Natural Language Processing with Deep Learning

Lecture 5: Fancy Recurrent Neural Networks

Lecture Plan

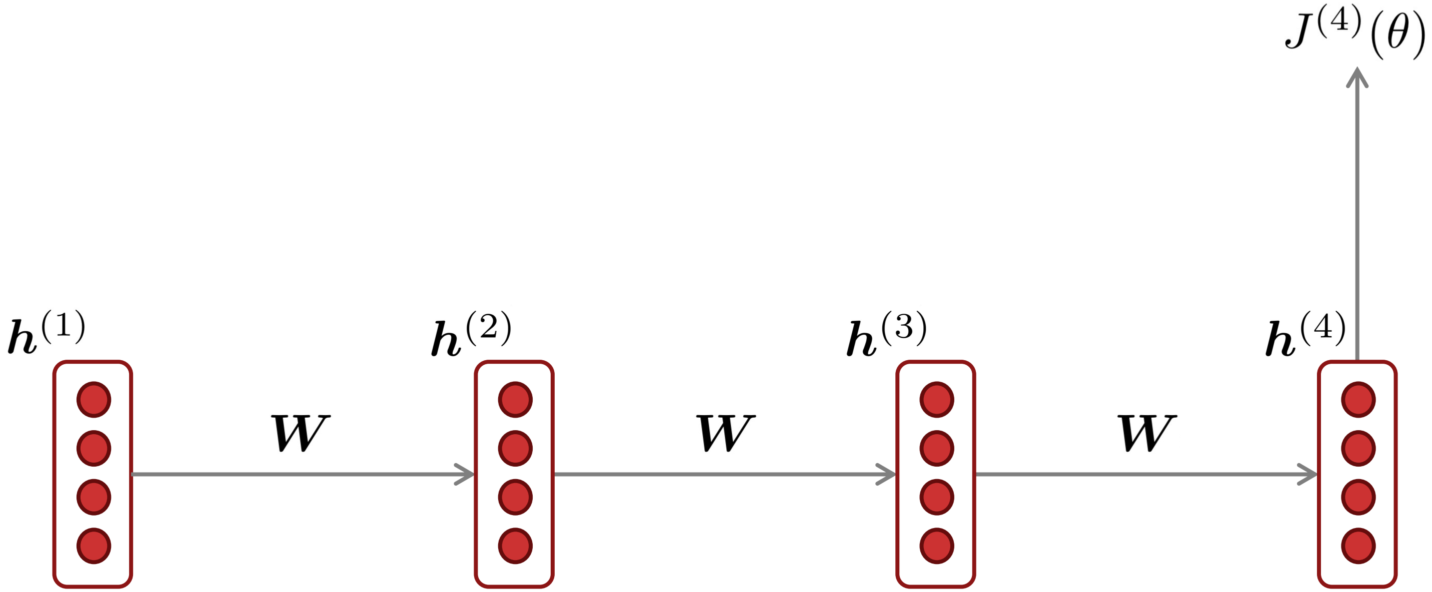
1. Exploding and vanishing gradients
2. LSTMs
3. Bidirectional and multi-layer RNNs

Overview

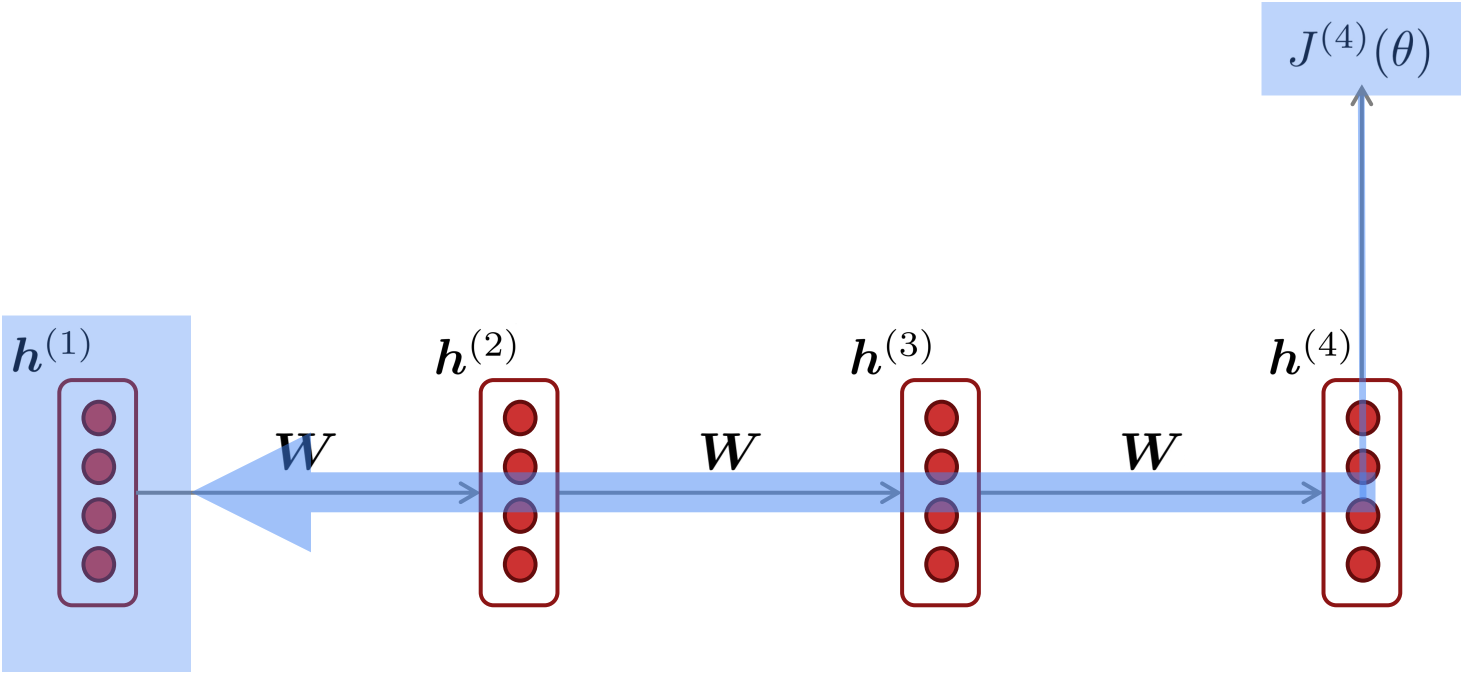
- Last lecture we learned:
  - Language models, n-gram language models, and Recurrent Neural Networks (RNNs)

- Today we'll learn how to get RNNs to work for you
  - Problems with RNNs (exploding and vanishing gradients) and how to fix them
  - These problems motivate a more sophisticated RNN architecture: LSTMs
  - And other more complex RNN options: bidirectional RNNs and multi-layer RNNs

