

10-701: Introduction to Machine Learning

# Lecture 12 - Recurrent Neural Networks

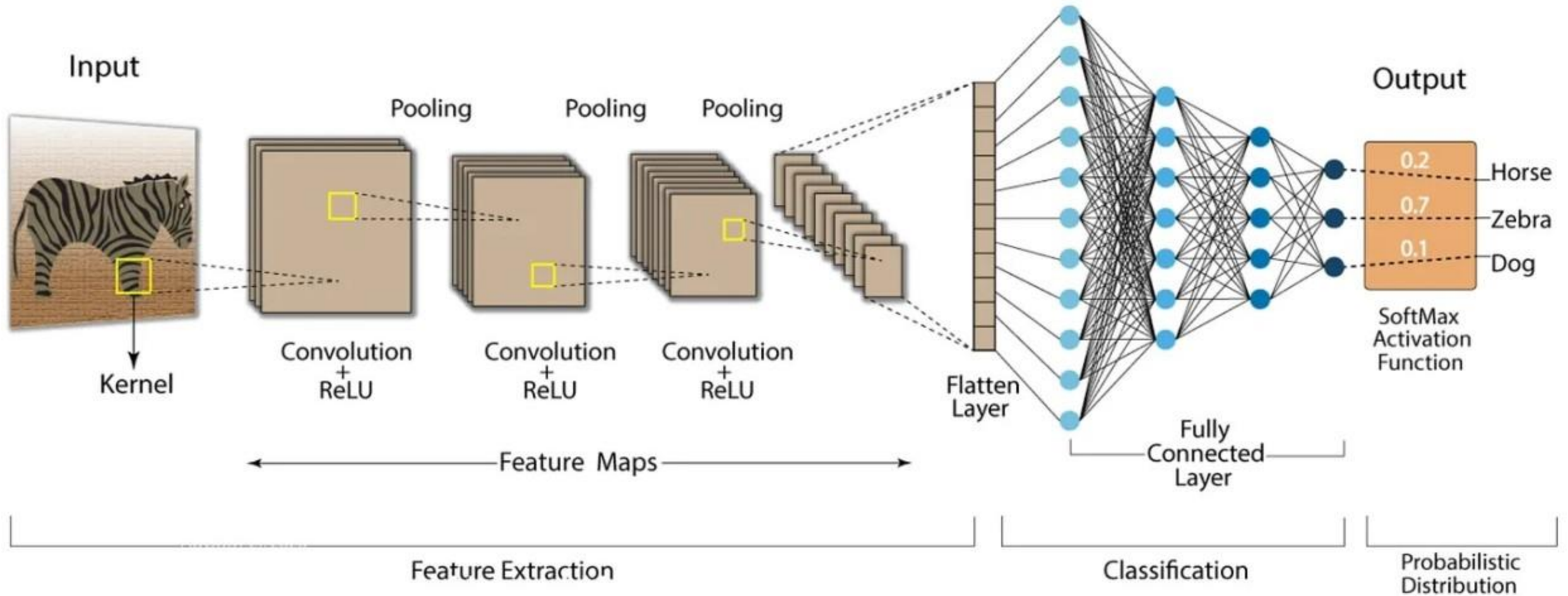
Hoda Heidari

\* Slides adopted from F24 offering of 10701 by Henry Chai.

# Convolutional Neural Networks

- Neural networks are frequently applied to inputs with some inherent spatial structure, **e.g., images**
- Idea: use the first few layers to identify relevant macro-features, **e.g., edges**
- Insight: for spatially-structured inputs, many useful macro-features are shift or location-invariant, **e.g., an edge in the upper left corner of a picture looks like an edge in the center**
- Strategy: learn a *filter* for macro-feature detection in a small window and apply it over the entire image

# Convolution Neural Network (CNN)



# Convolutional Filters

- Images can be represented as matrices: each element corresponds to a pixel and its value is the intensity
- A **filter/kernel** is just a small matrix that is convolved with same-sized sections of the image matrix

0	0	0	0	0	0
0	1	2	2	1	0
0	2	4	4	2	0
0	1	3	3	1	0
0	1	2	3	1	0
0	0	1	1	0	0

 \* 

0	1	0
1	-4	1
0	1	0

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0	1	2	2	1	0
0	2	4	4	2	0
0	1	3	3	1	0
0	1	2	3	1	0
0	0	1	1	0	0

 $*$ 

0	1	0
1	-4	1
0	1	0

 $=$ 

0			

$$(0 * 0) + (0 * 1) + (0 * 0) + (0 * 1) + (1 * -4) + (2 * 1) + (0 * 0) + (2 * 1) + (4 * 0) = 0$$

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0	0	0	0	0	0
0	1	2	2	1	0
0	2	4	4	2	0
0	1	3	3	1	0
0	1	2	3	1	0
0	0	1	1	0	0

 $*$ 

0	1	0
1	-4	1
0	1	0

 $=$ 

0	-1		

$$(0 * 0) + (0 * 1) + (0 * 0) + (1 * 1) + (2 * -4) + (2 * 1) + (2 * 0) + (4 * 1) + (4 * 0) = -1$$

# Convolutional Filters

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- A **filter/kernel** is just a small matrix that is convolved with same-sized sections of the image matrix

0	0	0	0	0	0
0	1	2	2	1	0
0	2	4	4	2	0
0	1	3	3	1	0
0	1	2	3	1	0
0	0	1	1	0	0






 $*$ 

0	1	0
1	-4	1
0	1	0

 $=$ 




0	-1	-1	0
-2	-5	-5	-2
2	-2	-1	3
-1	0	-5	0

# Convolutional Filters

Operation	Kernel $\omega$	Image result $g(x,y)$
Identity	$\begin{bmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix}$	 
Edge detection	$\begin{bmatrix} 1 & 0 & -1 \\ 0 & 0 & 0 \\ -1 & 0 & 1 \end{bmatrix}$	
	$\begin{bmatrix} \cancel{0} & \textcircled{1} & \cancel{0} \\ \textcircled{1} & \textcircled{-4} & \textcircled{1} \\ \cancel{0} & \textcircled{1} & \cancel{0} \end{bmatrix}$	
	$\begin{bmatrix} -1 & -1 & -1 \\ -1 & \textcircled{8} & -1 \\ -1 & -1 & -1 \end{bmatrix}$	

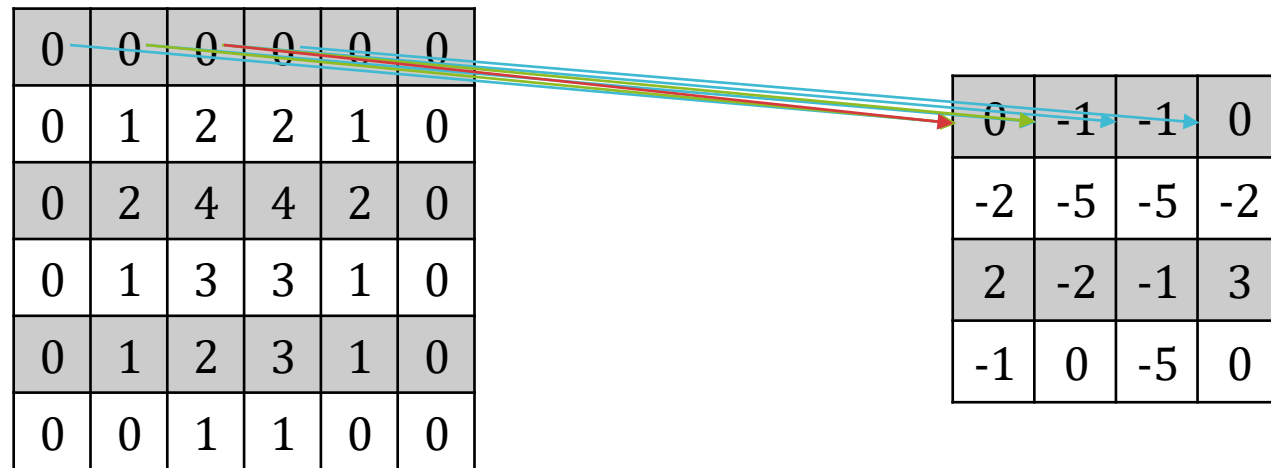


# More Filters

Operation	Kernel $\omega$	Image result $g(x,y)$
Identity	$\begin{bmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix}$	
<u>Sharpen</u>	$\begin{bmatrix} 0 & \underline{-1} & 0 \\ \underline{-1} & \textcircled{5} & \underline{-1} \\ 0 & \underline{-1} & 0 \end{bmatrix}$	
<b>Box blur</b> (normalized)	$\frac{1}{9} \begin{bmatrix} \underline{1} & \underline{1} & \underline{1} \\ \underline{1} & \underline{1} & \underline{1} \\ \underline{1} & \underline{1} & \underline{1} \end{bmatrix}$	

# Convolutional Filters

- Convolutions can be represented by a feed forward neural network where:
  1. Nodes in the input layer are only connected to some nodes in the next layer but not all nodes.
  2. Many of the weights have the same value.



- Many fewer weights than a fully connected layer!
- **Convolution weights are learned using gradient descent/backpropagation, not prespecified**

# Convolutional Filters: Padding

- What if relevant features exist at the border of our image?
- Add zeros around the image to allow for the filter to be applied “everywhere” e.g. a *padding* of 1 with a 3x3 filter preserves image size and allows every pixel to be the center

0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0
0	0	1	2	2	1	0	0
0	0	2	4	4	2	0	0
0	0	1	3	3	1	0	0
0	0	1	2	3	1	0	0
0	0	0	1	1	0	0	0
0	0	0	0	0	0	0	0

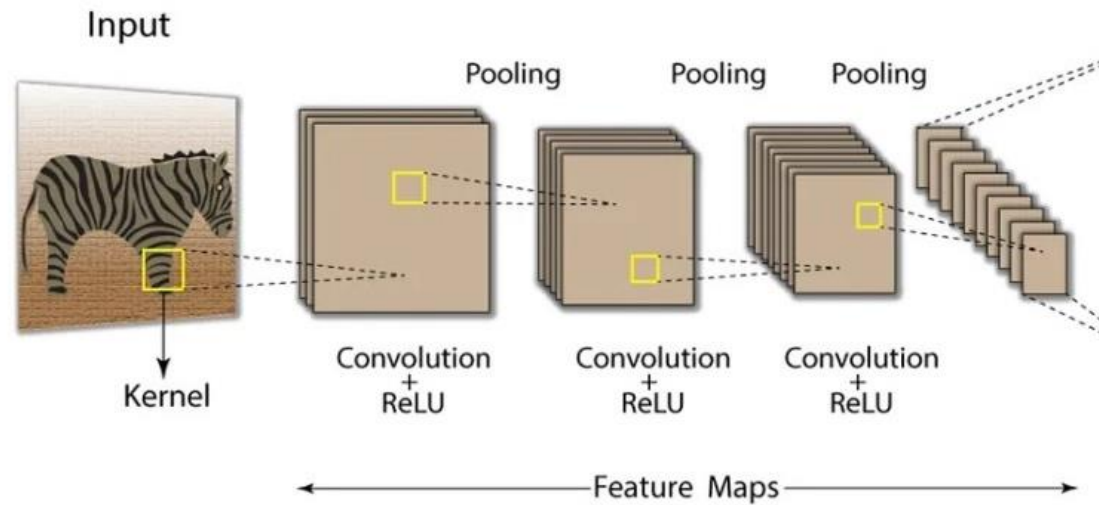
 $*$ 

0	1	0
1	-4	1
0	1	0

 $=$ 

0	1	2	2	1	0
1	0	-1	-1	0	1
2	-2	-5	-5	-2	2
1	2	-2	-1	3	1
1	-1	0	-5	0	1
0	2	-1	0	2	0

# Downsampling



- **Idea:** reduce the spatial size of the feature maps to
  - cut down the number of parameters and computations in later layers
  - reduce the risk of overfitting
  - make the model less sensitive to small shifts in input

# Downsampling: Stride

- Only apply the convolution to some subset of the image  
e.g., every other column and row = a *stride* of 2

