

### Lecture 6: Recurrent Neural Networks Efstratios Gavves

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- o Sequential data
- Recurrent Neural Networks
- Backpropagation through time
- Exploding and vanishing gradients
- o LSTMs and variants
- o Encoder-Decoder Architectures

#### Sequence data

#### Sequence applications

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o Videos

 $\circ$  Other?

#### o Videos

#### $\circ$ Other?

#### • Time series data

- Stock exchange
- Biological measurements
- Climate measurements
- Market analysis
- o Speech/Music
- User behavior in websites

#### 0 .....

- Machine translation
- o Image captioning
- Ouestion answering
- Video generation
- Speech synthesis
- Speech recognition

 $\circ$  Sequence  $\rightarrow$  Chain rule of probabilities

$$p(x) = \prod_{i} p(x_i | x_1, \dots, x_{i-1})$$

o For instance, let's model that "This is the best course!"

<mark>0</mark>???

Sequences might be of arbitrary or even infinite lengths
 Infinite parameters?

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• No, better share and reuse parameters

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can be reused also for

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For a ConvNet that is not straightforward
Why?

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• For a ConvNet that is not straightforward

• Why? Fixed dimensionalities

## Some properties of sequences?

• Data inside a sequence are non identically, independently distributed (IID)

- The next "word" depends on the previous "words"
- Ideally on all of them

• We need context, and we need memory!

• **Big question:** How to model context and memory ?



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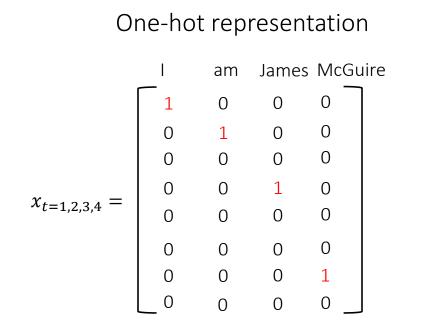
• **Big question:** How to model context and memory ?



○ A vector with all zeros except for the active dimension
○ 12 words in a sequence → 12 One-hot vectors
○ After the one-hot vectors apply an embedding
○ Word2Vec, GloVE

Vocabulary	One-hot vectors							
Ι	I	1		0		0		0
am	am	0	am	1	am	0	am	0
Bond	Bond	0	Bond	0	Bond	1	Bond	0
James	James	0	James	0	James	0	James	1
tired	tired	0	tired	0	tired	0	tired	0
,	1	0	,	0	,	0	,	0
McGuire	McGuire	0	McGuire	0	McGuire	0	McGuire	0
!	]	0	!	0	!	0		0

## Why not indices instead of one-hot vectors?



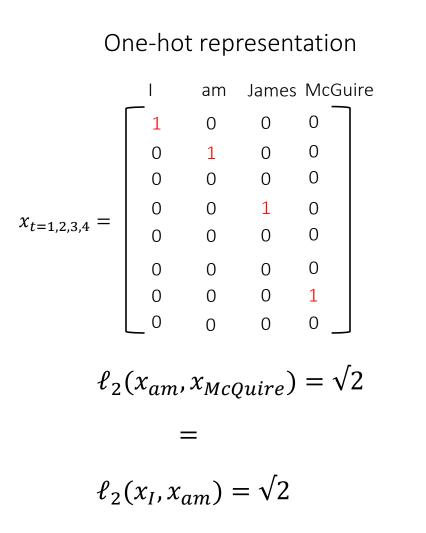
Index representation

OR?

I am James McGuire

$$x_{"I"} = 1$$
$$x_{"am"} = 2$$
$$x_{"James"} = 4$$
$$x_{"McGuire"} = 7$$

## Why not indices instead of one-hot vectors?



Index representation

OR?

