

10-701: Introduction to Machine Learning

Lecture 12 - Recurrent Neural Networks

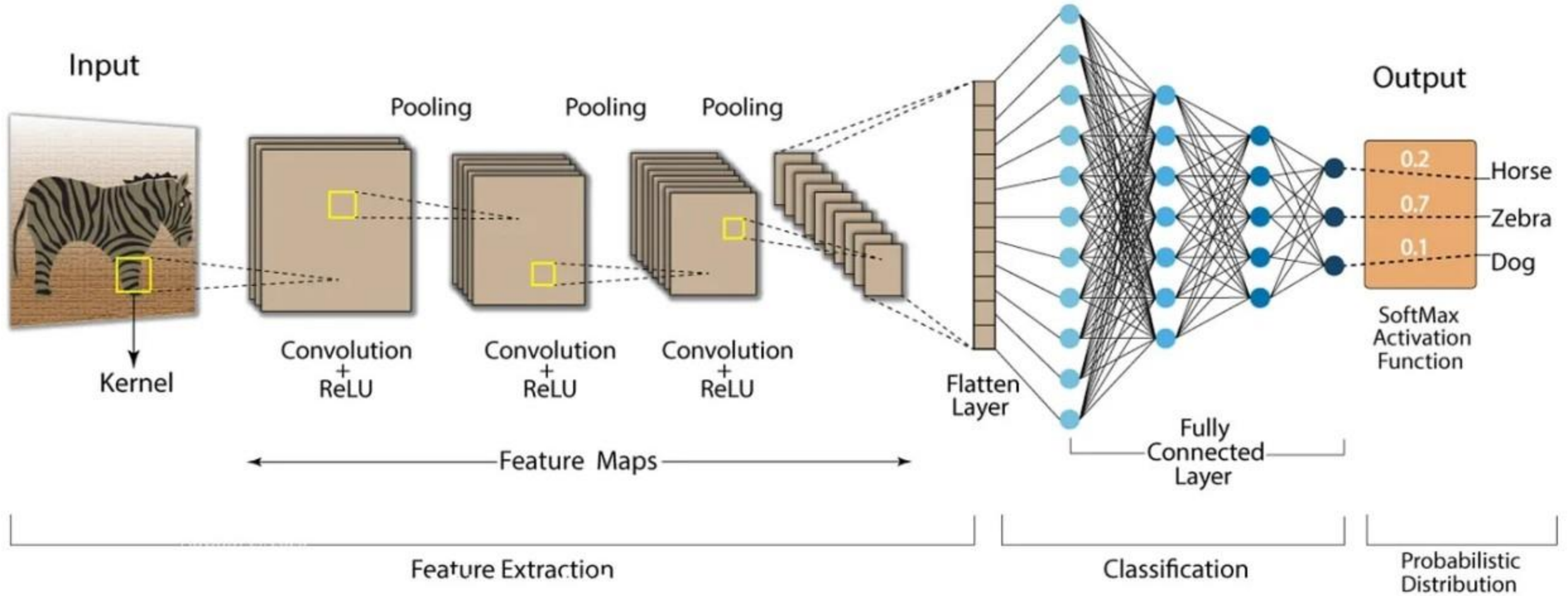
Hoda Heidari

* 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

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			

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

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

 $=$

0	-1		

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

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




 $=$

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

Convolutional Filters

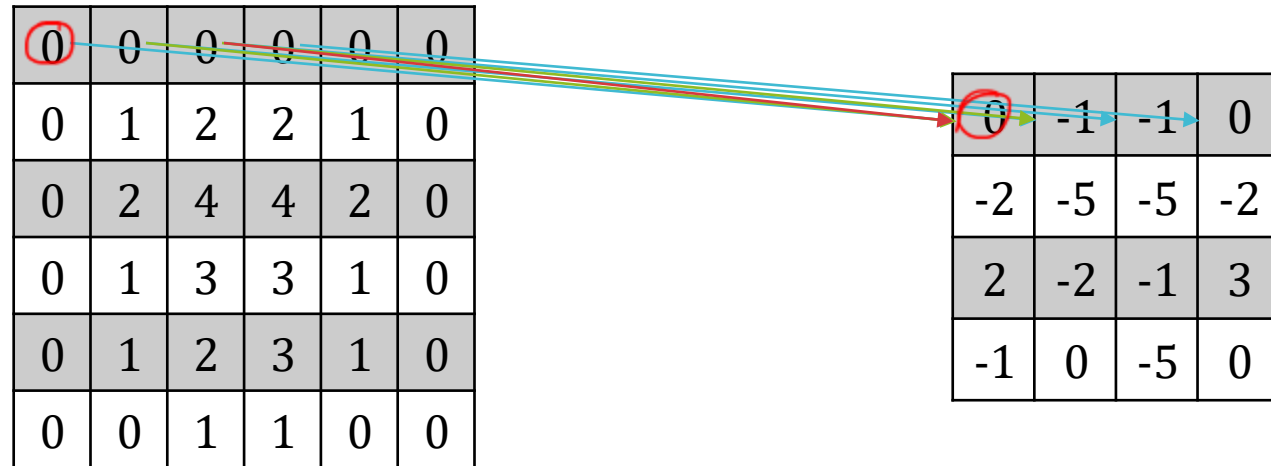
Operation	Kernel ω	Image result $g(x,y)$
Identity	$\begin{bmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix}$	 ✓
Edge detection	2 $\begin{bmatrix} 1 & 0 & -1 \\ 0 & 0 & 0 \\ -1 & 0 & 1 \end{bmatrix}$	
	2 $\begin{bmatrix} \cancel{0} & \textcircled{1} & \cancel{0} \\ \textcircled{1} & \textcircled{-4} & \textcircled{1} \\ \cancel{0} & \textcircled{1} & \cancel{0} \end{bmatrix}$ ←	
	3 $\begin{bmatrix} \textcircled{-1} & \textcircled{-1} & \textcircled{-1} \\ \textcircled{-1} & \textcircled{8} & \textcircled{-1} \\ \textcircled{-1} & \textcircled{-1} & \textcircled{-1} \end{bmatrix}$	

