## Lecture 9 - Networks for Sequential Data

RNNs \& LSTMs

DD2424

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- RNNs are a family of networks for processing sequential data.
- A RNN applies the same function recursively when traversing network's graph structure.
- RNN encodes a sequence $\mathbf{x}_{1}, \mathbf{x}_{2}, \ldots, \mathbf{x}_{\tau}$ into fixed length hidden vector $\mathbf{h}_{\tau}$.
- The size of $\mathbf{h}_{\tau}$ is independent of $\tau$.
- Amazingly flexible and powerful high-level architecture.

- Graph displays processing of information for each time step.
- Information from input $\mathbf{x}$ is incorporated into state $\mathbf{h}$.

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- Information from input $\mathbf{x}$ is incorporated into state $\mathbf{h}$.
- State $\mathbf{h}$ is passed forward in time.
- Most recurrent neural networks have a function $f$

$$
\mathbf{h}_{t}=f\left(\mathbf{h}_{t-1}, \mathbf{x}_{t} ; \boldsymbol{\theta}\right)
$$

that defines their hidden state over time where

- $\mathbf{h}_{t}$ is the hidden state at time $t$ (a vector)
- $\mathbf{x}_{t}$ is the input vector at time $t$
- $\boldsymbol{\theta}$ is the parameters of $f$.
- $\theta$ remains constant as $t$ changes.

Apply the same function with the same parameter values at each iteration.

## RNN: How hidden states generated

- Most recurrent neural networks have a function $f$

$$
\mathbf{h}_{t}=f\left(\mathbf{h}_{t-1}, \mathbf{x}_{t} ; \boldsymbol{\theta}\right)
$$

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- $\boldsymbol{\theta}$ is the parameters of $f$.
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Unrolled visualization of the RNN
Apply the same function with the same parameter values
at each iteration.


- Usually also predict an output vector at each time step

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## Back to Vanilla RNN

- The state consists of a single hidden vector $\mathbf{h}_{t}$ :
- Initial hidden state $\mathbf{h}_{0}$ is assumed given.
- For $t=1, \ldots, \tau$ the RNN equations are

$$
\begin{aligned}
\mathbf{a}_{t} & =W \mathbf{h}_{t-1}+U \mathbf{x}_{t}+\mathbf{b} \\
\mathbf{h}_{t} & =\tanh \left(\mathbf{a}_{t}\right) \\
\mathbf{o}_{t} & =V \mathbf{h}_{t}+\mathbf{c} \\
\mathbf{p}_{t} & =\operatorname{softmax}\left(\mathbf{o}_{t}\right)
\end{aligned}
$$

## Network's input

- $\mathbf{h}_{0}$ initial hidden state has size $m \times 1$
- $\mathbf{x}_{t}$ input vector at time $t$ has size $d \times 1$
- The state consists of a single hidden vector $\mathbf{h}_{t}$ :
- Initial hidden state $\mathbf{h}_{0}$ is assumed given.
- For $t=1, \ldots, \tau$ the RNN equations are

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\mathrm{o}_{t} & =V \mathbf{h}_{t}+\mathbf{c} \\
\mathrm{p}_{t} & =\operatorname{softmax}\left(\mathrm{o}_{t}\right)
\end{aligned}
$$

## Network's output and hidden vectors

- $\mathbf{a}_{t}$ hidden state at time $t$ of size $m \times 1$ before non-linearity
- $\mathbf{h}_{t}$ hidden state at time $t$ of size $m \times 1$
- $\mathbf{o}_{t}$ output vector (of unnormalized log probabilities for each class) at time $t$ of size $C \times 1$
- $\mathbf{p}_{t}$ output probability vector at time $t$ of size $C \times 1$


## Character-level language model example

Vocabulary: [h,e,l,o]

Example training sequence:
"hello"


## Character-level language model example

Vocabulary:
[h,e,l,o]
Example training sequence:
"hello"

$$
h_{t}=\tanh \left(W_{h h} h_{t-1}+W_{x h} x_{t}\right)
$$



Character-level language model example

Vocabulary:
[h,e,l,o]
Example training sequence:
"hello"


Extend this simple approach to full alphabet and punctuation characters


## Sonnet 116 - Let me not ...

by William Shakespeare
Let me not to the marriage of true minds Admit impediments. Love is not love
Which alters when it alteration finds,
o! it is an ever-fixed mark
That looks on tempests and is never shaken
It is the star to every wandering bark,
Whose worth's unknown, although his height be taken.
Love's not Time's fool, though rosy lips and cheeks
althin his bending sickle's compass come
But bears it out even to the edge of doom.
If this be error and upon me proved.
I never writ, nor no man ever loved.
tyntd-iafhatawiaoihrdenot lytdws e,tfti, astai fogoh eoase rrranbyne 'nhthnee e plia tklirgd toldoe ns, sntt $h$ ne etie $h$, hregtrs nigtike, aoaenns ing

## train more

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

## train more

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 15 so overetical 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.
pardaras:
Alas, I think se ahall be cocee approached and the day
When little arain would bo attain'd into being sever fod
Ans uho is but a chain and subjects of mis death:
I ahould not almop.