1. Problems with RNNs: Vanishing and Exploding Gradients

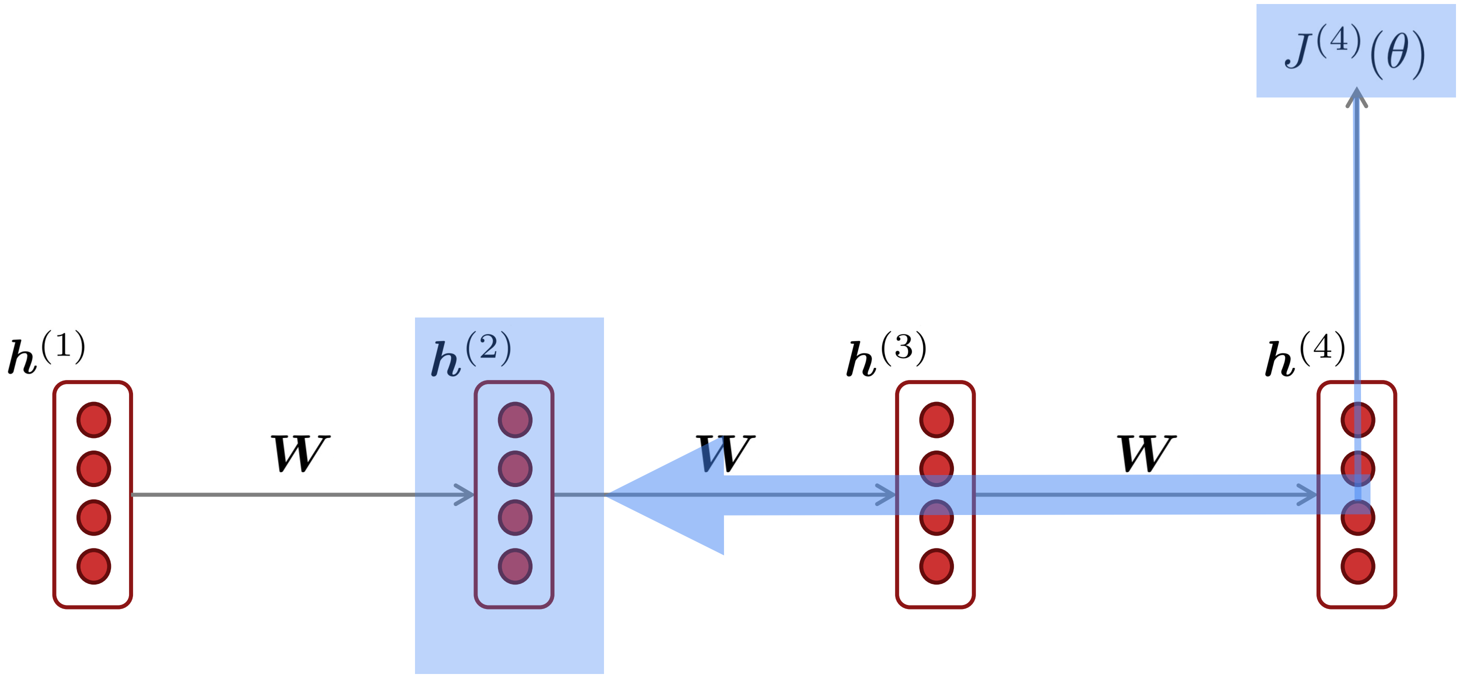


Vanishing gradient intuition



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

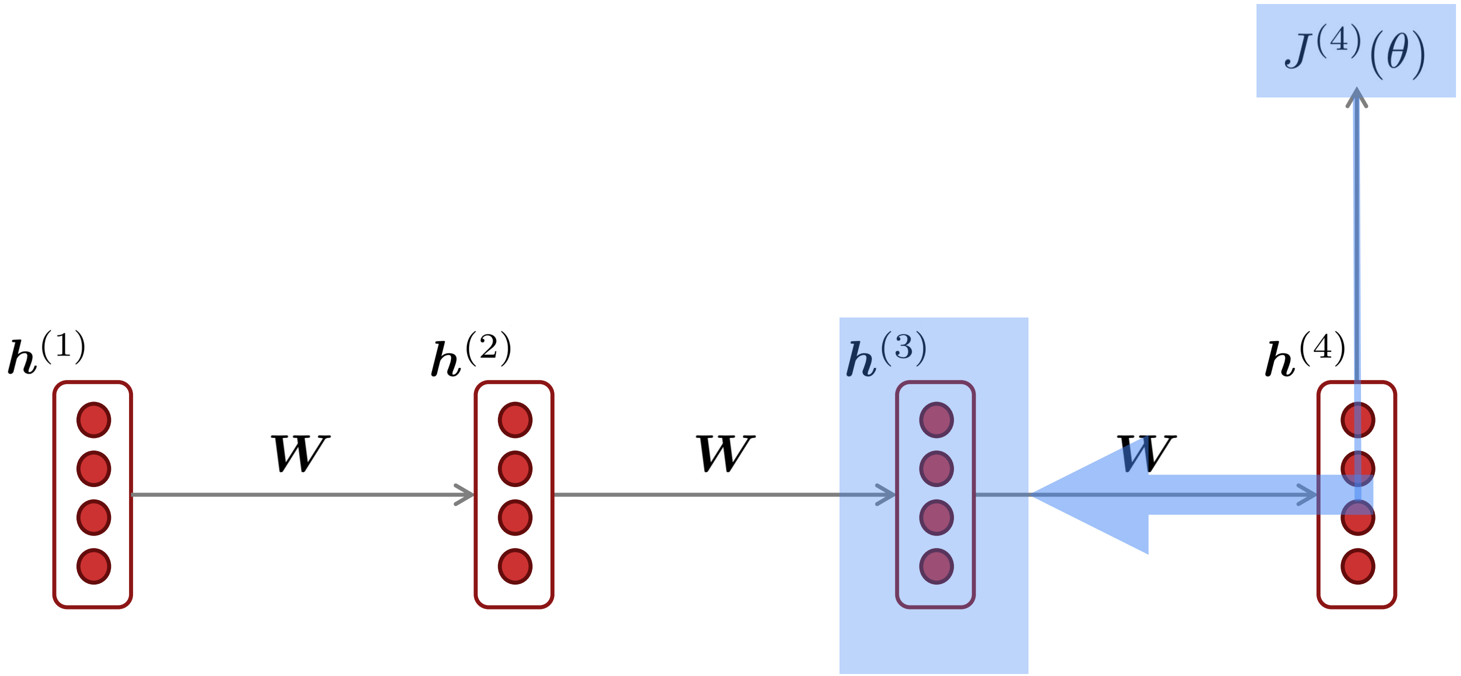
Vanishing gradient intuition



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

chain rule!

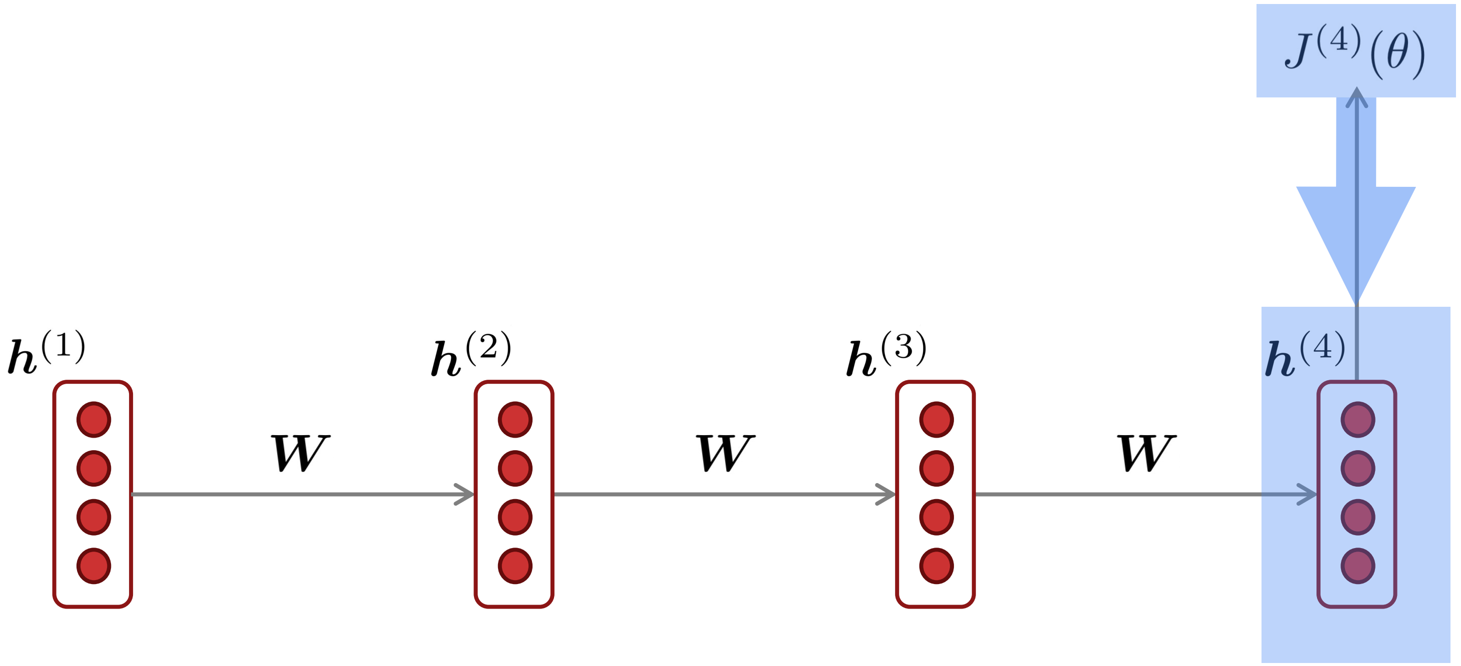
Vanishing gradient intuition



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

chain rule!