More Filters

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

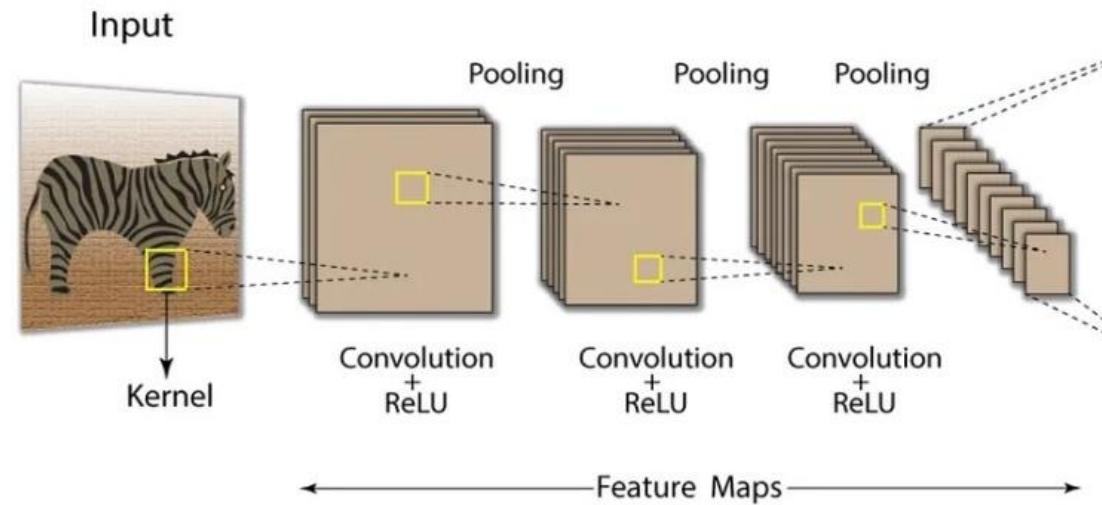
 $*$

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

- 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	-2	

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	-2	1

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	-2	1
0		

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

=

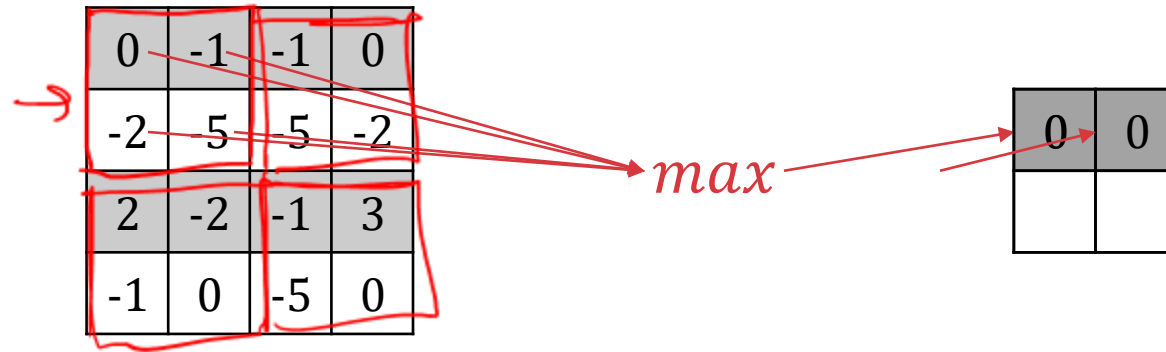
-2	-2	1
0	1	1
1	2	0

$$0 \cdot 0 + 0 \cdot 1 + 0 \cdot 1 + 1 \cdot (-2) = -2$$

- 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

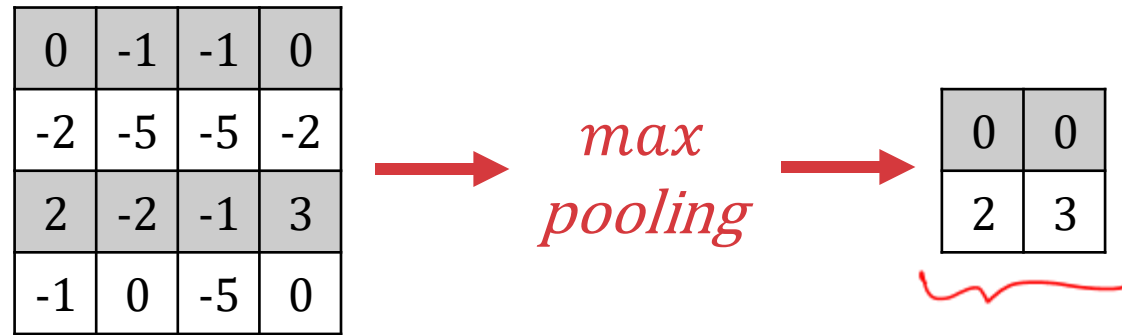
Downsampling: Pooling

- Combine multiple adjacent nodes into a single node

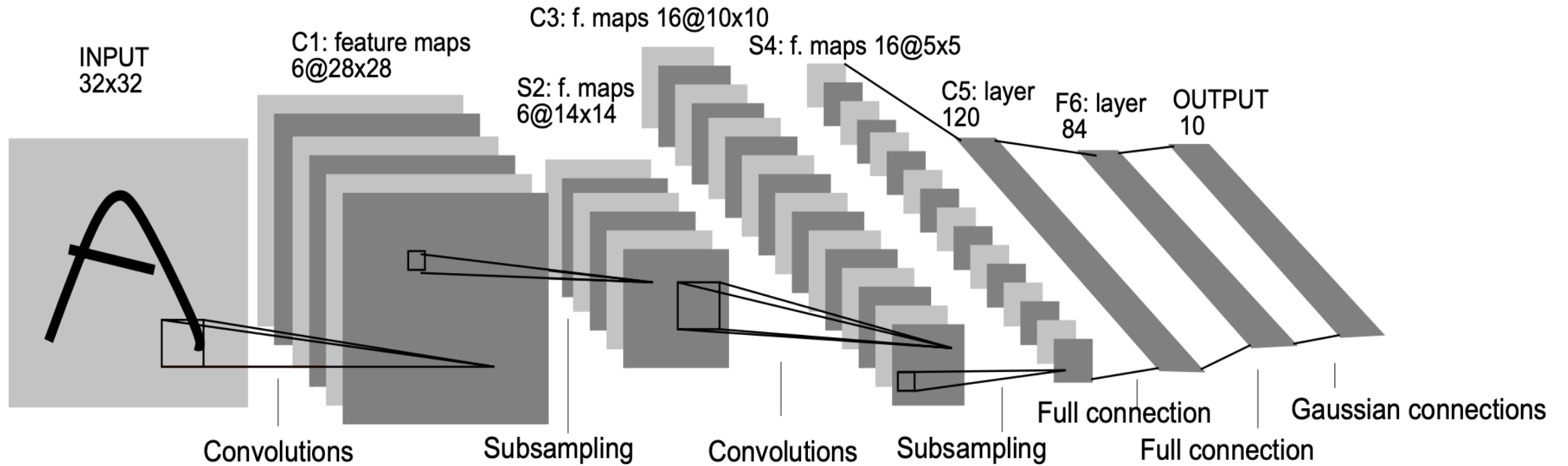


Downsampling: Pooling

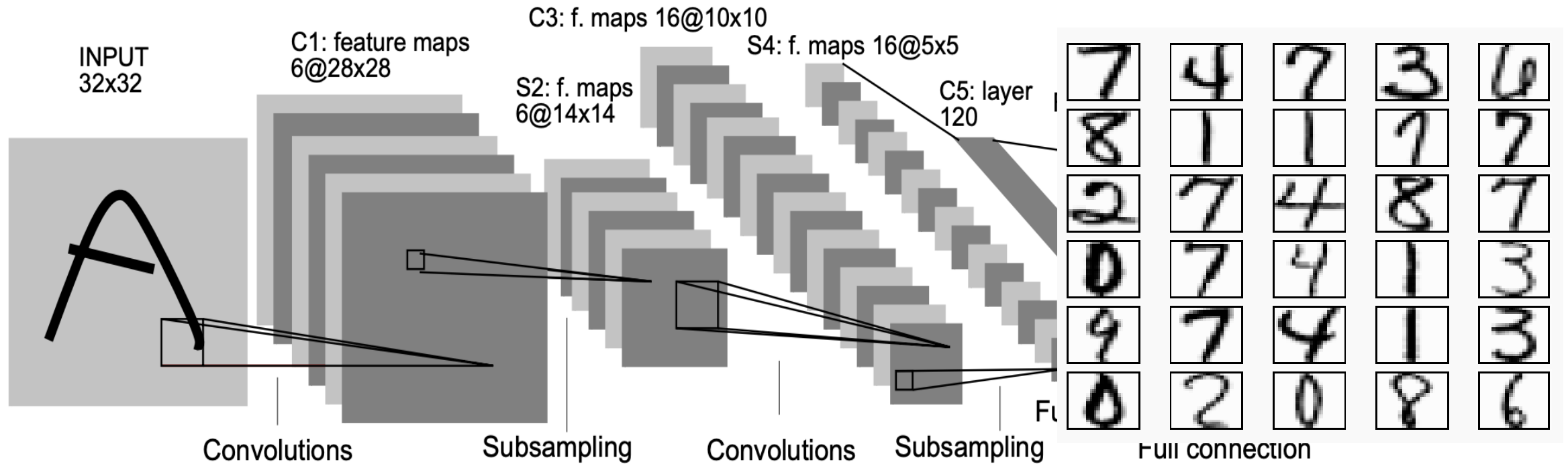
- Combine multiple adjacent nodes into a single node



- **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.



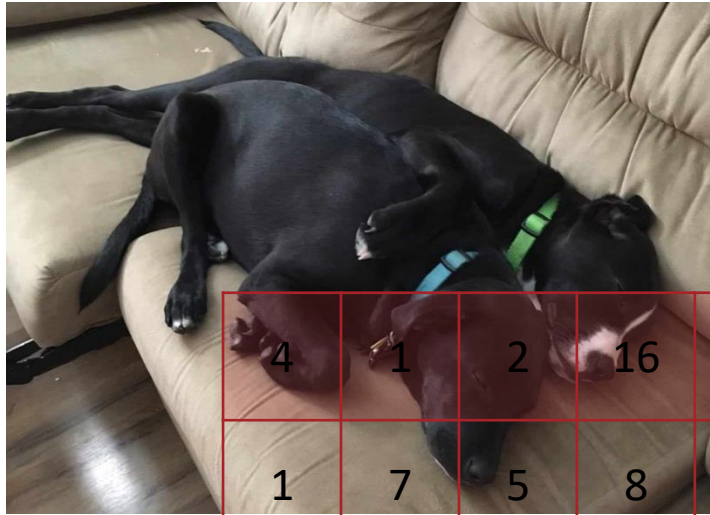
LeNet (LeCun et al., 1998)



- 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

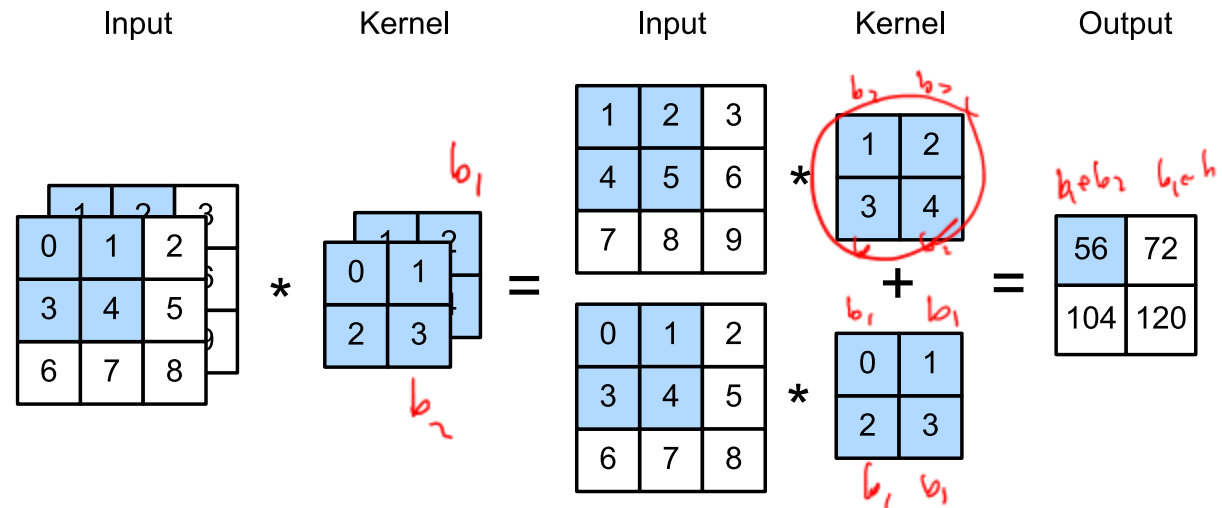
5	2	6	14	15	8
26	3	6	8	4	9
0	15	24	6	1	8
7	4	9	5	24	17

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

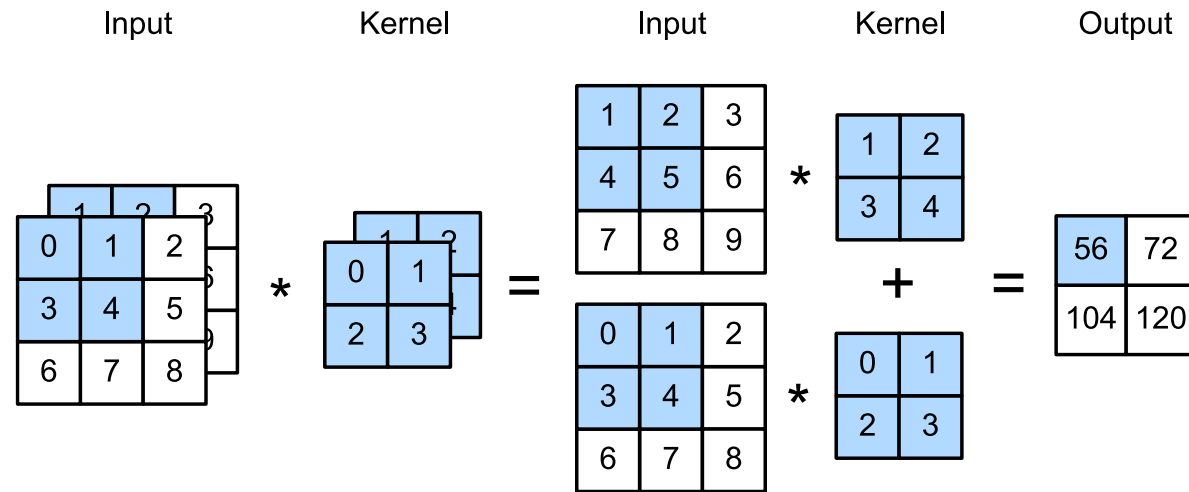


- For c channels and $h \times w$ -sized filters, we have $chw + c$ learnable parameters (each filter has a bias term)

