AIE1007: Natural Language Processing

L10: Recurrent neural networks - 2

Autumn 2024

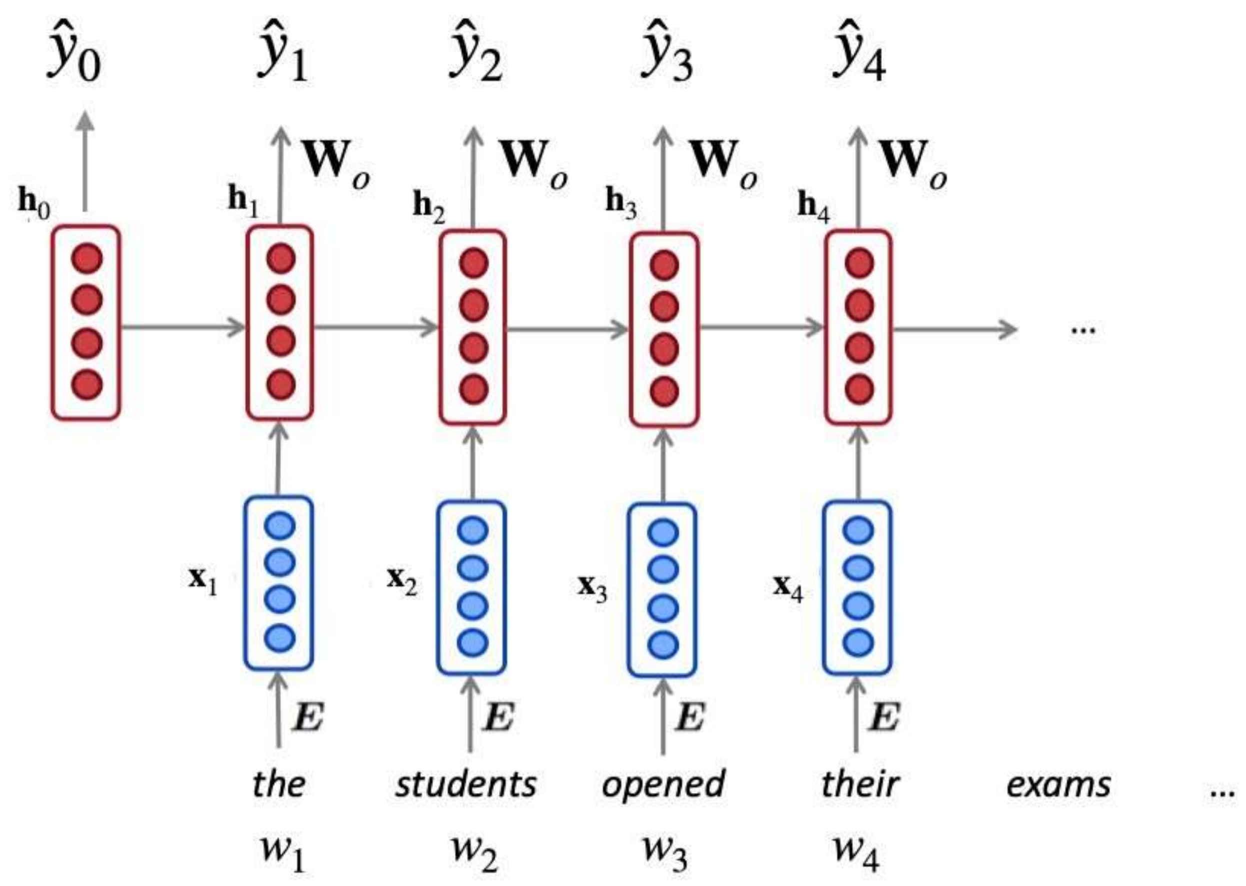
Recap: Recurrent neural networks

$\mathbf{h}_0 \in \mathbb{R}^h$ is an initial state

$$\boxed{\mathbf{h}_t = f(\mathbf{h}_{t-1}, \mathbf{x}_t) \in \mathbb{R}^h}$$

$\mathbf{h}_t$: hidden states which store information from $\mathbf{x}_1$ to $\mathbf{x}_t$

RNNLMs:



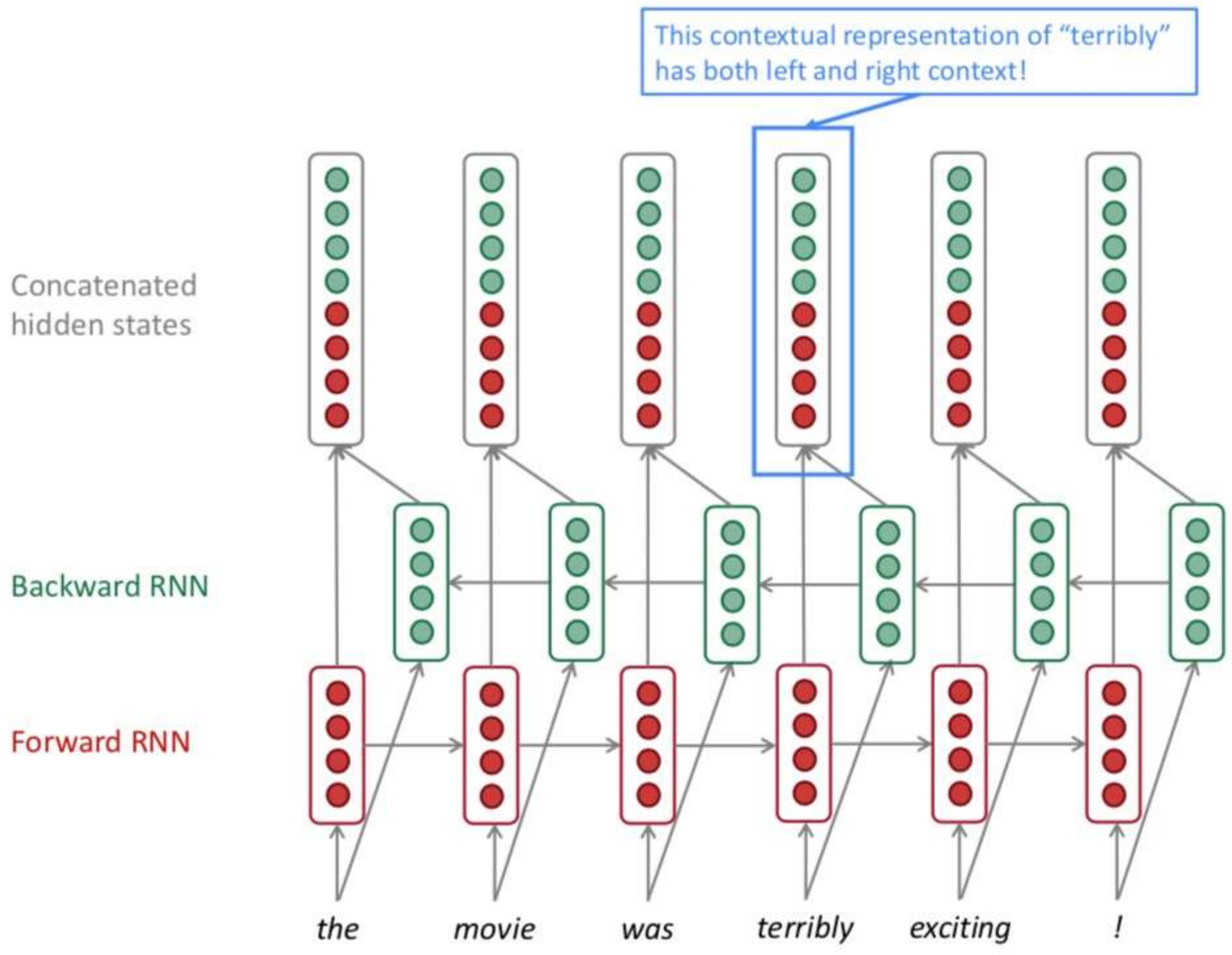
Simple RNNs:

$$\boxed{\mathbf{h}_t = g(\mathbf{W}\mathbf{h}_{t-1} + \mathbf{U}\mathbf{x}_t + \mathbf{b}) \in \mathbb{R}^h}$$

g: nonlinearity (e.g. tanh, ReLU),

$$\mathbf{W} \in \mathbb{R}^{h \times h}, \mathbf{U} \in \mathbb{R}^{h \times d}, \mathbf{b} \in \mathbb{R}^h$$

Bidirectional RNNs



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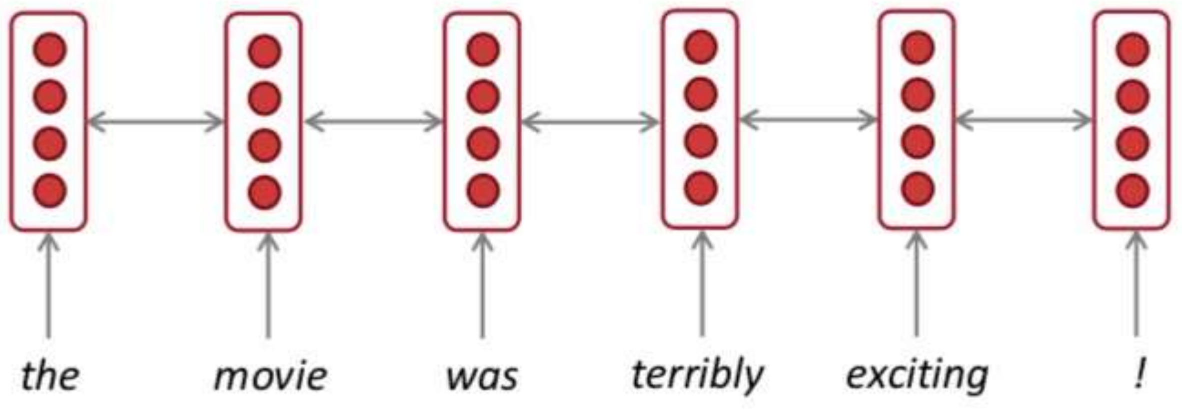


$$\overrightarrow{\mathbf{h}}_t = f_1(\overrightarrow{\mathbf{h}}_{t-1}, \mathbf{x}_t), t = 1,2,\ldots n$$

$$\overleftarrow{\mathbf{h}}_t = f_2(\overleftarrow{\mathbf{h}}_{t+1}, \mathbf{x}_t), t = n, n-1,\ldots 1$$

$$\mathbf{h}_t = [\overleftarrow{\mathbf{h}}_t, \overrightarrow{\mathbf{h}}_t] \in \mathbb{R}^{2h}$$

