Lecture 2: Recurrent Neural Network

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Tianyuan Mathematical Center in Central China

Introduction

Recurrent neural networks

- Dates back to (Rumelhart *et al.*, 1986)
- A family of neural networks for handling sequential data, which involves variable length inputs or outputs

- Especially, for natural language processing (NLP)

Sequential data

- Each data point: A sequence of vectors $x^{(t)}$, for $1 \leq t \leq \tau$
- Batch data: many sequences with different lengths τ
- Label: can be a scalar, a vector, or even a sequence

- Example
  - Sentiment analysis
  - Machine translation

Example: machine translation

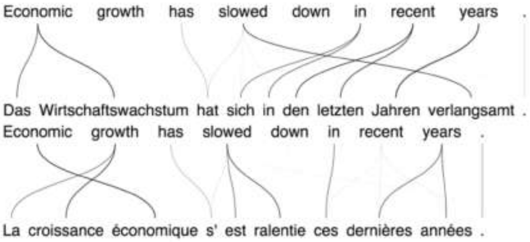


Figure from: devblogs.nvidia.com

More complicated sequential data

- Data point: two dimensional sequences like images
- Label: different type of sequences like text sentences

- Example: image captioning

Image captioning

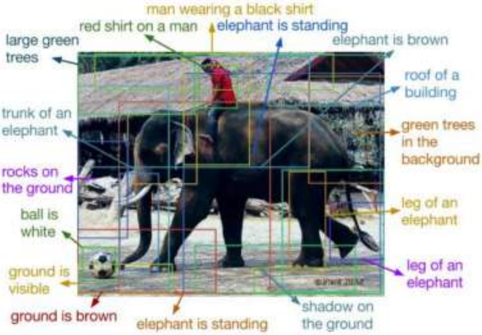
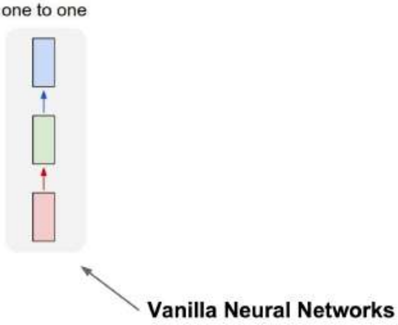
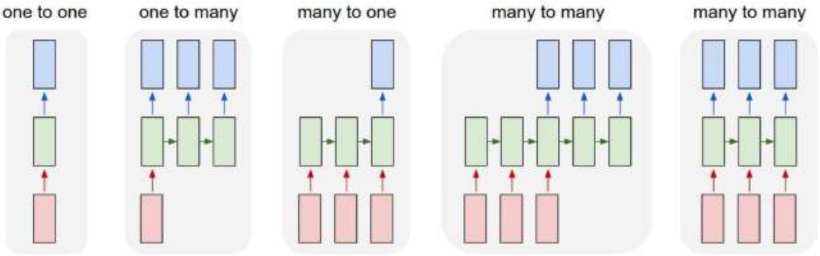


Figure from the paper "DenseCap: Fully Convolutional Localization Networks for Dense Captioning", by Justin Johnson, Andrej Karpathy, Li Fei-Fei

"Vanilla" Neural Network

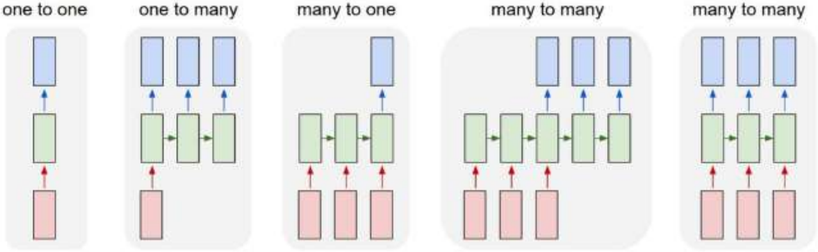


Recurrent Neural Networks: Process Sequences



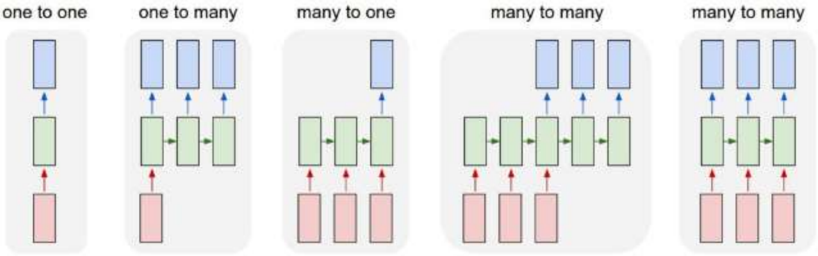
e.g. **Image Captioning**
image -> sequence of words