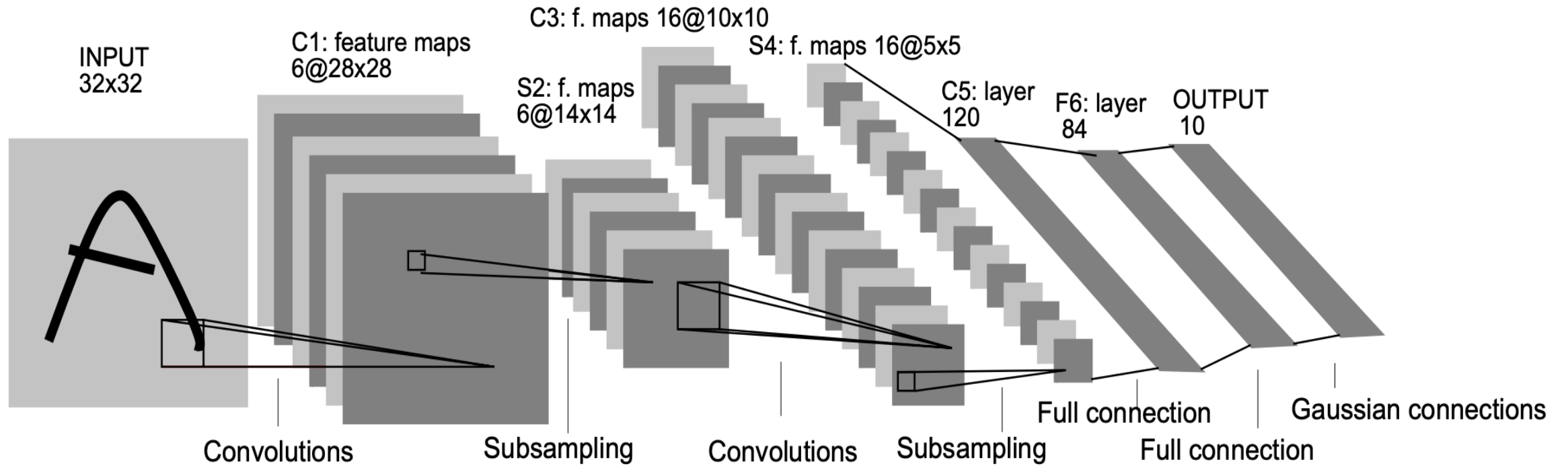
bias terms ?
why not combine them

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



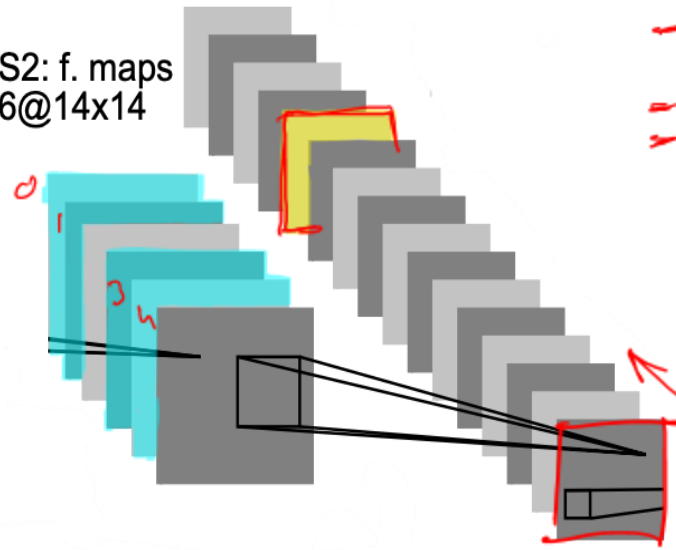
- Questions:
 - Why might we want a different filter for each input?
 - Why do we combine them together into a single output channel?



- 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

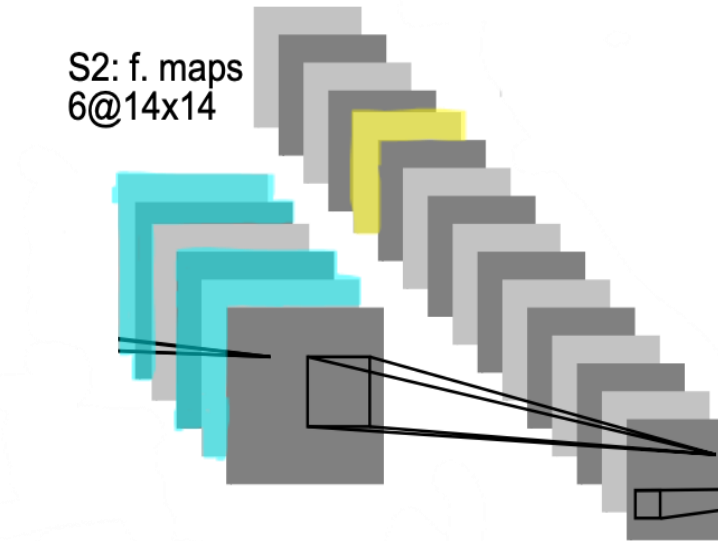
TABLE I

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

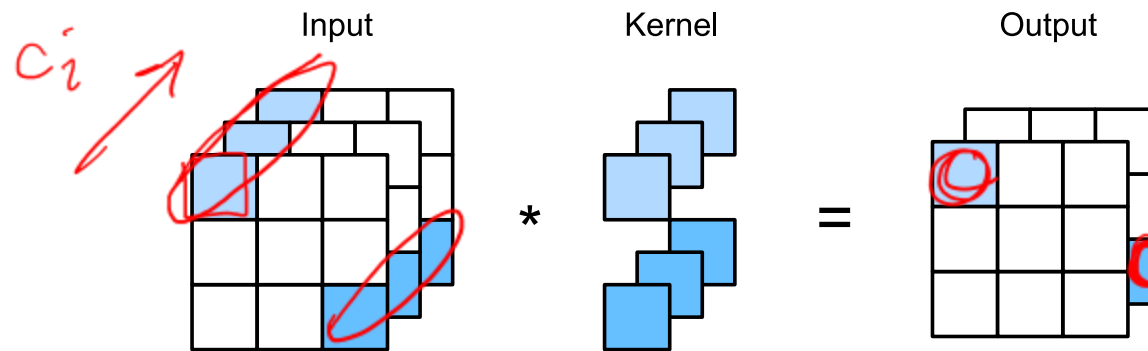
TABLE I

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: 1×1 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: 1×1 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 1×1 convolutions are used to downsample intermediate representations.