I am James McGuire

$$x_{"I"} = 1$$
$$x_{"am"} = 2$$
$$x_{"James"} = 4$$
$$x_{"McGuire"} = 7$$

$$\ell_2(x_{am}, x_{McQuire}) = (7 - 2)^2 = 5$$

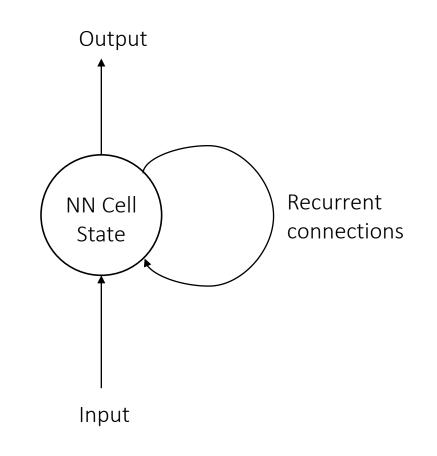
$$\neq$$

$$\ell_2(x_I, x_{am}) = (2 - 1)^2 = 1$$

Recurrent Neural Networks

Backprop through time

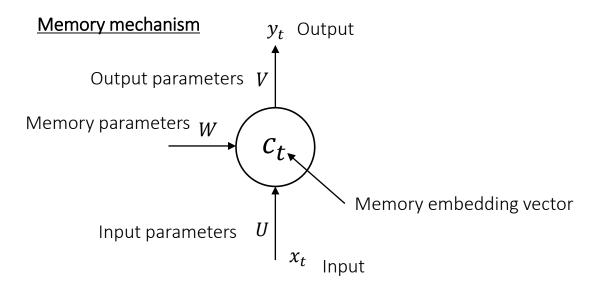
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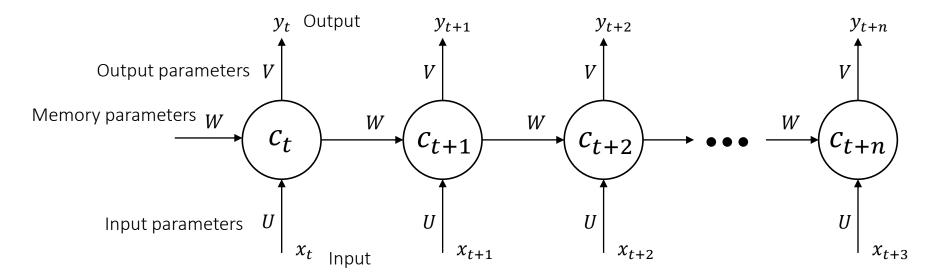
- o Memory is a mechanism that learns a representation of the past
- At timestep t project all previous information 1, ..., t onto a latent space  $c_t$ • Memory controlled by a neural network  $h_{\theta}$  with shared parameters  $\theta$
- o Then, at timestep t+1 re-use the parameters  $\theta$  and the previous  $c_t$   $c_{t+1} = h_\theta(x_{t+1},c_t)$

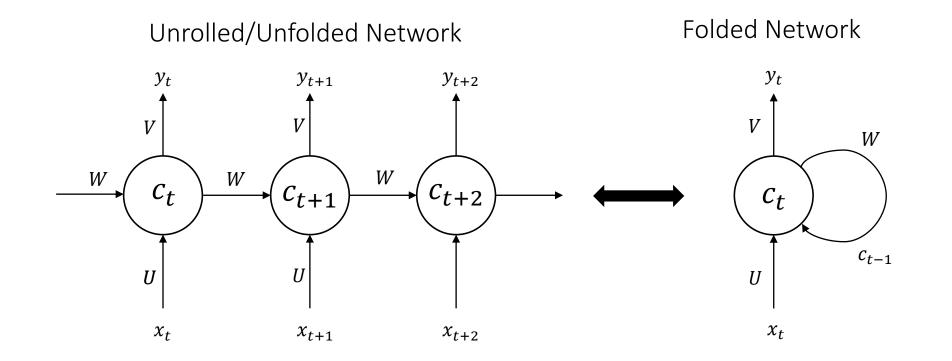
 $c_{t+1} = h_{\theta}(x_{t+1}, h_{\theta}(x_t, h_{\theta}(x_{t-1}, \dots h_{\theta}(x_1, c_0))))$ 

In the simplest case, what are the Inputs/Outputs of our system
Sequence inputs → we model them with parameters U
Sequence outputs → we model them with parameters V
Memory I/O → we model it with parameters W



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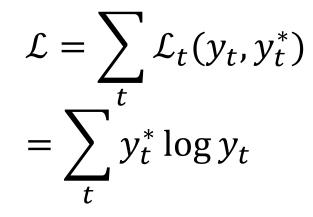


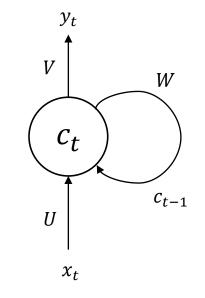
• Basically, two equations

$$c_t = \tanh(U x_t + W c_{t-1})$$
  

$$y_t = \operatorname{softmax}(V c_t)$$

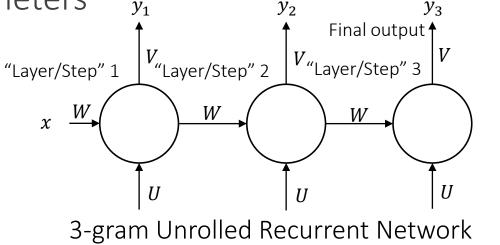
• And a loss function

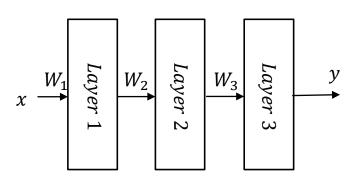




assuming the cross-entropy loss function

- o Is there a big difference?
- $_{\circ}$  Instead of layers  $\rightarrow$  Steps
- $_{\odot}$  Outputs at every step  $\rightarrow$  MLP outputs in every layer possible
- Main difference: Instead of layer-specific parameters  $\rightarrow$  Layer-shared parameters  $y_1$   $y_2$   $y_3$





3-layer Neural Network

• How is the training done? Does Backprop remain the same?

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- Basically, chain rule
- So, again the same concept

• Yet, a bit more tricky this time, as the gradients survive over time

Backpropagation through time

$$c_{t} = \tanh(U x_{t} + W c_{t-1})$$
  

$$y_{t} = \operatorname{softmax}(V c_{t})$$
  

$$\mathcal{L} = \sum_{t} y_{t}^{*} \log y_{t}$$

• Let's say we focus on the third timestep loss

$$\frac{\partial \mathcal{L}}{\partial V} = \cdots$$
$$\frac{\partial \mathcal{L}}{\partial \mathcal{L}} = \cdots$$
$$\frac{\partial \mathcal{L}}{\partial \mathcal{L}} = \cdots$$

