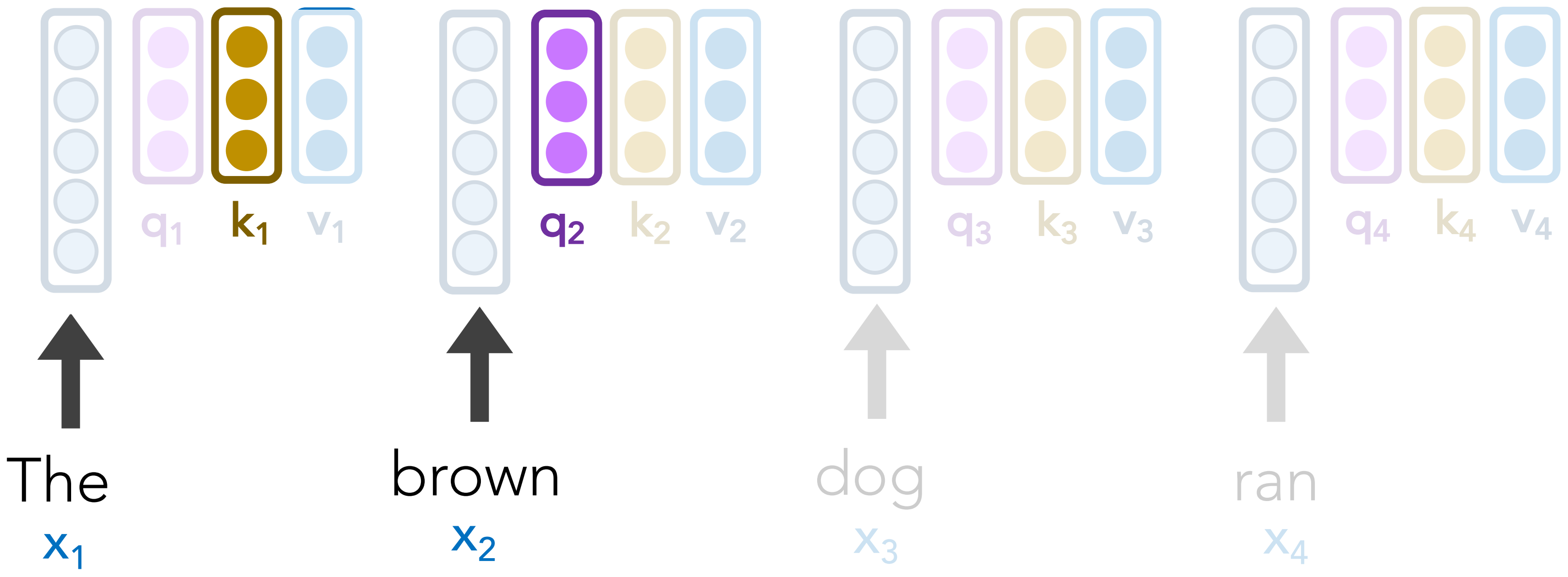
Under the hood, each x_i has 3 small, associated vectors. For example, x_1 has:

- Query $\mathbf{q_1}$
- Key $\mathbf{k_1}$
- Value $\mathbf{v_1}$

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

$s_1 = q_2 \cdot k_1 = 92$

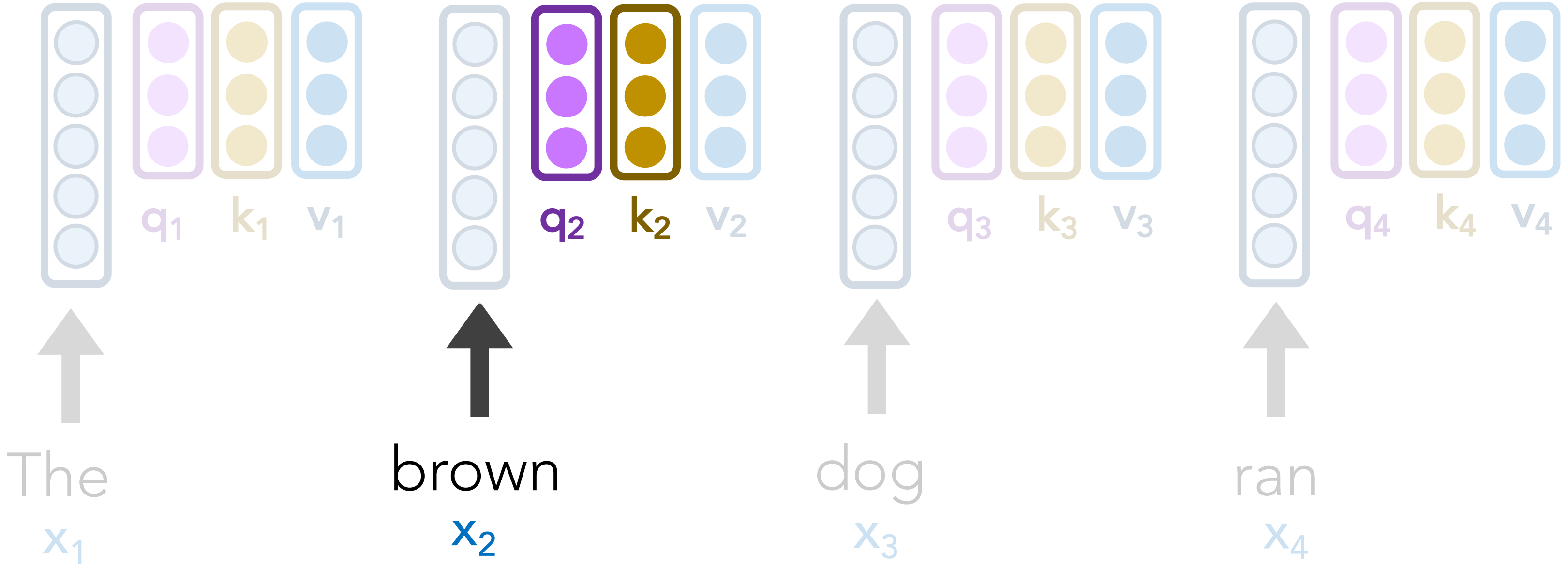


Self-Attention

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

$s_2 = q_2 \cdot k_2 = 124$

$s_1 = q_2 \cdot k_1 = 92$



