

# RNN problems, LSTM, GRU and other variants of RNN


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Slides adapted from Stanford's NLP with Deep Learning  
course

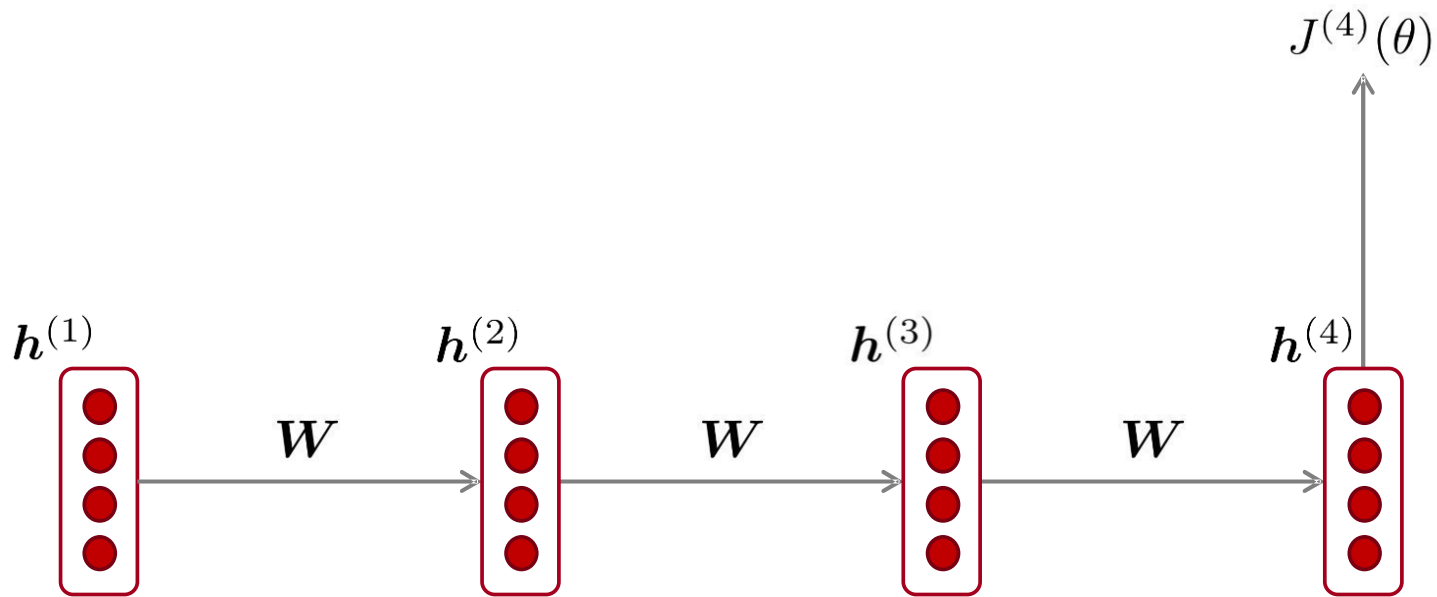
# Overview

- Last class we learned:
  - Recurrent Neural Networks (RNNs) and why they're great for Language Modeling (LM).
- Today we'll learn:
  - Problems with RNNs and how to fix them
  - More complex RNN variants

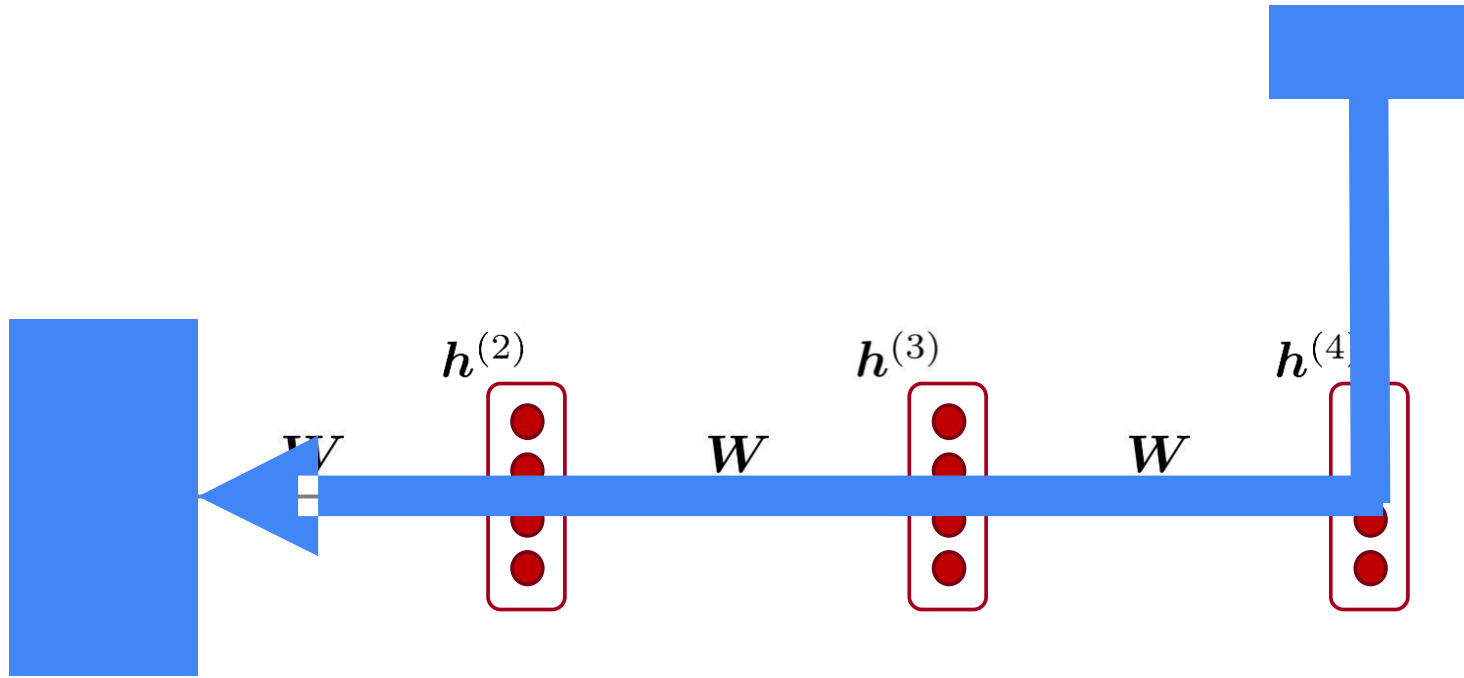
# Today's class

- Vanishing gradient problem
  - Two new types of RNN: LSTM and GRU
  - Other fixes for vanishing (or exploding) gradient:
    - Gradient clipping
    - Skip connections
  - More fancy RNN variants:
    - Bidirectional RNNs
    - Multi-layer RNNs
- motivates
- 

# Vanishing gradient intuition

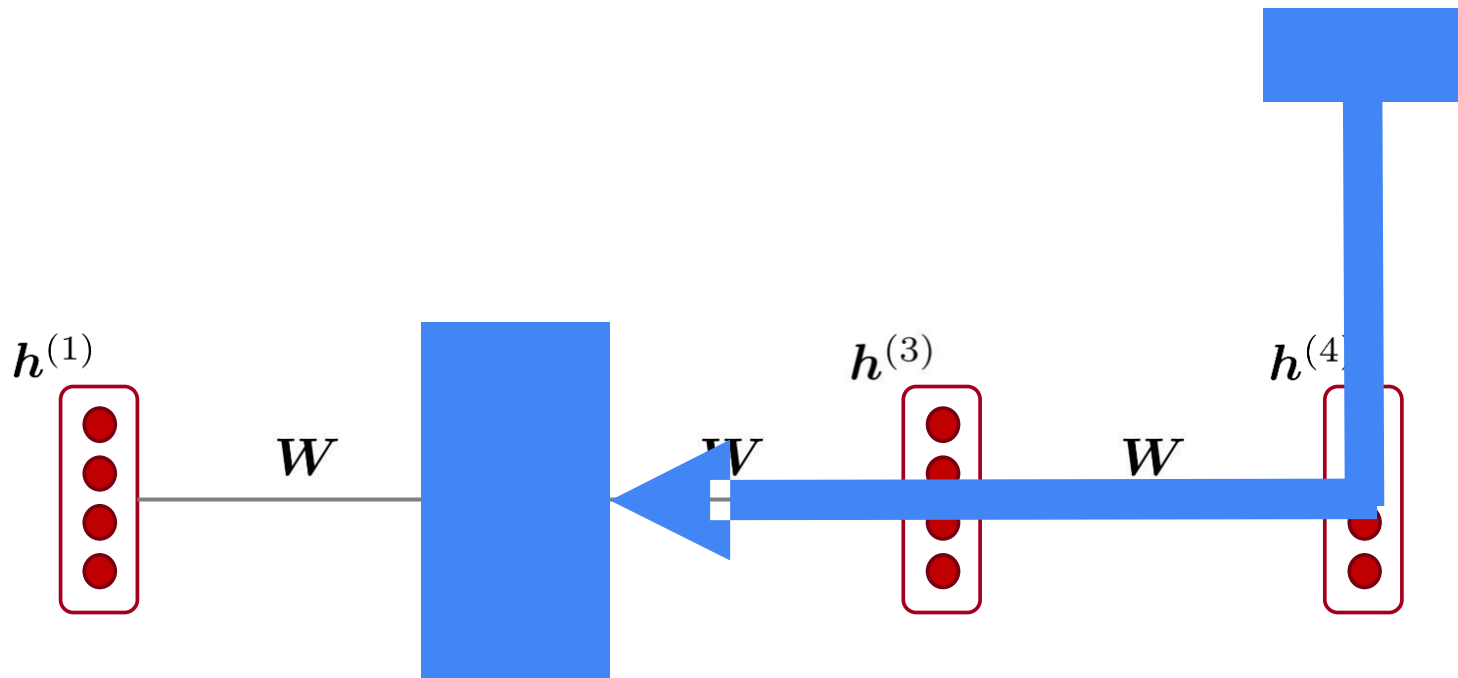


# Vanishing gradient intuition



$$\frac{\partial J^{(4)}}{\partial h^{(1)}} = ?$$

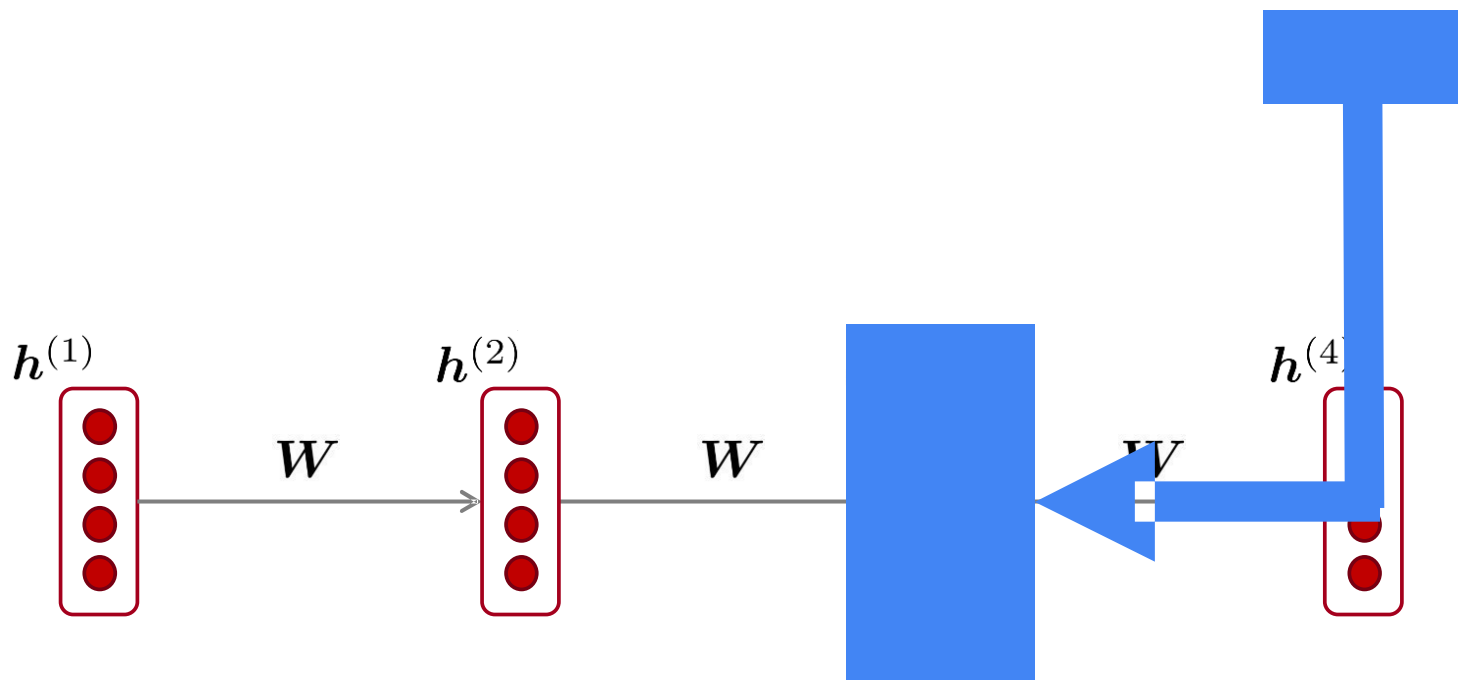
# Vanishing gradient intuition



$$\frac{\partial J^{(4)}}{\partial h^{(1)}} = \frac{\partial h^{(2)}}{\partial h^{(1)}} \times \frac{\partial J^{(4)}}{\partial h^{(2)}}$$

chain rule!