0	0	0	0	0	0
0	1	2	2	1	0
0	2	4	4	2	0
0	1	3	3	1	0
0	1	2	3	1	0
0	0	1	1	0	0

 $*$ 

0	1
1	-2

 $=$ 

-2		

# Downsampling: Stride

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0	0	0	0	0	0
0	1	2	2	1	0
0	2	4	4	2	0
0	1	3	3	1	0
0	1	2	3	1	0
0	0	1	1	0	0

 $*$ 

0	1
1	-2

 $=$ 

-2	-2	

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0	1	3	3	1	0
0	1	2	3	1	0
0	0	1	1	0	0

 $*$ 

0	1
1	-2

 $=$ 

-2	-2	1

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0	1	2	2	1	0
0	2	4	4	2	0
0	1	3	3	1	0
0	1	2	3	1	0
0	0	1	1	0	0

 $*$ 

0	1
1	-2

 $=$ 

-2	-2	1
0		



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0	1	3	3	1	0
0	1	2	3	1	0
0	0	1	1	0	0

 \* 

0	1
1	-2

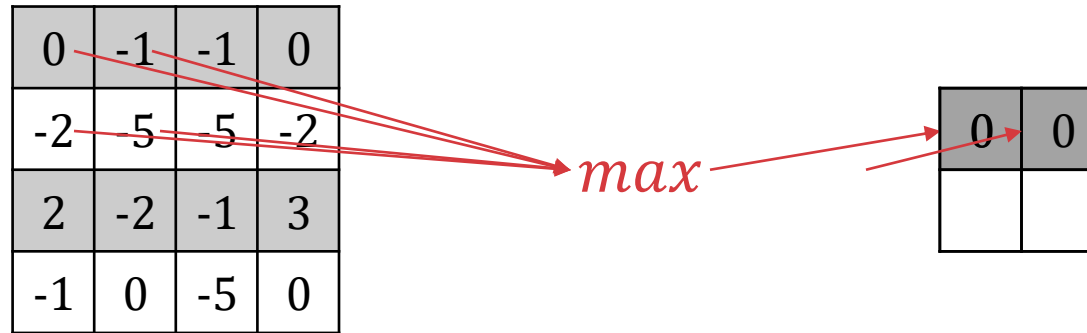
 = 

-2	-2	1
0	1	1
1	2	0

- Reduces the dimensionality of the input to subsequent layers and thus, the number of weights to be learned
- Many relevant macro-features will tend to span large portions of the image, so taking strides with the convolution tends not to miss out on too much

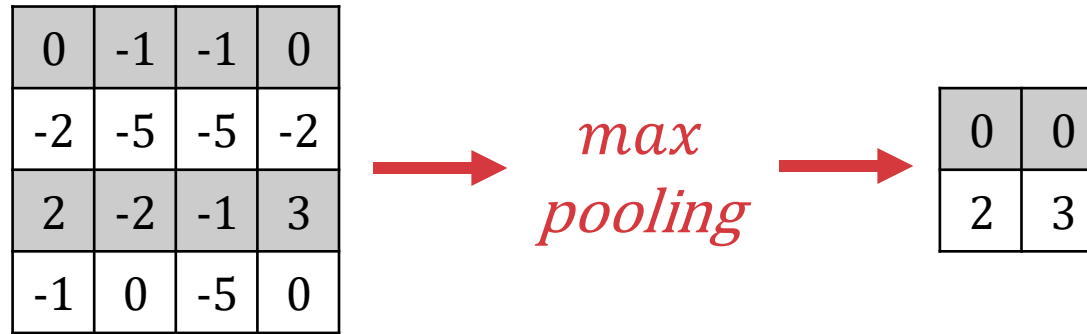
# Downsampling: Pooling

- Combine multiple adjacent nodes into a single node

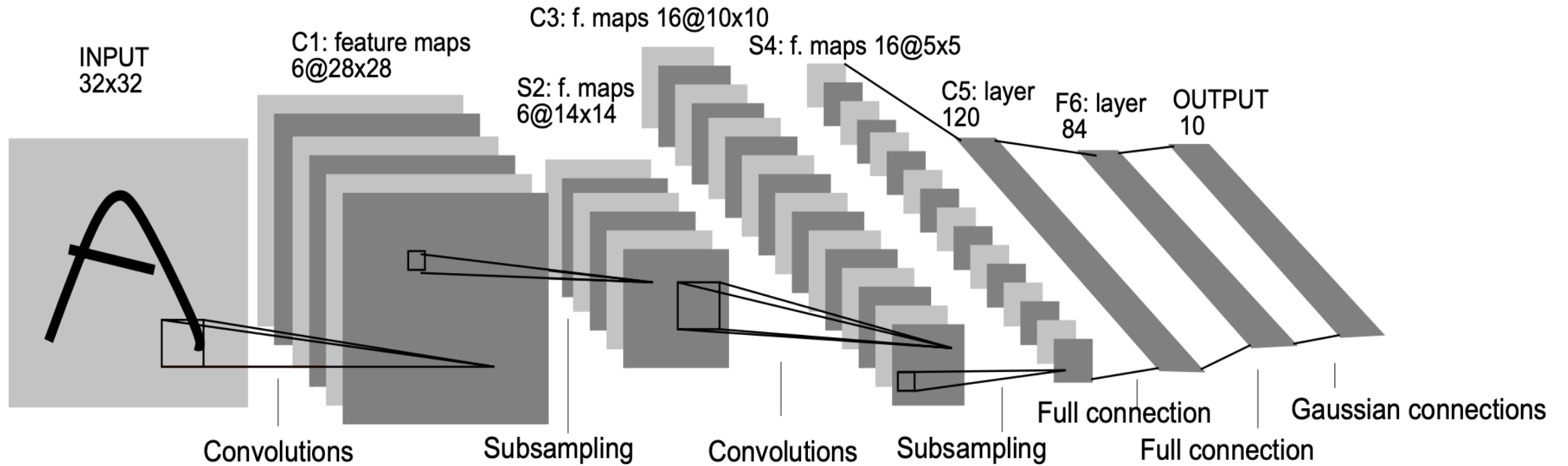


# Downsampling: Pooling

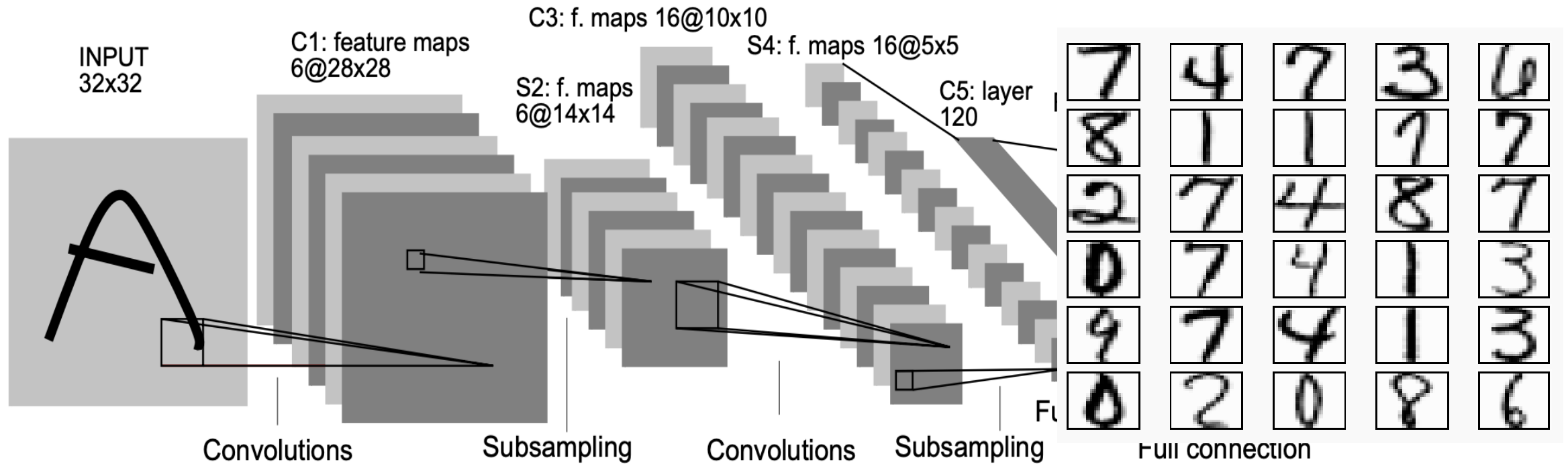
- Combine multiple adjacent nodes into a single node



- **Max Pooling** keeps the strongest activation in each region, focusing on the most prominent features.
- **Average Pooling** computes the average of the region, providing a smoother, more generalized representation.



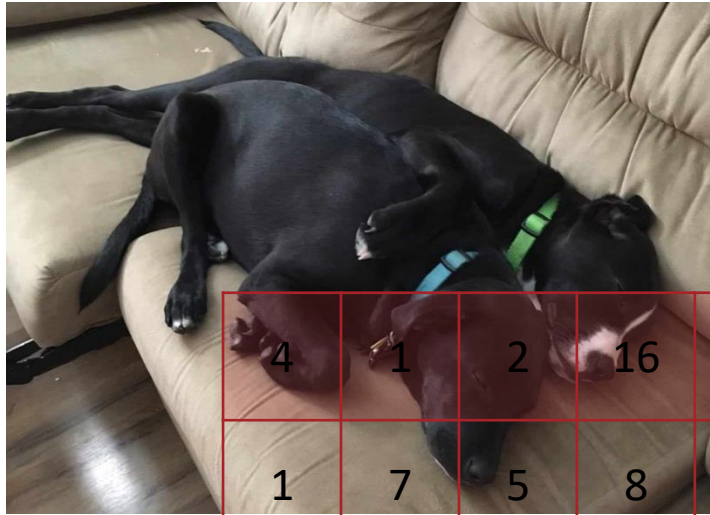
# LeNet (LeCun et al., 1998)



- One of the earliest, most famous deep learning models – achieved remarkable performance at handwritten digit recognition (< 1% test error rate on MNIST)
- Used sigmoid (or logistic) activation functions between layers and mean-pooling, both of which are pretty uncommon in modern architectures



# Colored Images and Channels



4	1	2	16	3	6
1	7	5	8	19	27
5	2	5	12	17	8
0	4	9	9	6	11

5	2	6	14	15	8
26	3	6	8	4	9
0	15	24	6	1	8
7	4	9	5	24	17

4	6	8	9	5	3
16	5	2	8	2	1
5	2	14	11	7	8
15	2	5	0	9	8

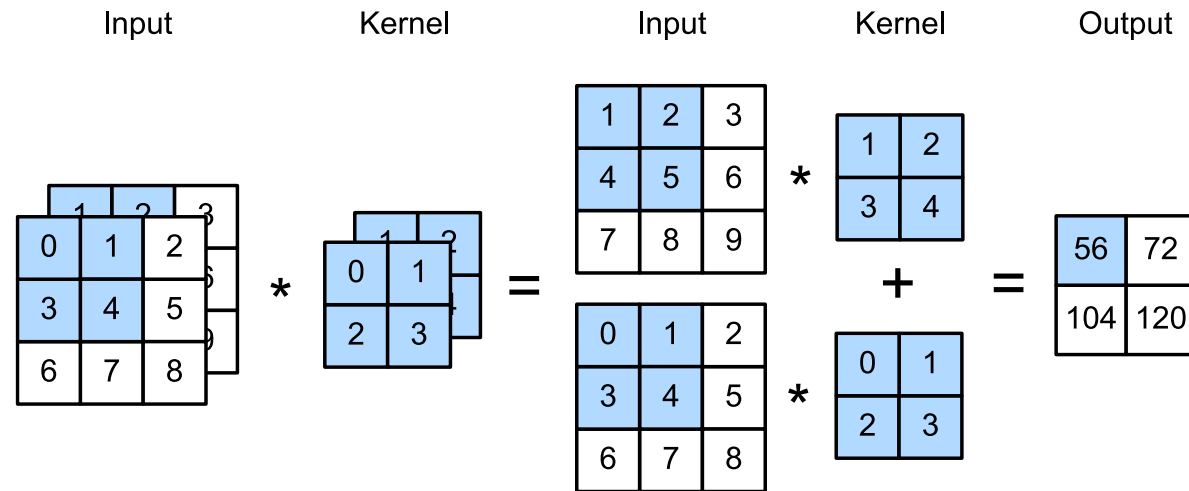
- An image can be represented as the sum of red, green and blue pixel intensities
- Each color corresponds to a *channel*