## Socosd Sonator:

They are oway this niseries, produced upon my soul, Breaxing and strongly should be buried, when I perish The earth and thoughts of many states.

## dere vinceritio

Well, your wit is in the care of side and that.
second tard
They would be ruled after this ohamber, and ny fair nues begun out of the fact, to be ocnveged moose noble souls I'll have the heart of the wars.
clom:
Cone, sir, I will make did behold your vorship.
viols:
I'11 drink it.

## viots:

kny, saliabury muat find hia fleak and thought That which I am not aps, not a nan and in fire,
to ahow the reining of the raven and the vars To show the reining of the raven and the vara To graen ar are haird, When I was heaven of presence and our fleets, we spare with hours, but eut thy council I an great, Murdered and by thy nastor' A ready thera my power to give thee but so much an bell Sone service in the noble bondman here, would show him to het vine.
xima lear:
0 , if you were a feeble sight, the courtesy of your law, your aight and several breath, will wear the geds With his hasda, and ny bands are vonder'd at the daeds, shall be against your honour.

## How do we train a vanilla RNN?

Supervised learning via a loss function \& mini-batch gradient descent.

## Loss defined for one training sequence.

- Have a sequence $\mathbf{x}_{1}, \mathbf{x}_{2}, \ldots, \mathbf{x}_{\tau}$ of input vectors.
- For each $\mathbf{x}_{t}$ in sequence have a target output $\mathbf{y}_{t}$.
- Define loss $l_{t}$ between the $y_{t}$ and $\mathbf{p}_{t}$ for each $t$.
- Sum the loss over all time-steps

$$
L\left(\mathbf{x}_{1}, \ldots, \mathbf{x}_{\tau}, y_{1}, \ldots, y_{\tau}, W, U, V, \mathbf{b}, \mathbf{c}\right)=\sum_{t=1}^{\tau} l_{t}
$$

Common to use the cross-entropy loss:

$$
l_{t}=-\log \left(\mathbf{y}_{t}^{T} \mathbf{p}_{t}\right)
$$

thus

$$
L\left(\mathbf{x}_{1: \tau}, y_{1: \tau}, W, U, V, \mathbf{b}, \mathbf{c}\right)=-\sum_{t=1}^{\tau} \log \left(\mathbf{y}_{t}^{T} \mathbf{p}_{t}\right)
$$

where $\mathbf{x}_{1: \tau}=\left\{\mathbf{x}_{1}, \ldots, \mathbf{x}_{\tau}\right\}$ and $\mathbf{y}_{1: \tau}=\left\{y_{1}, \ldots, y_{\tau}\right\}$.

- To implement mini-batch gradient descent need to compute

$$
\frac{\partial L\left(\mathbf{x}_{1: \tau}, y_{1: \tau}, W, U, V, \mathbf{b}, \mathbf{c}\right)}{\partial W}, \frac{\partial L\left(\mathbf{x}_{1: \tau}, y_{1: \tau}, W, U, V, \mathbf{b}, \mathbf{c}\right)}{\partial U}, \cdots
$$

- You've guessed it, use back-prop...

- Loss for one labelled training sequence $\mathbf{x}_{1}, \ldots \mathbf{x}_{\tau}$
- Bias vectors have been omitted for clarity.

Gradient of loss for the cross-entropy \& softmax layers


Know from prior dealings with cross-entropy loss:
for $t=1, \ldots \tau$
$\frac{\partial L}{\partial l_{t}}=1$
$\frac{\partial L}{\partial \mathbf{p} t}=\frac{\partial L}{\partial l_{t}} \frac{\partial l_{t}}{\partial \mathbf{p} t}=-\frac{\mathbf{y}_{t}^{T}}{\mathbf{y}_{t}^{T} \mathbf{p}_{t}}$
$\frac{\partial L}{\partial \mathbf{o}_{t}}=\frac{\partial L}{\partial \mathbf{p}_{t}} \frac{\partial \mathbf{p}_{t}}{\partial \mathbf{o}_{t}}=-\frac{\mathbf{y}_{t}^{T}}{\mathbf{y}_{t}^{T} \mathbf{p}_{t}}\left(\operatorname{diag}\left(\mathbf{p}_{t}\right)-\mathbf{p}_{t} \mathbf{p}_{t}^{T}\right)$


