Using RNNs to generate Super Mario Maker levels, Adam Geitgey

COMP541 ² DEEP LEARNING

KOÇ

UNIVERSITY

Lecture #07 – Recurrent Neural Networks

Aykut Erdem // Koç University // Fall 2024

Previously on COMP541

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



Lecture overview

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

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

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

Sequence modeling

Sequential data

- "I took the dog for a walk this morning." sentence
- Multimeter and a for a second and a second

medical signals

speech waveform



video frames

Modeling sequential data

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



• Activity recognition from a video sequence



 $P(y_1,\ldots,y_M|I)$

Modeling sequential data

• Speech recognition

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



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

→ Hey Siri



Modeling sequential data

• Generate natural sentences to describe a video



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

\rightarrow A man is riding a bike

Machine translation



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



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!

[00010010010010000000000000001]

On Monday it was snowing

VS

[1000010000100010001000100]

It was snowing on Monday

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

Markov Models



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

Markov Models

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

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

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

To model sequences, we need

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

Recurrent Neural Networks

Recurrent Neural Networks

Feed Forward Network



Recurrent Network



t = n

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

Unrolled RNN



Sample RNN



The Vanilla RNN Cell



$$h_t = \tanh W \begin{pmatrix} x_t \\ h_{t-1} \end{pmatrix}$$
 cell state

The Vanilla RNN Forward



$$h_{t} = \tanh W \begin{pmatrix} x_{t} \\ h_{t-1} \end{pmatrix}$$
$$y_{t} = F(h_{t})$$
$$C_{t} = Loss(y_{t}, GT_{t})$$

The Vanilla RNN Forward



$$h_{t} = \tanh W \begin{pmatrix} x_{t} \\ h_{t-1} \end{pmatrix}$$
$$y_{t} = F(h_{t})$$
$$C_{t} = \text{Loss}(y_{t}, \text{GT}_{t})$$

----- indicates shared weights

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

 Classify a restaurant review from Yelp! OR movie review from IMDB OR

as positive or negative

- Inputs: Multiple words, one or more sentences
- Outputs: Positive / Negative classification
- "The food was really good"
- "The chicken crossed the road because it was uncooked"











Language Modeling

Language Modeling

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



KING LEAR:

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

http://karpathy.github.io/2015/05/21/rnn-effectiveness/

$$h_n = g(V[x_n; h_{n-1}] + c)$$
$$\hat{y}_n = Wh_n + b$$





$$h_n = g(V[x_n; h_{n-1}] + c)$$
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$$\hat{y}_n = Wh_n + b$$



$$h_n = g(V[x_n; h_{n-1}] + c)$$
$$\hat{y}_n = Wh_n + b$$




Pierre aking his soul came to the packs and drove up his father-in-law women.

http://karpathy.github.io/2015/05/21/rnn-effectiveness/

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.

http://karpathy.github.io/2015/05/21/rnn-effectiveness/

More Language Modeling Fun eepDrumpf



DeepDrumpf

@DeepDrumpf

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

& deepdrumpf2016.com

Joined March 2016

Photos and videos



https://twitter.com/deepdrumpf

TWEETS	FOLLOWING	FOLLOWERS	LIKES
284	7	29.4K	19



Tweets Tweets & replies Media In reply to Thomas Paine DeepDrumpf @DeepDrumpf · Mar 20 There will be no amnesty. It is going to pass because the people are going to be gone. I'm giving a mandate. #ComeyHearing @Thomas1774Paine 23 12 17 4 1 4 In reply to David Yankovich DeepDrumpf @DeepDrumpf · Feb 19

2+ Follow



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

In reply to Glenn Thrush

4 1

13 22



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:

								 		-
??					-###?	-^####	#??#	 		

#^#?#			_pp	#^##	###	-??#	##	 ##?#		
			_PD					 		
			00							
PP		-PP						 =PP	PP-=====	
PP	PP @	-pp@@	-pp		8		0000auso	 pp	@@PP======	