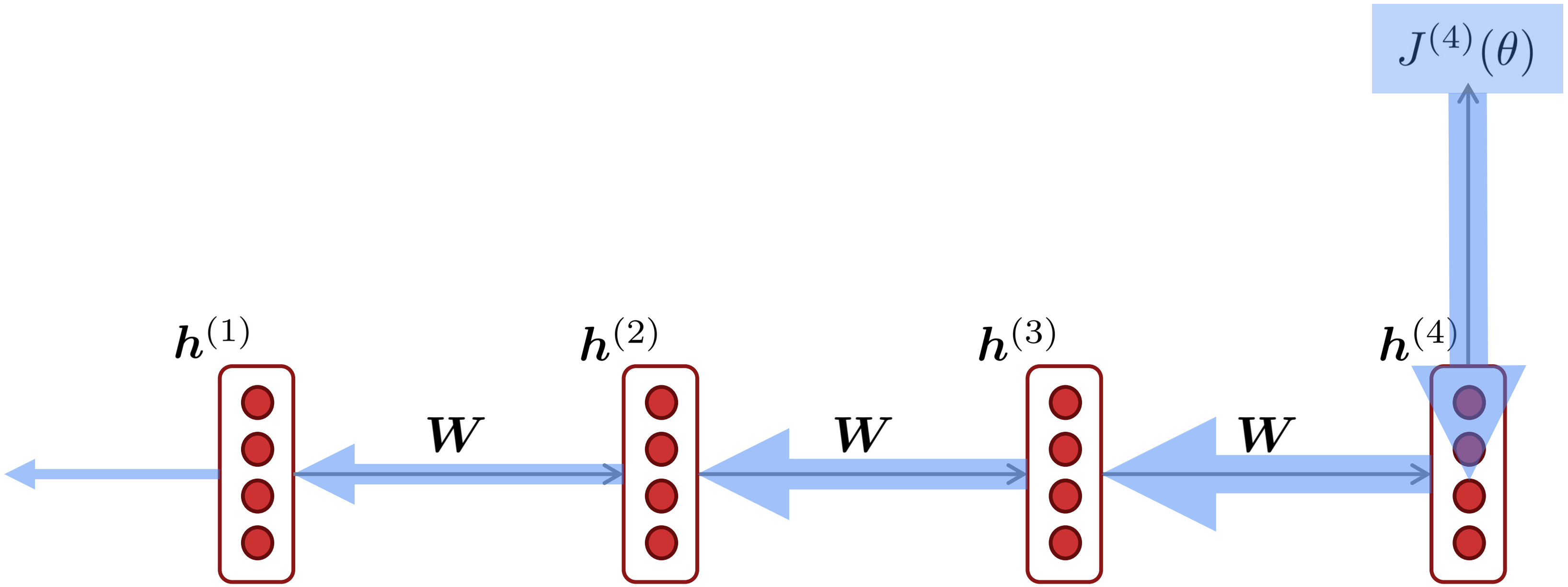
Vanishing gradient intuition



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

chain rule!

Vanishing gradient intuition



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

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 (linear case)

- Recall: $$\boldsymbol{h}^{(t)} = \sigma\left(\boldsymbol{W}_h \boldsymbol{h}^{(t-1)} + \boldsymbol{W}_x \boldsymbol{x}^{(t)} + \boldsymbol{b}_1\right)$$
- What if σ were the identity function, $\sigma(x) = x$?

$$\frac{\partial \boldsymbol{h}^{(t)}}{\partial \boldsymbol{h}^{(t-1)}} = \operatorname{diag}\left(\sigma'\left(\boldsymbol{W}_h \boldsymbol{h}^{(t-1)} + \boldsymbol{W}_x \boldsymbol{x}^{(t)} + \boldsymbol{b}_1\right)\right)\boldsymbol{W}_h \qquad \text{(chain rule)}$$

$$= \boldsymbol{I}\ \boldsymbol{W}_h = \boldsymbol{W}_h$$

- Consider the gradient of the loss $J^{(i)}(\theta)$ on step i, with respect to the hidden state $\boldsymbol{h}^{(j)}$ on some previous step j. *Let* $\ell = i - j$

$$\frac{\partial J^{(i)}(\theta)}{\partial \boldsymbol{h}^{(j)}} = \frac{\partial J^{(i)}(\theta)}{\partial \boldsymbol{h}^{(i)}} \prod_{j<t\leq i} \frac{\partial \boldsymbol{h}^{(t)}}{\partial \boldsymbol{h}^{(t-1)}} \qquad \text{(chain rule)}$$

$$= \frac{\partial J^{(i)}(\theta)}{\partial \boldsymbol{h}^{(i)}} \prod_{j<t\leq i} \boldsymbol{W}_h = \frac{\partial J^{(i)}(\theta)}{\partial \boldsymbol{h}^{(i)}} \boxed{\boldsymbol{W}_h^{\ell}} \qquad \text{(value of } \frac{\partial \boldsymbol{h}^{(t)}}{\partial \boldsymbol{h}^{(t-1)}}\text{)}$$

If W_h is “small”, then this term gets exponentially problematic as ℓ becomes large

Source: “On the difficulty of training recurrent neural networks”, Pascanu et al, 2013. http://proceedings.mlr.press/v28/pascanu13.pdf (and supplemental materials), at http://proceedings.mlr.press/v28/pascanu13-supp.pdf

Vanishing gradient proof sketch (linear case)

- What's wrong with $\boldsymbol{W}_h^\ell$?
- Consider if the eigenvalues of $\boldsymbol{W}_h$ are $\underbrace{\text{all less than 1}}_{\text{sufficient but not necessary}}$:

$$\lambda_1, \lambda_2, \ldots, \lambda_n < 1$$
$$\boldsymbol{q}_1, \boldsymbol{q}_2, \ldots, \boldsymbol{q}_n \text{ (eigenvectors)}$$

- We can write $\frac{\partial J^{(i)}(\theta)}{\partial \boldsymbol{h}^{(i)}} \boldsymbol{W}_h^\ell$ using the eigenvectors of $\boldsymbol{W}_h$ as a basis:

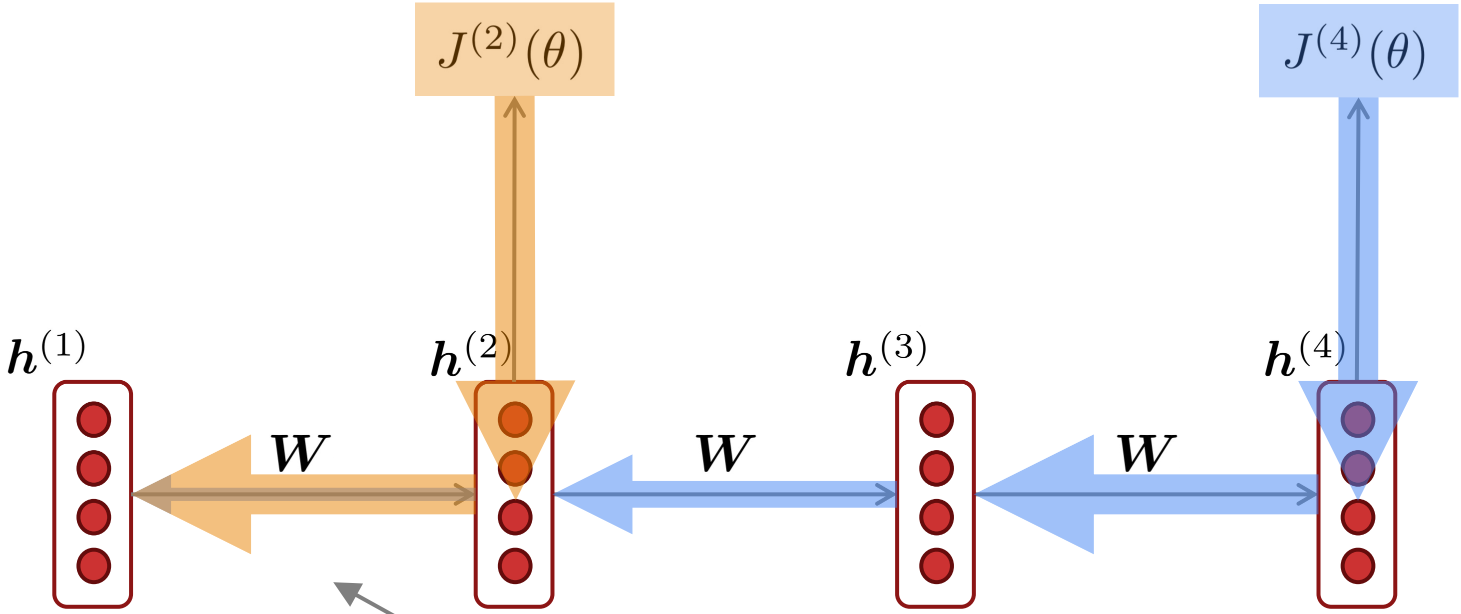
$$\frac{\partial J^{(i)}(\theta)}{\partial \boldsymbol{h}^{(i)}} \boldsymbol{W}_h^\ell = \sum_{i=1}^{n} c_i \boxed{\lambda_i^\ell} \boldsymbol{q}_i \approx \boldsymbol{0} \text{ (for large } \ell)$$

Approaches 0 as ℓ grows, so gradient vanishes

- What about nonlinear activations σ (i.e., what we use?)
  - Pretty much the same thing, except the proof requires $\lambda_i < \gamma$ for some γ dependent on dimensionality and σ

Source: "On the difficulty of training recurrent neural networks", Pascanu et al, 2013. http://proceedings.mlr.press/v28/pascanu13.pdf (and supplemental materials), at http://proceedings.mlr.press/v28/pascanu13-supp.pdf

Why is vanishing gradient a problem?



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

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

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 7th step and the target word *"tickets"* at the end.

- But if the gradient is small, the model can't learn this dependency
  - So, the model is unable to predict similar long-distance dependencies at test time

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 weird and bad parameter configuration (with large loss)
  - You think you've found a hill to climb, but suddenly you're in Iowa

- 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

Algorithm 1 Pseudo-code for norm clipping

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

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

- In practice, remembering to clip gradients is important, but exploding gradients are an easy problem to solve

Source: "On the difficulty of training recurrent neural networks", Pascanu et al, 2013. http://proceedings.mlr.press/v28/pascanu13.pdf

How to fix the 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

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

- How about an RNN with separate memory which is added to?

2. Long Short-Term Memory RNNs (LSTMs)

- A type of RNN proposed by Hochreiter and Schmidhuber in 1997 as a solution to the vanishing gradients problem.
  - Everyone cites that paper but really a crucial part of the modern LSTM is from Gers et al. (2000) 💜

- On step *t*, there is a hidden state $\boldsymbol{h}^{(t)}$ *and* a cell state $\boldsymbol{c}^{(t)}$
  - Both are vectors length *n*
  - The cell stores long-term information
  - The LSTM can read, erase, and write information from the cell
    - The cell becomes conceptually rather like RAM in a computer

- The selection of which information is erased/written/read is controlled by three corresponding gates
  - The gates are also vectors of 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", Hochreiter and Schmidhuber, 1997. https://www.bioinf.jku.at/publications/older/2604.pdf
"Learning to Forget: Continual Prediction with LSTM", Gers, Schmidhuber, and Cummins, 2000. https://dl.acm.org/doi/10.1162/089976600300015015

Long Short-Term Memory (LSTM)

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

Sigmoid function: all gate values are between 0 and 1

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

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

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

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

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

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

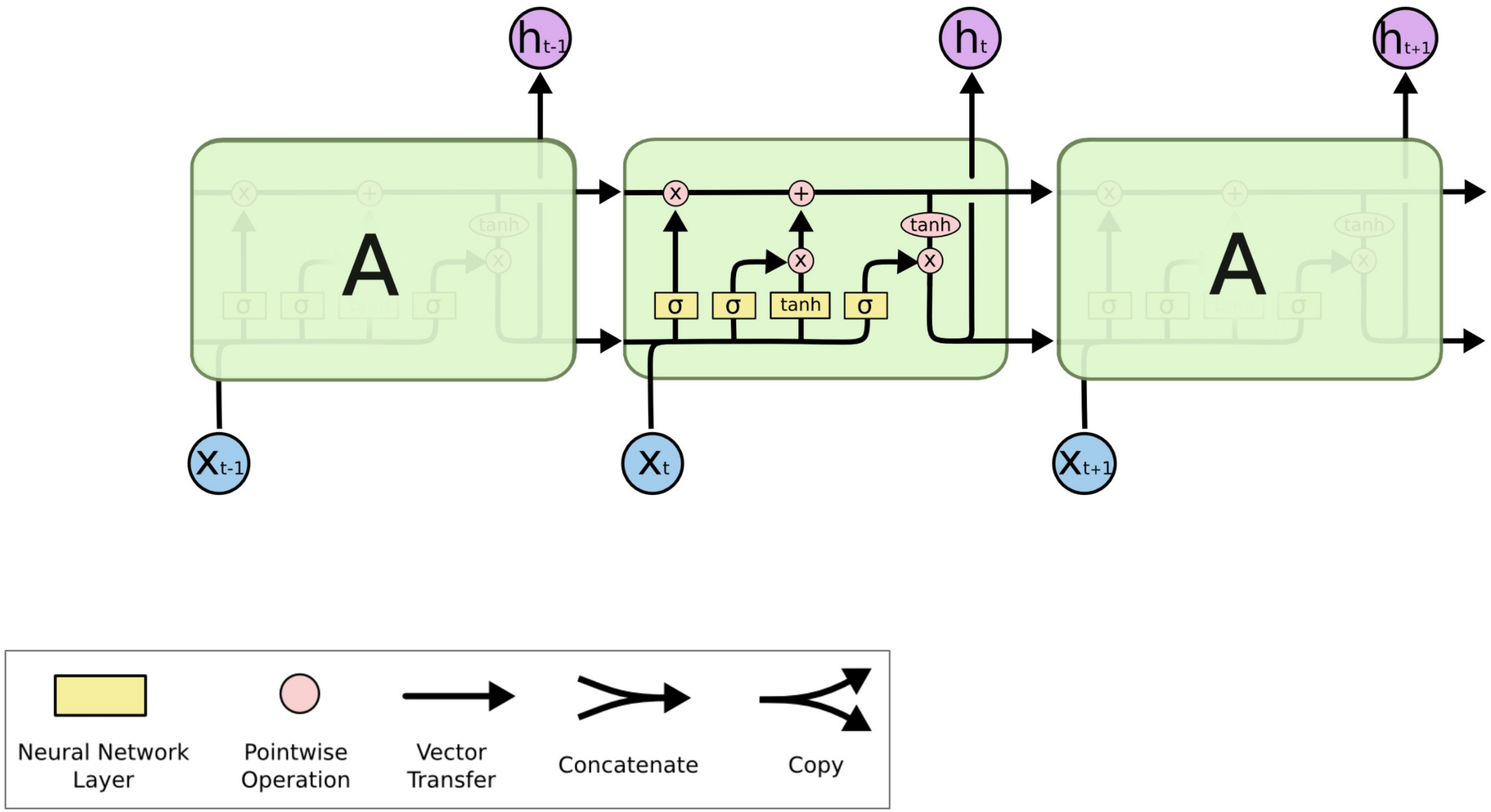
$$\boldsymbol{h}^{(t)} = \boldsymbol{o}^{(t)} \circ \tanh \boldsymbol{c}^{(t)}$$

