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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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 - Sensor data (speed, temperature, energy consumption, ...)

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

Motivation (cont.)

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 - Inefficient memory usage
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 - Difference between spatial and temporal dimensions?
 - **Not real-time!** (translation, ...)
- Better approach: Model sequential behavior within the architecture:
→ **Recurrent neural networks (RNNs)**

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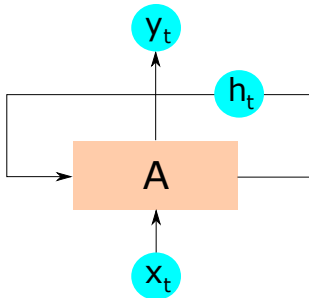


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Simple Recurrent Networks



Simple Recurrent Neural Networks



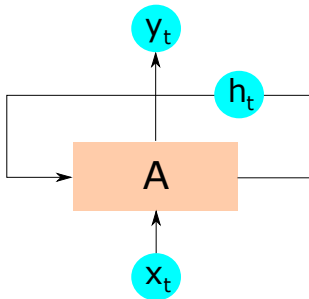
Simple RNN unit

- 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

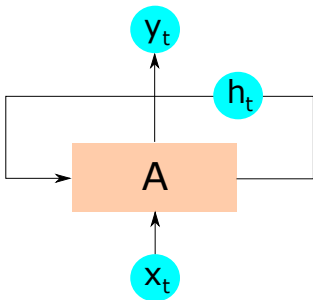
Basic Structure of RNNs



Simple RNN unit

- Current input x_t multiplied by weight

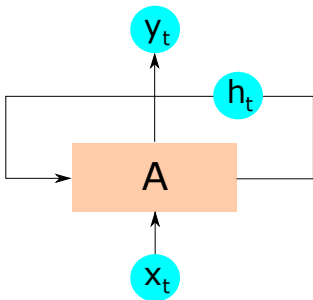
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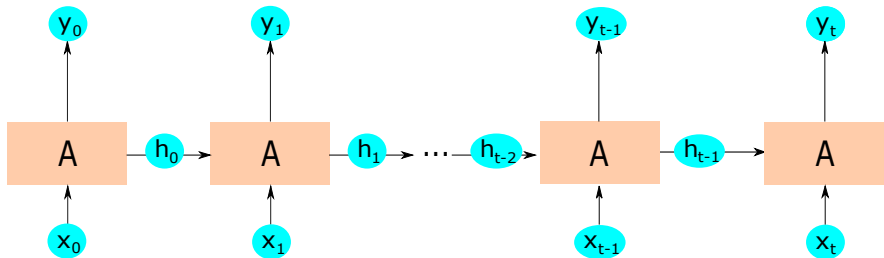


Simple RNN unit

- 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

Basic Structure of RNNs (cont.)

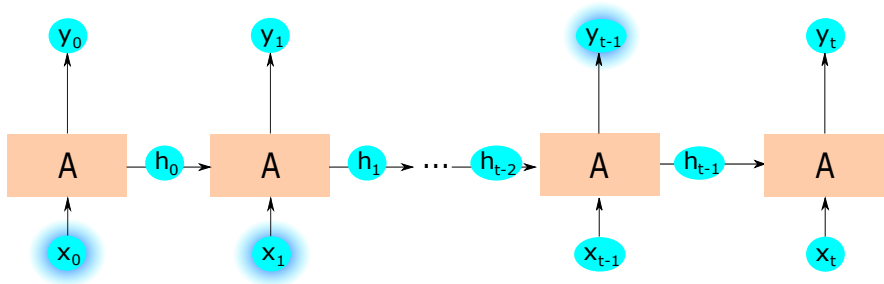
- “Unfolded” RNN unit: sequence of copies of the **same** unit (= same weights)
- Each unit passes hidden state as additional input to successor



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



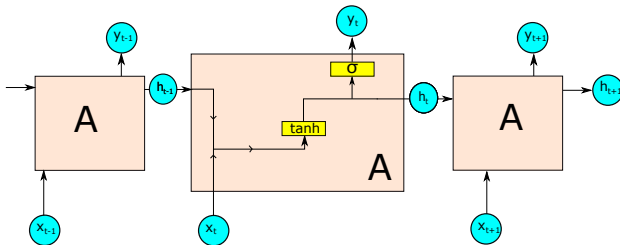
Basic RNN unfolded

Close-up of a basic RNN unit

- Question 1: How do we update the hidden state?
- Question 2: How do we combine input and hidden state to compute output?

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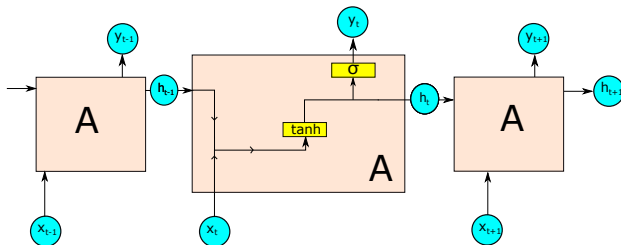


Two activation functions:

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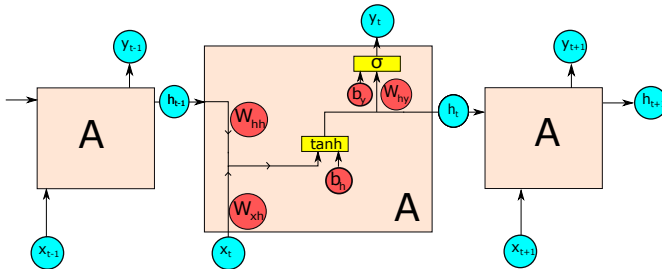
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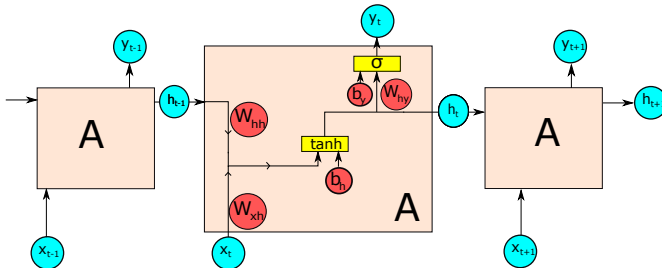
Two activation functions:

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

Closer-up: How to update the hidden state?