Children of node $V$ are $\mathbf{o}_{1}, \mathbf{o}_{2}, \ldots, \mathbf{o}_{7}$. Thus

$$
\frac{\partial L}{\partial \mathrm{vec}(V)}=\sum_{t=1}^{\tau} \frac{\partial L}{\partial \mathbf{o}_{t}} \frac{\partial \mathbf{o}_{t}}{\partial \mathrm{vec}(V)}
$$

Know

$$
\begin{aligned}
\mathbf{o}_{t}=V \mathbf{h}_{t} & \Longrightarrow \mathbf{o}_{t}=\left(I_{C} \otimes \mathbf{h}_{t}^{T}\right) \operatorname{vec}(V) \\
& \Longrightarrow \frac{\partial \mathbf{o}_{t}}{\partial \operatorname{vec}(V)}=I_{C} \otimes \mathbf{h}_{t}^{T}
\end{aligned}
$$

From prior reshapings know:

$$
\frac{\partial L}{\partial V}=\sum_{t=1}^{\tau} \mathbf{g}_{t}^{T} \mathbf{h}_{t}^{T}
$$

where $\mathrm{g}_{t}=\frac{\partial L}{\partial \mathrm{O}_{t}}$.


Children of node $V$ are $\mathbf{o}_{1}, \mathbf{o}_{2}, \ldots, \mathbf{o}_{\tau}$. Thus

$$
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Know

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& \Longrightarrow \frac{\partial \mathbf{o}_{t}}{\partial \mathrm{vec}(V)}=I_{C} \otimes \mathbf{h}_{t}^{T}
\end{aligned}
$$

From prior reshapings know:

$$
\frac{\partial L}{\partial V}=\sum_{t=1}^{\tau} \mathbf{g}_{t}^{T} \mathbf{h}_{t}^{T} \leftarrow \text { gradient needed for training network }
$$

where $\mathrm{g}_{t}=\frac{\partial L}{\partial \mathbf{o}_{t}}$.

$\mathbf{h}_{\tau}$ (last hidden state) has one child $\mathbf{o}_{\tau}$ thus

$$
\frac{\partial L}{\partial \mathbf{h}_{\tau}}=\frac{\partial L}{\partial \mathbf{o}_{\tau}} \frac{\partial \mathbf{o}_{\tau}}{\partial \mathbf{h}_{\tau}}
$$

Know

$$
\mathbf{o}_{\tau}=V \mathbf{h}_{\tau} \Longrightarrow \frac{\partial \mathbf{o}_{\tau}}{\partial \mathbf{h}_{\tau}}=V
$$

Thus

$$
\frac{\partial L}{\partial \mathbf{h}_{\tau}}=\frac{\partial L}{\partial \mathbf{o}_{\tau}} V
$$



If $1 \leq t \leq \tau-1$ then $\mathbf{h}_{t}$ has children $\mathbf{o}_{t}$ and $\mathbf{a}_{t+1}$

$$
\frac{\partial L}{\partial \mathbf{h}_{t}}=\frac{\partial L}{\partial \mathbf{o}_{t}} \frac{\partial \mathbf{o}_{t}}{\partial \mathbf{h}_{t}}+\frac{\partial L}{\partial \mathbf{a}_{t+1}} \frac{\partial \mathbf{a}_{t+1}}{\partial \mathbf{h}_{t}}
$$

Know

$$
\mathbf{o}_{t}=V \mathbf{h}_{t} \Longrightarrow \frac{\partial \mathbf{o}_{t}}{\partial \mathbf{h}_{t}}=V
$$

and

$$
\mathbf{a}_{t+1}=W \mathbf{h}_{t}+U \mathbf{x}_{t+1} \Longrightarrow \frac{\partial \mathbf{a}_{t+1}}{\partial \mathbf{h}_{t}}=W
$$

Thus

$$
\frac{\partial L}{\partial \mathbf{h}_{t}}=\frac{\partial L}{\partial \mathbf{o}_{t}} V+\frac{\partial L}{\partial \mathbf{a}_{t+1}} W
$$



If $1 \leq t \leq \tau-1$ then $\mathbf{h}_{t}$ has children $\mathbf{o}_{t}$ and $\mathbf{a}_{t+1}$

$$
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$$

Know

$$
\mathbf{o}_{t}=V \mathbf{h}_{t} \Longrightarrow \frac{\partial \mathbf{o}_{t}}{\partial \mathbf{h}_{t}}=V
$$

and

$$
\mathbf{a}_{t+1}=W \mathbf{h}_{t}+U \mathbf{x}_{t+1} \Longrightarrow \frac{\partial \mathbf{a}_{t+1}}{\partial \mathbf{h}_{t}}=W
$$