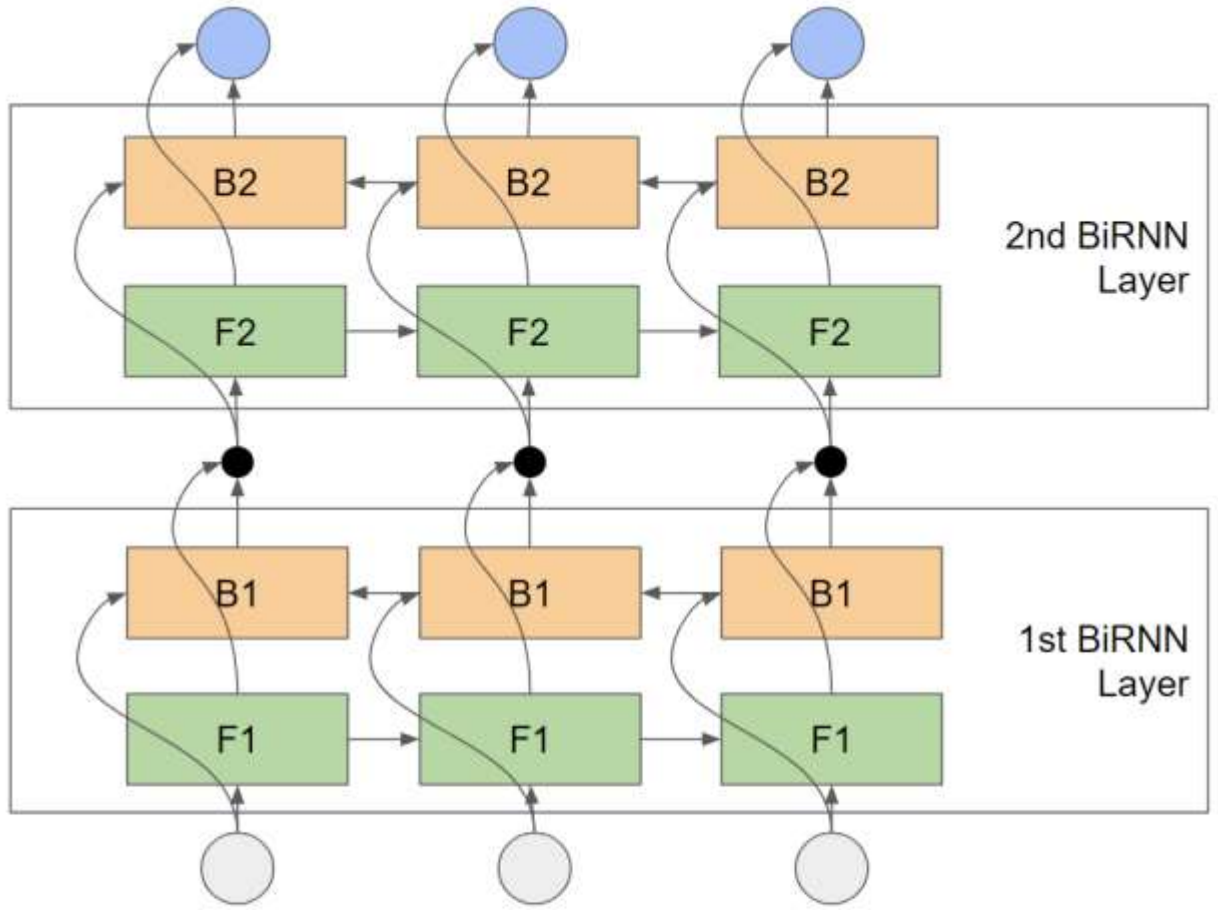
Bidirectional RNNs

- Bidirectional RNNs are only applicable if you have access to the **entire input sequence** (= they can't do text generation!)

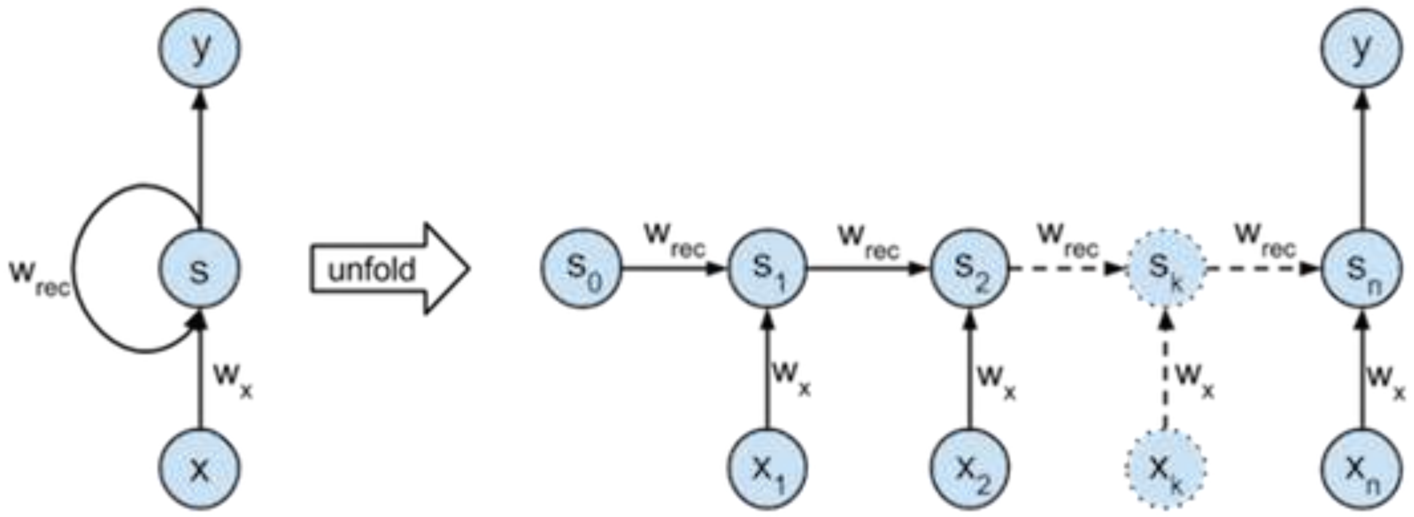
- If you do have entire input sequence, bidirectionality is powerful (and you should use it by default)

- Modeling the bidirectionality is the key idea behind BERT (BERT = **Bidirectional** Encoder Representations from Transformers)
    - We will learn Transformers and BERT in a few weeks!

- A very common choice for sentence/document modeling: multi-layer bidirectional RNNs



Advanced RNN variants



$$\mathbf{h}_t = f(\mathbf{h}_{t-1}, \mathbf{x}_t) \in \mathbb{R}^h$$

$$\mathbf{h}_t = \tanh(\mathbf{W}\mathbf{h}_{t-1} + \mathbf{U}\mathbf{x}_t + \mathbf{b}) \in \mathbb{R}^h$$

LSTMs

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

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

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

$$\mathbf{g}_t = \tanh(\mathbf{W}^g\mathbf{h}_{t-1} + \mathbf{U}^g\mathbf{x}_t + \mathbf{b}^g)$$

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

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

GRUs

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

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

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

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

Long Short-Term Memory RNNs (LSTMs)

A type of RNN proposed by Hochreiter and Schmidhuber in 1997 as a solution to the **vanishing gradients problem**.

- Everyone cites that paper but really a crucial part of the modern LSTM is from Gers et al. (2000)

LONG SHORT-TERM MEMORY

NEURAL COMPUTATION 9(8):1735–1780, 1997

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Learning to Forget: Continual Prediction with LSTM

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Recap: Vanishing Gradient Problem

$$\mathbf{h}_2 = g(\mathbf{W}\mathbf{h}_1 + \mathbf{U}\mathbf{x}_2 + \mathbf{b})$$
$$\mathbf{h}_3 = g(\mathbf{W}\mathbf{h}_2 + \mathbf{U}\mathbf{x}_3 + \mathbf{b})$$
$$L_3 = -\log \hat{\mathbf{y}}_3(w_4)$$

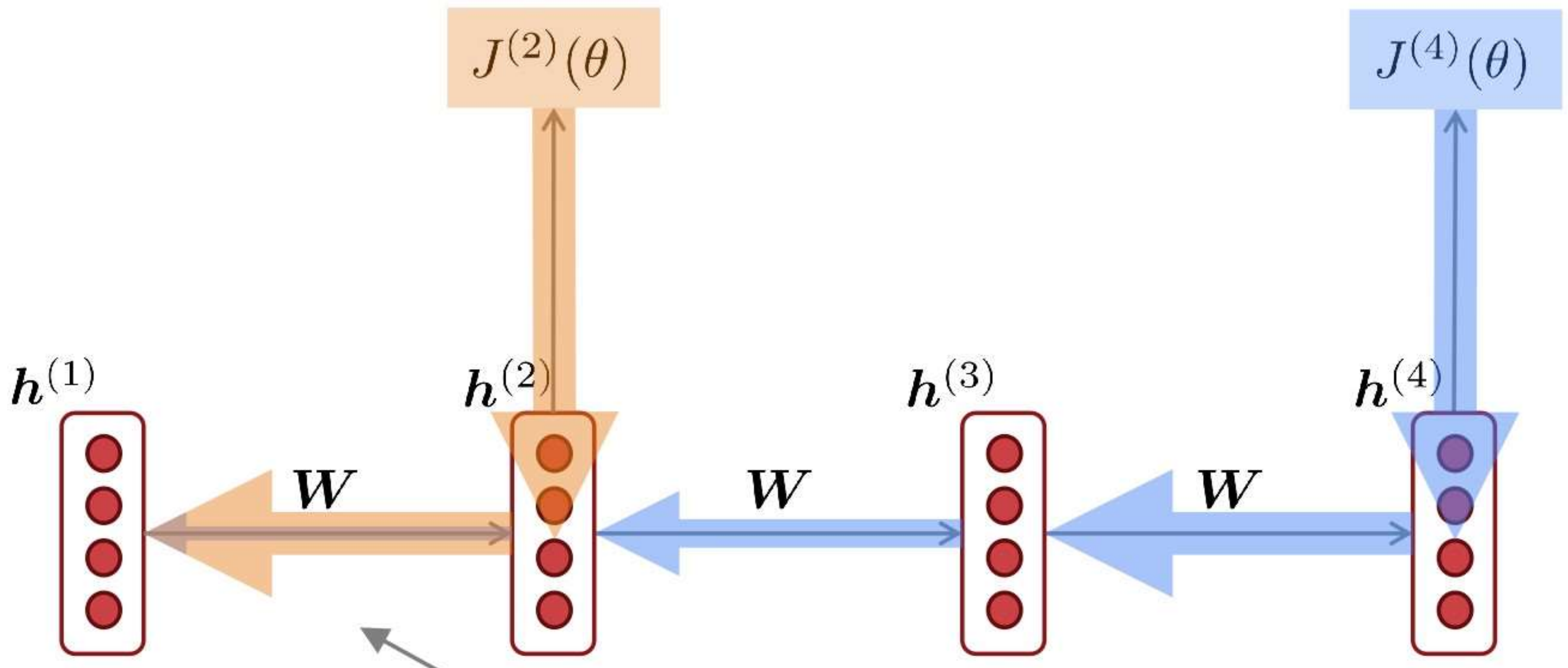
Vanishing gradient problem:
When these are small, the gradient signal gets smaller and smaller as it backpropagates further

$$\frac{\partial L_3}{\partial \mathbf{W}} = \frac{\partial L_3}{\partial \mathbf{h}_3}\frac{\partial \mathbf{h}_3}{\partial \mathbf{W}} + \frac{\partial L_3}{\partial \mathbf{h}_3}\boxed{\frac{\partial \mathbf{h}_3}{\partial \mathbf{h}_2}}\frac{\partial \mathbf{h}_2}{\partial \mathbf{W}} + \frac{\partial L_3}{\partial \mathbf{h}_3}\boxed{\frac{\partial \mathbf{h}_3}{\partial \mathbf{h}_2}\frac{\partial \mathbf{h}_2}{\partial \mathbf{h}_1}}\frac{\partial \mathbf{h}_1}{\partial \mathbf{W}}$$

$$\boxed{\frac{\partial L}{\partial \mathbf{W}} = -\frac{1}{n}\sum_{t=1}^{n}\sum_{k=1}^{t}\frac{\partial L_t}{\partial \mathbf{h}_t}\left(\prod_{j=k+1}^{t}\frac{\partial \mathbf{h}_j}{\partial \mathbf{h}_{j-1}}\right)\frac{\partial \mathbf{h}_k}{\partial \mathbf{W}}}$$

If k and t are far away, the gradients are very easy to grow/shrink exponentially
(called the gradient exploding or gradient vanishing problem)

Recap: Vanishing Gradient Problem



Gradient signal from far away is lost because it's much smaller than gradient signal from close-by.

So, model weights are basically updated only with respect to near effects, not long-term effects.