All these are vectors of same length *n*

Gates are applied using element-wise (or Hadamard) product: $\odot$

Long Short-Term Memory (LSTM)

You can think of the LSTM equations visually like this:



Source: http://colah.github.io/posts/2015-08-Understanding-LSTMs/

Long Short-Term Memory (LSTM)

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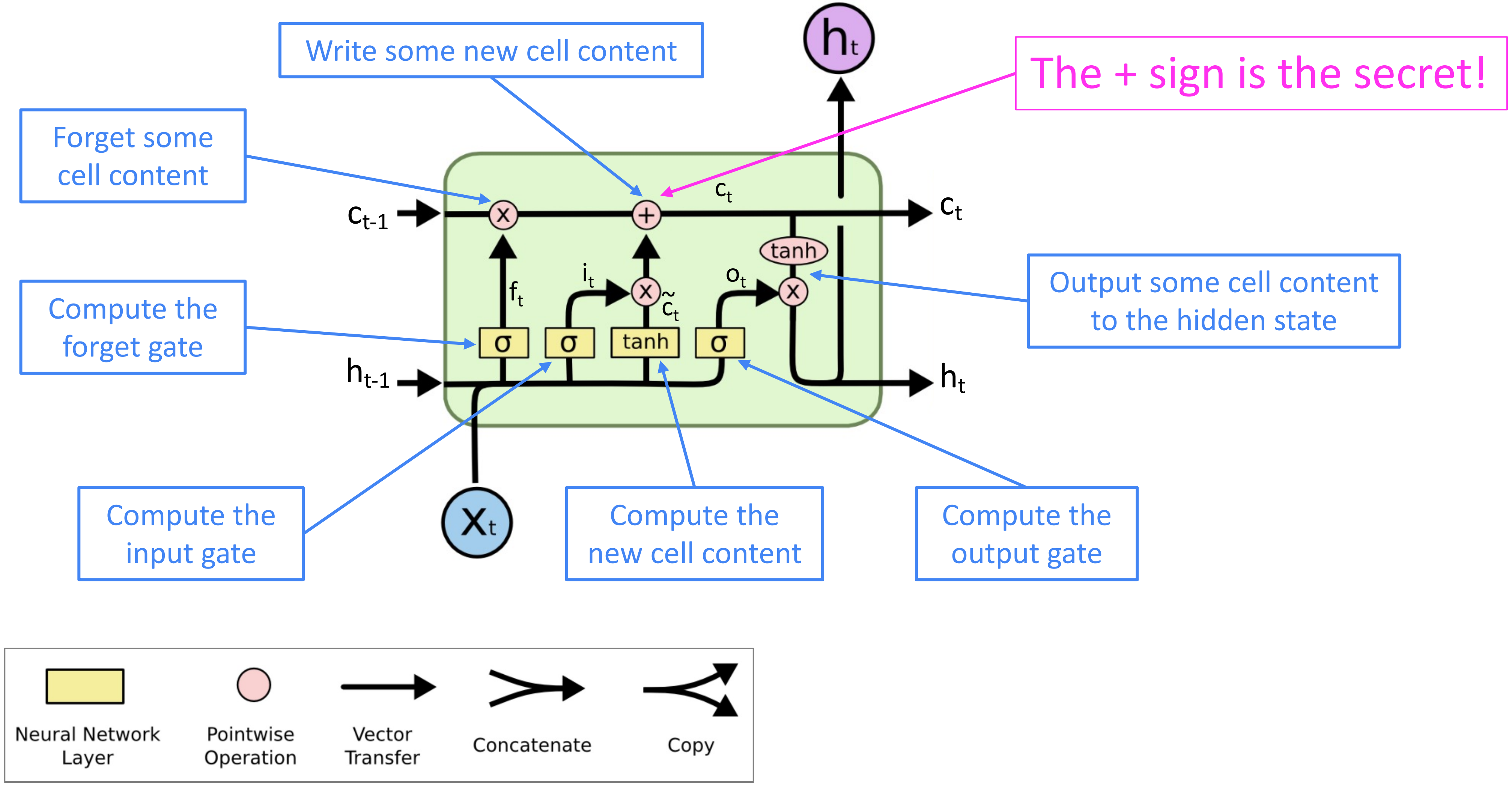


Source: http://colah.github.io/posts/2015-08-Understanding-LSTMs/

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 $\boldsymbol{x}^{(t)}$ and hidden state $\boldsymbol{h}^{(t)}$ (no cell state).

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

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

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

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

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

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

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

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

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)

"Learning Phrase Representations using RNN Encoder–Decoder for Statistical Machine Translation", Cho et al. 2014, https://arxiv.org/pdf/1406.1078v3.pdf

LSTM vs GRU

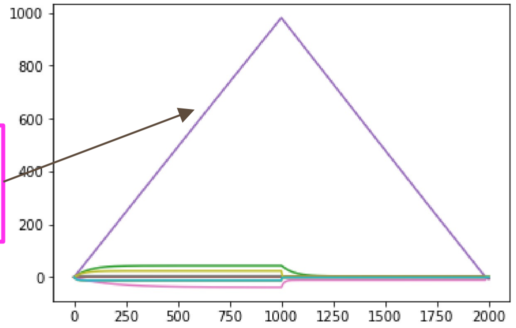
- Researchers have proposed many gated RNN variants, but LSTM and GRU are the most widely-used

- <u>Rule of thumb:</u> LSTM is a good default choice (especially if your data has particularly long dependencies, or you have lots of training data); Switch to GRUs for speed and fewer parameters.

- **Note**: LSTMs can store unboundedly* large values in memory cell dimensions, and relatively easily learn to count. (Unlike GRUs.)

LSTM

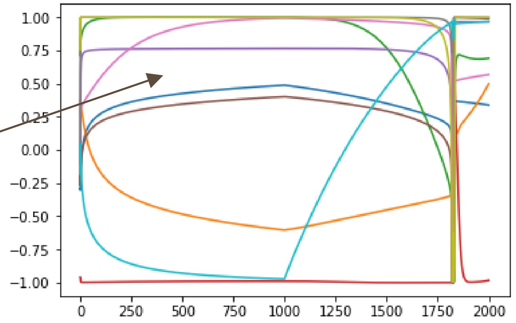
Single dimension used as counter



(a) $a^n b^n$-LSTM on $a^{1000}b^{1000}$

GRU

???



