

Deep Learning

Recurrent Neural Networks

Technische Hochschule Rosenheim Sommer 2023 Prof. Dr. Jochen Schmidt

Acknowledgements



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https://lme.tf.fau.de/

Overview



- Simple Recurrent Neural Networks (RNNs)
- Long Short-Term Memory Units (LSTMs)
- Gated Recurrent Units (GRUs)
- Comparison of simple RNN units, LSTM units and GRUs



Simple Recurrent Neural Networks (RNNs)

Motivation



- So far: **One** input, e.g., single image
- Feed forward neural networks: input → processing → result
- But: there are lots of sequential or time-dependent signals, e.g.
 - Speech/Music (translation, music classification)
 - Video (object detection/face recognition)
 - Sensor data (speed, temperature, energy consumption,...)
- "Snapshots" often not informative (single word → translation?)
- → **Temporal context** is important!

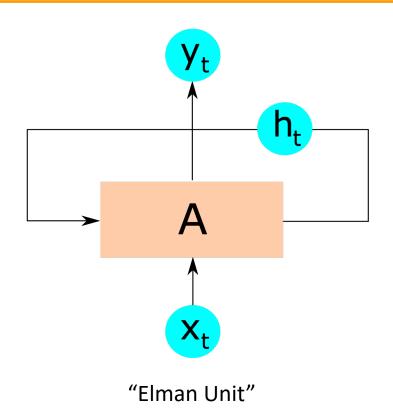
Motivation



- How can we integrate this context in the network?
- Simple approach: Feed the whole sequence to a big network → Bad idea!
 - Inefficient memory usage
 - Difficult/impossible to train
 - Difference between spatial and temporal dimensions?
 - Not real-time! (translation,...)
- Better approach: Model sequential behavior within the architecture:
 - → Recurrent Neural Networks (RNNs)

Basic RNN Structure (Elman Unit)





- Current input x_t multiplied by weight
- Additional input: Hidden state h_{t-1} of the unit
- → Feedback loop:

use information from present and recent past to compute output y_t

- First models in 1970's [Lit74] and early 1980's [Hop82] (Hopfield Network)
- Simple recurrent neural network or Elman network introduced in *Finding Structure in Time* by Jeff Elman in 1990 [Elm90]

RNNs vs Feed-forward Networks

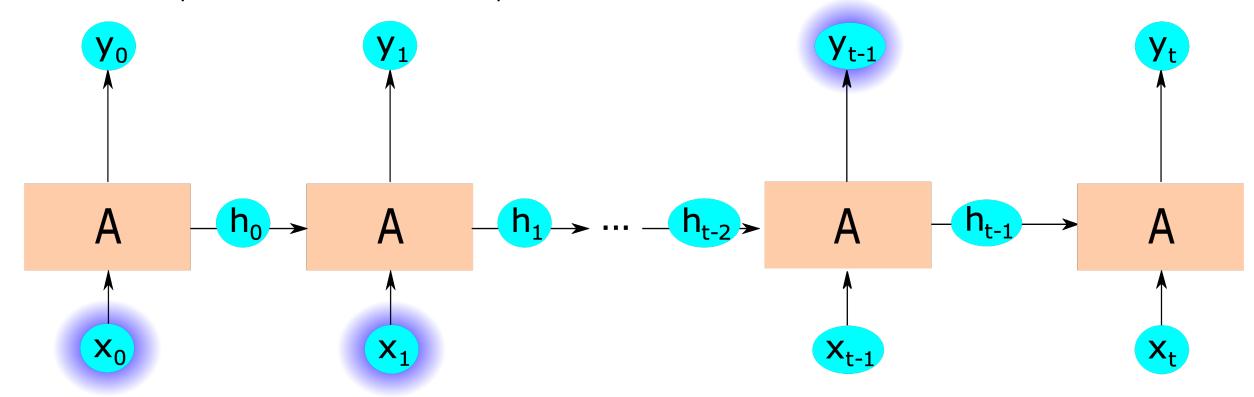


- Feed-forward networks only feed information forward through the net
 - they do not have an internal state
- With recurrent neural networks, we can:
 - model loops
 - model memory and experience
 - learn sequential relationships
 - provide continuous predictions as data comes in → real-time

Unfolded RNN



- "Unfolded" RNN unit: sequence of copies of the **same** unit (= same weights)
 - Parameter-sharing over time
- Each unit passes hidden state as additional input to successor
- → Previous input can influence current output



Types of Sequences



one to one

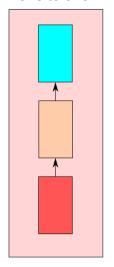


image classification
in: image
out: class label
(fixed-size vector)
classic feed-forward

one to many

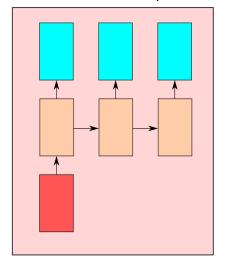
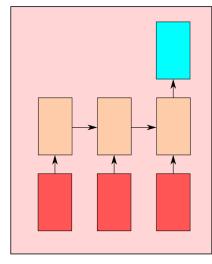


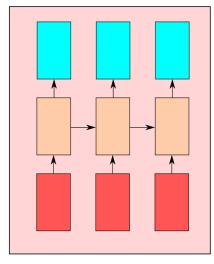
image captioningin: imageout: text description (sequence)

many to one



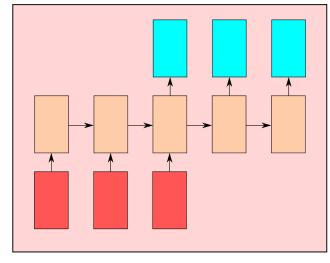
sentiment analysisin: text (sequence)out: class label (fixed-size vector)

many to many (sync)



video classificationin: image stream (sequence)out: label for each frame (sequence)

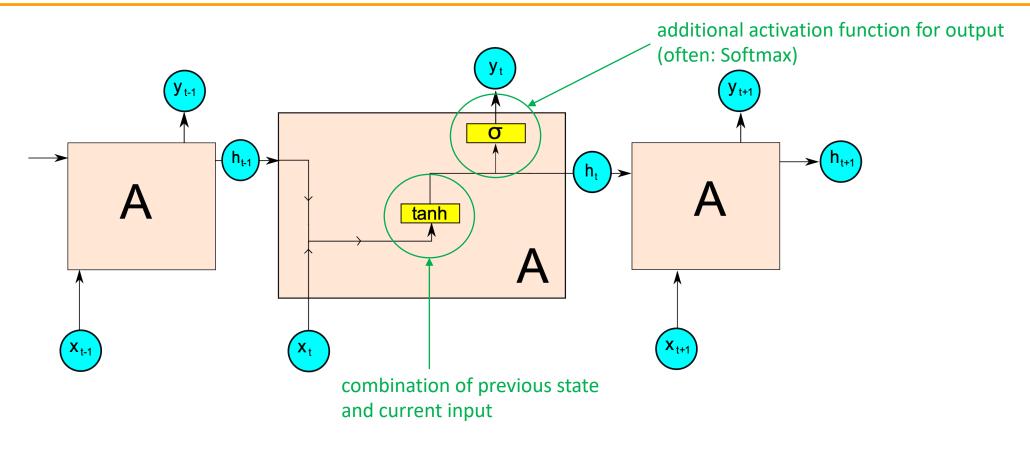
many to many (no sync)



machine translation
in: German text (sequence)
out: English text (sequence)
input and output sequences
not necessarily of same length