Closer-up: How to update the hidden state?



Update hidden state:

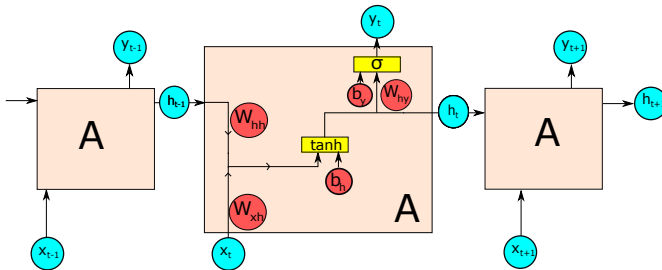
$$\mathbf{h}_t = \tanh(\mathbf{W}_{hh} \cdot \mathbf{h}_{t-1} + \mathbf{W}_{xh} \cdot \mathbf{x}_t + \mathbf{b}_h)$$

\mathbf{W}_{hh} : Weight matrix for previous hidden state \mathbf{h}_{t-1}

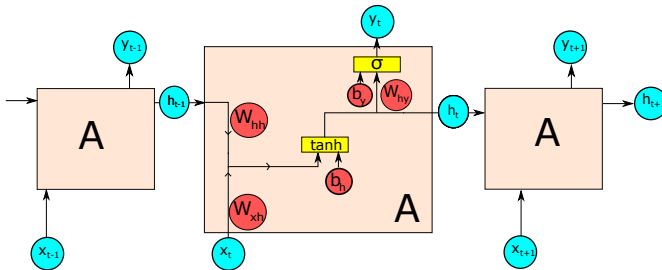
\mathbf{W}_{xh} : Weight matrix for current input \mathbf{x}_t

\mathbf{b}_h : Update bias

Closer-up: How to compute the output?



Closer-up: How to compute the output?



Output formula:

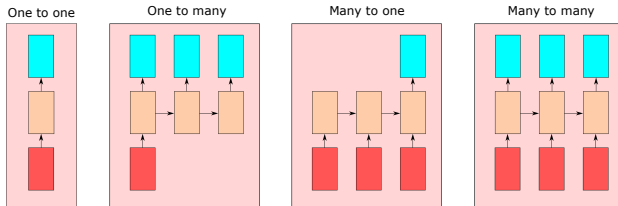
$$\mathbf{y}_t = \sigma(\mathbf{W}_{hy} \cdot \mathbf{h}_t + \mathbf{b}_y)$$

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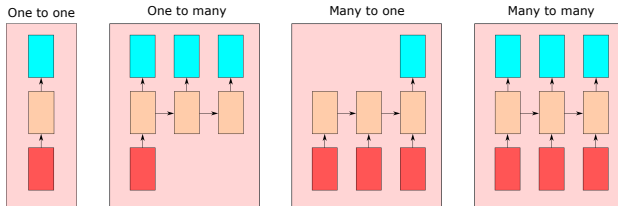
RNN Basic Architectures

Type of sequential relationship \leftrightarrow architecture:



RNN Basic Architectures

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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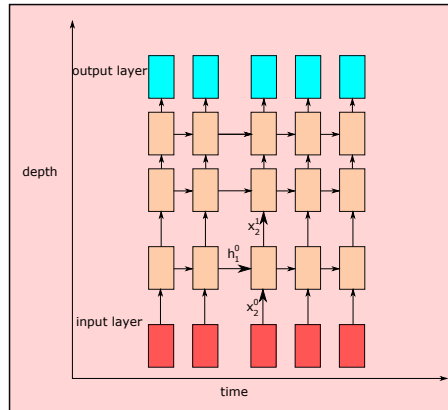
Deep RNNs (cont.)

Similar to CNNs, stack multiple units for
deep RNNs

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

t : time point

l : layer index



NEXT TIME

ON DEEP LEARNING



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Recurrent Neural Networks - Part 2

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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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Given ‘*h*’ as first input, the network should generate sequence “*hello*”

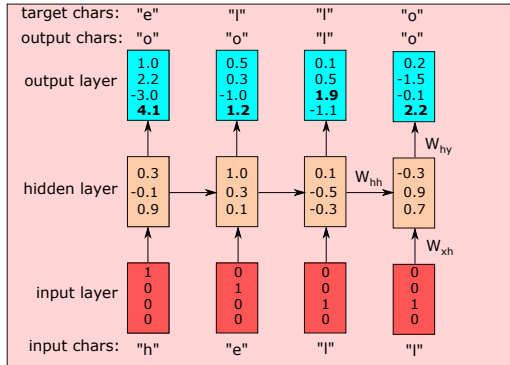
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Given ‘*h*’ as first input, the network should generate sequence “*hello*”
- Network needs to know **previous inputs** when presented with ‘*l*’:
Do we need another ‘*l*’ or an ‘*o*’?

Simple Example: Character Level Language Model (cont.)

Prediction with random initialization:

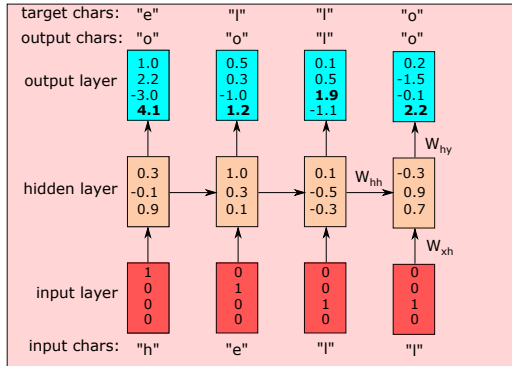


- Goal: Maximize prediction for correct component
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Source: Adapted from <http://karpathy.github.io/2015/05/21/rnn-effectiveness>