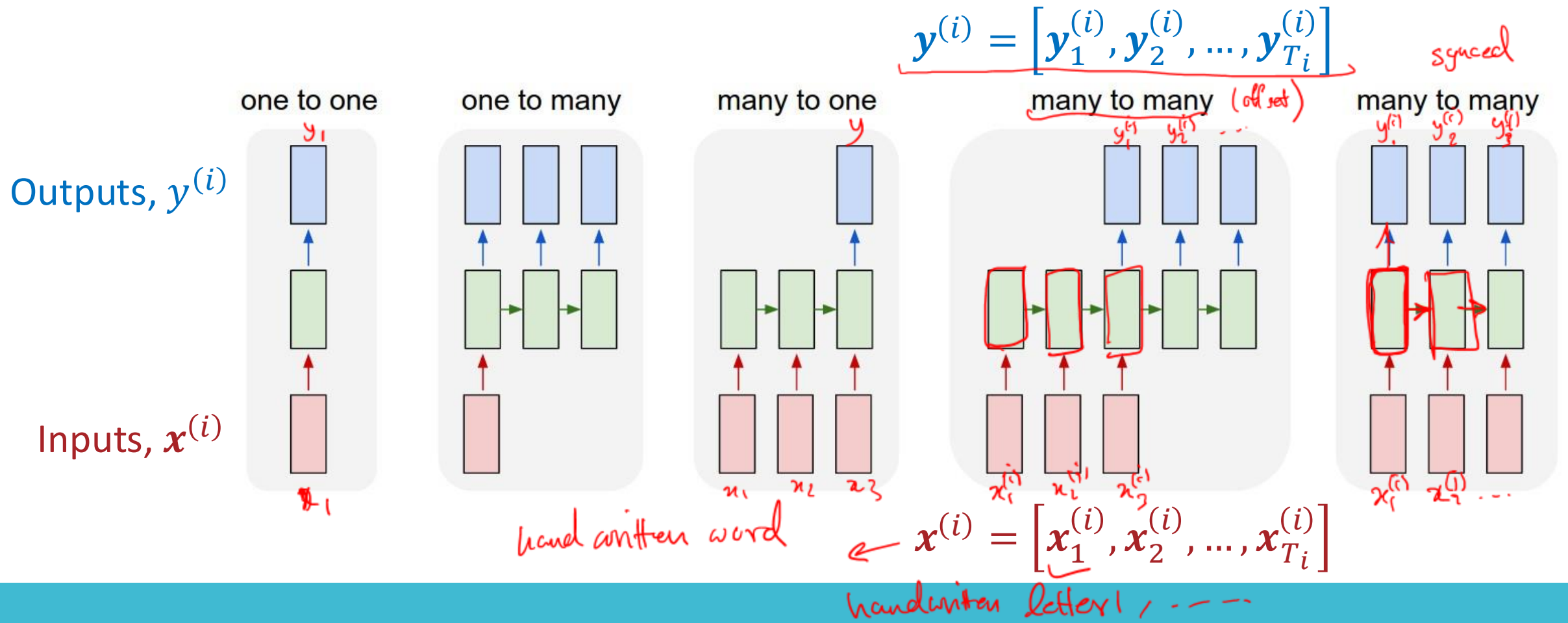
Example: Handwriting Recognition

U N E X P E C T E D

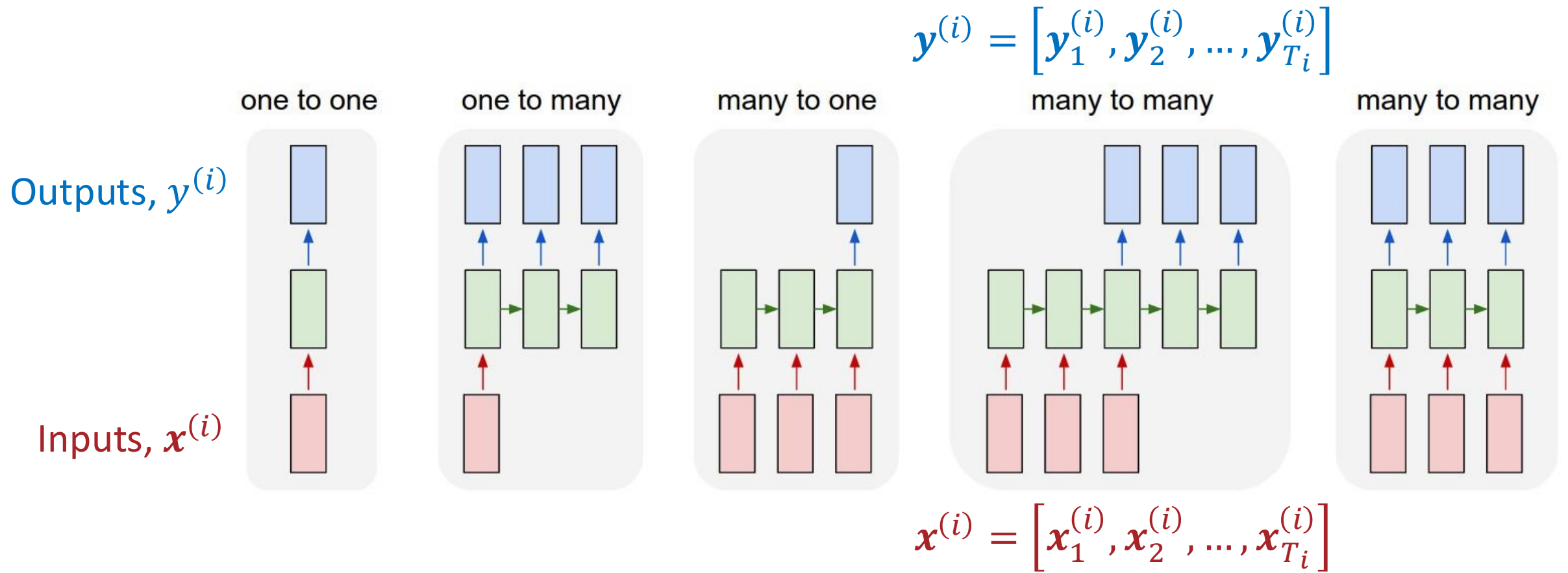
V O L C A N I C

E M B R A C E S

C K N
B



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**

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

$$\rightarrow \mathbf{x}^{(n)} = [\underbrace{x_1^{(n)}}_{\text{red bracket}}, \dots, \underbrace{x_{T_n}^{(n)}}_{\text{red bracket}}]$$

$$\mathbf{y}^{(n)} = [\underbrace{y_1^{(n)}}_{\text{red bracket}}, \dots, \underbrace{y_{T_n}^{(n)}}_{\text{red bracket}}]$$

Recurrent Neural Networks

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

hidden rep state $x_t^{(i)}$

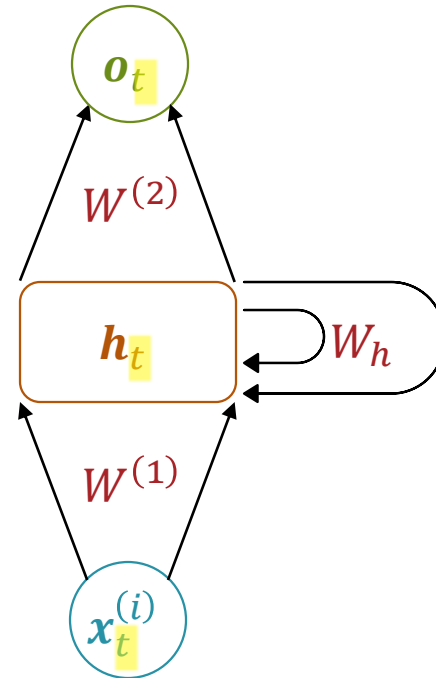
$$\leftarrow \underline{h}_t = \left[1, \theta \left(\underline{W^{(1)}} \underline{x_t^{(i)}} + \underline{W_h} \underline{h_{t-1}} \right) \right]^T \text{ and } \underline{o}_t = \underline{\hat{y}_t^{(i)}} = \underline{\tilde{\theta}} \left(\underline{W^{(2)}} \underline{h_t} \right)$$

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

- The same parameters $\underline{W^{(1)}}$, $\underline{W_h}$ and $\underline{W^{(2)}}$ 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

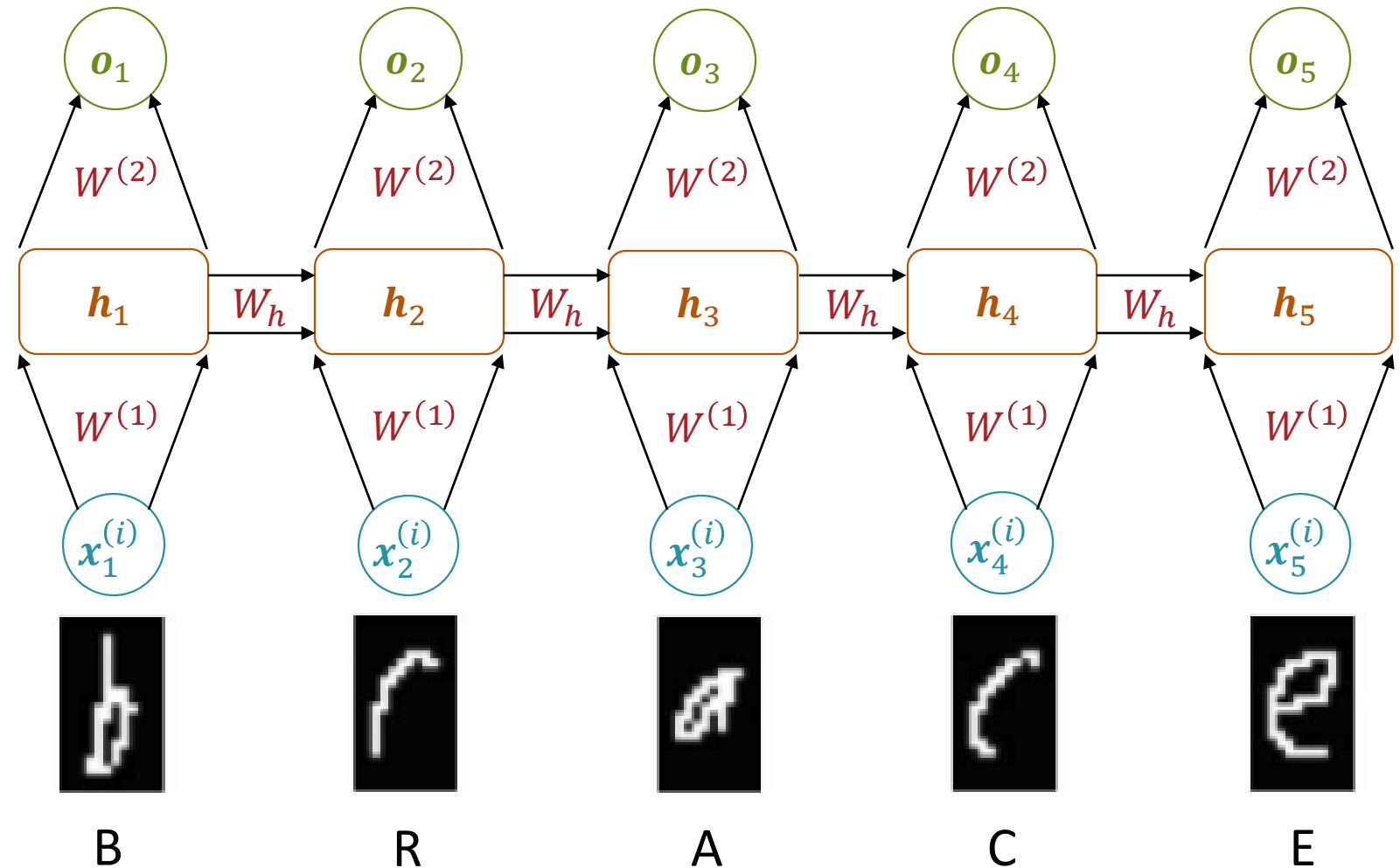
$$\mathbf{h}_t = \left[1, \theta \left(W^{(1)} \mathbf{x}_t^{(i)} + W_h \mathbf{h}_{t-1} \right) \right]^T \text{ and } \mathbf{o}_t = \hat{y}_t^{(i)} = \theta(W^{(2)} \mathbf{h}_t)$$