Internal Structure of RNN Unit



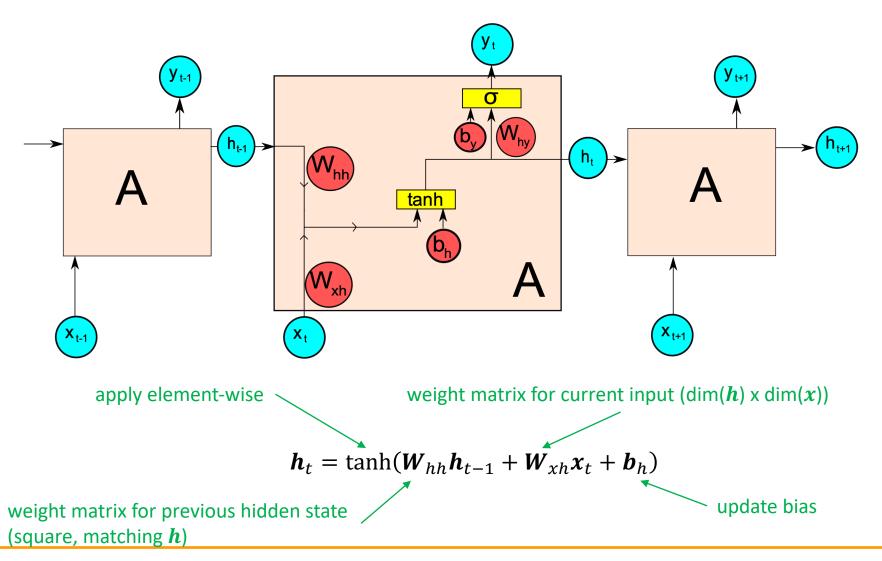


Question 1: How do we update the hidden state?

Question 2: How do we combine input and hidden state to compute output?

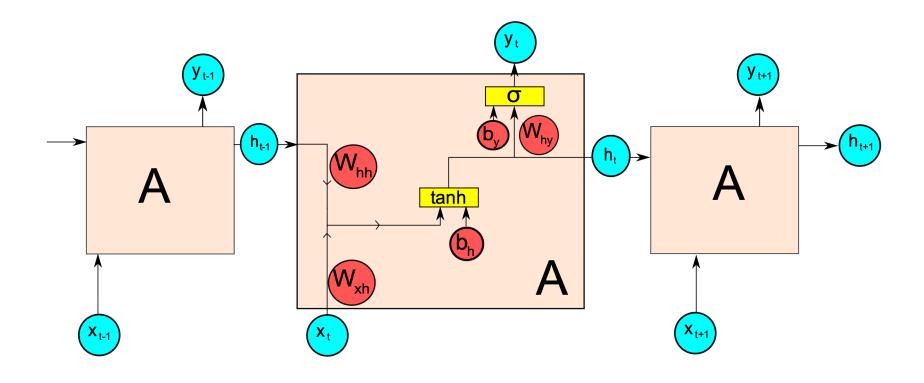
Close-up: How to Update the Hidden State?





Close-up: How to Compute the Output?



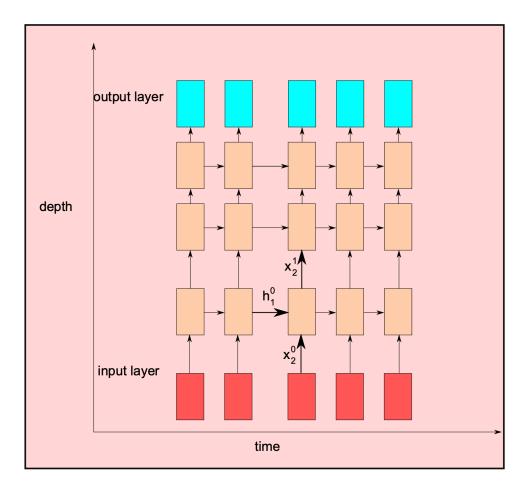


$$\mathbf{y}_t = \sigma \big(\mathbf{W}_{hy} \mathbf{h}_t + \mathbf{b}_y \big)$$
 weight matrix for current hidden state — output bias

Deep RNNs



Stack multiple Elman units



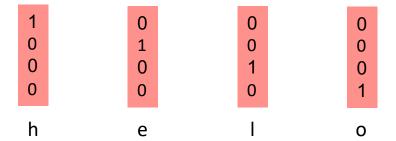
- as in feed-forward networks: additional layers for each time step
- higher learning capacity
- more training data required
- in practice you find deep RNNs only very rarely, if at all

Example: Character Level Language Model



Task: Learn character probability distribution from input text

- Vocabulary: {h, e, l, o}
- Characters encoded as one-hot vectors:

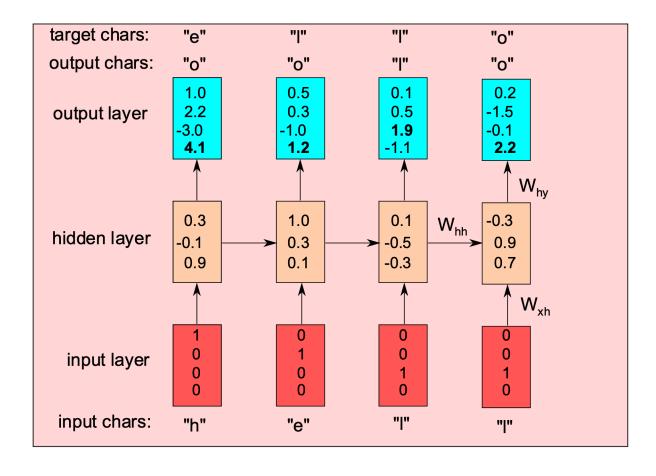


- Train RNN on the sequence "hello":
 Given 'h' as first input, the network should generate the sequence "hello"
- Network needs to know previous inputs
 - when presented with 'l': Do we need another 'l' or an 'o'?
- Adapted from http://karpathy.github.io/2015/05/21/rnn-effectiveness

Example: Character Level Language Model



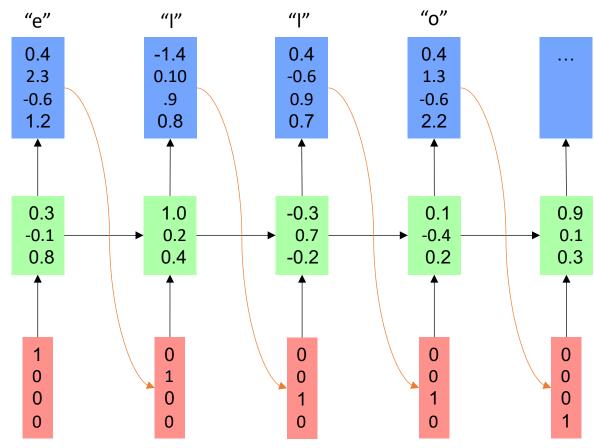
Prediction with random initialization:



Character Level Language Models at Runtime



Desired result after training (example) – Goal: Maximize prediction for correct component



How can we now train this network? "h'

→ Backpropagation through time (BPTT): train "unfolded" network

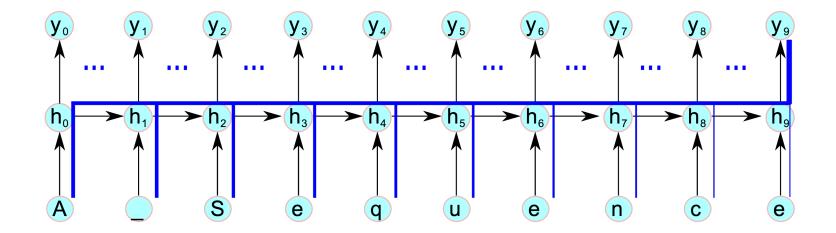
based on silde courtesy of Tobias Bocklet [Boc20]

Backpropagation Through Time (BPTT)



Concept: Train the unfolded network

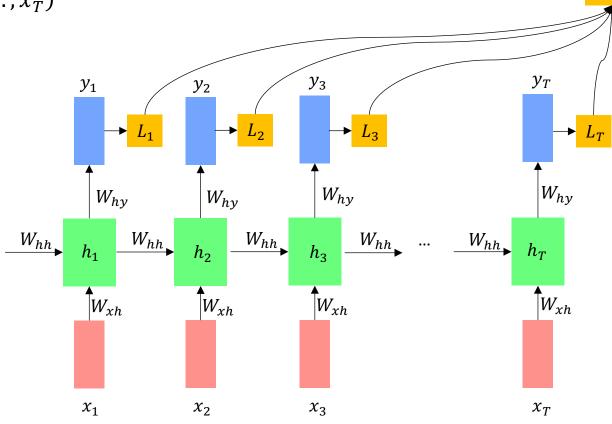
- Compute forward pass for the full sequence → loss
- Compute backward pass for the full sequence to get gradients → weight update



BPTT – Forward Pass



Forward pass: Computation of hidden states and output using input sequence $(x_1, x_2, ..., x_T)$



 $L(\widehat{\mathbf{y}}, \mathbf{y}) = \sum_{t=1}^{T} L_t(\widehat{\mathbf{y}_t}, \mathbf{y}_t)$

 $\widehat{m{y}}$: predicted output

y: ground truth

based on silde courtesy of Tobias Bocklet [Boc20]

BPTT – Backward Pass



• Loss function, e.g., cross-entropy loss: L(j)

$$L(\widehat{\mathbf{y}}, \mathbf{y}) = \sum_{t=1}^{T} L_t(\widehat{\mathbf{y}_t}, \mathbf{y}_t)$$

• Compute gradient of the loss function L with respect to network parameters $oldsymbol{ heta}$

$$\nabla_{\boldsymbol{\theta}} L = \left[\nabla_{\boldsymbol{W}_{xh}} L, \ \nabla_{\boldsymbol{W}_{hh}} L, \ \nabla_{\boldsymbol{W}_{hy}} L, \ \nabla_{\boldsymbol{b}_h} L, \ \nabla_{\boldsymbol{b}_y} L, \ \nabla_{\boldsymbol{h}_0} L \right]$$

• Update parameters using a learning rate α

$$\boldsymbol{\theta} = \boldsymbol{\theta} - \alpha \nabla_{\boldsymbol{\theta}} L$$

How do we get these derivatives?
 Go "back in time" through the network

BPTT – Backward Pass



Go "backwards" through the unfolded unit, starting at final time step t=T and iteratively compute gradients for $t=T,\ldots,1$

Reminder:
$$\hat{y}_t = \sigma(o_t) = \sigma(W_{hy}h_t + b_y)$$
 $h_t = \tanh(W_{hh}h_{t-1} + W_{xh}x_t + b_h)$

$$\nabla_{\boldsymbol{o}_{t}}L = \frac{\partial \widehat{\boldsymbol{y}}}{\partial \boldsymbol{o}_{t}} \frac{\partial L}{\partial \widehat{\boldsymbol{y}}} = \sigma'(\boldsymbol{o}_{t}) \frac{\partial L}{\partial \widehat{\boldsymbol{y}}} \qquad \qquad \underline{\nabla_{\boldsymbol{w}_{hy,t}}L} = \frac{\partial \widehat{\boldsymbol{y}}}{\partial \boldsymbol{o}_{t}} \frac{\partial L}{\partial \widehat{\boldsymbol{y}}} \frac{\partial \boldsymbol{o}_{t}}{\partial \boldsymbol{W}_{hy}} = \nabla_{\boldsymbol{o}_{t}}L \, \boldsymbol{h}_{t}^{T} \qquad \qquad \underline{\nabla_{\boldsymbol{b}_{y,t}}L} = \frac{\partial \widehat{\boldsymbol{y}}}{\partial \boldsymbol{o}_{t}} \frac{\partial L}{\partial \widehat{\boldsymbol{y}}} \frac{\partial \boldsymbol{o}_{t}}{\partial \boldsymbol{b}_{y}} = \nabla_{\boldsymbol{o}_{t}}L \, \boldsymbol{h}_{t}^{T}$$

The gradient $\nabla_{h_t}L$ depends on two elements – the hidden state influences o_t as well as the next hidden state h_{t+1}

$$\underline{\nabla_{\boldsymbol{h}_{t}}L} = \left(\frac{\partial \boldsymbol{h}_{t+1}}{\partial \boldsymbol{h}_{t}}\right)^{T} \nabla_{\boldsymbol{h}_{t+1}}L + \left(\frac{\partial \boldsymbol{o}_{t}}{\partial \boldsymbol{h}_{t}}\right)^{T} \nabla_{\boldsymbol{o}_{t}}L$$

$$= \boldsymbol{W}_{hh}^{T} \tanh'(\boldsymbol{W}_{hh}\boldsymbol{h}_{t} + \boldsymbol{W}_{xh}\boldsymbol{x}_{t+1} + \boldsymbol{b}_{h}) \nabla_{\boldsymbol{h}_{t+1}}L + \boldsymbol{W}_{hy}^{T} \nabla_{\boldsymbol{o}_{t}}L$$

Note: For t = 0 (to get $\nabla_{h_0} L$) and t = T, we only need one element of the sum.

BPTT – Backward Pass



Using $\nabla_{h_t} L$ we get the remaining gradients.