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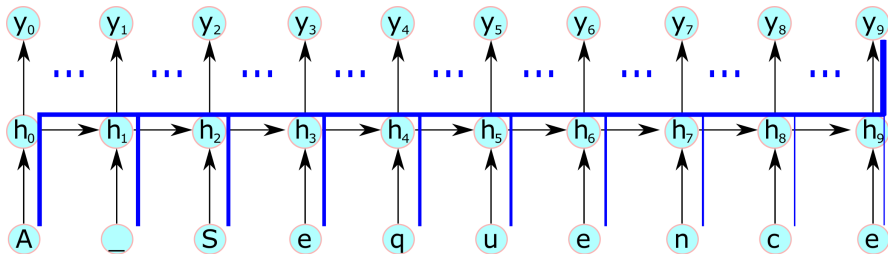
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- **Backpropagation through time (BPTT):** train “unfolded” network

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Backpropagation through Time (BPTT)

Concept: Train the unfolded network

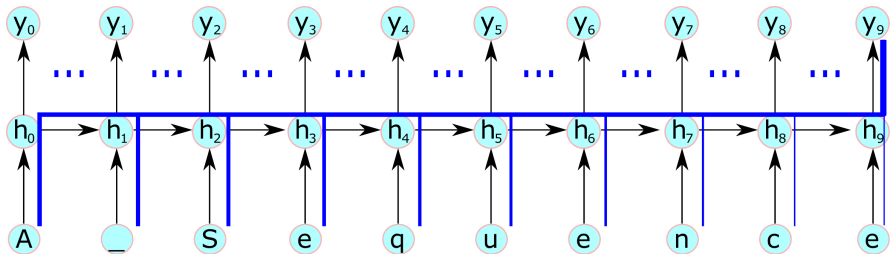
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Backpropagation through Time (BPTT)

Concept: Train the unfolded network

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

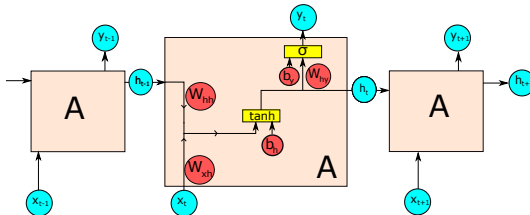


Backpropagation through Time (BPTT) (cont.)

Forward pass: Computation of hidden states and output

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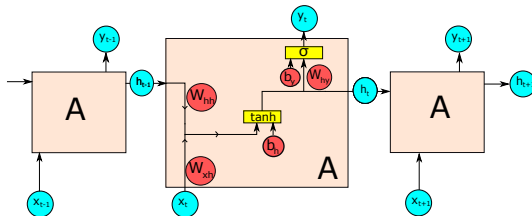


Input sequence: $\mathbf{X} = \{\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_T\}$

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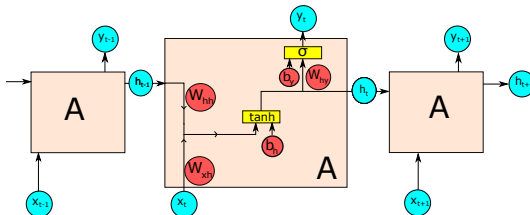
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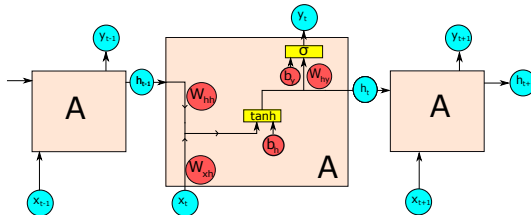
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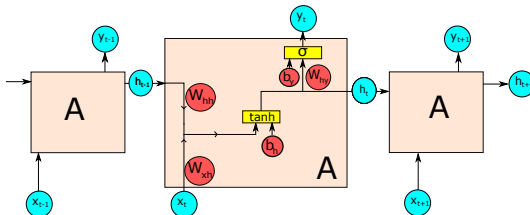


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- 5: $\hat{\mathbf{y}}_t = \sigma(\mathbf{o}_t)$

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 η

$$\theta = \theta - \eta \nabla \theta$$

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

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

$$\nabla \mathbf{W}_{hy,t} = \nabla \mathbf{o}_t \mathbf{h}_t^\top$$

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Backpropagation through Time (BPTT) (cont.)

- Note: For $t = 0$ and $t = T$, we only need one element of the sum.

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- Currently, gradient depends on t . How do we get the gradient for the sequence?

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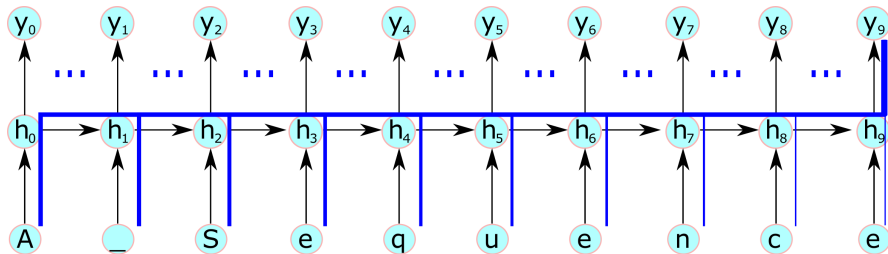
$$\nabla \mathbf{W}_{hh,t} = \nabla \mathbf{h}_t \cdot \tanh'(\mathbf{u}_t) \cdot \mathbf{h}_{t-1}^\top$$

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$$\nabla \mathbf{b}_{h,t} = \nabla \mathbf{h}_t \cdot \tanh'(\mathbf{u}_t)$$

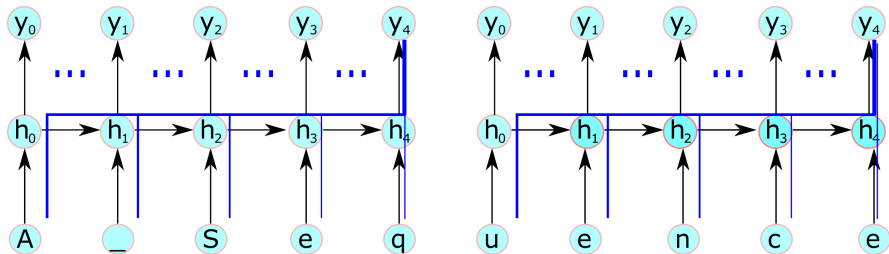
- Currently, gradient depends on t . How do we get the gradient for the sequence?
 - Unrolled unit is a network with **shared weights**
- For each gradient, simply **sum over all time-steps** $t = \{1, \dots, T\}$!