Thus

$$
\frac{\partial L}{\partial \mathbf{h}_{t}}=\frac{\partial L}{\partial \mathbf{o}_{t}} V+\frac{\partial L}{\partial \mathbf{a}_{t+1}} W
$$

Have two different time steps in expression $\Longrightarrow$ must iterate backwards in time to compute all $\frac{\partial L}{\partial h_{t}}$


The gradient w.r.t. $\mathbf{a}_{t}$

$$
\frac{\partial L}{\partial \mathbf{a}_{t}}=\frac{\partial L}{\partial \mathbf{h}_{t}} \frac{\partial \mathbf{h}_{t}}{\partial \mathbf{a}_{t}}
$$

Know

$$
\begin{aligned}
\mathbf{h}_{t}=\tanh \left(\mathbf{a}_{t}\right) \Longrightarrow \frac{\partial \mathbf{h}_{t}}{\partial \mathbf{a}_{t}} & =\operatorname{diag}\left(\tanh ^{\prime}\left(\mathbf{a}_{t}\right)\right) \\
& =\operatorname{diag}\left(1-\tanh ^{2}\left(\mathbf{a}_{t}\right)\right)
\end{aligned}
$$

Thus

$$
\frac{\partial L}{\partial \mathbf{a}_{t}}=\frac{\partial L}{\partial \mathbf{h}_{t}} \operatorname{diag}\left(1-\tanh ^{2}\left(\mathbf{a}_{t}\right)\right)
$$



- Assume $\frac{\partial L}{\partial \mathbf{o}_{t}}$ calculated for $1 \leq t \leq \tau$.
- Calculate

$$
\frac{\partial L}{\partial \mathbf{h}_{\tau}}=\frac{\partial L}{\partial \mathbf{o}_{\tau}} V \quad \& \quad \frac{\partial L}{\partial \mathbf{a}_{\tau}}=\frac{\partial L}{\partial \mathbf{h}_{\tau}} \operatorname{diag}\left(1-\tanh ^{2}\left(\mathbf{a}_{\tau}\right)\right)
$$

- for $t=\tau-1, \tau-2, \ldots, 1$


## - Compute

$$
\frac{\partial L}{\partial \mathbf{h}_{t}}=\frac{\partial L}{\partial \mathbf{o}_{t}} V+\frac{\partial L}{\partial \mathbf{a}_{t+1}} W
$$

- Compute

$$
\frac{\partial L}{\partial \mathbf{a}_{t}}=\frac{\partial L}{\partial \mathbf{h}_{t}} \operatorname{diag}\left(1-\tanh ^{2}\left(\mathbf{a}_{t}\right)\right)
$$



The gradient of the loss w.r.t. node $W$.
Children of $W$ are $\mathbf{a}_{1}, \ldots \mathbf{a}_{\tau}$ thus

$$
\frac{\partial L}{\partial \operatorname{vec}(W)}=\sum_{t=1}^{\tau} \frac{\partial L}{\partial \mathbf{a}_{t}} \frac{\partial \mathbf{a}_{t}}{\partial \operatorname{vec}(W)}
$$

## Know

$$
\begin{aligned}
\mathbf{a}_{t}=W \mathbf{h}_{t-1}+U \mathbf{x}_{t} & \Longrightarrow \mathbf{a}_{t}=\left(I_{m} \otimes \mathbf{h}_{t-1}^{T}\right) \operatorname{vec}(W)+U \mathbf{x}_{t} \\
& \Longrightarrow \frac{\partial \mathbf{a}_{t}}{\partial \operatorname{vec}(W)}=I_{m} \otimes \mathbf{h}_{t-1}^{T}
\end{aligned}
$$

From prior reshapings know:

$$
\frac{\partial L}{\partial W}=\sum_{t=1}^{\tau} \mathbf{g}_{t}^{T} \mathbf{h}_{t-1}^{T}
$$

where $\mathbf{g}_{t}=\frac{\partial L}{\partial \mathbf{a}_{t}}$.


The gradient of the loss w.r.t. node $W$.
Children of $W$ are $\mathbf{a}_{1}, \ldots \mathbf{a}_{\tau}$ thus

$$
\frac{\partial L}{\partial \operatorname{vec}(W)}=\sum_{t=1}^{\tau} \frac{\partial L}{\partial \mathbf{a}_{t}} \frac{\partial \mathbf{a}_{t}}{\partial \operatorname{vec}(W)}
$$

## Know

$\mathbf{a}_{t}=W \mathbf{h}_{t-1}+U \mathbf{x}_{t} \Longrightarrow \mathbf{a} t=\left(I_{m} \otimes \mathbf{h}_{t-1}^{T}\right) \operatorname{vec}(W)+U \mathbf{x}_{t}$

$$
\Longrightarrow \frac{\partial \mathbf{a}_{t}}{\partial \mathrm{vec}(W)}=I_{m} \otimes \mathbf{h}_{t-1}^{T}
$$

From prior reshapings know:
$\frac{\partial L}{\partial W}=\sum_{t=1}^{\top} \mathbf{g}_{t}^{T} \mathbf{h}_{t-1}^{T} \leftarrow$ gradient needed for training network
where $\mathbf{g}_{t}=\frac{\partial L}{\partial \mathbf{a}_{t}}$.

