## CMP784 <br>  DEEP LEARNING



Lecture \#07 - Recurrent Neural Networks

- 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 $P\left(x_{1}, \ldots, x_{N}\right)$
- Generate natural sentences to describe an image $P\left(y_{1}, \ldots, y_{M} \mid I\right)$

- Activity recognition from a video sequence

$P\left(y \mid x_{1}, \ldots, x_{N}\right)$
Running
Jumping
Dancing
Fighting
Eating


## Modeling sequential data

- Speech recognition

$$
P\left(y_{1}, \ldots, y_{N} \mid x_{1}, \ldots, x_{N}\right)
$$



- Object tracking

$$
P\left(y_{1}, \ldots, y_{N} \mid x_{1}, \ldots, x_{N}\right)
$$



## Modeling sequential data

- Generate natural sentences to describe a video

$$
P\left(y_{1}, \ldots, y_{M} \mid x_{1}, \ldots, x_{N}\right)
$$


$\rightarrow$ A man is riding a bike

- Machine translation

$$
P\left(y_{1}, \ldots, y_{M} \mid x_{1}, \ldots, x_{N}\right)
$$



# 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!

$$
\begin{gathered}
\text { [0001000100100000100000001] } \\
\text { On Monday it was snowing } \\
{[1000001000000010001000100 \text { ] }} \\
\text { It was snowing on Monday }
\end{gathered}
$$

- 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



$$
h_{t}=\tanh W\binom{x_{t}}{h_{t-1}}
$$

cell state

## The Vanilla RNN Forward



## The Vanilla RNN Forward



$$
\begin{aligned}
& h_{t}=\tanh W\binom{x_{t}}{h_{t-1}} \\
& y_{t}=\mathrm{F}\left(h_{t}\right) \\
& C_{t}=\operatorname{Loss}\left(y_{t}, \mathrm{GT}_{t}\right)
\end{aligned}
$$

------ 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


## Sentiment Classification

## Sentiment Classification

- 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"


## Sentiment Classification



The

## Sentiment Classification



## Sentiment Classification



## Sentiment Classification



## Sentiment Classification



## Language Modeling

## Language Modeling

- Language models aim to represent the history of observed text ( $w_{1}, \ldots, w_{\mathrm{t}-1}$ ) succinctly in order to predict the next word $\left(w_{t}\right)$ :
all the works of shakespeare
KING LEAR:
O, if you were a feeble sight,
the courtesy of your law,
language

model $\longrightarrow$| 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. |

## RNN Language Models

$$
\begin{aligned}
& h_{n}=g\left(V\left[x_{n} ; h_{n-1}\right]+c\right) \\
& \hat{y}_{n}=W h_{n}+b
\end{aligned}
$$


a probability distribution over possible next words, aka a softmax

## RNN Language Models

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$$


tyntd-iafhatawiaoihrdemot lytdws e ,tfti, astai fogoh eoase rranbyne 'nhthnee e plia tklrgd to idoe ns,smtt h ne etie h,hregtrs nigtike,aoaenns lng

## train more

"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."

## 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 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 Fwo -




## 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.
fo deepdrumpf2016.com
自 Joined March 2016

0 Photos and videos

https://twitter.com/deepdrumpf

## Tweets

## Tweets \& replies

Media
4. 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

4 1
1212

- 17

4. 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
4 1
1272

- 45

4. 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


## More Language Modeling Fun Generating Super Mario Levels

Original Level:


Textual Representation:

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




conv-64
maxpool

| conv-128 |
| :---: |
| conv-128 |
| maxpool |


| conv-256 |
| :---: |
| conv-256 |
| maxpool |







## Beam Search $(K=3)$



For $t=1 \ldots T$ :

- For all $k$ and for all possible output words $w$ :

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

- Update beam:

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

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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 <br> [Tsung-Yi Lin et al. 2014] <br> mscoco.org

## currently: <br> ~120K images <br> ~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."

"a young boy is holding a baseball bat."

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

"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."

"boy is doing backflip on wakeboard."

"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 $\rightarrow$ Comment tu t'appelle
- Is the below architecture suitable for this problem?