Normal BPTT



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

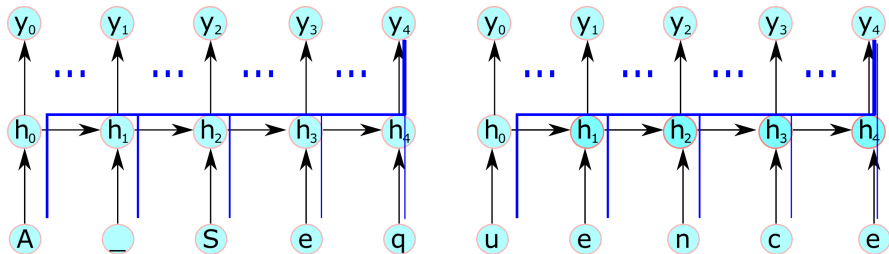
Naive BPTT



Naive Solution:

- Split long sequences into batches of smaller parts

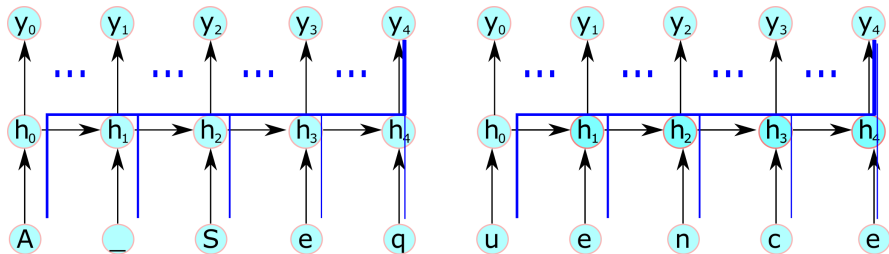
Naive BPTT



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!

Naive BPTT



Naive Solution:

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→ **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

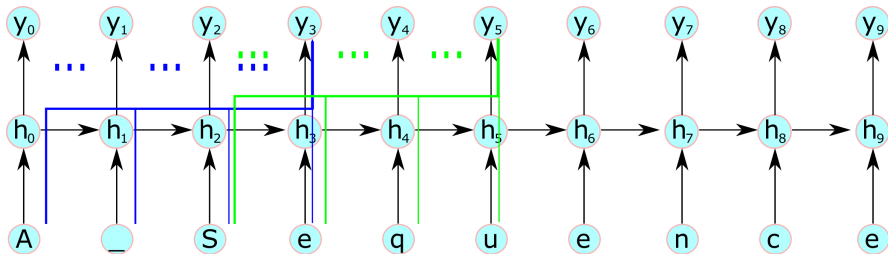
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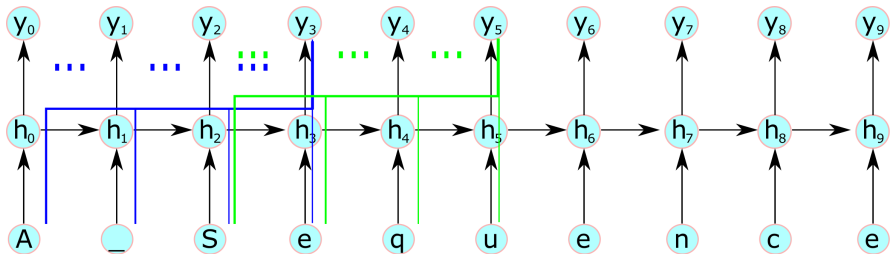
Algorithm:

- 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



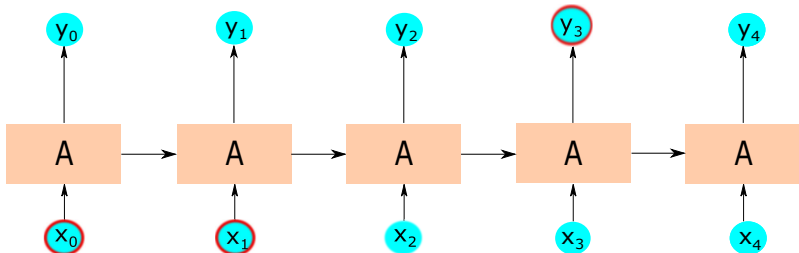
Truncated BPTT



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

The Long-Term Dependency Problem with Basic RNNs

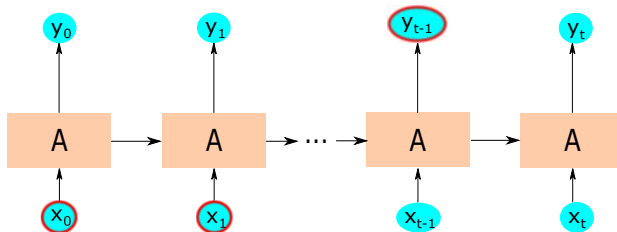
- Short term dependencies work fine
- Example: Predict next word in "the clouds are in the [sky]"



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

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

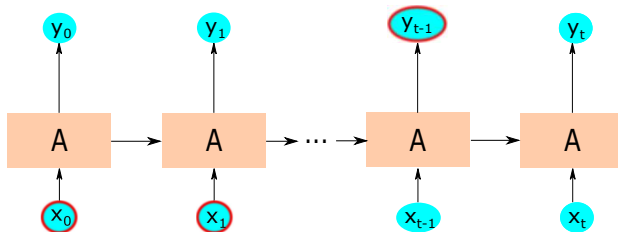
- Harder to connect relevant past and present inputs for longer time spans
- Example: Predict next word in "I grew up in Germany ... I speak fluent [German]"



- Contextual information far away

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

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- 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 (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])

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

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- **Vanishing gradient** harder to solve!