# Vanishing gradient intuition

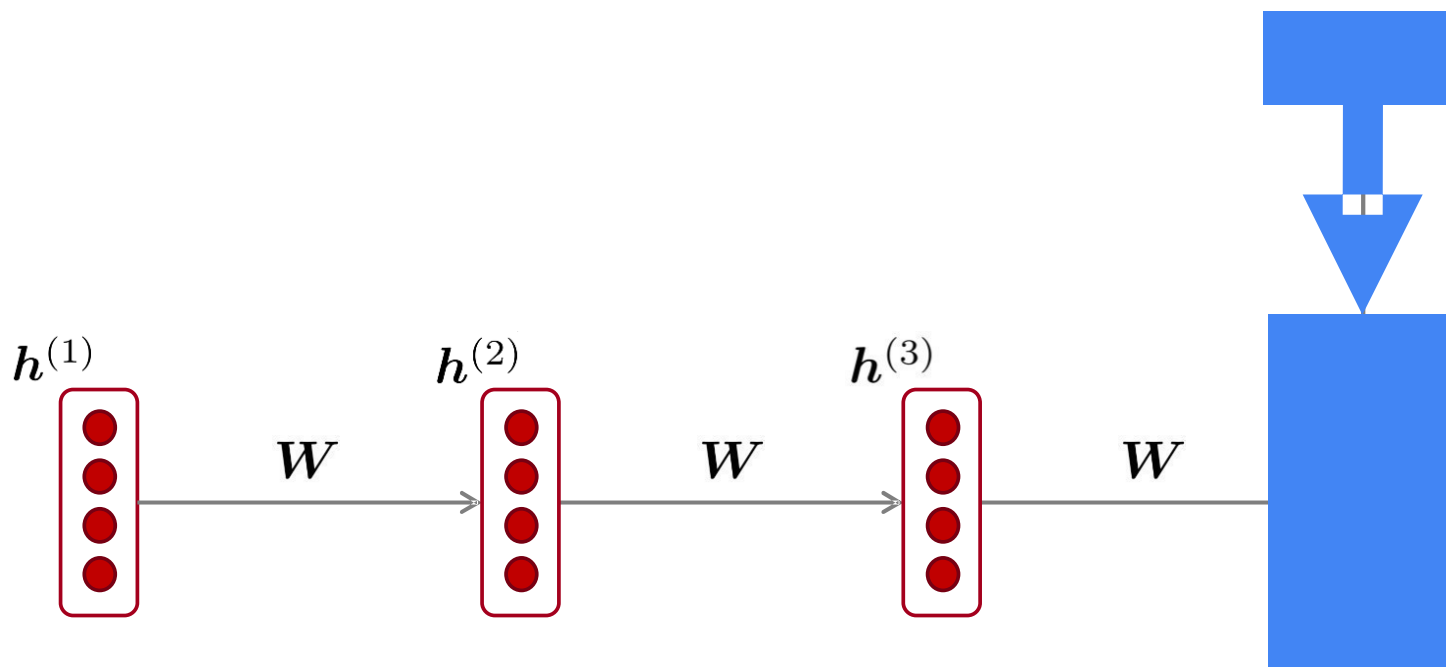


$$\frac{\partial J^{(4)}}{\partial h^{(1)}} = \frac{\partial h^{(2)}}{\partial h^{(1)}} \times$$

$$\frac{\partial h^{(3)}}{\partial h^{(2)}} \times \frac{\partial J^{(4)}}{\partial h^{(3)}}$$

chain rule!

# Vanishing gradient intuition



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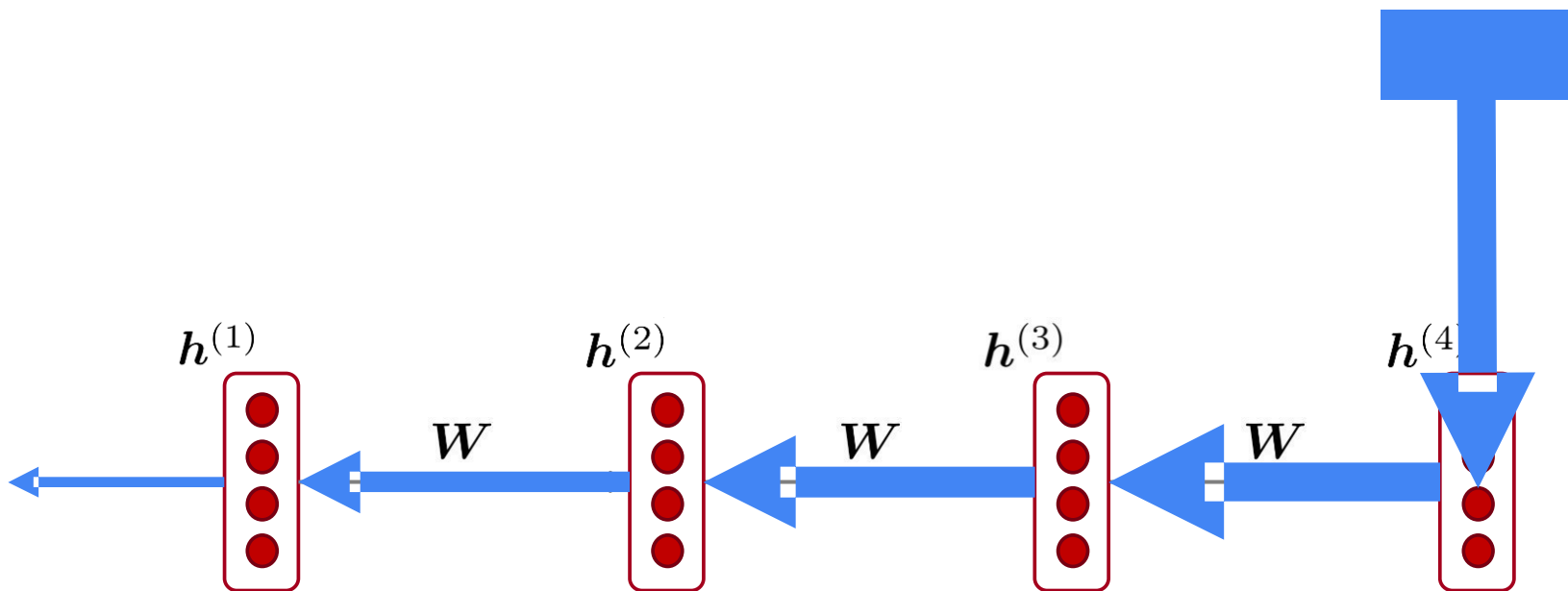
$$\frac{\partial h^{(3)}}{\partial h^{(2)}} \times$$

$$\frac{\partial h^{(4)}}{\partial h^{(3)}} \times \frac{\partial J^{(4)}}{\partial h^{(4)}}$$

chain rule!



# Vanishing gradient intuition



$$\frac{\partial J^{(4)}}{\partial h^{(1)}} = \boxed{\frac{\partial h^{(2)}}{\partial h^{(1)}}} \times \boxed{\frac{\partial h^{(3)}}{\partial h^{(2)}}} \times \boxed{\frac{\partial h^{(4)}}{\partial h^{(3)}}} \times \frac{\partial J^{(4)}}{\partial h^{(4)}}$$

What happens if these are small?

Vanishing gradient problem:  
When these are small, the gradient signal gets smaller and smaller as it backpropagates further

# Vanishing gradient proof sketch

- Recall:  $\mathbf{h}^{(t)} = \sigma \left( \mathbf{W}_h \mathbf{h}^{(t-1)} + \mathbf{W}_x \mathbf{x}^{(t)} + \mathbf{b}_1 \right)$
- Therefore:  $\frac{\partial \mathbf{h}^{(t)}}{\partial \mathbf{h}^{(t-1)}} = \text{diag} \left( \sigma' \left( \mathbf{W}_h \mathbf{h}^{(t-1)} + \mathbf{W}_x \mathbf{x}^{(t)} + \mathbf{b}_1 \right) \right) \mathbf{W}_h$  (chain rule)
- Consider the gradient of the loss  $J^{(i)}(\theta)$  on step  $i$ , with respect to the hidden state  $\mathbf{h}^{(j)}$  on some previous step  $j$ .

$$\begin{aligned} \frac{\partial J^{(i)}(\theta)}{\partial \mathbf{h}^{(j)}} &= \frac{\partial J^{(i)}(\theta)}{\partial \mathbf{h}^{(i)}} \prod_{j < t \leq i} \frac{\partial \mathbf{h}^{(t)}}{\partial \mathbf{h}^{(t-1)}} && \text{(chain rule)} \\ &= \frac{\partial J^{(i)}(\theta)}{\partial \mathbf{h}^{(i)}} \boxed{\mathbf{W}_h^{(i-j)}} \prod_{j < t \leq i} \text{diag} \left( \sigma' \left( \mathbf{W}_h \mathbf{h}^{(t-1)} + \mathbf{W}_x \mathbf{x}^{(t)} + \mathbf{b}_1 \right) \right) && \left( \text{value of } \frac{\partial \mathbf{h}^{(t)}}{\partial \mathbf{h}^{(t-1)}} \right) \end{aligned}$$

If  $\mathbf{W}_h$  is small, then this term gets vanishingly small as  $i$  and  $j$  get further apart

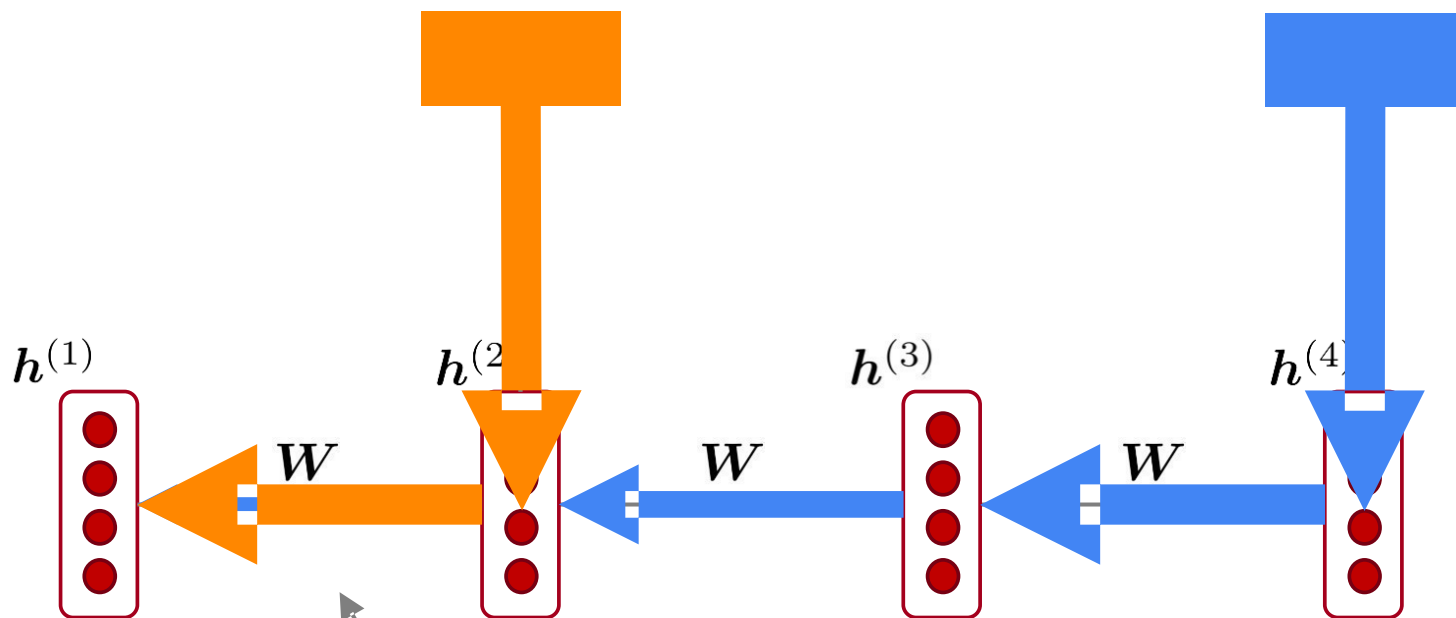
# Vanishing gradient proof sketch

- Consider matrix L2 norms:

$$\left\| \frac{\partial J^{(i)}(\theta)}{\partial \mathbf{h}^{(j)}} \right\| \leq \left\| \frac{\partial J^{(i)}(\theta)}{\partial \mathbf{h}^{(i)}} \right\| \|\mathbf{W}_h\|^{(i-j)} \prod_{j < t \leq i} \left\| \text{diag} \left( \sigma' \left( \mathbf{W}_h \mathbf{h}^{(t-1)} + \mathbf{W}_x \mathbf{x}^{(t)} + \mathbf{b}_1 \right) \right) \right\|$$

- Pascanu et al showed that that if the **largest eigenvalue** of  $\mathbf{W}_h$  is **less than 1**, then the gradient  $\left\| \frac{\partial J^{(i)}(\theta)}{\partial \mathbf{h}^{(j)}} \right\|$  will **shrink** exponentially
  - Here the bound is 1 because we have sigmoid nonlinearity
- There's a similar proof relating a **largest eigenvalue  $> 1$**  to **exploding gradients**

# Why is vanishing gradient a problem?



Gradient signal from faraway is lost because it's much smaller than gradient signal from close-by.

So model weights are only updated only with respect to near effects, not long-term effects.

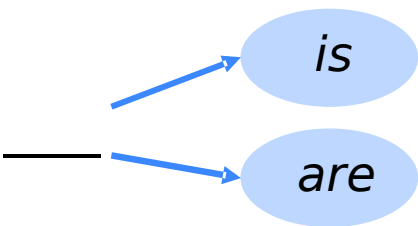


# Why is vanishing gradient a problem?

- Another explanation: Gradient can be viewed as a measure of the *effect of the past on the future*
- If the gradient becomes vanishingly small over longer distances (step  $t$  to step  $t+n$ ), then we can't tell whether:
  1. There's **no dependency** between step  $t$  and  $t+n$  in the data
  2. We have **wrong parameters** to capture the true dependency between  $t$  and  $t+n$

# Effect of vanishing gradient on RNN-LM

- **LM task:** *When she tried to print her tickets, she found that the printer was out of toner. She went to the stationery store to buy more toner. It was very overpriced. After installing the toner into the printer, she finally printed her \_\_\_\_\_*
- To learn from this training example, the RNN-LM needs to model **the dependency** between “*tickets*” on the 7<sup>th</sup> step and the target word “*tickets*” at the end.
- But if gradient is small, the model **can't learn this dependency**
  - So the model is **unable to predict similar long-distance dependencies** at test time

# Effect of vanishing gradient on RNN-LM

- **LM task:** *The writer of the books \_\_\_\_* 
- **Correct answer:** *The writer of the books is planning a sequel*
- **Syntactic recency:** *The writer of the books is* (correct) 
- **Sequential recency:** *The writer of the books are* (incorrect) 
- Due to vanishing gradient, RNN-LMs are better at learning from **sequential recency** than **syntactic recency**, so they make this type of error more often than we'd like [Linzen et al 2016]

# Why is exploding gradient a problem?

- If the gradient becomes too big, then the SGD update step becomes too big:

$$\theta^{new} = \theta^{old} - \overbrace{\alpha}^{\text{learning rate}} \underbrace{\nabla_{\theta} J(\theta)}_{\text{gradient}}$$

- This can cause **bad updates**: we take too large a step and reach a bad parameter configuration (with large loss)
- In the worst case, this will result in **Inf** or **NaN** in your network (then you have to restart training from an earlier checkpoint)



# Gradient clipping: solution for exploding gradient

- Gradient clipping: if the norm of the gradient is greater than some threshold, scale it down before applying SGD update

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**Algorithm 1** Pseudo-code for norm clipping

