Understanding Large Language Models

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Session 03: LSTMs & Transformers

Main learning goals

1. Recap
   - backpropagation through time (BTTP)
   - vanishing (and exploding 💥) gradients
2. Long Short-Term Memory
   - intuition, architecture, variants
3. Bi-LSTM
   - model architecture, stacked Bi-LSTMs, ELMo
4. Attention
   - intuition, architecture, early transparency
5. Self-Attention
   - contextualized word embeddings, architecture
6. Transformers
   - transformer encoders, multi-headed self-attention, decoders, BERT

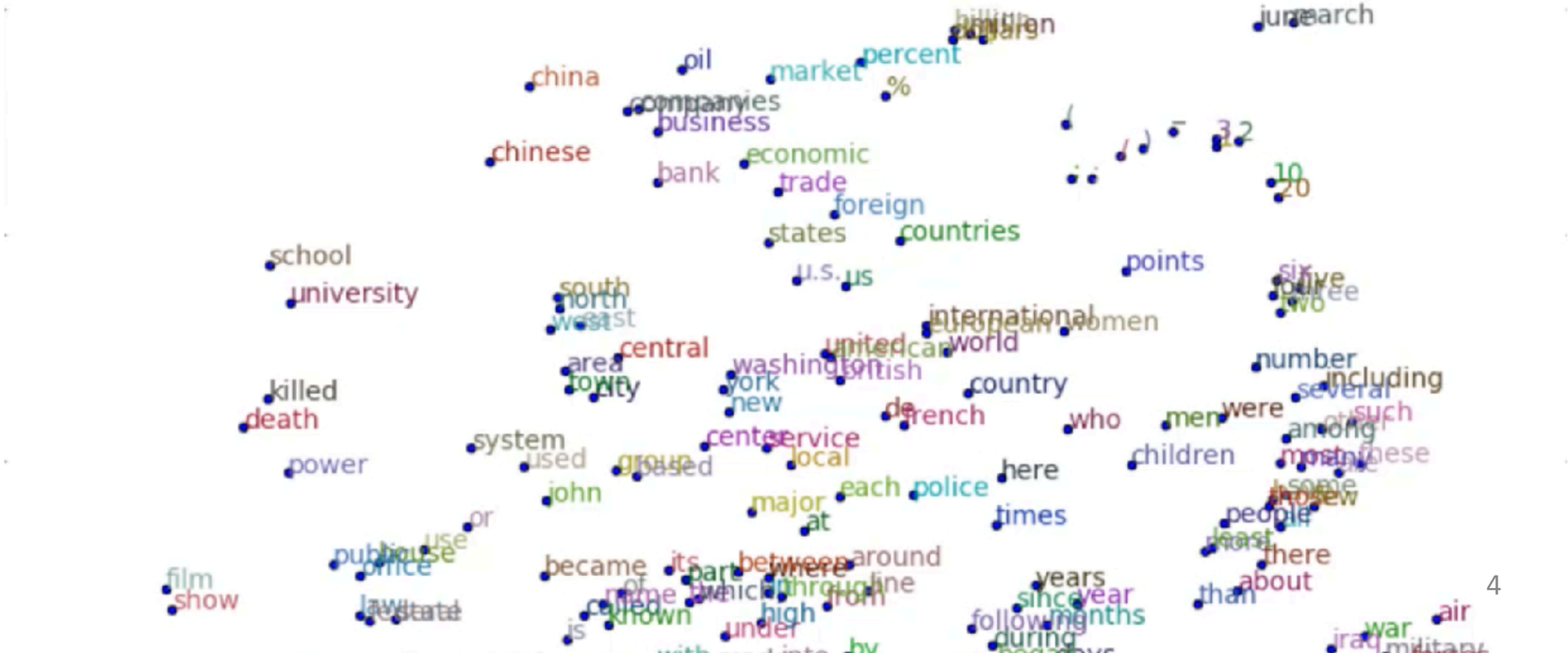
Slides adapted from: Chris Tanner CS287r

Recap

Recap: Embeddings

Distributed Representations: dense vectors (aka embeddings) that aim to convey the meaning of tokens:

- "word embeddings" refer to when you have type-based representations
- "contextualized embeddings" refer to when you have token-based representations



Recap: Language Modeling

An auto-regressive LM is one that only has access to the previous tokens (and the outputs become the inputs).

Evaluation: Perplexity

A masked LM can peak ahead, too. It "masks" a word within the context (e.g., the center word).

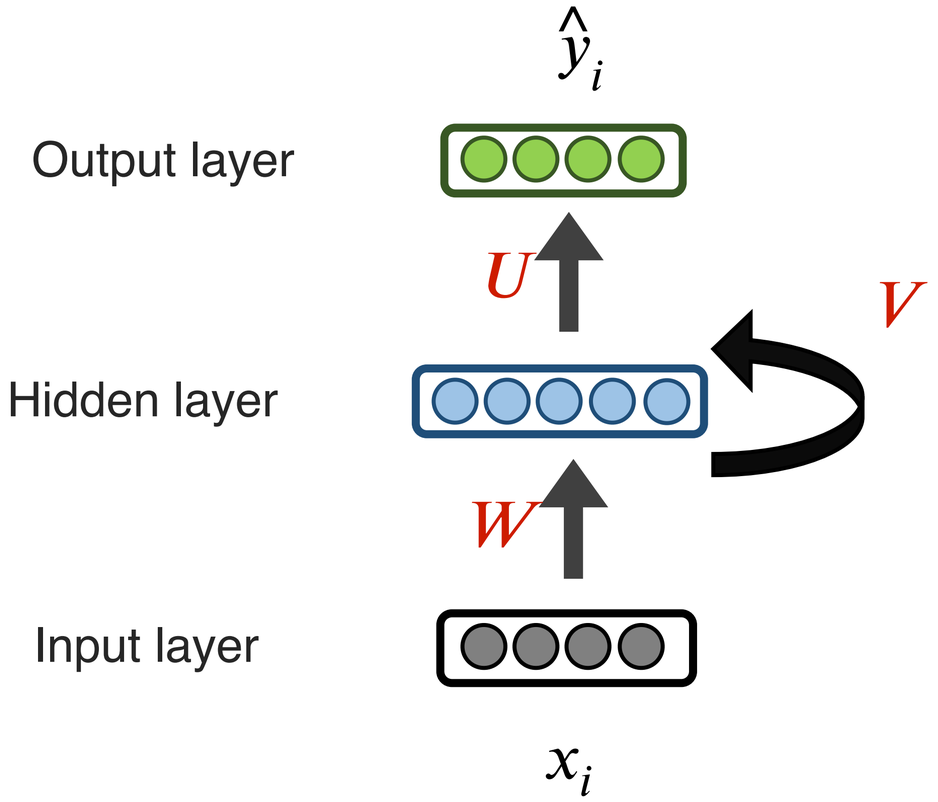
Evaluation: downstream NLP tasks that use the learned embeddings.

Both of these can produce useful word embeddings!

Recap: RNNs

- RNNs help capture more context while avoiding sparsity, storage, and compute issues!

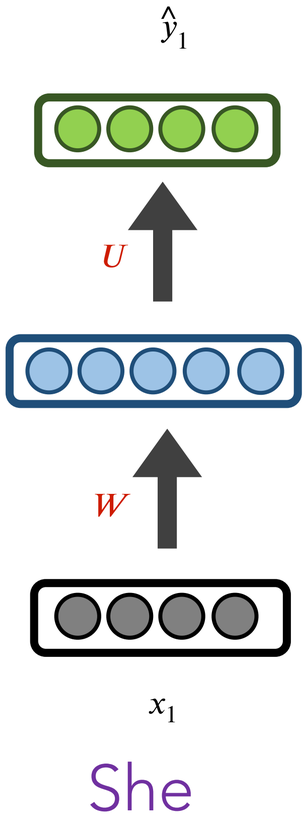
- The hidden layer is what we care about. It represents the word's "meaning".



Training Process

$$CE\left(y^i, \hat{y}^i\right) = -\sum_{w \in V} y^i_w \log(\hat{y}^i_w)$$

Error $CE\left(y^1, \hat{y}^1\right)$



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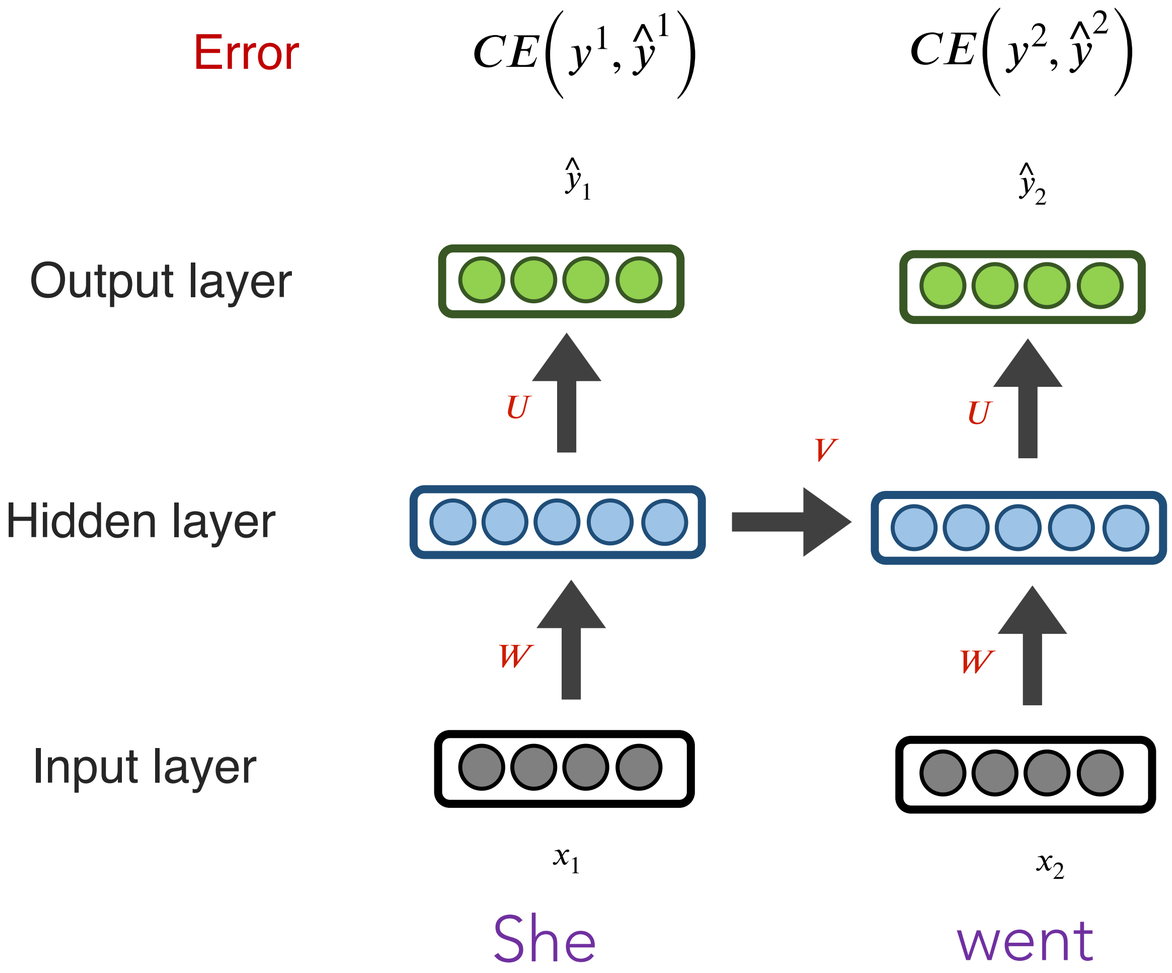
$$CE\left(y^i, \hat{y}^i\right) = -\sum_{w \in V} y_w^i \log(\hat{y}_w^i)$$



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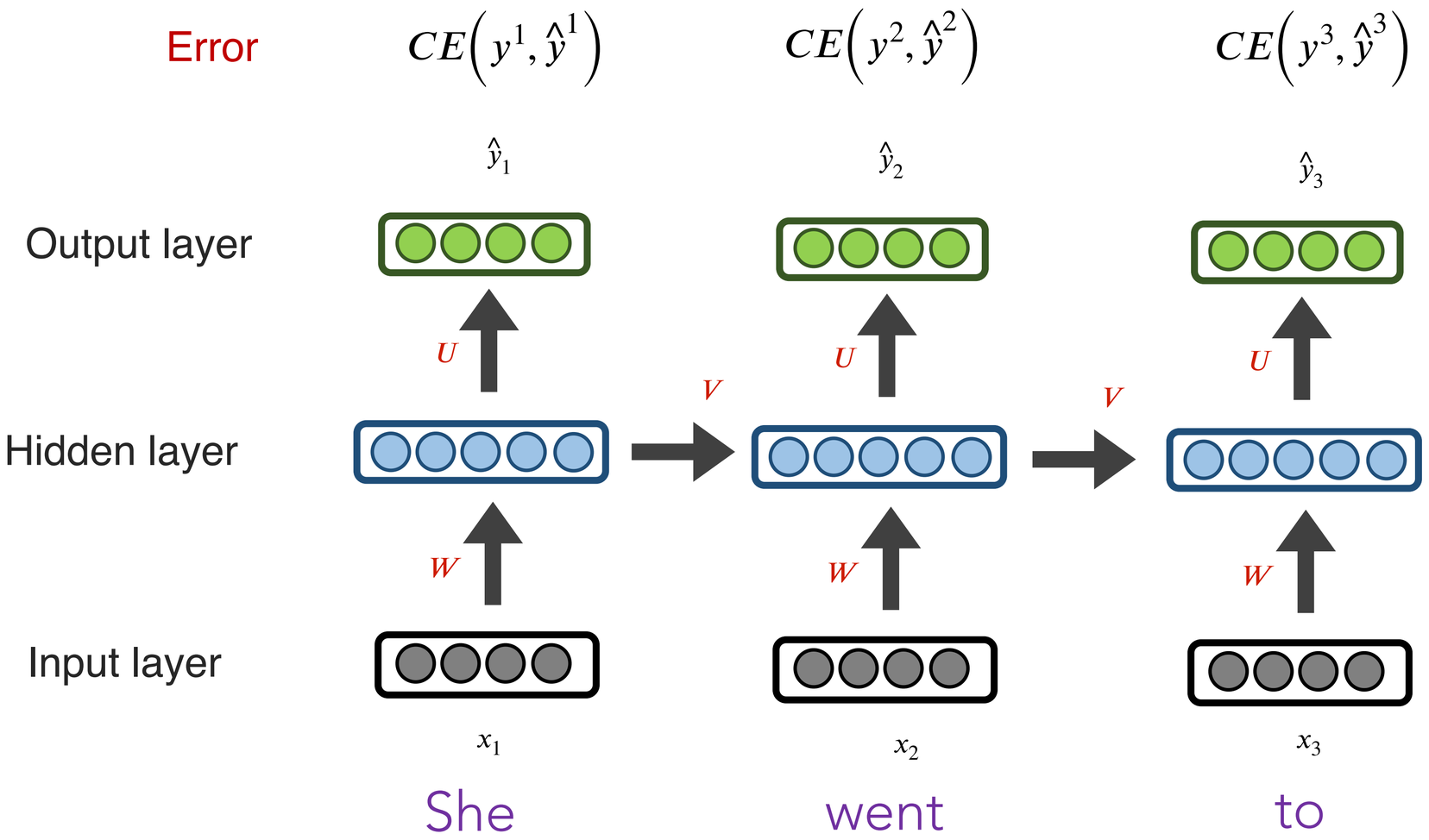

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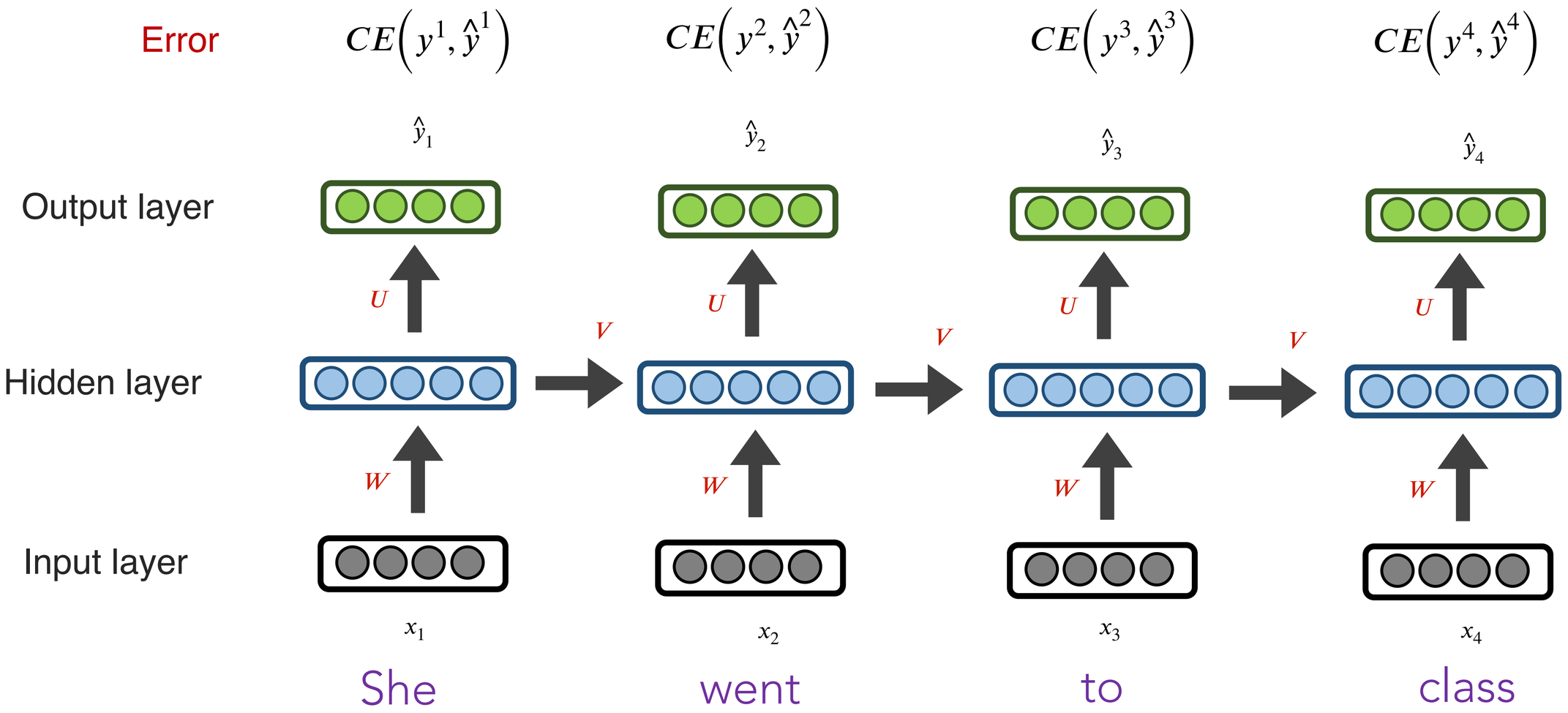

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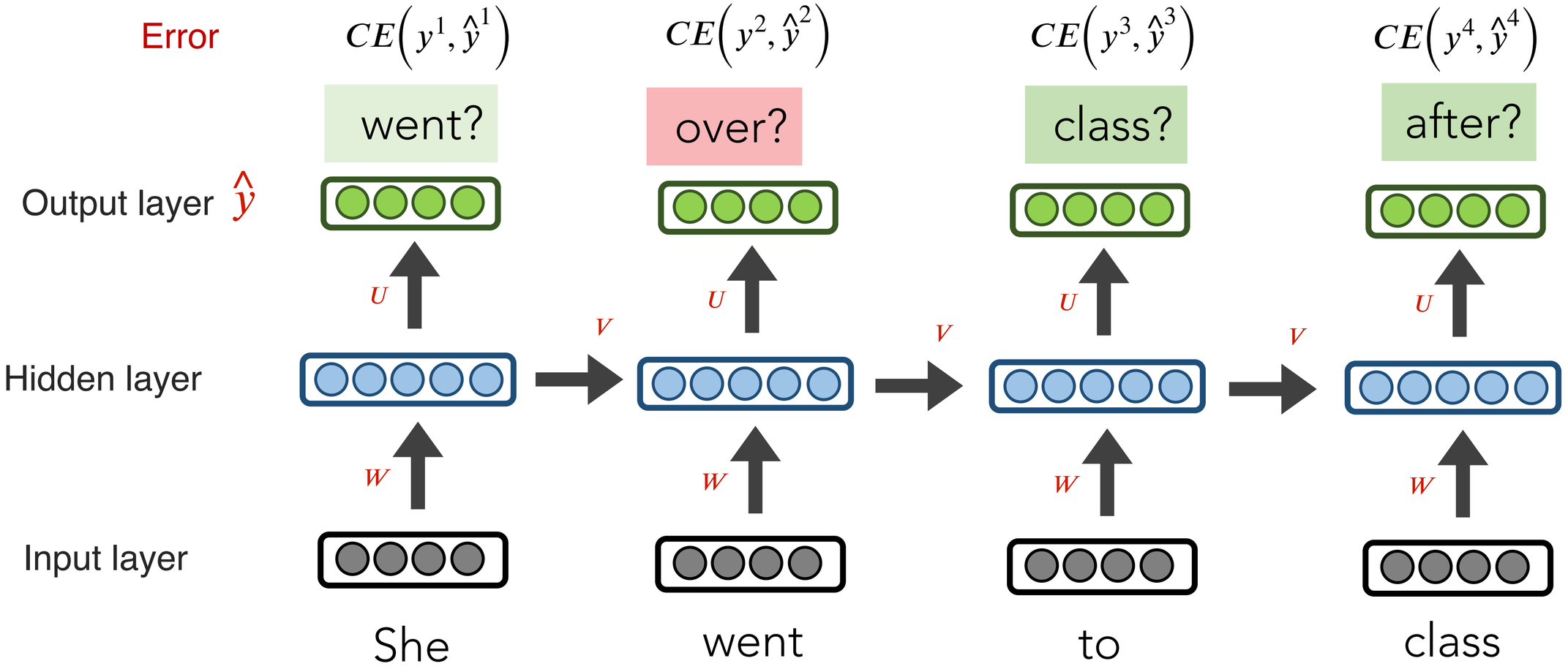

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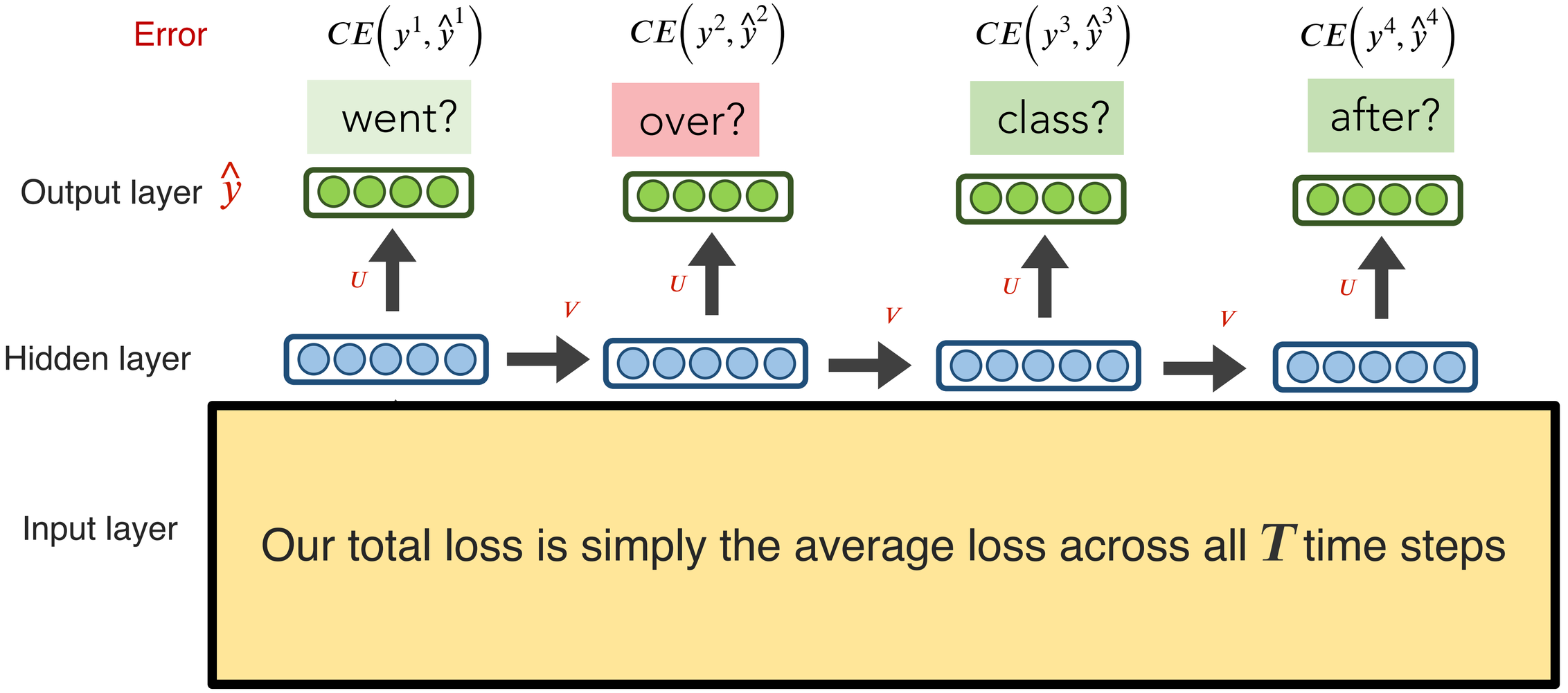
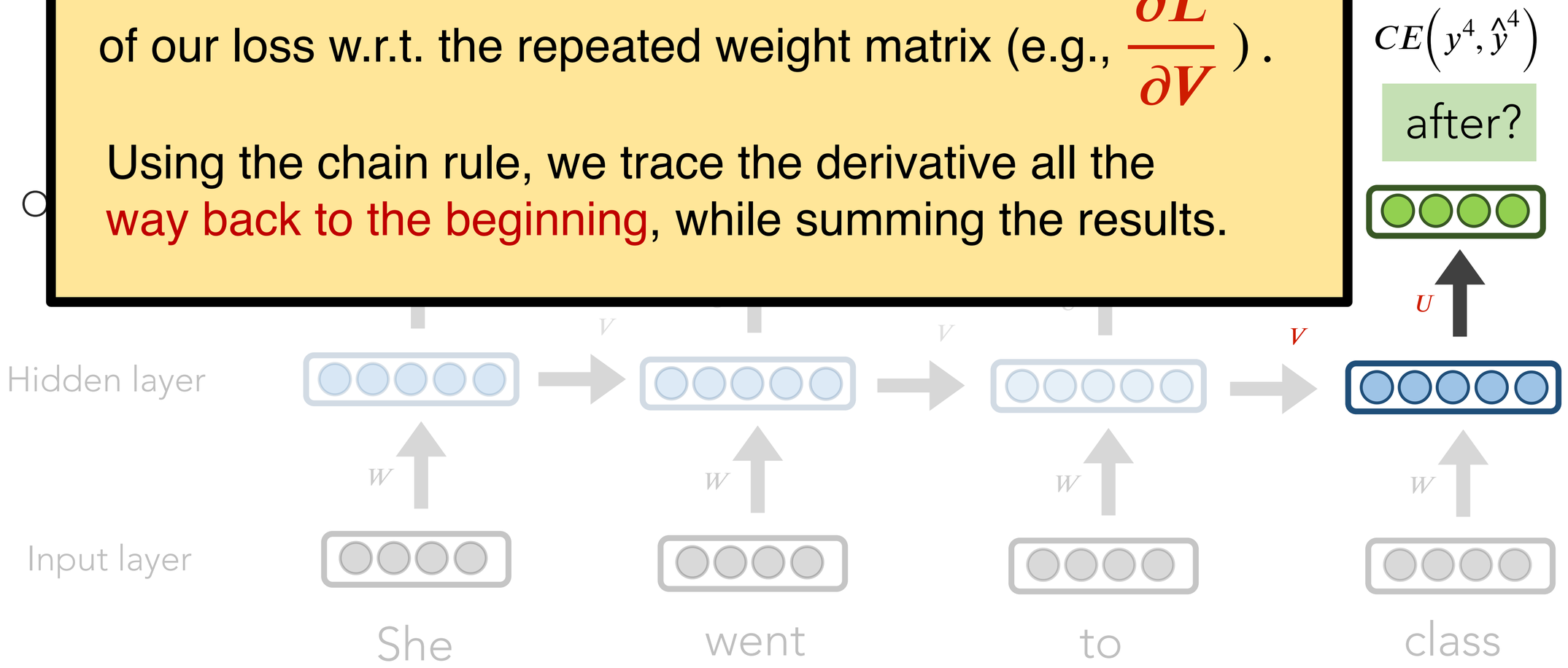


Training Details

To update our weights (e.g. V), we calculate the gradient of our loss w.r.t. the repeated weight matrix (e.g., $\frac{\partial L}{\partial V}$).

Using the chain rule, we trace the derivative all the way back to the beginning, while summing the results.



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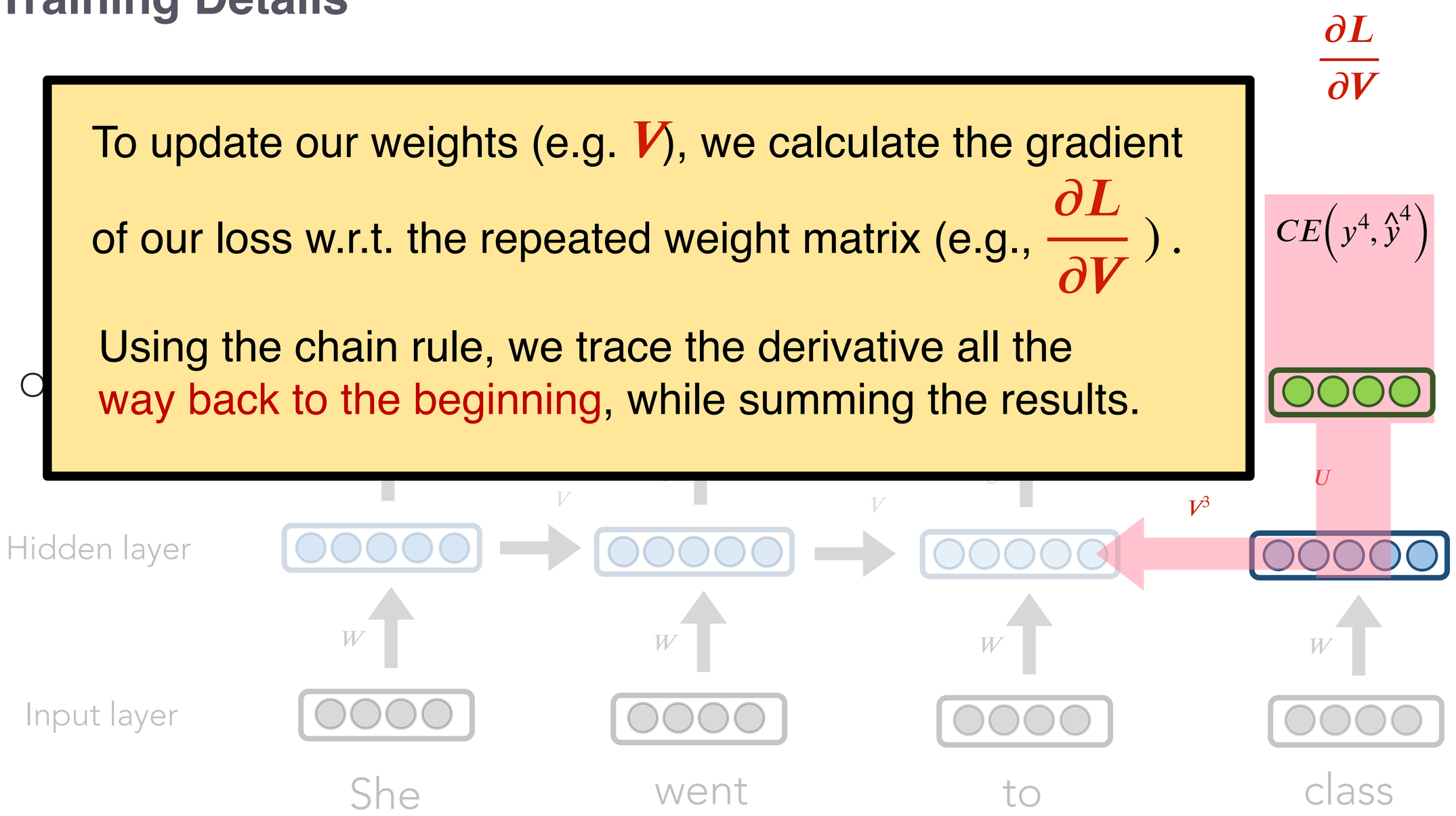

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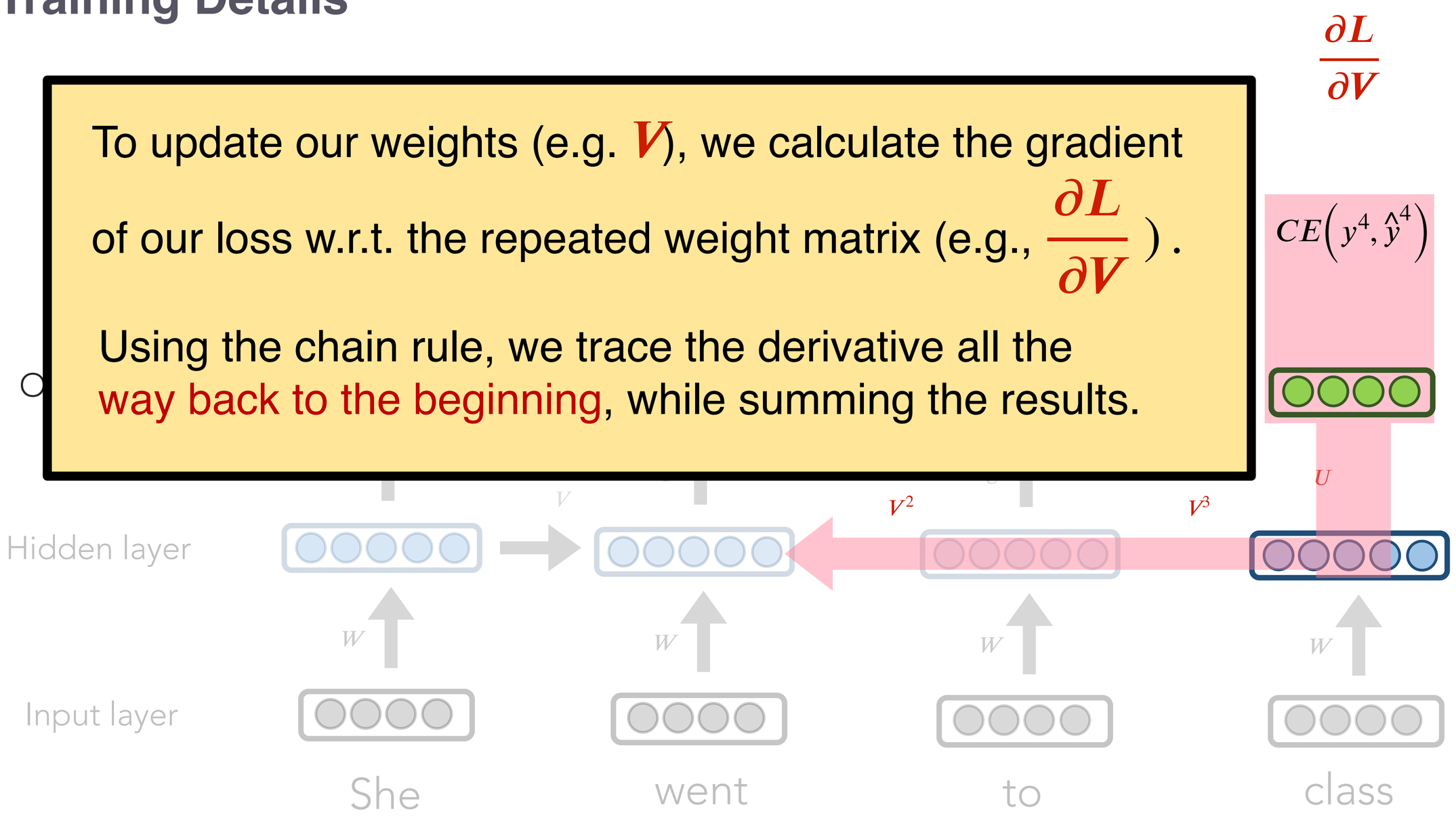

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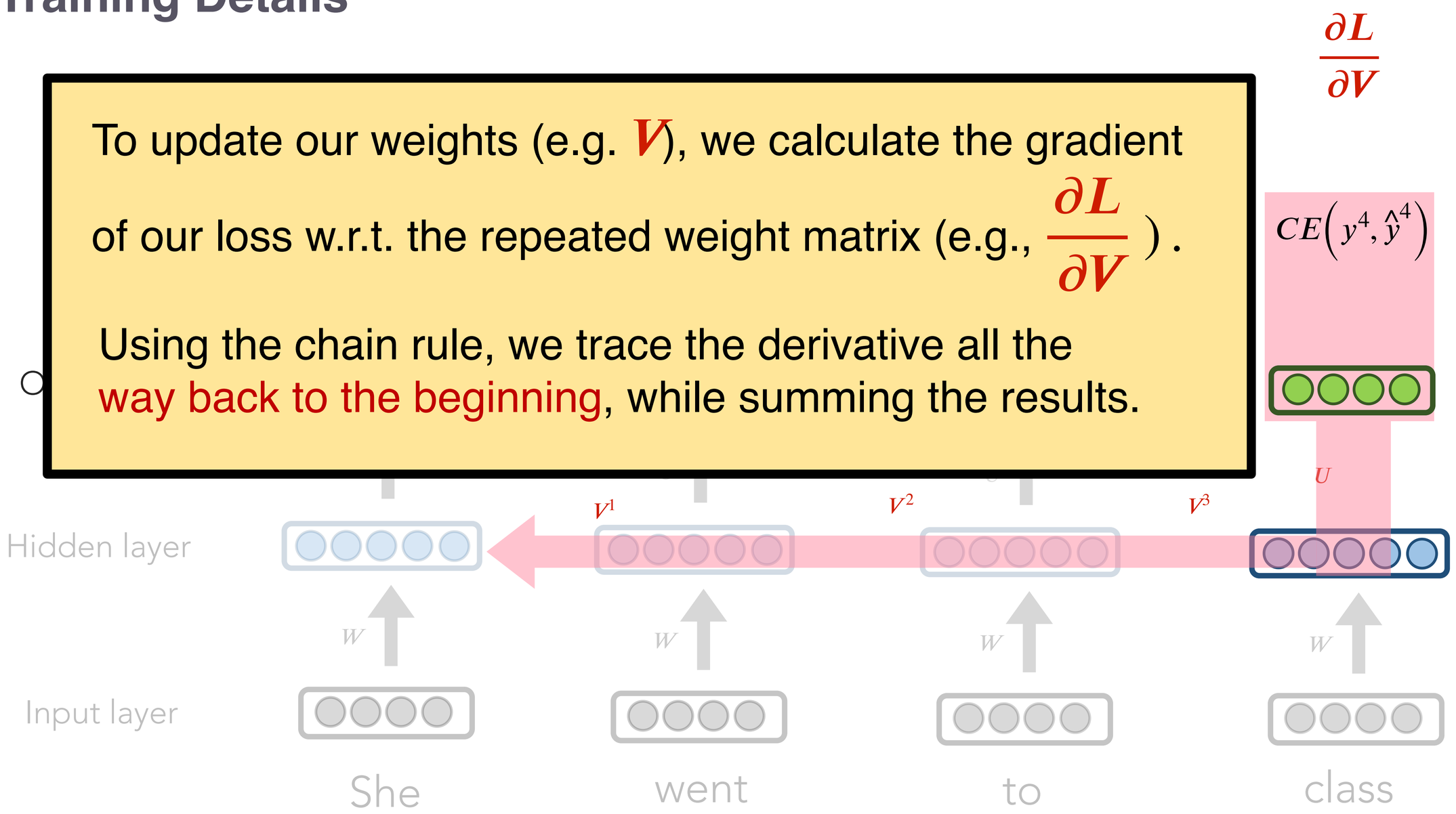


Training Details

- This backpropagation through time (BPTT) process is expensive
- Instead of updating after every time step, we tend to do so every T steps (e.g., every sentence or paragraph)
- This is not equivalent to using only a window size T (a la n-grams) because we still have “infinite memory”

Examples: Training on Harry Potter

"Sorry," Harry shouted, panicking—"I'll leave those brooms in London, are they?"

"No idea," said Nearly Headless Nick, casting low close by Cedric, carrying the last bit of treacle Charms, from Harry's shoulder, and to answer him the common room perched upon it, four arms held a shining knob from when the spider hadn't felt it seemed. He reached the teams too.

Source: https://medium.com/deep-writing/harry-potter-written-by-artificial-intelligence-8a9431803da6

Examples: Training on Recipes


```
      Title: CHOCOLATE RANCH BARBECUE
Categories: Game, Casseroles, Cookies, Cookies
      Yield: 6 Servings

      2 tb Parmesan cheese -- chopped
      1 c  Coconut milk
      3    Eggs, beaten

  Place each pasta over layers of lumps. Shape mixture into the moderate oven and simmer
  until firm. Serve hot in bodied fresh, mustard, orange and cheese.

  Combine the cheese and salt together the dough in a large skillet; add the ingredients
  and stir in the chocolate and pepper.
```

Source: https://gist.github.com/nylki/1efbaa36635956d35bcc

RNN Summary

Strengths

- Can handle infinite-length sequences (not just a fixed-window)
- Has a “memory” of the context (thanks to the hidden layer’s recurrent loop)
- Same weights used for all inputs, so positionality is not wonky/overwritten (like FFNN)

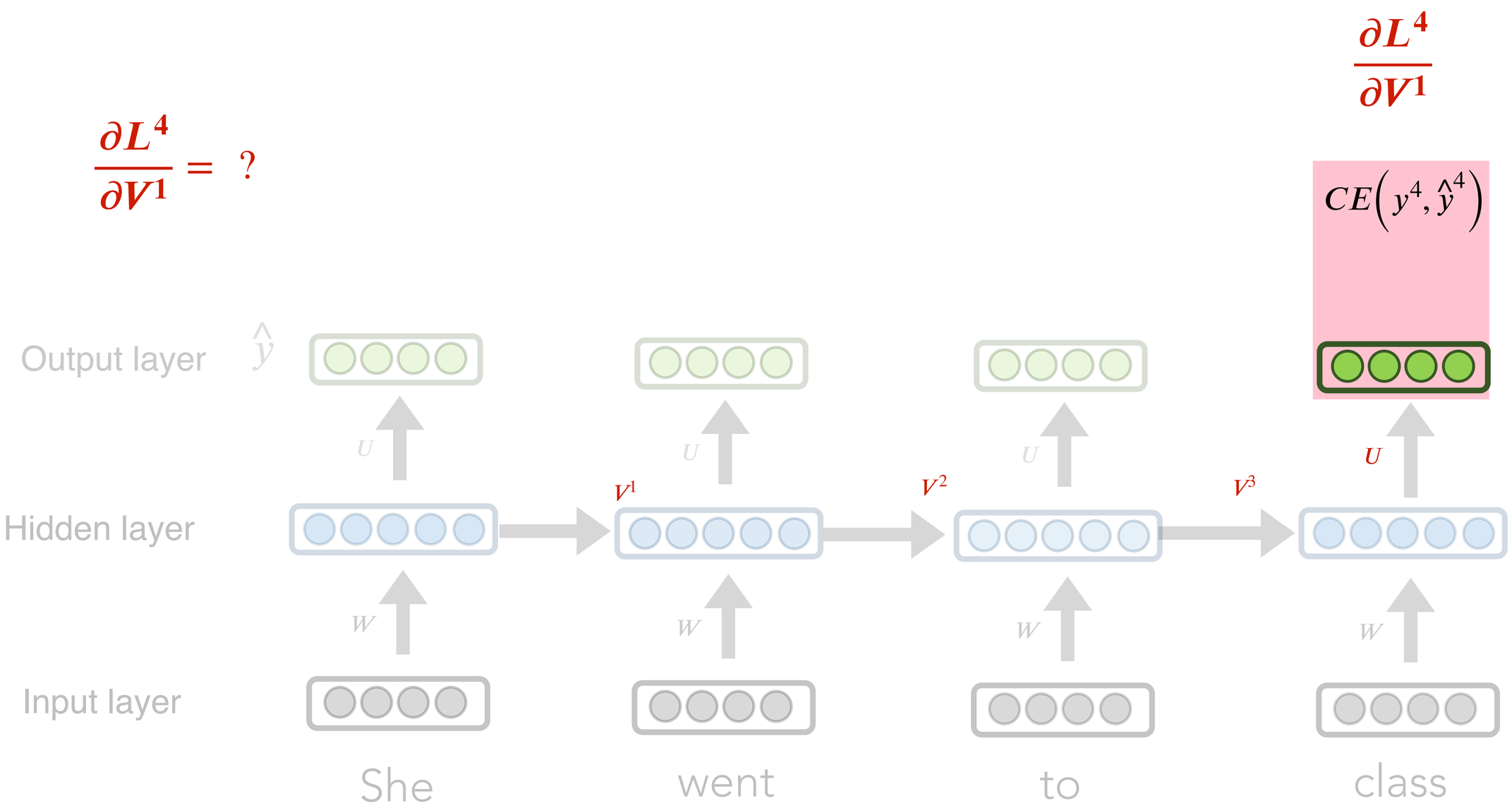
Issues?

