Deep Learning for NLP



Lecture 8 – Recurrent Neural Nets

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Natural Language Learning Group (NLLG)

Previous lectures:



- Introduction (MLPs, loss functions, batch size, activation functions, etc.)
- Embeddings continuous representations of words, letters, sentences, etc.
- More elaborate architecture: CNN

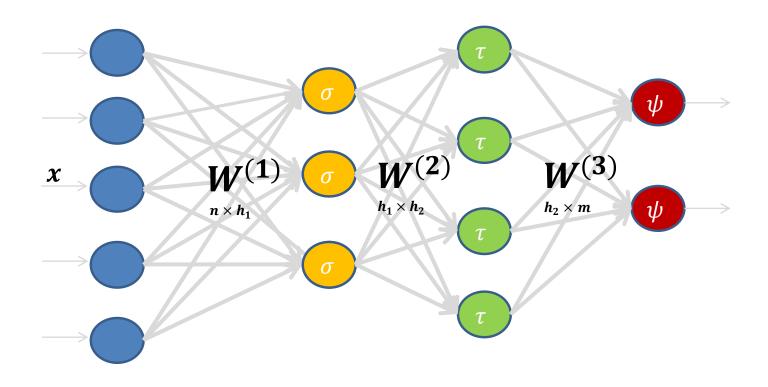
This lecture:



- Recurrent Neural Nets (RNNs)
 - Basic principles
 - Extensions (Bidirectional, etc.)
 - NLP applications: Sequence tagging & sentence classification
- Vanishing gradients
 - Simple Remedies
 - GRUs & LSTMs