# Convolutions on Multiple Input Channels

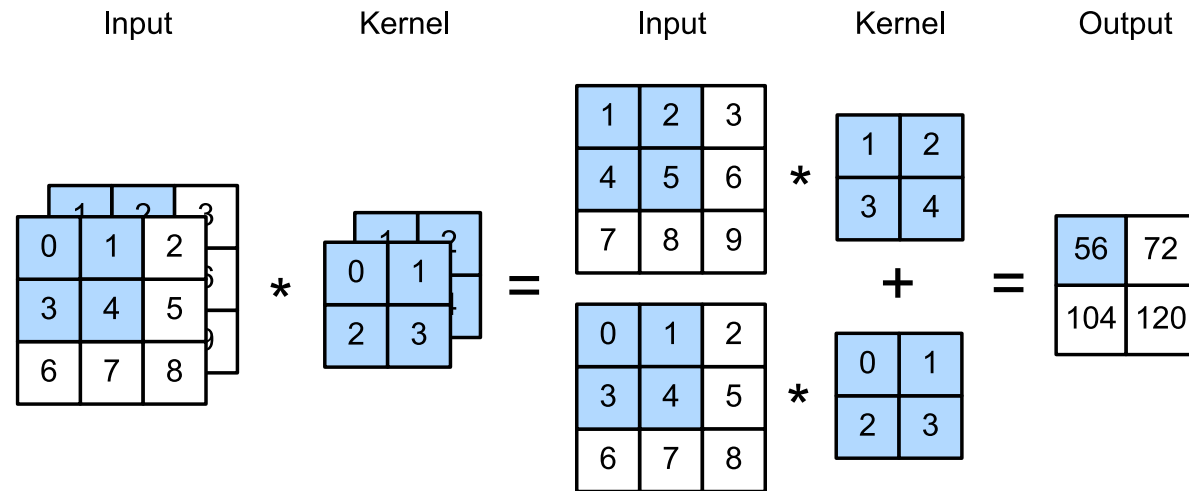
- Given multiple input channels, we can specify a filter for each one and sum the results to get a 2-D output tensor



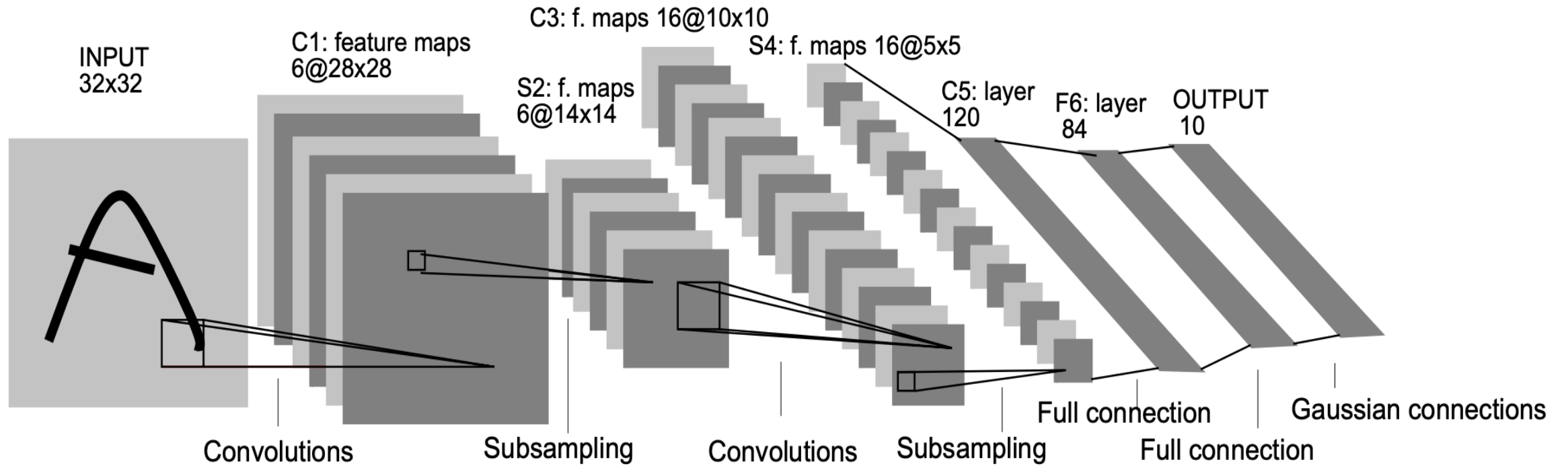
- For  $c$  channels and  $h \times w$ -sized filters, we have  $chw + c$  learnable parameters (each filter has a bias term)

# Convolutions on Multiple Input Channels

- Given multiple input channels, we can specify a filter for each one and sum the results to get a 2-D output tensor



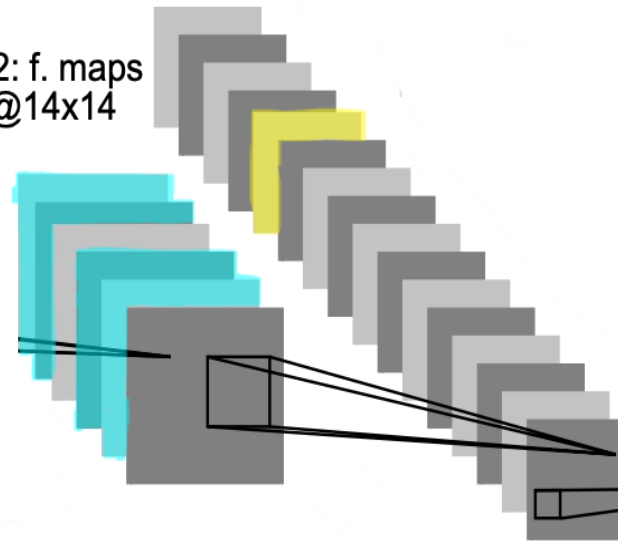
- Questions:
  - Why might we want a different filter for each input?
  - Why do we combine them together into a single output channel?



- Channels in hidden layers correspond to different macro-features, which we might want to manipulate differently → one filter per channel

C3: f. maps 16@10x10

S2: f. maps  
6@14x14



	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
0	X				X	X	X			X	X	X	X		X	X
1	X	X				X	X	X			X	X	X	X		X
2	X	X	X				X	X	X			X		X	X	X
3		X	X	X			X	X	X	X			X		X	X
4			X	X	X			X	X	X	X		X	X		X
5				X	X	X			X	X	X	X		X	X	X

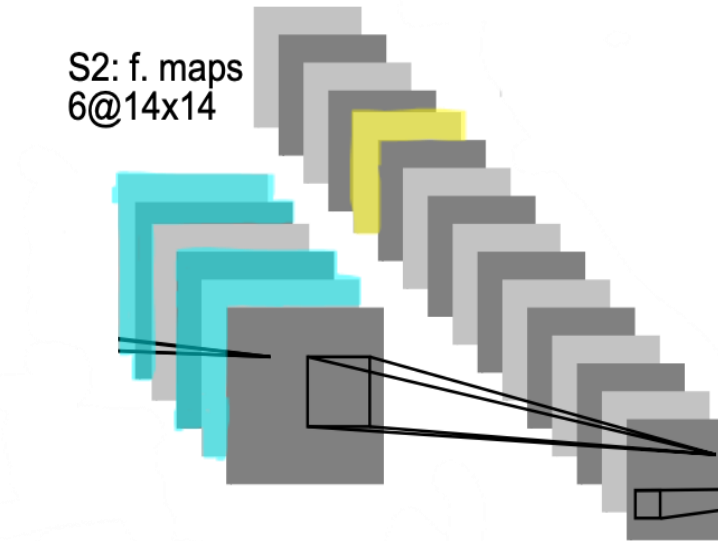
TABLE I

EACH COLUMN INDICATES WHICH FEATURE MAP IN S2 ARE COMBINED BY THE UNITS IN A PARTICULAR FEATURE MAP OF C3.

- We can combine these macro-features into a new, interesting, “higher-level” feature
  - But we don’t always need to combine all of them!
  - Different combinations → multiple output channels
  - Common pattern: more output channels and smaller outputs in deeper layers

C3: f. maps 16@10x10

S2: f. maps  
6@14x14



	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
0	X				X	X	X			X	X	X	X		X	X
1	X	X				X	X	X			X	X	X	X		X
2	X	X	X				X	X	X			X		X	X	X
3		X	X	X			X	X	X	X			X		X	X
4			X	X	X			X	X	X	X		X	X		X
5				X	X	X			X	X	X	X	X	X	X	X

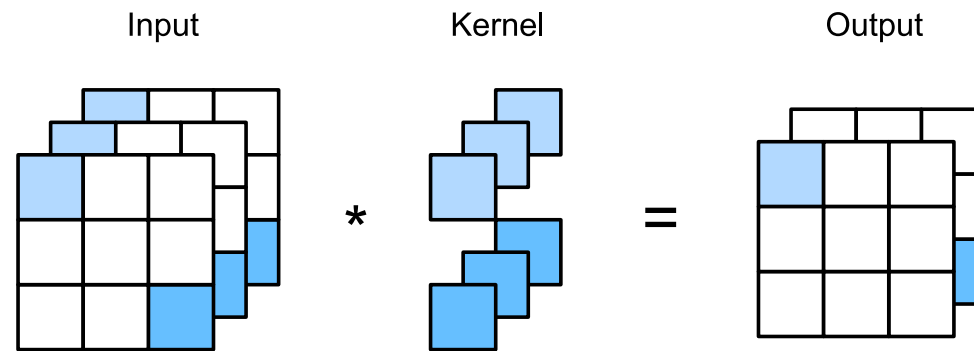
TABLE I

EACH COLUMN INDICATES WHICH FEATURE MAP IN S2 ARE COMBINED BY THE UNITS IN A PARTICULAR FEATURE MAP OF C3.

# Okay, but what if our layers become too big in the channel dimension?

# Downsampling: $1 \times 1$ Convolutions

- Convolutional layers can be represented as 4-D tensors of size  $c_o \times c_i \times h \times w$  where  $c_o$  is the number of output channels and  $c_i$  is the number of input channels
- Layers of size  $c_o \times c_i \times 1 \times 1$  can condense many input channels into fewer output channels (if  $c_o < c_i$ )



- Practical note:  $1 \times 1$  convolutions are typically followed by a nonlinear activation function; otherwise, they could simply be folded into other convolutions

# Key Takeaways

- Convolutional neural networks use convolutions to learn macro-features.
  - Can be thought of as slight modifications to the fully-connected feed-forward neural network.
  - Can still be learned using SGD.
  - Padding is used to preserve spatial dimensions.
  - Pooling, stride and  $1 \times 1$  convolutions are used to downsample intermediate representations.

