COSC 4368 Fundamentals of Artificial Intelligence

Recurrent Neural Networks

October 25th, 2023

(slides modified from Stanford cs321n)

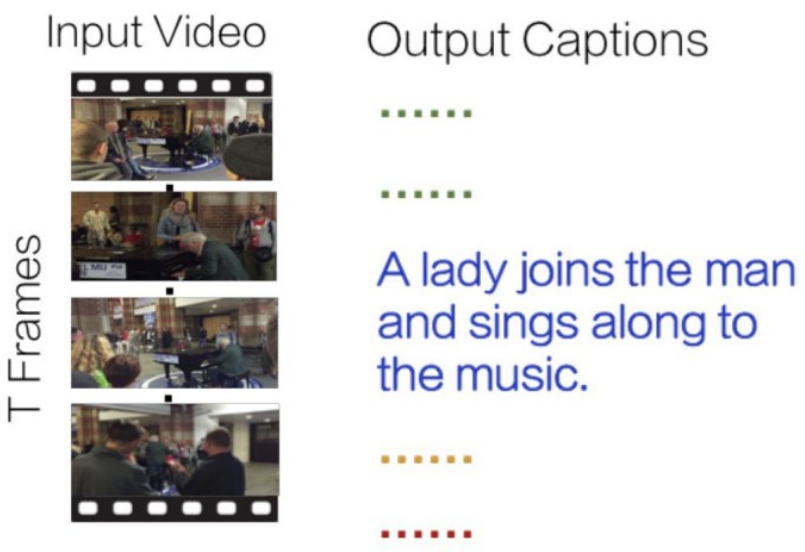
Why existing convets are insufficient?

Variable sequence length inputs and outputs!

Example task: video captioning

Input video can have variable number of frames

Output captions can be variable length.



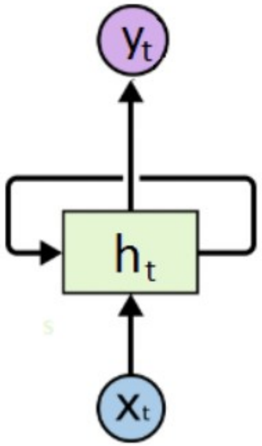
Krishna, Hata, Ren, Fei-Fei, Niebles. Dense captioning Events in Videos. ICCV 2019

The sequence of inputs also matters in many applications, not i.i.d.

Recurrent neural networks

Recurrent neural networks (RNNs) are networks with loops, allowing information to persist [Rumelhart et al., 1986].

$$\underbrace{\boxed{h_t}}_{\text{new state}} = \underbrace{\boxed{f_W}}_{\substack{\text{some function}\\ \text{with parameters W}}}(\underbrace{\boxed{h_{t-1}}}_{\text{old state}}, \underbrace{\boxed{x_t}}_{\substack{\text{input vector at}\\ \text{some time step}}})$$

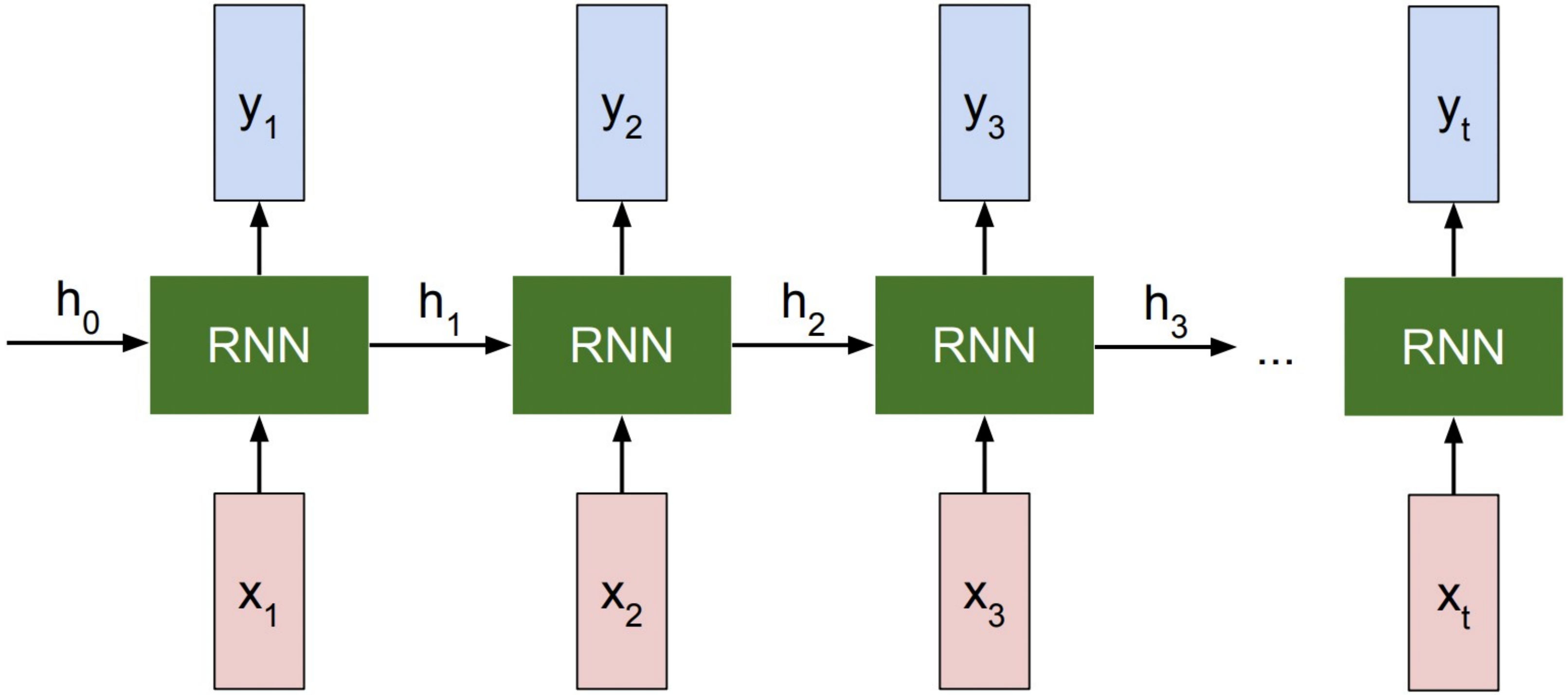


Have **memory** that keeps track of information observed so far

Maps from the entire history of previous inputs to each output

Handle sequential data

Unrolled RNN



RNN hidden state update

We can process a sequence of vectors **x** by applying a **recurrence formula** at every time step:

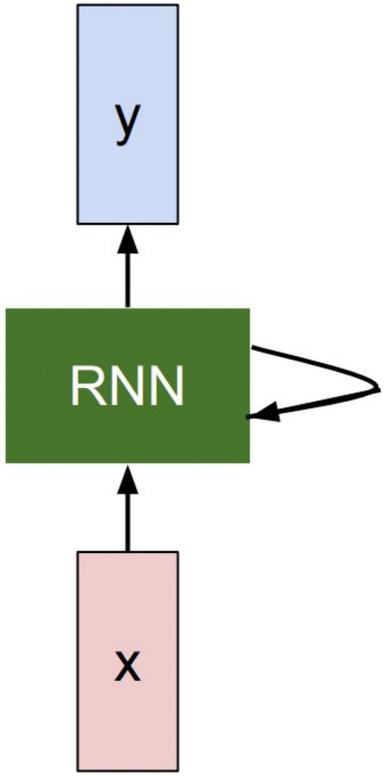
$$\boxed{h_t} = \boxed{f_W}(\boxed{h_{t-1}}, \boxed{x_t})$$

new state

old state

input vector at some time step

some function with parameters W

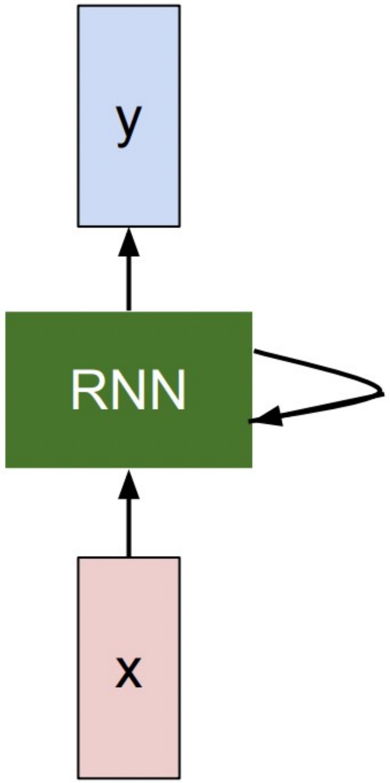


The same function and the same set of parameters are used at each time step

RNN output generation

We can process a sequence of vectors **x** by applying a **recurrence formula** at every time step:

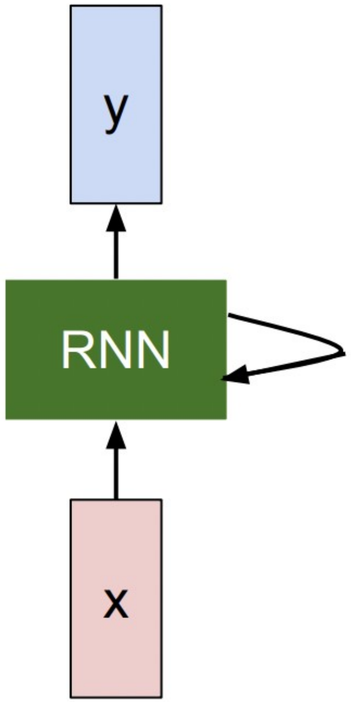
$$\underbrace{\boxed{y_t}}_{\text{output}} = \underbrace{\boxed{f_{W_{hy}}}}_{\text{another function with parameters } W_o}(\underbrace{\boxed{h_t}}_{\text{new state}})$$



The same function and the same set of parameters are used at each time step

(Simple) Recurrent neural network

The state consists of a single *"hidden"* vector **h**:



$$h_t = f_W(h_{t-1}, x_t)$$

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

$$y_t = W_{hy} h_t$$

Input-output scenarios

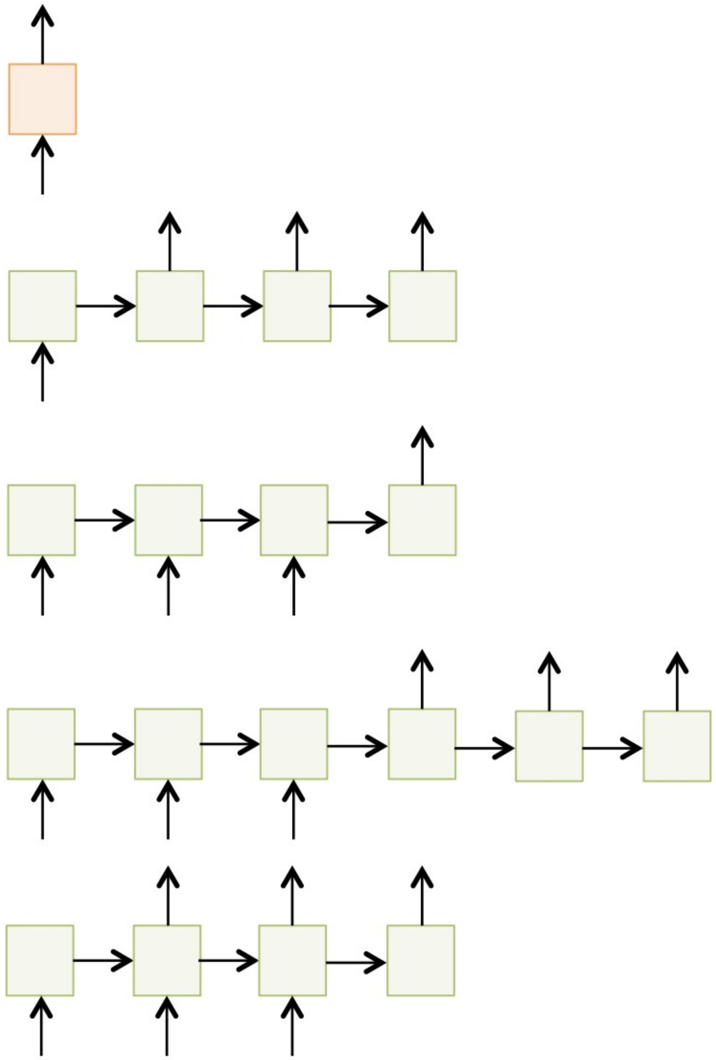
Single - Single — Feed-forward Network

Single - Multiple — Image Captioning