Reminder:
$$\boldsymbol{h}_t = \tanh(\boldsymbol{u}_t) = \tanh(\boldsymbol{W}_{hh}\boldsymbol{h}_{t-1} + \boldsymbol{W}_{xh}\boldsymbol{x}_t + \boldsymbol{b}_h)$$

$$\nabla_{\boldsymbol{W}_{hh,t}} L = \nabla_{\boldsymbol{h}_t} L \cdot \tanh'(\boldsymbol{u}_t) \cdot \boldsymbol{h}_{t-1}^T$$

$$\nabla_{\boldsymbol{W}_{xh,t}}L = \nabla_{\boldsymbol{h}_t}L \cdot \tanh'(\boldsymbol{u}_t) \cdot \boldsymbol{x}_t^T$$

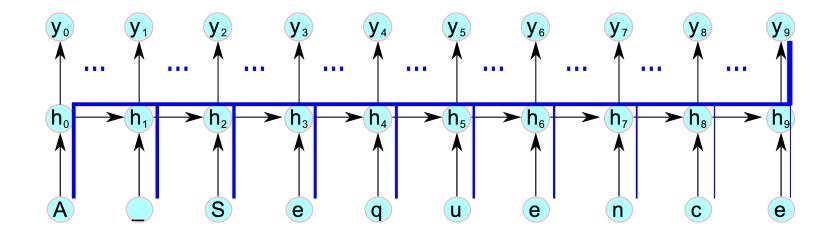
$$\nabla_{\boldsymbol{b}_{h,t}} L = \nabla_{\boldsymbol{h}_t} L \cdot \tanh'(\boldsymbol{u}_t)$$

Currently, the gradients depend on t. How do we get the gradient for the sequence?

- The unrolled unit is a network with shared weights (over time)
- For each gradient, simply sum over all time-steps t = 1, ..., T

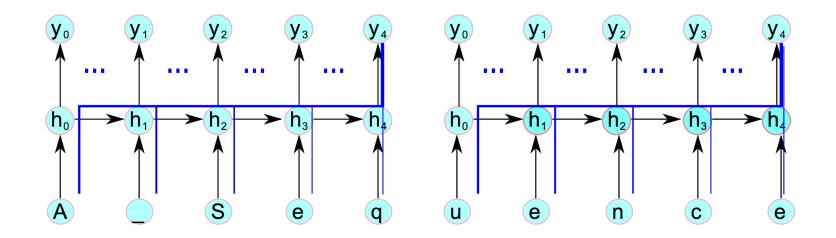
Normal BPTT





One update requires backpropagation through a complete sequence

→ Single parameter update is very expensive!

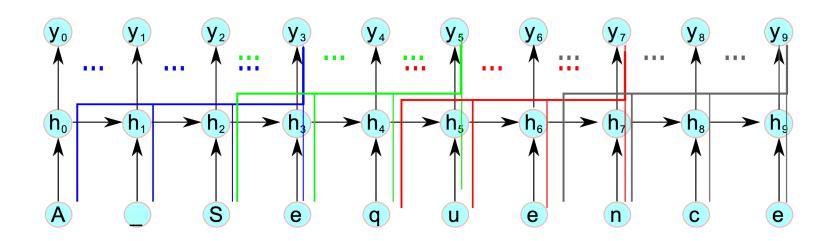


Naive Solution:

- Split long sequences into batches of smaller parts
- Might work ok in practice, but blind to long-term dependencies
- Can we do better? Yes!
- → Truncated backpropagation through time (TBPTT)

Truncated Backpropagation Through Time (TBPTT)





- Main idea: Keep processing sequence as a whole
- Adapt frequency and depth of update:
 - Every k_1 time steps, run BPTT for k_2 time steps
 - Parameter update cheap if k_2 small
- Hidden states are still exposed to many time steps

Algorithm:

for t = 1 to T do:

Run RNN for one step, computing h_t and \hat{y}_t if $t \mod k_1 == 0$:

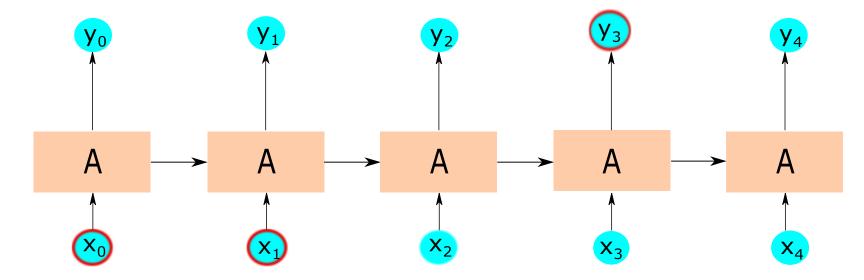
Run BPTT from t down to $t - k_2$

So can we successfully train RNNs now? Still no...

The Long-Term Dependency Problem with Basic RNNs



- Short term dependencies work fine
- Example: Predict next word in "the clouds are in the [sky]"

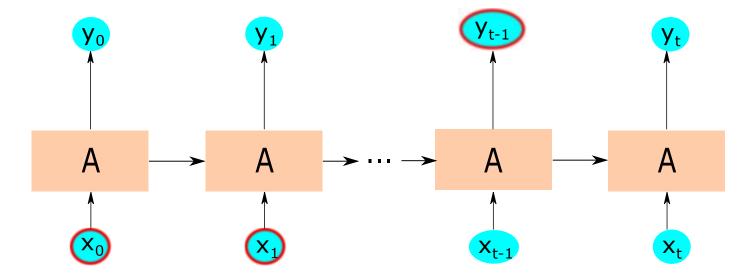


Contextual information nearby → can be encoded in hidden state easily

The Long-Term Dependency Problem with Basic RNNs



- It is harder to connect relevant past and present inputs for longer time spans
- Example: Predict next word in "I grew up in Germany ... I speak fluent [German]"



Contextual information far away Why does this make a difference?

The Long-Term Dependency Problem with Basic RNNs



Old acquaintances: vanishing and exploding gradients

- Layers and time steps of deep RNNs are related through multiplication
 - → Gradients prone to vanishing or exploding
- Exploding gradient relatively easy to solve by clipping gradient
- Vanishing gradient harder to solve!

Additional problem: memory overwriting

- Hidden state is overwritten each time step
 - → Detecting long-term dependencies even more difficult
- Can we do better? Again, yes!



Long Short-Term Memory Units (LSTMs)

LSTM Motivation



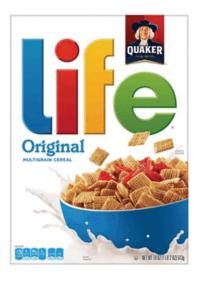
Customers Review 2,491



Thanos

September 2018
Verified Purchase

Amazing! This box of cereal gave me a perfectly balanced breakfast, as all things should be. I only ate half of it but will definitely be buying again!