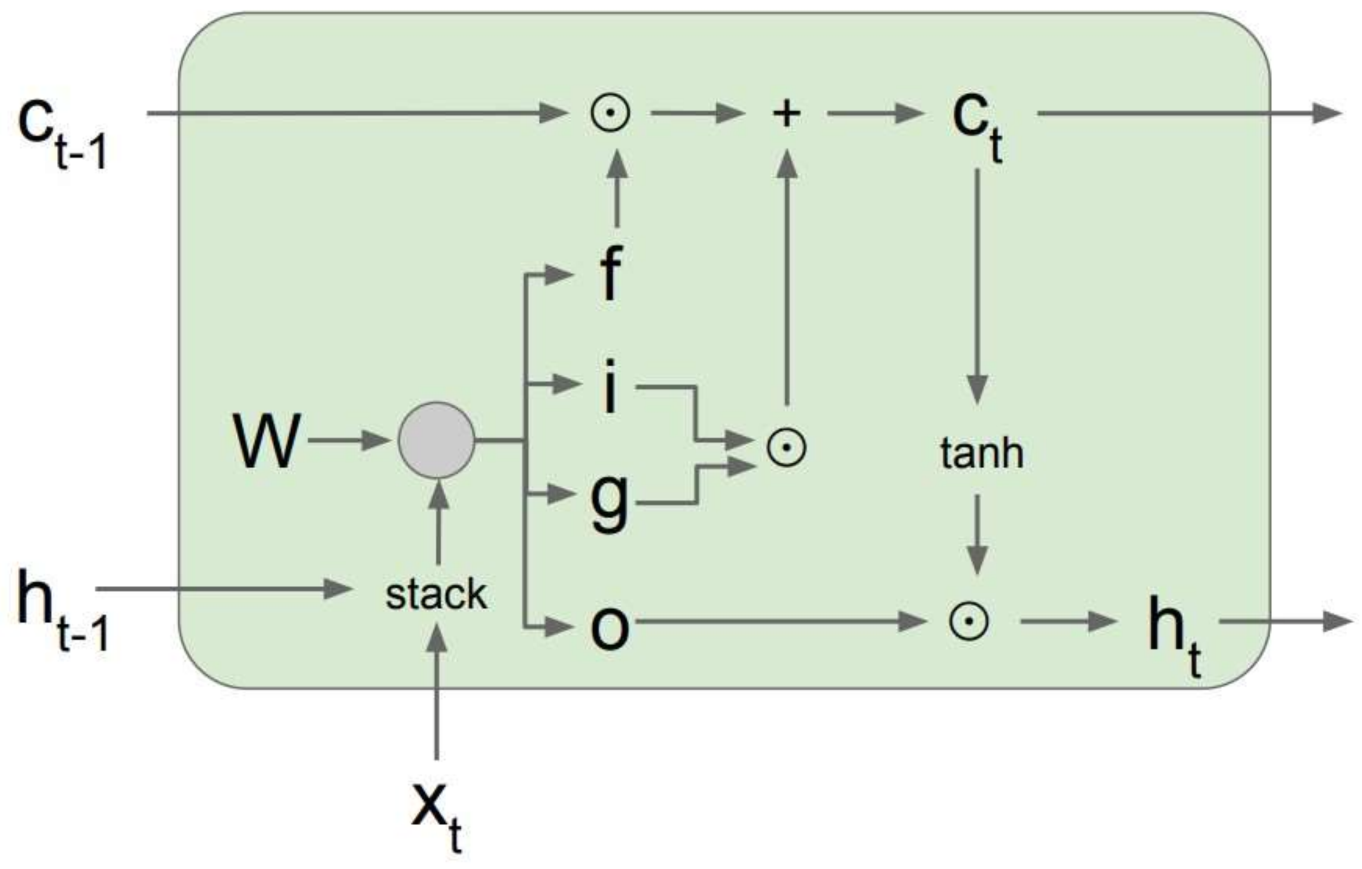
(Slide credit: Chris Manning)

LSTMs: The intuition

- Key idea: turning **multiplication** into **addition** and using "**gates**" to control how much information to add/erase

- At each time step, instead of re-writing the hidden state $\mathbf{h}_t = g(\mathbf{W}\mathbf{h}_{t-1} + \mathbf{U}\mathbf{x}_t + \mathbf{b})$, there is also a cell state $\mathbf{c}_t \in \mathbb{R}^h$ which stores **long-term information**

  - We write to/erase information from $\mathbf{c}_t$ after each step
  - We read $\mathbf{h}_t$ from $\mathbf{c}_t$



LSTMs: the formulation

- Input gate **(how much to write)**:
  $\mathbf{i}_t = \sigma(\mathbf{W}^i\mathbf{h}_{t-1} + \mathbf{U}^i\mathbf{x}_t + \mathbf{b}^i) \in \mathbb{R}^h$

- Forget gate **(how much to erase)**:
  $\mathbf{f}_t = \sigma(\mathbf{W}^f\mathbf{h}_{t-1} + \mathbf{U}^f\mathbf{x}_t + \mathbf{b}^f) \in \mathbb{R}^h$

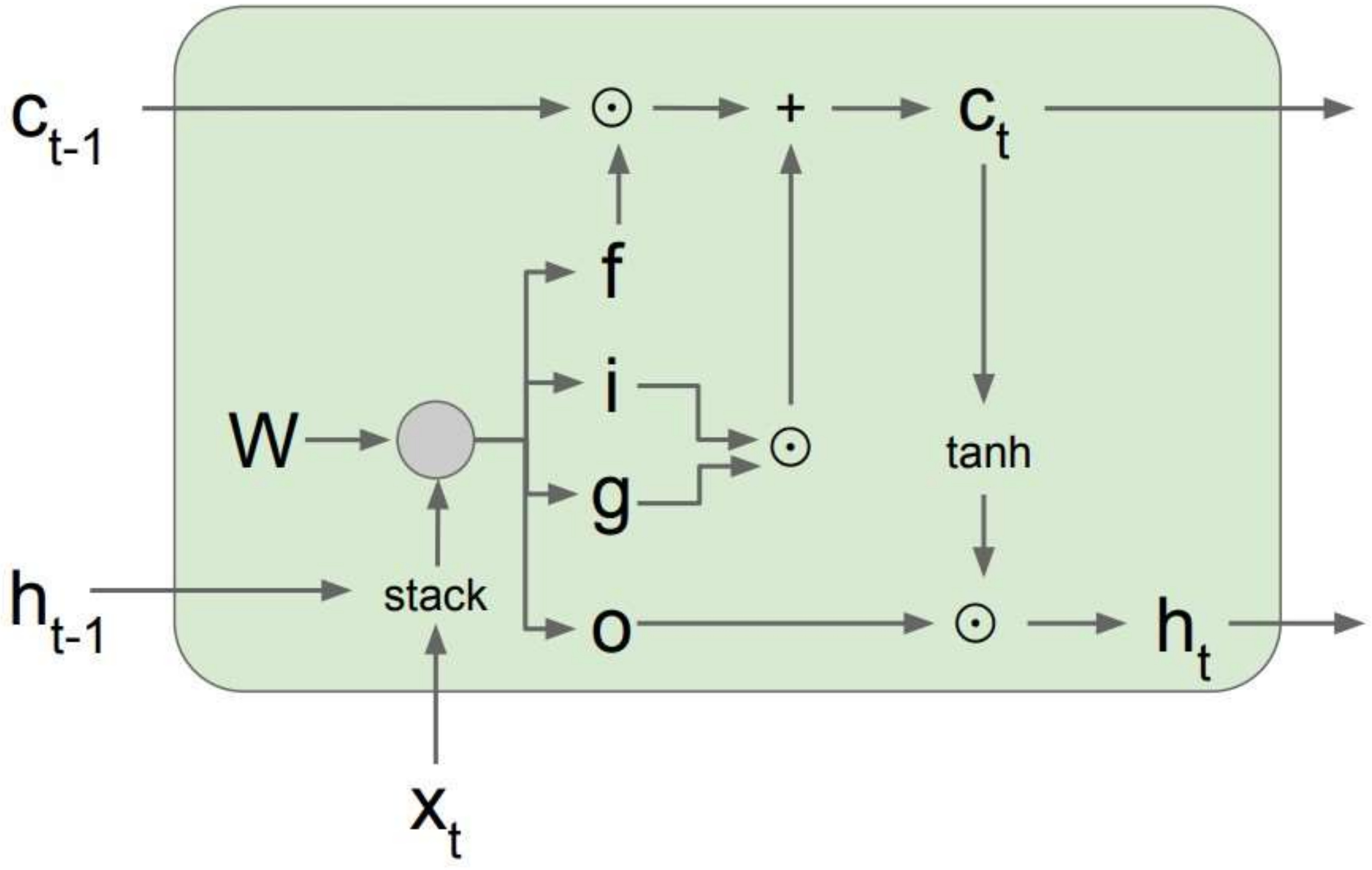
- Output gate **(how much to reveal)**:
  $\mathbf{o}_t = \sigma(\mathbf{W}^o\mathbf{h}_{t-1} + \mathbf{U}^o\mathbf{x}_t + \mathbf{b}^{(o)}) \in \mathbb{R}^h$

- New memory cell **(what to write)**:
  $\mathbf{g}_t = \tanh(\mathbf{W}^g\mathbf{h}_{t-1} + \mathbf{U}^g\mathbf{x}_t + \mathbf{b}^g) \in \mathbb{R}^h$

- Final memory cell: $\mathbf{c}_t = \mathbf{f}_t \odot \mathbf{c}_{t-1} + \mathbf{i}_t \odot \mathbf{g}_t$

  element-wise product

- Final hidden cell: $\mathbf{h}_t = \mathbf{o}_t \odot \tanh(\mathbf{c}_t)$



$\mathbf{h}_0, \mathbf{c}_0 \in \mathbb{R}^h$ are initial states (usually set to $\mathbf{0}$)

LSTMs: the formulation

LSTMs has 4x parameters compared to simple RNNs:

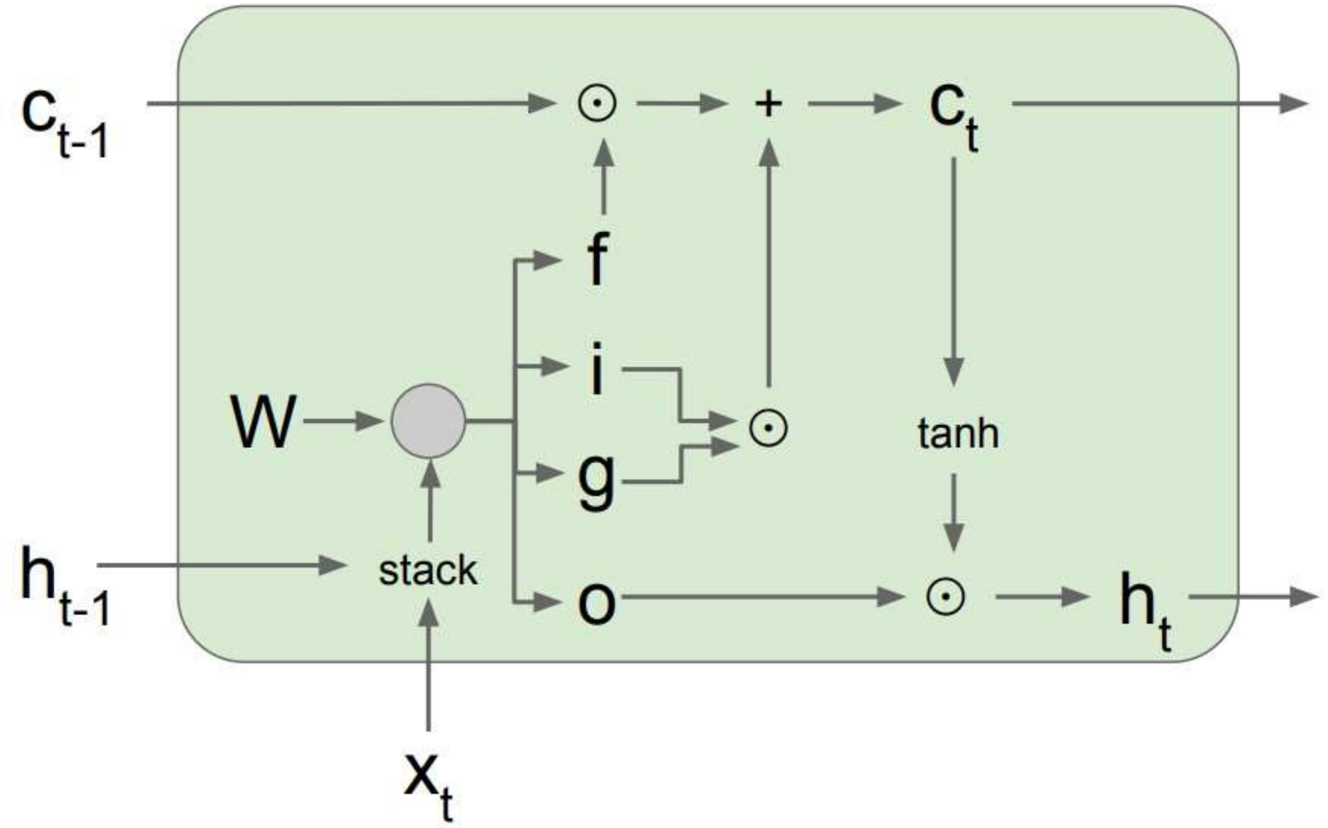
Input dimension: d, hidden size: h

$$\boxed{\mathbf{h}_t = g(\mathbf{W}\mathbf{h}_{t-1} + \mathbf{U}\mathbf{x}_t + \mathbf{b}) \in \mathbb{R}^h}$$