- Slow to train (BPTT)
- Due to ”infinite sequence”, gradients can easily vanish or explode
- Has trouble actually making use of long-range context

Vanishing Gradients

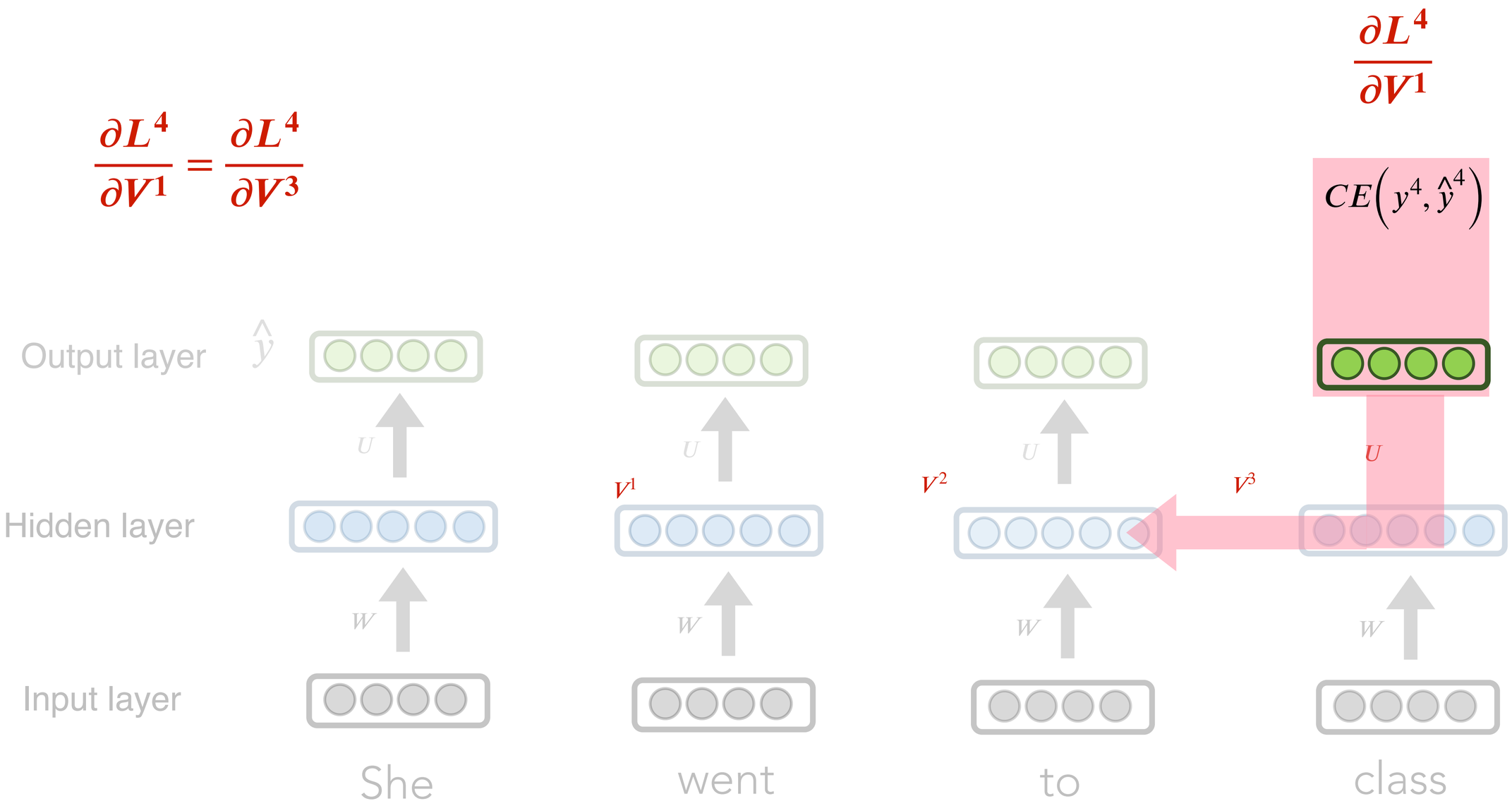
$$\frac{\partial L^4}{\partial V^1} = \ ?$$

$$\frac{\partial L^4}{\partial V^1}$$



Vanishing Gradients

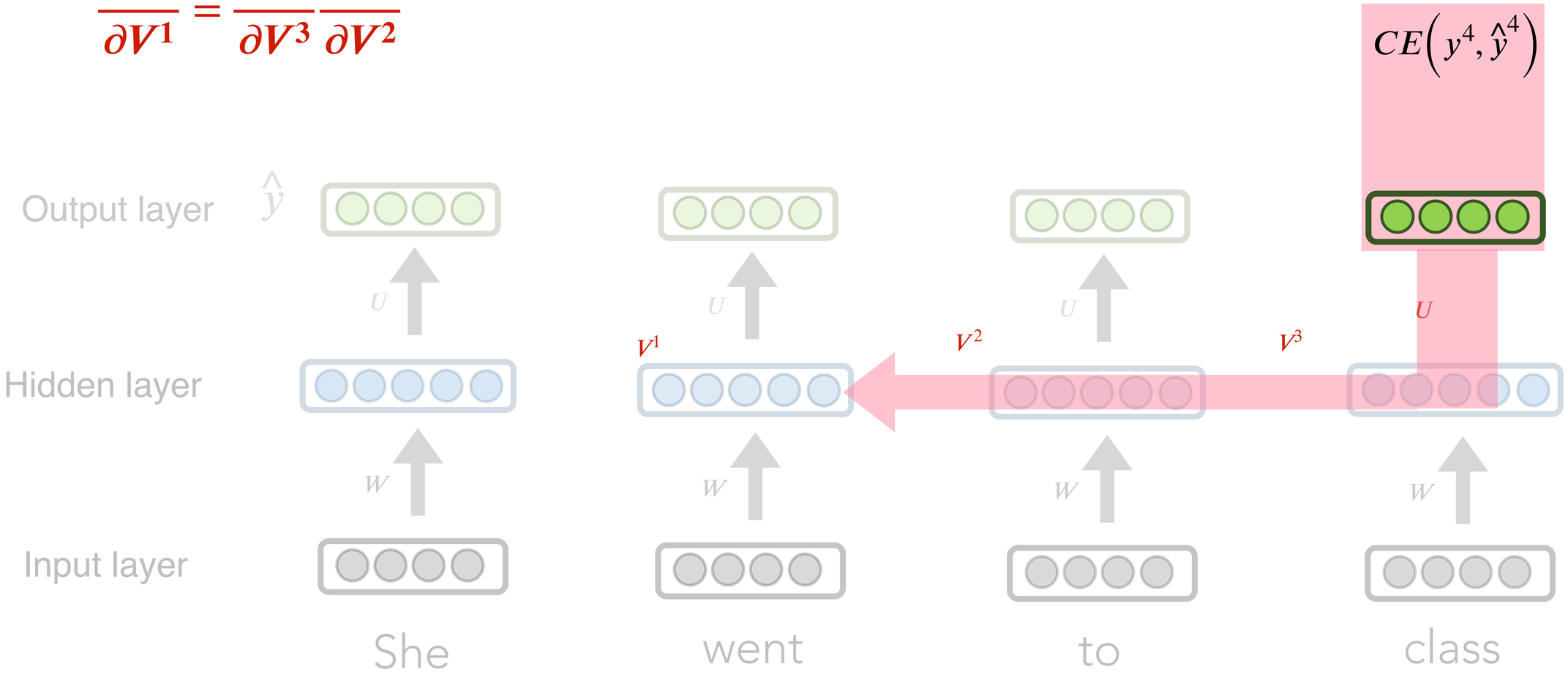
$$\frac{\partial L^4}{\partial V^1} = \frac{\partial L^4}{\partial V^3}$$



Vanishing Gradients

$$\frac{\partial L^4}{\partial V^1} = \frac{\partial L^4}{\partial V^3}\frac{\partial V^3}{\partial V^2}$$

$$\frac{\partial L^4}{\partial V^1}$$



Vanishing Gradients

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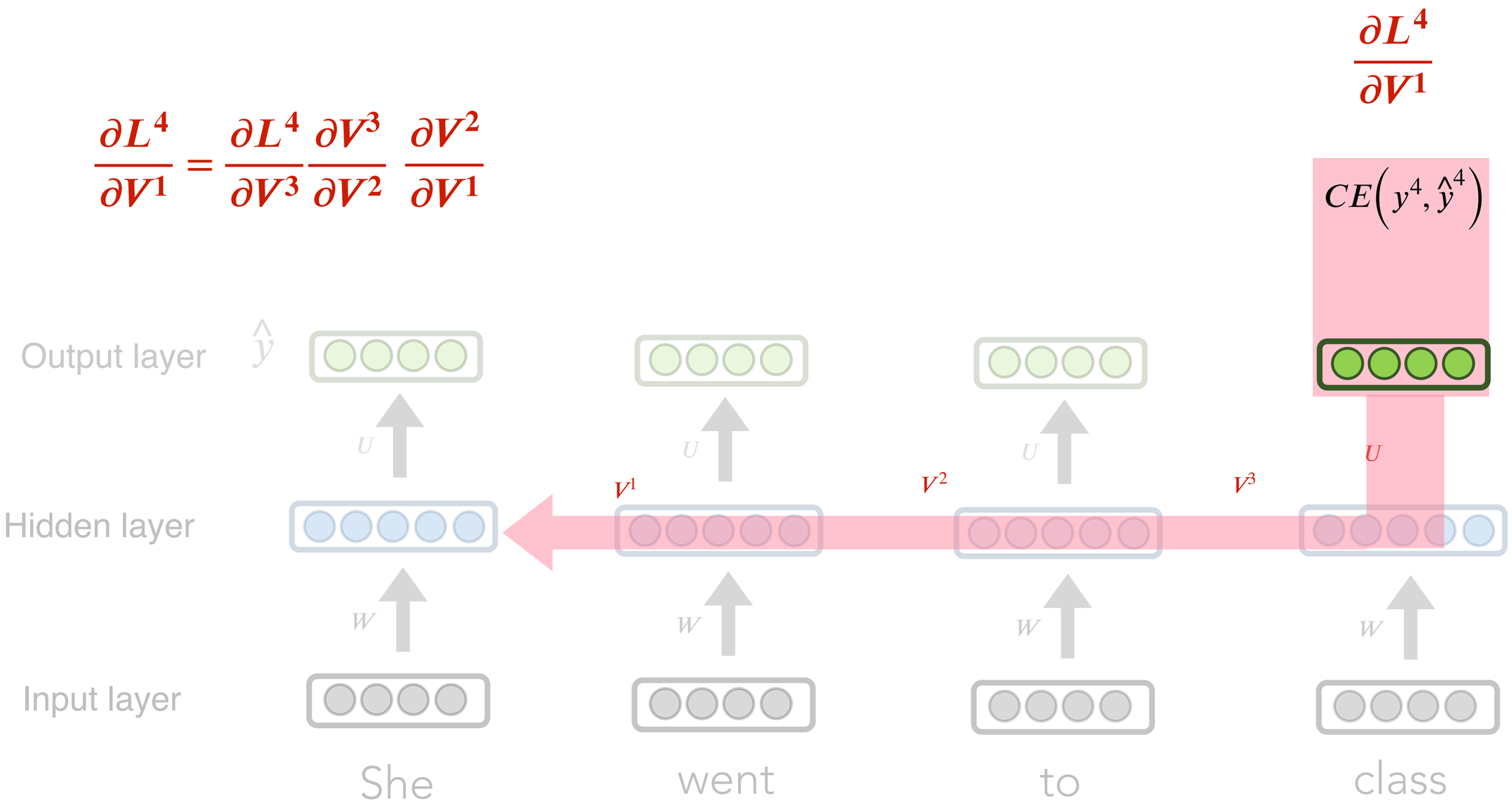

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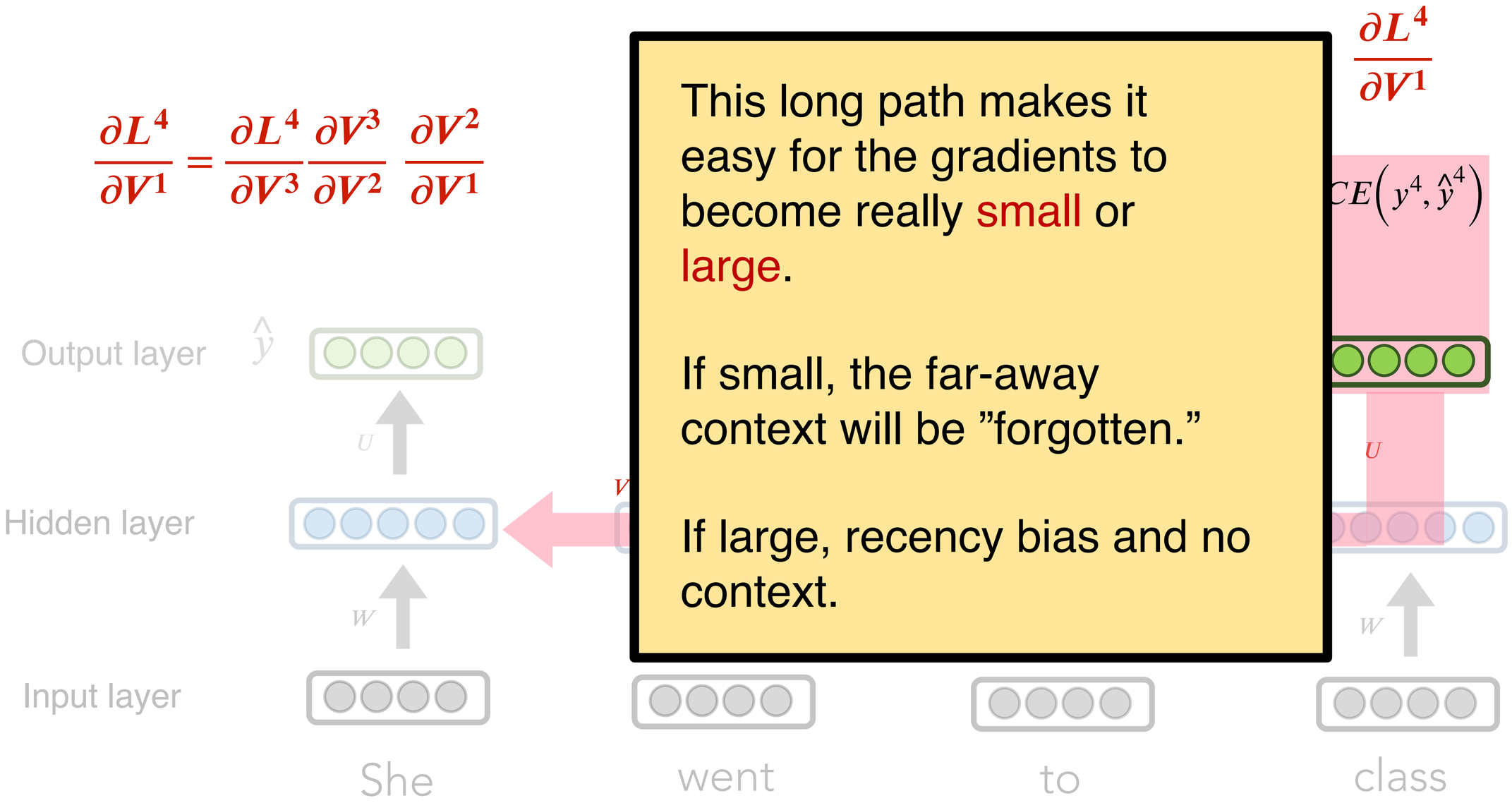


This long path makes it easy for the gradients to become really small or large.

If small, the far-away context will be ”forgotten.”

If large, recency bias and no context.

LSTM

LSTM Motivation

- A type of RNN that is designed to better handle long-range dependencies
- In ”vanilla” RNNs, the hidden state is perpetually being rewritten
- In addition to a traditional hidden state h, let’s have a dedicated memory cell c for long-term events. More power to relay sequence information.

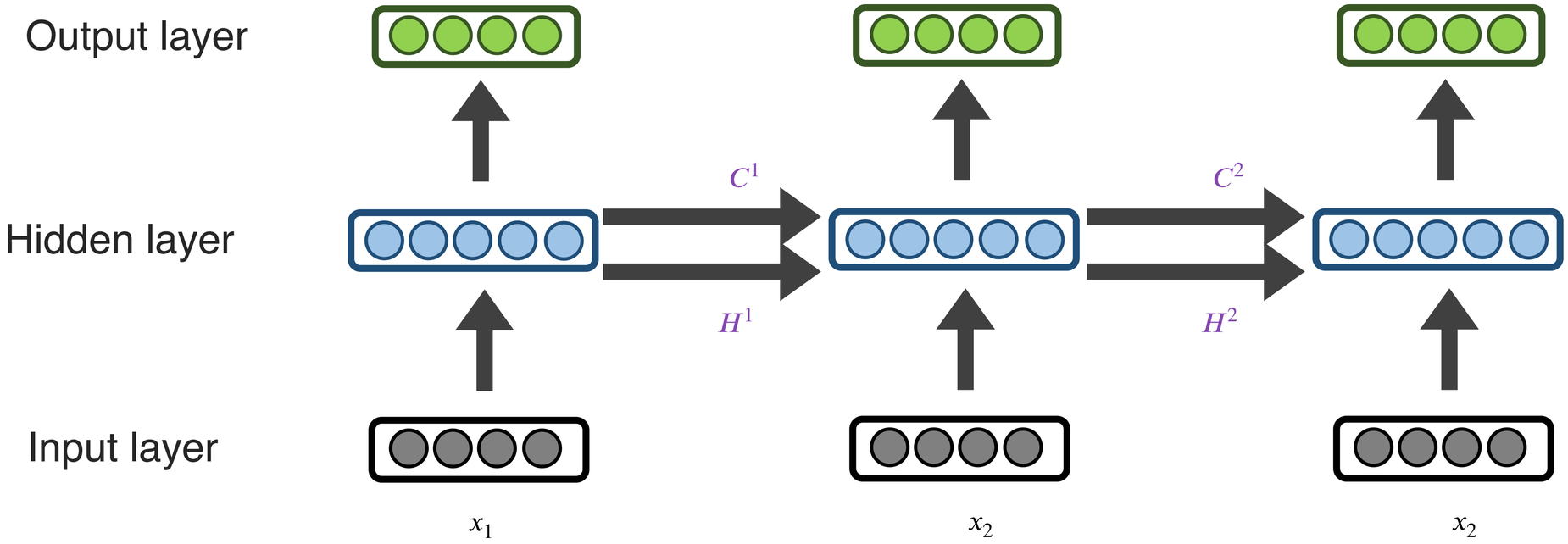
LSTM Intuition

At each each time step t, we have a hidden state h^t and cell state c^t:

- Both are vectors of length n
- cell state c^t stores long-term information
- At each time step t, the LSTM erases, writes, and reads information from the cell c^t
  - c^t never undergoes a nonlinear activation though, just $-$ and $+$
  - $+$ of two things does not modify the gradient; simply adds the gradients

LSTM Intuition

C and H relay long- and short-term memory to the hidden layer, respectively. Inside the hidden layer, there are many weights.



LSTM Architecture

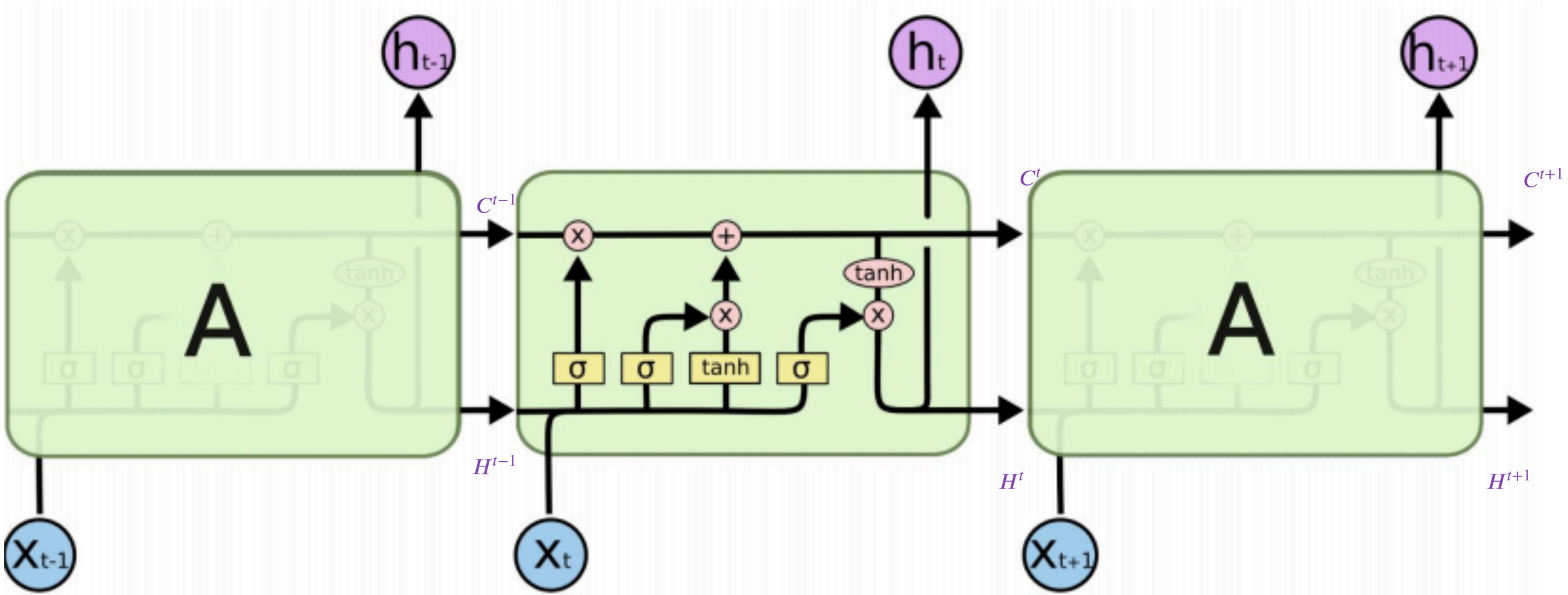


Diagram: https://colah.github.io/posts/2015-08-Understanding-LSTMs/

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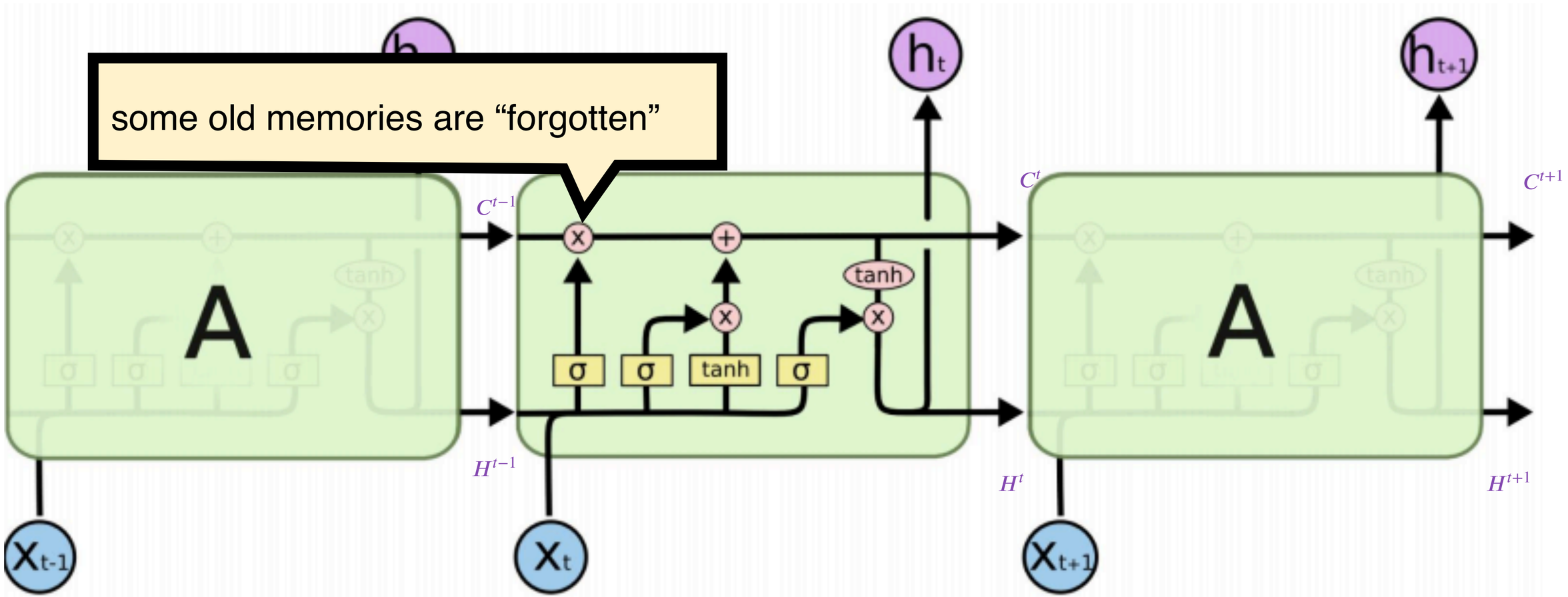

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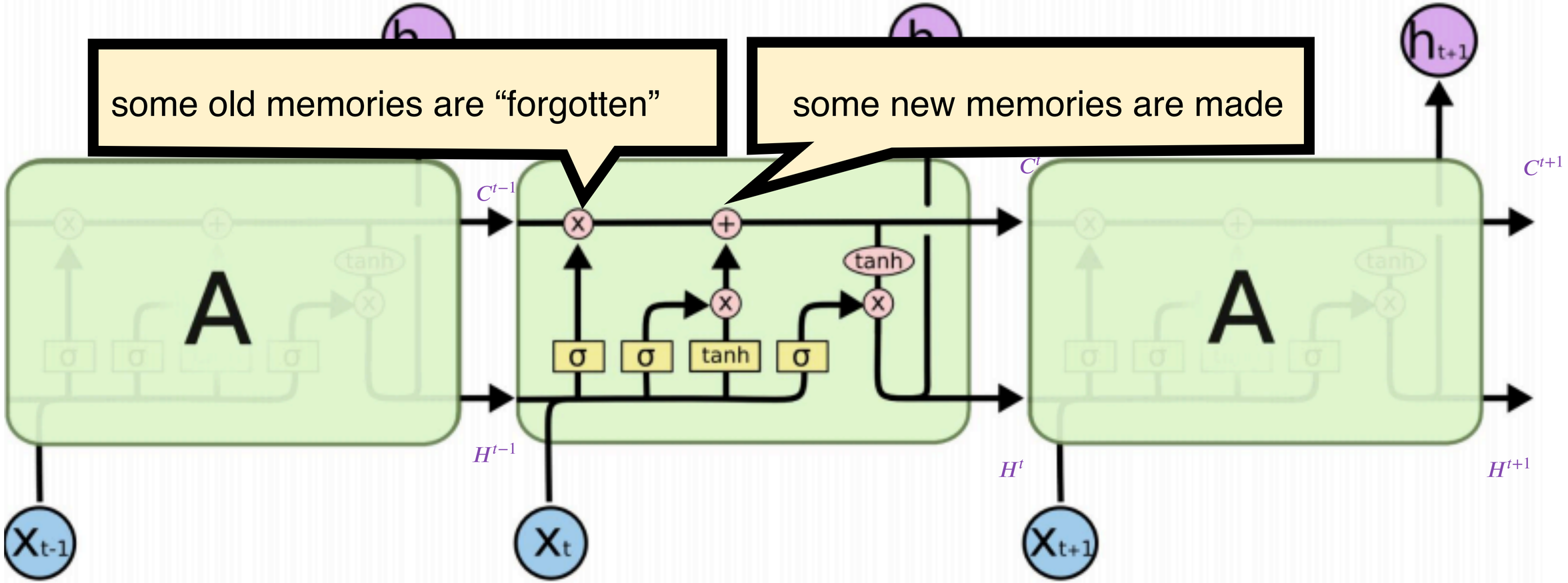

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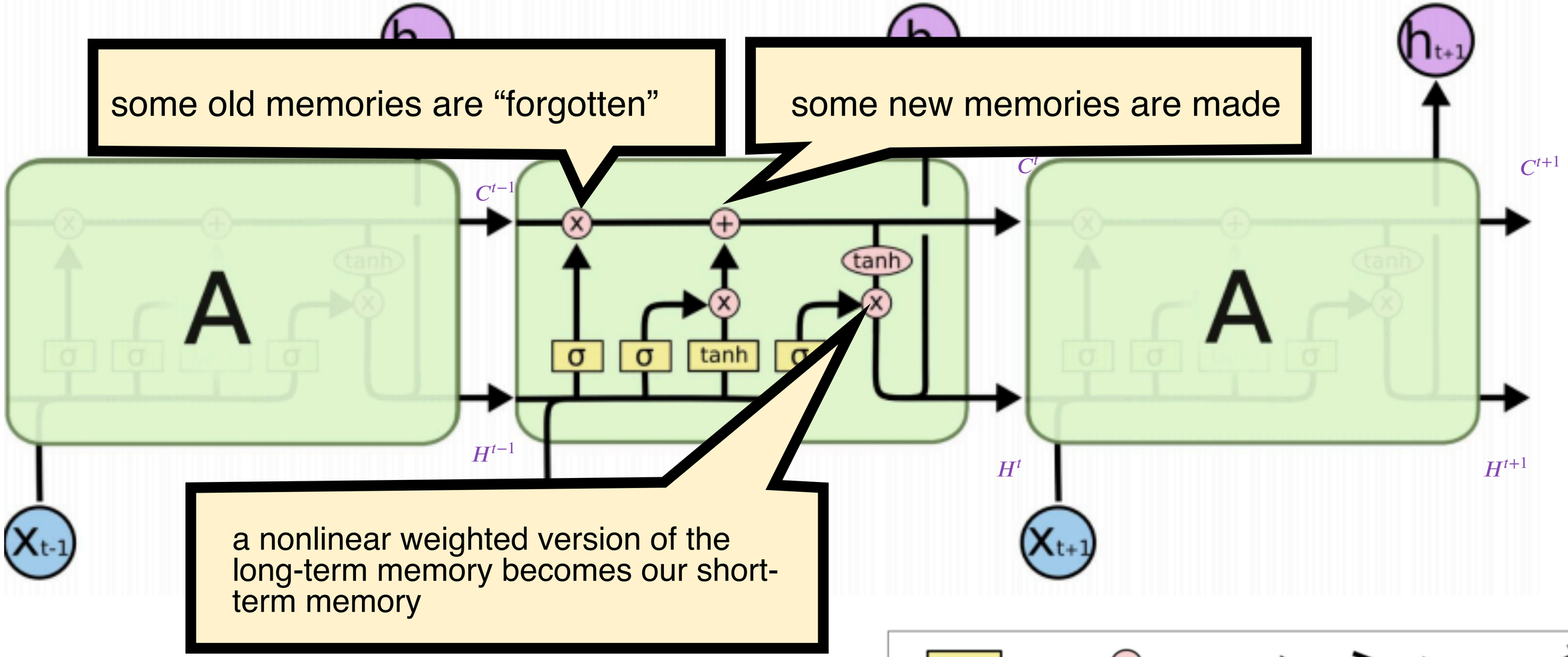

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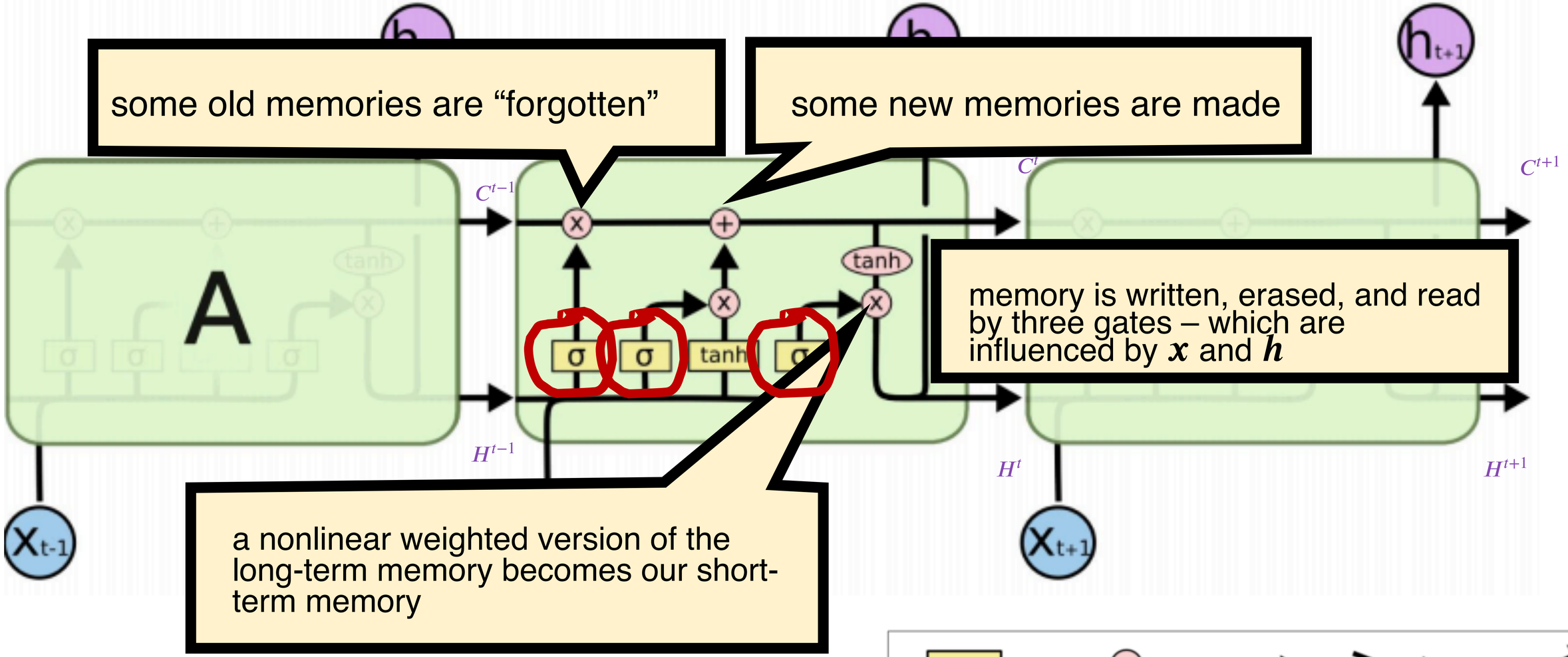

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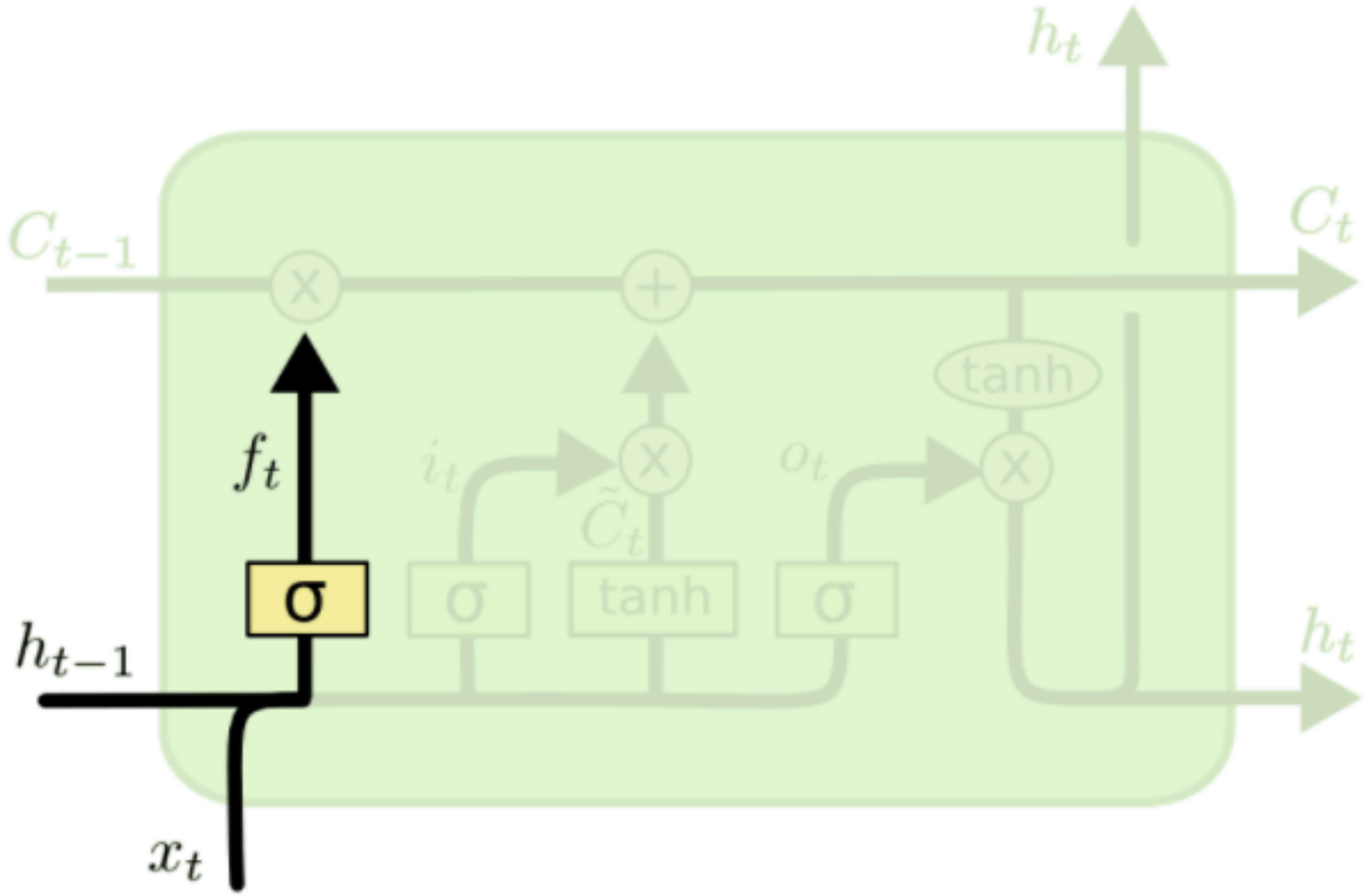
LSTM Architecture (Forget Gate)

$$f_t = \sigma\left(W_f \cdot [h_{t-1}, x_t] \; + \; b_f\right)$$



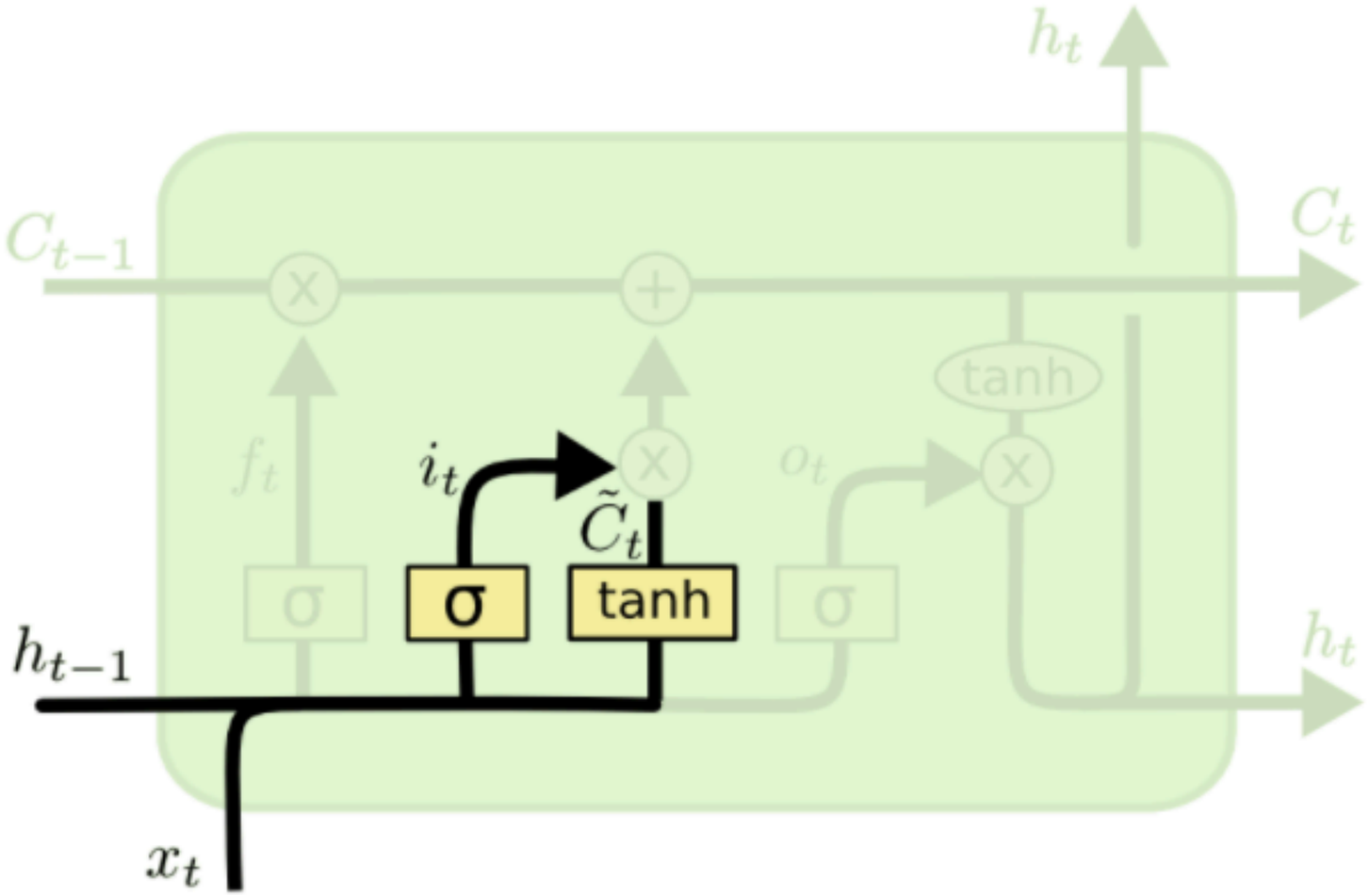
Imagine the cell state currently has values related to a previous topic.
But now the conversation shifts. We need to forget things!

LSTM Architecture (Input Gate)

$$f_t = \sigma\left(W_f \cdot [h_{t-1}, x_t] \; + \; b_f\right)$$

$$i_t = \sigma\left(W_i \cdot [h_{t-1}, x_t] \; + \; b_i\right)$$

$$\tilde{C}_t = \tanh(W_C \cdot [h_{t-1}, x_t] \; + \; b_C)$$



Decides which values to update (by scaling each of the new, incoming info).

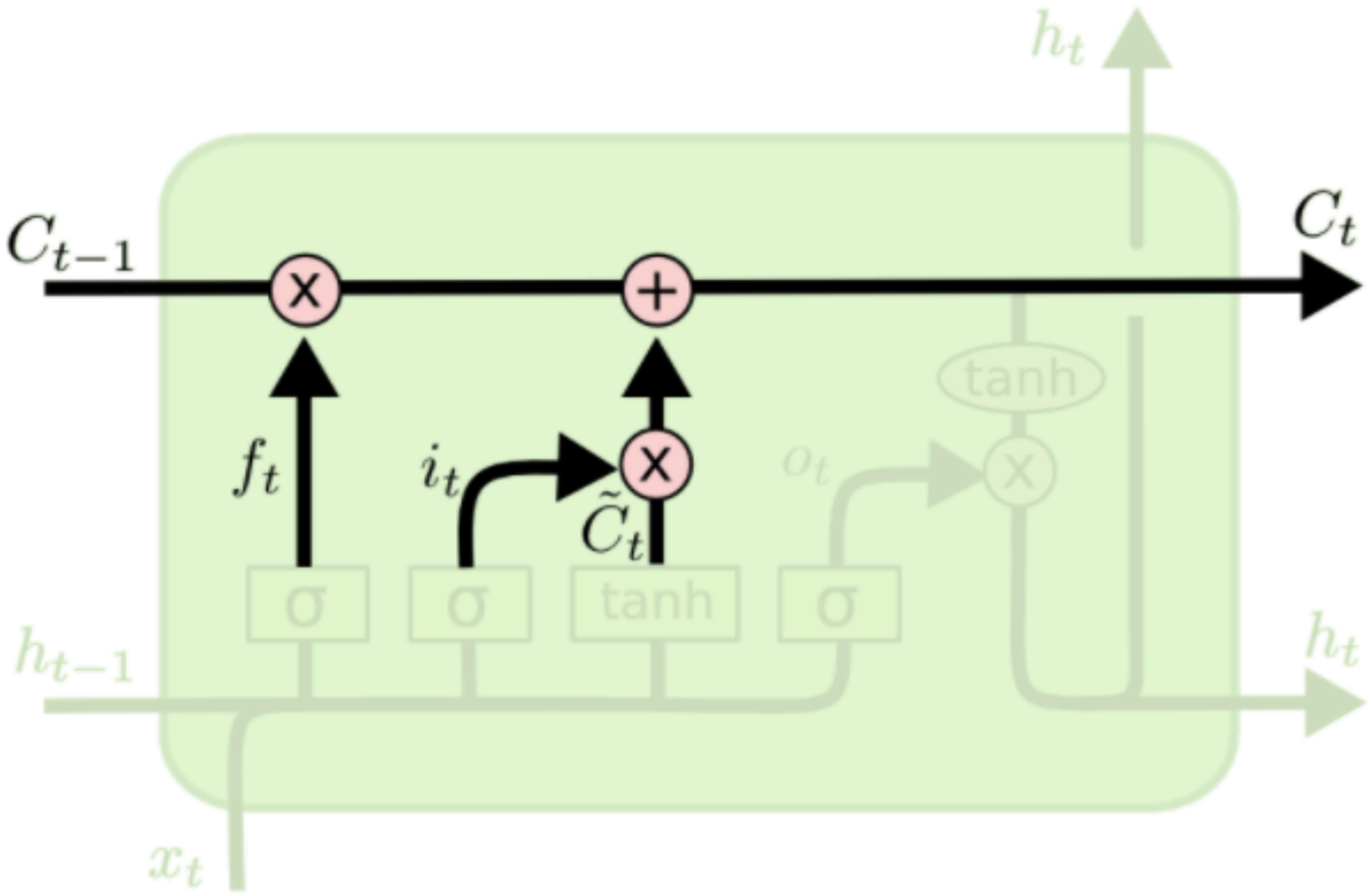
LSTM Architecture

$$f_t = \sigma\left(W_f \cdot [h_{t-1}, x_t] \; + \; b_f\right)$$

$$i_t = \sigma\left(W_i \cdot [h_{t-1}, x_t] \; + \; b_i\right)$$

$$\tilde{C}_t = \tanh(W_C \cdot [h_{t-1}, x_t] \; + \; b_C)$$

$$C_t = f_t * C_{t-1} + i_t * \tilde{C}_t$$



The cell state forgets some info, then it is simultaneously updated by us adding to it.

LSTM Architecture (Output Gate)

$$f_t = \sigma\left(W_f \cdot [h_{t-1}, x_t] \; + \; b_f\right)$$

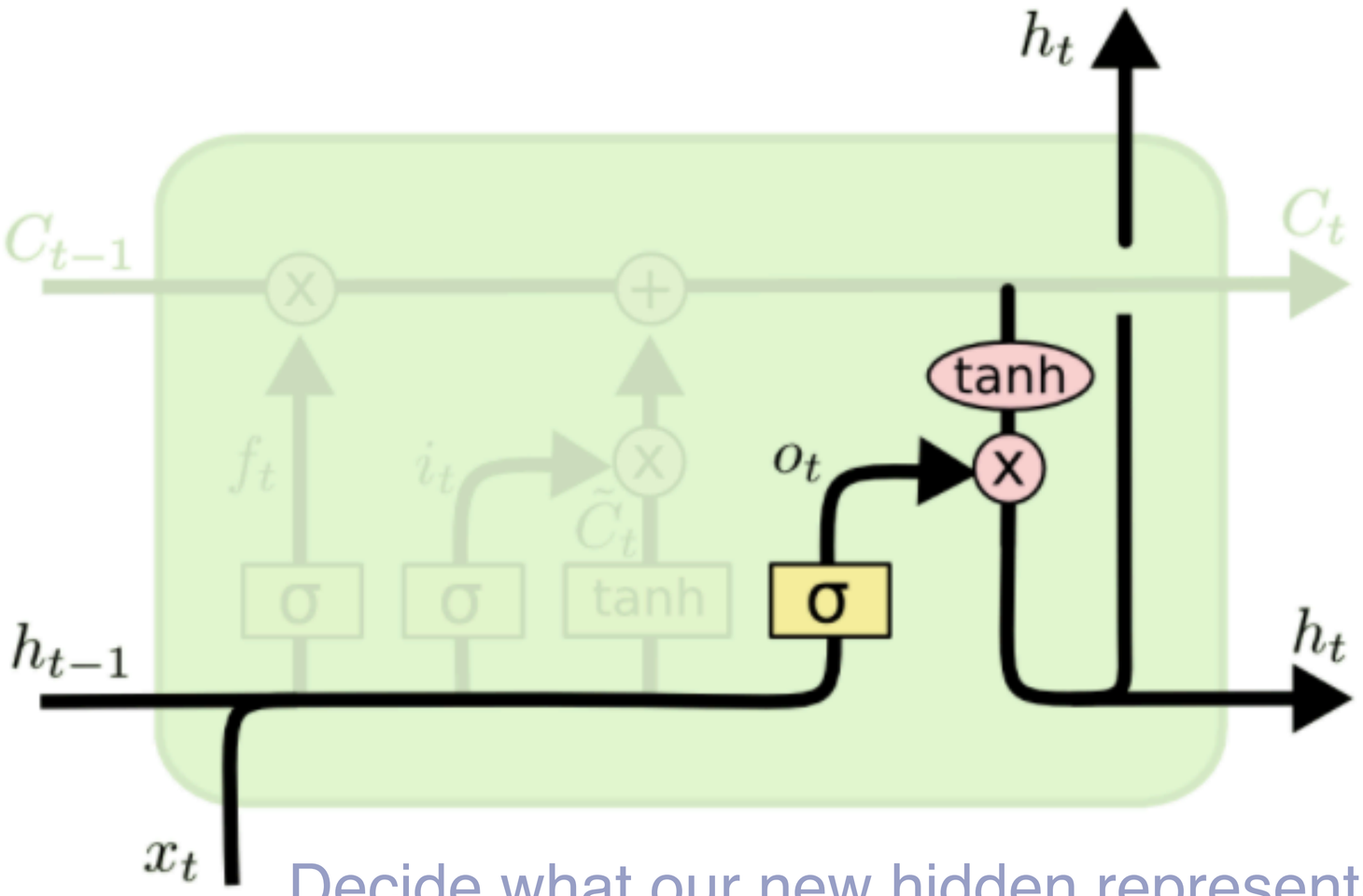
$$i_t = \sigma\left(W_i \cdot [h_{t-1}, x_t] \; + \; b_i\right)$$

$$\tilde{C}_t = \tanh(W_C \cdot [h_{t-1}, x_t] \; + \; b_C)$$

$$C_t = f_t * C_{t-1} + i_t * \tilde{C}_t$$

$$o_t = \sigma\left(W_o \; [h_{t-1}, x_t] \; + \; b_o\right)$$

$$h_t = o_t * \tanh\left(C_t\right)$$



Decide what our new hidden representation will be. Based on:
- filtered version of the cell state, and
- weighted version of recurrent, hidden layer

Total Recall?

It is still possible for LSTMs to suffer from vanishing/exploding gradients, but it's way less likely than with vanilla RNNs:

- If RNNs wish to preserve info over long contexts, it must delicately find a recurrent weight matrix W_h that isn't too large or small
- LSTMs have 3 separate mechanism that adjust the flow of information (e.g., forget gate, if turned off, will preserve all info)

Cell sensitive to position in line:

```
The sole importance of the crossing of the Berezina lies in the fact
that it plainly and indubitably proved the fallacy of all the plans for
cutting off the enemy's retreat and the soundness of the only possible
line of action--the one Kutuzov and the general mass of the army
demanded--namely, simply to follow the enemy up. The French crowd fled
at a continually increasing speed and all its energy was directed to
reaching its goal. It fled like a wounded animal and it was impossible
to block its path. This was shown not so much by the arrangements it
made for crossing as by what took place at the bridges. When the bridges
broke down, unarmed soldiers, people from Moscow and women with children
who were with the French transport, all--carried on by vis inertiae--
pressed forward into boats and into the ice-covered water and did not,
surrender.
```

Cell that turns on inside quotes:

```
"You mean to imply that I have nothing to eat out of.... On the
contrary, I can supply you with everything even if you want to give
dinner parties," warmly replied Chichagov, who tried by every word he
spoke to prove his own rectitude and therefore imagined Kutuzov to be
animated by the same desire.

Kutuzov, shrugging his shoulders, replied with his subtle penetrating
smile: "I meant merely to say what I said."
```

Cell that robustly activates inside if statements:

```
static int __dequeue_signal(struct sigpending *pending, sigset_t *mask,
        siginfo_t *info)
{
  int sig = next_signal(pending, mask);
  if (sig) {
    if (current->notifier) {
      if (sigismember(current->notifier_mask, sig)) {
        if (!(current->notifier)(current->notifier_data)) {
          clear_thread_flag(TIF_SIGPENDING);
          return 0;
        }
      }
    }
    collect_signal(sig, pending, info);
  }
  return sig;
}
```

A large portion of cells are not easily interpretable. Here is a typical example:

```
/* Unpack a filter field's string representation from user-space
 * buffer. */
char *audit_unpack_string(void **bufp, size_t *remain, size_t len)
{
  char *str;
  if (!*bufp || (len == 0) || (len > *remain))
    return ERR_PTR(-EINVAL);
  /* Of the currently implemented string fields, PATH_MAX
   * defines the longest valid length.
   */
```

The cell learns an operative time to “turn on”.

Cell that turns on inside comments and quotes:

```
/* Duplicate LSM field information.  The lsm_rule is opaque, so
 * re-initialized. */
static inline int audit_dupe_lsm_field(struct audit_field *df,
           struct audit_field *sf)
{
  int ret = 0;
  char *lsm_str;
  /* our own copy of lsm_str */
  lsm_str = kstrdup(sf->lsm_str, GFP_KERNEL);
  if (unlikely(!lsm_str))
    return -ENOMEM;
  df->lsm_str = lsm_str;
  /* our own (refreshed) copy of lsm_rule */
  ret = security_audit_rule_init(df->type, df->op, df->lsm_str,
             (void **)&df->lsm_rule);
  /* Keep currently invalid fields around in case they
   * become valid after a policy reload. */
  if (ret == -EINVAL) {
    pr_warn("audit rule for LSM \'%s\' is invalid\n",
      df->lsm_str);
    ret = 0;
  }
  return ret;
}
```

Cell that is sensitive to the depth of an expression:

```
#ifdef CONFIG_AUDITSYSCALL
static inline int audit_match_class_bits(int class, u32 *mask)
{
  int i;
  if (classes[class]) {
    for (i = 0; i < AUDIT_BITMASK_SIZE; i++)
      if (mask[i] & classes[class][i])
        return 0;
  }
  return 1;
}
```

The cell learns an operative time to “turn on”.

LSTM Summary

Strengths

- Almost always outperforms RNNs
- Captures long-range dependencies very well

Issues?