# Example: Handwriting Recognition

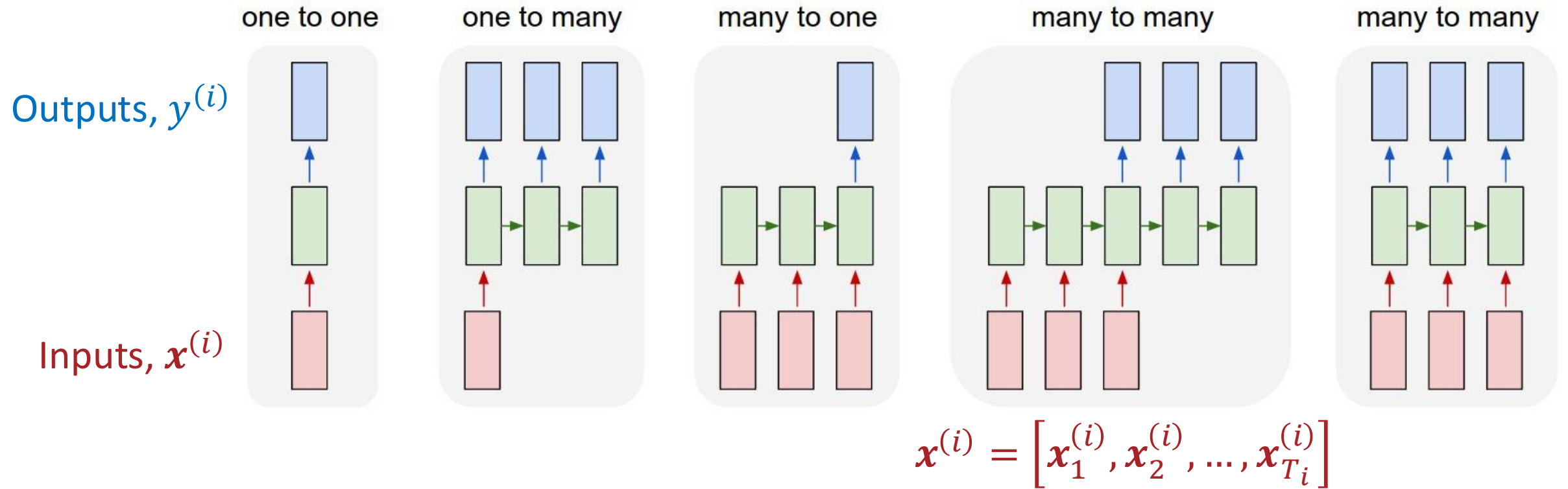
U N E X P E C T E D

V O L C A N I C

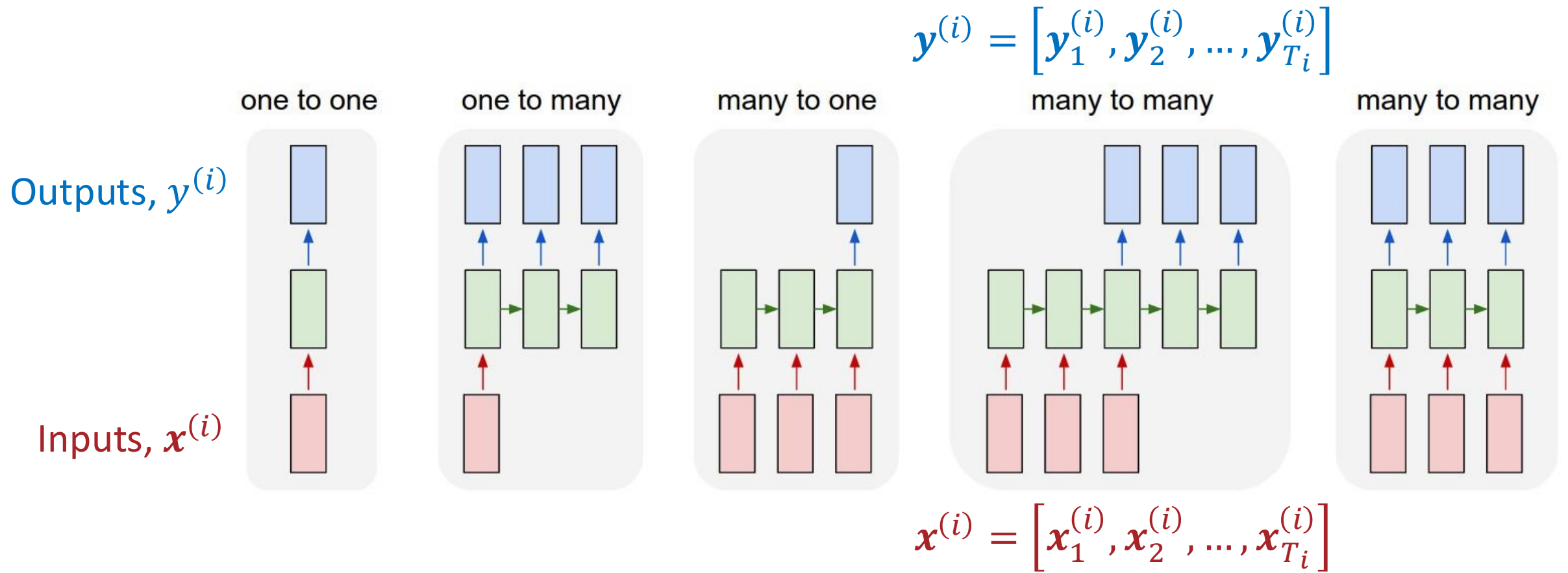
E M B R A C E S



$$\mathbf{y}^{(i)} = [\mathbf{y}_1^{(i)}, \mathbf{y}_2^{(i)}, \dots, \mathbf{y}_{T_i}^{(i)}]$$



# Sequential Data



Poll:  
formulate a hand-written digit recognition task

# Recurrent Neural Networks

- Neural networks are frequently applied to inputs with some inherent **temporal or sequential** structure (**e.g., text or video**) of **variable length**
- Idea: use the information from previous parts of the input to inform subsequent predictions
- Insight: the hidden layers learn a useful representation (relative to the task)
- Approach: incorporate the output from earlier hidden layers into later ones.

# Recurrent Neural Networks

- Data points consists of (input **sequence**, label **sequence**) pairs, potentially of **varying lengths**

$$\mathcal{D} = \{(\mathbf{x}^{(n)}, \mathbf{y}^{(n)})\}_{n=1}^N$$

$$\mathbf{x}^{(n)} = [\mathbf{x}_1^{(n)}, \dots, \mathbf{x}_{T_n}^{(n)}]$$

$$\mathbf{y}^{(n)} = [\mathbf{y}_1^{(n)}, \dots, \mathbf{y}_{T_n}^{(n)}]$$

# Recurrent Neural Networks

- RNNs process inputs one time step at a time, using **recurrence**:

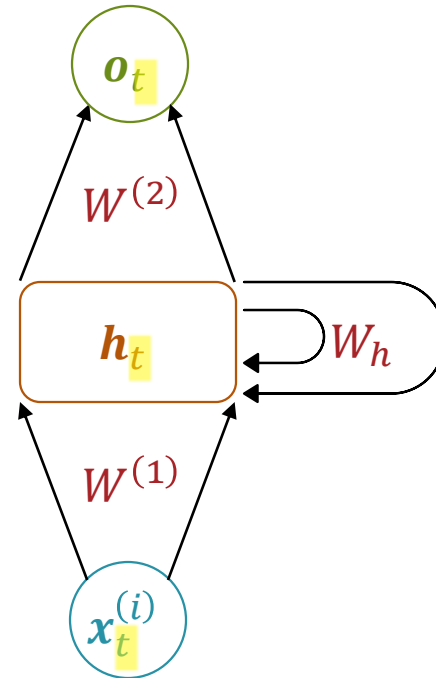
$$\mathbf{h}_t = \left[ 1, \theta \left( W^{(1)} \mathbf{x}_t^{(i)} + W_h \mathbf{h}_{t-1} \right) \right]^T \text{ and } \mathbf{o}_t = \hat{y}_t^{(i)} = \theta(W^{(2)} \mathbf{h}_t)$$

Where  $\mathbf{h}_t$  serves as a summary or latent representation of the sequence up to time  $t$ .

- The same parameters  $W^{(1)}$ ,  $W_h$  and  $W^{(2)}$  are reused at every step.
- We can unroll the RNN for as many time steps as the sequence requires.
- So, at training and inference time, the RNN can run for different numbers of steps depending on the input length.

# Recurrent Neural Networks

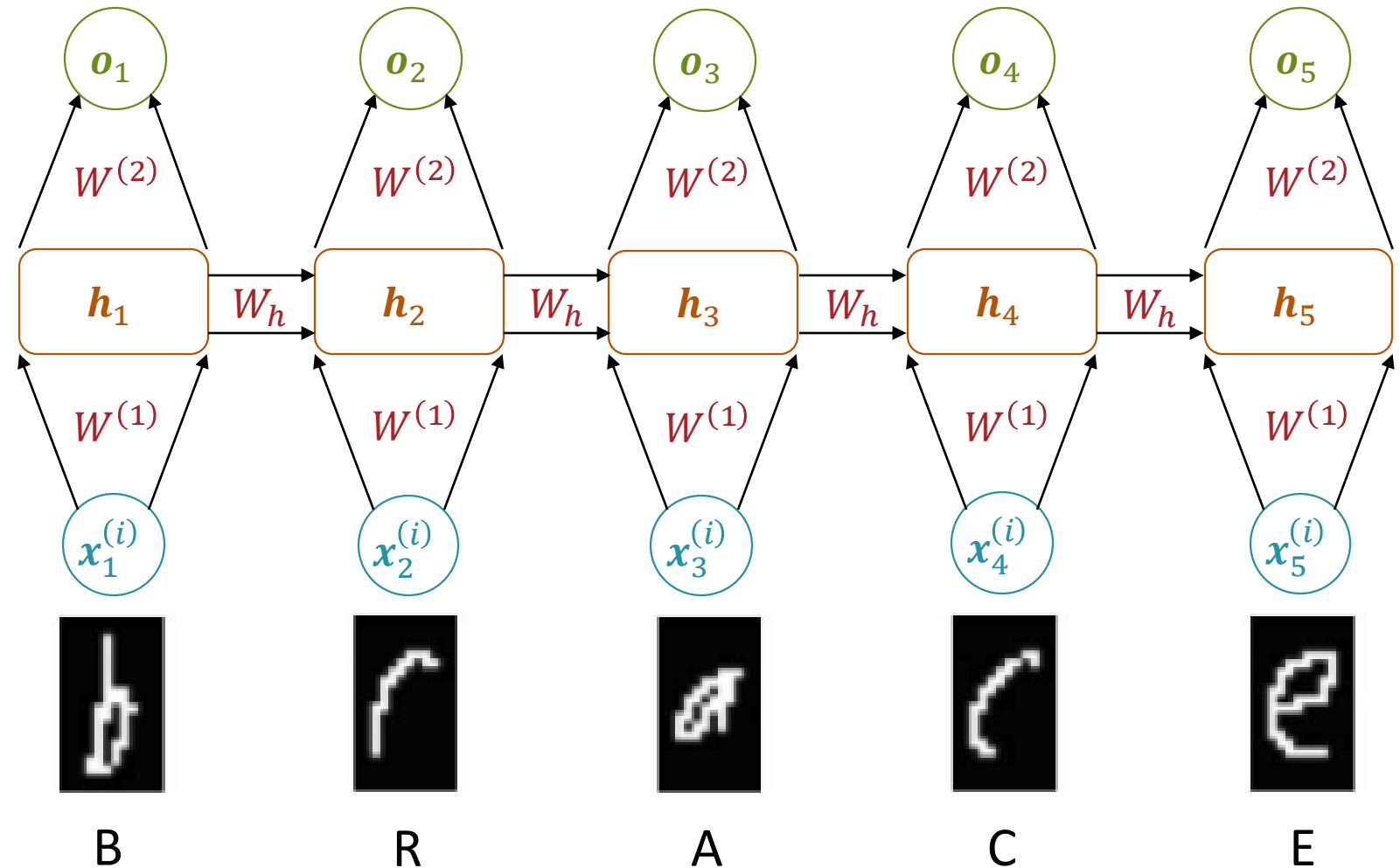
$$\mathbf{h}_t = \left[ 1, \theta \left( W^{(1)} \mathbf{x}_t^{(i)} + W_h \mathbf{h}_{t-1} \right) \right]^T \text{ and } \mathbf{o}_t = \hat{y}_t^{(i)} = \theta(W^{(2)} \mathbf{h}_t)$$



- This model requires an initial value for the hidden representation,  $\mathbf{h}_0$ , typically a vector of all zeros

