23. Recurrent Neural Networks STA3142 Statistical Machine Learning

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Applied Statistics / Statistics and Data Science
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* Slides adapted from EECS498/598 @ Univ. of Michigan by Justin Johnson



Rest of the Course Schedule

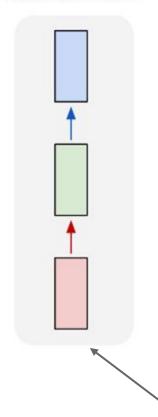
- 6/4 Tue: 22. Generative Models
- 6/6 Thu: 23. Recurrent Neural Networks (We have a class!)
- 6/9 Tue: 24. Transformers & 25. Reinforcement Learning
- **6/13 Thu**: 26. ML Advice
- 6/14 Fri: Final Assignment Deadline

Assignment 5 (Final Exam Replacement)

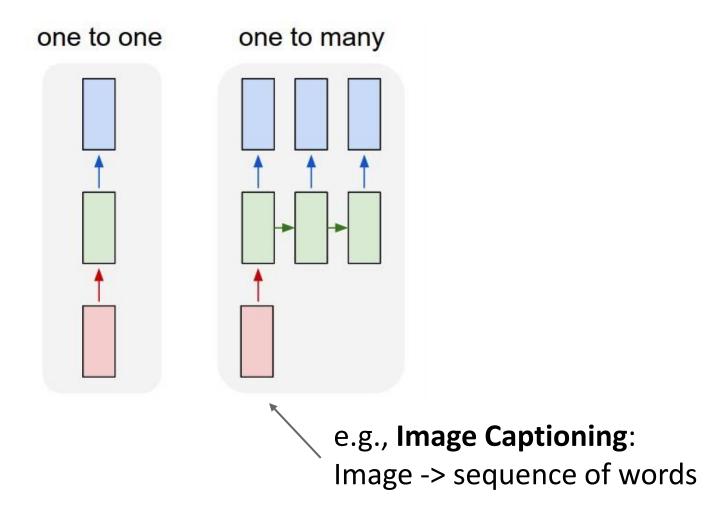
- Due Friday 6/14, 11:59pm
- Topic: Convolutional Neural Networks
 - Derive gradients for NN layers
 - Implement layers for CNNs
 - Train a CNN classifier for MNIST digit recognition
- Please read the instruction carefully!
 - Submit one pdf and one zip file separately
 - Write your code only in the designated spaces
 - Do not import additional libraries
 - ...
- If you feel difficult, consider to take option 2.

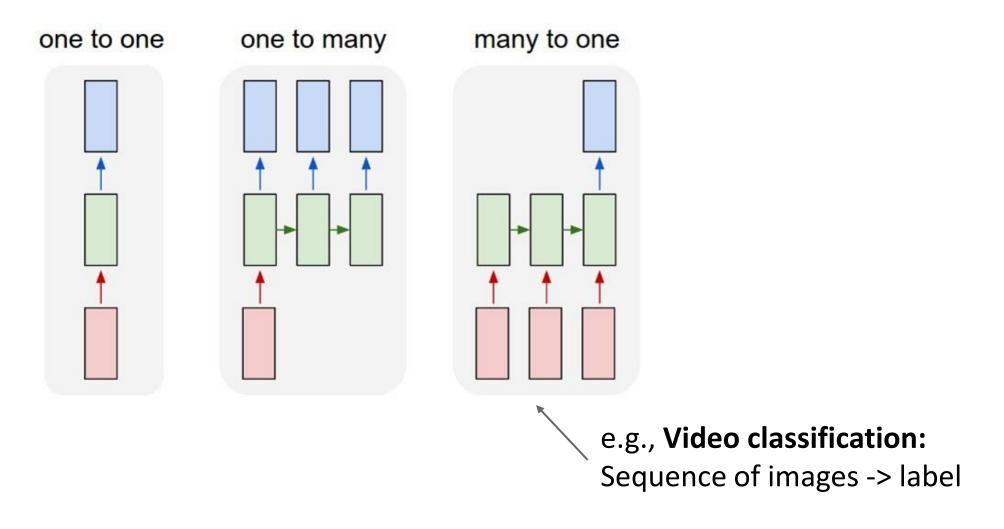
So far: "Feedforward" Neural Networks

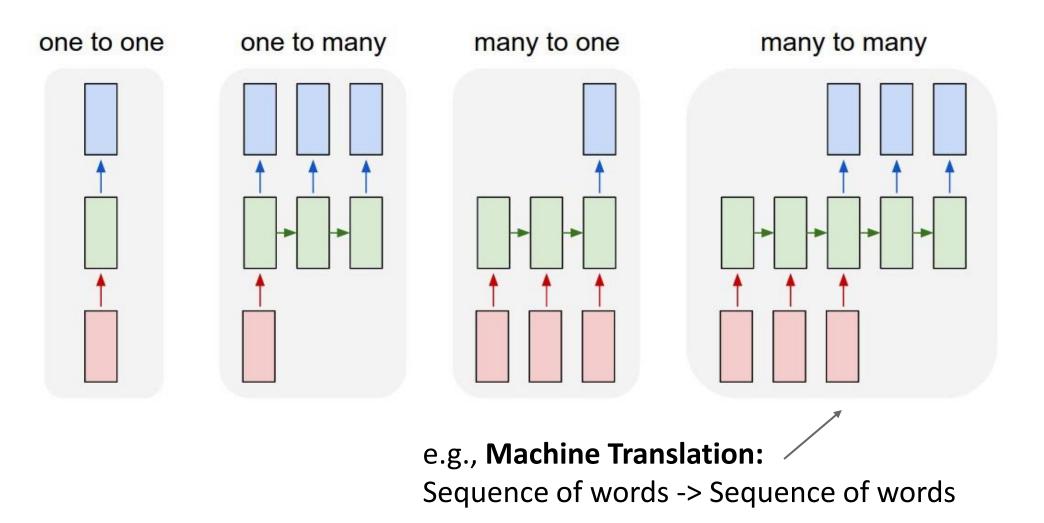
one to one

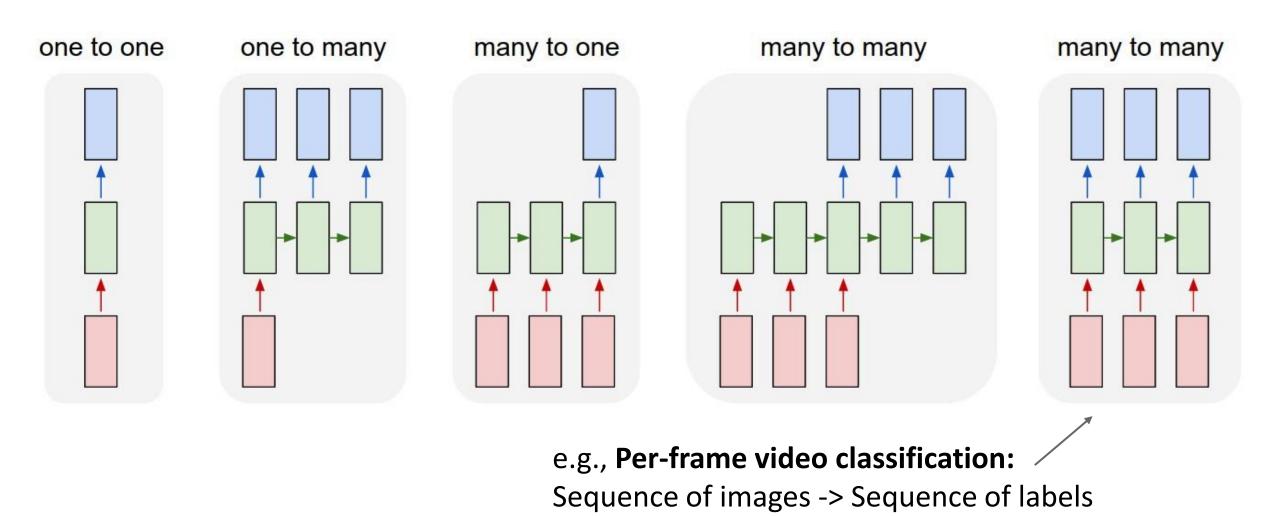


e.g., Image classification

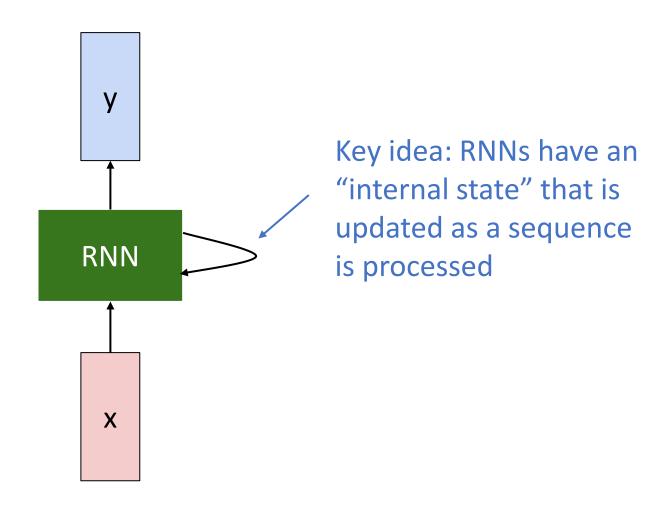






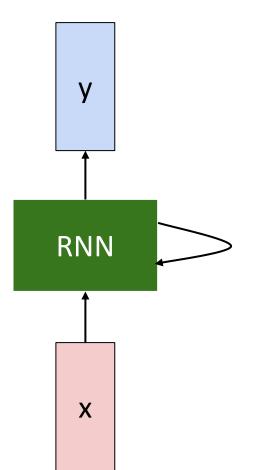


Recurrent Neural Networks

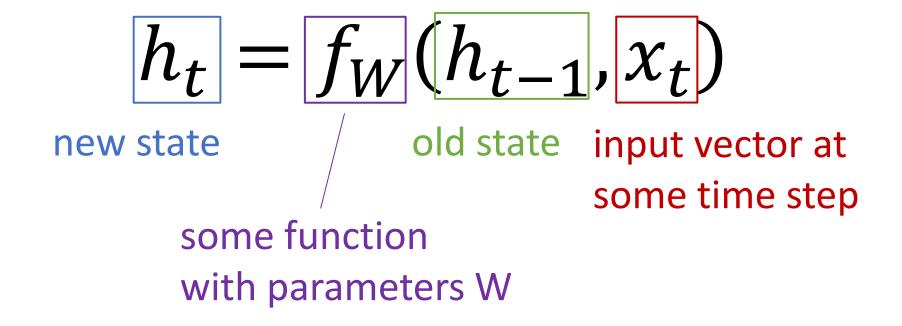


Recurrent Neural Networks

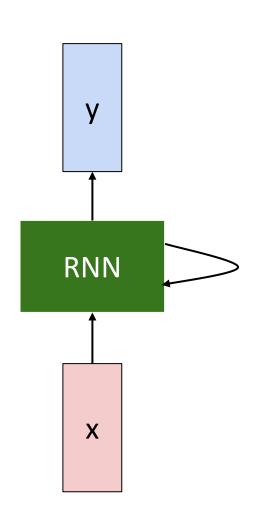
Note: the same function and the same set of parameters are used at every time step.