Multiple - Single — Sentiment Classification

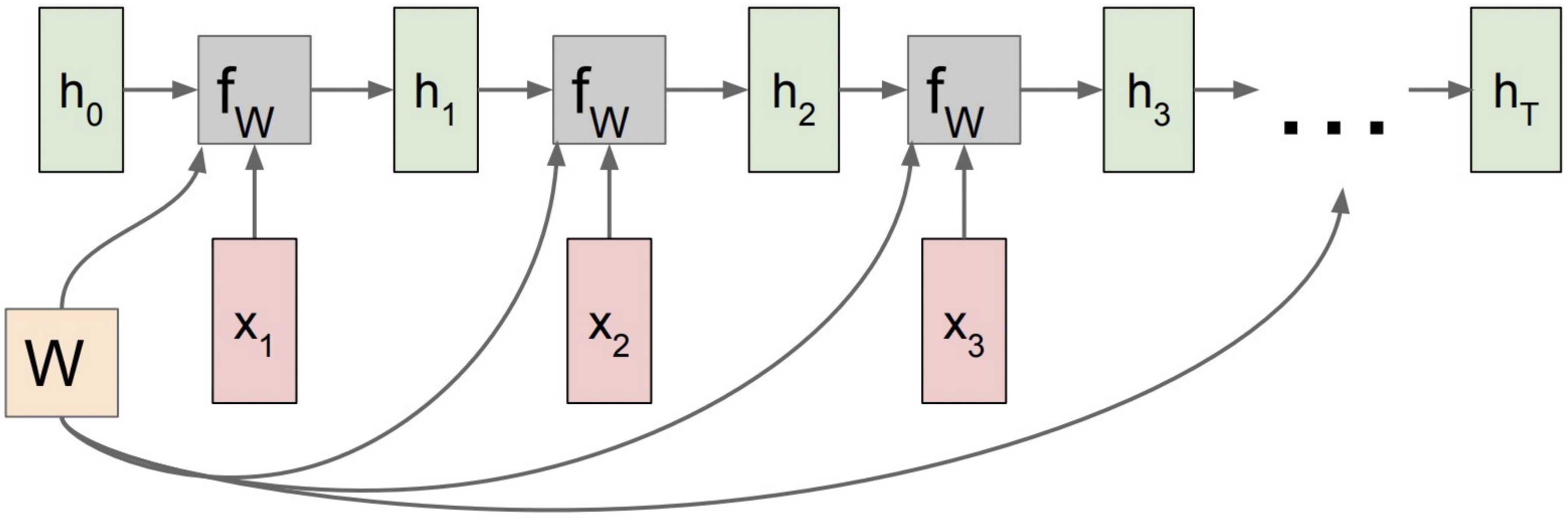
Multiple - Multiple — Translation

Image Captioning

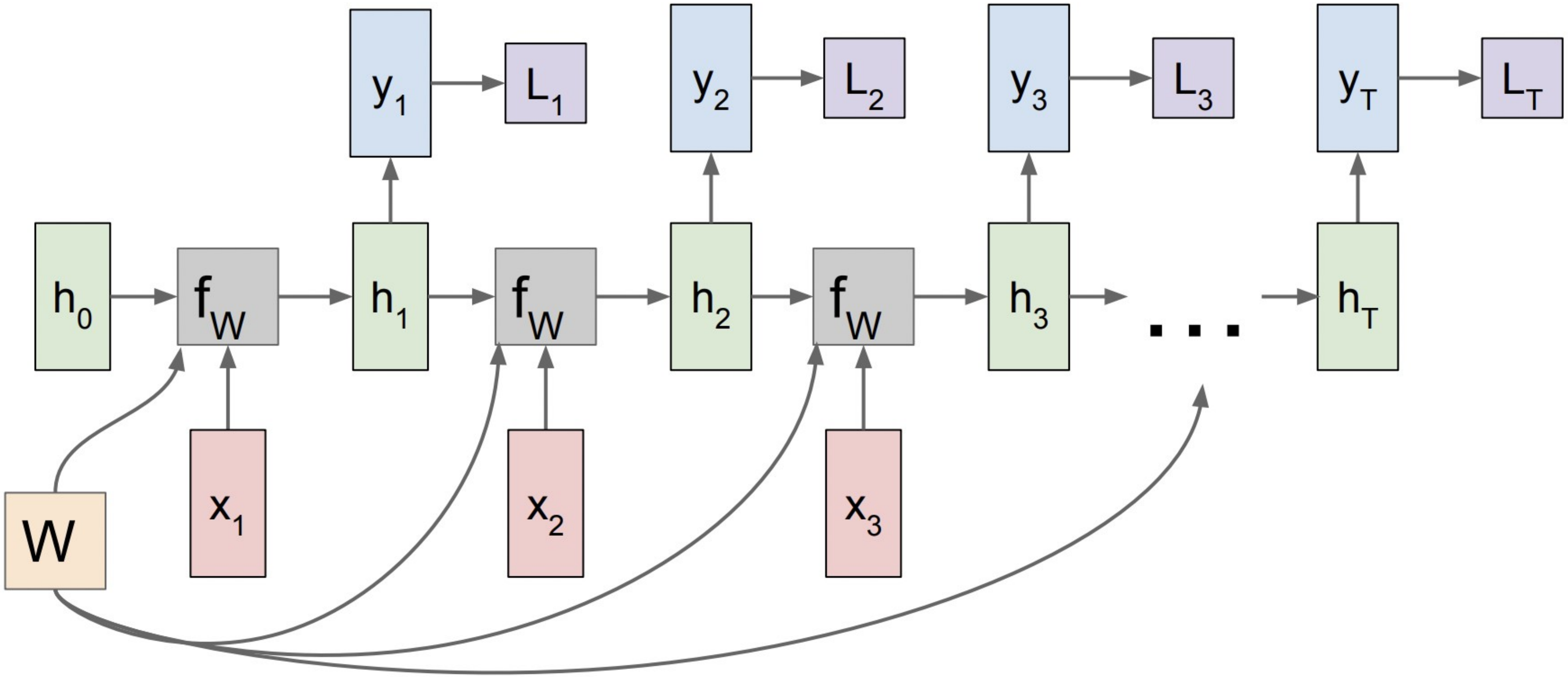


RNN: computational graph

Re-use the same weight matrix at every time-step



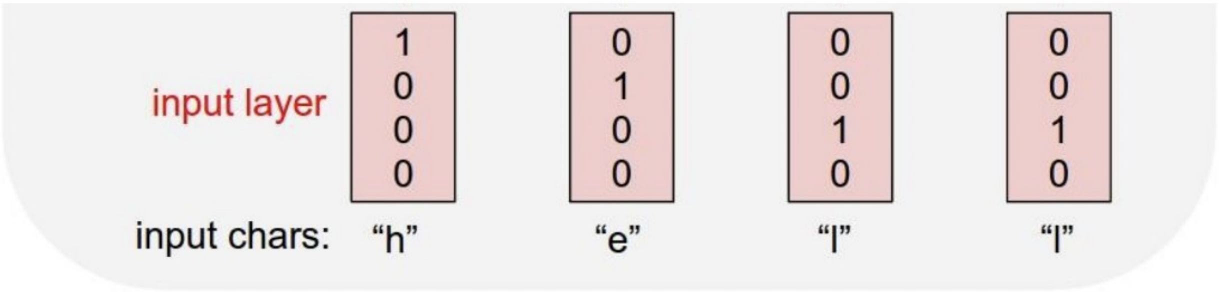
RNN: computational graph: many to many



Example: character-level language model

Vocabulary:
[h,e,l,o]

Example training sequence:
“hello”



Example: character-level language model

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

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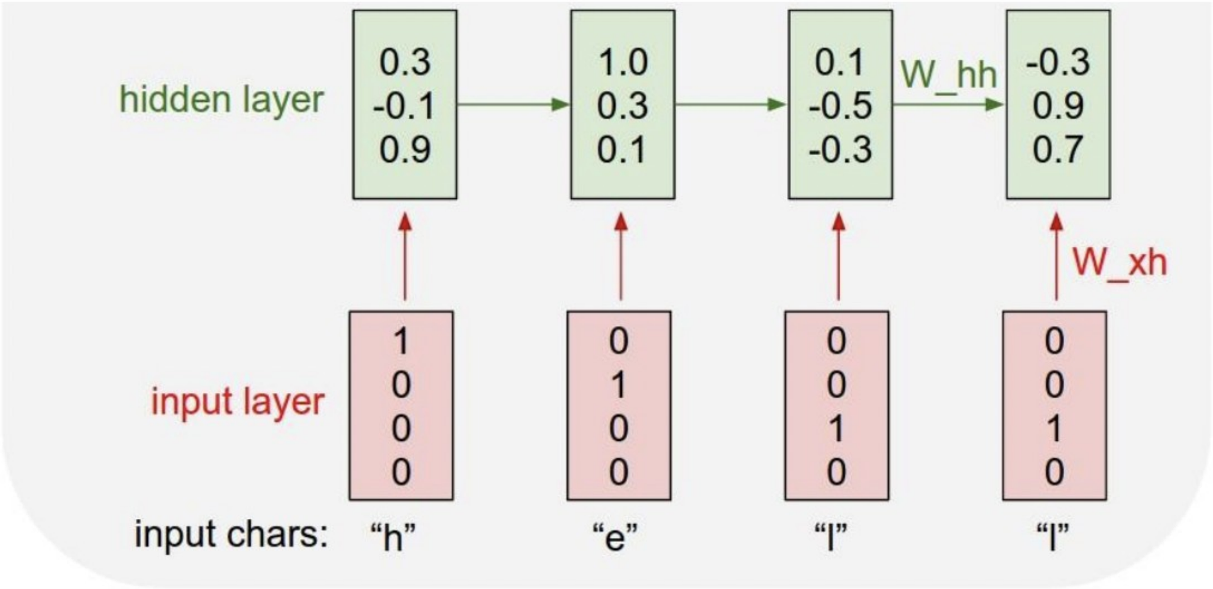