A Box of Cereal \$3.99

https://towardsdatascience.com/illustrated-guide-to-lstms-and-gru-s-a-step-by-step-explanation-44e9eb85bf21

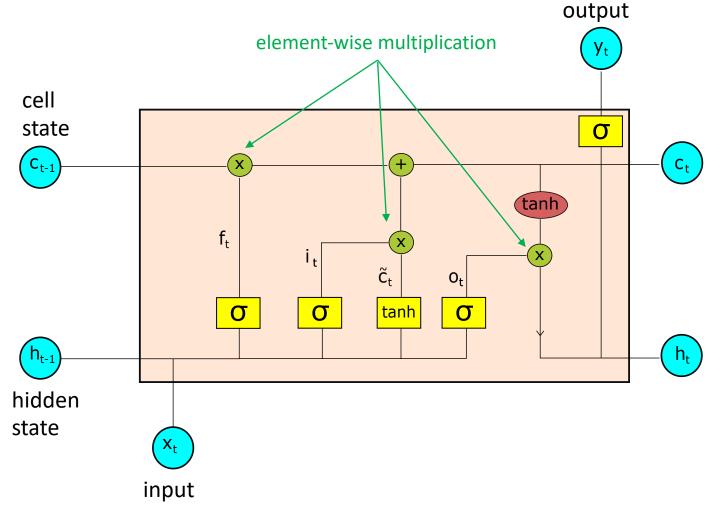
Background



- Long Short-Term Memory Units (LSTMs) introduced by Sepp Hochreiter & Jürgen Schmidhuber in 1997 [Hoc97]
- Designed to solve vanishing gradient and learning long-term dependencies
- Main idea: introduction of gates that control writing and accessing "memory" in additional cell state
 - "forgetting" and "memorizing" information in separate steps

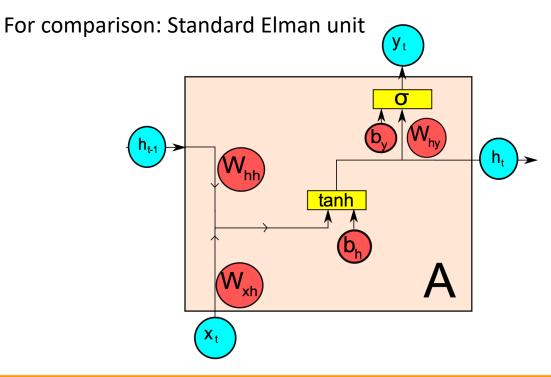
Overview LSTM Unit





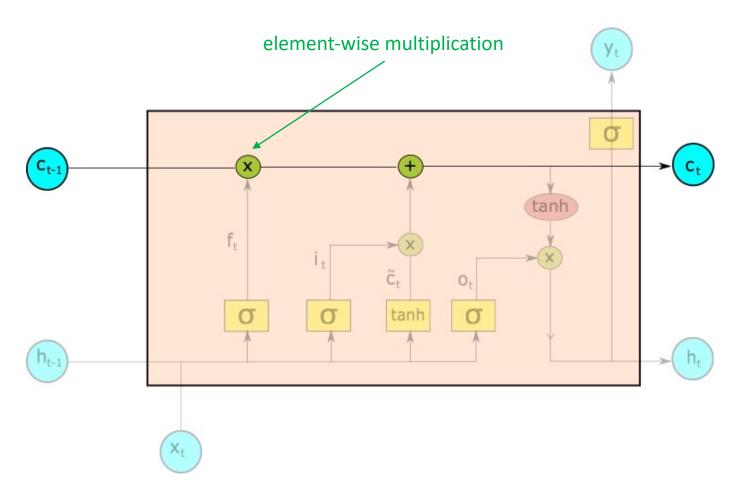
Update of internal states in multiple steps:

- 1) Forget gate: Forgetting old information in cell state
- 2) Input gate: Deciding on new input for cell state
- 3) Computing the updated cell state
- 4) Computing the updated hidden state



LSTM Cell State



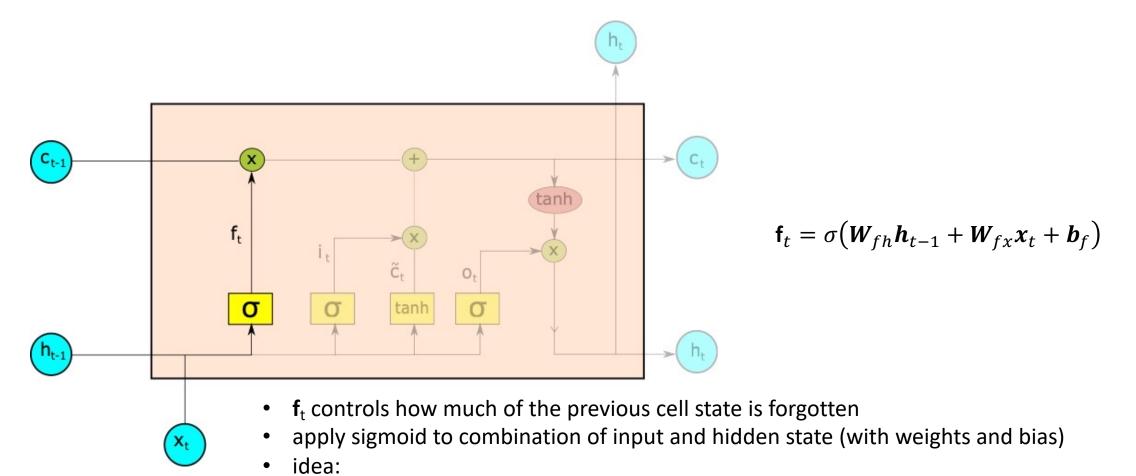


Cell state after time step t

- Undergoes only linear changes: no activation function!
- can flow through a unit unchanged → cell state can stay constant for multiple time steps
- this is the memory of the network

