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SCHOOL OF ENGINEERING

# Recurrent Neural Networks

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## Outline

Motivation

Simple Recurrent Networks

Long Short-Term Memory Units (LSTMs)

Gated Recurrent Units

Comparison of Simple RNN units, LSTM units and GRUs

Sampling strategies for RNNs

Examples

Summary



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# Motivation



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  - “Snapshots” often not informative (single word → translation?)
- **Temporal context** is important!

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  - **Not real-time!** (translation, ...)
- Better approach: Model sequential behavior within the architecture:  
→ **Recurrent neural networks (RNNs)**

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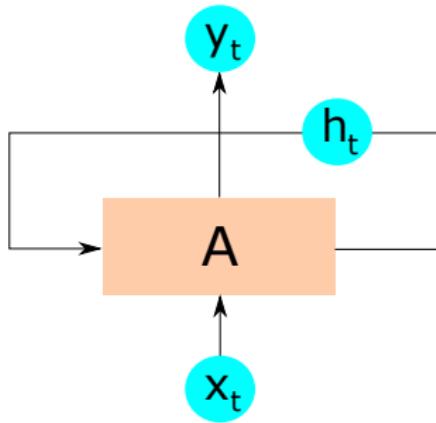
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# Simple Recurrent Networks



# Simple Recurrent Neural Networks



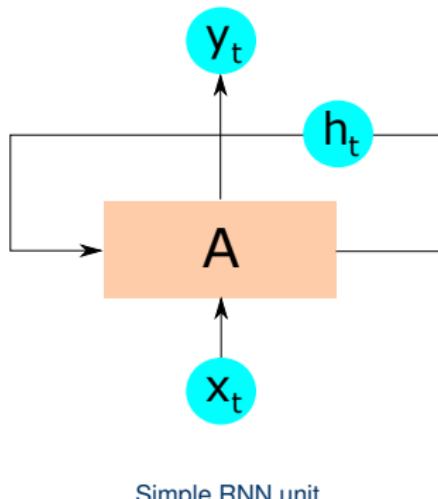
Simple RNN unit

- First models in 1970's [11] and early 1980's [10] (Hopfield Network)
- **Simple recurrent neural network** or **Elman network** introduced in *Finding Structure in Time* by Jeff Elman in 1990 [5]

# Difference between Recurrent Neural Networks and Feedforward Neural Networks

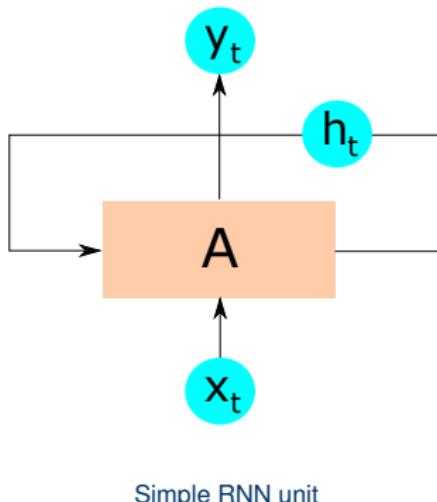
- Feedforward networks only **feed** information **forward**
- With recurrent neural networks, we can:
  - model loops
  - model memory and experience
  - learn sequential relationships
  - provide continuous predictions as data comes in → real-time

## Basic Structure of RNNs



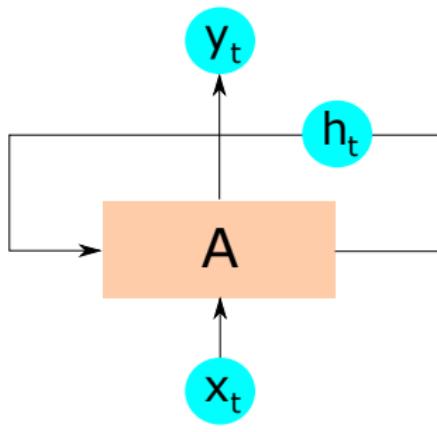
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## Basic Structure of RNNs



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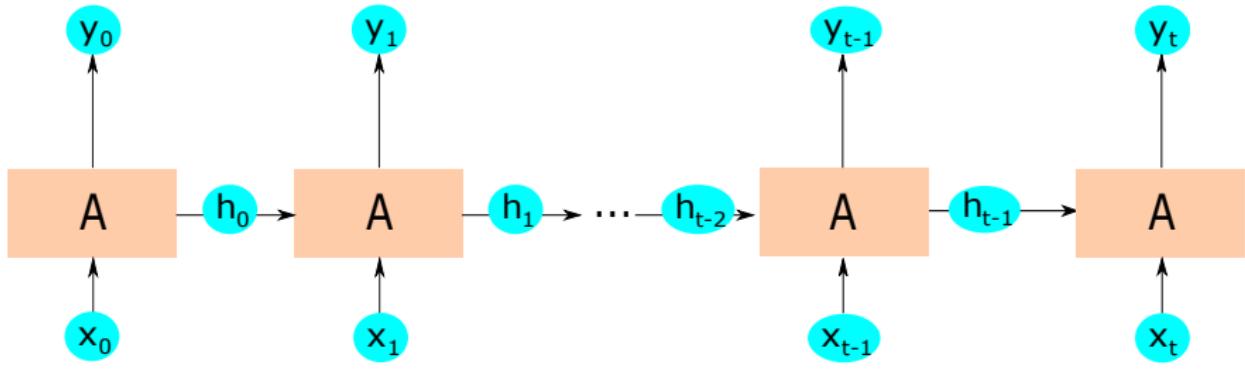
## Basic Structure of RNNs



- 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  $y_t$

## Basic Structure of RNNs (cont.)

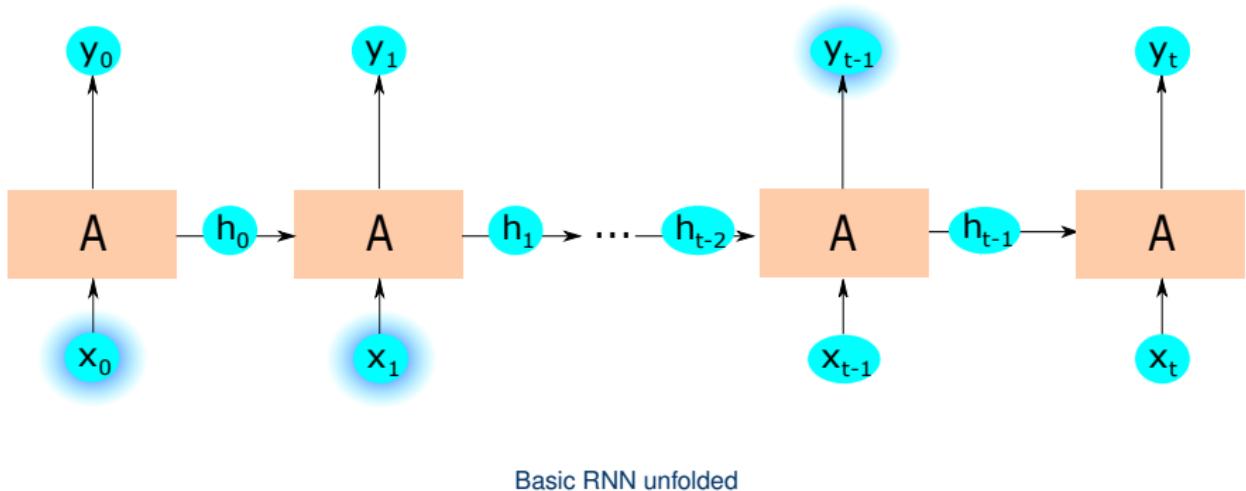
- “Unfolded” RNN unit: sequence of copies of the **same** unit (= same weights)
- Each unit passes hidden state as additional input to successor



Basic RNN unfolded

## Basic Structure of RNNs (cont.)

- “Unfolded” RNN unit: sequence of copies of the **same** unit (= same weights)
- Each unit passes hidden state as additional input to successor
- Previous input can influence current output

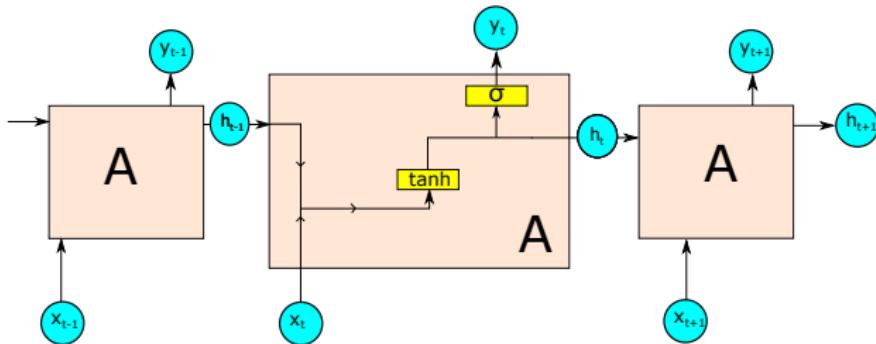


## Close-up of a basic RNN unit

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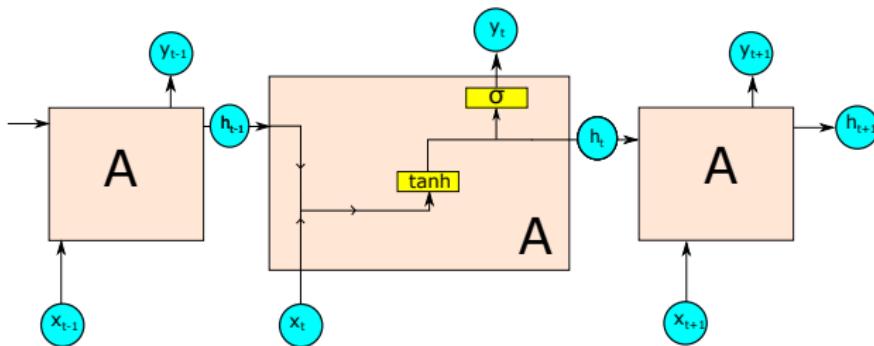