- More weights to learn, thus:
- Higher training data demand
- Can still suffer from vanishing/exploding gradients

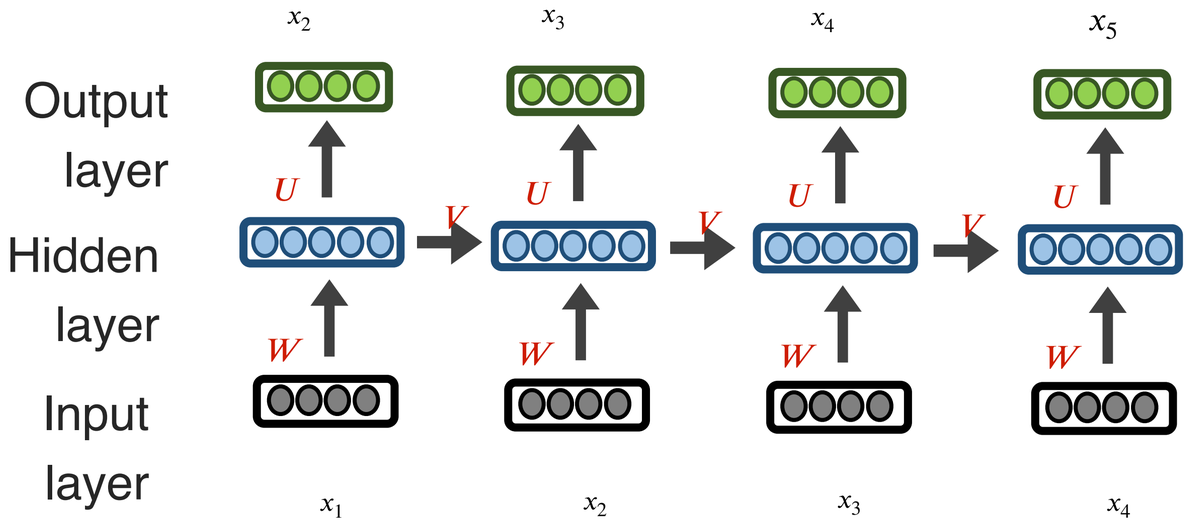
LSTM Applications

If your goal isn't to predict the next item in a sequence, and you rather do some other classification or regression task using the sequence, then you can:

- Train an aforementioned model (e.g., LSTM) as a language model
- Use the hidden layers that correspond to each item in your sequence

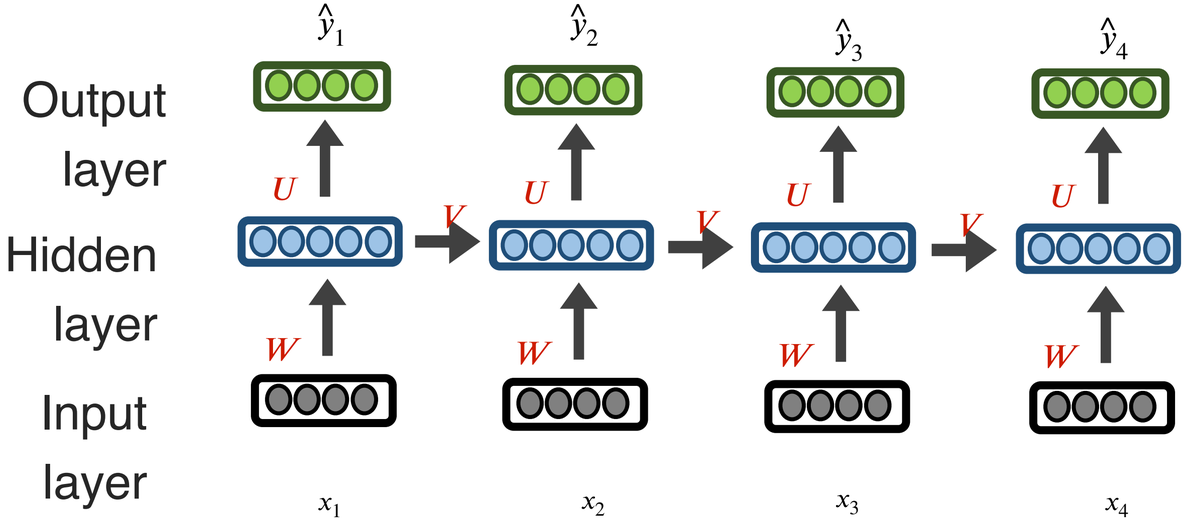
LSTM Applications

Language Modeling



Auto-regressive

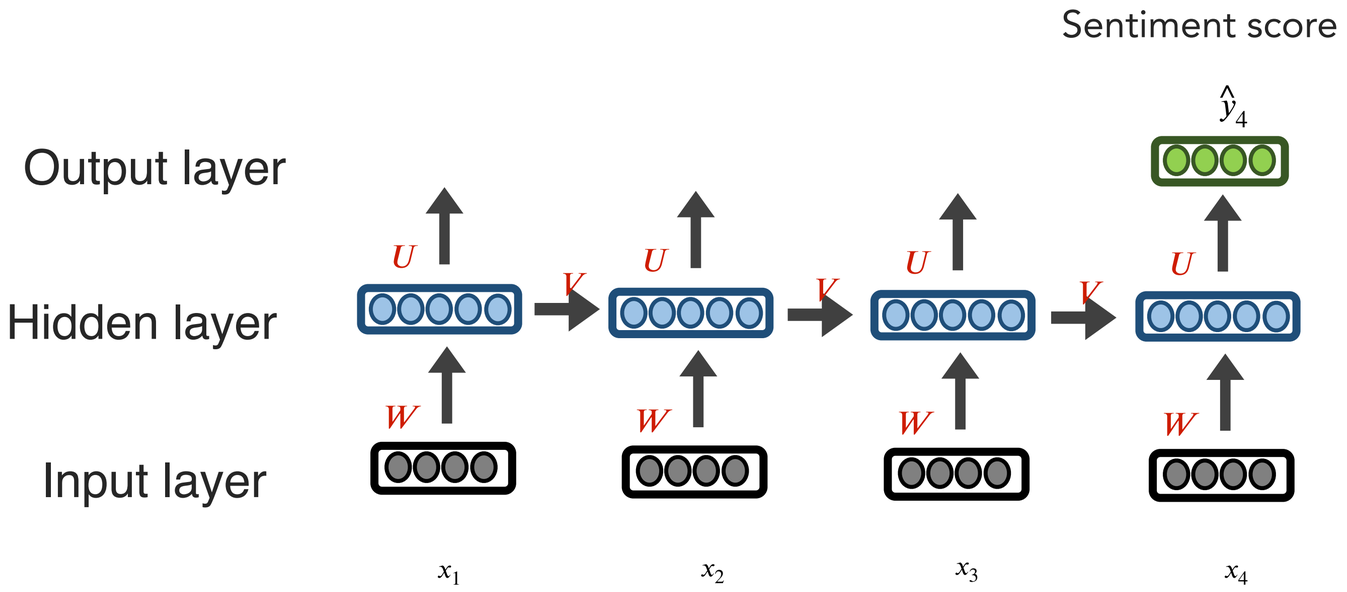
1-to-1 tagging/classification



Non-Auto-regressive

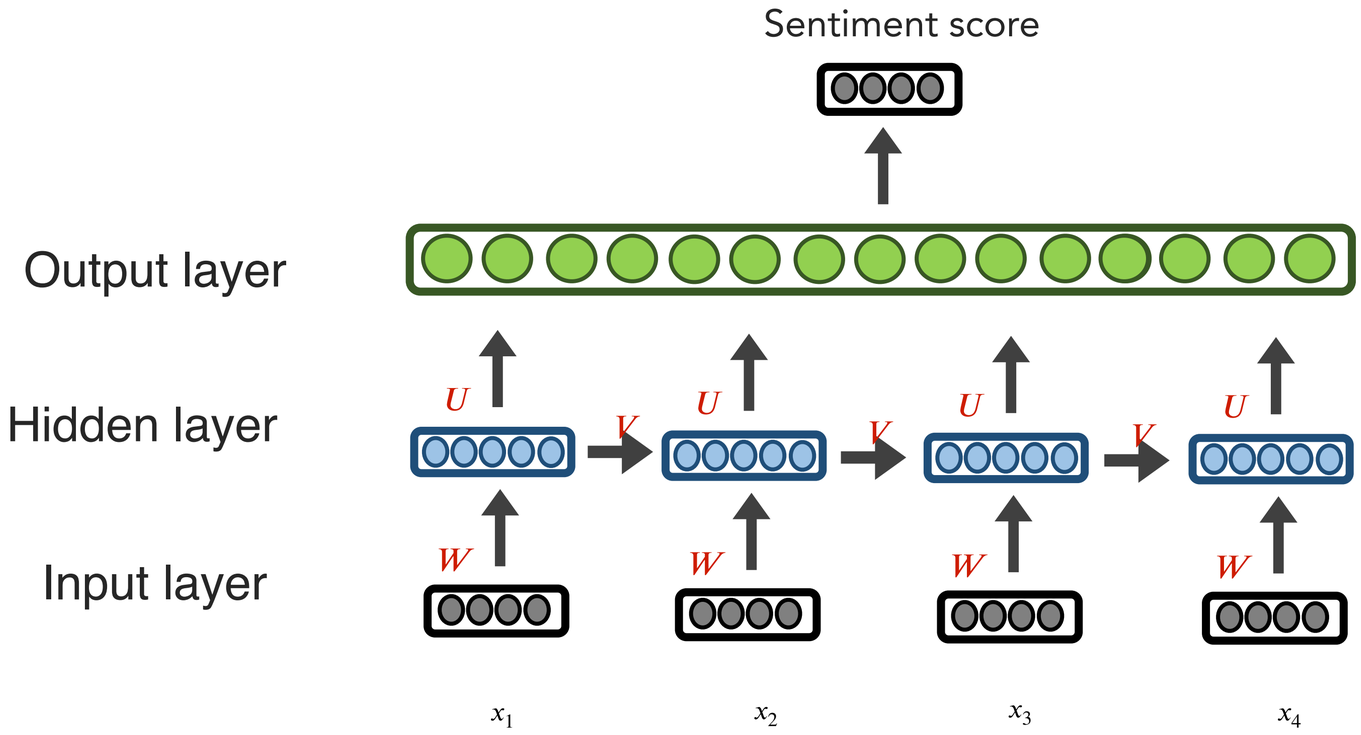
LSTM Applications

Many-to-1 classification



LSTM Applications

Many-to-1 classification



Bi-LSTM

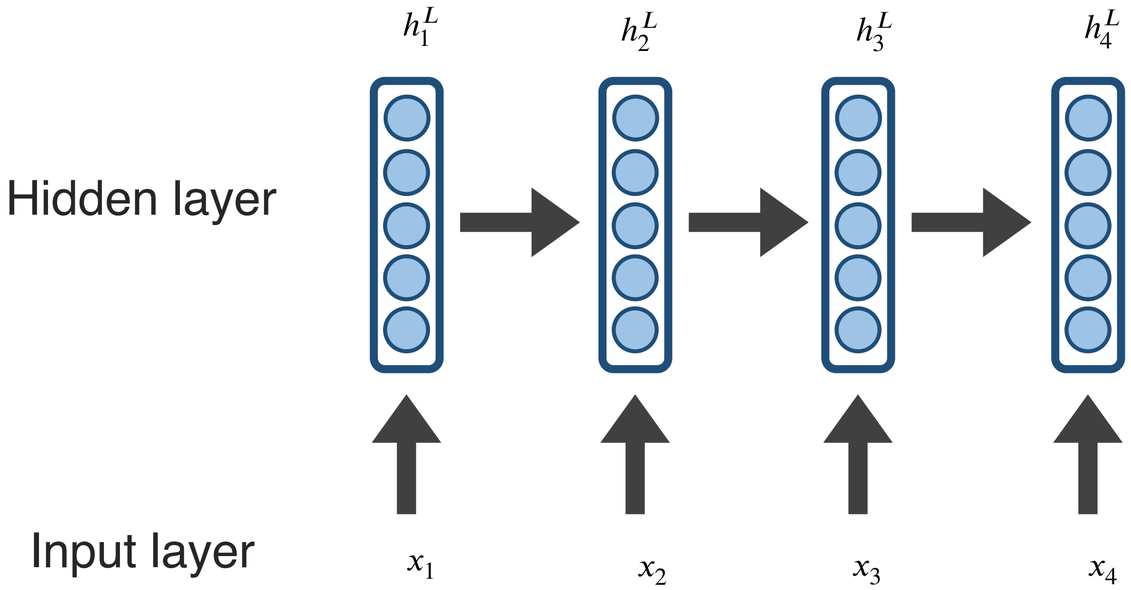
Reading Bidirectionally

RNNs/LSTMs use the left-to-right context and sequentially process data.

If you have full access to the data at testing time, why not make use of the flow of information from right-to-left, also?

Reading Bidirectionally

For brevity, let's use the follow schematic to represent an RNN



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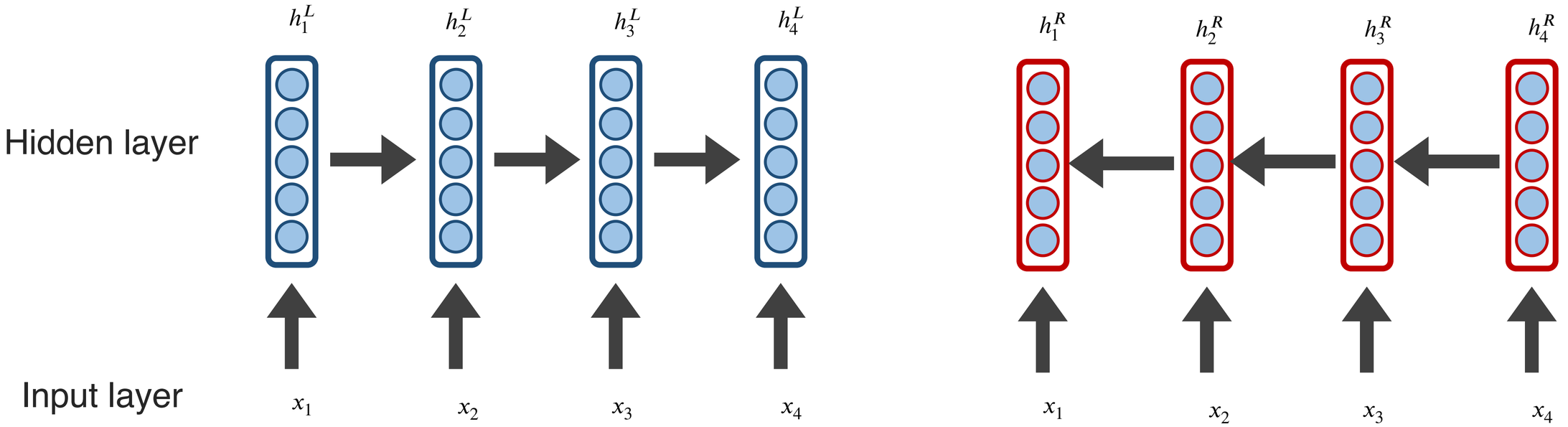
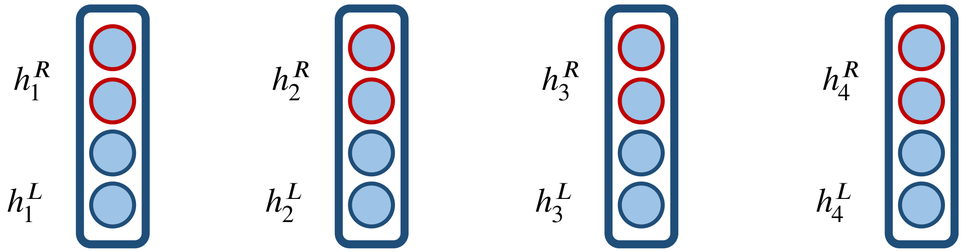


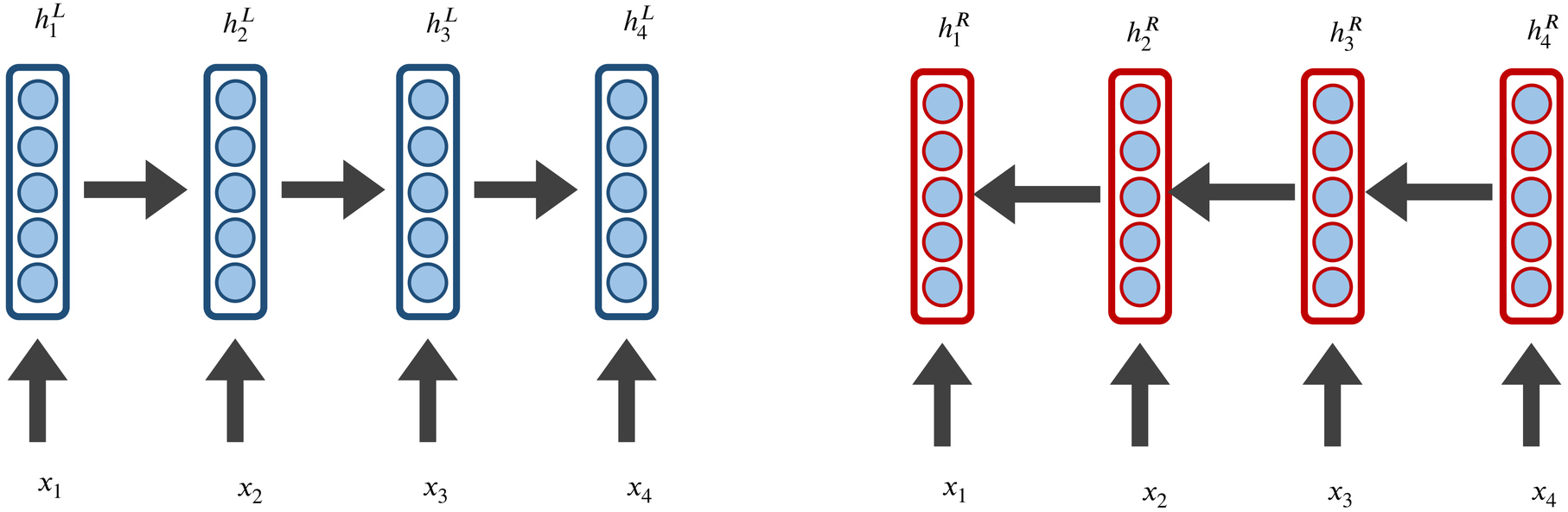
Reading Bidirectionally

Concatenate the hidden layers

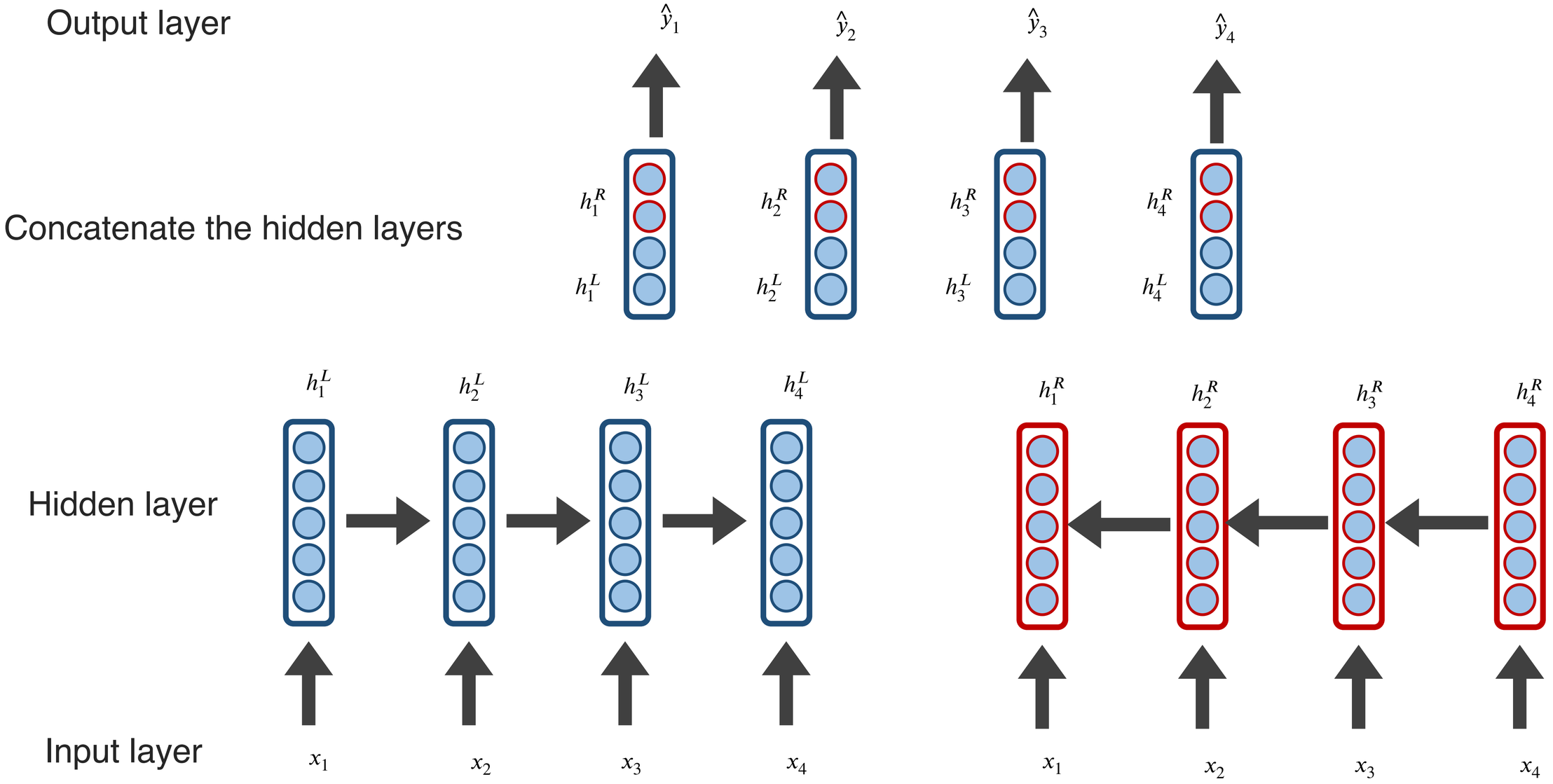


Hidden layer

Input layer



Reading Bidirectionally



Bi-LSTM Summary

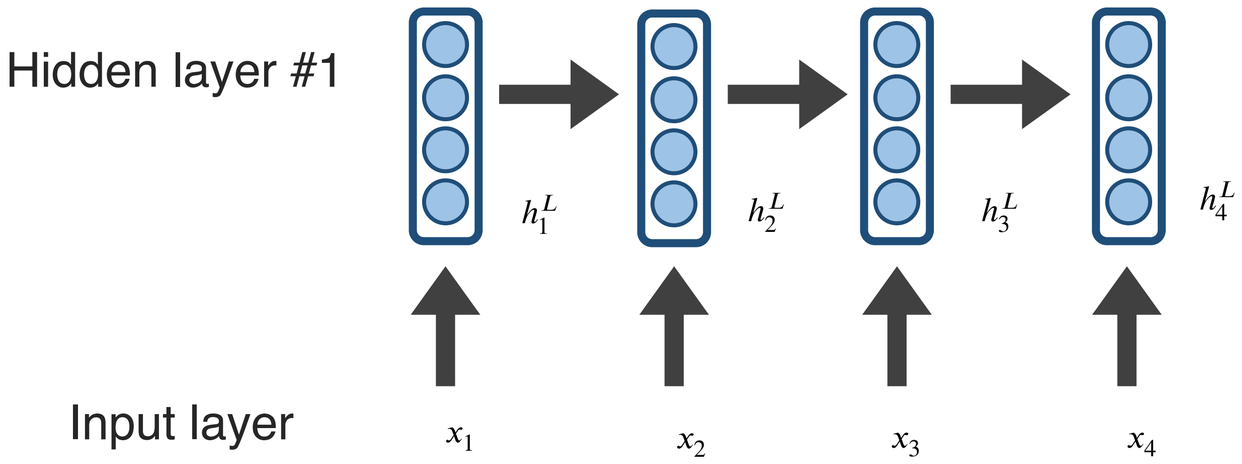
Strengths

- Usually performs at least as well as uni-directional RNNs/LSTMs

Issues?

- Slower to train
- Only possible if access to full data is allowed

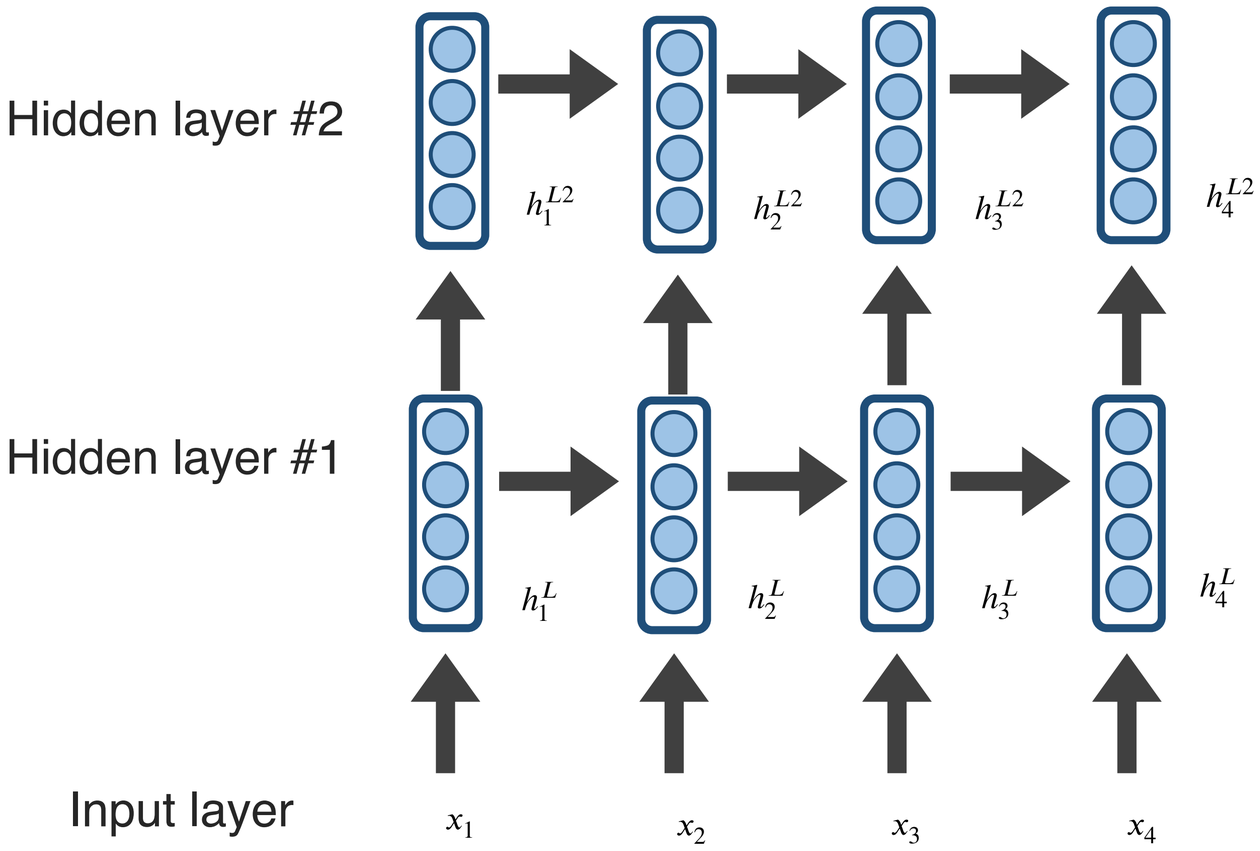
Stacked LSTMs



Hidden layers provide an abstraction (hold “meaning”).

Stacking hidden layers provides increased abstractions.

Stacked LSTMs



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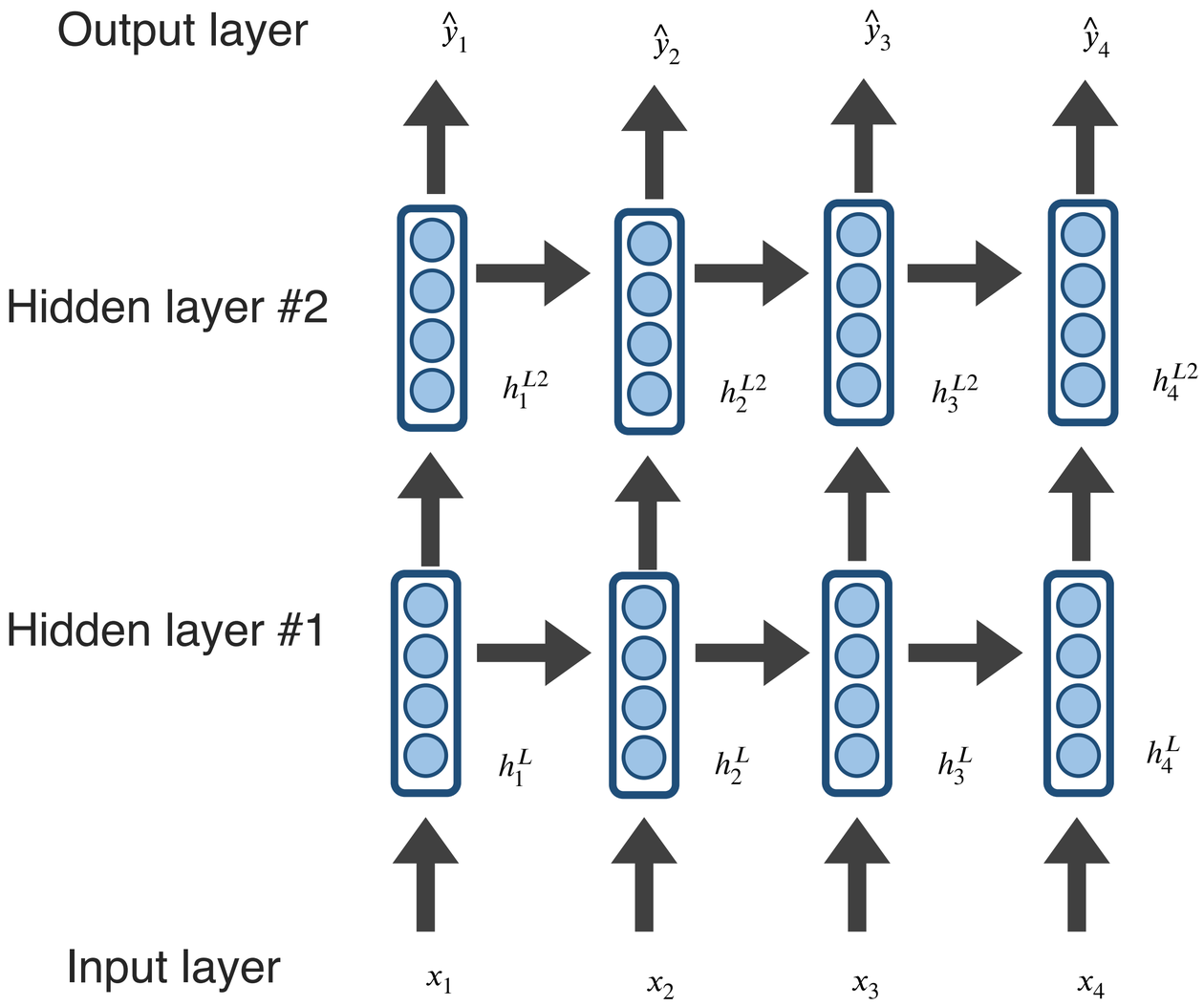
Stacked LSTMs



Hidden layers provide an abstraction (holds “meaning”).

Stacking hidden layers provides increased abstractions.

ELMo

General Idea:

- Goal is to obtain highly rich embeddings for each word (unique type)
- Use both directions of context (bi-directional), with increasing abstractions (stacked)
- Linearly combine all abstract representations (hidden layers) and optimize w.r.t. a particular task (e.g., sentiment classification)

ELMo Slides: https://www.slideshare.net/shuntaroy/a-review-of-deep-contextualized-word-representations-peters-2018

ELMo

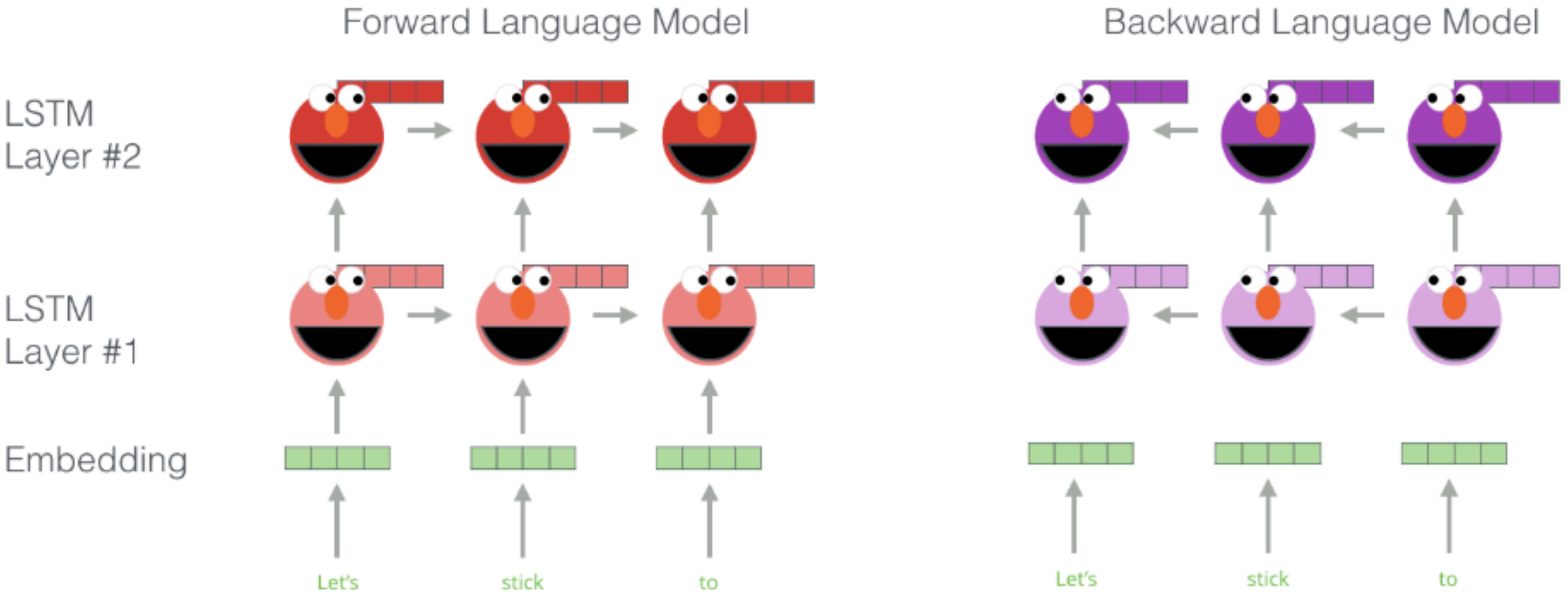


Illustration: http://jalammar.github.io/illustrated-bert/

Embedding of “stick” in “Let’s stick to” - Step #2

1- Concatenate hidden layers

2- Multiply each vector by a weight based on the task

x s_2

x s_1

x s_0

3- Sum the (now weighted) vectors

ELMo embedding of “stick” for this task in this context

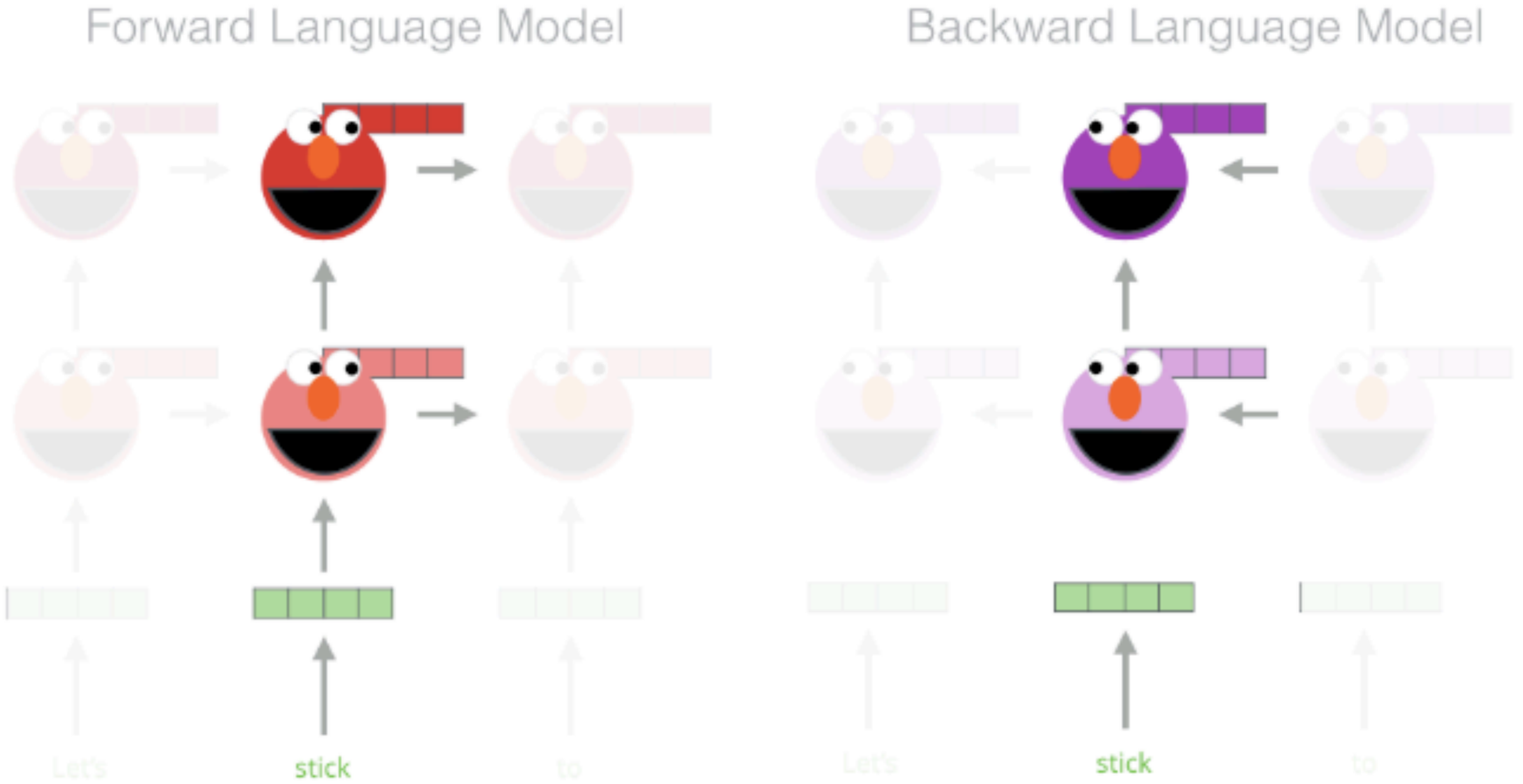


Illustration: http://jalammar.github.io/illustrated-bert/

ELMo

Task	Previous SOTA		Our baseline	ELMo + baseline	Increase (absolute/ relative)
SQuAD	Liu et al. (2017)	84.4	81.1	85.8	4.7 / 24.9%
SNLI	Chen et al. (2017)	88.6	88.0	88.7 ± 0.17	0.7 / 5.8%
SRL	He et al. (2017)	81.7	81.4	84.6	3.2 / 17.2%
Coref	Lee et al. (2017)	67.2	67.2	70.4	3.2 / 9.8%
NER	Peters et al. (2017)	91.93 ± 0.19	90.15	92.22 ± 0.10	2.06 / 21%
SST-5	McCann et al. (2017)	53.7	51.4	54.7 ± 0.5	3.3 / 6.8%

Deep contextualized word representations. Peters et al. NAACL 2018.

ELMo

- ELMo yielded very good contextualized embeddings, which re-defined SOTA when applied to many NLP tasks.
- Main ELMo takeaway: given enough training data, having tons of explicit connections between your vectors is useful (the system can determine how to best use context)

ELMo Slides: https://www.slideshare.net/shuntaroy/a-review-of-deep-contextualized-word-representations-peters-2018

ELMo

- Distributed Representations can be:
  - Type-based (“word embeddings”)
  - Token-based (“contextualized representations/embeddings”)
- Type-based models include Bengio’s 2003 and word2vec 2013
- Token-based models include RNNs/LSTMs, which:
  - demonstrated profound results from 2015 onward.
  - can be used for essentially any NLP task.

Attention

Attention Motivation

What if the decoder (component that produces outputs), at each step, pays attention to a distribution of all of the encoder's (component that receives inputs) hidden states?

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What if the decoder (component that produces outputs), at each step, pays attention to a distribution of all of the encoder's (component that receives inputs) hidden states?

Intuition: when we (humans) translate a sentence, we don't just consume the original sentence, reflect on the meaning of the last word, then regurgitate in a new language; we continuously think back at the original sentence while focusing on different parts.

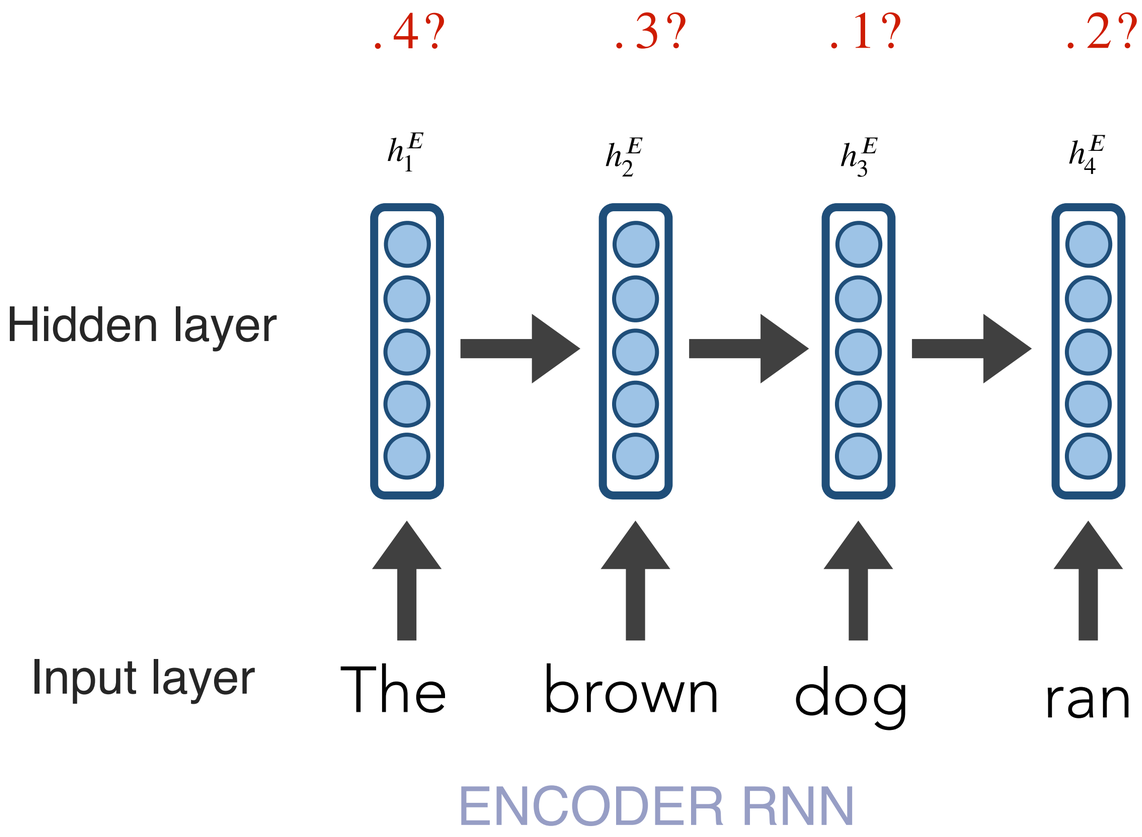
Attention Motivation

The concept of attention within cognitive neuroscience and psychology dates back to the 1800s. [William James, 1890].

Nadaray-Watson kernel regression proposed in 1964. It locally weighted its predictions.

Attention Architecture

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



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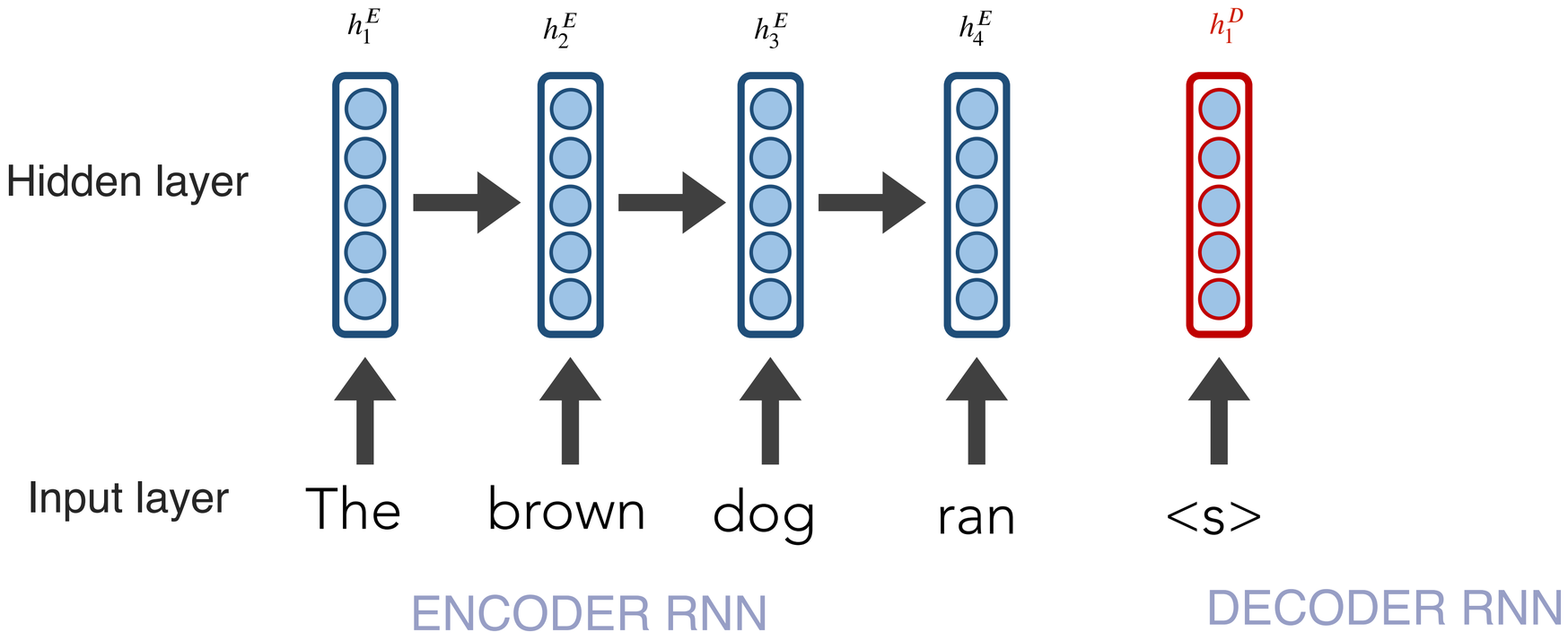
A: Let's base it on our decoder's current hidden state (our current representation of meaning) and all of the encoder's hidden layers!