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



(Vanilla) Recurrent Neural Networks



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

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

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

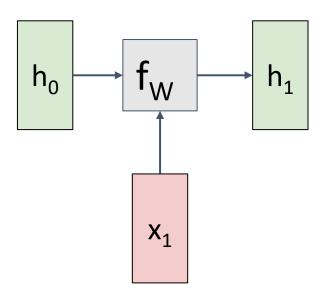
$$y_t = W_{hy}h_t + b_y$$

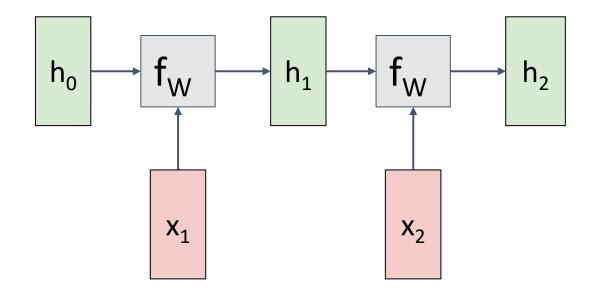
Sometimes called a "Vanilla RNN" or an "Elman RNN" after Prof. Jeffrey Elman

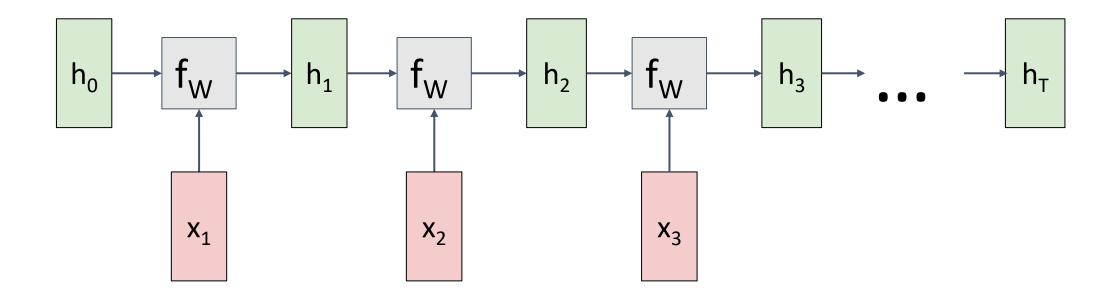
Initial hidden state Either set to all 0, Or learn it

h₀

x₁

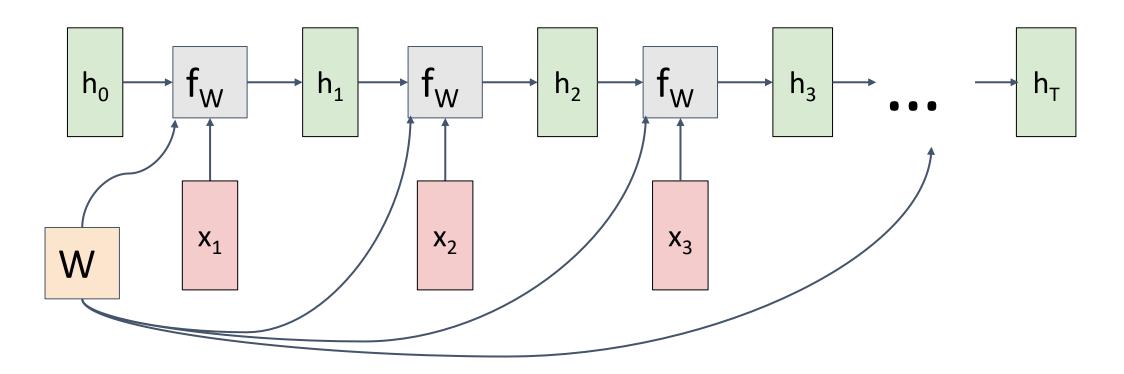




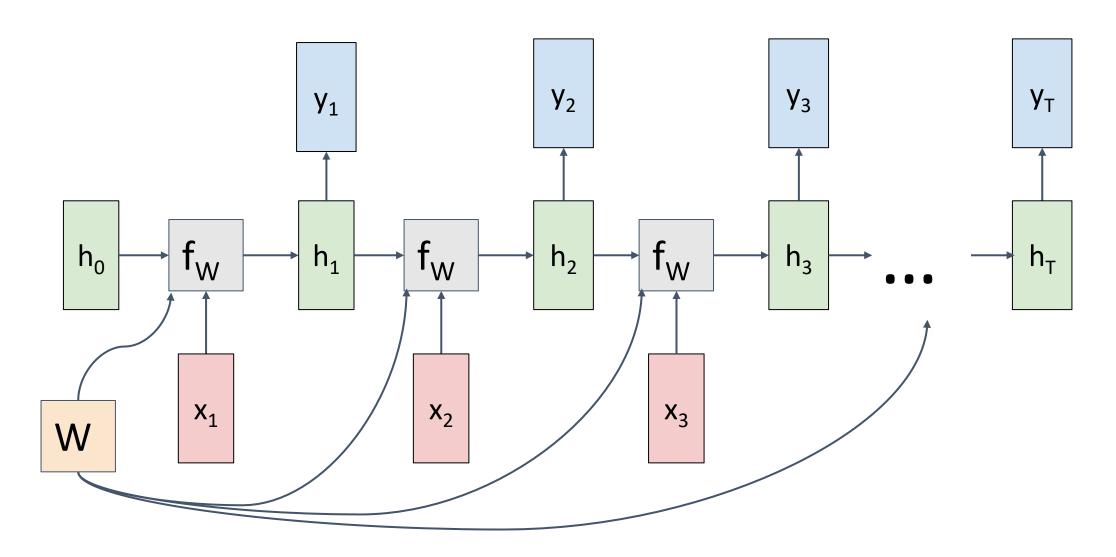


Statistical Machine Learning

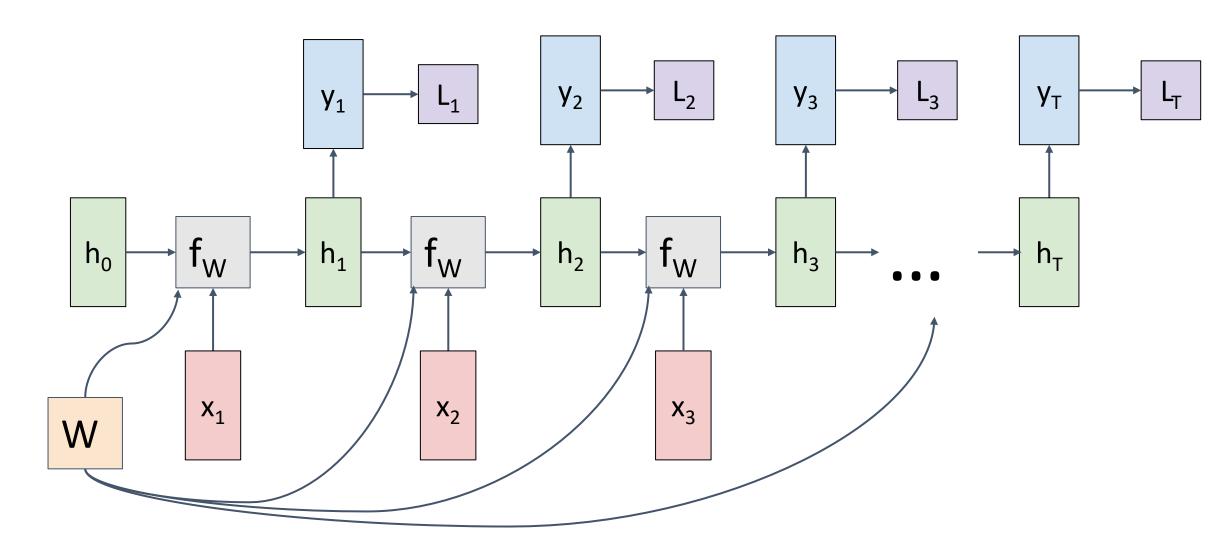
Re-use the same weight matrix at every time-step

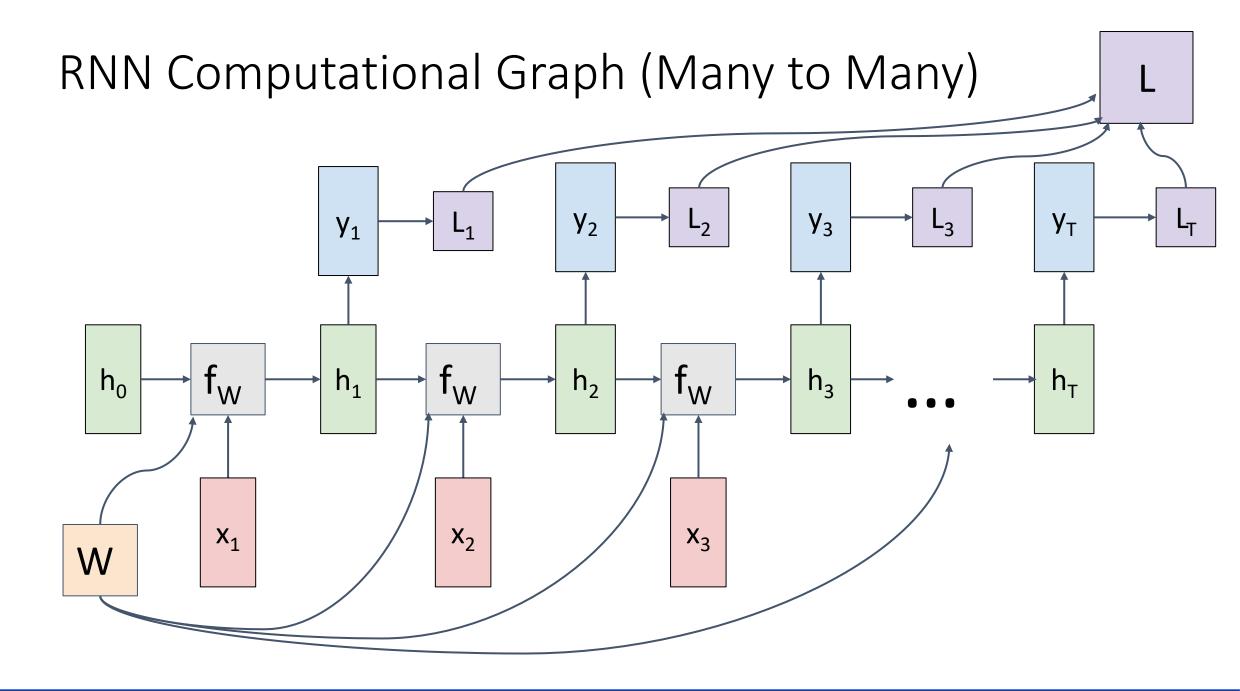


RNN Computational Graph (Many to Many)