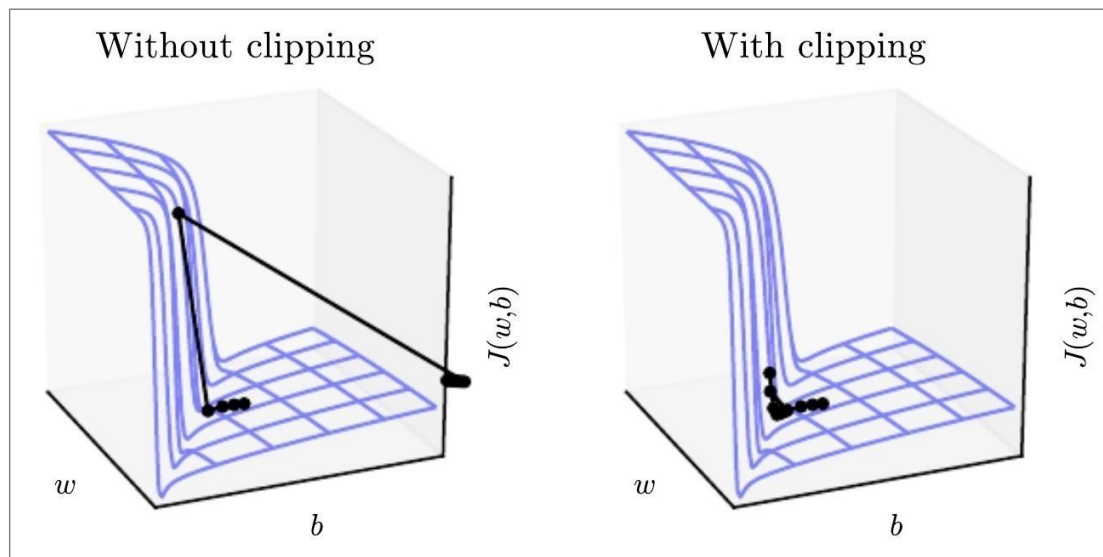
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$$\begin{aligned} \hat{\mathbf{g}} &\leftarrow \frac{\partial \mathcal{E}}{\partial \theta} \\ \text{if } \|\hat{\mathbf{g}}\| &\geq \textit{threshold} \text{ then} \\ &\quad \hat{\mathbf{g}} \leftarrow \frac{\textit{threshold}}{\|\hat{\mathbf{g}}\|} \hat{\mathbf{g}} \\ \text{end if} \end{aligned}$$

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- Intuition: take a step in the same direction, but a smaller step

# Gradient clipping: solution for exploding gradient



- This shows the loss surface of a simple RNN (hidden state is a scalar not a vector)
- The “cliff” is dangerous because it has steep gradient
- On the left, gradient descent takes two very big steps due to steep gradient, resulting in climbing the cliff then shooting off to the right (both bad updates)
- On the right, gradient clipping reduces the size of those steps, so effect is less drastic

# How to fix vanishing gradient problem?

- The main problem is that *it's too difficult for the RNN to learn to preserve information over many timesteps.*

- In a vanilla RNN, the hidden state is constantly being rewritten

$$\mathbf{h}^{(t)} = \sigma \left( \mathbf{W}_h \mathbf{h}^{(t-1)} + \mathbf{W}_x \mathbf{x}^{(t)} + \mathbf{b} \right)$$

- How about a RNN with separate memory?

# Long Short-Term Memory (LSTM)

- A type of RNN proposed by Hochreiter and Schmidhuber in 1997 as a solution to the vanishing gradients problem.
- On step  $t$ , there is a **hidden state**  $h^{(t)}$  and a **cell state**  $c^{(t)}$ 
  - Both are vectors length  $n$
  - The cell stores **long-term information**
  - The LSTM can **erase**, **write** and **read** information from the cell
- The selection of which information is erased/written/read is controlled by three corresponding **gates**
  - The gates are also vectors length  $n$
  - On each timestep, each element of the gates can be **open** (1), **closed** (0), or somewhere in-between.
  - The gates are **dynamic**: their value is computed based on the current context

# Long Short-Term Memory (LSTM)

We have a sequence of inputs  $\mathbf{x}^{(t)}$ , and we will compute a sequence of hidden states  $\mathbf{h}^{(t)}$  and cell states  $\mathbf{c}^{(t)}$ . On timestep  $t$ :

**Forget gate:** controls what is kept vs forgotten, from previous cell state

**Input gate:** controls what parts of the new cell content are written to cell

**Output gate:** controls what parts of cell are output to hidden state

**New cell content:** this is the new content to be written to the cell

**Cell state:** erase (“forget”) some content from last cell state, and write (“input”) some new cell content

**Hidden state:** read (“output”) some content from the cell

**Sigmoid function:** all gate values are between 0 and 1

$$\mathbf{f}^{(t)} = \sigma \left( \mathbf{W}_f \mathbf{h}^{(t-1)} + \mathbf{U}_f \mathbf{x}^{(t)} + \mathbf{b}_f \right)$$

$$\mathbf{i}^{(t)} = \sigma \left( \mathbf{W}_i \mathbf{h}^{(t-1)} + \mathbf{U}_i \mathbf{x}^{(t)} + \mathbf{b}_i \right)$$

$$\mathbf{o}^{(t)} = \sigma \left( \mathbf{W}_o \mathbf{h}^{(t-1)} + \mathbf{U}_o \mathbf{x}^{(t)} + \mathbf{b}_o \right)$$

$$\tilde{\mathbf{c}}^{(t)} = \tanh \left( \mathbf{W}_c \mathbf{h}^{(t-1)} + \mathbf{U}_c \mathbf{x}^{(t)} + \mathbf{b}_c \right)$$

$$\mathbf{c}^{(t)} = \mathbf{f}^{(t)} \circ \mathbf{c}^{(t-1)} + \mathbf{i}^{(t)} \circ \tilde{\mathbf{c}}^{(t)}$$

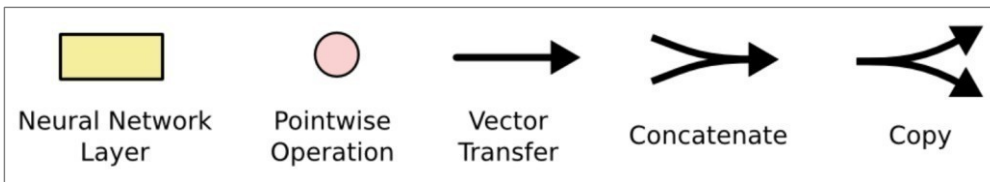
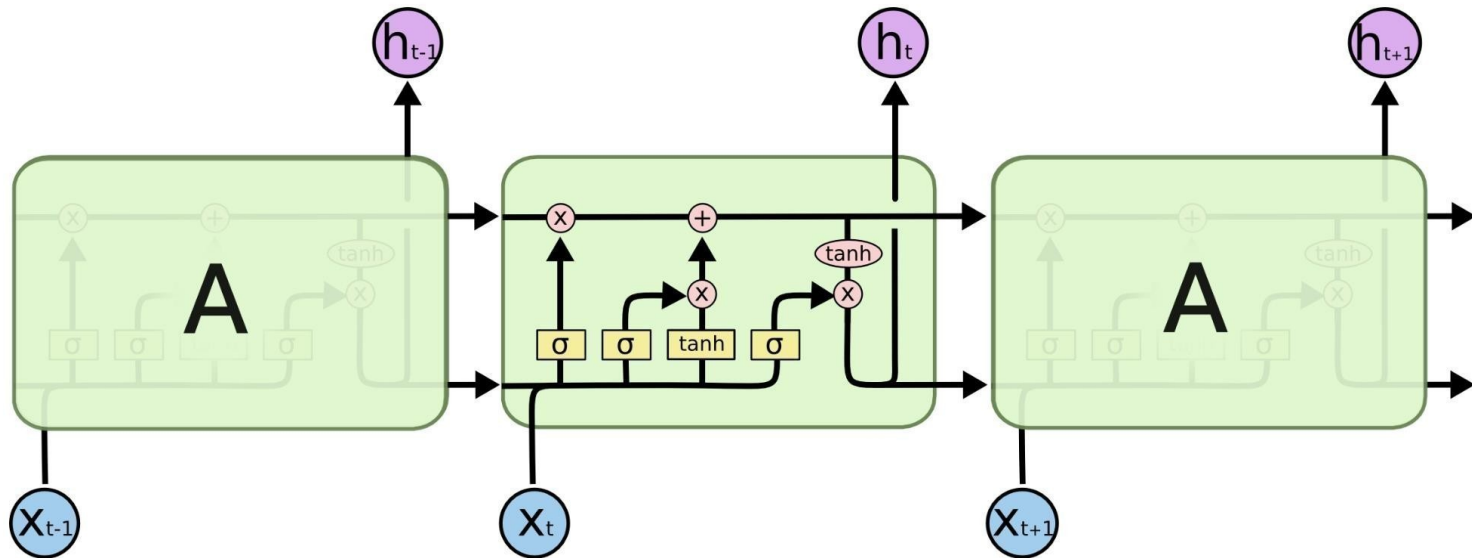
$$\mathbf{h}^{(t)} = \mathbf{o}^{(t)} \circ \tanh \mathbf{c}^{(t)}$$

Gates are applied using element-wise product

All these are vectors of same length  $n$

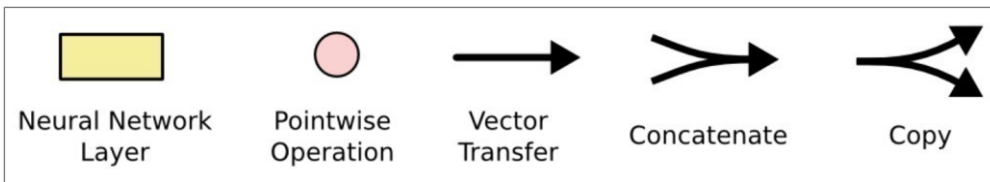
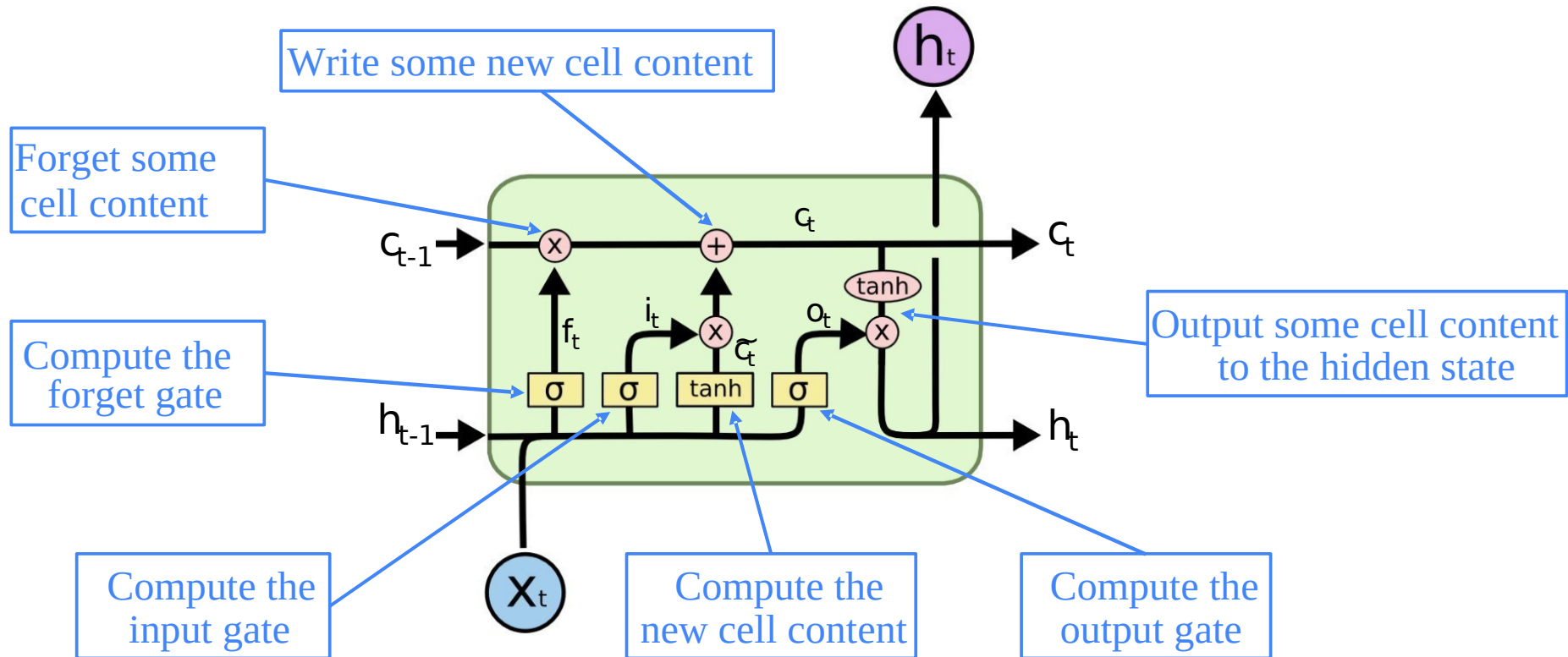
# Long Short-Term Memory (LSTM)

You can think of the LSTM equations visually like this:



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# How does LSTM solve vanishing gradients?

- The LSTM architecture makes it **easier** for the RNN to **preserve information over many timesteps**
  - e.g. if the forget gate is set to remember everything on every timestep, then the info in the cell is preserved indefinitely
  - By contrast, it's harder for vanilla RNN to learn a recurrent weight matrix  $W_h$  that preserves info in hidden state
- LSTM doesn't *guarantee* that there is no vanishing/exploding gradient, but it does provide an easier way for the model to learn long-distance dependencies



# LSTMs: real-world success

- In 2013-2015, LSTMs started achieving state-of-the-art results
  - Successful tasks include: handwriting recognition, speech recognition, machine translation, parsing, image captioning
  - LSTM became the dominant approach
- Now (2019), other approaches (e.g. Transformers) have become more dominant for certain tasks.
  - For example in WMT (a MT conference + competition):
  - In WMT 2016, the summary report contains "RNN" 44 times
  - In WMT 2018, the report contains "RNN" 9 times and "Transformer" 63 times

Source: "Findings of the 2016 Conference on Machine Translation (WMT16)", Bojar et al. 2016, <http://www.statmt.org/wmt16/pdf/W16-2301.pdf>

Source: "Findings of the 2018 Conference on Machine Translation (WMT18)", Bojar et al. 2018, <http://www.statmt.org/wmt18/pdf/WMT028.pdf>

# Gated Recurrent Units (GRU)

- Proposed by Cho et al. in 2014 as a simpler alternative to the LSTM.
- On each timestep  $t$  we have input  $\mathbf{x}^{(t)}$  and hidden state  $\mathbf{h}^{(t)}$  (no cell state).