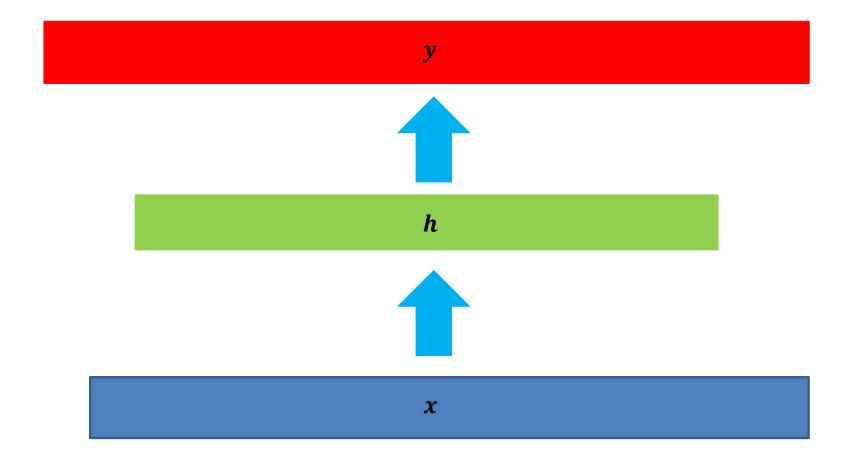
Recurrent Neural Nets Basic principles

Remember FF Nets / MLP

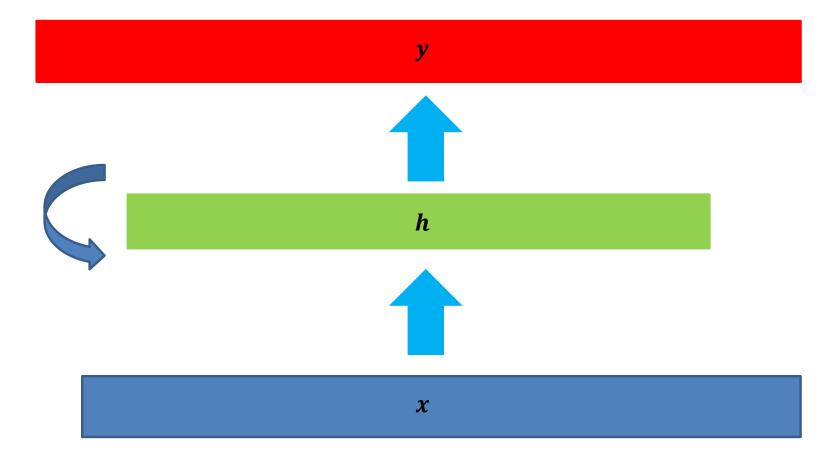


Feedforward / MLP

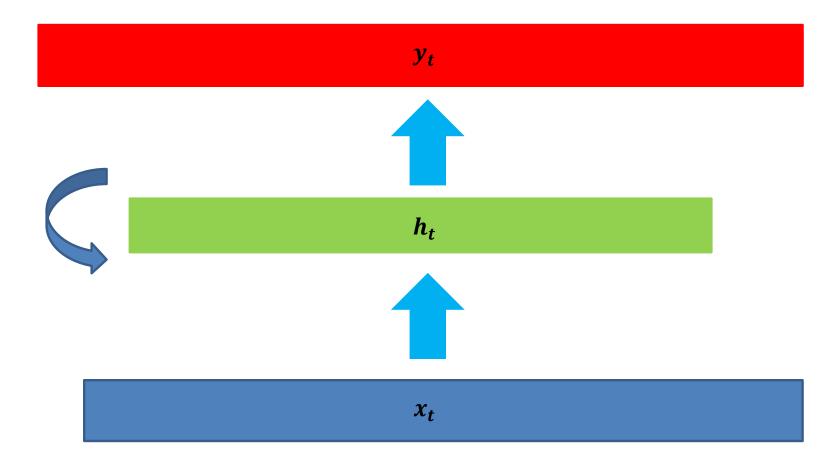




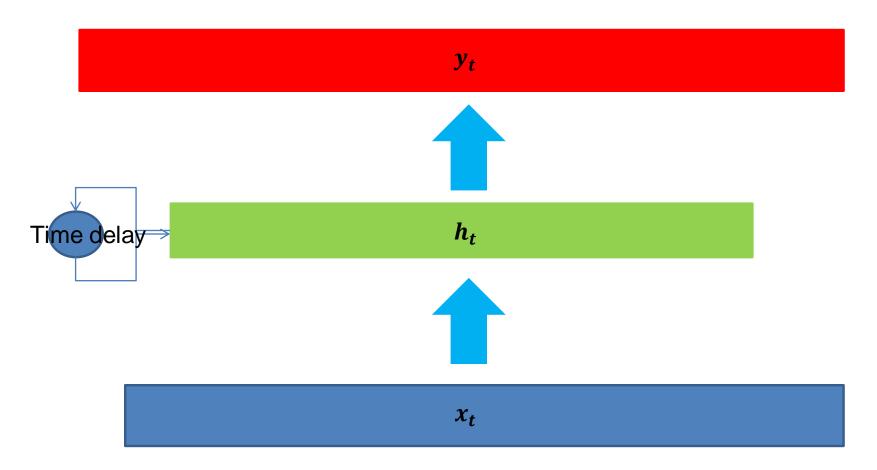




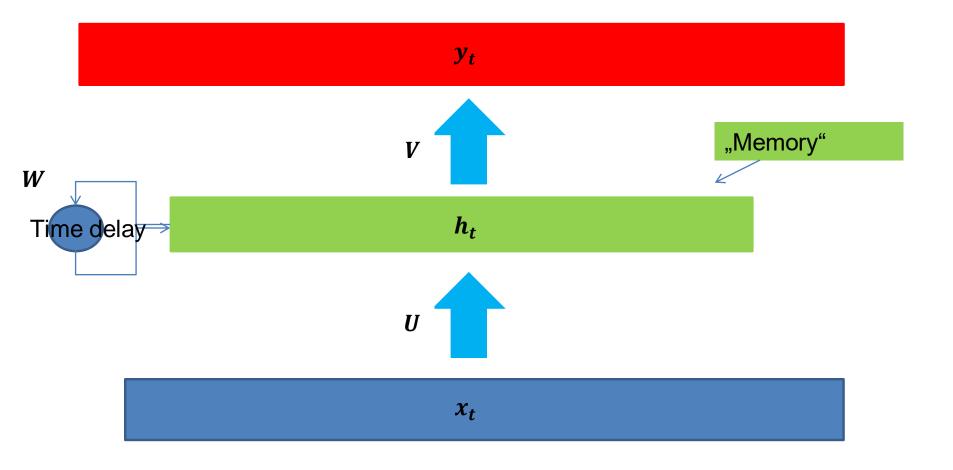












Input vectors x_t , t = 1,2,3,... lie in $R^{1 \times n}$

$$\bullet \quad \boldsymbol{h}_t = \sigma_H(\boldsymbol{x}_t \boldsymbol{U} + \boldsymbol{h}_{t-1} \boldsymbol{W} + \boldsymbol{b})$$

- Where $\boldsymbol{U} \in R^{n \times d}$, $\boldsymbol{W} \in R^{d \times d}$, $\boldsymbol{h}_t \in R^{1 \times d}$
 - d is hidden dimensionality

• Where $V \in \mathbb{R}^{d \times m}$

What we want to optimize is

- lacktriangle Average loss E over individual time losses E_t
 - E.g. $E_t = ce(\boldsymbol{y}_t, \boldsymbol{t}_t) = -\sum_j t_{t,j} \log y_{t,j}$
 - $\bullet \quad E = \frac{1}{T} \sum_{t} E_{t}$



- Input: "A rusty can"
- Embeddings: $x_1 = (1,0,0), x_2 = (1,1,2), x_3 = (1,-1,1)$
- Truth: DET,ADJ,NOUN, encoded as 1-hot vectors (in a 4-d label space)
- Activations: ReLU for hidden layer, Softmax for output layer

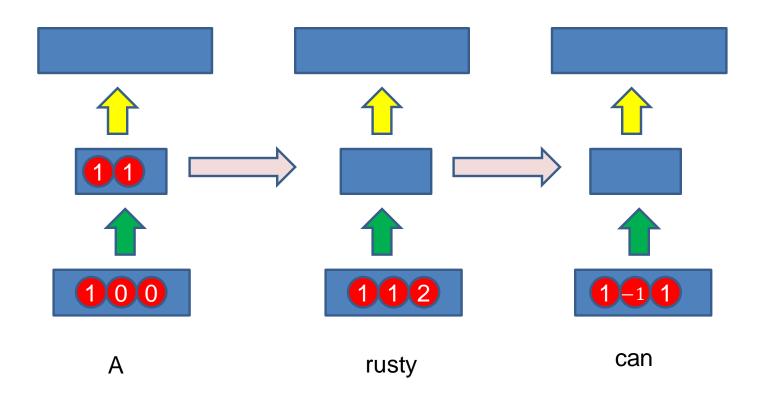
Initialization:

$$U = \begin{pmatrix} 1 & 1 \\ 2 & 0 \\ 0.5 & 1 \end{pmatrix}$$

- b = c =zero-vectors of appropriate size
- $h_0 = (0,0)$

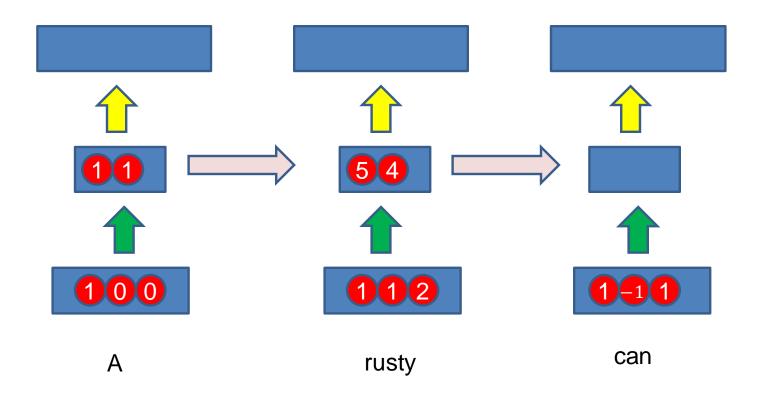
$$h_1 = \sigma_H(x_1U + h_0W + b)$$

$$h_1 = (1,1)$$



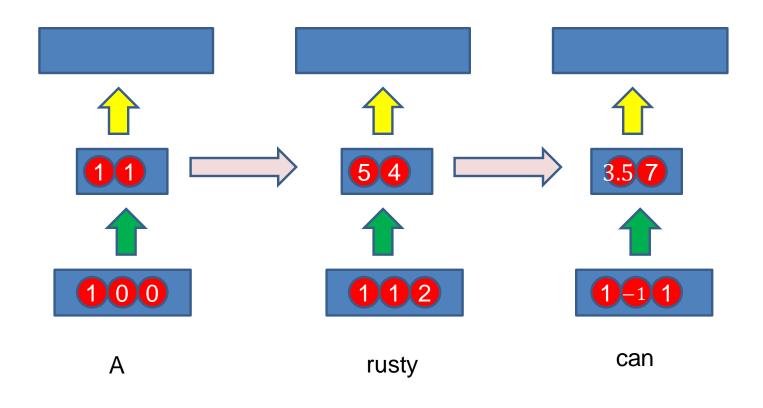
$$h_2 = \sigma_H(x_2U + h_1W + b)$$

 $h_2 = (5,4)$

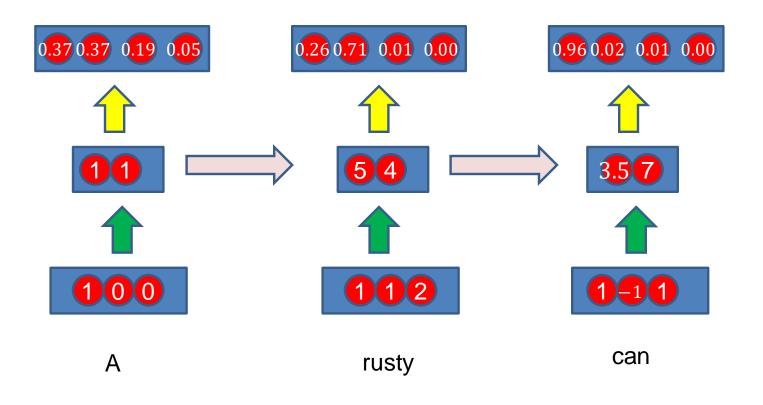


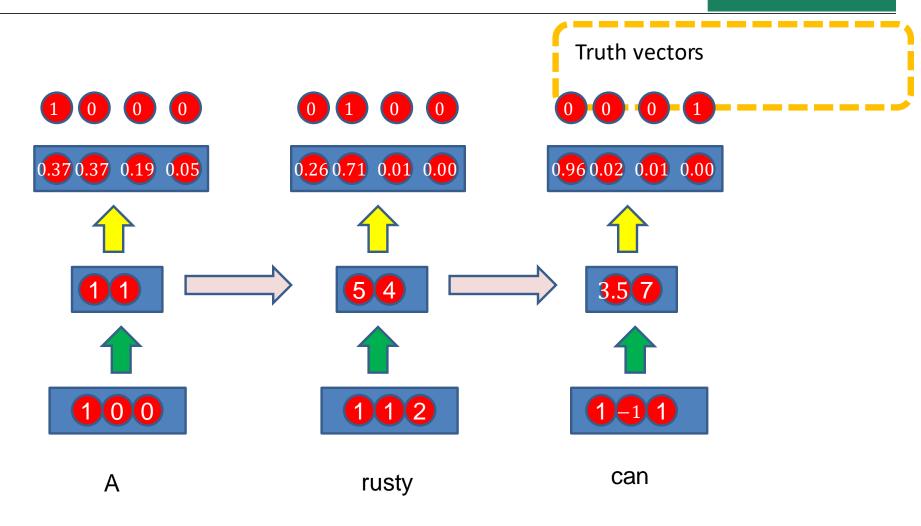
$$h_3 = \sigma_H(x_3 U + h_2 W + b)$$

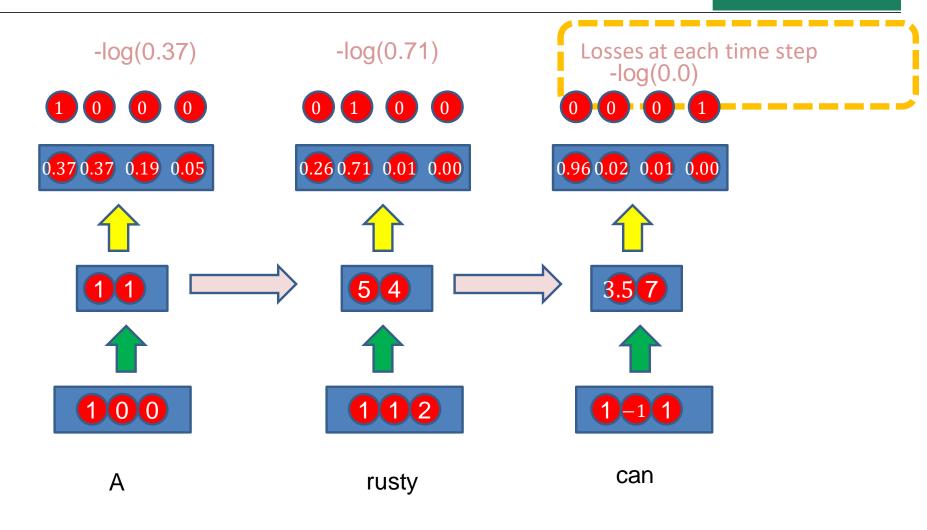
 $h_3 = (3.5,7)$



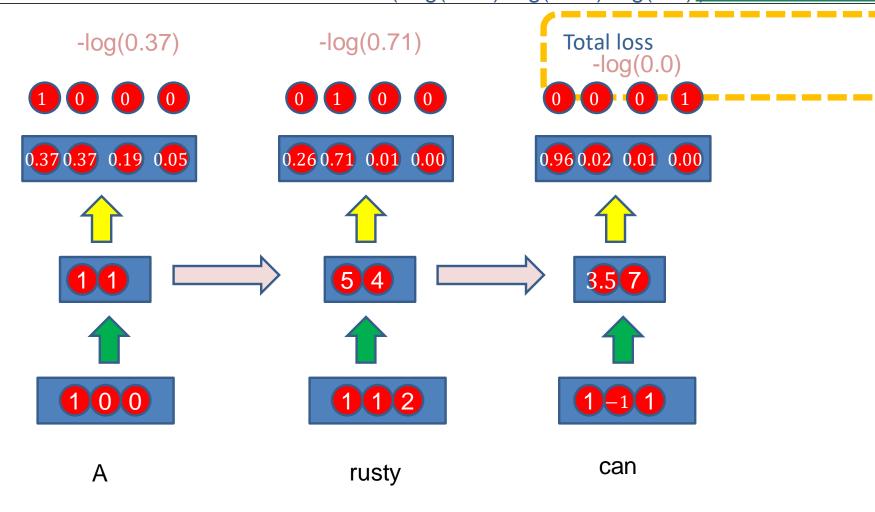
$$\mathbf{y}_t = \sigma_{\mathbf{Y}}(\mathbf{h}_t \mathbf{V} + \mathbf{c})$$



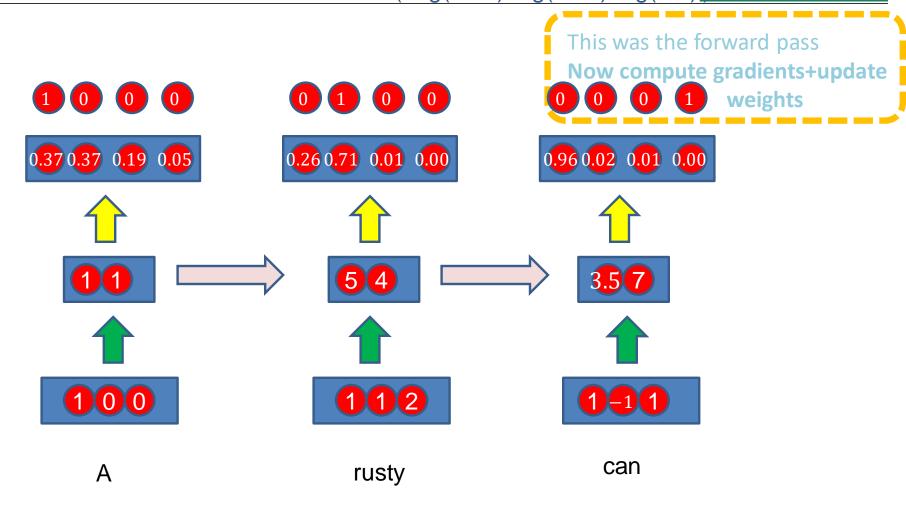




1/3·(-log(0.37)-log(0.71)-log(6.6) Universität Bielefeld



1/3·(-log(0.37)-log(0.71)-log(6.6) Universität Bielefeld



RNN – Weight update / Gradient computation

- Computation of gradient is similar as in standard MLP
 - But: Need to keep in mind that several parameters are shared
 - Some people call backprop for RNNs "backpropagation through time" (BPTT)
 - No need to go through, TensorFlow does it for you
- If you want to do it brute-force, can also do it numerically
 - i.e., for each individual weight w, compute $\frac{f(w+h)-f(w)}{h}$
 - Where f is the loss function
- Weight update after gradient computation is $\mathbf{w} \leftarrow \mathbf{w} \alpha \ \nabla f$ as usual