$$\mathbf{W} \in \mathbb{R}^{h\times h}, \mathbf{U} \in \mathbb{R}^{h\times d}, \mathbf{b} \in \mathbb{R}^h$$

$$\downarrow$$

$$\mathbf{W}^i, \mathbf{W}^f, \mathbf{W}^g, \mathbf{W}^o \in \mathbb{R}^{h\times h}$$
$$\mathbf{U}^i, \mathbf{U}^f, \mathbf{U}^g, \mathbf{U}^o \in \mathbb{R}^{h\times d}$$
$$\mathbf{b}^i, \mathbf{b}^f, \mathbf{b}^g, \mathbf{b}^o \in \mathbb{R}^h$$



$$\begin{pmatrix} i \\ f \\ o \\ g \end{pmatrix} = \begin{pmatrix} \sigma \\ \sigma \\ \sigma \\ \tanh \end{pmatrix} \underbrace{W}_{\mathbb{R}^{4h\times(h+d)}} \begin{pmatrix} h_{t-1} \\ x_t \end{pmatrix}$$

$$c_t = f \odot c_{t-1} + i \odot g$$
$$h_t = o \odot \tanh(c_t)$$

Simple RNNs:

$$h_t = (\tanh) W \begin{pmatrix} h^t \\ x_t \end{pmatrix}$$

What is the range of values?

Q: What is the range of values for each element in the hidden representations $\mathbf{h}_t$?

(a) 0 to

(b) 0 to 1

(c) -1 to 1

(d) to

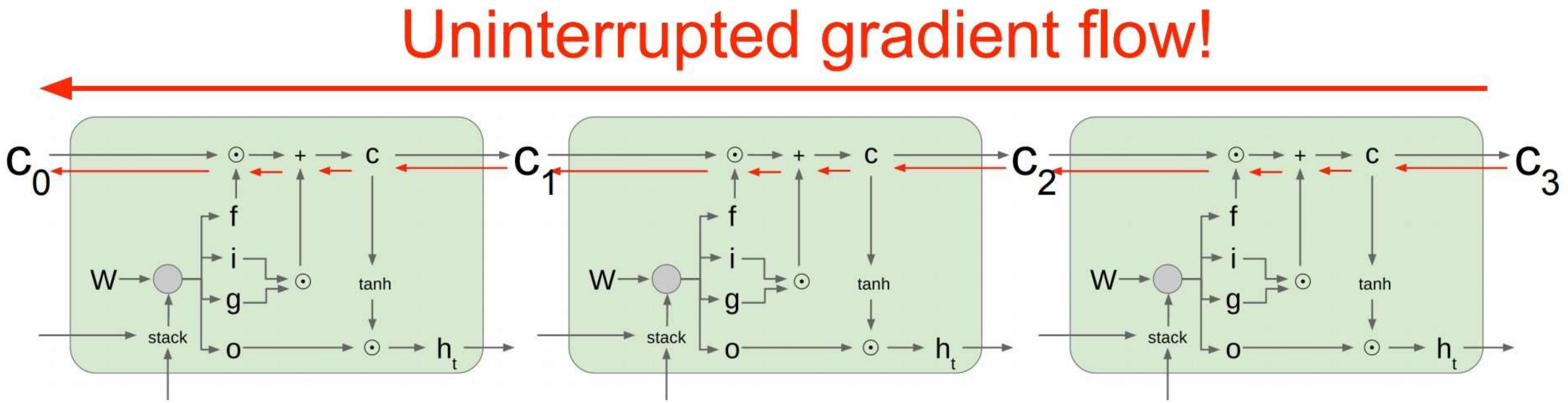
The answer is (c).

$$\begin{pmatrix} i \\ f \\ o \\ g \end{pmatrix} = \begin{pmatrix} \sigma \\ \sigma \\ \sigma \\ \tanh \end{pmatrix} W \begin{pmatrix} h_{t-1} \\ x_t \end{pmatrix}$$

$$c_t = f \odot c_{t-1} + i \odot g$$

$$h_t = o \odot \tanh(c_t)$$

LSTMs: the formulation



- LSTM doesn’t guarantee that there is no vanishing/exploding gradient, but it does provide an easier way for the model to learn long-distance dependencies

- LSTMs were invented in 1997 but finally got working from 2013-2015.

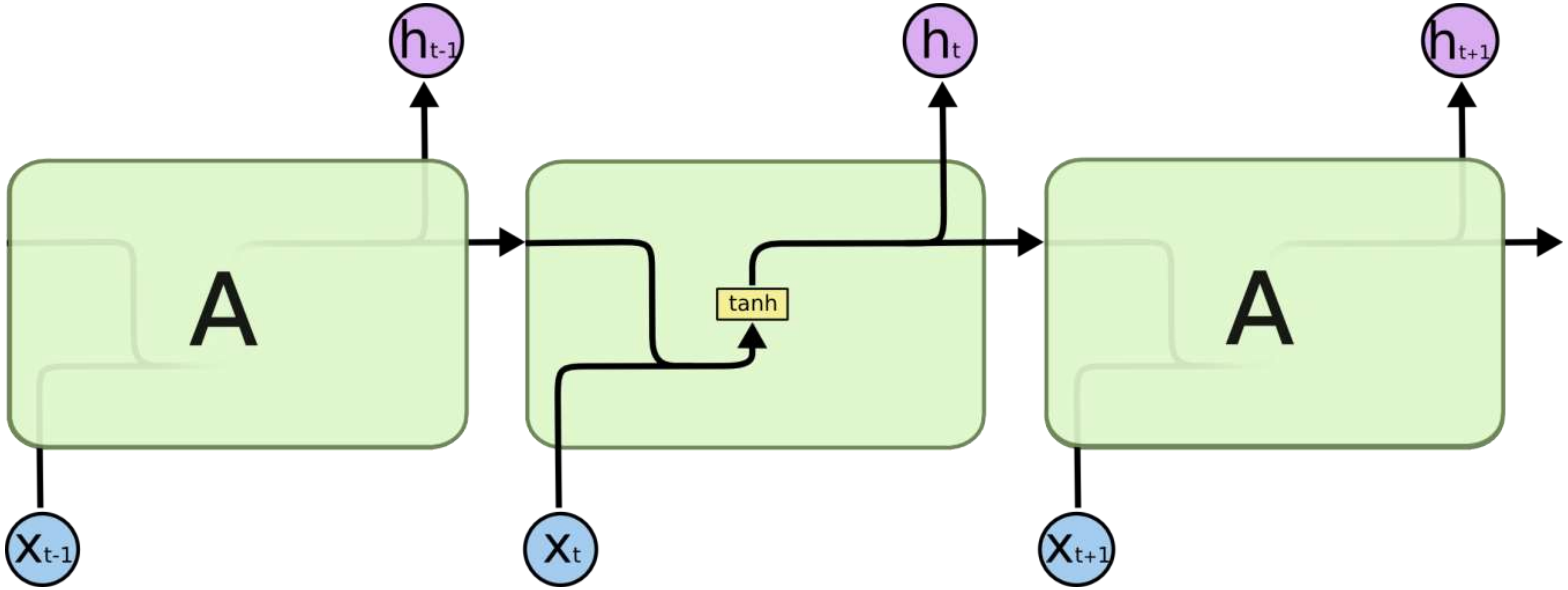
Visualization of LSTMs

Understanding LSTM Networks

Posted on August 27, 2015

https://colah.github.io/posts/2015-08-Understanding-LSTMs/

Christopher Olah



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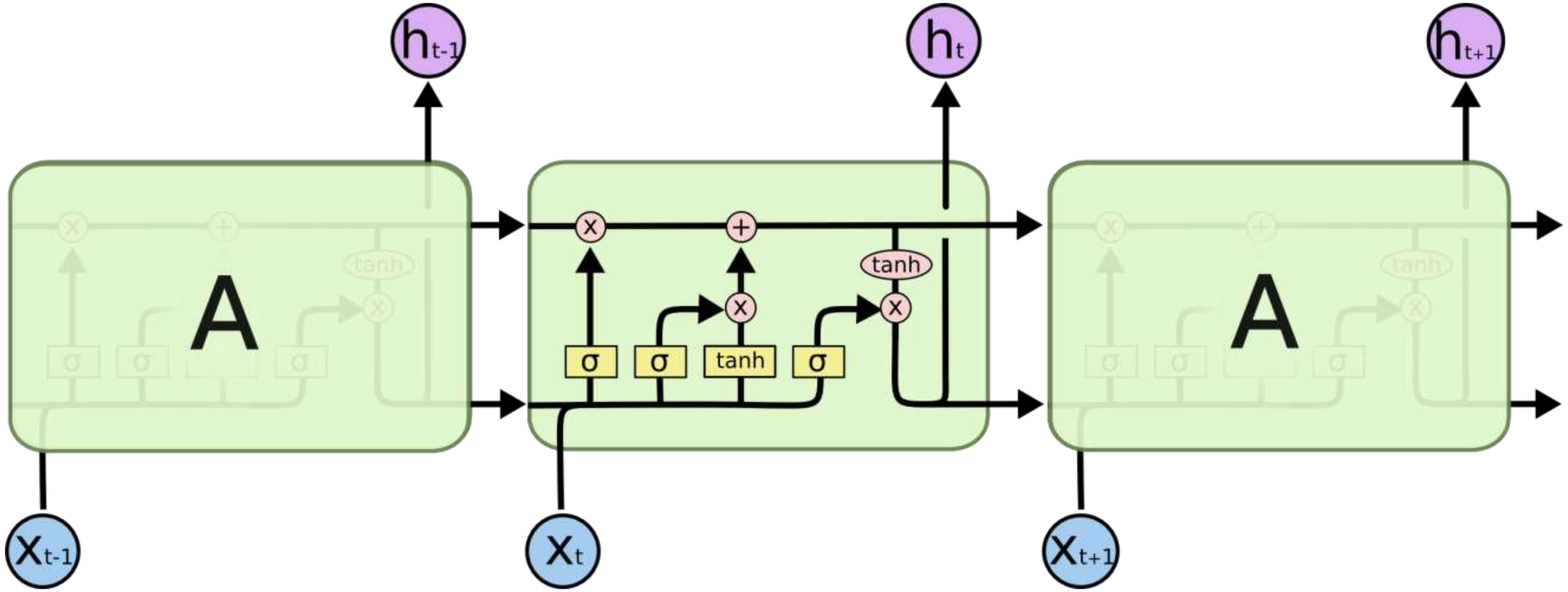