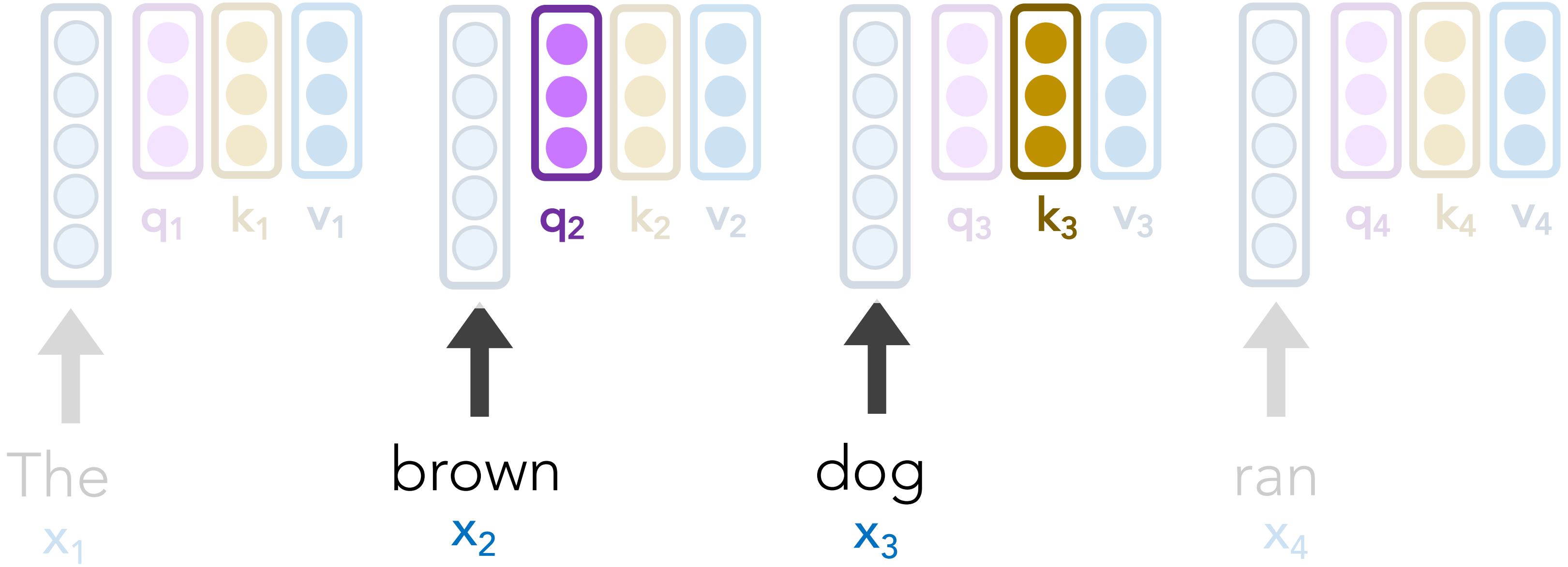
Self-Attention

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

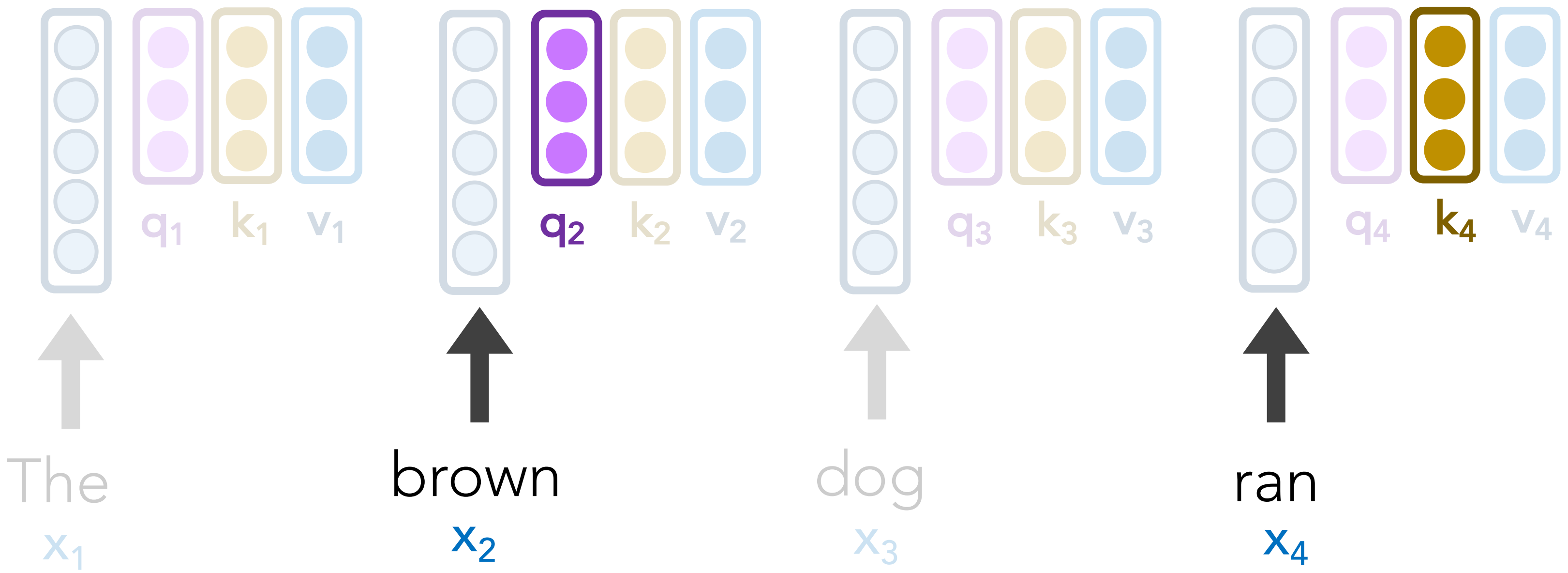
Step 2: For word x_2, let's calculate the scores s_1, s_2, s_3, s_4, which represent how much attention to pay to each respective "word" v_i