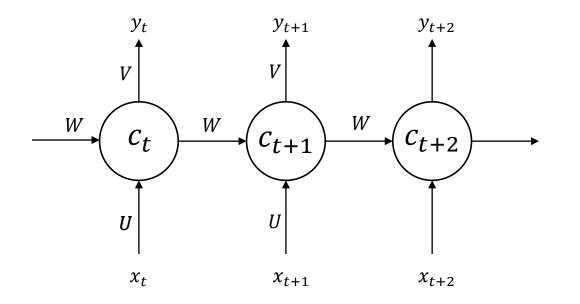
# Backpropagation through time: $\partial \mathcal{L}_t / \partial V$

o Expanding the chain rule

$$\frac{\partial \mathcal{L}_{t}}{\partial V} = \frac{\partial \mathcal{L}_{t}}{\partial y_{t_{k}}} \frac{\partial y_{t_{k}}}{\partial q_{t_{l}}} \frac{\partial q_{t_{l}}}{\partial V_{ij}} = \cdots$$
$$= (y_{t} - y_{t}^{*}) \otimes c_{t}$$

- All terms depend only on the current timestep *t*
- Then, we should sum up all the gradients for all time steps

$$\frac{\partial \mathcal{L}}{\partial V} = \sum_{t} \frac{\partial \mathcal{L}_{t}}{\partial V}$$



# Backpropagation through time: $\partial \mathcal{L}_t / \partial W$

- Expanding with the chain rule
  - $\frac{\partial \mathcal{L}_t}{\partial W} = \frac{\partial \mathcal{L}_t}{\partial y_t} \frac{\partial y_t}{\partial c_t} \frac{\partial c_t}{\partial W}$
- However,  $c_t$  itself depends on  $c_{t-1} \rightarrow \frac{\partial c_t}{\partial W}$  depends also on  $c_{t-1} \rightarrow$ The current dependency of  $c_t$  to W is recurrent
  - And continuing till we reach  $c_{-1} = [0]$
- o So, in the end we have

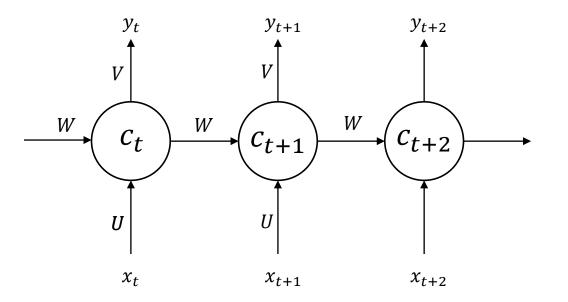
$$\frac{\partial \mathcal{L}_t}{\partial W} = \sum_{k=0}^t \frac{\partial \mathcal{L}_t}{\partial y_t} \frac{\partial y_t}{\partial c_t} \frac{\partial c_t}{\partial c_k} \frac{\partial c_k}{\partial W}$$

• The gradient  $\frac{\partial c_t}{\partial c_k}$  itself is subject to the chain rule

$$\frac{\partial c_t}{\partial c_k} = \frac{\partial c_t}{\partial c_{t-1}} \frac{\partial c_{t-1}}{\partial c_{t-2}} \dots \frac{\partial c_{k+1}}{\partial c_k} = \prod_{j=k+1}^t \frac{\partial c_j}{\partial c_{j-1}}$$

• Then, we should sum up all the gradients for all time steps

 $c_t = \tanh(U x_t + W c_{t-1})$  $y_t = \operatorname{softmax}(V c_t)$ 

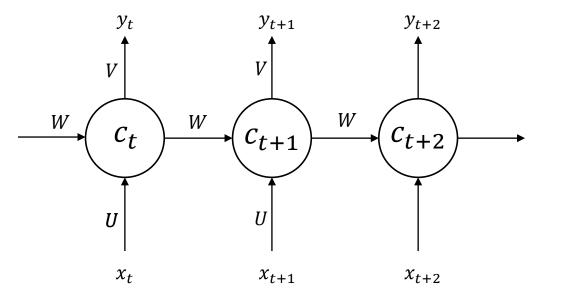


Backpropagation through time:  $\partial \mathcal{L}_t / \partial U$ 

 $\circ$  For parameter matrix U a similar process

$$\frac{\partial \mathcal{L}_t}{\partial W} = \sum_{k=0}^t \frac{\partial \mathcal{L}_t}{\partial y_t} \frac{\partial y_t}{\partial c_t} \frac{\partial c_t}{\partial c_k} \frac{\partial c_k}{\partial W}$$

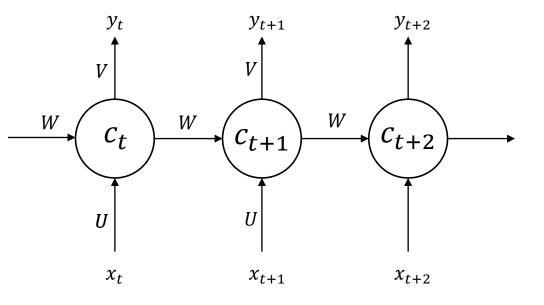
 $c_t = \tanh(U x_t + W c_{t-1})$  $y_t = \operatorname{softmax}(V c_t)$ 



# Trading off Weight Update Frequency & Gradient Accuracy

- At time t we use current weights  $w_t$  to compute states  $c_t$  and outputs  $y_t$
- $_{\rm O}$  Then, we use the states and outputs to backprop and get  $w_{t+1}$
- $_{\rm o}$  Then, at t+1 we use  $w_{t+1}$  and the current state  $c_t$  to  $y_{t+1}$  and  $c_{t+1}$
- Then we update the weights again with  $y_{t+1}$ .
- The problem is  $y_{t+1}$  was computed with  $c_t$  in mind, which in turns depends on the old weights  $w_t$ , not the current ones  $w_{t+1}$ . So, the new gradients are only an estimate
- Getting worse and worse, the more we backprop through time