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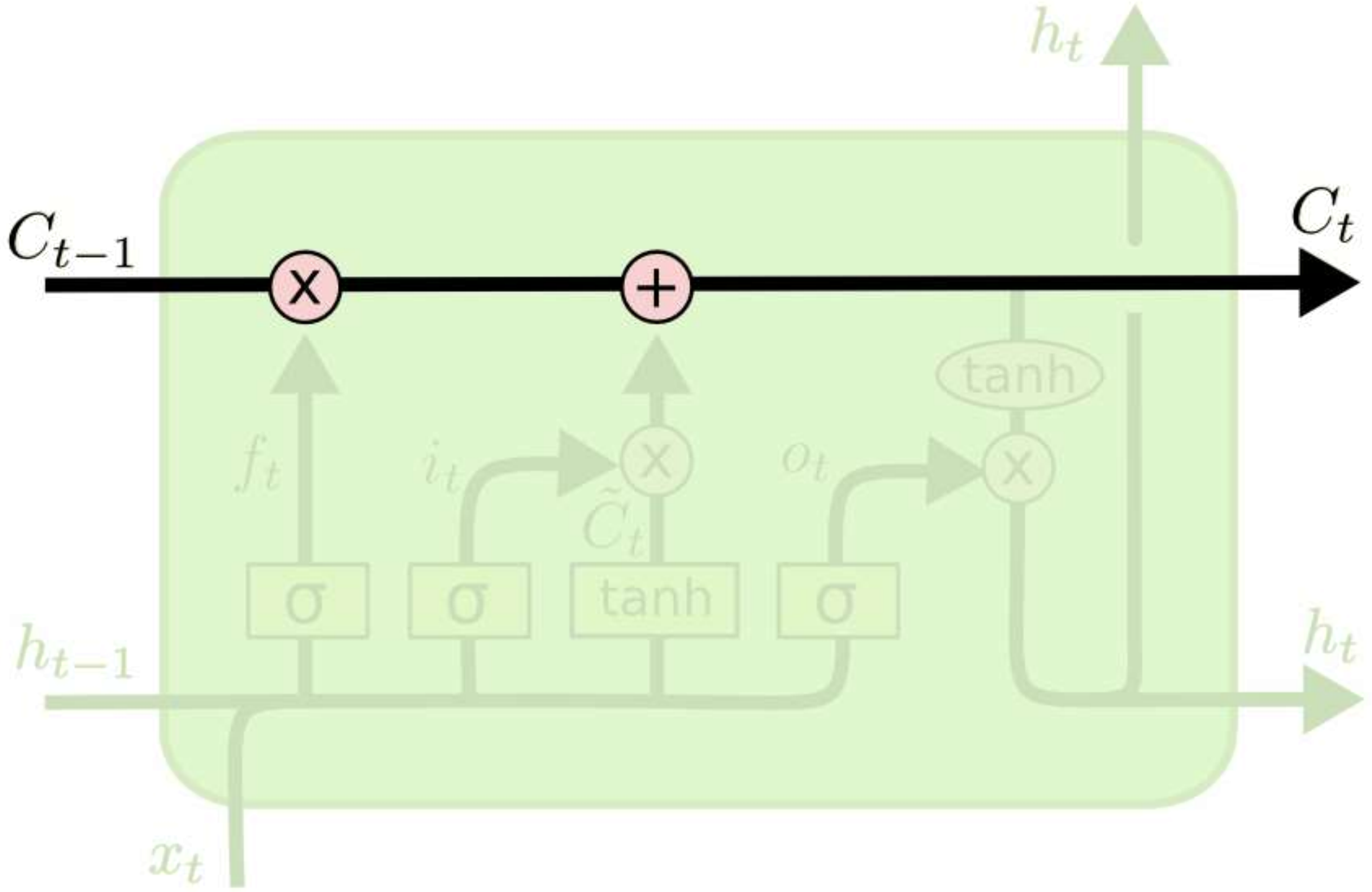
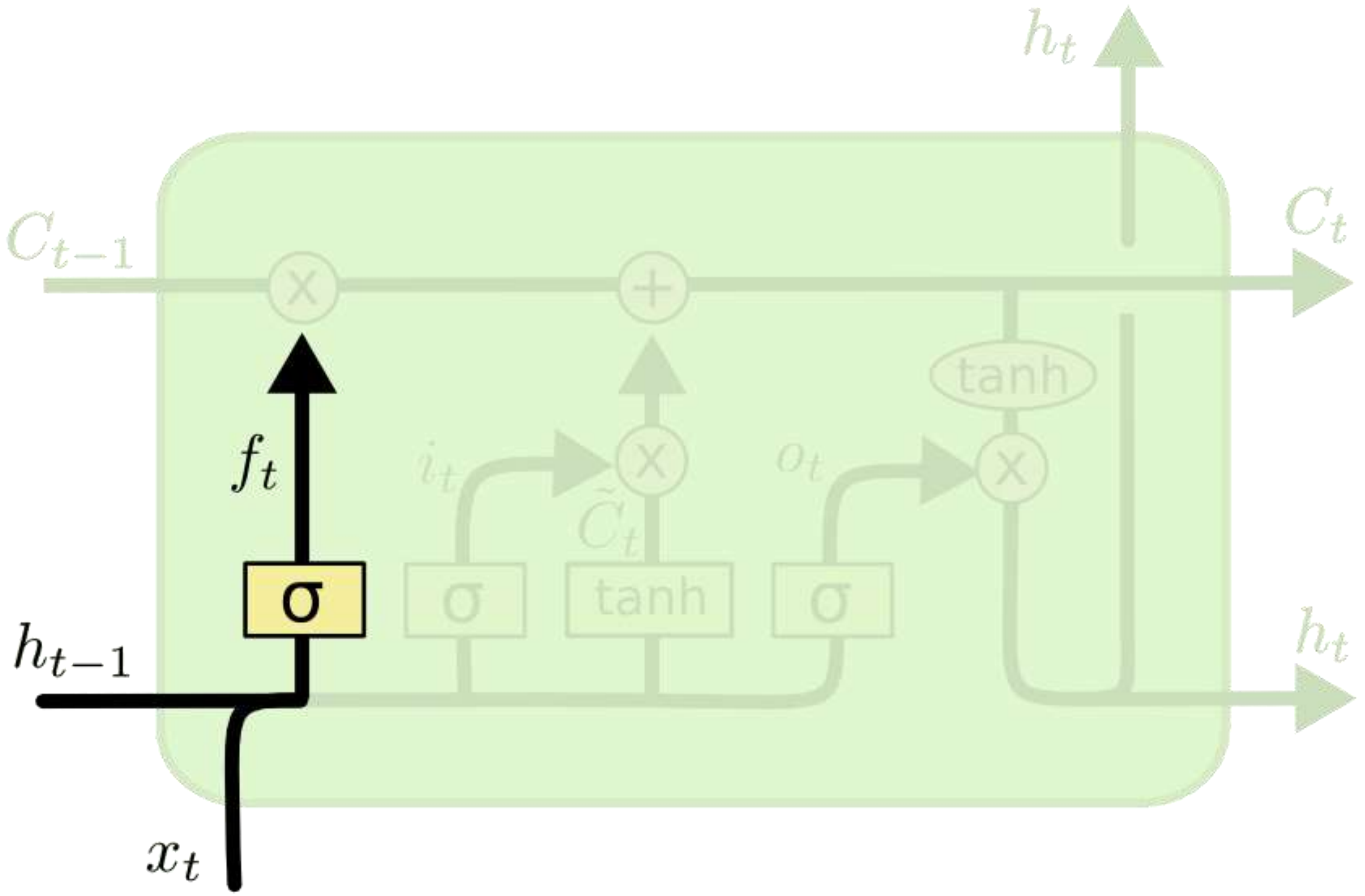


Cell state = a conveyor belt

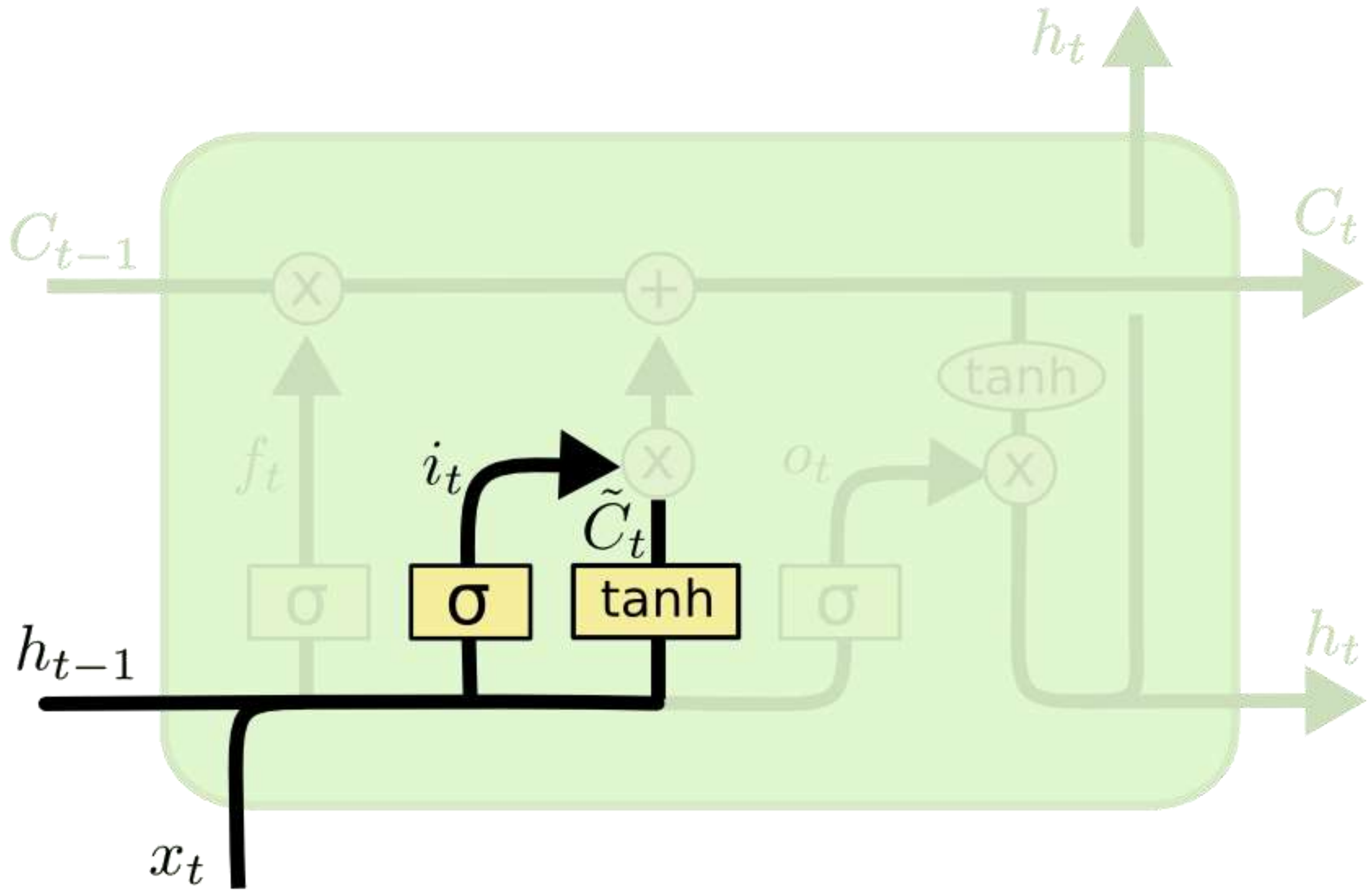
It allows **adding** or **removing** information, carefully regulated by gates

