



# Recurrent Neural Networks (RNN) and Long-Short-Term-Memory (LSTM)

Yuan YAO

HKUST



# Summary

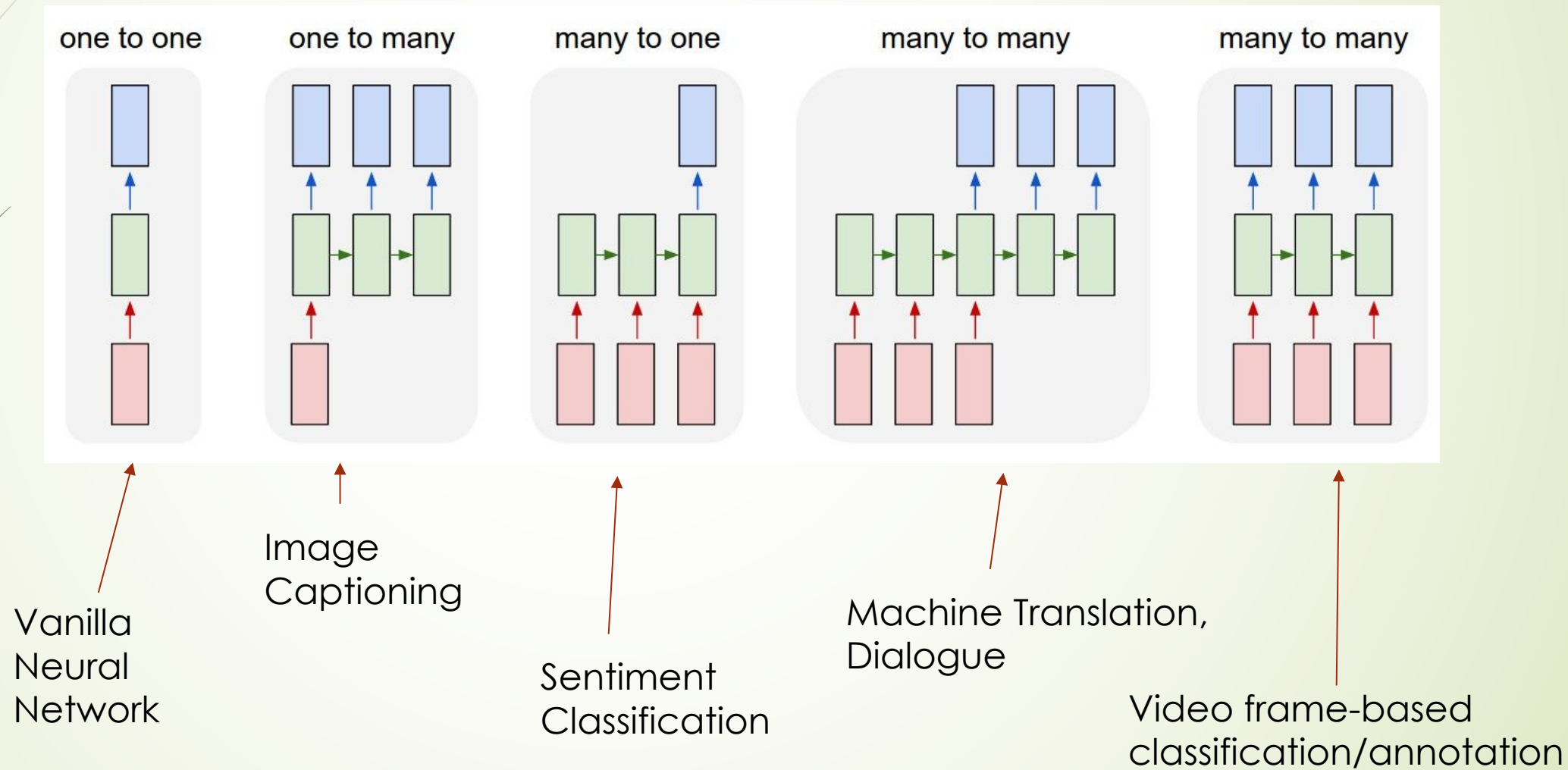


- ▶ We have shown:
  - ▶ CNN Architectures: LeNet5, Alexnet, VGG, GoogleNet, Resnet
- ▶ Today:
  - ▶ **Recurrent Neural Networks**
  - ▶ **LSTM/GRU**
- ▶ Reference:
  - ▶ Feifei Li, Stanford cs231n
  - ▶ Chris Manning, Stanford cs224n

A decorative graphic on the left side of the slide. It features a solid red arrow pointing to the right, positioned horizontally. Behind the arrow and extending upwards and to the right are several thin, dark grey, curved lines that resemble stylized grass or reeds. The background of the slide is a light, pale green color.

# Recurrent Neural Networks

# Recurrent Neural Networks: Sequence Processing



# Sequential Processing of Non-Sequence Data

Classify images by taking a series of “glimpses”

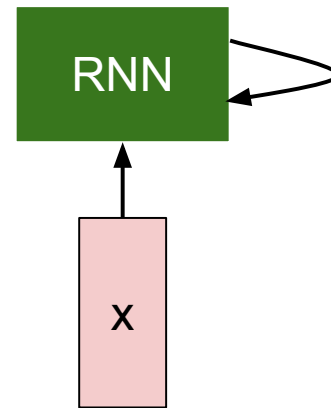


Ba, Mnih, and Kavukcuoglu, “Multiple Object Recognition with Visual Attention”, ICLR 2015.

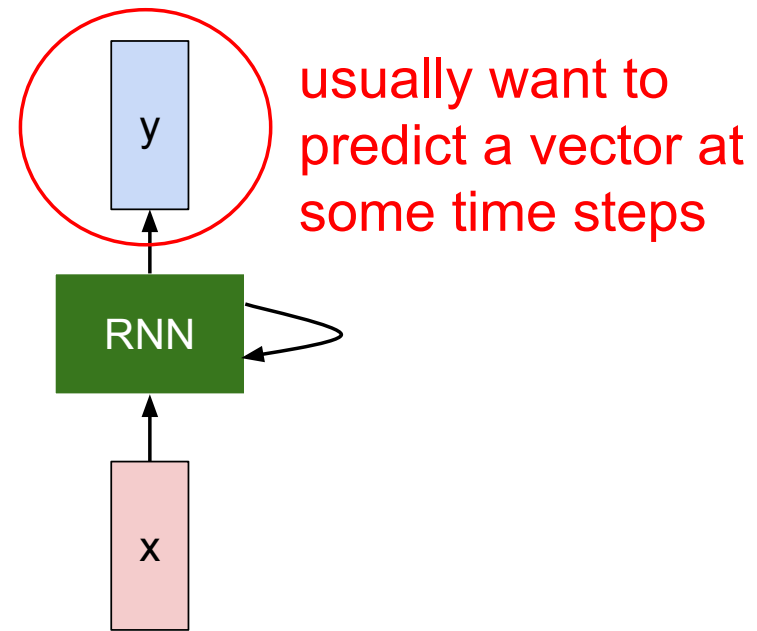
Gregor et al, “DRAW: A Recurrent Neural Network For Image Generation”, ICML 2015

Figure copyright Karol Gregor, Ivo Danihelka, Alex Graves, Danilo Jimenez Rezende, and Daan Wierstra, 2015. Reproduced with permission

# Recurrent Neural Network



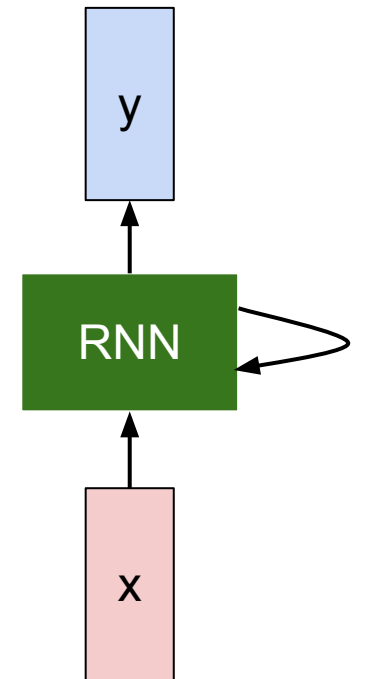
# Recurrent Neural Network



We can process a sequence of vectors  $\mathbf{x}$  by applying a **recurrence formula** at every time step:

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

new state                      some function with parameters  $W$                       old state                      input vector at some time step

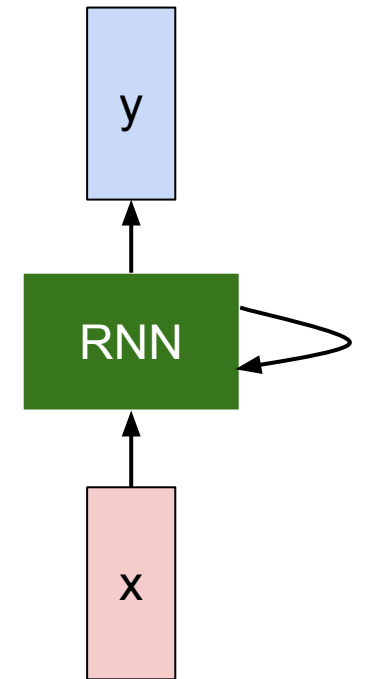




We can process a sequence of vectors  $\mathbf{x}$  by applying a **recurrence formula** at every time step:

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

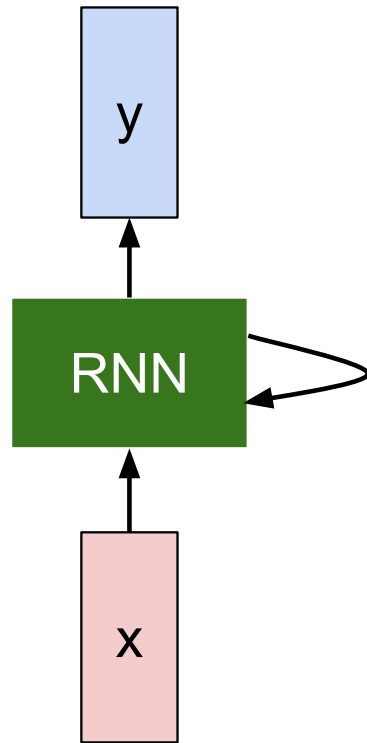
Notice: the same function and the same set of parameters are used at every time step.



# Vanilla Recurrent Neural Networks

State Space equations in feedback dynamical systems

The state consists of a single “*hidden*” vector  $\mathbf{h}$ :



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



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

$$y_t = W_{hy}h_t$$

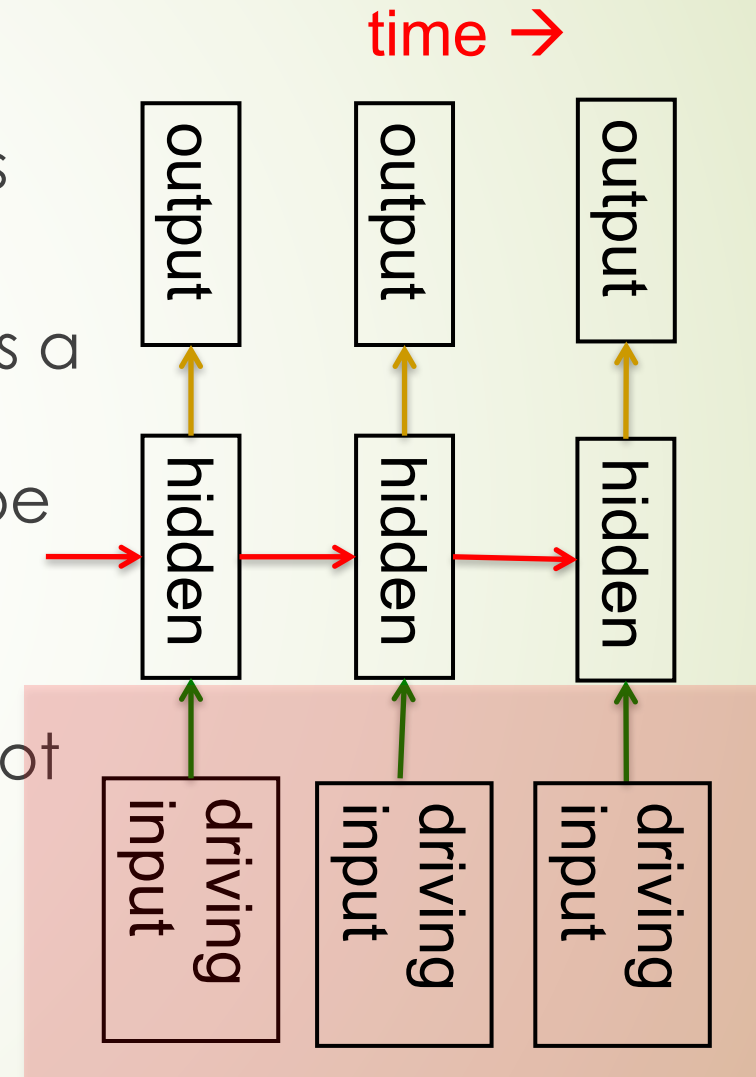
Or, 
$$y_t = \text{softmax}(W_{hy}h_t)$$

# Linear Dynamical Systems (1940s-)

- ▶ The hidden state has linear dynamics with Gaussian noise and produces the observations using a linear model with Gaussian noise.
- ▶ Kalman Filter: A linearly transformed Gaussian is a Gaussian. So the distribution over the hidden state given the data so far is Gaussian. It can be computed using “Kalman filtering” (a.k.a. **recursive least square**).
- ▶ To predict the next output (so that we can shoot down the missile) we need to infer the hidden state.

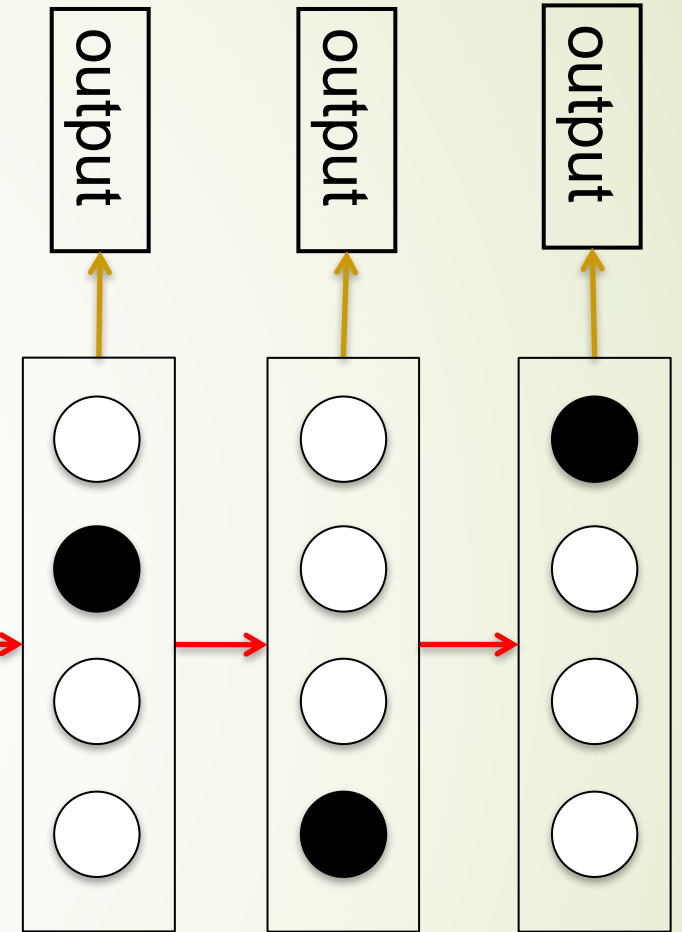
$$h_t = W_{hh}h_{t-1} + W_{hx}x_t + \epsilon_t^h$$

$$y_t = W_{yh}h_t + W_{yx}x_t + \epsilon_t^y$$

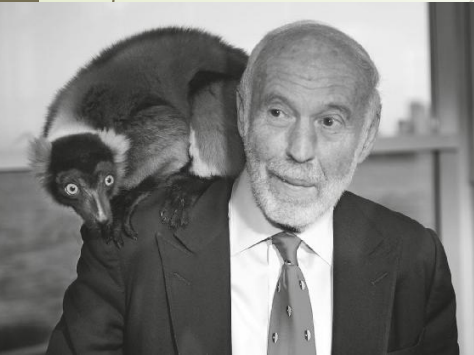


# Hidden Markov Models (1970s-)

- Hidden Markov Models have a discrete one-of-N hidden state. Transitions between states are stochastic and controlled by a transition matrix. The outputs produced by a state are stochastic.
- We cannot be sure which state produced a given output. So the state is “hidden”.
- It is easy to represent a probability distribution across N states with N numbers.
- To predict the next output we need to infer the probability distribution over hidden states.
  - HMMs have efficient algorithms (**Baum-Welch or EM Algorithm**) for inference and learning.
  - **Jim Simons** hires Lenny Baum as the founding member of Renaissance Technologies in 1979

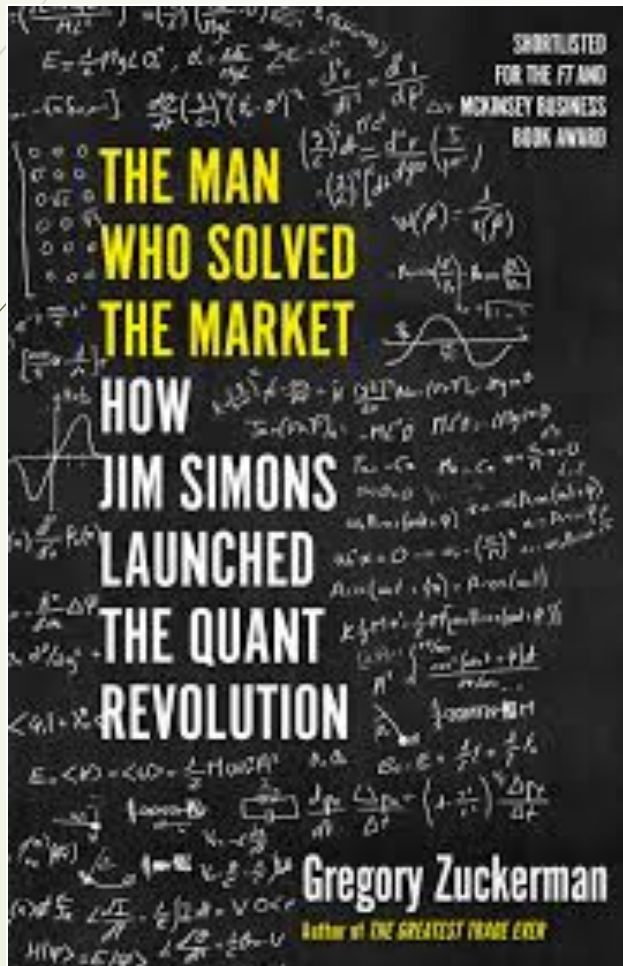


time →



Lenny Baum became a devoted Go player despite his deteriorating eyesight.

# Jim Simons and Renaissance Technology in 1990s



- “A golden age for traditional investing had dawned as George Soros, Peter Lynch, Bill Gross, and others divined the direction of investments, financial markets, and global economies, producing enormous profits with intelligence, intuition, and old-fashioned economic and corporate research.
- Unlike his rivals, Simons didn't have a clue how to estimate cash flows, identify new products, or forecast interest rates. He was digging through reams of price information. There wasn't even a proper name for this kind of trading, which involved **data cleansing, signals, and backtesting**, terms most Wall Street pros were wholly unfamiliar with. “

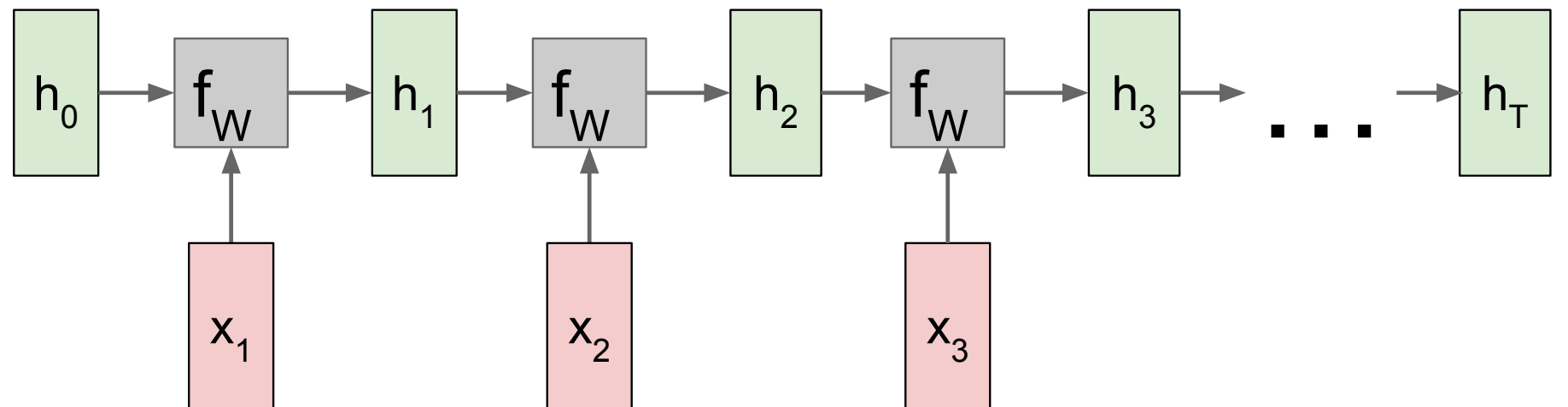


# Recurrent Neural Networks



- ▶ **The issue of a hidden Markov model (HMM):**
  - ▶ At each time step it must select one of its hidden states. So with  $N$  hidden states it can only remember  $\log(N)$  bits about what it generated so far.
- ▶ RNNs are very powerful, because they combine two properties:
  - ▶ Distributed hidden state that allows them to store a lot of information about the past efficiently.
  - ▶ Non-linear dynamics that allows them to update their hidden state in complicated ways.
- ▶ With enough neurons and time, RNNs can compute anything that can be computed by your computer.