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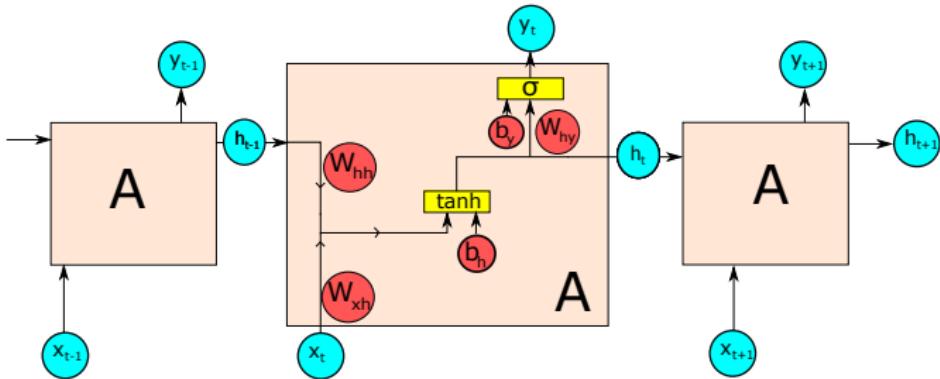
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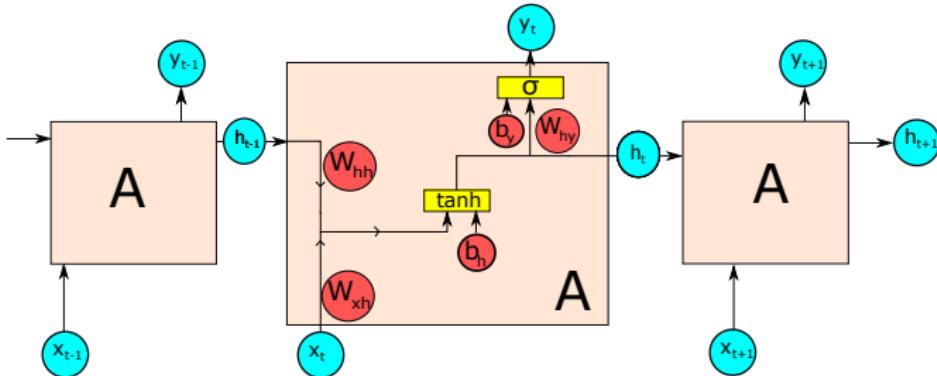
Two activation functions:

- $\tanh$ : Combination of previous state and current input
- $\sigma$ : Additional non-linearity for output

## Closer-up: How to update the hidden state?



## Closer-up: How to update the hidden state?



Update hidden state:

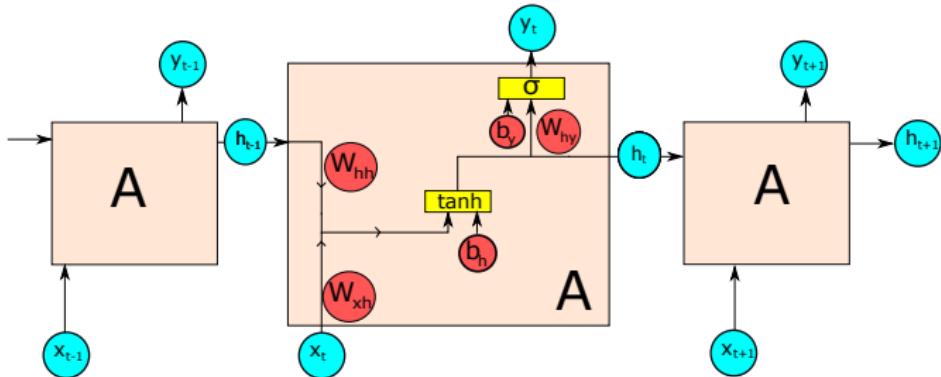
$$h_t = \tanh(W_{hh} \cdot h_{t-1} + W_{xh} \cdot x_t + b_h)$$

$W_{hh}$ : Weight matrix for previous hidden state  $h_{t-1}$

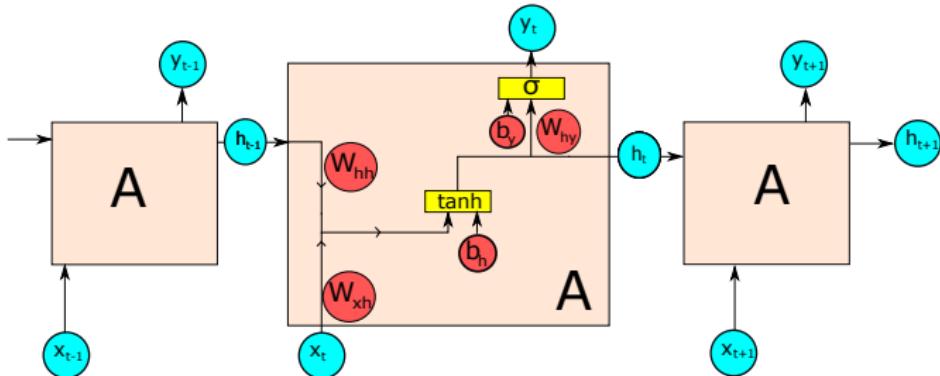
$W_{xh}$ : Weight matrix for current input  $x_t$

$b_h$ : Update bias

## Closer-up: How to compute the output?



## Closer-up: How to compute the output?



Output formula:

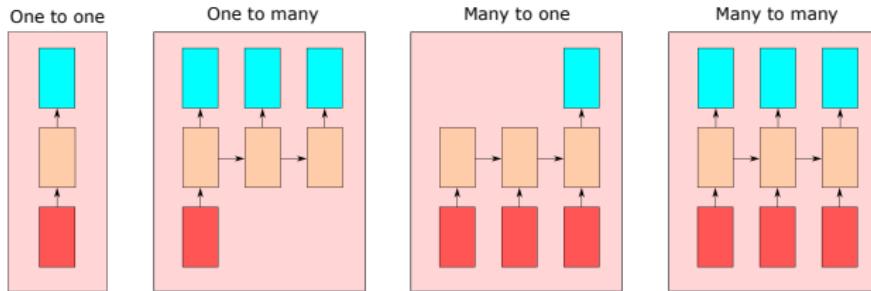
$$\mathbf{y}_t = \sigma (\mathbf{W}_{hy} \cdot \mathbf{h}_t + \mathbf{b}_y)$$

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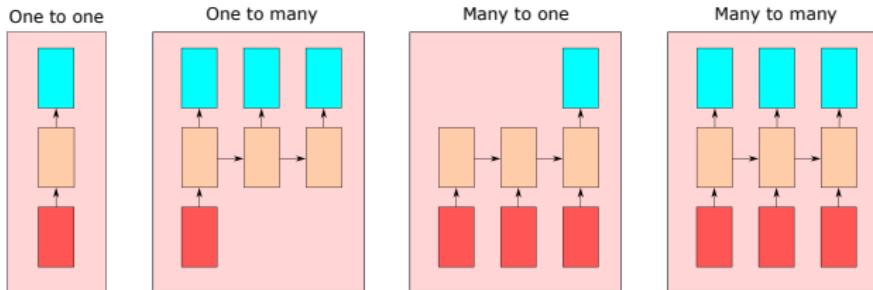
# RNN Basic Architectures

Type of sequential relationship  $\leftrightarrow$  architecture:



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Type of sequential relationship  $\leftrightarrow$  architecture:



- Examples:
  - One to one: Image classification (classic feed-forward)
  - One to many: Image captioning
  - Many to one: Sentiment analysis
  - Many to many: Video classification

## Deep RNNs

- So far, only one hidden layer

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- So far, only one hidden layer
- Recurring (ha!) motto:



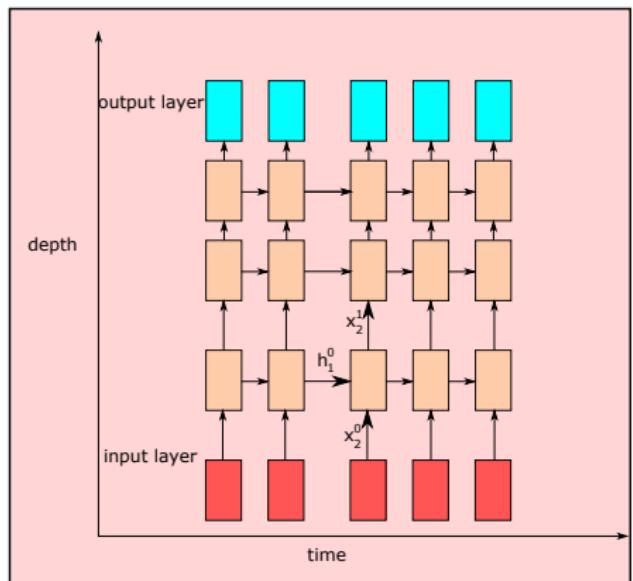
## Deep RNNs (cont.)

Similar to CNNs, stack multiple units for  
**deep RNNs**

$$\mathbf{h}_t^l = \tanh(\mathbf{W}_{xh}^l \cdot \mathbf{x}_t + \mathbf{W}_{hh}^l \cdot \mathbf{h}_{t-1}^l + \mathbf{b}^l)$$

*t*: time point

*l*: layer index



## Simple Example: Character Level Language Model

Task: Learn character probability distribution from input text

- Vocabulary of  $\{h, e, l, o\}$
- Characters encoded as one-hot vectors, e.g.,  $h = (1, 0, 0, 0)$

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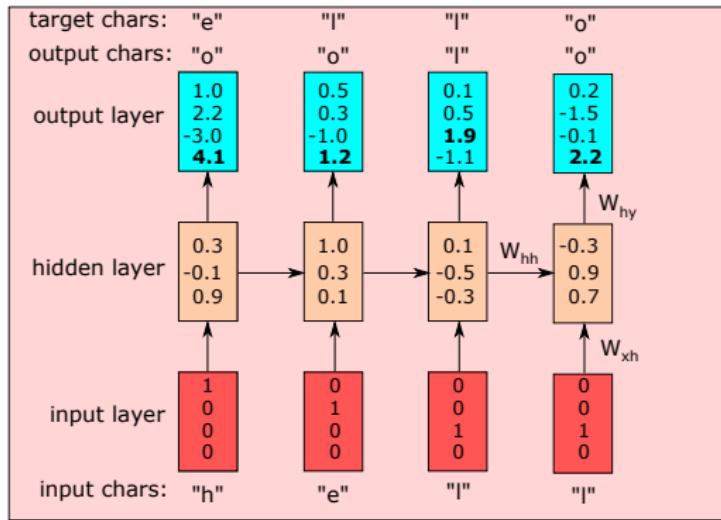
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- Train RNN on the sequence “hello”:  
Given ‘h’ as first input, the network should generate sequence “hello”
- Network needs to know **previous inputs** when presented with ‘l’:  
Do we need another ‘l’ or an ‘o’?