A level generated by a RNN:



https://medium.com/@ageitgey/machine-learning-is-fun-part-2-a26a10b68df3

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





FC-1000

softmax







conv-512 conv-512

maxpool

FC-4096 FC-4096





before: h = tanh(Wxh*x+Whh*h)

now: h = tanh(Wxh*x+Whh*h+Wih*v)











Beam Search (K = 3)



For t = 1...T:

• For all k and for all possible output words w:

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

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

Beam Search (K = 3)



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Image Description Datasets

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



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

currently: ~120K images ~5 sentences each



"man in black shirt is playing guitar."



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



"two young girls are playing with lego toy."



"boy is doing backflip on wakeboard."



"man in black shirt is playing guitar."



"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." 64

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?



Adapted from http://www.cs.toronto.edu/~rgrosse/csc321/lec10.pdf

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?



• 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

Seq2Seq Learning with Neural Networks. Sutskever et al., NIPS 2014



Vanilla Neural Networks



image -> sequence of words

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sequence of words -> sentiment



many to many many to many

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



Multi-layer RNNs

• We can of course design RNNs with multiple hidden layers



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

Bi-directional RNNs

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



• Popular in speech recognition and machine translation
How to Train Recurrent Neural Networks

BackPropagation Refresher



Multiple Layers



Chain Rule for Gradient Computation



Chain Rule for Gradient Computation

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



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



Intrinsic to the layer are:

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

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

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

Chain Rule for Gradient Computation

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Extension to Computational Graphs



Extension to Computational Graphs



Extension to Computational Graphs



• RNNs remember their previous state:



 x_0 : vector representing first word s_0 : cell state at t = 0 (some initialization) s_1 : cell state at t = 1

 $s_1 = tanh(Wx_0 + Us_0)$

W, U: weight matrices

• RNNs remember their previous state:



W, U: weight matrices

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 x_1 : vector representing second word

 s_1 : cell state at t = 1

 s_2 : cell state at t = 2

 $s_2 = tanh(Wx_1 + Us_1)$

• "unfolding" the RNN across time:





notice that W and U stay the same!

• "unfolding" the RNN across 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:





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



$$\frac{\partial J}{\partial W} = \sum_t \frac{\partial J_t}{\partial W}$$



$$\frac{\partial J}{\partial W} = \sum_t \frac{\partial J_t}{\partial W}$$

so let's take a single timestep t:

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



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

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



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

∂J_2 _	$\partial J_2 \ \partial y_2$
$\overline{\partial W}$ –	$\overline{\partial y2}\overline{\partial s_2}$



$$\frac{\partial J}{\partial W} = \sum_t \frac{\partial J_t}{\partial W}$$

∂J_2	∂J_2	∂y_2	∂s_2
$\overline{\partial W}$ –	$\overline{\partial y2}$	$\overline{\partial s_2}$	$\overline{\partial W}$



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

so let's take a single timestep t:

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

but wait...



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

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...

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



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

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...

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

 s_1 also depends on W so we can't just treat $\frac{\partial s_2}{\partial W}$ as a constant!





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



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



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

Backpropagation through time:

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

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

Backpropagation through time:

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

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

Why are RNNs hard to train?

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



 x_{o}

 $\frac{\partial J_n}{\partial W} = \sum_{k=0}^n \frac{\partial J_n}{\partial y_n} \frac{\partial y_n}{\partial s_n} \frac{\partial s_n}{\partial s_k} \frac{\partial s_k}{\partial W}$ $\frac{\partial s_n}{\partial s_{n-1}} \frac{\partial s_{n-1}}{\partial s_{n-2}} \cdots \frac{\partial s_3}{\partial s_2} \frac{\partial s_2}{\partial s_1} \frac{\partial s_1}{\partial s_0}$ as the gap between timesteps gets bigger, this product gets longer and longer!



we're multiplying a lot of small numbers together.
Vanishing Gradient Problem

we're multiplying a lot of **small numbers** together.

so what?

errors due to further back timesteps have increasingly **smaller gradients**.

so what?

parameters become biased to **capture shorter-term** dependencies.