Forget Gate: Forgetting Old Information



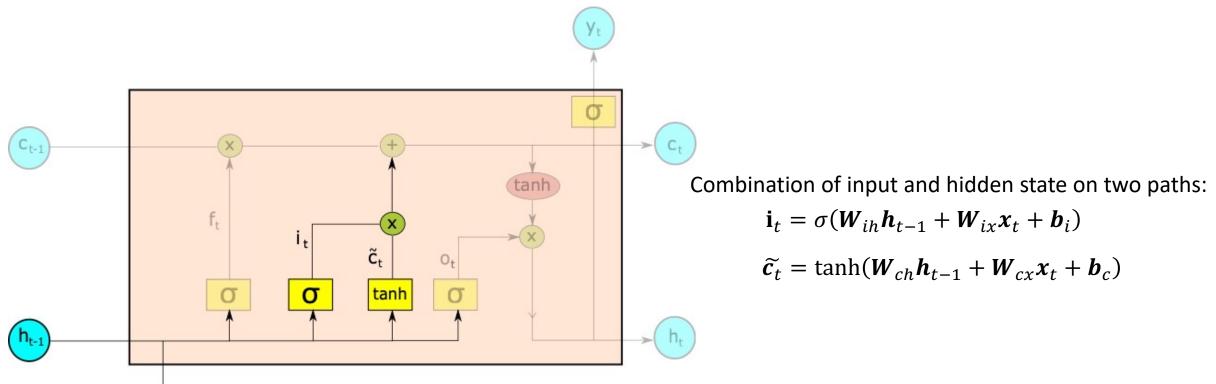


Sigmoid output = $0 \rightarrow$ forget

Sigmoid output = $1 \rightarrow$ remember

Input Gate: Deciding on New Input



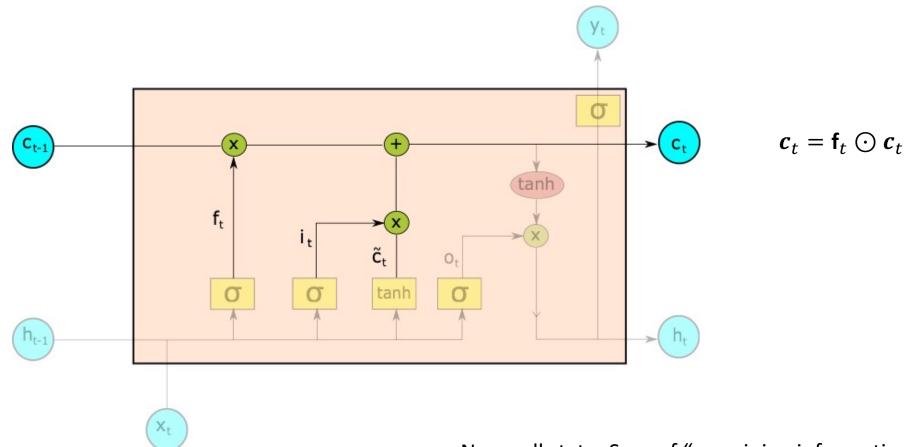


Input gate controls which new information is to be stored in cell state

- 1. Sigmoid applied to combination of input and hidden state; decides which values are to be updated
- 2. tanh generates new candidate vector
- 3. The sigmoid decides which parts of the candidate are to be kept and added to the cell state

Updating the Cell State



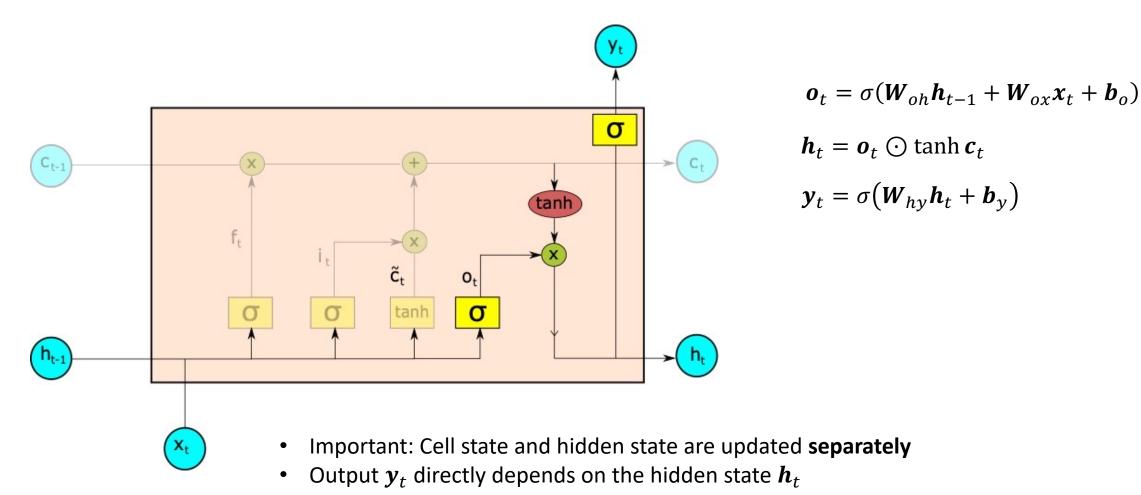


$$c_t = \mathbf{f}_t \odot c_{t-1} + \mathbf{i}_t \odot \widetilde{c}_t$$

New cell state: Sum of "remaining information" from $oldsymbol{c}_{t-1}$ and new information from input and hidden state (⊙: element-wise multiplication)

Updating the Hidden State and Computing the Output







Gated Recurrent Units (GRUs)

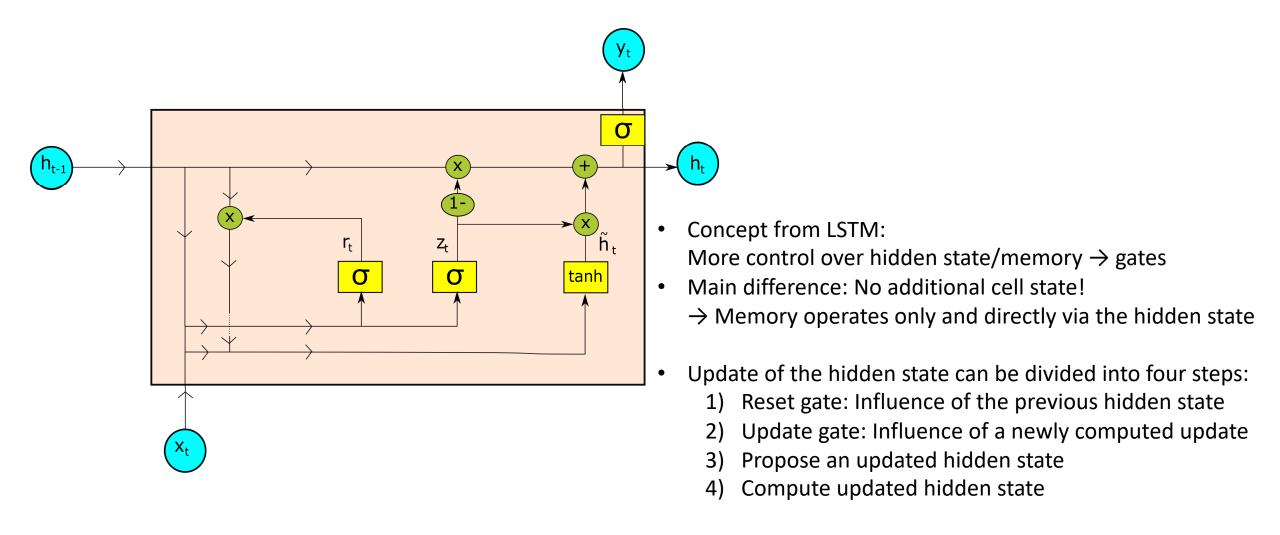
Motivation

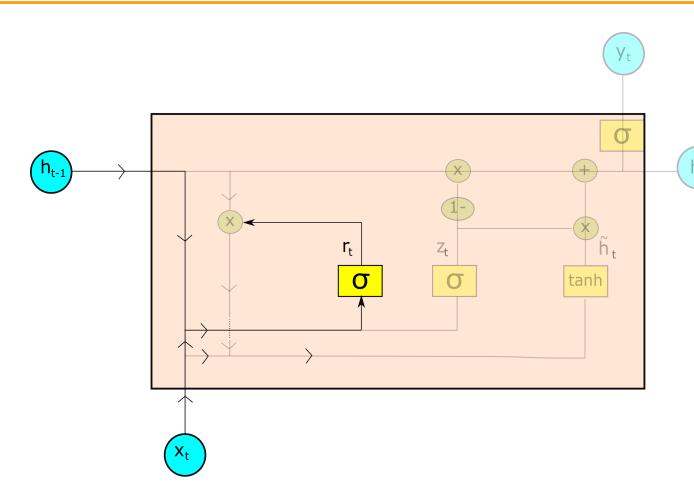


- LSTM great idea, but many parameters and difficult to train
 - → Gated Recurrent Unit (GRU)
- Originally introduced by Cho et al. in 2014 for statistical machine translation [Cho14]
- Variant of the LSTM unit, but simpler and fewer parameters