 $c_t = \tanh(U x_t + W c_{t-1})$  $y_t = \operatorname{softmax}(V c_t)$ 



- Do fewer updates
- That might slow down training

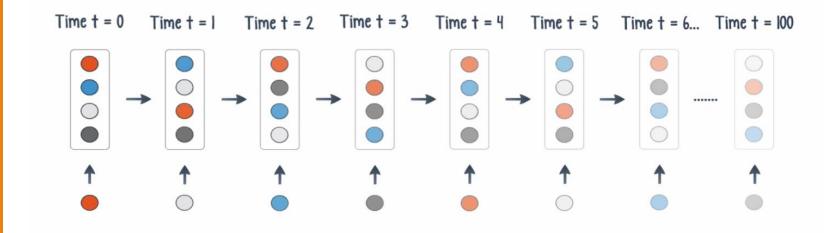
 We can also make sure we do not backprop through more steps than our frequency of updates

- But then we do not compute the full gradients
- $^{\circ}$  Bias again  $\rightarrow$  not really gaining much

#### Vanishing gradients Exploding gradients Truncated backprop

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# Decay of information through time



• Easier for mathematical analysis, and doesn't change the mechanics of the recurrent neural network

$$c_{t} = W \cdot \tanh(c_{t-1}) + U \cdot x_{t} + b$$
$$\mathcal{L} = \sum_{t} \mathcal{L}_{t}(c_{t})$$
$$\theta = \{W, U, b\}$$

• As we just saw, the gradient  $\frac{\partial c_t}{\partial c_k}$  itself is subject to the chain rule

$$\frac{\partial c_t}{\partial c_k} = \frac{\partial c_t}{\partial c_{t-1}} \frac{\partial c_{t-1}}{\partial c_{t-2}} \dots \frac{\partial c_{k+1}}{\partial c_k} = \prod_{\substack{j=k+1}}^t \frac{\partial c_j}{\partial c_{j-1}}$$

• Product of ever expanding Jacobians

• Ever expanding because we multiply more and more for longer dependencies

## Let's look again the gradients

• Minimize the total loss over all time steps

$$\arg\min_{\theta} \sum_{t} \mathcal{L}_{t}(c_{t,\theta})$$
$$\frac{\partial \mathcal{L}_{t}}{\partial W}^{t} = \cdots$$

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$$\frac{\partial \mathcal{L}_{t}}{\partial W} = \sum_{\tau=1}^{t} \frac{\partial \mathcal{L}_{t}}{\partial c_{t}} \frac{\partial c_{\tau}}{\partial c_{\tau}} \frac{\partial c_{\tau}}{\partial W}$$

$$\frac{\partial \mathcal{L}}{\partial c_{t}} \frac{\partial c_{t}}{\partial c_{\tau}} = \frac{\partial \mathcal{L}}{\frac{\partial c_{t}}{\partial c_{t}}} \cdot \frac{\partial c_{t}}{\partial c_{t-1}} \cdot \frac{\partial c_{t-1}}{\partial c_{t-2}} \cdot \dots \cdot \frac{\partial c_{\tau+1}}{\partial c_{\tau}} \leq \eta^{t-\tau} \frac{\partial \mathcal{L}_{t}}{\partial c_{t}}$$
NN gradients expanding product of  $\frac{\partial c_{t}}{\partial c_{t-1}}$ 

o With  $\eta < 1$  long-term factors ightarrow 0 exponentially fast

Pascanu, Mikolov, Bengio, On the difficulty of training recurrent neural networks, JMLR 2013

 $\circ R$ 

• Let's assume we have 10 time steps and  $\frac{\partial c_t}{\partial c_{t-1}} > 1$ , e.g.  $\frac{\partial c_t}{\partial c_{t-1}} = 1.5$ • What would happen to the total  $\frac{\partial \mathcal{L}_t}{\partial W}$ ? • Let's assume we have 100 time steps and  $\frac{\partial c_t}{\partial c_{t-1}} > 1$ , e.g.  $\frac{\partial c_t}{\partial c_{t-1}} = 1.5$ • What would happen to the total  $\frac{\partial \mathcal{L}_t}{\partial W}$ ?  $\frac{\partial \mathcal{L}}{\partial c_t} \frac{\partial c_t}{\partial c_\tau} \propto 1.5^{10} = 4.06 \cdot 10^{17}$ 

• Let's assume now that 
$$\frac{\partial c_t}{\partial c_{t-1}} < 1$$
, e.g.  $\frac{\partial c_t}{\partial c_{t-1}} = 0.5$   
• What would happen to the total  $\frac{\partial \mathcal{L}_t}{\partial W}$ ?

• Let's assume now that 
$$\frac{\partial c_t}{\partial c_{t-1}} < 1$$
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 $\frac{\partial \mathcal{L}}{\partial c_t} \frac{\partial c_t}{\partial c_\tau} \propto 0.5^{10} = 9.7 \cdot 10^{-5}$ 

#### • Do you think our optimizers like these kind of gradients?

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○ Do you think our optimizers like these kind of gradients?
○ Too large → unstable training, oscillations, divergence
○ Too small → very slow training, has it converged?