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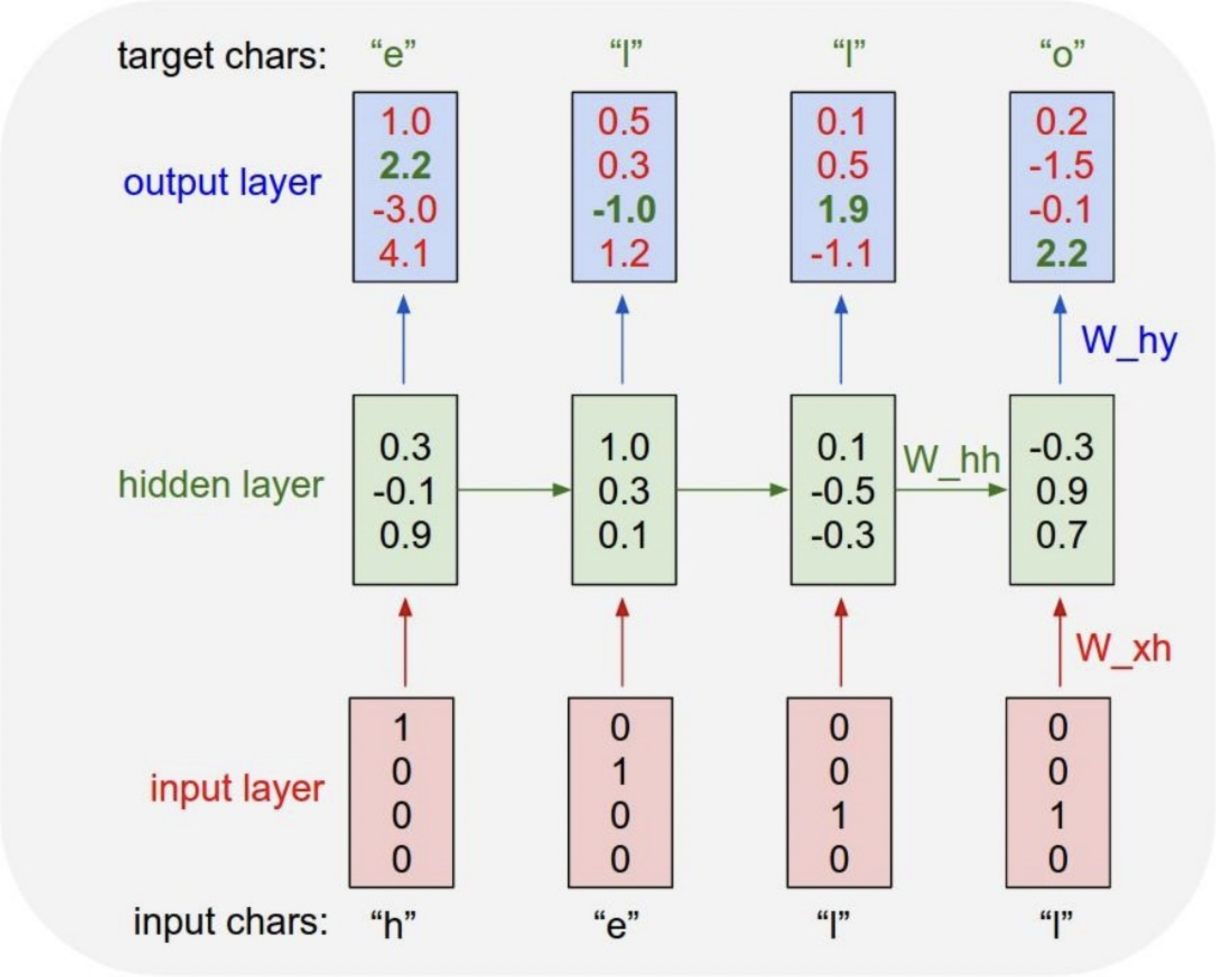
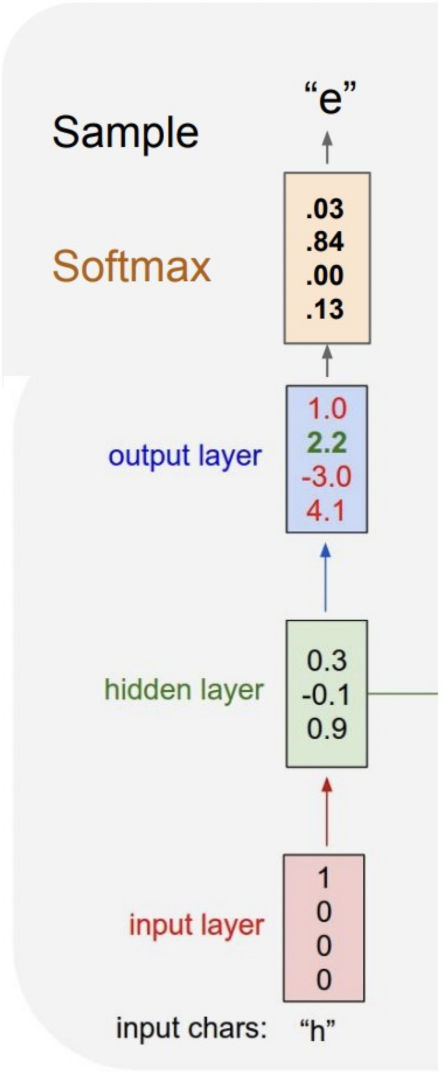


Example: character-level language model

**Example:
Character-level
Language Model
Sampling**

Vocabulary:
[h,e,l,o]

At test-time sample characters one at a time, feed back to model



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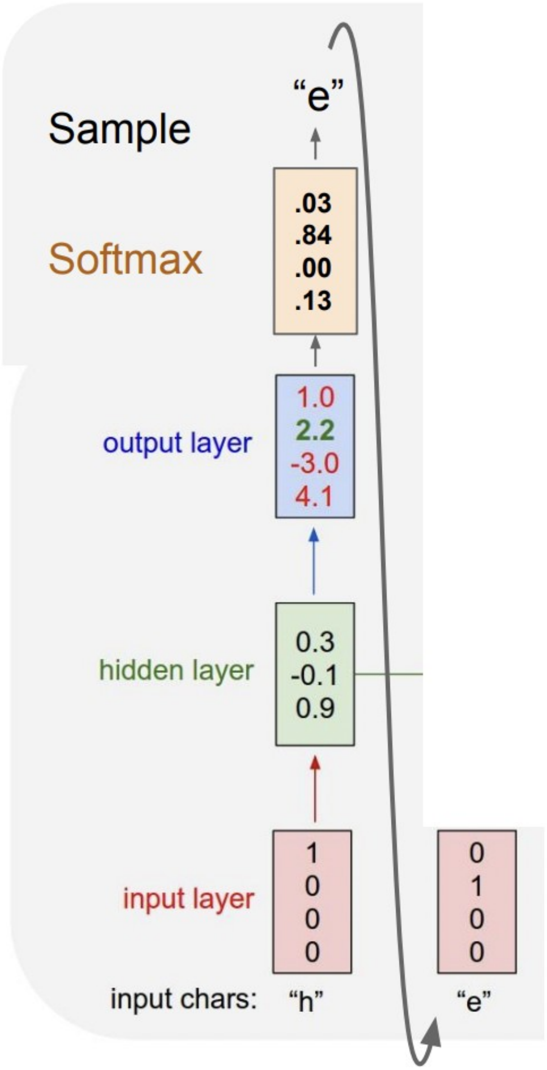

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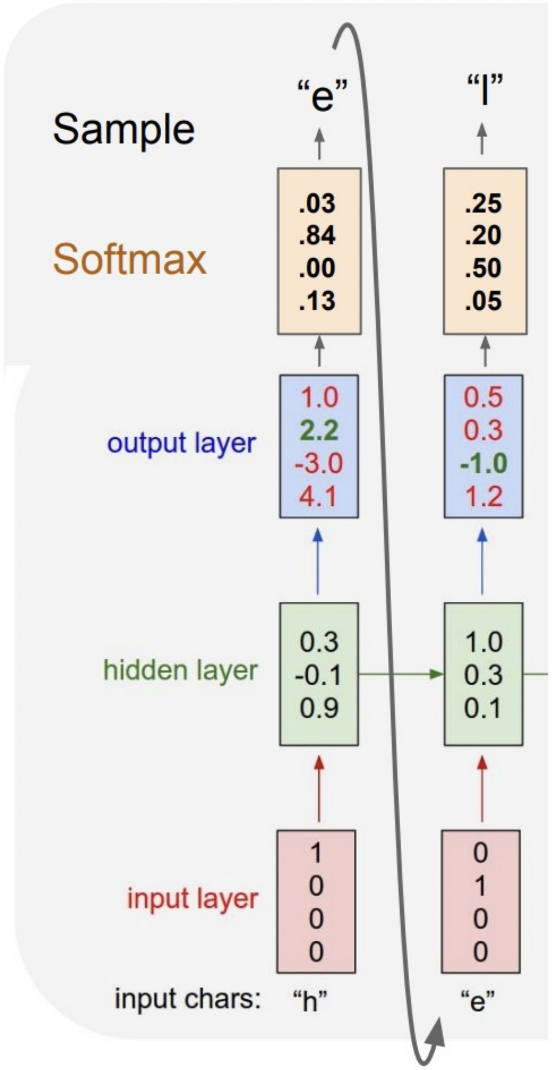