## Gradient of loss w.r.t. $U$

The gradient of the loss w.r.t. node $U$.
Children of $V$ are $\mathbf{a}_{1}, \ldots \mathbf{a}_{\tau}$ thus

$$
\frac{\partial L}{\partial \operatorname{vec}(U)}=\sum_{t=1}^{T} \frac{\partial L}{\partial \mathbf{a}_{t}} \frac{\partial \mathbf{a}_{t}}{\partial \operatorname{vec}(U)}
$$

## Know

$$
\begin{aligned}
\mathbf{a}_{t}=W \mathbf{h}_{t-1}+U \mathbf{x}_{t} & \Longrightarrow \mathbf{a}_{t}=W \mathbf{h}_{t-1}+\left(I_{m} \otimes \mathbf{x}_{t}^{T}\right) \operatorname{vec}(U) \\
& \Longrightarrow \frac{\partial \mathbf{a}_{t}}{\partial \operatorname{vec}(U)}=I_{m} \otimes \mathbf{x}_{t}^{T}
\end{aligned}
$$

From prior reshapings know:

$$
\begin{aligned}
& \quad \frac{\partial L}{\partial U}=\sum_{t=1}^{\tau} \mathbf{g}_{t}^{T} \mathbf{x}_{t}^{T} \leftarrow \text { gradient needed for training network } \\
& \text { where } \mathbf{g}_{t}=\frac{\partial L}{\partial \mathbf{a}_{t}} \text {. }
\end{aligned}
$$

The gradient of the loss w.r.t. node $U$.
Children of $V$ are $\mathbf{a}_{1}, \ldots \mathbf{a}_{\tau}$ thus

$$
\frac{\partial L}{\partial \operatorname{vec}(U)}=\sum_{t=1}^{\tau} \frac{\partial L}{\partial \mathbf{a}_{t}} \frac{\partial \mathbf{a}_{t}}{\partial \operatorname{vec}(U)}
$$

## Know

$$
\mathbf{a}_{t}=W \mathbf{h}_{t-1}+U \mathbf{x}_{t} \Longrightarrow \mathbf{a}_{t}=W \mathbf{h}_{t-1}+\left(I_{m} \otimes \mathbf{x}_{t}^{T}\right) \operatorname{vec}(U)
$$

$$
\Longrightarrow \frac{\partial \mathbf{a}_{t}}{\partial \mathrm{vec}(U)}=I_{m} \otimes \mathbf{x}_{t}^{T}
$$

From prior reshapings know:

$$
\frac{\partial L}{\partial U}=\sum_{t=1}^{\tau} \mathbf{g}_{t}^{T} \mathbf{x}_{t}^{T}
$$

where $\mathbf{g}_{t}=\frac{\partial L}{\partial \mathbf{a}_{t}}$.

RNNs in Translation Applications

- Given a sentence in on language translate it to another language
- le chien sur la plage $\rightarrow$ Dog on the beach



## Language Technologies Institute

RNN-based Sentence Generation (Decoder)


## Image Captioning

## Recurrent Neural Network



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


test image




"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.

"two young girls are playing with
lego toy.

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


Evaluation of text translation results

- Tricky to do automatically!
- Ideally want humans to evaluate
- What do you ask?
- Can't use human evaluation for validating models - too slow and expensive.
- Use standard machine translation metrics instead
- BLEU
- ROUGE CIDER
- Meteor


## Image Sentence Datasets



## Microsoft COCO

[Tsung-Yi Lin et al. 2014] mscoco.org
currently:
~120K images
$\sim 5$ sentences each

Problem of exploding and vanishing gradients in an RNN

- Take a closer look at

$$
\frac{\partial L}{\partial W}=\sum_{t=1}^{\tau} \mathbf{g}_{t}^{T} \mathbf{h}_{t-1}^{T} \quad \text { where } \mathbf{g}_{t}=\frac{\partial L}{\partial \mathbf{a}_{t}}
$$