 In recurrent networks, and in very deep networks in general (an RNN is not very different from an MLP), gradients are much affected by depth

$$\frac{\partial \mathcal{L}}{\partial c_{t}} = \frac{\partial \mathcal{L}}{\partial c_{T}} \cdot \frac{\partial c_{T}}{\partial c_{T-1}} \cdot \frac{\partial c_{T-1}}{\partial c_{T-2}} \cdot \dots \cdot \frac{\partial c_{t+1}}{\partial c_{c_{t}}} \text{ and } \frac{\partial c_{t+1}}{\partial c_{t}} < 1 \Rightarrow \frac{\partial \mathcal{L}}{\partial W} \ll 1 \Rightarrow \text{Vanishing gradient}$$
$$\frac{\partial \mathcal{L}}{\partial c_{t}} = \frac{\partial \mathcal{L}}{\partial c_{T}} \cdot \frac{\partial c_{T}}{\partial c_{T-1}} \cdot \frac{\partial c_{T-1}}{\partial c_{T-2}} \cdot \dots \cdot \frac{\partial c_{t+1}}{\partial c_{c_{t}}} \text{ and } \frac{\partial c_{t+1}}{\partial c_{t}} > 1 \Rightarrow \frac{\partial \mathcal{L}}{\partial W} \gg 1 \Rightarrow \text{Exploding gradient}$$

• Vanishing gradients are particularly a problem for long sequences
 • Why?

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 • Why?

• Exponential decay

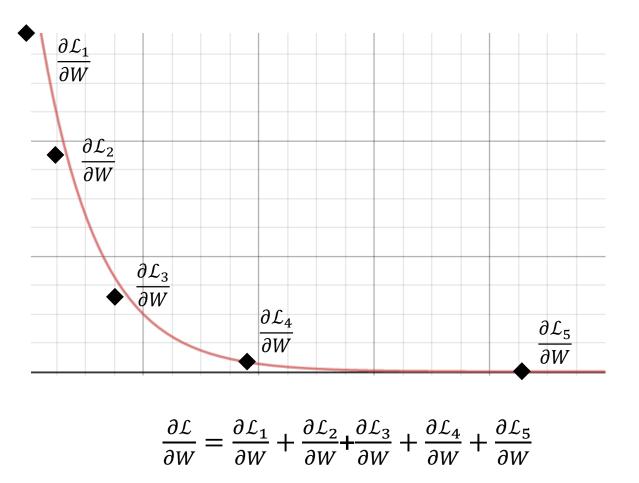
$$\frac{\partial \mathcal{L}}{\partial c_t} = \prod_{k \ge \tau} \frac{\partial c_k}{\partial c_{k-1}} = \prod_{k \ge \tau} W \cdot \partial \tanh(c_{k-1})$$

 The further back we look (long-term dependencies), the smaller the weights automatically become

• exponentially smaller weights

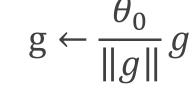
# Why are vanishing gradients bad?

- The weight changes of earlier time steps become exponentially smaller
- Bad, even if we train the model exponentially longer
- The weights will quickly learn to "model" short-term transitions and ignore long-term transitions
- At best, even after longer training, they will try "fine-tune" the whatever bad "modelling" of long-term transitions
- But, as the short-term transitions are inherently more prevalent, they will dominate the learning and gradients

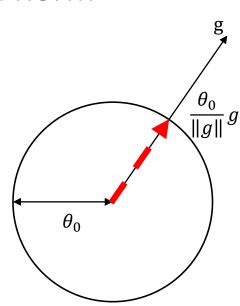


Quick fix for exploding gradients: Rescaling!

- First, get the gradient  $g \leftarrow \frac{\partial \mathcal{L}}{\partial W}$
- $_{
  m O}$  Check if the norm is larger than a threshold  $heta_{
  m 0}$
- o If it is, rescale it to have same direction and threshold norm



• Simple, but works!



oNo!

• The nature of the problem is different

- $_{\odot}$  Exploding gradients ightarrow you might have bouncing and unstable optimization
- Vanishing gradients → you simply do not have a gradient to begin with
   Rescaling of what exactly?
- In any case, even with re-scaling we would still focus on the short-term gradients
  - Long-term dependencies would still be ignored

• Backpropagating all the way till infinity is unrealistic

- We would backprop forever (or simply it would be computationally very expensive)
- And in case, the gradients would be inaccurate because of intermediate updates

• What about truncating backprop to the last K steps

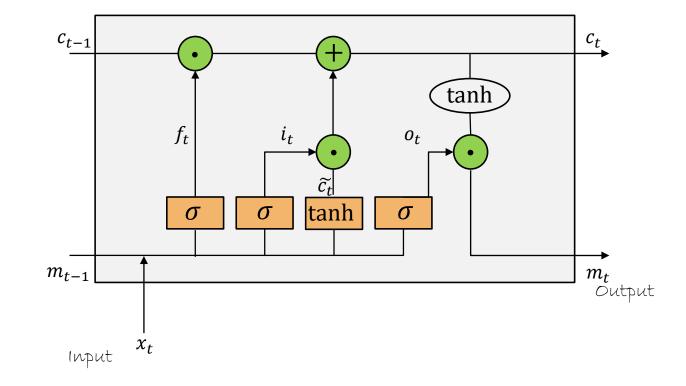
$$\tilde{g}_{t+1} \propto \frac{\partial \mathcal{L}}{\partial w} \Big|_{t=0}^{t=k}$$