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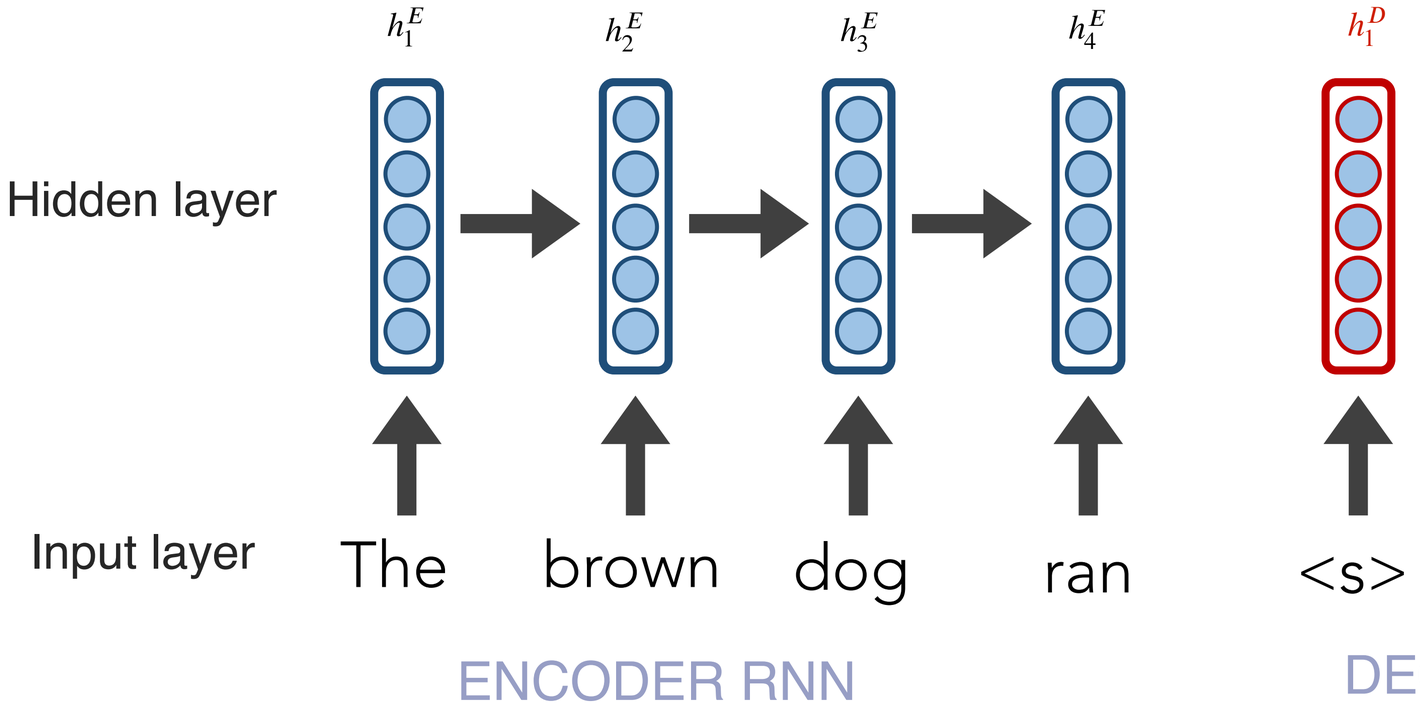

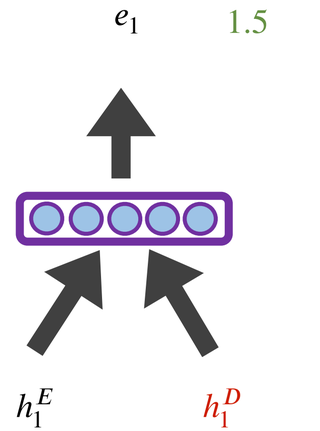

Separate FFNN

Attention Architecture

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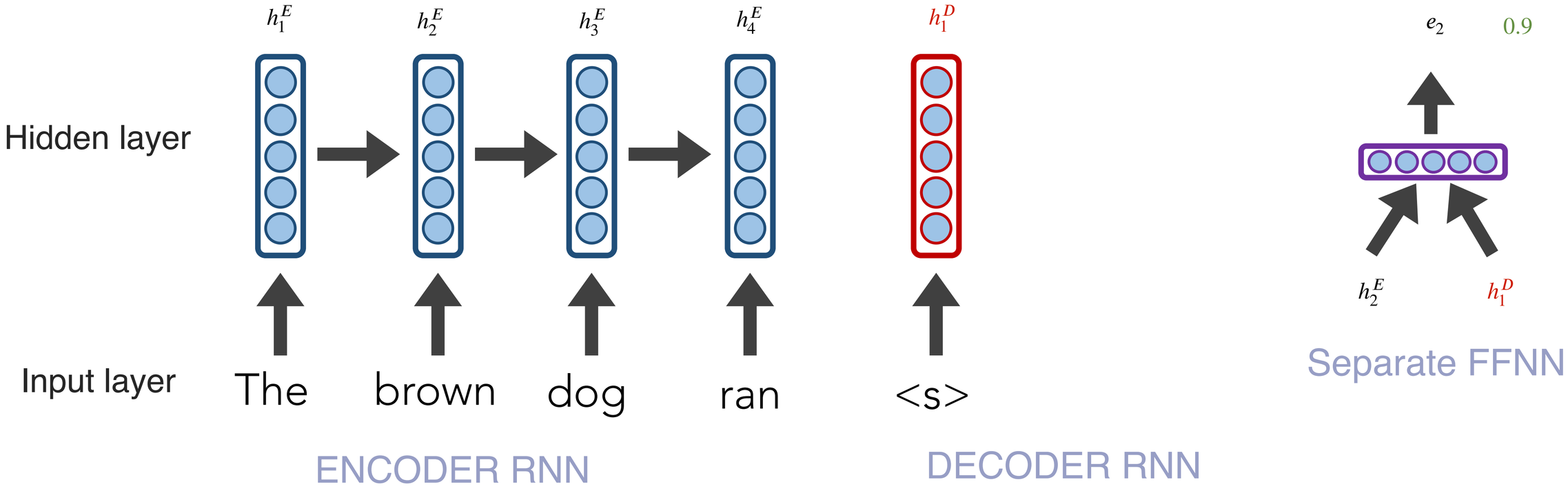

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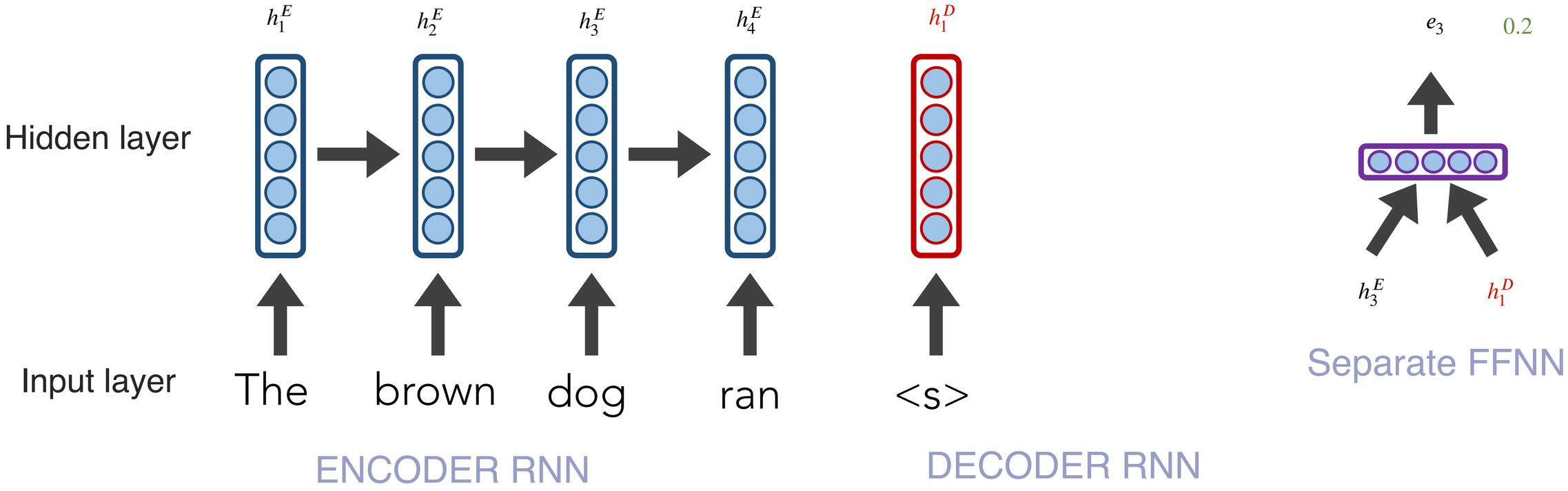

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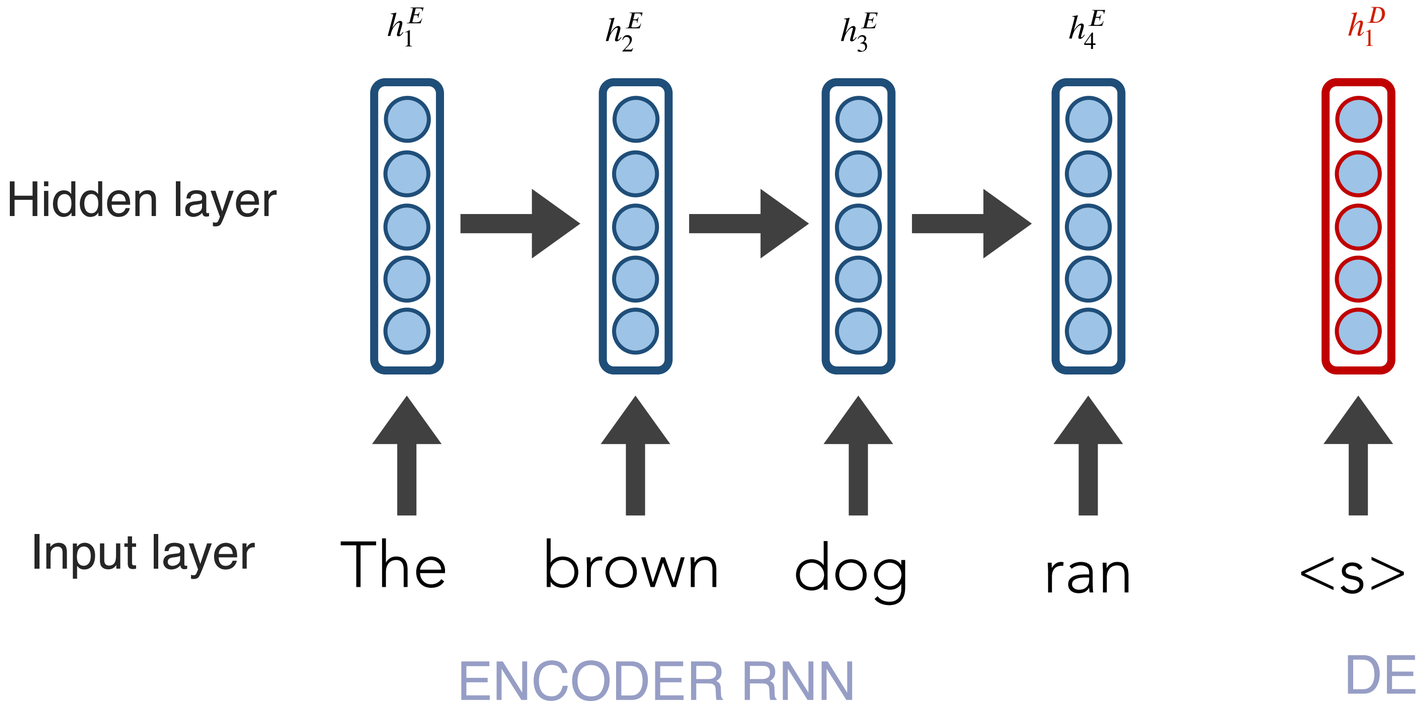

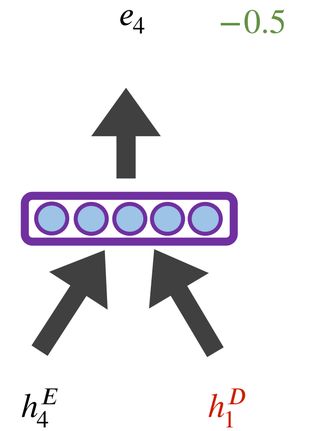

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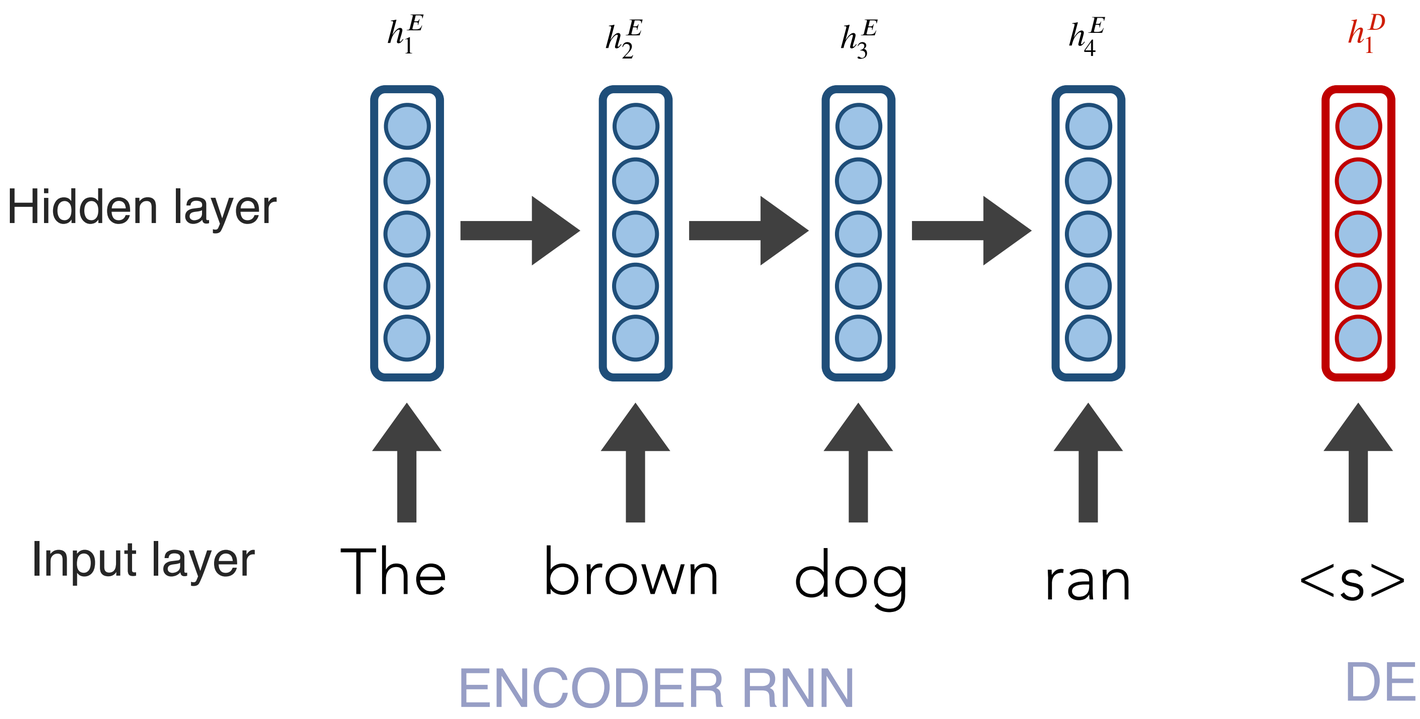

Attention (raw scores)

e_1	1.5
e_2	0.9
e_3	0.2
e_4	−0.5

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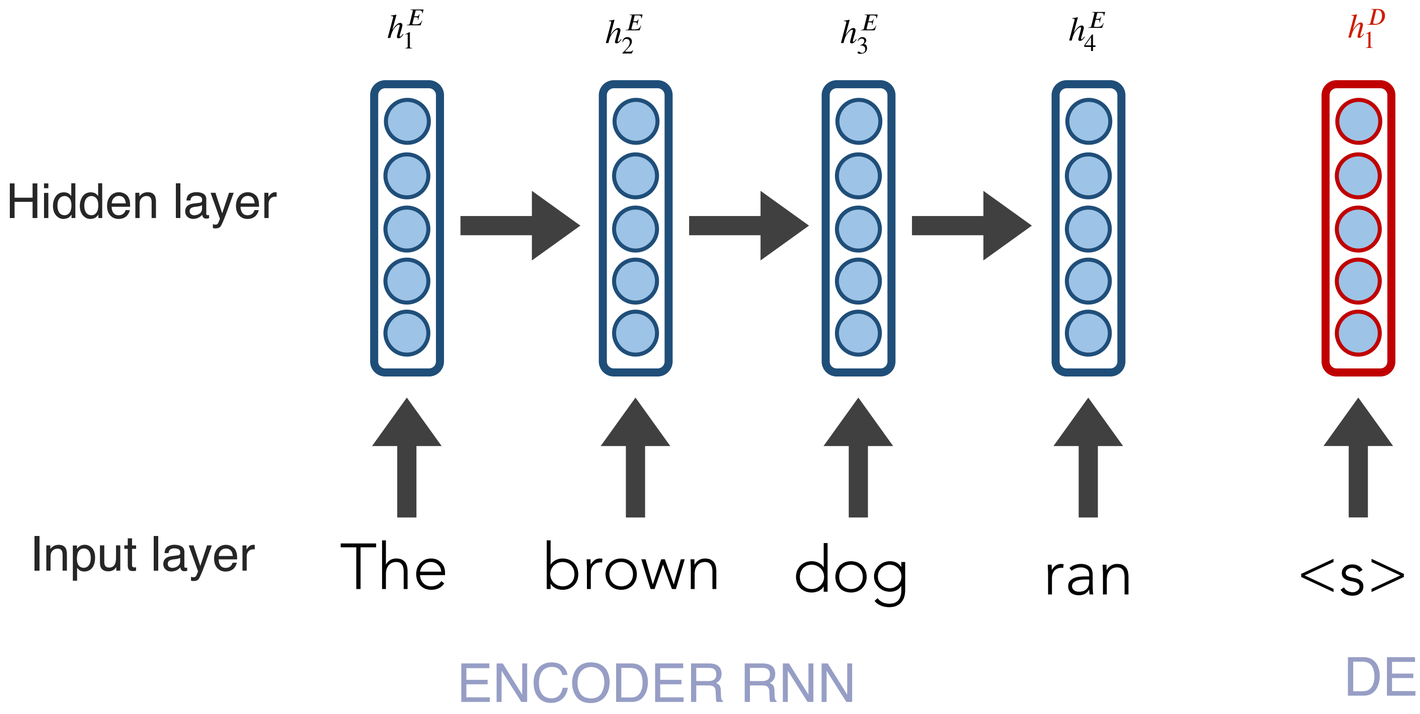

Attention (raw scores)

e_1	1.5
e_2	0.9
e_3	0.2
e_4	−0.5

Attention (softmax'd)

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

Attention Architecture

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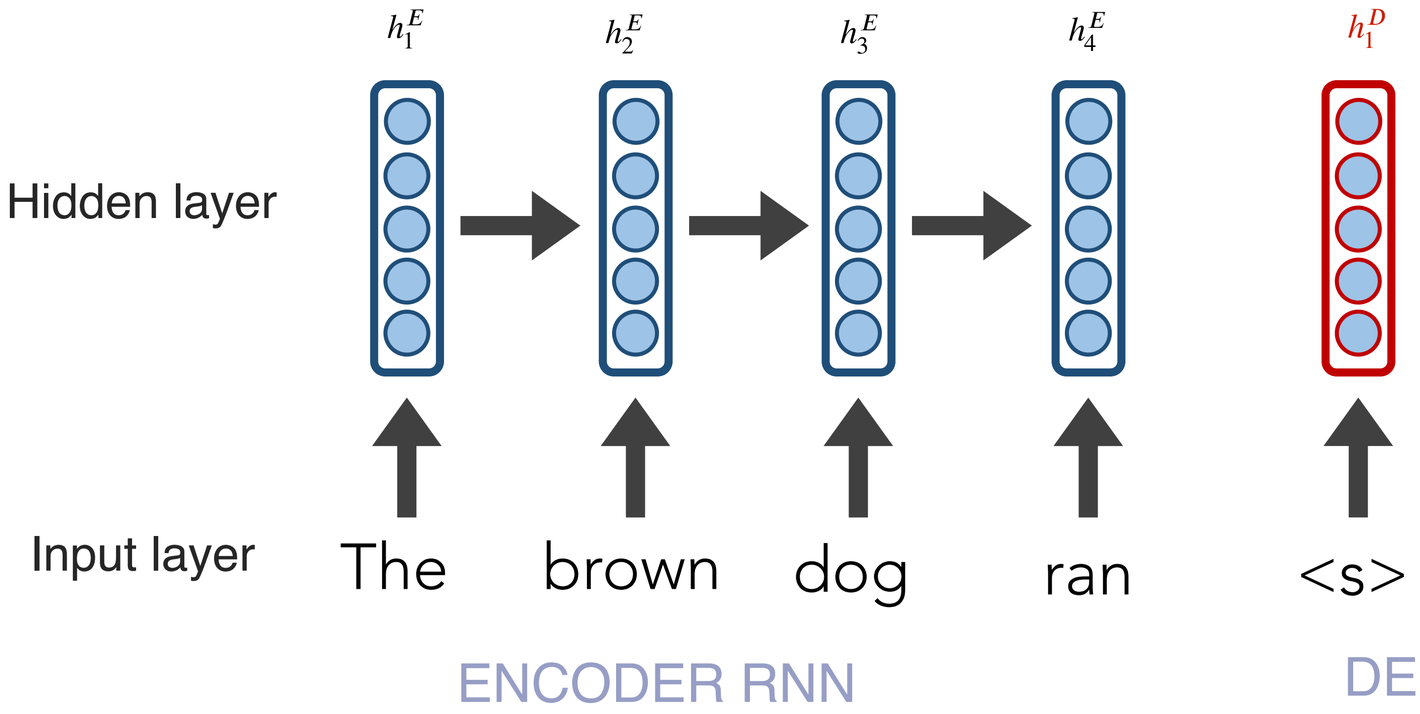

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Attention (softmax'd)

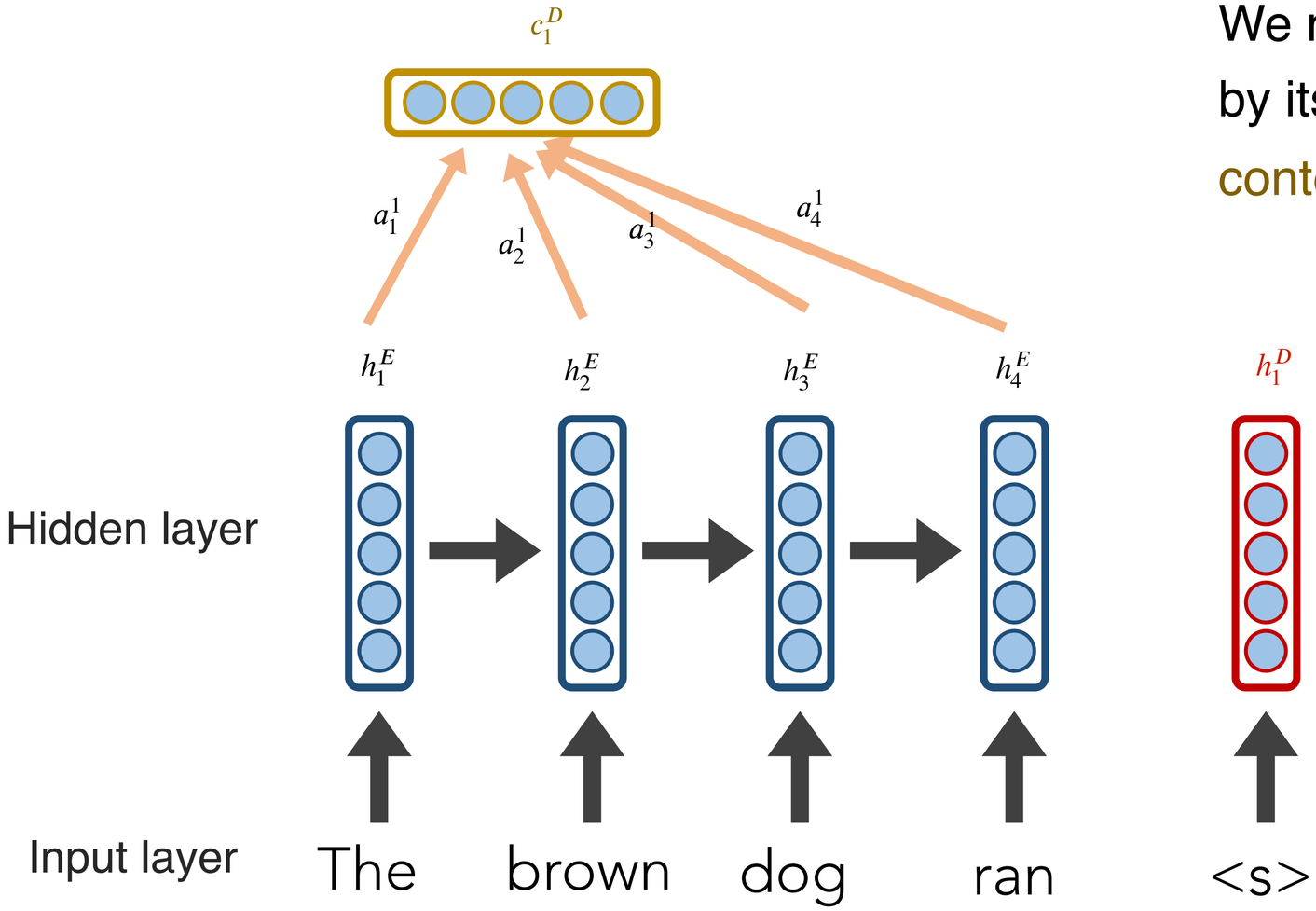
$a_1^1 = 0.51$

$a_2^1 = 0.28$

$a_3^1 = 0.14$

$a_3^1 = 0.07$

Attention Architecture



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)

$a_1^1 = 0.51$

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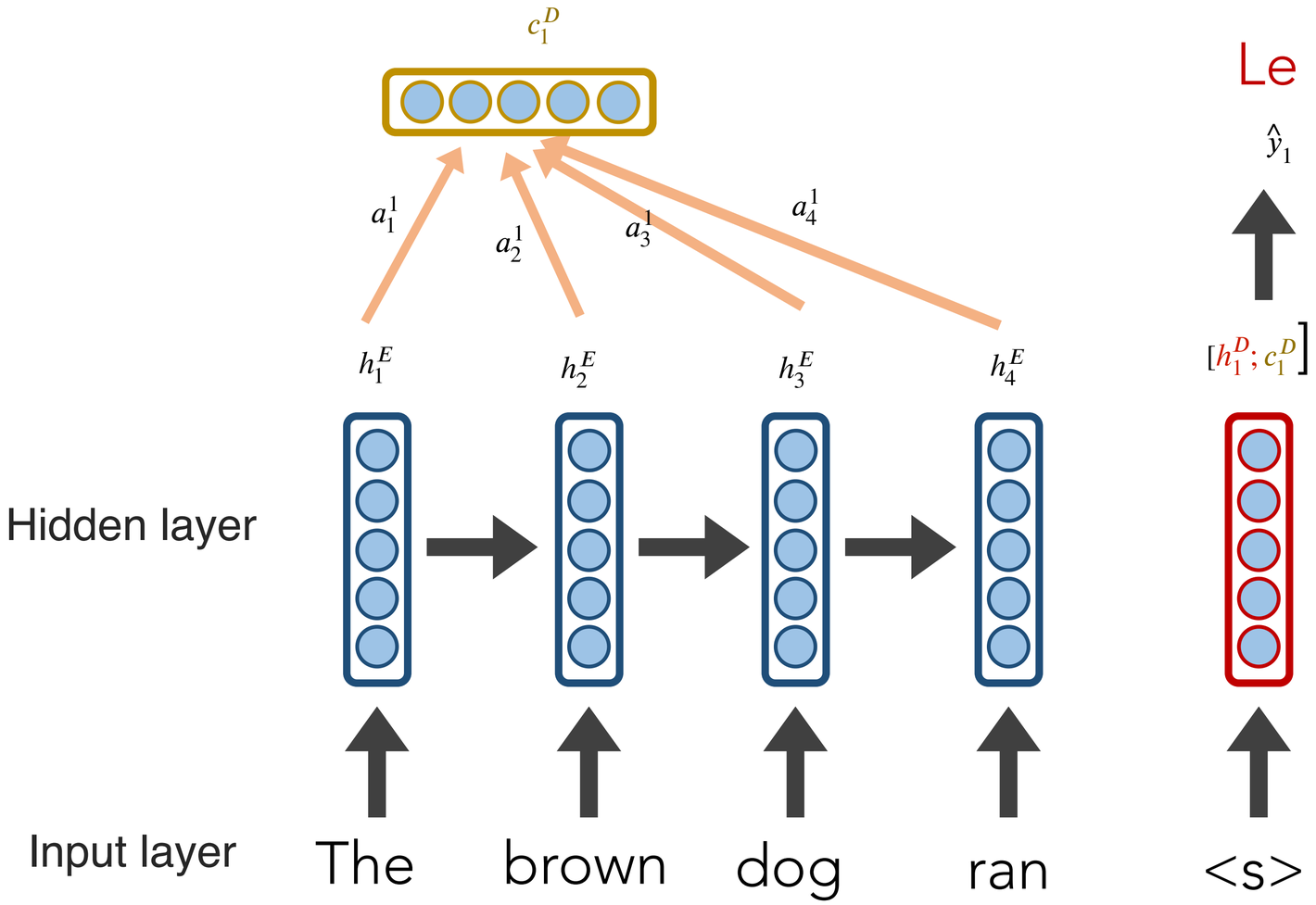
$a_3^1 = 0.07$

Attention Architecture

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



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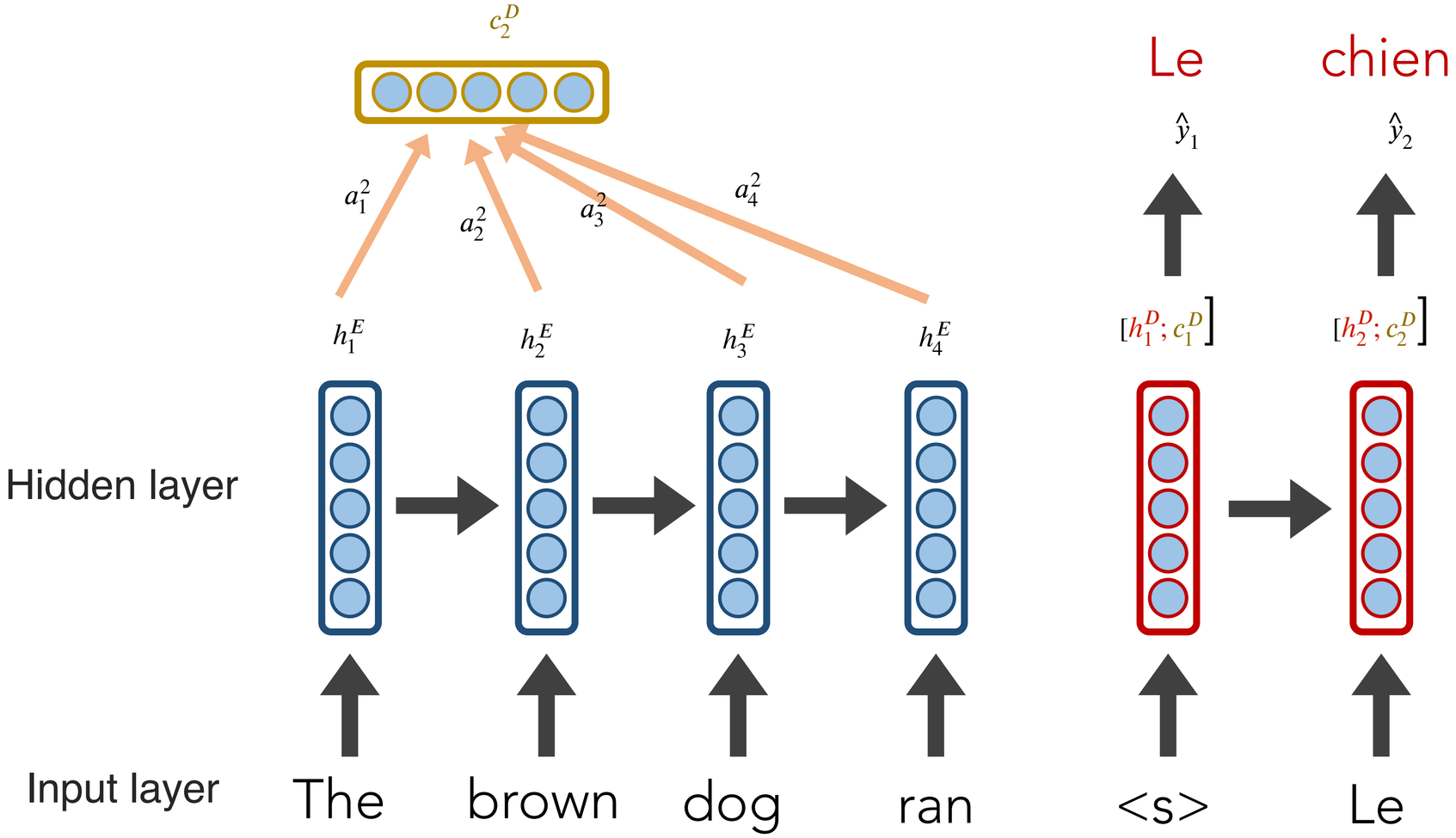

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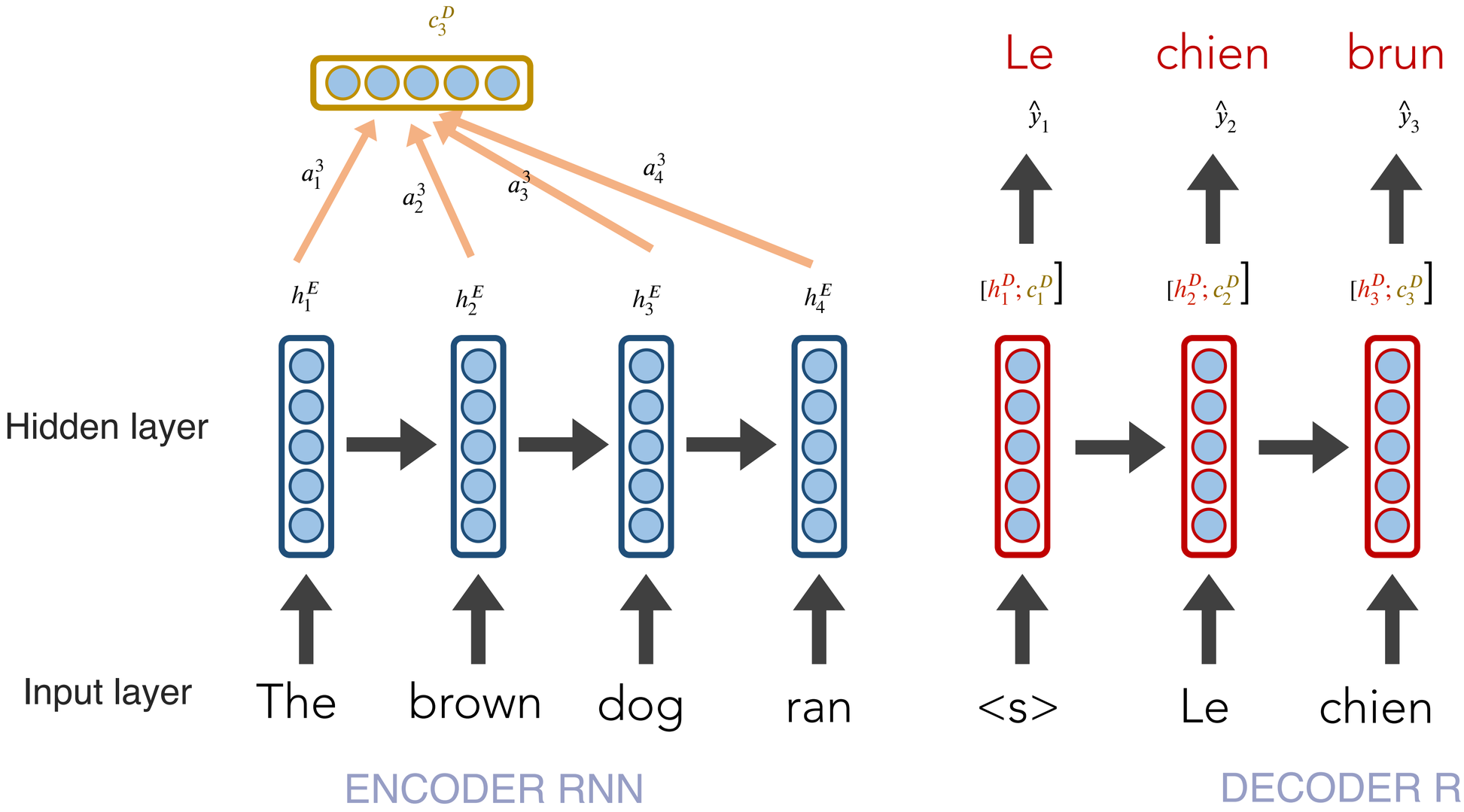

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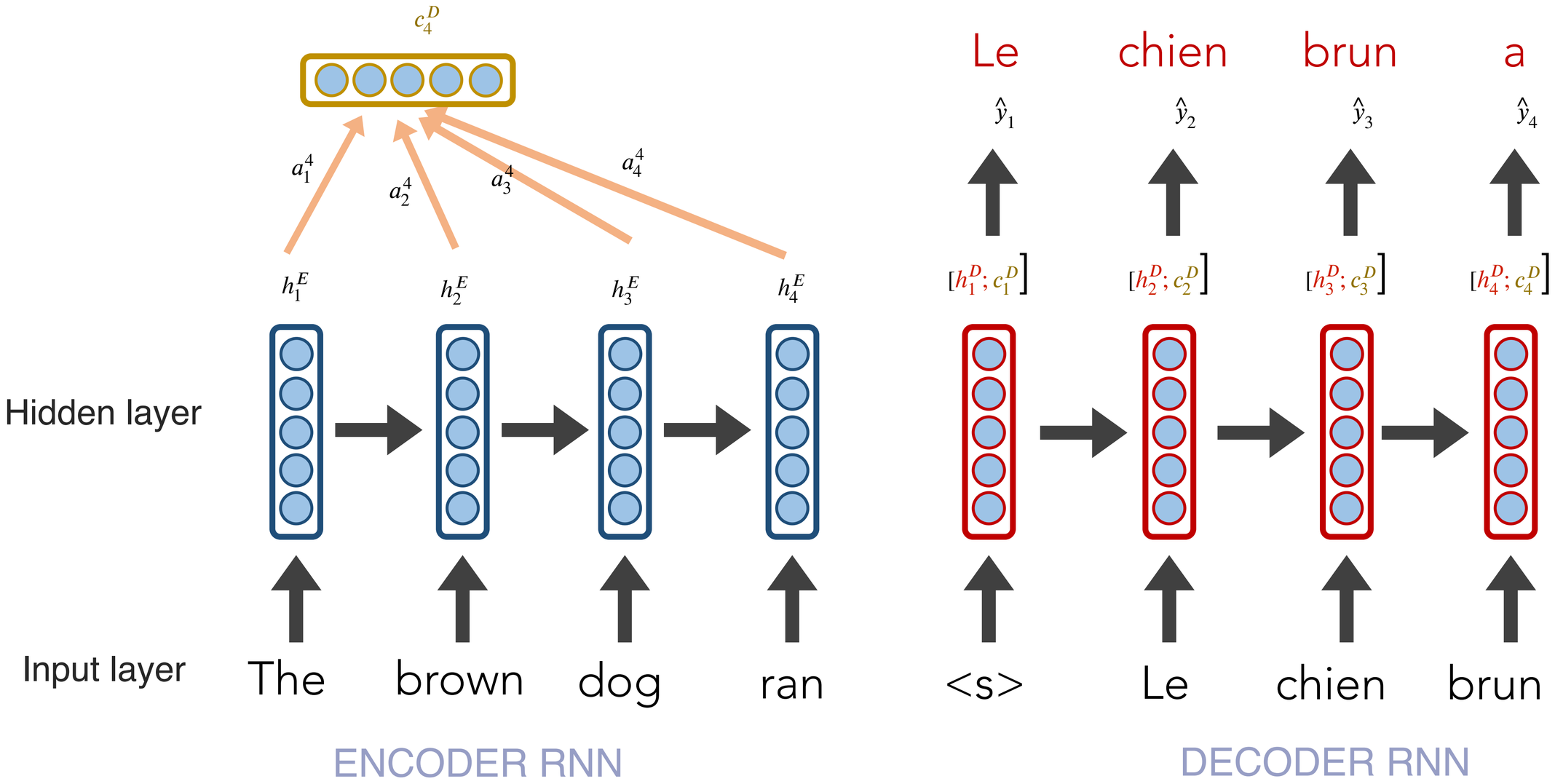

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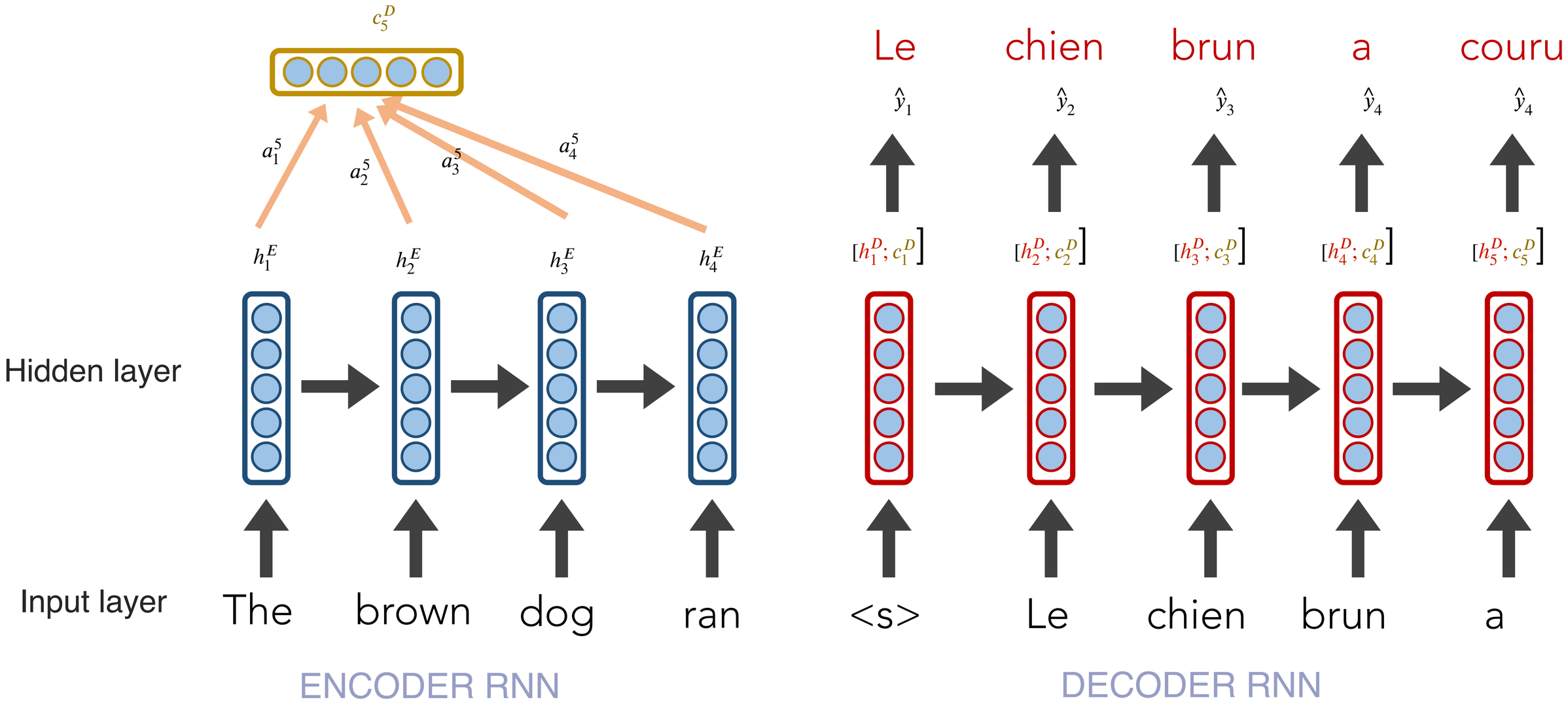


Attention Summary

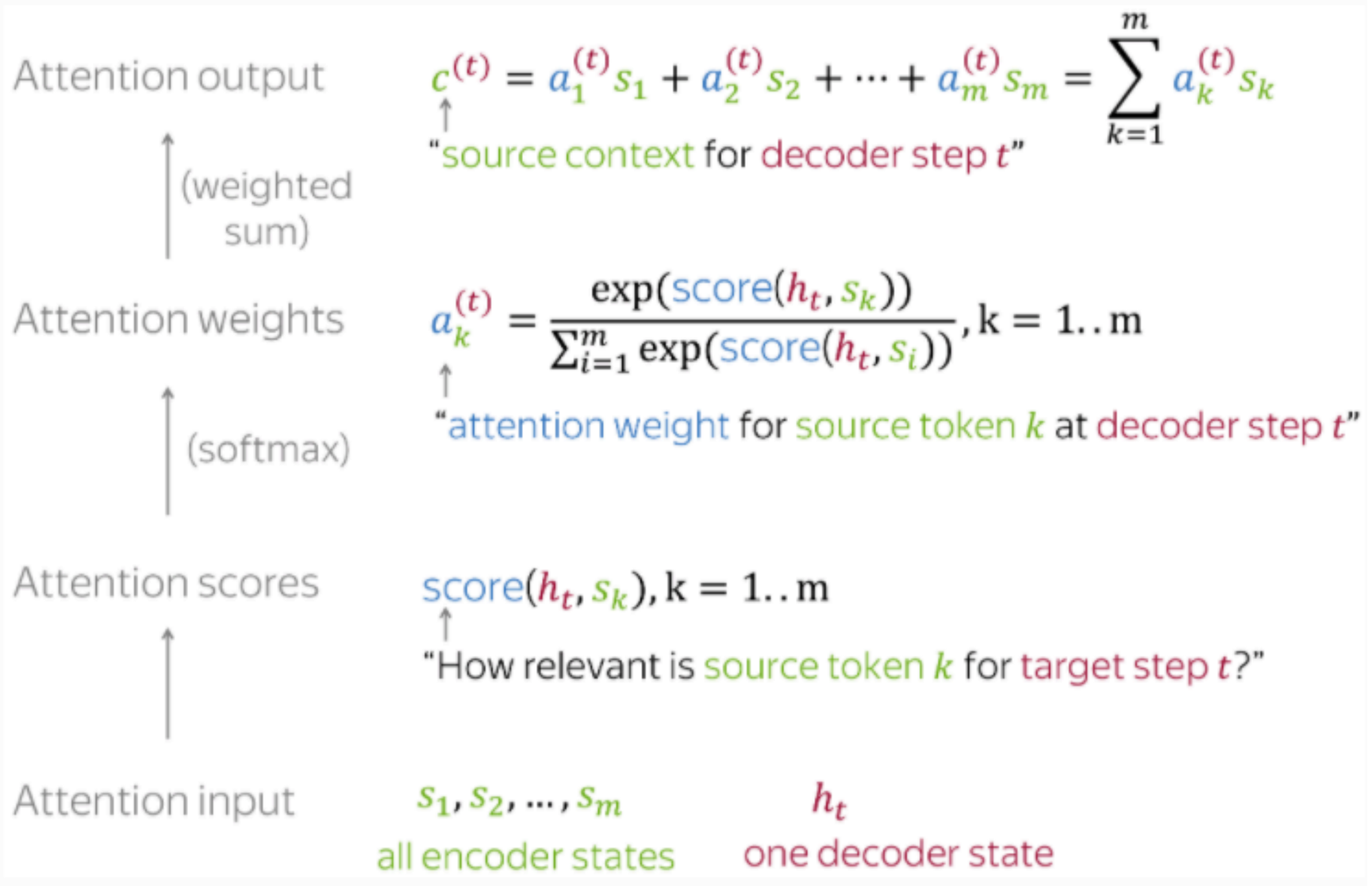
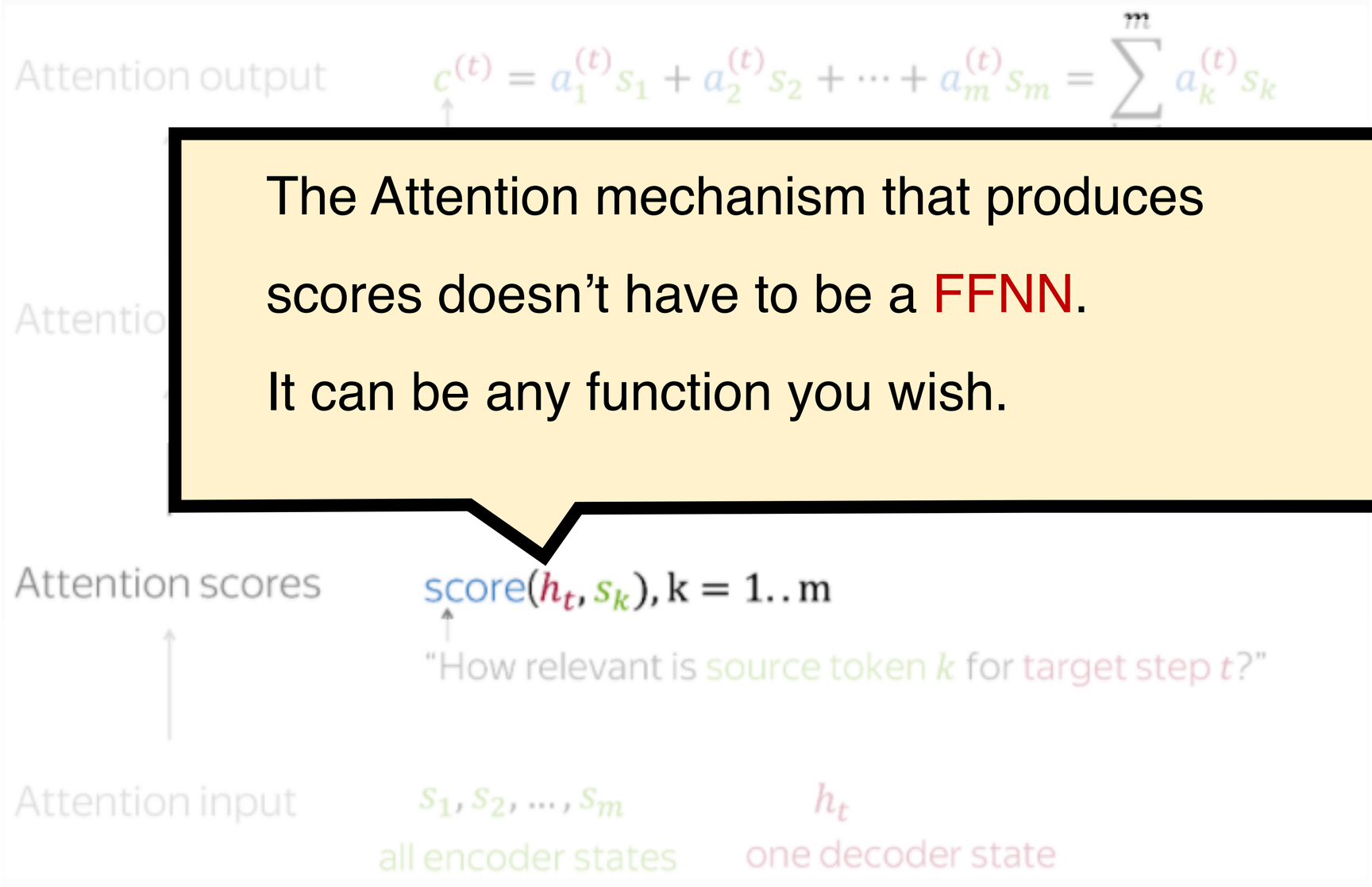


Photo credit: https://lena-voita.github.io/nlp_course/seq2seq_and_attention.html

Attention Summary



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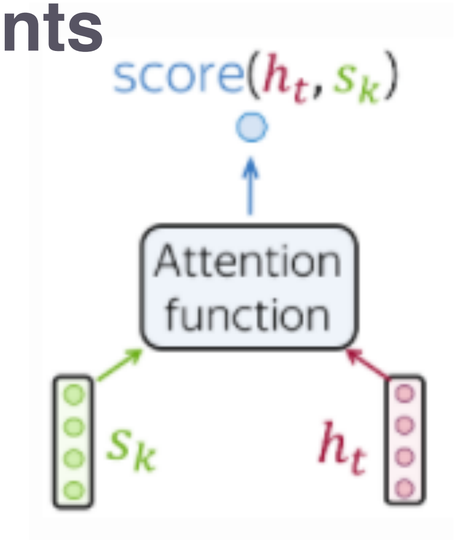
Attention Variants



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

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

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

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

Attention Summary

Attention:

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

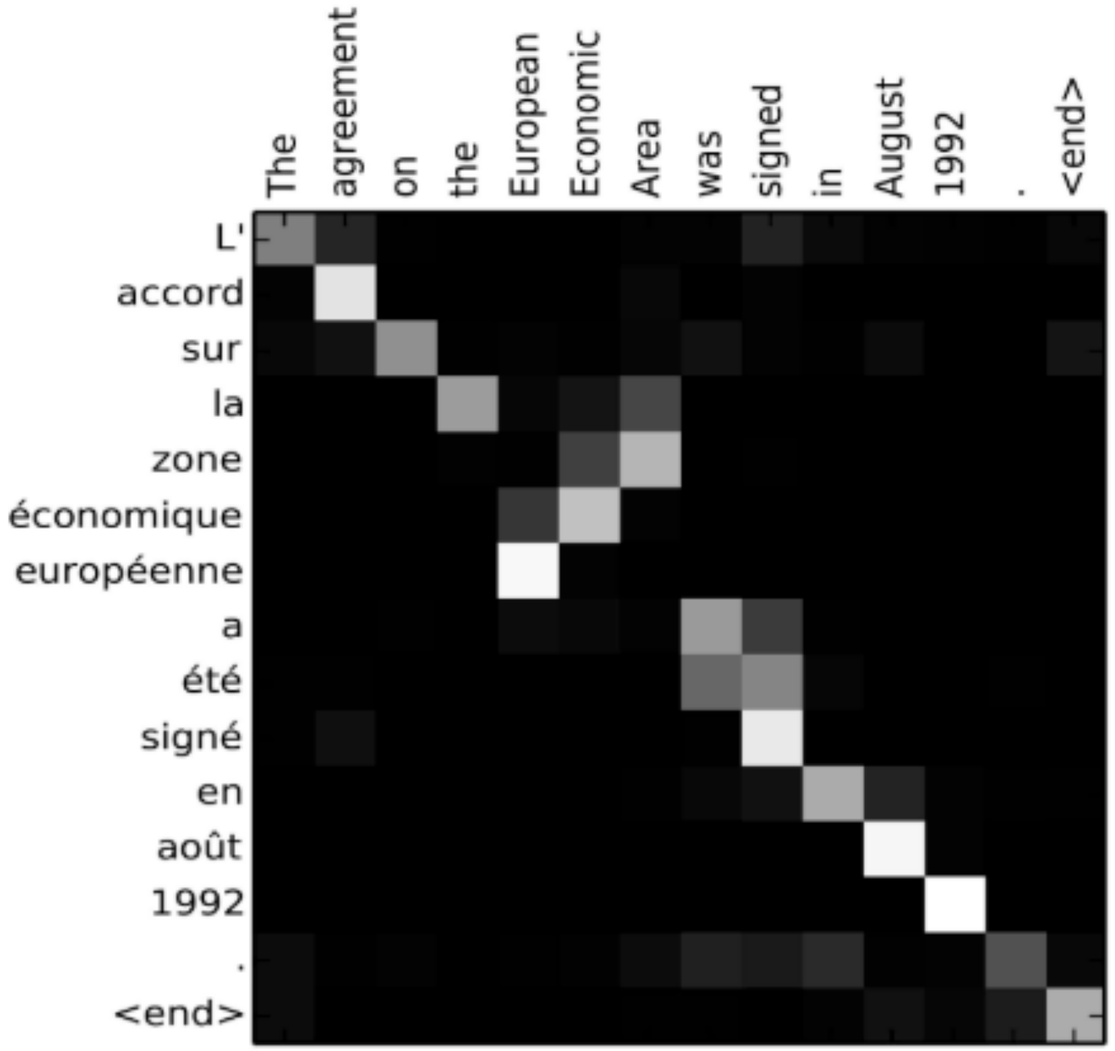
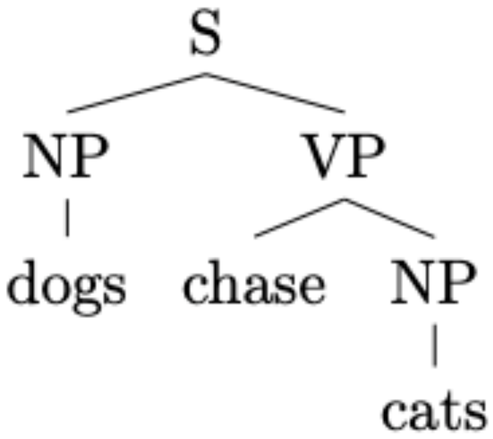


Image source: Fig 3 in [Bahdanau et al., 2015]

Attention Applications

Input: dogs chase cats

Output:



or a flattened representation

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

Attention Applications

Input: I shot an elephant in my pajamas

Output:

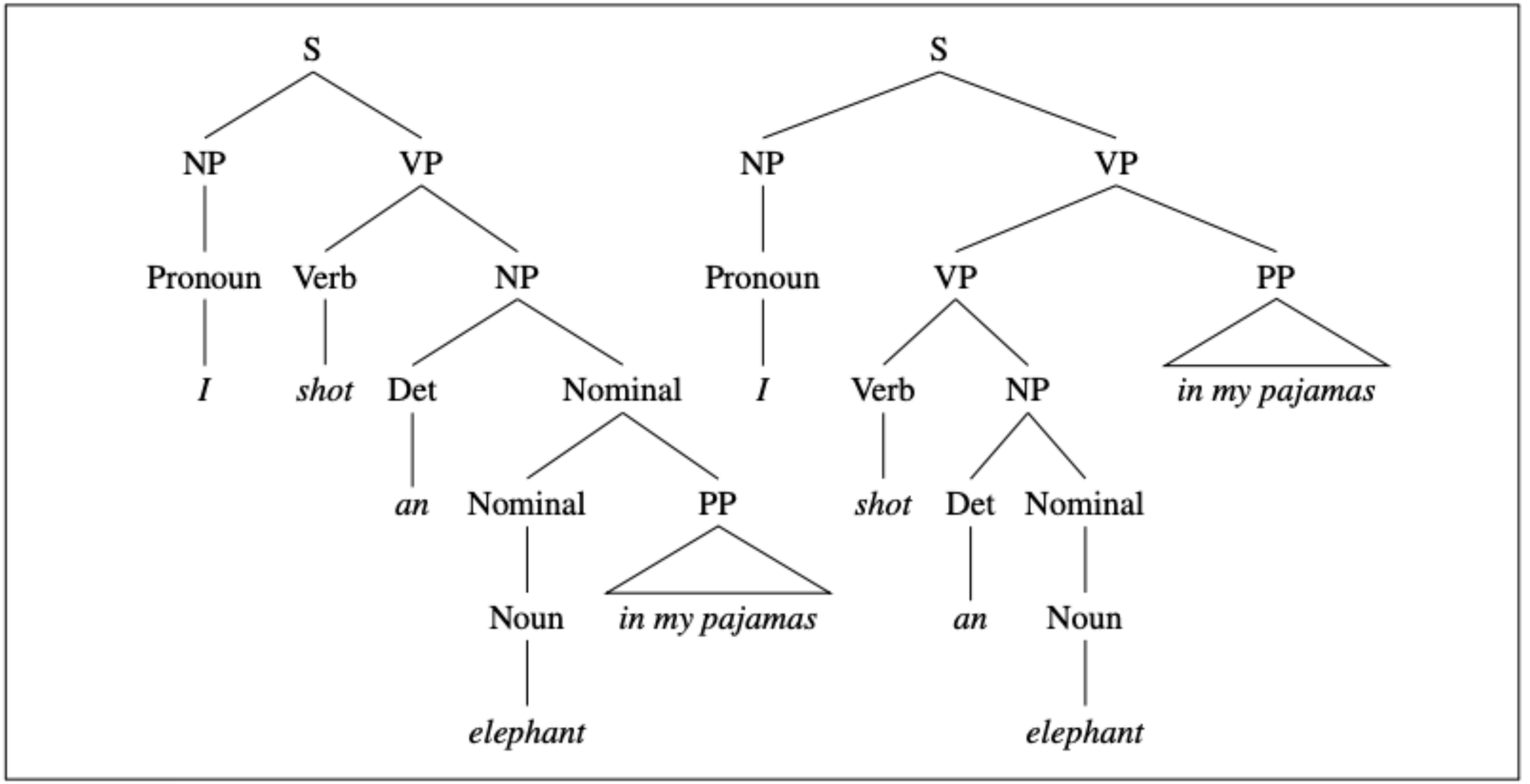


Figure 13.2 Two parse trees for an ambiguous sentence. The parse on the left corresponds to the humorous reading in which the elephant is in the pajamas, the parse on the right corresponds to the reading in which Captain Spaulding did the shooting in his pajamas.