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

- 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 $\rightarrow$ 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


## Recurrent Networks offer a lot of flexibility:



## Recurrent Networks offer a lot of flexibility:

one to one

one to many

many to one

many to many

many to many

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

## Recurrent Networks offer a lot of flexibility:

one to one

one to many

many to one

many to many

many to many


## e.g. Sentiment Classification

 sequence of words -> sentiment
## Recurrent Networks offer a lot of flexibility:

one to one

many to many

many to many

e.g. Machine Translation seq of words -> seq of words

## Recurrent Networks offer a lot of flexibility:



## 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



$$
\begin{aligned}
y & =f(x ; W) \\
C & =\operatorname{Loss}\left(y, y_{G T}\right)
\end{aligned}
$$

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



$$
\begin{aligned}
& y_{1}=f_{1}\left(x ; W_{1}\right) \\
& y_{2}=f_{2}\left(y_{1} ; W_{2}\right) \\
& C=\operatorname{Loss}\left(y_{2}, y_{G T}\right)
\end{aligned}
$$

## SGD Update

$$
\begin{aligned}
W_{2} & \leftarrow W_{2}-\eta \frac{\partial C}{\partial W_{2}} \\
W_{1} & \leftarrow W_{1}-\eta \frac{\partial C}{\partial W_{1}}
\end{aligned}
$$

## Chain Rule for Gradient Computation



$$
\begin{array}{lr}
y_{1}=f_{1}\left(x ; W_{1}\right) & \text { Find } \frac{\partial C}{\partial W_{1}} \\
y_{2}=f_{2}\left(y_{1} ; W_{2}\right) \\
C=\operatorname{Loss}\left(y_{2}, y_{G T}\right) & \frac{\partial C}{\partial W_{2}}
\end{array}=\left(\frac{\partial C}{\partial y_{2}}\right)\left(\frac{\partial y_{2}}{\partial W_{2}}\right) .
$$

## Chain Rule for Gradient Computation

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


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

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

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$$

## Extension to Computational Graphs



## Extension to Computational Graphs



## Extension to Computational Graphs



## Sample RNN

- RNNs remember their previous state:

$W, U$ : weight matrices


## Sample RNN

- RNNs remember their previous state:

$$
t=1
$$

$x_{1}$ : vector representing second word
$s_{1}$ : cell state at $t=1$
$s_{2}$ : cell state at $t=2$
$s_{2}=\tanh \left(W x_{1}+U s_{1}\right)$
$W, U$ : weight matrices

## Sample RNN

- "unfolding" the RNN across time:

> time


## Sample RNN

- "unfolding" the RNN across time:

> 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)


# We have a loss at each timestep: 

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


## We sum the losses across time:



## Let's try it our for W with the chain rule:



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

## Let's try it our for W with the chain rule:



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

so let's take a single timestep t:

## Let's try it our for W with the chain rule:



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

so let's take a single timestep t:
$\frac{\partial J_{2}}{\partial W}$

## Let's try it our for W with the chain rule:



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

so let's take a single timestep t:

$$
\frac{\partial J_{2}}{\partial W}=\frac{\partial J_{2}}{\partial y 2}
$$

## Let's try it our for W with the chain rule:



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

so let's take a single timestep t:

$$
\frac{\partial J_{2}}{\partial W}=\frac{\partial J_{2}}{\partial y 2} \frac{\partial y_{2}}{\partial s_{2}}
$$

## Let's try it our for W with the chain rule:



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

so let's take a single timestep t:

$$
\frac{\partial J_{2}}{\partial W}=\frac{\partial J_{2}}{\partial y 2} \frac{\partial y_{2}}{\partial s_{2}} \frac{\partial s_{2}}{\partial W}
$$

## Let's try it our for W with the chain rule:



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

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..

## Let's try it our for W with the chain rule:



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

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..

$$
s_{2}=\tanh \left(U s_{1}+W x_{2}\right)
$$

## Let's try it our for W with the chain rule:



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

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...

$$
\begin{aligned}
& s_{2}=\tanh \left(U s_{1}+W x_{2}\right) \\
& s_{1} \text { also depends on } W \text { so we can't just } \\
& \text { treat } \frac{\partial s_{2}}{\partial W} \text { as a constant! }
\end{aligned}
$$

## Let's try it our for W with the chain rule:



## Let's try it our for W with the chain rule:



## Let's try it our for W with the chain rule:



$$
\begin{gathered}
\frac{\partial s_{2}}{\partial W} \\
+\frac{\partial s_{2}}{\partial s_{1}} \frac{\partial s_{1}}{\partial W}
\end{gathered}
$$

## Let's try it our for W with the chain rule:



$$
\begin{gathered}
\frac{\partial s_{2}}{\partial W} \\
+\frac{\partial s_{2}}{\partial s_{1}} \frac{\partial s_{1}}{\partial W} \\
+\frac{\partial s_{2}}{\partial s_{0}} \frac{\partial s_{0}}{\partial W}
\end{gathered}
$$