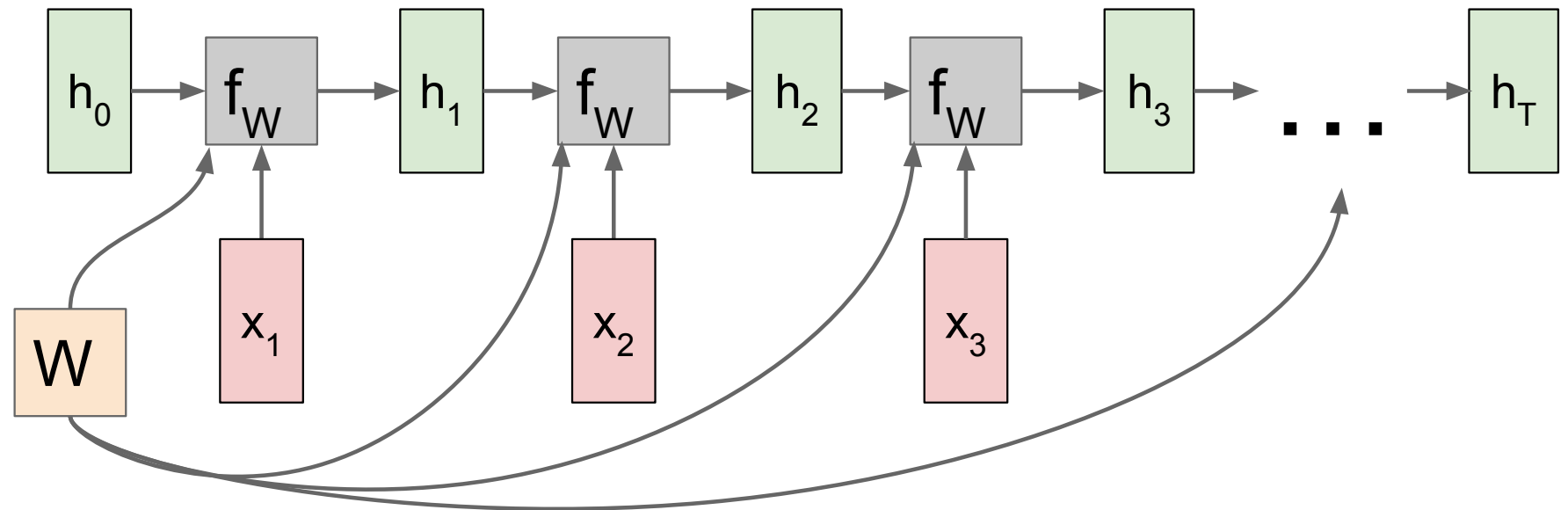
# RNN: Computational Graph



# Time invariant systems

## RNN: Computational Graph

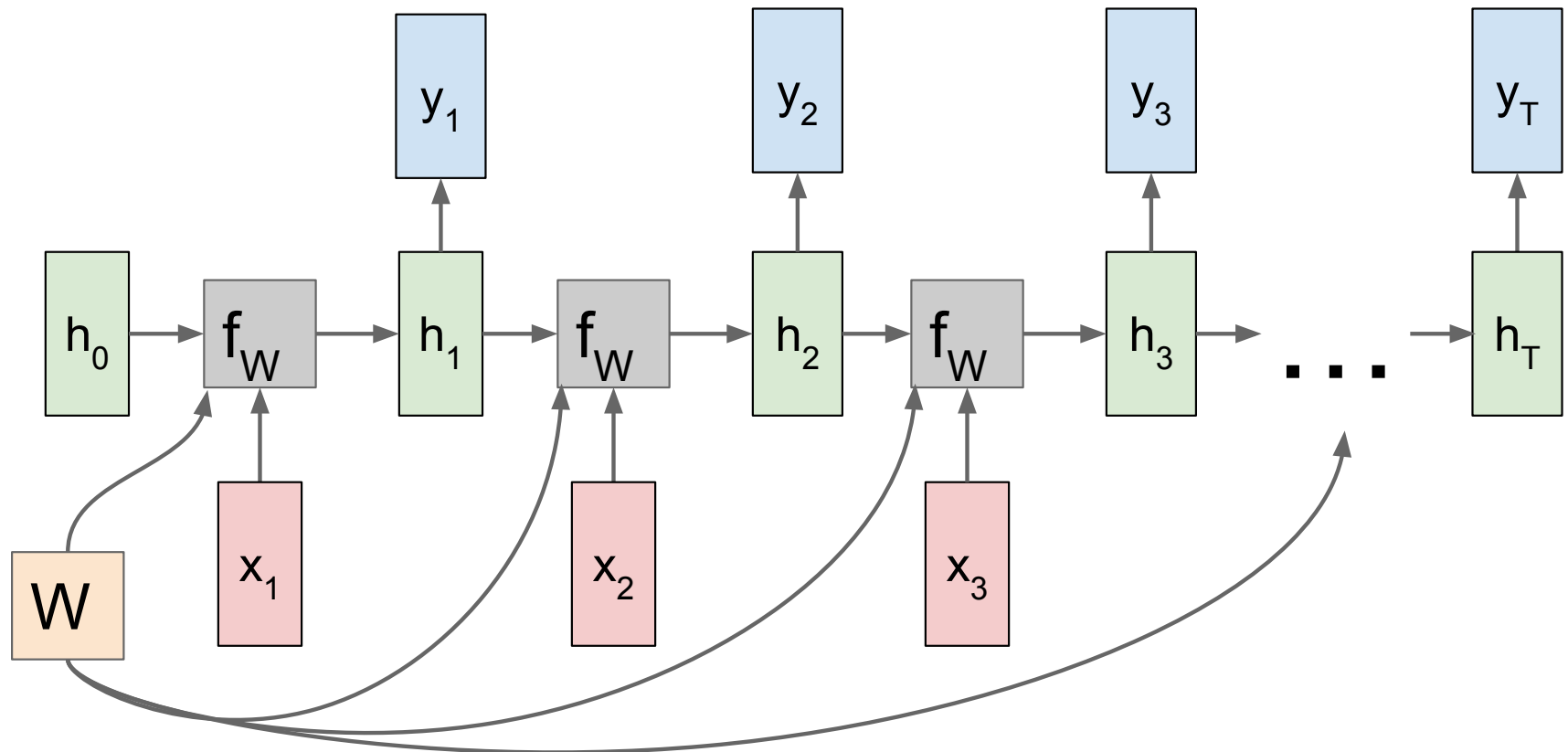
Re-use the same weight matrix at every time-step





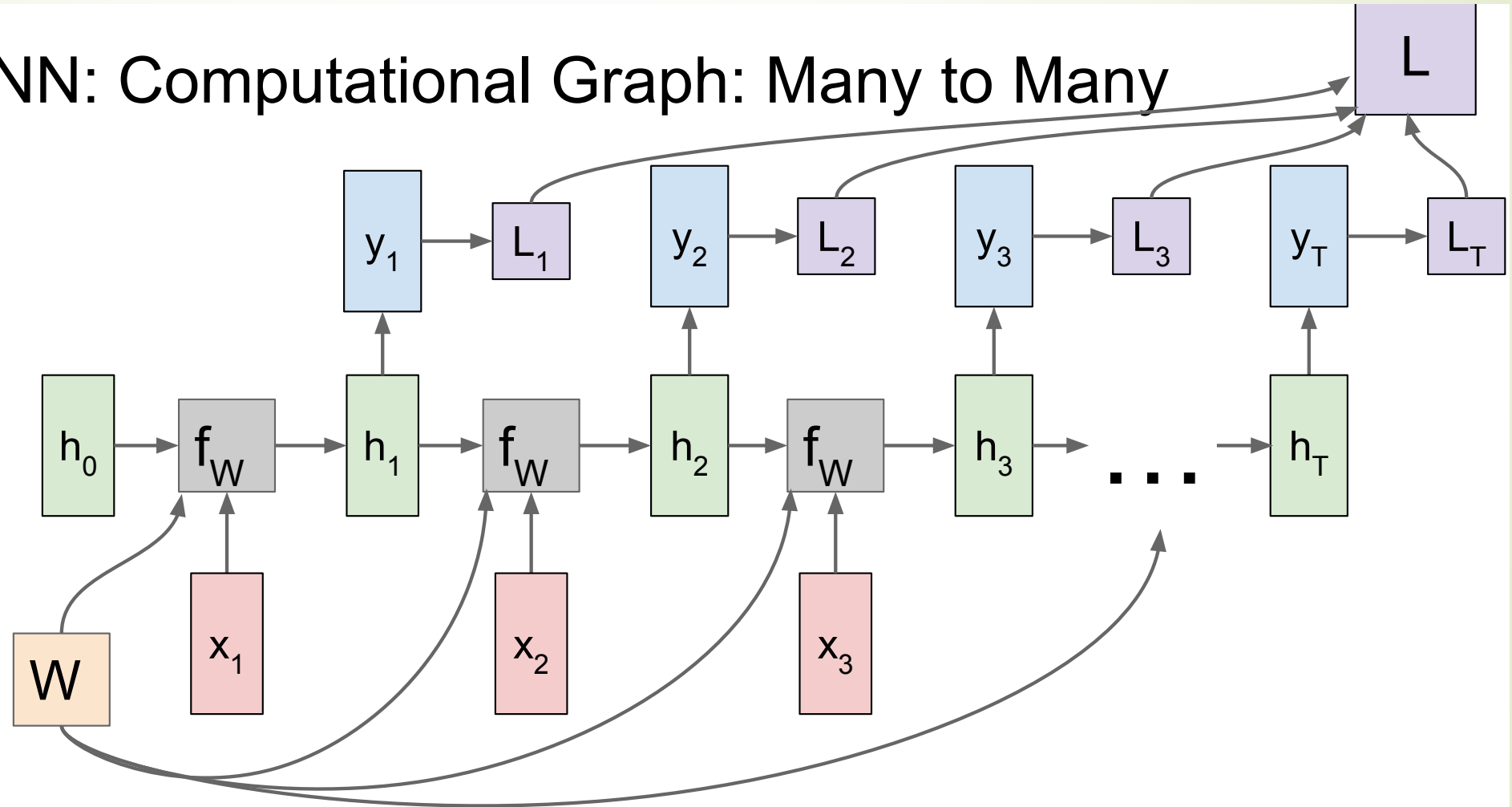
# Outputs added

## RNN: Computational Graph: Many to Many

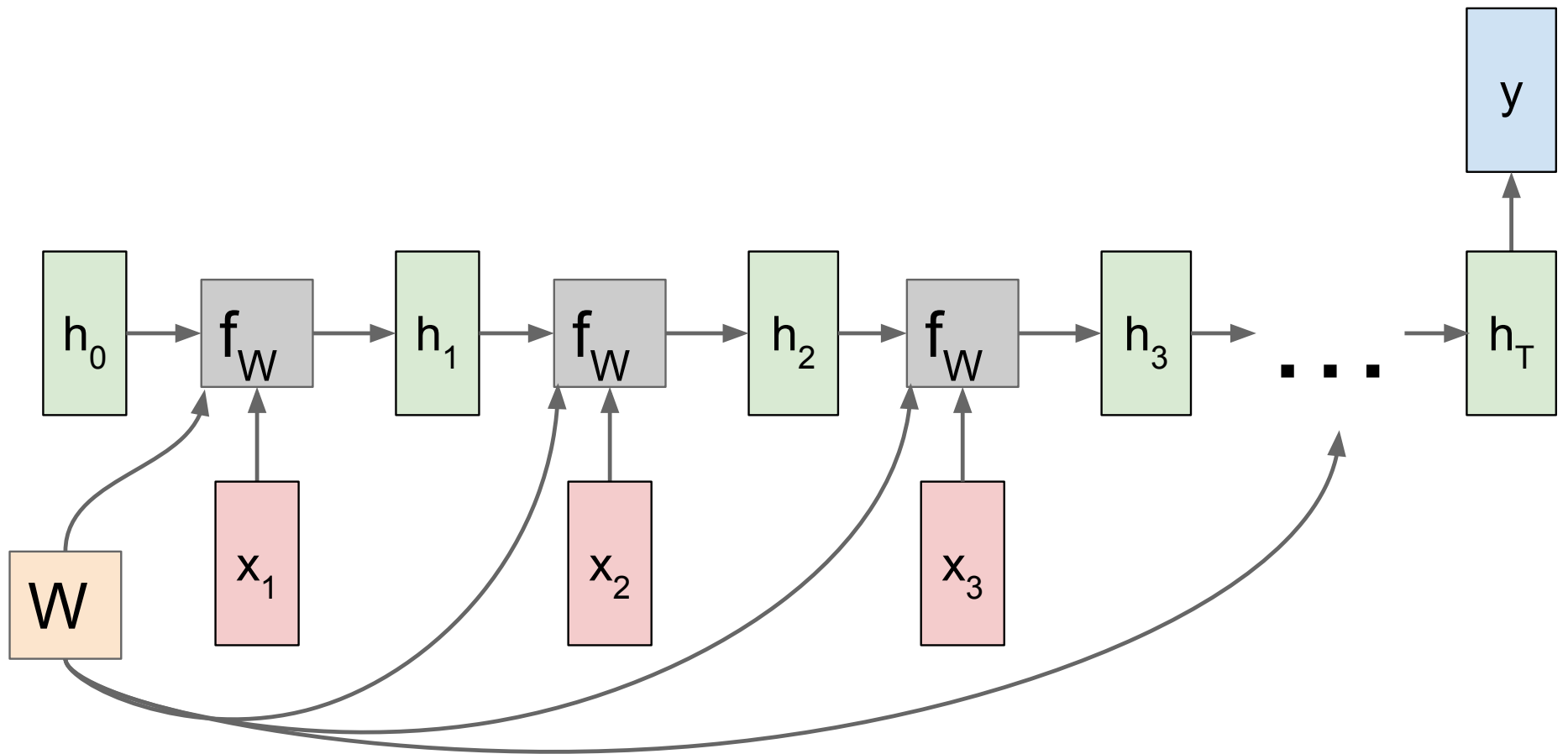


# Loss modules

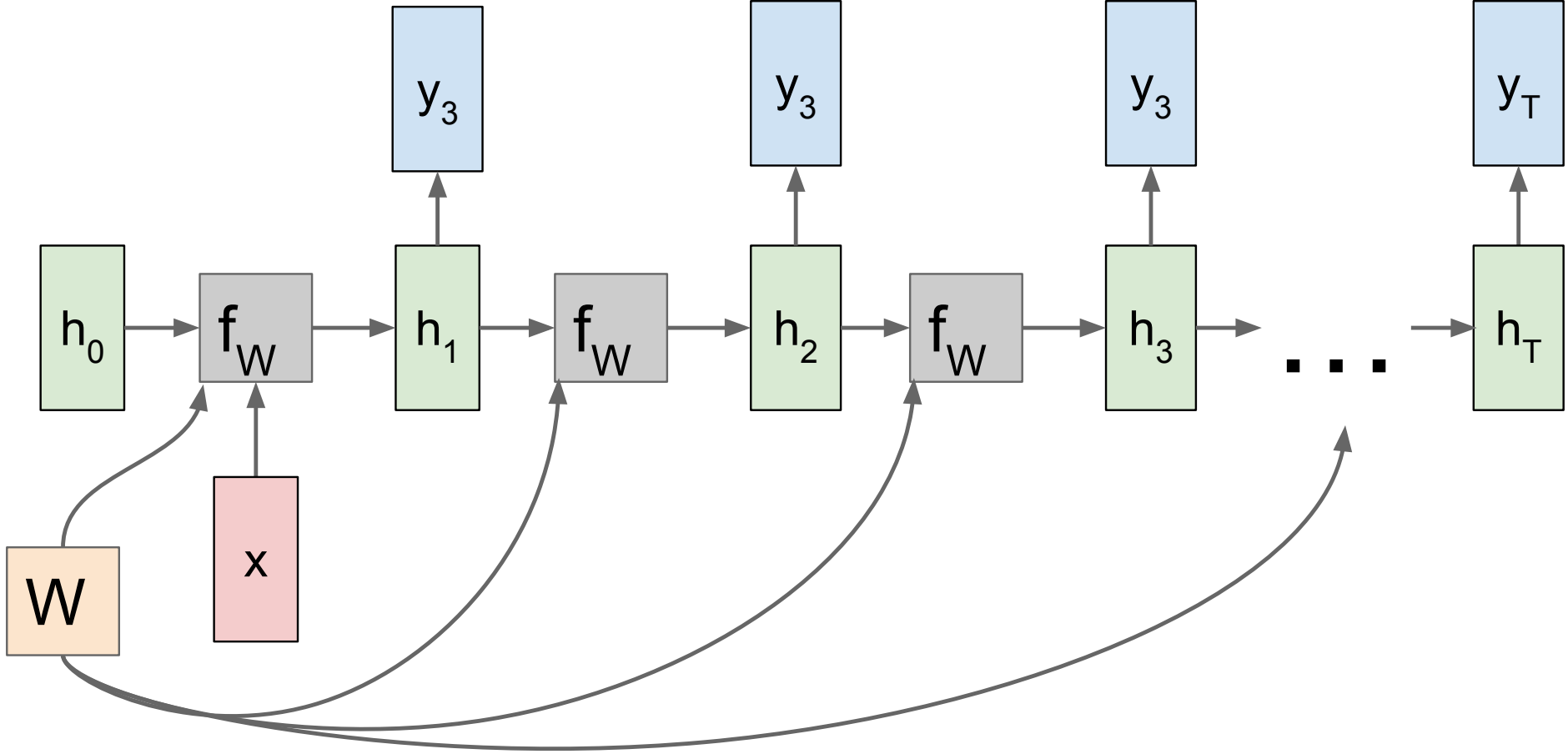
## RNN: Computational Graph: Many to Many



