# COMP541 DEEP LEARNING

Lecture #07 – Recurrent Neural Networks



Aykut Erdem // Koç University // Fall 2022

## Previously on COMP541

- more on transfer learning
- interpretability
- visualizing neuron activations
- visualizing class activations
- pre-images
- adversarial examples
- adversarial training



#### Lecture overview

- sequence modeling
- recurrent neural networks (RNNs)
- the vanilla RNN unit
- how to train RNNs
- the long short-term memory (LSTM) unit and its variants
- gated recurrent unit (GRU)

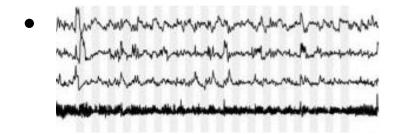
**Disclaimer:** Much of the material and slides for this lecture were borrowed from

- —Harini Suresh's MIT 6.S191 slides
- —Arun Mallya's tutorial on Recurrent Neural Networks
- —Phil Blunsom's Oxford Deep NLP class
- —Fei-Fei Li, Andrej Karpathy and Justin Johnson's CS231n class

# Sequence modeling

## Sequential data

• "I took the dog for a walk this morning." sentence



medical signals



speech waveform



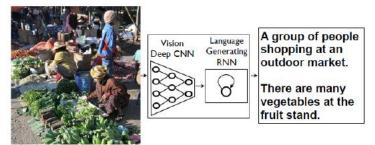




video frames

## Modeling sequential data

- Sample data sequences from a certain distribution  $P(x_1,\ldots,x_N)$
- Generate natural sentences to describe an image  $P(y_1,\ldots,y_M|I)$



• Activity recognition from a video sequence



 $P(y|x_1,\ldots,x_N)$ 

## Modeling sequential data

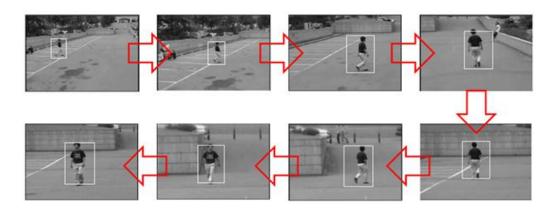
Speech recognition

$$P(y_1,\ldots,y_N|x_1,\ldots,x_N)$$



Object tracking

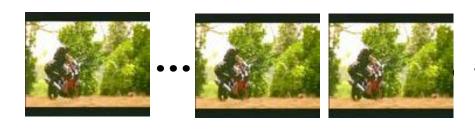
$$P(y_1,\ldots,y_N|x_1,\ldots,x_N)$$



## Modeling sequential data

Generate natural sentences to describe a video

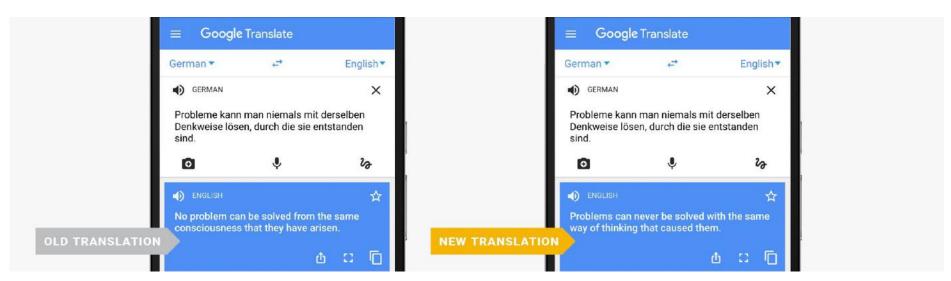
$$P(y_1,\ldots,y_M|x_1,\ldots,x_N)$$



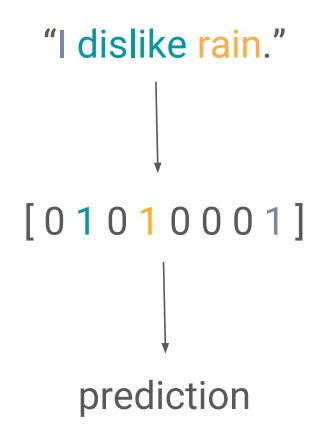
#### → A man is riding a bike

Machine translation





## Represent a sequence as a bag of words



• Problem: Bag of words does not preserve order

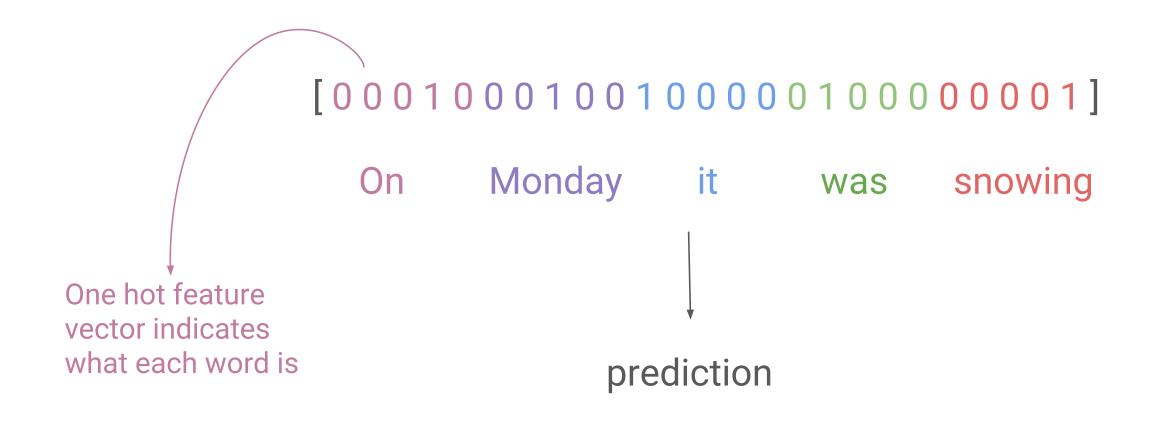
## Bag of words does not preserve order!

"The food was good, not bad at all."

vs

"The food was bad, not good at all."

## Maintain an ordering within feature vector



• Problem: Hard to deal with different word orders!

## Hard to deal with different word orders!

```
"On Monday, it was snowing." vs
```

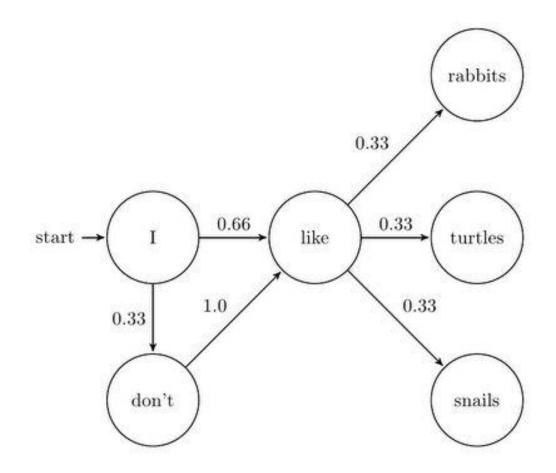
"It was snowing on Monday."

#### Hard to deal with different word orders!

```
[000100010010000010000001]
      Monday it was snowing
             VS
[1000001000000010001000100]
      was snowing on Monday
```

 we would have to relearn the rules of language at each point in the sentence

## Markov Models



• Problem: we can't model long-term dependencies

### **Markov Models**

Markov assumption: Each state depends only on the last state.

"In France, I had a great time and I learnt some of the \_\_\_\_\_language."

• We need information from the far past and future to accurately guess the correct word.

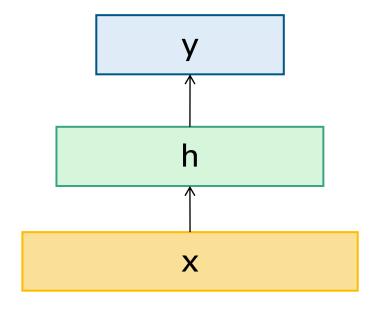
## To model sequences, we need

- 1. to deal with variable length sequences
- 2. to maintain sequence order
- 3. to keep track of long-term dependencies
- 4. to share parameters across the sequence

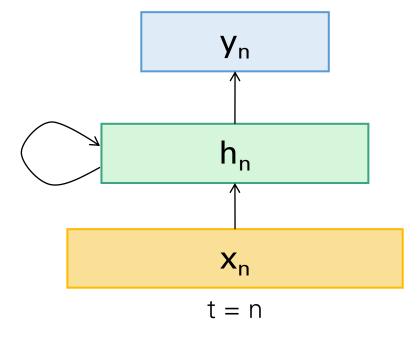
## Recurrent Neural Networks

## Recurrent Neural Networks

Feed Forward Network

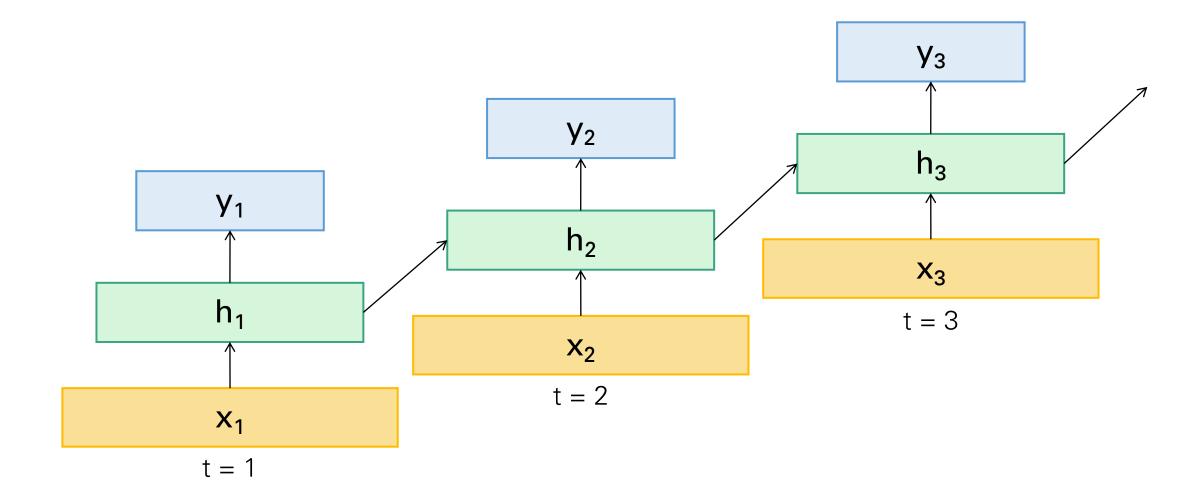


Recurrent Network

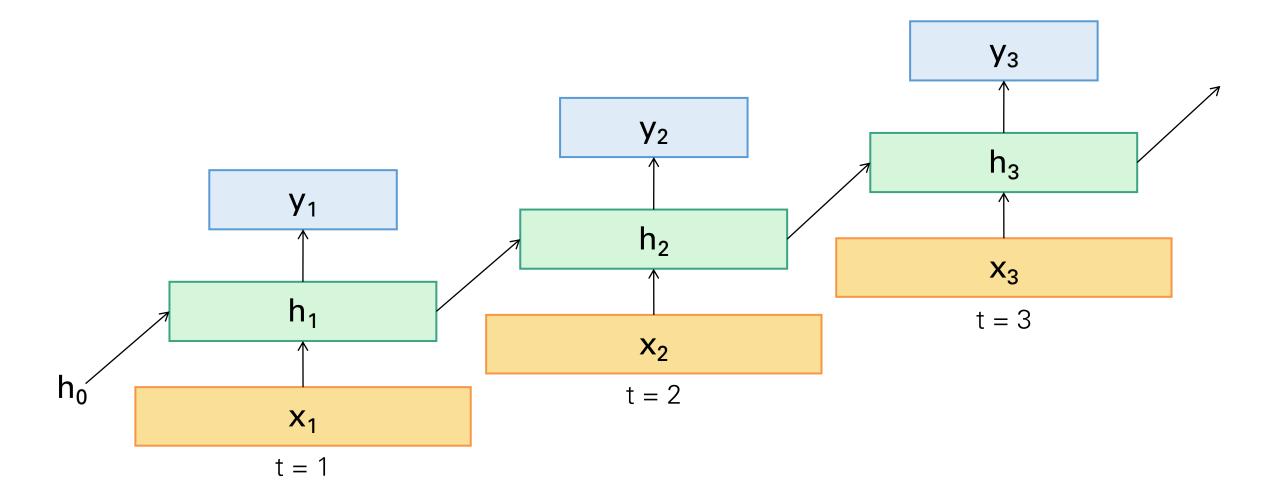


Notice: the same function and the same set of parameters are used at every time step.

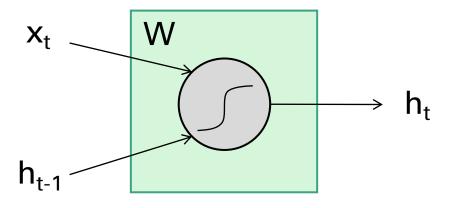
## **Unrolled RNN**



## Sample RNN

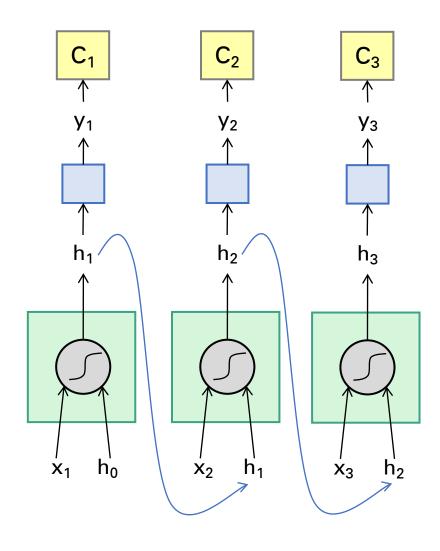


## The Vanilla RNN Cell



$$h_{t} = \tanh W \begin{pmatrix} x_{t} \\ h_{t-1} \end{pmatrix} \qquad \text{cell state}$$

## The Vanilla RNN Forward

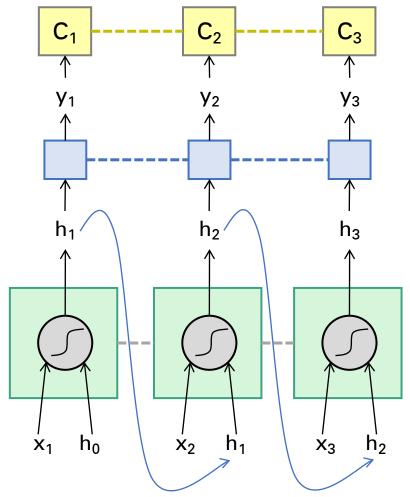


$$h_{t} = \tanh W \begin{pmatrix} x_{t} \\ h_{t-1} \end{pmatrix}$$

$$y_{t} = F(h_{t})$$

$$C_{t} = Loss(y_{t}, GT_{t})$$

## The Vanilla RNN Forward



$$h_{t} = \tanh W \begin{pmatrix} x_{t} \\ h_{t-1} \end{pmatrix}$$
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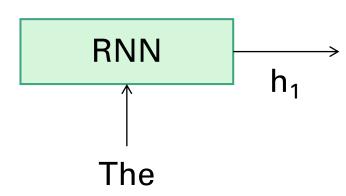
---- indicates shared weights

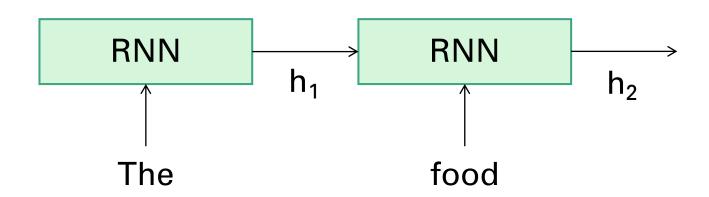
- Note that the weights are shared over time
- Essentially, copies of the RNN cell are made over time (unrolling/unfolding), with different inputs at different time steps

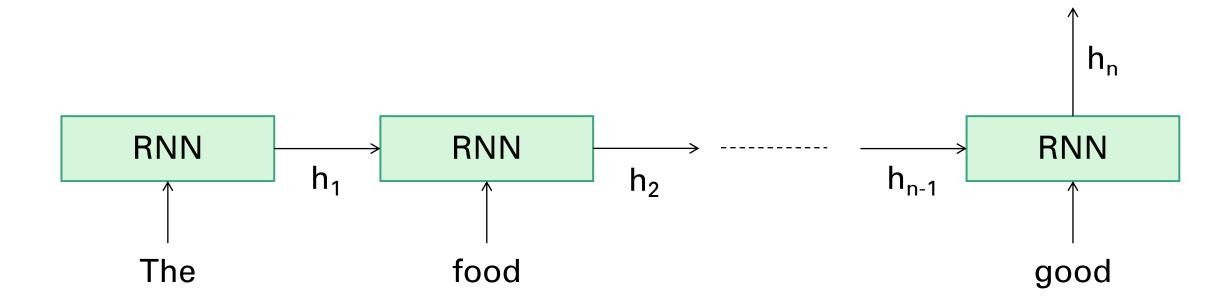
Classify a restaurant review from Yelp! OR movie review from IMDB OR ...
 as positive or negative

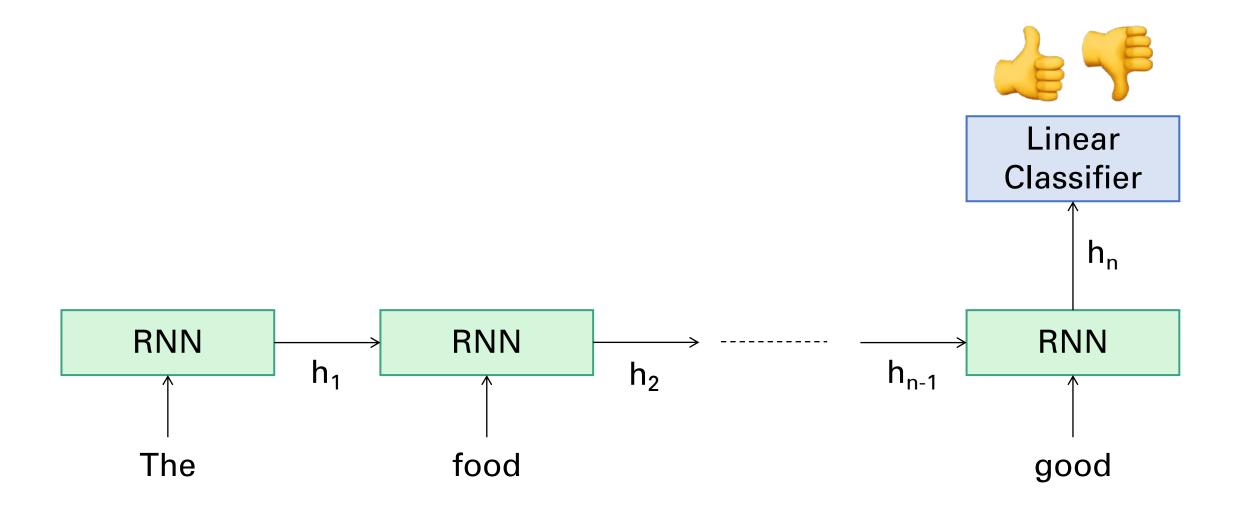
- Inputs: Multiple words, one or more sentences
- Outputs: Positive / Negative classification

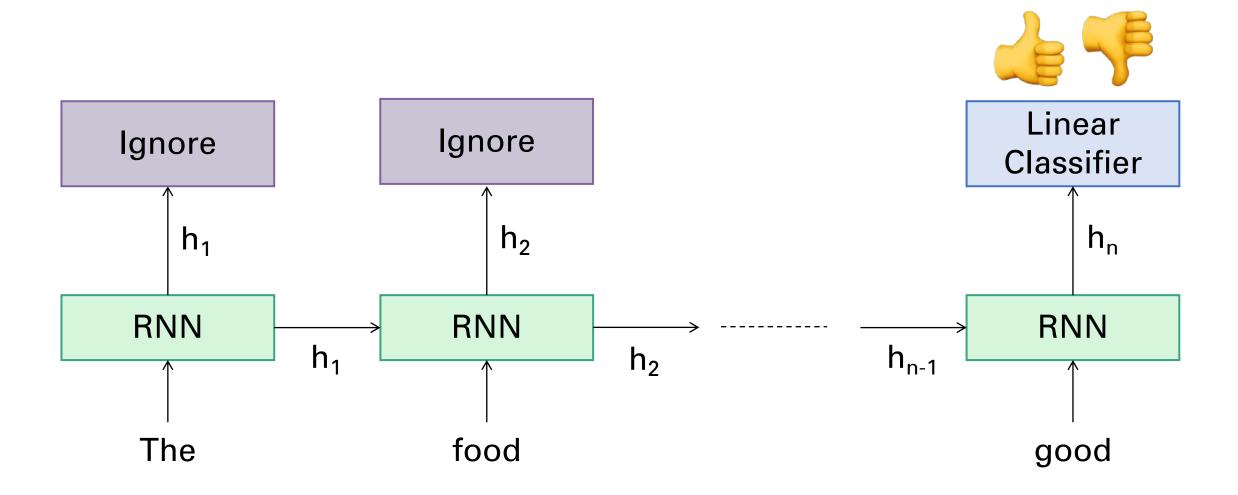
- "The food was really good"
- "The chicken crossed the road because it was uncooked"