Recurrent Neural Networks: Process Sequences



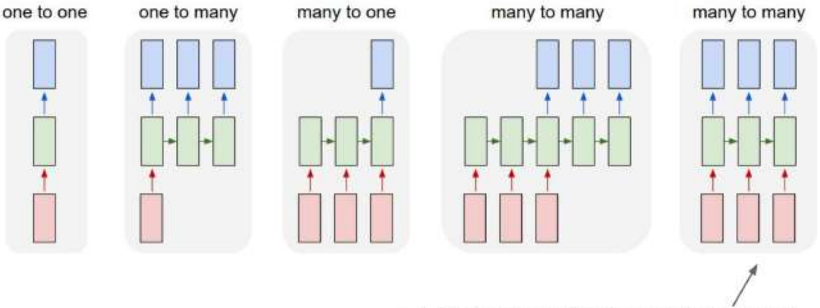
e.g. **Sentiment Classification**
sequence of words -> sentiment

Recurrent Neural Networks: Process Sequences



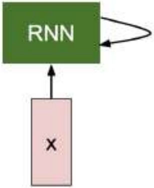
e.g. **Machine Translation**
seq of words -> seq of words

Recurrent Neural Networks: Process Sequences

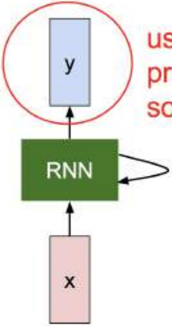


e.g. **Video classification on frame level**

Recurrent Neural Network



Recurrent Neural Network



usually want to predict a vector at some time steps

Recurrent Neural Network

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

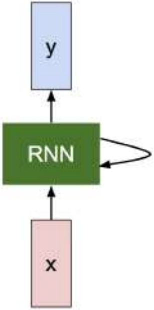
$$\boxed{h_t} = \boxed{f_W}(\boxed{h_{t-1}}, \boxed{x_t})$$

new state

old state

input vector at some time step

some function with parameters W

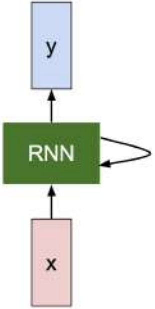


Recurrent Neural Network

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

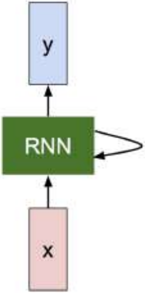
$$h_t = f_W(h_{t-1}, x_t)$$

Notice: the same function and the same set of parameters are used at every time step.



(Vanilla) Recurrent Neural Network

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

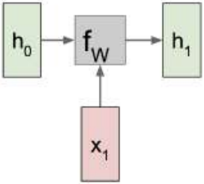


$$h_t = f_W(h_{t-1}, x_t)$$

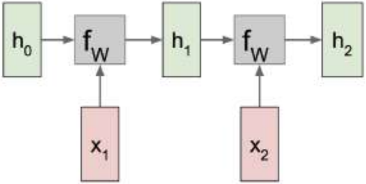
$$h_t = \tanh(W_{hh}h_{t-1} + W_{xh}x_t)$$