**Update gate:** controls what parts of hidden state are updated vs preserved

$$\mathbf{u}^{(t)} = \sigma \left( \mathbf{W}_u \mathbf{h}^{(t-1)} + \mathbf{U}_u \mathbf{x}^{(t)} + \mathbf{b}_u \right)$$

**Reset gate:** controls what parts of previous hidden state are used to compute new content

$$\mathbf{r}^{(t)} = \sigma \left( \mathbf{W}_r \mathbf{h}^{(t-1)} + \mathbf{U}_r \mathbf{x}^{(t)} + \mathbf{b}_r \right)$$

**New hidden state content:** reset gate selects useful parts of prev hidden state. Use this and current input to compute new hidden content.

$$\tilde{\mathbf{h}}^{(t)} = \tanh \left( \mathbf{W}_h (\mathbf{r}^{(t)} \circ \mathbf{h}^{(t-1)}) + \mathbf{U}_h \mathbf{x}^{(t)} + \mathbf{b}_h \right)$$

$$\mathbf{h}^{(t)} = (1 - \mathbf{u}^{(t)}) \circ \mathbf{h}^{(t-1)} + \mathbf{u}^{(t)} \circ \tilde{\mathbf{h}}^{(t)}$$

**Hidden state:** update gate simultaneously controls what is kept from previous hidden state, and what is updated to new hidden state content

**How does this solve vanishing gradient?**

Like LSTM, GRU makes it easier to retain info long-term (e.g. by setting update gate to 0)

# LSTM vs GRU

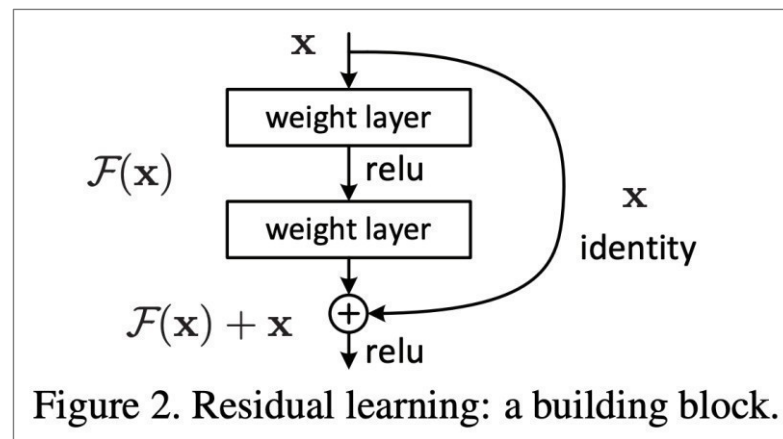
- Researchers have proposed many gated RNN variants, but LSTM and GRU are the most widely-used
- The biggest difference is that GRU is quicker to compute and has fewer parameters
- There is no conclusive evidence that one consistently performs better than the other
- LSTM is a good default choice (especially if your data has particularly long dependencies, or you have lots of training data)
- Rule of thumb: start with LSTM, but switch to GRU if you want something more efficient

# Is vanishing/exploding gradient just a RNN problem?

- No! It can be a problem for all neural architectures (including feed-forward and convolutional), especially deep ones.
  - Due to chain rule / choice of nonlinearity function, gradient can become vanishingly small as it backpropagates
  - Thus lower layers are learnt very slowly (hard to train)
  - Solution: lots of new deep feedforward/convolutional architectures that add more direct connections (thus allowing the gradient to flow)

For example:

- Residual connections aka “ResNet”
- Also known as skip-connections
- The identity connection preserves information by default
- This makes deep networks much easier to train

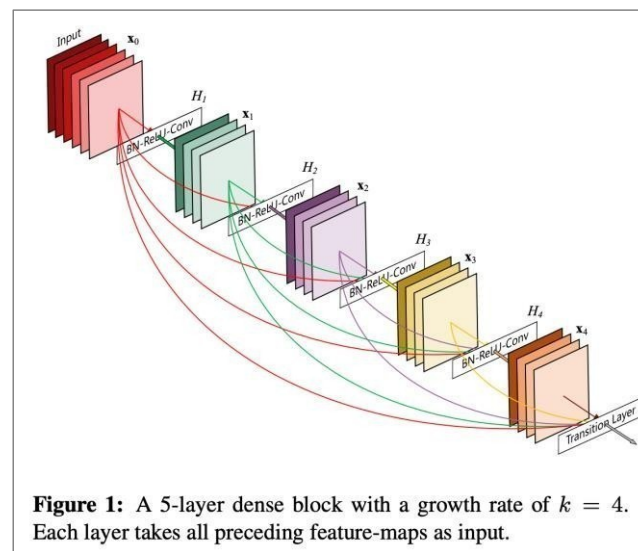


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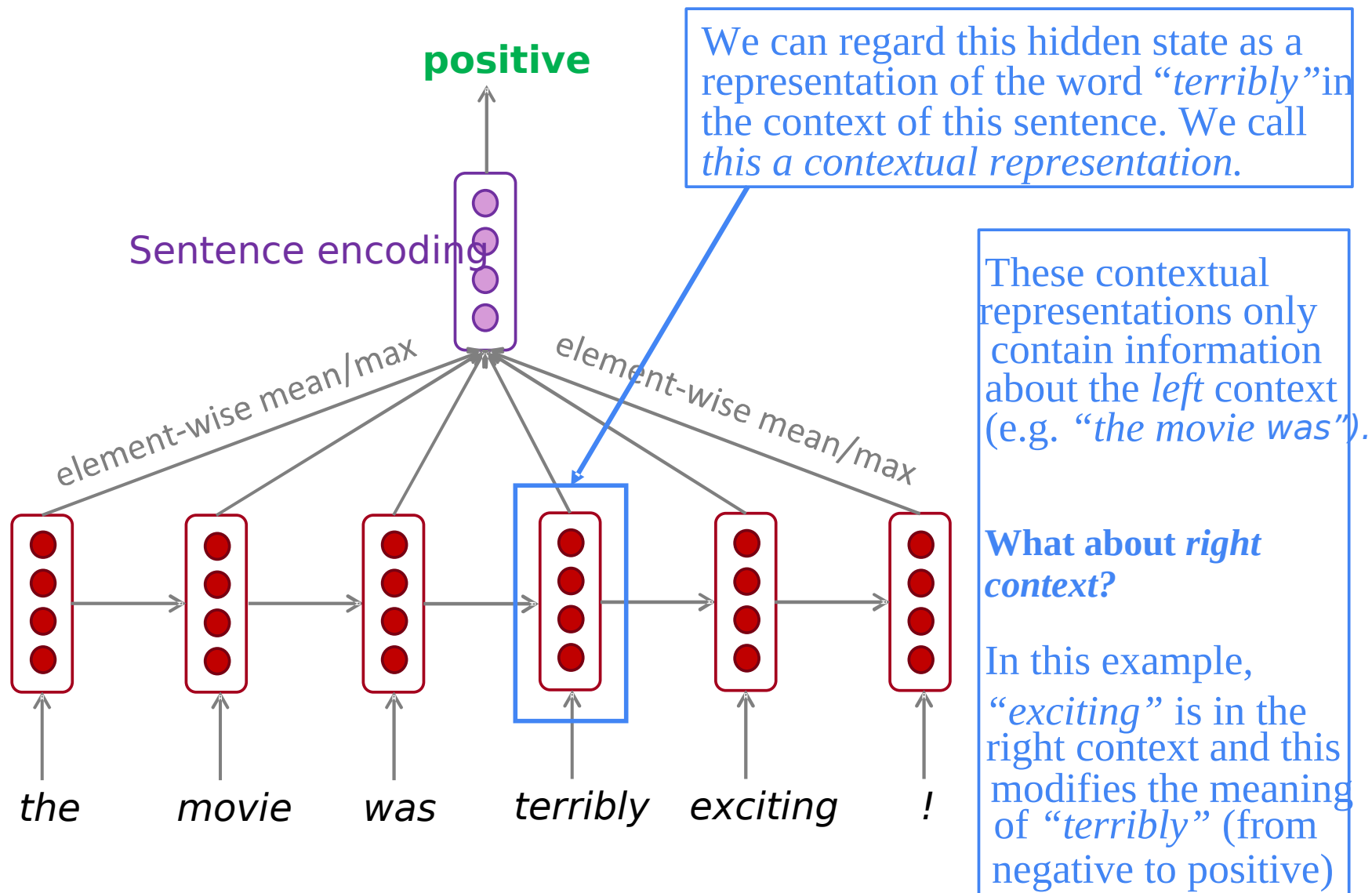
For example:

- Dense connections aka “DenseNet”
- Directly connect everything to everything!



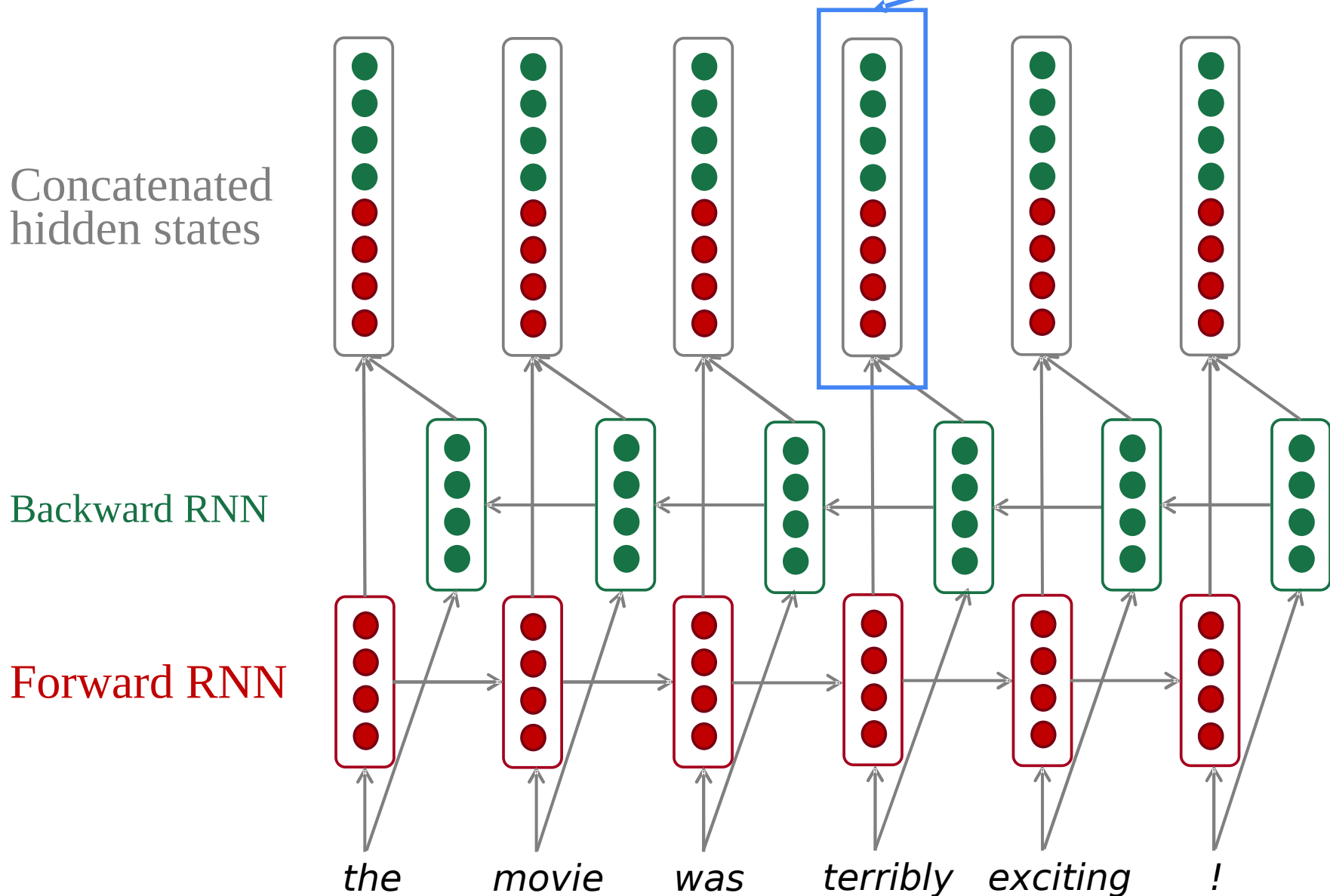
# Bidirectional RNNs: motivation

## Task: Sentiment Classification

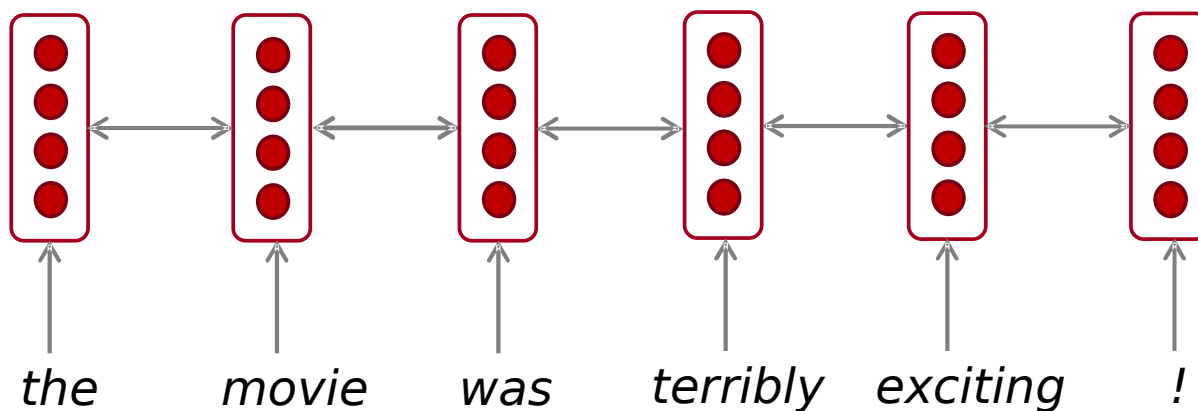


# Bidirectional RNNs

This contextual representation of “terribly”  
has both left and right context!



# Bidirectional RNNs: simplified diagram



The two-way arrows indicate bidirectionality and the depicted hidden states are assumed to be the concatenated forwards+backwards states.