$s_4 = q_2 \cdot k_4 = 8$

$s_3 = q_2 \cdot k_3 = 22$

$s_2 = q_2 \cdot k_2 = 124$

$s_1 = q_2 \cdot k_1 = 92$



Self-Attention

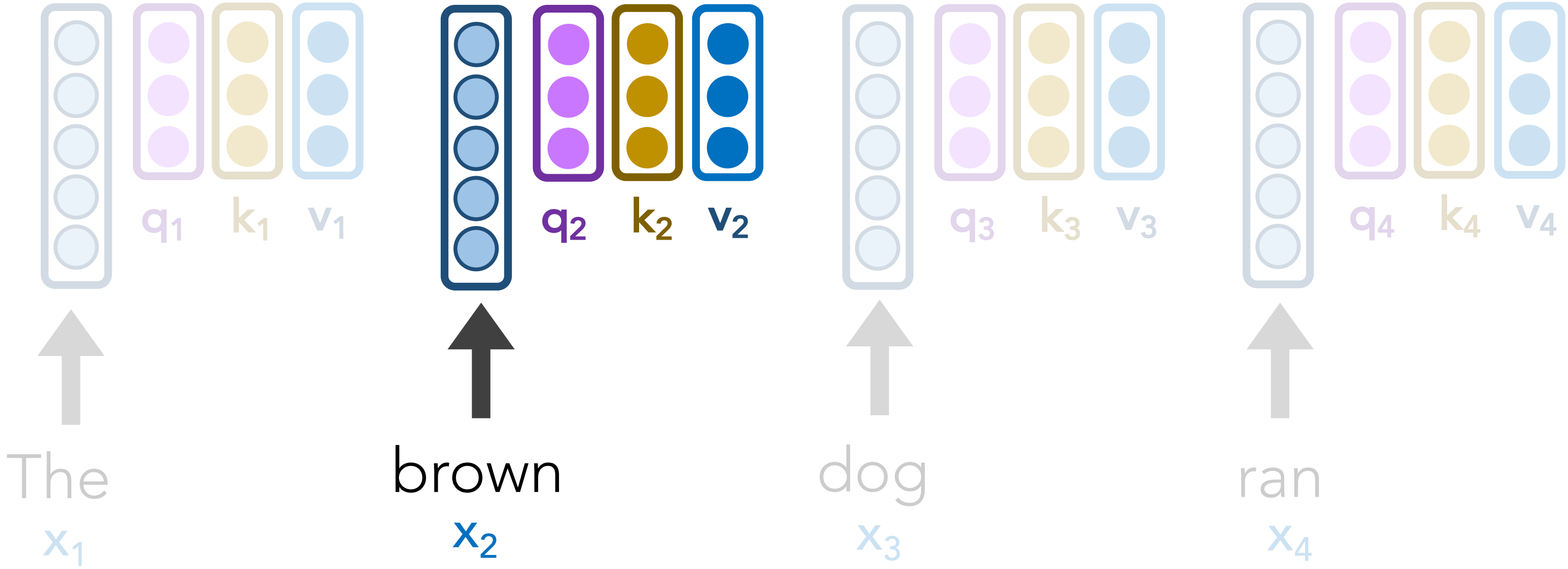
Step 3: Our scores s_1, s_2, s_3, s_4 don't sum to 1. Let's divide by $\sqrt{len(k_i)}$ and softmax it