- $\Longrightarrow \frac{\partial L}{\partial W}$ depends on $\mathbf{h}_{t-1}$ and $\frac{\partial L}{\partial \mathbf{a}_{t}}$ for $t=1, \ldots, \tau$.
- Let's take a closer look at $\frac{\partial L}{\partial \mathbf{a}_{t}} \cdots$
- Denote

$$
\mathrm{g}_{o_{t}}=\frac{\partial L}{\partial \mathbf{o}_{t}} \quad \text { and } \quad D\left(\mathbf{a}_{t}\right)=\operatorname{diag}\left(1-\tanh ^{2}\left(\mathbf{a}_{t}\right)\right)
$$

- Remember

$$
\frac{\partial L}{\partial \mathbf{h}_{\tau}}=\mathbf{g}_{\mathbf{o}_{\tau}} V \Longrightarrow \frac{\partial L}{\partial \mathbf{a}_{\tau}}=\mathbf{g}_{\mathbf{o}_{\tau}} V D\left(\mathbf{a}_{\tau}\right)
$$

and for $t=\tau-1, \tau-2, \ldots, 1$ :

$$
\frac{\partial L}{\partial \mathbf{h}_{t}}=\mathbf{g}_{\mathbf{o}_{t}} V+\frac{\partial L}{\partial \mathbf{a}_{t+1}} W \quad \text { and } \quad \frac{\partial L}{\partial \mathbf{a}_{t}}=\frac{\partial L}{\partial \mathbf{h}_{t}} D\left(\mathbf{a}_{t}\right)
$$

- Then you can show by recursive substitution that

$$
\frac{\partial L}{\partial \mathbf{h}_{t}}=\sum_{j=t}^{\tau} \mathbf{g}_{\mathbf{o}_{j}} V\left(\prod_{k=1}^{j-t} D\left(\mathbf{a}_{t+k}\right)\right) W^{j-t}
$$

and

$$
\frac{\partial L}{\partial \mathbf{a}_{t}}=\sum_{j=t}^{\tau} \mathbf{g}_{\mathbf{o}_{j}} V\left(\prod_{k=0}^{j-t} D\left(\mathbf{a}_{t+k}\right)\right) W^{j-t}
$$

- Denote

$$
\mathbf{g}_{\mathbf{o}_{t}}=\frac{\partial L}{\partial \mathbf{o}_{t}} \quad \text { and } \quad D\left(\mathbf{a}_{t}\right)=\operatorname{diag}\left(1-\tanh ^{2}\left(\mathbf{a}_{t}\right)\right)
$$

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$$
\frac{\partial L}{\partial \mathbf{h}_{t}}=\sum_{j=t}^{\tau} \mathbf{g}_{\mathbf{o}_{j}} V\left(\prod_{k=1}^{j-t} D\left(\mathbf{a}_{t+k}\right)\right) W^{j-t}
$$

and

$$
\frac{\partial L}{\partial \mathbf{a}_{t}}=\sum_{j=t}^{\tau} \mathbf{g}_{\mathbf{o}_{j}} V \underbrace{\left(\prod_{k=0}^{j-t} D\left(\mathbf{a}_{t+k}\right)\right)}_{\text {likely has small values on diagonal }} W^{j-t}
$$

Why? Each matrix $D\left(\mathbf{a}_{t+k}\right)$ has $\tanh ^{\prime}\left(\mathbf{a}_{t+k}\right)$ on its diagonal and
$0 \leq \tanh ^{\prime}(a) \leq 1$. Thus $\left(\tanh ^{\prime}(a)\right)^{j-t+1}$ is highly likely to have a small value even for not too large $j-t+1$.
$\Longrightarrow \frac{\partial L}{\partial \mathbf{a}_{t}}$ only depends on first few entries in the sum.

- Denote

$$
\mathrm{g}_{o_{t}}=\frac{\partial L}{\partial \mathbf{o}_{t}} \quad \text { and } \quad D\left(\mathbf{a}_{t}\right)=\operatorname{diag}\left(1-\tanh ^{2}\left(\mathbf{a}_{t}\right)\right)
$$

- Then you can show by recursive substitution that

$$
\frac{\partial L}{\partial \mathbf{h}_{t}}=\sum_{j=t}^{\tau} \mathbf{g}_{\mathbf{o}_{j}} V\left(\prod_{k=1}^{j-t} D\left(\mathbf{a}_{t+k}\right)\right) W^{j-t}
$$

and

$$
\frac{\partial L}{\partial \mathbf{a}_{t}}=\sum_{j=t}^{\tau} \mathbf{g}_{\mathbf{o}_{j}} V\left(\prod_{k=0}^{j-t} D\left(\mathbf{a}_{t+k}\right)\right)_{\text {potentially has very large or small values }}^{W^{j-t}}
$$

Why? ......

- Remember $W$ has size $m \times m$.
- Assume $W$ is diagonalizable.
- Let its eigen-decomposition be

$$
W=Q \Lambda Q^{T}
$$

where $Q$ is orthogonal and $\Lambda$ is a diagonal matrix containing the eigenvalues of $W$.