(c) $a^n b^n$-GRU on $a^{1000}b^{1000}$

*bounded if assuming finite precision, but still, large

<u>Source:</u> "On the Practical Computational Power of Finite Precision RNNs for Language Recognition", Weiss et al., 2018. https://arxiv.org/pdf/1805.04908.pdf

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 1 for a cell dimension and the input gate set to 0, then the information of that cell is preserved indefinitely.
  - In contrast, it's harder for a vanilla RNN to learn a recurrent weight matrix W_h that preserves info in the hidden state
  - In practice, you get about 100 timesteps rather than about 7

- 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, and image captioning, as well as language models
  - LSTMs became the dominant approach for most NLP tasks

- Now (2019–2022), other approaches (e.g., Transformers) have become dominant for many tasks
  - For example, in **WMT** (a Machine Translation conference + competition):
    - In WMT 2014, there were 0 neural machine translation systems (!)
    - In WMT 2016, the summary report contains "RNN" 44 times (and these systems won)
    - In WMT 2019: "RNN" 7 times, "Transformer" 105 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
Source: "Findings of the 2019 Conference on Machine Translation (WMT19)", Barrault et al. 2019, http://www.statmt.org/wmt18/pdf/WMT028.pdf

Is vanishing/exploding gradient just a RNN problem?

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

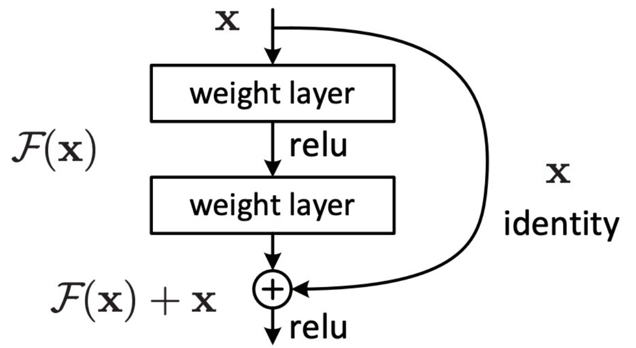


Figure 2. Residual learning: a building block.

"Deep Residual Learning for Image Recognition", He et al, 2015. https://arxiv.org/pdf/1512.03385.pdf

Is vanishing/exploding gradient just a RNN problem?

Other methods:

- Dense connections aka "DenseNet"
- Directly connect each layer to all future layers!

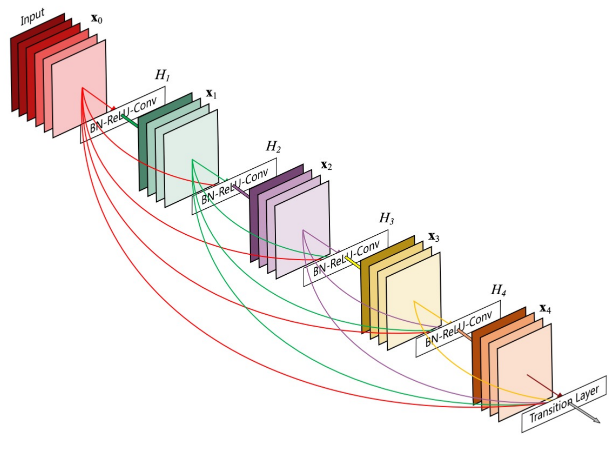
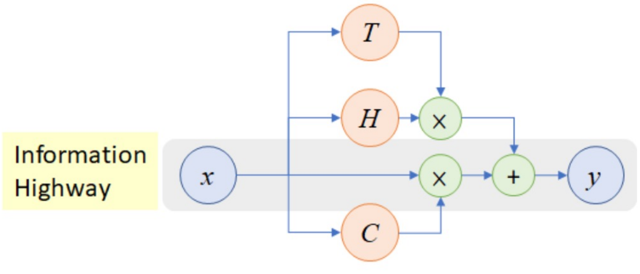


Figure 1: A 5-layer dense block with a growth rate of $k = 4$. Each layer takes all preceding feature-maps as input.

- Highway connections aka "HighwayNet"
- Similar to residual connections, but the identity connection vs the transformation layer is controlled by a dynamic gate
- Inspired by LSTMs, but applied to deep feedforward/convolutional networks



Highway Circuit

- **Conclusion**: Though vanishing/exploding gradients are a general problem, RNNs are particularly unstable due to the repeated multiplication by the same weight matrix [Bengio et al, 1994]

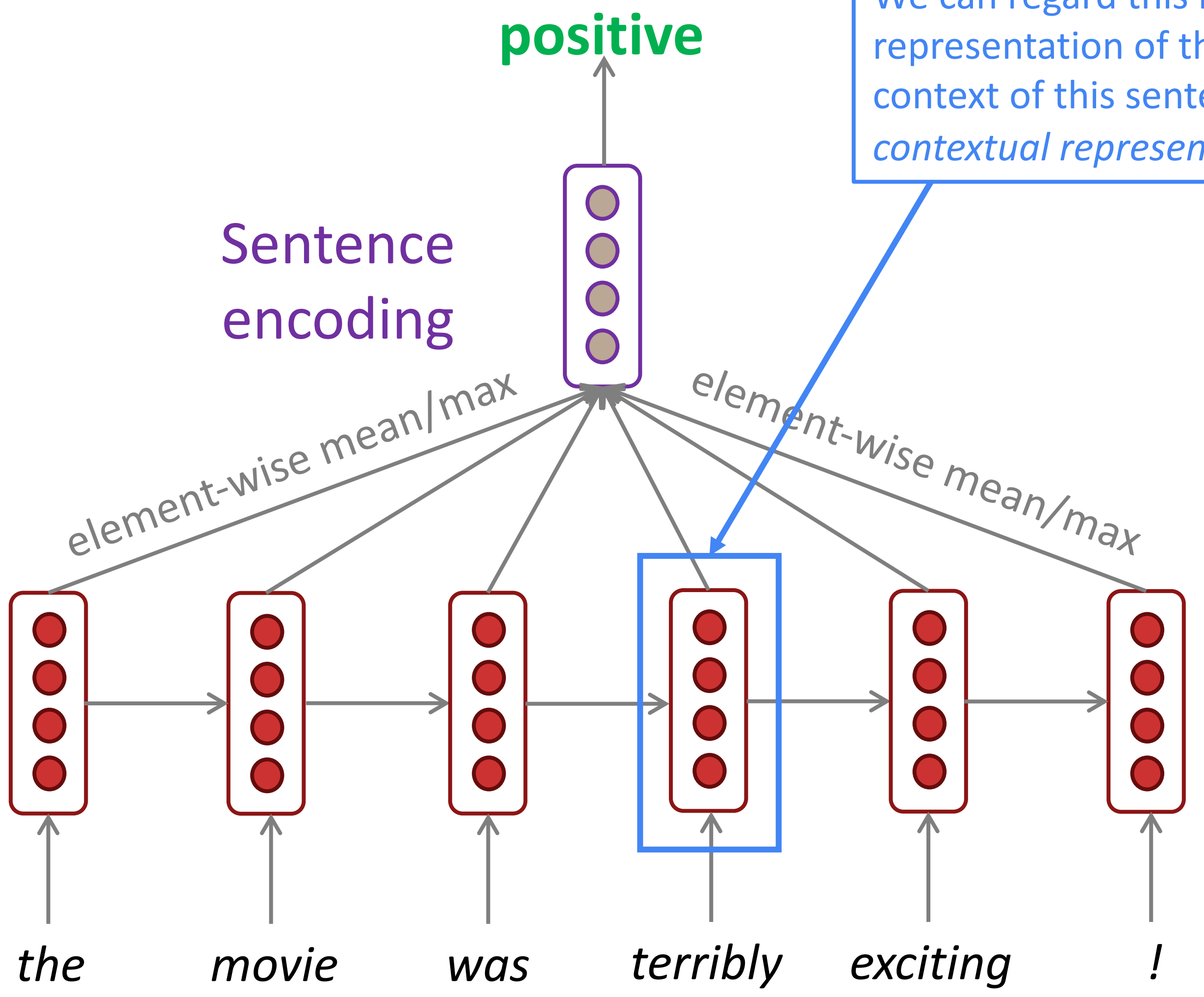
"Densely Connected Convolutional Networks", Huang et al, 2017. https://arxiv.org/pdf/1608.06993.pdf