RNN – Properties

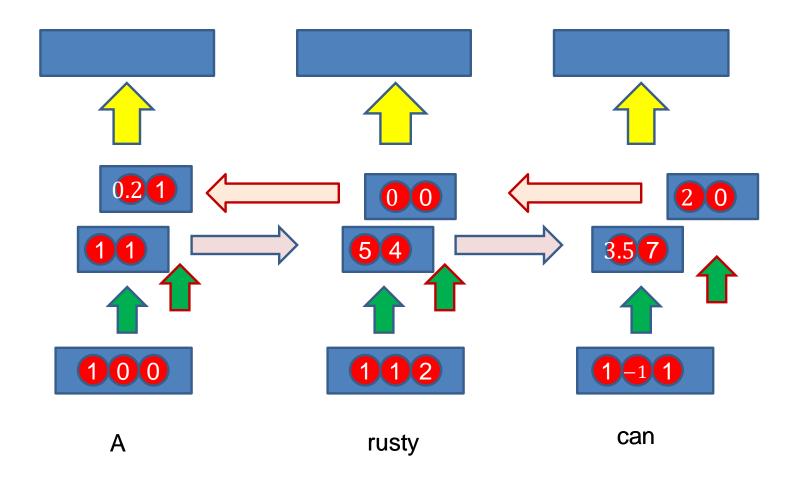


- Infinite window size "from the left"
 - Memory can (in principle) store everything from the past
- That's good, but we also want to base our decision on future words/tokens
 - → Bidirectional RNN:
 - run a second RNN from "right to left"
 - With independent weights
 - Concatenate the forward and backward hidden states
 - $\boldsymbol{h}_t = [\overrightarrow{\boldsymbol{h}}_t; \overleftarrow{\boldsymbol{h}}_t]$
 - Note that V is of dimension $2d \times m$ in this case

Recurrent Neural Nets Extensions

Bidirectional RNN - Illustration

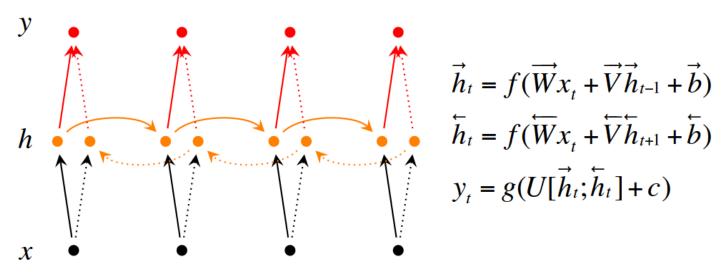




Extensions of simple RNNs

Bidirectional RNNs

Problem: For classification you want to incorporate information from words both preceding and following

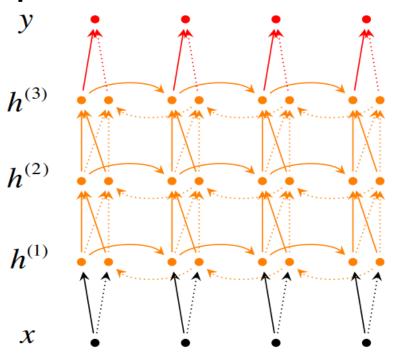


 $h = [\vec{h}; \vec{h}]$ now represents (summarizes) the past and future around a single token.

Extensions of simple RNNs

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Deep Bidirectional RNNs



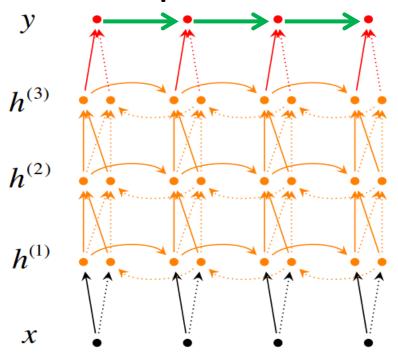
$$\vec{h}_{t}^{(i)} = f(\vec{W}^{(i)} h_{t}^{(i-1)} + \vec{V}^{(i)} \vec{h}_{t-1}^{(i)} + \vec{b}^{(i)})$$

$$\vec{h}_{t}^{(i)} = f(\vec{W}^{(i)} h_{t}^{(i-1)} + \vec{V}^{(i)} \vec{h}_{t+1}^{(i)} + \vec{b}^{(i)})$$

$$y_{t} = g(U[\vec{h}_{t}^{(L)}; \vec{h}_{t}^{(L)}] + c)$$

Each memory layer passes an intermediate sequential representation to the next.

RNNs with output connections



$$\vec{h}_{t}^{(i)} = f(\vec{W}^{(i)} h_{t}^{(i-1)} + \vec{V}^{(i)} \vec{h}_{t-1}^{(i)} + \vec{b}^{(i)})$$

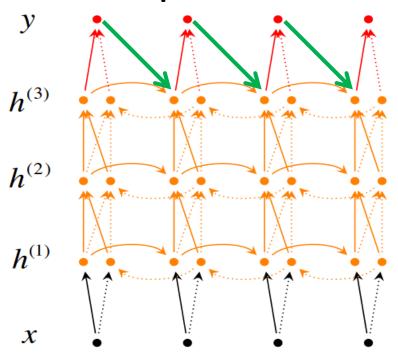
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Equations?

Each memory layer passes an intermediate sequential representation to the next.

RNNs with output connections



$$\vec{h}_{t}^{(i)} = f(\vec{W}^{(i)} h_{t}^{(i-1)} + \vec{V}^{(i)} \vec{h}_{t-1}^{(i)} + \vec{b}^{(i)})$$

$$\vec{h}_{t}^{(i)} = f(\vec{W}^{(i)} h_{t}^{(i-1)} + \vec{V}^{(i)} \vec{h}_{t+1}^{(i)} + \vec{b}^{(i)})$$

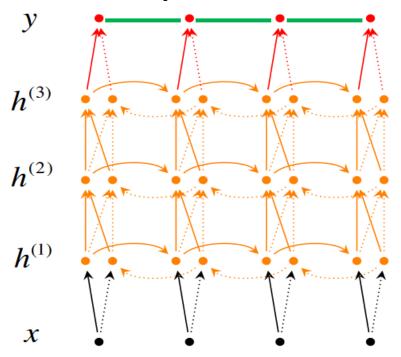
$$y_{t} = g(U[\vec{h}_{t}^{(L)}; \vec{h}_{t}^{(L)}] + c)$$

Equations?