A Toy Example

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



Vanishing Gradient Problem

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

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

Long-Term Dependencies



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

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

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

RNN Tricks

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

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

Mini-batching in RNNs

- Mini-batching makes things much faster!
- But mini-batching in RNNs is harder than in feed-forward networks
 - Each word depends on the previous word
 - Sequences are of various length
- Padding: this is an example </s>
 this is another </s>
 </r>
- 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

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

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

0 ___ 0∟ 5M 0 5M 1M 2M 3M 4M 1M 2M 3M 4M 5M 10M 15M 20M Mini-batching in RNNs



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

trg_src

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.

Dropout: A Simple Way to Prevent Neural Networks from Overfitting. Srivastava et al. JMLR 2014.

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



Recurrent neural network regularization. Zaremba et al., arXiv 2014.

Regularization: Dropout

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



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

A Theoretically Grounded Application of Dropout in Recurrent Neural Networks. Gal and Ghahramani. NIPS 2016

Regularization: Norm-stabilizer

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

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

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



Regularizing RNNs by Stabilizing Activations. Krueger and Memisevic, ICLR 2016

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





Layer Normalization [Ba, Kiros & Hinton, 2016]

Scheduled Sampling

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



Scheduled Sampling for Sequence Prediction with Recurrent Neural Networks. Bengio et al., NIPS 2015

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



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Scheduled Sampling for Sequence Prediction with Recurrent Neural Networks. Bengio et al., NIPS 2015

Gated Cells

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



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











The LSTM Idea



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

* Dashed line indicates time-lag

The Original LSTM Cell















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



* Dashed line indicates time-lag

Extension I: Peephole LSTM



* Dashed line indicates time-lag

Other minor variants

• Coupled Input and Forget Gate $f_t = 1 - i_t$

• Full Gate Recurrence

$$f_{t} = \boldsymbol{\sigma} \left(W_{f} \begin{pmatrix} x_{t} \\ h_{t-1} \\ C_{t-1} \\ i_{t-1} \\ f_{t-1} \\ f_{t-1} \\ O_{t-1} \end{pmatrix} + b_{f} \right)$$
LSTM: A Search Space Odyssey

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

LSTM: A Search Space Odyssey [Greff et al., 2015]

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

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



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

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

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

 $h_t = (1 - z_t) \otimes h_{t-1} + z_t \otimes h'_t$





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



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

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

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

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



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

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

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

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



$$r_{t} = \sigma \left(W_{r} \begin{pmatrix} x_{t} \\ h_{t-1} \end{pmatrix} + b_{f} \right)$$
$$h'_{t} = \tanh W \begin{pmatrix} x_{t} \\ r_{t} \otimes h_{t-1} \end{pmatrix}$$
$$z_{t} = \sigma \left(W_{z} \begin{pmatrix} x_{t} \\ h_{t-1} \end{pmatrix} + b_{f} \right)$$
$$h_{t} = z_{t} \otimes h_{t-1} + (1 - z_{t}) \otimes \tilde{h}_{t}$$

Final memory at timestep t combines both current and previous timesteps



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

An Empirical Exploration of Recurrent Network Architectures

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

• They use an evolutionary search for better architectures

Evolutionary Architecture Search

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

Evolutionary Architecture Search

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

Evolutionary Architecture Search

- 3 novel architectures are presented in the paper
- Very similar to GRU, but slightly outperform it
- LSTM initialized with a large positive forget gate bias outperformed both the basic LSTM and the GRU!

LSTM initialized with large positive forget gate bias?

• Recall

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

$$\delta c_{t-1} = \delta c_t \otimes f_t$$

- Gradients will vanish if f is close to 0. Using a large positive bias ensures that f has values close to 1, especially when training begins
- Helps learn long-range dependencies
- Originally stated in 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 Transformers