"Highway Networks", Srivastava et al, 2015. https://arxiv.org/pdf/1505.00387.pdf

"Learning Long-Term Dependencies with Gradient Descent is Difficult", Bengio et al. 1994, http://ai.dinfo.unifi.it/paolo//ps/tnn-94-gradient.pdf

3. Bidirectional and Multi-layer RNNs: motivation

<u>Task: Sentiment Classification</u>



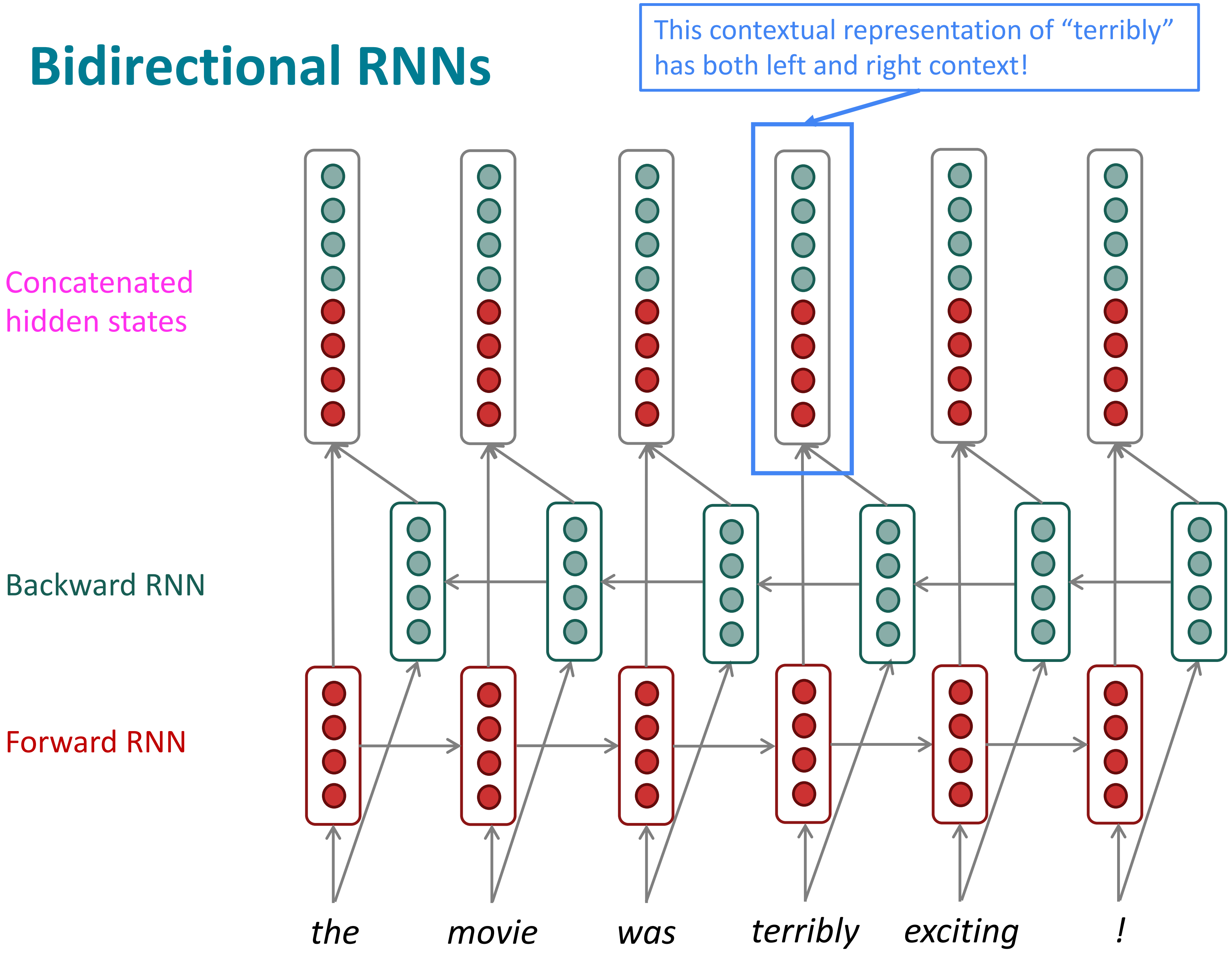
We can regard this hidden state as a representation of the word "*terribly*" in the context of this sentence. We call this a *contextual representation.*

These contextual representations only contain information about the *left* context (e.g. *"the movie was"*).

What about *right* context?

In this example, *"exciting"* is in the right context and this modifies the meaning of *"terribly"* (from negative to positive)

Bidirectional RNNs



Bidirectional RNNs

On timestep *t*:

This is a general notation to mean "compute one forward step of the RNN" – it could be a simple, LSTM, or other (e.g., GRU) RNN computation.

Forward RNN $\overrightarrow{\boldsymbol{h}}^{(t)} = \boxed{\mathrm{RNN}_{\mathrm{FW}}}(\overrightarrow{\boldsymbol{h}}^{(t-1)}, \boldsymbol{x}^{(t)})$

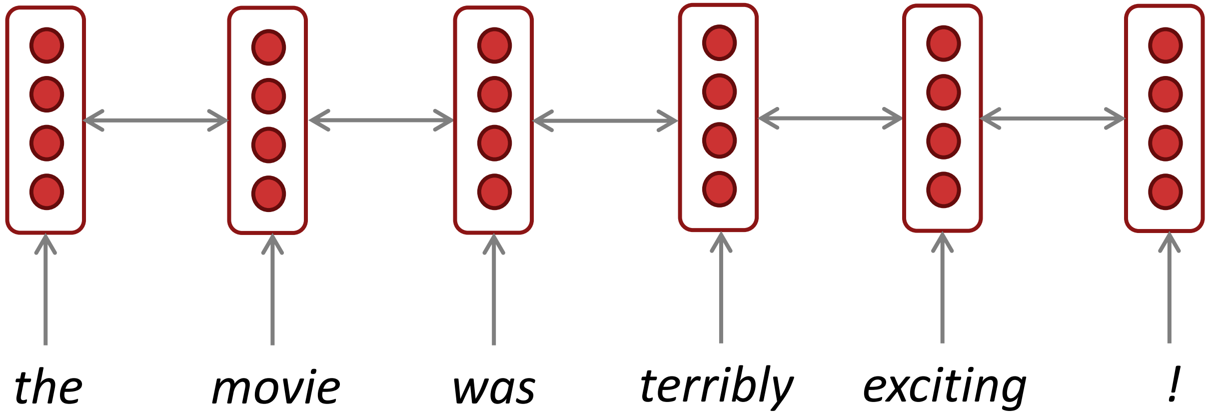
Backward RNN $\overleftarrow{\boldsymbol{h}}^{(t)} = \mathrm{RNN}_{\mathrm{BW}}(\overleftarrow{\boldsymbol{h}}^{(t+1)}, \boldsymbol{x}^{(t)})$

Generally, these two RNNs have separate weights

Concatenated hidden states $\boxed{\boldsymbol{h}^{(t)}} = [\overrightarrow{\boldsymbol{h}}^{(t)}; \overleftarrow{\boldsymbol{h}}^{(t)}]$

We regard this as "the hidden state" of a bidirectional RNN. This is what we pass on to the next parts of the network.

Bidirectional RNNs: simplified diagram



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

Bidirectional RNNs

- Note: bidirectional RNNs are only applicable if you have access to the entire input sequence
  - They are **not** applicable to Language Modeling, because in LM you *only* have left context available.

- If you do have entire input sequence (e.g., any kind of encoding), bidirectionality is powerful (you should use it by default).

- For example, BERT (**Bidirectional** Encoder Representations from Transformers) is a powerful pretrained contextual representation system built on bidirectionality.
  - You will learn more about transformers, including BERT, in a couple of weeks!