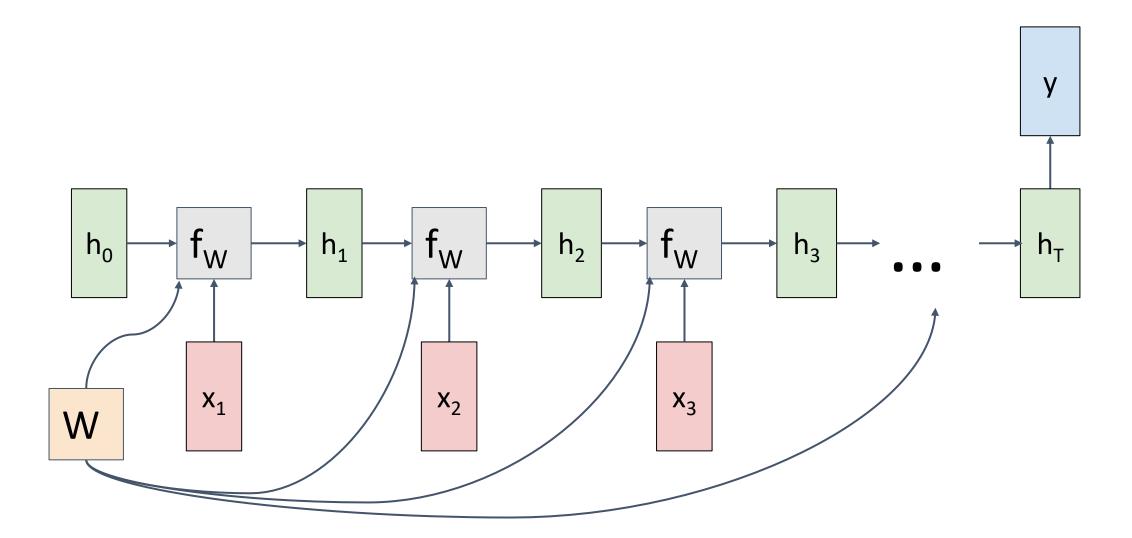


RNN Computational Graph (Many to Many)

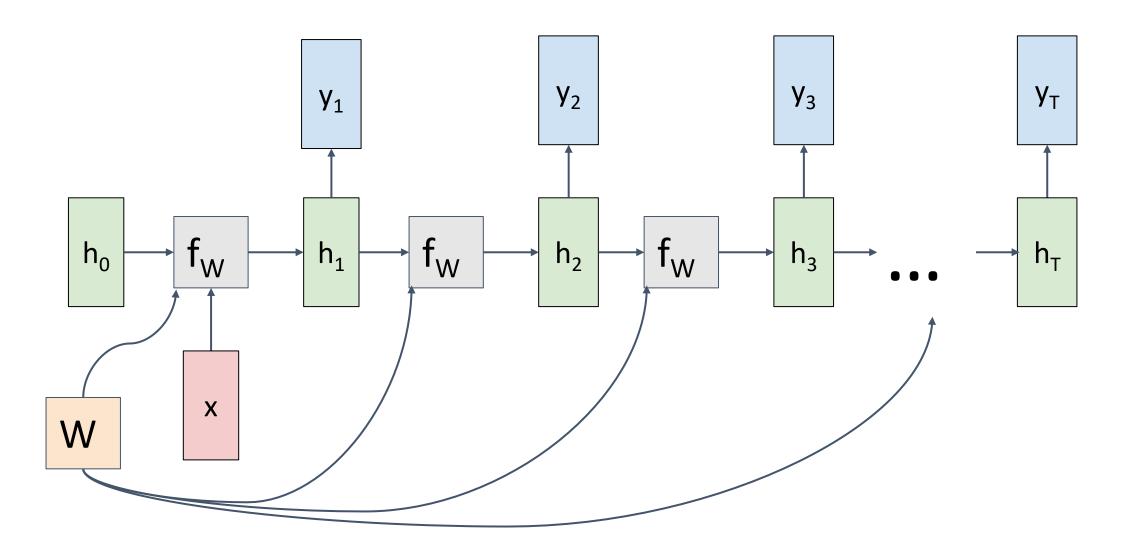




RNN Computational Graph (Many to One)

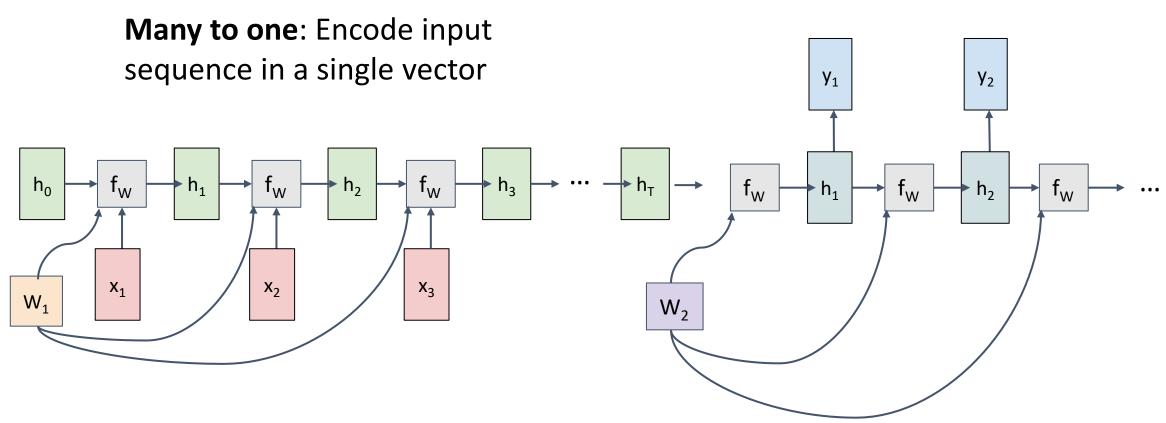


RNN Computational Graph (One to Many)



Sequence to Sequence (seq2seq) (Many to one) + (One to many)

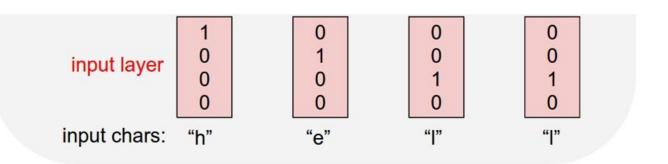
One to many: Produce output sequence from single input vector



Sutskever et al, "Sequence to Sequence Learning with Neural Networks", NIPS 2014

Given characters 1, 2, ..., t-1, model predicts character t

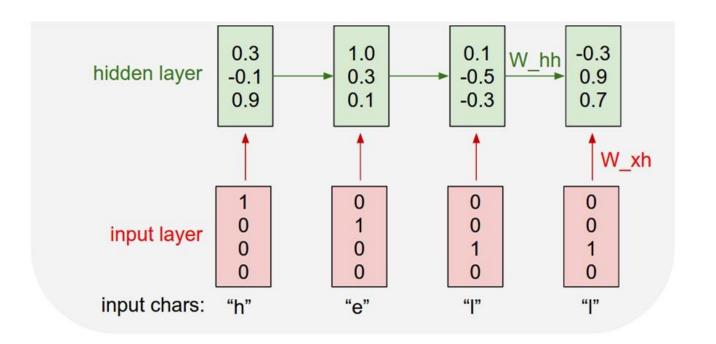
Training sequence: "hello"



Given characters 1, 2, ..., t-1, model predicts character t

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

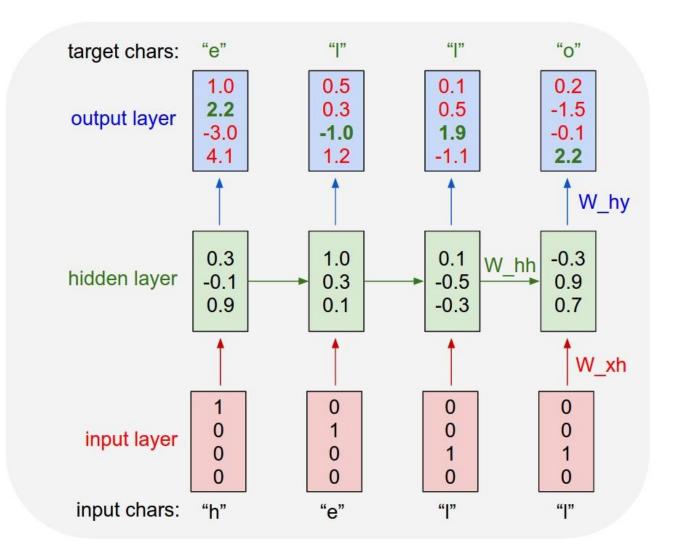
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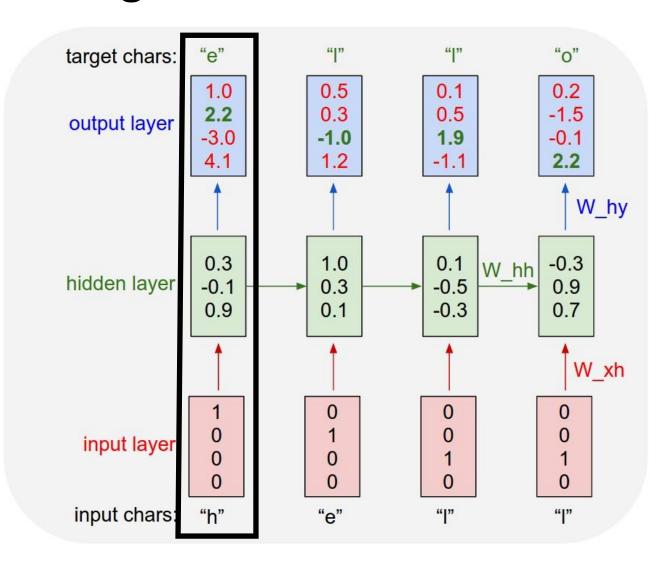


Given "h", predict "e"

Given characters 1, 2, ..., t-1, model predicts character t

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

Training sequence: "hello"

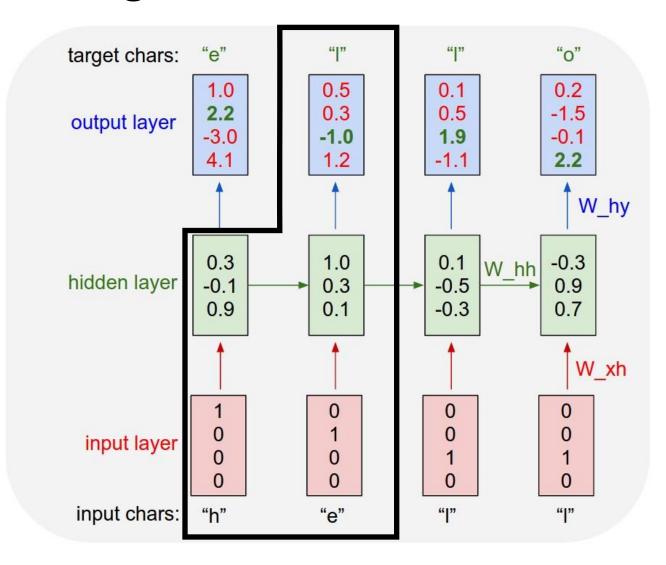


Given "he", predict "l"

Given characters 1, 2, ..., t-1, model predicts character t

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

Training sequence: "hello"

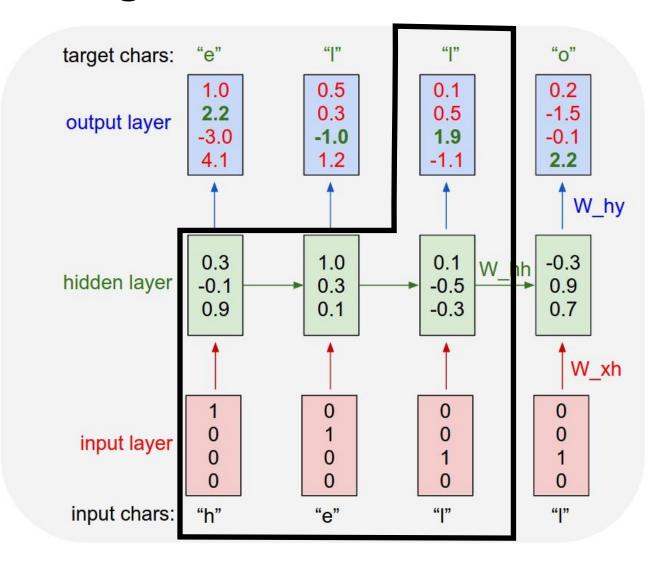


Given "hel", predict "l"