## Simple Example: Character Level Language Model (cont.)

Prediction with random initialization:

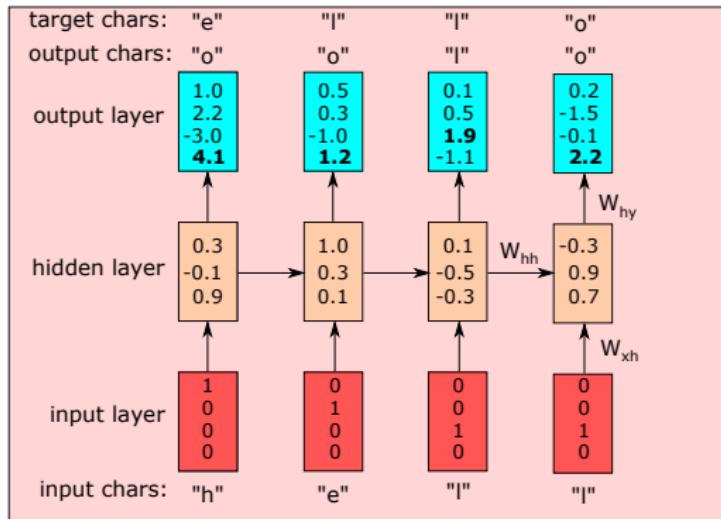


- Goal: Maximize prediction for correct component
- How can we now train this network?

Source: Adapted from <http://karpathy.github.io/2015/05/21/rnn-effectiveness>

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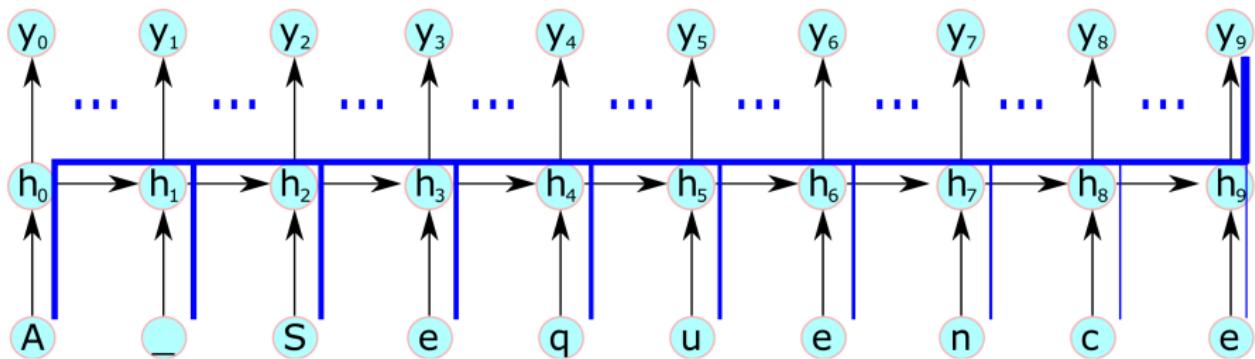
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- **Backpropagation through time (BPTT)**: train “unfolded” network

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# Backpropagation through Time (BPTT)

Concept: Train the unfolded network

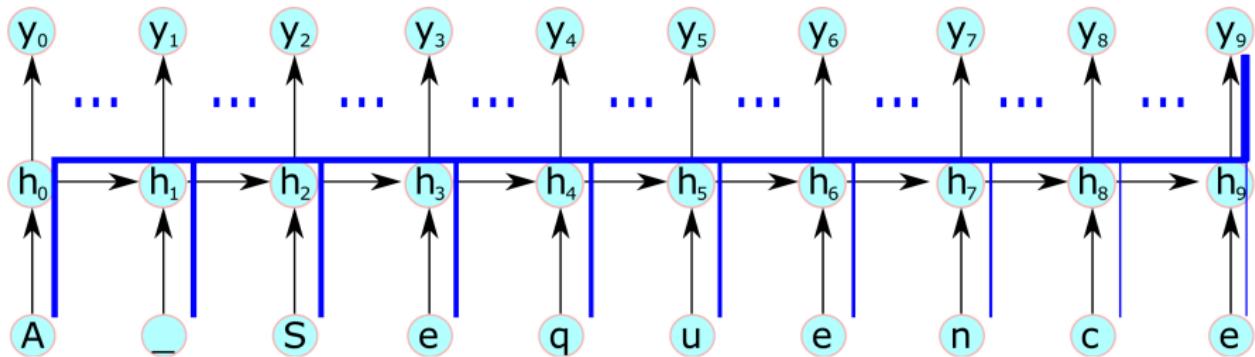
- Compute the forward pass for the full sequence → loss



# Backpropagation through Time (BPTT)

Concept: Train the unfolded network

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

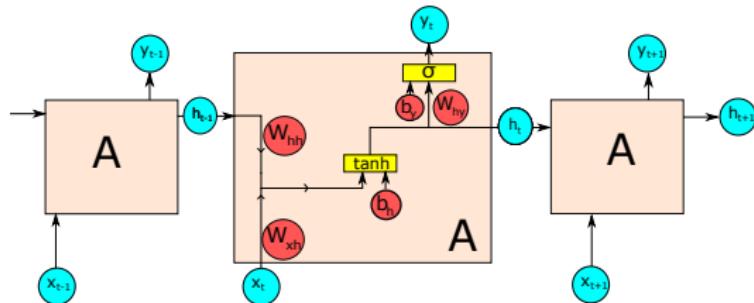


## Backpropagation through Time (BPTT) (cont.)

Forward pass: Computation of hidden states and output

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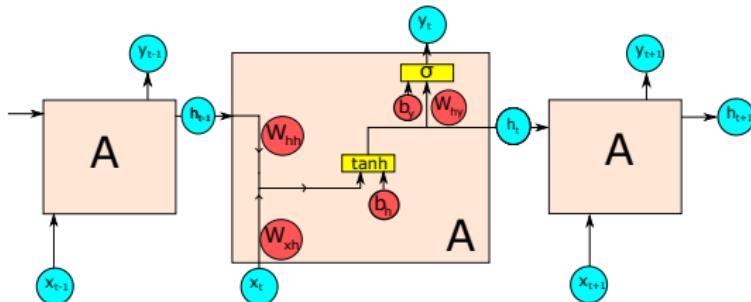


Input sequence:  $\mathbf{X} = \{x_1, x_2, \dots, x_T\}$

1: **for**  $t$  from 1 to  $T$  **do:**

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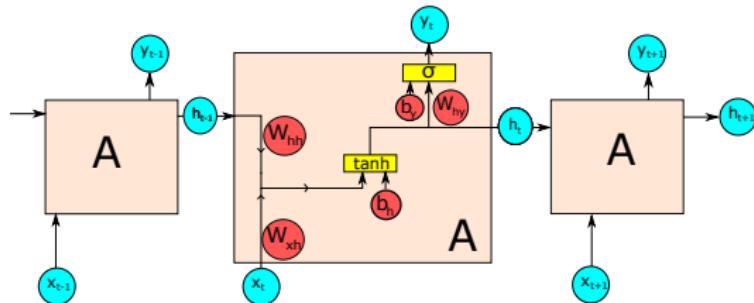


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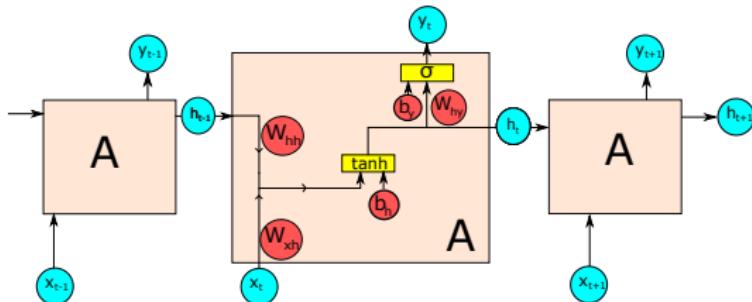


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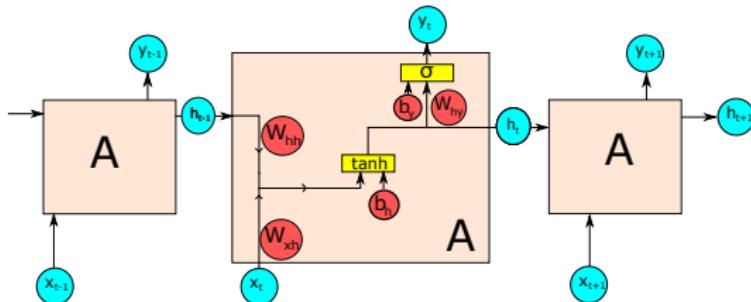


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- 5:    $\hat{\mathbf{y}}_t = \sigma(\mathbf{o}_t)$

## Backpropagation through Time (BPTT) (cont.)

- Loss function, e.g., cross-entropy loss:  $L(\hat{\mathbf{y}}, \mathbf{y}) = \sum_{t=1}^T L(\hat{\mathbf{y}}_t, \mathbf{y}_t)$ 
  - $\hat{\mathbf{y}}$ : predicted output
  - $\mathbf{y}$ : ground truth
- Compute gradient of the loss function

$$\nabla \theta = [\nabla \mathbf{W}_{xh}, \nabla \mathbf{W}_{hh}, \nabla \mathbf{W}_{hy}, \nabla \mathbf{b}_h, \nabla \mathbf{b}_y, \nabla \mathbf{h}_0]$$

- Update parameters using a learning rate  $\eta$

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- Question: How do we get these derivatives?
- Go “back in time” through the network

## Backpropagation through Time (BPTT) (cont.)

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

Reminder:  $\hat{\mathbf{y}}_t = \sigma(\mathbf{o}_t) = \sigma(\mathbf{W}_{hy} \cdot \mathbf{h}_t + \mathbf{b}_y)$

$$\nabla \mathbf{o}_t = \sigma'(\mathbf{o}_t) \cdot \frac{\partial L}{\partial \hat{\mathbf{y}}_t} (\hat{\mathbf{y}}_t, \mathbf{y}_t)$$

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- Currently, gradient depends on  $t$ . How do we get the gradient for the sequence?
- Unrolled unit is a network with **shared weights**
- For each gradient, simply **sum over all time-steps**  $t = \{1, \dots, T\}$ !

## Backpropagation through Time (BPTT) (cont.)

- BPTT: One update requires backpropagation through a **complete sequence**  
→ Single parameter update is very expensive!