## Backpropagation through time:

$$
\frac{\partial J_{2}}{\partial W}=\sum_{k=0}^{2} \frac{\partial J_{2}}{\partial y_{2}} \frac{\partial y_{2}}{\partial s_{2}} \underbrace{\frac{\partial s_{2}}{\partial s_{k}} \frac{\partial s_{k}}{\partial W}}_{\begin{array}{c}
\text { Contributions of } W \text { in previous } \\
\text { timesteps to the error at timestep } t
\end{array}}
$$

# Backpropagation through time: 

$$
\frac{\partial J_{t}}{\partial W}=\sum_{k=0}^{t} \frac{\partial J_{t}}{\partial y_{t}} \frac{\partial y_{t}}{\partial s_{t}} \underbrace{\frac{\partial s_{t}}{\partial s_{k}} \frac{\partial s_{k}}{\partial W}}_{\begin{array}{c}
\text { Contributions of } W \text { in previous } \\
\text { timesteps to the error at timestep } t
\end{array}}
$$

## Why are RNNs hard to train?

## Vanishing Gradient Problem

$$
\frac{\partial J_{2}}{\partial W}=\sum_{k=0}^{2} \frac{\partial J_{2}}{\partial y_{2}} \frac{\partial y_{2}}{\partial s_{2}} \frac{\partial s_{2}}{\partial s_{k}} \frac{\partial s_{k}}{\partial W}
$$

## Vanishing Gradient Problem

$$
\frac{\partial J_{2}}{\partial W}=\sum_{k=0}^{2} \frac{\partial J_{2}}{\partial y_{2}} \frac{\partial y_{2}}{\partial s_{2}} \frac{\partial s_{2}}{\partial s_{k}} \frac{\partial s_{k}}{\partial W}
$$



## Vanishing Gradient Problem

$$
\frac{\partial J_{n}}{\partial W}=\sum_{k=0}^{n} \frac{\partial J_{n}}{\partial y_{n}} \frac{\partial y_{n}}{\partial s_{n}} \frac{\partial s_{n}}{\partial s_{k}} \frac{\partial s_{k}}{\partial W} \underbrace{\frac{\partial s_{n}}{\partial s_{n-1}} \frac{\partial s_{n-1}}{\partial s_{n-2}} \ldots \frac{\partial s_{3}}{\partial s_{2}} \frac{\partial s_{2}}{\partial s_{1}} \frac{\partial s_{1}}{\partial s_{0}}}_{\begin{array}{l}
\text { as the gap between timesteps } \\
\text { gets bigger, this product gets } \\
\text { longer and longer! }
\end{array}}
$$



## Vanishing Gradient Problem


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?

$$
\begin{aligned}
& x_{t}=f\left(a_{t}\right)=\tanh \left(a_{t}\right) \\
& a_{t}=w x_{t-1}+h_{t}
\end{aligned}
$$




## 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].

$$
\begin{aligned}
& L=L\left(s_{T}\left(s_{T-1}\left(\ldots s_{t+1}\left(s_{t}, \ldots\right)\right)\right)\right) \\
& \frac{\partial L}{\partial s_{t}}=\frac{\partial L}{\partial s_{T}} \frac{\partial s_{T}}{\partial s_{T-1}} \ldots \frac{\partial s_{t+1}}{\partial s_{t}}
\end{aligned}
$$

- Problems:
- sing. values of Jacobians $>1 \rightarrow$ gradients explode
- or sing. values $<\rightarrow$ gradients shrink \& vanish
- or random $\rightarrow$ 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> </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:

1. 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
    \(C \leftarrow\) Training corpus
    \(\boldsymbol{C} \leftarrow \operatorname{sort}(\boldsymbol{C})\) or shuffle \((\boldsymbol{C}) \triangleright\) sort or shuffle
    the whole corpus
    \(\boldsymbol{B} \leftarrow\} \quad \triangleright\) mini-batches
    \(i \leftarrow 0, j \leftarrow 0\)
    while \(i<\boldsymbol{C}\).size() do
        \(\boldsymbol{B}[j] \leftarrow \boldsymbol{B}[j]+\boldsymbol{C}[i]\)
        if \(B[j]\).size ()\(\geq\) max mini-batch size then
                \(\boldsymbol{B}[j] \leftarrow \operatorname{padding}(\boldsymbol{B}[j])\)
            -
    Padding tokens to the longest sentence in the
    mini-batch
        \(j \leftarrow j+1\)
        end if
        \(i \leftarrow i+1\)
    end while
    \(\boldsymbol{B} \leftarrow \operatorname{shuffle}(\boldsymbol{B}) \quad \triangleright\) shuffle the order of the
    mini-batches
```


## Mini-batching in RNNs

- Many

1. Sh





rt or shuffle
nini-batches
ch size then

tence in the
order of the

- May affect performance!
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



## 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.
(a) Naive dropout RNN

(b) Variational RNN

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

$$
\beta \frac{1}{T} \sum_{t=1}^{T}\left(\left\|h_{t}\right\|_{2}-\left\|h_{t-1}\right\|_{2}\right)^{2}
$$

- 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

$$
\begin{aligned}
& \mathbf{h}^{t}=f\left[\frac{\mathbf{g}}{\sigma^{t}} \odot\left(\mathbf{a}^{t}-\mu^{t}\right)+\mathbf{b}\right] \\
& \mu^{t}=\frac{1}{H} \sum_{i=1}^{H} a_{i}^{t} \\
& \sigma^{t}=\sqrt{\frac{1}{H} \sum_{i=1}^{H}\left(a_{i}^{t}-\mu^{t}\right)^{2}}
\end{aligned}
$$



## 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."


$$
P\left(y_{t} \mid h_{t}\right) \text { with } h_{t}=f\left(h_{t-1}, y_{t-1}\right)
$$

## 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."
- During training, randomly replace a conditioning ground truth token by the model's previous prediction



## 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


RNN


LSTM, GRU, etc

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

## Long Short-Term Memory (LSTM)



## Long Short-Term Memory (LSTM)



## Long Short-Term Memory (LSTM)



## Long Short-Term Memory (LSTM)


output certain
parts of cell
state

## Long Short-Term Memory (LSTM)



## The LSTM Idea



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

## The Original LSTM Cell


$c_{t}=c_{t-1}+i_{t} \otimes \tanh W\binom{x_{t}}{h_{t-1}}$
$h_{t}=o_{t} \otimes \tanh c_{t}$
$i_{t}=\sigma\left(W_{i}\binom{x_{t}}{h_{t-1}}+b_{i}\right)$
Similarly for $O_{t}$

## The Popular LSTM Cell



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

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

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

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

## The Popular LSTM Cell


$i_{t}=\sigma\left(W_{i}\binom{x_{t}}{h_{t-1}}+b_{i}\right)$
$c_{t}=f_{t} \otimes c_{t-1}+i_{t} \otimes \tanh W\binom{x_{t}}{h_{t-1}}$

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

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

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

## The Popular LSTM Cell



$$
\begin{gathered}
i_{t}=\sigma\left(W_{i}\binom{x_{t}}{h_{t-1}}+b_{i}\right) \\
c_{t}=f_{t} \otimes c_{t-1}+i_{t} \otimes \tanh W\binom{x_{t}}{h_{t-1}} \\
f_{t}=\sigma\left(W_{f}\binom{x_{t}}{h_{t-1}}+b_{f}\right) \\
h_{t}=o_{t} \otimes \tanh c_{t}
\end{gathered}
$$

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

## The Popular LSTM Cell



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

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

$$
\begin{aligned}
& f_{t}=\sigma\left(W_{f}\binom{x_{t}}{h_{t-1}}+b_{f}\right) \\
& h_{t}=o_{t} \otimes \tanh c_{t}
\end{aligned}
$$

Update the old cell state with the new one.

## The Popular LSTM Cell



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

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