# RNN: Computational Graph: Many to One



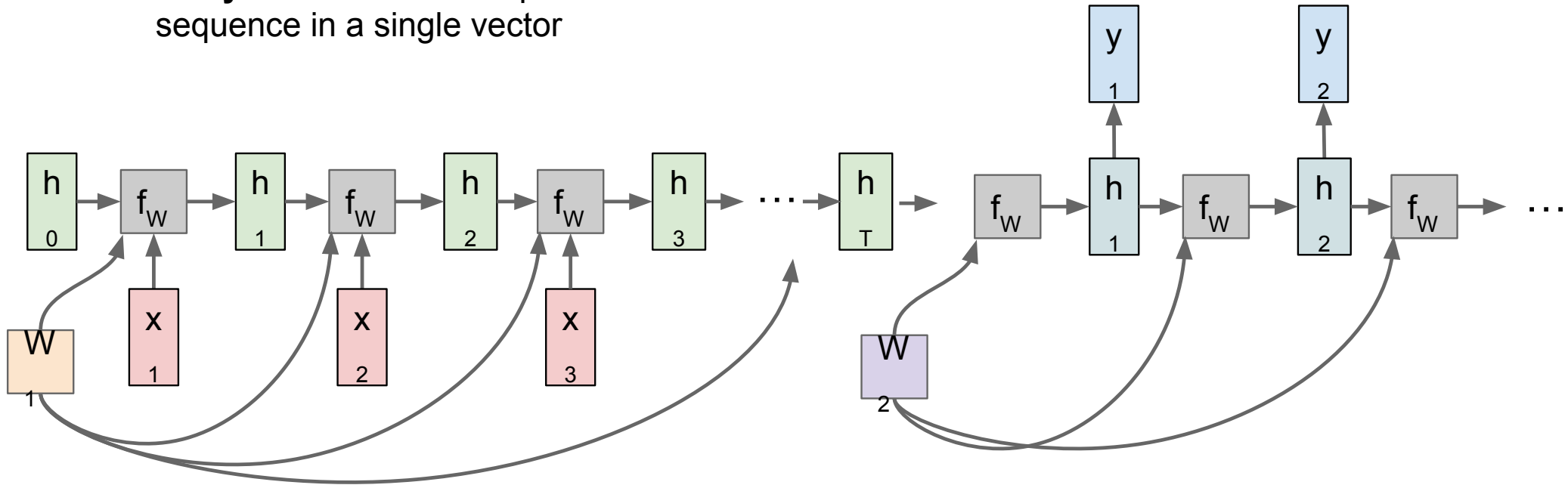
# RNN: Computational Graph: One to Many



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

**Many to one:** Encode input sequence in a single vector

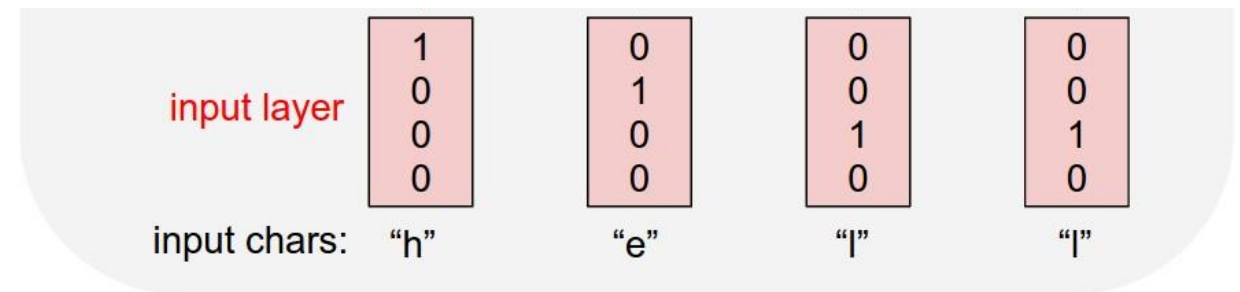
**One to many:** Produce output sequence from single input vector



# Example: Character-level Language Model

Vocabulary:  
[h,e,l,o]

Example training  
sequence:  
“hello”

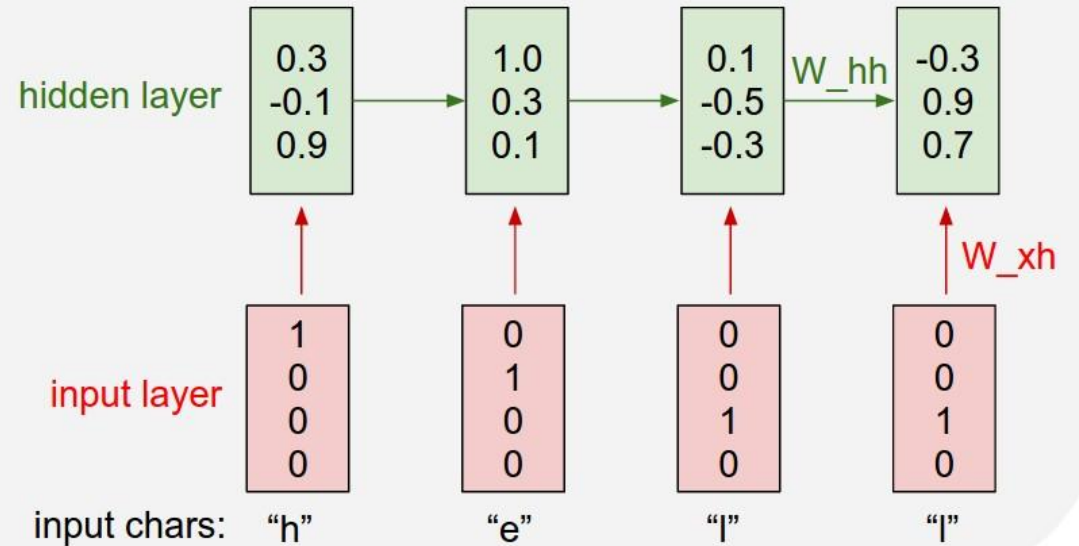


## Example: Character-level Language Model

Vocabulary:  
[h,e,l,o]

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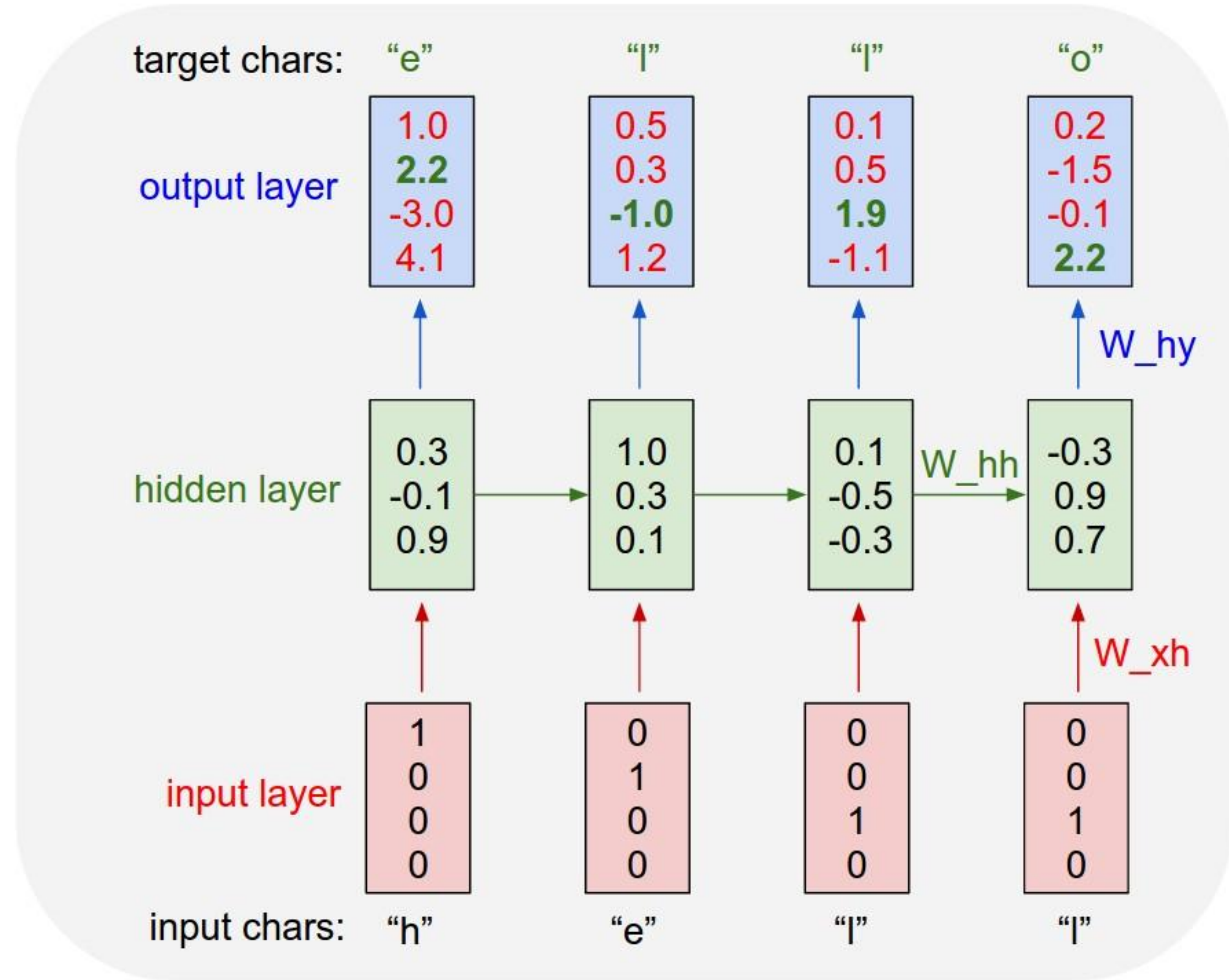
$$h_t = \tanh(W_{hh}h_{t-1} + W_{xh}x_t)$$



# Example: Character-level Language Model

Vocabulary:  
[h,e,l,o]

Example training  
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“hello”

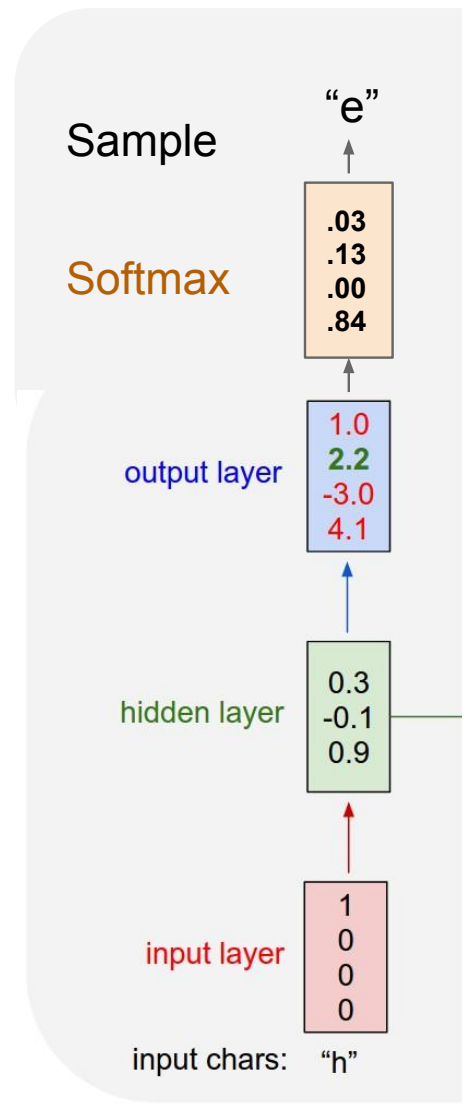




# Example: Character-level Language Model Sampling

Vocabulary:  
[h,e,l,o]

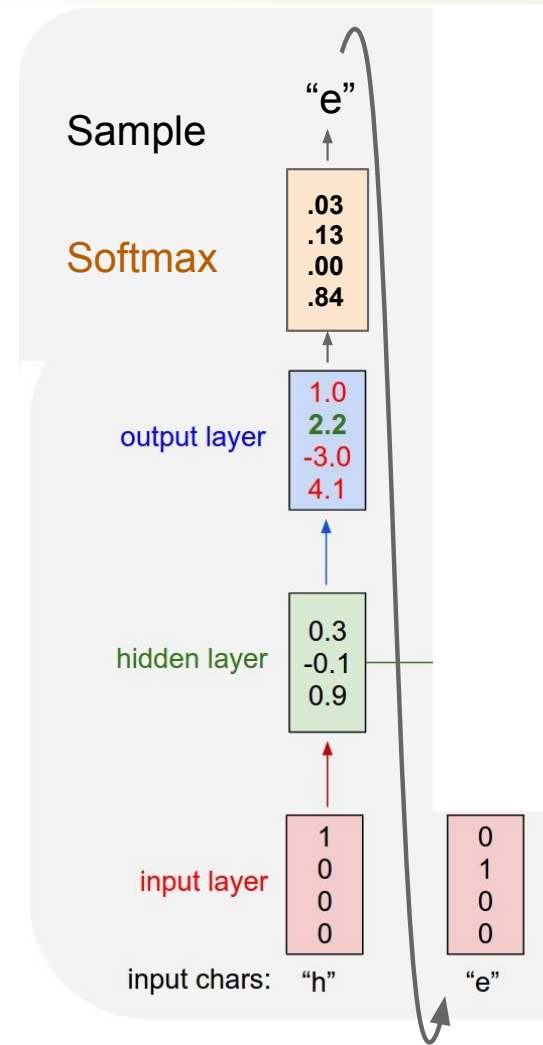
At test-time sample  
characters one at a time,  
feed back to model



# Example: Character-level Language Model Sampling

Vocabulary:  
[h,e,l,o]

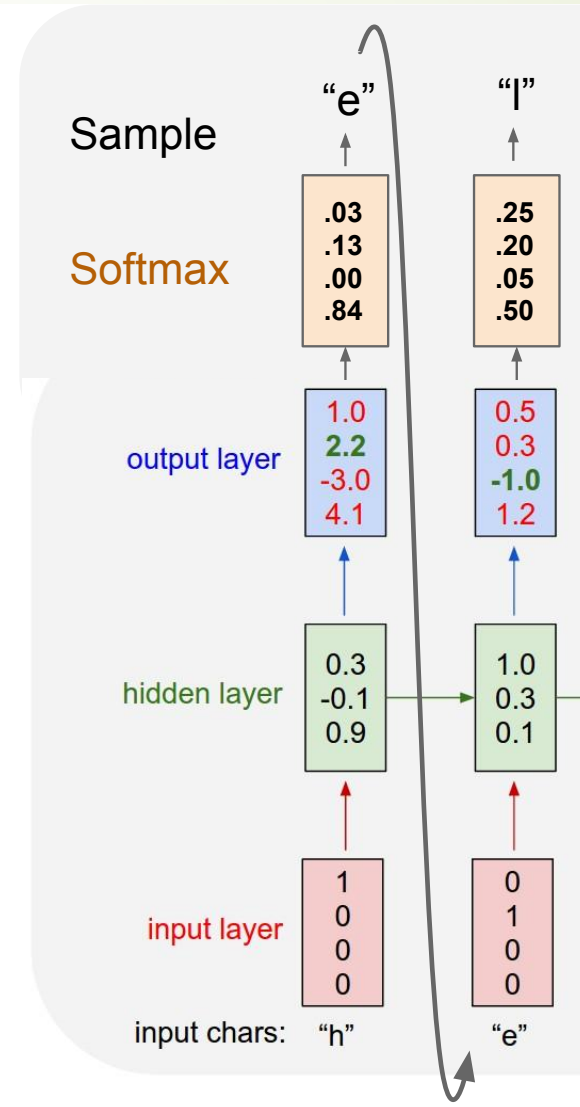
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# Example: Character-level Language Model Sampling

Vocabulary:  
[h,e,l,o]

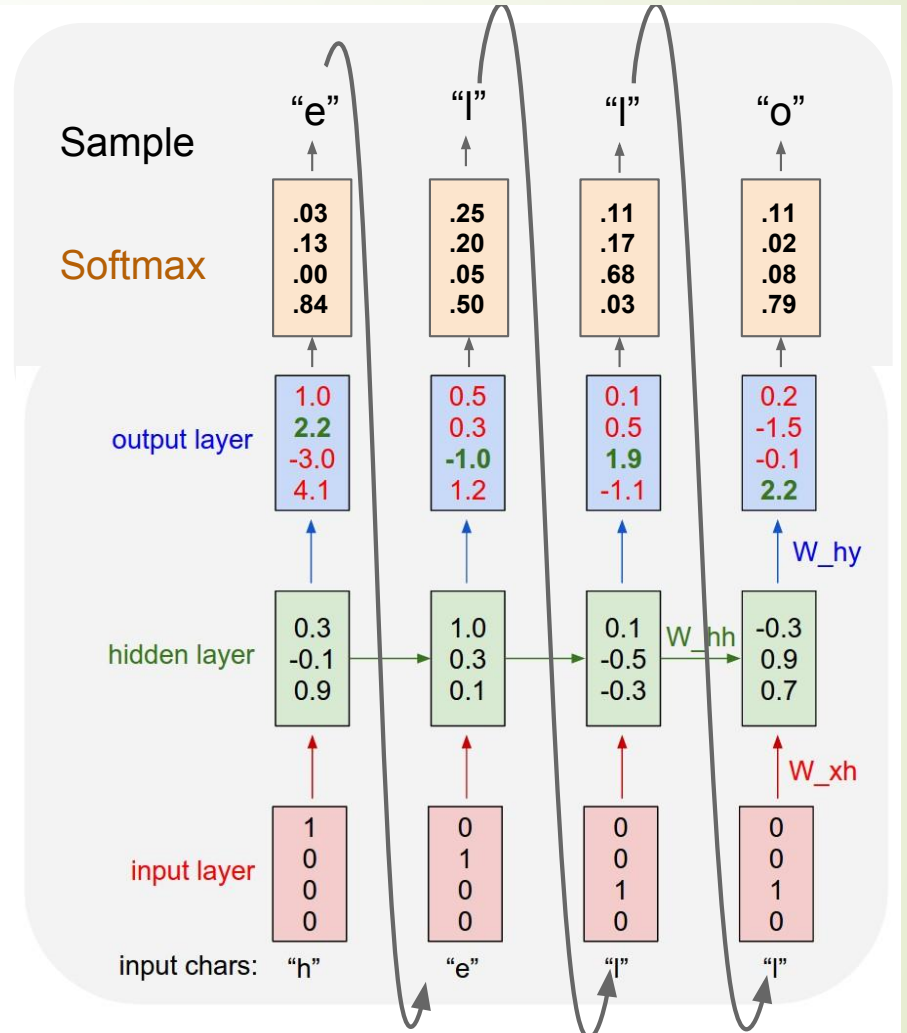
At test-time sample  
characters one at a time,  
feed back to model



# Example: Character-level Language Model Sampling

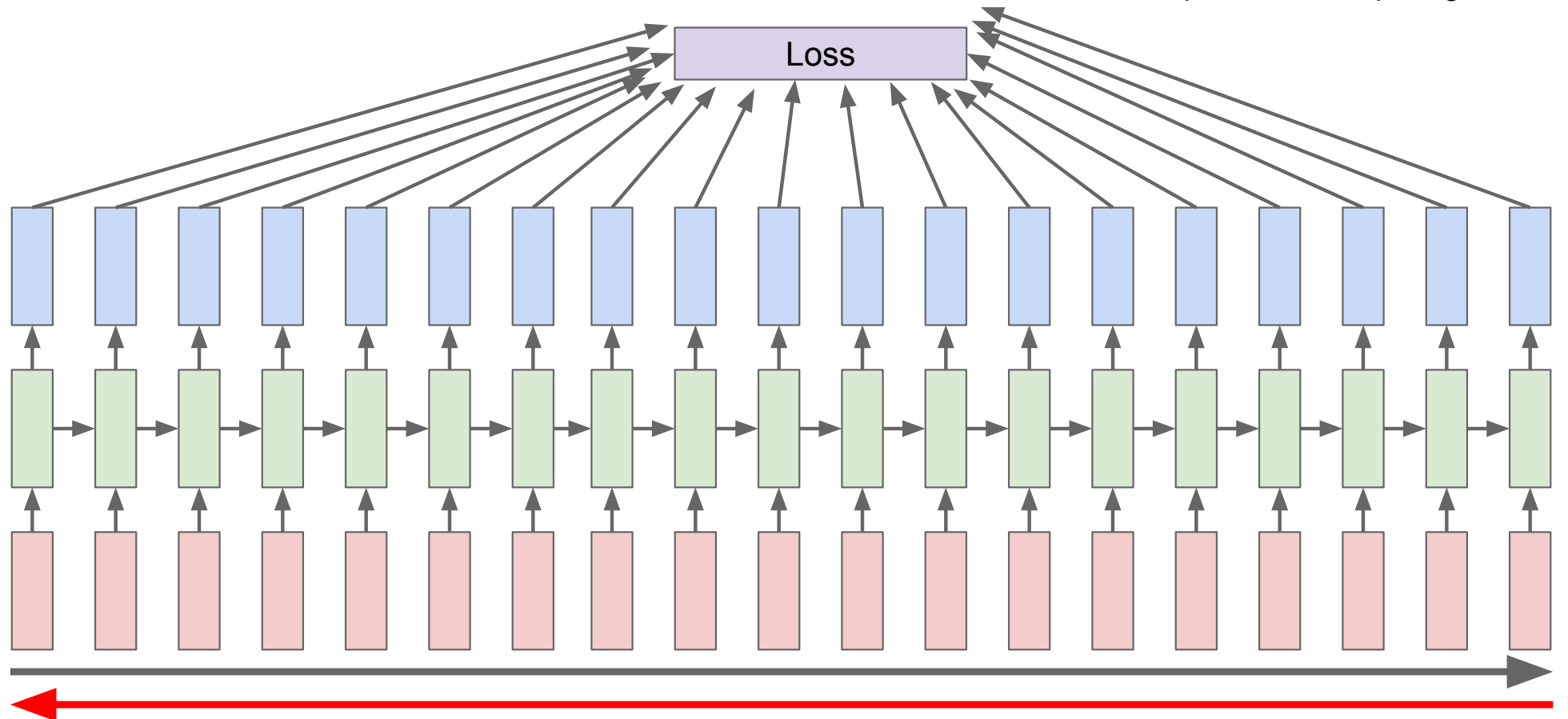
Vocabulary:  
[h,e,l,o]