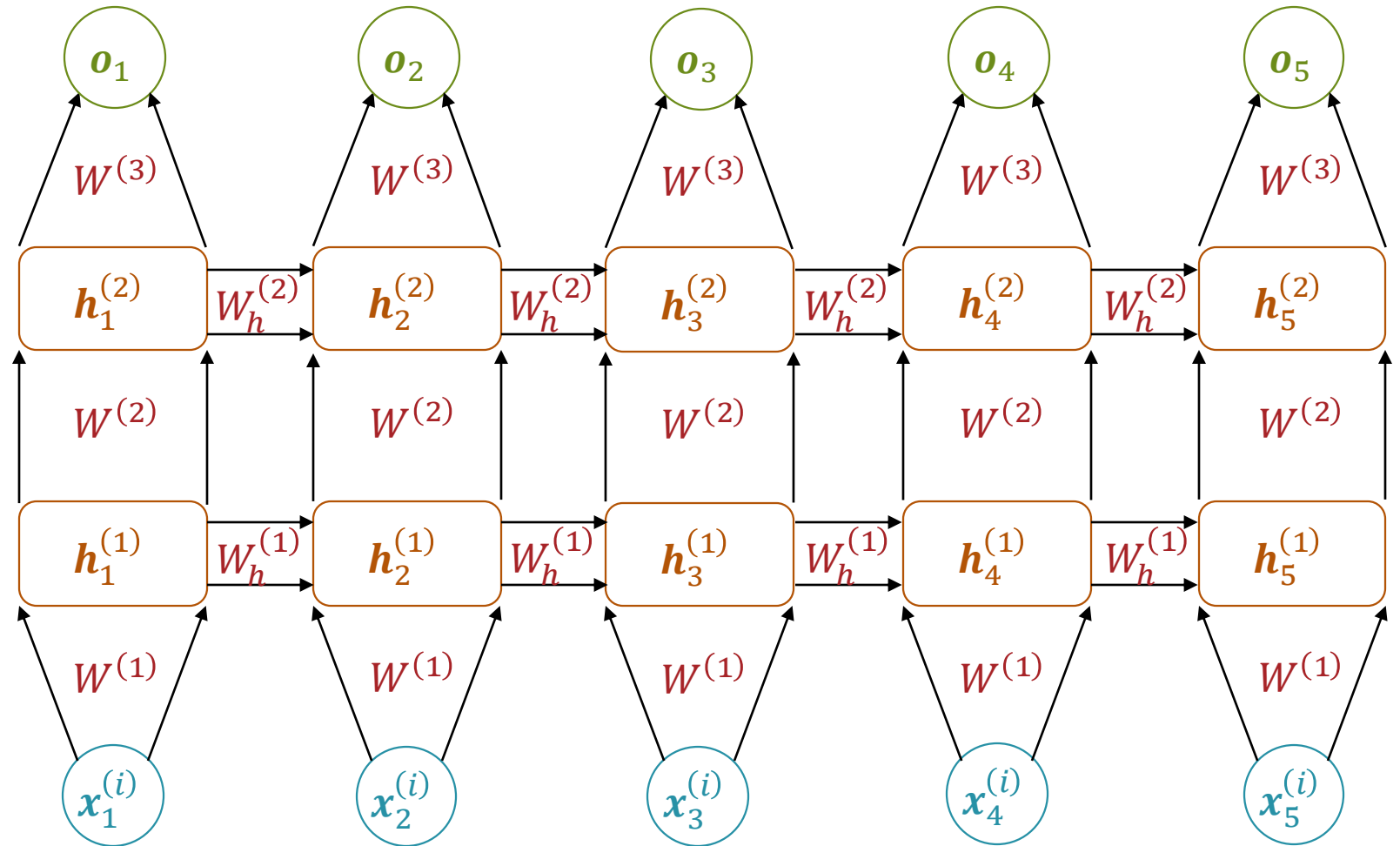
# Unrolling Recurrent Neural Networks

$$\mathbf{h}_t = \left[ 1, \theta \left( W^{(1)} \mathbf{x}_t^{(i)} + W_h \mathbf{h}_{t-1} \right) \right]^T \text{ and } \mathbf{o}_t = \hat{y}_t^{(i)} = \theta(W^{(2)} \mathbf{h}_t)$$



# Deep Recurrent Neural Networks

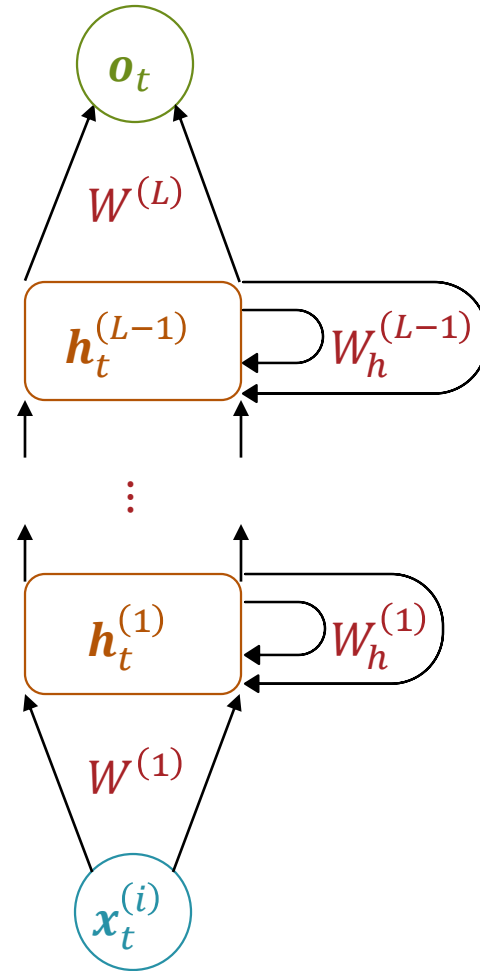
$$\mathbf{h}_t^{(l)} = \left[ 1, \theta \left( W^{(l)} \mathbf{h}_t^{(l-1)} + W_h^{(l)} \mathbf{h}_{t-1}^{(l)} \right) \right]^T \text{ and } \mathbf{o}_t = \hat{y}_t^{(i)} = \theta \left( W^{(L)} \mathbf{h}_t^{(L-1)} \right)$$





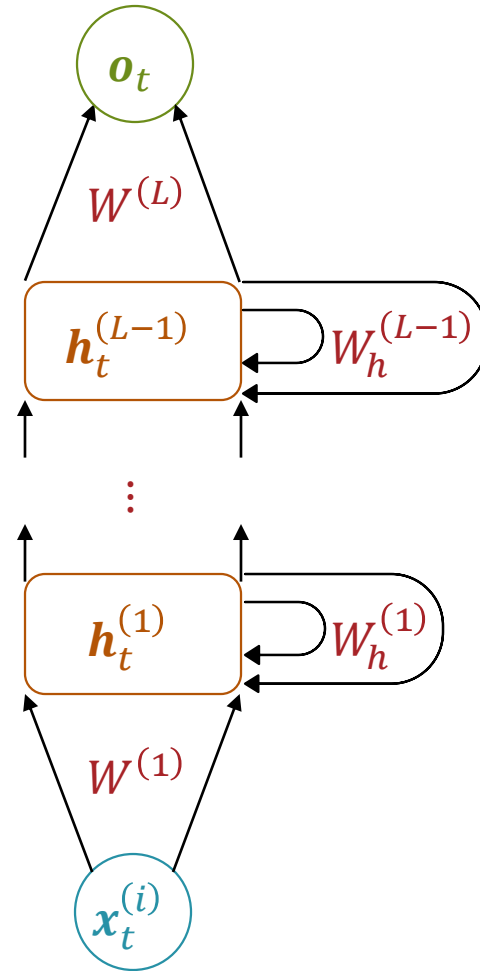
# Deep Recurrent Neural Networks

$$\mathbf{h}_t^{(l)} = \left[ 1, \theta \left( W^{(l)} \mathbf{h}_t^{(l-1)} + W_h^{(l)} \mathbf{h}_{t-1}^{(l)} \right) \right]^T \text{ and } \mathbf{o}_t = \hat{y}_t^{(i)} = \theta \left( W^{(L)} \mathbf{h}_t^{(L-1)} \right)$$



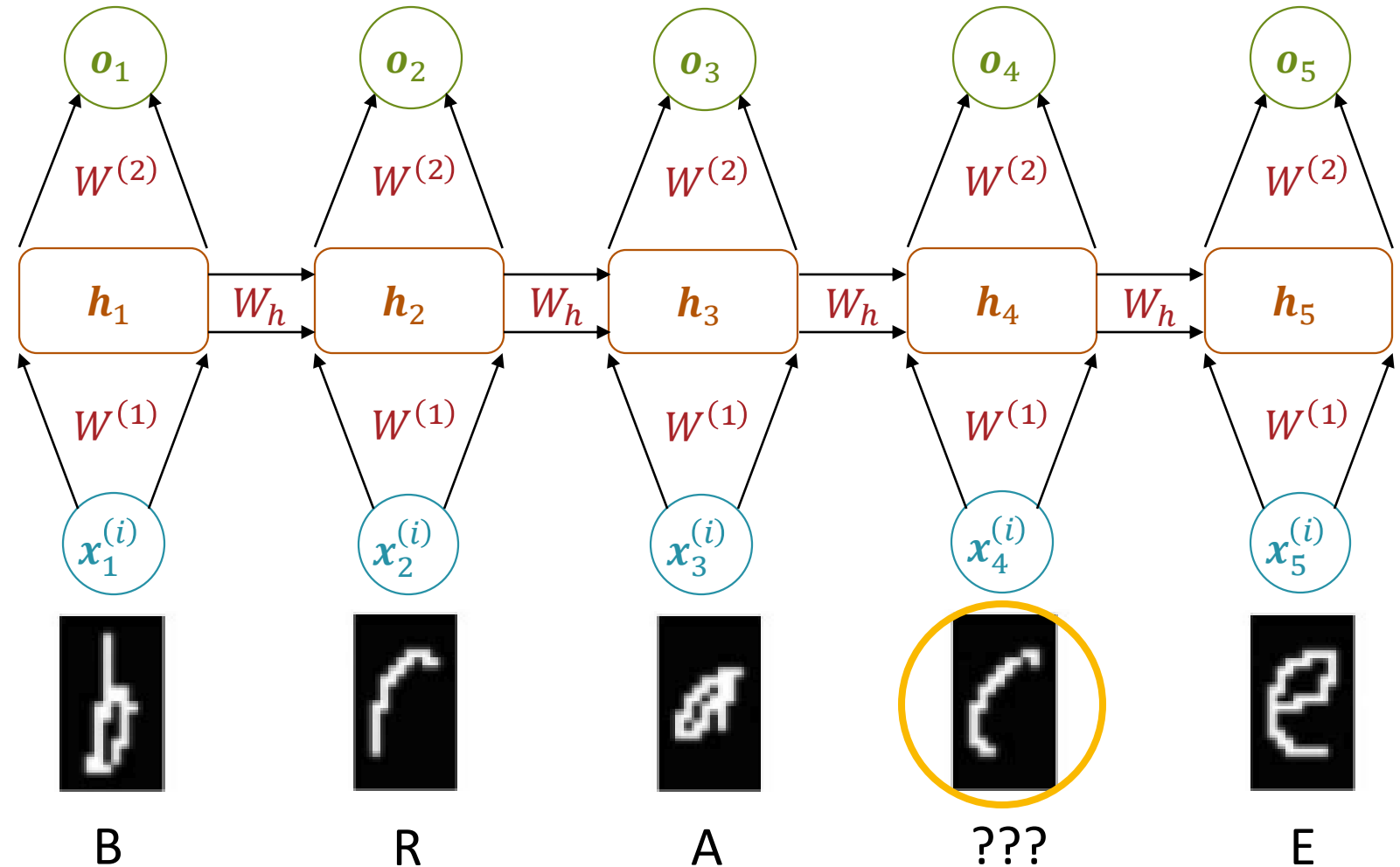
But why do we only pass information forward?  
What if later time steps have useful information as well?

$$\mathbf{h}_t^{(l)} = \left[ 1, \theta \left( W^{(l)} \mathbf{h}_t^{(l-1)} + W_h^{(l)} \mathbf{h}_{t-1}^{(l)} \right) \right]^T \text{ and } \mathbf{o}_t = \hat{y}_t^{(i)} = \theta \left( W^{(L)} \mathbf{h}_t^{(L-1)} \right)$$