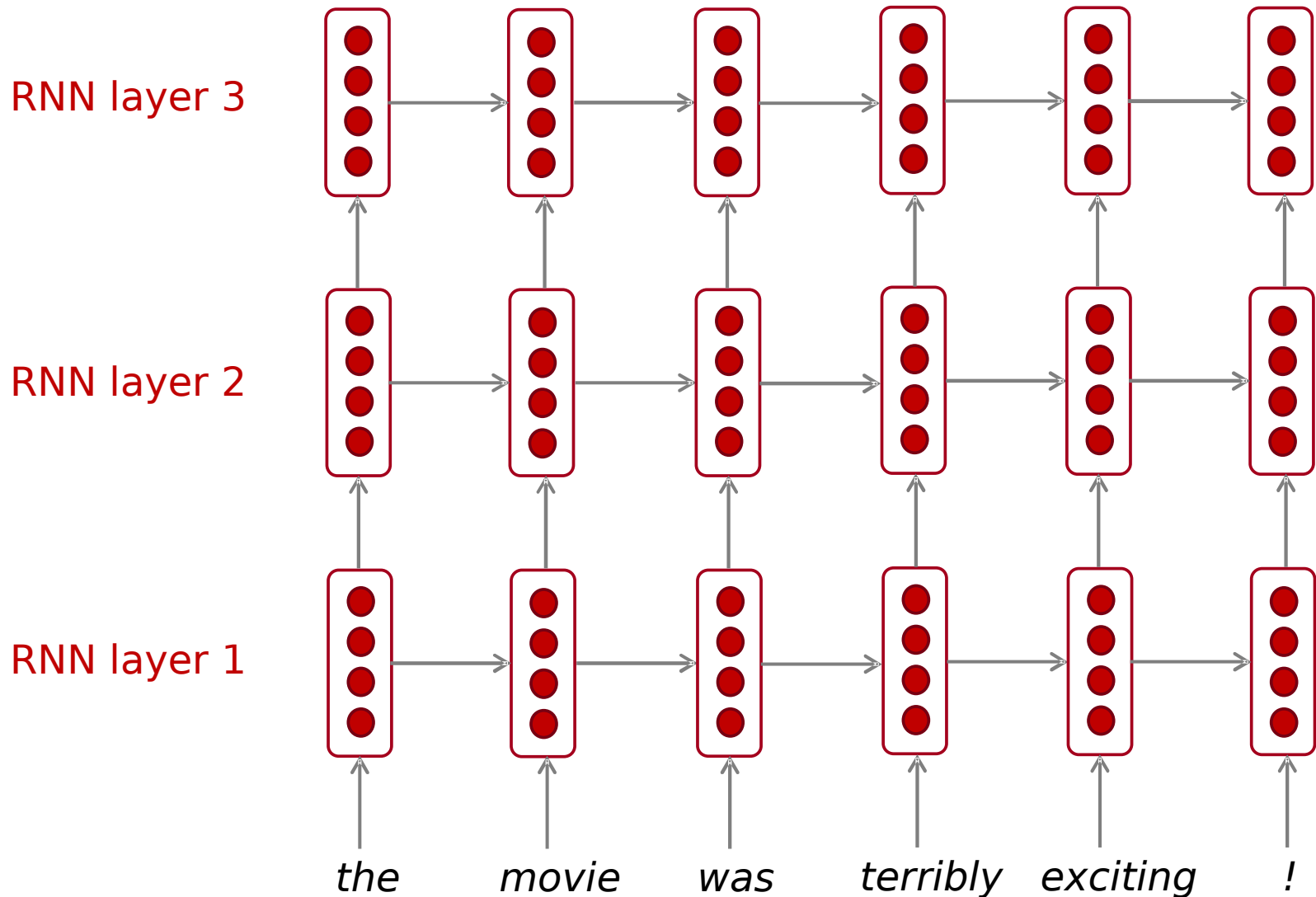


# Multi-layer RNNs

- RNNs are already “deep” on one dimension (they unroll over many timesteps)
- We can also make them “deep” in another dimension by **applying multiple RNNs** – this is a multi-layer RNN.
- This allows the network to compute **more complex representations**
- Multi-layer RNNs are also called *stacked RNNs*.

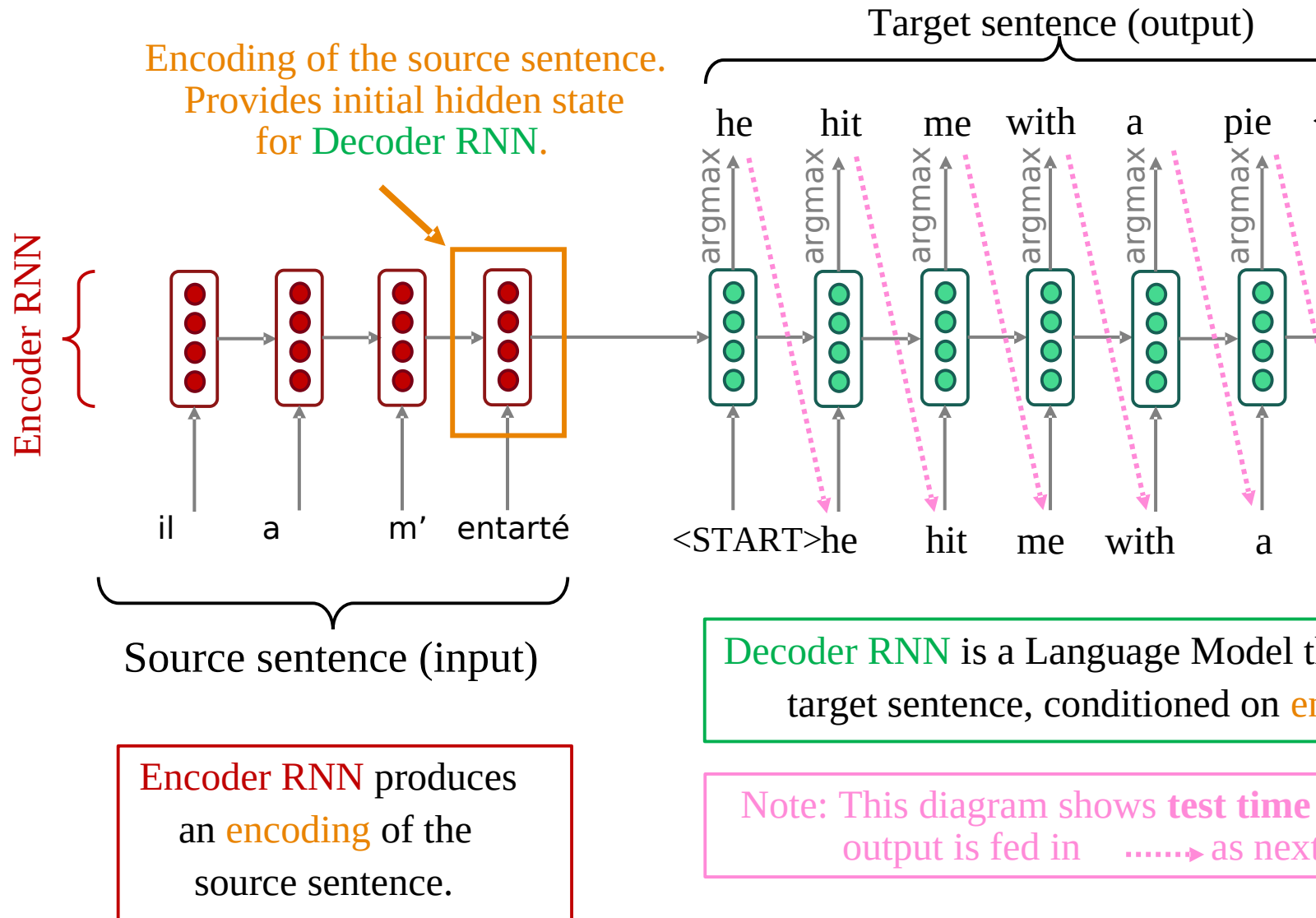
# Multi-layer RNNs

The hidden states from RNN layer  $i$  are the inputs to RNN layer  $i+1$



# Sequence-to-sequence model

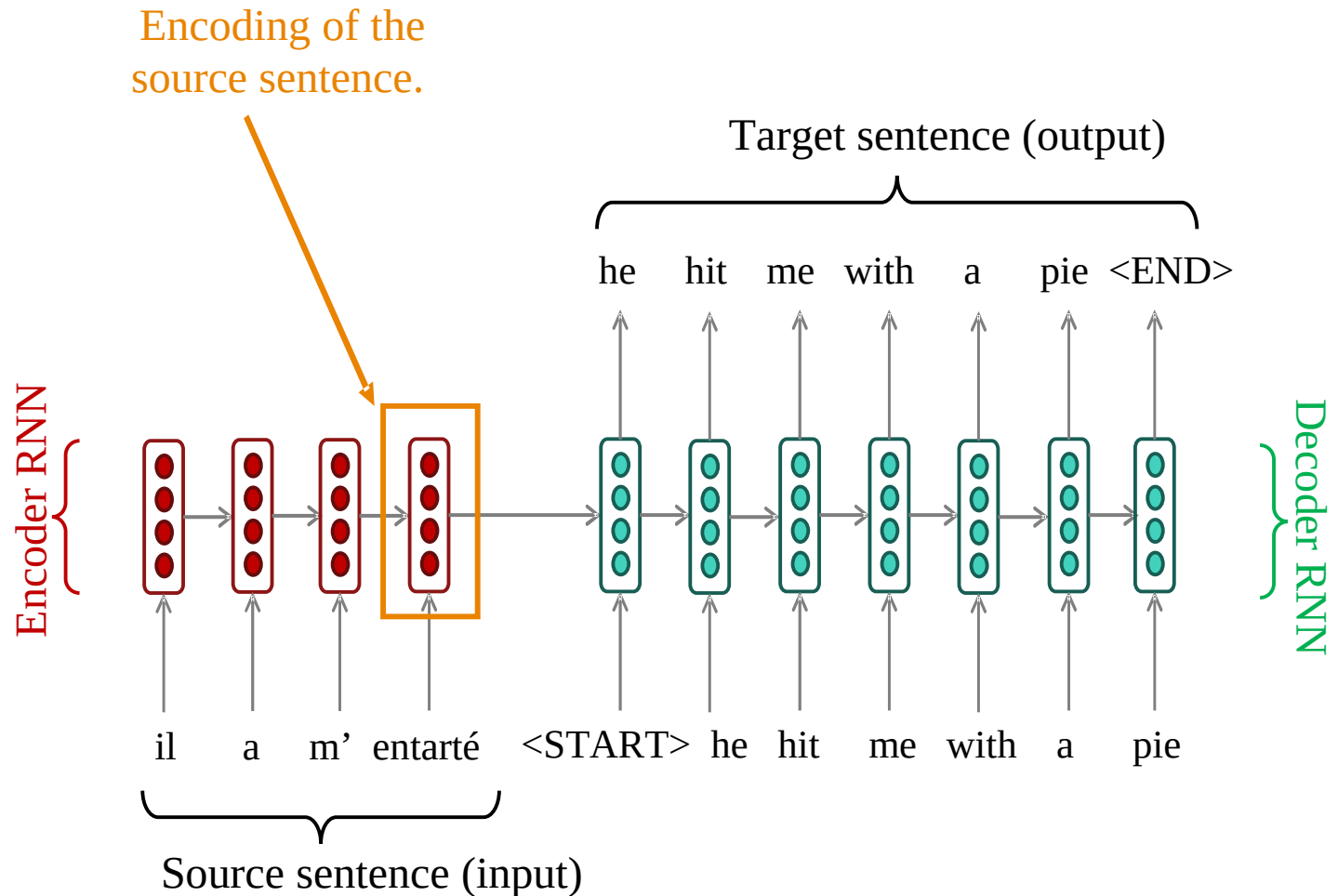
## Neural Machine Translation (NMT)



# Sequence-to-sequence is versatile!

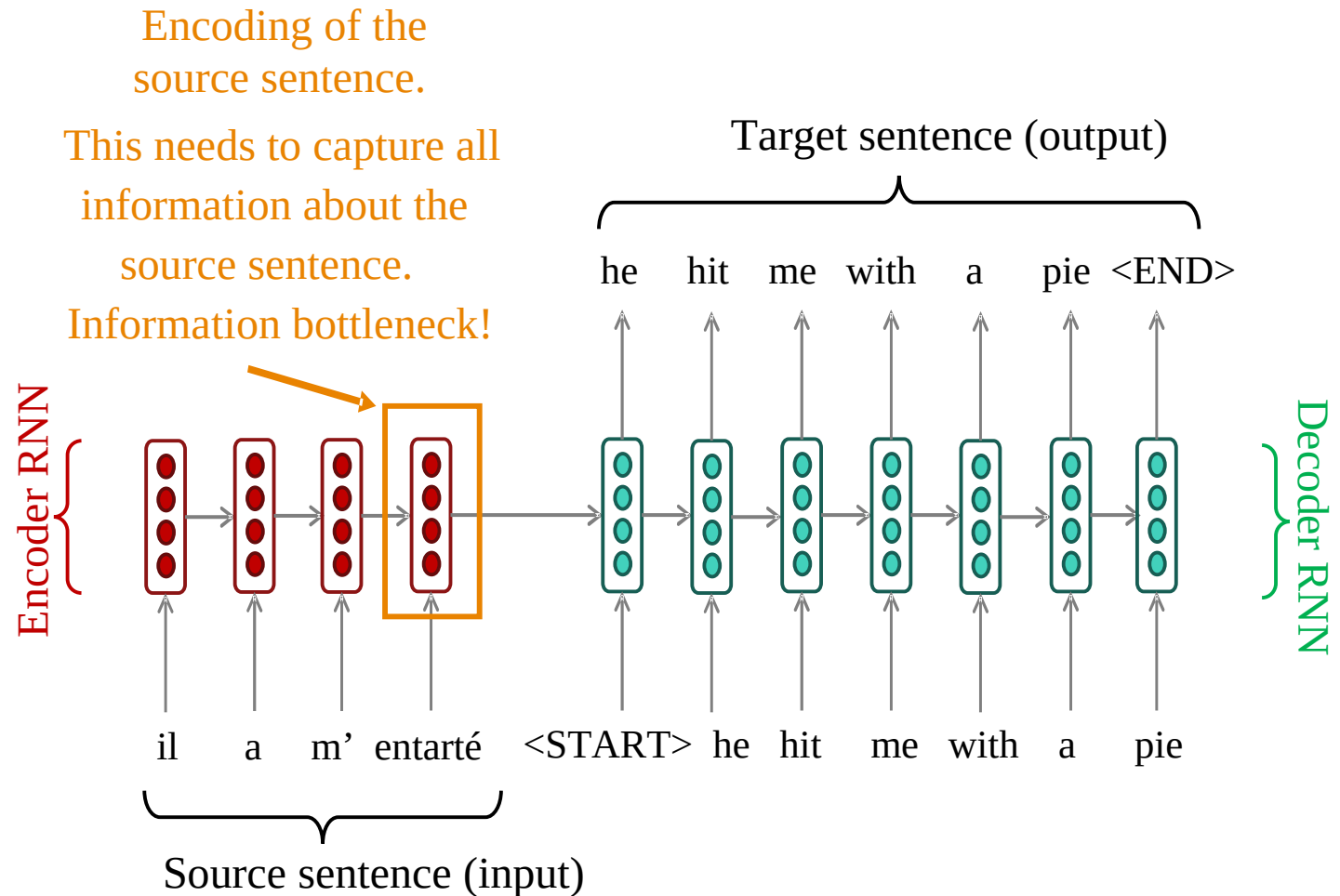
- Sequence-to-sequence is useful for more than just MT
- Many NLP tasks can be phrased as sequence-to-sequence:
  - Summarization (long text → short text)
  - Dialogue (previous utterances → next utterance)
  - Parsing (input text → output parse as sequence)
  - Code generation (natural language → Python code)

# Sequence-to-sequence: the bottleneck problem



Problems with this architecture?