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

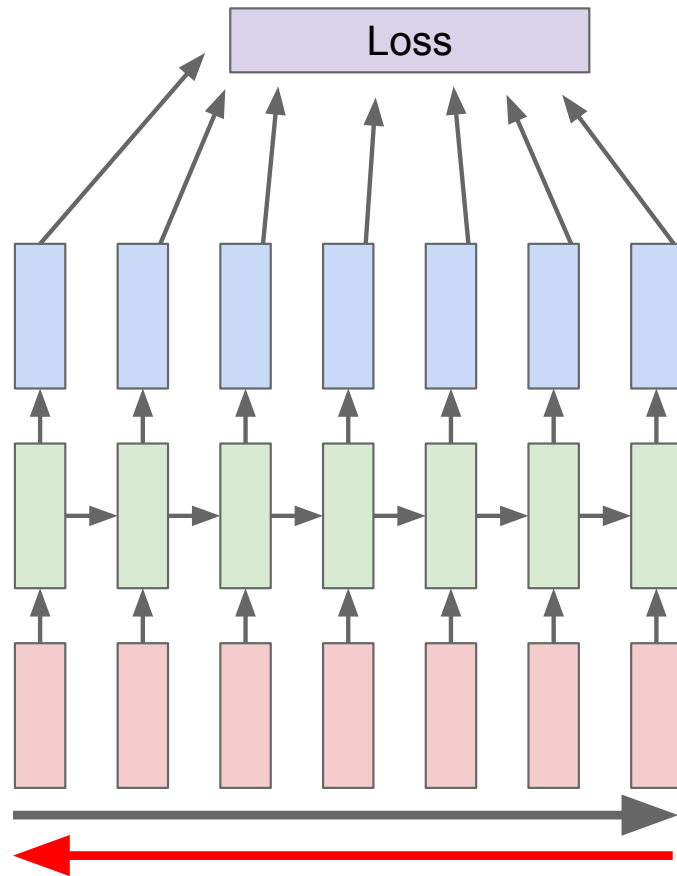


# Backpropagation through time

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

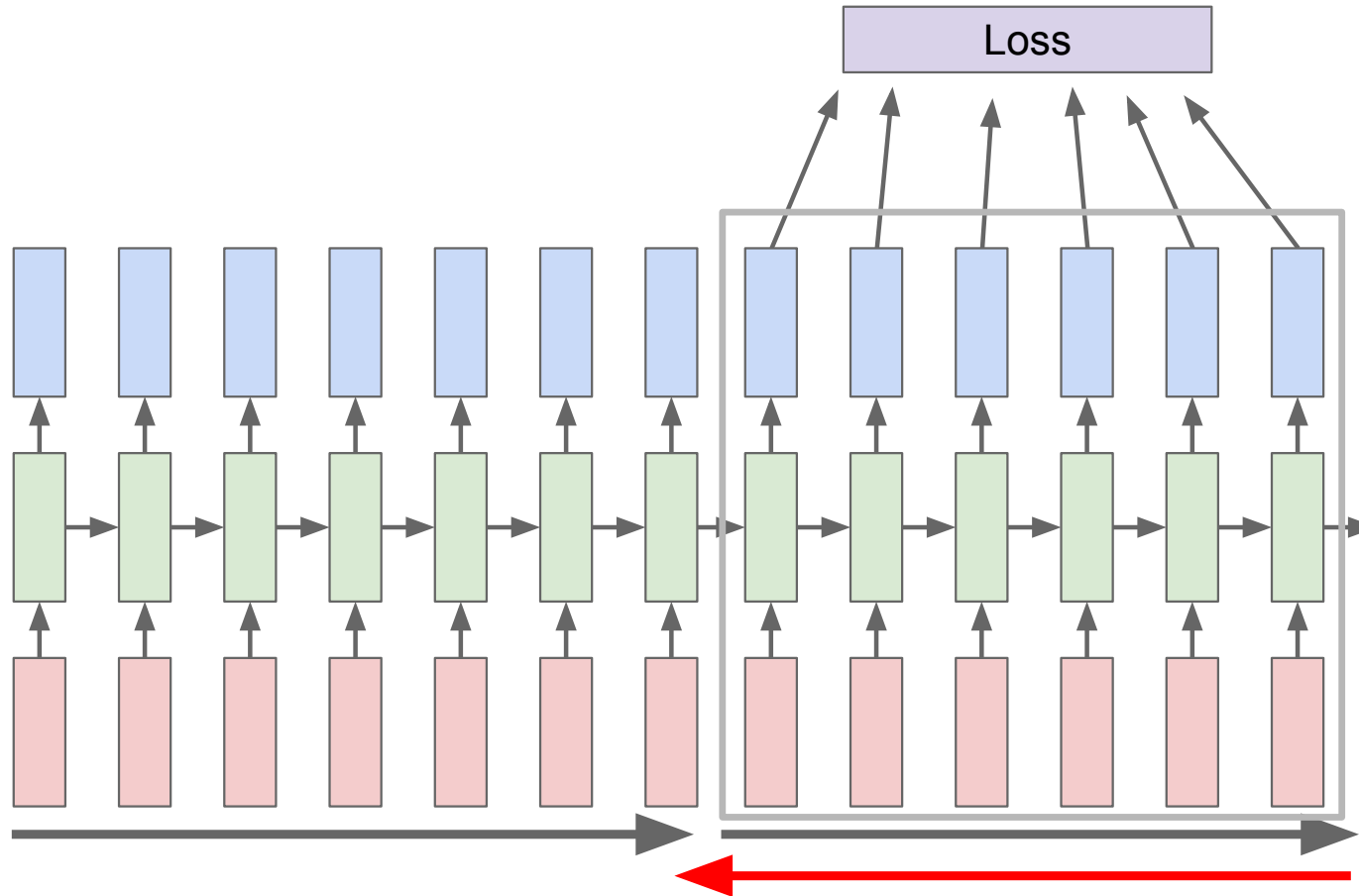


# Truncated Backpropagation through time



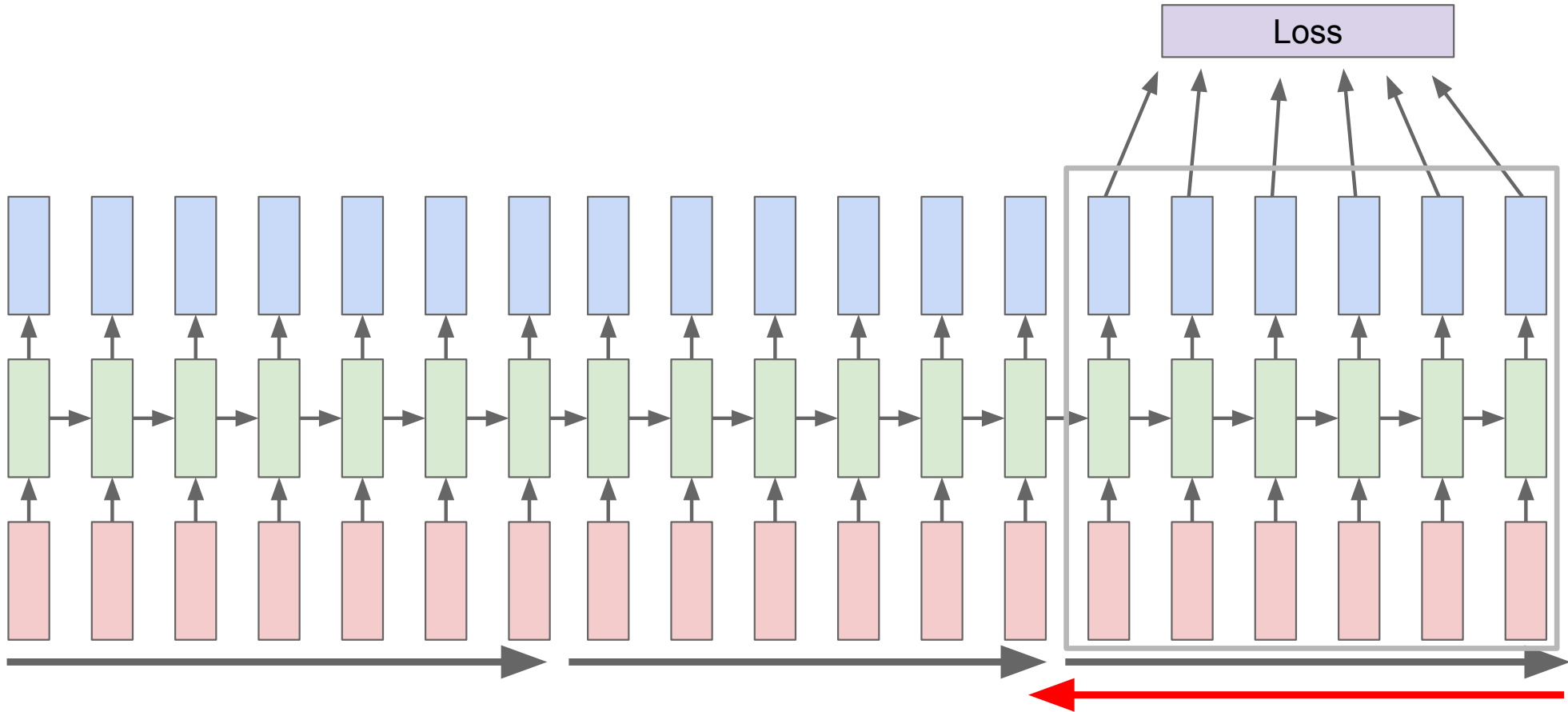
Run forward and backward through chunks of the sequence instead of whole sequence

# Truncated Backpropagation through time



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

# Truncated Backpropagation through time





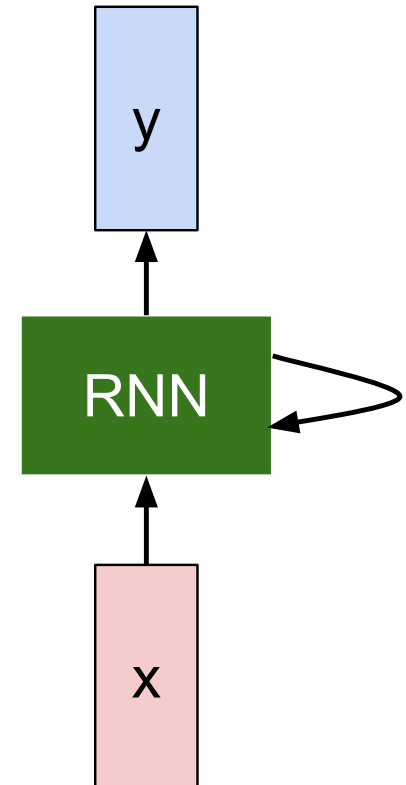
# Example: Text->RNN

## THE SONNETS

by William Shakespeare

From fairest creatures we desire increase,  
That thereby beauty's rose might never die,  
But as the ripper 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.





at first:

tyntd-iafhatawiaoahrdemot lytdws e ,tfti, astai f ogoh eoase rrranbyne 'nhthnee e  
plia tkllrgd 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 shuw y 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 offer.

↓ train more

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

# Image Captioning

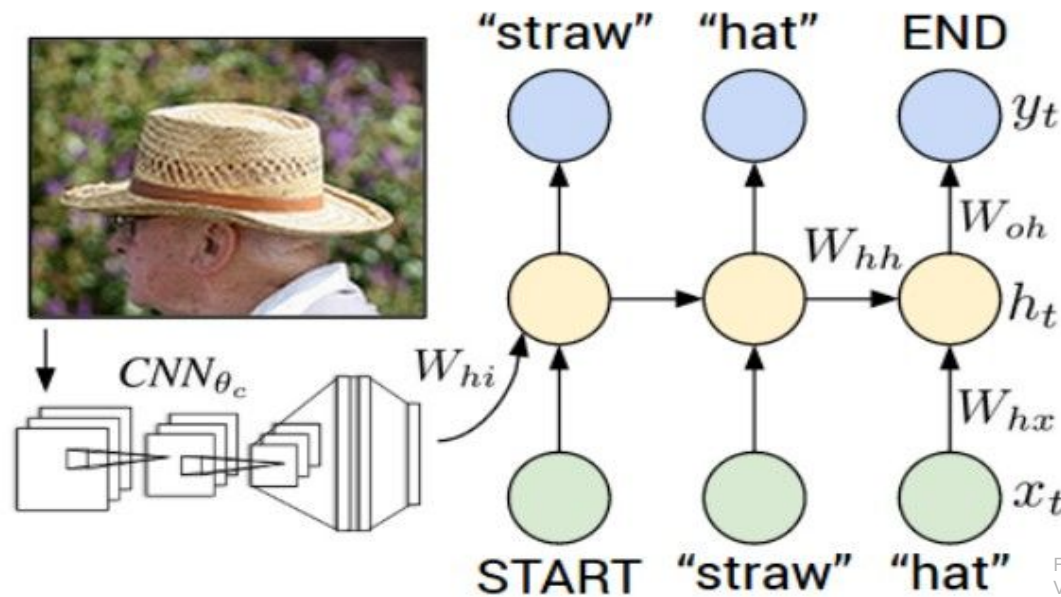


Figure from Karpathy et al, "Deep Visual-Semantic Alignments for Generating Image Descriptions", CVPR 2015; figure copyright IEEE, 2015. Reproduced for educational purposes.

Explain Images with Multimodal Recurrent Neural Networks, Mao et al.

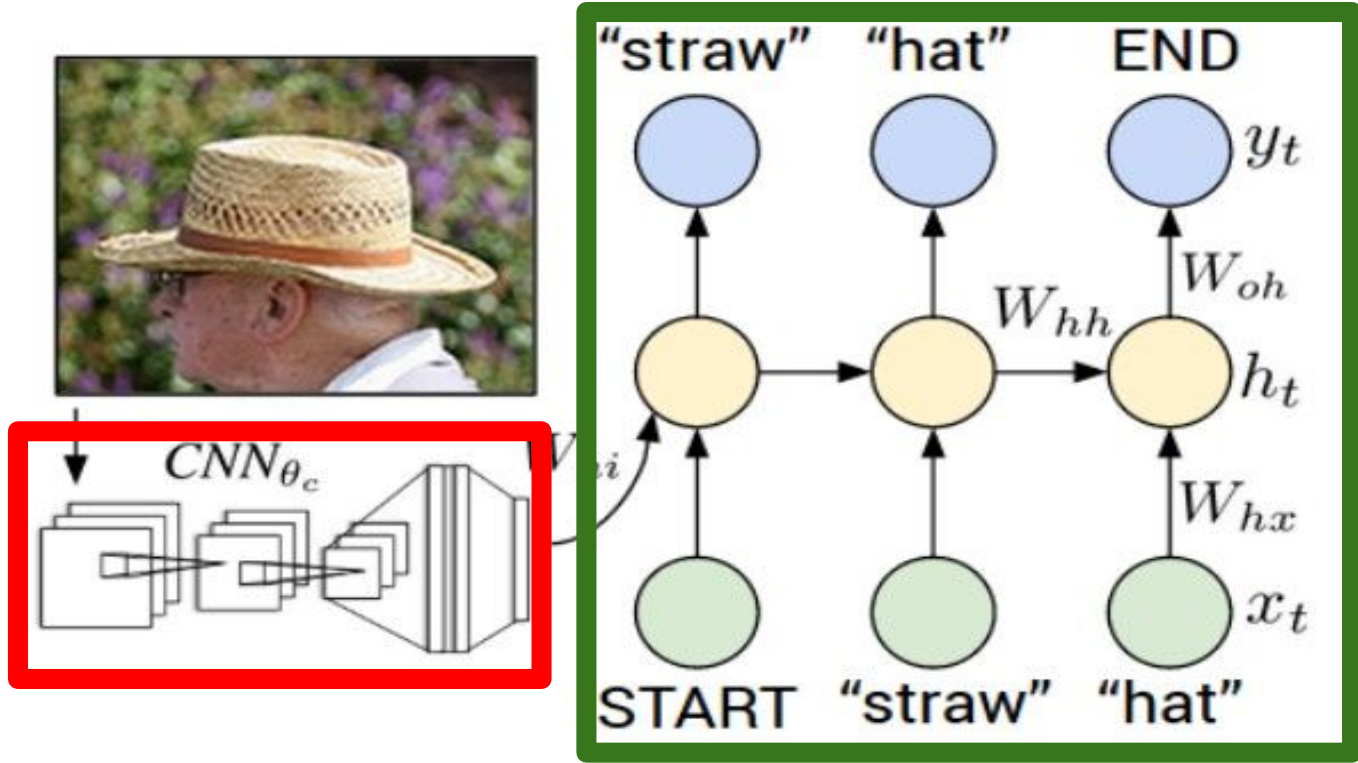
Deep Visual-Semantic Alignments for Generating Image Descriptions, Karpathy and Fei-Fei

Show and Tell: A Neural Image Caption Generator, Vinyals et al.

Long-term Recurrent Convolutional Networks for Visual Recognition and Description, Donahue et al.

Learning a Recurrent Visual Representation for Image Caption Generation, Chen and Zitnick

# Recurrent Neural Network



# Convolutional Neural Network



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

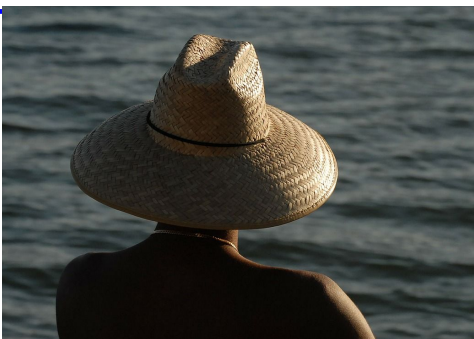
maxpool

FC-4096

FC-4096

FC-1000

softmax



test image



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

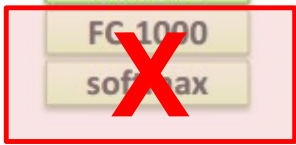
maxpool

FC-4096

FC-4096

FC-1000

softmax



test image



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

V



test image

y0

h0

x0  
<START>

<START>

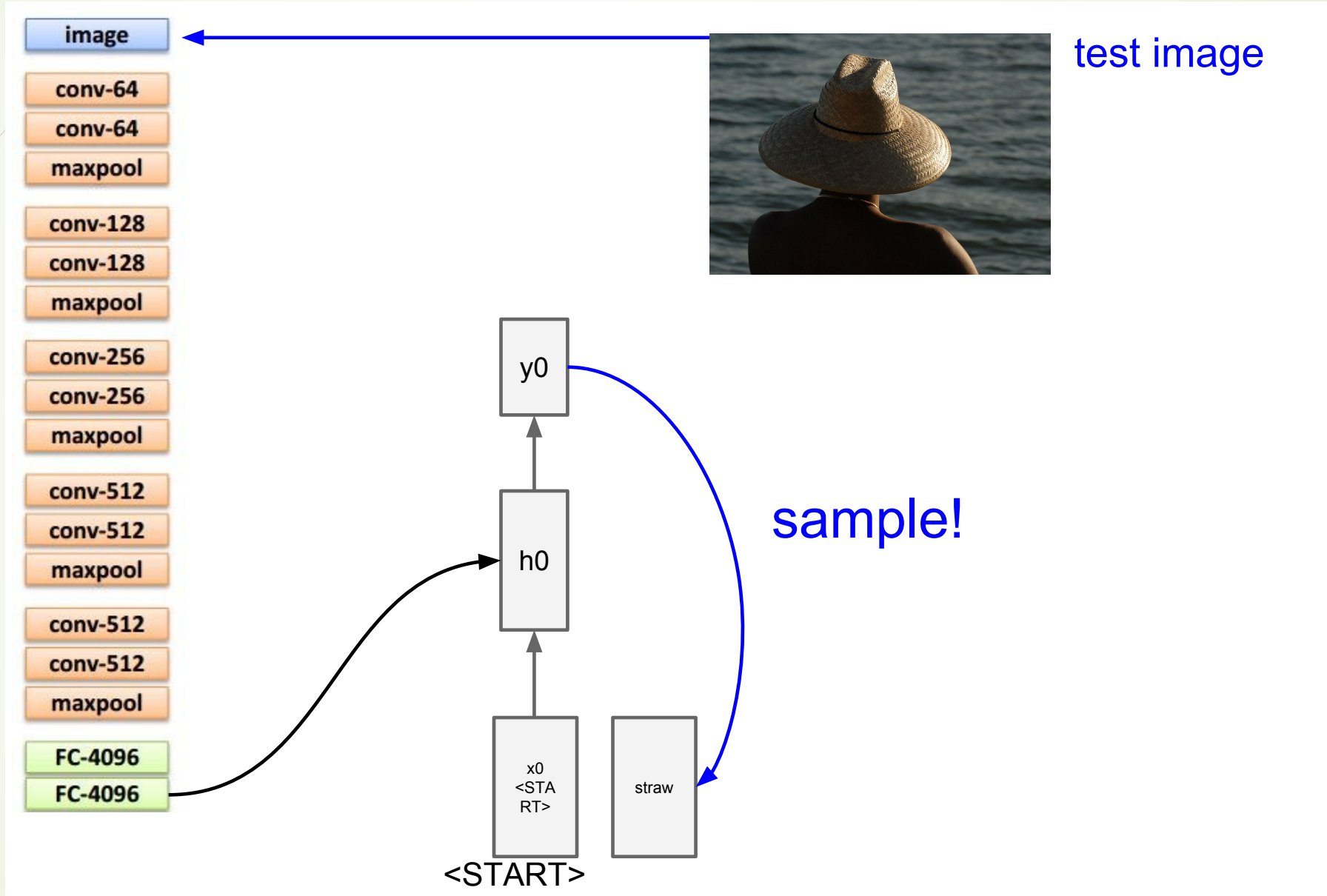
Wih

before:

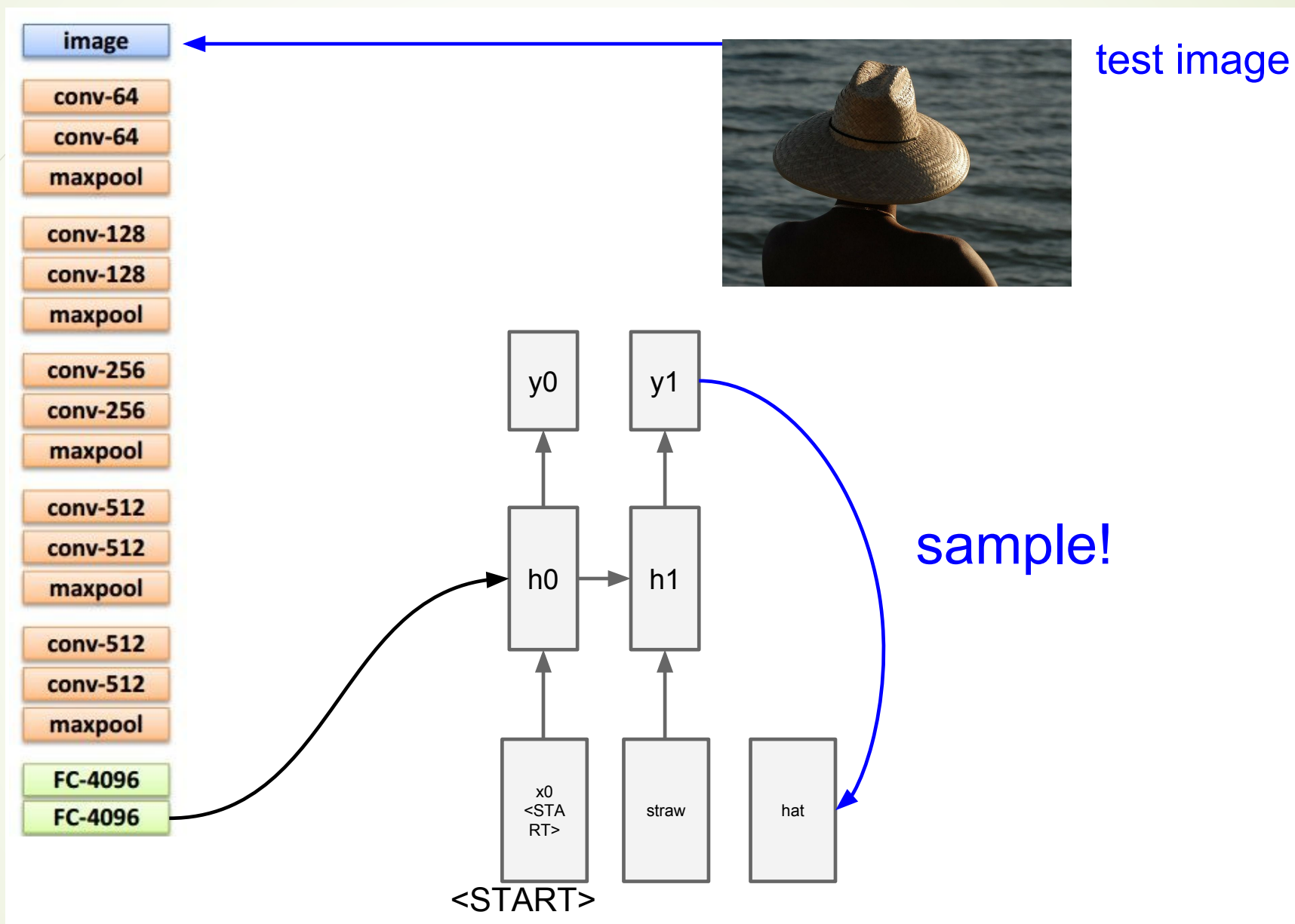
$$h = \tanh(W_{xh} * x + W_{hh} * h)$$

now:

$$h = \tanh(W_{xh} * x + W_{hh} * h + W_{ih} * v)$$





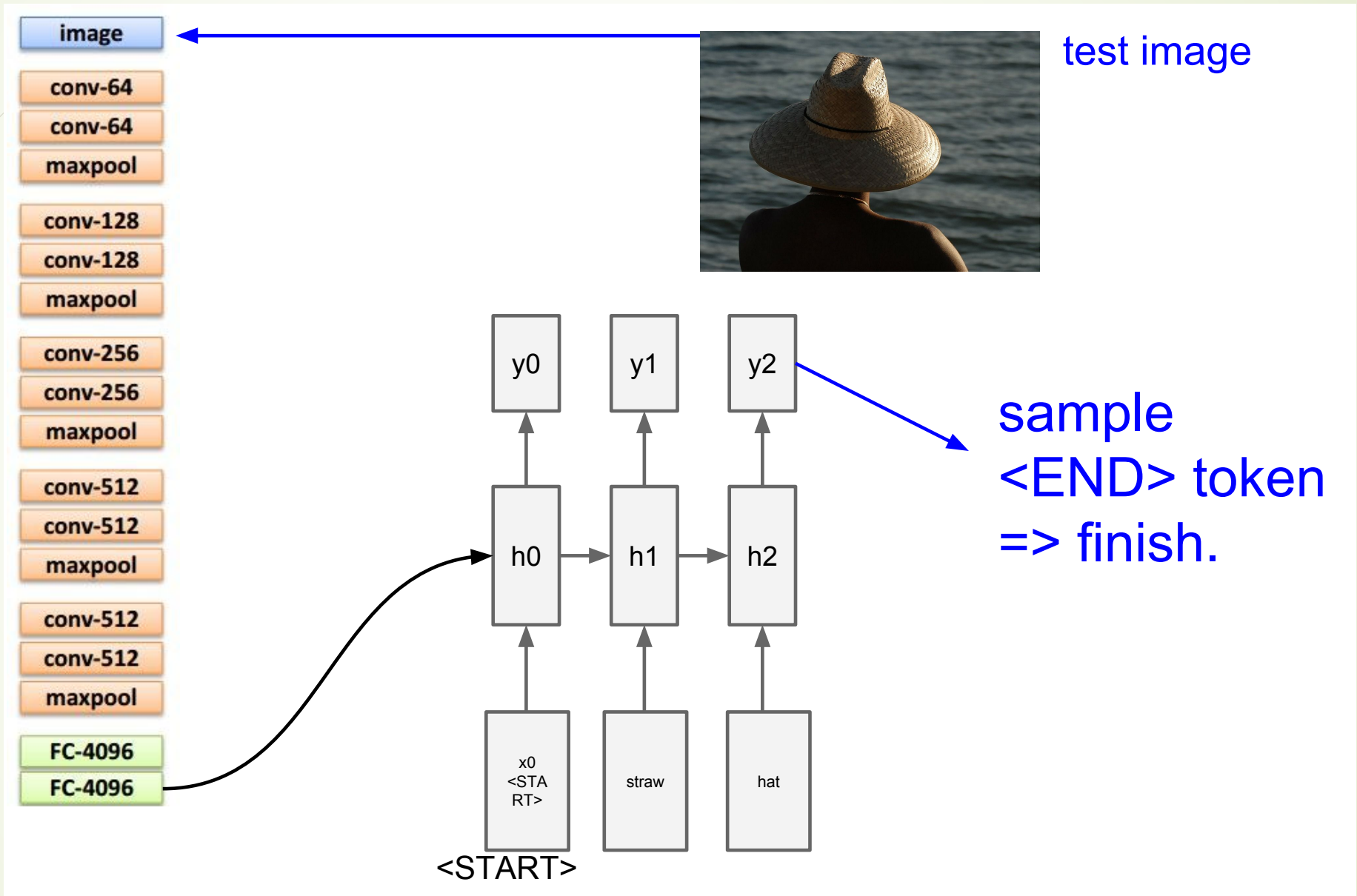


test image



sample!

<START>



image

conv-64

conv-64

maxpool

conv-128

conv-128

maxpool

conv-256

conv-256

maxpool

conv-512

conv-512

maxpool

conv-512

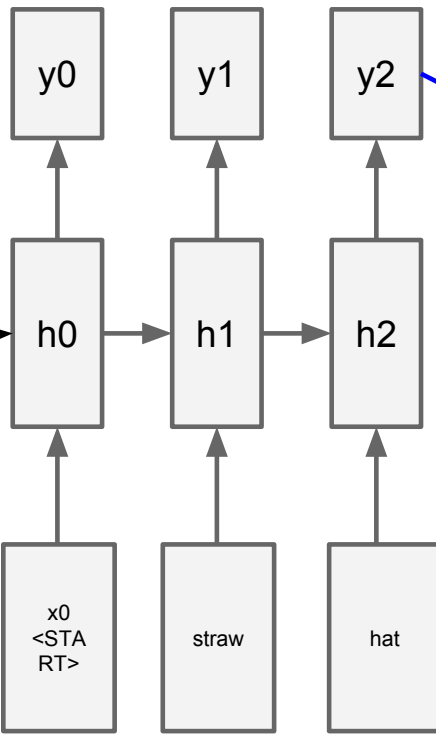
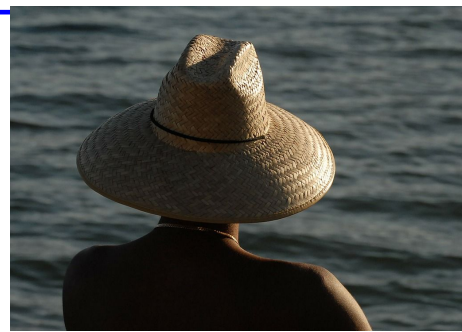
conv-512

maxpool

FC-4096

FC-4096

test image



sample  
<END> token  
=> finish.

<START>

# Image Captioning: Example Results

Captions generated using [neuraltalk2](#)  
All images are [CC0 Public domain](#):  
[cat](#), [suitcase](#), [cat tree](#), [dog](#), [bear](#),  
[surfers](#), [tennis](#), [giraffe](#), [motorcycle](#)



*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*



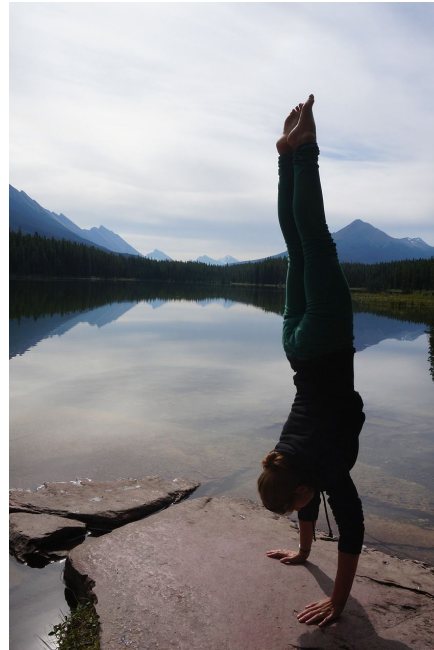
*A man riding a dirt bike on a dirt track*

# Image Captioning: Failure Cases

Captions generated using [neuraltalk2](#)  
All images are [CC0](#) Public domain: [fur coat](#), [handstand](#), [spider web](#), [baseball](#)



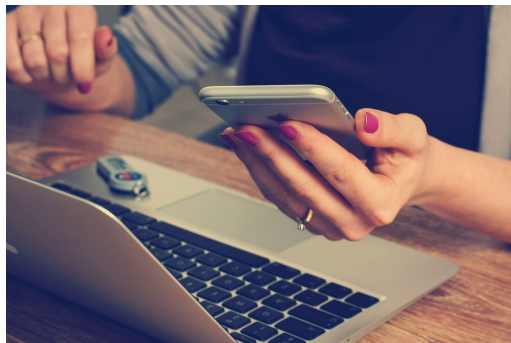
*A woman is holding a cat in her hand*



*A woman standing on a beach holding a surfboard*



*A bird is perched on a tree branch*



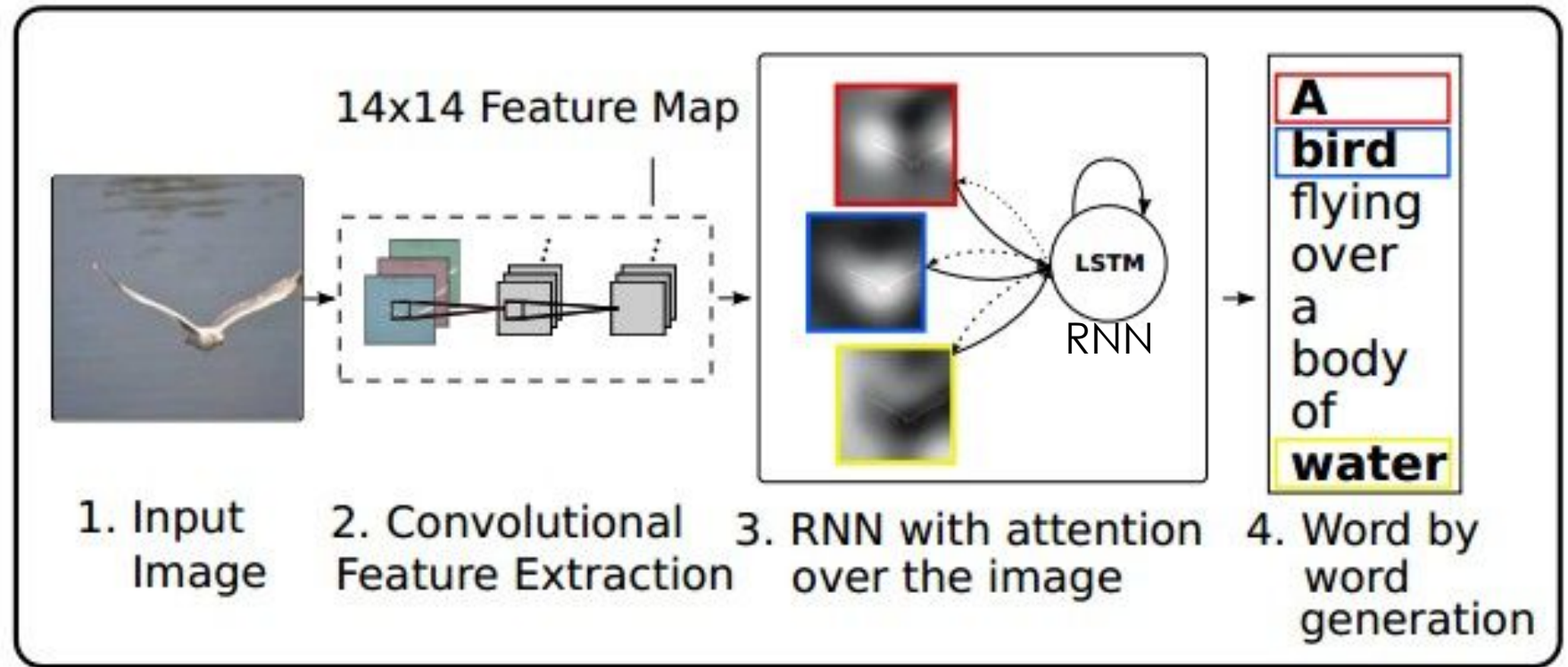
*A person holding a computer mouse on a desk*



*A man in a baseball uniform throwing a ball*

# Image Captioning with Attention

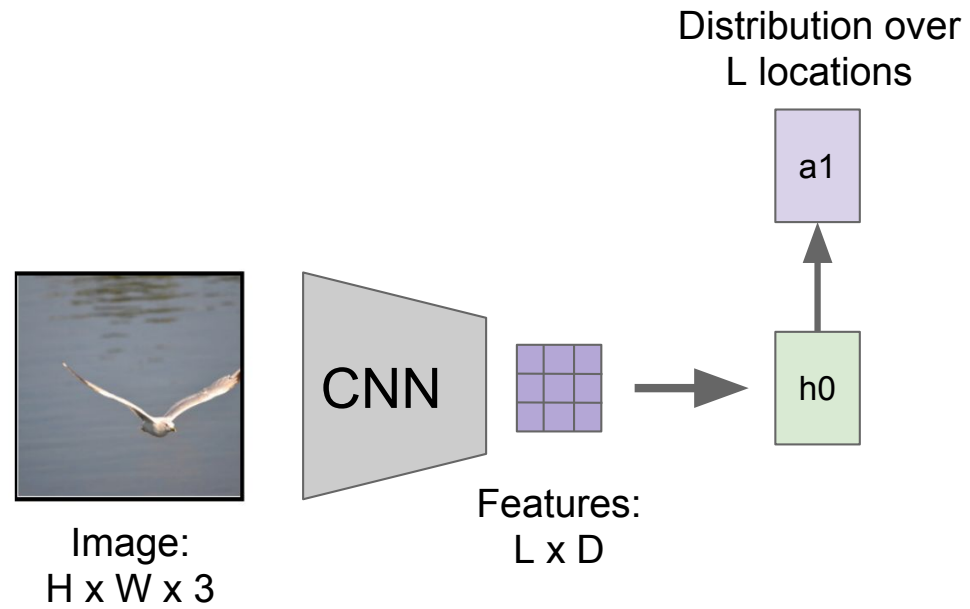
RNN focuses its attention at a different spatial location when generating each word



Xu et al, "Show, Attend, and Tell: Neural Image Caption Generation with Visual Attention", ICML 2015

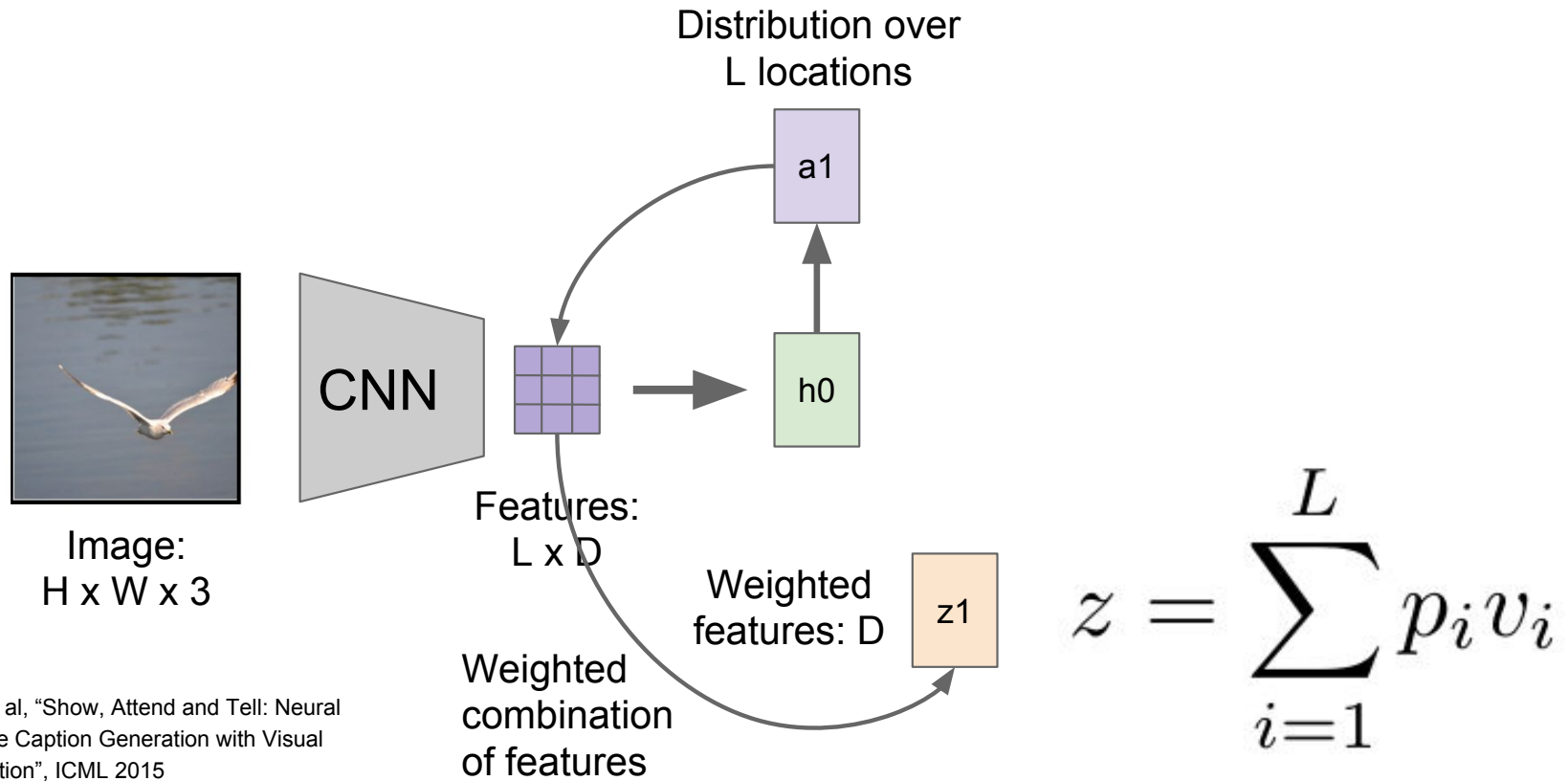
Figure copyright Kelvin Xu, Jimmy Lei Ba, Jamie Kiros, Kyunghyun Cho, Aaron Courville, Ruslan Salakhutdinov, Richard S. Zemel, and Yoshua Bengio, 2015. Reproduced with permission.