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

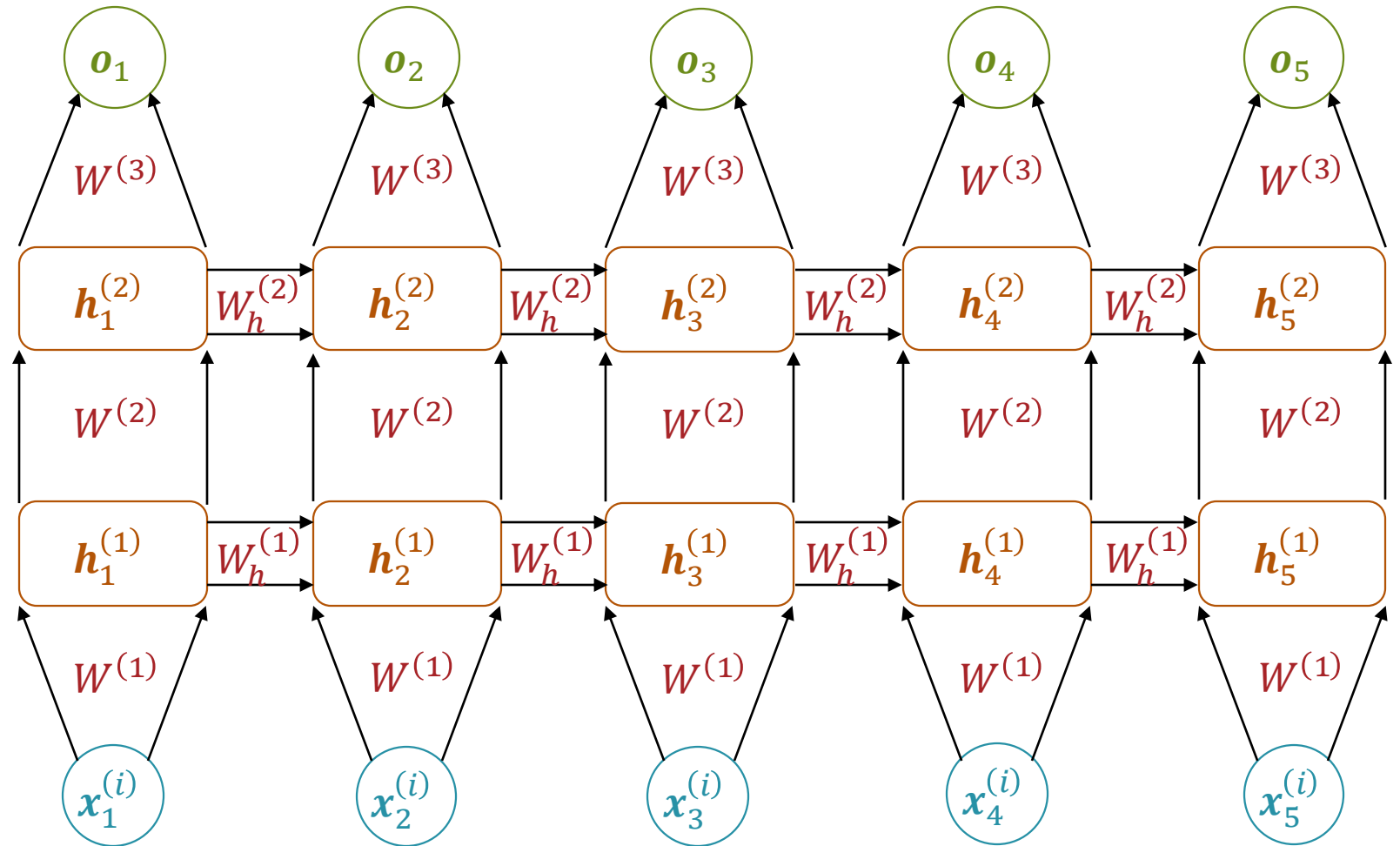
Unrolling Recurrent Neural Networks

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



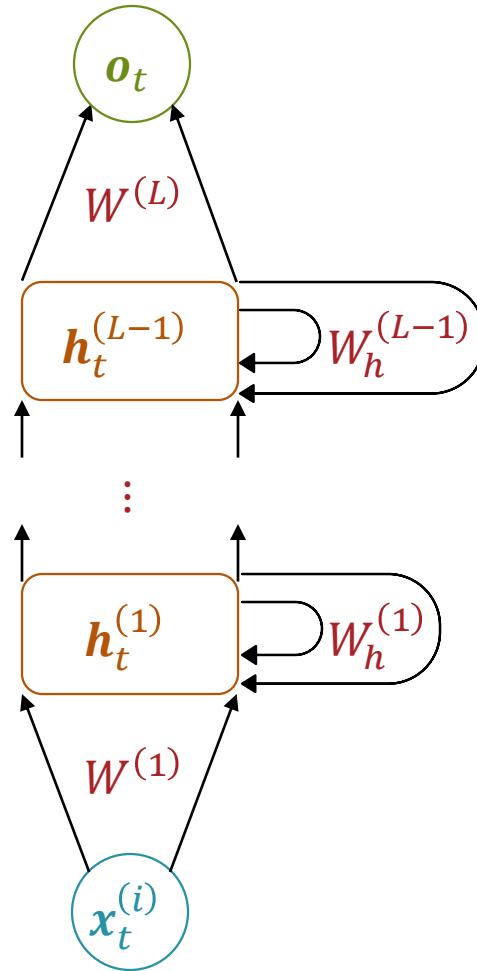
Deep Recurrent Neural Networks

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



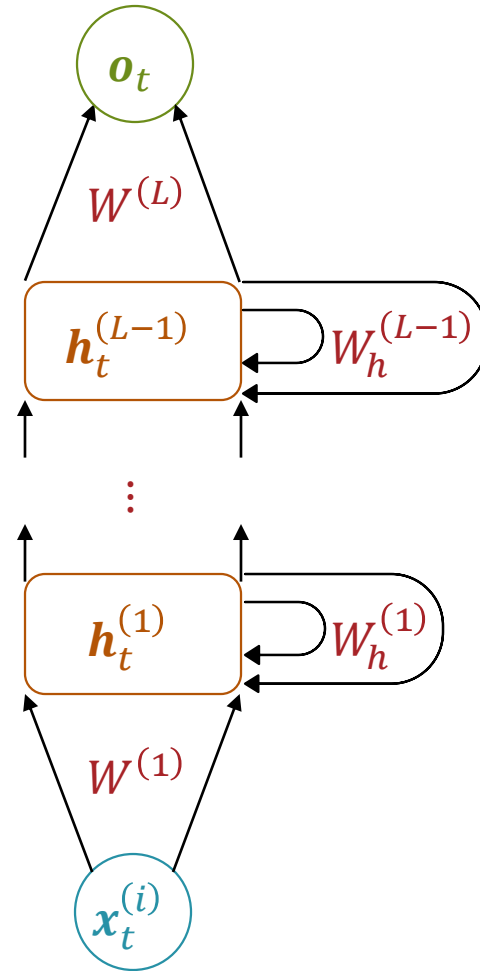
Deep Recurrent Neural Networks

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



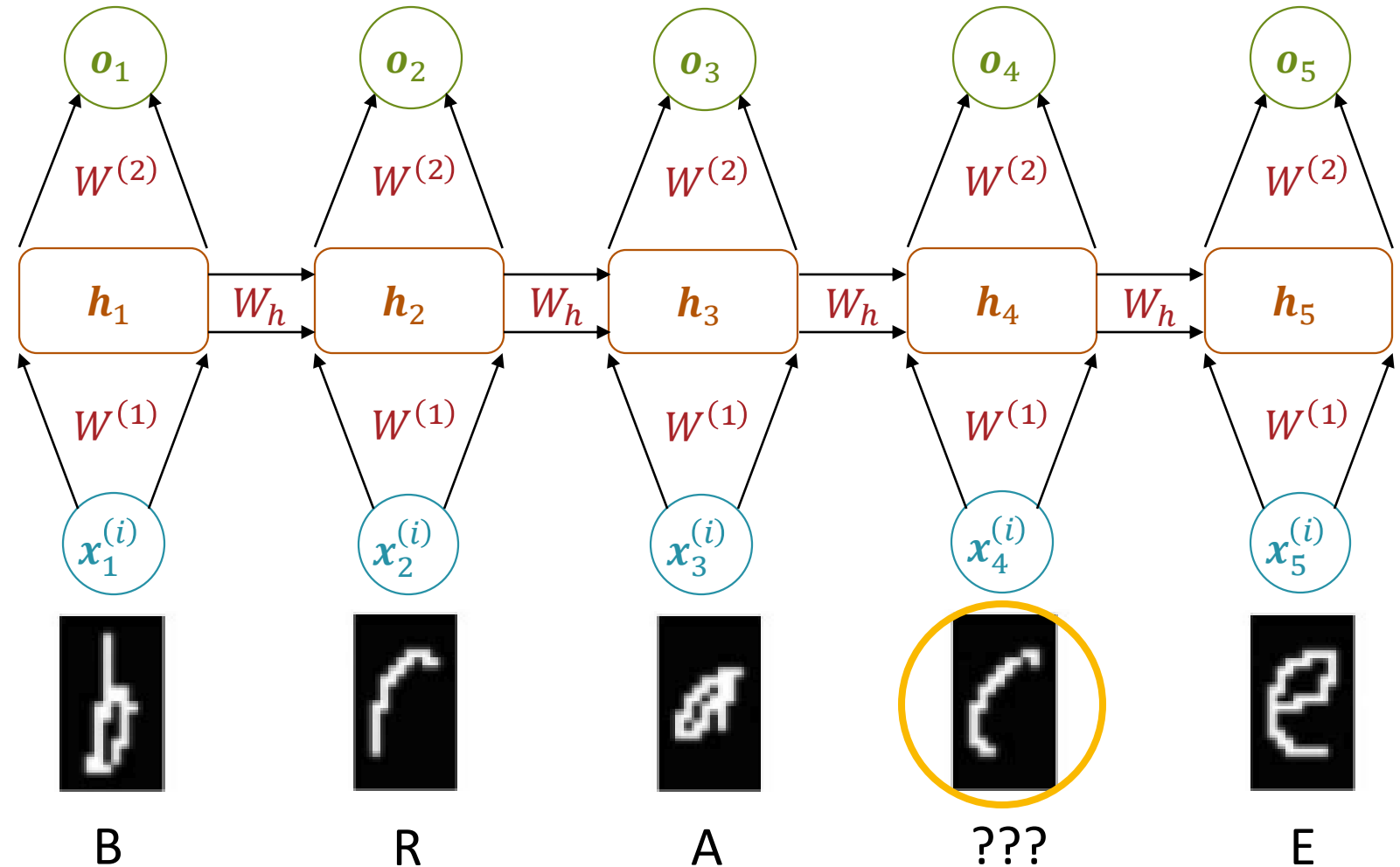
But why do we only pass information forward?
What if later time steps have useful information as well?