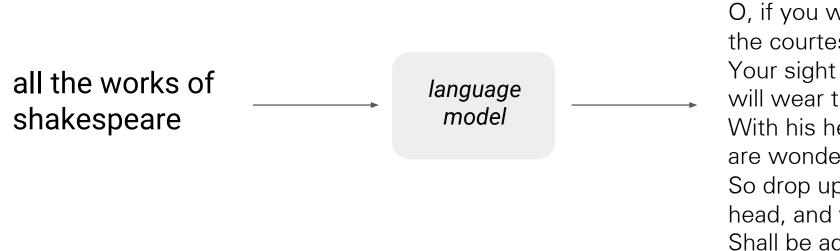




## Language Modeling

## Language Modeling

• Language models aim to represent the history of observed text  $(w_1,...,w_{t-1})$  succinctly in order to predict the next word  $(w_t)$ :

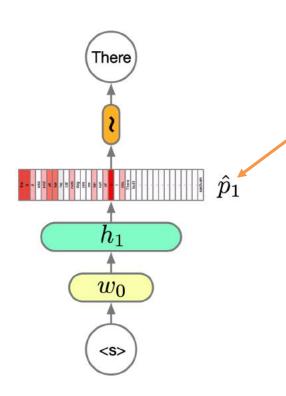


#### KING LEAR:

O, if you were a feeble sight, the courtesy of your law, Your sight and several breath, will wear the gods
With his heads, and my hands are wonder'd at the deeds,
So drop upon your lordship's head, and your opinion
Shall be against your honour.

$$h_n = g(V[x_n; h_{n-1}] + c)$$

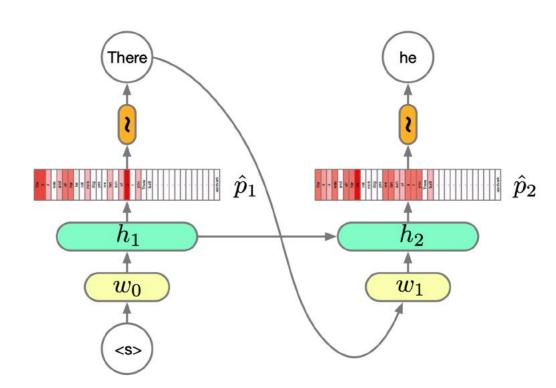
$$\hat{y}_n = Wh_n + b$$



a probability distribution over possible next words, aka a softmax

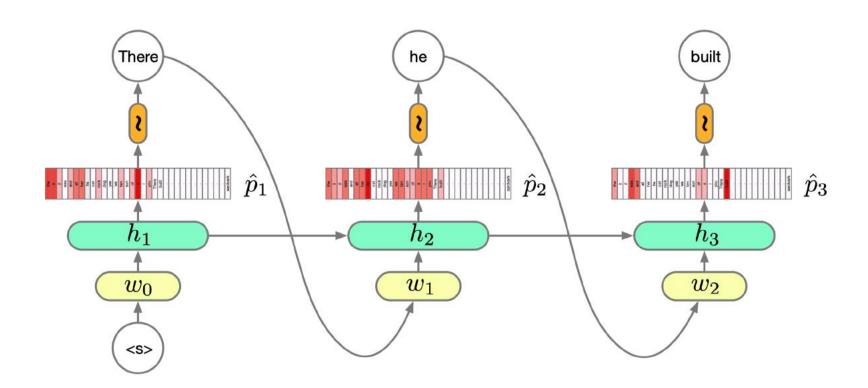
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$$\hat{y}_n = Wh_n + b$$

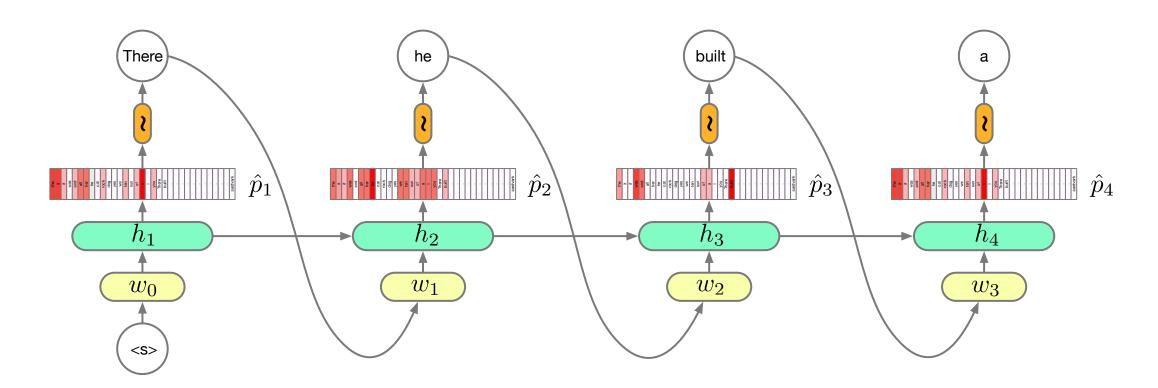


$$h_n = g(V[x_n; h_{n-1}] + c)$$

$$\hat{y}_n = Wh_n + b$$

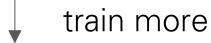


$$h_n = g(V[x_n; h_{n-1}] + c)$$
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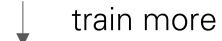


#### at first:

tyntd-iafhatawiaoihrdemot lytdws e ,tfti, astai f ogoh eoase rrranbyne 'nhthnee e plia tklrgd t o idoe ns,smtt h ne etie h,hregtrs nigtike,aoaenns lng



"Tmont thithey" fomesscerliund
Keushey. Thom here
sheulke, anmerenith ol sivh I lalterthend Bleipile shuwy fil on aseterlome
coaniogennc Phe lism thond hon at. MeiDimorotion in ther thize."



Aftair fall unsuch that the hall for Prince Velzonski's that me of her hearly, and behs to so arwage fiving were to it beloge, pavu say falling misfort how, and Gogition is so overelical and ofter.

#### train more

"Why do what that day," replied Natasha, and wishing to himself the fact the princess, Princess Mary was easier, fed in had oftened him. Pierre aking his soul came to the packs and drove up his father-in-law women.

#### PANDARUS:

Alas, I think he shall be come approached and the day When little srain would be attain'd into being never fed, And who is but a chain and subjects of his death, I should not sleep.

#### Second Senator:

They are away this miseries, produced upon my soul, Breaking and strongly should be buried, when I perish The earth and thoughts of many states.

#### DUKE VINCENTIO:

Well, your wit is in the care of side and that.

#### Second Lord:

They would be ruled after this chamber, and my fair nues begun out of the fact, to be conveyed, Whose noble souls I'll have the heart of the wars.

#### Clown:

Come, sir, I will make did behold your worship.

#### VIOLA:

I'll drink it.

#### VIOLA:

Why, Salisbury must find his flesh and thought
That which I am not aps, not a man and in fire,
To show the reining of the raven and the wars
To grace my hand reproach within, and not a fair are hand,
That Caesar and my goodly father's world;
When I was heaven of presence and our fleets,
We spare with hours, but cut thy council I am great,
Murdered and by thy master's ready there
My power to give thee but so much as hell:
Some service in the noble bondman here,
Would show him to her wine.

#### KING LEAR:

O, if you were a feeble sight, the courtesy of your law, Your sight and several breath, will wear the gods With his heads, and my hands are wonder'd at the deeds, So drop upon your lordship's head, and your opinion Shall be against your honour.

# More Language Modeling Fun -

eepDrumpi



TWEETS 284

FOLLOWING

FOLLOWERS 29.4K

LIKES 19



#### DeepDrumpf

@DeepDrumpf

I'm a Neural Network trained on Trump's transcripts. Priming text in []s. Donate (gofundme.com/deepdrumpf) to interact! Created by @hayesbh.

& deepdrumpf2016.com

Joined March 2016

Photos and videos



Tweets Tweets & replies Media

♠ In reply to Thomas Paine



DeepDrumpf @DeepDrumpf · Mar 20

There will be no amnesty. It is going to pass because the people are going to be gone. I'm giving a mandate. #ComeyHearing @Thomas1774Paine

12 12

W 17

A In reply to David Yankovich



DeepDrumpf @DeepDrumpf · Feb 19

Media hurting and left behind, I say: it looked like a million people.It's imploding as we sit with my steak. #swedenincident @DavidYankovich

♠ In reply to Glenn Thrush



DeepDrumpf @DeepDrumpf · Feb 13

Mike. Fantastic guy. Today I heard it. Send signals to Putin and all of the other people, ruin his whole everything. @GlennThrush @POTUS

https://twitter.com/deepdrumpf



More Language Modeling Fun – Generating Super Mario Levels

Original Level:

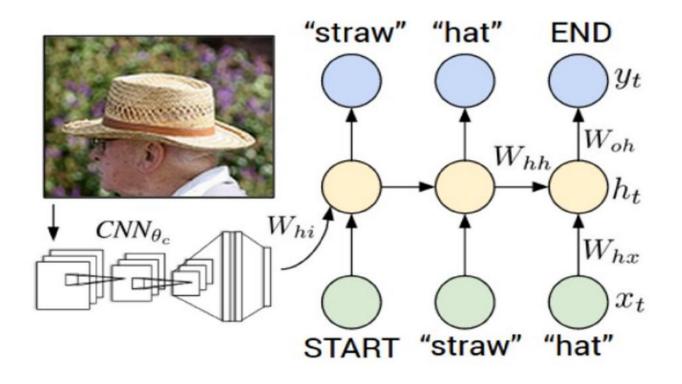


A level generated by a RNN:



# Image Captioning

# **Image Captioning**



Explain Images with Multimodal Recurrent Neural Networks [Mao et al.]

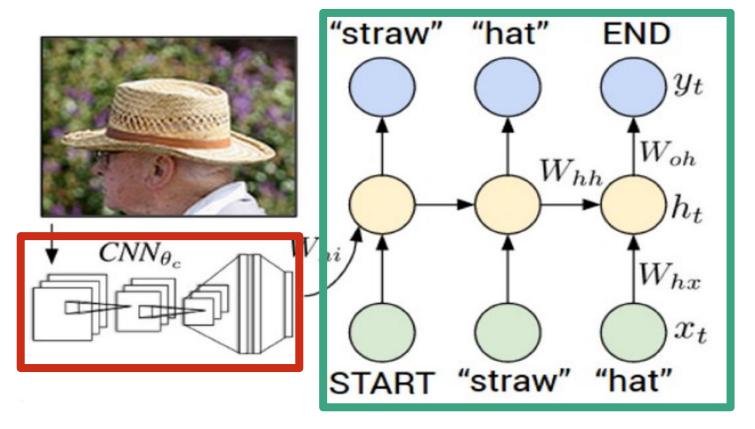
Deep Visual-Semantic Alignments for Generating Image Descriptions [Karpathy and Fei-Fei]

Show and Tell: A Neural Image Caption Generator [Vinyals et al.]

Long-term Recurrent Convolutional Networks for Visual Recognition and Description [Donahue et al.]

Learning a Recurrent Visual Representation for Image Caption Generation [Chen and Zitnick]