- Then

$$
W^{n}=Q \Lambda^{n} Q^{T}
$$

- Let $\lambda_{1}, \ldots, \lambda_{m}$ be the e-values of $W$. Thus
- If $\lambda_{i}>1 \Longrightarrow \lambda_{i}^{n}$ will explode as $n$ increases.
- If $\lambda_{i}<1 \Longrightarrow \lambda_{i}^{n} \rightarrow 0$ as $n$ increases.
- Denote

$$
\mathbf{g}_{\mathbf{o}_{t}}=\frac{\partial L}{\partial \mathbf{o}_{t}} \quad \text { and } \quad D\left(\mathbf{a}_{t}\right)=\operatorname{diag}\left(1-\tanh ^{2}\left(\mathbf{a}_{t}\right)\right)
$$

- Then you can show by recursive substitution that

$$
\frac{\partial L}{\partial \mathbf{h}_{t}}=\sum_{j=t}^{\tau} \mathbf{g}_{\mathbf{o}_{j}} V\left(\prod_{k=1}^{j-t} D\left(\mathbf{a}_{t+k}\right)\right) W^{j-t}
$$

and

$$
\frac{\partial L}{\partial \mathbf{a}_{t}}=\sum_{j=t}^{\tau} \mathbf{g}_{\mathbf{o}_{j}} V\left(\prod_{k=0}^{j-t} D\left(\mathbf{a}_{t+k}\right)\right) \underbrace{W^{j-t}}_{\text {potentially has very large or small values }}
$$

Thus for sufficiently large $j-t$ either entries in $W^{j-t}$ can explode or vanish.

- Denote

$$
\mathbf{g}_{\mathbf{o}_{t}}=\frac{\partial L}{\partial \mathbf{o}_{t}} \quad \text { and } \quad D\left(\mathbf{a}_{t}\right)=\operatorname{diag}\left(1-\tanh ^{2}\left(\mathbf{a}_{t}\right)\right)
$$

- Then you can show by recursive substitution that

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$$

and

$$
\frac{\partial L}{\partial \mathbf{a}_{t}}=\sum_{j=t}^{\tau} \mathbf{g}_{\mathbf{o}_{j}} V\left(\prod_{k=0}^{j-t} D\left(\mathbf{a}_{t+k}\right)\right) W^{j-t}
$$

- If $W^{j-t}$ explodes for $j-t>N \Longrightarrow \frac{\partial L}{\partial \mathbf{a}_{t}}$ explodes $\Longrightarrow \frac{\partial L}{\partial W}$ explodes.
- If $W^{j-t}$ vanishes for $j-t>N$
$\Longrightarrow \frac{\partial L}{\partial \mathbf{a}_{t}}$ only has contributions from nearby $\mathrm{go}_{\mathrm{o}^{\prime}}$ where $t \leq t^{\prime} \leq t+N$
$\Longrightarrow \frac{\partial L}{\partial W}$ is based on aggregation of gradients from subsets of temporally nearby states.
- Denote

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\mathrm{g}_{\mathrm{o}_{t}}=\frac{\partial L}{\partial \mathbf{o}_{t}} \quad \text { and } \quad D\left(\mathbf{a}_{t}\right)=\operatorname{diag}\left(1-\tanh ^{2}\left(\mathbf{a}_{t}\right)\right)
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- Then you can show by recursive substitution that

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\frac{\partial L}{\partial \mathbf{h}_{t}}=\sum_{j=t}^{\tau} \mathbf{g o}_{\mathbf{o}_{j}} V\left(\prod_{k=1}^{j-t} D\left(\mathbf{a}_{t+k}\right)\right) w^{j-t}
$$

and

$$
\frac{\partial L}{\partial \mathbf{a}_{t}}=\sum_{j=t}^{\top} \mathbf{g}_{\mathbf{o}_{j}} V\left(\prod_{k=0}^{j-t} D\left(\mathbf{a}_{t+k}\right)\right) W^{j-t}
$$

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$\Longrightarrow \frac{\partial L}{\partial \mathrm{a}_{t}}$ only has contributions from nearby $\mathrm{g}_{\mathrm{o}^{\prime}}$ where $t \leq t^{\prime} \leq t+N$
$\Longrightarrow \frac{\partial L}{\partial W}$ is based on aggregation of gradients from subsets of temporally nearby states.
$\Longrightarrow$ Cannot learn long-range dependencies between states.


## Easy solution to exploding gradients

## - Gradient clipping

Let $G=\frac{\partial L}{\partial W}$ then

$$
G= \begin{cases}\frac{\theta}{\|G\|} G & \text { if }\|G\| \geq \theta \\ G & \text { otherwise }\end{cases}
$$

where $\theta$ is some sensible threshold.