$s_4 = q_2 \cdot k_4 = 8$ $\quad a_4 = \sigma(s_4/8) = 0$

$s_3 = q_2 \cdot k_3 = 22$ $\quad a_3 = \sigma(s_3/8) = .01$

$s_2 = q_2 \cdot k_2 = 124$ $\quad a_2 = \sigma(s_2/8) = .91$

$s_1 = q_2 \cdot k_1 = 92$ $\quad a_1 = \sigma(s_1/8) = .08$



Self-Attention

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

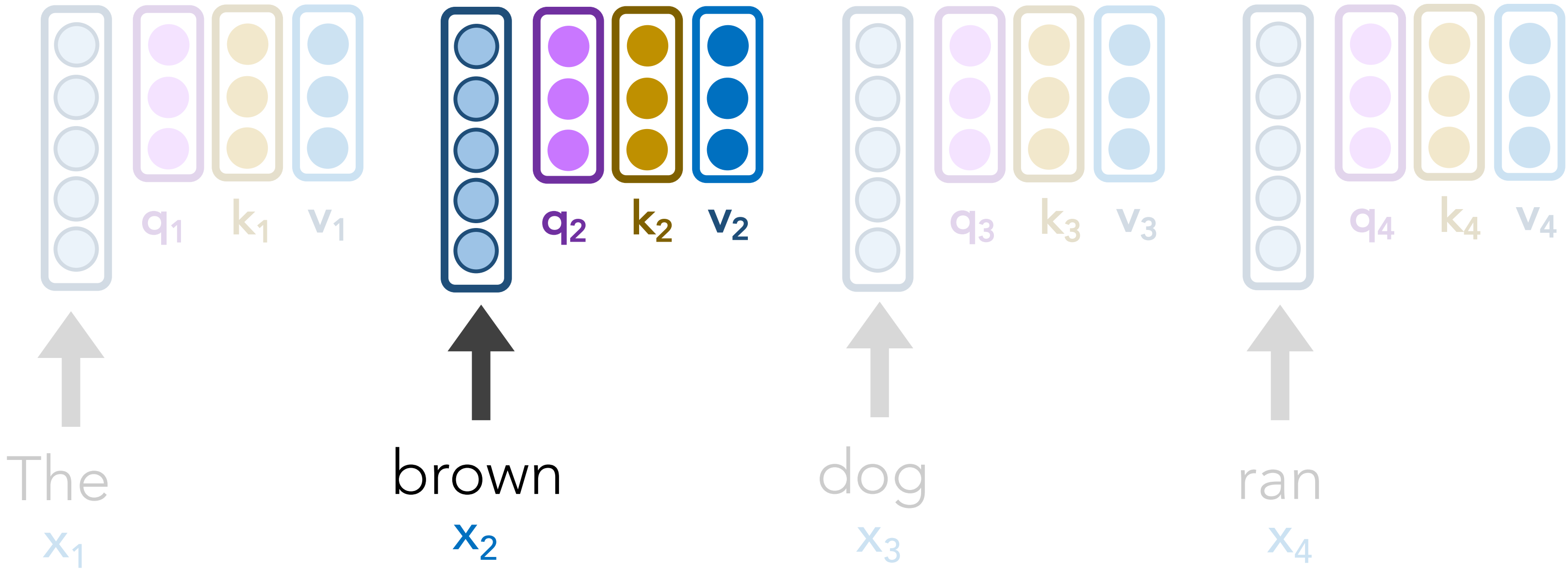
$s_4 = q_2 \cdot k_4 = 8$ $\quad a_4 = \sigma(s_4/8) = 0$