#### Recurrent Neural Network



**Convolutional Neural Network** 



test image

image

conv-64

conv-64

maxpool

conv-128

conv-128

maxpool

conv-256

conv-256

maxpool

conv-512

conv-512

maxpool

conv-512

conv-512

maxpool

FC-4096

FC-4096

FC-1000

softmax



test image

image

conv-64

conv-64

maxpool

conv-128

conv-128

maxpool

conv-256

conv-256

maxpool

conv-512

conv-512

maxpool

conv-512

conv-512

maxpool

FC-4096

FC-4096





test image

image

conv-64

conv-64

maxpool

conv-128

conv-128

maxpool

conv-256

conv-256

maxpool

conv-512

conv-512

maxpool

conv-512

conv-512

maxpool

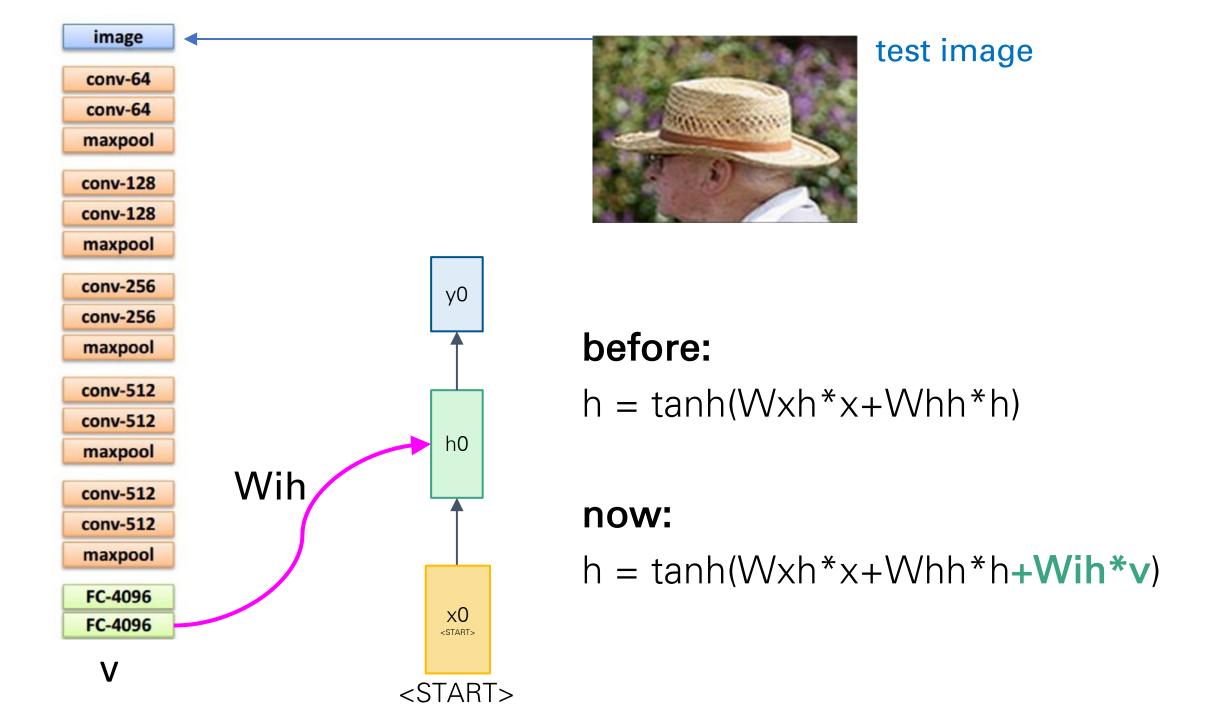
FC-4096

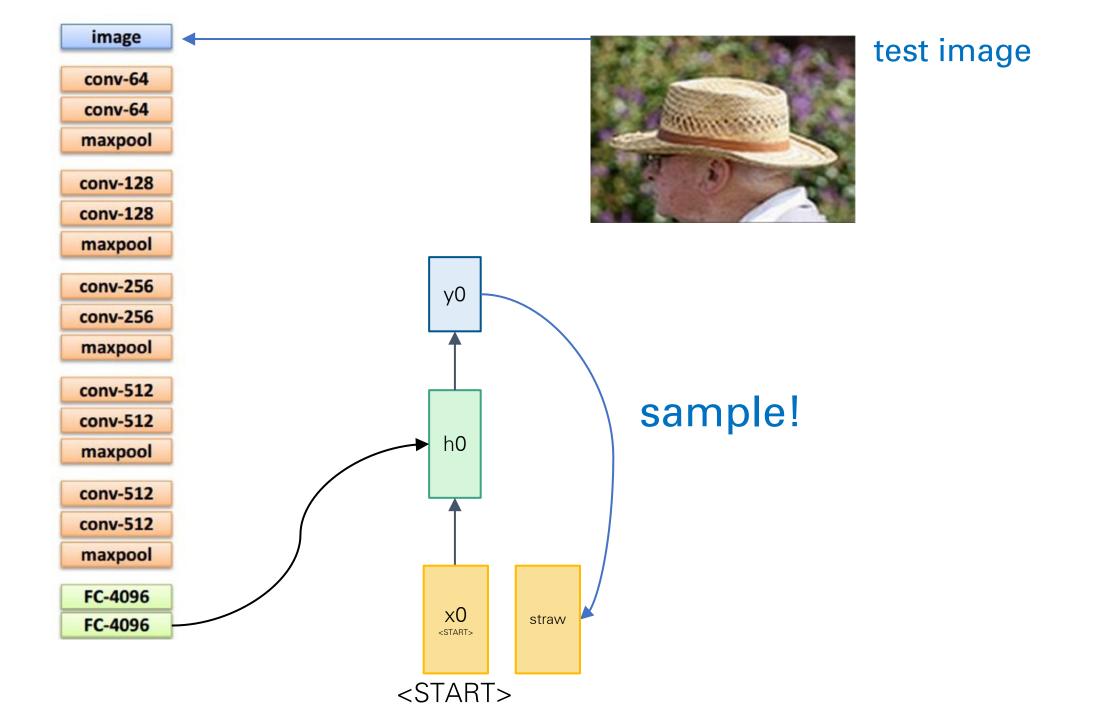
FC-4096

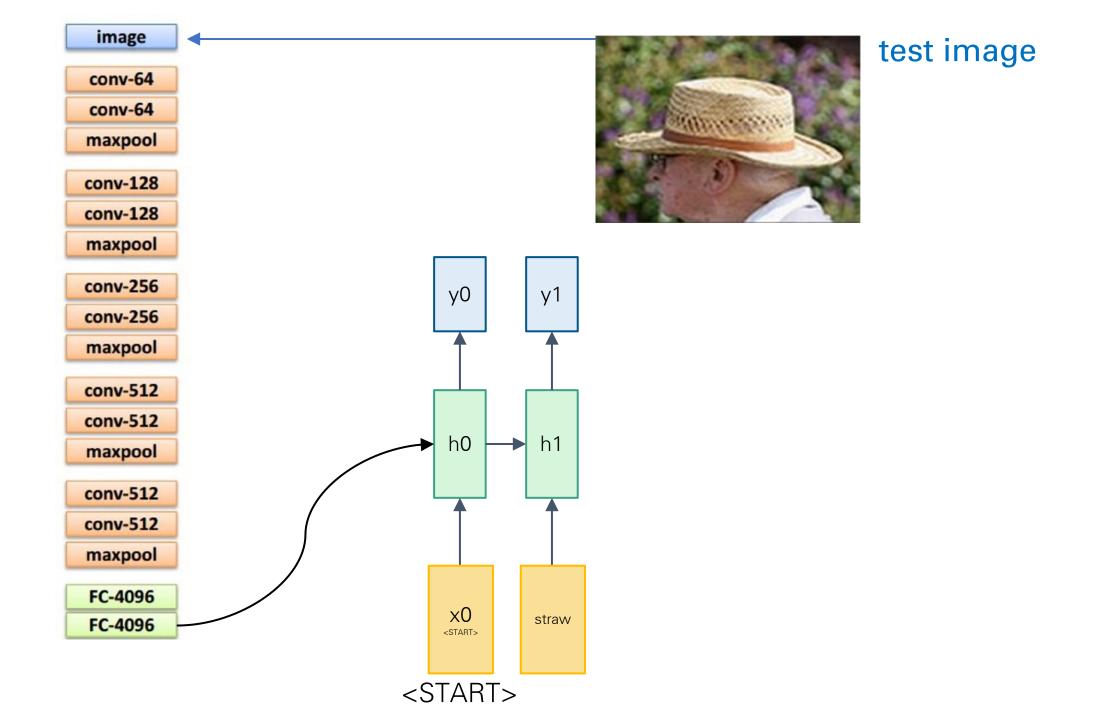


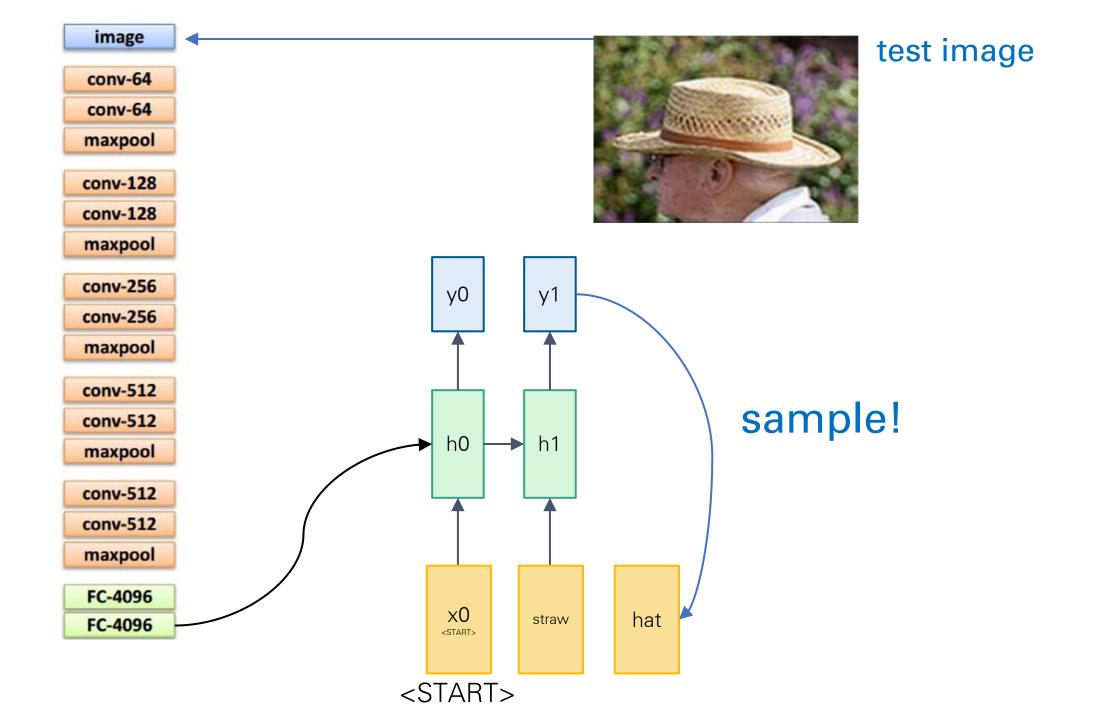
test image

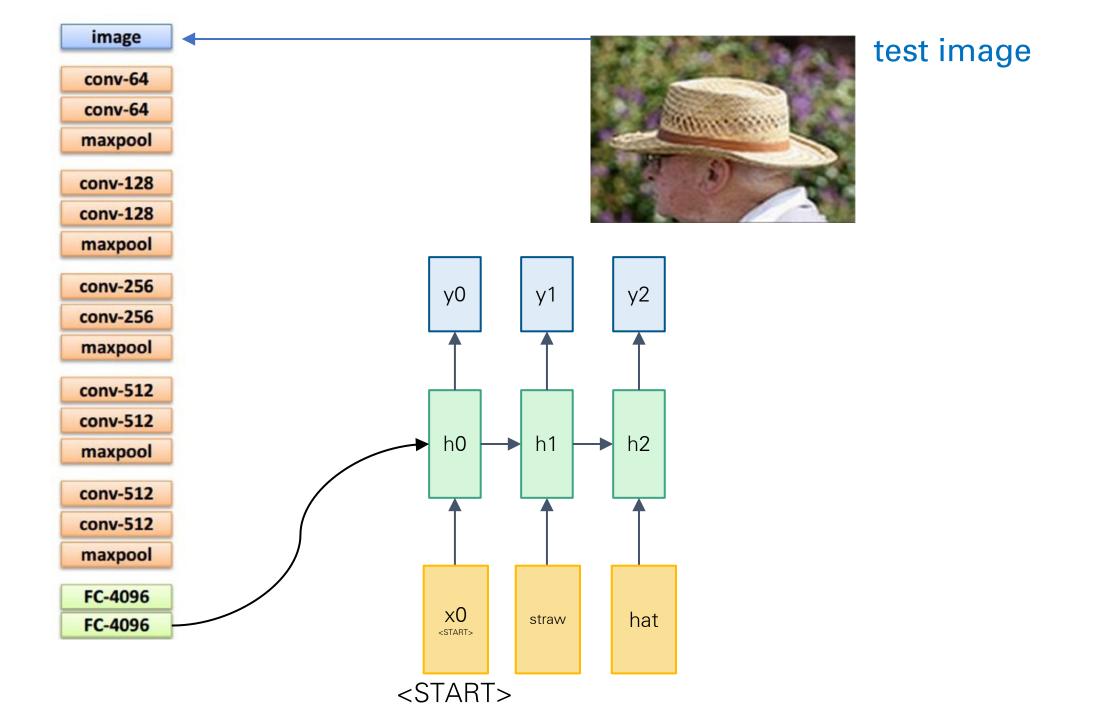


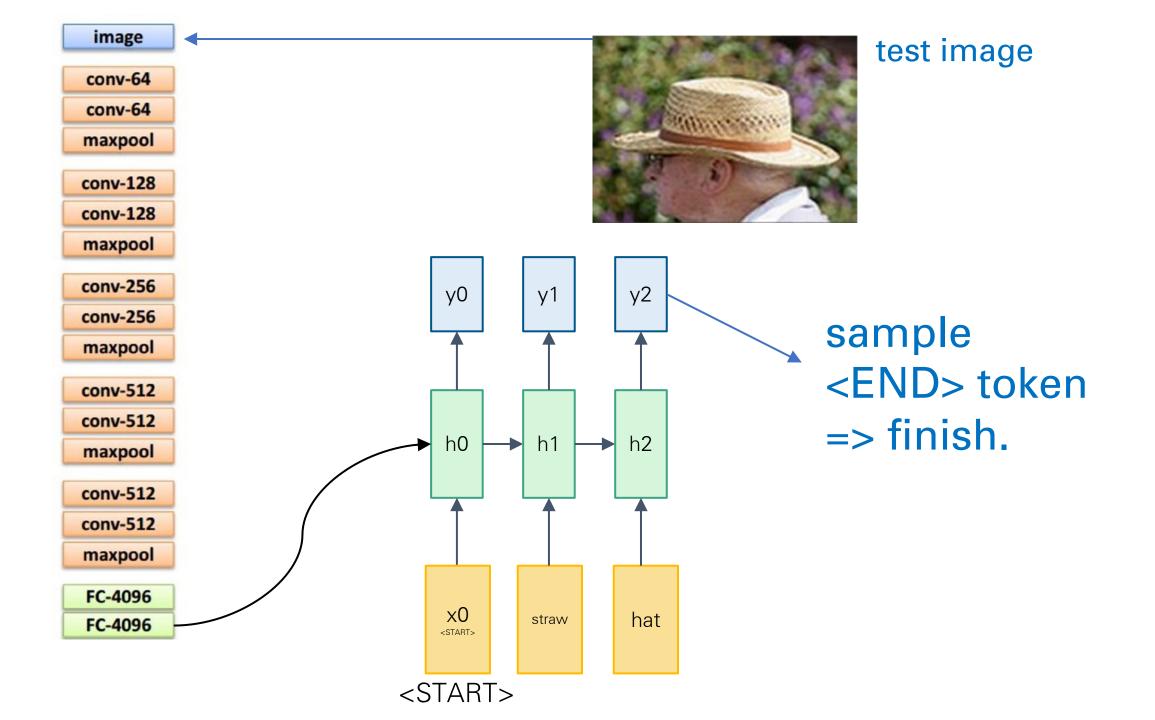


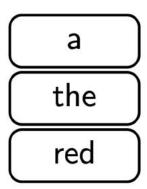










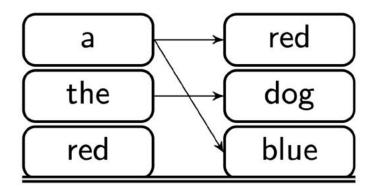


For t = 1...T:

For all k and for all possible output words w:

$$s(w, \hat{y}_{1:t-1}^{(k)}) \leftarrow \log p(\hat{y}_{1:t-1}^{(k)}|x) + \log p(w|\hat{y}_{1:t-1}^{(k)}, x)$$

$$\hat{y}_{1:t}^{(1:K)} \leftarrow \text{K-arg max } s(w, \hat{y}_{1:t-1}^{(k)})$$

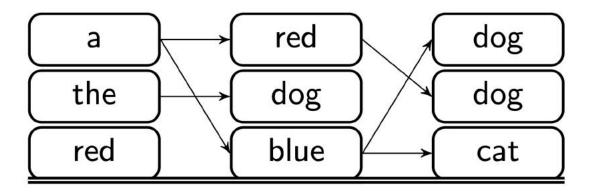


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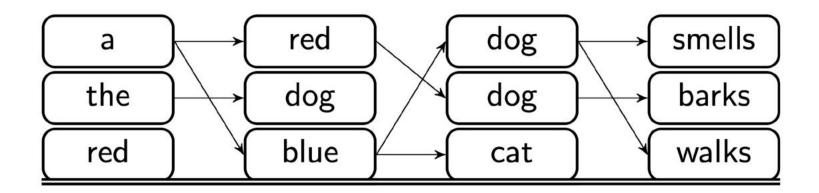


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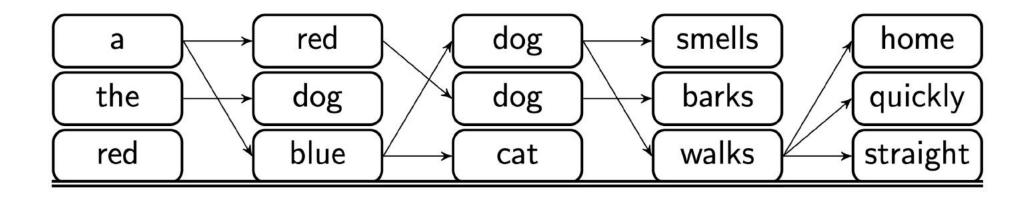


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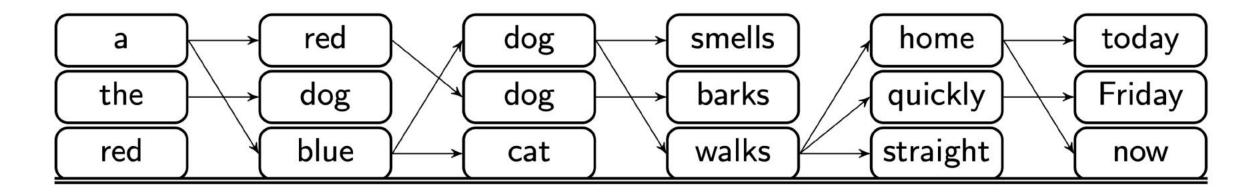


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### Image Description Datasets

a man riding a bike on a dirt path through a forest. bicyclist raises his fist as he rides on desert dirt trail. this dirt bike rider is smiling and raising his fist in triumph. a man riding a bicycle while pumping his fist in the air. a mountain biker pumps his fist in celebration.



Microsoft COCO
[Tsung-Yi Lin et al. 2014]
mscoco.org

currently:

~120K images

~5 sentences each



"man in black shirt is playing guitar."



"construction worker in orange safety vest is working on road."



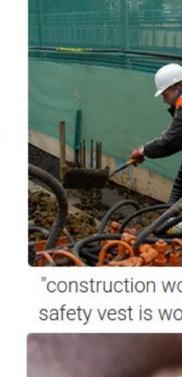
"two young girls are playing with lego toy."



"boy is doing backflip on wakeboard."



"man in black shirt is playing guitar."



"construction worker in orange safety vest is working on road."



"two young girls are playing with lego toy."



"boy is doing backflip on wakeboard."



"a young boy is holding a baseball bat."



"a cat is sitting on a couch with a remote control."



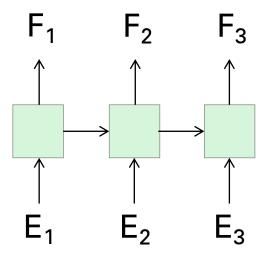
"a woman holding a teddy bear in front of a mirror."



"a horse is standing in the middle of a road."

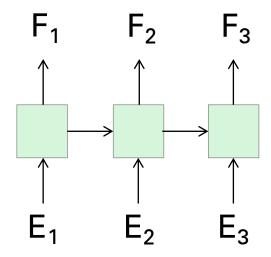
#### Class Exercise

- Consider the problem of translation of English to French
- E.g. What is your name → Comment tu t'appelle
- Is the below architecture suitable for this problem?



#### Class Exercise

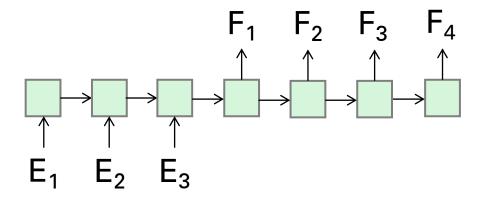
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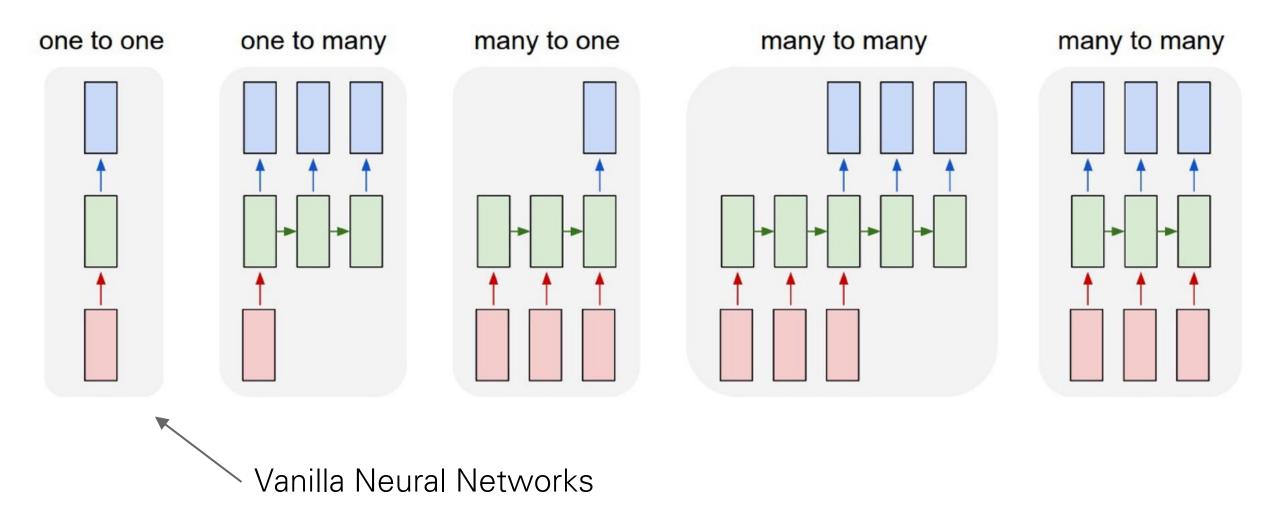
 No, sentences might be of different length and words might not align. Need to see entire sentence before translating

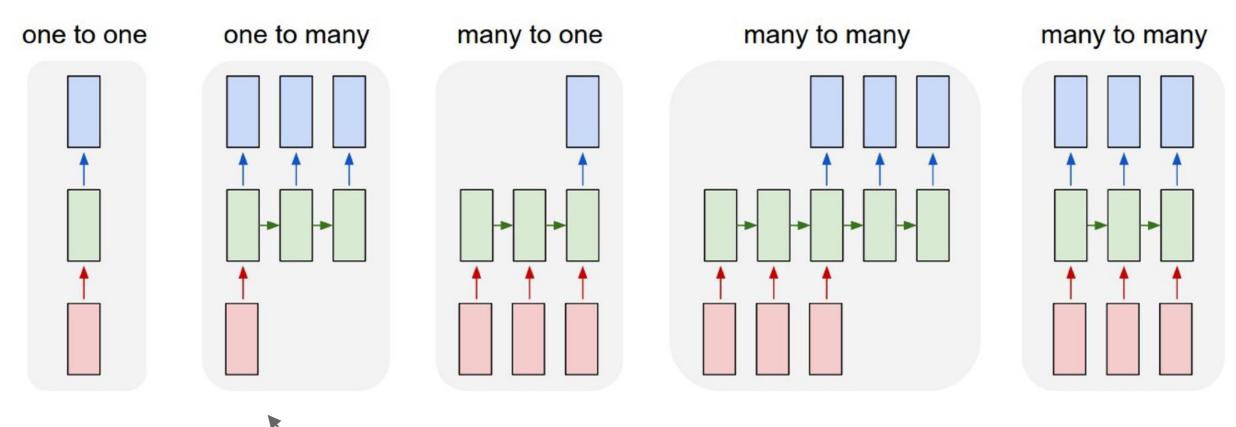
## Encoder-Decoder Seq2Seq Model

- Consider the problem of translation of English to French
- E.g. What is your name → Comment tu t'appelle
- Sentences might be of different length and words might not align.
   Need to see entire sentence before translating

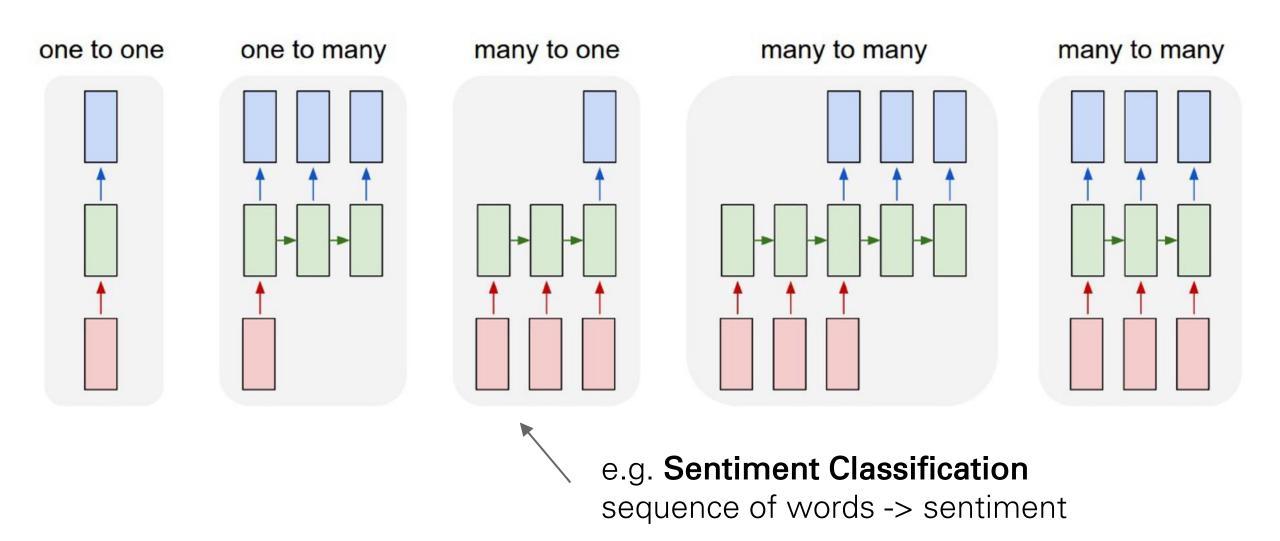


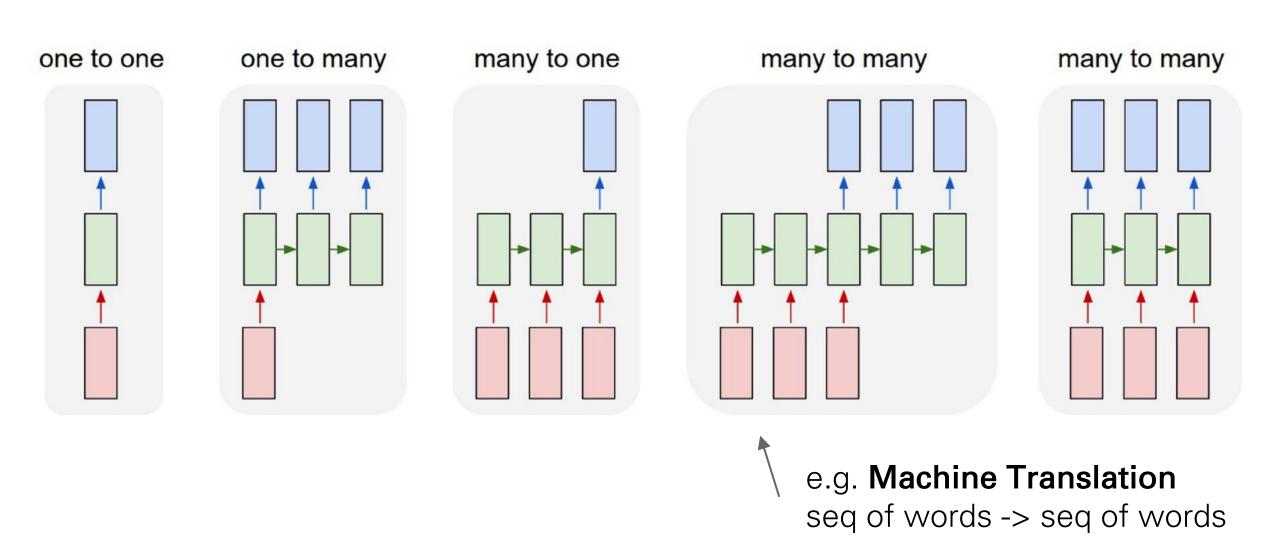
Input-Output nature depends on the structure of the problem at hand