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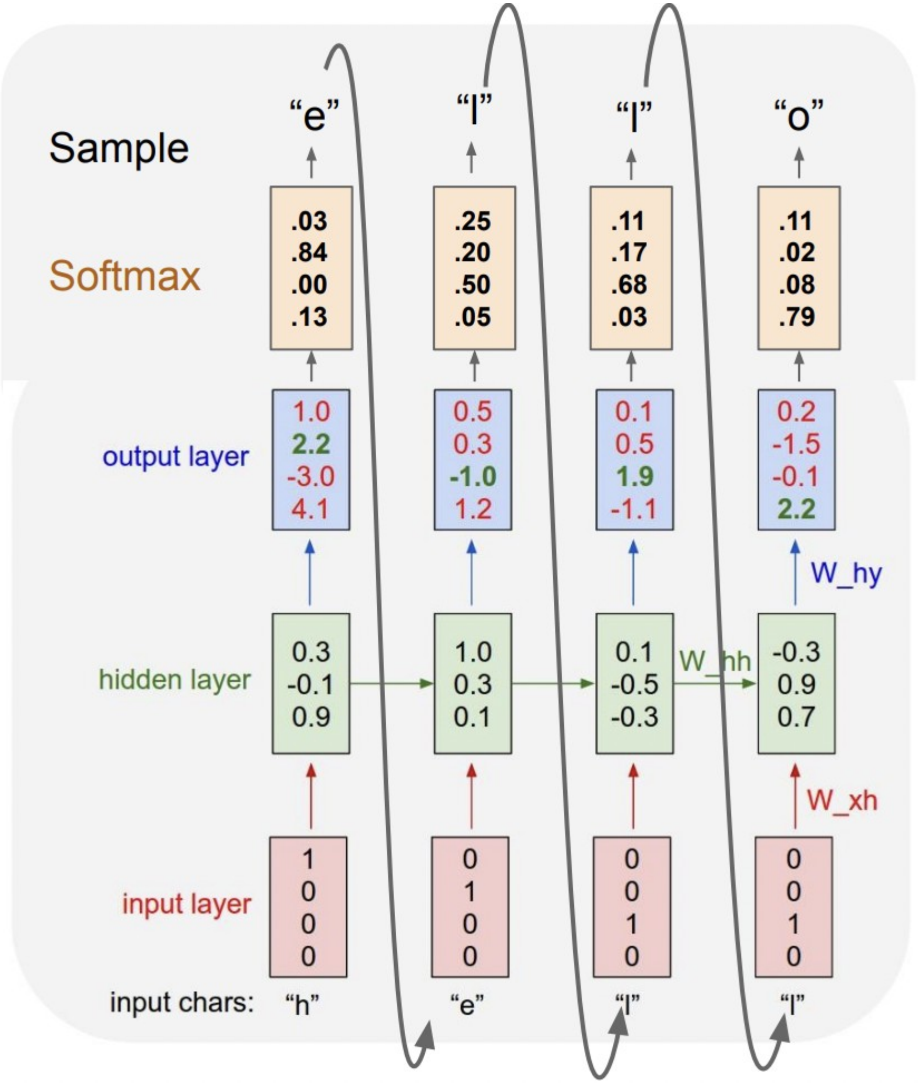
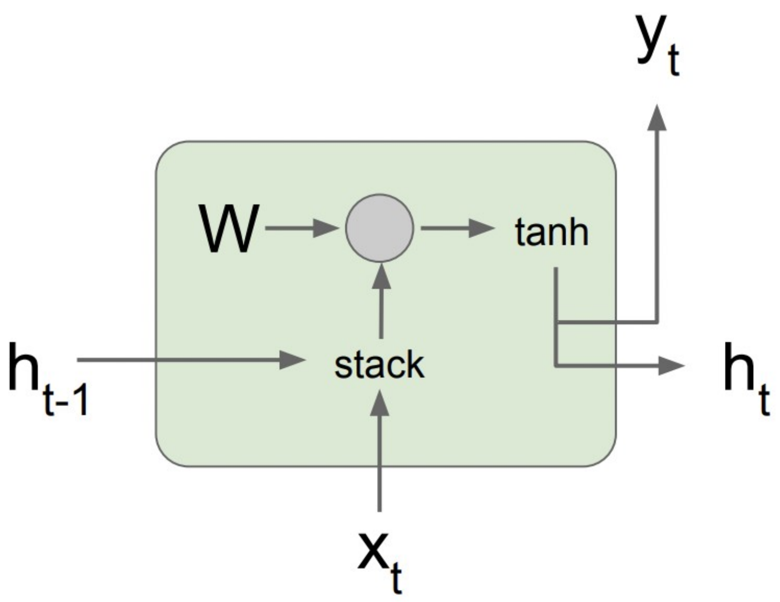
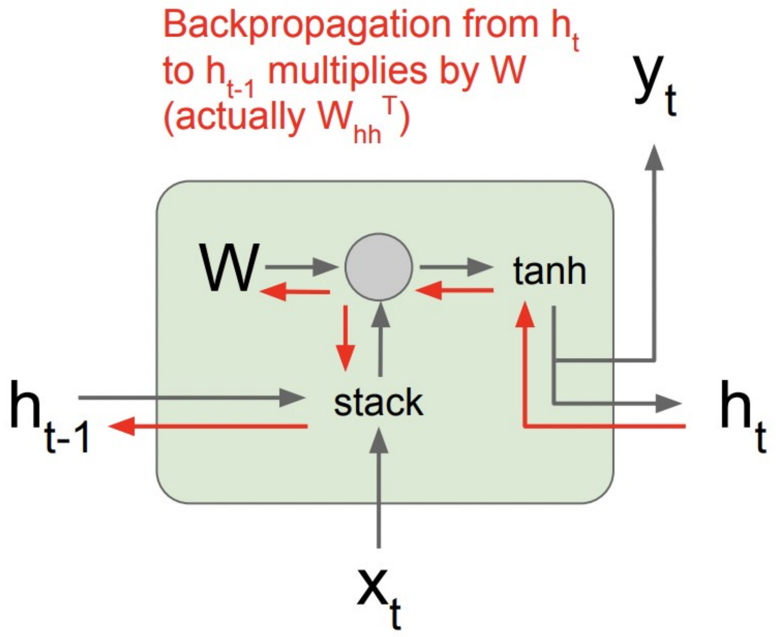


Vanilla RNN gradient flow



$$
\begin{aligned}
h_t &= \tanh(W_{hh}h_{t-1} + W_{xh}x_t) \\
&= \tanh\left(\begin{pmatrix} W_{hh} & W_{hx} \end{pmatrix} \begin{pmatrix} h_{t-1} \\ x_t \end{pmatrix}\right) \\
&= \tanh\left(W \begin{pmatrix} h_{t-1} \\ x_t \end{pmatrix}\right)
\end{aligned}
$$