$s_3 = q_2 \cdot k_3 = 22$ $\quad a_3 = \sigma(s_3/8) = .01$

$s_2 = q_2 \cdot k_2 = 124$ $\quad a_2 = \sigma(s_2/8) = .91$

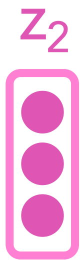
$s_1 = q_2 \cdot k_1 = 92$ $\quad a_1 = \sigma(s_1/8) = .08$

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



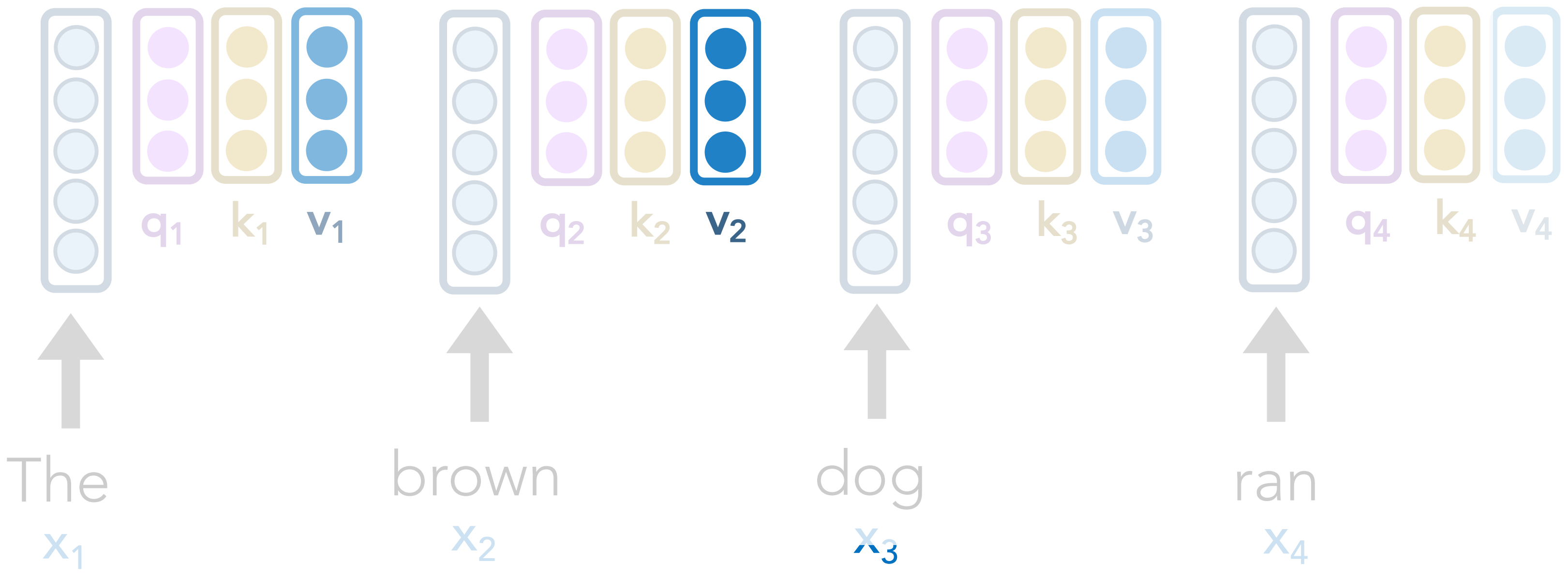
Self-Attention

Step 4: Let's weight our v_i vectors and simply sum them up!