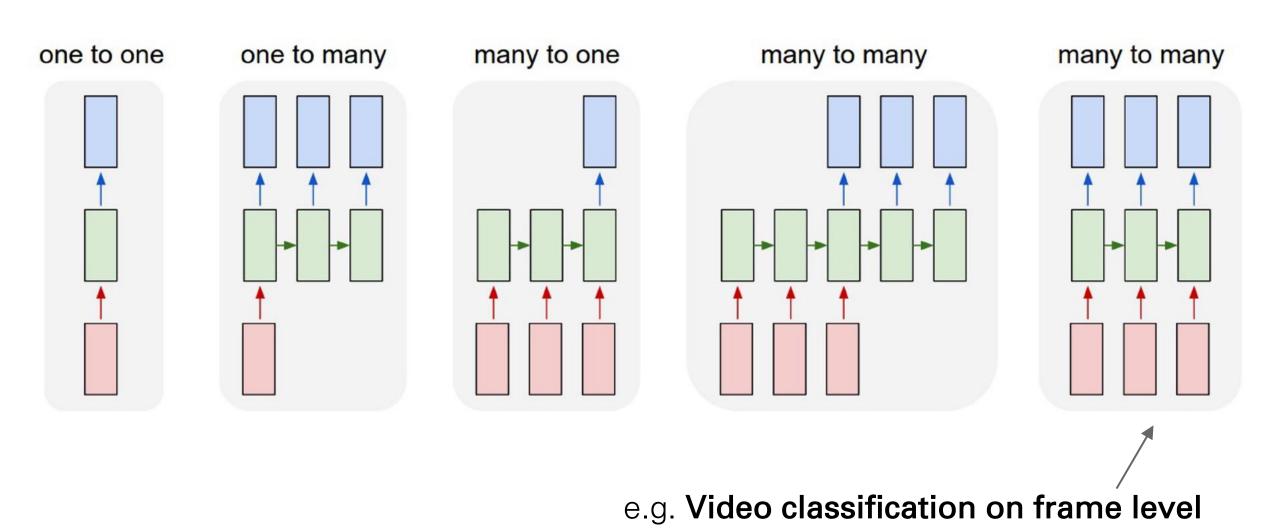




e.g. **Image Captioning** image -> sequence of words

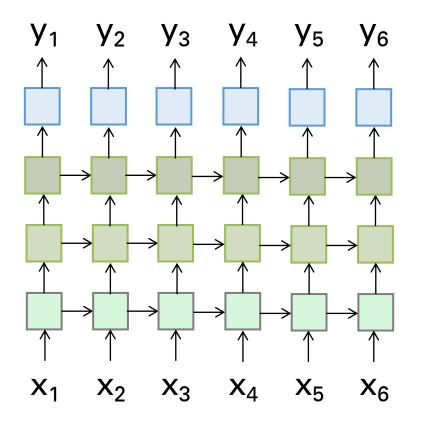






# Multi-layer RNNs

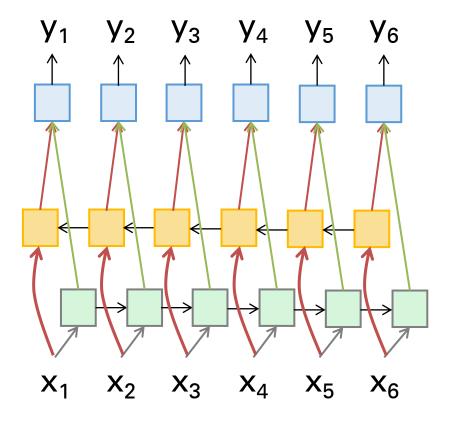
We can of course design RNNs with multiple hidden layers



• Think exotic: Skip connections across layers, across time, ...

#### **Bi-directional RNNs**

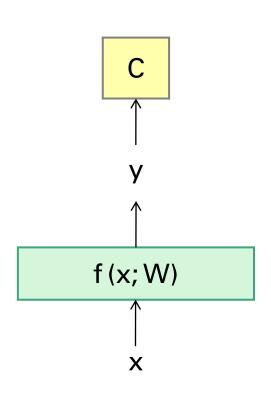
 RNNs can process the input sequence in forward and in the reverse direction



Popular in speech recognition and machine translation

# How to Train Recurrent Neural Networks

### BackPropagation Refresher



$$y = f(x; W)$$

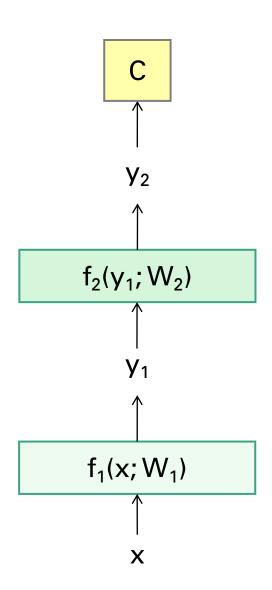
$$C = \text{Loss}(y, y_{GT})$$

SGD Update

$$W \leftarrow W - \eta \frac{\partial C}{\partial W}$$

$$\frac{\partial C}{\partial W} = \left(\frac{\partial C}{\partial y}\right) \left(\frac{\partial y}{\partial W}\right)$$

### Multiple Layers



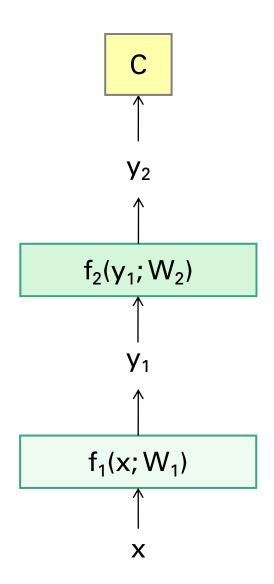
$$y_1 = f_1(x; W_1)$$
  
 $y_2 = f_2(y_1; W_2)$   
 $C = \text{Loss}(y_2, y_{GT})$ 

SGD Update

$$W_2 \leftarrow W_2 - \eta \frac{\partial C}{\partial W_2}$$

$$W_1 \leftarrow W_1 - \eta \frac{\partial C}{\partial W_1}$$

### Chain Rule for Gradient Computation



$$y_1 = f_1(x; W_1)$$
  
 $y_2 = f_2(y_1; W_2)$   
 $C = \text{Loss}(y_2, y_{GT})$ 

Find 
$$\frac{\partial C}{\partial W_1}$$
,  $\frac{\partial C}{\partial W_2}$ 

$$\frac{\partial C}{\partial W_2} = \left(\frac{\partial C}{\partial y_2}\right) \left(\frac{\partial y_2}{\partial W_2}\right)$$

$$\frac{\partial C}{\partial W_1} = \left(\frac{\partial C}{\partial y_1}\right) \left(\frac{\partial y_1}{\partial W_1}\right)$$

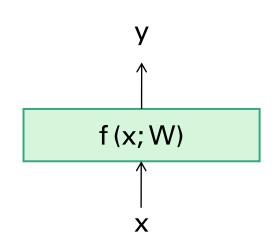
$$= \left(\frac{\partial C}{\partial y_2}\right) \left(\frac{\partial y_2}{\partial y_1}\right) \left(\frac{\partial y_2}{\partial W_1}\right)$$

$$= \left(\frac{\partial C}{\partial y_2}\right) \left(\frac{\partial y_2}{\partial y_1}\right) \left(\frac{\partial y_1}{\partial W_1}\right)$$

Application of the Chain Rule

### Chain Rule for Gradient Computation

Given: 
$$\left(\frac{\partial C}{\partial y}\right)$$



We are interested in computing: 
$$\left(\frac{\partial C}{\partial W}\right), \left(\frac{\partial C}{\partial x}\right)$$

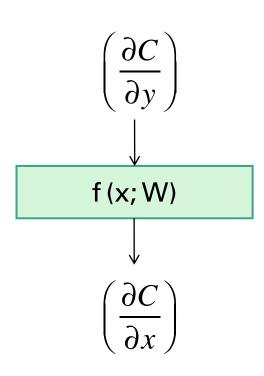
Intrinsic to the layer are:

$$\left(\frac{\partial y}{\partial W}\right)$$
 – How does output change due to params

$$\left(\frac{\partial y}{\partial x}\right)$$
 – How does output change due to inputs

$$\left(\frac{\partial C}{\partial W}\right) = \left(\frac{\partial C}{\partial y}\right) \left(\frac{\partial y}{\partial W}\right) \quad \left(\frac{\partial C}{\partial x}\right) = \left(\frac{\partial C}{\partial y}\right) \left(\frac{\partial y}{\partial x}\right)$$

## Chain Rule for Gradient Computation



Given: 
$$\left(\frac{\partial C}{\partial y}\right)$$

We are interested in computing:  $\left(\frac{\partial C}{\partial W}\right), \left(\frac{\partial C}{\partial x}\right)$ 

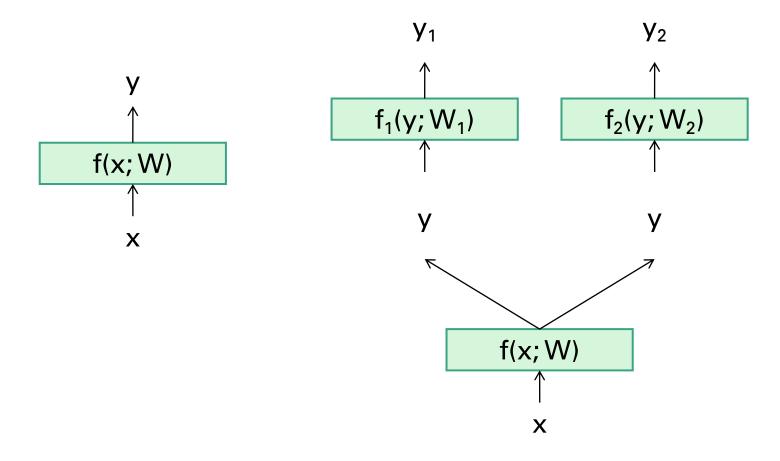
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 - How does output change due to params

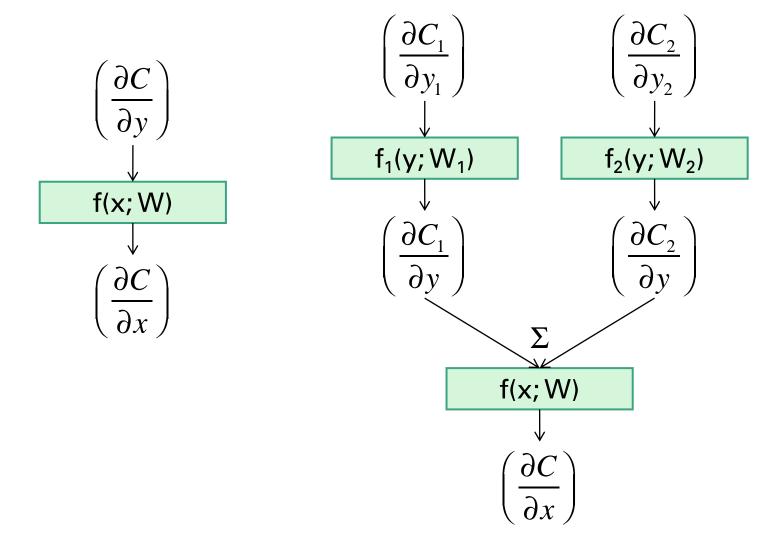
$$\left(\frac{\partial y}{\partial x}\right)$$
 – How does output change due to inputs

$$\left(\frac{\partial C}{\partial W}\right) = \left(\frac{\partial C}{\partial y}\right) \left(\frac{\partial y}{\partial W}\right) \quad \left(\frac{\partial C}{\partial x}\right) = \left(\frac{\partial C}{\partial y}\right) \left(\frac{\partial y}{\partial x}\right)$$

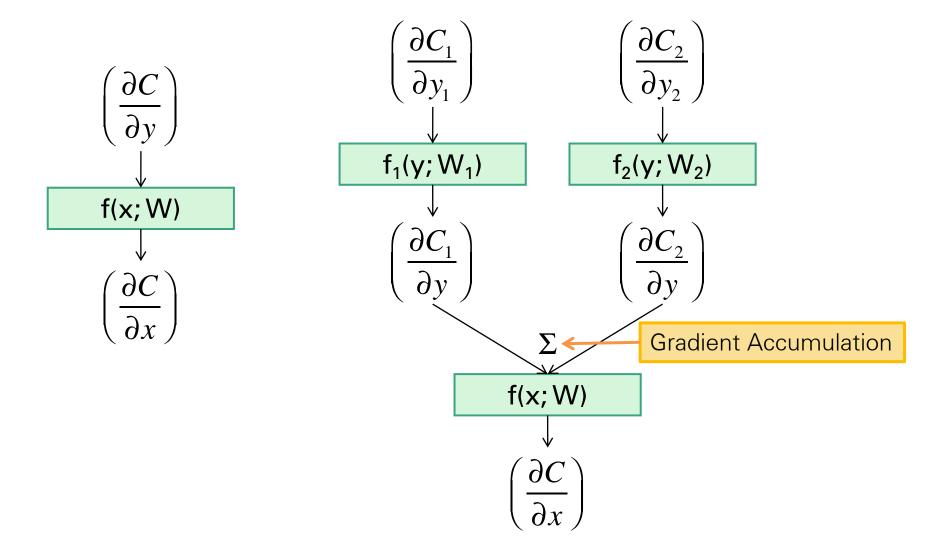
## Extension to Computational Graphs



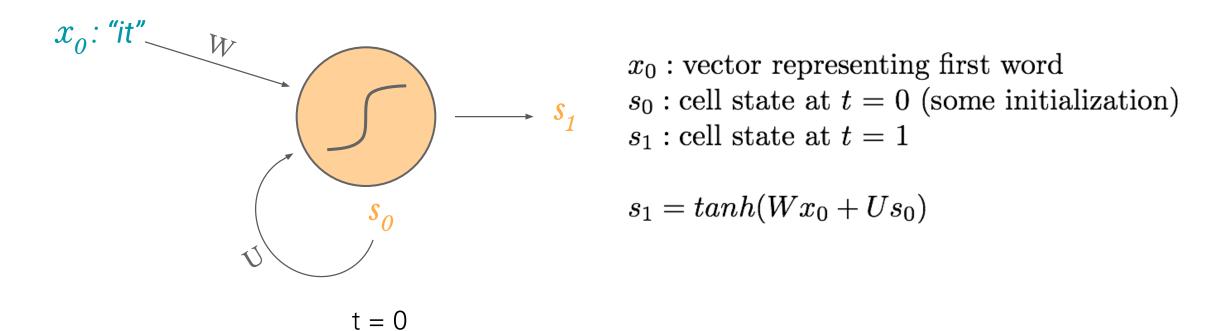
### Extension to Computational Graphs



### Extension to Computational Graphs

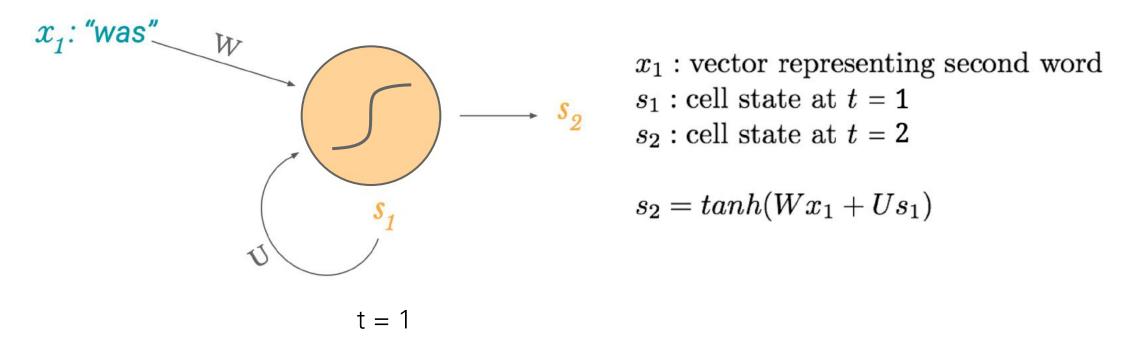


• RNNs remember their previous state:



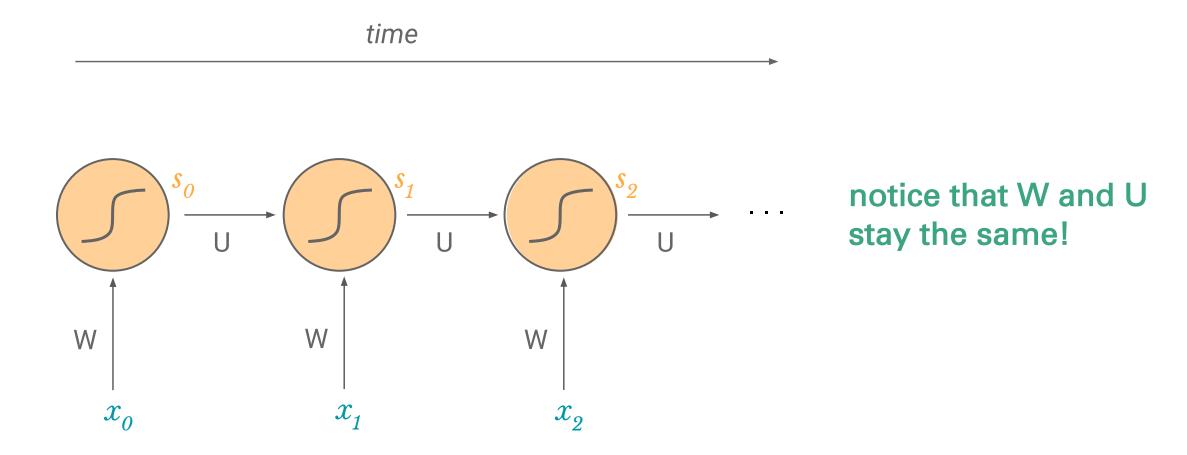
W, U: weight matrices

• RNNs remember their previous state:

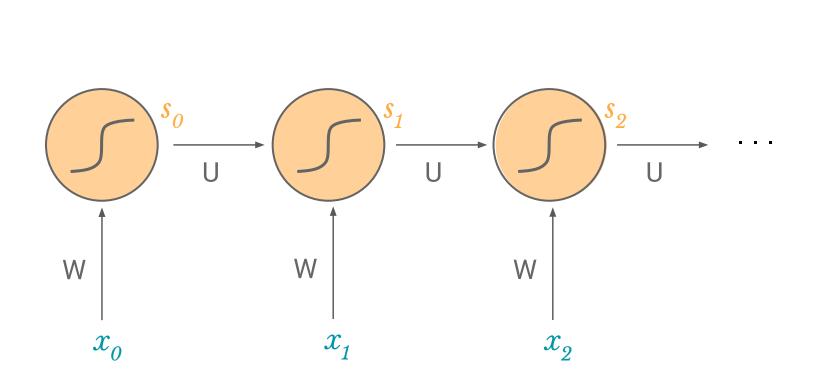


W, U: weight matrices

• "unfolding" the RNN across time:



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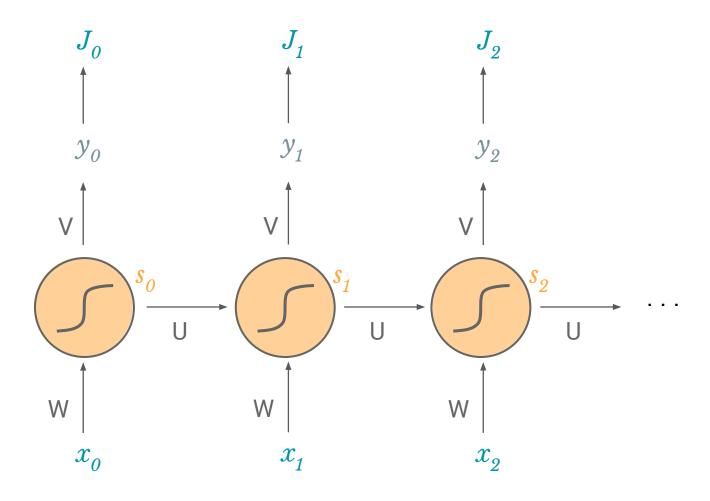


time

 $s_n$  can contain information from all past timesteps

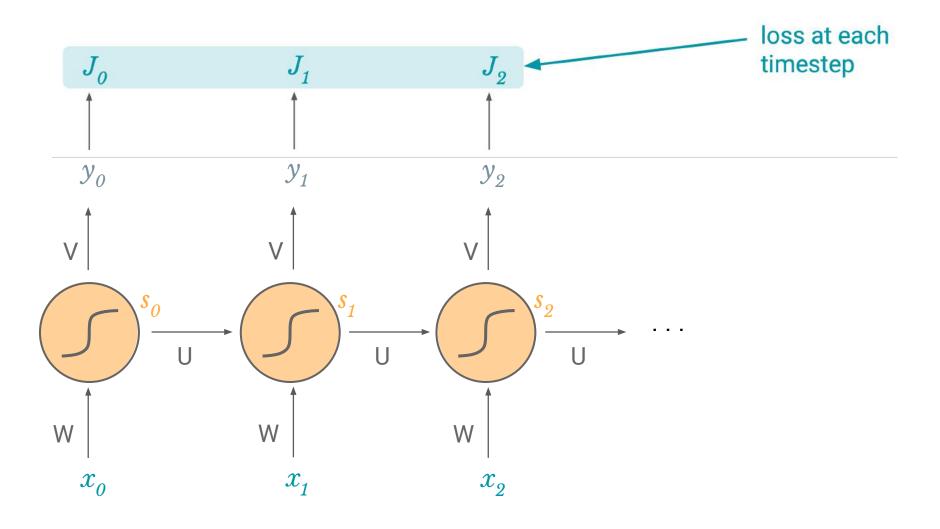
#### We have a loss at each timestep:

(since we're making a prediction at each timestep)

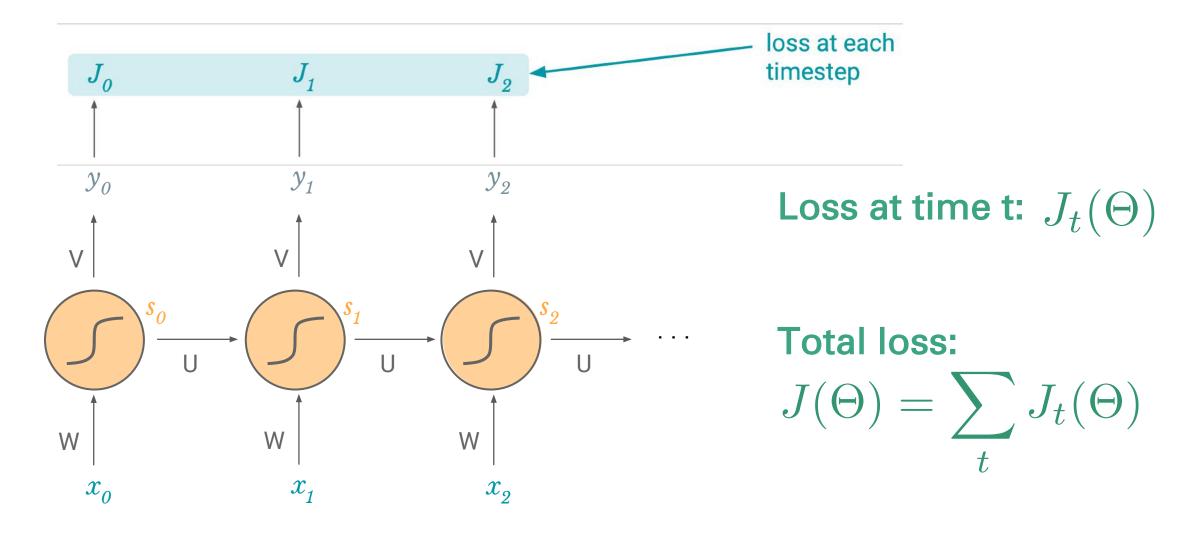


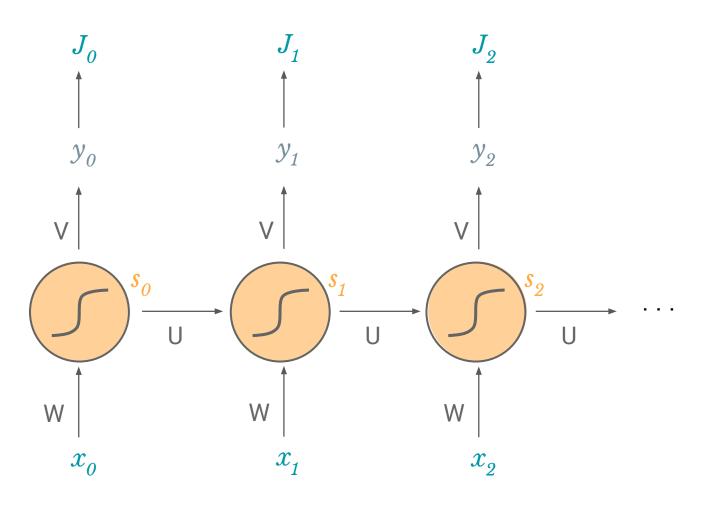
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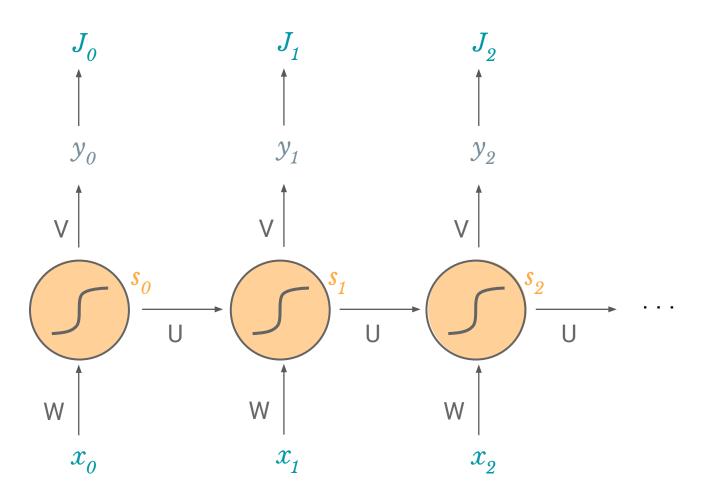


#### We sum the losses across time:

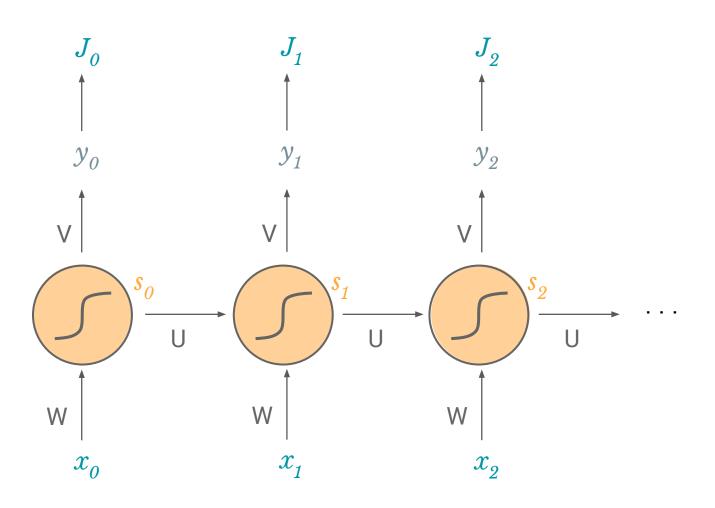




$$\frac{\partial J}{\partial W} = \sum_{t} \frac{\partial J_{t}}{\partial W}$$

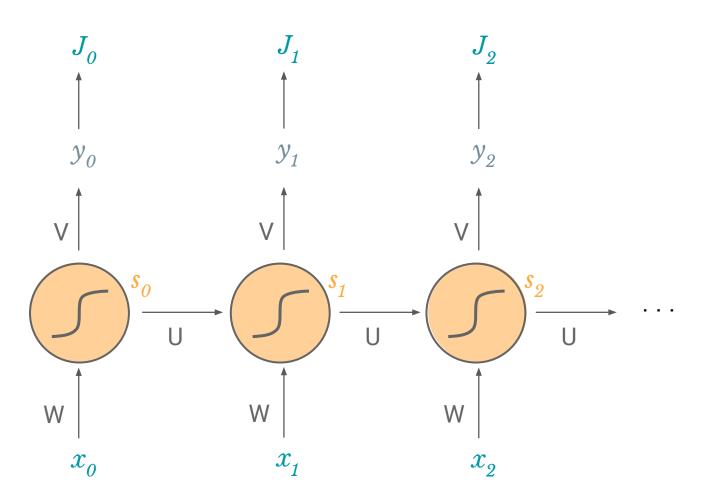


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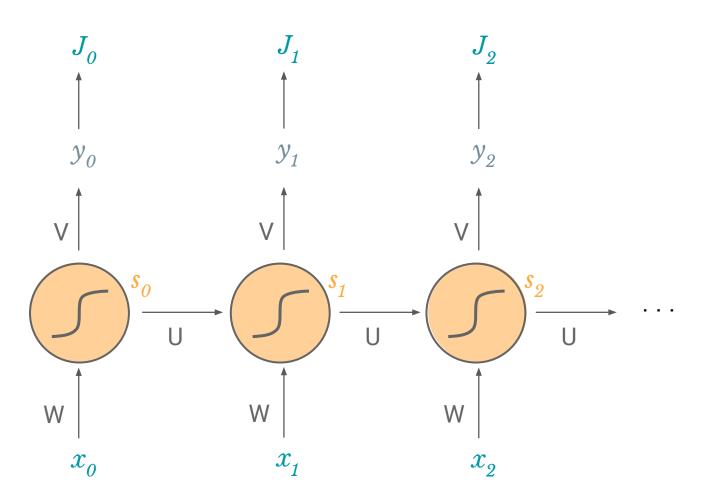
$$\frac{\partial J}{\partial W} = \sum_{t} \frac{\partial J_{t}}{\partial W}$$

$$\frac{\partial J_2}{\partial W}$$



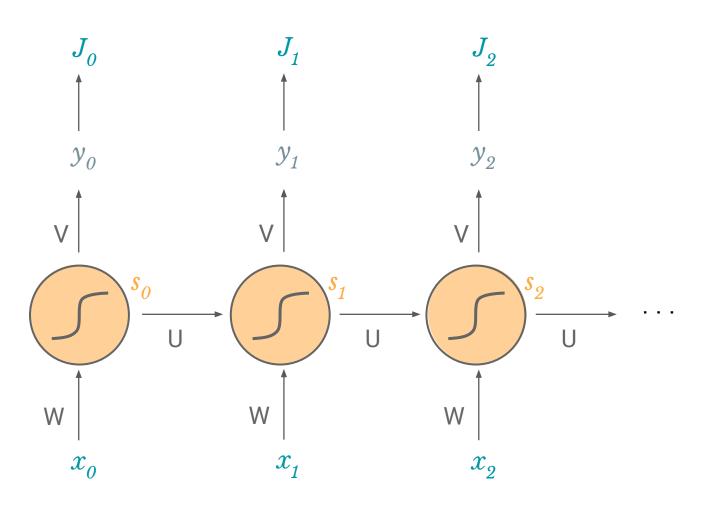
$$\frac{\partial J}{\partial W} = \sum_{t} \frac{\partial J_{t}}{\partial W}$$

$$\frac{\partial J_2}{\partial W} = \frac{\partial J_2}{\partial y^2}$$



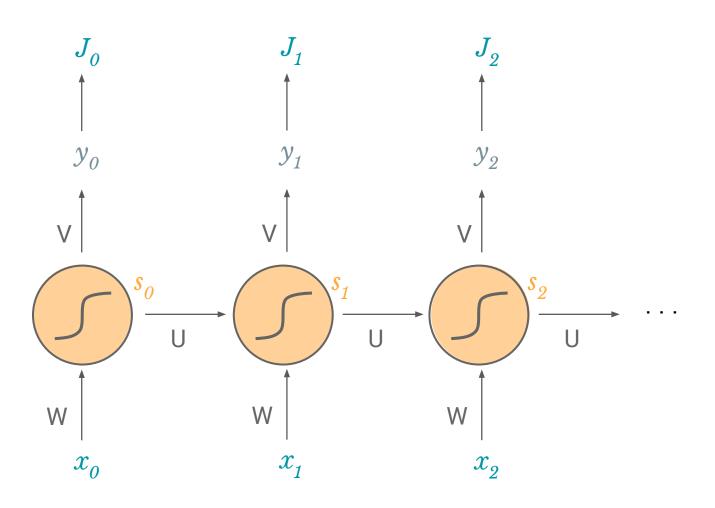
$$\frac{\partial J}{\partial W} = \sum_{t} \frac{\partial J_{t}}{\partial W}$$

$$\frac{\partial J_2}{\partial W} = \frac{\partial J_2}{\partial y_2} \frac{\partial y_2}{\partial s_2}$$



$$\frac{\partial J}{\partial W} = \sum_{t} \frac{\partial J_{t}}{\partial W}$$

$$\frac{\partial J_2}{\partial W} = \frac{\partial J_2}{\partial y_2} \frac{\partial y_2}{\partial s_2} \frac{\partial s_2}{\partial W}$$

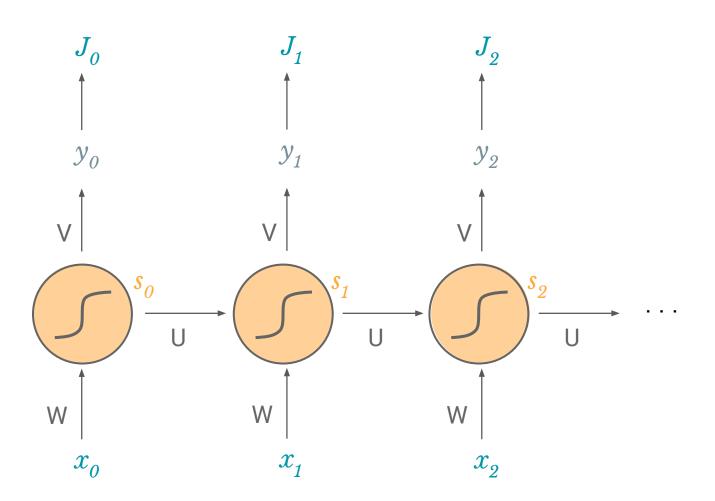


$$\frac{\partial J}{\partial W} = \sum_{t} \frac{\partial J_{t}}{\partial W}$$

so let's take a single timestep t:

$$\frac{\partial J_2}{\partial W} = \frac{\partial J_2}{\partial y_2} \frac{\partial y_2}{\partial s_2} \frac{\partial s_2}{\partial W}$$

but wait...



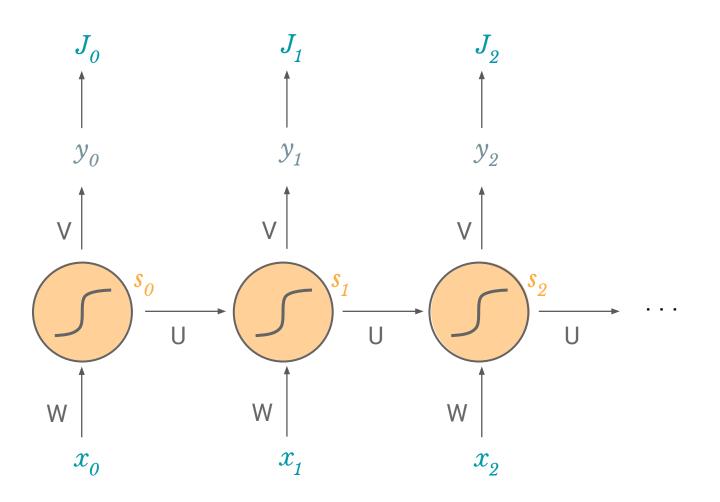
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$$\frac{\partial J_2}{\partial W} = \frac{\partial J_2}{\partial y_2} \frac{\partial y_2}{\partial s_2} \frac{\partial s_2}{\partial W}$$

but wait...

$$s_2 = tanh(Us_1 + Wx_2)$$



$$\frac{\partial J}{\partial W} = \sum_{t} \frac{\partial J_{t}}{\partial W}$$

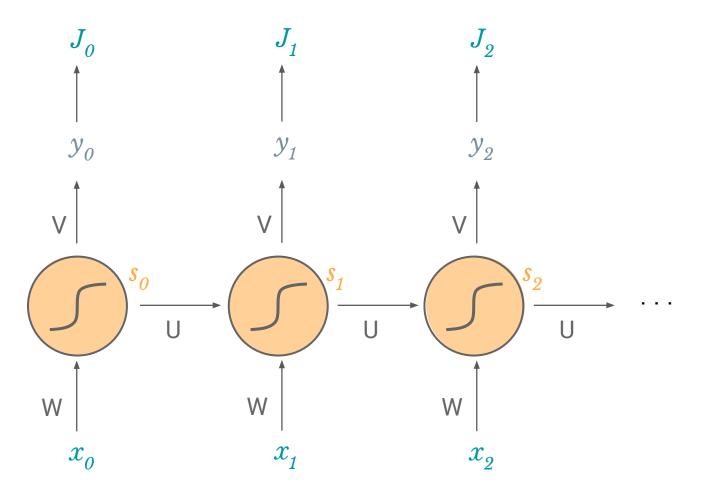
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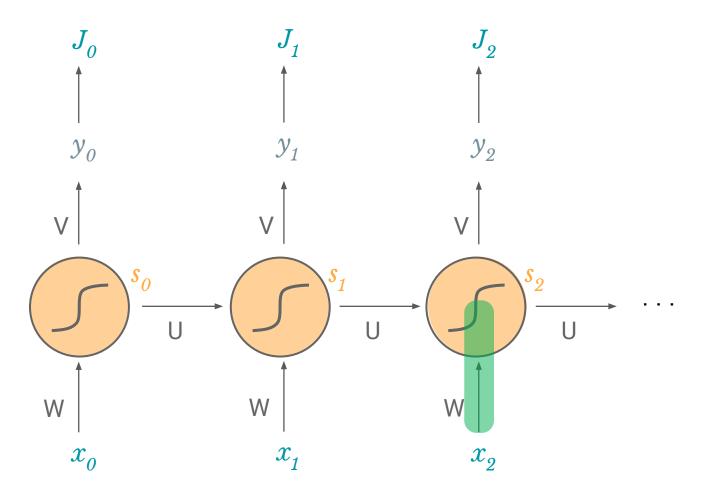
$$\frac{\partial J_2}{\partial W} = \frac{\partial J_2}{\partial y_2} \frac{\partial y_2}{\partial s_2} \frac{\partial s_2}{\partial W}$$

but wait...

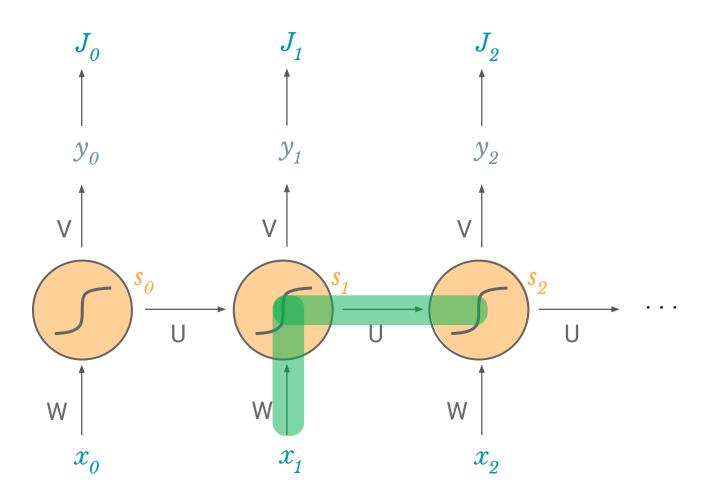
$$s_2 = tanh(Us_1 + Wx_2)$$

 $s_{\rm I}$  also depends on W so we can't just treat  $\frac{\partial s_2}{\partial W}$  as a constant!