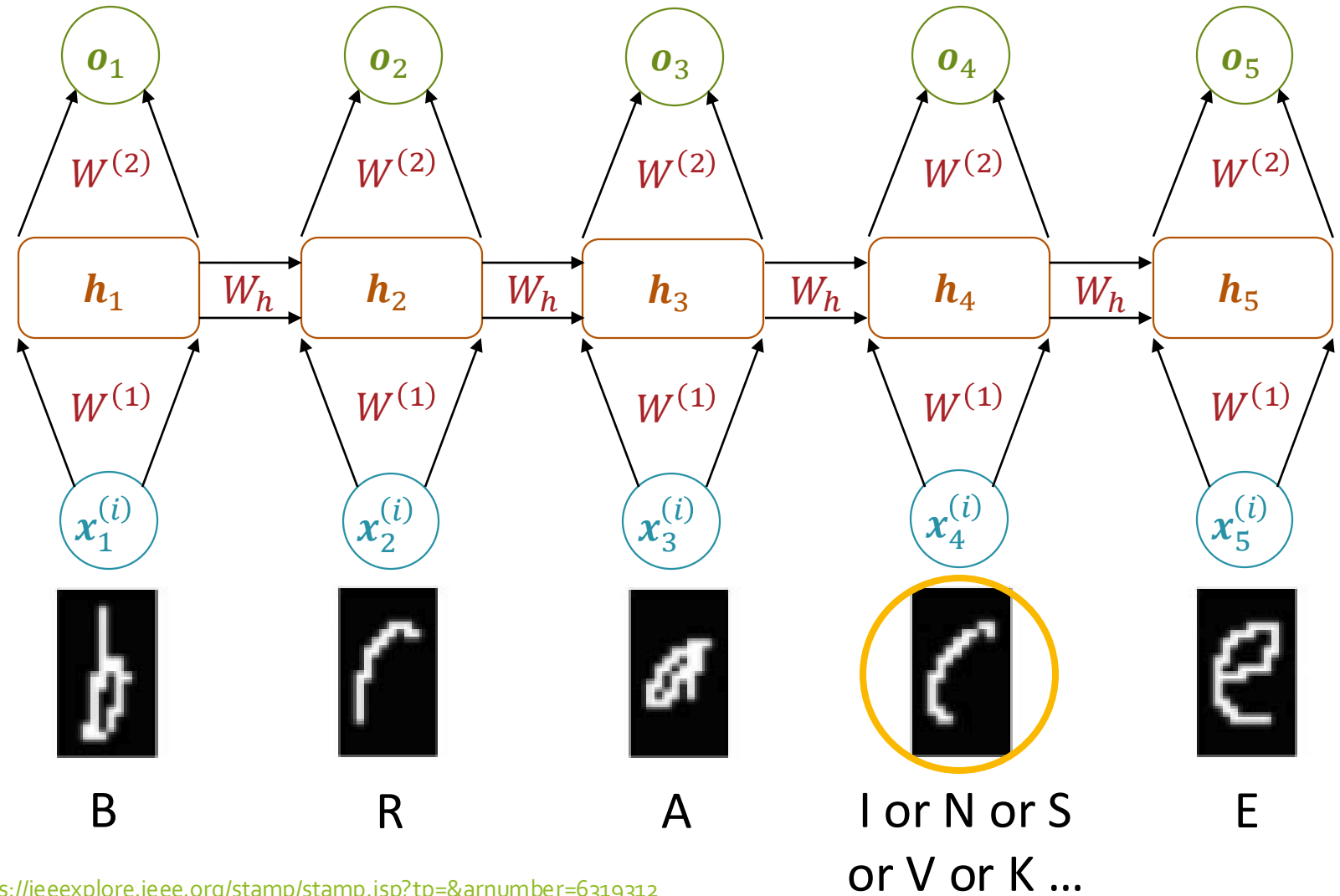
But why do we only pass information forward?  
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$$\mathbf{h}_t = \left[ 1, \theta \left( W^{(1)} \mathbf{x}_t^{(i)} + W_h \mathbf{h}_{t-1} \right) \right]^T \text{ and } \mathbf{o}_t = \hat{y}_t^{(i)} = \theta(W^{(2)} \mathbf{h}_t)$$



But why do we only pass information forward?  
What if later time steps have useful information as well?

$$\mathbf{h}_t = \left[ 1, \theta \left( W^{(1)} \mathbf{x}_t^{(i)} + W_h \mathbf{h}_{t-1} \right) \right]^T \text{ and } \mathbf{o}_t = \hat{y}_t^{(i)} = \theta(W^{(2)} \mathbf{h}_t)$$

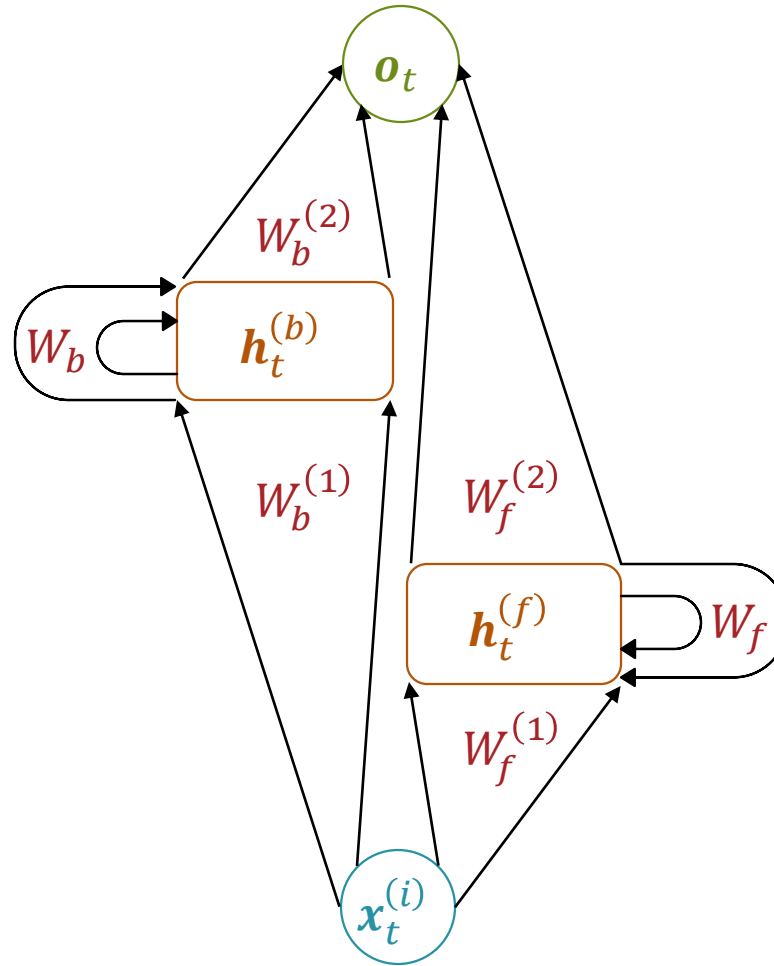


# Bidirectional Recurrent Neural Networks

- Bidirectional Recurrent Neural Networks (BiRNNs) capture **context from both the past and the future** of a sequence.
- A BiRNN has two RNNs:
  - one  $\mathbf{h}_t^{(f)}$  processes the sequence **forward in time**
  - one  $\mathbf{h}_t^{(b)}$  processes it **backward in time**
  - The combination contains information from the entire sequence centered around position  $t$ .

# Bidirectional Recurrent Neural Networks

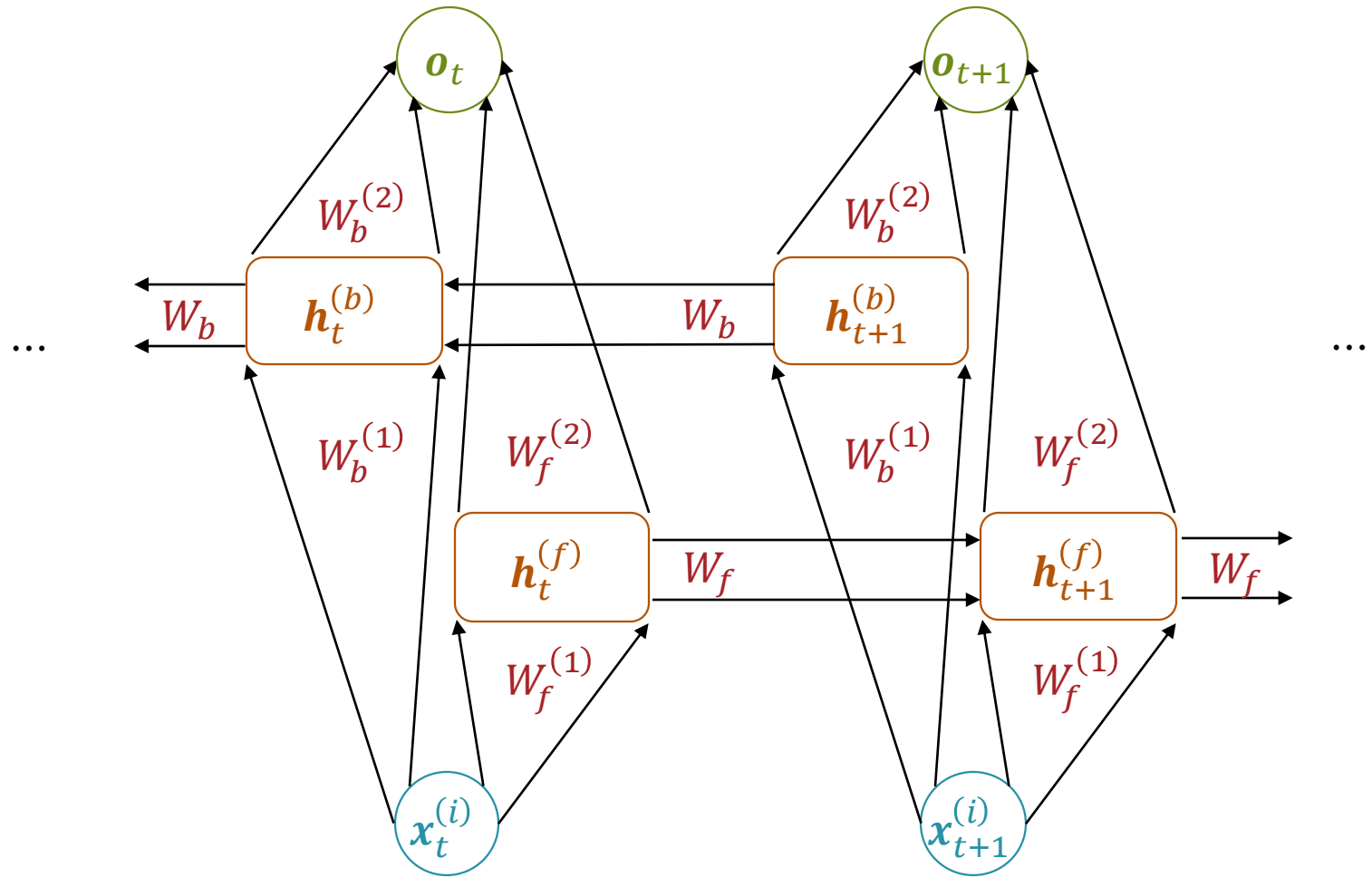
$$\mathbf{h}_t^{(f)} = \left[ 1, \theta \left( W_f^{(1)} \mathbf{x}_t^{(i)} + W_f \mathbf{h}_{t-1} \right) \right]^T \text{ and } \mathbf{h}_t^{(b)} = \left[ 1, \theta \left( W_b^{(1)} \mathbf{x}_t^{(i)} + W_b \mathbf{h}_{t+1} \right) \right]^T$$
$$\mathbf{o}_t = \hat{y}_t^{(i)} = \theta \left( W_f^{(2)} \mathbf{h}_t^{(f)} + W_b^{(2)} \mathbf{h}_t^{(b)} \right)$$



# Unrolling Bidirectional Recurrent Neural Networks

$$\mathbf{o}_t = \hat{y}_t^{(i)} = \theta \left( W_f^{(2)} \mathbf{h}_t^{(f)} + W_b^{(2)} \mathbf{h}_t^{(b)} \right)$$

$$\mathbf{h}_t^{(f)} = \left[ 1, \theta \left( W_f^{(1)} \mathbf{x}_t^{(i)} + W_f \mathbf{h}_{t-1} \right) \right]^T \text{ and } \mathbf{h}_t^{(b)} = \left[ 1, \theta \left( W_b^{(1)} \mathbf{x}_t^{(i)} + W_b \mathbf{h}_{t+1} \right) \right]^T$$