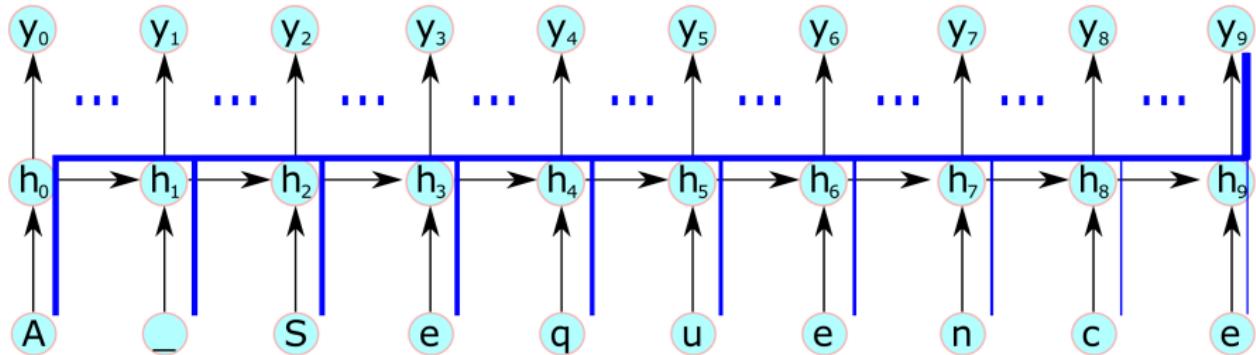
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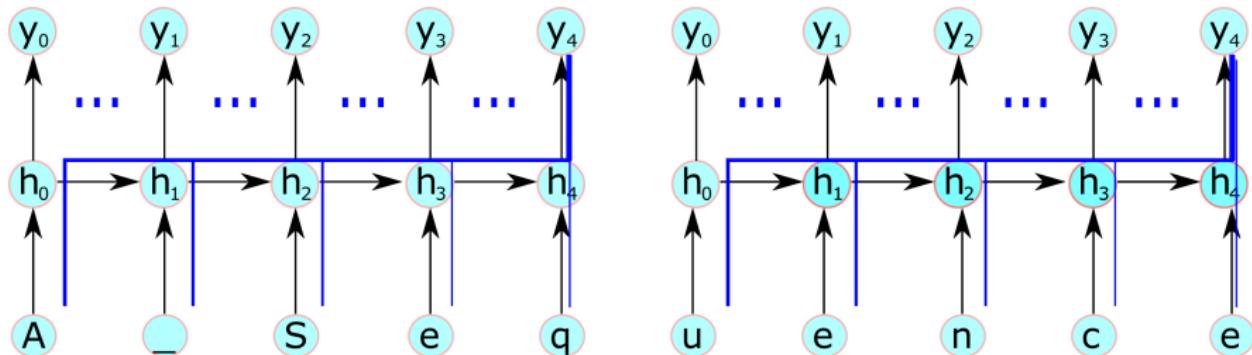
Naive Solution:

- Split long sequences into batches of smaller sequences

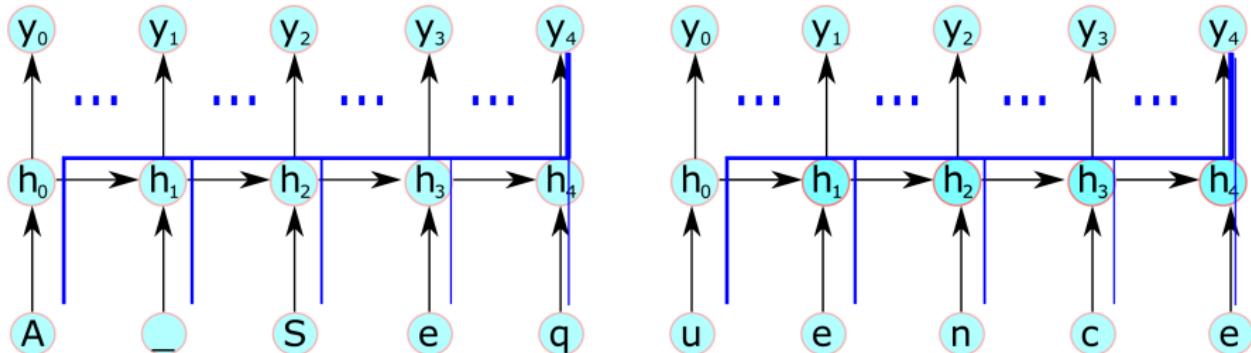
## Normal BPTT



## Naive BPTT

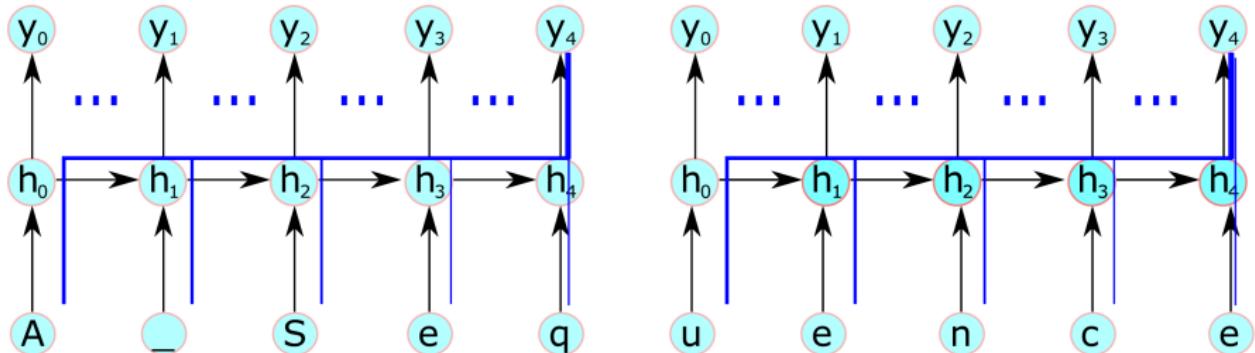


## Naive BPTT



- Might work ok in practice, but blind to long-term dependencies
- Can we do better? Yes!

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- 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

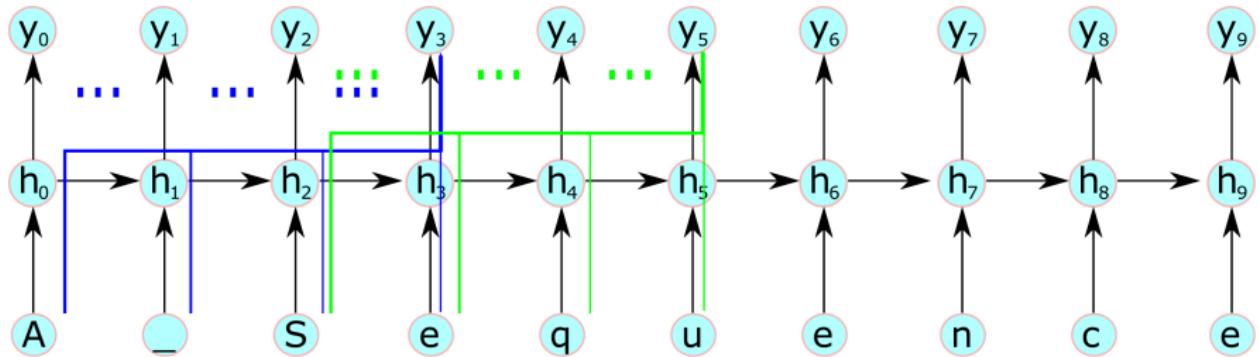
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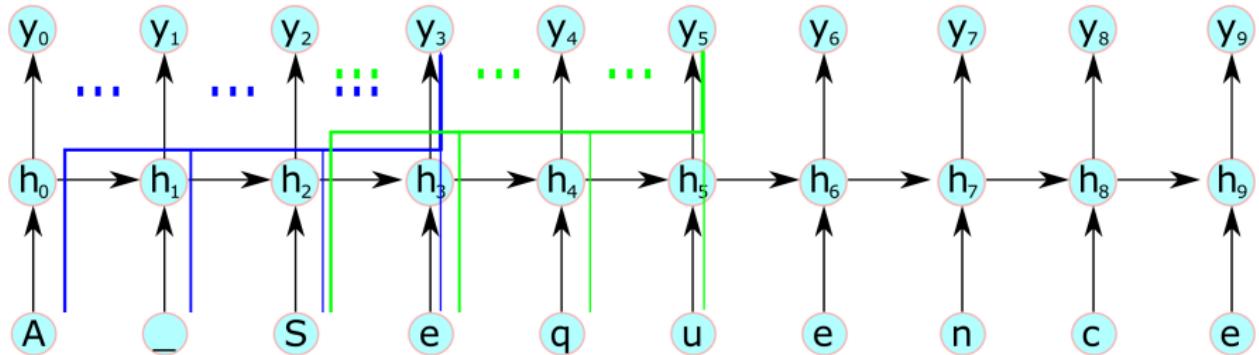
Algorithm:

- 1: **for**  $t$  **from** 1 **to**  $T$  **do**:
- 2:   Run RNN for one step, computing  $h_t$  and  $y_t$
- 3:   **if**  $t \bmod k_1 == 0$ :
- 4:     Run BPTT from  $t$  down to  $t - k_2$

## Truncated BPTT



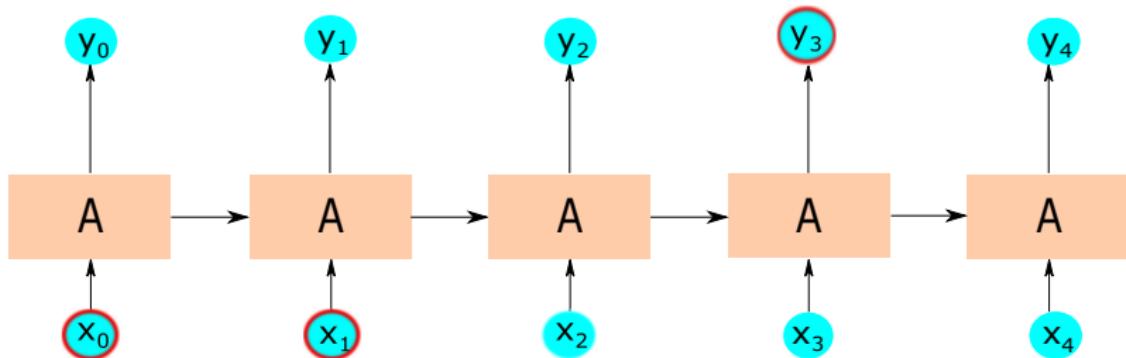
## Truncated BPTT



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

## The Long-Term Dependency Problem with Basic RNNs

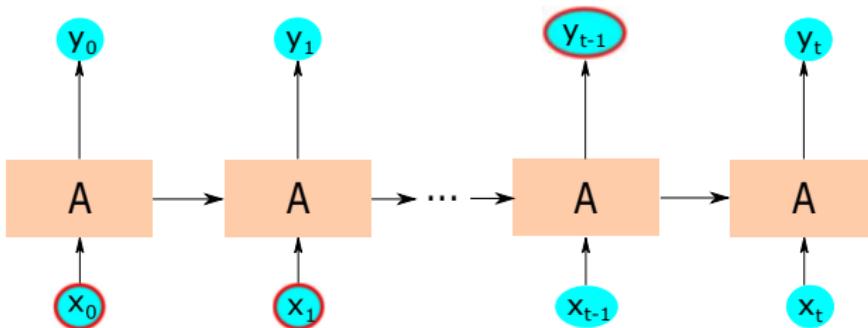
- Short term dependencies work fine
- Example: Predict next word in "the clouds are in the *sky*"