Given characters 1, 2, ..., t-1, model predicts character t

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

Training sequence: "hello"

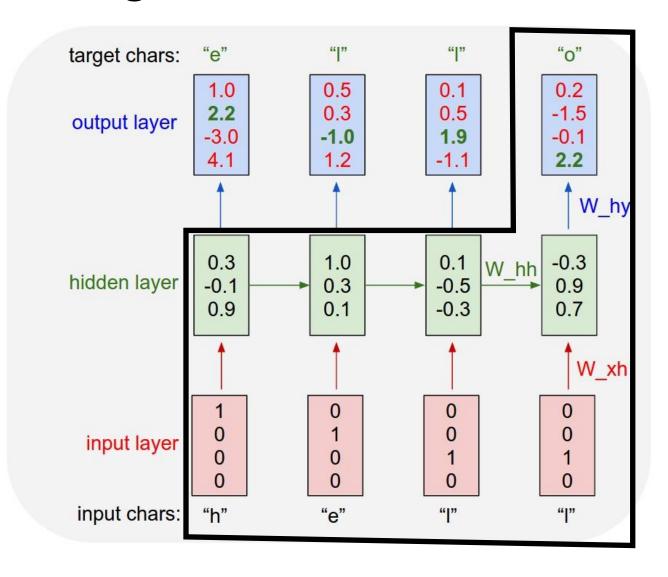


Given "hell", predict "o"

Given characters 1, 2, ..., t-1, model predicts character t

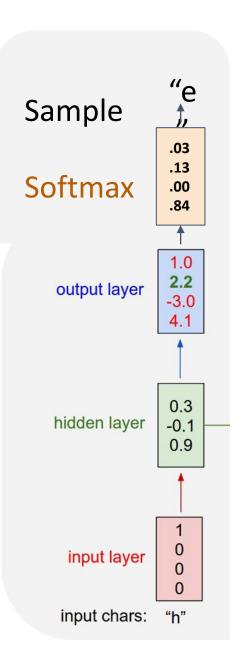
$$h_t = anh(W_{hh}h_{t-1} + W_{xh}x_t)$$

Training sequence: "hello"



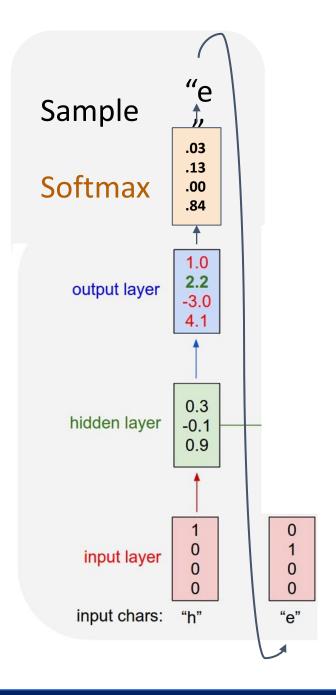
At test-time, **generate** new text: sample characters one at a time, feed back to model

Training sequence: "hello"



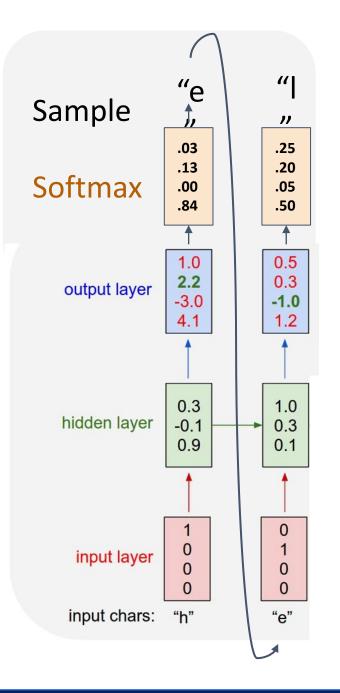
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Training sequence: "hello"



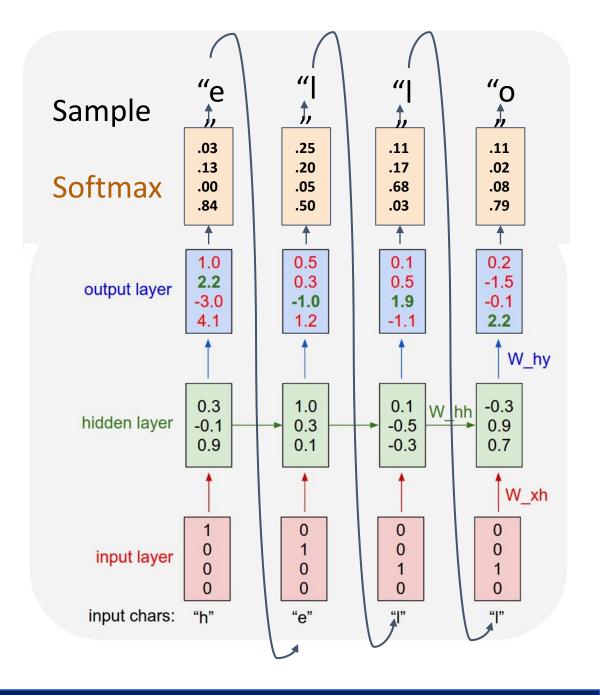
At test-time, **generate** new text: sample characters one at a time, feed back to model

Training sequence: "hello"



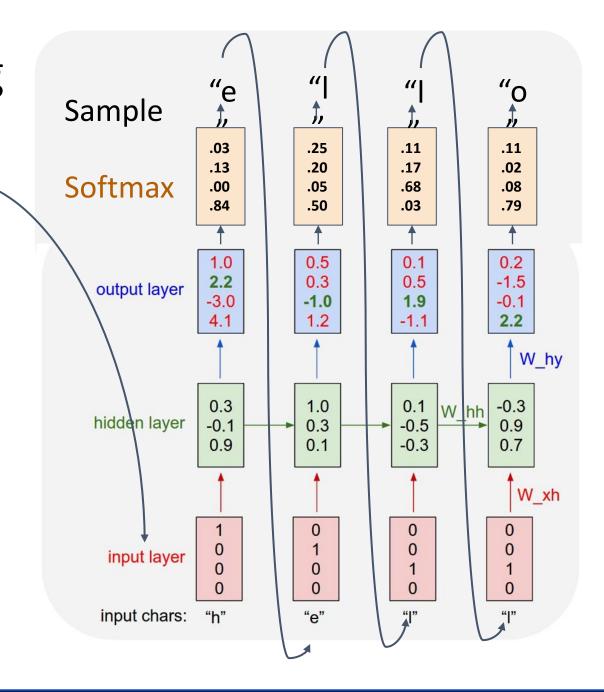
At test-time, **generate** new text: sample characters one at a time, feed back to model

Training sequence: "hello"



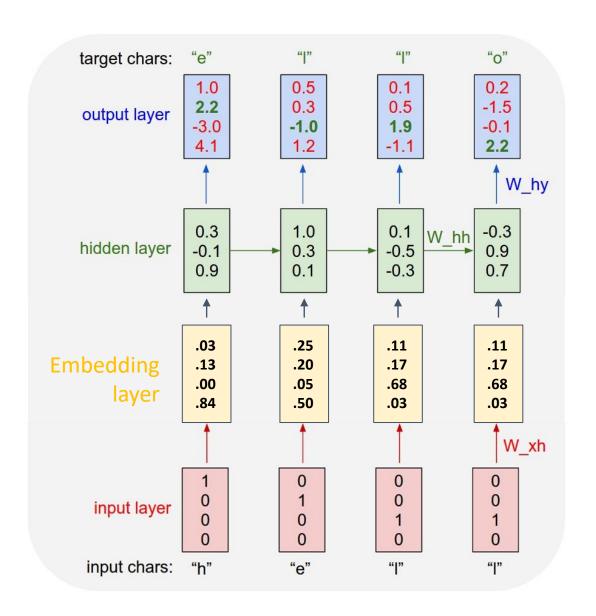
So far: encode inputs as **one-hot-vector**

Matrix multiply with a one-hot vector just extracts a column from the weight matrix. Often extract this into a separate **embedding** layer



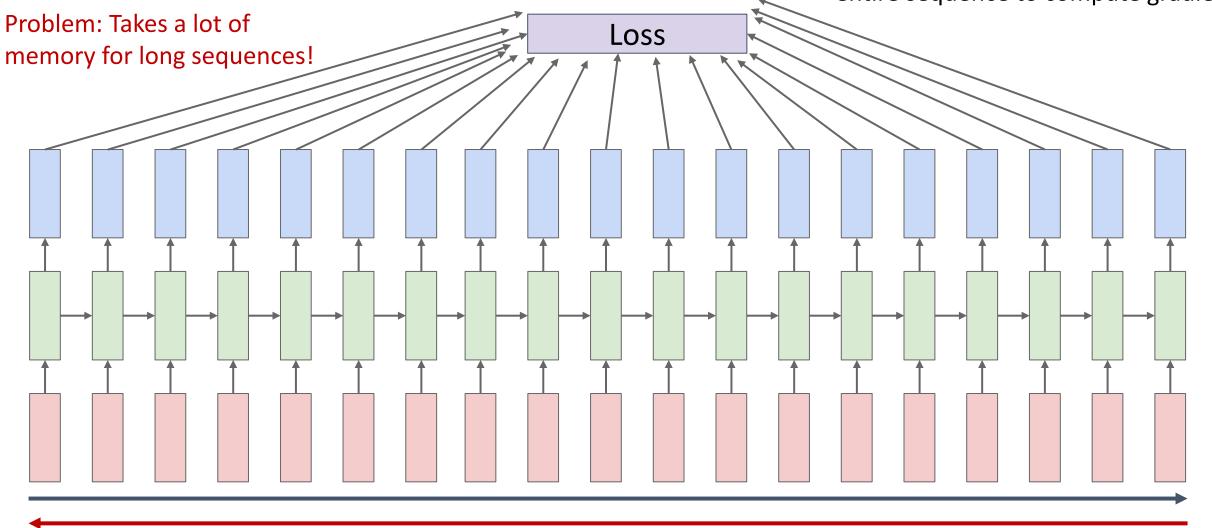
So far: encode inputs as **one-hot-vector**

Matrix multiply with a one-hot vector just extracts a column from the weight matrix. Often extract this into a separate **embedding** layer