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

Attention Applications

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

Visualizing Attention

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)

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

Visualizing Attention

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)

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

Visualizing Attention

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)

Visualizing Attention

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.

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

Self Attention

Self Attention Motivation

- Word meaning is contextual!
  - *The shirt is green*
  - *The recruits are green*
  - *Green policy has wrecked the economy*
- But word (type) embeddings conflate all of these meanings
- Every occurrence (token) of “green” carries the same semantic mix
- Instead: embed individual term occurrences

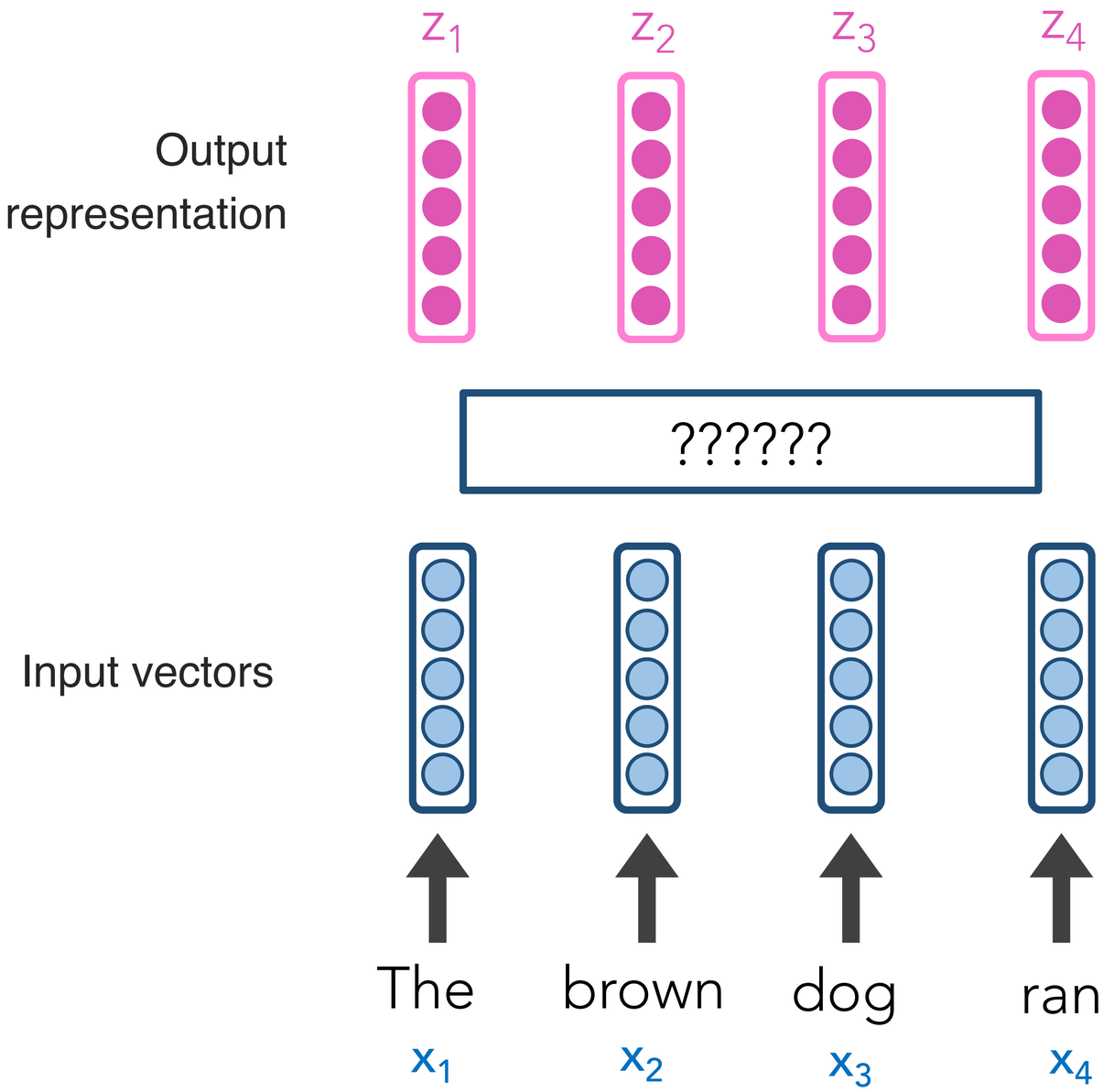
Self Attention Motivation

- Each word in a sequence is 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”

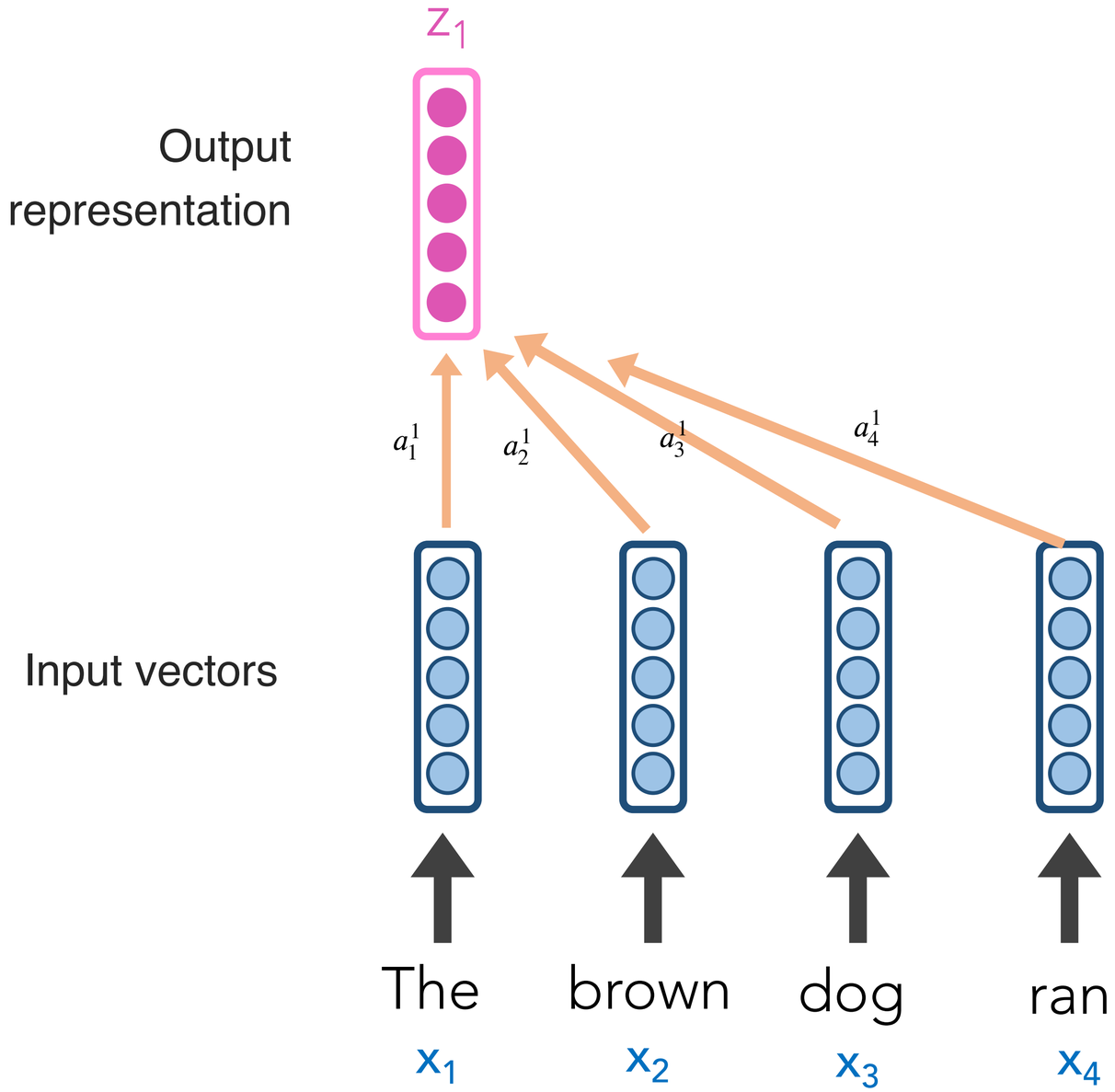
- We want (explicit) positionality

Self Attention Motivation



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

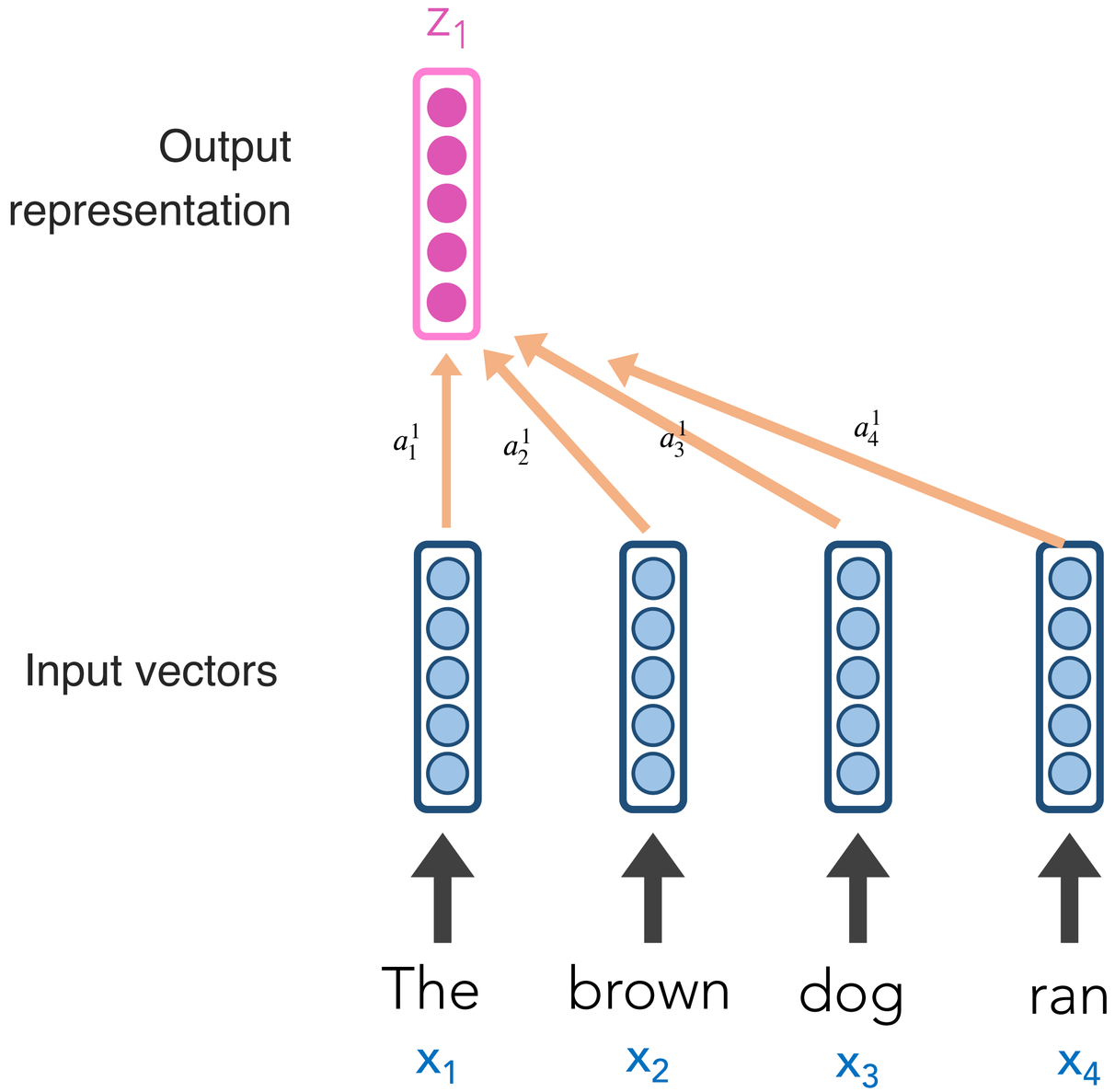
Self Attention Motivation



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 Motivation

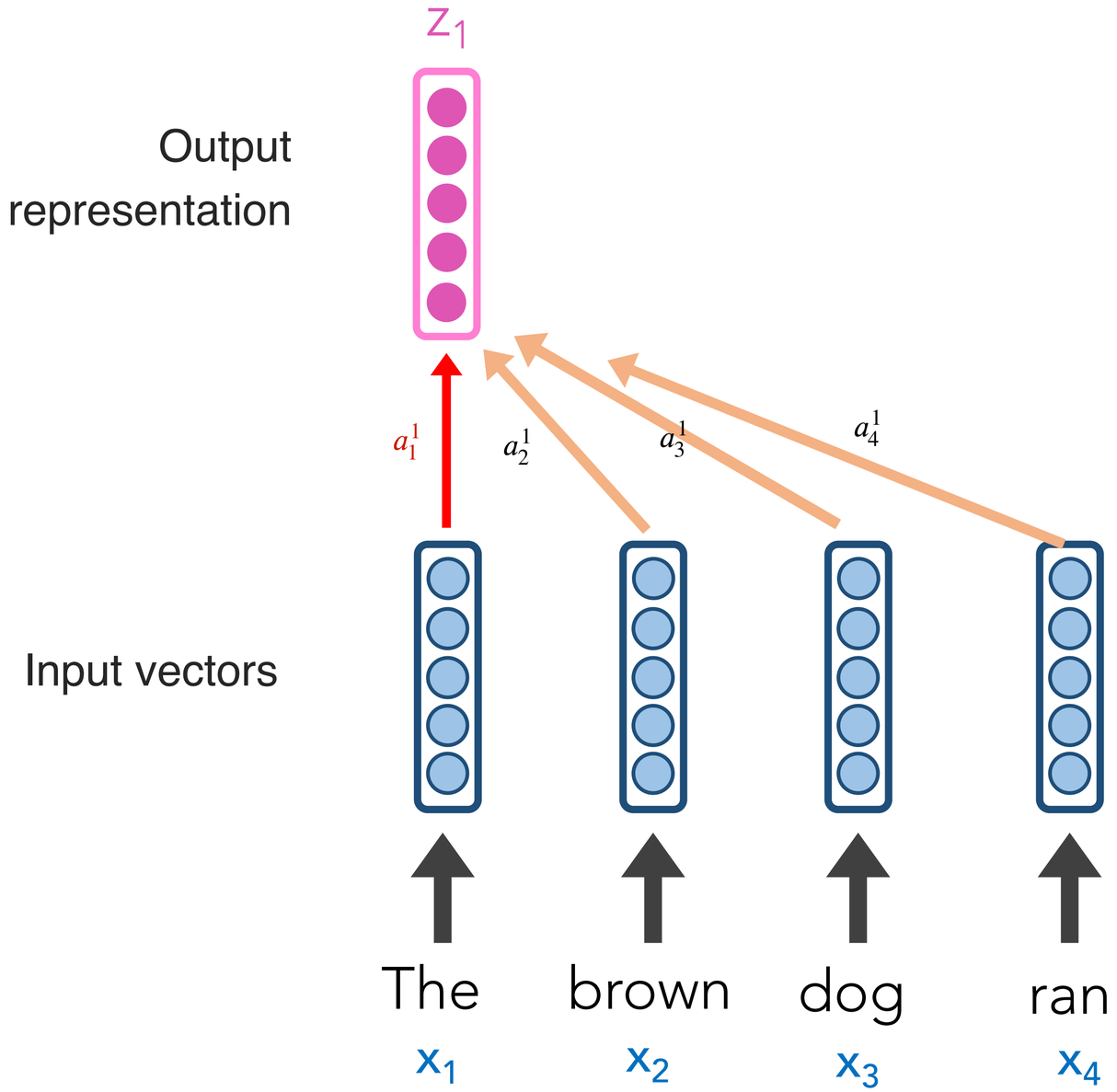


Self-Attention's goal is to create great representations, z_i, of the input

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 Motivation



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 Architecture

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:

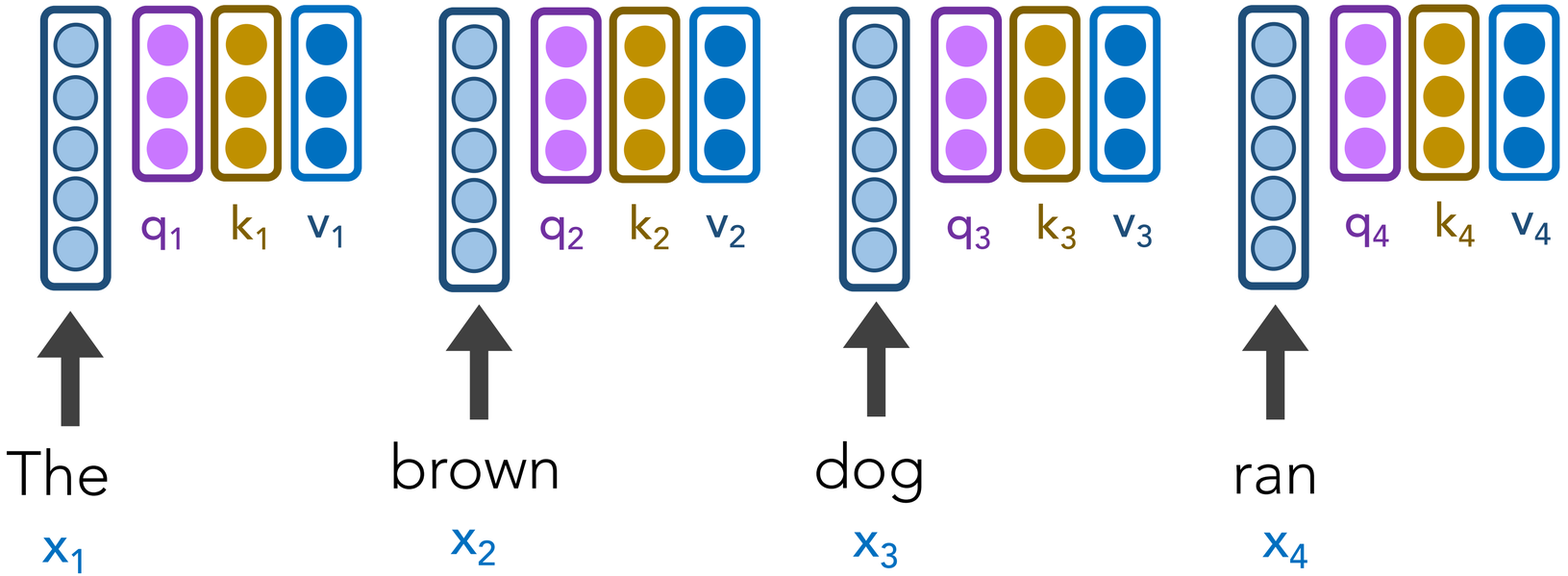
$$q_i = w_q x_i$$

$$k_i = w_k x_i$$

$$v_i = w_v x_i$$

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

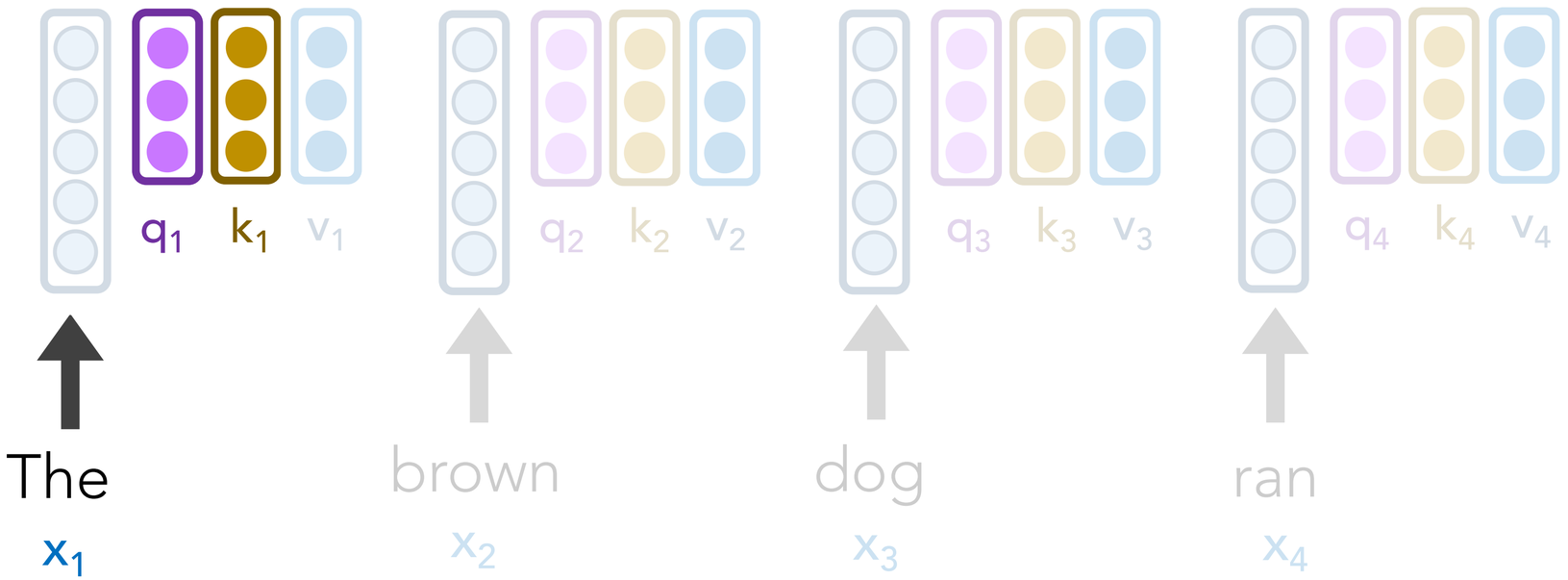
- Query q_1
- Key k_1
- Value v_1



Self-Attention Architecture

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

$s_1 = q_1 . k_1 = 112$

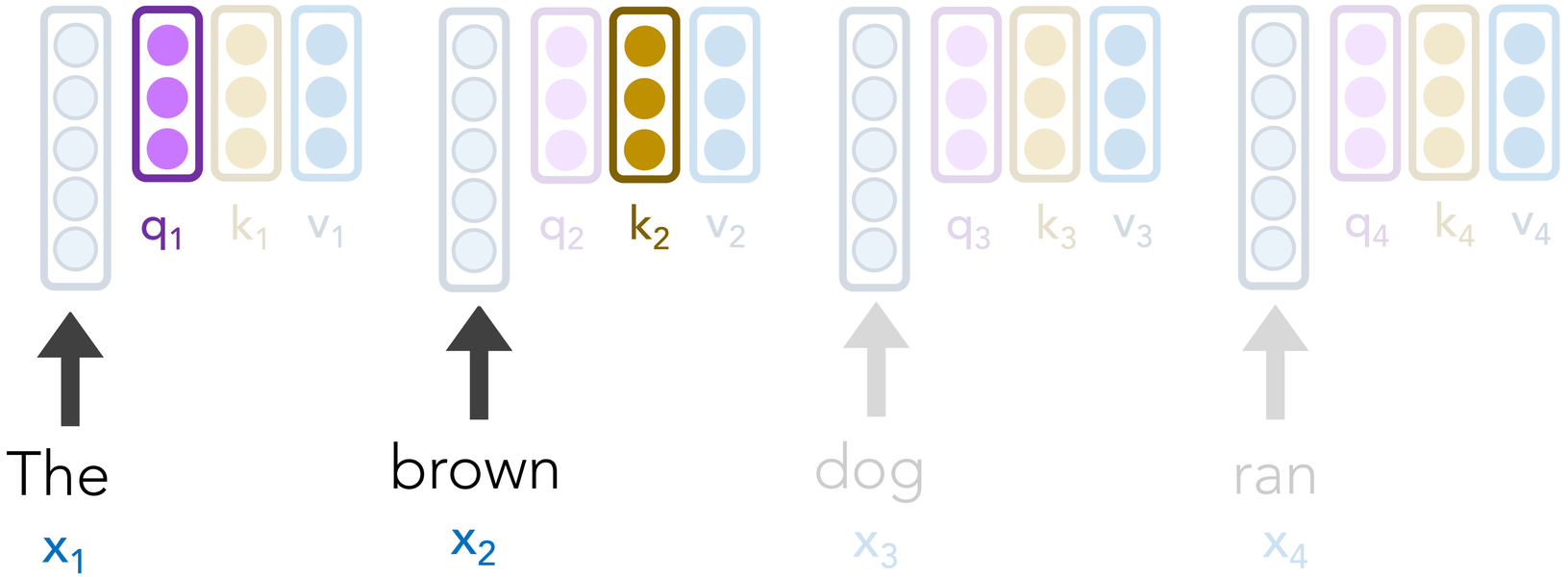


Self-Attention Architecture

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

$s_2 = q_1 . k_2 = 96$

$s_1 = q_1 . k_1 = 112$



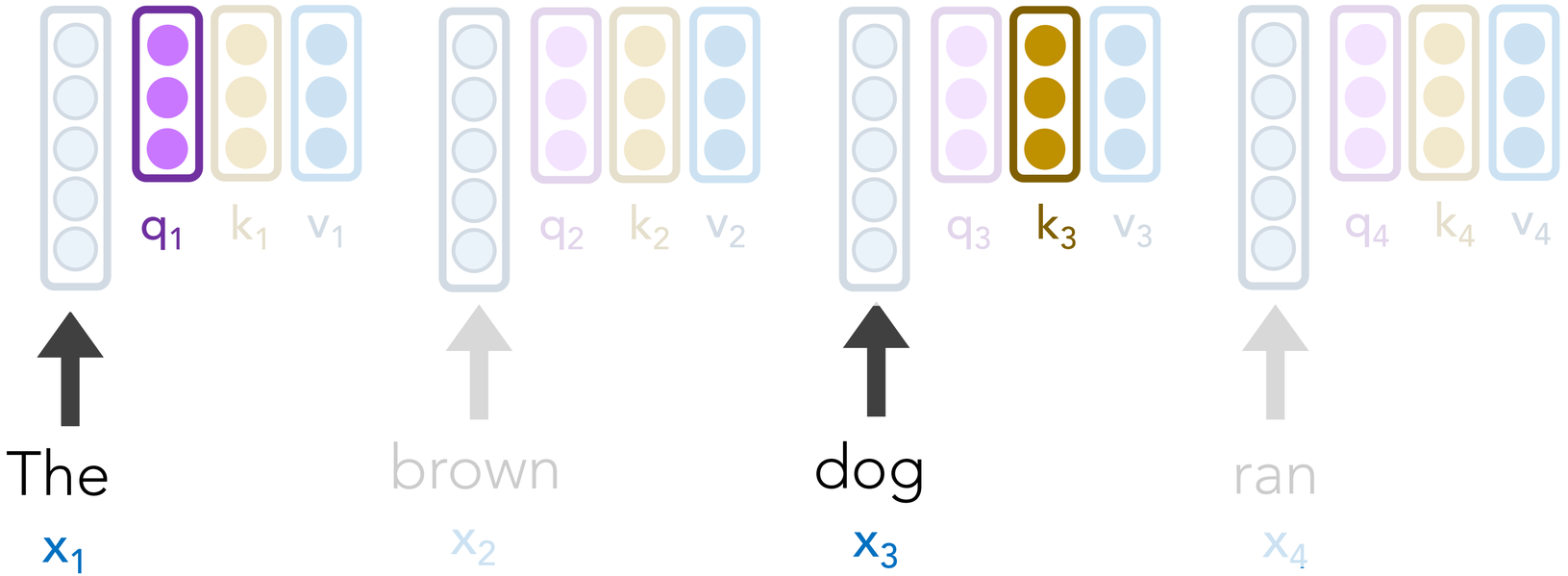
Self-Attention Architecture

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

$s_3 = q_1 . k_3 = 16$

$s_2 = q_1 . k_2 = 96$

$s_1 = q_1 . k_1 = 112$



Self-Attention Architecture

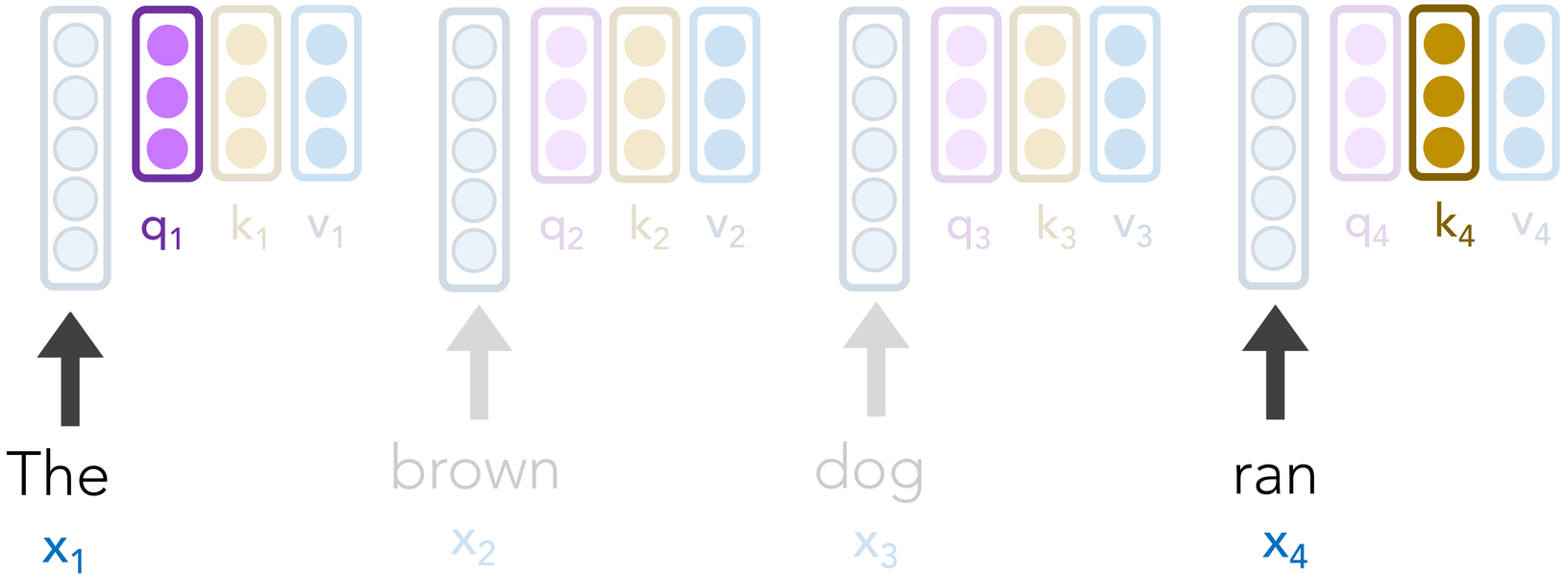
Step 2: For word x_1, let's calculate the scores s_1, s_2, s_3, s_4, which represent how much attention to pay to each respective "word" v_i

$s_4 = q_1 . k_4 = 8$

$s_3 = q_1 . k_3 = 16$

$s_2 = q_1 . k_2 = 96$

$s_1 = q_1 . k_1 = 112$



Self-Attention Architecture

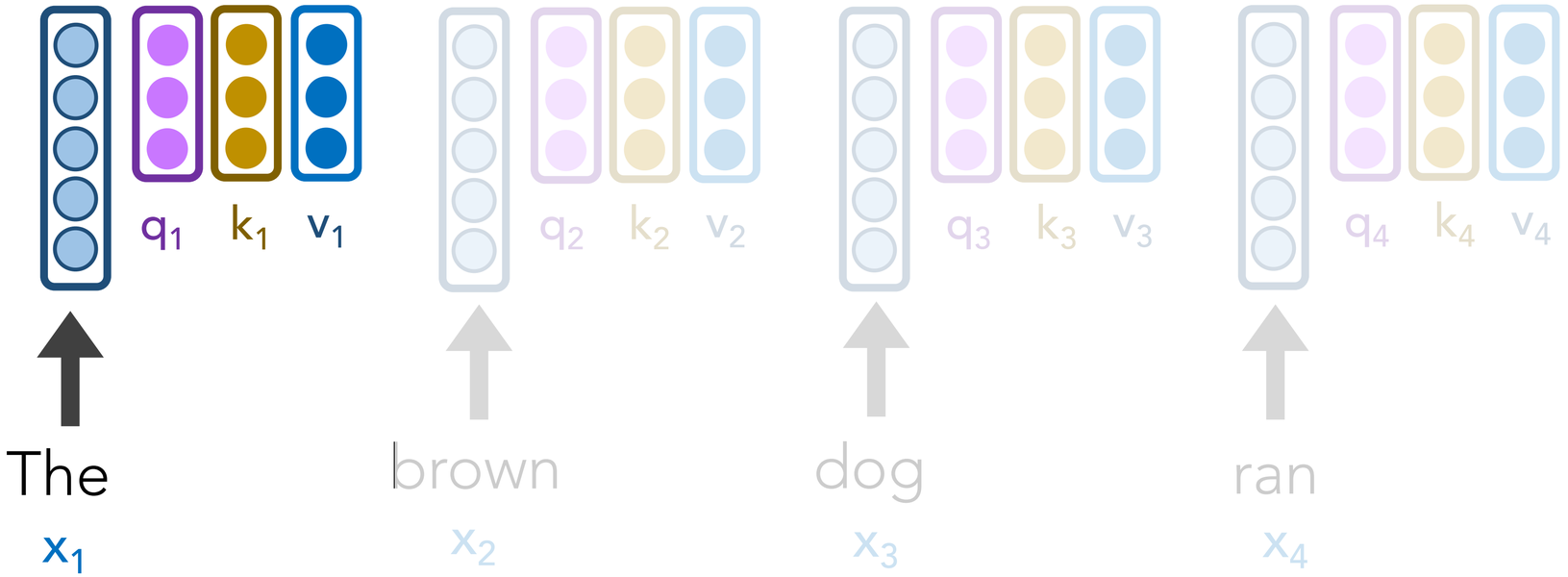
Step 3: Our scores s_1, s_2, s_3, s_4 don't sum to 1. Let's divide by $\sqrt{len(k_i)}$ and softmax it

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

$s_3 = q_1 . k_3 = 16$ $\quad a3 = \sigma(s_3/8) = .01$

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

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



Self-Attention Architecture

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

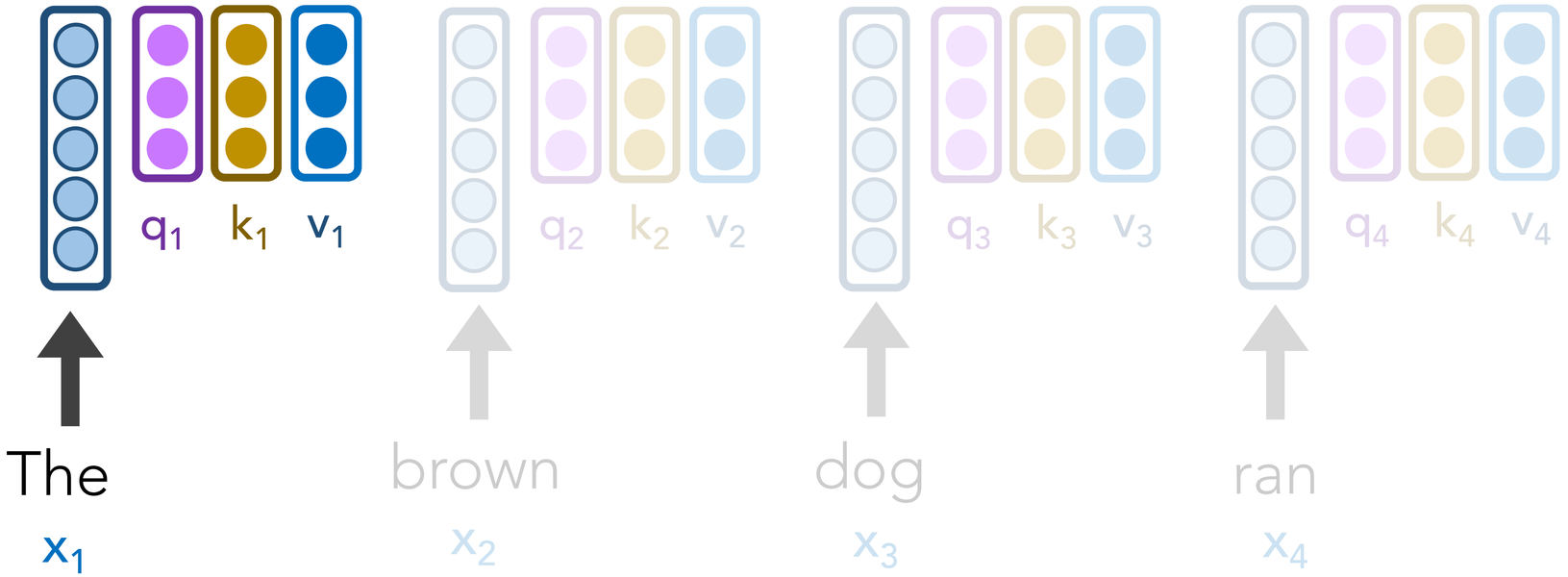
$s_4 = q_1 \cdot k_4 = 8$ $\quad a_4 = \sigma(s_4/8) = 0$

$s_3 = q_1 \cdot k_3 = 16$ $\quad a3 = \sigma(s_3/8) = .01$

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

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

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

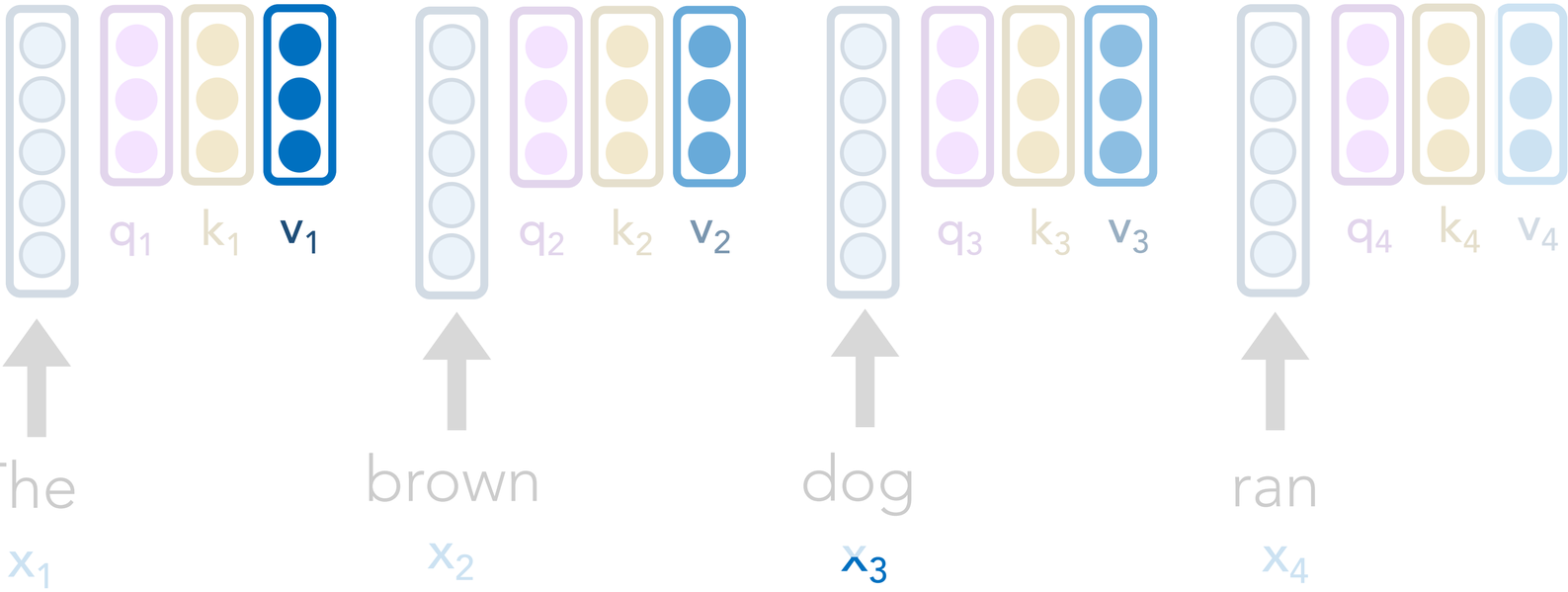


Self-Attention Architecture

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

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

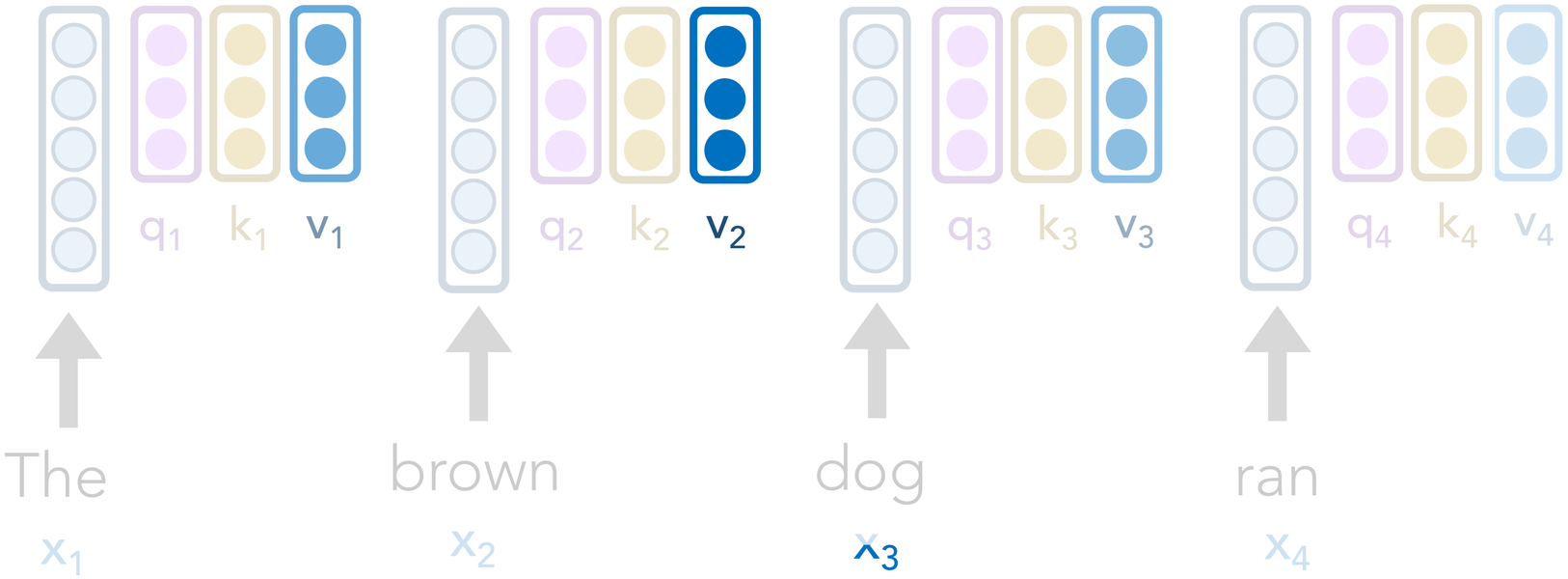
$$= 0.87 \cdot v_1 + \mathbf{0.12} \cdot v_2 + \mathbf{0.01} \cdot v_3 + \mathbf{0} \cdot v_4$$



Self-Attention Architecture

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

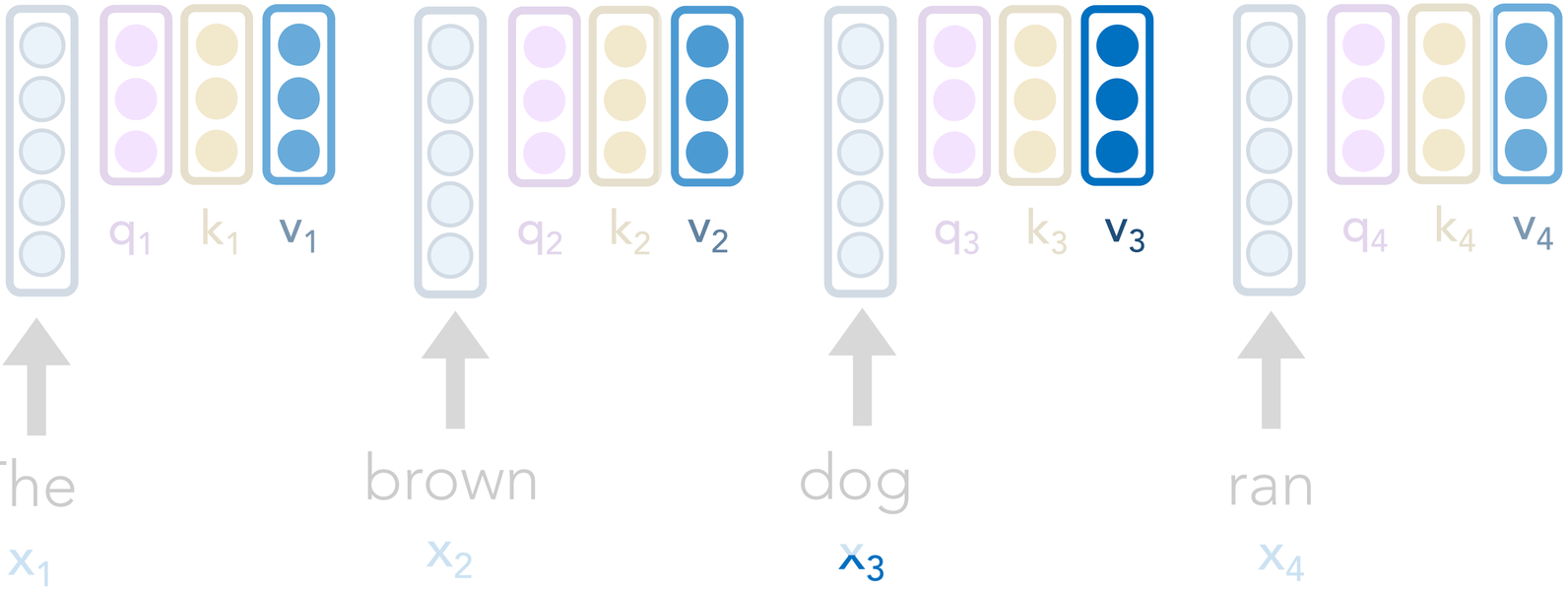
$$z_2 = a_1 \cdot v_1 + a_2 \cdot v_2 + a_3 \cdot v_3 + a_4 \cdot v_4$$