- A simple heuristic first introduced by Thomas Mikolov.


Dashed arrow shows what happens when the gradient is rescaled to a
fixed size when its norm is above a threshold.

- Solution 1: Initialize $W$ as the identity matrix as opposed a random initialization.
- Solution 2: Use ReLU instead of tanh as the non-linear activation function.
- Solution 1: Initialize $W$ as the identity matrix as opposed a random initialization.
- Solution 2: Use ReLU instead of tanh as the non-linear activation function.

Still hard for an RNN to capture long-term dependencies.

Long-Short-Term-Memories (LSTMs) - capturing long-range dependencies


## High-level graphic of an RNN

- LSTMs similar to RNN but they introduce a memory cell state $\mathbf{c}_{t}$.



## High-level graphic of a LSTM

- LSTMs similar to RNN but they introduce a memory cell state $\mathbf{c}_{t}$.
- LSTMs have the ability to remove or add information to $\mathbf{c}_{t}$ regulated by structures called gates based on context.
- Update of $\mathbf{c}_{t}$ designed so gradients flows these nodes backward in time easily.
- $\mathbf{c}_{t}$ then controls what information from $\mathbf{h}_{t-1}$ and $\mathbf{x}_{t}$ and $\mathbf{c}_{t-1}$ should be used to generate $\mathbf{h}_{t}$.
- LSTMs (Hochreiter \& Schmidhuer, 1997) better at capturing long term dependencies.
- Introduces gates to calculate $\mathbf{h}_{t}, \mathbf{c}_{t}$ from $\mathbf{c}_{t-1}, \mathbf{h}_{t-1}$ and $\mathbf{x}_{t}$.
- Formal description of a LSTM unit:

$$
\begin{aligned}
\mathbf{i}_{t} & =\sigma\left(W_{i} \mathbf{x}_{t}+U_{i} \mathbf{h}_{t-1}\right) \quad \text { Input gate } \\
\mathbf{f}_{t} & =\sigma\left(W_{f} \mathbf{x}_{t}+U_{f} \mathbf{h}_{t-1}\right) \quad \text { Forget gate } \\
\mathbf{o}_{t} & =\sigma\left(W_{o} \mathbf{x}_{t}+U_{o} \mathbf{h}_{t-1}\right) \quad \text { Outpur/Exposure gate } \\
\tilde{\mathbf{c}}_{t} & =\tanh \left(W_{c} \mathbf{x}_{t}+U_{c} \mathbf{h}_{t-1}\right) \quad \text { New memory cell } \\
\mathbf{c}_{t} & =\mathbf{f}_{t} \odot \mathbf{c}_{t-1}+\mathbf{i}_{t} \odot \tilde{\mathbf{c}}_{t} \quad \text { Final memory cell } \\
\mathbf{h}_{t} & =\mathbf{o}_{t} \odot \tanh \left(\mathbf{c}_{t}\right)
\end{aligned}
$$

where

- $\sigma(\cdot)$ is the sigmoid function and
- $\odot$ denotes element by element multiplication.

- New temporary memory: Use $\mathrm{x}_{t}$ and $\mathbf{h}_{t-1}$ to generate new memory that includes aspects of $\mathbf{x}_{t}$.
- Input gate: Use $x_{t}$ and $h_{t-1}$ to determine whether the temporary memory $\hat{\mathrm{c}}_{2}$ is worth preserving.
- Forget gate: Assess whether the past memory cell $c_{t-1}$ should be included in $\mathbf{c}_{t}$.
- Updated memory state: Use the forget and input gates to combine the new temporary memory and the current memory cell state to get ct
- Output gate: Decides which part of $\mathbf{c}_{t}$ should be exposed to $\mathbf{h}_{\boldsymbol{t}}$.

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- Updated memory state: Use the forget and input gates to combine the new temporary memory and the current memory cell state to get $\mathbf{c}_{t}$
- Output gate: Decides which part of $\mathrm{C}_{t}$ should be exposed to $\mathrm{h}_{1}$

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- Updated memory state: Use the forget and input gates to combine the new temporary memory and the current memory cell state to get $\mathbf{c}_{t}$.
- Output gate: Decides which part of $\mathbf{c}_{t}$ should be exposed to $\mathbf{h}_{t}$.


## Deep LSTM Network



## Bi-directional LSTM Network



## Summary

- RNNs allow a lot of flexibility in architecture design
- Backward flow of gradients in RNN can explode or vanish.
- Vanilla RNNs are simple but find it hard to learn long-term dependencies.
- Exploding is controlled with gradient clipping. Vanishing is controlled with additive interactions (LSTM)
- Common to use LSTMs: their additive interactions improve gradient flow