Structure of a GRU Cell





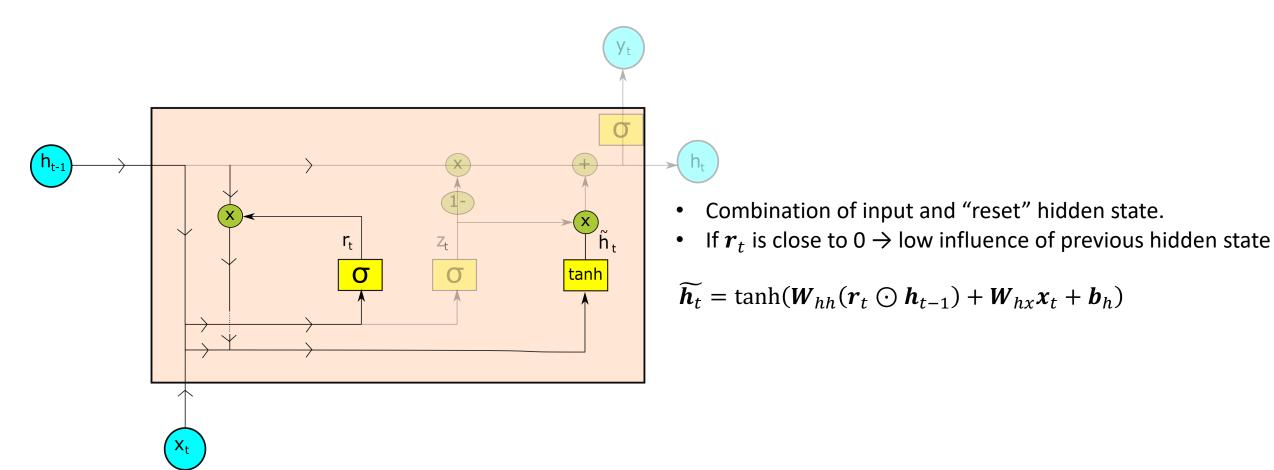


Determines the influence of the previous hidden state

$$\boldsymbol{r}_t = \sigma(\boldsymbol{W}_{rh}\boldsymbol{h}_{t-1} + \boldsymbol{W}_{rx}\boldsymbol{x}_t + \boldsymbol{b}_r)$$

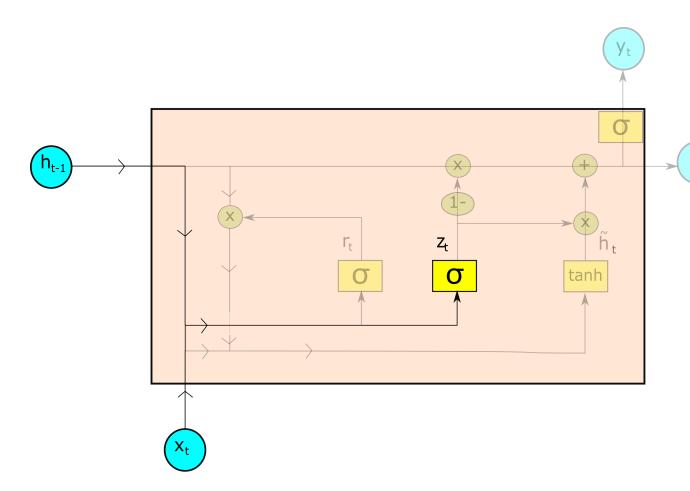
Proposing an Update





Update Gate



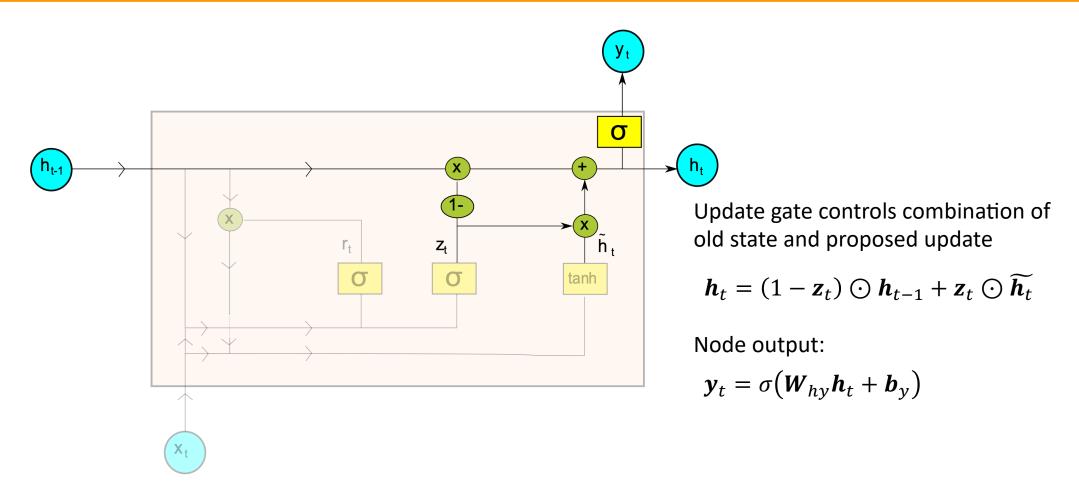


Determines the influence of an "update proposal" on the new hidden state

$$\mathbf{z}_t = \sigma(\mathbf{W}_{zh}\mathbf{h}_{t-1} + \mathbf{W}_{zx}\mathbf{x}_t + \mathbf{b}_z)$$

Finally: Compute the Updated Hidden State





Remarks



- Add ("+") essential for preservation of error in backpropagation
 - resolves vanishing gradient problem (which originates from multiplication)
- Gates allow capturing diverse time scales and remote dependencies
- Units learning **short-term** dependencies have restrictive reset gates $\rightarrow r_t$ close to 0: ignore previous hidden state
- Units learning **long-term** dependencies have restrictive update gates $\rightarrow z_t$ close to 0: ignore new input
- → Gates have varying "rhythm" depending on the type of information

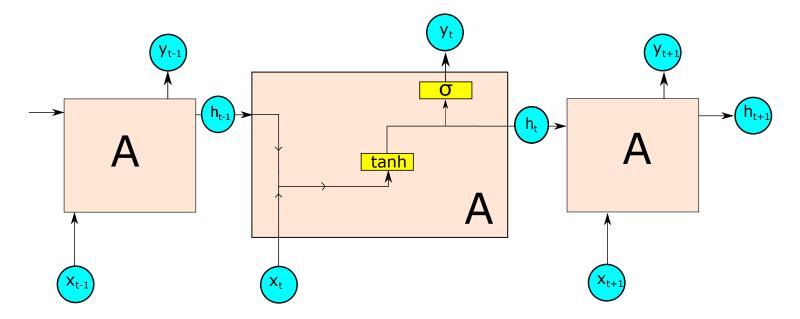


Comparison

Recap: Simple RNNs



- Gradient-based training difficult (vanishing/exploding gradients)
- Short-term dependencies hide long-term dependencies due to exponentially small gradients
- Hidden state is overwritten in each time step