$$y_t = W_{hy}h_t$$

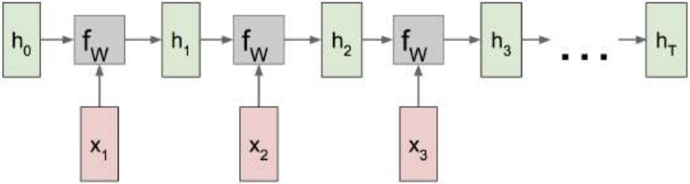
RNN: Computational Graph



RNN: Computational Graph

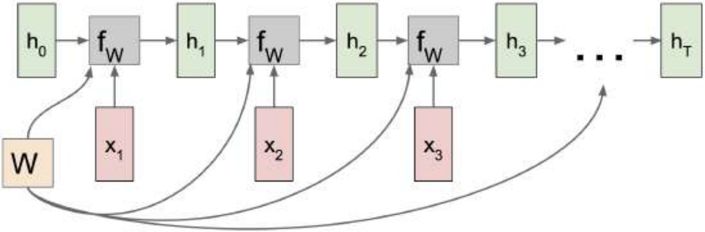


RNN: Computational Graph

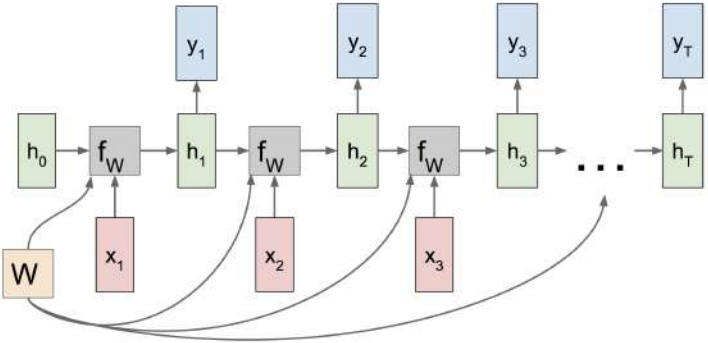


RNN: Computational Graph

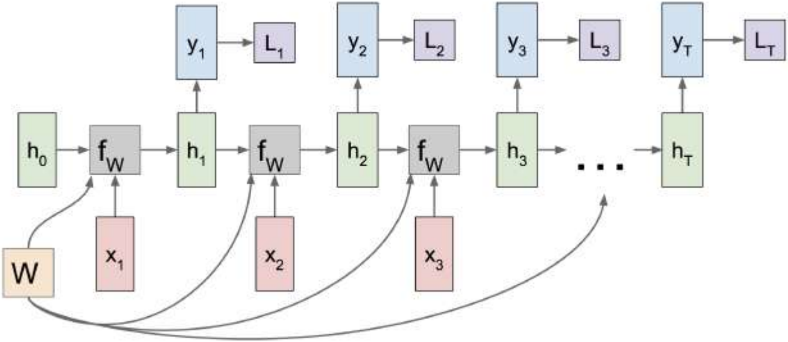
Re-use the same weight matrix at every time-step