# Image Captioning with Attention



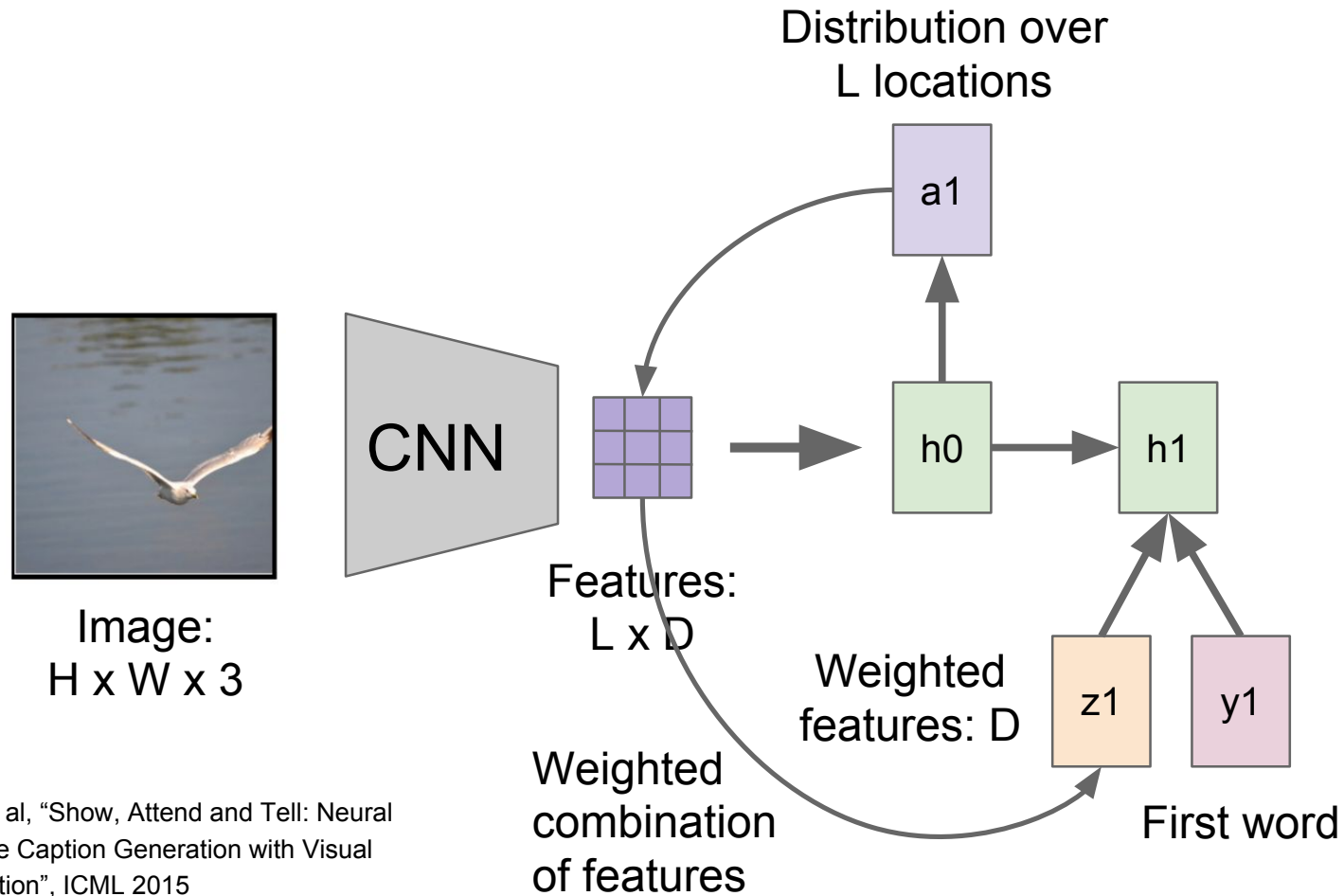
Xu et al, "Show, Attend and Tell: Neural Image Caption Generation with Visual Attention", ICML 2015

# Image Captioning with Attention



Xu et al, "Show, Attend and Tell: Neural Image Caption Generation with Visual Attention", ICML 2015

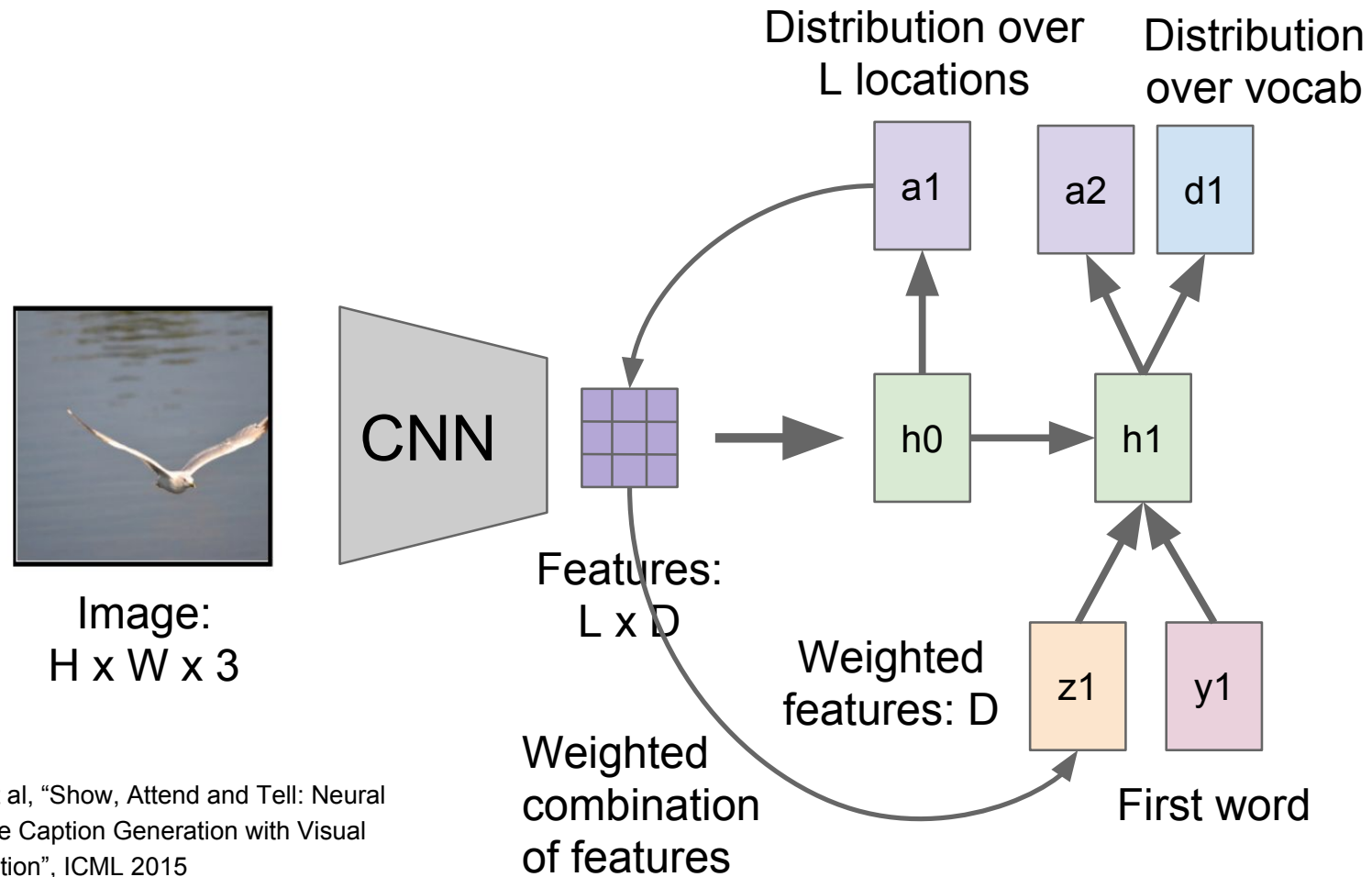
# Image Captioning with Attention



Xu et al, "Show, Attend and Tell: Neural Image Caption Generation with Visual Attention", ICML 2015

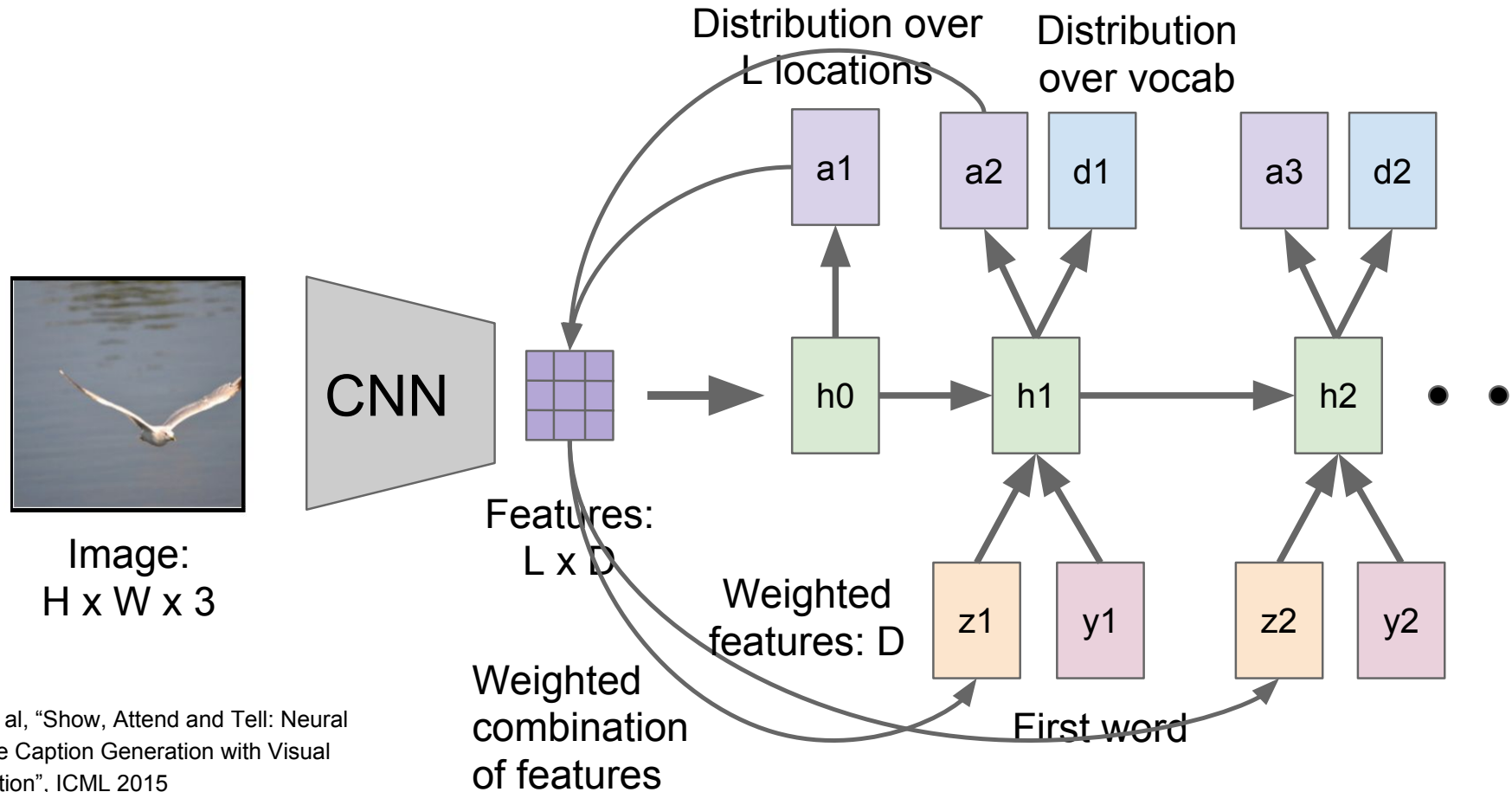


# Image Captioning with Attention



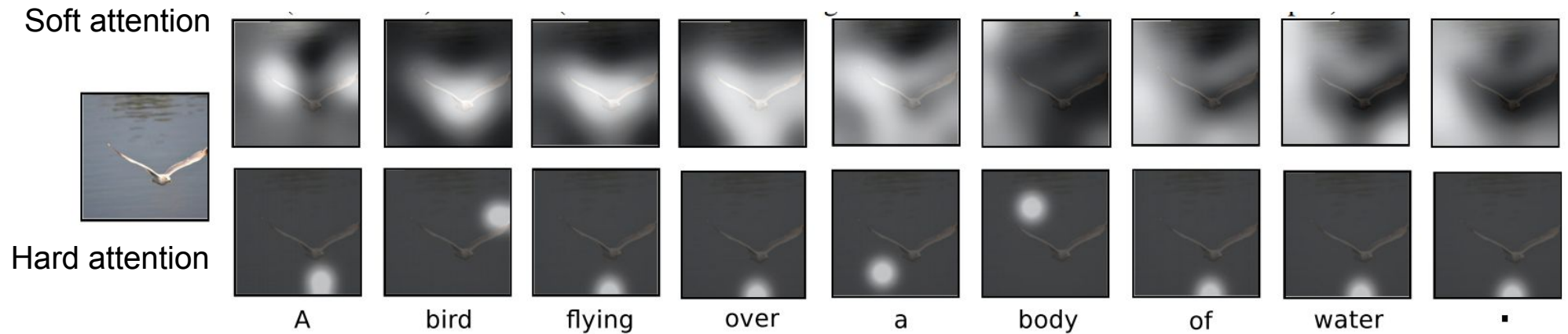
Xu et al, "Show, Attend and Tell: Neural Image Caption Generation with Visual Attention", ICML 2015

# Image Captioning with Attention



Xu et al, "Show, Attend and Tell: Neural Image Caption Generation with Visual Attention", ICML 2015

# Image Captioning with Attention



Xu et al, "Show, Attend, and Tell: Neural Image Caption Generation with Visual Attention", ICML 2015

Figure copyright Kelvin Xu, Jimmy Lei Ba, Jamie Kiros, Kyunghyun Cho, Aaron Courville, Ruslan Salakhutdinov, Richard S. Zemel, and Yoshua Bengio, 2015. Reproduced with permission.

# Image Captioning with Attention



A woman is throwing a frisbee in a park.



A dog is standing on a hardwood floor.



A stop sign is on a road with a mountain in the background.



A little girl sitting on a bed with a teddy bear.



A group of people sitting on a boat in the water.

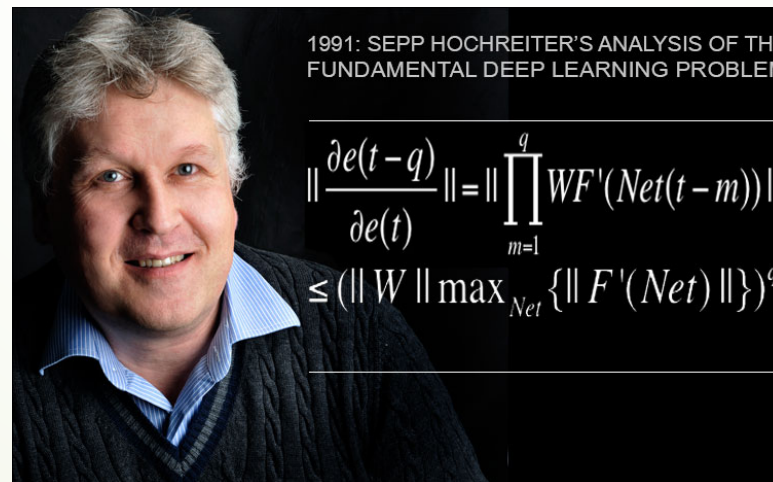


A giraffe standing in a forest with trees in the background.

Xu et al, "Show, Attend, and Tell: Neural Image Caption Generation with Visual Attention", ICML 2015

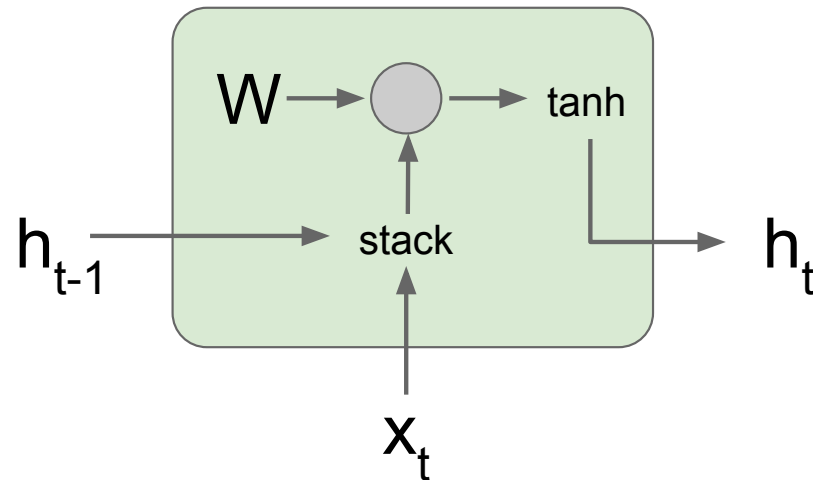
Figure copyright Kelvin Xu, Jimmy Lei Ba, Jamie Kiros, Kyunghyun Cho, Aaron Courville, Ruslan Salakhutdinov, Richard S. Zemel, and Yoshua Benchio, 2015. Reproduced with permission.