• Unfortunately, this leads to biased gradients

$$g_{t+1} = \frac{\partial \mathcal{L}}{\partial w} \Big|_{t=0}^{t=\infty} \neq \tilde{g}_{t+1}$$

Other algorithms exist but they are not as successful
 We will visit them later

### LSTM and variants



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o Let's have a look at the loss function

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$$\frac{\partial \mathcal{L}_{t}}{\partial W} = \sum_{\tau=1}^{t} \frac{\partial \mathcal{L}_{r}}{\partial y_{t}} \frac{\partial y_{t}}{\partial c_{t}} \frac{\partial c_{t}}{\partial c_{\tau}} \frac{\partial c_{\tau}}{\partial W}$$
$$\frac{\partial c_{t}}{\partial c_{\tau}} = \prod_{t \ge k \ge \tau} \frac{\partial c_{k}}{\partial c_{k-1}}$$

o How to make the product roughly the same no matter the length?

• Error signal over time must have not too large, not too small norm

o Let's have a look at the loss function

$$\frac{\partial \mathcal{L}_{t}}{\partial W} = \sum_{\tau=1}^{t} \frac{\partial \mathcal{L}_{r}}{\partial y_{t}} \frac{\partial y_{t}}{\partial c_{t}} \frac{\partial c_{t}}{\partial c_{\tau}} \frac{\partial c_{\tau}}{\partial W}$$
$$\frac{\partial c_{t}}{\partial c_{\tau}} = \prod_{t \ge k \ge \tau} \frac{\partial c_{k}}{\partial c_{k-1}}$$

How to make the product roughly the same no matter the length?
Use the identity function with gradient of 1

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• Over time the state change is  $c_{t+1} = c_t + \Delta c_{t+1}$ 

• This constant over-writing over long time steps leads to chaotic behavior

o Input weight conflict

• Are all inputs important enough to write them down?

Output conflict

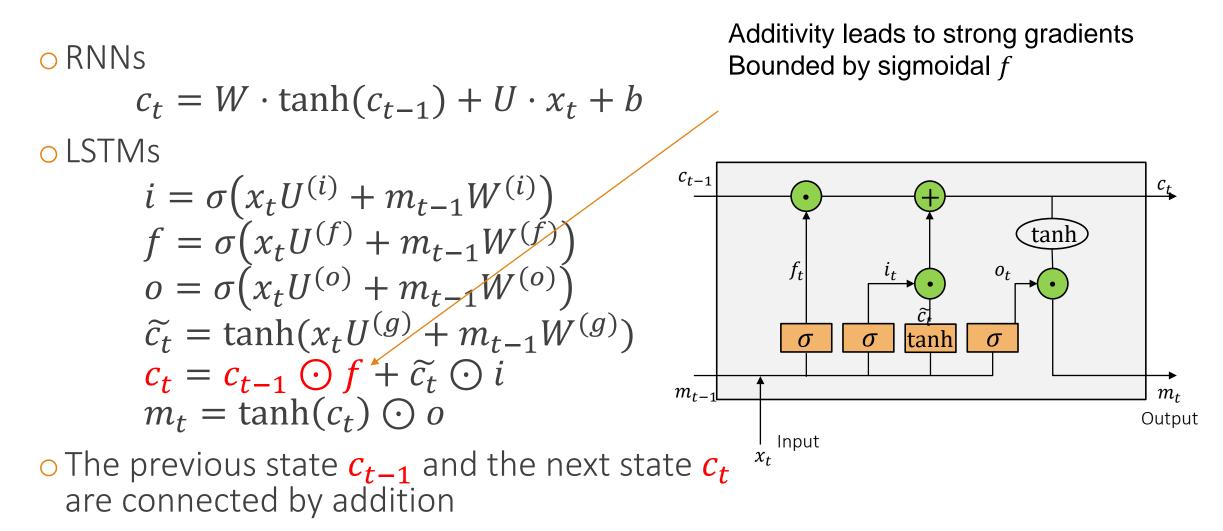
• Are all outputs important enough to be read?

• Forget conflict

• Is all information important enough to be remembered over time?

LSTMs

**O**RNNs  $c_t = W \cdot \tanh(c_{t-1}) + U \cdot x_t + b$ **o** LSTMs  $C_{t-1}$  $C_t$  $i = \sigma(x_t U^{(i)} + m_{t-1} W^{(i)})$  $f = \sigma (x_t U^{(f)} + m_{t-1} W^{(f)})$   $o = \sigma (x_t U^{(o)} + m_{t-1} W^{(o)})$ tanh  $f_t$  $0_t$  $\widetilde{c_t} = \tanh(x_t U^{(g)} + m_{t-1} W^{(g)})$ ltanh  $\sigma$  $\sigma$  $\sigma$  $c_t = c_{t-1} \odot f + \widetilde{c_t} \odot i$  $m_{t-}$  $m_{t}$  $m_t = \tanh(c_t) \odot o$ Output Input  $x_t$ 