Each memory layer passes an intermediate sequential representation to the next.

Extensions of simple RNNs

RNNs with output connections: CRF instead of forward conn.



$$\vec{h}_{t}^{(i)} = f(\vec{W}^{(i)} h_{t}^{(i-1)} + \vec{V}^{(i)} \vec{h}_{t-1}^{(i)} + \vec{b}^{(i)})$$

$$\vec{h}_{t}^{(i)} = f(\vec{W}^{(i)} h_{t}^{(i-1)} + \vec{V}^{(i)} \vec{h}_{t+1}^{(i)} + \vec{b}^{(i)})$$

$$y_{t} = g(U[\vec{h}_{t}^{(L)}; \vec{h}_{t}^{(L)}] + c)$$

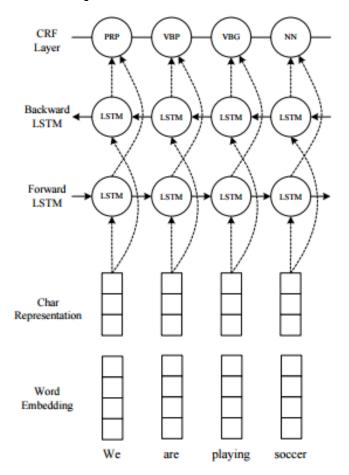
Equations?

Each memory layer passes an intermediate sequential representation to the next.

Extensions of simple RNNs



RNNs with output connections and character information

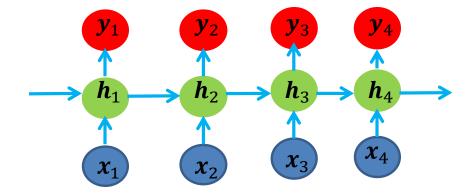


Why character information?
Ma and Hovy (2016)
Lample et al. (2016)

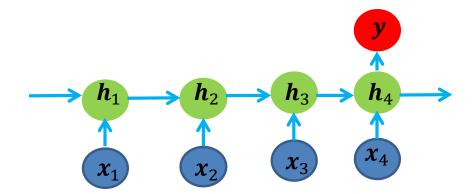
Recurrent Neural Nets For sequence tagging & for classification

RNNs for sequence tagging (aka sequence labeling)





RNNs for sentence classification



Code for RNNs



- Many implementations out there
- Lample et al (2016), Ma and Hovy (2016), and also newer stuff
- Nils Reimers has a nice Keras implementation
 - See: https://github.com/UKPLab/emnlp2017-bilstm-cnn-crf
 - He also has one for ELMo embeddings
- We also have a TensorFlow implementation (using Multi-Task Learning, etc.)
 - See: https://github.com/UKPLab/thesis2018-tk
 tk mtl sequence tagging

Recurrent Neural Nets NLP applications

- RNNs are "natural" forms for sequence labeling tasks
 - POS tagging

- RNNs are "natural" forms for sequence labeling tasks
 - POS tagging



We	love	cold	beer
PRON	V	ADJ	Noun

Label space = y = {PRON,V,DET,ADVERB,...} encoded as 1-hot vectors Input space = x = natural language words = {I,you,he,she,run,...} encoded as embeddings RNNs are "natural" forms for sequence labeling tasks

NER



Angela	Merkel	loves	New	York
B-PER	I-PER	0	B-LOC	I-LOC

Label space = y = {B-PER,I-PER,O,B-LOC,I-LOC,....} encoded as 1-hot vectors Input space = x = natural language words = {I,you,he,she,run,...} encoded as embeddings

- RNNs are "natural" forms for sequence labeling tasks
 - Grapheme-to-Phoneme Conversion (s c h u h → S U:)

Χ
У

S	С	h	u	h
S	Ø	Ø	U:	Ø

Label space = $y = \{S,a,a:,\emptyset,...\}$ encoded as 1-hot vectors Input space = $x = \text{chars} = \{a,b,c,...\}$ encoded as char embeddings or 1-hot

- RNNs are "natural" forms for sequence labeling tasks
 - Lemmatization (g e l i e b t → l i e b e n)



g	е	1	i	е	b	t
Ø	Ø	1	i	е	b	en

Label space = $y = \{a,b,c,st,en,...\}+\{\emptyset\}$ encoded as 1-hot vectors Input space = $x = chars = \{a,b,c,...\}$ encoded as char embeddings or 1-hot

RNNs are "natural" forms for sequence labeling tasks

Language Modeling



<sos></sos>	Here	comes	а	new	year
Here	comes	а	new	year	<eos></eos>

Label space = $y = \{words\}+padding encoded as 1-hot vectors lnput space = <math>x = \{words\}+padding encoded as embeddings$

Vanishing Gradients Introduction

- (following mostly the lecture slides of Richard Socher, <u>https://cs224d.stanford.edu/lectures/CS224d-Lecture8.pdf</u>
- See also de Freitas' video: https://www.youtube.com/watch?v=56TYLaQN4N8

The chain rule



- Newton notation: f(g(x))' = f'(g(x))g'(x)
- Leibniz notation: $\frac{df}{dx} = \frac{df}{dy} \cdot \frac{dy}{dx}$
- In higher dimensions, multiplication becomes scalar product or matrix multiplication
 - And $\frac{\partial f}{\partial x}$ is a vector (=gradient) when x is a vector:

•
$$\frac{\partial f}{\partial x} = \left(\frac{\partial f}{\partial x_1}, \dots, \frac{\partial f}{\partial x_n}\right)$$

• And $\frac{\partial y}{\partial x}$ is a matrix (=Jacobian) when y, x are vectors

•
$$\frac{\partial y}{\partial x} = (\frac{\partial y_1}{\partial x}, \dots, \frac{\partial y_m}{\partial x})$$

vector

Back to RNNs

- RNN formulation:
 - $\boldsymbol{h}_t = \sigma_H(\boldsymbol{x}_t \boldsymbol{U} + \boldsymbol{h}_{t-1} \boldsymbol{W})$
 - $\mathbf{y}_t = \sigma_Y(\mathbf{h}_t \mathbf{V})$

• Interested in:

$$rac{\partial m{h}_t}{\partial m{h}_{m{k}}}$$

$$\frac{\partial \boldsymbol{h}_{t}}{\partial \boldsymbol{h}_{k}} = \frac{\partial \boldsymbol{h}_{t}}{\partial \boldsymbol{h}_{t-1}} \frac{\partial \boldsymbol{h}_{t-1}}{\partial \boldsymbol{h}_{t-2}} \cdots \frac{\partial \boldsymbol{h}_{k+1}}{\partial \boldsymbol{h}_{k}}$$

- Remember:
 - $\boldsymbol{h}_t = \sigma_H(\boldsymbol{x}_t \boldsymbol{U} + \boldsymbol{h}_{t-1} \boldsymbol{W})$