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



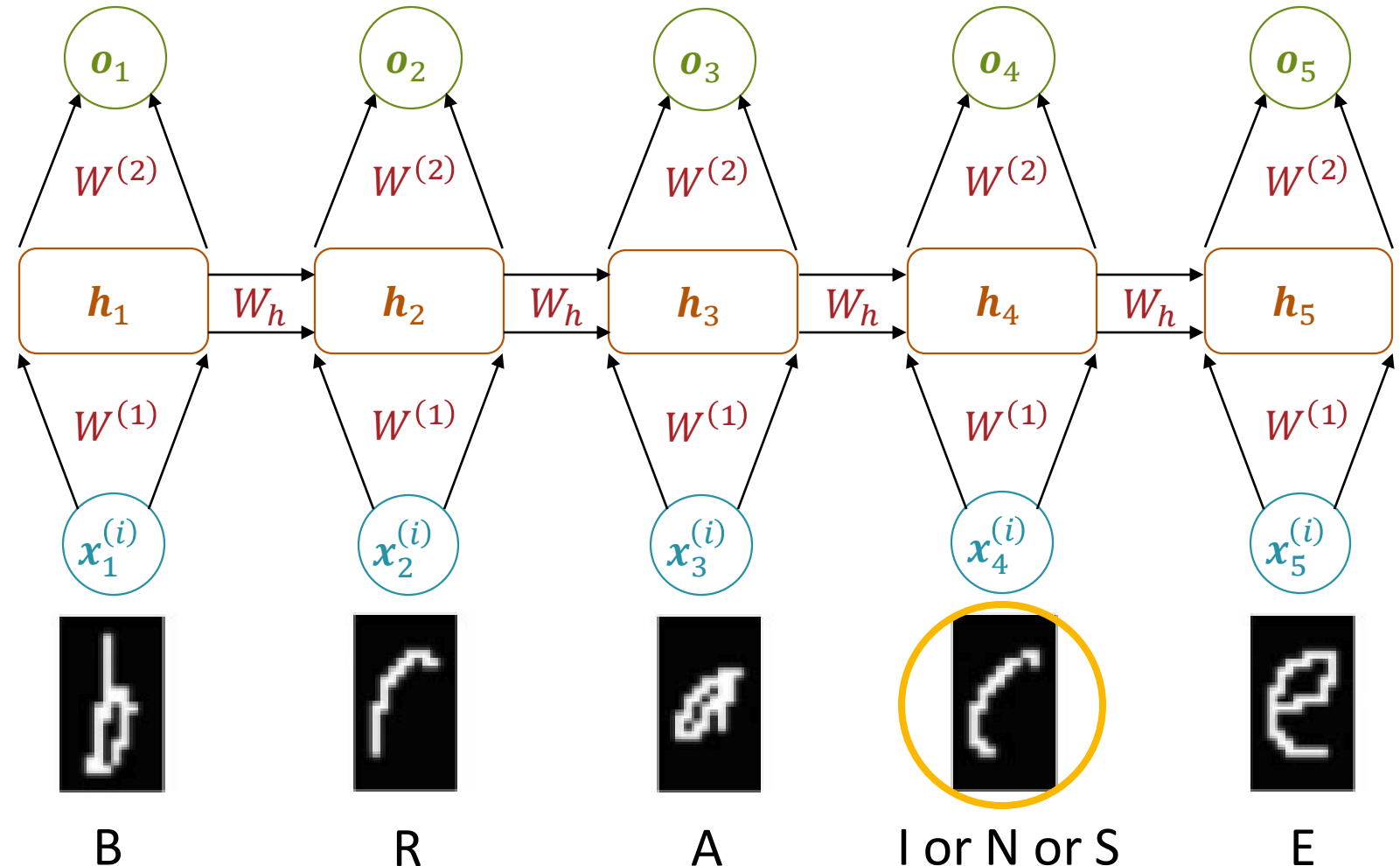
But why do we only pass information forward?
What if later time steps have useful information as well?

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



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

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

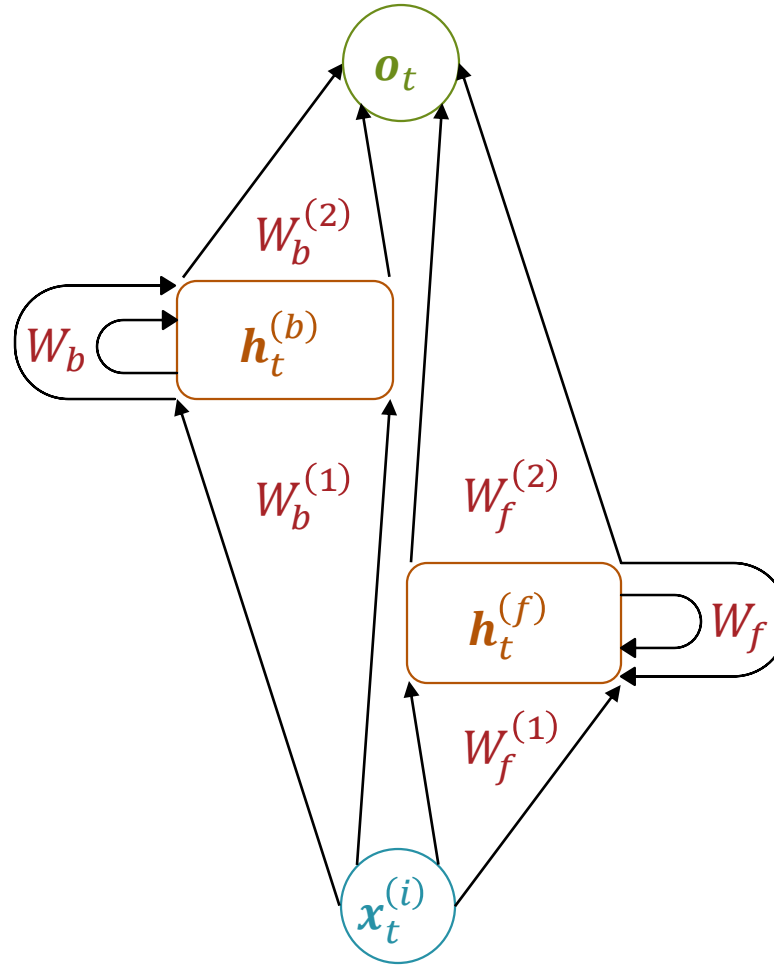


Bidirectional Recurrent Neural Networks

- 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

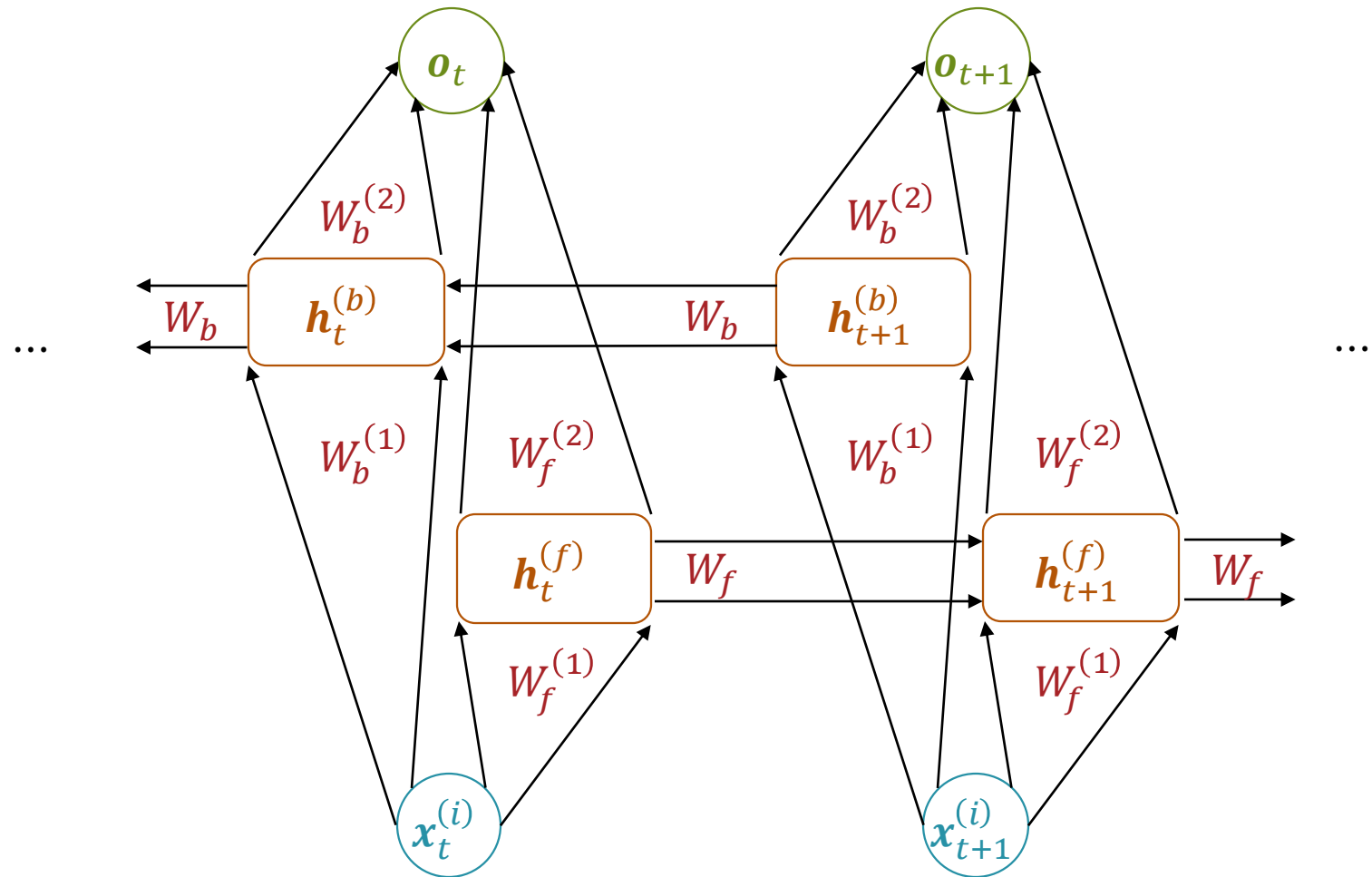
$$\mathbf{h}_t^{(f)} = \left[1, \theta \left(W_f^{(1)} \mathbf{x}_t^{(i)} + W_f \mathbf{h}_{t-1} \right) \right]^T \text{ and } \mathbf{h}_t^{(b)} = \left[1, \theta \left(W_b^{(1)} \mathbf{x}_t^{(i)} + W_b \mathbf{h}_{t+1} \right) \right]^T$$
$$\mathbf{o}_t = \hat{y}_t^{(i)} = \theta \left(W_f^{(2)}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