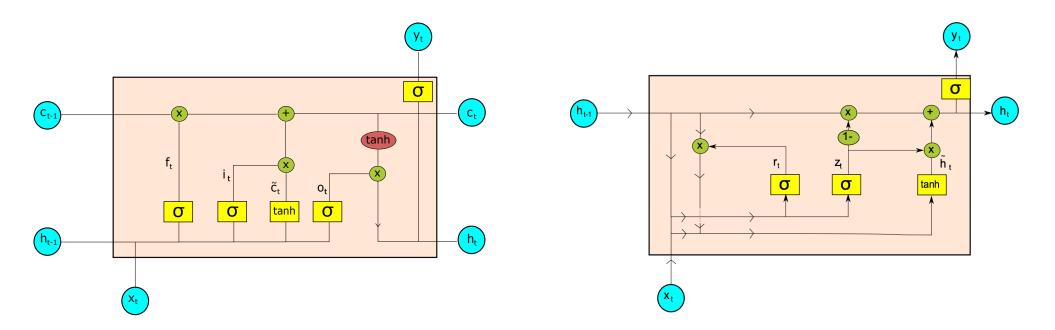


Recap: Advanced structures – LSTM and GRU



Both

- introduce gates that control information flow and operate on memory
- can capture dependencies at different time scales
- additive calculation of state preserves error during backpropagation
 → more efficient training possible



Recap: LSTM and GRU – Differences



LSTM	GRU
Separate hidden and cell state	Combined hidden and cell state
Controlled exposure of memory content through output gate	Full exposure of memory content without control
Independent input and forget gate: $c_t = \mathbf{f}_t \odot c_{t-1} + \mathbf{i}_t \odot \widetilde{c_t}$	Joint update gate: $m{h}_t = (1 - m{z}_t) \odot m{h}_{t-1} + m{z}_t \odot \widetilde{m{h}_t}$

Comparison of Recurrent Units: What Should We Use? Hochschule



- LSTM and GRU outperform simple RNN units [Agg18]
- LSTM vs GRU inconclusive
 - roughly similar in performance
 - GRU is simpler and more efficient
 - GRU might generalize slightly better with less data due to less parameters
 - LSTM might be preferable with more data



Application Examples

Character-based Language Modeling with RNNs



- Great blog post by Andrej Karpathy: http://karpathy.github.io/2015/05/21/rnn-effectiveness/
- Character-level RNN for text generation trained on Shakespeare
- Example for generated text:

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.

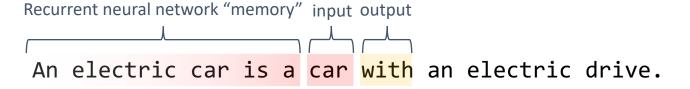
VIOLA:

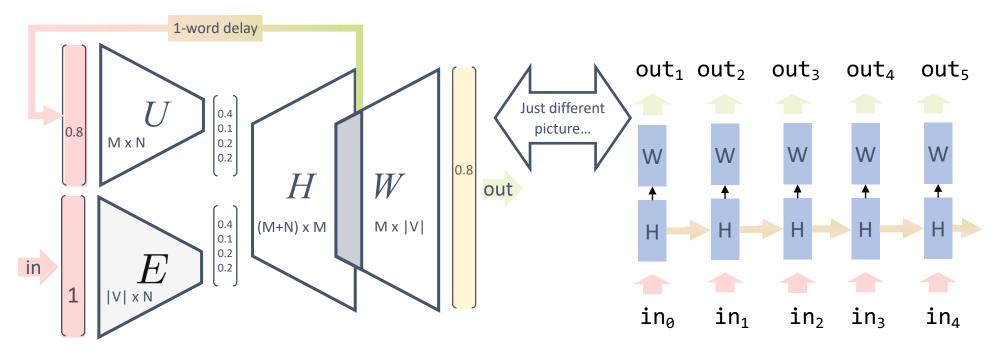
I'll drink it.

Experiments with LATEX, Linux code and Wikipedia entries in the blog post

Language Modeling – How Probable is the Next Word? Hochschule



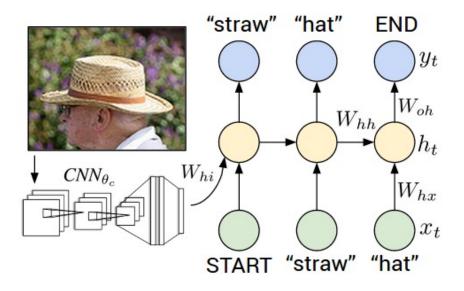




based on silde courtesy of Tobias Bocklet [Boc20]

Image Captioning





• Encoder:

- encode image using CNN
- similar to transfer-learning based on Imagenet trained network using the second to last layer

• Decoder:

- RNN models language
- START and END as special tokens

Andrej Karpathy Li Fei-Fei, Deep Visual-Semantic Alignments for Generating Image Descriptions, CVPR 2015 https://arxiv.org/abs/1412.2306

Composing Folk Music



- Music composition tackled frequently with RNNs (e.g. 1989 by Todd [Tod89], 2002 by Eck and Schmidhuber [Eck02], ...)
- Sturm and Ben-Tal [Stu15] use bigger/deeper networks to generate Folk music
- Character-level RNN using ABC format, including generating title
- Example:

 Bornity Horse



• Audio examples online, e.g., https://themachinefolksession.org/tune/31



Concluding Remarks

Summary



- Recurrent neural networks are able to directly model sequential algorithms
- Training via (truncated) backpropagation through time
- Simple units suffer extremely from exploding/vanishing gradients
- LSTM & GRU as improved RNN units that explicitly model "forgetting" and "remembering"
- Many more architectures we have not discussed
 - Memory Networks [Wes14, Suk15]
 - Neural Turing Machines [Gra14]
 - Neural GPUs [Kai16]
 - Transformer [Vas17]

Computational Power



- Recurrent networks are Turing complete!
 - not using the simple structures presented here, but with feedback loops in the network
 - proof by Siegelmann and Sontag 1992 [Sie92]
 - 886 neurons with rational weights are sufficient to build a universal neural network [Sie95]
 - this is a conservative estimate; there are probably smaller universal networks
 - this does not mean that we have an algorithm for training
- Neural Turing Machines, Neural GPUs, and Transformers can also be shown to be Turing complete [Per19]
- Simple Elman-Unit RNNs have at least the power of deterministic finite automata (DFAs) [Sie96]
- Allowing infinite precision, [Kor19]
 - RNNs with just one hidden layer and ReLU activation are at least as powerful as pushdown automata (PDAs)
 - GRUs are at least as powerful as DFAs

Links



RNN Folk Music

FolkRNN.org
MachineFolkSession.com
The Glass Herry Comment 14128

Further Reading

Character RNNs
CNNs for Machine Translation
Composing Music with RNNs

References



[Agg18]	C. Aggarwal. Neural Networks and Deep Learning, Springer 2018
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