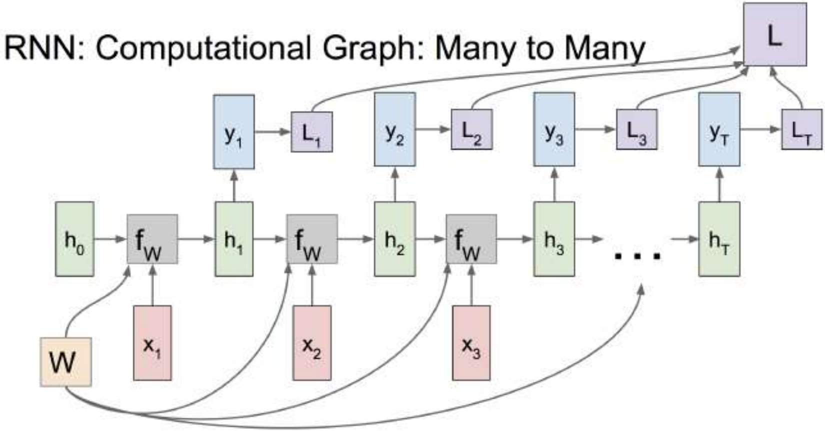


RNN: Computational Graph: Many to Many

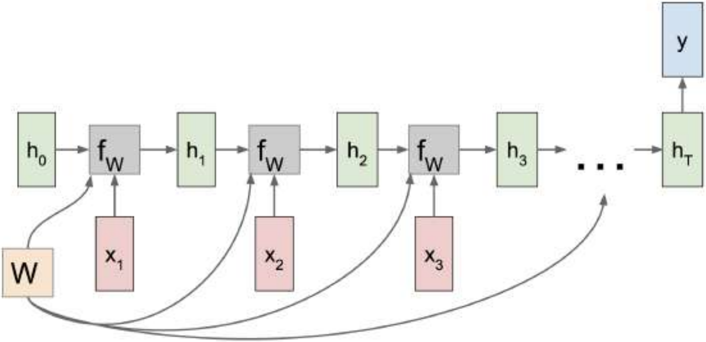


RNN: Computational Graph: Many to Many

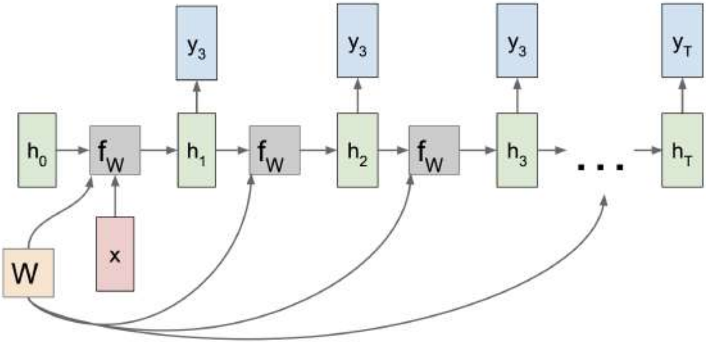



RNN: Computational Graph: Many to Many
L
y_1
L_1
y_2
L_2
y_3
L_3
y_T
L_T
h_0
f_W
h_1
f_W
h_2
f_W
h_3
...
h_T
W
x_1
x_2
x_3

RNN: Computational Graph: Many to One

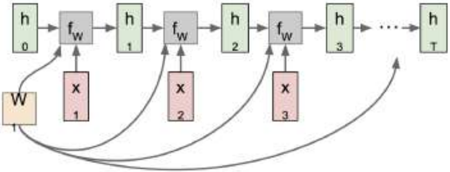


RNN: Computational Graph: One to Many

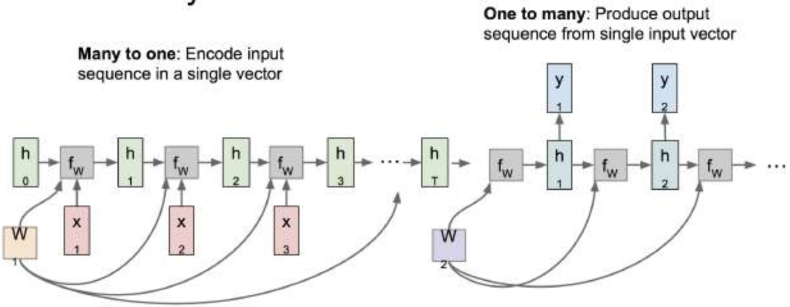


Sequence to Sequence: Many-to-one + one-to-many

Many to one: Encode input sequence in a single vector



Sequence to Sequence: Many-to-one + one-to-many



Bidirectional RNNs

- Many applications: output at time t may depend on the whole input sequence
- Example in speech recognition: correct interpretation of the current sound may depend on the next few phonemes, potentially even the next few words