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Additional problem: memory overwriting

- Hidden state is overwritten each time step
- Detecting long-term dependencies even more difficult

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 - Detecting long-term dependencies even more difficult
- Can we do better? Again, yes!

NEXT TIME

ON DEEP LEARNING



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Recurrent Neural Networks - Part 3

A. Maier, V. Christlein, K. Breininger, Z. Yang, L. Rist, M. Nau, S. Jaganathan, C. Liu, N. Maul, L. Folle,
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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**

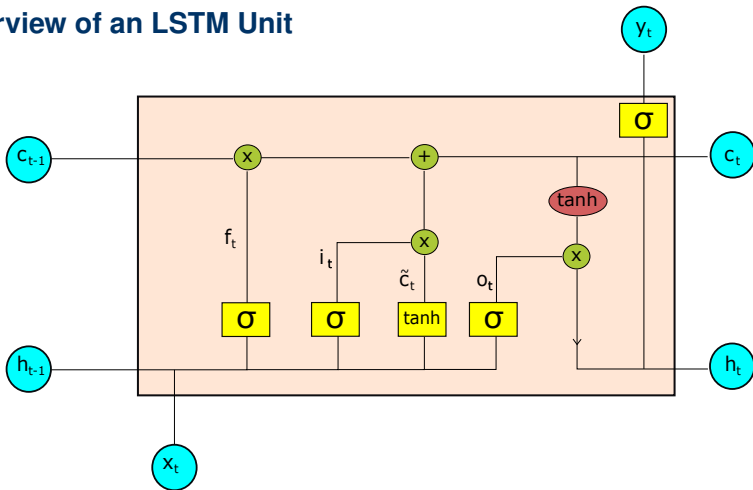


Sepp Hochreiter



Jürgen Schmidhuber

Overview of an LSTM Unit



LSTM unit workflow

Elements of LSTM units:

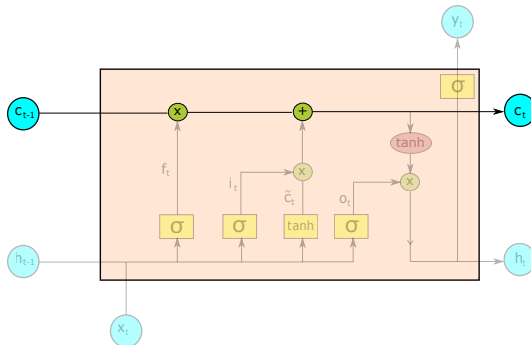
- Input \mathbf{x}_t
- Hidden state $\mathbf{h}_{t-1}/\mathbf{h}_t$
- Cell state $\mathbf{c}_{t-1}/\mathbf{c}_t$
- Output \mathbf{y}_t

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

LSTM Cell State

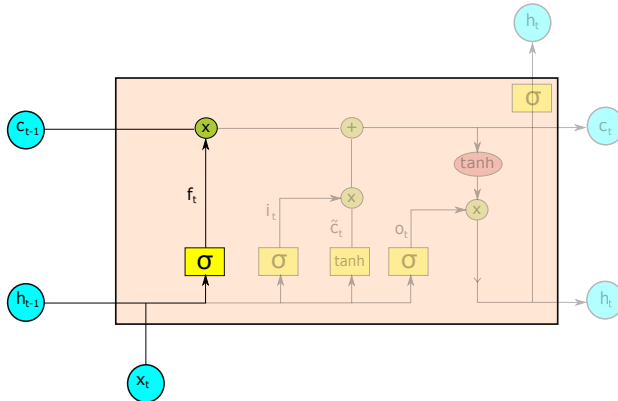
- c_t : **Cell state** after time point t
- Undergoes only **linear changes**: no activation function!
- c_t can flow through a unit unchanged \rightarrow cell state can be constant for multiple time steps



Forget Gate: Forgetting Old Information

- Key idea: “forgetting” and “memorizing” information in separate steps
- \mathbf{f}_t controls how much of the previous cell state is forgotten:

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

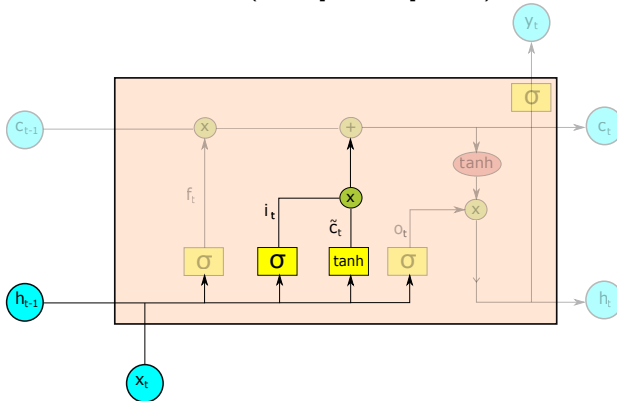


Input Gate: Deciding on New Input

Combination of input and hidden state on two paths:

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

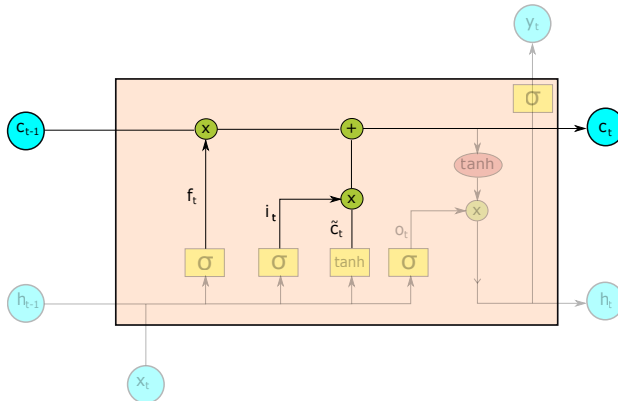
$$\tilde{\mathbf{c}}_t = \tanh(\mathbf{W}_c \cdot [\mathbf{h}_{t-1}, \mathbf{x}_t] + \mathbf{b}_c)$$