Each $\frac{\partial h_s}{\partial h_{s-1}}$ is a matrix (called Jacobian)

Hence,

•
$$\frac{\partial h_S}{\partial h_{S-1}} = \operatorname{diag}(\sigma'_H(x_S U + h_{S-1} W)) \cdot W$$

Definition for diag:

• Let
$$\mathbf{z} = \mathbf{x}_{\scriptscriptstyle S} \mathbf{U} + \mathbf{h}_{\scriptscriptstyle S-1} \mathbf{W}$$

$$\bullet \operatorname{diag}([z_1 \cdots z_n]) = \begin{bmatrix} z_1 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & z_n \end{bmatrix}$$



$$||\frac{\partial h_{S}}{\partial h_{S-1}}|| = ||\operatorname{diag}(\sigma'_{H}(\mathbf{z})) \cdot \mathbf{W}||$$

$$\leq ||\operatorname{diag}(\sigma'_{H}(\mathbf{z}))|| \cdot ||\mathbf{W}||$$

- Assume β_H is an upper bound for the norm of diag and β_W is an upper bound for the norm of W
- Similarly, assume that the norm of $\mathbf{Q}=\mathrm{diag}ig(\sigma_H'(\mathbf{z})ig)\cdot \mathbf{W}$ is bounded from below by α

Then:

$$\alpha \le \left| \left| \frac{\partial \boldsymbol{h}_{S}}{\partial \boldsymbol{h}_{S-1}} \right| \right| \le \left| \left| \operatorname{diag}(\sigma'_{H}(\boldsymbol{z})) \right| \cdot \left| |\boldsymbol{W}| \right| \le \beta_{H} \beta_{W}$$

$$\left| \frac{\partial \boldsymbol{h}_{t}}{\partial \boldsymbol{h}_{k}} \right| = \left| \frac{\partial \boldsymbol{h}_{t}}{\partial \boldsymbol{h}_{t-1}} \frac{\partial \boldsymbol{h}_{t-1}}{\partial \boldsymbol{h}_{t-2}} \cdots \frac{\partial \boldsymbol{h}_{k+1}}{\partial \boldsymbol{h}_{k}} \right| \leq (\beta_{H} \beta_{W})^{(t-k)}$$

- This can become very large (exploding gradients) or very small (vanishing gradients) quickly (Bengio et al. 1994)
 - If very large:

- If very small:
 - $m{h}_k$ (and all that goes into it) has no effect on $m{h}_t$

- Vanishing gradient problem for language models/sequence labeling, etc.
 - Time steps far away are not taken into consideration
- "Jane walked into the room. John walked in too. It was late in the day. John said hi to XX"
- "Berlin_(_the_very_beautiful_...._capital_of _XX"

Rule of thumb:

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• A note on the term β_H :

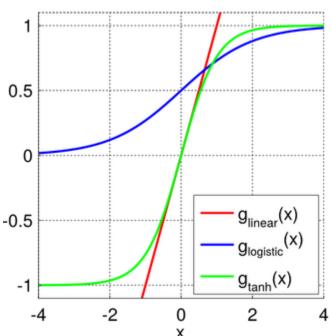
$$\left| \left| \operatorname{diag} \left(\sigma'_{H} (\boldsymbol{x}_{s} \boldsymbol{U} + \boldsymbol{h}_{s-1} \boldsymbol{W}) \right) \right| \right| \leq \beta_{H}$$

 $\sigma' > 1$ exploding gradient

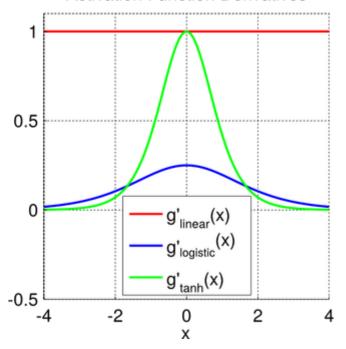
 $\sigma' < 1$ vanishing gradient

 $\sigma' = 1$ good region





Activation Function Derivatives

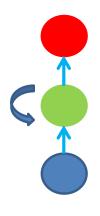


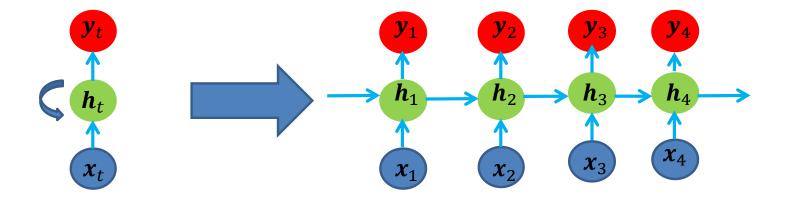
Vanishing gradients in MLPs

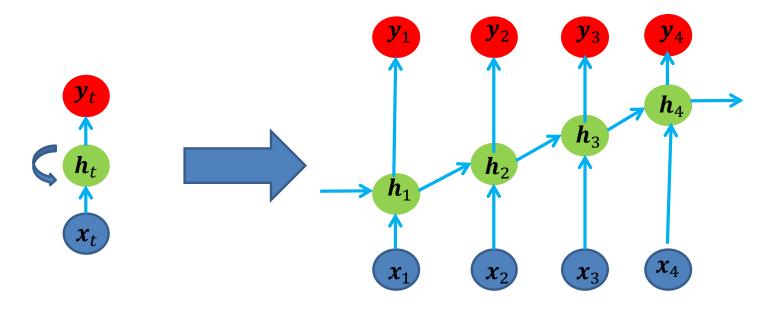


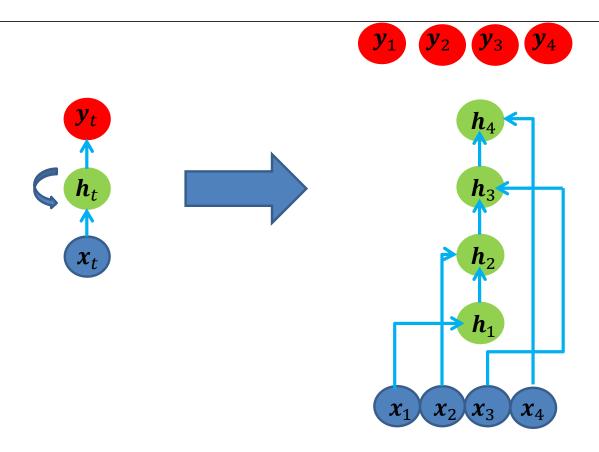
- Note that the vanishing gradient problem is not specific to RNNs
- It occurs in all deep networks, also in deep MLPs
- Also behold that RNNs are a form of deep neural nets:

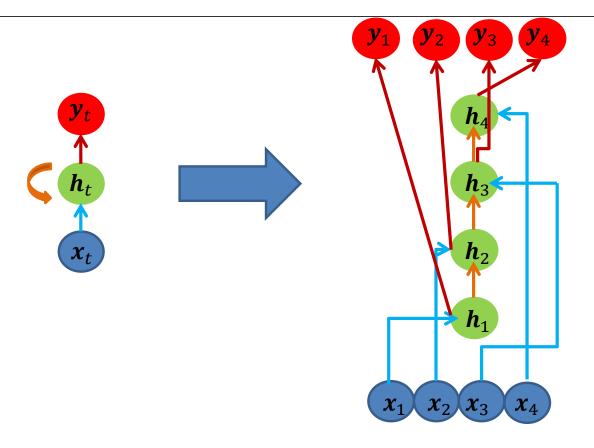




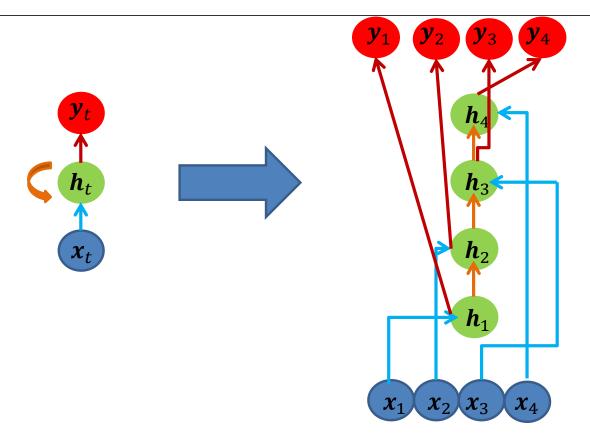












- RNNs are deep MLPs
- With weight sharing
- And sparse connectivity
- And skip connections

Vanishing gradients Simple Remedies

Regularization & Norm clipping



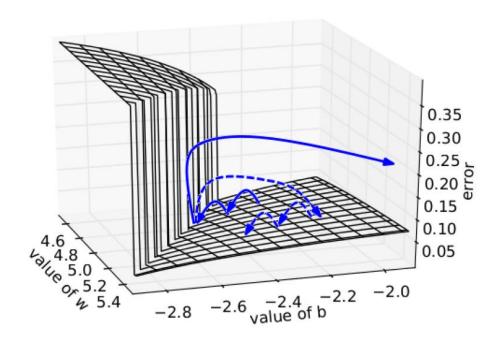
Exploding gradients:

- L1 or L2 regularization on recurrent weights \rightarrow keeps W small
- Gradient clipping (first introduced by Mikolov)
 - If error derivative $\frac{\partial E}{\partial w_{ik}}$ is too large, set it to some fixed constant

Norm clipping



Gradient clipping intuition:



From: On the difficulty of training RNNs, Pascanu et al. 2013

- Solid lines: standard gradient descent trajectories
- Dashed lines: gradients rescaled to fixed size

IRNNs



Vanishing (/exploding) gradients

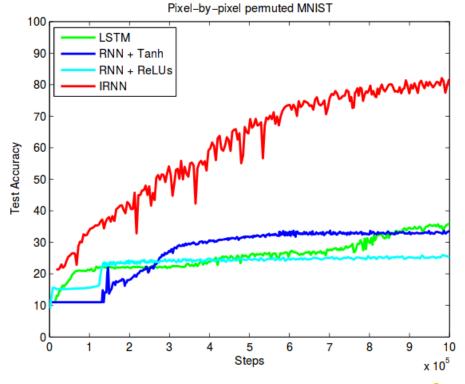
- ReLU and initialization, Le et al., 2015
 - Initialize W's to identity matrix I
 - $\sigma_H(z) = \max(0, z)$

IRNNs



Vanishing (/exploding) gradients

- ReLU and initialization, Le et al., 2015
 - Initialize $oldsymbol{W}$'s to identity matrix $oldsymbol{I}$
 - $\sigma_H(z) = \max(0, z)$
 - They call this IRNNs (I = identity matrix)



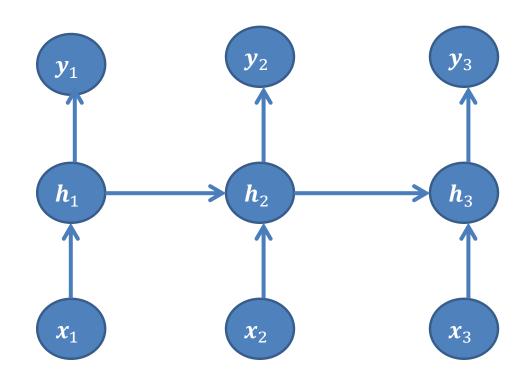
Vanishing gradients GRUs & LSTMs

GRUs

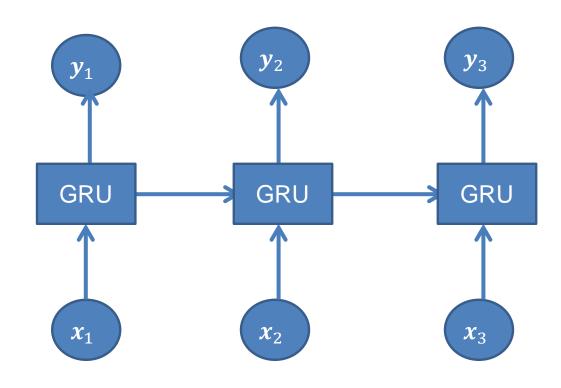


- More complex hidden unit computation in recurrence
- Gated Recurrent Units (GRU) introduced by Cho et al. (2014)
- Main idea:
 - Gates to control the flow of information

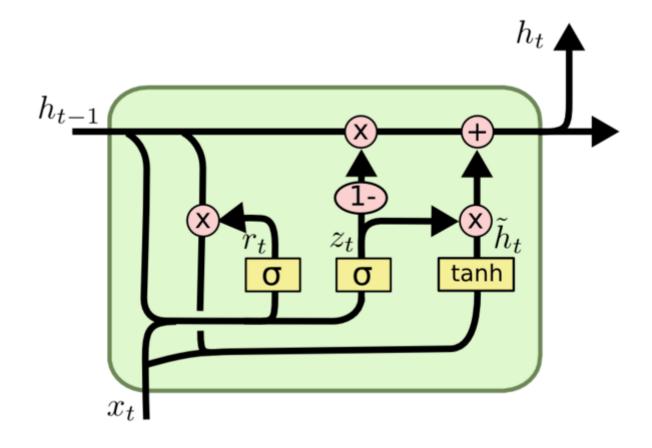
GRUs



GRUs



GRU illustration



Some notation

- Conventions for the following slides
 - σ is the sigmoid (=logistic) non-linearity
 - ⊙ is the *Hadamard* (=point-wise) product
 - $\boldsymbol{a} \odot \boldsymbol{b} = (a_1 \cdot b_1, \dots, a_n \cdot b_n)$

GRU memory unit

Update gate

•
$$\mathbf{z}_t = \sigma(\mathbf{x}_t \mathbf{U}^{(z)} + \mathbf{h}_{t-1} \mathbf{W}^{(z)})$$

Reset gate

•
$$\mathbf{r}_t = \sigma(\mathbf{x}_t \mathbf{U}^{(r)} + \mathbf{h}_{t-1} \mathbf{W}^{(r)})$$