Visualization of LSTMs (Warning: notation change!)



$$f_t = \sigma\left(W_f \cdot [h_{t-1}, x_t] \ + \ b_f\right)$$

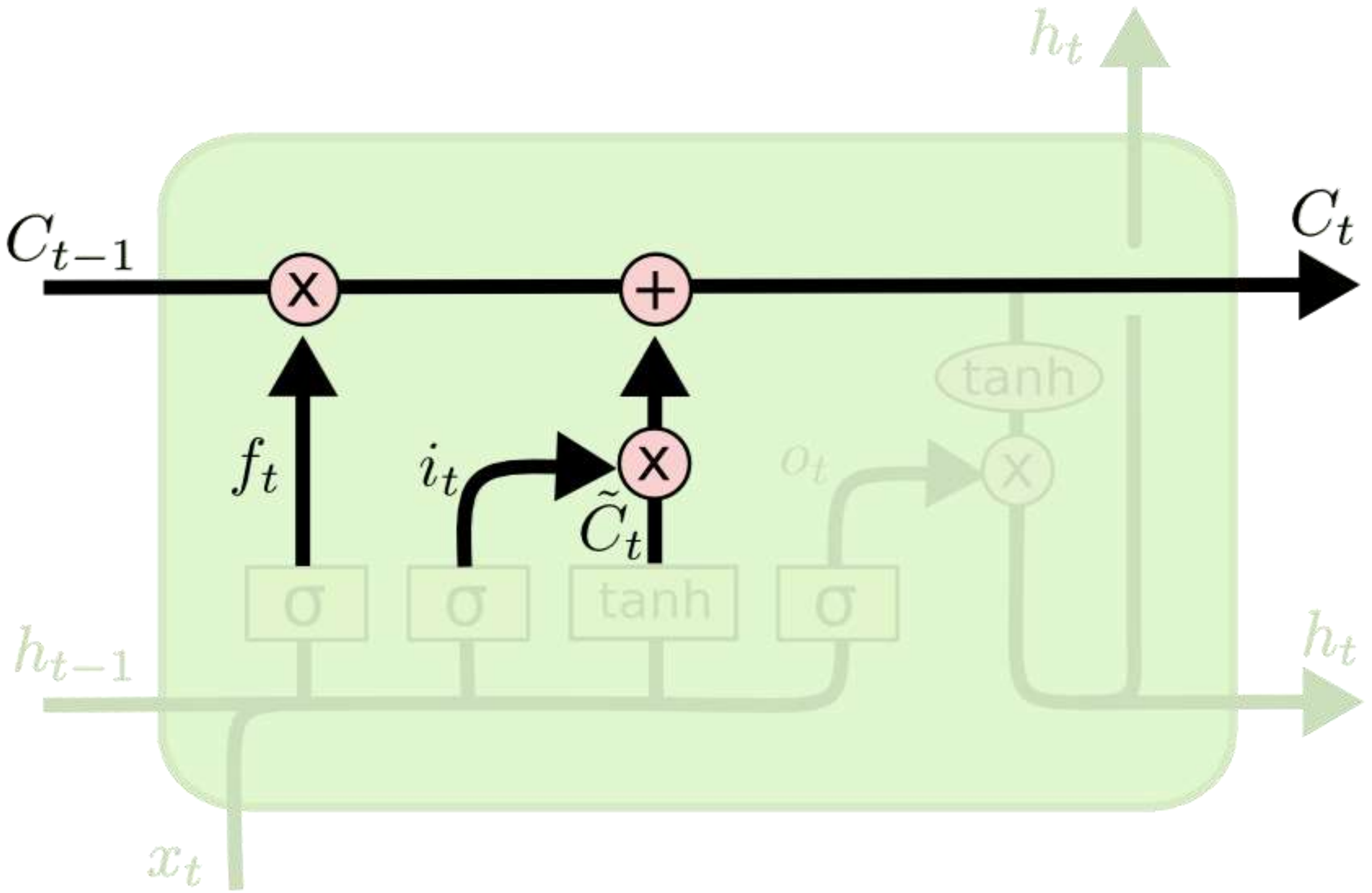
Visualization of LSTMs (Warning: notation change!)



$$i_t = \sigma\left(W_i \cdot [h_{t-1}, x_t] \ + \ b_i\right)$$

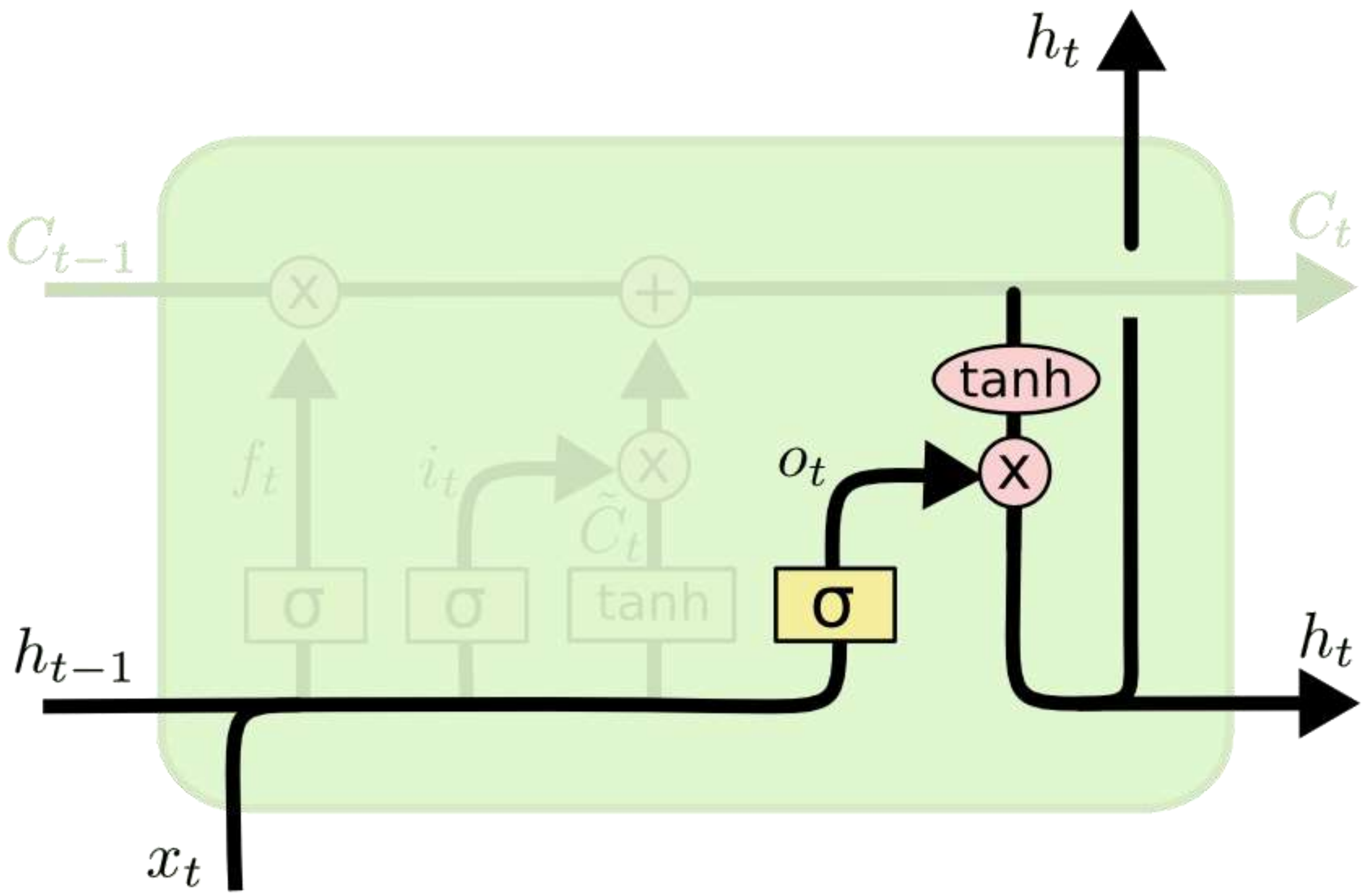
$$\tilde{C}_t = \tanh(W_C \cdot [h_{t-1}, x_t] \ + \ b_C)$$

Visualization of LSTMs (Warning: notation change!)



$$C_t = f_t * C_{t-1} + i_t * \tilde{C}_t$$

Visualization of LSTMs (Warning: notation change!)



$$o_t = \sigma\left(W_o\ [h_{t-1}, x_t]\ +\ b_o\right)$$

$$h_t = o_t * \tanh\left(C_t\right)$$

Gated Recurrent Units (GRUs)

- Introduced by Kyunghyun Cho et al. in 2014:

Learning Phrase Representations using RNN Encoder–Decoder for Statistical Machine Translation

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- Simplified 3 gates to 2 gates: **reset** gate and **update** gate, without an explicit cell state

Gated Recurrent Units (GRUs)

- Reset gate:

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

- Update gate:

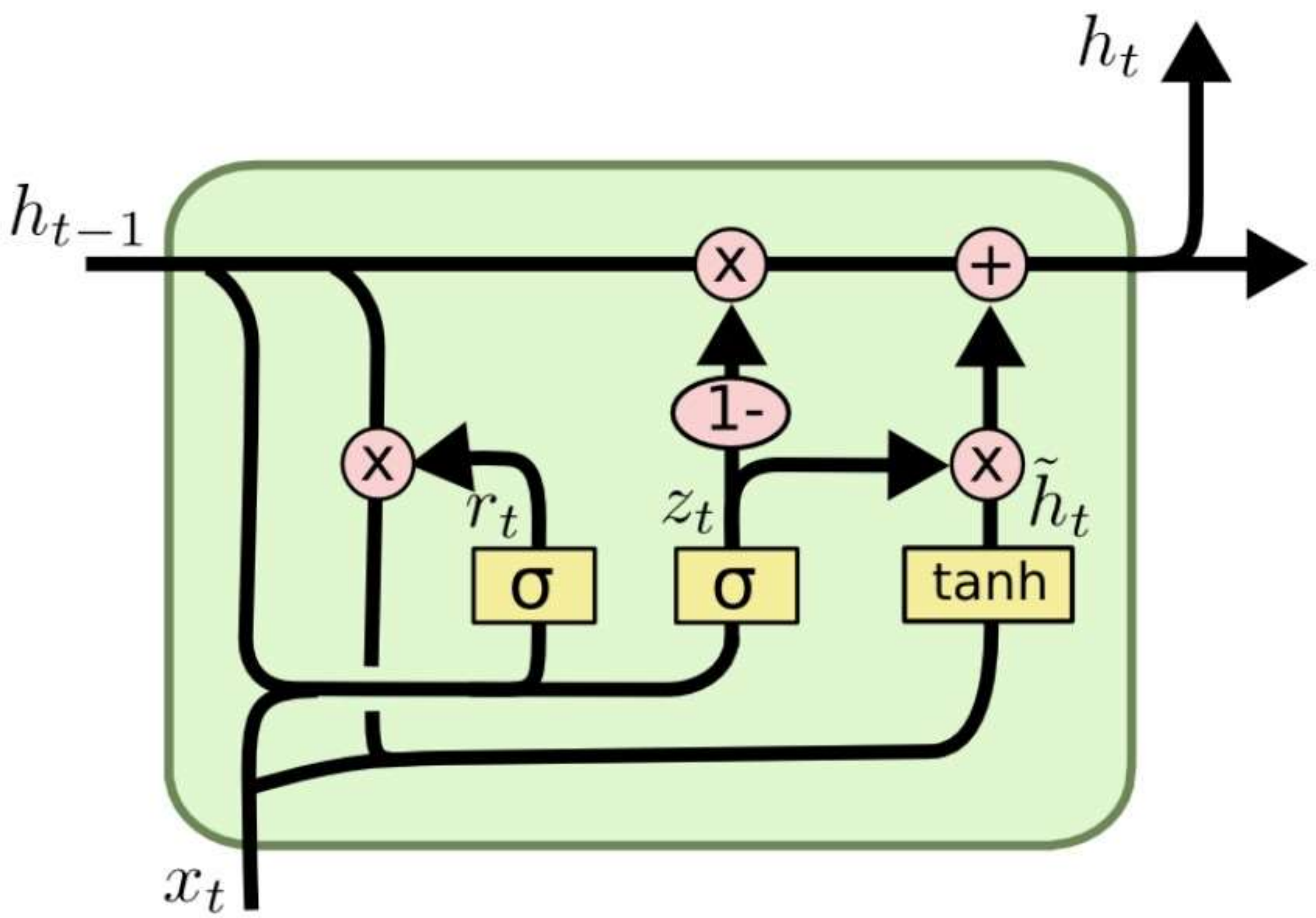
$$\mathbf{z}_t = \sigma(\mathbf{W}^z\mathbf{h}_{t-1} + \mathbf{U}^z\mathbf{x}_t + \mathbf{b}^z)$$

- New hidden state:

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

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

merge input and forget gate!