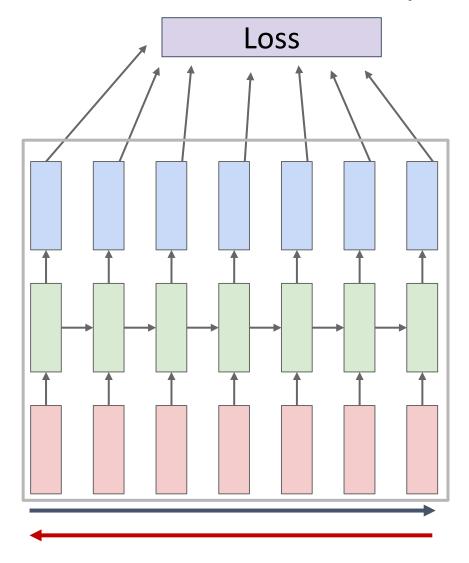


Backpropagation Through Time

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

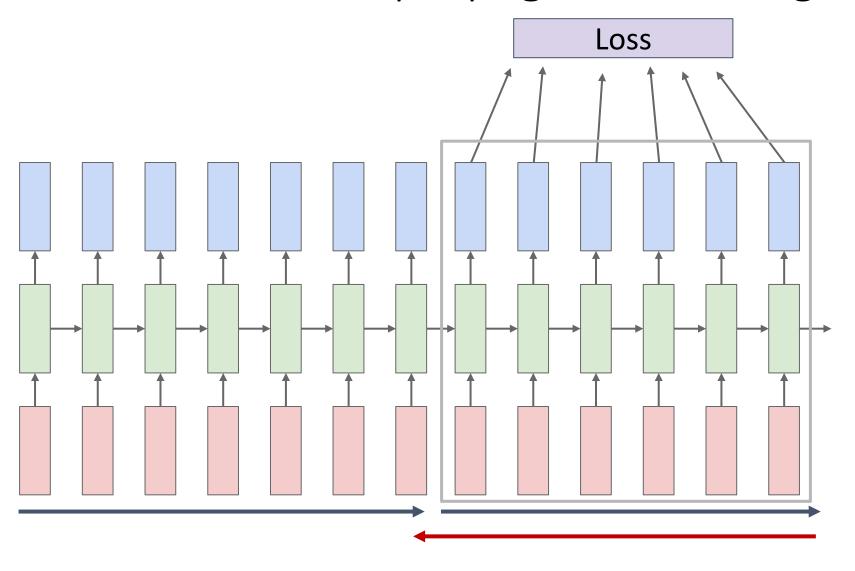


Truncated Backpropagation Through Time



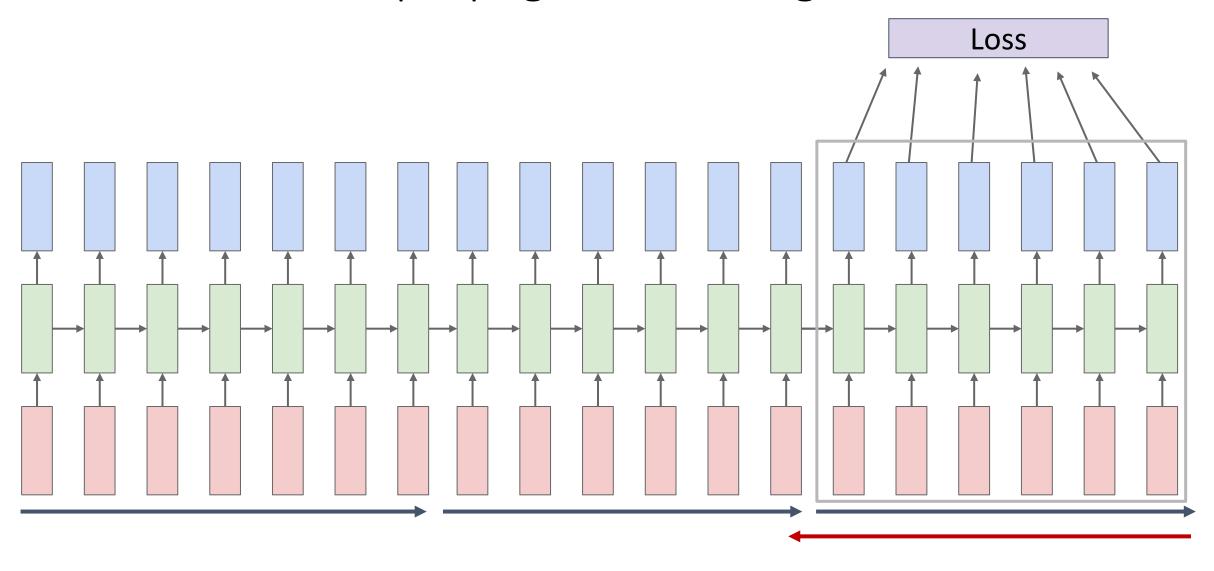
Run forward and backward through chunks of the sequence instead of whole sequence

Truncated Backpropagation Through Time



Carry hidden states forward in time forever, but only backpropagate for some smaller number of steps

Truncated Backpropagation Through Time

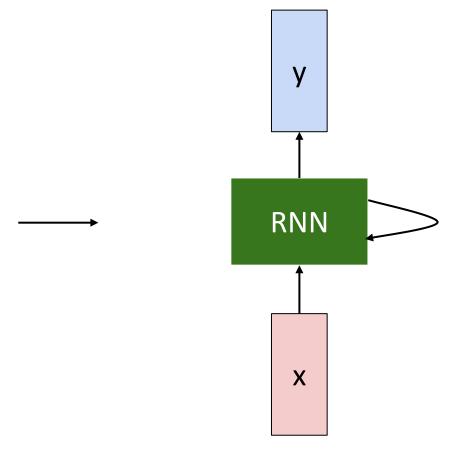


THE SONNETS

by William Shakespeare

From fairest creatures we desire increase,
That thereby beauty's rose might never die,
But as the riper should by time decease,
His tender heir might bear his memory:
But thou, contracted to thine own bright eyes,
Feed'st thy light's flame with self-substantial fuel,
Making a famine where abundance lies,
Thyself thy foe, to thy sweet self too cruel:
Thou that art now the world's fresh ornament,
And only herald to the gaudy spring,
Within thine own bud buriest thy content,
And tender churl mak'st waste in niggarding:
Pity the world, or else this glutton be,
To eat the world's due, by the grave and thee.

When forty winters shall besiege thy brow,
And dig deep trenches in thy beauty's field,
Thy youth's proud livery so gazed on now,
Will be a tatter'd weed of small worth held:
Then being asked, where all thy beauty lies,
Where all the treasure of thy lusty days;
To say, within thine own deep sunken eyes,
Were an all-eating shame, and thriftless praise.
How much more praise deserv'd thy beauty's use,
If thou couldst answer "This fair child of mine
Shall sum my count, and make my old excuse,'
Proving his beauty by succession thine!
This were to be new made when thou art old,
And see thy blood warm when thou feel'st it cold.



Source: Karpathy, "The Unreasonable Effectiveness of Recurrent Neural Networks", 2015. http://karpathy.github.io/2015/05/21/rnn-effectiveness/

at first:

tyntd-iafhatawiaoihrdemot lytdws e ,tfti, astai f ogoh eoase rrranbyne 'nhthnee e plia tklrgd t o idoe ns,smtt h ne etie h,hregtrs nigtike,aoaenns lng

train more

"Tmont thithey" fomesscerliund
Keushey. Thom here
sheulke, anmerenith ol sivh I lalterthend Bleipile shuwy fil on aseterlome
coaniogennc Phe lism thond hon at. MeiDimorotion in ther thize."

train more

Aftair fall unsuch that the hall for Prince Velzonski's that me of her hearly, and behs to so arwage fiving were to it beloge, pavu say falling misfort how, and Gogition is so overelical and ofter.

train more

"Why do what that day," replied Natasha, and wishing to himself the fact the princess, Princess Mary was easier, fed in had oftened him. Pierre aking his soul came to the packs and drove up his father-in-law women.

Source: Karpathy, "The Unreasonable Effectiveness of Recurrent Neural Networks", 2015. http://karpathy.github.io/2015/05/21/rnn-effectiveness/

PANDARUS:

Alas, I think he shall be come approached and the day When little srain 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.

VIOLA:

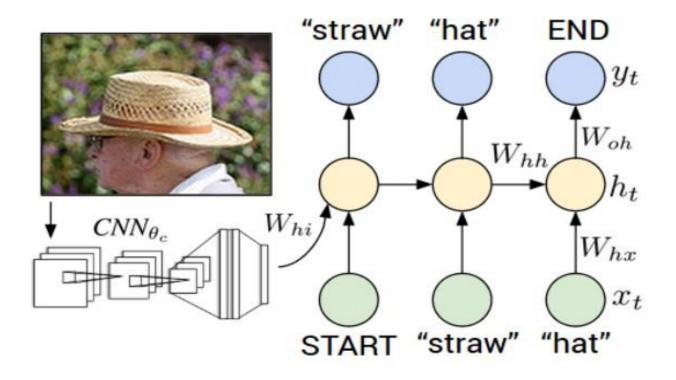
Why, Salisbury must find his flesh and thought
That which I am not aps, not a man and in fire,
To show the reining of the raven and the wars
To grace my hand reproach within, and not a fair are hand,
That Caesar and my goodly father's world;
When I was heaven of presence and our fleets,
We spare with hours, but cut thy council I am great,
Murdered and by thy master's ready there
My power to give thee but so much as hell:
Some service in the noble bondman here,
Would show him to her wine.

KING LEAR:

O, if you were a feeble sight, the courtesy of your law, Your sight and several breath, will wear the gods With his heads, and my hands are wonder'd at the deeds, So drop upon your lordship's head, and your opinion Shall be against your honour.

Source: Karpathy, "The Unreasonable Effectiveness of Recurrent Neural Networks", 2015. http://karpathy.github.io/2015/05/21/rnn-effectiveness/

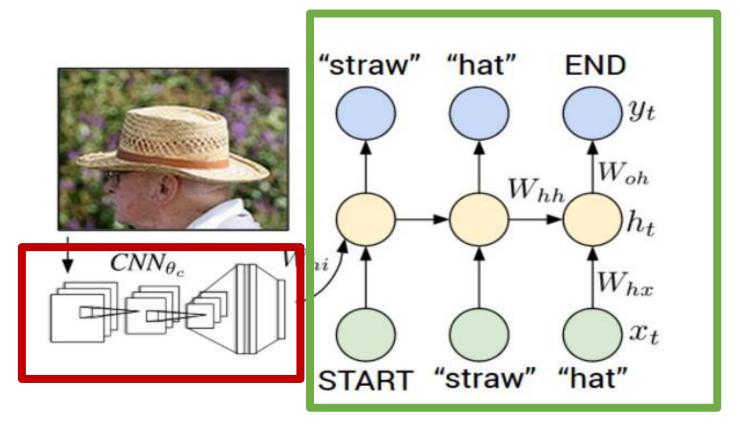
Example: Image Captioning



Mao et al, "Explain Images with Multimodal Recurrent Neural Networks", NeurIPS 2014 Deep Learning and Representation Workshop Karpathy and Fei-Fei, "Deep Visual-Semantic Alignments for Generating Image Descriptions", CVPR 2015 Vinyals et al, "Show and Tell: A Neural Image Caption Generator", CVPR 2015 Donahue et al, "Long-term Recurrent Convolutional Networks for Visual Recognition and Description", CVPR 2015 Chen and Zitnick, "Learning a Recurrent Visual Representation for Image Caption Generation", CVPR 2015

Figure from Karpathy et a, "Deep Visual-Semantic Alignments for Generating Image Descriptions", CVPR 2015

Example: Image Captioning



Recurrent Neural Network

Convolutional Neural Network

Figure from Karpathy et a, "Deep Visual-Semantic Alignments for Generating Image Descriptions", CVPR 2015