Self-Attention Architecture

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

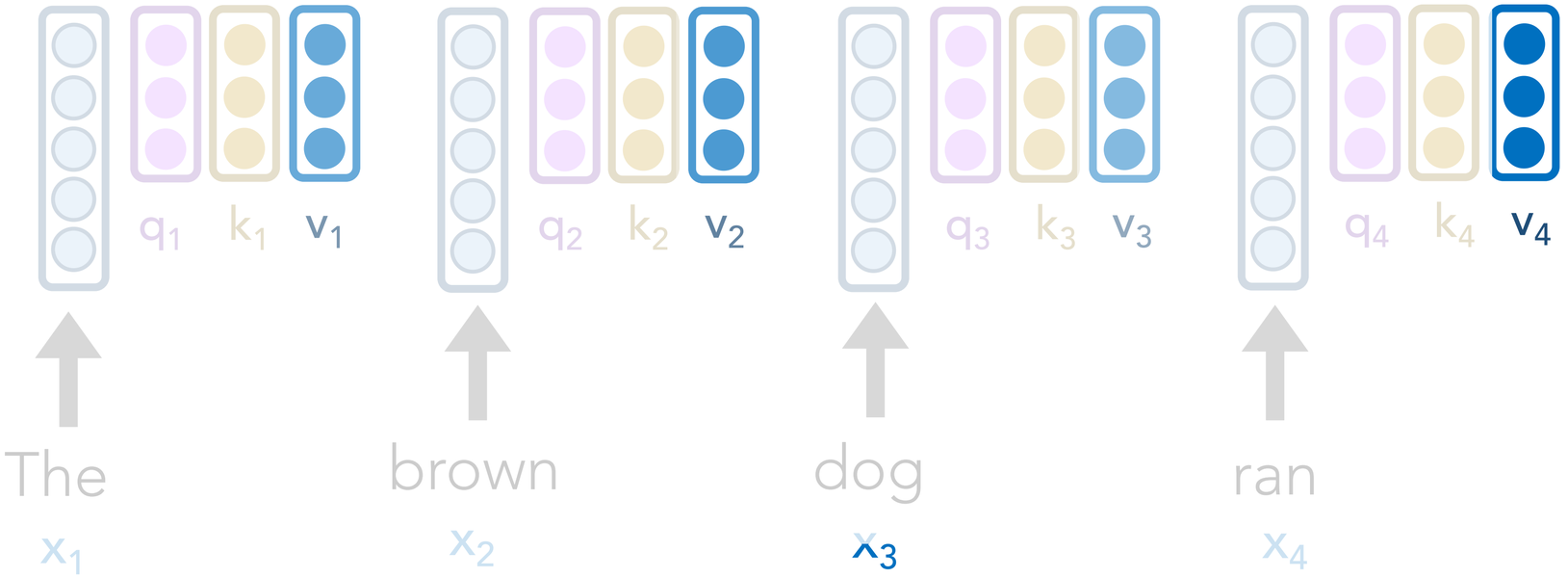
$$z_3 = a_1 \cdot v_1 + a_2 \cdot v_2 + a_3 \cdot v_3 + a_4 \cdot v_4$$



Self-Attention Architecture

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

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



Self-Attention Architecture

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 Architecture

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:

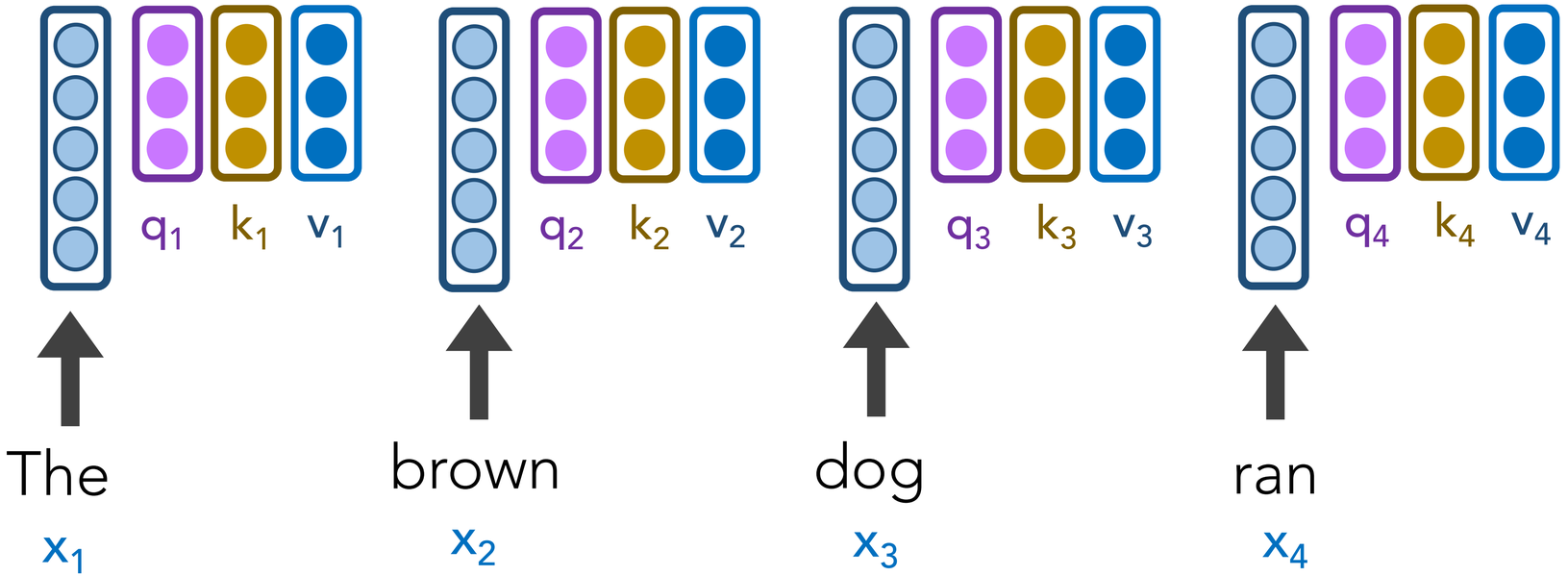
$$q_i = w_q x_i$$

$$k_i = w_k x_i$$

$$v_i = w_v x_i$$

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

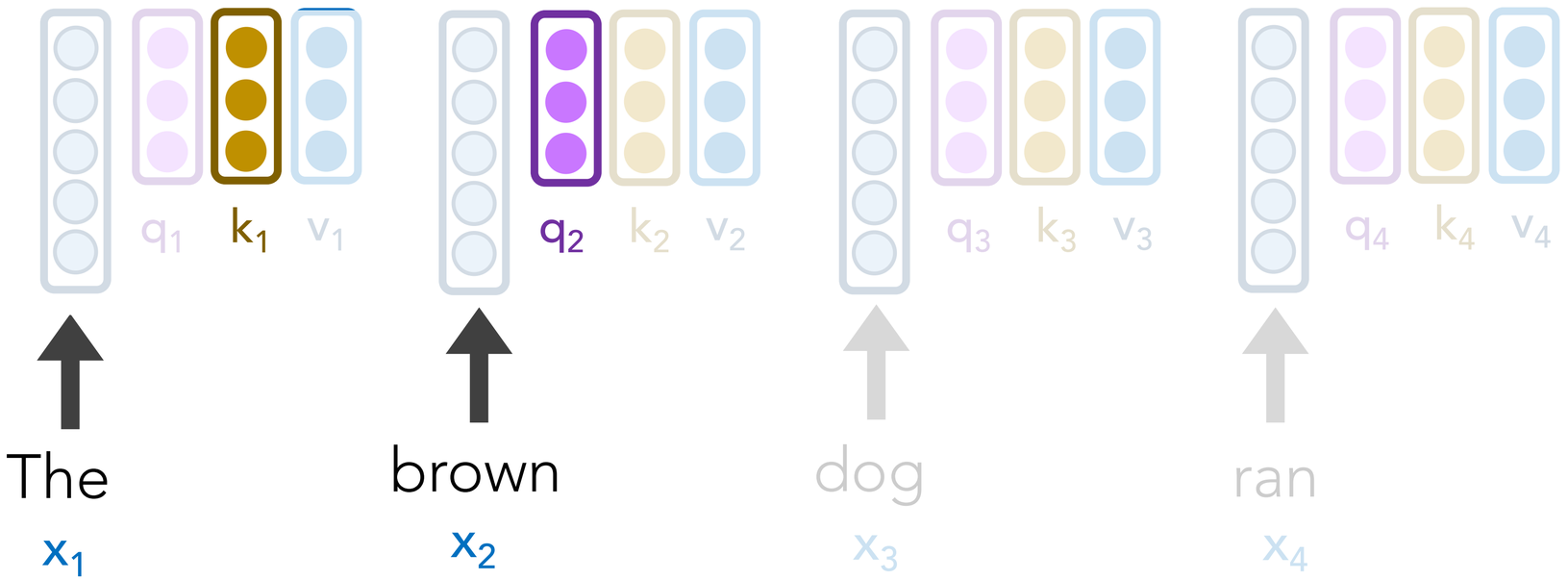
- Query q_1
- Key k_1
- Value v_1



Self-Attention Architecture

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

$s_1 = q_2 \cdot k_1 = 92$

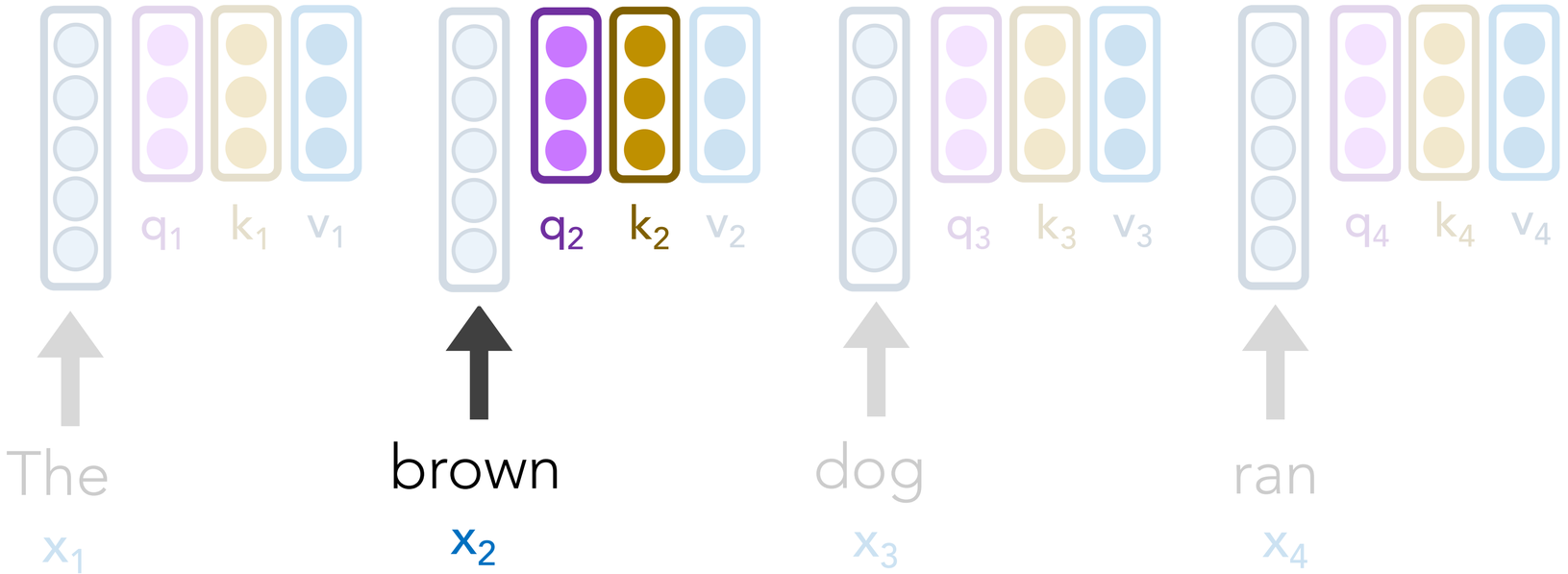


Self-Attention Architecture

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

$s_2 = q_2 \cdot k_2 = 124$

$s_1 = q_2 \cdot k_1 = 92$



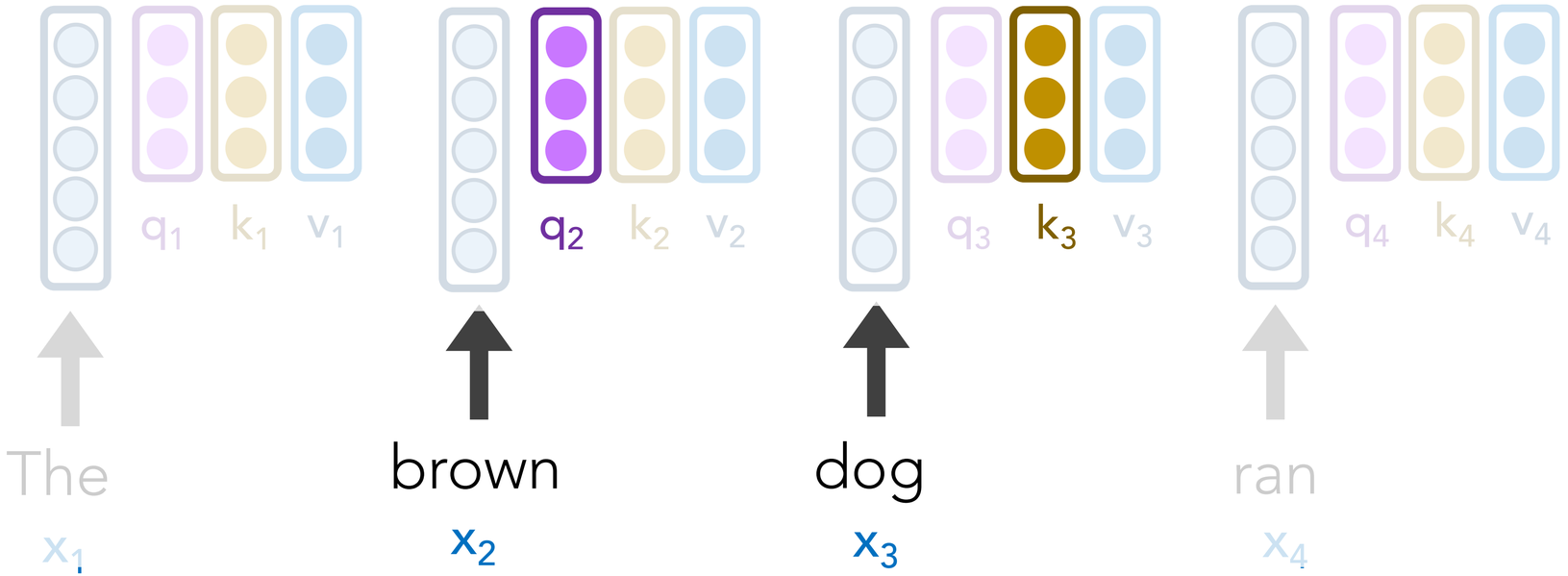
Self-Attention Architecture

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 Architecture

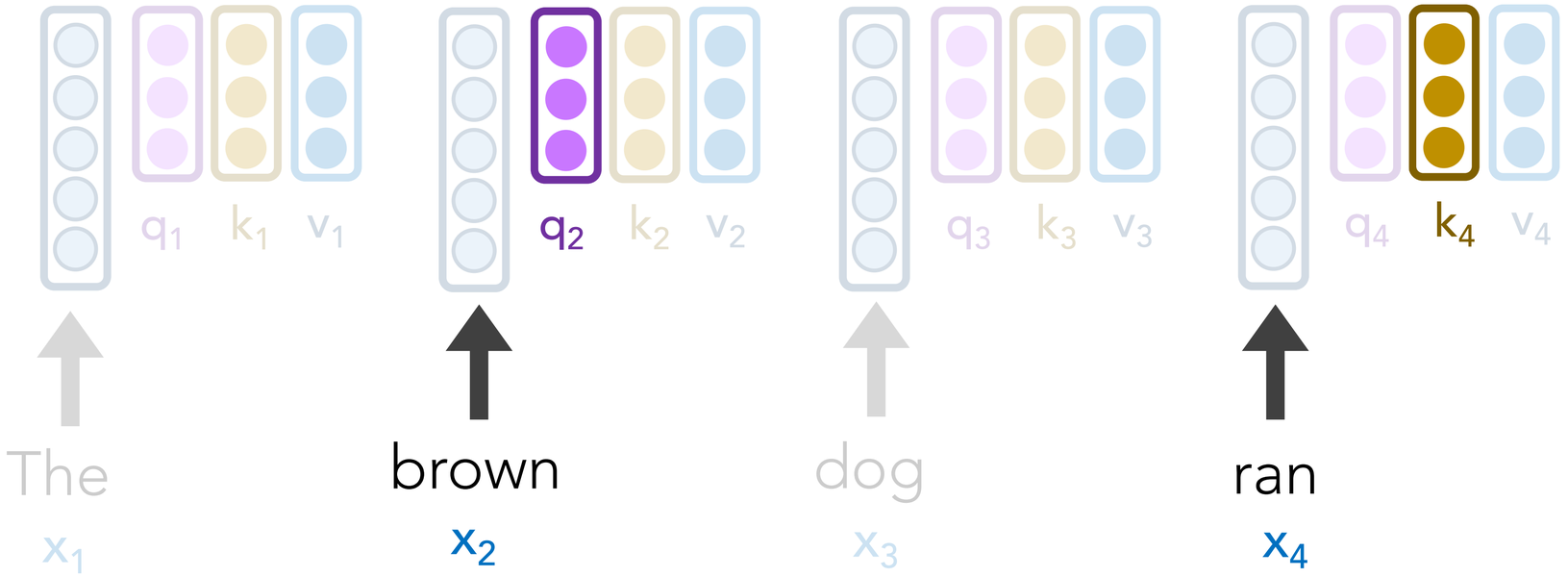
Step 2: For word x_2, let's calculate the scores s_1, s_2, s_3, s_4, which represent how much attention to pay to each respective "word" v_i

$s_4 = q_2 . k_4 = 8$

$s_3 = q_2 . k_3 = 22$

$s_2 = q_2 . k_2 = 124$

$s_1 = q_2 . k_1 = 92$



Self-Attention Architecture

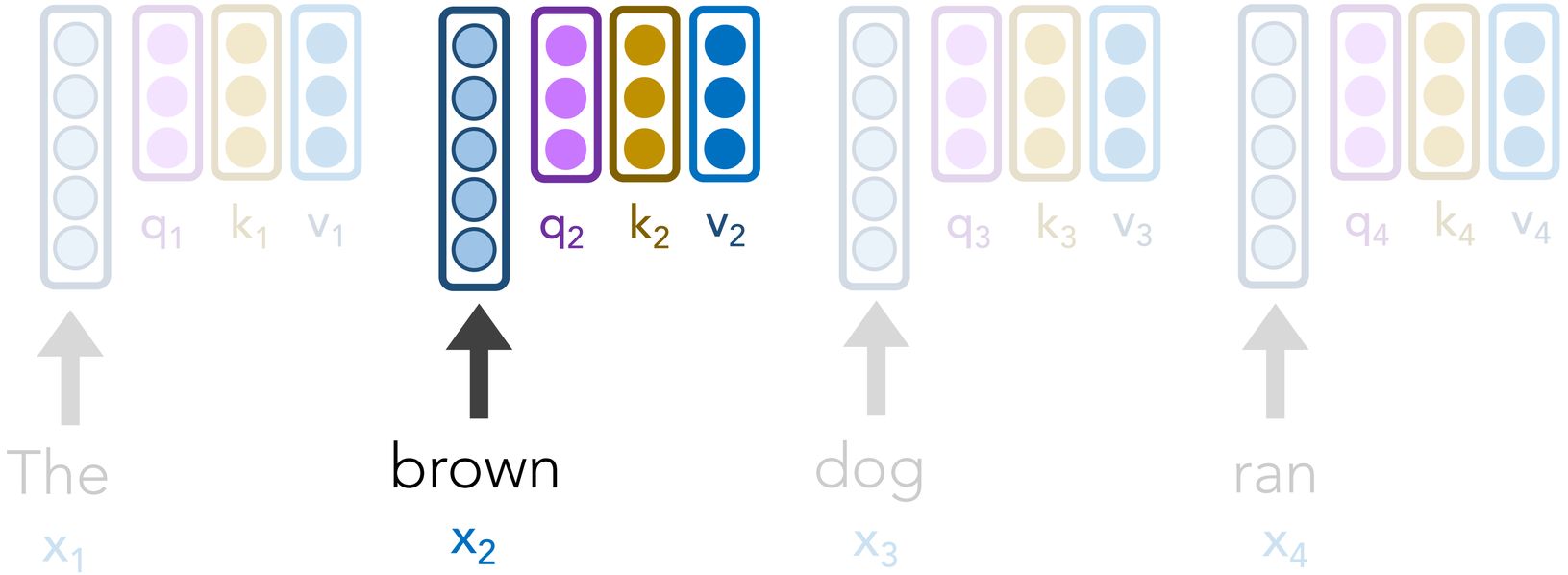
Step 3: Our scores s_1, s_2, s_3, s_4 don't sum to 1. Let's divide by $\sqrt{len(k_i)}$ and softmax it

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

$s_3 = q_2 \cdot k_3 = 22$ $\quad a3 = \sigma(s_3/8) = .01$

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

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



Self-Attention Architecture

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

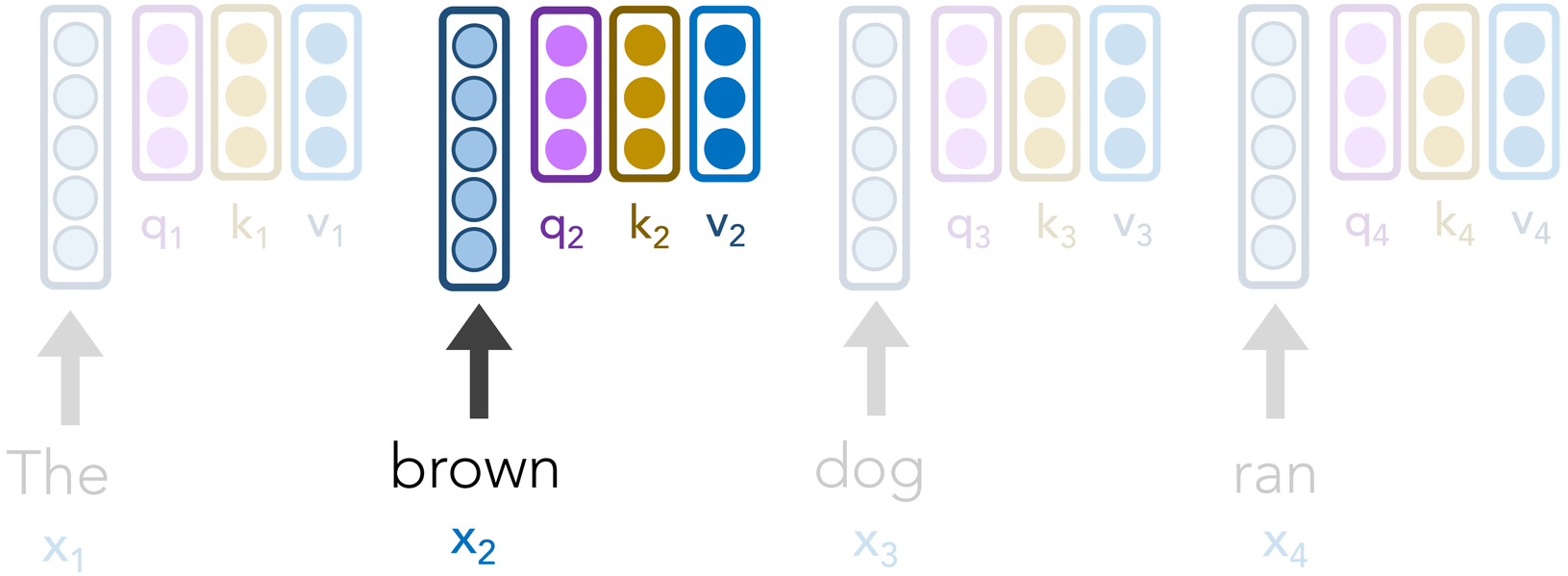
$s_4 = q_2 \cdot k_4 = 8$ $\quad$ $a_4 = \sigma(s_4/8) = 0$

$s_3 = q_2 \cdot k_3 = 22$ $\quad$ $a3 = \sigma(s_3/8) = .01$

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

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

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

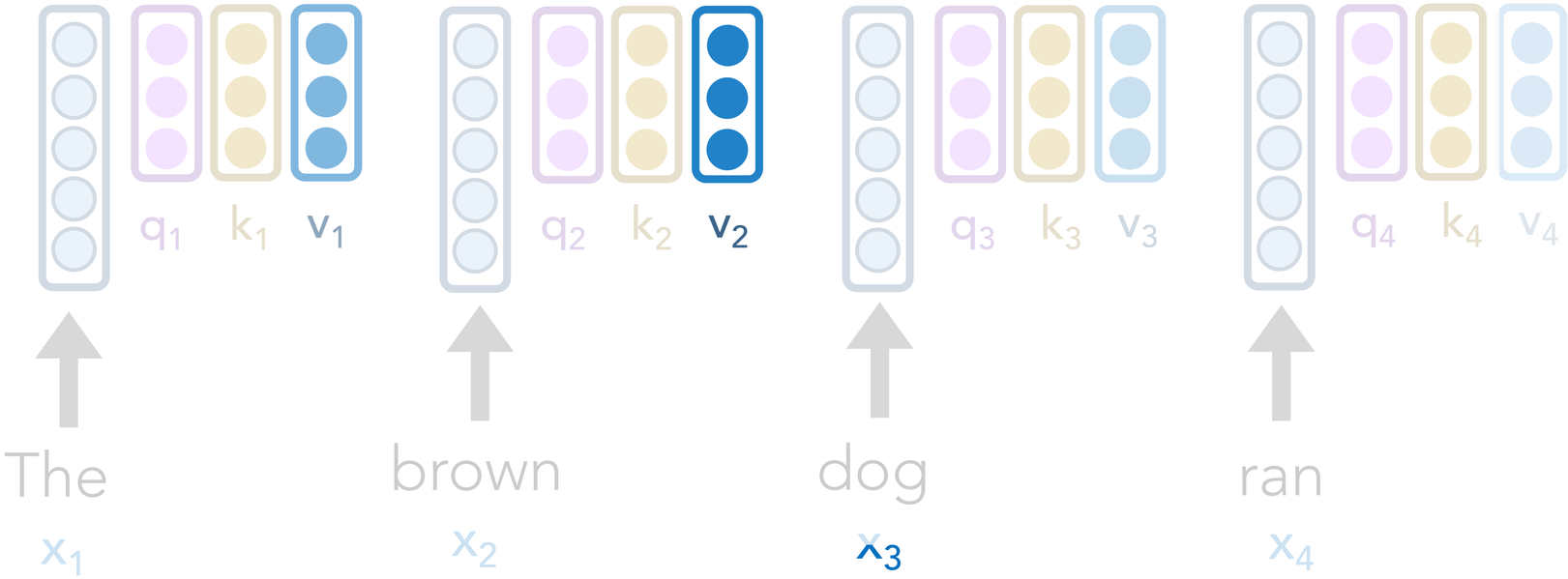


Self-Attention Architecture

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

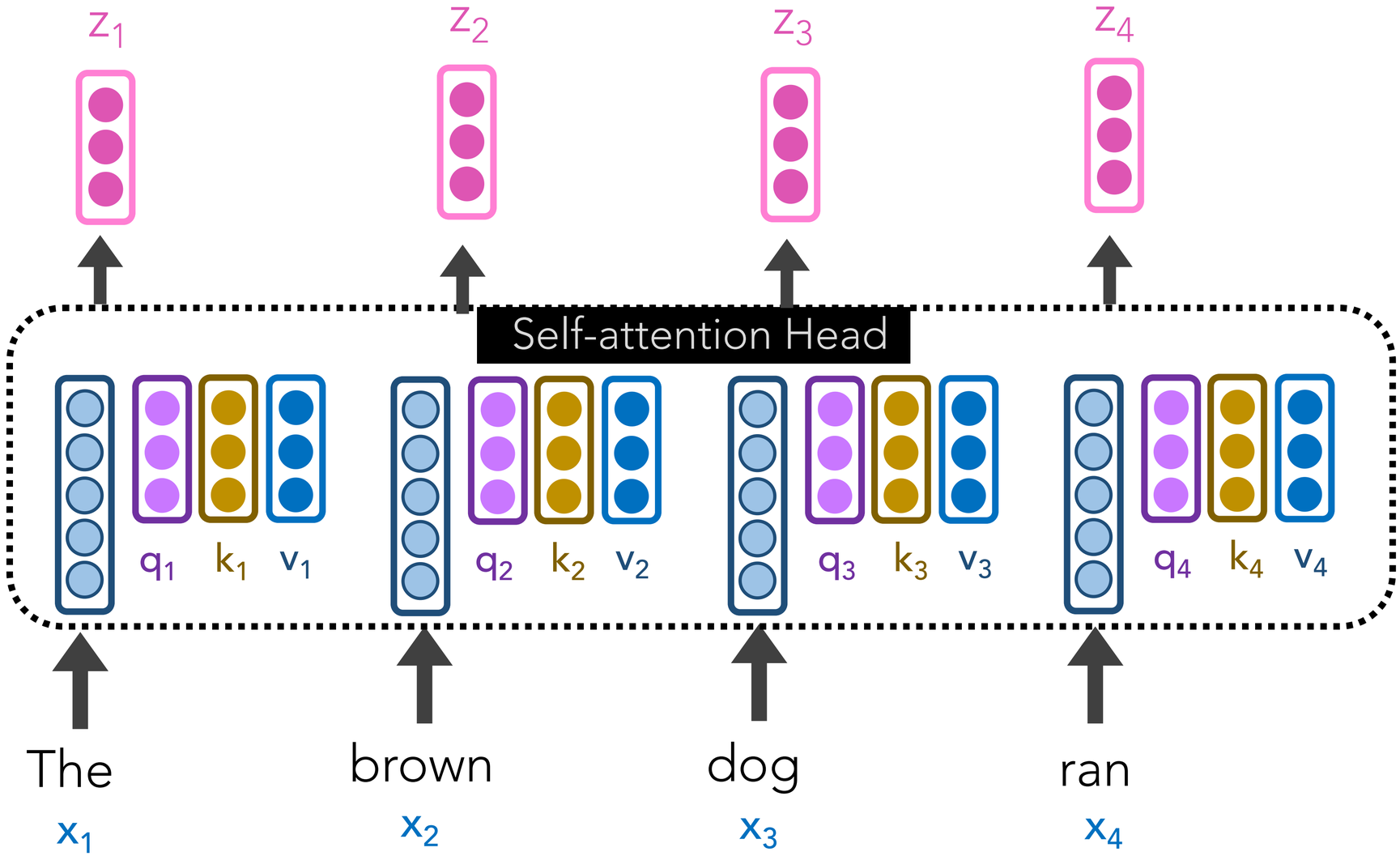
$$z_2 = a_1 \cdot v_1 + a_2 \cdot v_2 + a_3 \cdot v_3 + a_4 \cdot v_4$$

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



Self-Attention Architecture

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



Self-Attention Summary

Strengths

- Context-aware
- Much more powerful than static embeddings

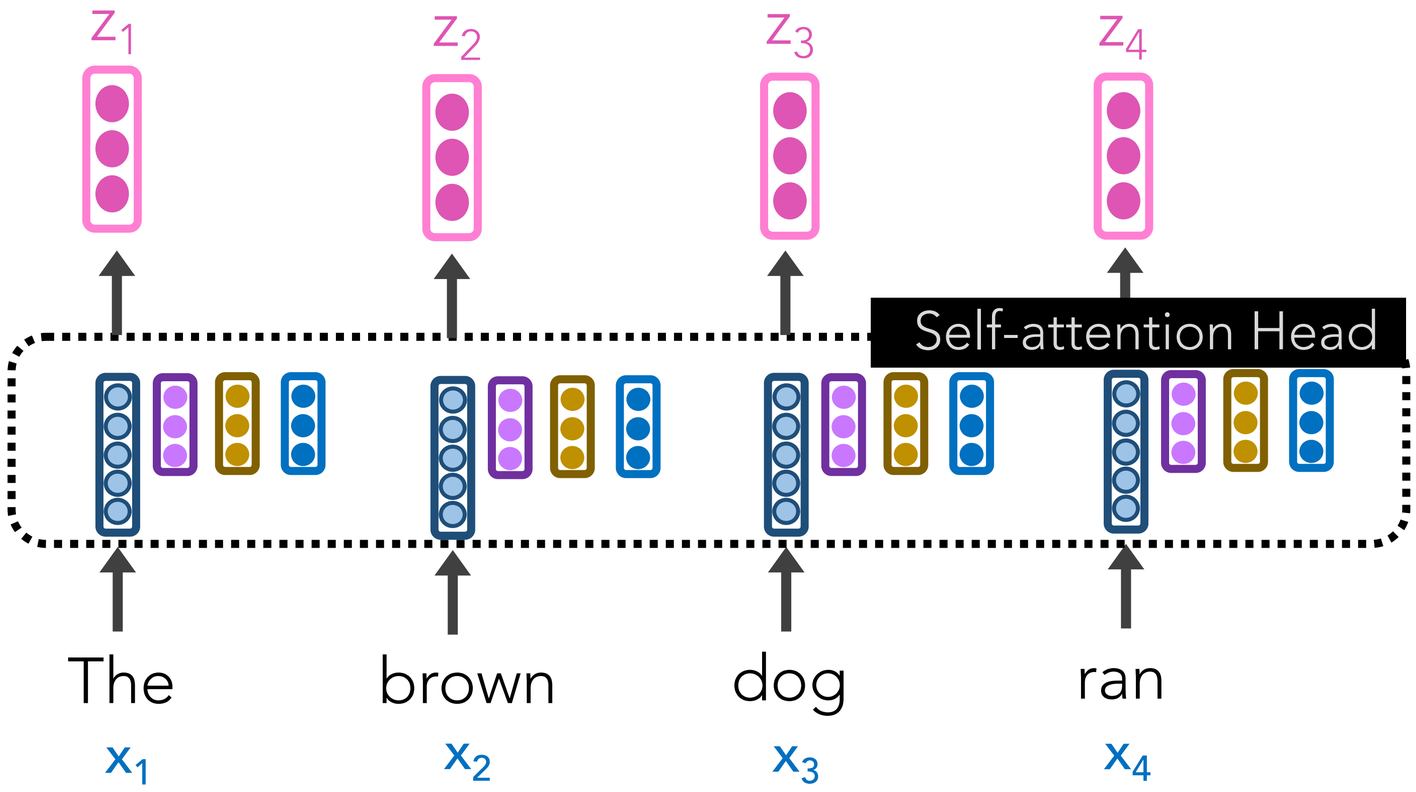
Issues?

- Slower to train
- Cannot easily be pre-computed

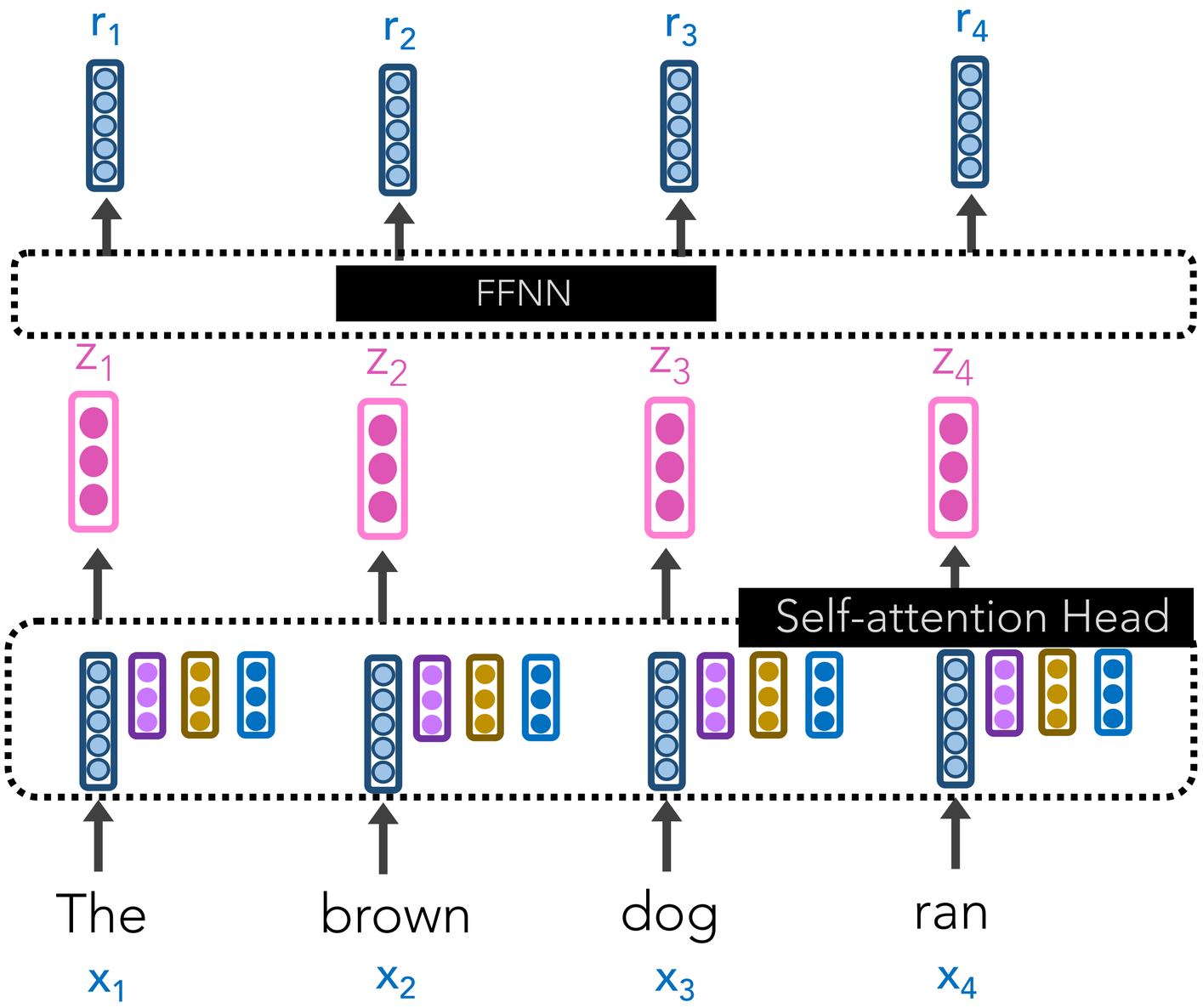
Transformers

Transformer Architecture

Let's further pass each z_i through a FFNN

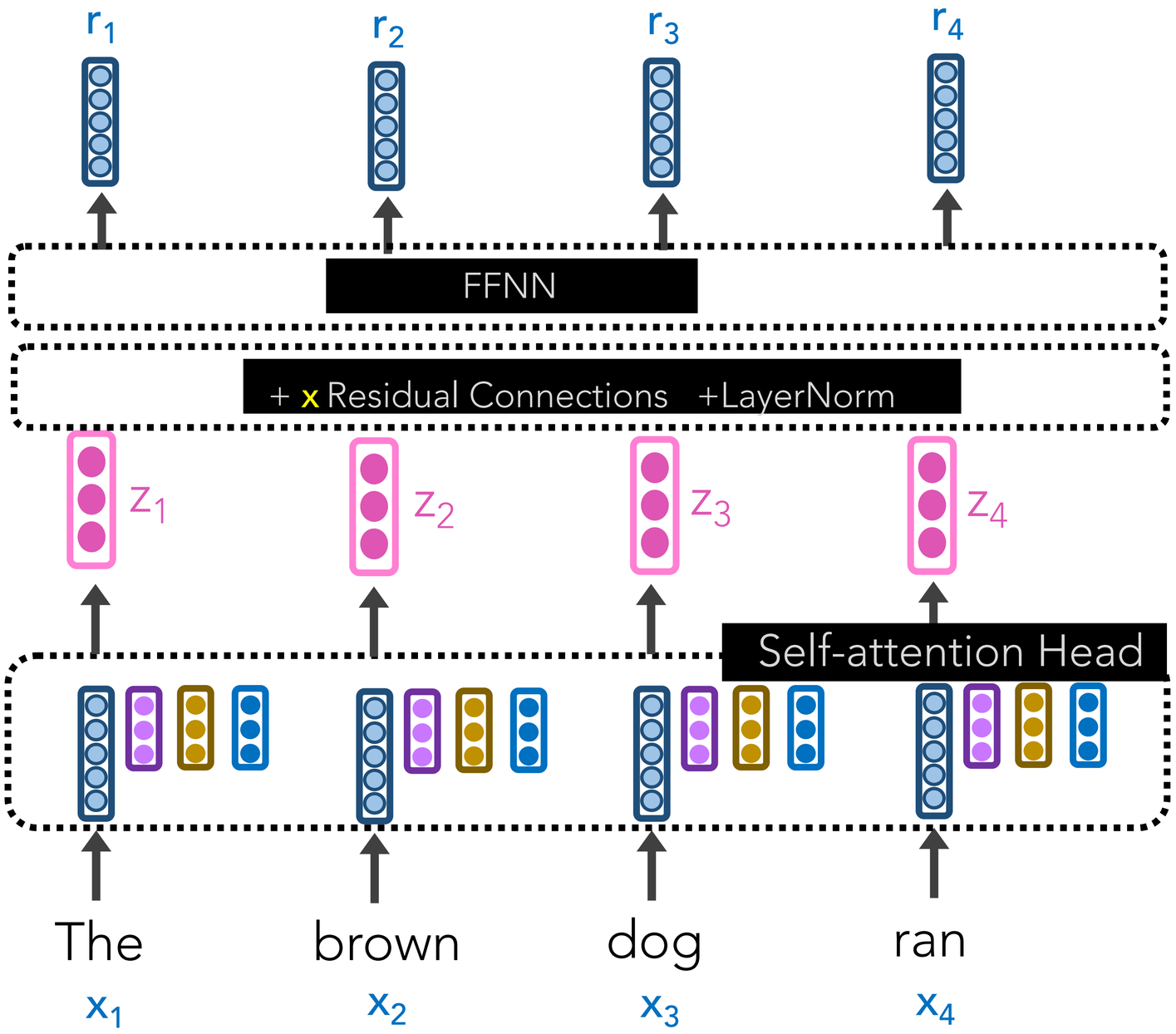


Transformer Architecture



Let's further pass each z_i through a FFNN

Transformer Architecture

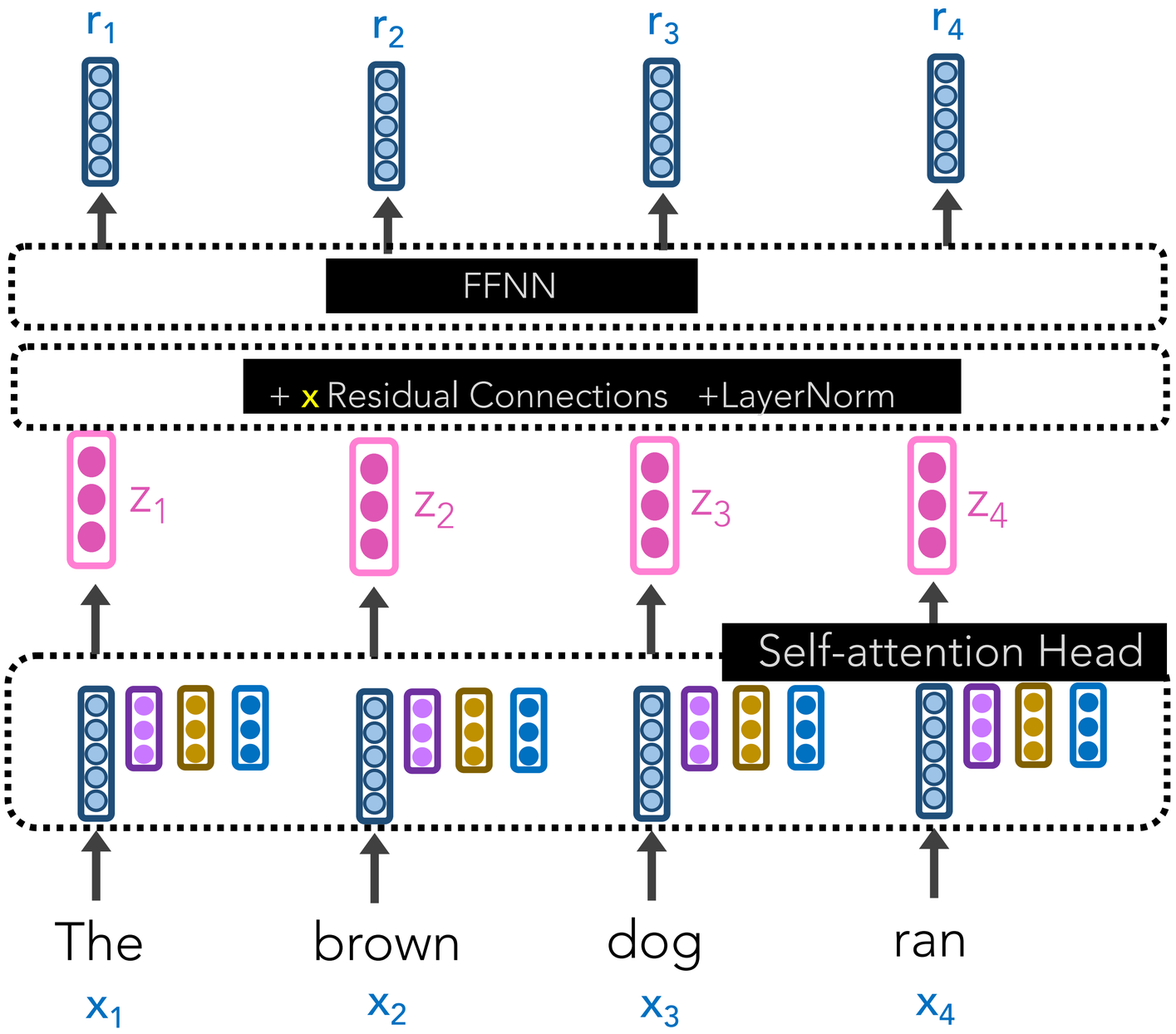


Let's further pass each z_i through a FFNN

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. You should do this after the FFNN, too.

Transformer Architecture



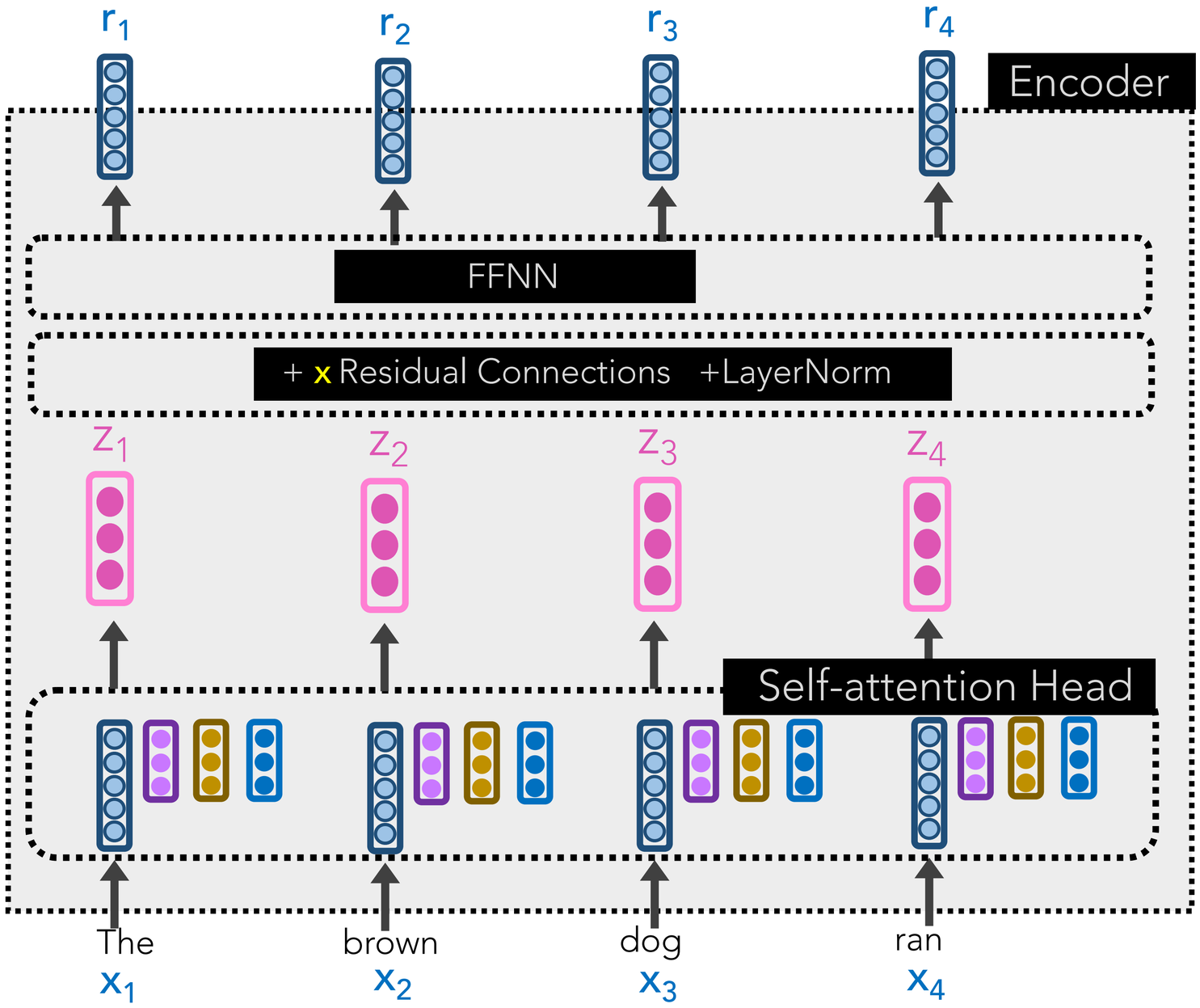
Let's further pass each z_i through a FFNN

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. You should do this after the FFNN, too.