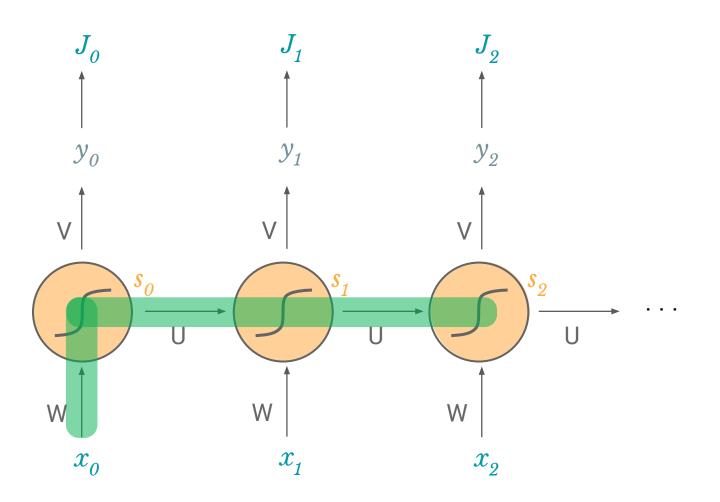








$$\frac{\partial s_2}{\partial W} + \frac{\partial s_2}{\partial s_1} \frac{\partial s_1}{\partial W}$$



$$\frac{\partial s_2}{\partial W} + \frac{\partial s_2}{\partial s_1} \frac{\partial s_1}{\partial W} + \frac{\partial s_2}{\partial s_0} \frac{\partial s_0}{\partial W}$$

#### Backpropagation through time:

$$\frac{\partial J_2}{\partial W} = \sum_{k=0}^{2} \frac{\partial J_2}{\partial y_2} \frac{\partial y_2}{\partial s_2} \frac{\partial s_2}{\partial s_k} \frac{\partial s_k}{\partial W}$$

Contributions of W in previous timesteps to the error at timestep t

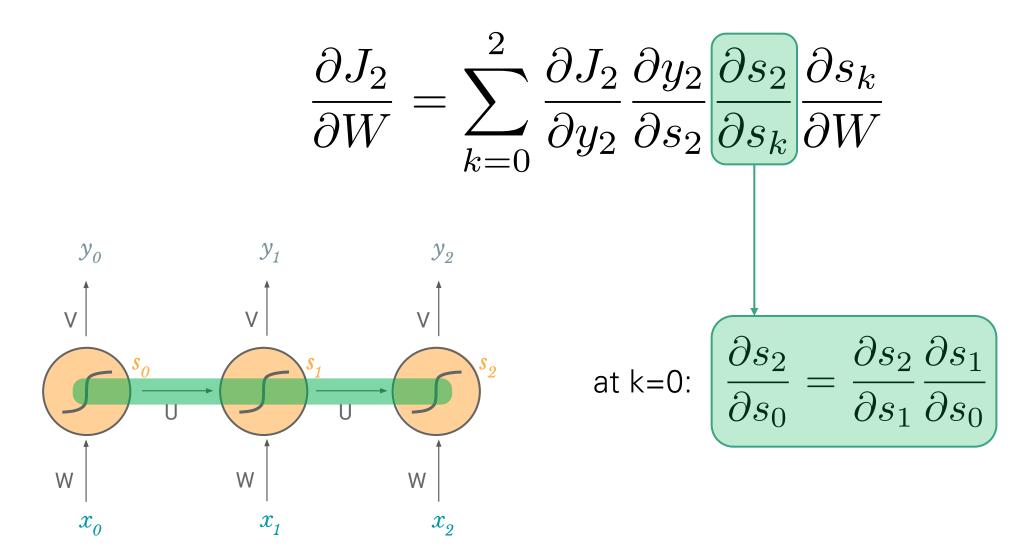
### Backpropagation through time:

$$\frac{\partial J_t}{\partial W} = \sum_{k=0}^t \frac{\partial J_t}{\partial y_t} \frac{\partial y_t}{\partial s_t} \frac{\partial s_t}{\partial s_k} \frac{\partial s_k}{\partial W}$$

Contributions of W in previous timesteps to the error at timestep t

## Why are RNNs hard to train?

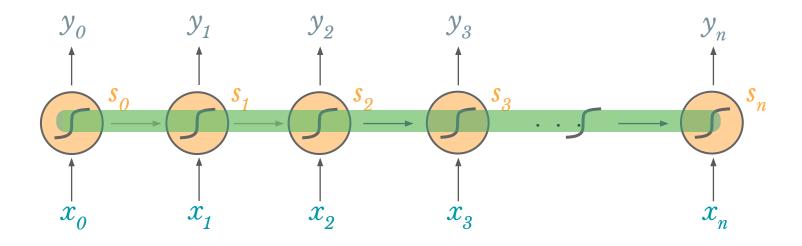
$$\frac{\partial J_2}{\partial W} = \sum_{k=0}^{2} \frac{\partial J_2}{\partial y_2} \frac{\partial y_2}{\partial s_2} \frac{\partial s_2}{\partial s_k} \frac{\partial s_k}{\partial W}$$

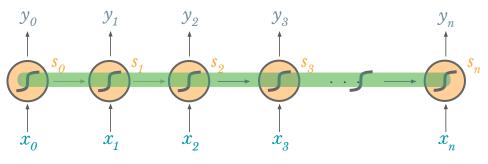


$$\frac{\partial J_n}{\partial W} = \sum_{k=0}^{n} \frac{\partial J_n}{\partial y_n} \frac{\partial y_n}{\partial s_n} \frac{\partial s_n}{\partial s_k} \frac{\partial s_k}{\partial W}$$

$$\frac{\partial s_n}{\partial s_{n-1}} \frac{\partial s_{n-1}}{\partial s_{n-2}} \cdots \frac{\partial s_3}{\partial s_2} \frac{\partial s_2}{\partial s_1} \frac{\partial s_1}{\partial s_0}$$

as the gap between timesteps gets bigger, this product gets longer and longer!





what are each of these terms?

what are each of these terms? 
$$\frac{\partial s_n}{\partial s_{n-1}} \frac{\partial s_{n-1}}{\partial s_{n-2}} \dots \frac{\partial s_3}{\partial s_2} \frac{\partial s_2}{\partial s_1} \frac{\partial s_1}{\partial s_0}$$

$$\frac{\partial s_n}{\partial s_{n-1}} = W^T \operatorname{diag} \left[ f'(W_{s_{j-1}+Ux_j}) \right]$$

$$W =$$
sampled from standard normal distribution = mostly < 1

$$f = \text{tanh or sigmoid so } f' < 1$$

we're multiplying a lot of small numbers together.

#### Vanishing Gradient Problem

we're multiplying a lot of small numbers together.

#### so what?

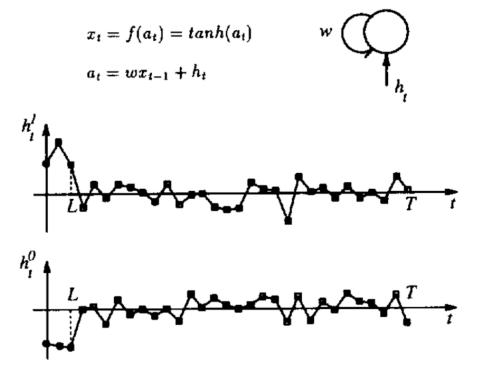
errors due to further back timesteps have increasingly smaller gradients.

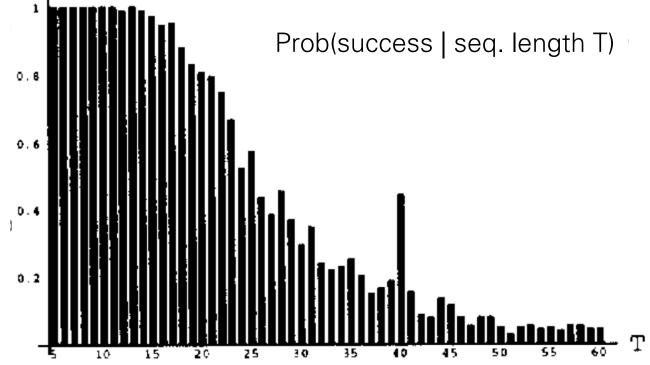
#### so what?

parameters become biased to capture shorter-term dependencies.

## A Toy Example

- 2 categories of sequences
- Can the single tanh unit learn to store for T time steps 1 bit of information given by the sign of initial input?





#### Vanishing Gradient Problem

"In France, I had a great time and I learnt some of the \_\_\_\_ language."

our parameters are not trained to capture long-term dependencies, so the word we predict will mostly depend on the previous few words, not much earlier ones

#### Long-Term Dependencies



• The RNN gradient is a product of Jacobian matrices, each associated with a step in the forward computation. To store information robustly in a finite-dimensional state, the dynamics must be contractive [Bengio et al 1994].

$$L = L(s_T(s_{T-1}(\dots s_{t+1}(s_t, \dots))))$$

$$\frac{\partial L}{\partial s_t} = \frac{\partial L}{\partial s_T} \frac{\partial s_T}{\partial s_{T-1}} \dots \frac{\partial s_{t+1}}{\partial s_t}$$

- Problems:
  - sing. values of Jacobians > 1 → gradients explode
  - or sing. values < → gradients shrink & vanish</li>
  - or random → variance grows exponentially

#### **RNN Tricks**

(Pascanu et al., 2013; Bengio et al., 2013; Gal and Ghahramani, 2016; Morishita et al., 2017)

- Mini-batch creation strategies (efficient computations)
- Clipping gradients (avoid exploding gradients)
- Leaky integration (propagate long-term dependencies)
- Momentum (cheap 2nd order)
- Dropout (avoid overfitting)
- Initialization (start in right ballpark avoids exploding/vanishing)
- Sparse Gradients (symmetry breaking)
- Gradient propagation regularizer (avoid vanishing gradient)
- Gated self-loops (LSTM & GRU, reduces vanishing gradient)

#### Mini-batching in RNNs

- Mini-batching makes things much faster!
- But mini-batching in RNNs is harder than in feed-forward networks
  - Each word depends on the previous word
  - Sequences are of various length

• Padding:

```
this is an example </s>
this is another </s>
```

- If we use sentences of different lengths, too much padding and sorting can result in decreased performance
- To remedy this: sort sentences so similarly-lengthed seqs are in the same batch

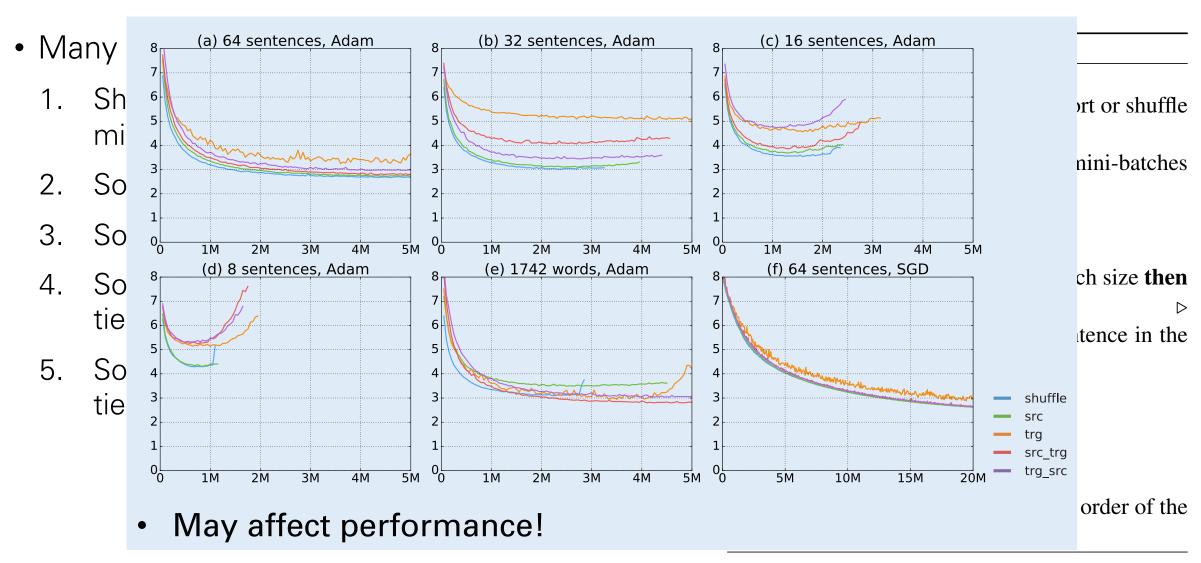
#### Mini-batching in RNNs

- Many alternatives:
  - Shuffle the corpus randomly before creating mini-batches (with no sorting).
  - 2. Sort based on the source sequence length.
  - 3. Sort based on the target sequence length.
  - 4. Sort using the source sequence length, break ties by sorting by target sequence length.
  - 5. Sort using the target sequence length, break ties by sorting by source sequence length.

#### **Algorithm 1** Create mini-batches

- 1:  $C \leftarrow \text{Training corpus}$
- 2:  $C \leftarrow \text{sort}(C)$  or shuffle $(C) \triangleright \text{sort or shuffle}$  the whole corpus
- 3:  $\boldsymbol{B} \leftarrow \{\}$   $\triangleright$  mini-batches
- 4:  $i \leftarrow 0, j \leftarrow 0$
- 5: while i < C.size() do
- 6:  $\boldsymbol{B}[j] \leftarrow \boldsymbol{B}[j] + \boldsymbol{C}[i]$
- 7: **if** B[j].size()  $\geq$  max mini-batch size **then**
- 8:  $B[j] \leftarrow \text{padding}(B[j])$   $\triangleright$  Padding tokens to the longest sentence in the mini-batch
- 9:  $j \leftarrow j + 1$
- 10: **end if**
- 11:  $i \leftarrow i + 1$
- 12: end while
- 13:  $B \leftarrow \text{shuffle}(B) \Rightarrow \text{shuffle the order of the mini-batches}$

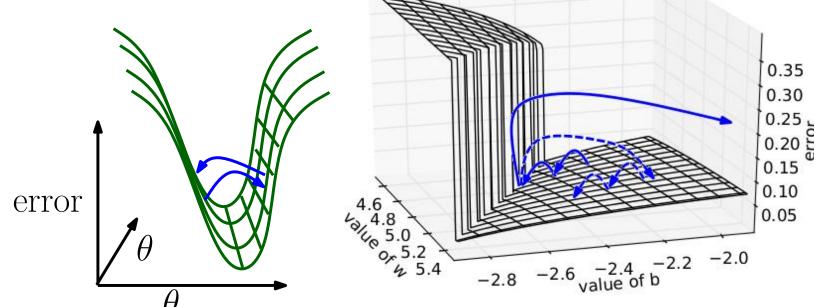
#### Mini-batching in RNNs



M. Morishita, Y. Oda, G. Neubig, K. Yoshino, K. Sudoh, and S. Nakamura. "An Empirical Study of Mini-Batch Creation Strategies for Neural Machine Translation". 1st Workshop on NMT 2017

#### Gradient Norm Clipping

$$\hat{\mathbf{g}} \leftarrow \frac{\partial error}{\partial \theta}$$
if  $\|\hat{\mathbf{g}}\| \geq threshold$  then
 $\hat{\mathbf{g}} \leftarrow \frac{threshold}{\|\hat{\mathbf{g}}\|} \hat{\mathbf{g}}$ 
end if

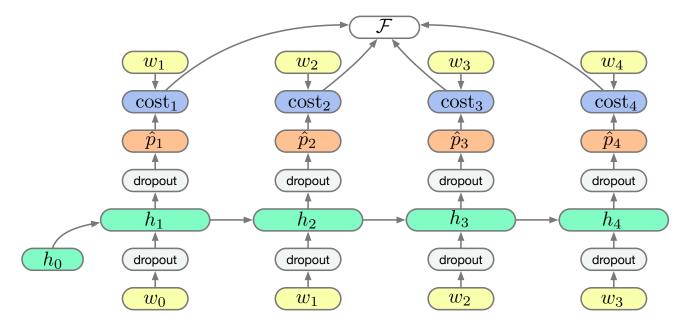


#### Regularization: Dropout

- Large recurrent networks often overfit their training data by memorizing the sequences observed. Such models generalize poorly to novel sequences.
- A common approach in Deep Learning is to overparametrize a model, such that it could easily memorize the training data, and then heavily regularize it to facilitate generalization.
- The regularization method of choice is often Dropout.

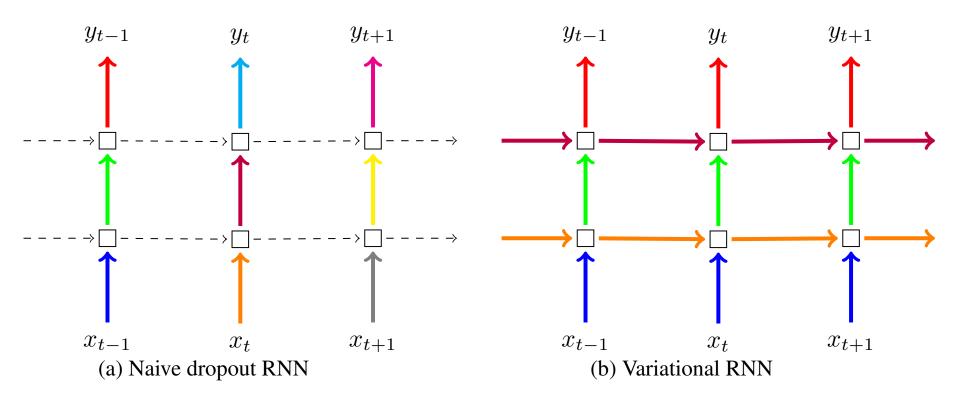
#### Regularization: Dropout

- Dropout is ineffective when applied to recurrent connections, as repeated random masks zero all hidden units in the limit.
- The most common solution is to only apply dropout to non-recurrent connections



#### Regularization: Dropout

• A Better Solution: Use the same dropout mask at each time step for both inputs, outputs, and recurrent layers.



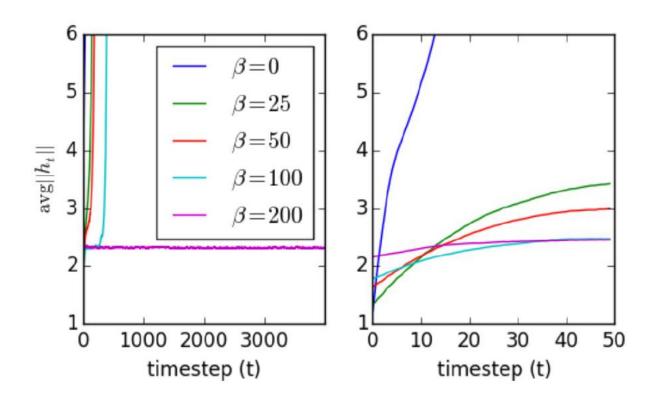
Each square represents an RNN unit, with horizontal arrows representing recurrent connections. Vertical arrows represent the input and output to each RNN unit. Coloured connections represent dropped-out inputs, with different colours corresponding to different dropout masks. Dashed lines correspond to standard connections with no dropout.

#### Regularization: Norm-stabilizer

 Stabilize the activations of RNNs by penalizing the squared distance between successive hidden states' norms

$$\beta \frac{1}{T} \sum_{t=1}^{T} (\|h_t\|_2 - \|h_{t-1}\|_2)^2$$

 Enforce the norms of the hidden layer activations approximately constant across time



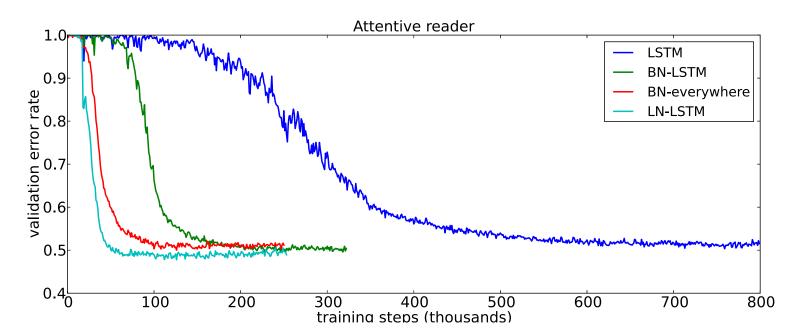
#### Regularization: Layer Normalization

- Similar to batch normalization
- Computes the normalization statistics separately at each time step
- Effective for stabilizing the hidden state dynamics in RNNs
- Reduces training time

$$\mathbf{h}^{t} = f \left[ \frac{\mathbf{g}}{\sigma^{t}} \odot \left( \mathbf{a}^{t} - \mu^{t} \right) + \mathbf{b} \right]$$

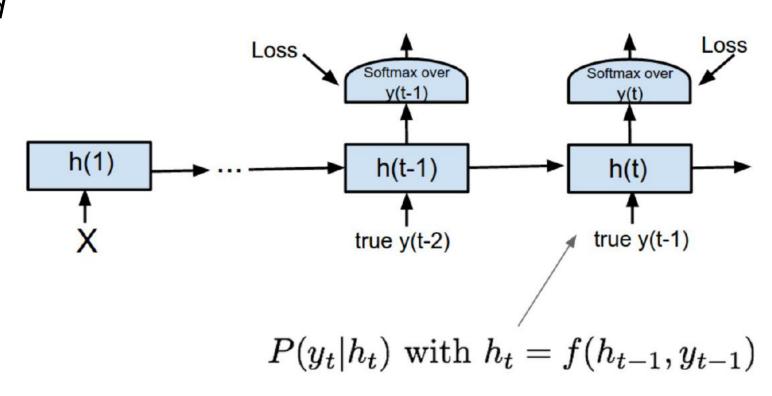
$$\mu^t = \frac{1}{H} \sum_{i=1}^H a_i^t$$

$$\sigma^t = \sqrt{\frac{1}{H} \sum_{i=1}^{H} \left(a_i^t - \mu^t\right)^2}$$



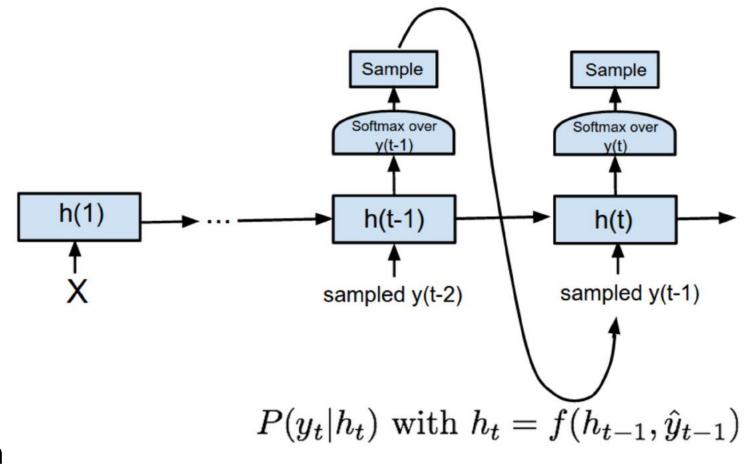
## Scheduled Sampling

 "change the training process from a fully guided scheme using the true previous token, towards a less guided scheme which mostly uses the generated token instead."