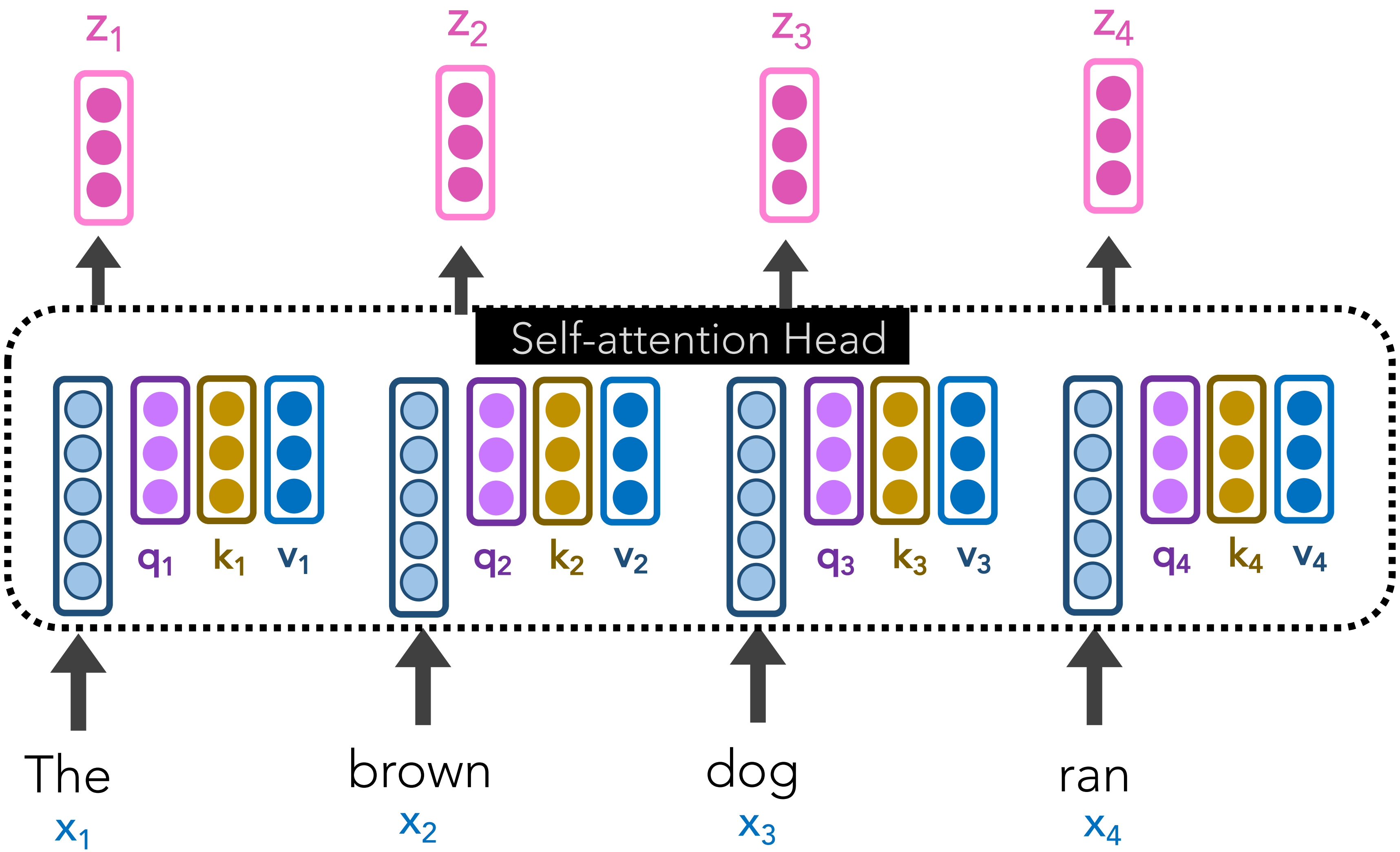
$$z_2 = a_1 \cdot v_1 + a_2 \cdot v_2 + a_3 \cdot v_3 + a_4 \cdot v_4$$

$$= 0.08 \cdot v_1 + 0.91 \cdot v_2 + 0.01 \cdot v_3 + 0 \cdot v_4$$



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