Multi-layer RNNs

- RNNs are already "deep" on one dimension (they unroll over many timesteps)

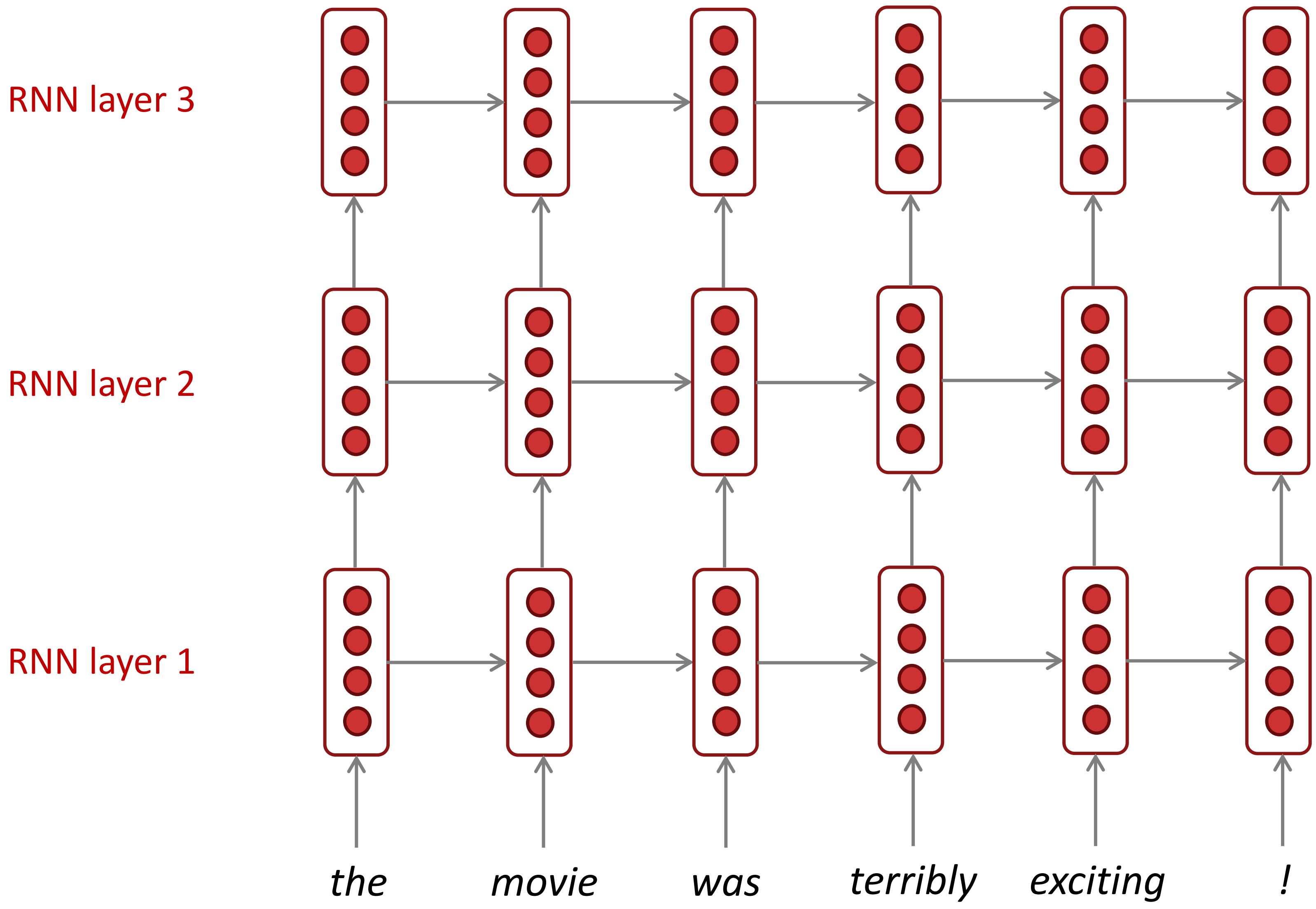
- We can also make them "deep" in another dimension by applying multiple RNNs – this is a multi-layer RNN.

- This allows the network to compute more complex representations
  - The lower RNNs should compute lower-level features and the higher RNNs should compute higher-level features.

- 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



Multi-layer RNNs in practice

- High-performing RNNs are usually multi-layer (but aren't as deep as convolutional or feed-forward networks)

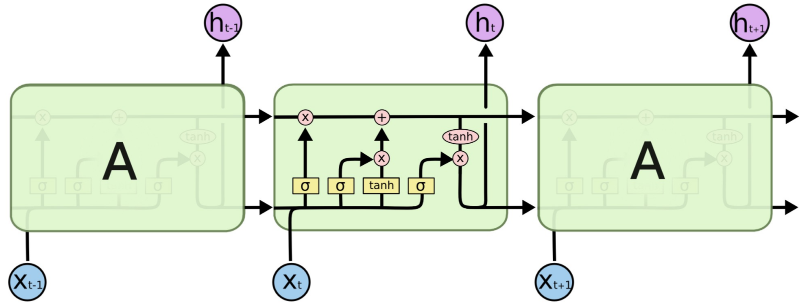
- For example: In a 2017 paper, Britz et al. find that for Neural Machine Translation, 2 to 4 layers is best for the encoder RNN, and 4 layers is best for the decoder RNN
  - Often 2 layers is a lot better than 1, and 3 might be a little better than 2
  - Usually, skip-connections/dense-connections are needed to train deeper RNNs (e.g., 8 layers)

- Transformer-based networks (e.g., BERT) are usually deeper, like 12 or 24 layers.
  - You will learn about Transformers later; they have a lot of skipping-like connections

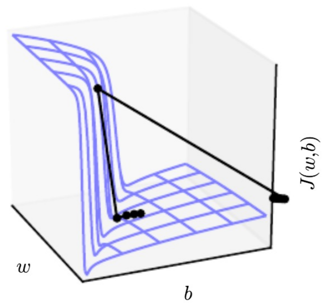
"Massive Exploration of Neural Machine Translation Architecutres", Britz et al, 2017. https://arxiv.org/pdf/1703.03906.pdf

In summary

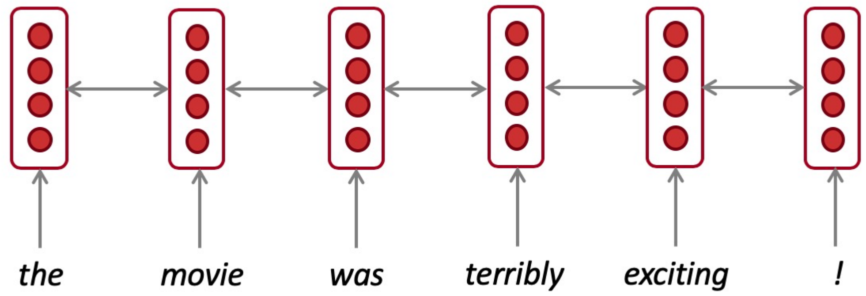
Lots of new information today! What are some of the practical takeaways?



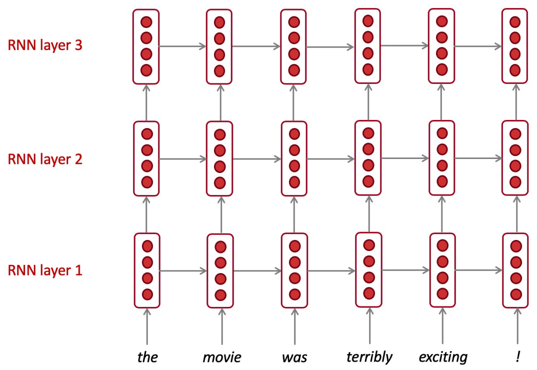
1. LSTMs are powerful



2. Clip your gradients



3. Use bidirectionality when possible



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