$h_{t} |$| input | forget <br> gate <br> gate | behavior |
| :---: | :---: | :--- |
| 0 | 1 | remember the <br> previous value <br> 1 |
| 1 | add to the previous |  |
| 0 | 0 | value |
| 1 | 0 | erase the value |
| overwrite the value |  |  |

## The Popular LSTM Cell



$$
\begin{aligned}
& i_{t}=\sigma\left(W_{i}\binom{x_{t}}{h_{t-1}}+b_{i}\right) \\
& c_{t}=f_{t} \otimes c_{t-1}+i_{t} \otimes \tanh W\binom{x_{t}}{t_{t-1}}
\end{aligned}
$$

$f_{t}=\sigma\left(W_{f}\binom{x_{t}}{h_{t-1}}+b_{f}\right)$
$h_{t}=o_{t} \otimes \tanh c_{t}$

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

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

## The Popular LSTM Cell


$f_{t}=\sigma\left(W_{f}\binom{x_{t}}{h_{t-1}}+b_{f}\right)$
Similarly for $i_{t}, o_{t}$
$c_{t}=f_{t} \otimes c_{t-1}+i_{t} \otimes \tanh W\binom{x_{t}}{h_{t-1}}$
$h_{t}=o_{t} \otimes \tanh c_{t}$

[^0]
## Extension I: Peephole LSTM


$f_{t}=\sigma\left(W_{f}\left(\begin{array}{c}x_{t} \\ h_{t-1} \\ c_{t-1}\end{array}\right)+b_{f}\right)$
Similarly for $i_{t}, o_{t}$ (uses $c_{t}$ )
$c_{t}=f_{t} \otimes c_{t-1}+i_{t} \otimes \tanh W\binom{x_{t}}{h_{t-1}}$
$h_{t}=o_{t} \otimes \tanh c_{t}$

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

[^1]
## Other minor variants

- Coupled Input and Forget Gate $f_{t}=1-i_{t}$
- Full Gate Recurrence

$$
f_{t}=\sigma\left(W_{f}\left(\begin{array}{c}
x_{t} \\
h_{t-1} \\
c_{t-1} \\
i_{t-1} \\
f_{t-1} \\
o_{t-1}
\end{array}\right)+b_{f}\right)
$$

## 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


## GRU



$$
\begin{aligned}
& r_{t}=\sigma\left(W_{r}\binom{x_{t}}{h_{t-1}}+b_{f}\right) \\
& h_{t}^{\prime}=\tanh W\binom{x_{t}}{r_{t} \otimes h_{t-1}} \\
& z_{t}=\sigma\left(W_{z}\binom{x_{t}}{h_{t-1}}+b_{f}\right)
\end{aligned}
$$

$$
h_{t}=\left(1-z_{t}\right) \otimes h_{t-1}+z_{t} \otimes h_{t}^{\prime}
$$

## GRU

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


computes a reset gate based on current input and hidden state

## GRU

$$
\begin{aligned}
& r_{t}=\sigma\left(W_{r}\binom{x_{t}}{h_{t-1}}+b_{f}\right) \\
& h_{t}^{\prime}=\tanh W\binom{x_{t}}{r_{t} \otimes h_{t-1}}
\end{aligned}
$$

computes the hidden state based on current input and hidden state
if reset gate unit is $\sim 0$, then this ignores previous memory and only stores the new input information

## GRU



$$
\begin{aligned}
& r_{t}=\sigma\left(W_{r}\binom{x_{t}}{h_{t-1}}+b_{f}\right) \\
& h_{t}^{\prime}=\tanh W\binom{x_{t}}{r_{t} \otimes h_{t-1}} \\
& z_{t}=\sigma\left(W_{z}\binom{x_{t}}{h_{t-1}}+b_{f}\right)
\end{aligned}
$$

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

## GRU



$$
\begin{aligned}
& r_{t}=\sigma\left(W_{r}\binom{x_{t}}{h_{t-1}}+b_{f}\right) \\
& h_{t}^{\prime}=\tanh W\binom{x_{t}}{r_{t} \otimes h_{t-1}} \\
& z_{t}=\sigma\left(W_{z}\binom{x_{t}}{h_{t-1}}+b_{f}\right) \\
& h_{t}=\left(1-z_{t}\right) \otimes h_{t-1}+z_{t} \otimes h_{t}^{\prime}
\end{aligned}
$$

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

## GRU Intuition



$$
\begin{aligned}
& r_{t}=\sigma\left(W_{r}\binom{x_{t}}{h_{t-1}}+b_{f}\right) \\
& h_{t}^{\prime}=\tanh W\binom{x_{t}}{r_{t} \otimes h_{t-1}} \\
& z_{t}=\sigma\left(W_{z}\binom{x_{t}}{h_{t-1}}+b_{f}\right) \\
& h_{t}=\left(1-z_{t}\right) \otimes h_{t-1}+z_{t} \otimes h_{t}^{\prime}
\end{aligned}
$$

- 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. p
- If node is a non-linearity, replace with $\{\tanh (x)$, $\operatorname{sigmoid}(x), \operatorname{ReLU}(x)$, 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


## 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? <br> - Recall <br> $$
\begin{aligned} & f_{t}=\sigma\left(W_{f}\binom{x_{t}}{h_{t-1}}+b_{f}\right) \\ & c_{t}=f_{t} \otimes c_{t-1}+i_{t} \otimes \tanh W\binom{x_{t}}{h_{t-1}} \\ & \delta c_{t-1}=\delta c_{t} \otimes f_{t} \end{aligned}
$$

- 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 Learning to forget: Continual prediction with LSTM [Gers et al., 2000], 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 Memory


[^0]:    * Dashed line indicates time-lag

[^1]:    * Dashed line indicates time-lag