Updating the Cell State

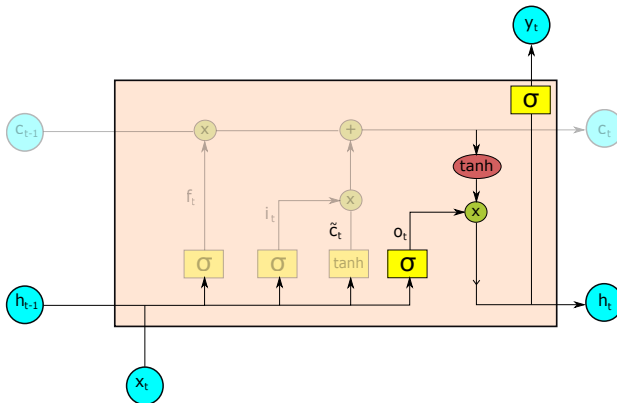
- New cell state: Sum of “remaining information” from \mathbf{c}_{t-1} and new information from input and hidden state (\odot : element-wise multiplication)

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



Updating the Hidden State and Computing the Output

- Important: Cell state and hidden state are updated **separately**
- Output \mathbf{y}_t directly depends on the hidden state \mathbf{h}_t

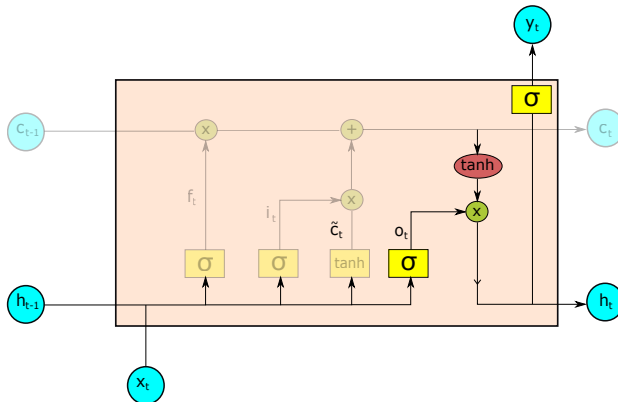


Updating the Hidden State and Computing the Output (cont.)

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

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

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



NEXT TIME

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Recurrent Neural Networks - Part 4

A. Maier, V. Christlein, K. Breininger, Z. Yang, L. Rist, M. Nau, S. Jaganathan, C. Liu, N. Maul, L. Folle,
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Gated Recurrent Units



Motivation

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

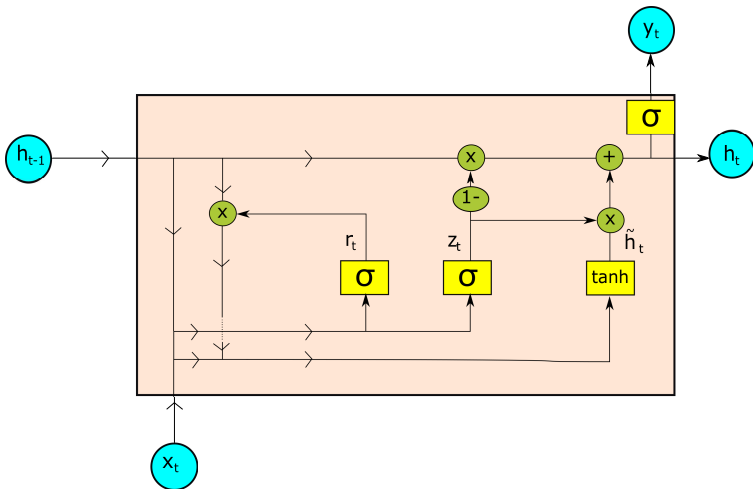
Motivation

- 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



Kyunghyung Cho

Structure of a GRU cell



GRU workflow

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

GRU workflow

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→ Memory operates only and directly via the hidden state

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 - 1) **Reset gate**: Influence of the previous hidden state

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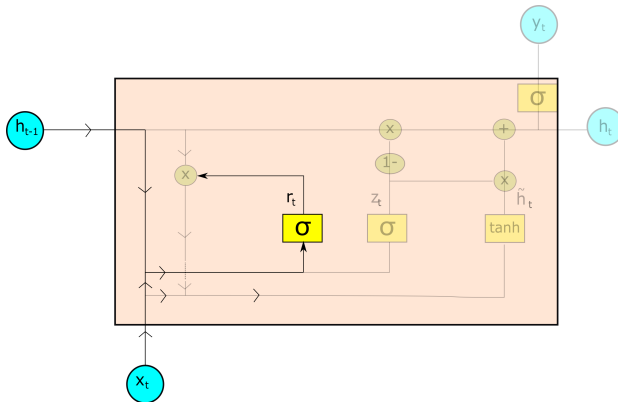
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 - 4) Computing updated hidden state

Reset gate

- Determines the influence of the previous hidden state

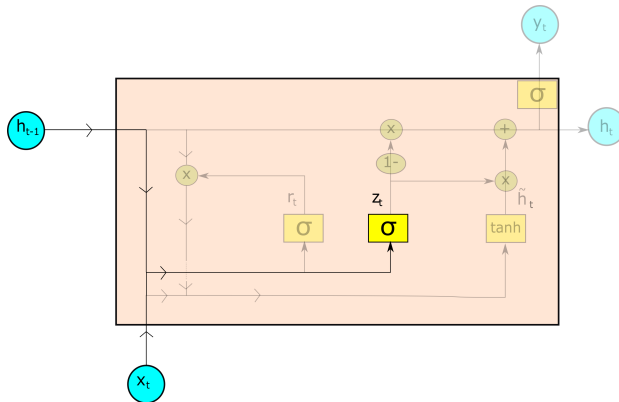
$$\mathbf{r}_t = \sigma(\mathbf{W}_r \cdot [\mathbf{h}_{t-1}, \mathbf{x}_t] + \mathbf{b}_r)$$