# Training RNNs

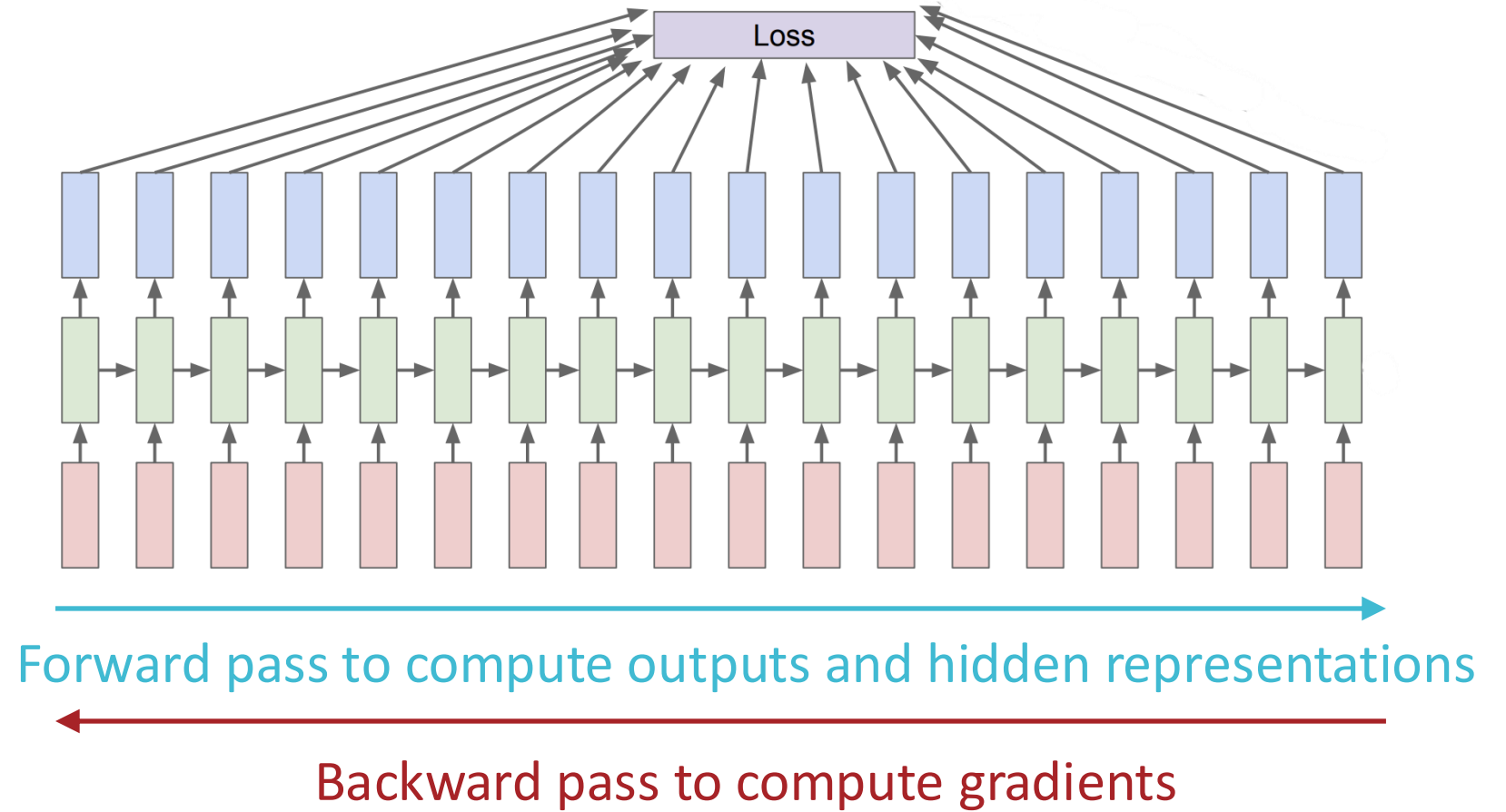
- A (deep/bidirectional) RNN simply represents a (somewhat complicated) computation graph
  - Weights ( $W^{(1)}$ ,  $W_h$  and  $W^{(2)}$ ) are shared between different timesteps, significantly reducing the number of parameters to be learned!
- Can be trained using (stochastic) gradient descent/backpropagation → “backpropagation through time”



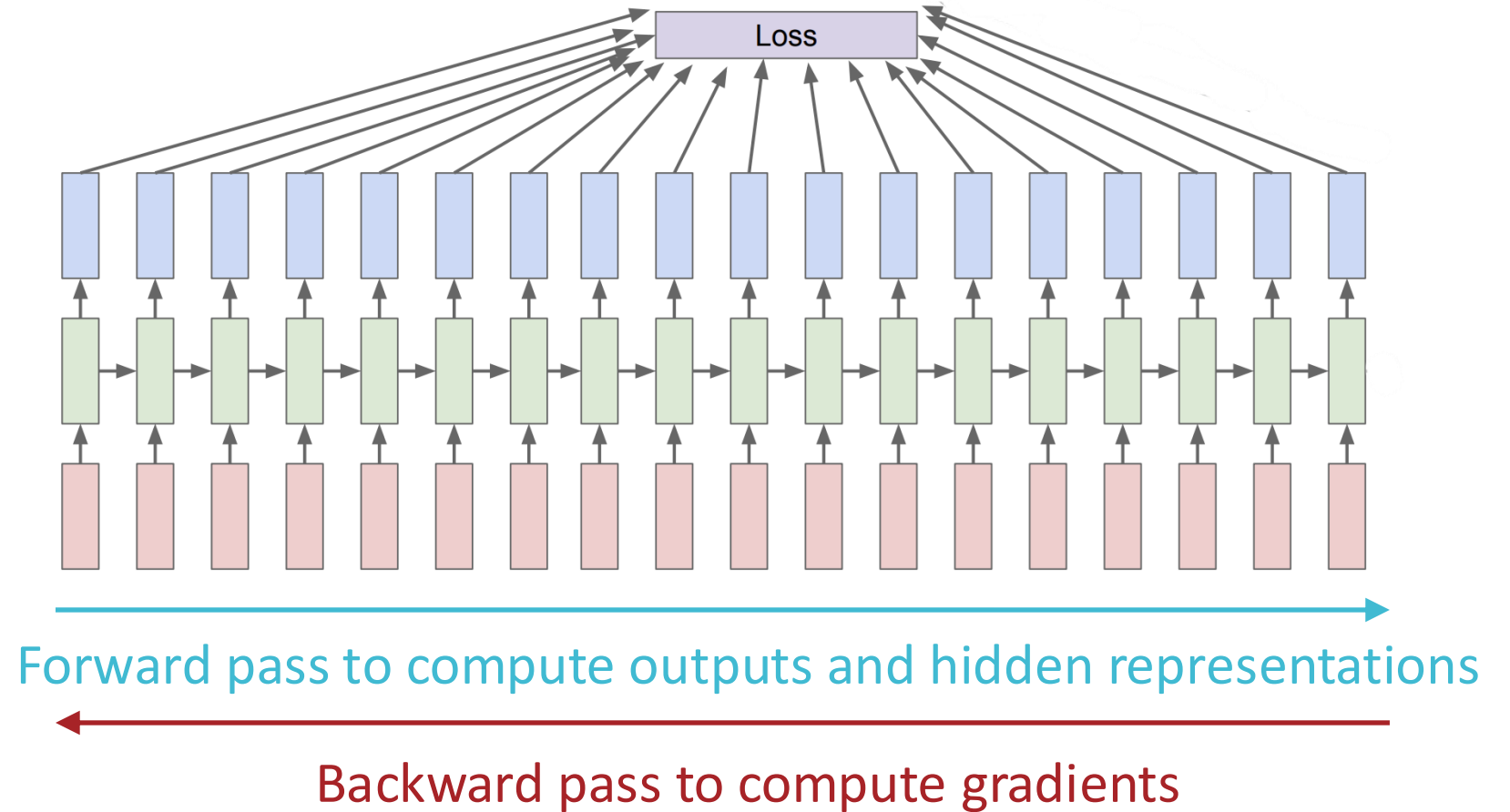
# Backprop Through Time

- Each hidden state  $h_t$  influences not only its immediate output  $y_t$ , but also all future hidden states  $h_{t+1}, h_{t+2}, \dots$
- Thus, each parameter affects the loss indirectly **through time**.
- So, during training, need to propagate the gradient back through all those time steps.
- To train the RNN, we unroll it over the sequence, treating it like a deep feed-forward network with  $T$  layers — one per time step — all sharing the same parameters.
- Then, we apply standard backpropagation over this unrolled network.

# Training RNNs



# Training RNNs: Challenges

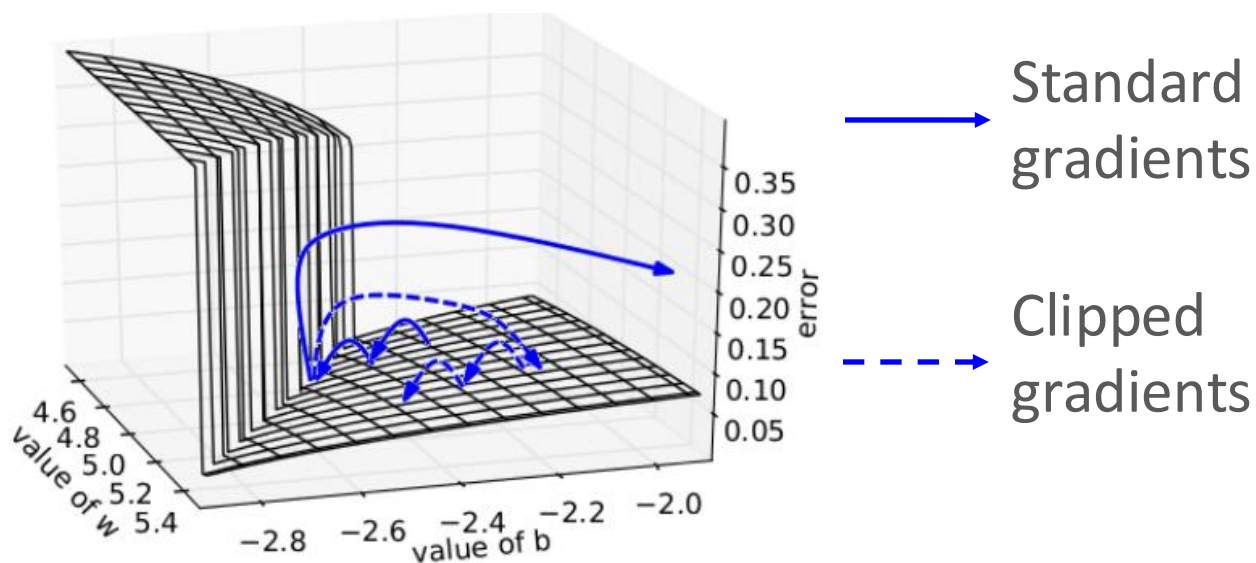


- Issue: as the sequence length grows, the gradient is more likely to explode or vanish