New memory content

•
$$\widetilde{\boldsymbol{h}}_t = \tanh(\boldsymbol{x}_t \boldsymbol{U} + \boldsymbol{h}_{t-1} \boldsymbol{W} \odot \boldsymbol{r}_t)$$

- Final memory at time step combines current and previous time steps
 - $\boldsymbol{h}_t = (1 \boldsymbol{z}_t) \odot \boldsymbol{h}_{t-1} + \boldsymbol{z}_t \odot \widetilde{\boldsymbol{h}}_t$



- Extreme cases: $z_t \in \{0,1\}, r_t \in \{0,1\}$
 - Note: \mathbf{z}_t and \mathbf{r}_t are vectors, but we look at individual components here



• Extreme cases: $z_t \in \{0,1\}, r_t \in \{0,1\}$

$$\boldsymbol{h}_t = (1 - \boldsymbol{z}_t) \odot \boldsymbol{h}_{t-1} + \boldsymbol{z}_t \odot \widetilde{\boldsymbol{h}}_t$$

- $z_t = 0$:
 - $h_t = h_{t-1} \rightarrow$ no update \rightarrow can keep memory from previous time step \rightarrow no vanishing gradient



• Extreme cases: $z_t \in \{0,1\}, r_t \in \{0,1\}$

$$\boldsymbol{h}_t = (1 - \boldsymbol{z}_t) \odot \boldsymbol{h}_{t-1} + \boldsymbol{z}_t \odot \widetilde{\boldsymbol{h}}_t$$

- $z_t = 1$:
 - $\boldsymbol{h}_t = \widetilde{\boldsymbol{h}}_t$



• Extreme cases: $z_t \in \{0,1\}, r_t \in \{0,1\}$

$$\boldsymbol{h}_t = (1 - \boldsymbol{z}_t) \odot \boldsymbol{h}_{t-1} + \boldsymbol{z}_t \odot \widetilde{\boldsymbol{h}}_t$$

- $z_t = 1$:
 - $\boldsymbol{h}_t = \widetilde{\boldsymbol{h}}_t$
 - $r_t = 0$:
 - $h_t = \tanh(x_t U) \rightarrow \text{Forget past}$
 - $r_t = 1$:
 - $h_t = \tanh(x_t U + h_{t-1} W) \rightarrow \text{Standard RNN}$

$$\widetilde{\boldsymbol{h}}_t$$

$$= \tanh(\boldsymbol{x}_t \boldsymbol{U} + \boldsymbol{h}_{t-1} \boldsymbol{W} \odot \boldsymbol{r}_t)$$



- Summary:
 - Can store memory at a cell indefinitely
 - Can also forget past memory, and reset everything
 - Can also go back to standard RNN mode, where memory is continuously updated based on past memory and current input

LSTM



Can make units even more complex



- Input gate (= write gate) $i_t = F(x_t, h_{t-1}; \theta_i)$
- Forget gate (= reset gate) $\boldsymbol{f}_t = F(\boldsymbol{x}_t, \boldsymbol{h}_{t-1}; \boldsymbol{\theta}_f)$
- Output gate (= read gate) $o_t = F(x_t, h_{t-1}; \theta_o)$
- New memory cell

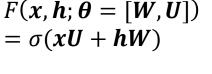
•
$$\tilde{\boldsymbol{c}}_t = \tanh(\boldsymbol{x}_t \boldsymbol{U} + \boldsymbol{h}_{t-1} \boldsymbol{W})$$

Final memory cell

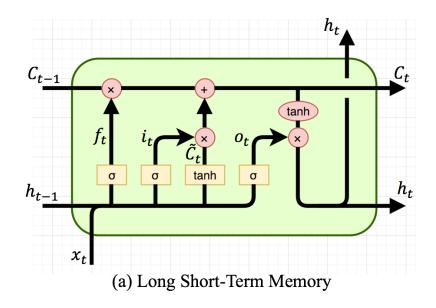
$$c_t = f_t \odot c_{t-1} + i_t \odot \tilde{c}_t$$

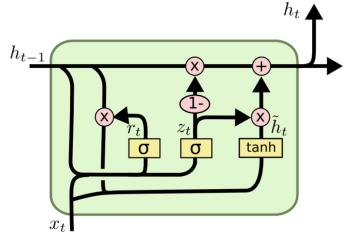
Final hidden state

•
$$\boldsymbol{h}_t = \boldsymbol{o}_t \odot \tanh(\boldsymbol{c}_t)$$









(b) Gated Recurrent Unit



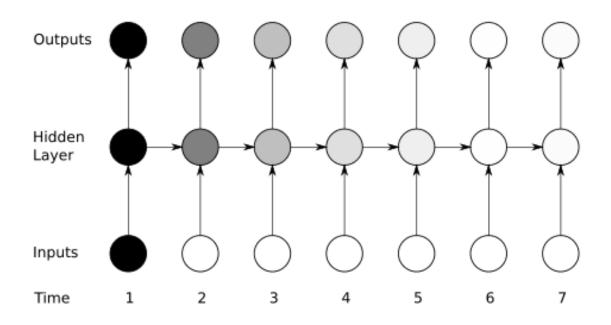


Figure 4.1: The vanishing gradient problem for RNNs. The shading of the nodes in the unfolded network indicates their sensitivity to the inputs at time one (the darker the shade, the greater the sensitivity). The sensitivity decays over time as new inputs overwrite the activations of the hidden layer, and the network 'forgets' the first inputs.

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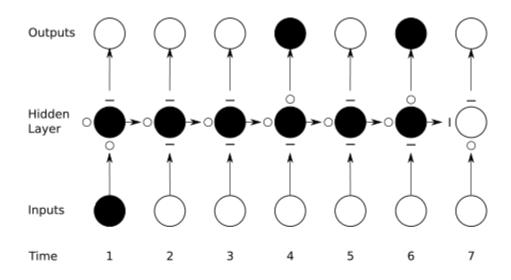


Figure 4.4: **Preservation of gradient information by LSTM.** As in Figure 4.1 the shading of the nodes indicates their sensitivity to the inputs at time one; in this case the black nodes are maximally sensitive and the white nodes are entirely insensitive. The state of the input, forget, and output gates are displayed below, to the left and above the hidden layer respectively. For simplicity, all gates are either entirely open ('O') or closed ('—'). The memory cell 'remembers' the first input as long as the forget gate is open and the input gate is closed. The sensitivity of the output layer can be switched on and off by the output gate without affecting the cell.

Source: Alex Graves, PhD thesis

GRU vs. LSTM



- LSTM much more popular (a lot has to do with bias)
- But follows same principles of controlling flow of information via gates

Summary



- Recurrent Neural Networks are powerful
- Gated Recurrent Units even better
- LSTMs maybe even better
- LSTMs in heavy use until 2018
- Problem: parallelization is difficult
 - Search for more efficient architectures (Transformers)

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