Update Gate

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

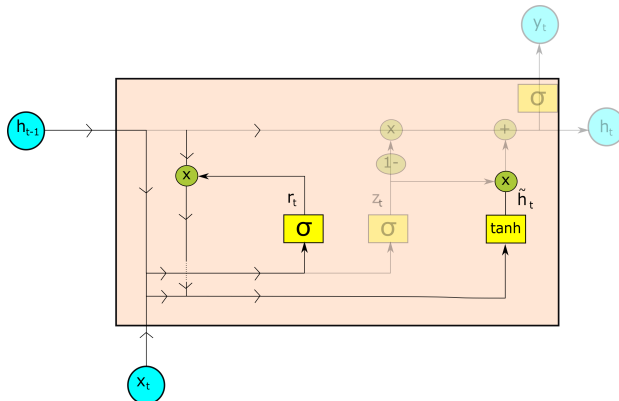
$$\mathbf{z}_t = \sigma(\mathbf{W}_z \cdot [\mathbf{h}_{t-1}, \mathbf{x}_t] + \mathbf{b}_z)$$



Proposing an Update

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

$$\tilde{h}_t = \tanh(W_h \cdot [r_t \odot h_{t-1}, x_t] + b_h)$$

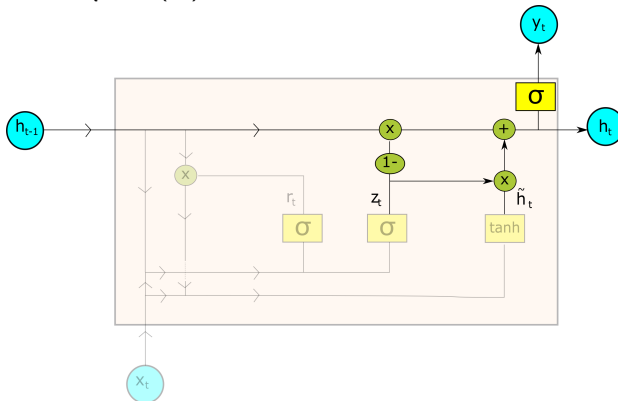


Finally: Computing the Updated Hidden State

- **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
→ z_t close to 0: ignore new input
- Gates have varying "rhythm" depending on the type of information



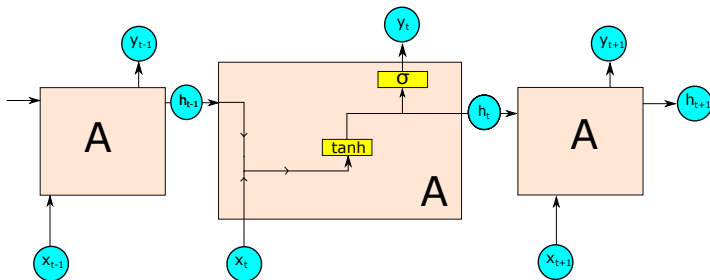
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Comparison of Simple RNN units, LSTM units and GRUs

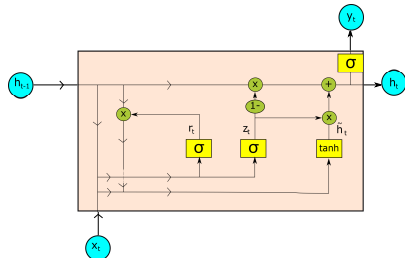
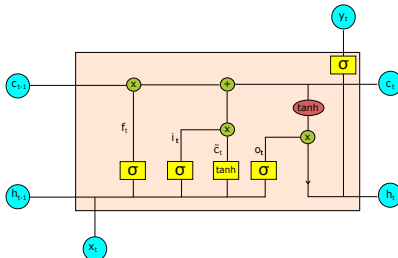


Recap: Simple RNNs

- 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
Seperate 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

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
- Gated recurrent units clearly outperformed regular recurrent unit
- Comparison between GRU and LSTM not conclusive, similar performance

NEXT TIME

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Recurrent Neural Networks - Part 5

A. Maier, V. Christlein, K. Breininger, Z. Yang, L. Rist, M. Nau, S. Jaganathan, C. Liu, N. Maul, L. Folle,
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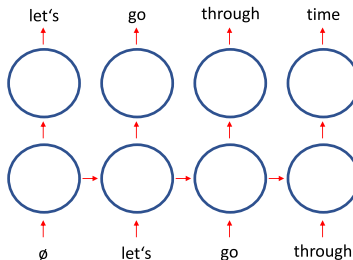
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Sampling strategies for RNNs



Why Sampling Strategies?

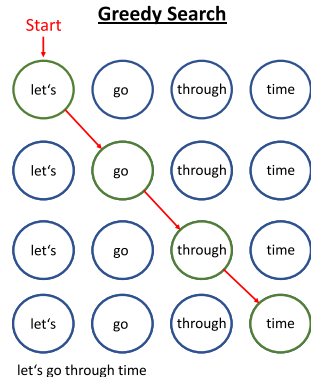
- RNN can generate sequences (words/notes/...)
- RNN actually computes **probability distribution** of the next element
- Question: How do we sample this distribution?



Ideal sequence - or?

Greedy search

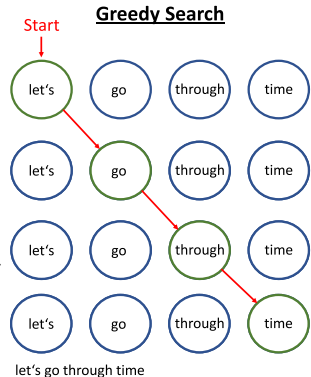
- **Concept:** At each point, pick the most likely element
- Generates exactly one sample sequence per experiment



Greedy search

Greedy search

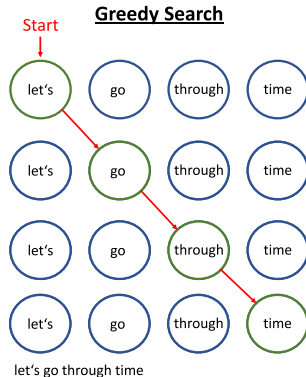
- **Concept:** At each point, pick the most likely element
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- **Drawback:** No **lookahead** possible!
 - Example: “let’s” may be most likely after “let’s go” → “let’s go let’s”
 - Cannot detect that “let’s go through time” has a higher total probability