- Bidirectional RNNs are introduced to address this

BiRNNs

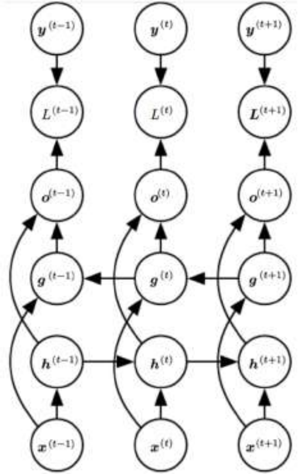


Figure from *Deep Learning*, Goodfellow, Bengio and Courville

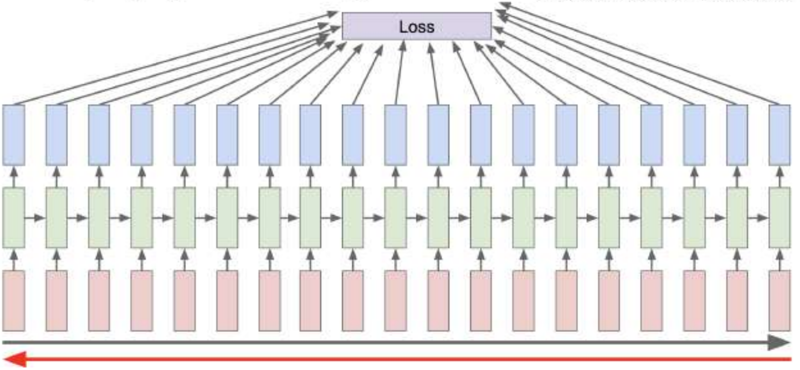
Advantage

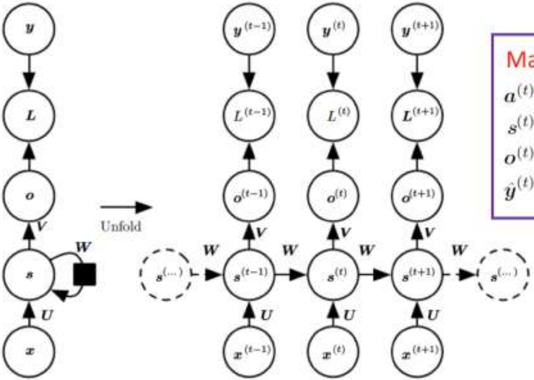
- Shared parameters: reduce the capacity and good for generalization in learning
- Hidden state: a lossy summary of the past for computational efficiency

Training RNN

Backpropagation through time

Forward through entire sequence to compute loss, then backward through entire sequence to compute gradient

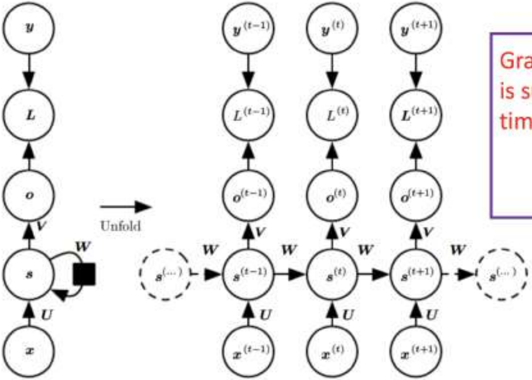




Math formula:

$$
\begin{aligned}
\boldsymbol{a}^{(t)} &= \boldsymbol{b} + \boldsymbol{W}\boldsymbol{s}^{(t-1)} + \boldsymbol{U}\boldsymbol{x}^{(t)} \\
\boldsymbol{s}^{(t)} &= \tanh(\boldsymbol{a}^{(t)}) \\
\boldsymbol{o}^{(t)} &= \boldsymbol{c} + \boldsymbol{V}\boldsymbol{s}^{(t)} \\
\hat{\boldsymbol{y}}^{(t)} &= \operatorname{softmax}(\boldsymbol{o}^{(t)})
\end{aligned}
$$

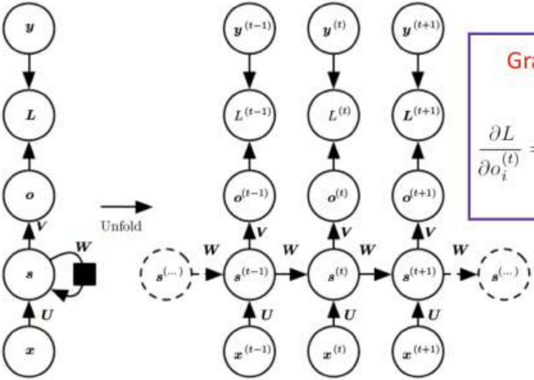
Figure from *Deep Learning*, Goodfellow, Bengio and Courville