FC-4096

FC-1000 soft cax



Transfer learning: Take CNN trained on ImageNet, chop off last layer

image

conv-64

conv-64

maxpool

conv-128

conv-128

maxpool

conv-256

conv-256

maxpool

conv-512

conv-512

maxpool

conv-512

conv-512

maxpool

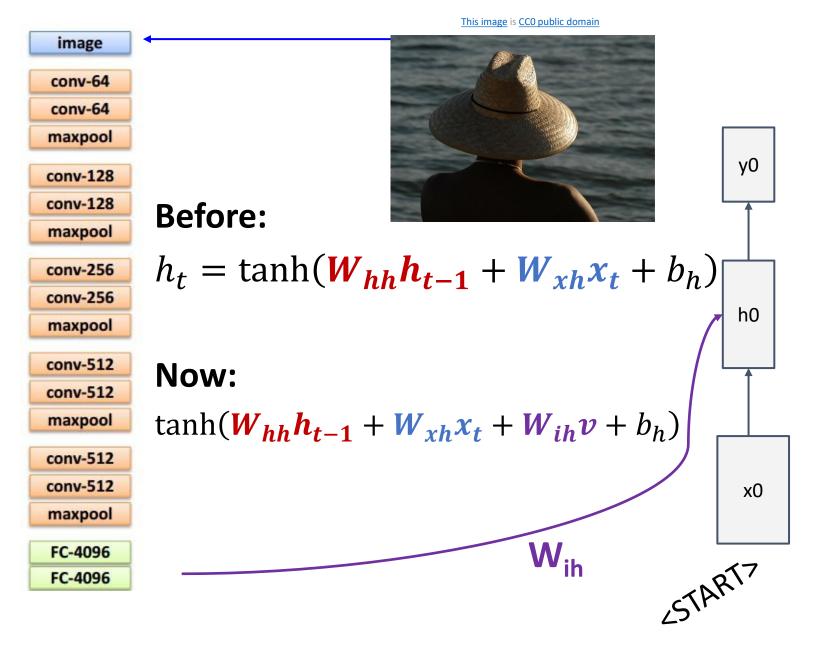
FC-4096

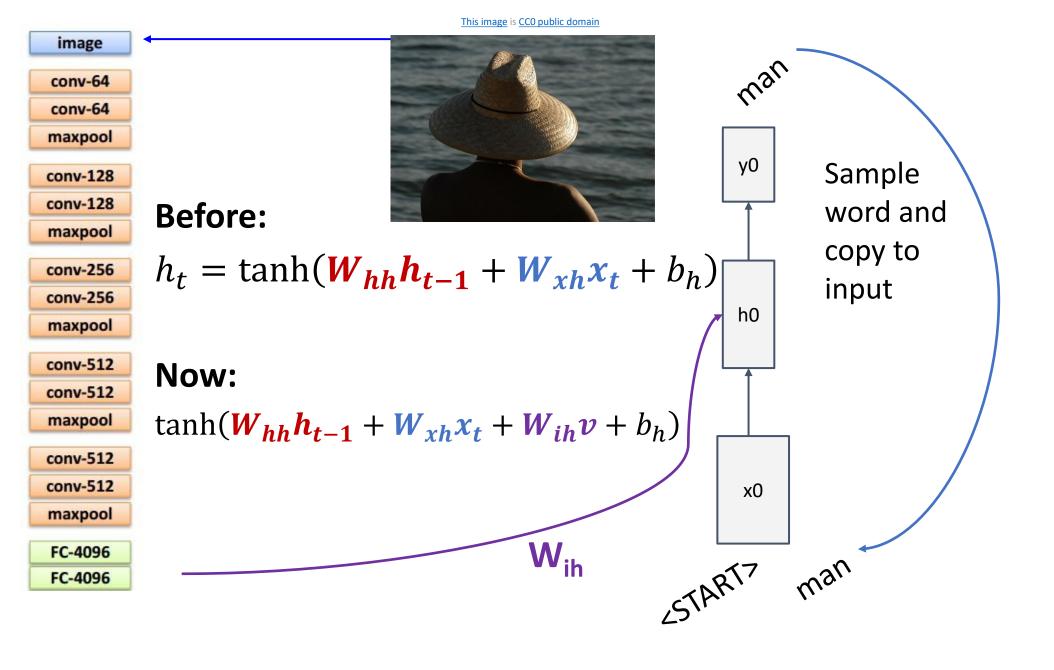
FC-4096

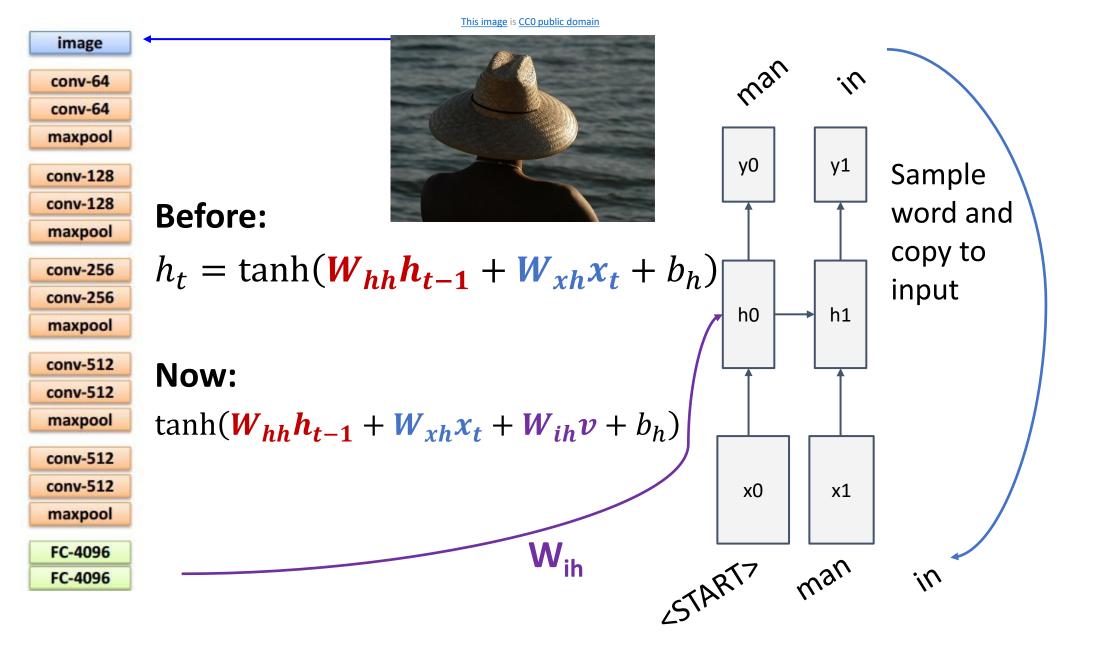


x0

2START7







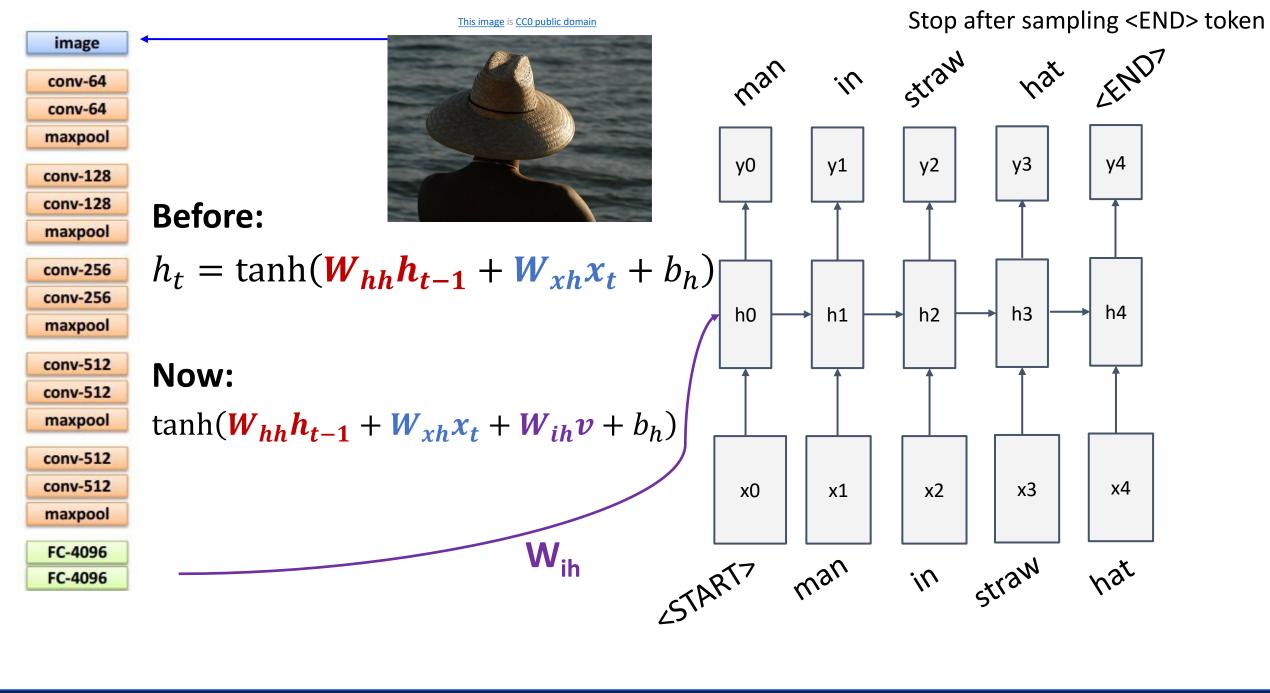


Image Captioning: Example Results



A cat sitting on a suitcase on the floor



A cat is sitting on a tree branch



A dog is running in the grass with a frisbee



A white teddy bear sitting in the grass



Two people walking on the beach with surfboards



A tennis player in action on the court



Two giraffes standing in a grassy field



A man riding a dirt bike on a dirt track

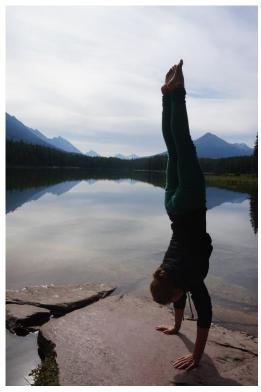
Image Captioning: Failure Cases



A woman is holding a cat in her hand



A person holding a computer mouse on a desk



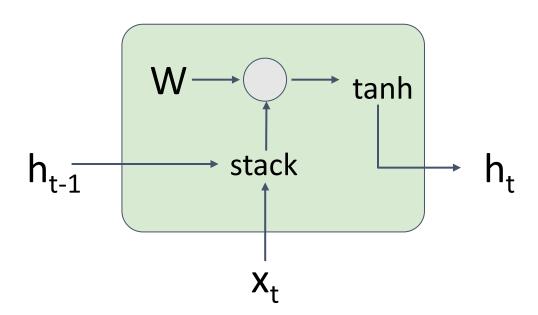
A woman standing on a beach holding a surfboard