Nice tutorial: <u>http://colah.github.io/posts/2015-08-Understanding-LSTMs/</u>

Cell state

$$i = \sigma \left( x_t U^{(i)} + m_{t-1} W^{(i)} \right)$$
  

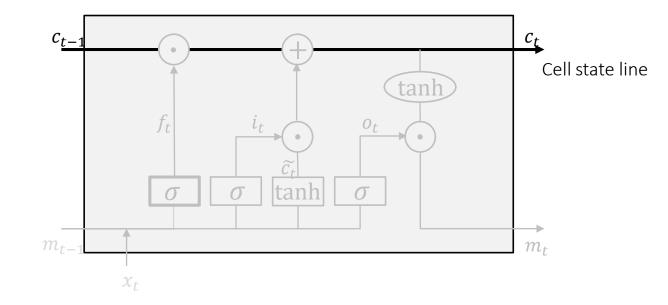
$$f = \sigma \left( x_t U^{(f)} + m_{t-1} W^{(f)} \right)$$
  

$$o = \sigma \left( x_t U^{(o)} + m_{t-1} W^{(o)} \right)$$
  

$$\widetilde{c}_t = \tanh(x_t U^{(g)} + m_{t-1} W^{(g)})$$
  

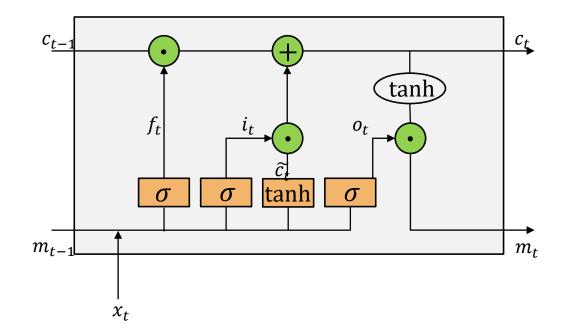
$$c_t = c_{t-1} \odot f + \widetilde{c}_t \odot i$$
  

$$m_t = \tanh(c_t) \odot o$$



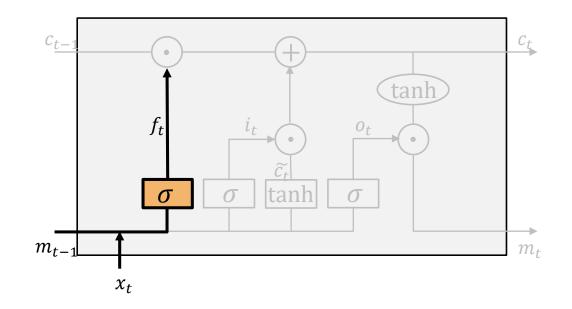
## LSTM nonlinearities

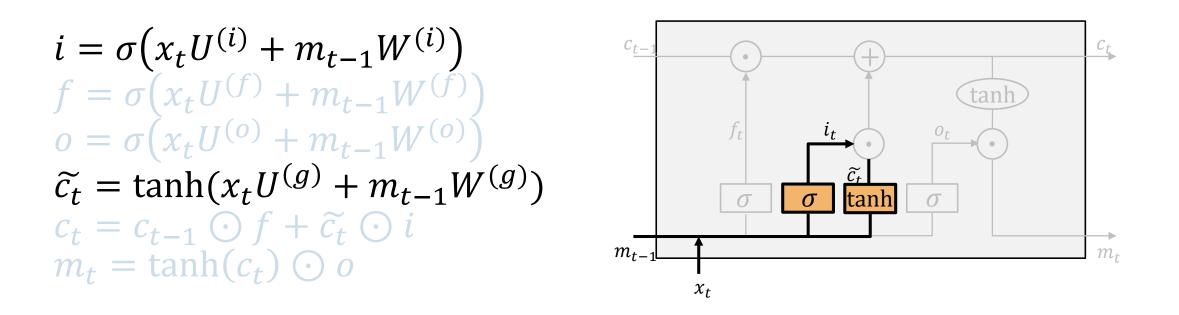
 $i = \sigma(x_t U^{(i)} + m_{t-1} W^{(i)})$   $f = \sigma(x_t U^{(f)} + m_{t-1} W^{(f)})$   $o = \sigma(x_t U^{(o)} + m_{t-1} W^{(o)})$   $\widetilde{c_t} = \tanh(x_t U^{(g)} + m_{t-1} W^{(g)})$   $c_t = c_{t-1} \odot f + \widetilde{c_t} \odot i$  $m_t = \tanh(c_t) \odot o$ 



 $\circ \sigma \in (0, 1)$ : control gate − something like a switch  $\circ \tanh \in (-1, 1)$ : recurrent nonlinearity

 $i = \sigma(x_t U^{(i)} + m_{t-1} W^{(i)})$  $f = \sigma \left( x_t U^{(f)} + m_{t-1} W^{(f)} \right)$  $o = \sigma(x_t U^{(o)} + m_{t-1} W^{(o)})$  $\widetilde{c_t} = \tanh(x_t U^{(g)} + m_{t-1} W^{(g)})$  $c_t = c_{t-1} \odot f + \widetilde{c_t} \odot i$  $m_t = \tanh(c_t) \odot o$ 

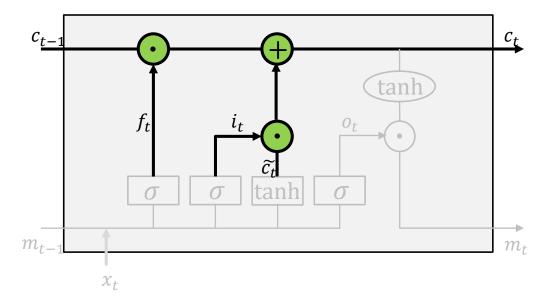




 Decide what new information is relevant from the new input and should be added to the new memory