# Sequence-to-sequence: the bottleneck problem

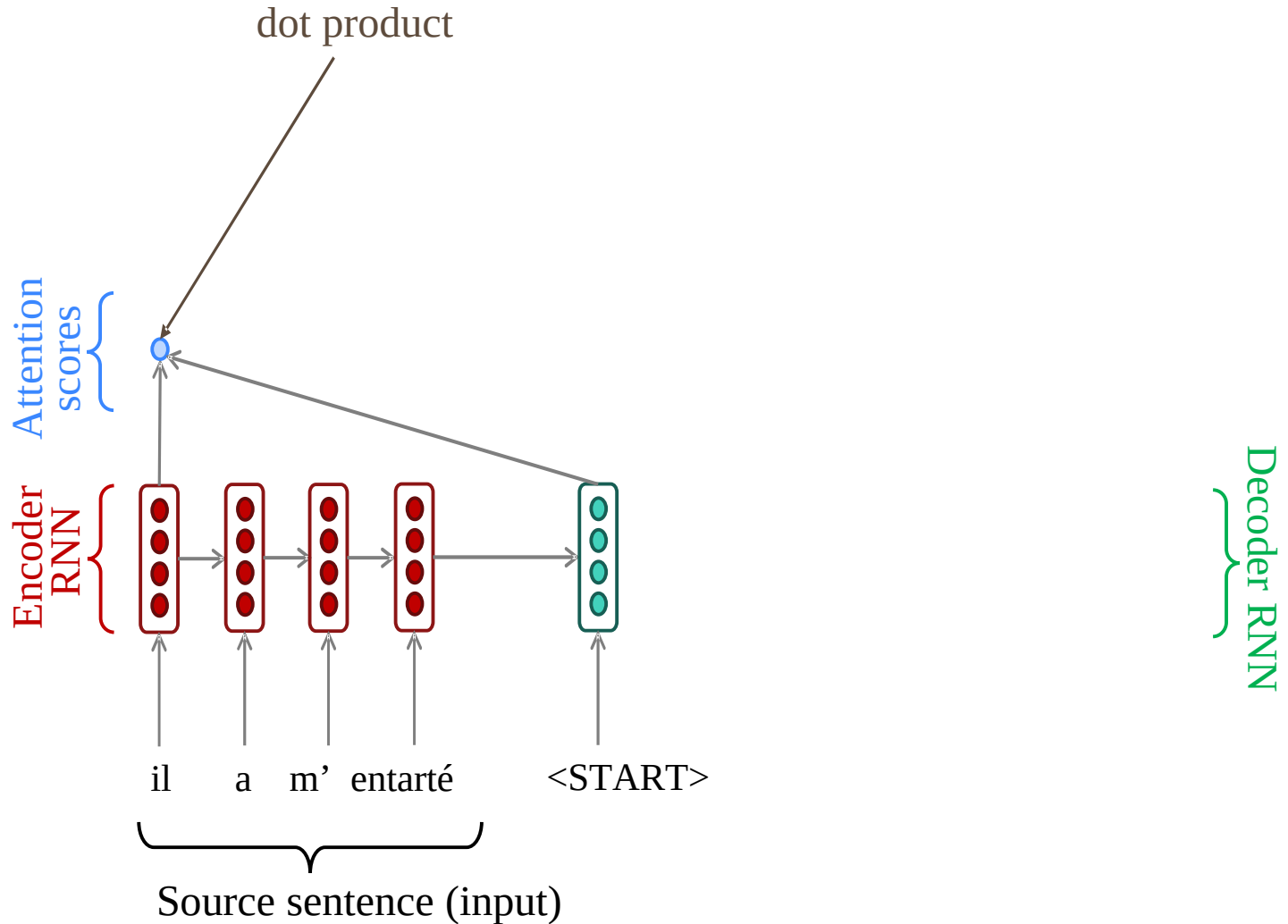


Problems with this architecture?

# Attention

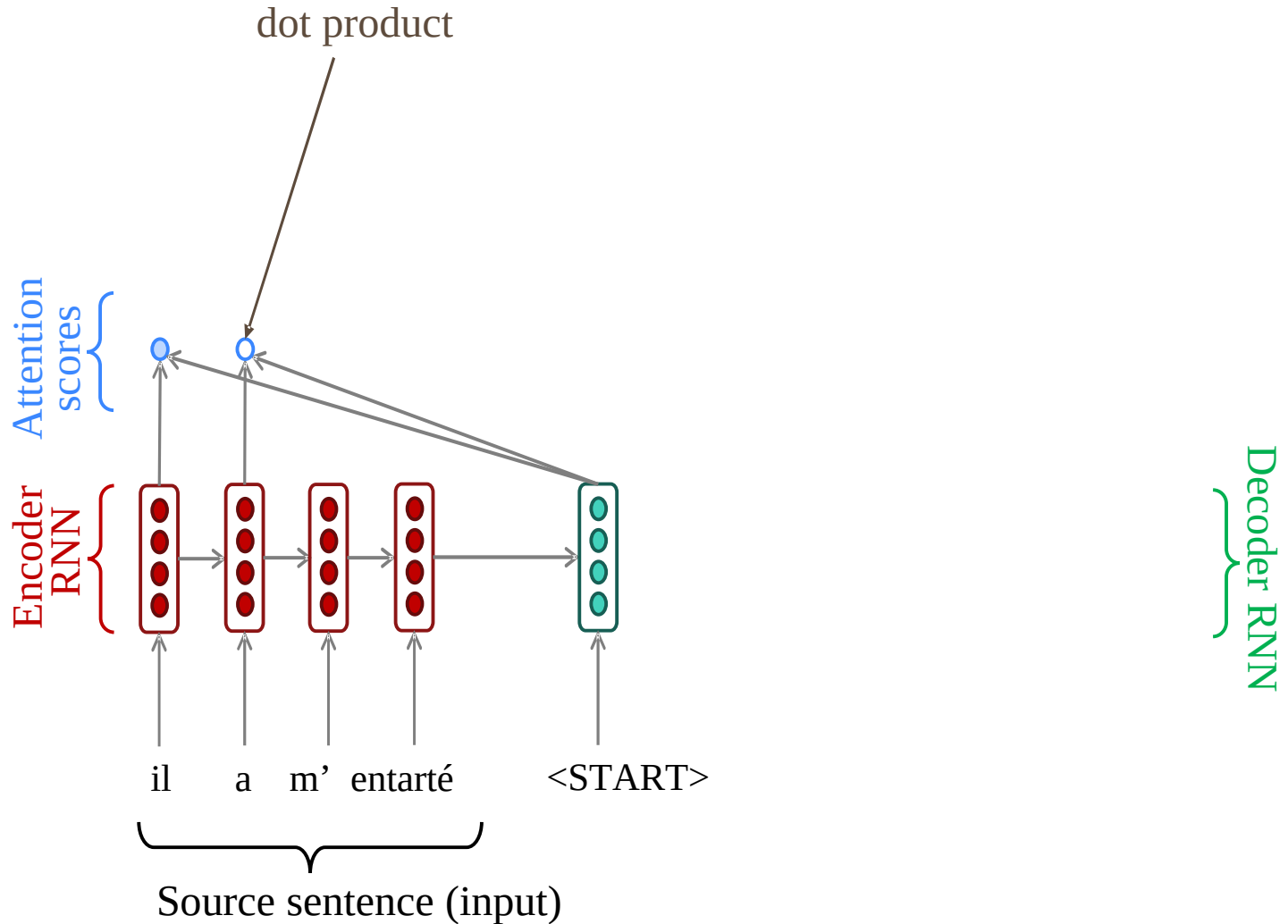
- **Attention** provides a solution to the bottleneck problem.
- Core idea: on each step of the decoder, use direct connection to the encoder to focus on a particular part of the source sequence.
- First, we will show via diagram (no equations), then we will show with equations.