Gradient at $L^{(t)}$: (total loss is sum of those at different time steps)

$$\frac{\partial L}{\partial L^{(t)}} = 1.$$

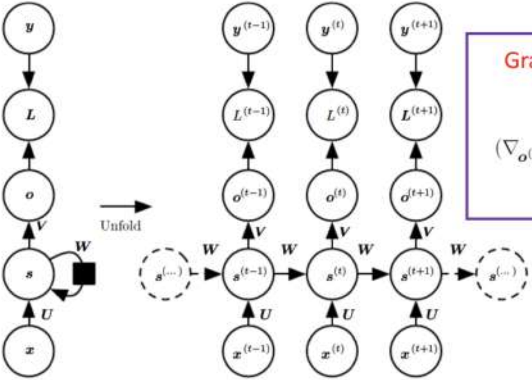
Figure from *Deep Learning*, Goodfellow, Bengio and Courville



Gradient at $o^{(t)}$:

$$\frac{\partial L}{\partial o_i^{(t)}} = \frac{\partial L}{\partial L^{(t)}} \frac{\partial L^{(t)}}{\partial o_i^{(t)}}$$

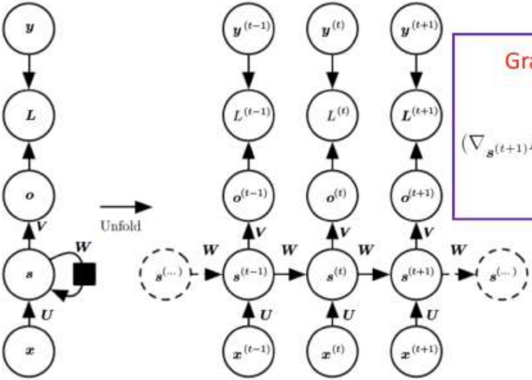
Figure from *Deep Learning*, Goodfellow, Bengio and Courville



Gradient at $s^{(\tau)}$:

$$(\nabla_{\boldsymbol{o}^{(\tau)}} L) \frac{\partial \boldsymbol{o}^{(\tau)}}{\partial \boldsymbol{s}^{(\tau)}} = (\nabla_{\boldsymbol{o}^{(\tau)}} L) \boldsymbol{V}$$

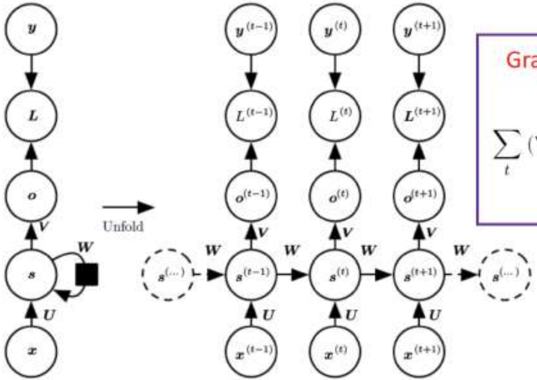
Figure from *Deep Learning*, Goodfellow, Bengio and Courville



Gradient at $s^{(t)}$:

$$(\nabla_{\boldsymbol{s}^{(t+1)}} L)\,\frac{\partial \boldsymbol{s}^{(t+1)}}{\partial \boldsymbol{s}^{(t)}} + (\nabla_{\boldsymbol{o}^{(t)}} L)\,\frac{\partial \boldsymbol{o}^{(t)}}{\partial \boldsymbol{s}^{(t)}}$$

Figure from *Deep Learning*, Goodfellow, Bengio and Courville



Gradient at parameter V:

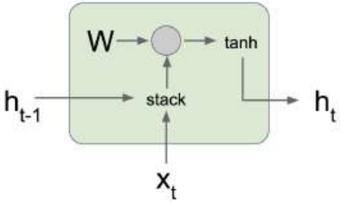
$$\sum_t (\nabla_{o^{(t)}} L) \frac{\partial o^{(t)}}{\partial V} = \sum_t (\nabla_{o^{(t)}} L)\, s^{(t)^\top}$$

Figure from *Deep Learning*,
Goodfellow, Bengio and Courville

We encounter numerical problems for gradient at W!