Greedy search

Greedy search

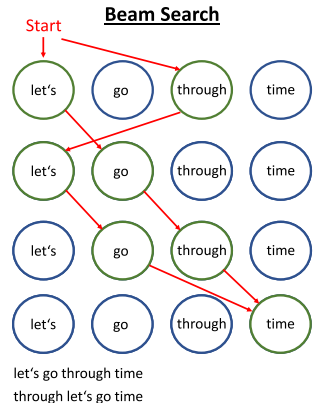
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 - Example: “let’s” may be most likely after “let’s go” → “let’s go let’s”
 - Cannot detect that “let’s go through time” has a higher total probability
- Tends to repeat sequences of frequent words, e.g., “and”, “the”, “some” in speech



Greedy search

Beam Search

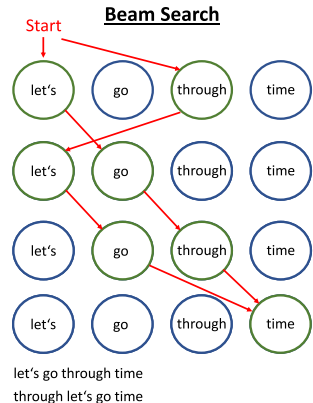
- **Concept:** Select k most likely elements (k : beam width or size)



Beam Search with $k = 2$

Beam Search

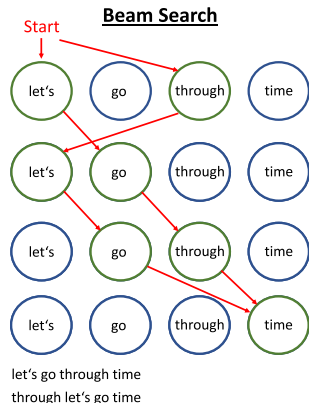
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Beam Search with $k = 2$

Beam Search

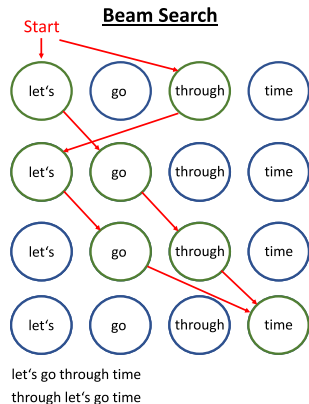
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Beam Search with $k = 2$

Beam Search

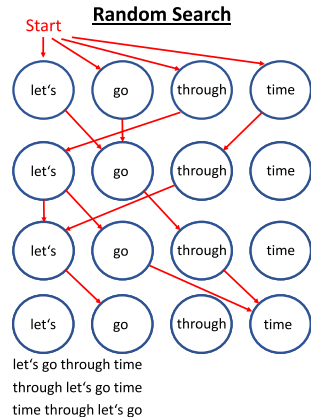
- **Concept:** Select k most likely elements (k : beam width or size)
- Out of all possible sequences that have one of these k elements as a **prefix**, take k most probable ones
- Iterate until end of sequence
- Can generate k sequences in one go
→ usually better than greedy search



Beam Search with $k = 2$

Random Sampling

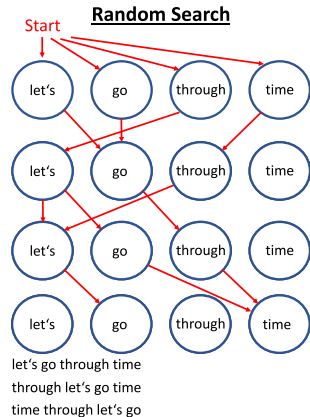
- **Idea:** Sample next word according to output probability distribution



Random Sampling

Random Sampling

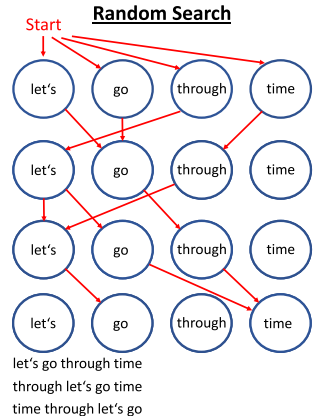
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Random Sampling

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- Creates very diverse results, can look too random



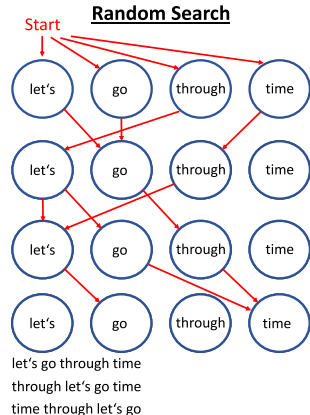
Random Sampling

Random Sampling

- **Idea:** Sample next word according to output probability distribution
- Example: If “let’s” 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 , τ : temperature



Random Sampling



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Examples



Character-based Language Modeling with RNNs

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

Character-based Language Modeling with RNNs

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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 nudes 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

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

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

Bornity Horse



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

Source: [14]

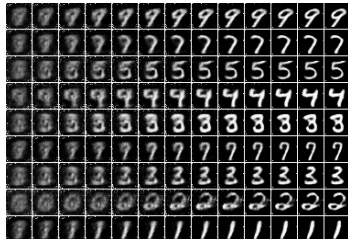
RNNs for Non-Sequential Tasks

- 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]

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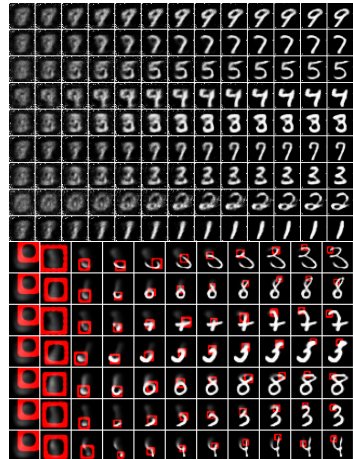
- RNNs can also be used for stationary inputs, e.g., image generation
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- Gregor et al. [8]: Drawing numbers
→ from blurry to sharp



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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]



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Summary



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- Recurrent neural networks are able to directly model sequential algorithms
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- 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
- 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”

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”.

Attention mechanisms

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 Andrej 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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