- Contextual information nearby → can be encoded in hidden state easily

## The Long-Term Dependency Problem with Basic RNNs (cont.)

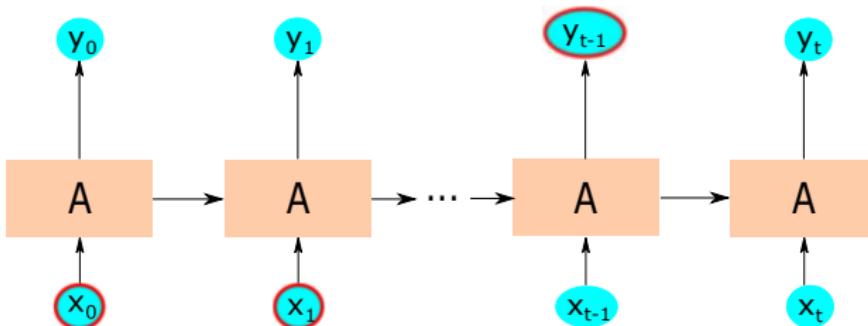
- Harder to connect relevant past and present inputs for longer time spans
- Example: Predict next word in "I grew up in Germany . . . I speak fluent German"



- Contextual information far away

## The Long-Term Dependency Problem with Basic RNNs (cont.)

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- Contextual information far away
- **Why** does this make a difference?

## The Long-Term Dependency Problem with Basic RNNs (cont.)

Old acquaintances: vanishing and exploding gradients

- Layers and time steps of deep RNNs are related through multiplication
- Gradients prone to vanishing or exploding (Hochreiter and Schmidhuber [12])

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# Long Short-Term Memory Units (LSTMs)



## Background

- **Long Short-Term Memory Units (LSTMs)**  
introduced by Hochreiter & Schmidhuber in 1997
- 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**

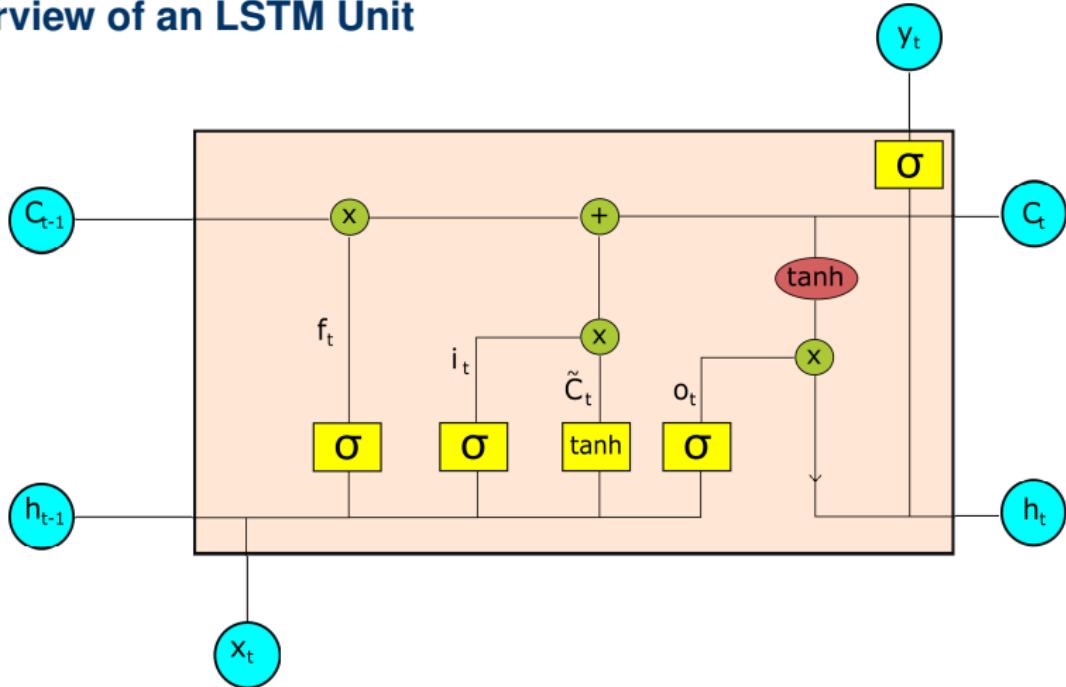


Sepp Hochreiter



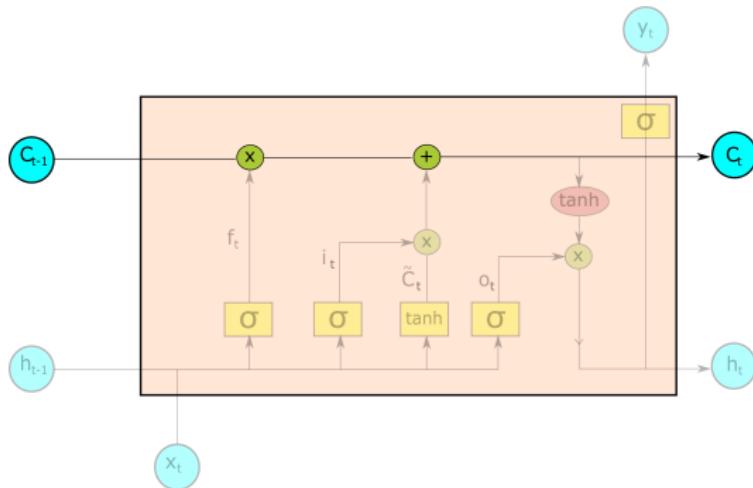
Jürgen Schmidhuber

## Overview of an LSTM Unit



## LSTM Cell State

- $C_t$ : **Cell state** after time point  $t$
- Undergoes only **linear changes**: no activation function!
- $C_t$  can flow through a unit unchanged → cell state can be constant for multiple time steps



## LSTM unit workflow

Elements of LSTM units:

- Input  $\mathbf{x}_t$
- Hidden state  $\mathbf{h}_{t-1}/\mathbf{h}_t$
- Cell state  $\mathbf{C}_{t-1}/\mathbf{C}_t$
- Output  $\mathbf{y}_t$

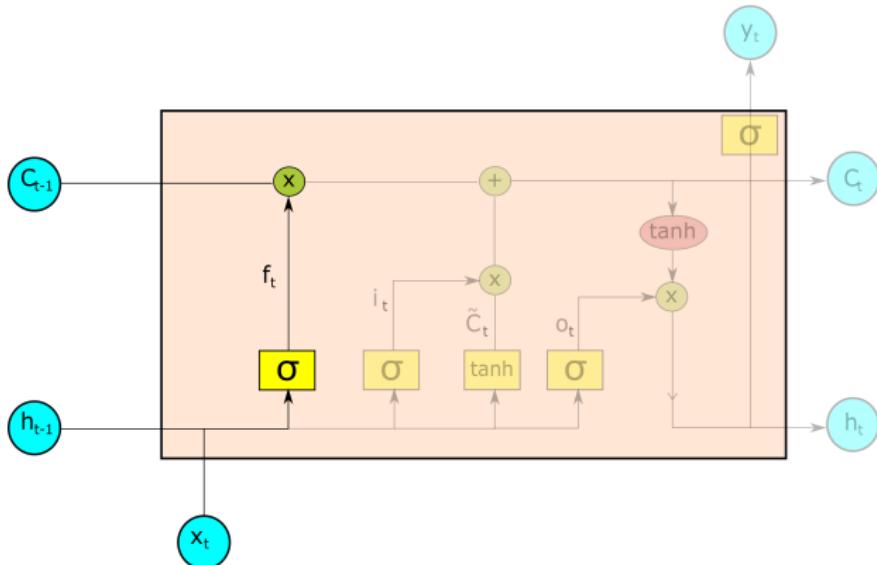
Update of internal states in multiple steps:

- 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

## Forget Gate: Forgetting Old Information

- Key idea: “forgetting” and “memorizing” information in separate steps
- $f_t$  controls how much of the previous cell state is forgotten:

$$f_t = \sigma(\mathbf{W}_f \cdot [\mathbf{h}_{t-1}, \mathbf{x}_t] + \mathbf{b}_f)$$

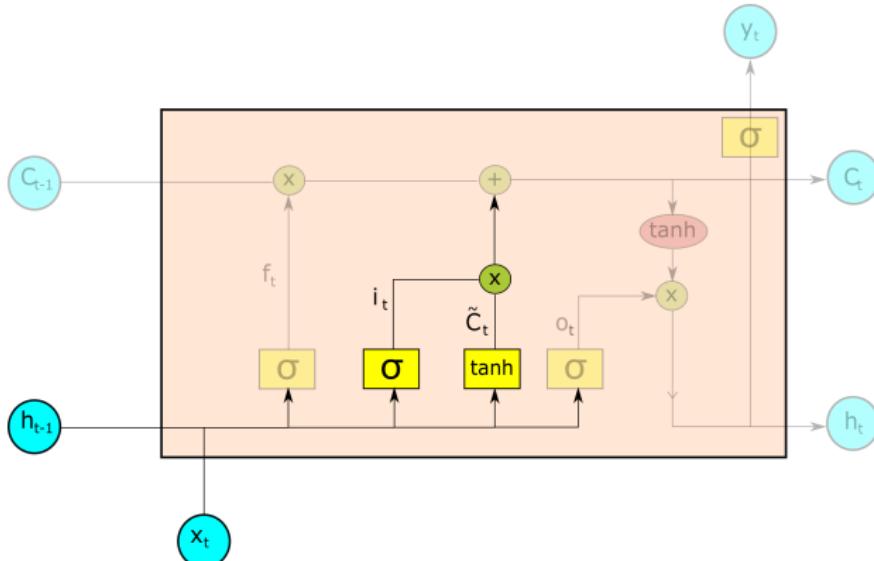


## Input Gate: Deciding on New Input

Combination of input and hidden state on two paths:

$$i_t = \sigma (\mathbf{W}_i \cdot [\mathbf{h}_{t-1}, \mathbf{x}_t] + \mathbf{b}_i)$$