- Modulate the input  $i_t$
- Generate candidate memories  $\widetilde{c_t}$

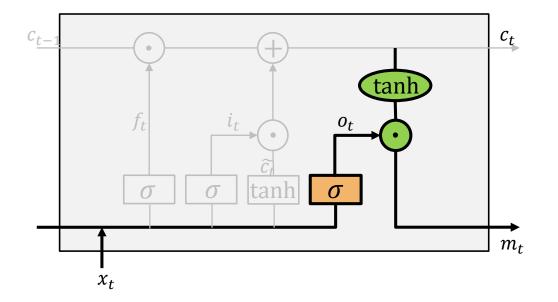
 $i = \sigma(x_t U^{(i)} + m_{t-1} W^{(i)})$   $f = \sigma(x_t U^{(f)} + m_{t-1} W^{(f)})$   $o = \sigma(x_t U^{(o)} + m_{t-1} W^{(o)})$   $\widetilde{c_t} = \tanh(x_t U^{(g)} + m_{t-1} W^{(g)})$   $c_t = c_{t-1} \odot f + \widetilde{c_t} \odot i$  $m_t = \tanh(c_t) \odot o$ 



 $\circ$  Compute and update the current cell state  $c_t$ 

- Depends on the previous cell state
- What we decide to forget
- What inputs we allow
- The candidate memories

 $i = \sigma(x_{t}U^{(i)} + m_{t-1}W^{(i)})$   $f = \sigma(x_{t}U^{(f)} + m_{t-1}W^{(f)})$   $o = \sigma(x_{t}U^{(o)} + m_{t-1}W^{(o)})$   $\widetilde{c_{t}} = \tanh(x_{t}U^{(g)} + m_{t-1}W^{(g)})$   $c_{t} = c_{t-1} \odot f + \widetilde{c_{t}} \odot i$  $m_{t} = \tanh(c_{t}) \odot o$ 



Modulate the output

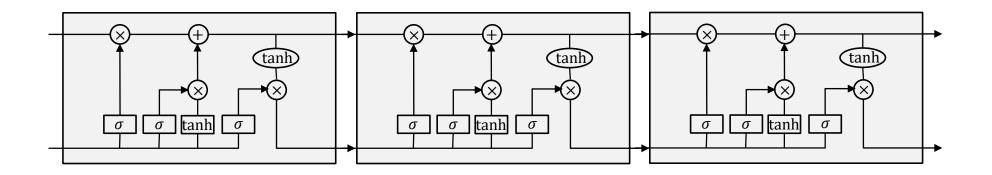
 $\circ$  Does the new cell state relevant?  $\rightarrow$  Sigmoid 1

• If not  $\rightarrow$  Sigmoid 0

• Generate the new memory

o Just the same like for RNNs

- The engine is a bit different (more complicated)
  - Because of their gates LSTMs capture long and short term dependencies



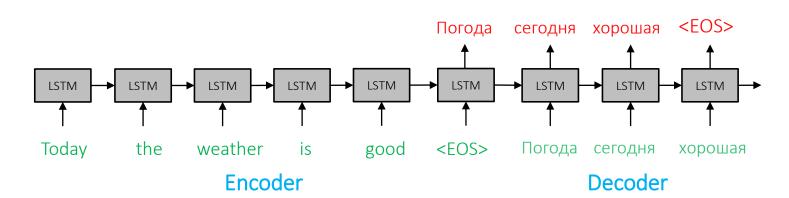
o LSTM with peephole connections

o Gates have access also to the previous cell states  $c_{(t-1)}$  (not only memories)

- Bi-directional recurrent networks
- Gated Recurrent Units (GRU)
- Phased LSTMs
- o Skip LSTMs
- And many more ...

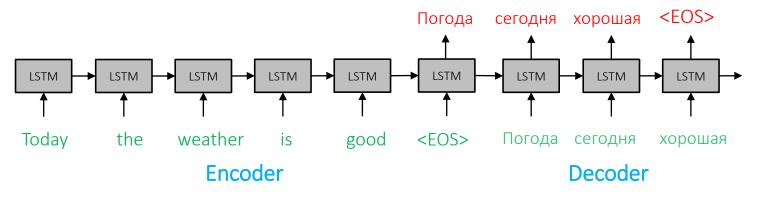
#### Encoder-Decoder Architectures

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• The phrase in the source language is one sequence

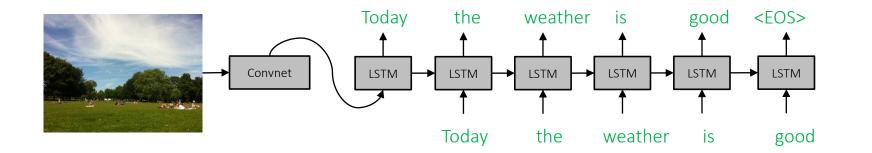
- "Today the weather is good"
- o It is captured by an Encoder LSTM
- The phrase in the target language is also a sequence
  - "Погода сегодня хорошая"
- o It is captured by a Decoder LSTM



• Similar to image translation

• The only difference is that the Encoder LSTM is an image ConvNet • VGG, ResNet, ...

• Keep decoder the same



### Image captioning demo

#### <u>Click to go to the video in Youtube</u>



NeuralTalk and Walk, recognition, text description of the image while walking

#### Summary

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- o Sequential data
- Recurrent Neural Networks
- Backpropagation through time
- Exploding and vanishing gradients
- o LSTMs and variants
- o Encoder-Decoder Architectures