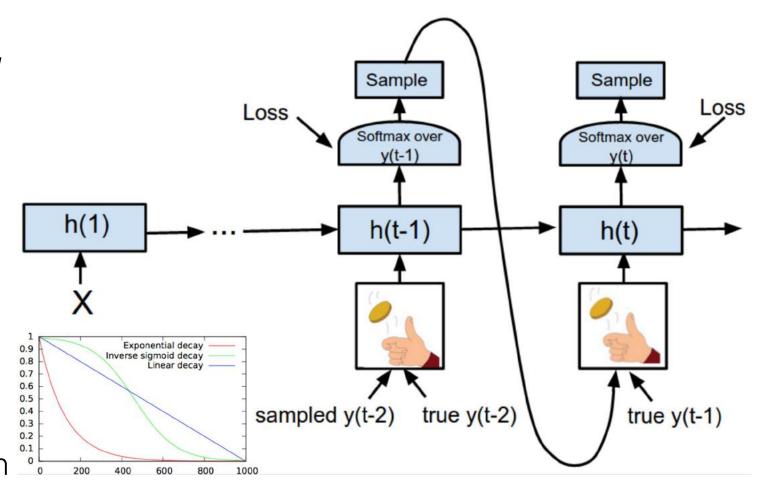
## Scheduled Sampling

- "change the training process from a fully guided scheme using the true previous token, towards a less guided scheme which mostly uses the generated token instead."
- During training, randomly replace a conditioning ground truth token by the model's previous prediction



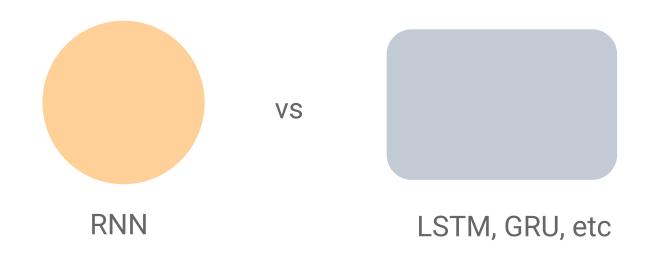
## Scheduled Sampling

- "change the training process from a fully guided scheme using the true previous token, towards a less guided scheme which mostly uses the generated token instead."
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#### **Gated Cells**

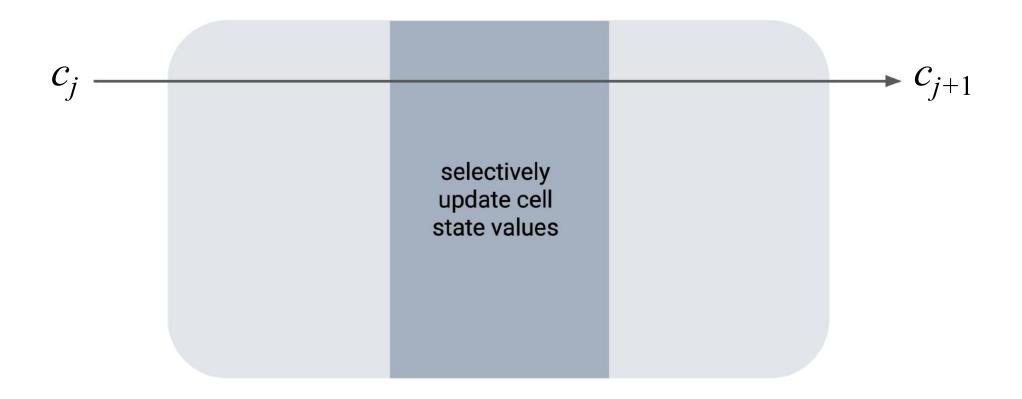
 rather each node being just a simple RNN cell, make each node a more complex unit with gates controlling what information is passed through

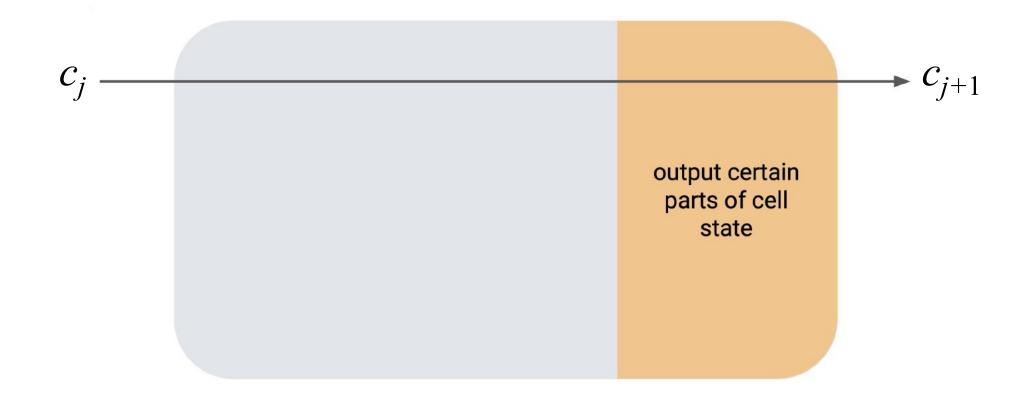


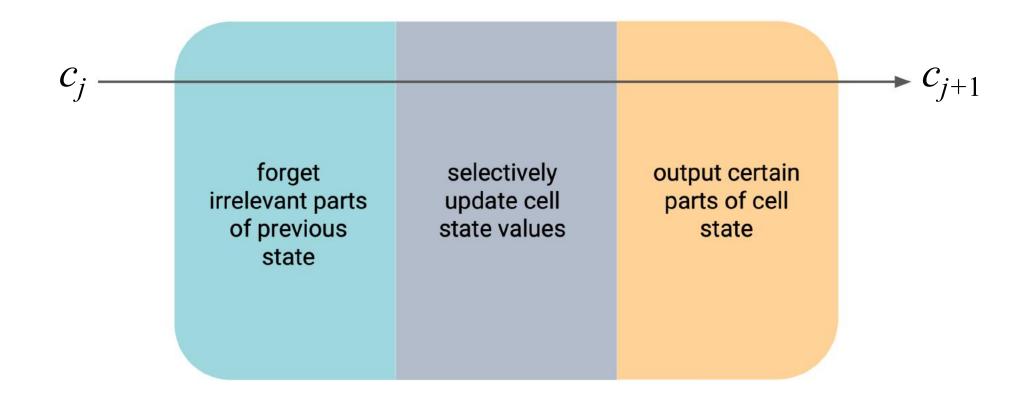
Long short term memory cells are able to keep track of information throughout many timesteps.



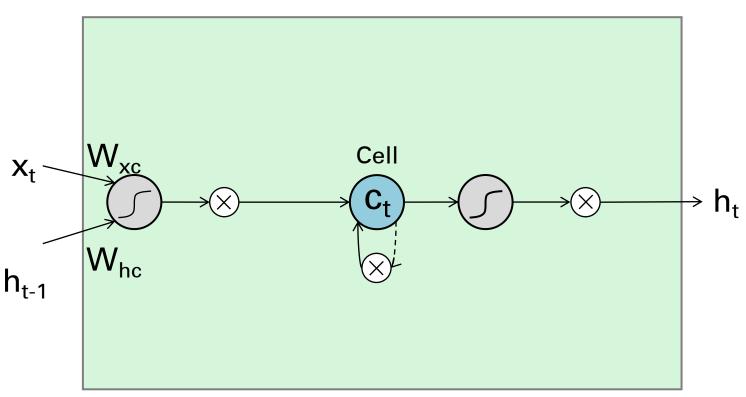








#### The LSTM Idea

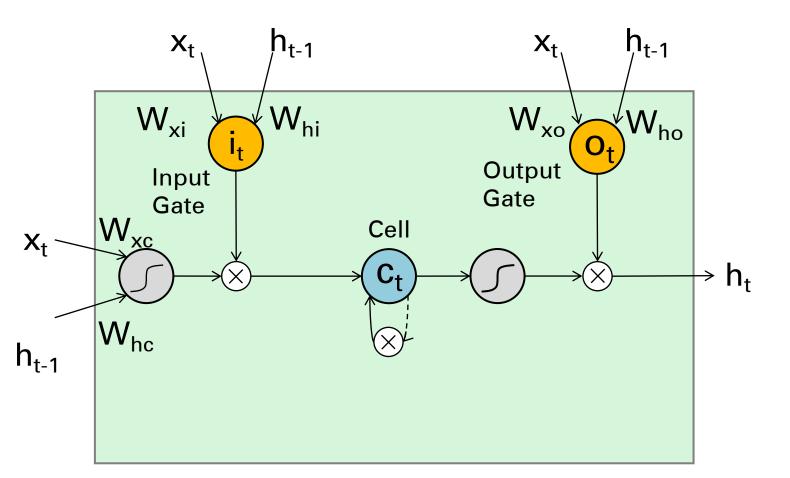


$$c_{t} = c_{t-1} + \tanh W \begin{pmatrix} x_{t} \\ h_{t-1} \end{pmatrix}$$

$$h_{t} = \tanh c_{t}$$

<sup>\*</sup> Dashed line indicates time-lag

## The Original LSTM Cell

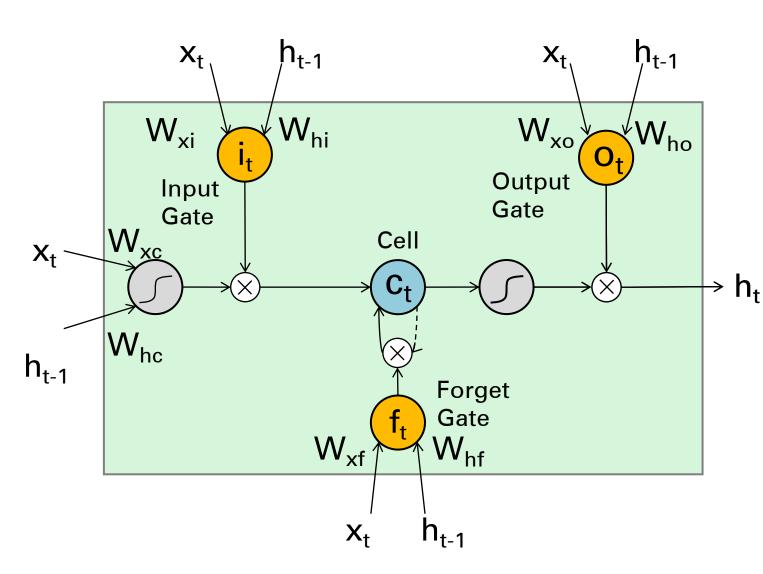


$$c_{t} = c_{t-1} + i_{t} \otimes \tanh W \begin{pmatrix} x_{t} \\ h_{t-1} \end{pmatrix}$$

$$h_t = o_t \otimes \tanh c_t$$

$$i_{t} = \sigma \left( W_{i} \begin{pmatrix} x_{t} \\ h_{t-1} \end{pmatrix} + b_{i} \right)$$

Similarly for ot

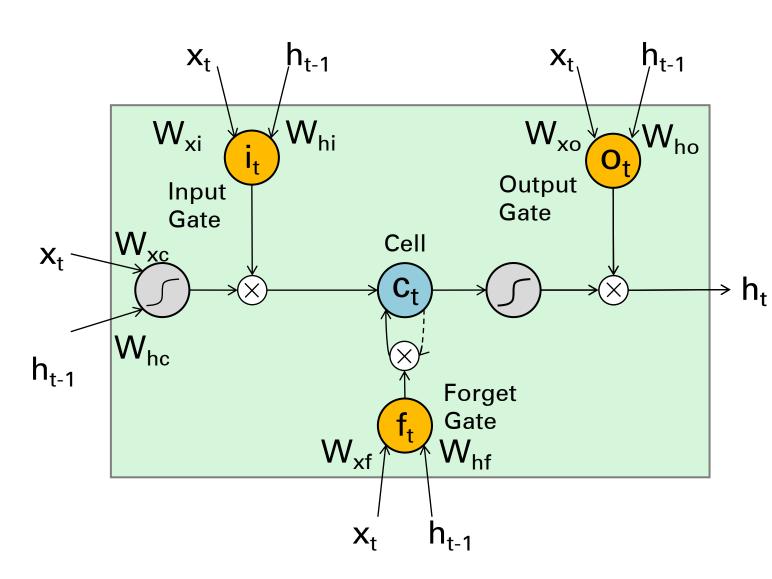


$$i_{t} = \sigma \left( W_{i} \begin{pmatrix} x_{t} \\ h_{t-1} \end{pmatrix} + b_{i} \right)$$

$$c_{t} = f_{t} \otimes c_{t-1} + i_{t} \otimes \tanh W \begin{pmatrix} x_{t} \\ h_{t-1} \end{pmatrix}$$

$$f_t = \sigma \left( W_f \begin{pmatrix} x_t \\ h_{t-1} \end{pmatrix} + b_f \right)$$

$$h_t = o_t \otimes \tanh c_t$$



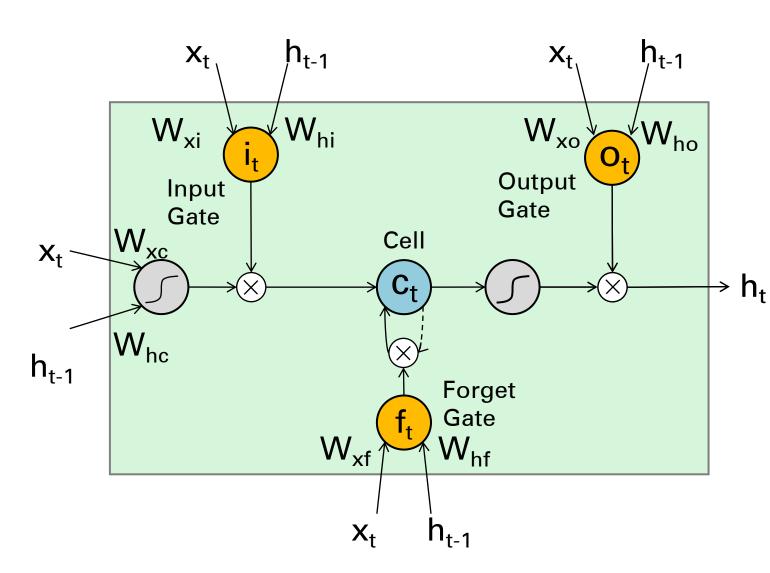
$$i_{t} = \sigma \left( W_{i} \begin{pmatrix} x_{t} \\ h_{t-1} \end{pmatrix} + b_{i} \right)$$

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$$f_t = \sigma \left( W_f \begin{pmatrix} x_t \\ h_{t-1} \end{pmatrix} + b_f \right)$$

$$h_t = o_t \otimes \tanh c_t$$

**forget gate** decides what information is going to be thrown away from the cell state



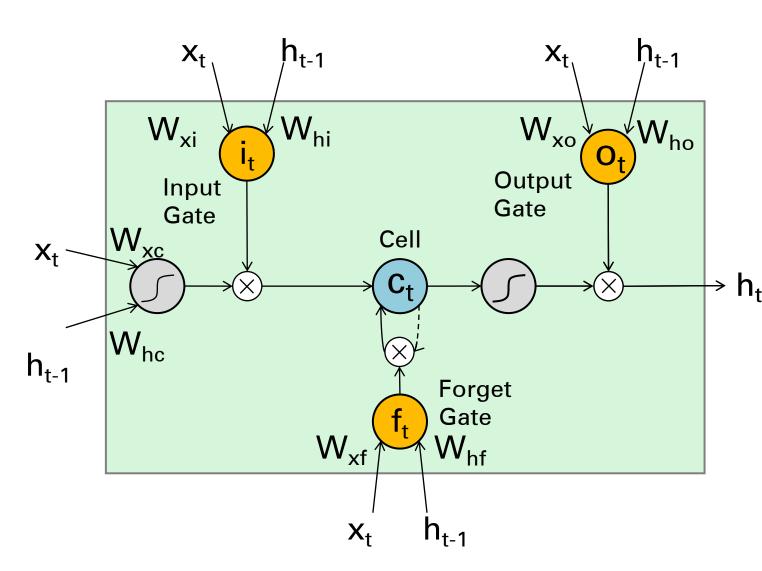
$$i_{t} = \sigma \left( W_{i} \begin{pmatrix} x_{t} \\ h_{t-1} \end{pmatrix} + b_{i} \right)$$

$$c_{t} = f_{t} \otimes c_{t-1} + i_{t} \otimes \tanh W \begin{pmatrix} x_{t} \\ h_{t-1} \end{pmatrix}$$

$$f_t = \sigma \left( W_f \begin{pmatrix} x_t \\ h_{t-1} \end{pmatrix} + b_f \right)$$

$$h_t = o_t \otimes \tanh c_t$$

input gate and a tanh layer decides what information is going to be stored in the cell state



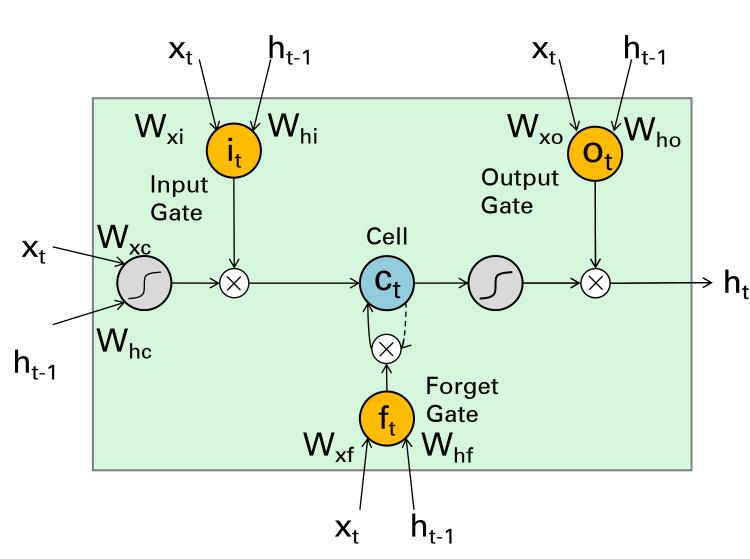
$$i_{t} = \sigma \left( W_{i} \begin{pmatrix} x_{t} \\ h_{t-1} \end{pmatrix} + b_{i} \right)$$

$$c_{t} = f_{t} \otimes c_{t-1} + i_{t} \otimes \tanh W \begin{pmatrix} x_{t} \\ h_{t-1} \end{pmatrix}$$

$$f_t = \sigma \left( W_f \begin{pmatrix} x_t \\ h_{t-1} \end{pmatrix} + b_f \right)$$

$$h_t = o_t \otimes \tanh c_t$$

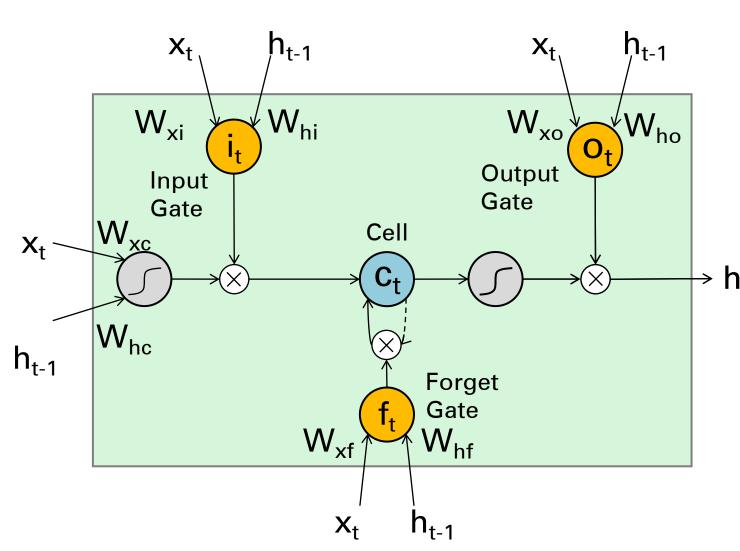
Update the old cell state with the new one.