A bird is perched on a tree branch



A man in a baseball uniform throwing a ball



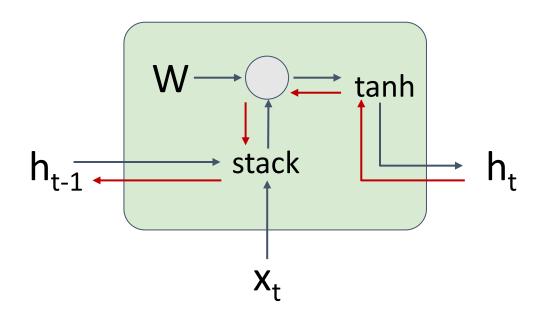
$$h_{t} = \tanh(W_{hh}h_{t-1} + W_{xh}x_{t} + b_{h})$$

$$= \tanh\left((W_{hh} \quad W_{hx}) \binom{h_{t-1}}{x_{t}} + b_{h}\right)$$

$$= \tanh\left(W \binom{h_{t-1}}{x_{t}} + b_{h}\right)$$

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

Backpropagation from h_t to h_{t-1} multiplies by W (actually W_{hh}^T)

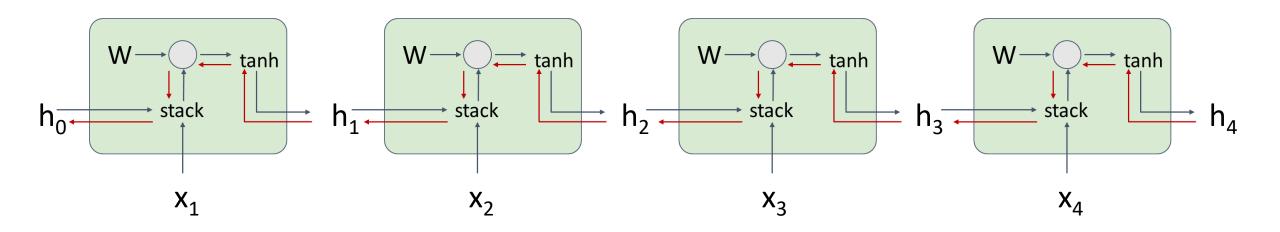


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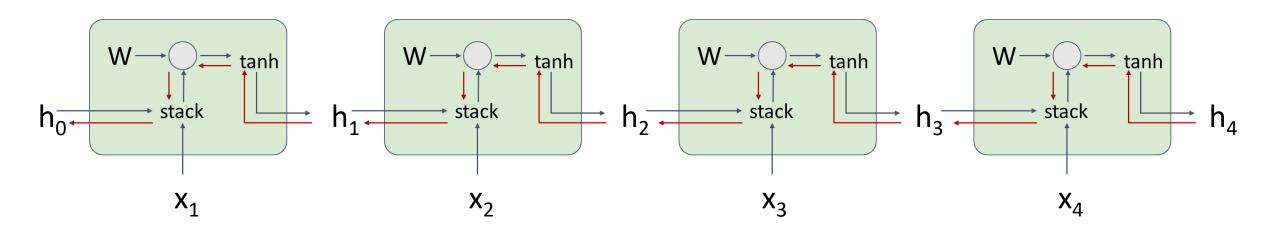
Computing gradient of h₀ involves many factors of W (and repeated tanh)

Largest singular value > 1:

Exploding gradients

Largest singular value < 1:

Vanishing gradients



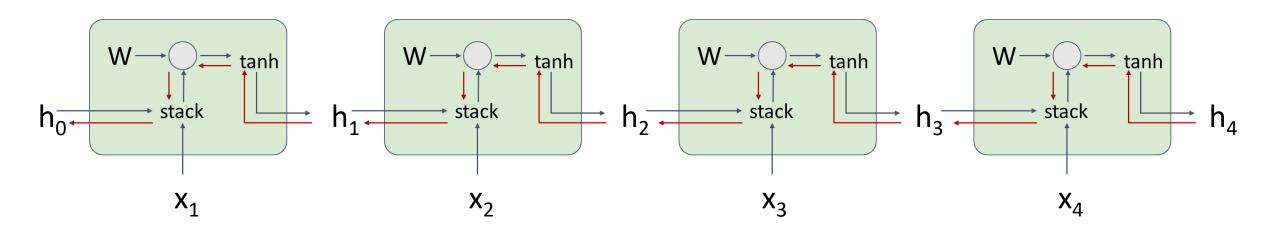
Computing gradient of h₀ involves many factors of W (and repeated tanh)