Vanilla RNN Gradient Flow

Bengio et al, "Learning long-term dependencies with gradient descent is difficult", IEEE Transactions on Neural Networks, 1994
Pascanu et al, "On the difficulty of training recurrent neural networks", ICML 2013



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

Vanilla RNN Gradient Flow

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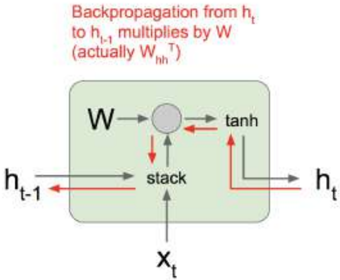

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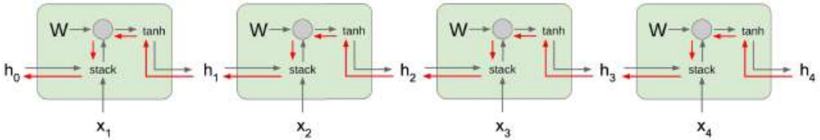

Computing gradient of h_0 involves many factors of W (and repeated tanh)

Vanilla RNN Gradient Flow

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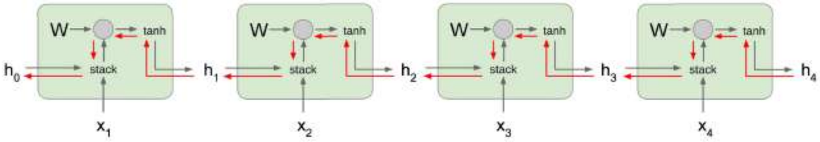

Computing gradient of h_0 involves many factors of W (and repeated tanh)

Largest singular value > 1:
Exploding gradients

Largest singular value < 1:
Vanishing gradients

Vanilla RNN Gradient Flow

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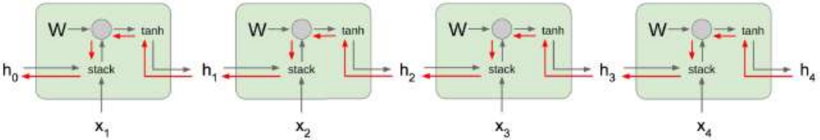
Pascanu et al, "On the difficulty of training recurrent neural networks", ICML 2013



Computing gradient of h_0 involves many factors of W (and repeated tanh)