Unrolling Bidirectional Recurrent Neural Networks

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

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



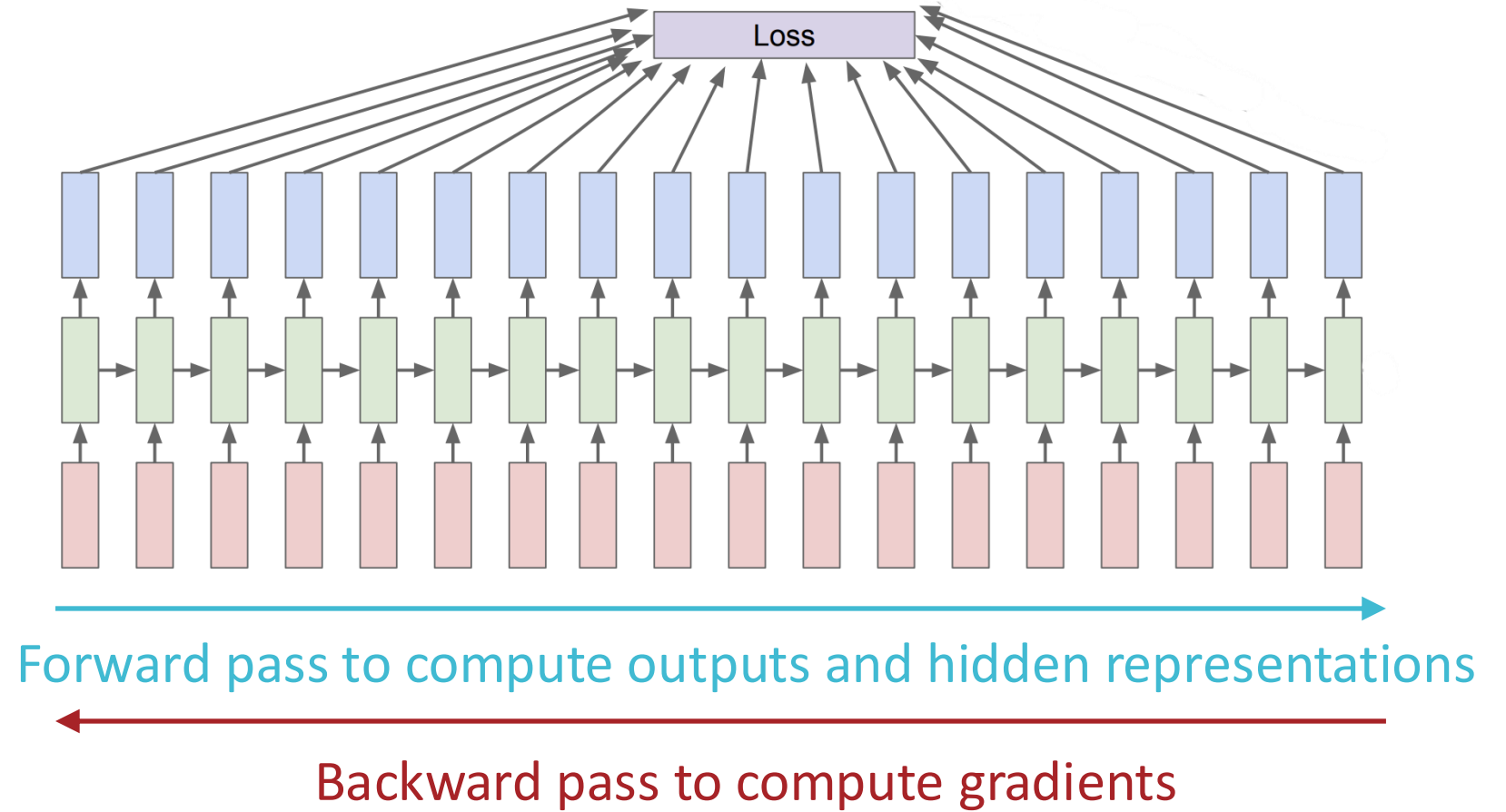
Training RNNs

- 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”

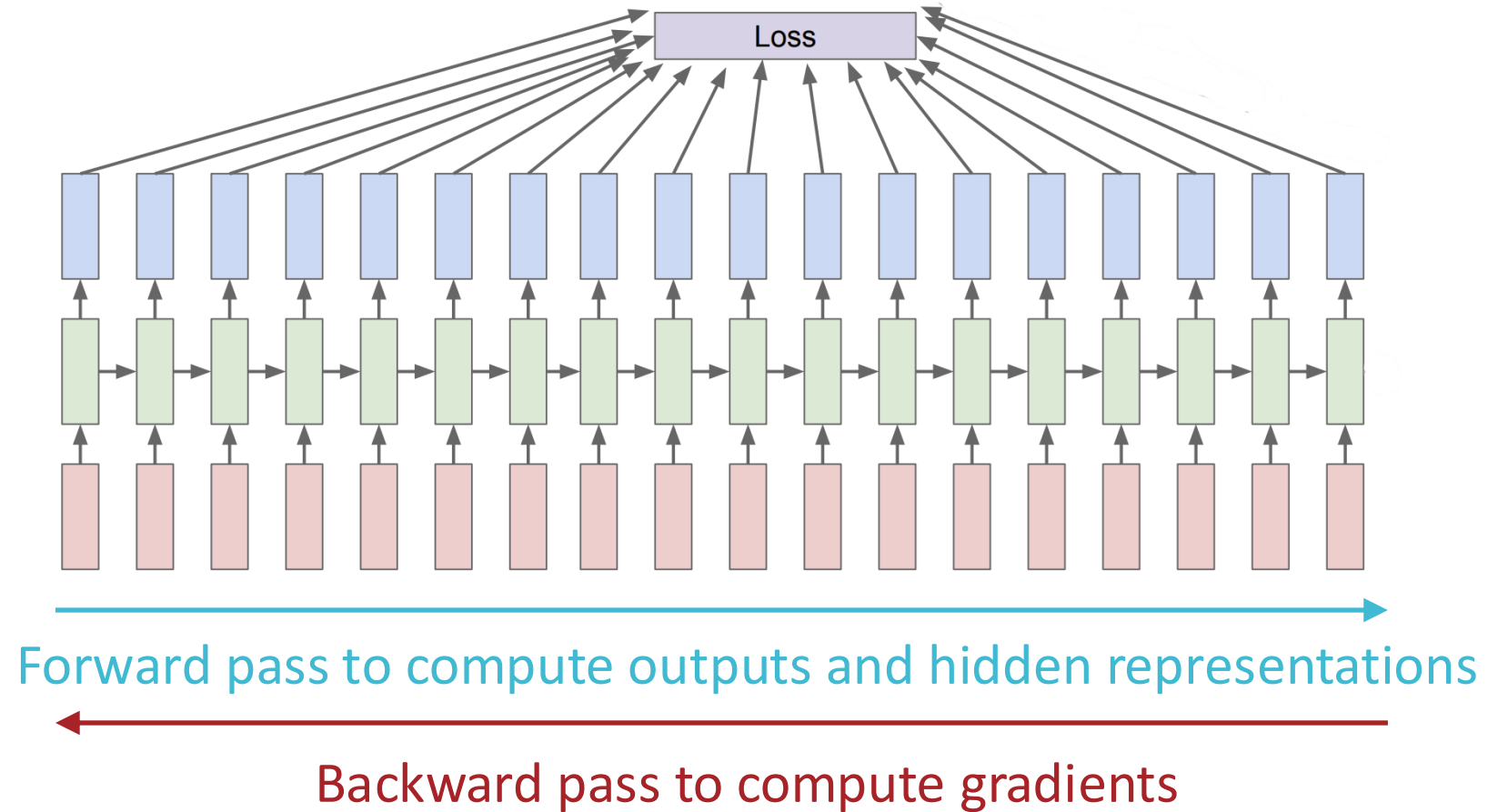
Backprop Through Time

- 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

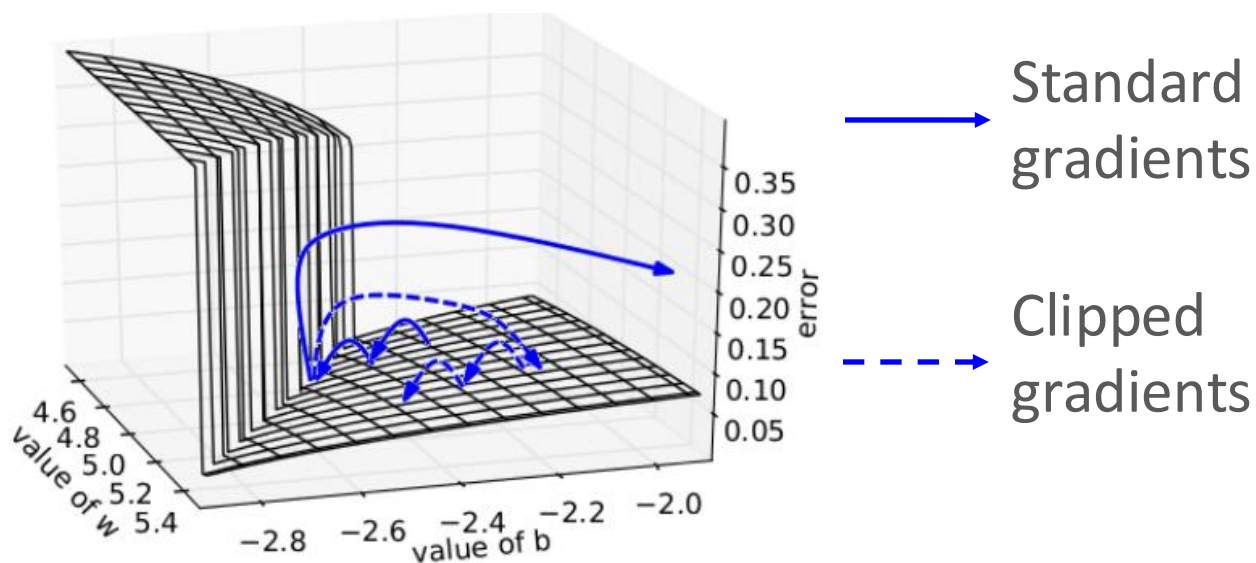


- Issue: as the sequence length grows, the gradient is more likely to explode or vanish