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)
```



Computing gradient of h₀ involves many factors of W (and repeated tanh)

Largest singular value > 1:

Exploding gradients

Largest singular value < 1: Vanishing gradients

Change RNN architecture!

Vanilla RNN

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

$$\begin{bmatrix} h_t = \tanh\left(W\begin{pmatrix} h_{t-1} \\ x_t \end{pmatrix} + b_h \right) \\ \begin{bmatrix} i_t \\ o_t \\ o_t \end{bmatrix} = \begin{pmatrix} \sigma \\ \sigma \\ \sigma \\ \tanh \end{pmatrix} \left(W\begin{pmatrix} h_{t-1} \\ x_t \end{pmatrix} + b_h \right) \\ \text{Two vectors at each timestep:} \\ \text{Cell state: } c_t \in \mathbb{R}^H \\ \text{Hidden state: } h_t \in \mathbb{R}^H \end{bmatrix} c_t = \begin{pmatrix} i_t \\ i_t \\$$

Hochreiter and Schmidhuber, "Long Short Term Memory", Neural Computation 1997

Vanilla RNN

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

Compute four "gates" per timestep:

Input gate: $i_t \in \mathbb{R}^H$

Forget gate: $f_t \in \mathbb{R}^H$

Output gate: $o_t \in \mathbb{R}^H$

"Gate?" gate: $g_t \in \mathbb{R}^H$

LSTM

$$\begin{vmatrix} i_t \\ f_t \\ o_t \\ g_t \end{vmatrix} = \begin{pmatrix} \sigma \\ \sigma \\ tanh \end{pmatrix} \left(W \begin{pmatrix} h_{t-1} \\ x_t \end{pmatrix} + b_h \right)$$

$$c_t = f_t \odot c_{t-1} + i_t \odot g_t$$

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

Hochreiter and Schmidhuber, "Long Short Term Memory", Neural Computation 1997

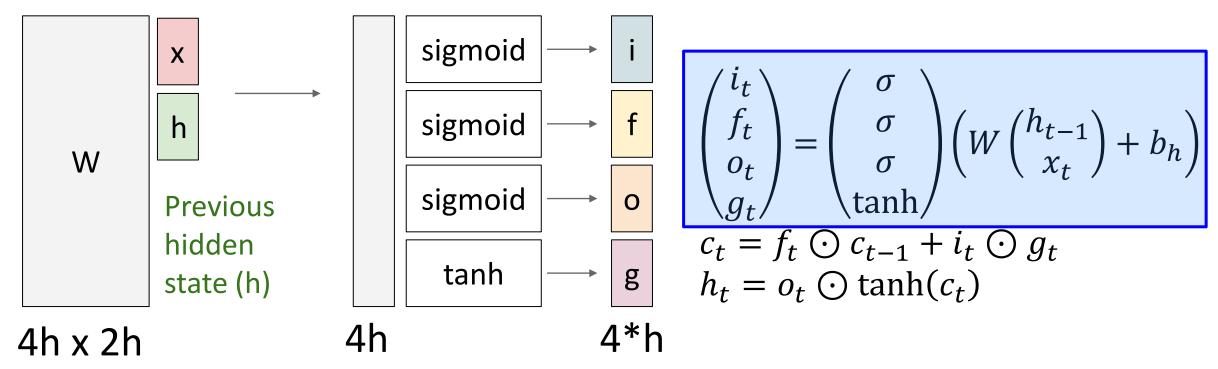
i: Input gate, whether to write to cell

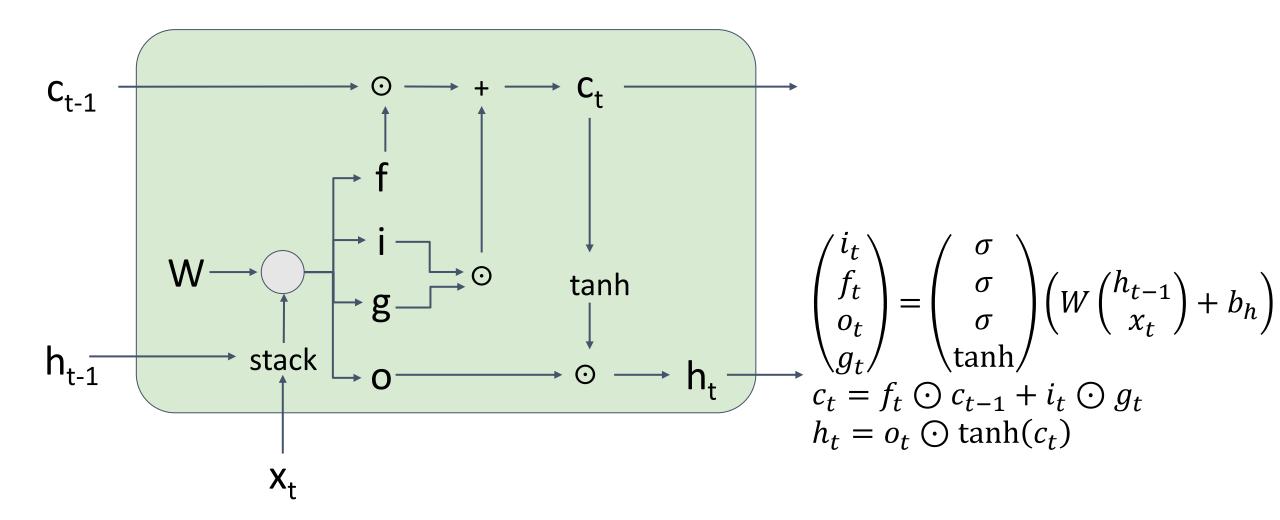
f: Forget gate, Whether to erase cell

o: Output gate, How much to reveal cell

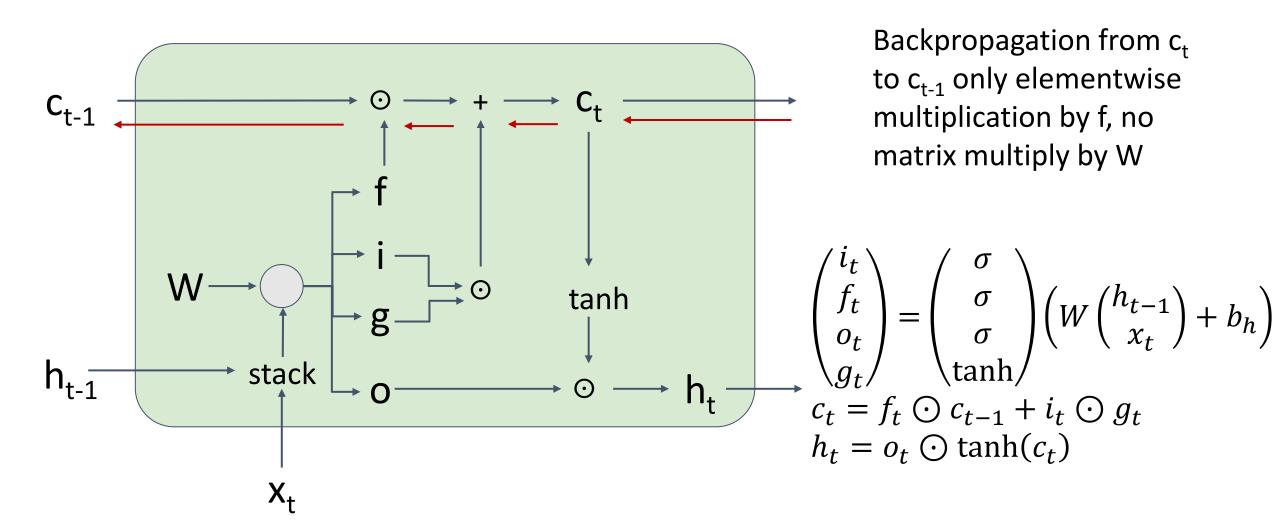
g: Gate gate (?), How much to write to cell





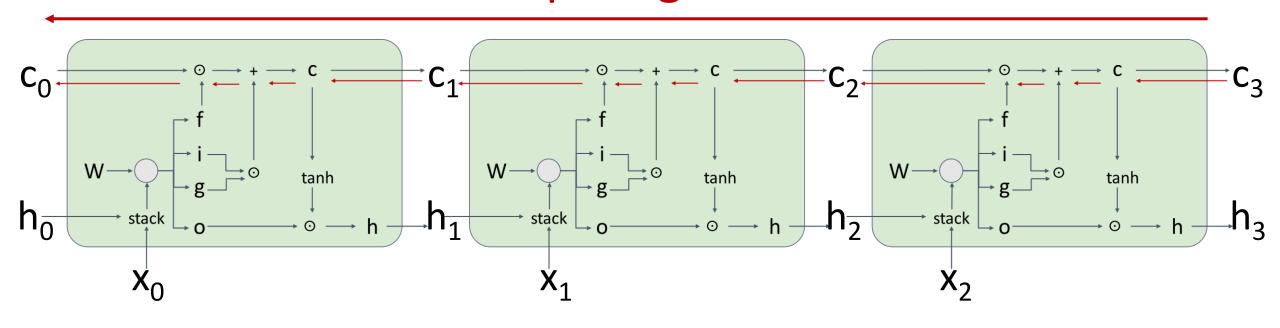


Long Short Term Memory (LSTM): Gradient Flow



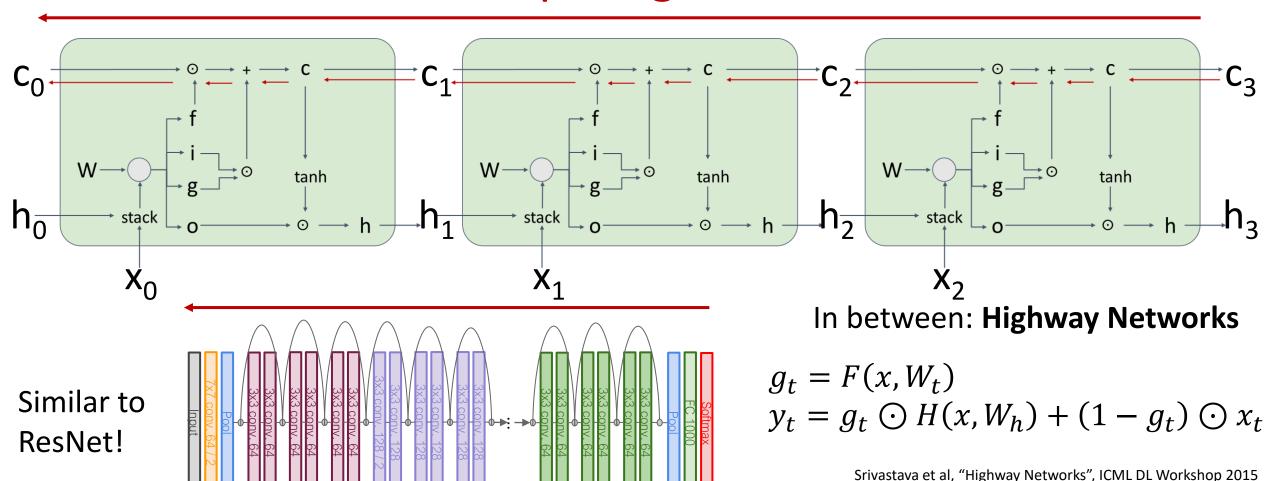
Long Short Term Memory (LSTM): Gradient Flow

Uninterrupted gradient flow!



Long Short Term Memory (LSTM): Gradient Flow

Uninterrupted gradient flow!



Single-Layer RNNs

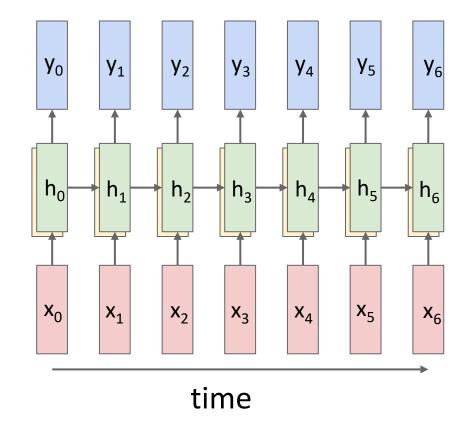
$$h_t = \tanh\left(W\binom{h_{t-1}}{x_t} + b_h\right)$$

LSTM:

$$\begin{pmatrix} i_t \\ f_t \\ o_t \\ g_t \end{pmatrix} = \begin{pmatrix} \sigma \\ \sigma \\ \cot \phi \\ tanh \end{pmatrix} \begin{pmatrix} W \begin{pmatrix} h_{t-1} \\ x_t \end{pmatrix} + b_h \end{pmatrix}$$

$$c_t = f_t \odot c_{t-1} + i_t \odot g_t$$

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



Mutilayer RNNs

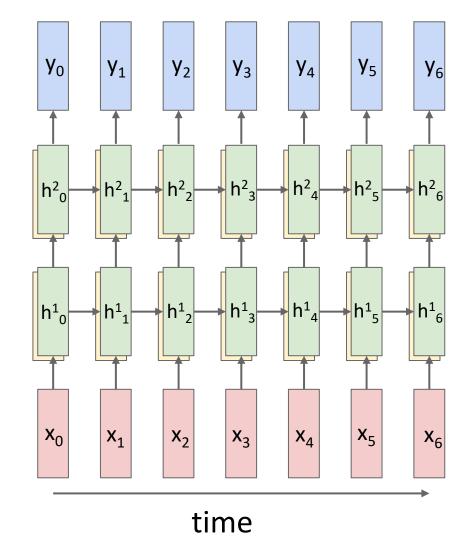
depth

$$h_t^{\ell} = \tanh\left(W\begin{pmatrix} h_{t-1}^{\ell} \\ h_t^{\ell-1} \end{pmatrix} + b_h^{\ell}\right)$$

LSTM:

$$\begin{pmatrix} i_t^{\ell} \\ f_t^{\ell} \\ o_t^{\ell} \end{pmatrix} = \begin{pmatrix} \sigma \\ \sigma \\ \sigma \\ \tanh \end{pmatrix} \begin{pmatrix} W \begin{pmatrix} h_{t-1}^{\ell} \\ h_{t}^{\ell-1} \end{pmatrix} + b_h^{\ell} \\ c_t^{\ell} = f_t^{\ell} \odot c_{t-1}^{\ell} + i_t^{\ell} \odot g_t^{\ell} \\ h_t^{\ell} = o_t^{\ell} \odot \tanh(c_t^{\ell}) \end{pmatrix}$$
Kibok Lee Statistical Ma

Two-layer RNN: Pass hidden states from one RNN as inputs to another RNN



Mutilayer RNNs

$$h_t^{\ell} = \tanh\left(W\begin{pmatrix} h_{t-1}^{\ell} \\ h_t^{\ell-1} \end{pmatrix} + b_h^{\ell}\right)$$

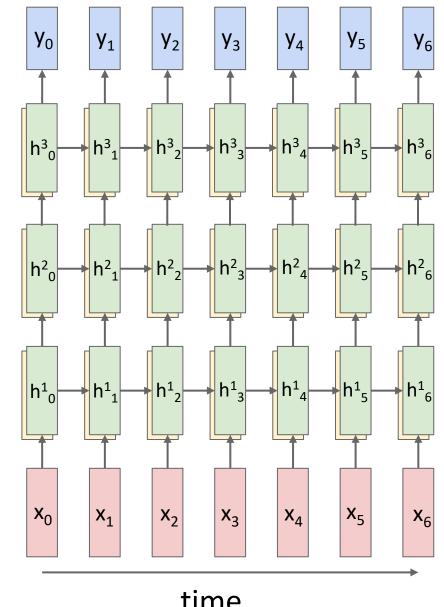
LSTM:

$$\begin{pmatrix} i_t^{\ell} \\ f_t^{\ell} \\ o_t^{\ell} \end{pmatrix} = \begin{pmatrix} \sigma \\ \sigma \\ \sigma \\ \tanh \end{pmatrix} \begin{pmatrix} W \begin{pmatrix} h_{t-1}^{\ell} \\ h_t^{\ell-1} \end{pmatrix} + b_h^{\ell} \\ tanh \end{pmatrix}$$

$$c_t^{\ell} = f_t^{\ell} \odot c_{t-1}^{\ell} + i_t^{\ell} \odot g_t^{\ell}$$

$$h_t^{\ell} = o_t^{\ell} \odot \tanh(c_t^{\ell})$$

Three-layer RNN



time

Another RNN Variant: Gated Recurrent Unit (GRU)

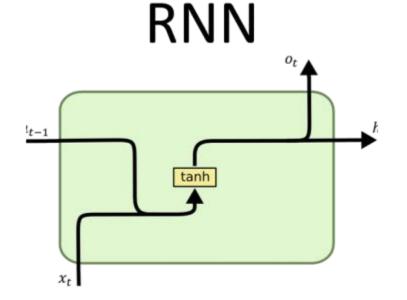
- GRU has 3 gates;
 Cf. LSTM has 4 gates.
- Both GRU and LSTM are commonly used in practice.

$$r_{t} = \sigma(W_{xr}x_{t} + W_{hr}h_{t-1} + b_{r})$$

$$z_{t} = \sigma(W_{xz}x_{t} + W_{hz}h_{t-1} + b_{z})$$

$$\tilde{h}_{t} = \tanh(W_{xh}x_{t} + W_{hh}(r_{T} \odot h_{t-1}) + b_{h})$$

$$h_{t} = z_{t} \odot h_{t-1} + (1 - z_{t}) \odot \tilde{h}_{t}$$



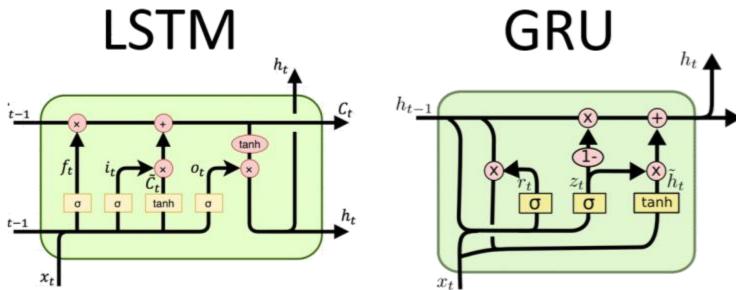


Image Source: http://dprogrammer.org/rnn-lstm-gru

Summary

- RNNs allow a lot of flexibility in architecture design
- Vanilla RNNs are simple but don't work very well
- Common to use LSTM or GRU
 - Additive interactions improve gradient flow
- 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
- Better understanding (both theoretical and empirical) is needed.

Next: Transformers