# The Fundamental Deep Learning Problem: **Vanishing / Exploding Gradients**



# 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

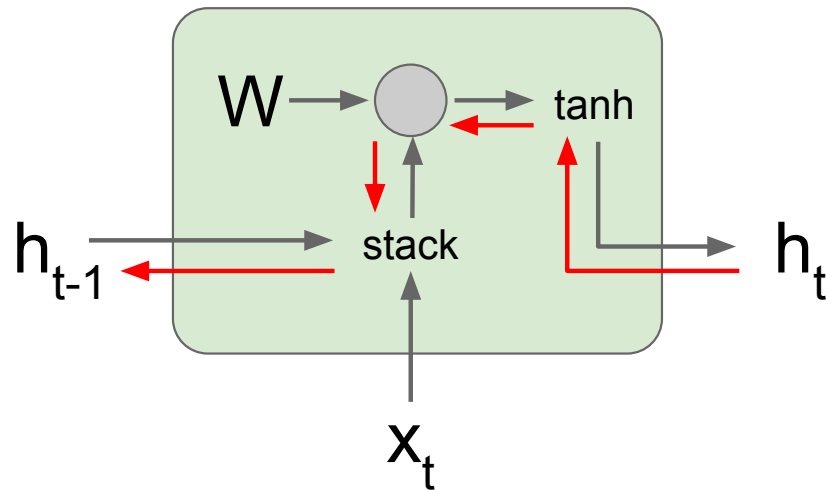


$$\begin{aligned} h_t &= \tanh(W_{hh}h_{t-1} + W_{hx}x_t) \\ &= \tanh\left(\begin{pmatrix} W_{hh} & W_{hx} \end{pmatrix} \begin{pmatrix} h_{t-1} \\ x_t \end{pmatrix}\right) \\ &= \tanh\left(W \begin{pmatrix} h_{t-1} \\ x_t \end{pmatrix}\right) \end{aligned}$$

# Vanilla RNN Gradient Flow

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

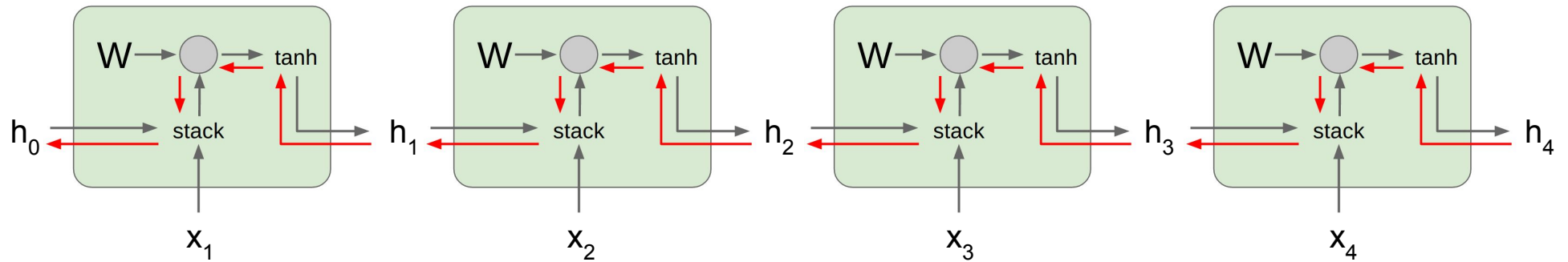
Backpropagation from  $h_t$   
to  $h_{t-1}$  multiplies by  $W$   
(actually  $W_{hh}^T$ )



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

# Vanilla RNN Gradient Flow

Bengio et al, "Learning long-term dependencies with gradient descent is difficult", IEEE Transactions on Neural Networks, 1994  
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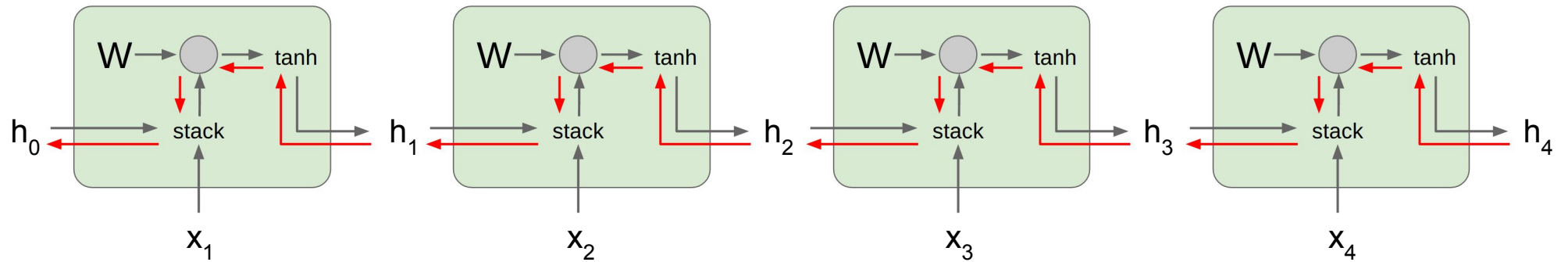


Computing gradient of  $h_0$  involves many factors of  $W$  (and repeated tanh)



# 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



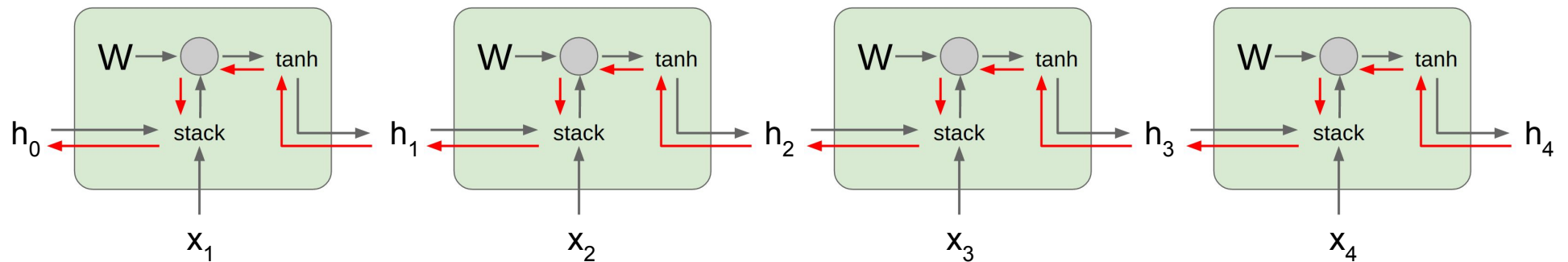
Computing gradient of  $h_0$  involves many factors of  $W$  (and repeated tanh)

Largest singular value  $> 1$ :  
**Exploding gradients**

Largest singular value  $< 1$ :  
**Vanishing gradients**

# Vanilla RNN Gradient Flow

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



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

Largest singular value  $> 1$ :  
**Exploding gradients**

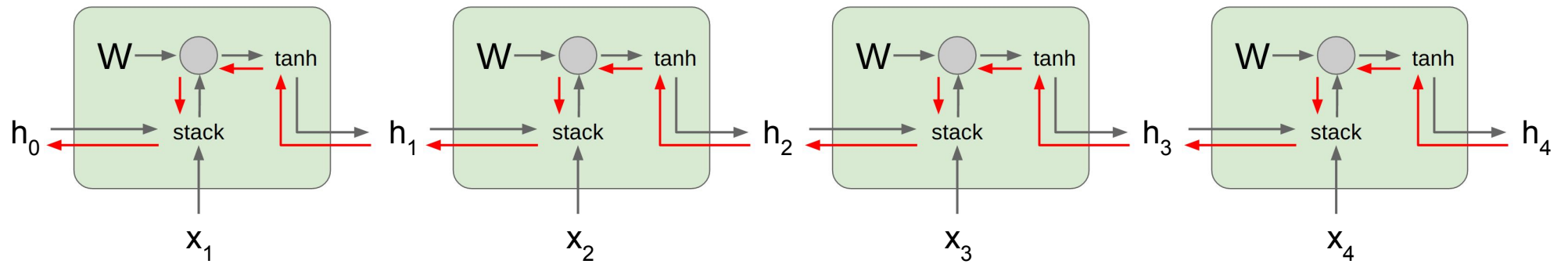
Largest singular value  $< 1$ :  
**Vanishing gradients**

**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

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



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

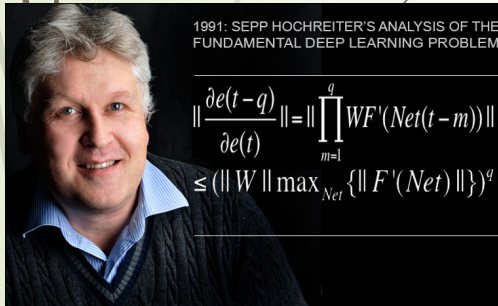
Largest singular value  $> 1$ :  
**Exploding gradients**

Largest singular value  $< 1$ :  
**Vanishing gradients**

→ Change RNN architecture

# Some Historical Remarks

- [VAN1] S. Hochreiter. Untersuchungen zu dynamischen neuronalen Netzen. Diploma thesis, TUM, 1991 (advisor [J. Schmidhuber](#)). Link: <http://www.idsia.ch/~juergen/SeppHochreiter1991ThesisAdvisorSchmidhuber.pdf>
- [VAN2] Y. Bengio, P. Simard, P. Frasconi. Learning long-term dependencies with gradient descent is difficult. IEEE TNN 5(2), p 157-166, 1994
- [VAN3] S. Hochreiter, Y. Bengio, P. Frasconi, J. Schmidhuber. Gradient flow in recurrent nets: the difficulty of learning long-term dependencies. In S. C. Kremer and J. F. Kolen, eds., A Field Guide to Dynamical Recurrent Neural Networks. IEEE press, 2001
- [VAN4] Y. Bengio. Neural net language models. Scholarpedia, 3(1):3881, 2008. Link: [http://www.scholarpedia.org/article/Neural\\_net\\_language\\_models?CachedSimilar13](http://www.scholarpedia.org/article/Neural_net_language_models?CachedSimilar13)
- **J. SchmidHuber** (<https://people.idsia.ch/~juergen/deep-learning-miraculous-year-1990-1991.html#Sec.%203>):
  - “As a part of his thesis, Sepp implemented the Neural History Compressor above (see [Sec. 1](#)) and other RNN-based systems (see [Sec. 11](#)). However, he did much more: His work formally showed that deep NNs suffer from the now famous problem of vanishing or exploding gradients: in typical deep or recurrent networks, back-propagated error signals either shrink rapidly, or grow out of bounds. In both cases, learning fails. This analysis led to basic principles of what's now called LSTM (see [Sec. 4](#)).”
  - “Interestingly, in 1994, others published results [\[VAN2\]](#) essentially identical to the 1991 vanishing gradient results of Sepp. [\[VAN1\]](#) Even after a [common publication](#) [\[VAN3\]](#) the first author of reference [\[VAN2\]](#) published papers [\[VAN4\]](#) that cited only their own 1994 paper but not Sepp's original work.”





# Long Short Term Memory (LSTM)

# Long-Short-Term-Memory (LSTM)

- ▶ A type of RNN proposed by Hochreiter and Schmidhuber in 1997 as a solution to the vanishing gradients problem.
  - ▶ “Long short-term memory”, Hochreiter and Schmidhuber, Neural Computation, 9(8):1735-1780, 1997. Link: <https://www.bioinf.jku.at/publications/older/2604.pdf>
- ▶ On time step  $t$ , there is a hidden state  $h$  and a cell state  $c$ 
  - ▶ Both are vectors length  $n$
  - ▶ The **cell stores long-term information**
  - ▶ The LSTM can erase, write and read information from the cell
- ▶ The selection of which information is erased/written/read is controlled by three corresponding **gates**
  - ▶ The gates are also vectors length  $n$
  - ▶ On each time step, each element of the gates can be open (1), closed (0),
  - ▶ or somewhere in-between.
  - ▶ The gates are **dynamic**: their value is computed based on the current context

# Long-Short-Term-Memory (LSTM)

We have a sequence of inputs  $\mathbf{x}^{(t)}$ , and we will compute a sequence of hidden states  $\mathbf{h}^{(t)}$  and cell states  $\mathbf{c}^{(t)}$ . On timestep  $t$ :

**Forget gate:** controls what is kept vs forgotten, from previous cell state

**Input gate:** controls what parts of the new cell content are written to cell

**Output gate:** controls what parts of cell are output to hidden state

**New cell content:** this is the new content to be written to the cell

**Cell state:** erase (“forget”) some content from last cell state, and write (“input”) some new cell content

**Hidden state:** read (“output”) some content from the cell

**Sigmoid function:** all gate values are between 0 and 1

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

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

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

$$\tilde{\mathbf{c}}^{(t)} = \tanh \left( \mathbf{W}_c \mathbf{h}^{(t-1)} + \mathbf{U}_c \mathbf{x}^{(t)} + \mathbf{b}_c \right)$$

$$\mathbf{c}^{(t)} = \mathbf{f}^{(t)} \circ \mathbf{c}^{(t-1)} + \mathbf{i}^{(t)} \circ \tilde{\mathbf{c}}^{(t)}$$

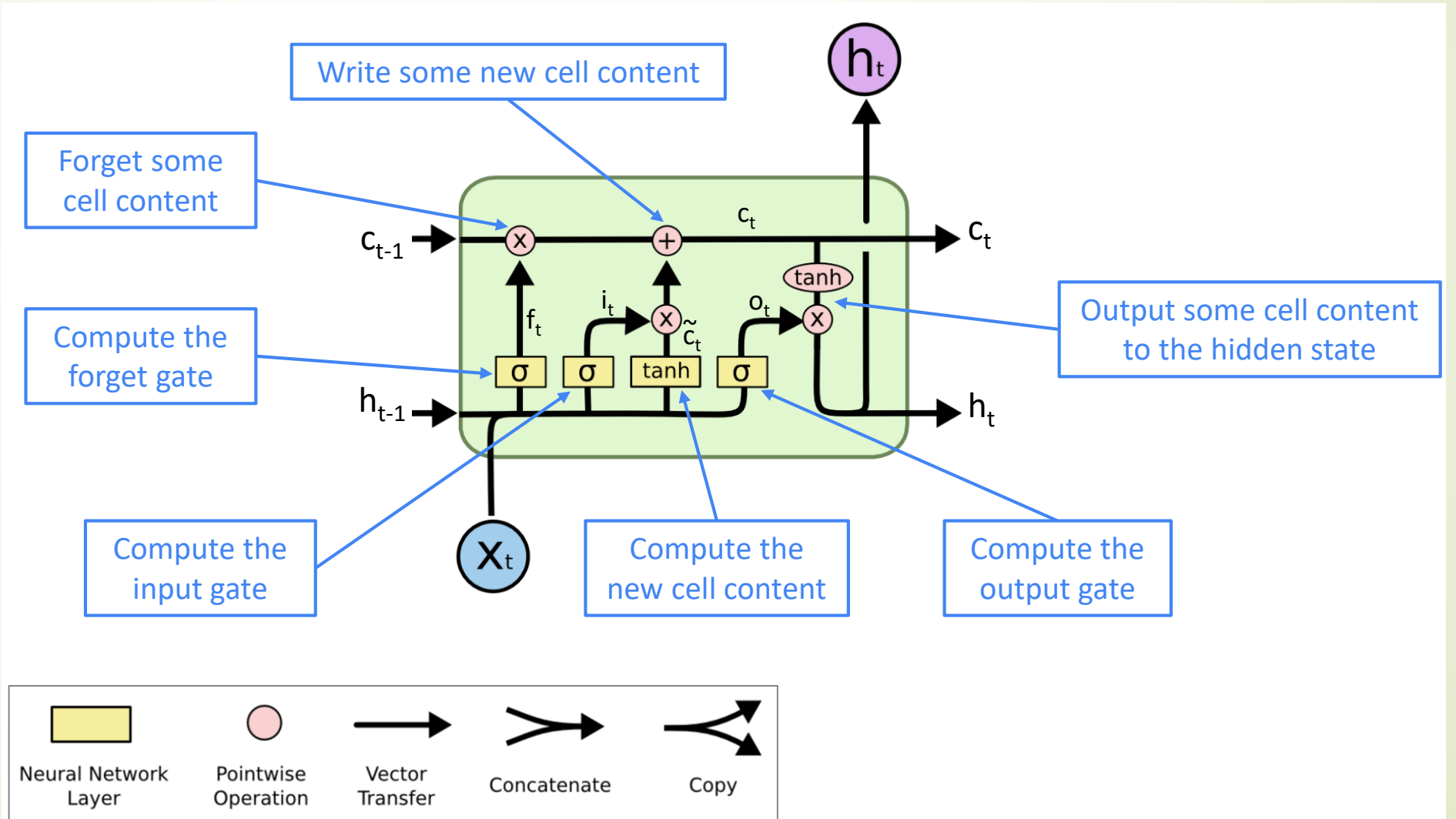
$$\mathbf{h}^{(t)} = \mathbf{o}^{(t)} \circ \tanh \mathbf{c}^{(t)}$$

All these are vectors of same length  $n$

Gates are applied using element-wise product

# LSTM Flowchart

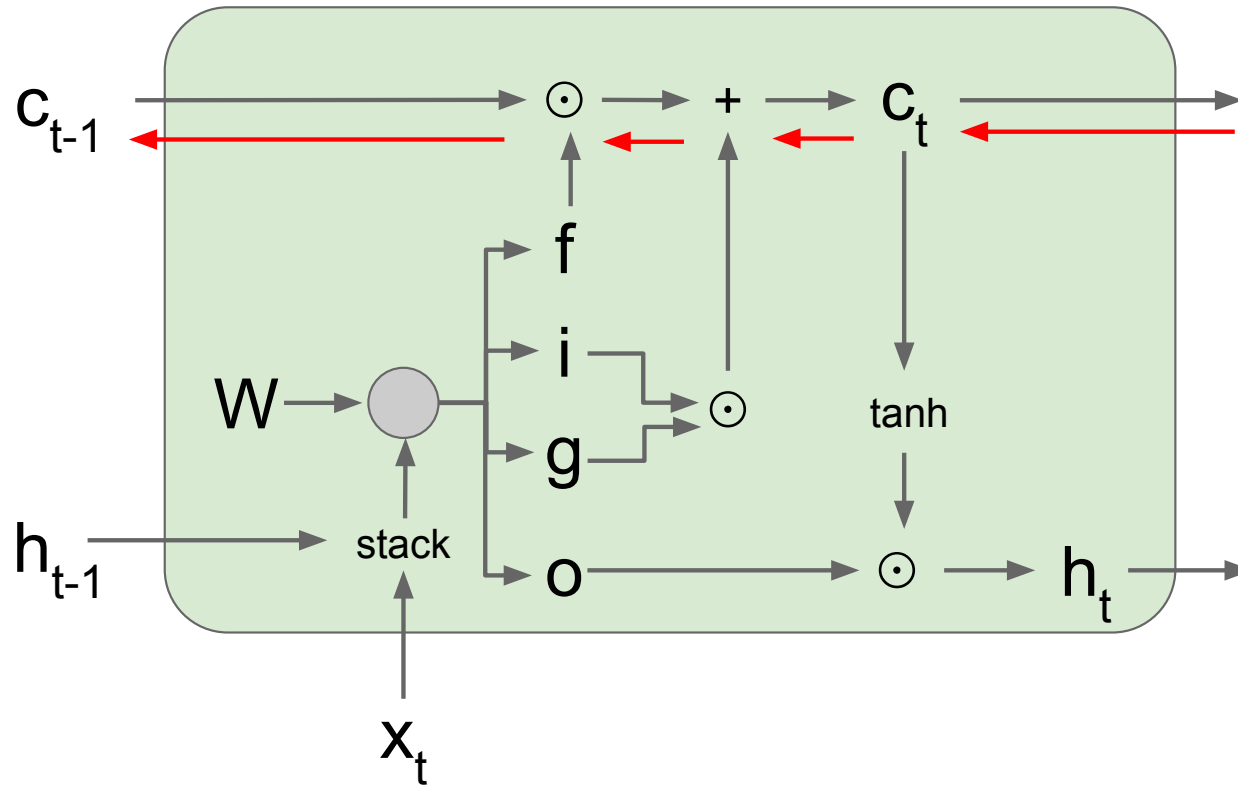
► **Source:** <http://colah.github.io/posts/2015-08-Understanding-LSTMs/>





# 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  $W$

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

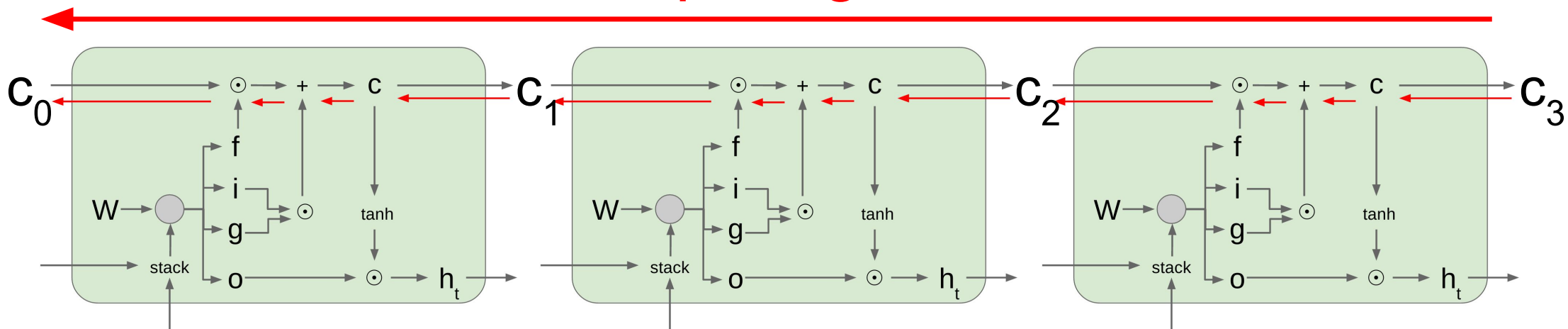
$$c_t = f \odot c_{t-1} + i \odot g$$

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

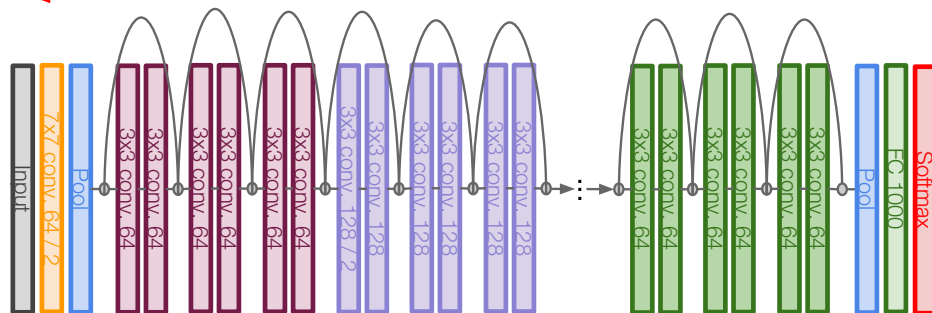
# Long Short Term Memory (LSTM): Gradient Flow

[Hochreiter et al., 1997]

## Uninterrupted gradient flow!



Similar to ResNet!