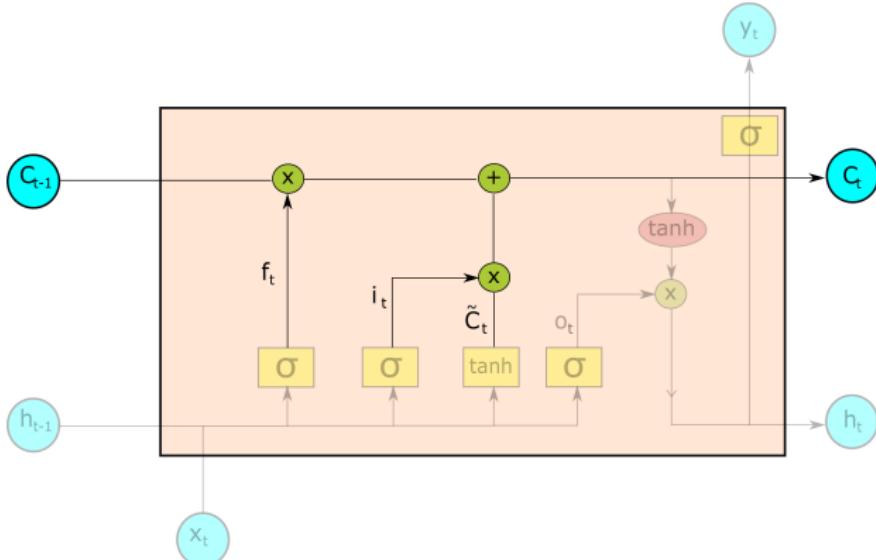
$$\tilde{\mathbf{c}}_t = \tanh (\mathbf{W}_C \cdot [\mathbf{h}_{t-1}, \mathbf{x}_t] + \mathbf{b}_C)$$



## Updating the Cell State

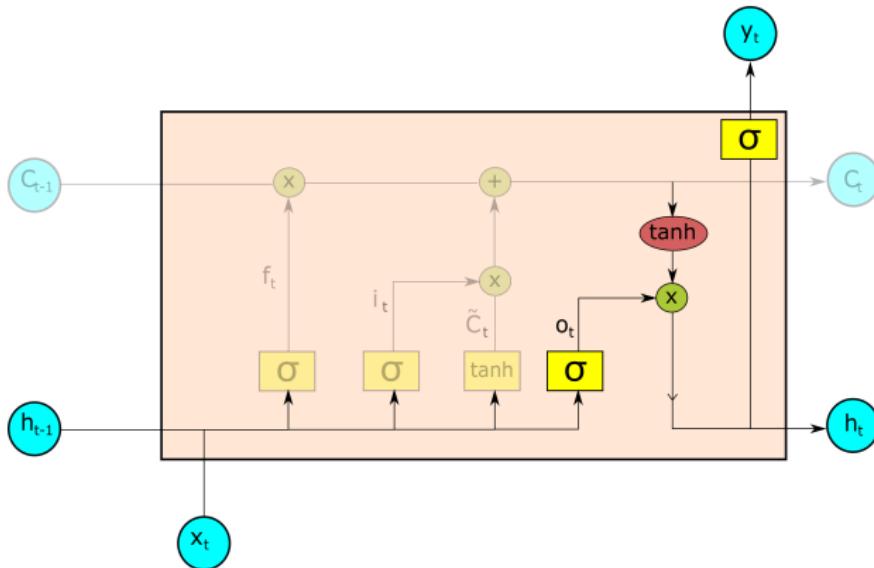
- New cell state: Sum of “remaining information” from  $\mathbf{C}_{t-1}$  and new information from input and hidden state ( $\odot$ : element-wise multiplication)

$$\mathbf{C}_t = \mathbf{f}_t \odot \mathbf{C}_{t-1} + \mathbf{i}_t \odot \tilde{\mathbf{C}}_t$$



## Updating the Hidden State and Computing the Output

- Important: Cell state and hidden state are updated **separately**
- Output  $y_t$  directly depends on the hidden state  $h_t$

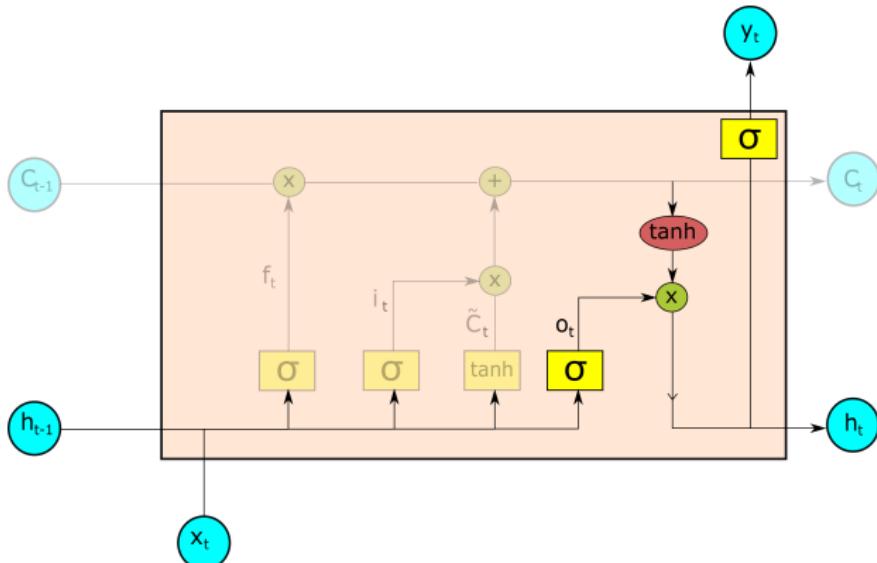


## Updating the Hidden State and Computing the Output (cont.)

$$\mathbf{o}_t = \sigma(\mathbf{W}_o[\mathbf{h}_{t-1}, \mathbf{x}_t] + \mathbf{b}_o)$$

$$\mathbf{h}_t = \mathbf{o}_t \odot \tanh(\mathbf{C}_t)$$

$$\mathbf{y}_t = \sigma(\mathbf{h}_t)$$





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# Gated Recurrent Units



## Motivation

- LSTM great idea, but many parameters and difficult to train

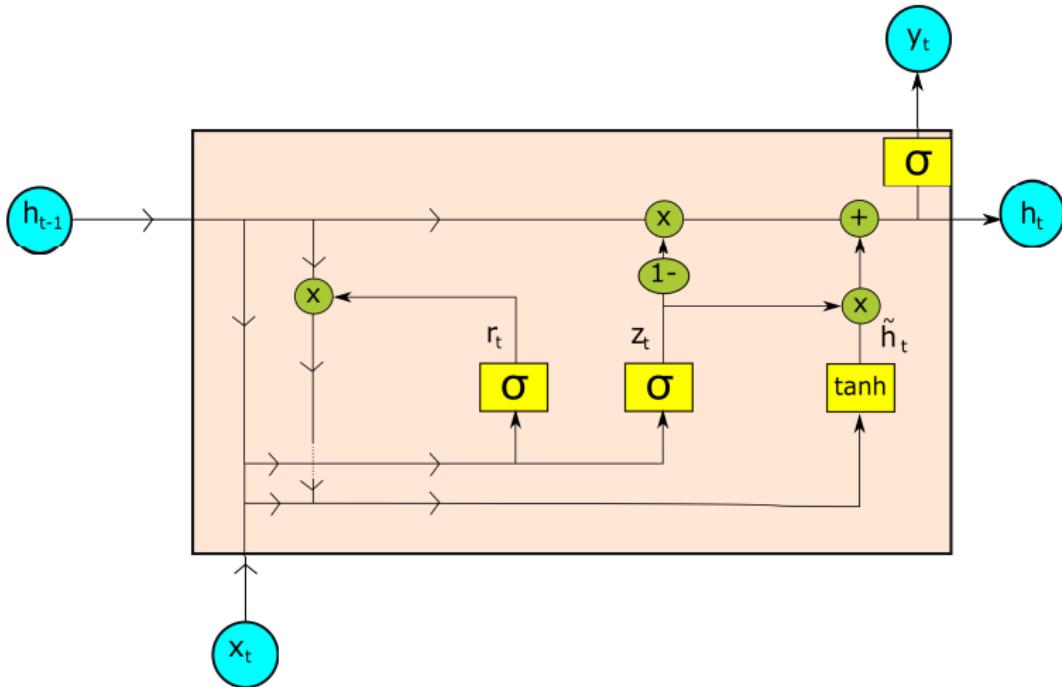
## Motivation

- 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
- Variant of the LSTM unit, but simpler and fewer parameters



Kyunghyun Cho

## Structure of a GRU cell



## GRU workflow

- Concept from LSTM: More control over hidden state/memory → **gates**

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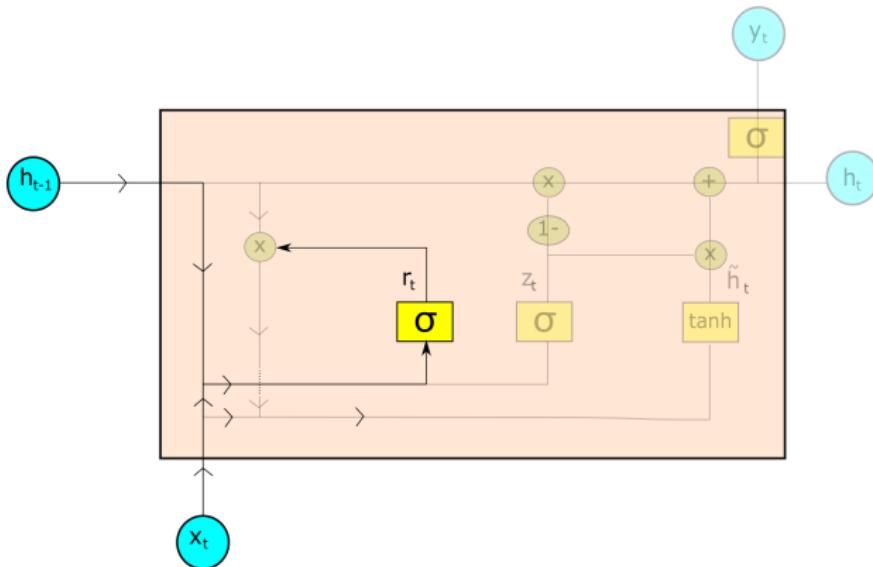
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## Reset gate