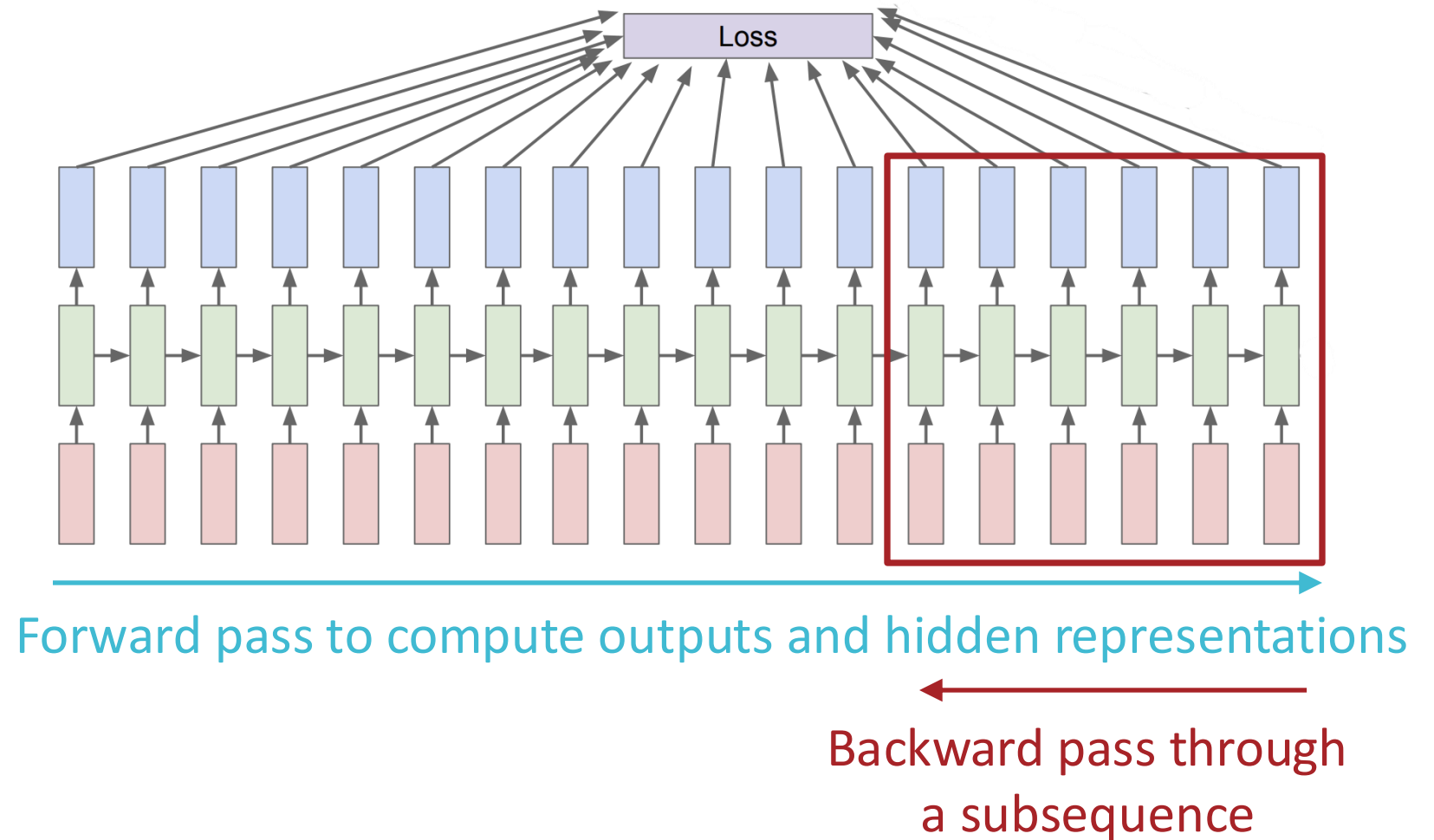
# Gradient Clipping (Pascanu et al., 2013)

- Common strategy to deal with exploding gradients: if the magnitude of the gradient ever exceeds some threshold, simply scale it down to the threshold

$$G = \begin{cases} \nabla_W \ell^{(i)} & \text{if } \|\nabla_W \ell^{(i)}\|_2 \leq \tau \\ \left( \frac{\tau}{\|\nabla_W \ell^{(i)}\|_2} \right) \nabla_W \ell^{(i)} & \text{otherwise} \end{cases}$$



# Truncated Backpropagation Through Time



- Idea: limit the number of time steps to backprop through

# Long Short-Term Memory (Hochreiter & Schmidhuber, 1997)

- LSTM networks address the vanishing gradient problem by replacing hidden layers with *memory cells*
- Each cell still computes a hidden representation  $\mathbf{h}_t$  but also maintains a separate internal *state*,  $\mathbf{c}_t$
- The flow of information through a cell is manipulated by three *gates*:
  - An input gate,  $\mathbf{I}_t$ , that controls how much the state looks like the normal RNN hidden layer
  - An output gate,  $\mathbf{O}_t$ , that “releases” the hidden representation to later timesteps
  - A forget gate,  $\mathbf{F}_t$ , that determines if the previous memory cell’s state affects the current internal state

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- Gates are implemented as sigmoids: a value of 0 would be a fully closed gate and 1 would be fully open

$$I_t = \sigma \left( W_{ix} \mathbf{x}_t^{(i)} + W_{ih} \mathbf{h}_{t-1} \right)$$

$$O_t = \sigma \left( W_{ox} \mathbf{x}_t^{(i)} + W_{oh} \mathbf{h}_{t-1} \right)$$

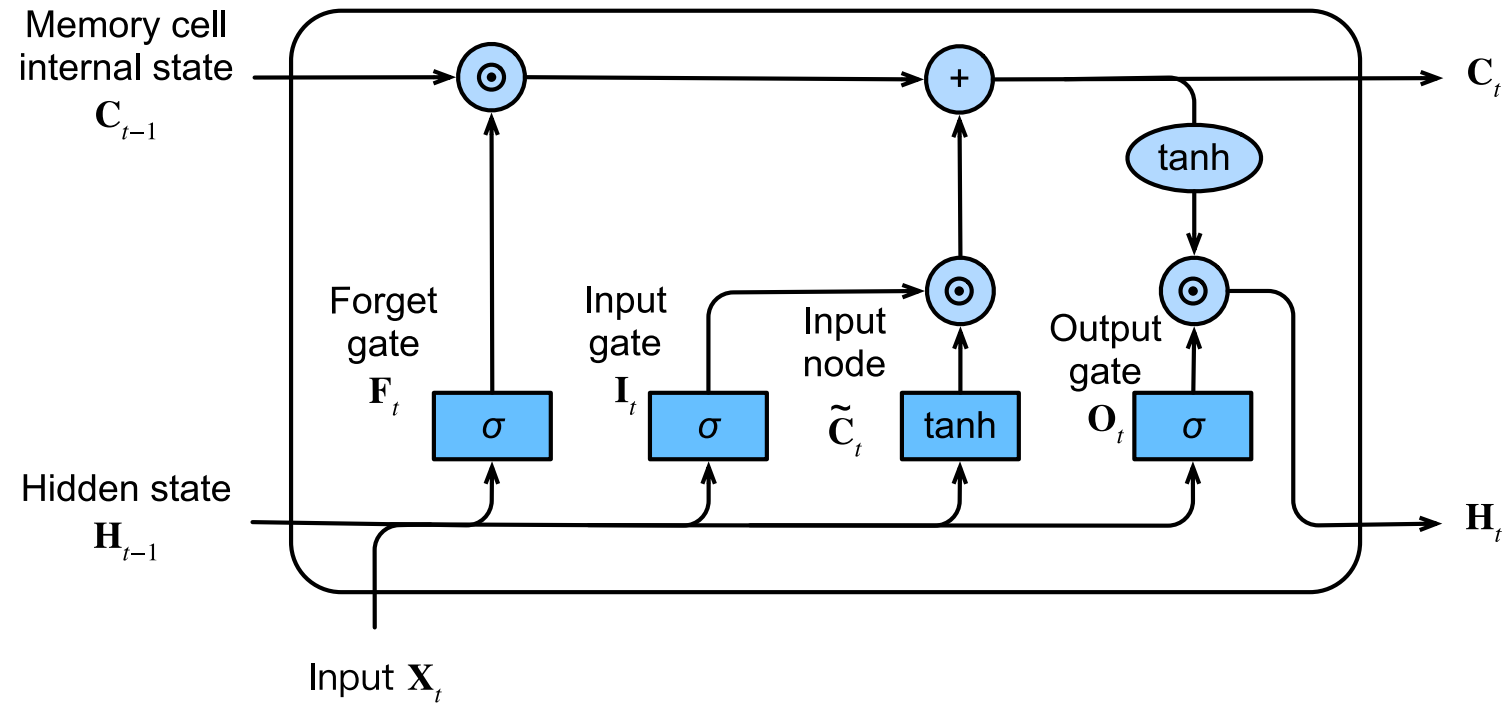
$$F_t = \sigma \left( W_{fx} \mathbf{x}_t^{(i)} + W_{fh} \mathbf{h}_{t-1} \right)$$

$$\mathbf{C}_t = F_t \odot \mathbf{C}_{t-1} + I_t \odot \theta \left( W^{(1)} \mathbf{x}_t^{(i)} + W_h \mathbf{h}_{t-1} \right)$$

$$\mathbf{h}_t = \mathbf{C}_t \odot \mathbf{O}_t$$

# Long Short-Term Memory (Hochreiter & Schmidhuber, 1997)

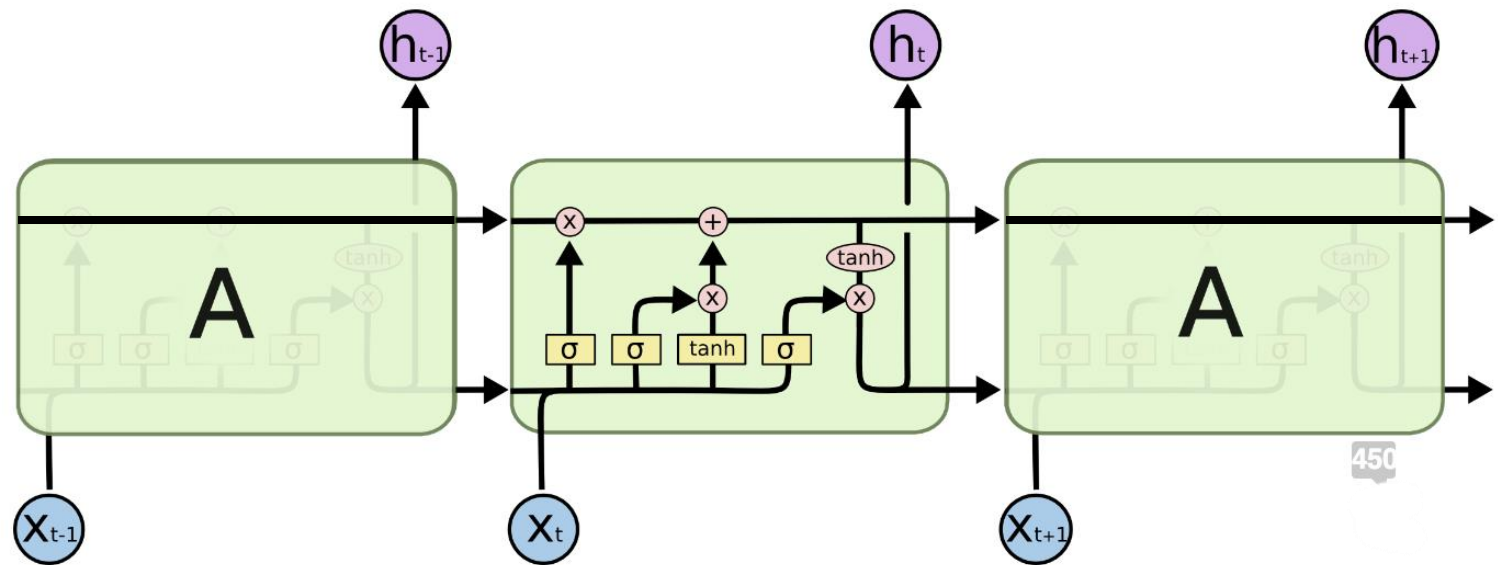
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- The internal state allows information to move through time without needing to affect the hidden representations!

# Applications of LSTMs



**2018:** [OpenAI](#) used LSTM trained by policy gradients to beat humans in the complex video game of Dota 2,<sup>[11]</sup> and to control a human-like robot hand that manipulates physical objects with unprecedented dexterity.<sup>[10][54]</sup>

**2019:** [DeepMind](#) used LSTM trained by policy gradients to excel at the complex video game of [Starcraft II](#).<sup>[12][54]</sup>

# Key Takeaways

- Recurrent neural networks use contextual information to reason about sequential data.
  - Can still be learned using backpropagation → backpropagation through time.
  - Susceptible to exploding/vanishing gradients for long training sequences.
  - LSTMs allow contextual information to reach later timesteps without directly affecting intermediate hidden representations.