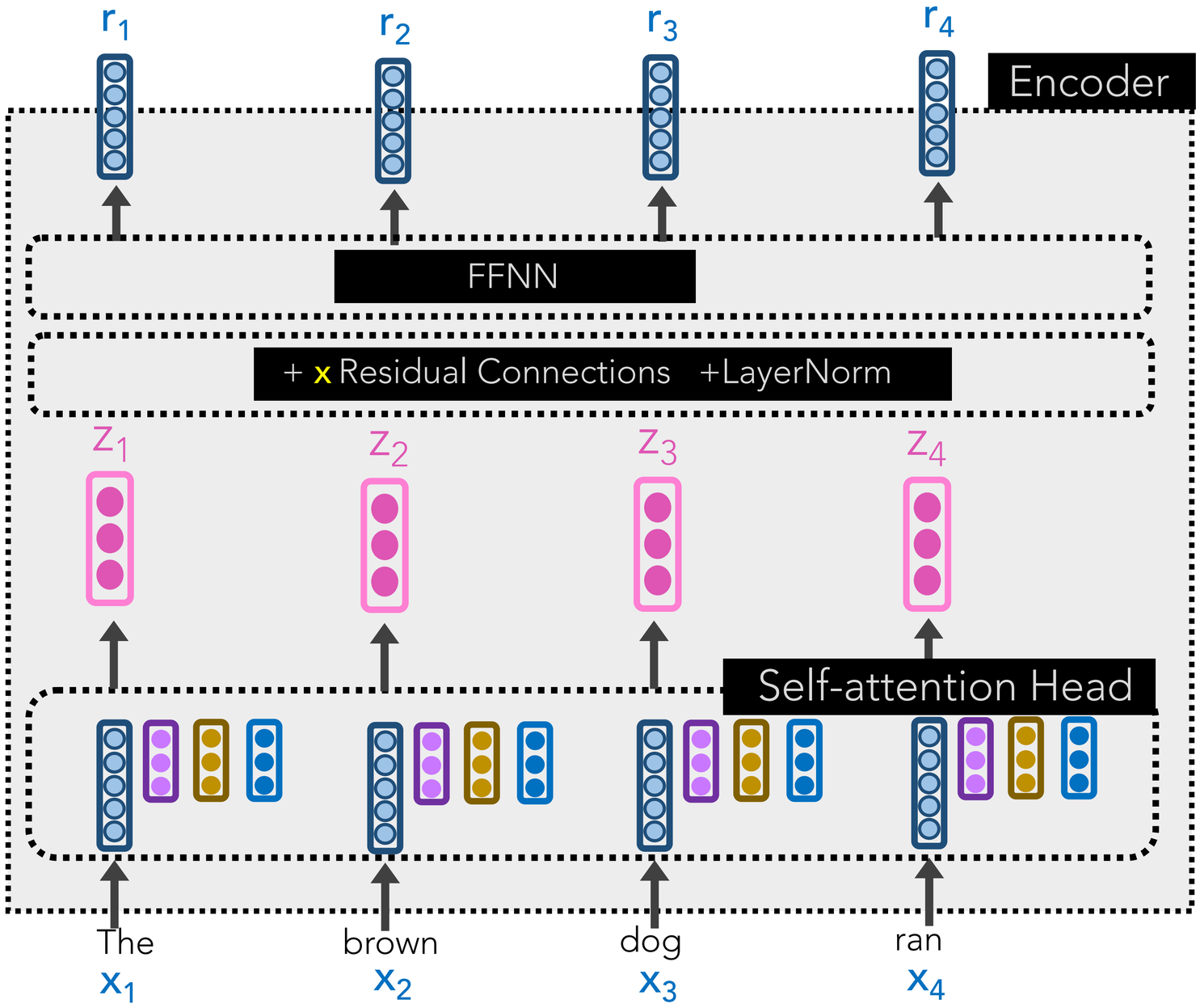
Each z_i can be computed in parallel, unlike LSTMs!

Transformer Architecture



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

Transformer Architecture



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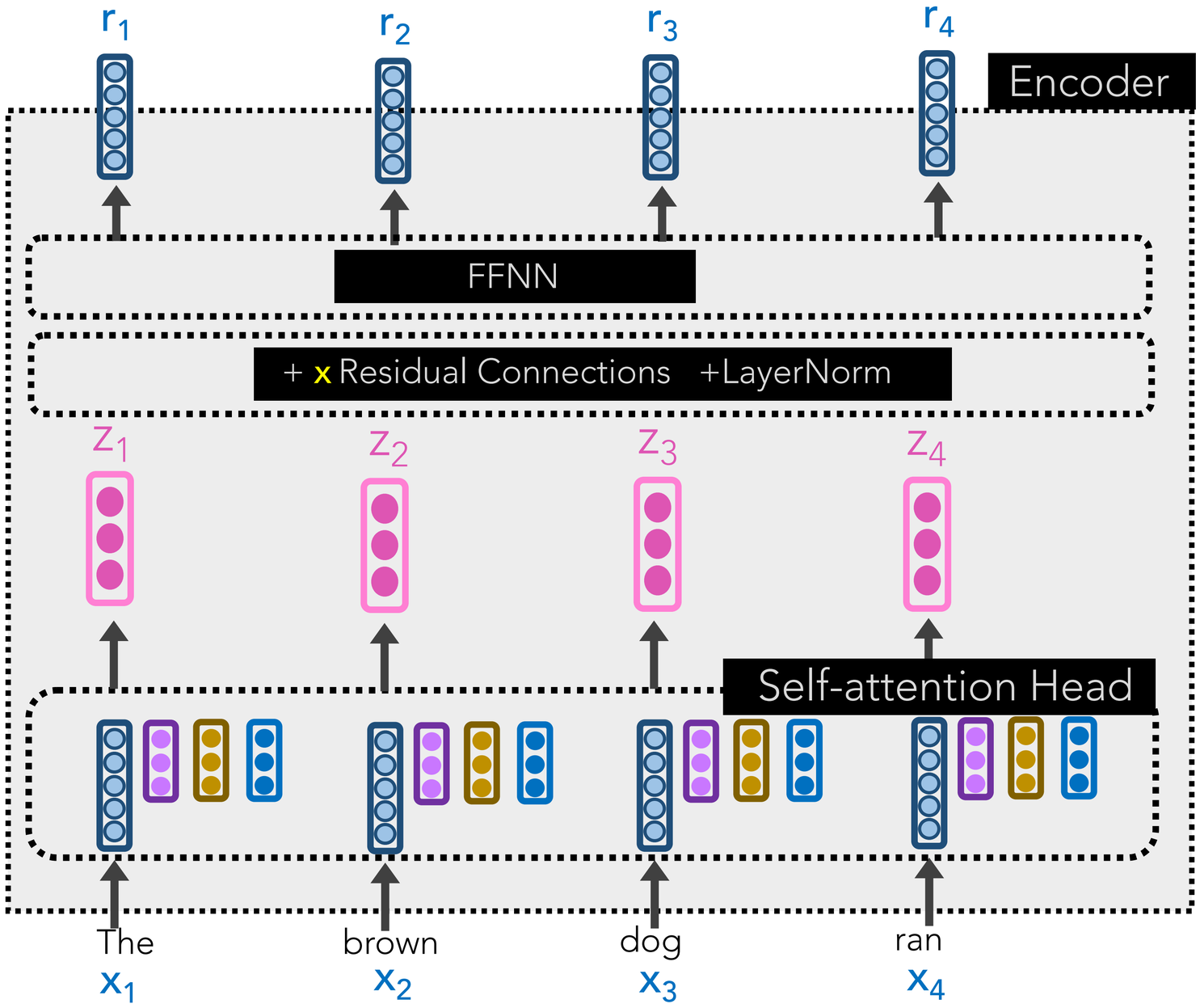
Problem: there is no concept of positionality. Words are weighted as if a “bag of words”

Transformer Architecture

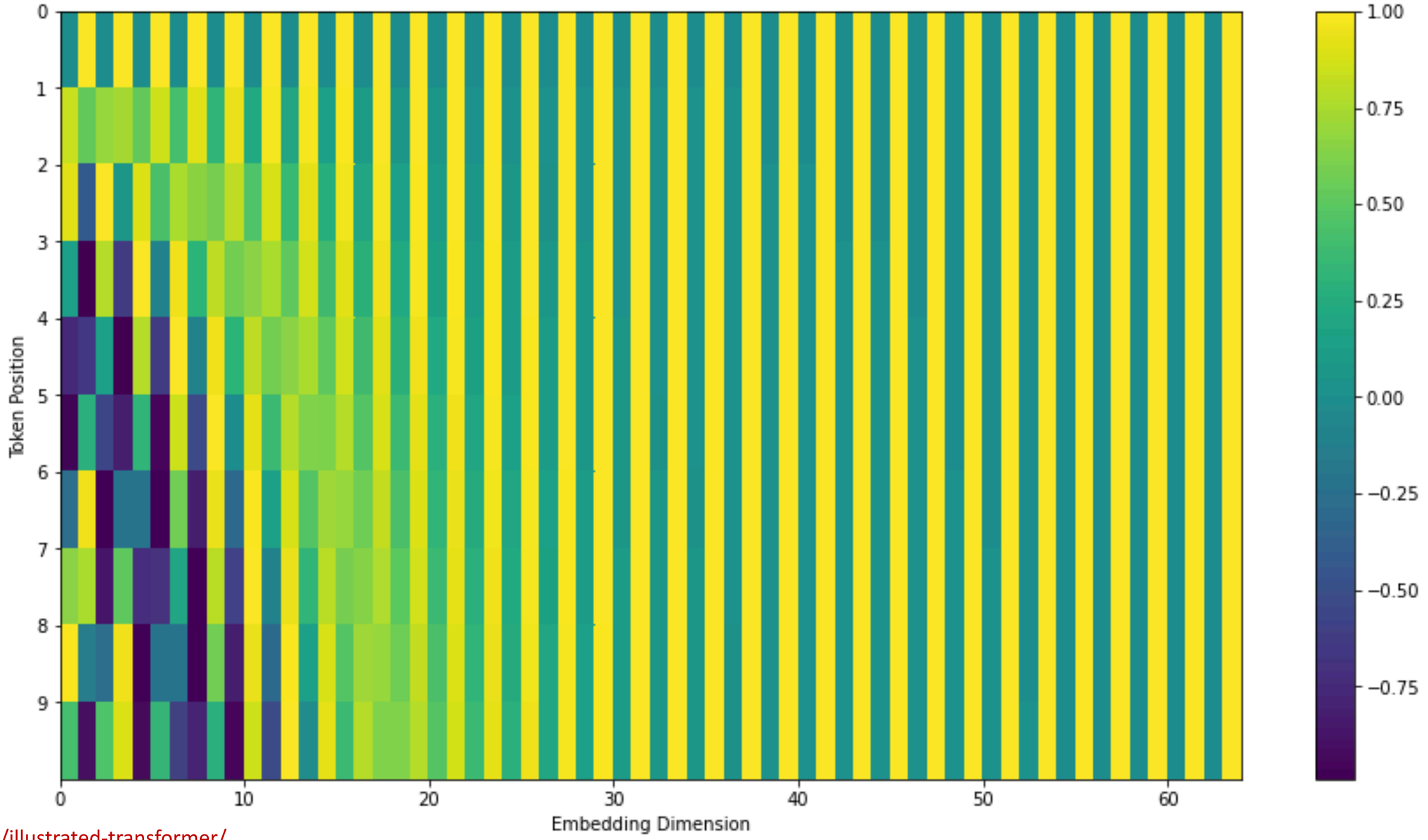


Yay! Our r_i vectors are our new representations, and this entire process is called a Transformer Encoder

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

Solution: add to each input word x_i a positional encoding $\sim \sin(i)\cos(i)$

Positional Encodings



https://jalammar.github.io/illustrated-transformer/

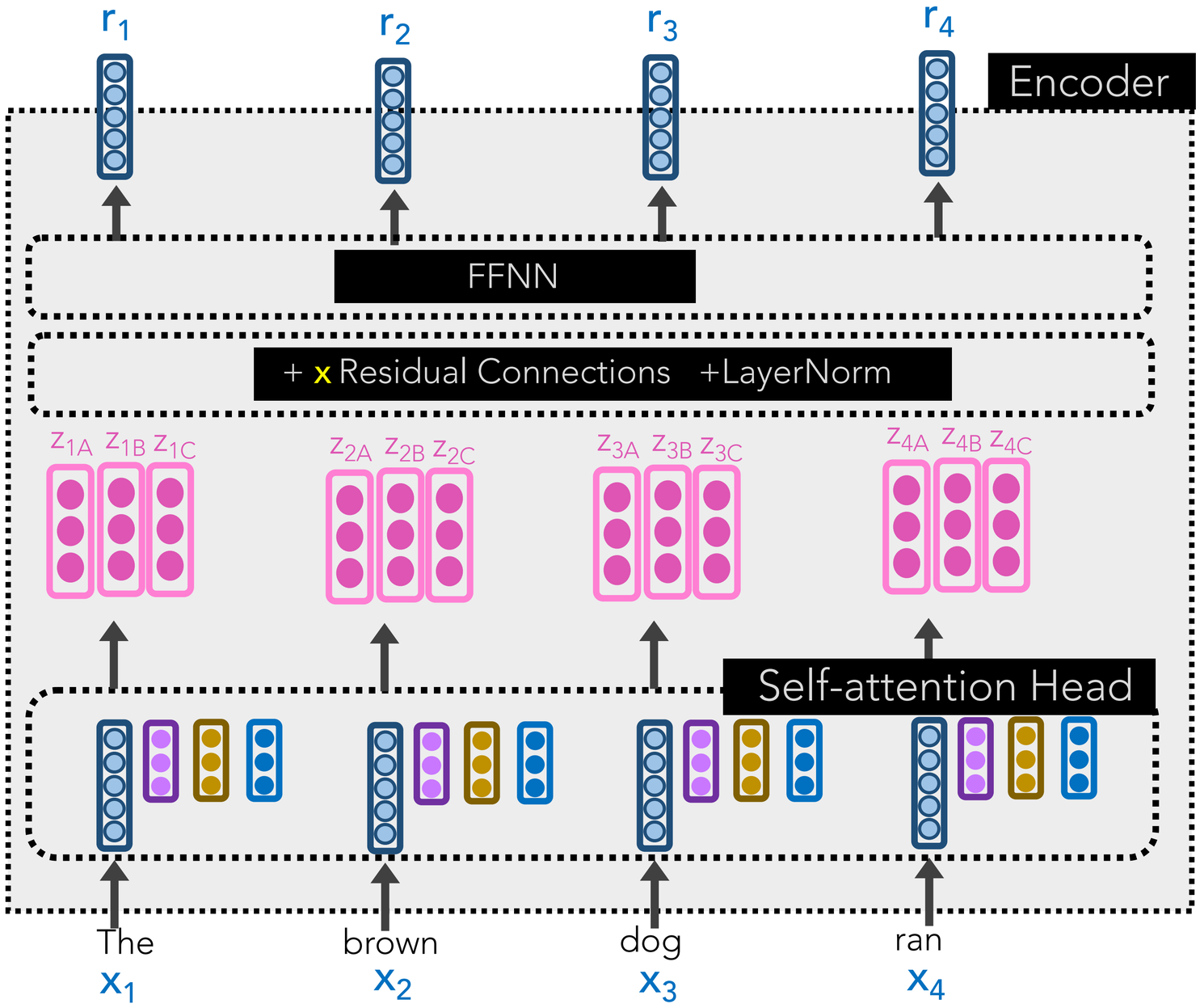
Transformer Architecture

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

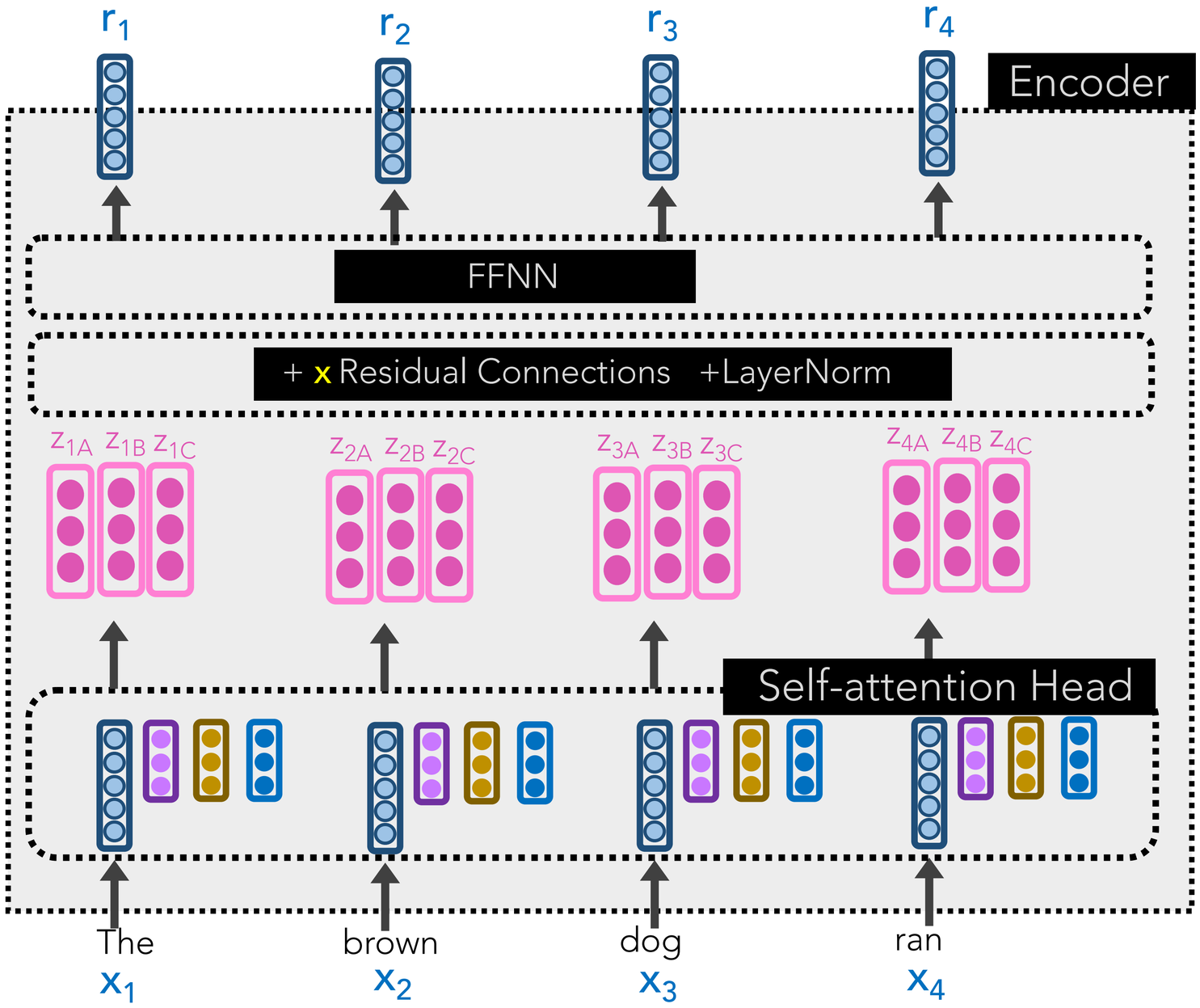
Transformer Architecture



Each Self-Attention Head produces a z_i vector.

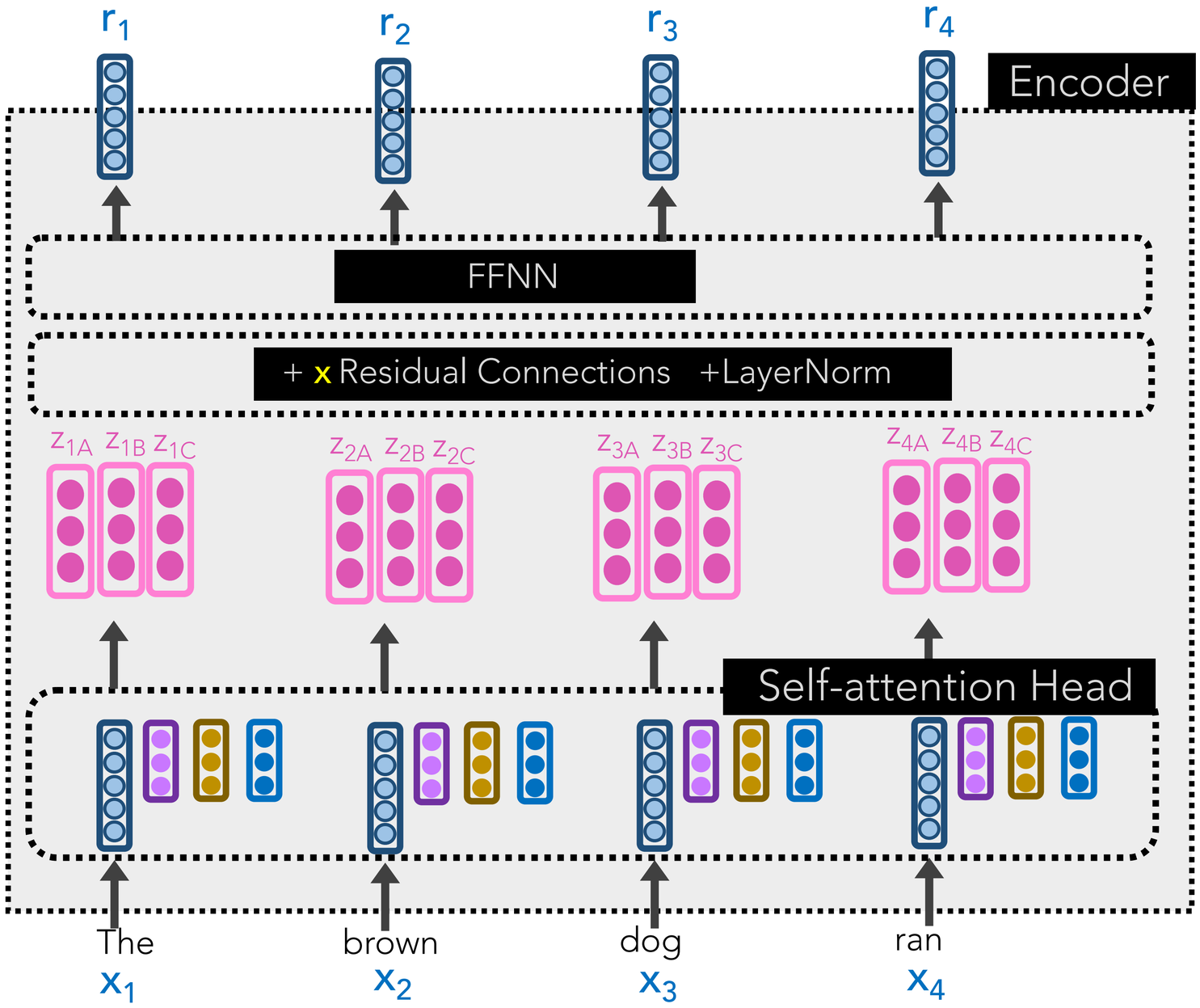
We can, in parallel, use multiple heads and concat the z_i's.

Transformer Architecture



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

Transformer Architecture



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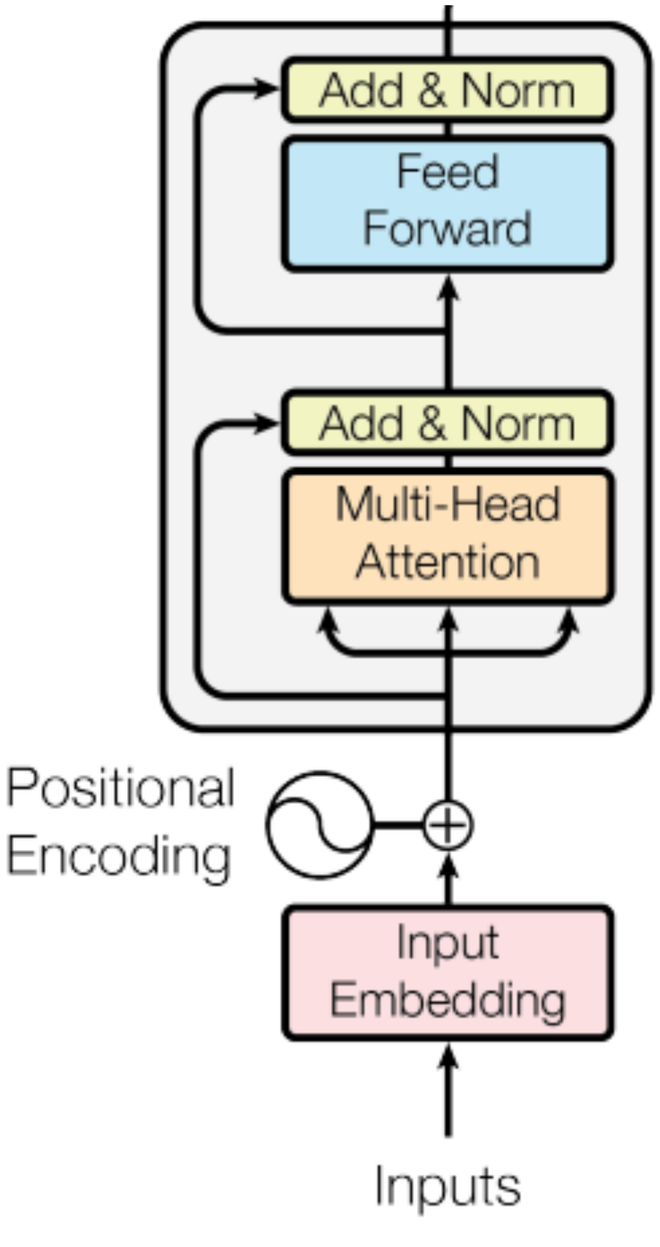
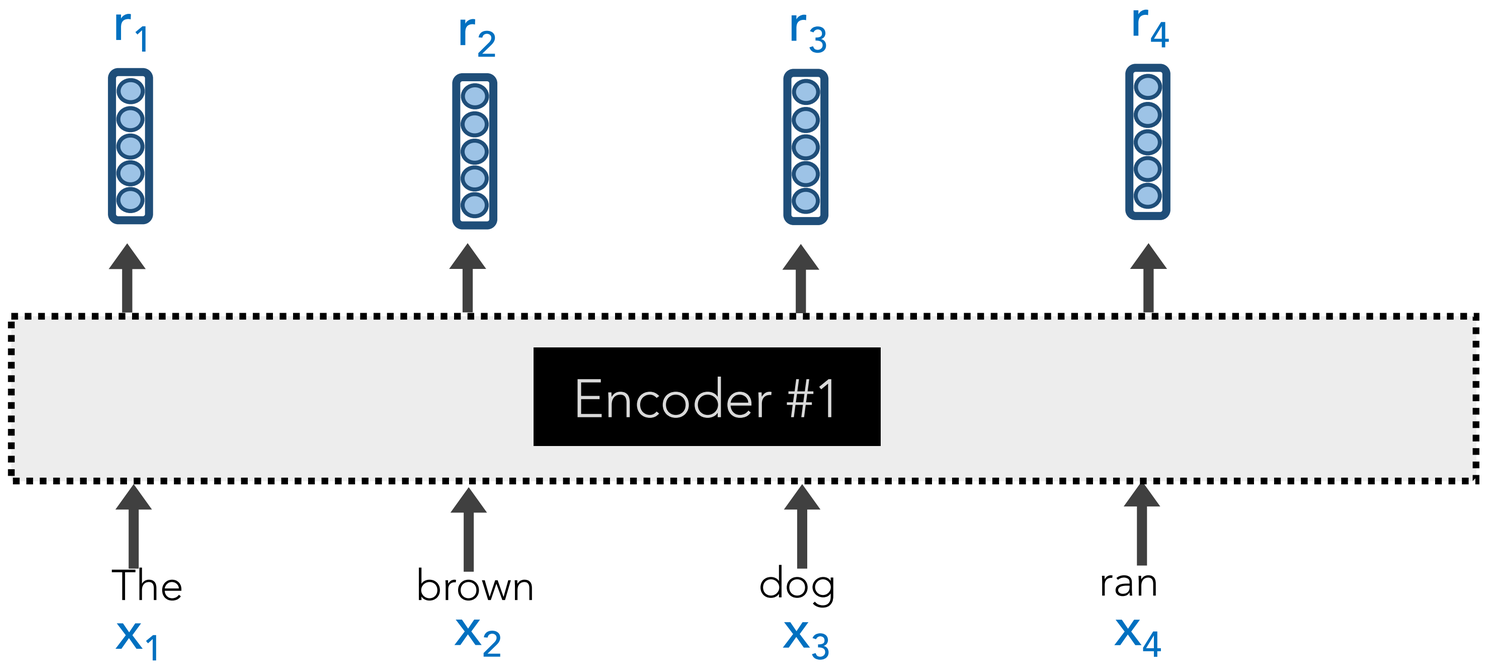


Transformer Architecture



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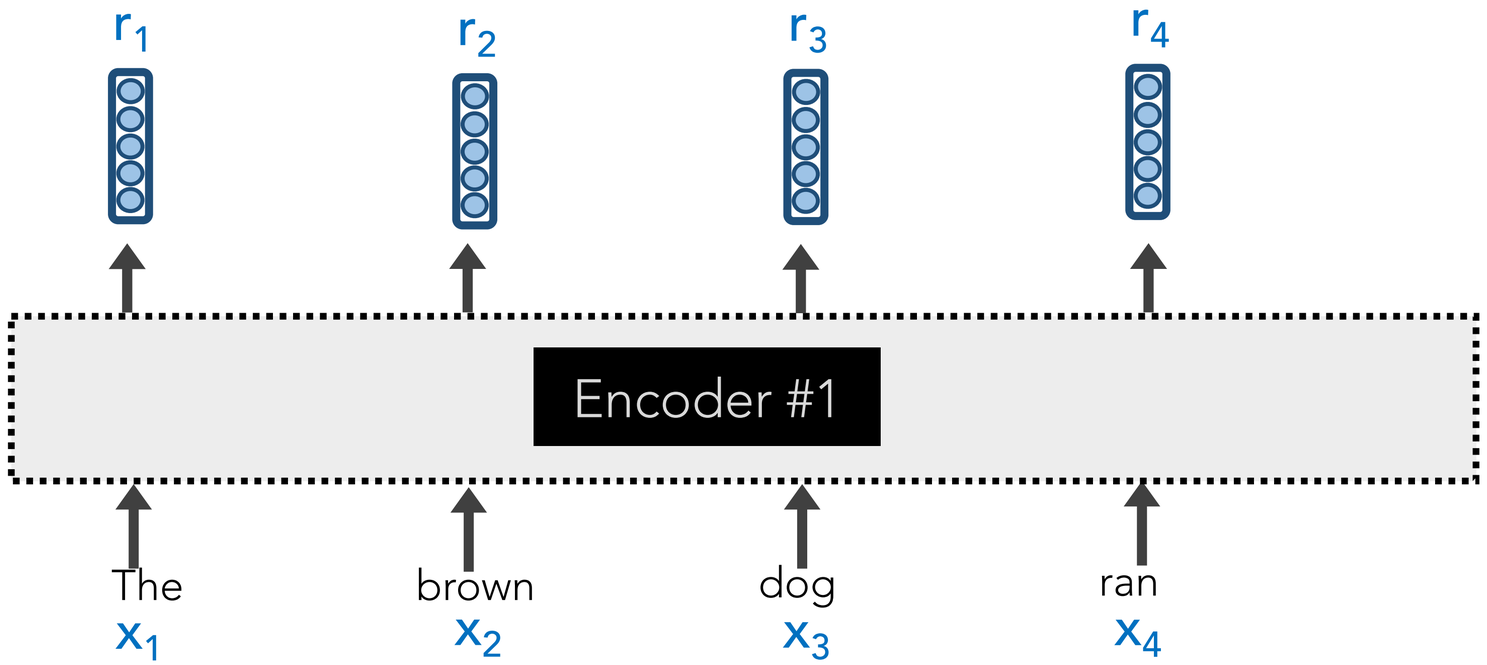
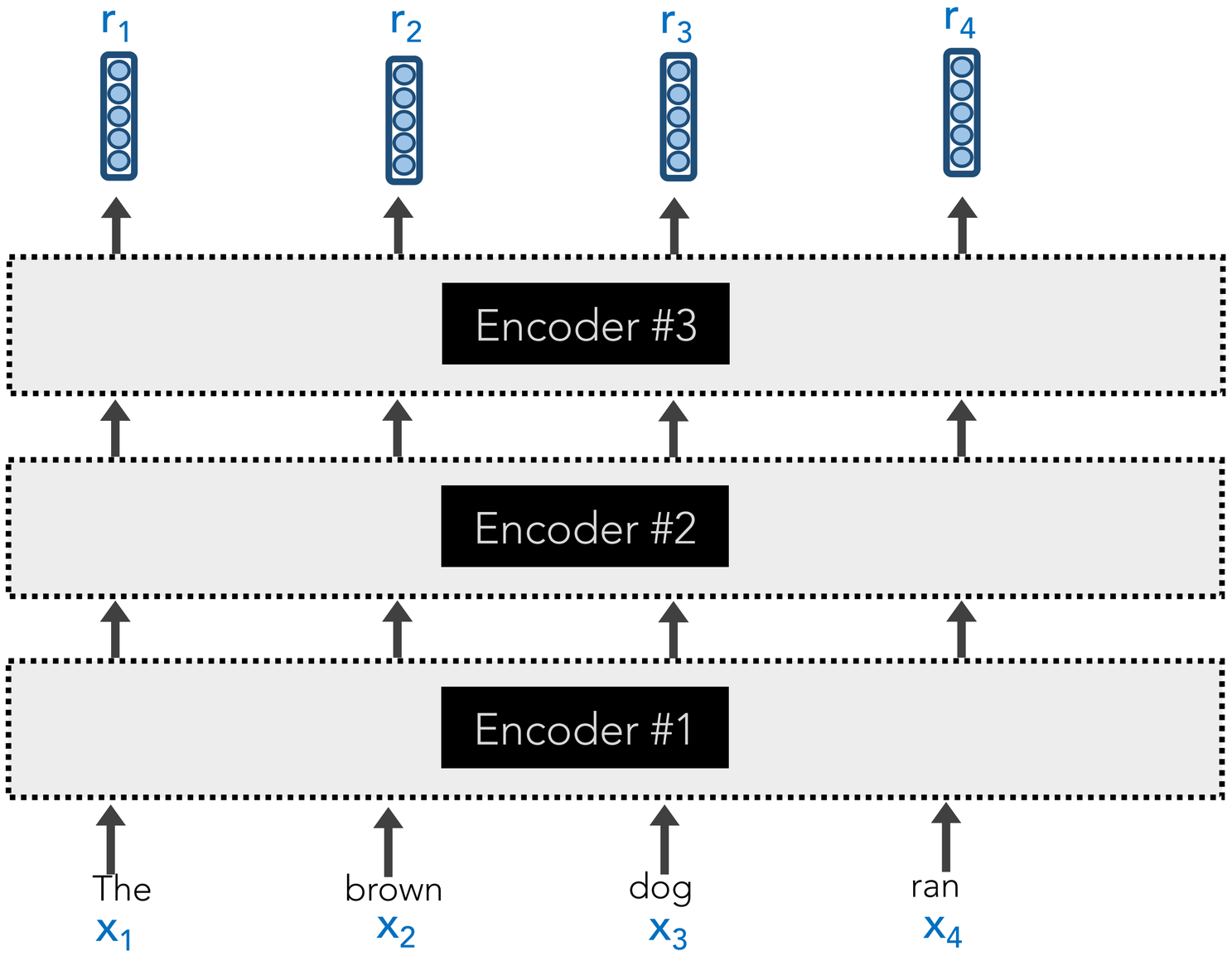
Transformer Architecture



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 Architecture



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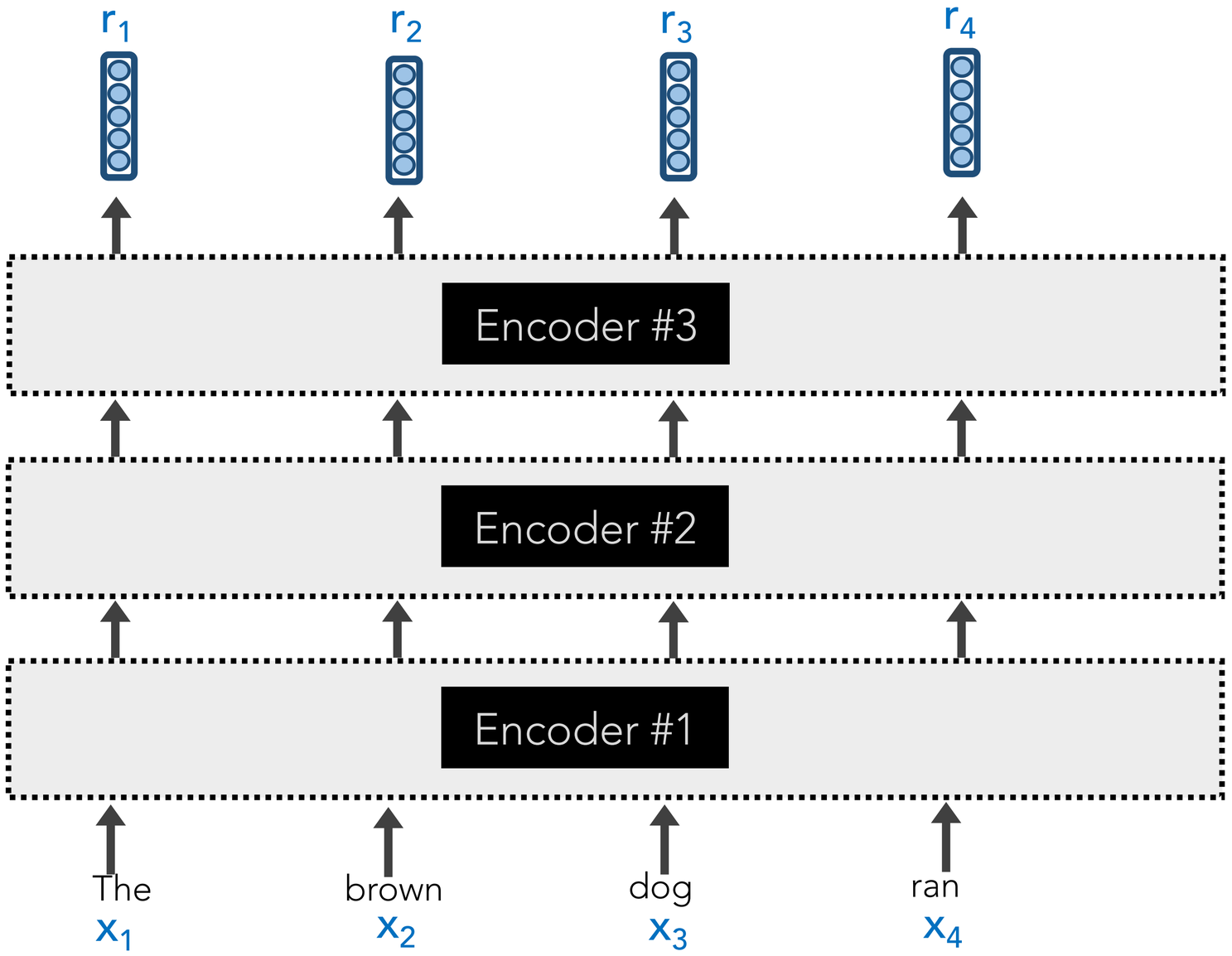
Transformer Architecture



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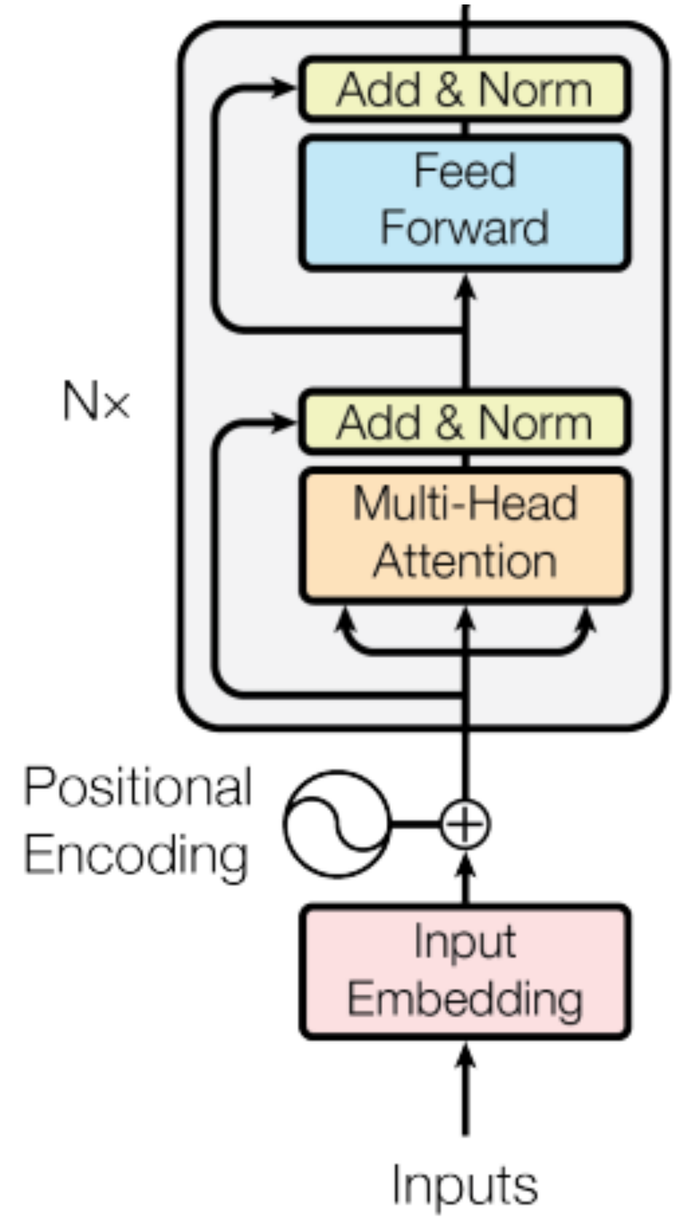
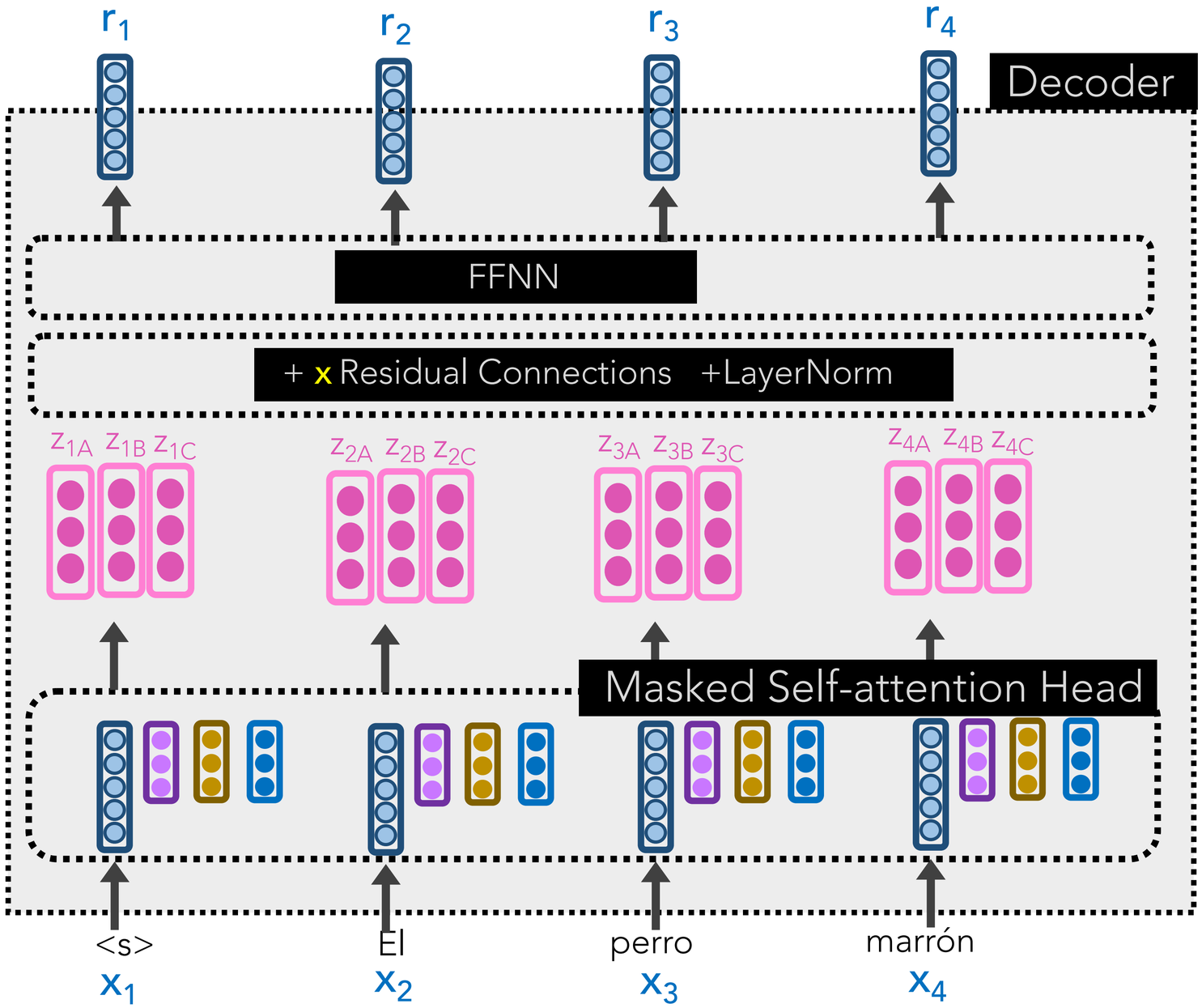


Transformer Decoders

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

Transformer Decoders



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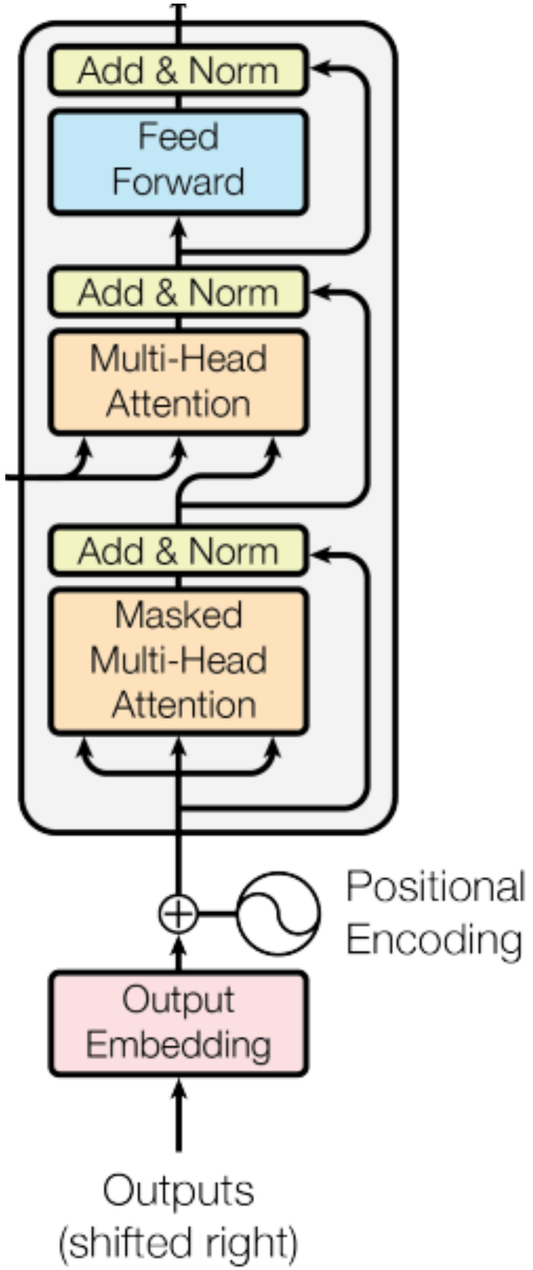
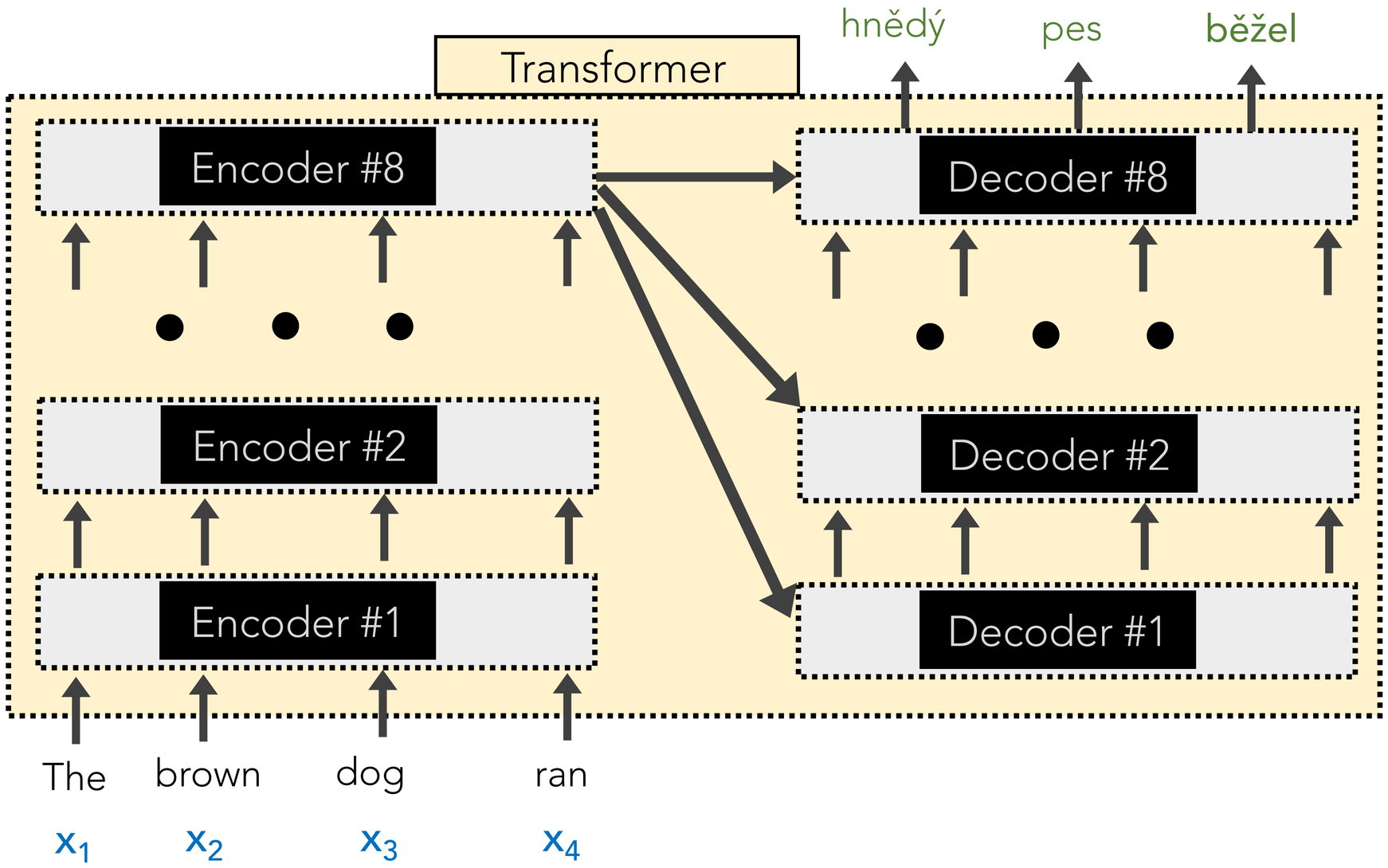