# Sequence-to-sequence with attention

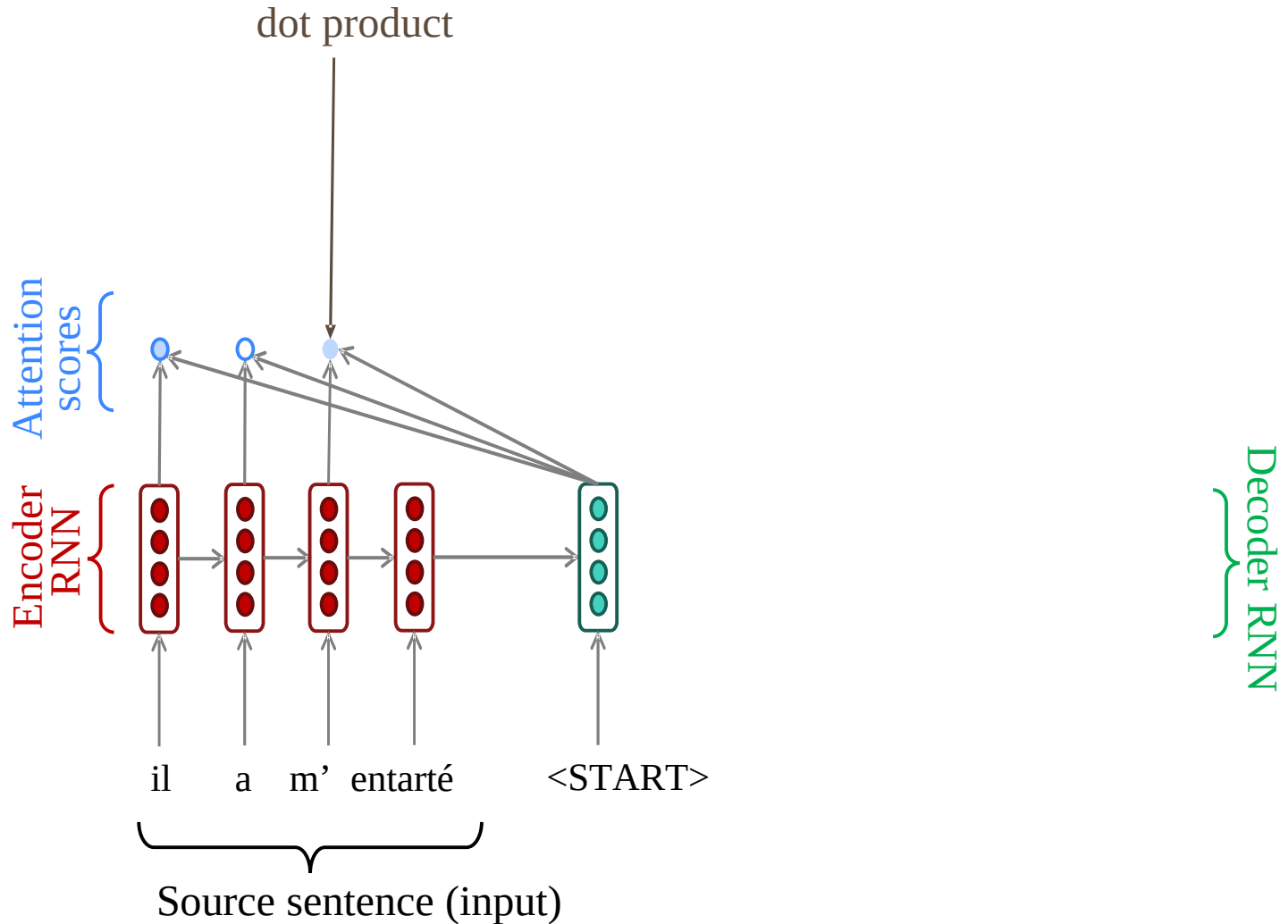




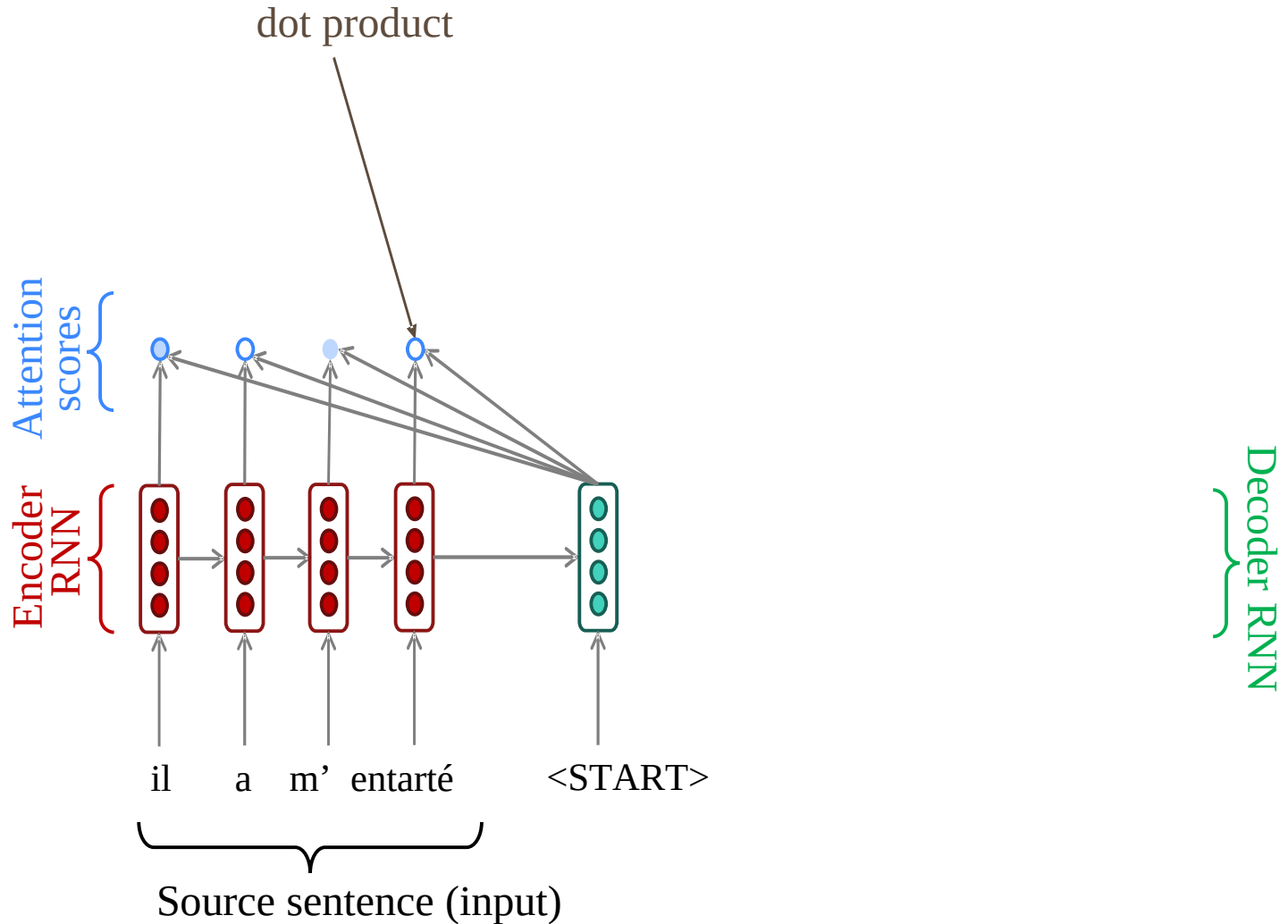
# Sequence-to-sequence with attention



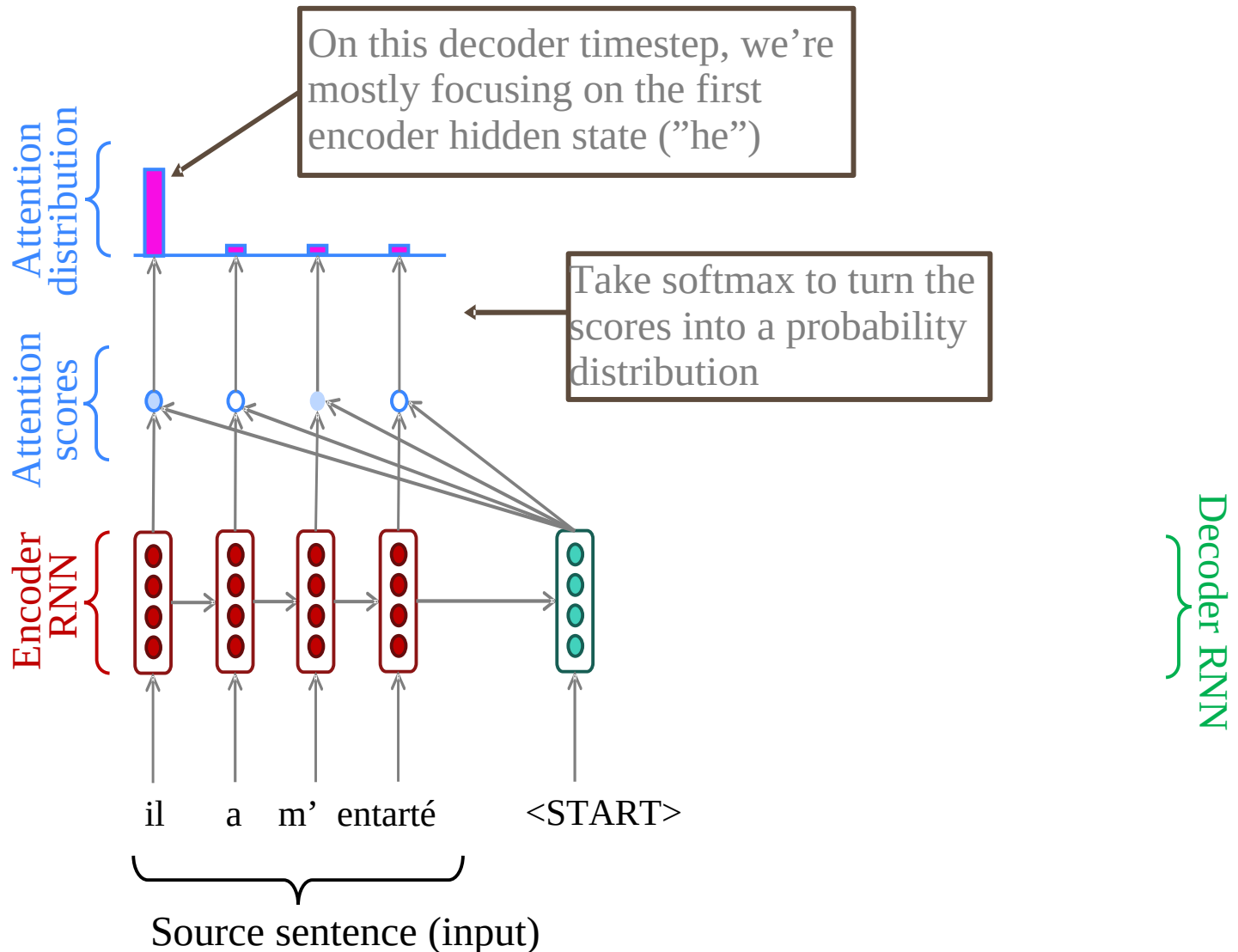
# Sequence-to-sequence with attention



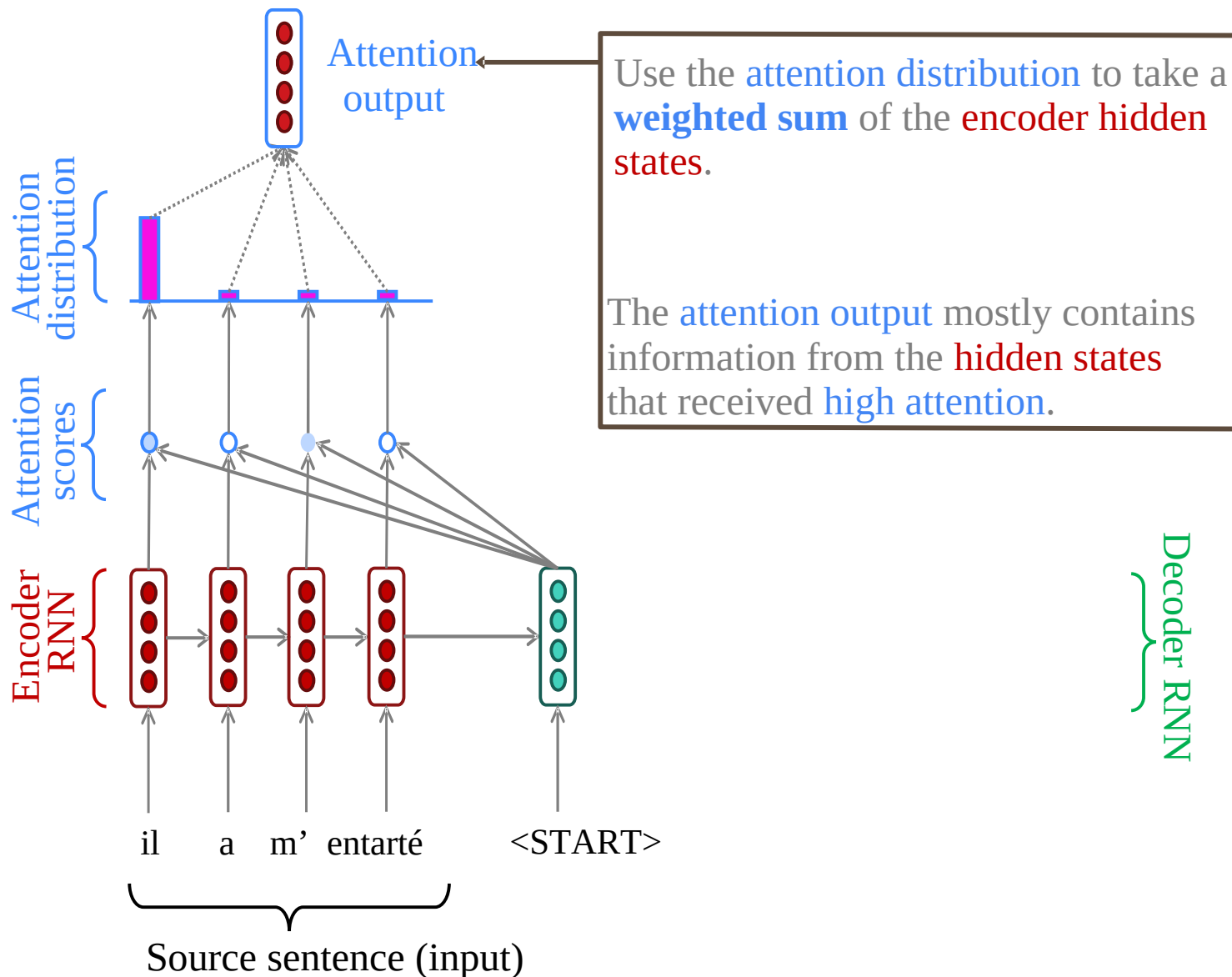
# Sequence-to-sequence with attention



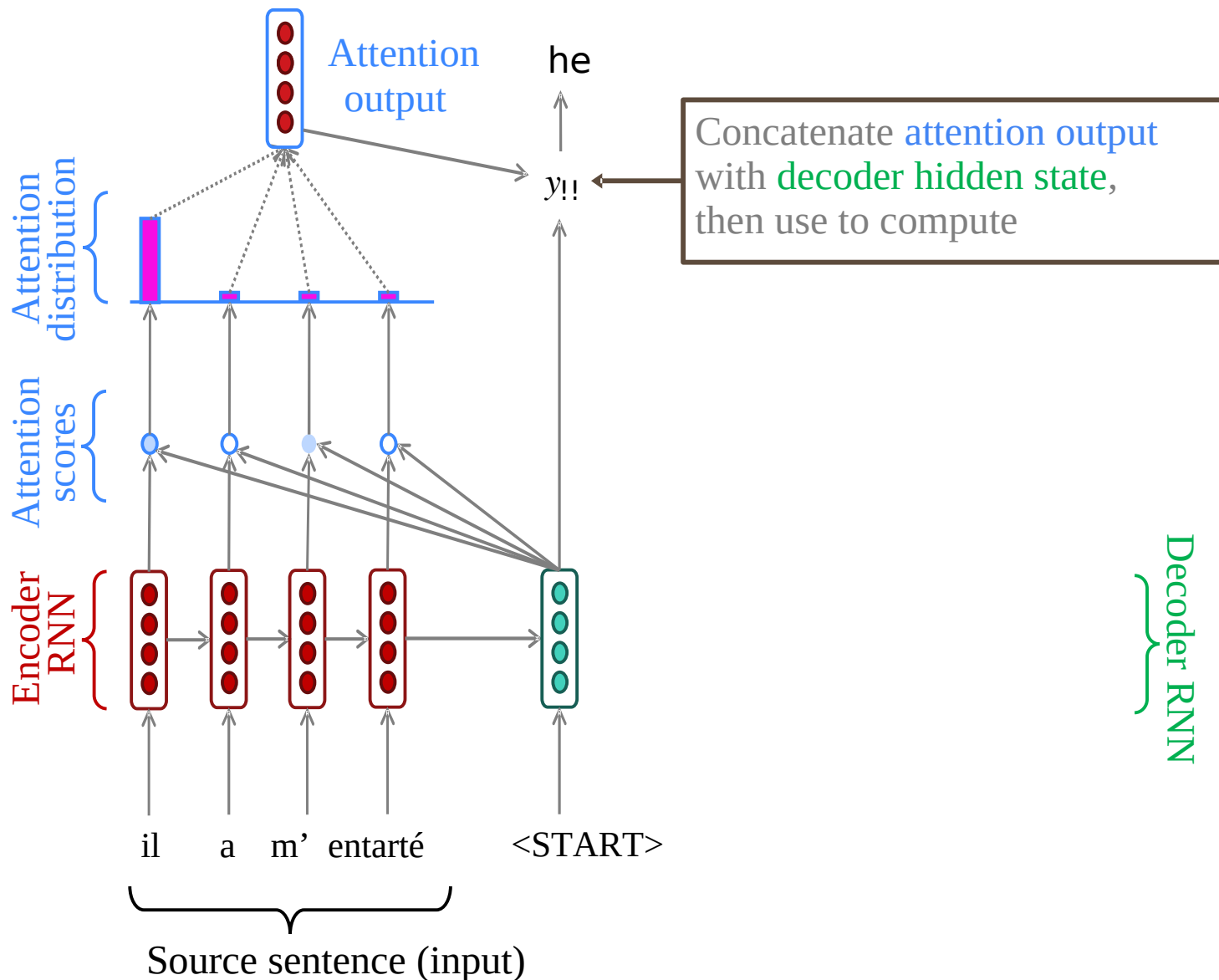
# Sequence-to-sequence with attention



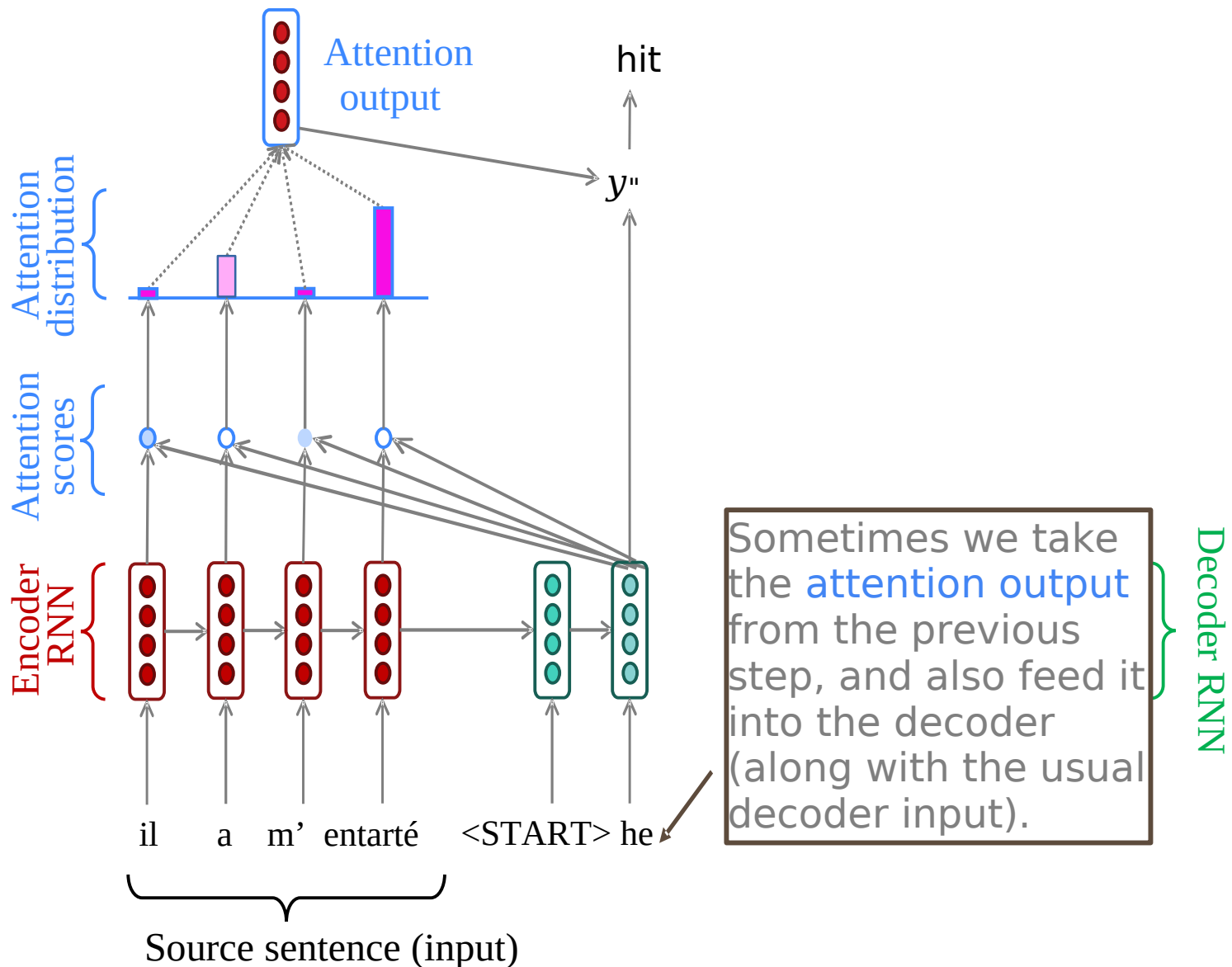
# Sequence-to-sequence with attention



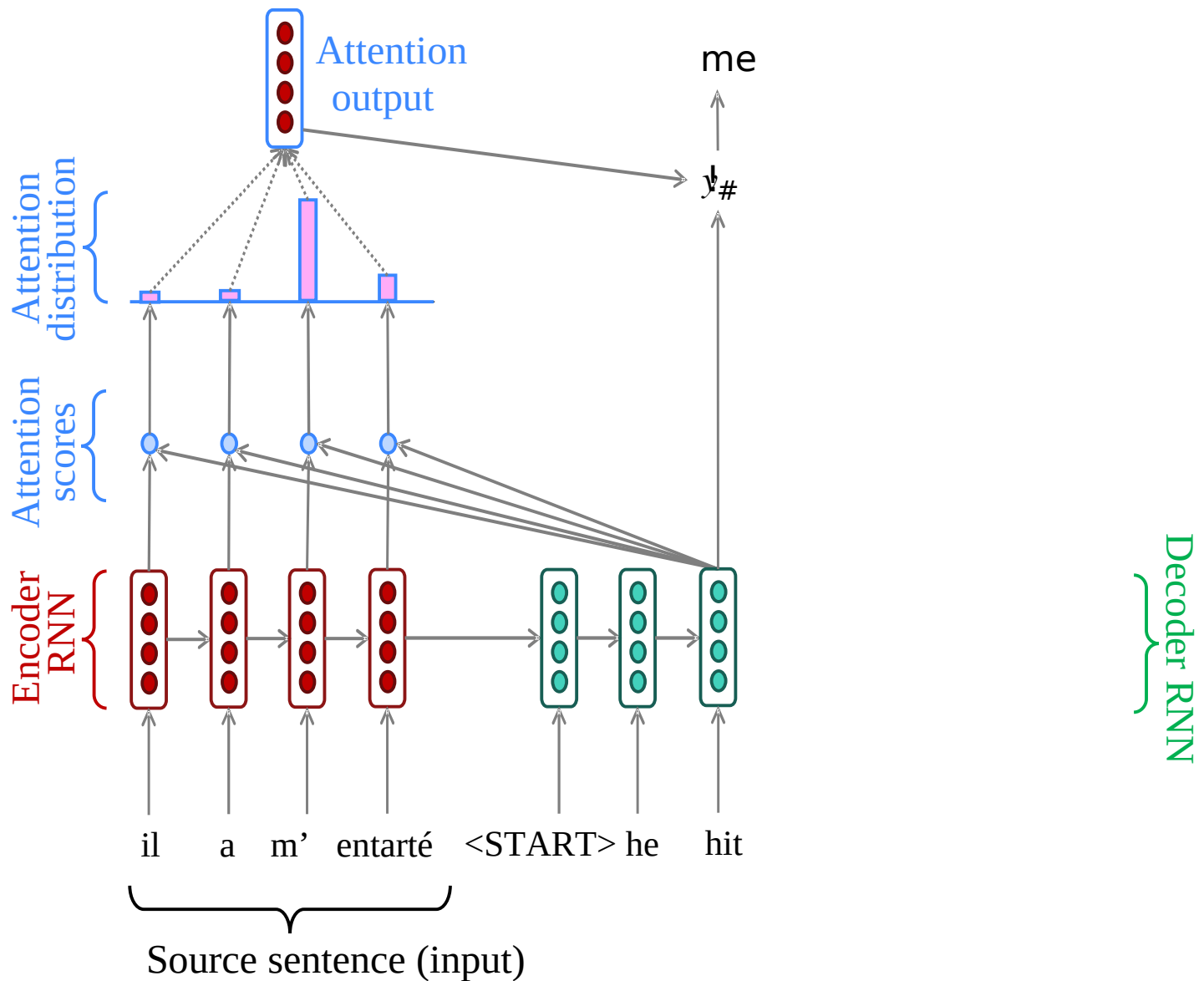
# Sequence-to-sequence with attention



# Sequence-to-sequence with attention

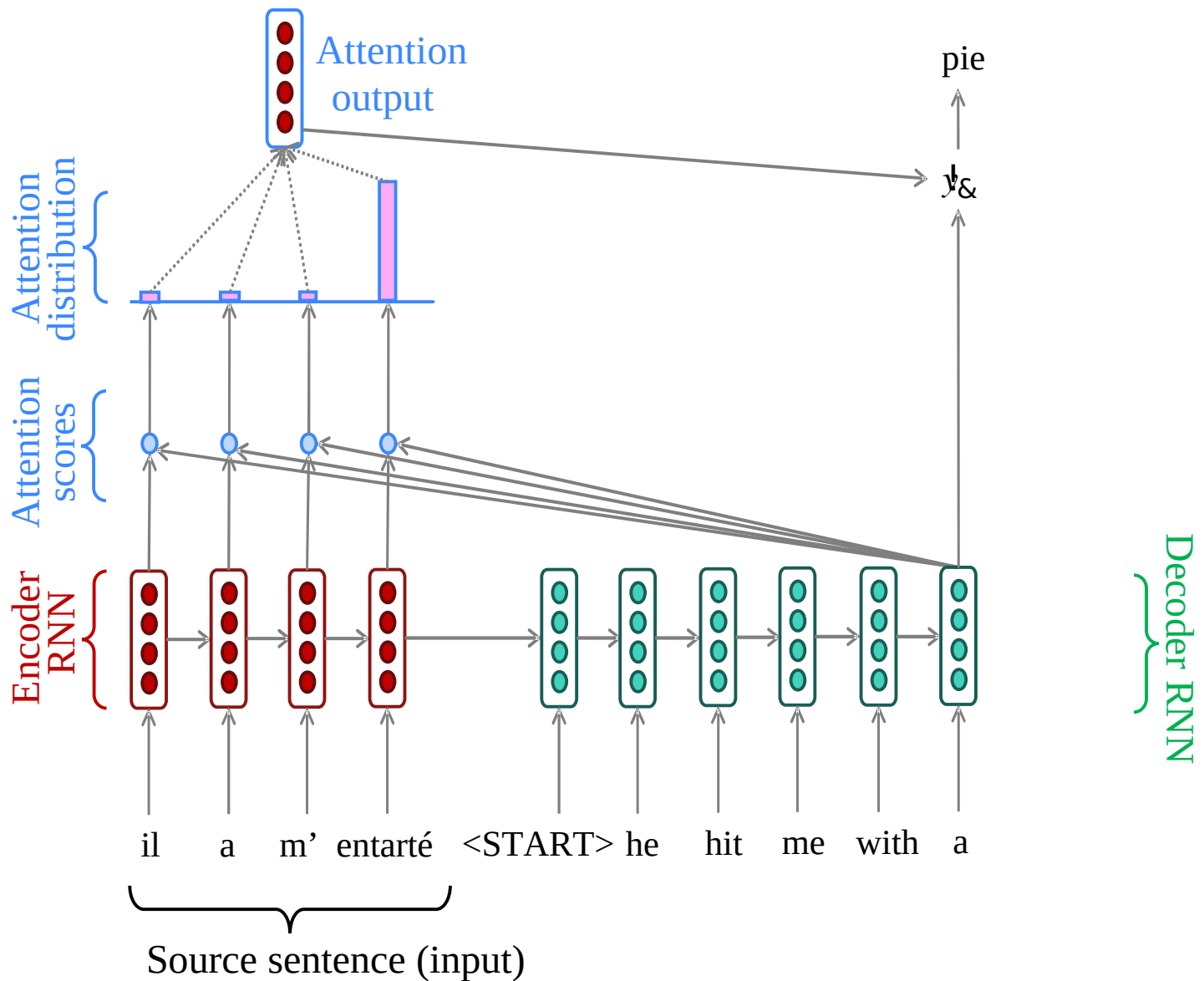


# Sequence-to-sequence with attention





# Sequence-to-sequence with attention



# Attention: in equations

- We have encoder hidden states  $h_1, \dots, h_N \in \mathbb{R}^h$
- On timestep  $t$ , we have decoder hidden  $s_t \in \mathbb{R}^h$
- We get the attention scores  $e^t = [s_t^T h_1, \dots, s_t^T h_N] \in \mathbb{R}^N$
- We take softmax to get the attention distribution  $\alpha^t = \text{softmax}(e^t) \in \mathbb{R}^N$  for this step (this is a probability distribution and sums to 1)
- We use  $\alpha^t = \text{softmax}(e^t) \in \mathbb{R}^N$  to take a weighted sum of the encoder hidden states to get the attention output

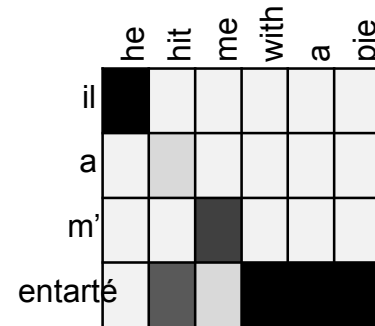
$$a_t = \sum_{i=1}^N \alpha_i^t h_i \in \mathbb{R}^h$$

- Finally we concatenate the attention output  $a_t = \sum_{i=1}^N \alpha_i^t h_i \in \mathbb{R}^h$  with the decoder hidden state  $s_t \in \mathbb{R}^h$  and proceed as in the non-attention seq2seq model

$$[a_t; s_t] \in \mathbb{R}^{2h}$$

# Attention is great

- Attention significantly **improves NMT performance**
  - It's very useful to allow decoder to focus on certain parts of the source
- Attention **solves the bottleneck problem**
  - Attention allows decoder to look directly at source; bypass bottleneck
- Attention **helps with vanishing gradient problem**
  - Provides shortcut to far away states
- Attention provides **some interpretability**
  - By inspecting attention distribution, we can see what the decoder was focusing on



# Attention is a general Deep Learning technique

## More general definition of attention:

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

## Intuition:

- The weighted sum is a **selective summary** of the information contained in the values, where the query determines which values to focus on.