Q: What is the range of the hidden representations $\mathbf{h}_t$?

Q: How many parameters are there compared to simple RNNs?

Comparison of LSTMs and GRUs

Let’s compare LSTMs and GRUs. Which of the following statements is correct?

(a) GRUs can be trained faster

(b) In theory LSTMs can capture long-term dependencies better

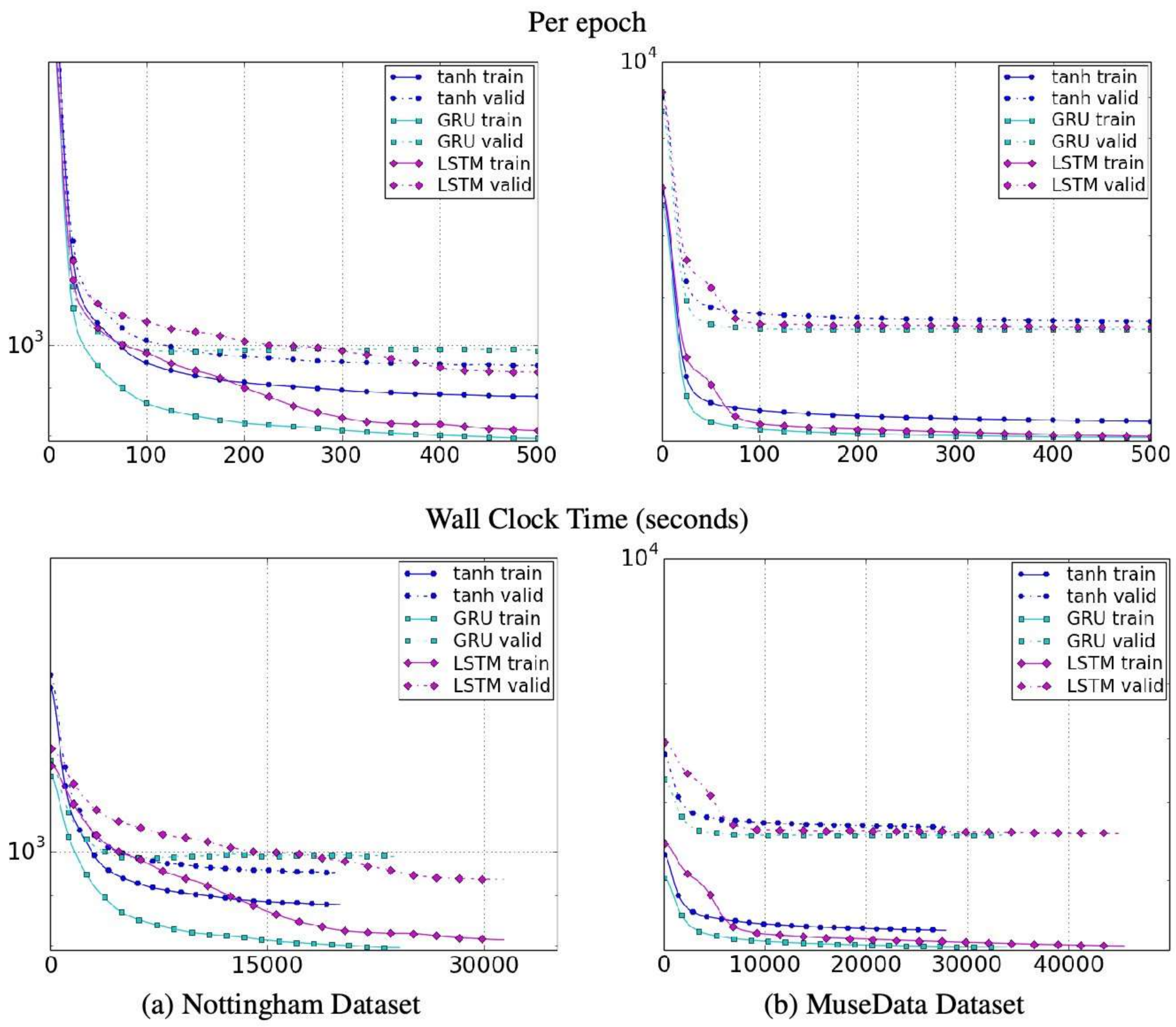
(c) LSTMs have a controlled exposure of memory content while GRUs don’t

(d) All of the above

The answer is (d). All of these are correct.

LSTMs vs GRUs

Music modeling

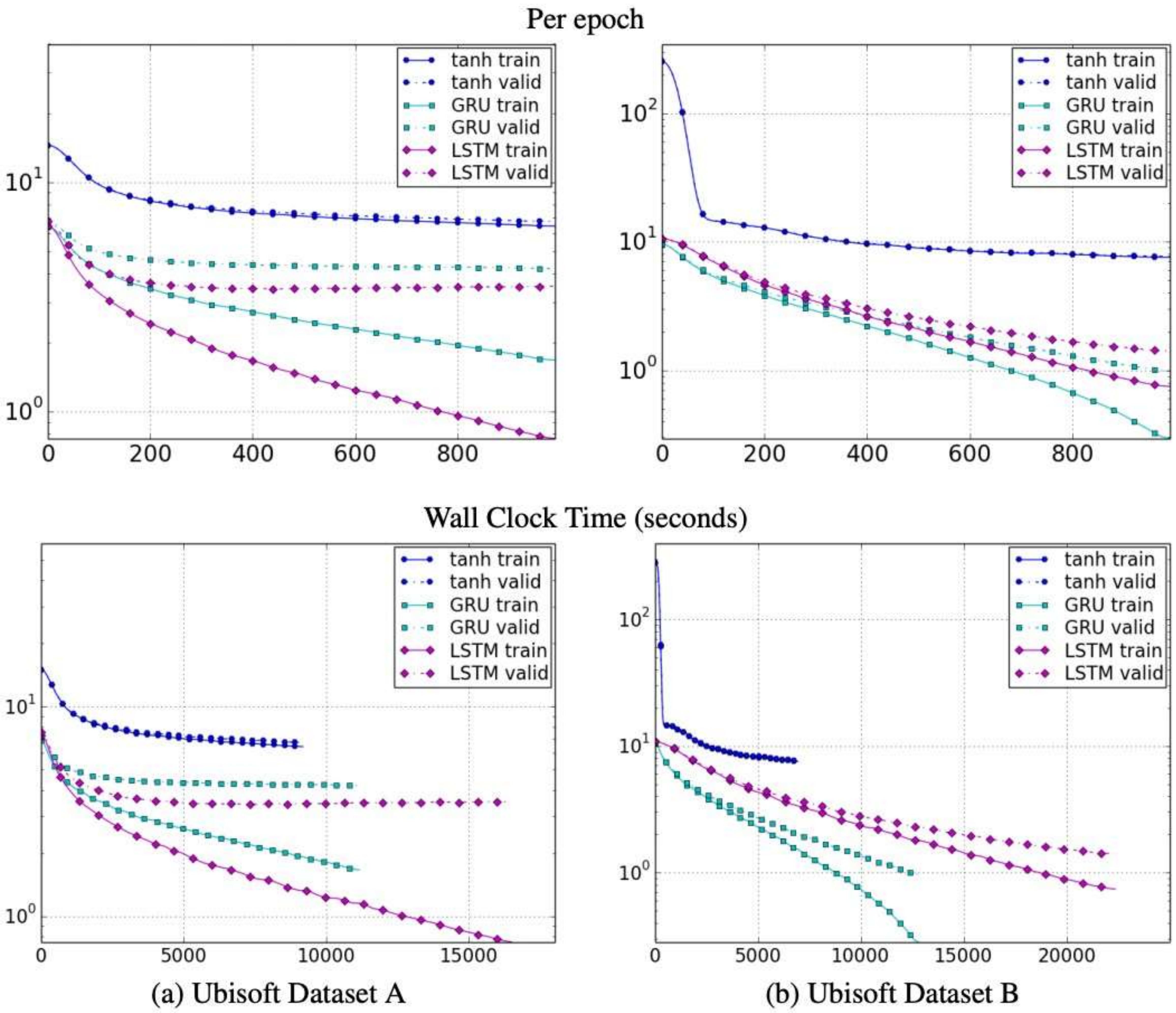


(Chung et al, 2014): Empirical Evaluation of Gated Recurrent Neural Networks on Sequence Modeling

LSTMs vs GRUs

Speech signal modeling

https://imgflip.com/i/495iim
(only for fun!!!)



(Chung et al, 2014): Empirical Evaluation of Gated Recurrent Neural Networks on Sequence Modeling

Are LSTMs and GRUs optimal?

MUT1:

$$\begin{aligned} z &= \mathrm{sigm}(W_{\mathrm{xz}} x_t + b_{\mathrm{z}}) \\ r &= \mathrm{sigm}(W_{\mathrm{xr}} x_t + W_{\mathrm{hr}} h_t + b_{\mathrm{r}}) \\ h_{t+1} &= \tanh(W_{\mathrm{hh}}(r \odot h_t) + \tanh(x_t) + b_{\mathrm{h}}) \odot z \\ &+ h_t \odot (1 - z) \end{aligned}$$

MUT2:

$$\begin{aligned} z &= \mathrm{sigm}(W_{\mathrm{xz}} x_t + W_{\mathrm{hz}} h_t + b_{\mathrm{z}}) \\ r &= \mathrm{sigm}(x_t + W_{\mathrm{hr}} h_t + b_{\mathrm{r}}) \\ h_{t+1} &= \tanh(W_{\mathrm{hh}}(r \odot h_t) + W_{xh} x_t + b_{\mathrm{h}}) \odot z \\ &+ h_t \odot (1 - z) \end{aligned}$$

MUT3:

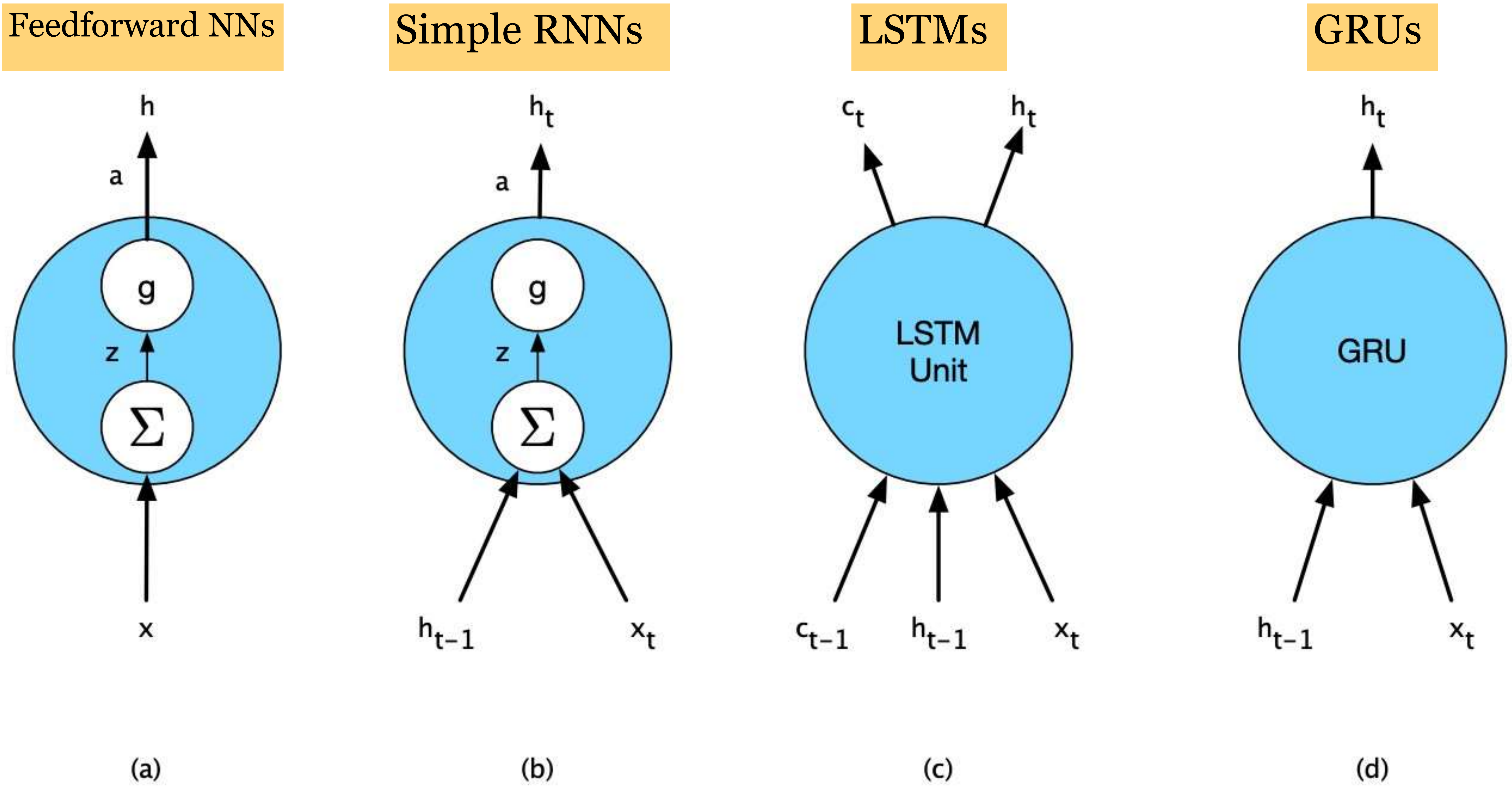
$$\begin{aligned} z &= \mathrm{sigm}(W_{\mathrm{xz}} x_t + W_{\mathrm{hz}} \tanh(h_t) + b_{\mathrm{z}}) \\ r &= \mathrm{sigm}(W_{\mathrm{xr}} x_t + W_{\mathrm{hr}} h_t + b_{\mathrm{r}}) \\ h_{t+1} &= \tanh(W_{\mathrm{hh}}(r \odot h_t) + W_{xh} x_t + b_{\mathrm{h}}) \odot z \\ &+ h_t \odot (1 - z) \end{aligned}$$

Arch.	Arith.	XML	PTB
Tanh	0.29493	0.32050	0.08782
LSTM	0.89228	0.42470	0.08912
LSTM-f	0.29292	0.23356	0.08808
LSTM-i	0.75109	0.41371	0.08662
LSTM-o	0.86747	0.42117	0.08933
LSTM-b	0.90163	0.44434	0.08952
GRU	0.89565	0.45963	0.09069
MUT1	**0.92135**	**0.47483**	0.08968
MUT2	0.89735	**0.47324**	0.09036
MUT3	0.90728	0.46478	**0.09161**

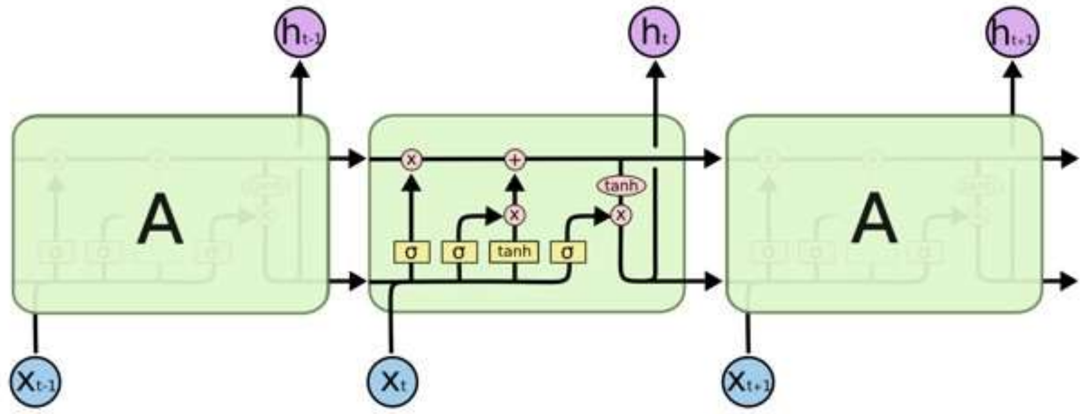
Arch.	5M-tst	10M-v	20M-v	20M-tst
Tanh	4.811	4.729	4.635	4.582 (97.7)
LSTM	4.699	4.511	4.437	4.399 (81.4)
LSTM-f	4.785	4.752	4.658	4.606 (100.8)
LSTM-i	4.755	4.558	4.480	4.444 (85.1)
LSTM-o	4.708	4.496	4.447	4.411 (82.3)
LSTM-b	4.698	4.437	4.423	**4.380 (79.83)**
GRU	4.684	4.554	4.559	4.519 (91.7)
MUT1	4.699	4.605	4.594	4.550 (94.6)
MUT2	4.707	4.539	4.538	4.503 (90.2)
MUT3	4.692	4.523	4.530	4.494 (89.47)

(Jozefowicz et al, 2015): An Empirical Exploration of Recurrent Network Architectures

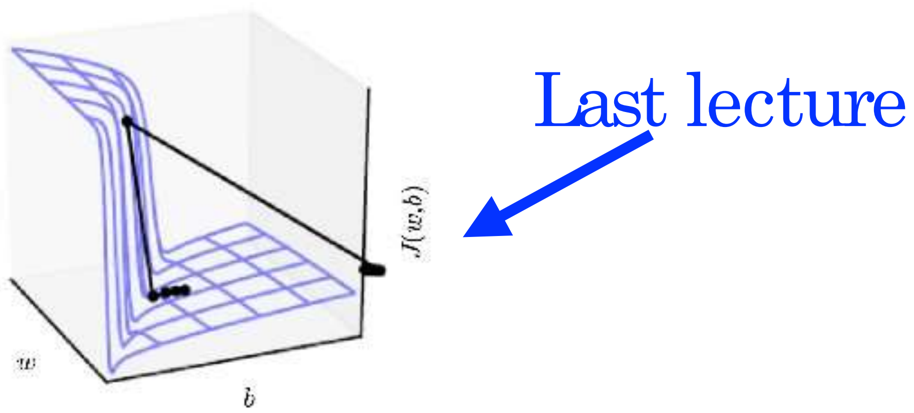
Comparison: FFNNs vs simple RNNs vs LSTMs vs GRUs



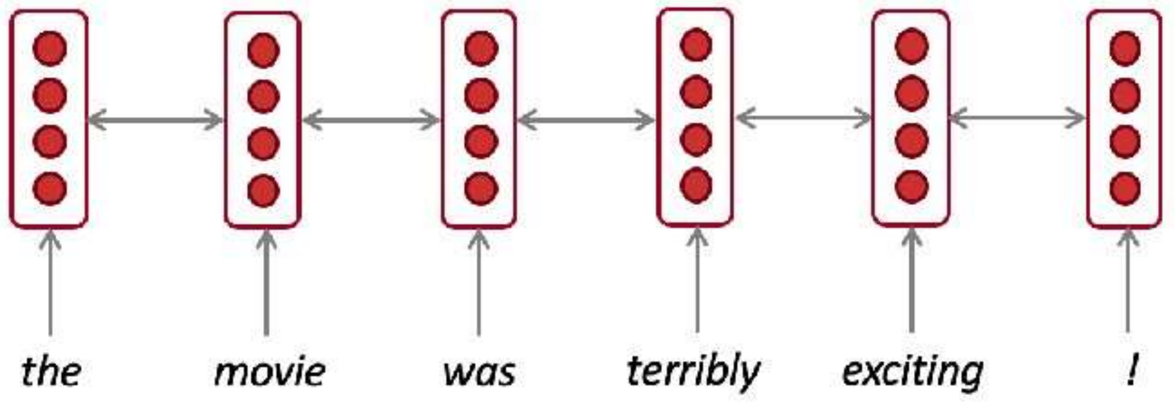
Practical takeaways



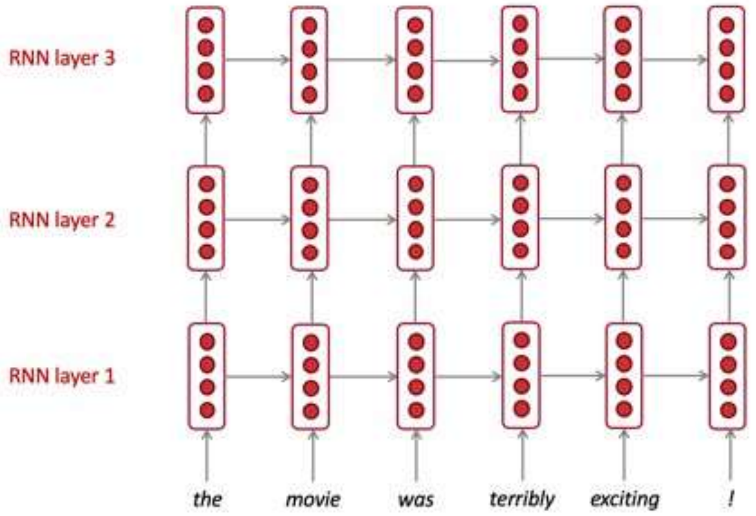
1. LSTMs are powerful



2. Clip your gradients



3. Use bidirectionality when possible



4. Multi-layer RNNs are more powerful, but you might need skip connections if it's deep

Simple recurrent units (SRU)

Simple Recurrent Units for Highly Parallelizable Recurrence

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2017

$$
\begin{aligned}
\mathbf{f}_t &= \sigma\left(\boxed{\mathbf{W}_f\mathbf{x}_t} + \boxed{\mathbf{v}_f} \odot \mathbf{c}_{t-1} + \mathbf{b}_f\right) \\
\mathbf{c}_t &= \mathbf{f}_t \odot \mathbf{c}_{t-1} + (1 - \mathbf{f}_t) \odot \boxed{(\mathbf{W}\mathbf{x}_t)} \\
\mathbf{r}_t &= \sigma\left(\boxed{\mathbf{W}_r\mathbf{x}_t} + \boxed{\mathbf{v}_r} \odot \mathbf{c}_{t-1} + \mathbf{b}_r\right) \\
\mathbf{h}_t &= \mathbf{r}_t \odot \mathbf{c}_t + (1 - \mathbf{r}_t) \odot \mathbf{x}_t
\end{aligned}
$$

- Lighter form of recurrent neural networks
- Enable high amounts of parallelism in computation, while maintaining expressivity of recurrent computation
- Use of CUDA kernels to maximize parallel operations

(Lei et al, 2017): Simple Recurrent Units for Highly Parallelizable Recurrence