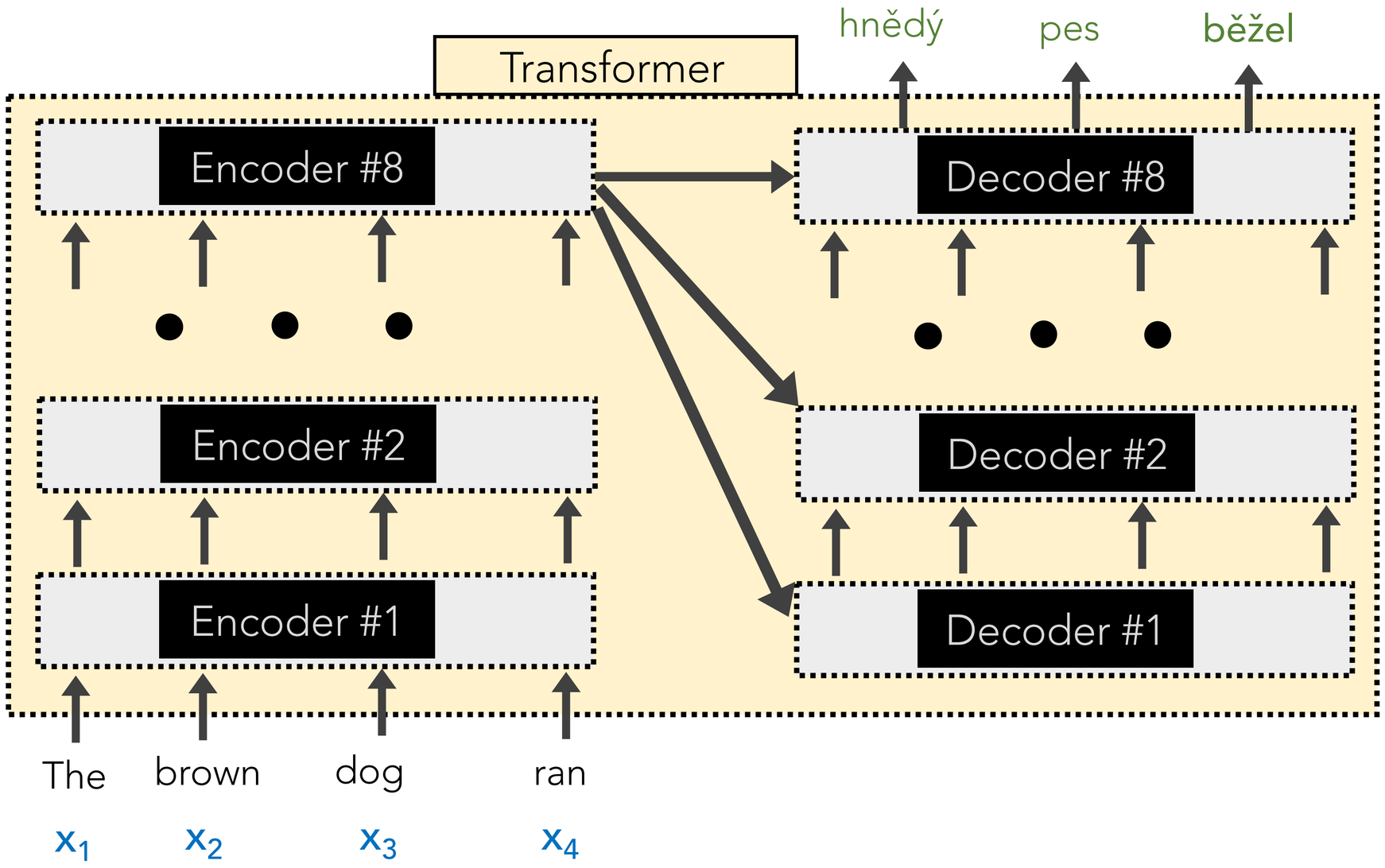
Transformer Decoders



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

Transformer Decoders generate new sequences of text

Transformer Decoders

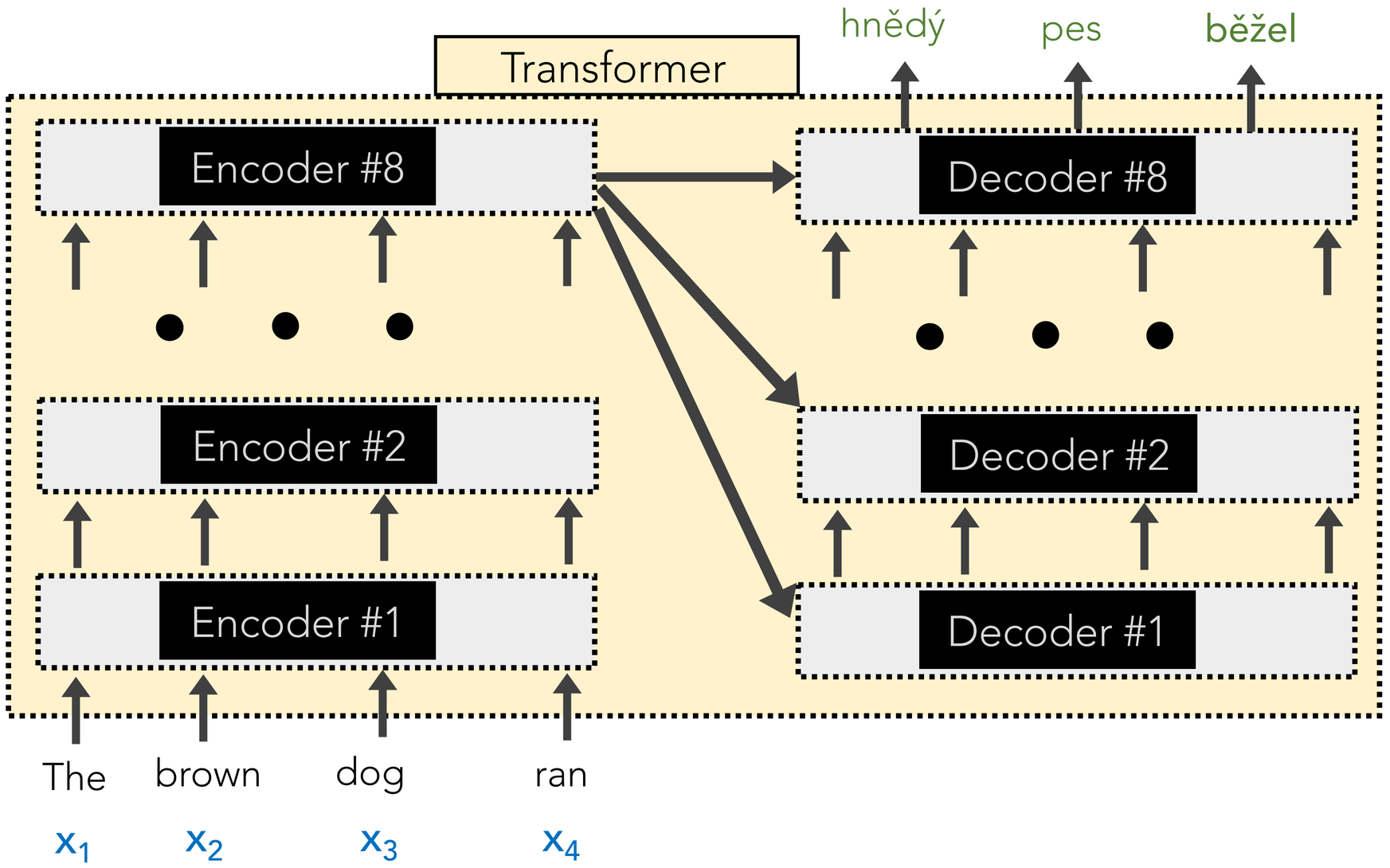


NOTE

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 Decoders

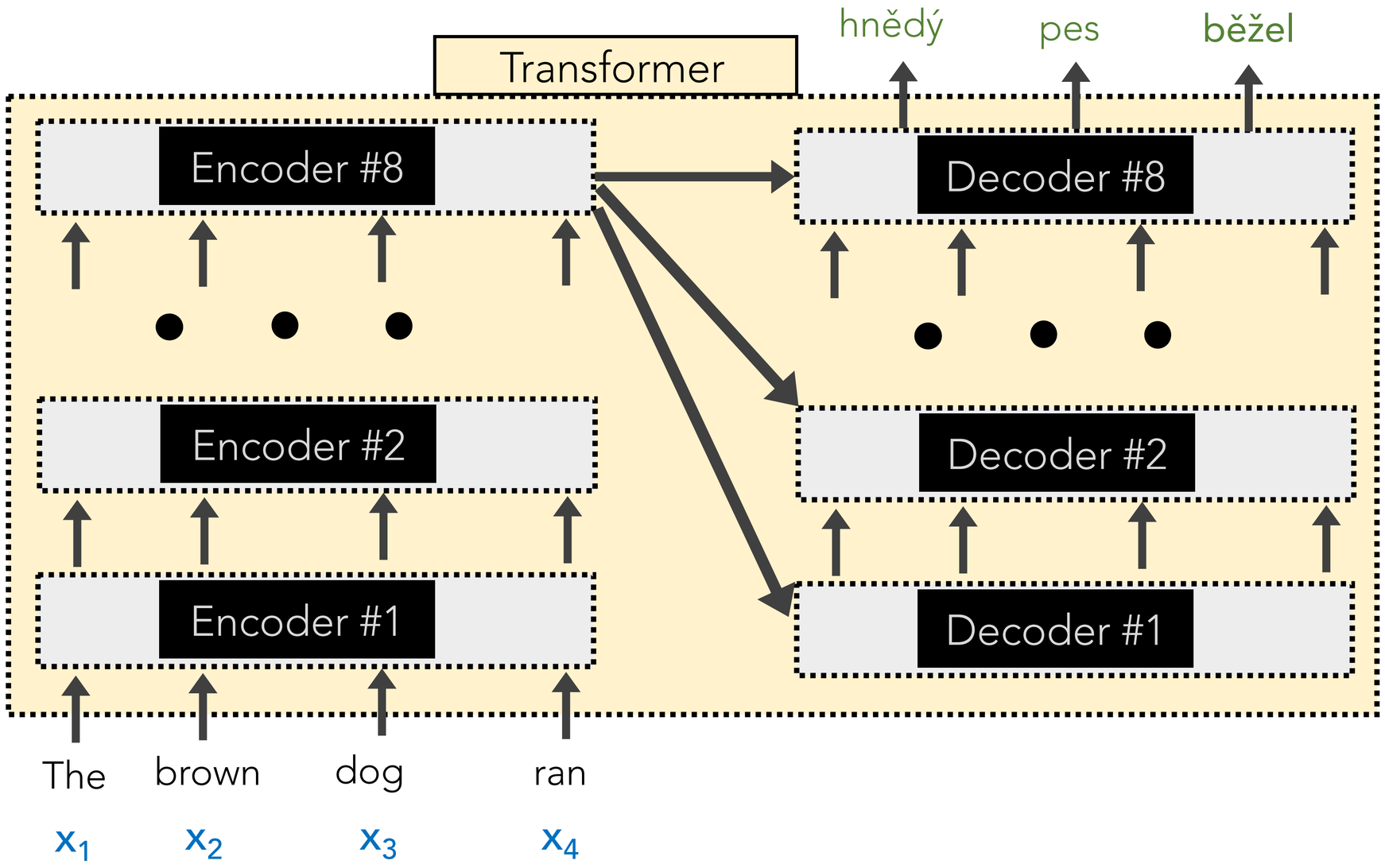


NOTE

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.

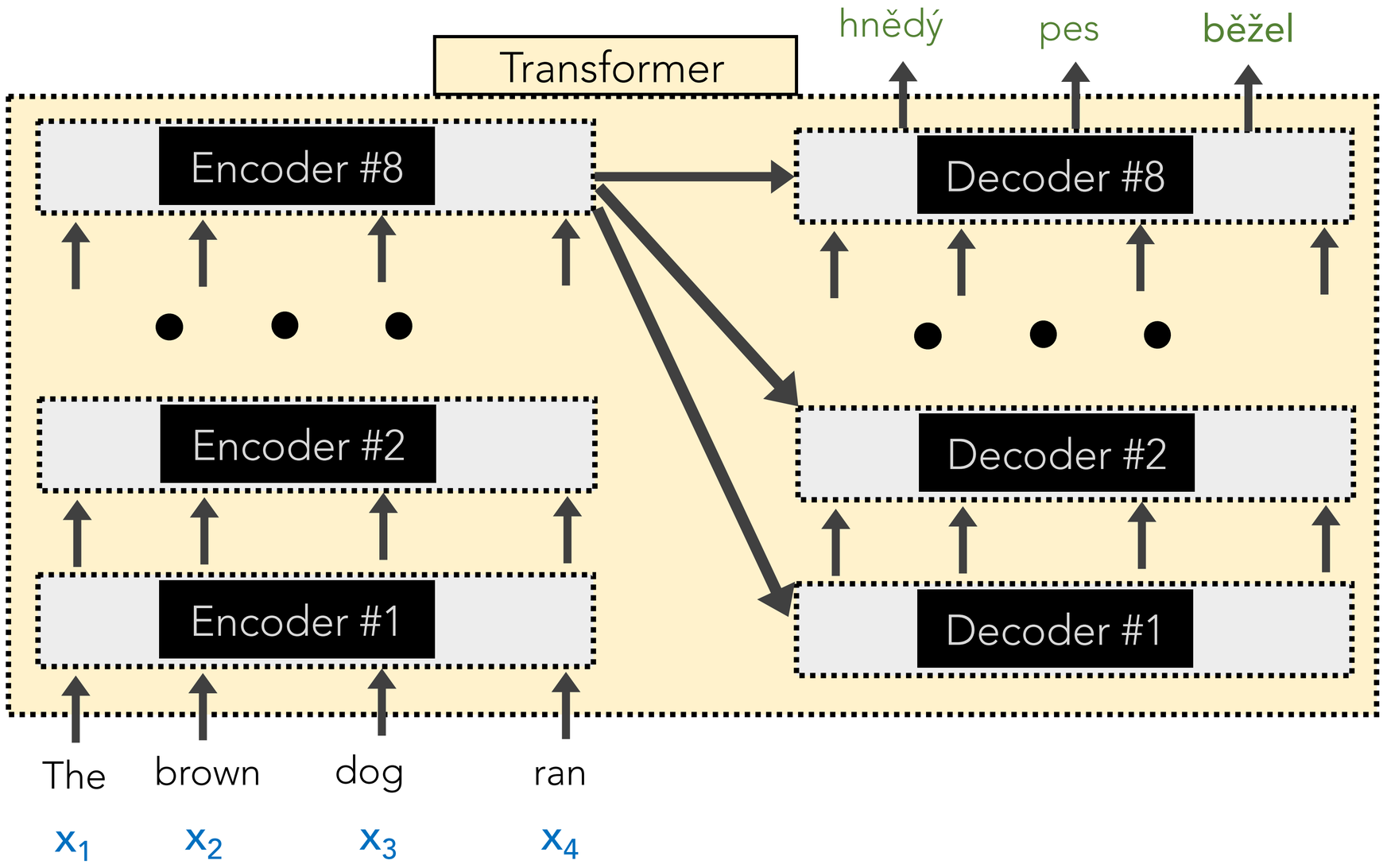
Transformer Decoders



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.

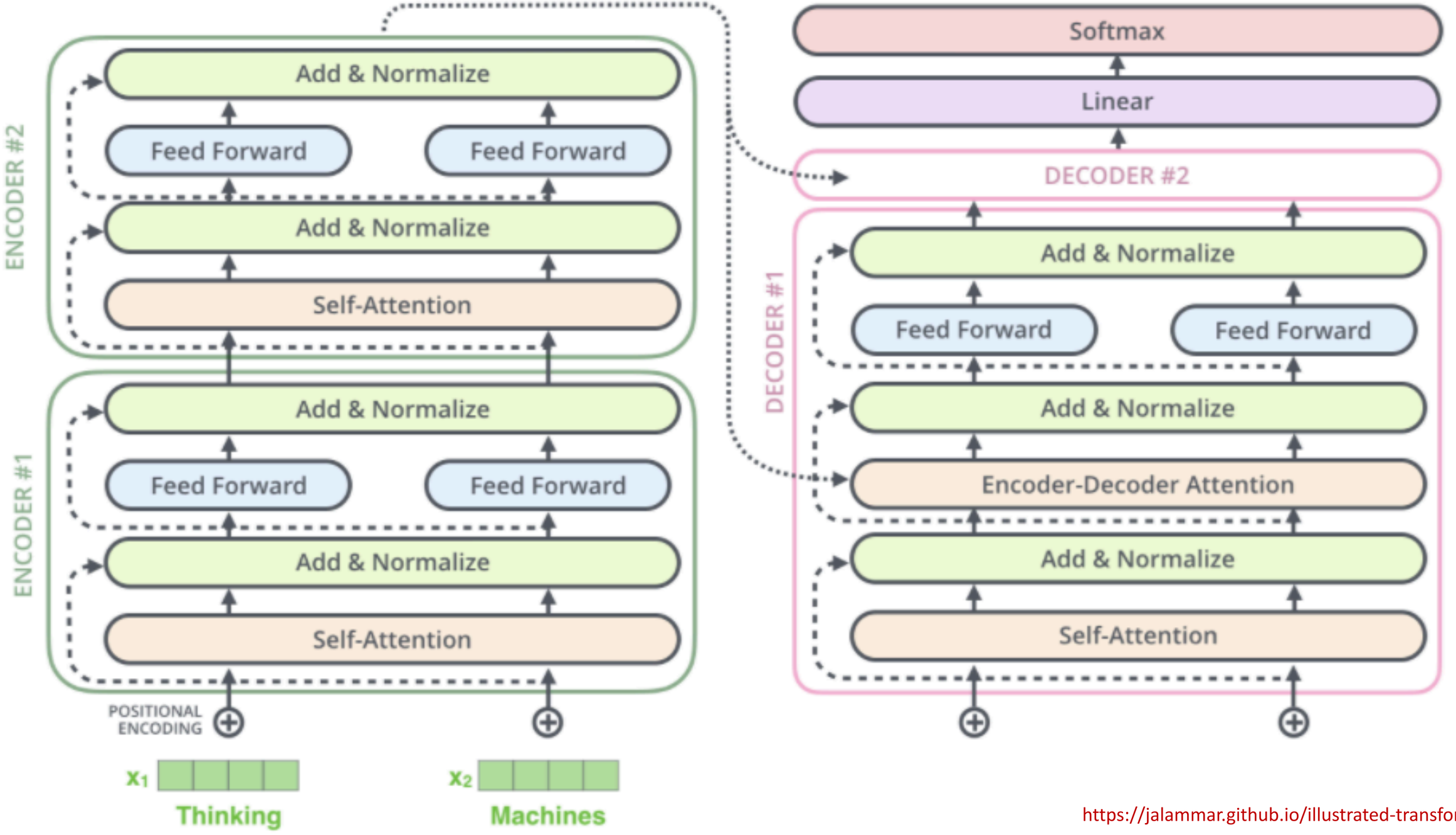
Transformer Decoders



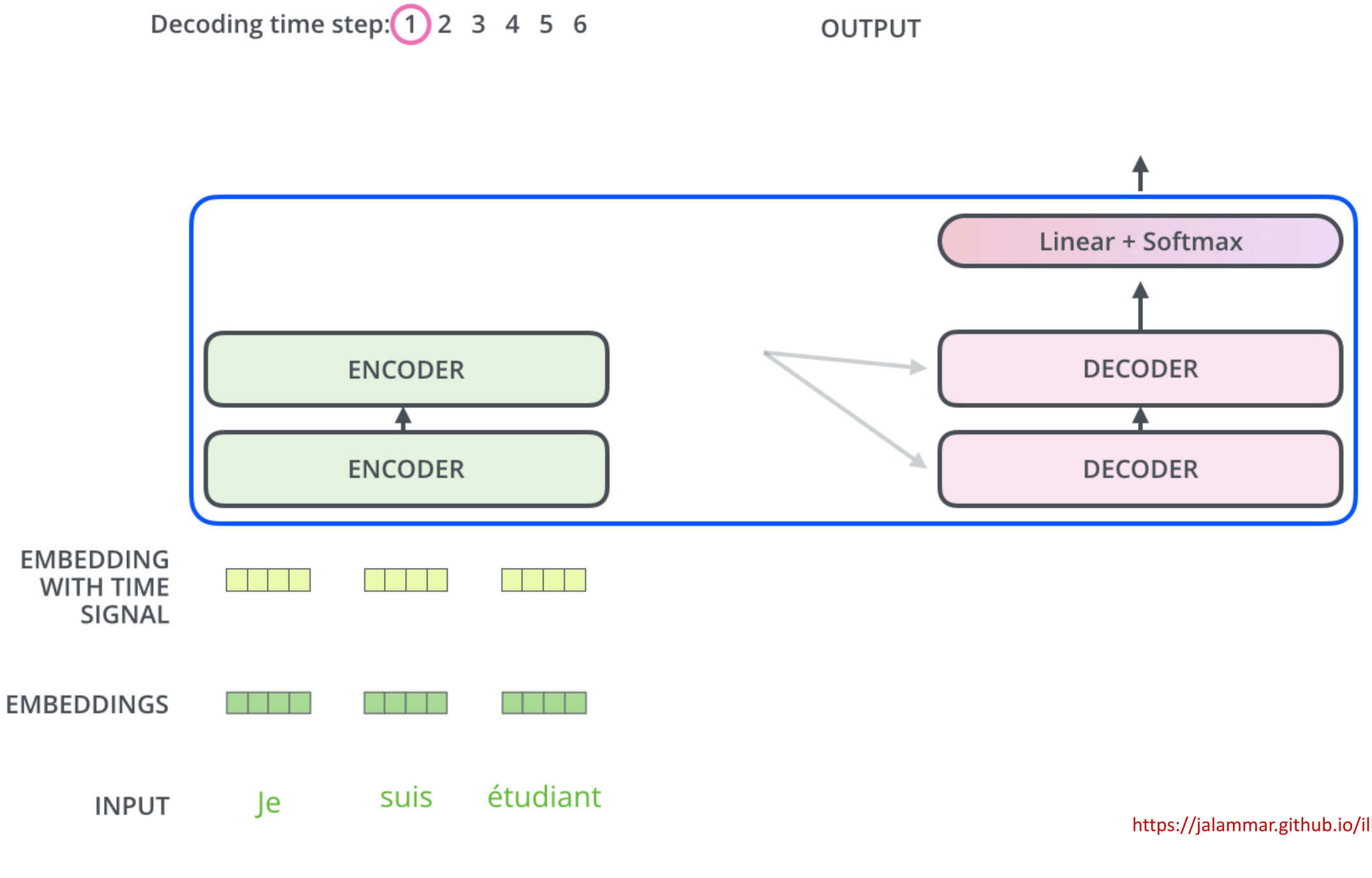
IMPORTANT

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.



https://jalammar.github.io/illustrated-transformer/



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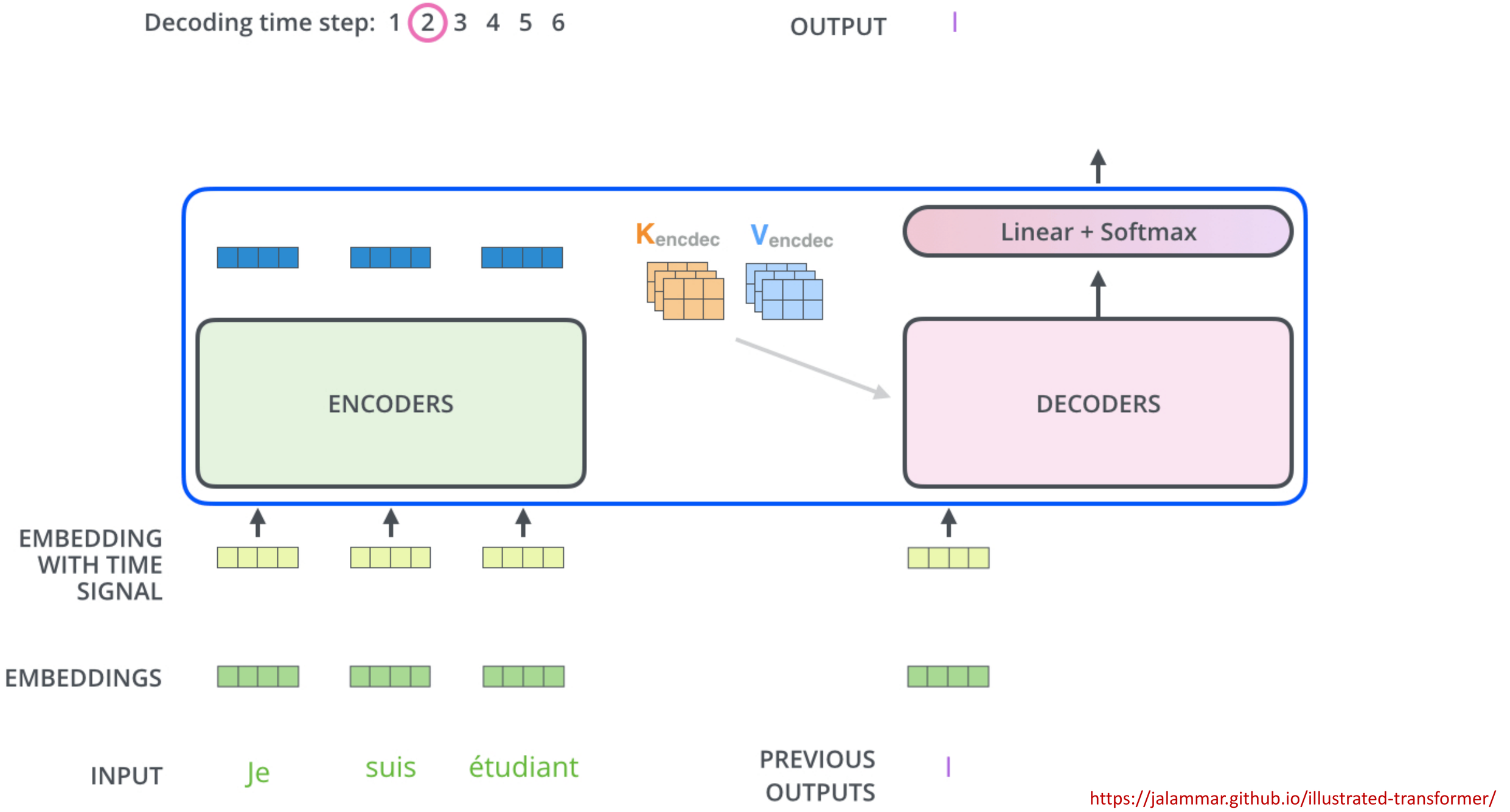

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Transformer Architecture

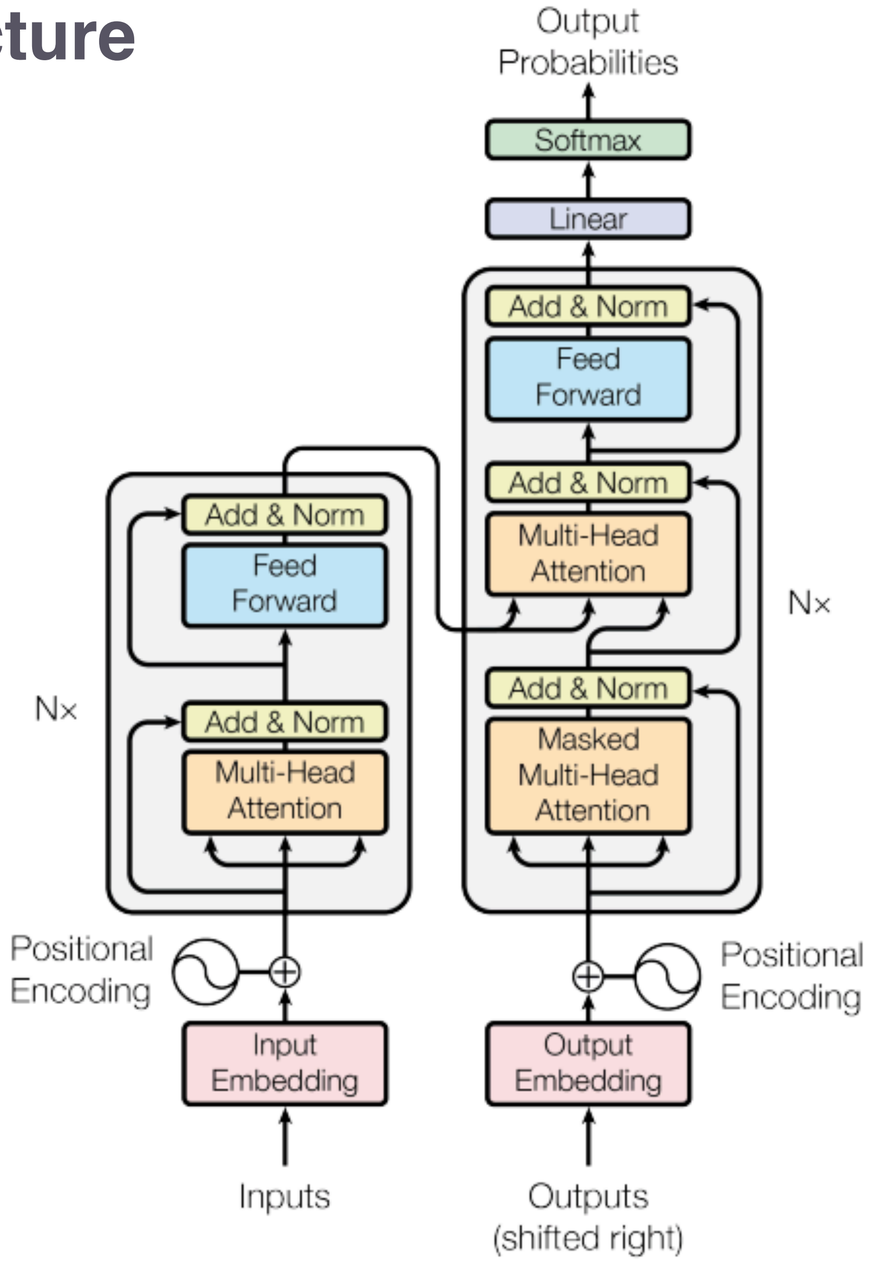

Figure 1: The Transformer - model architecture.

Attention is All you Need (2017) https://arxiv.org/pdf/1706.03762.pdf

Complexity

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)	$O(r \cdot n \cdot d)$	$O(1)$	$O(n/r)$

Complexity

n = sequence length

d = length of representation (vector)

Q: Is the complexity of self-attention good?

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

Complexity

Important: when learning dependencies b/w words, you don't want long paths. Shorter is better.

Self-attention connects all positions with a constant # of sequentially executed operations, whereas RNNs require $O(n)$.

Layer Type	Complexity per Layer	Sequential Operations	Maximum Path Length
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https://arxiv.org/pdf/1706.03762.pdf

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

Performance

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

BERT Motivation

- 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)

BERT Motivation

Bidirectional Encoder Representations from Transformers

BERT Motivation

Bidirectional Encoder Representations from Transformers

Like Bidirectional LSTMs, let's look in both directions

BERT Motivation

Bidirectional Encoder Representations from Transformers

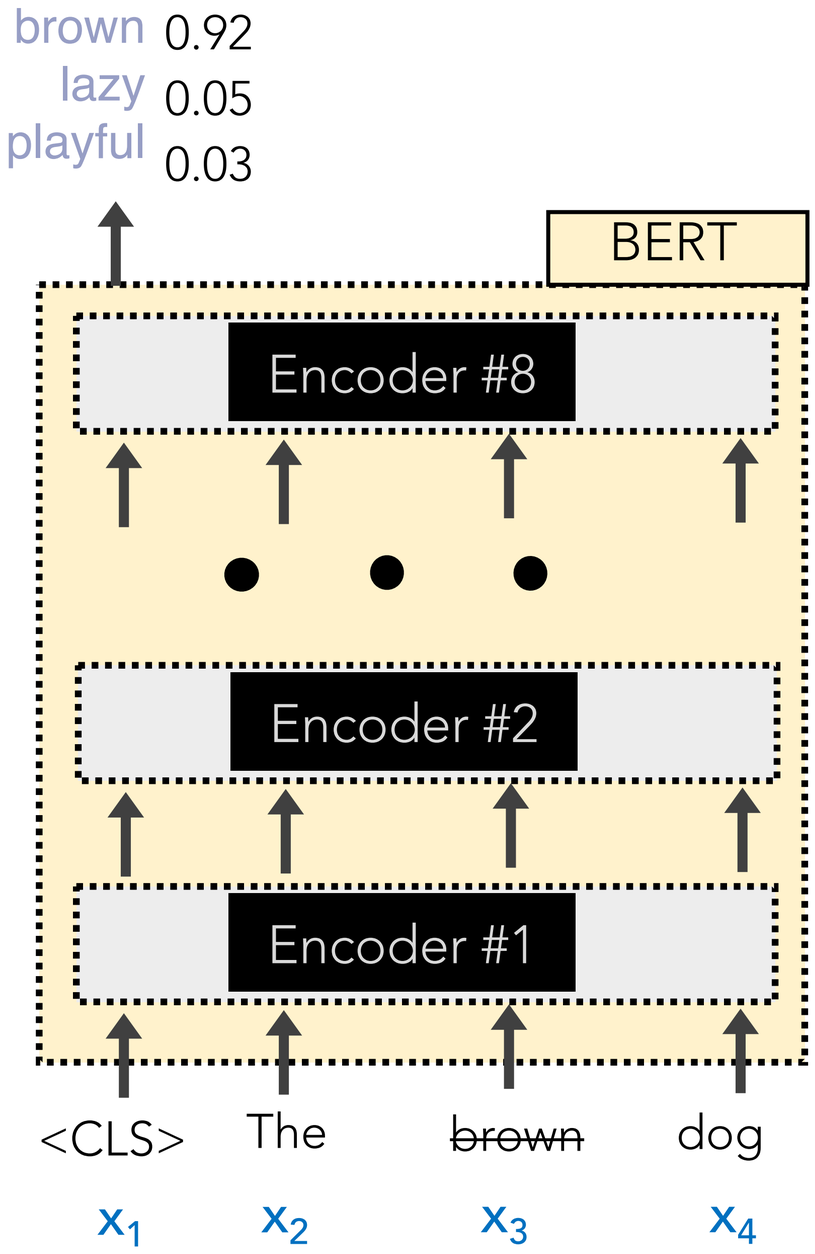
Let’s only use Transformer Encoders, no Decoders

BERT Motivation

Bidirectional Encoder Representations from Transformers

It’s a language model that builds rich representations

BERT Architecture



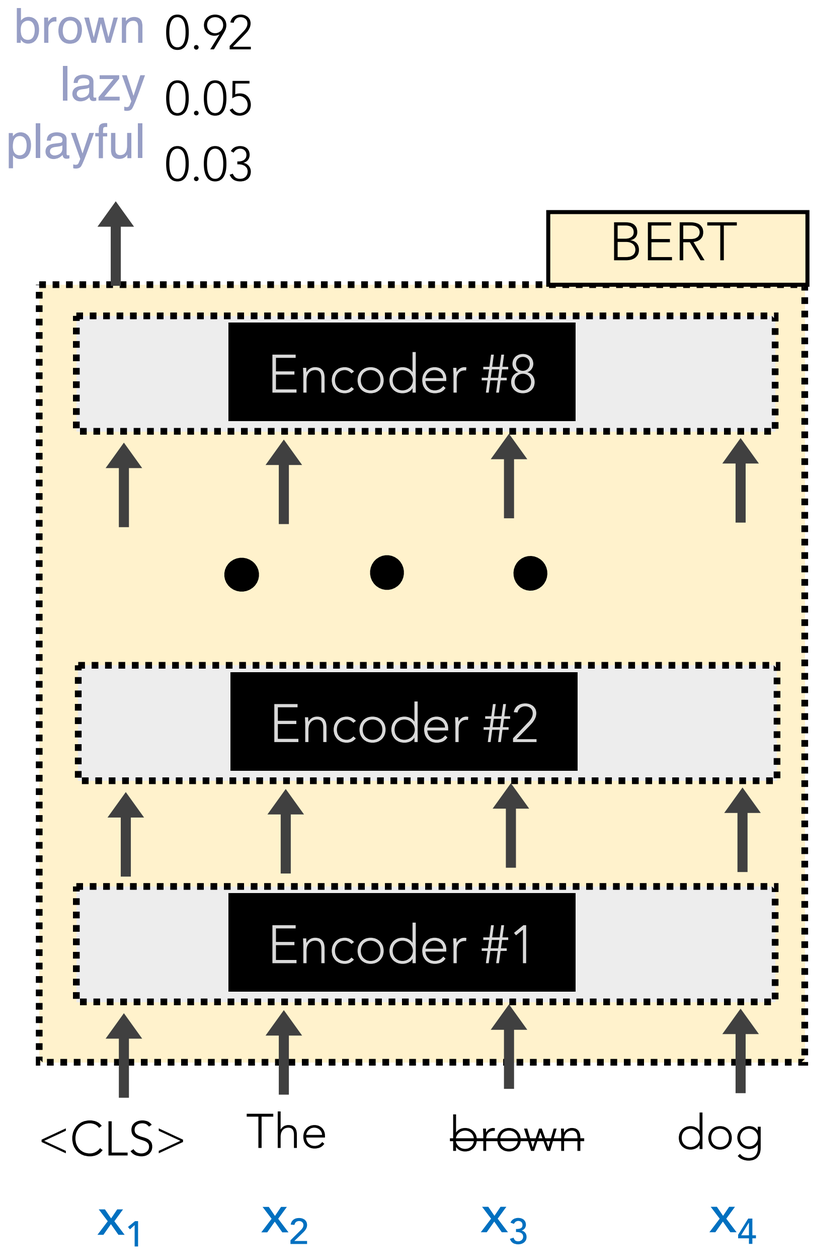
BERT has 2 training objectives:

1. Predict the **Masked word** (a la CBOW)

15% of all input words are randomly masked.

- 80% become [MASK]
- 10% become unmasked again
- 10% are deliberately corrupted as wrong words

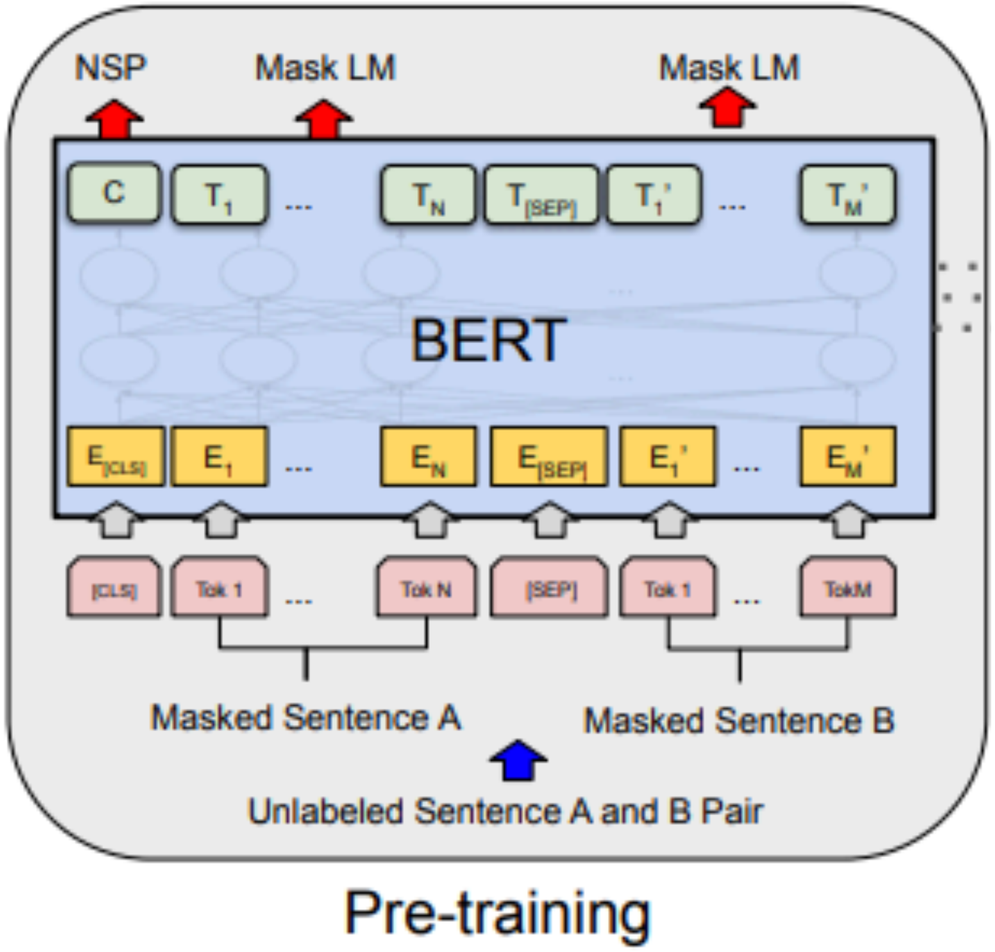
BERT Architecture



BERT has 2 training objectives:

2. Two sentences are fed in at a time. Predict if the second sentence of input truly follows the first one or not.

BERT Architecture



Pre-training

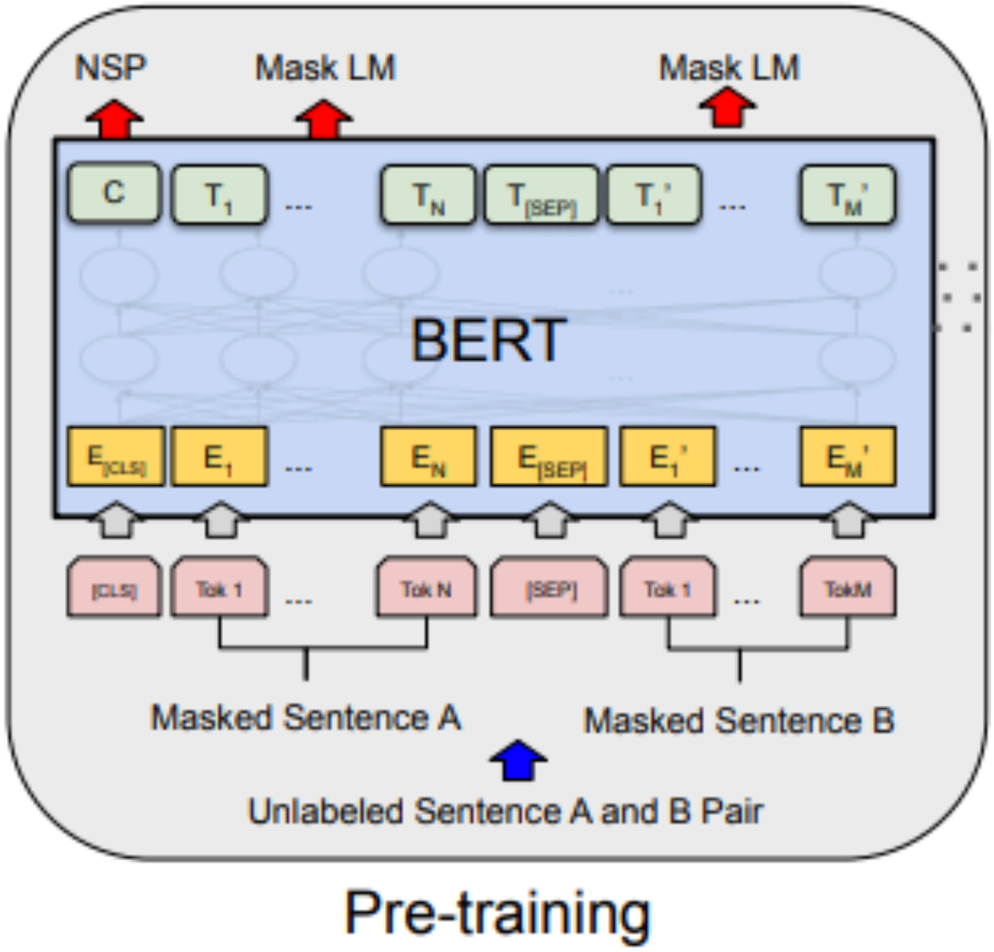
Every two sentences are separated by a **<SEP>** token.

50% of the time, the 2nd sentence is a randomly selected sentence from the corpus.

50% of the time, it truly follows the first sentence in the corpus.

Source: original BERT paper: https://arxiv.org/pdf/1810.04805.pdf

BERT Architecture



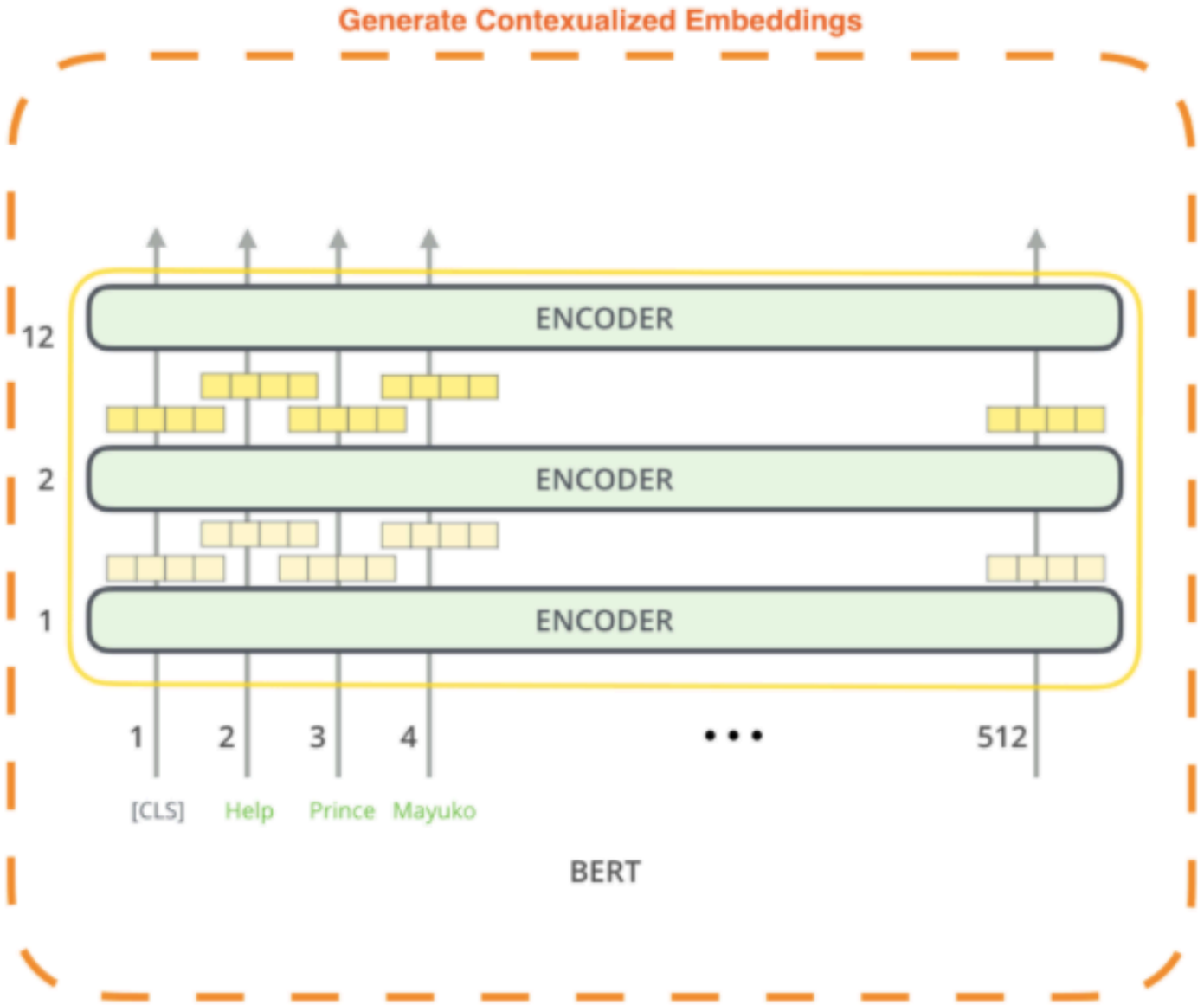
Pre-training

NOTE: BERT also embeds the inputs by their **WordPiece** embeddings.

WordPiece is a **sub-word tokenization** that learns to merge and use characters based on which pairs maximize the likelihood of the training data if added to the vocab.

Source: original BERT paper: https://arxiv.org/pdf/1810.04805.pdf

One could extract the contextualized embeddings



The output of each encoder layer along each token's path can be used as a feature representing that token.

But which one should we use?

Picture: https://jalammar.github.io/illustrated-bert/

Later layers have the best contextualized embeddings

		Dev F1 Score
First Layer	Embedding	91.0
Last Hidden Layer	12	94.9
Sum All 12 Layers	12 + ... + 2 + 1 =	95.5
Second-to-Last Hidden Layer	11	95.6
Sum Last Four Hidden	12 + 11 + 10 + 9 =	95.9
Concat Last Four Hidden	9 10 11 12	96.1

Picture: https://jalammar.github.io/illustrated-bert/

BERT yields state-of-the-art (SOTA) results on many tasks

System	MNLI-(m/mm) 392k	QQP 363k	QNLI 108k	SST-2 67k	CoLA 8.5k	STS-B 5.7k	MRPC 3.5k	RTE 2.5k	**Average** -
Pre-OpenAI SOTA	80.6/80.1	66.1	82.3	93.2	35.0	81.0	86.0	61.7	74.0
BiLSTM+ELMo+Attn	76.4/76.1	64.8	79.8	90.4	36.0	73.3	84.9	56.8	71.0
OpenAI GPT	82.1/81.4	70.3	87.4	91.3	45.4	80.0	82.3	56.0	75.1
$\text{BERT}_{\text{BASE}}$	84.6/83.4	71.2	90.5	93.5	52.1	85.8	88.9	66.4	79.6
$\text{BERT}_{\text{LARGE}}$	**86.7/85.9**	**72.1**	**92.7**	**94.9**	**60.5**	**86.5**	**89.3**	**70.1**	**82.1**

Table 1: GLUE Test results, scored by the evaluation server (https://gluebenchmark.com/leaderboard).

Source: original BERT paper: https://arxiv.org/pdf/1810.04805.pdf

BERT Summary

Strengths

- Great for embedding learning
- Powerful for transfer learning to other tasks

Issues?

- Not easily generative (no decoders)

What just happened!?

- RNN
- LSTM
- Attention
- Self-Attention
- Transformers

What is to come…

- Tutorials **May 3rd** + **May 10th**
- Next lecture. In two weeks! **May 14th**
- LLMs
- In-context Learning
- Prompt Engineering
- HW1 due!