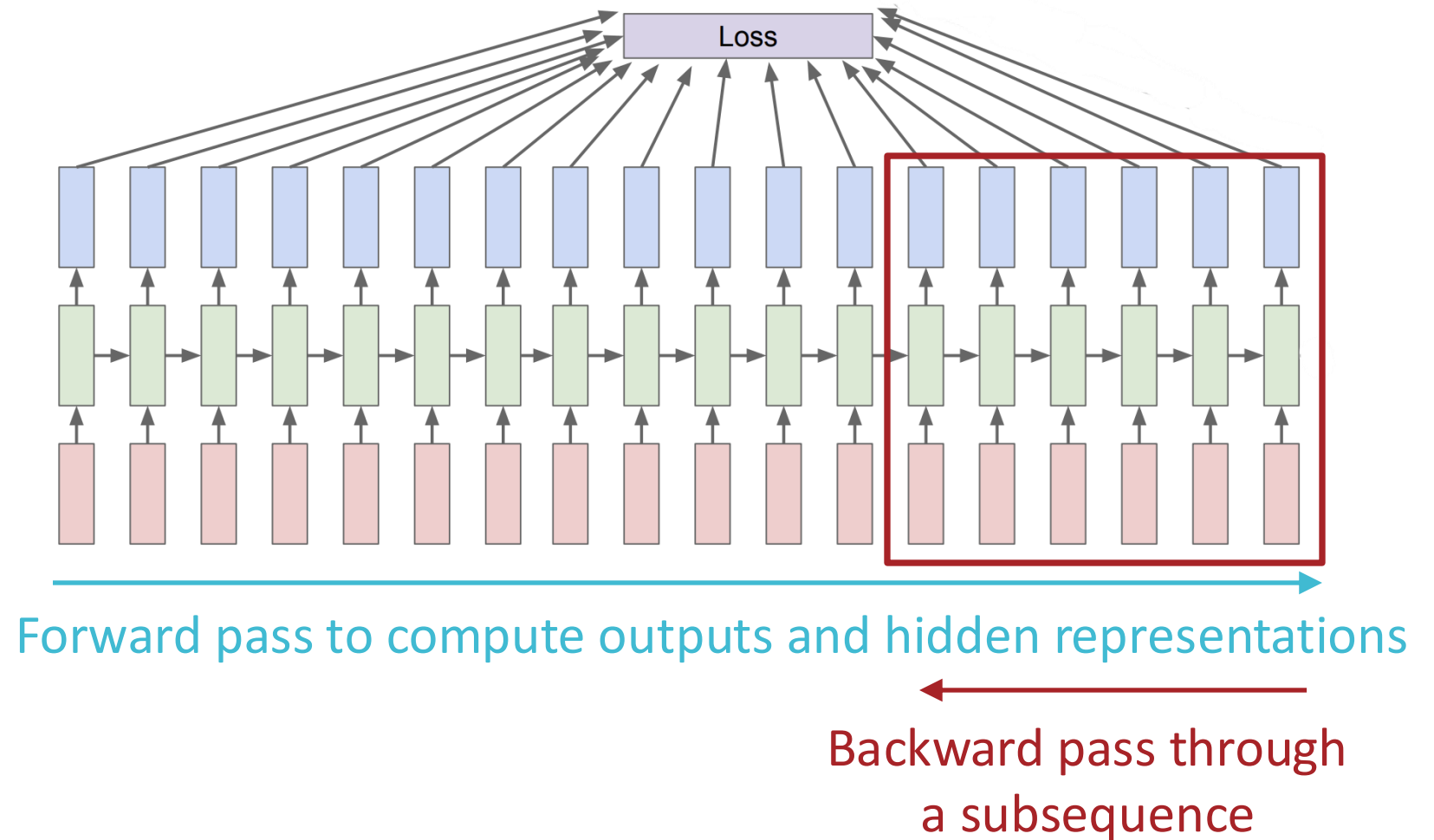
Gradient Clipping (Pascanu et al., 2013)

- 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

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

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

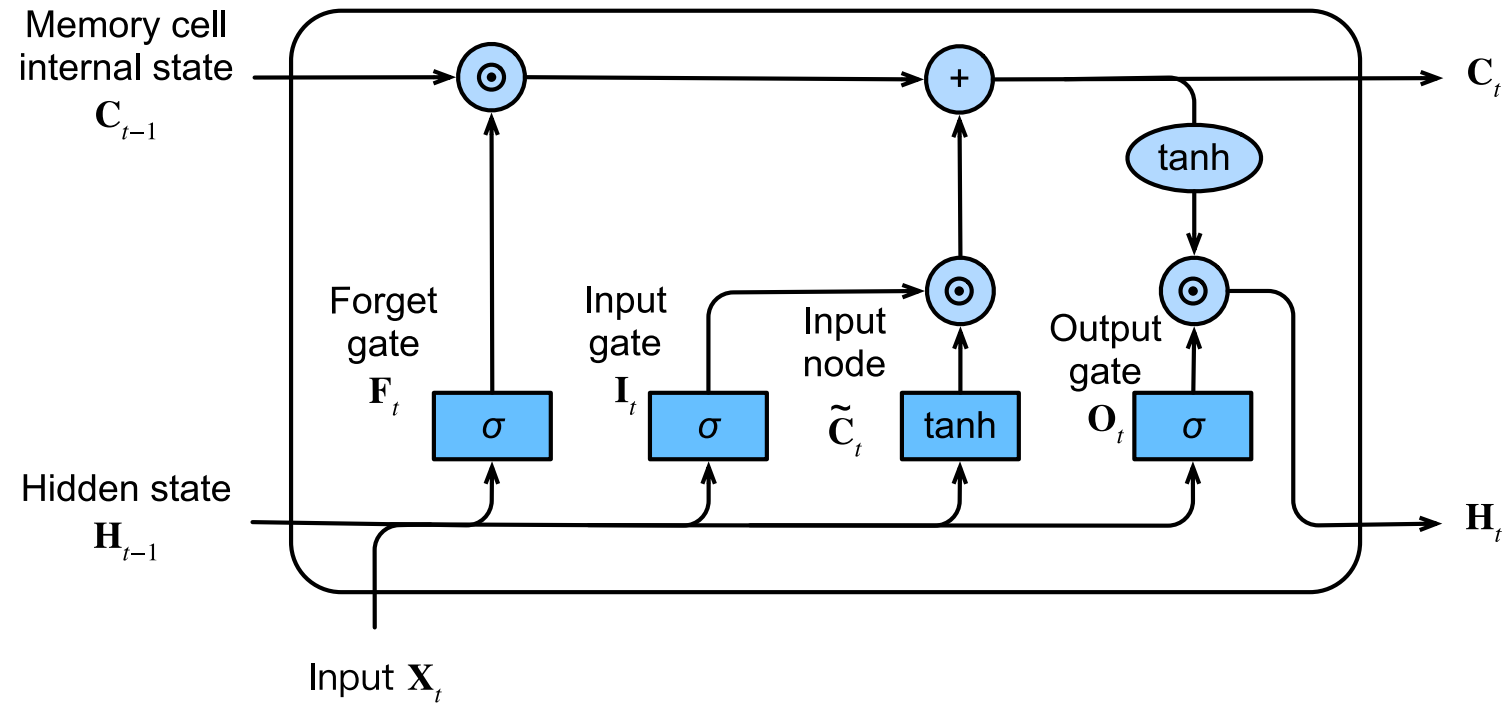
$$F_t = \sigma \left(W_{fx} \mathbf{x}_t^{(i)} + W_{fh} \mathbf{h}_{t-1} \right)$$

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

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

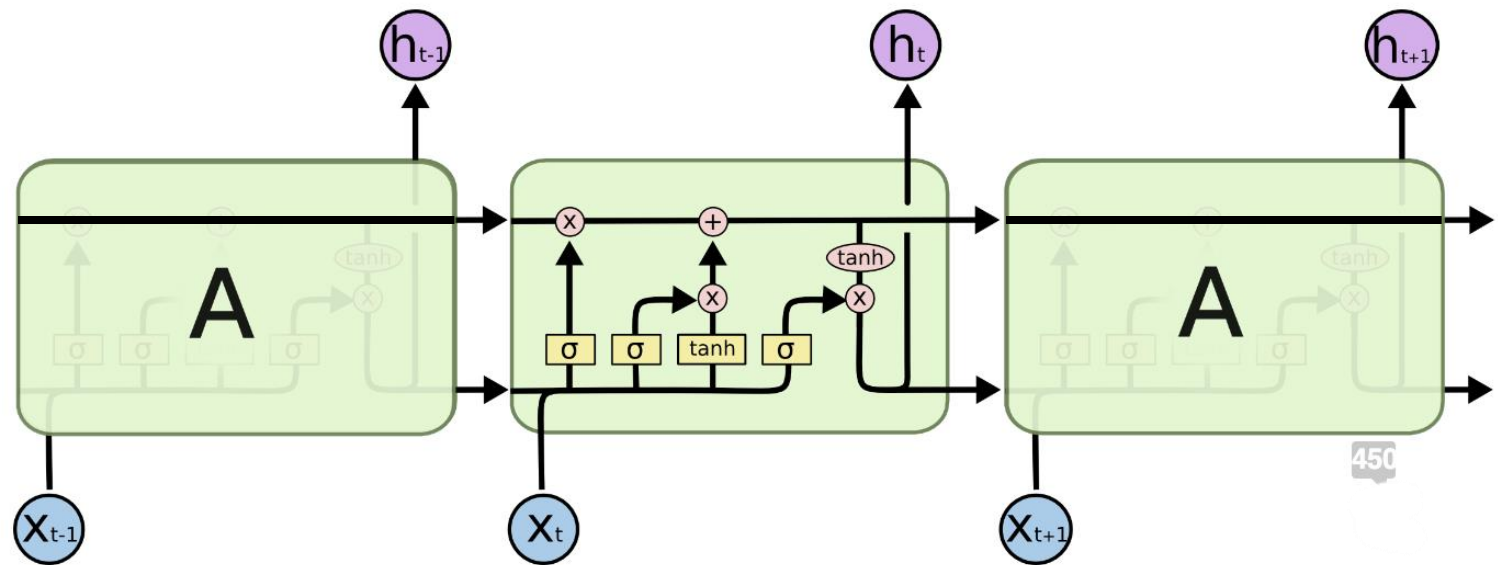
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- The internal state allows information to move through time without needing to affect the hidden representations!

Applications of LSTMs



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

2019: [DeepMind](#) used LSTM trained by policy gradients to excel at the complex video game of [Starcraft II](#).^{[12][54]}

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.