- Determines the influence of the previous hidden state

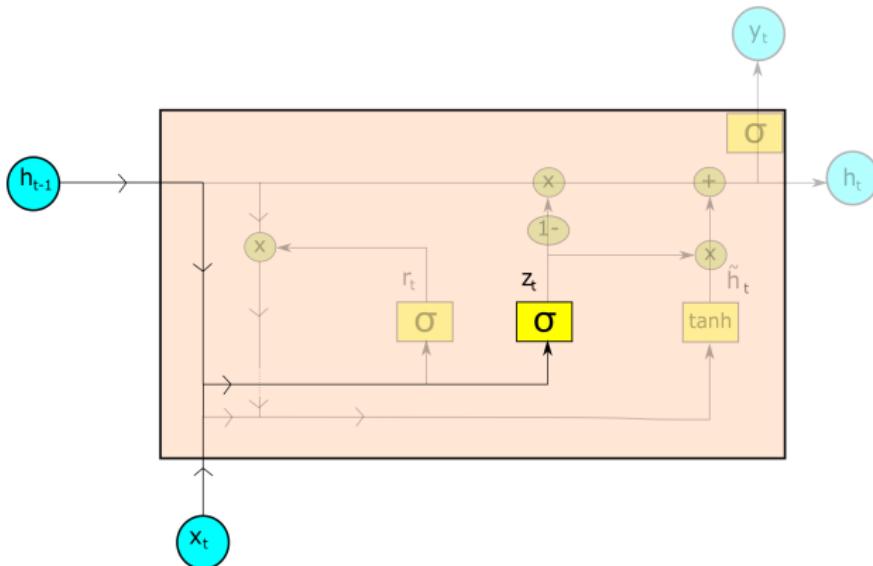
$$r_t = \sigma(\mathbf{W}_r \cdot [\mathbf{h}_{t-1}, \mathbf{x}_t] + \mathbf{b}_r)$$



## Update Gate

- Determines the influence of an “update proposal” on the new hidden state

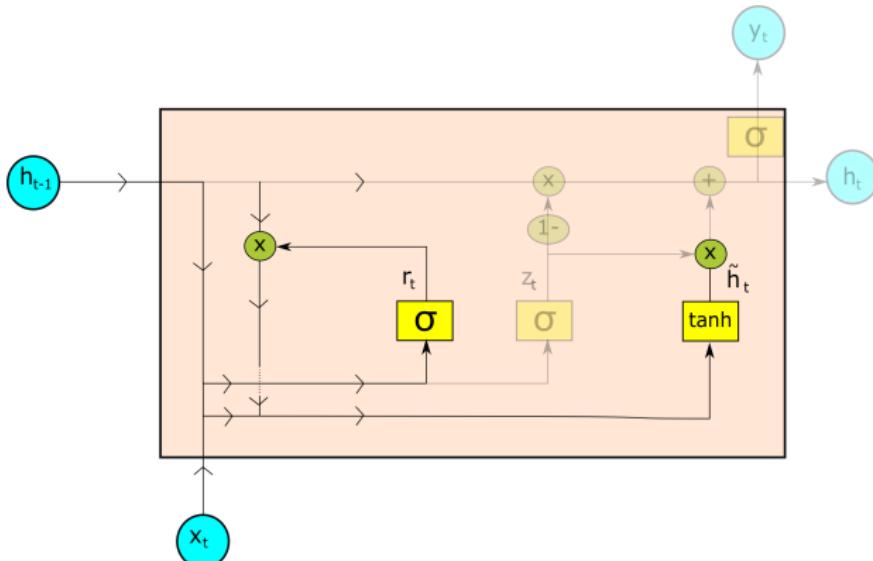
$$\mathbf{z}_t = \sigma (\mathbf{W}_z \cdot [\mathbf{h}_{t-1}, \mathbf{x}_t] + \mathbf{b}_z)$$



## Proposing an Update

- Combination of input and “reset” hidden state.
- If  $r_t$  is close to 0 → low influence of previous hidden state

$$\tilde{h}_t = \tanh(\mathbf{W}_h \cdot [r_t \odot h_{t-1}, x_t] + \mathbf{b}_h)$$

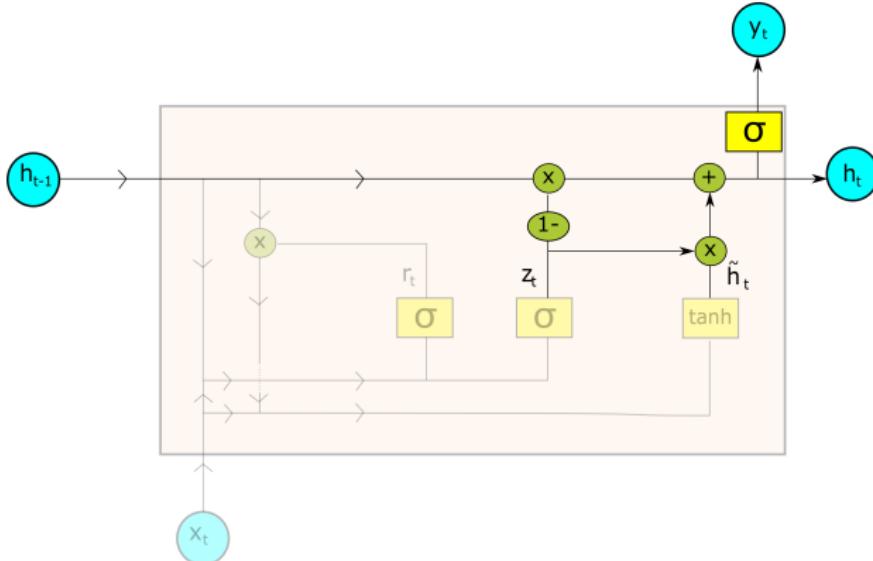


## Finally: Computing the Updated Hidden State

- **Update gate** controls combination of old state and proposed update

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

- Node output:  $\hat{\mathbf{y}}_t = \sigma(\mathbf{h}_t)$



## Remarks

- Add ("+") essential for preservation of error in backpropagation
- Gates allow capturing diverse time scales and remote dependencies

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- Units learning **long-term** dependencies have restrictive update gates  
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- Gates have varying "rhythm" depending on the type of information



**FAU**

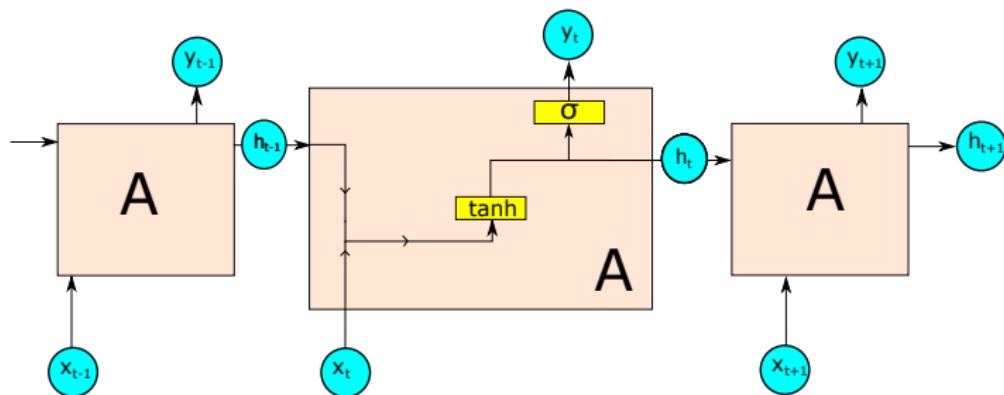
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# Comparison of Simple RNN units, LSTM units and GRUs

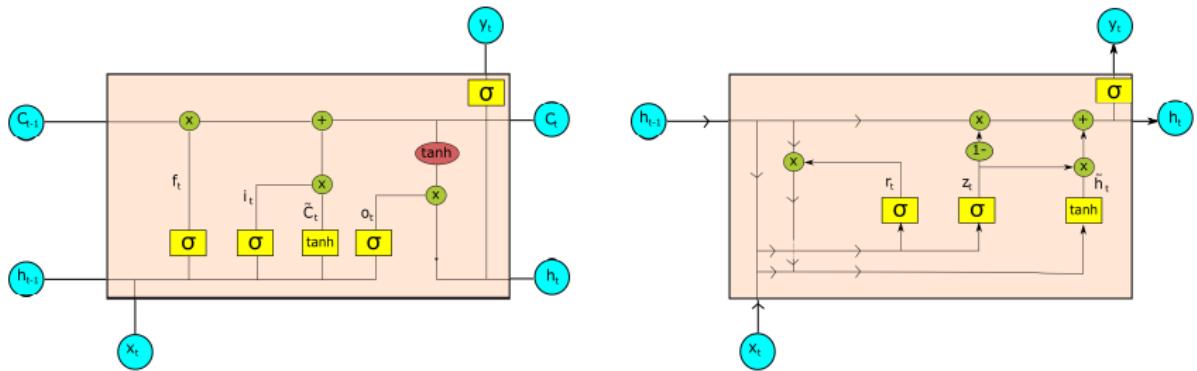


## Recap: Simple RNNs

- 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



# Advanced structures: LSTM and GRU



## Advanced structures: LSTM and GRU

### Similarities

- Control information flow via gates
- Ability to capture dependencies of different time scales
- Additive calculation of state preserves error during backpropagation  
→ more efficient training possible

## Advanced structures: 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: $C_t = f_t \odot C_{t-1} + i_t \odot \tilde{C}_t$ → New memory content independent of current memory	Common update gate: $h_t = (1 - z_t) \odot h_{t-1} + z_t \odot \tilde{h}_t$ → New memory content depends on current memory

## Comparison of Recurrent Units: So what should we use?

Empirical Evaluation of Gated Recurrent Neural Networks on Sequence Modeling [3]

- Comparison of simple RNN, LSTM and GRU networks
- Tasks: Polyphonic music modeling and speech signal modeling

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Empirical Evaluation of Gated Recurrent Neural Networks on Sequence Modeling [3]

- Comparison of simple RNN, LSTM and GRU networks
- Tasks: Polyphonic music modeling and speech signal modeling
- Gated recurrent units clearly outperformed regular recurrent unit
- Comparison between GRU and LSTM not conclusive, similar performance



**FAU**

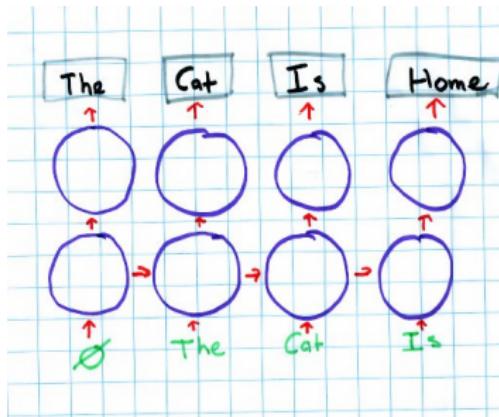
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# Sampling strategies for RNNs



# Why Sampling Strategies?

- RNN can generate sequences (words/notes/...)
- RNN actually computes **probability distribution** of the next element
- Question: How do we sample this distribution?



Ideal sequence - or?