$$i_{t} = \sigma \left( W_{i} \begin{pmatrix} x_{t} \\ h_{t-1} \end{pmatrix} + b_{i} \right)$$

$$c_{t} = f_{t} \otimes c_{t-1} + i_{t} \otimes \tanh W \begin{pmatrix} x_{t} \\ h_{t-1} \end{pmatrix}$$

input gate	forget gate	behavior
0	1	remember the previous value
1	1	add to the previous value
0	0	erase the value
1	0	overwrite the value



$$i_{t} = \sigma \left( W_{i} \begin{pmatrix} x_{t} \\ h_{t-1} \end{pmatrix} + b_{i} \right)$$

$$c_{t} = f_{t} \otimes c_{t-1} + i_{t} \otimes \tanh W \begin{pmatrix} x_{t} \\ h_{t-1} \end{pmatrix}$$

$$f_t = \sigma \left( W_f \begin{pmatrix} x_t \\ h_{t-1} \end{pmatrix} + b_f \right)$$

$$h_{t} = o_{t} \otimes \tanh c_{t}$$

$$o_{i} = \sigma \left( W_{o} \begin{pmatrix} x_{t} \\ h_{t-1} \end{pmatrix} + b_{o} \right)$$

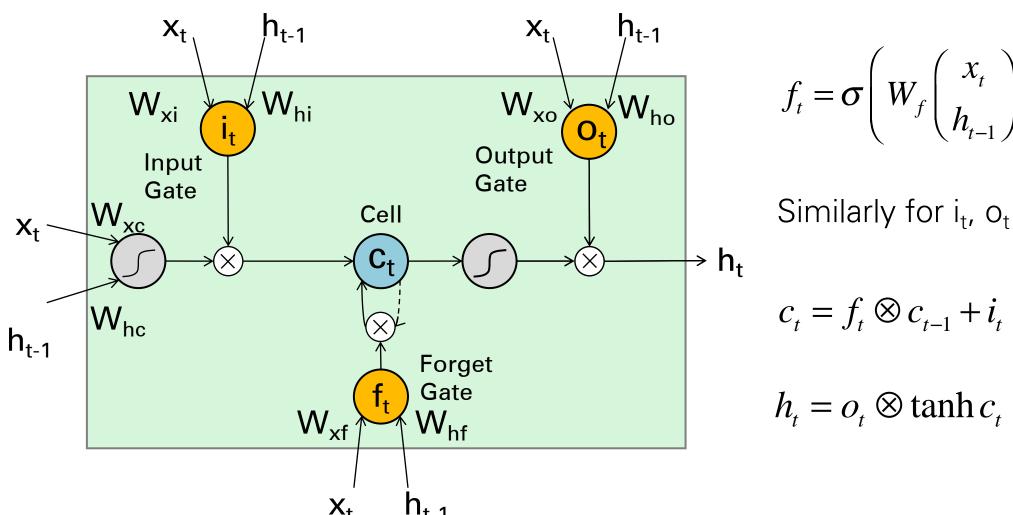
**Output gate** decides what is going to be outputted. The final output is based on cell state and output of sigmoid gate.

#### LSTM - Forward/Backward

Illustrated LSTM Forward and Backward Pass

http://arunmallya.github.io/writeups/nn/lstm/index.html

# LSTM variants

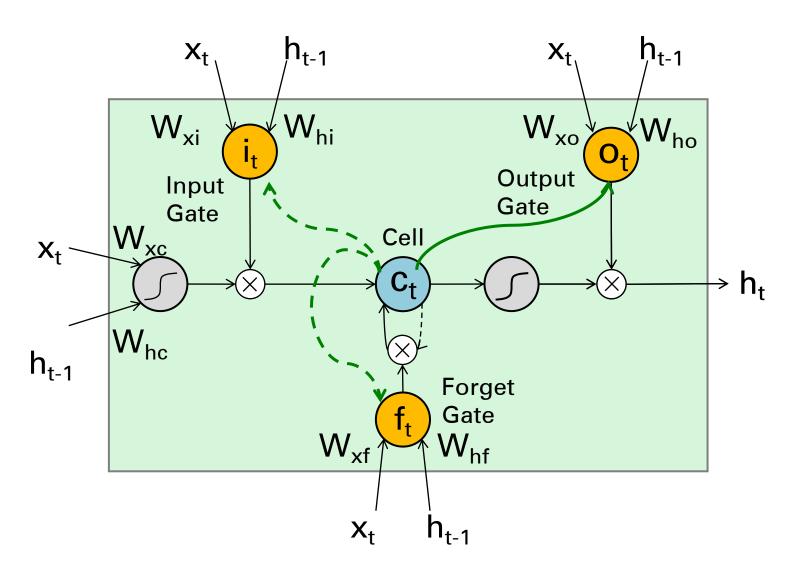


$$f_t = \sigma \left( W_f \begin{pmatrix} x_t \\ h_{t-1} \end{pmatrix} + b_f \right)$$

$$c_{t} = f_{t} \otimes c_{t-1} + i_{t} \otimes \tanh W \begin{pmatrix} x_{t} \\ h_{t-1} \end{pmatrix}$$

<sup>\*</sup> Dashed line indicates time-lag

#### Extension I: Peephole LSTM



$$f_t = \sigma \left( W_f \begin{pmatrix} x_t \\ h_{t-1} \\ C_{t-1} \end{pmatrix} + b_f \right)$$

Similarly for  $i_t$ ,  $o_t$  (uses  $c_t$ )

$$c_{t} = f_{t} \otimes c_{t-1} + i_{t} \otimes \tanh W \begin{pmatrix} x_{t} \\ h_{t-1} \end{pmatrix}$$

$$h_t = o_t \otimes \tanh c_t$$

- Add peephole connections.
- All gate layers look at the cell state!

<sup>\*</sup> Dashed line indicates time-lag

#### Other minor variants

Coupled Input and Forget Gate

$$f_t = 1 - i_t$$

• Full Gate Recurrence

$$f_t = \sigma \left( W_f \begin{pmatrix} x_t \\ h_{t-1} \\ c_{t-1} \\ \vdots \\ f_{t-1} \\ f_{t-1} \\ O_{t-1} \end{pmatrix} + b_f \right)$$

### LSTM: A Search Space Odyssey

- Tested the following variants, using Peephole LSTM as standard:
  - 1. No Input Gate (NIG)
  - 2. No Forget Gate (NFG)
  - 3. No Output Gate (NOG)
  - 4. No Input Activation Function (NIAF)
  - 5. No Output Activation Function (NOAF)
  - 6. No Peepholes (NP)
  - 7. Coupled Input and Forget Gate (CIFG)
  - 8. Full Gate Recurrence (FGR)
- On the tasks of:
  - Timit Speech Recognition: Audio frame to 1 of 61 phonemes
  - IAM Online Handwriting Recognition: Sketch to characters
  - JSB Chorales: Next-step music frame prediction

### LSTM: A Search Space Odyssey

- The standard LSTM performed reasonably well on multiple datasets and none of the modifications significantly improved the performance
- Coupling gates and removing peephole connections simplified the LSTM without hurting performance much
- The forget gate and output activation are crucial

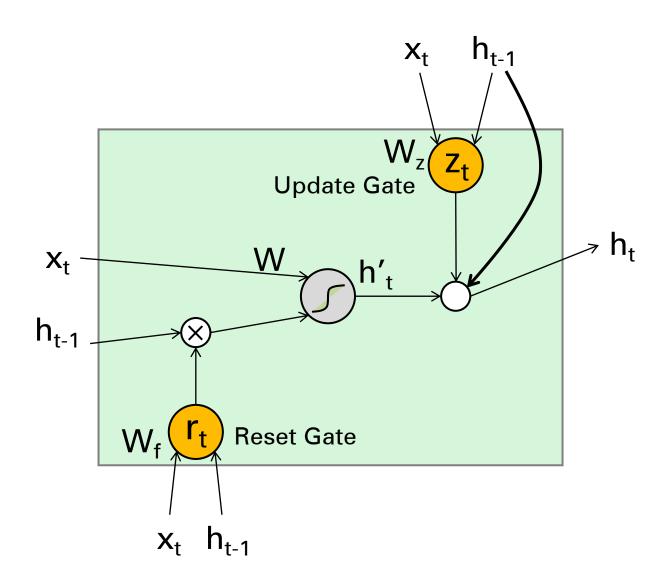
 Found interaction between learning rate and network size to be minimal – indicates calibration can be done using a small network first

### Gated Recurrent Unit

### Gated Recurrent Unit (GRU)

- A very simplified version of the LSTM
  - Merges forget and input gate into a single 'update' gate
  - Merges cell and hidden state
- Has fewer parameters than an LSTM and has been shown to outperform LSTM on some tasks

<u>Learning Phrase Representations using RNN Encoder-Decoder for Statistical Machine Translation</u>
[Cho et al.,14]

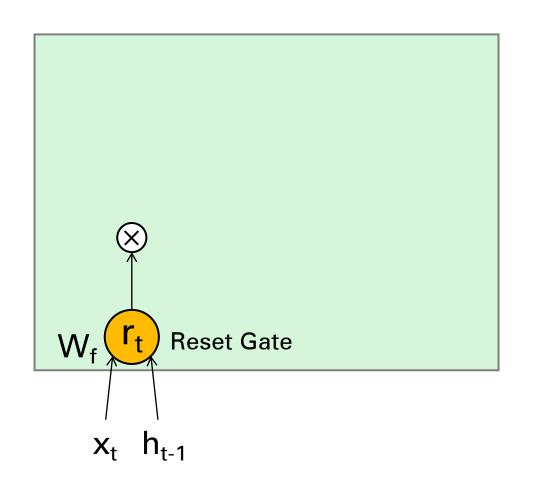


$$r_{t} = \sigma \left( W_{r} \begin{pmatrix} x_{t} \\ h_{t-1} \end{pmatrix} + b_{f} \right)$$

$$h'_{t} = \tanh W \begin{pmatrix} x_{t} \\ r_{t} \otimes h_{t-1} \end{pmatrix}$$

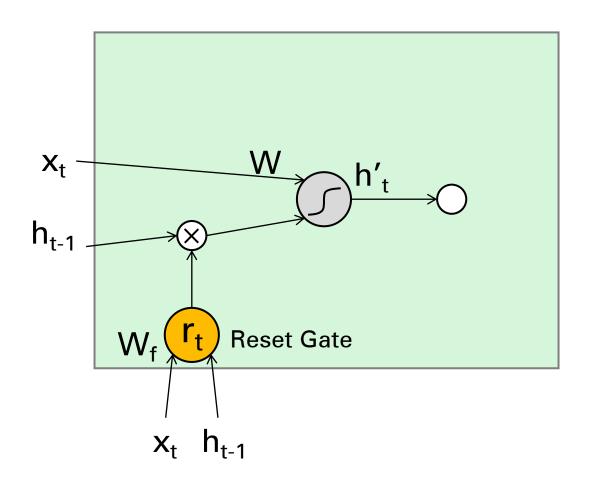
$$z_{t} = \sigma \left( W_{z} \begin{pmatrix} x_{t} \\ h_{t-1} \end{pmatrix} + b_{f} \right)$$

$$h_{t} = (1 - z_{t}) \otimes h_{t-1} + z_{t} \otimes h'_{t}$$



$$r_{t} = \sigma \left( W_{r} \begin{pmatrix} x_{t} \\ h_{t-1} \end{pmatrix} + b_{f} \right)$$

computes a **reset gate** based on current input and hidden state

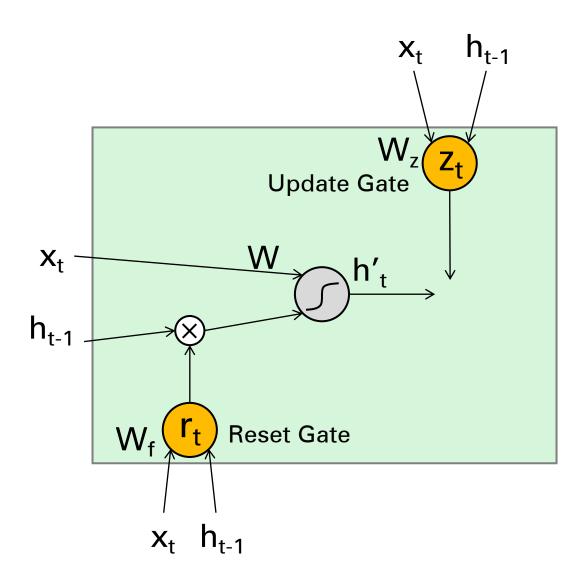


$$r_{t} = \sigma \left( W_{r} \begin{pmatrix} x_{t} \\ h_{t-1} \end{pmatrix} + b_{f} \right)$$

$$h'_{t} = \tanh W \begin{pmatrix} x_{t} \\ r_{t} \otimes h_{t-1} \end{pmatrix}$$

computes the **hidden state** based on current input and hidden state

if reset gate unit is ~0, then this ignores previous memory and only stores the new input information

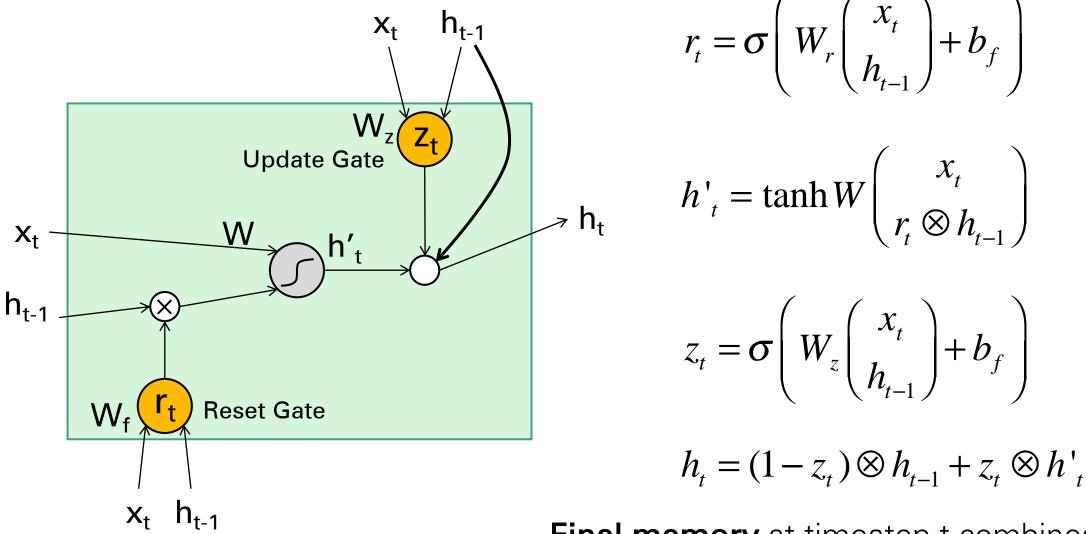


$$r_{t} = \sigma \left( W_{r} \begin{pmatrix} x_{t} \\ h_{t-1} \end{pmatrix} + b_{f} \right)$$

$$h'_{t} = \tanh W \begin{pmatrix} x_{t} \\ r_{t} \otimes h_{t-1} \end{pmatrix}$$

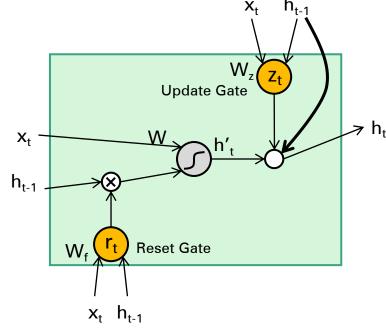
$$z_{t} = \sigma \left( W_{z} \begin{pmatrix} x_{t} \\ h_{t-1} \end{pmatrix} + b_{f} \right)$$

computes an **update gate** again based on current input and hidden state



**Final memory** at timestep t combines both current and previous timesteps

### GRU Intuition



$$r_{t} = \sigma \left( W_{r} \begin{pmatrix} x_{t} \\ h_{t-1} \end{pmatrix} + b_{f} \right)$$

$$h'_{t} = \tanh W \begin{pmatrix} x_{t} \\ r_{t} \otimes h_{t-1} \end{pmatrix}$$

$$z_{t} = \sigma \left( W_{z} \begin{pmatrix} x_{t} \\ h_{t-1} \end{pmatrix} + b_{f} \right)$$

$$h_{t} = (1 - z_{t}) \otimes h_{t-1} + z_{t} \otimes h'_{t}$$

- If reset is close to 0, ignore previous hidden state
  - > Allows model to drop information that is irrelevant in the future
- Update gate z controls how much of past state should matter now.
  - If z close to 1, then we can copy information in that unit through many time steps! Less vanishing gradient!
- Units with short-term dependencies often have reset gates very active

## An Empirical Exploration of Recurrent Network Architectures

 Given the rather ad-hoc design of the LSTM, the authors try to determine if the architecture of the LSTM is optimal

They use an evolutionary search for better architectures

### **Evolutionary Architecture Search**

- A list of top-100 architectures so far is maintained, initialized with the LSTM and the GRU
- The GRU is considered as the baseline to beat
- New architectures are proposed, and retained based on performance ratio with GRU
- All architectures are evaluated on 3 problems
  - Arithmetic: Compute digits of sum or difference of two numbers provided as inputs.
     Inputs have distractors to increase difficulty
     3e36d9-h1h39f94eeh43keg3c = 3369 13994433 = -13991064
  - XML Modeling: Predict next character in valid XML modeling
  - Penn Tree-Bank Language Modeling: Predict distributions over words

### **Evolutionary Architecture Search**

- At each step
  - Select 1 architecture at random, evaluate on 20 randomly chosen hyperparam settings.
  - Alternatively, propose a new architecture by mutating an existing one. Choose prob. p from [0,1] uniformly and apply a transformation to each node with prob.
    - If node is a non-linearity, replace with {tanh(x), sigmoid(x), ReLU(x), Linear(0, x), Linear(1, x), Linear(0.9, x), Linear(1.1, x)}
    - If node is an elementwise op, replace with {multiplication, addition, subtraction}
    - Insert random activation function between node and one of its parents
    - Replace node with one of its ancestors (remove node)
    - Randomly select a node (node A). Replace the current node with either the sum, product, or difference of a random ancestor of the current node and a random ancestor of A.
  - Add architecture to list based on minimum relative accuracy wrt GRU on 3 different tasks

An Empirical Exploration of Recurrent Network Architectures [Jozefowicz et al., 2015]

### **Evolutionary Architecture Search**

- 3 novel architectures are presented in the paper
- Very similar to GRU, but slightly outperform it

 LSTM initialized with a large positive forget gate bias outperformed both the basic LSTM and the GRU!

## LSTM initialized with large positive forget gate bias?

Recall

$$f_{t} = \sigma \left( W_{f} \begin{pmatrix} x_{t} \\ h_{t-1} \end{pmatrix} + b_{f} \right)$$

$$c_{t} = f_{t} \otimes c_{t-1} + i_{t} \otimes \tanh W \begin{pmatrix} x_{t} \\ h_{t-1} \end{pmatrix}$$

$$\delta c_{t-1} = \delta c_{t} \otimes f_{t}$$

- Gradients will vanish if f is close to 0. Using a large positive bias ensures that f has values close to 1, especially when training begins
- Helps learn long-range dependencies
- Originally stated in <u>Learning to forget: Continual prediction with LSTM [Gers et al., 2000</u>], but forgotten over time

### LSTMs and GRUs

#### Good

• Careful initialization and optimization of vanilla RNNs can enable them to learn long(ish) dependencies, but gated additive cells, like the LSTM and GRU, often just work.

#### Bad

 LSTMs and GRUs have considerably more parameters and computation per memory cell than a vanilla RNN, as such they have less memory capacity per parameter\*

An LSTM with large positive forget gate bias works best!

\*Capacity and Trainability in Recurrent Neural Networks. [Collins et al., arXiv 2016]

# Next lecture: Attention and Transformers