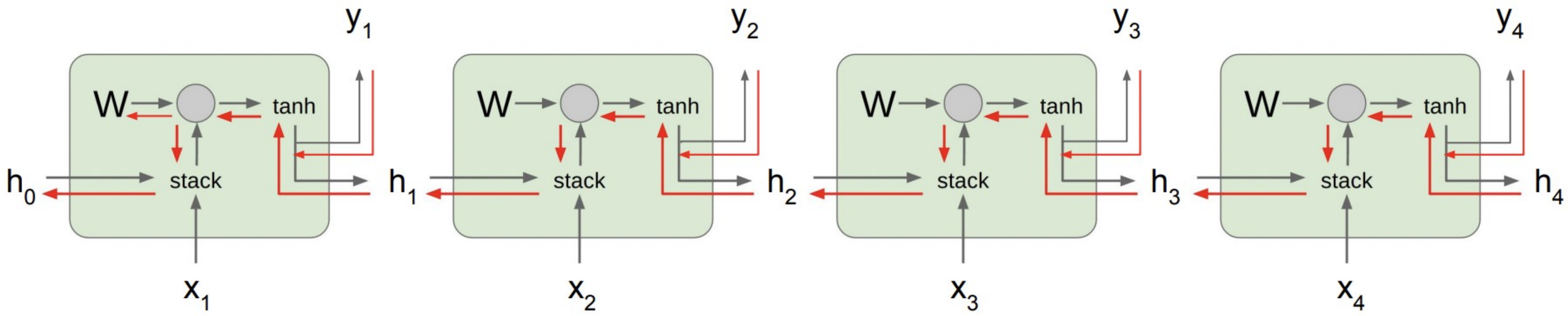
Vanilla RNN gradient flow



$$h_t = \tanh(W_{hh}h_{t-1} + W_{xh}x_t)$$
$$= \tanh\left(\begin{pmatrix} W_{hh} & W_{hx} \end{pmatrix} \begin{pmatrix} h_{t-1} \\ x_t \end{pmatrix}\right)$$
$$= \tanh\left(W \begin{pmatrix} h_{t-1} \\ x_t \end{pmatrix}\right)$$

$$\frac{\partial h_t}{\partial h_{t-1}} = tanh'(W_{hh}h_{t-1} + W_{xh}x_t)W_{hh}$$

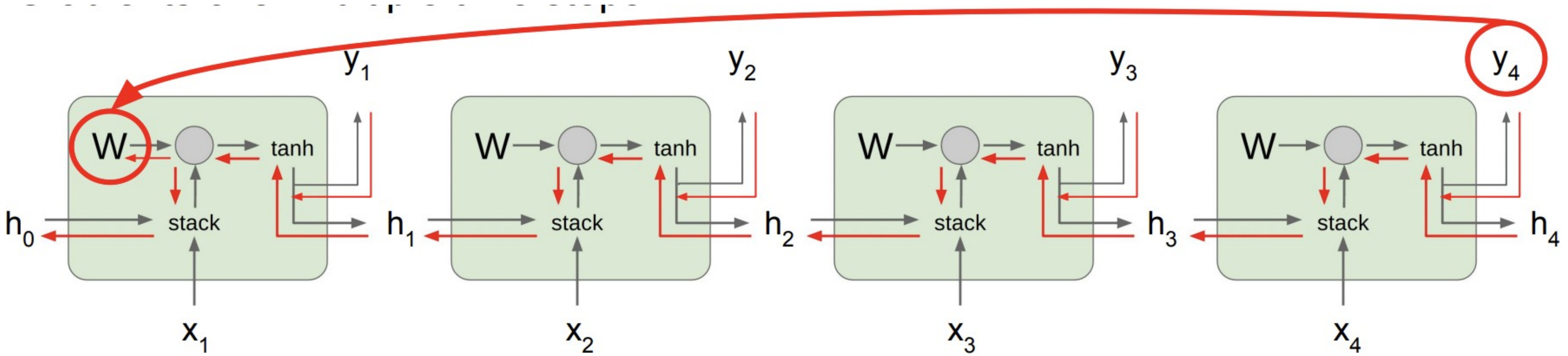
Vanilla RNN gradient flow



$$\frac{\partial L}{\partial W} = \sum_{t=1}^{T} \frac{\partial L_t}{\partial W}$$

Vanilla RNN gradient flow

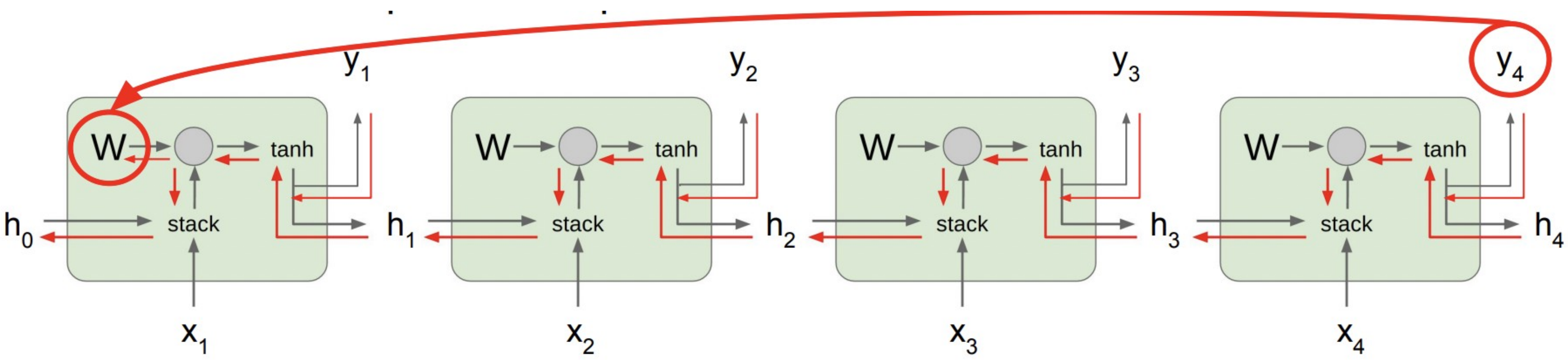
Backpropagation through time



$$\frac{\partial L}{\partial W} = \sum_{t=1}^{T} \frac{\partial L_t}{\partial W} \qquad \boxed{\frac{\partial h_t}{\partial h_{t-1}} = tanh'(W_{hh}h_{t-1} + W_{xh}x_t)W_{hh}}$$

$$\frac{\partial L_T}{\partial W} = \frac{\partial L_T}{\partial h_T}\frac{\partial h_t}{\partial h_{t-1}} \cdots \frac{\partial h_1}{\partial W} = \frac{\partial L_T}{\partial h_T}\left(\prod_{t=2}^{T} \boxed{\frac{\partial h_t}{\partial h_{t-1}}}\right)\frac{\partial h_1}{\partial W}$$

Vanilla RNN gradient flow



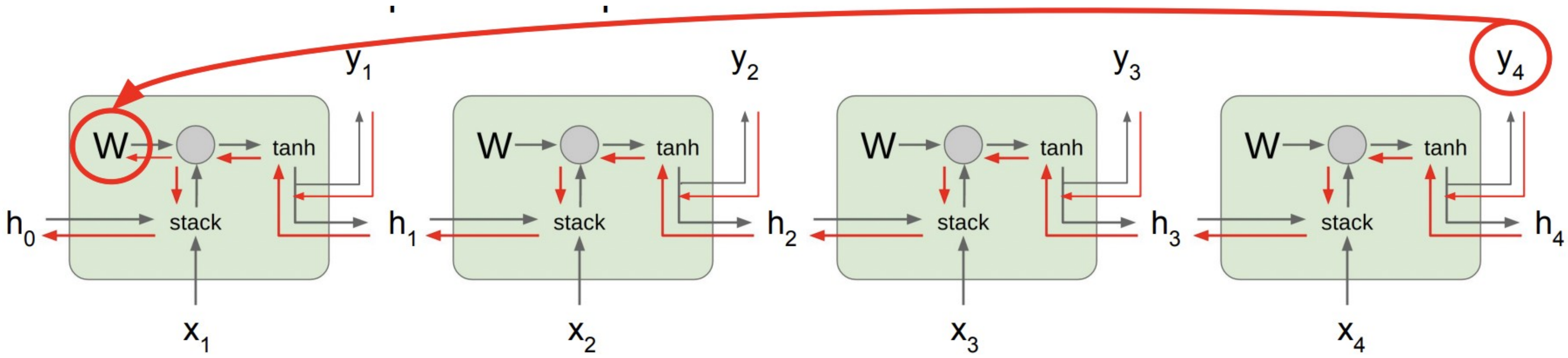
$$\frac{\partial L}{\partial W} = \sum_{t=1}^{T} \frac{\partial L_t}{\partial W}$$

Almost always < 1

Vanishing gradients

$$\frac{\partial L_T}{\partial W} = \frac{\partial L_T}{\partial h_T}\left(\prod_{t=2}^{T} \boxed{tanh'(W_{hh}h_{t-1} + W_{xh}x_t)}\right)W_{hh}^{T-1}\frac{\partial h_1}{\partial W}$$