Source: <https://medium.com/machine-learning-at-petiteprogrammer/sampling-strategies-for-recurrent-neural-networks-9aea02a6616f>

## Greedy search

- **Concept:** At each point, pick the most likely element
- Generates exactly one sample sequence per experiment

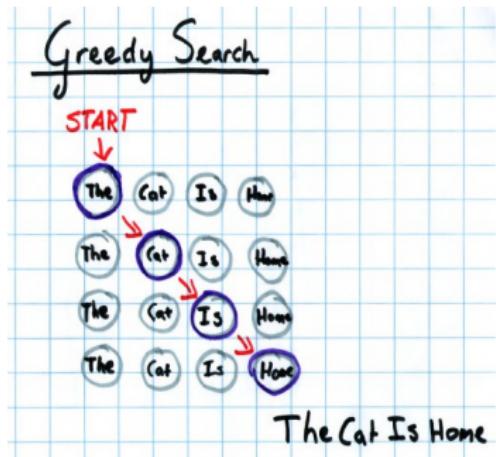


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  - Example: “The” may be most likely word after “The Cat” → “The Cat The”
  - Cannot detect that “The Cat Is Home” has a higher total probability



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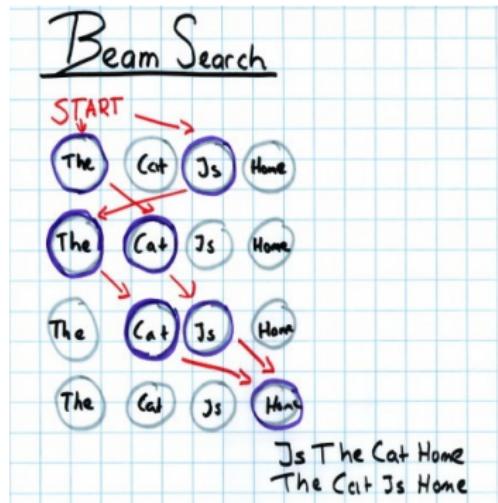
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  - Example: “The” may be most likely word after “The Cat” → “The Cat The”
  - Cannot detect that “The Cat Is Home” has a higher total probability
- Tends to repeat sequences of frequent words, e.g., “and”, “the”, “some” in speech



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# Beam Search

- **Concept:** Select  $k$  most likely words ( $k$ : beam width or size)

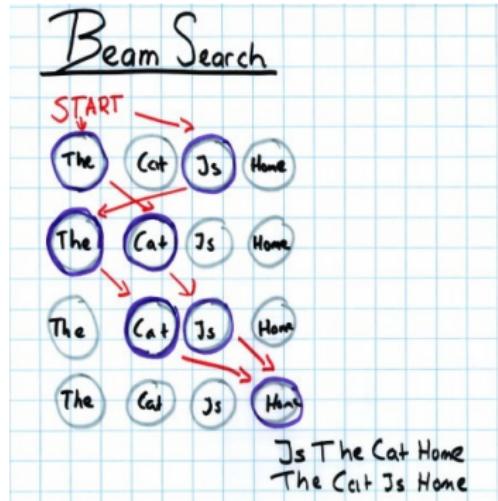


Beam Search with  $k = 2$

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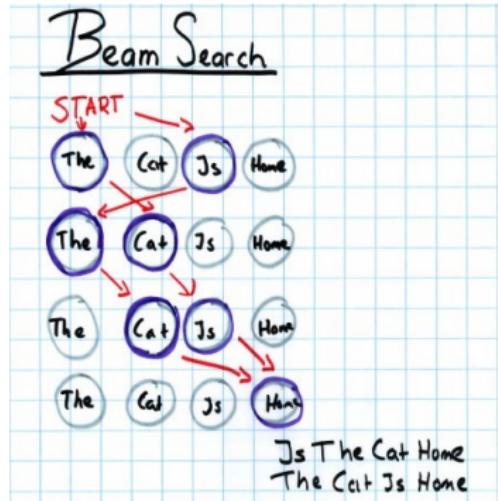


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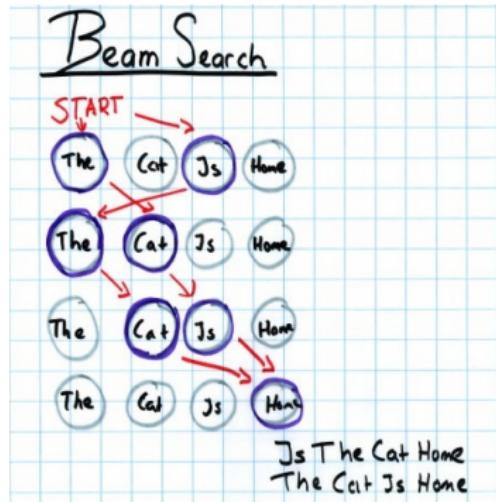


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- Iterate until end of sequence
- Can generate  $k$  sequences in one go  
→ usually better than greedy search



Beam Search with  $k = 2$

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# Random Sampling

- **Idea:** Sample next word according to output probability distribution



Random Sampling

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# Random Sampling

- **Idea:** Sample next word according to output probability distribution
- Example: If “The” has output probability 0.8, it is sampled 8 out of 10 times as the next word
- Creates very diverse results, can look too random
- To reduce randomness, increase/decrease probability of probable/less probable words  
 → **Temperature sampling**

$$\tilde{p}_i = f_\tau(p_i) = \frac{p_i^{1/\tau}}{\sum_j p_j^{1/\tau}}$$

$p_i$ : output probability for word  $i$ ,  $\tau$ : temperature



Random Sampling



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# Examples



## Character-based Language Modeling with RNNs

- Great blog post ([link](#)) by Andrew Karpathy (now director of AI at Tesla)
- Character-level RNN for text generation trained on Shakespeare

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- 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 strain 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  $\text{\LaTeX}$ , Linux code and Wikipedia entries in the blog post

## Composing Folk Music

- Music composition tackled frequently with RNNs (e.g. 1989 by Todd [16], 2002 by Eck and Schmidhuber [4], ...)
- Sturm and Ben-Tal [14] use bigger/deeper networks to generate Folk music
- Character-level RNN using ABC format, including generating title

# Composing Folk Music

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- Character-level RNN using ABC format, including generating title
- Example:

Bornity Horse



The image shows a musical score for a folk song titled "Bornity Horse". The score consists of two staves of music. The top staff uses a treble clef and a common time signature, featuring a sequence of eighth-note patterns. The bottom staff also uses a treble clef and common time, showing a different pattern of eighth notes. The music is divided into measures by vertical bar lines. Some measures have numerical superscripts above them: '3' over the first measure of the top staff, and '1' and '2' over the first two measures of the bottom staff. The score is presented in a clean, professional style with clear lines and standard musical notation.

- Audio examples online, e.g., [click here](#)

Source: [14]

## RNNs for Non-Sequencial Tasks

- RNNs can also be used for stationary inputs, e.g., image generation
- Idea: Model progress from rough sketch to final image

Source: Adapted from [8]

## RNNs for Non-Sequencial Tasks

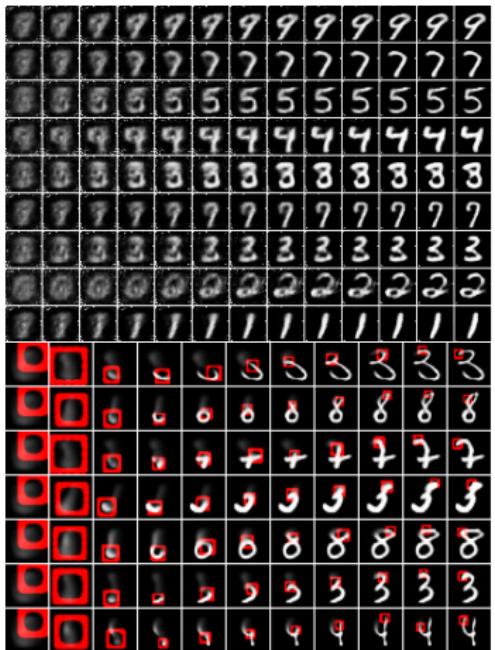
- RNNs can also be used for stationary inputs, e.g., image generation
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- Gregor et al. [8]: Drawing numbers  
→ from blurry to sharp



Source: Adapted from [8]

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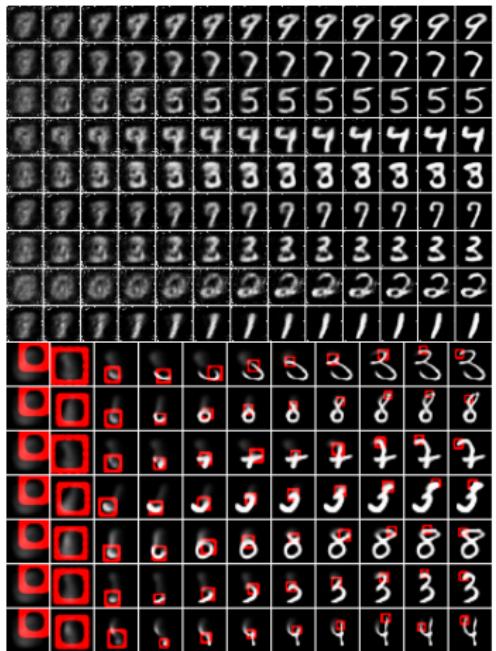
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- Additional “attention mechanism” telling the network where to look → like brushstrokes
- Uses (variational) **autoencoder** → Lecture 10: Unsupervised Deep Learning



Source: Adapted from [8]



**FAU**

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# Summary



## 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”

## Summary

- Recurrent neural networks are able to directly model sequential algorithms
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We haven't talked about:

- Memory networks [15], [19]
- Neural turing machines [7]
- Only grazed: Attention + recurrent networks [1], [13]
- ...

**NEXT TIME  
ON DEEP LEARNING**

# Coming Up: Visualization

Visualization of ...

- network architecture
- the training process
- the “inner workings” of a network
- neural network “art”

## Comprehensive Questions

- What is the strength of RNNs compared to feed-forward networks?
- What role does the hidden state play in RNNs?
- How do you train RNNs? What are the challenges?
- What is the main idea behind LSTMs and what is the main difference to simple RNN units?
- What are the differences between LSTMs and GRUs?
- In which scenarios would LSTMs be beneficial compared to GRUs?
- Name three applications where many-to-one and one-to-many RNNs would be beneficial.

## Further Reading

- Again, the great blog post by Andrew Karpathy on RNNs:  
[The Unreasonable Effectiveness of Recurrent Neural Networks](#)
- Blog post by facebook on CNNs for machine translation:  
[A novel approach to machine translation](#)
- Blog post on music generation:  
[Composing Music With Recurrent Neural Networks](#)



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