- Attention is a way to obtain a **fixed-size representation** of an arbitrary set of representations (the values), dependent on some other representation (the query).

# There are several attention variants

- We have some values  $h_1, \dots, h_N \in \mathbb{R}^{d_1}$  and a query  $s \in \mathbb{R}^{d_2}$

- Attention always involves:

1. Computing the attention scores  $e \in \mathbb{R}^N$
2. Taking softmax to get attention distribution  $\alpha$

There are  
multiple ways  
to do this

$$\alpha = \text{softmax}(e) \in \mathbb{R}^N$$

3. Using attention distribution to take weighted sum of values:

$$a = \sum_{i=1}^N \alpha_i h_i \in \mathbb{R}^{d_1}$$

thus obtaining the attention output  $a$  (sometimes called the context vector)

# Attention variants

There are several ways you can compute  $e \in \mathbb{R}^N$  from  $h_1, \dots, h_N \in \mathbb{R}^{d_1}$  and  $s \in \mathbb{R}^{d_2}$

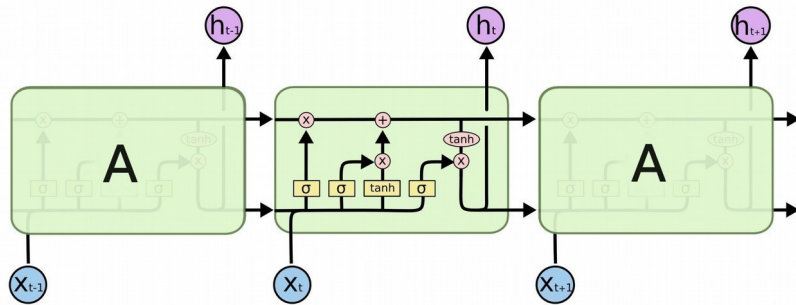
- Basic dot-product attention:  $e_i = s^T h_i \in \mathbb{R}$ 
  - Note: this assumes  $d_1 = d_2$
  - This is the version we saw earlier
- Multiplicative attention:  $e_i = s^T W h_i \in \mathbb{R}$ 
  - Where  $W \in \mathbb{R}^{d_2 \times d_1}$  is a weight matrix
- Additive attention:  $e_i = v^T \tanh(W_1 h_i + W_2 s) \in \mathbb{R}$ 
  - Where  $W_1 \in \mathbb{R}^{d_3 \times d_1}, W_2 \in \mathbb{R}^{d_3 \times d_2}$  are weight matrices and  $v \in \mathbb{R}^{d_3}$  is a weight vector.
  - $d$ (the attention dimensionality) is a hyperparameter

**More information:** “Deep Learning for NLP Best Practices”, Ruder, 2017. <http://ruder.io/deep-learning-nlp-best-practices/index.html#attention>

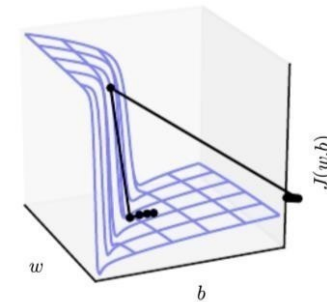
“Massive Exploration of Neural Machine Translation Architectures”, Britz et al, 2017, <https://arxiv.org/pdf/1703.03906.pdf>

# In summary

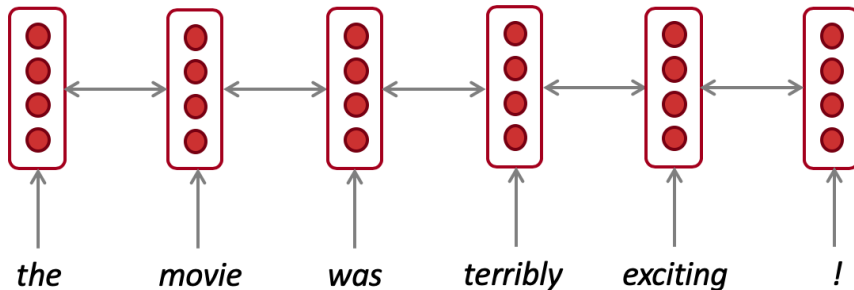
Lots of new information today! What are the **practical takeaways**?



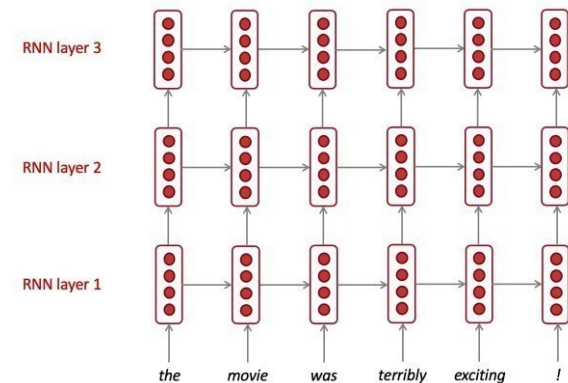
1. LSTMs are powerful but GRUs are faster



2. Clip your gradients



3. Use bidirectionality when possible



4. Multi-layer RNNs are powerful, but you might need skip/dense-connections if it's deep

5. **Attention** is a way to focus on particular parts of the input
- Improves sequence-to-sequence a lot!



**Thanks!**