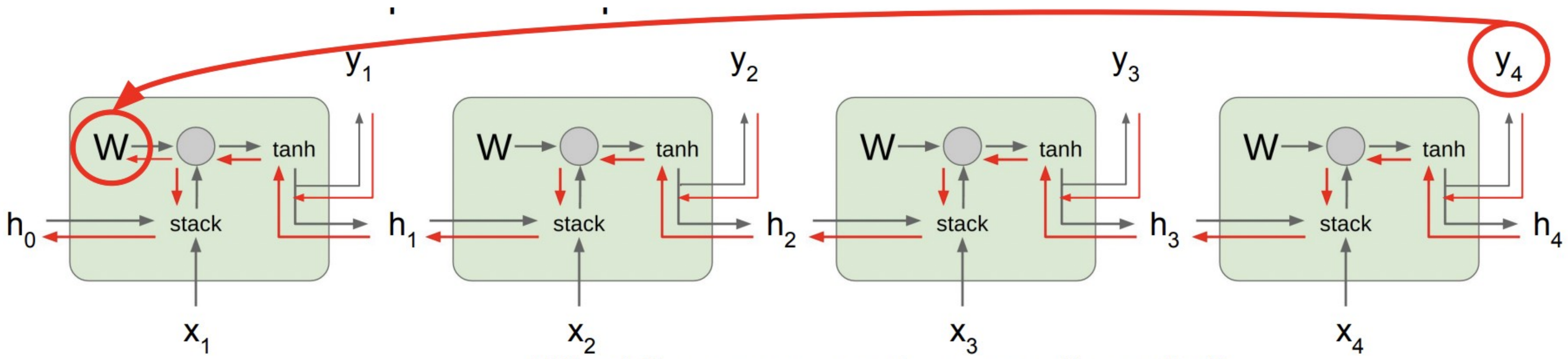
Vanilla RNN gradient flow



$$\frac{\partial L}{\partial W} = \sum_{t=1}^{T} \frac{\partial L_t}{\partial W}$$

What if we assumed no non-linearity?

Vanilla RNN gradient flow



What if we assumed no non-linearity?

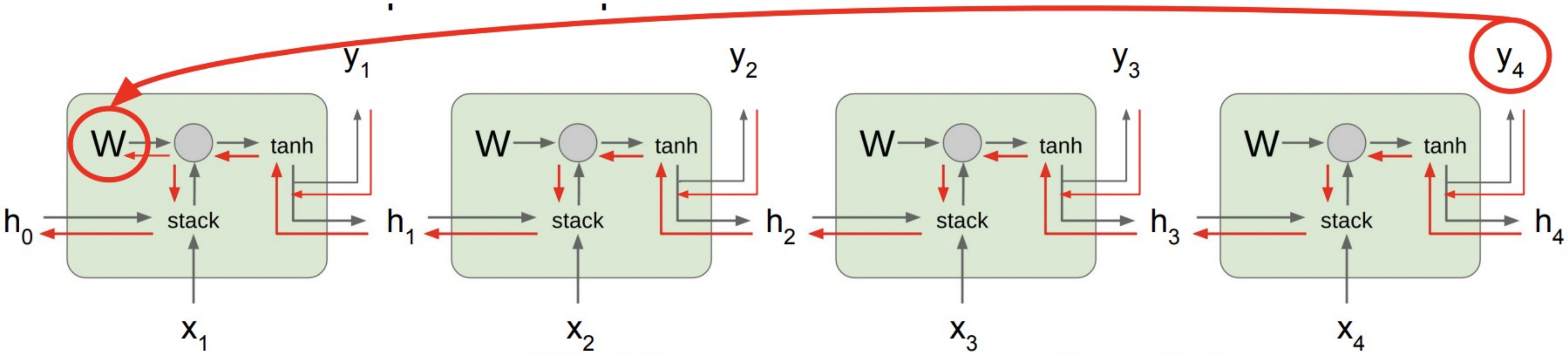
$$\frac{\partial L}{\partial W} = \sum_{t=1}^{T} \frac{\partial L_t}{\partial W}$$

$$\frac{\partial L_T}{\partial W} = \frac{\partial L_T}{\partial h_T} \boxed{W_{hh}^{T-1}} \frac{\partial h_1}{\partial W}$$

Largest singular value > 1:
Exploding gradients

Largest singular value < 1:
Vanishing gradients

Vanilla RNN gradient flow



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$$\frac{\partial L_T}{\partial W} = \frac{\partial L_T}{\partial h_T} \boxed{W_{hh}^{T-1}} \frac{\partial h_1}{\partial W}$$

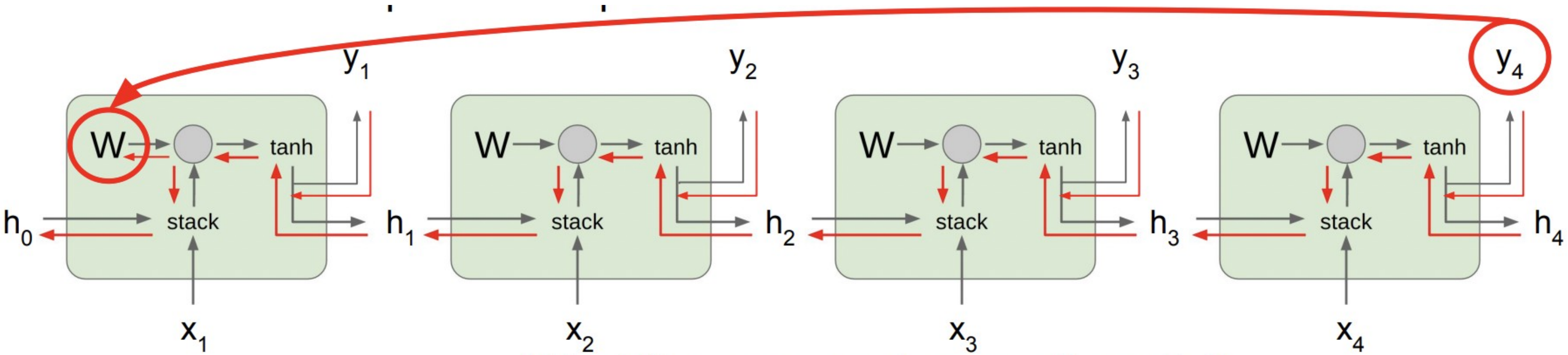
Largest singular value > 1:
Exploding gradients

→ **Gradient clipping**: Scale gradient if its norm is too big

```
grad_norm = np.sum(grad * grad)
if grad_norm > threshold:
  grad *= (threshold / grad_norm)
```

Largest singular value < 1:
Vanishing gradients

Vanilla RNN gradient flow



What if we assumed no non-linearity?

$$\frac{\partial L}{\partial W} = \sum_{t=1}^{T} \frac{\partial L_t}{\partial W}$$

$$\frac{\partial L_T}{\partial W} = \frac{\partial L_T}{\partial h_T} \boxed{W_{hh}^{T-1}} \frac{\partial h_1}{\partial W}$$

Largest singular value > 1:
Exploding gradients

Largest singular value < 1:
Vanishing gradients

→ Change RNN architecture

Long Short Term Memory (LSTM)