Largest singular value > 1:
Exploding gradients

Largest singular value < 1:
Vanishing 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)
```

Vanilla RNN Gradient Flow

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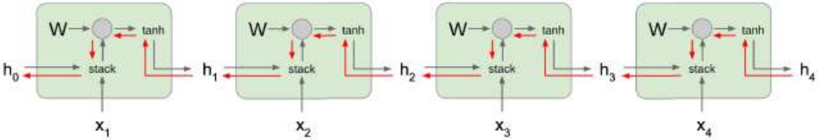
Pascanu et al, "On the difficulty of training recurrent neural networks", ICML 2013



Computing gradient of h_0 involves many factors of W (and repeated tanh)

Largest singular value > 1:
Exploding gradients

Largest singular value < 1:
Vanishing gradients

→ Change RNN architecture

Long Short Term Memory (LSTM)

Vanilla RNN

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

LSTM

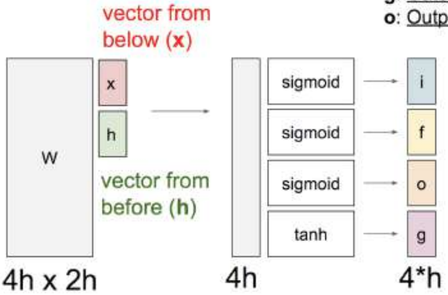
$$\boxed{\begin{aligned} \begin{pmatrix} i \\ f \\ o \\ g \end{pmatrix} &= \begin{pmatrix} \sigma \\ \sigma \\ \sigma \\ \tanh \end{pmatrix} W \begin{pmatrix} h_{t-1} \\ x_t \end{pmatrix} \\ c_t &= f \odot c_{t-1} + i \odot g \\ h_t &= o \odot \tanh(c_t) \end{aligned}}$$

Hochreiter and Schmidhuber, "Long Short Term Memory", Neural Computation

Long Short Term Memory (LSTM)

[Hochreiter et al., 1997]

f: Forget gate, Whether to erase cell
i: Input gate, whether to write to cell
g: Gate gate (?), How much to write to cell
o: Output gate, How much to reveal cell



f, i, and o are in [0,1] most likely 1 or 0
g is in [-1,1] most likely 1 or -1

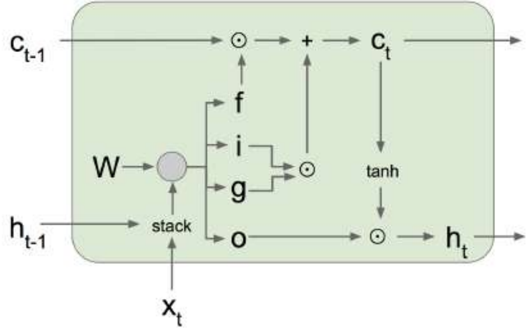
$$\boxed{\begin{pmatrix} i \\ f \\ o \\ g \end{pmatrix} = \begin{pmatrix} \sigma \\ \sigma \\ \sigma \\ \tanh \end{pmatrix} W \begin{pmatrix} h_{t-1} \\ x_t \end{pmatrix}}$$

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

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

Long Short Term Memory (LSTM)

[Hochreiter et al., 1997]



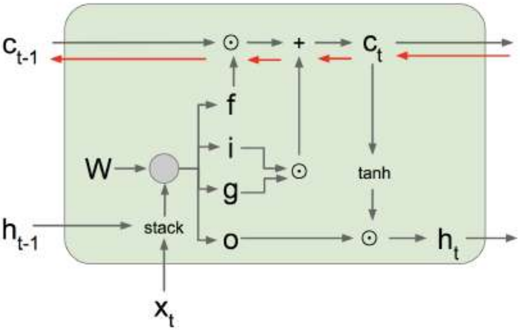
$$\begin{pmatrix} i \\ f \\ o \\ g \end{pmatrix} = \begin{pmatrix} \sigma \\ \sigma \\ \sigma \\ \tanh \end{pmatrix} W \begin{pmatrix} h_{t-1} \\ x_t \end{pmatrix}$$

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

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

Long Short Term Memory (LSTM): Gradient Flow

[Hochreiter et al., 1997]



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

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

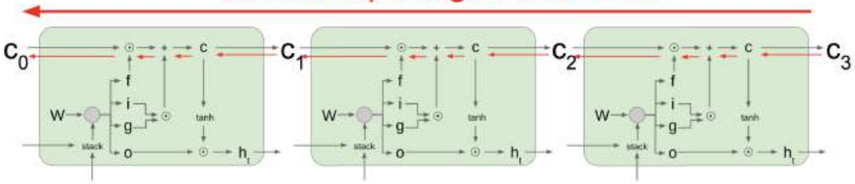
$$c_t = f \odot c_{t-1} + i \odot g$$

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

Long Short Term Memory (LSTM): Gradient Flow

[Hochreiter et al., 1997]

Uninterrupted gradient flow!



c: highway network

h: local network

Deep RNN

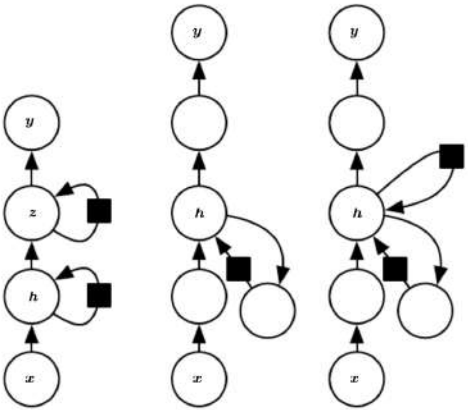


Figure: (a) More hidden units. (b) Deep NN instead of a single linear transform from input to hidden units, from hidden to hidden units, from hidden to output units. (c) Skipping algorithm.

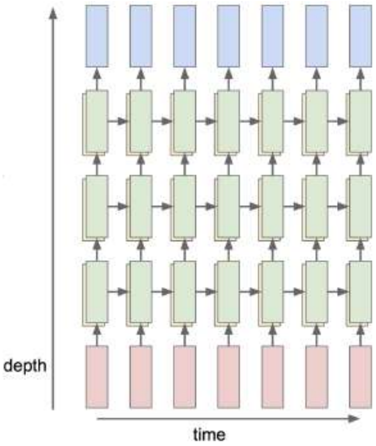


Figure: Example: more hidden units.