Vanilla RNN

$$h_t = \tanh\left(W \begin{pmatrix} h_{t-1} \\ x_t \end{pmatrix}\right)$$

LSTM

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

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

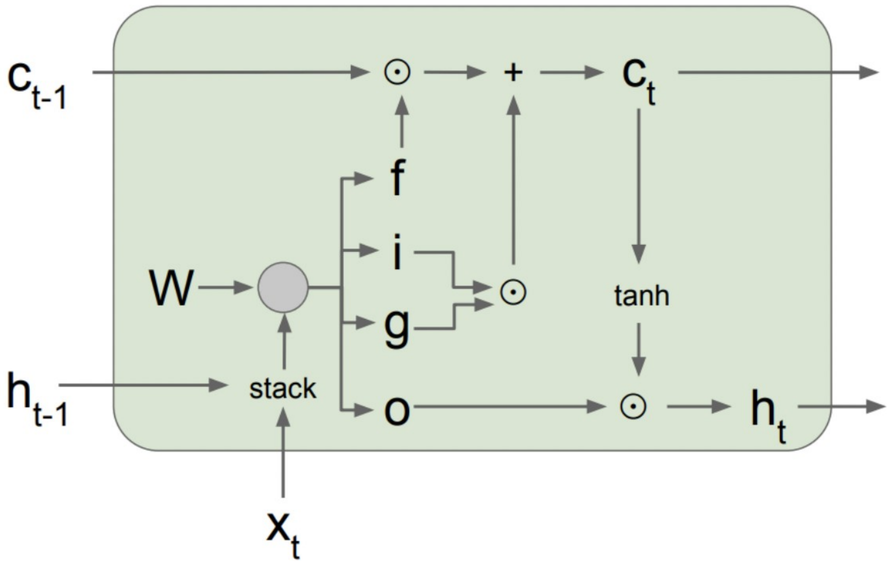
$$h_t = o \odot \tanh(c_t)$$

Long Short Term Memory (LSTM)

- A type of RNN proposed by Hochreiter and Schmidhuber in 1997 as a solution to the vanishing gradients problem
- Work extremely well in practice
- **Basic idea**: turning multiplication into addition
- Use "gates" to control how much information to add/erase

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

- At each timestep, there is a hidden state $\mathbf{h}_t \in \mathbb{R}^d$ and also a cell state $\mathbf{c}_t \in \mathbb{R}^d$
  - $\mathbf{c}_t$ stores **long-term information**
  - We write/erase $\mathbf{c}_t$ after each step
  - We read $\mathbf{h}_t$ from $\mathbf{c}_t$



Long Short Term Memory (LSTM)

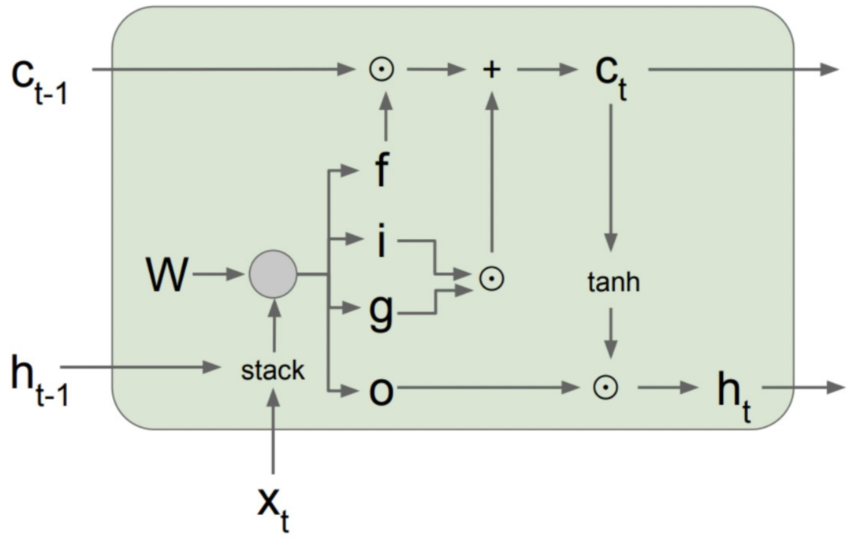
There are 4 gates:

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

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

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

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

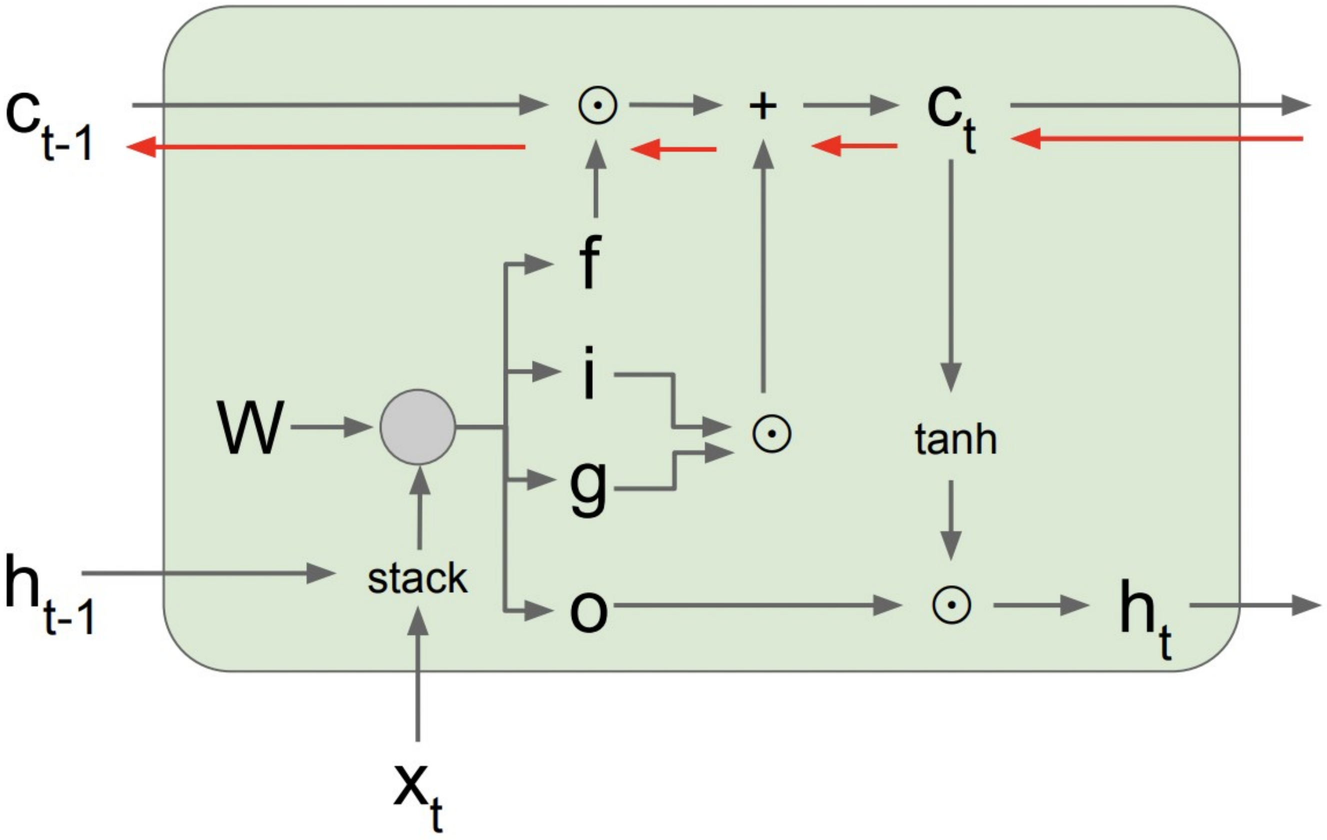


- Final memory cell: $\mathbf{c}_t = \mathbf{f}_t \odot \mathbf{c}_{t-1} + \mathbf{i}_t \odot \tilde{\mathbf{c}}_t$

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

element-wise product

LSTM gradient flow



Backpropagation from c_t to c_{t-1} only elementwise multiplication by f, no matrix multiply by W

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

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

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

Does LSTM solve the vanishing gradient problems?

The LSTM architecture makes it easier for the RNN to preserve information over many timesteps

- e.g. **if the f = 1 and the i = 0**, then the information of that cell is preserved indefinitely.
- By contrast, it's harder for vanilla RNN to learn a recurrent weight matrix Wh that preserves info in hidden state

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

Summary

- RNNs allow a lot of flexibility in architecture design
- Vanilla RNNs are simple but don’t work very well
- Backward flow of gradients in RNN can explode or vanish. Exploding is controlled with gradient clipping. Vanishing is controlled with additive interactions (LSTM)
- Better/simpler architectures are a hot topic of current research, as well as new paradigms for reasoning over sequences
- Better understanding (both theoretical and empirical) is needed