In between:  
**Highway Networks**

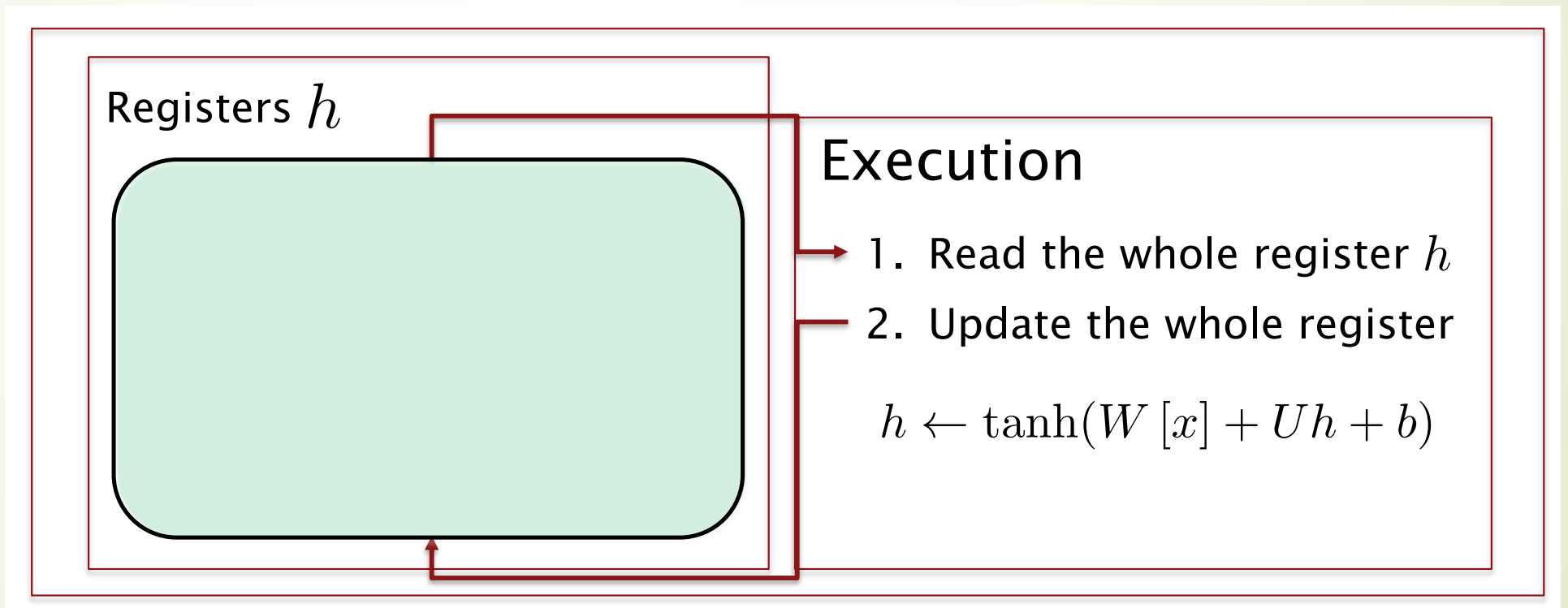
$$g = T(x, W_T)$$

$$y = g \odot H(x, W_H) + (1 - g) \odot x$$

Srivastava et al, "Highway Networks",  
 ICML DL Workshop 2015

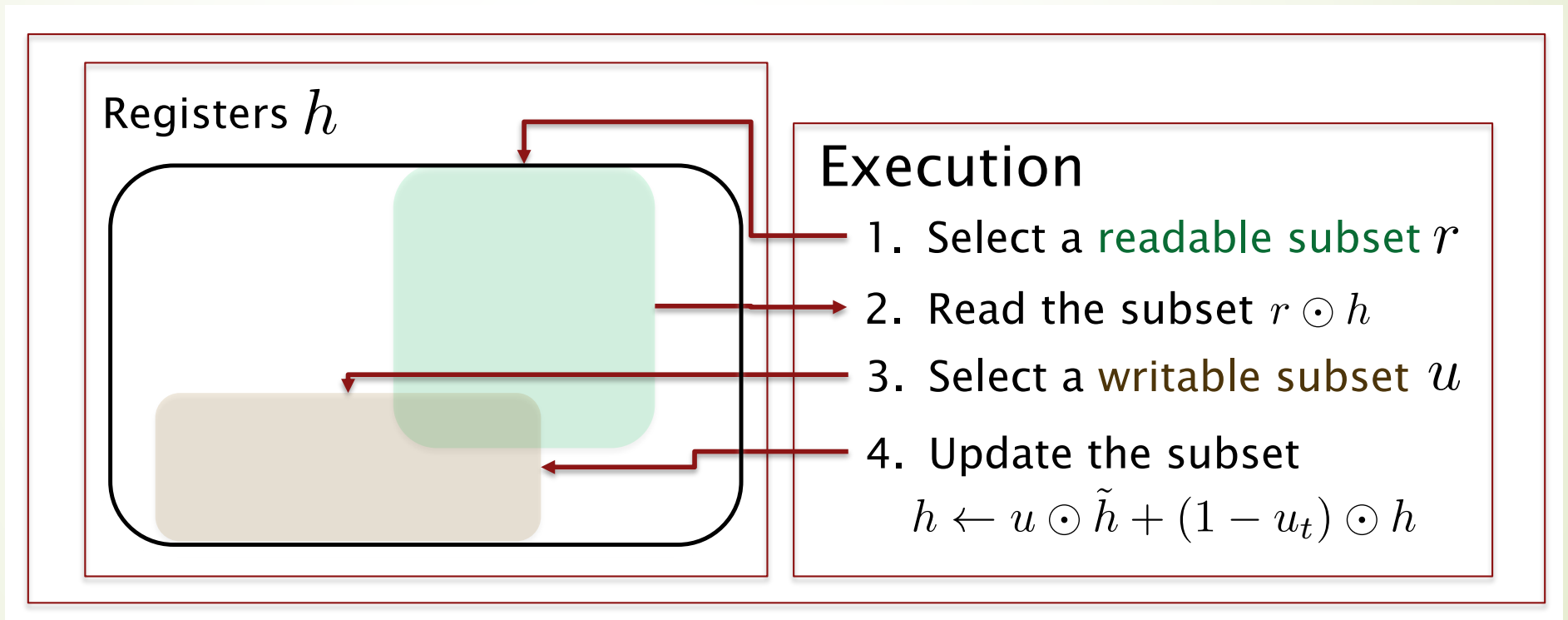
# Gated Recurrent Unit: tanh RNN

- ▶ (tanh) RNN is expensive in exploiting the whole register



# Gated Recurrent Unit (GRU)

- GRU is much more economic for computation!



# Gated Recurrent Unit (GRU)

- ▶ "Learning Phrase Representations using RNN Encoder–Decoder for Statistical Machine Translation", Cho et al. 2014, <https://arxiv.org/pdf/1406.1078v3.pdf>

**Update gate:** controls what parts of hidden state are updated vs preserved

$$\mathbf{u}^{(t)} = \sigma \left( \mathbf{W}_u \mathbf{h}^{(t-1)} + \mathbf{U}_u \mathbf{x}^{(t)} + \mathbf{b}_u \right)$$

**Reset gate:** controls what parts of previous hidden state are used to compute new content

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

**New hidden state content:** reset gate selects useful parts of prev hidden state. Use this and current input to compute new hidden content.

$$\tilde{\mathbf{h}}^{(t)} = \tanh \left( \mathbf{W}_h (\mathbf{r}^{(t)} \circ \mathbf{h}^{(t-1)}) + \mathbf{U}_h \mathbf{x}^{(t)} + \mathbf{b}_h \right)$$

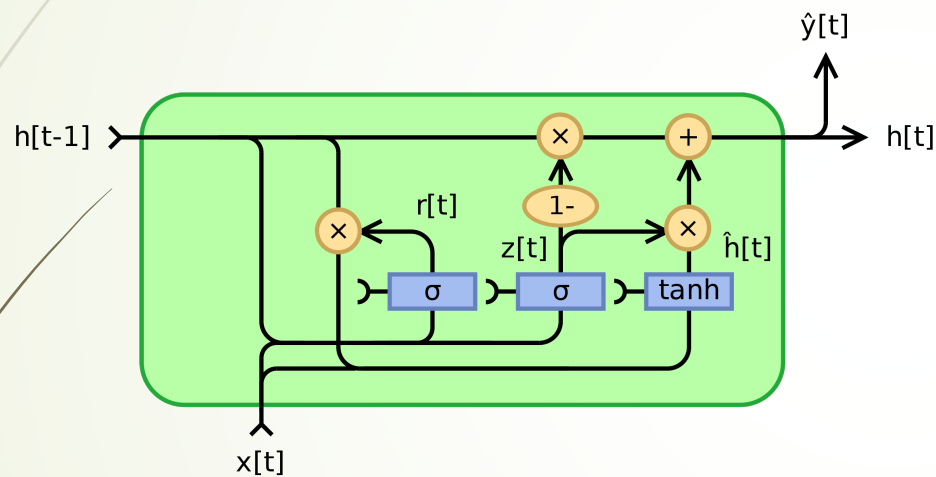
$$\mathbf{h}^{(t)} = (1 - \mathbf{u}^{(t)}) \circ \mathbf{h}^{(t-1)} + \mathbf{u}^{(t)} \circ \tilde{\mathbf{h}}^{(t)}$$

**Hidden state:** update gate simultaneously controls what is kept from previous hidden state, and what is updated to new hidden state content

**How does this solve vanishing gradient?**

Like LSTM, GRU makes it easier to retain info long-term (e.g. by setting update gate to 0)

# Diagram of GRU



**GRU** [*Learning phrase representations using rnn encoder-decoder for statistical machine translation*, Cho et al. 2014]

$$r_t = \sigma(W_{xr}x_t + W_{hr}h_{t-1} + b_r)$$

$$z_t = \sigma(W_{xz}x_t + W_{hz}h_{t-1} + b_z)$$

$$\tilde{h}_t = \tanh(W_{xh}x_t + W_{hh}(r_t \odot h_{t-1}) + b_h)$$

$$h_t = z_t \odot h_{t-1} + (1 - z_t) \odot \tilde{h}_t$$

Here

$$z_t = 1 - u^{(t)}$$

# GRU and LSTM

## Gated Recurrent Unit

[Cho et al., EMNLP2014;  
Chung, Gulcehre, Cho, Bengio,  
DLUFL2014]

$$h_t = u_t \odot \tilde{h}_t + (1 - u_t) \odot h_{t-1}$$

$$\tilde{h}_t = \tanh(W [x_t] + U(r_t \odot h_{t-1}) + b)$$

$$u_t = \sigma(W_u [x_t] + U_u h_{t-1} + b_u)$$

$$r_t = \sigma(W_r [x_t] + U_r h_{t-1} + b_r)$$

## Long Short-Term Memory

[Hochreiter & Schmidhuber, NC1999;  
Gers, Thesis2001]

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

$$c_t = f_t \odot c_{t-1} + i_t \odot \tilde{c}_t$$

$$\tilde{c}_t = \tanh(W_c [x_t] + U_c h_{t-1} + b_c)$$

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

$$i_t = \sigma(W_i [x_t] + U_i h_{t-1} + b_i)$$


$$f_t = \sigma(W_f [x_t] + U_f h_{t-1} + b_f)$$



# LSTM vs. GRU

- ▶ Researchers have proposed many gated RNN variants, but LSTM and GRU are the most widely-used
- ▶ The biggest difference is that GRU is quicker to **compute** and has fewer parameters
- ▶ There is no conclusive evidence that one consistently performs better than the other
- ▶ LSTM is a good default choice (especially if your data has particularly long dependencies, or you have lots of training data)
- ▶ **Rule of thumb:** start with LSTM, but switch to GRU if you want something more efficient





# Is vanishing/exploding gradient just a RNN problem?

- ▶ No! It can be a problem for all neural architectures (including **feed-forward** and **convolutional**), especially **deep** ones.
  - ▶ Due to chain rule / choice of nonlinearity function, gradient can become vanishingly small as it backpropagates
  - ▶ Thus lower layers are learnt very slowly (hard to train)
  - ▶ Solution: lots of new deep feedforward/convolutional architectures that add more **direct connections** (thus allowing the gradient to flow)
- ▶ For example:
  - ▶ “**HighwayNet**” with highway connections:
    - ▶ Similar to residual connections, but the identity connection vs the transformation layer is controlled by a dynamic gate
    - ▶ Inspired by LSTMs, but applied to deep feedforward/convolutional networks
  - ▶ **ResNet** with residual connections, inspired by **HighwayNet**
  - ▶ **DenseNet** directly connect everything to everything!

# Some Historical Remarks on LSTM

- **[LSTM0]** S. Hochreiter and J. Schmidhuber. [Long Short-Term Memory](https://people.idsia.ch/~juergen/FKI-207-95ocr.pdf). TR FKI-207-95, TUM, August 1995. Link: <https://people.idsia.ch/~juergen/FKI-207-95ocr.pdf>
- **[LSTM1]** S. Hochreiter, J. Schmidhuber. Long Short-Term Memory. *Neural Computation*, 9(8):1735-1780, 1997. Based on [LSTM0].
- **[LSTM2]** F. A. Gers, J. Schmidhuber, F. Cummins. Learning to Forget: Continual Prediction with LSTM. *Neural Computation*, 12(10):2451-2471, 2000. *The "vanilla LSTM architecture" with forget gates that everybody is using today, e.g., in Google's Tensorflow.*
- **[LSTM3]** A. Graves, J. Schmidhuber. Framewise phoneme classification with bidirectional LSTM and other neural network architectures. *Neural Networks*, 18:5-6, pp. 602-610, 2005.



**Schmidhuber:** "In 2020 we celebrated the quarter-century anniversary of [LSTM's first failure to pass peer review](#). After the main peer-reviewed publication in 1997 [\[LSTM1\]](#) (now the most cited article in the history of *Neural Computation*), LSTM and its training procedures were further improved on my Swiss LSTM grants at IDSIA through the work of my later students Felix Gers, Alex Graves, and others. A milestone was the "vanilla LSTM architecture" with forget gate [\[LSTM2\]](#)—the LSTM variant of 1999-2000 that everybody is using today, e.g., in Google's Tensorflow. 2005 saw the first publication of LSTM with full backpropagation through time and of bi-directional LSTM [\[LSTM3\]](#) (now widely used)."

# Some Historical Remarks on HighwayNet

- ▶ **[HW1]** R. K. Srivastava, K. Greff, J. Schmidhuber. Highway networks. Preprints [arXiv:1505.00387](https://arxiv.org/abs/1505.00387) (May 2015) and [arXiv:1507.06228](https://arxiv.org/abs/1507.06228) (July 2015). Also at NIPS 2015. *The first working very deep feedforward nets with over 100 layers (previous NNs had at most a few tens of layers). Let  $g, t, h$ , denote non-linear differentiable functions. Each non-input layer of a highway net computes  $g(x)x + t(x)h(x)$ , where  $x$  is the data from the previous layer. (Like LSTM with forget gates [\[LSTM2\]](#) for RNNs.) Resnets [\[HW2\]](#) are a special case of this where the gates are always open:  $g(x)=t(x)=\text{const}=1$ . Highway Nets perform roughly as well as ResNets [\[HW2\]](#) on ImageNet. [\[HW3\]](#) Highway layers are also often used for natural language processing, where the simpler residual layers do not work as well. [\[HW3\]](#)*
- ▶ **[HW2]** He, K., Zhang, X., Ren, S., Sun, J. Deep residual learning for image recognition. Preprint [arXiv:1512.03385](https://arxiv.org/abs/1512.03385) (Dec 2015). *Residual nets are a special case of Highway Nets [\[HW1\]](#) where the gates are always open:  $g(x)=1$  (a typical highway net initialization) and  $t(x)=1$ .*
- ▶ **[HW3]** K. Greff, R. K. Srivastava, J. Schmidhuber. Highway and Residual Networks learn Unrolled Iterative Estimation. Preprint [arxiv:1612.07771](https://arxiv.org/abs/1612.07771) (2016). Also at ICLR 2017.





# Summary



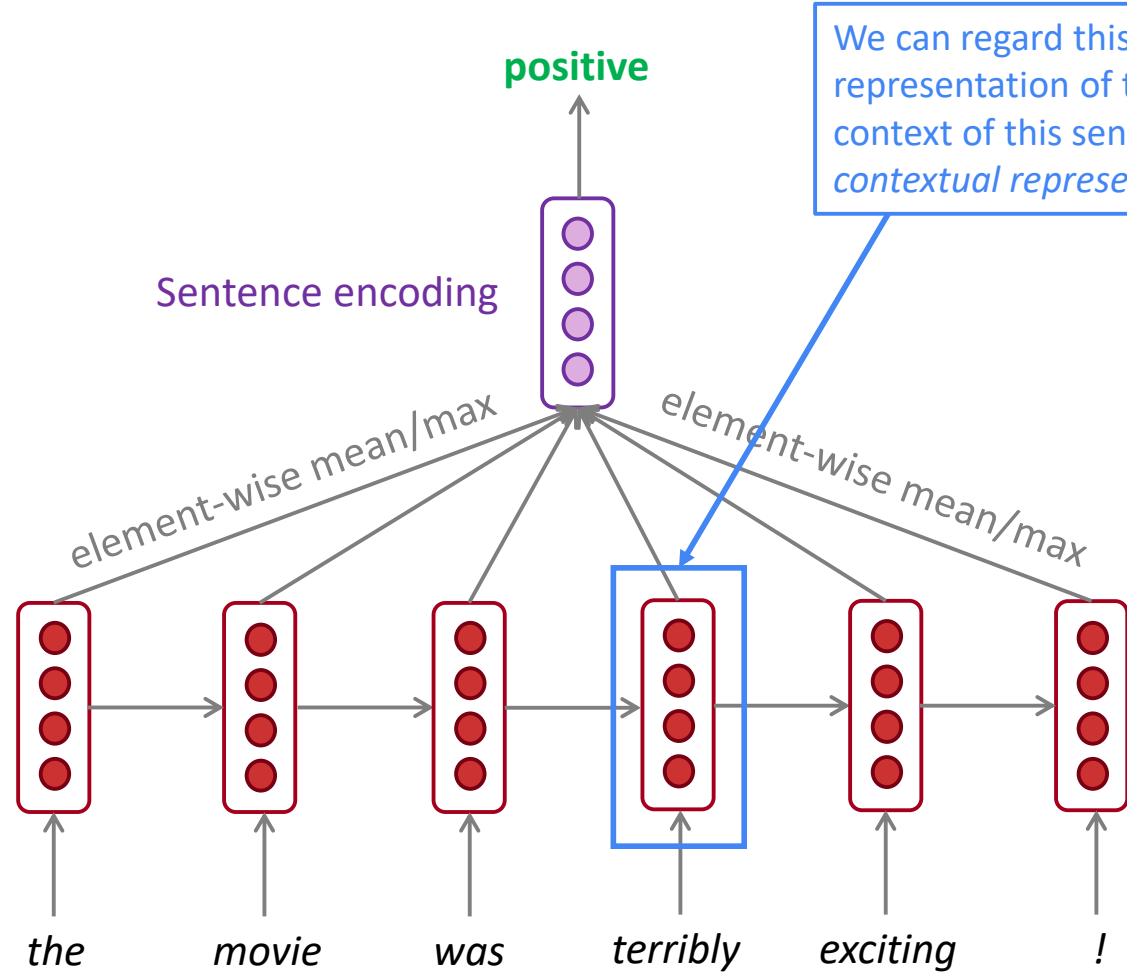
- RNN is flexible in architectures
- Vanilla RNNs are simple but don't work very well for deep nets
- Common to use LSTM or GRU: their additive interactions improve gradient flow
  - Backward flow of gradients in RNN can explode or vanish.
  - Exploding is controlled with gradient clipping.
  - Vanishing is controlled with additive interactions

A decorative graphic on the left side of the slide. It features a solid red arrow pointing to the right, positioned horizontally. Behind the arrow and extending upwards and to the right are several thin, dark grey, curved lines that resemble stylized grass or abstract brushstrokes.

Bi-Direction

# Motivation of Bidirection

Task: Sentiment Classification



We can regard this hidden state as a representation of the word "terribly" in the context of this sentence. We call this a contextual representation.

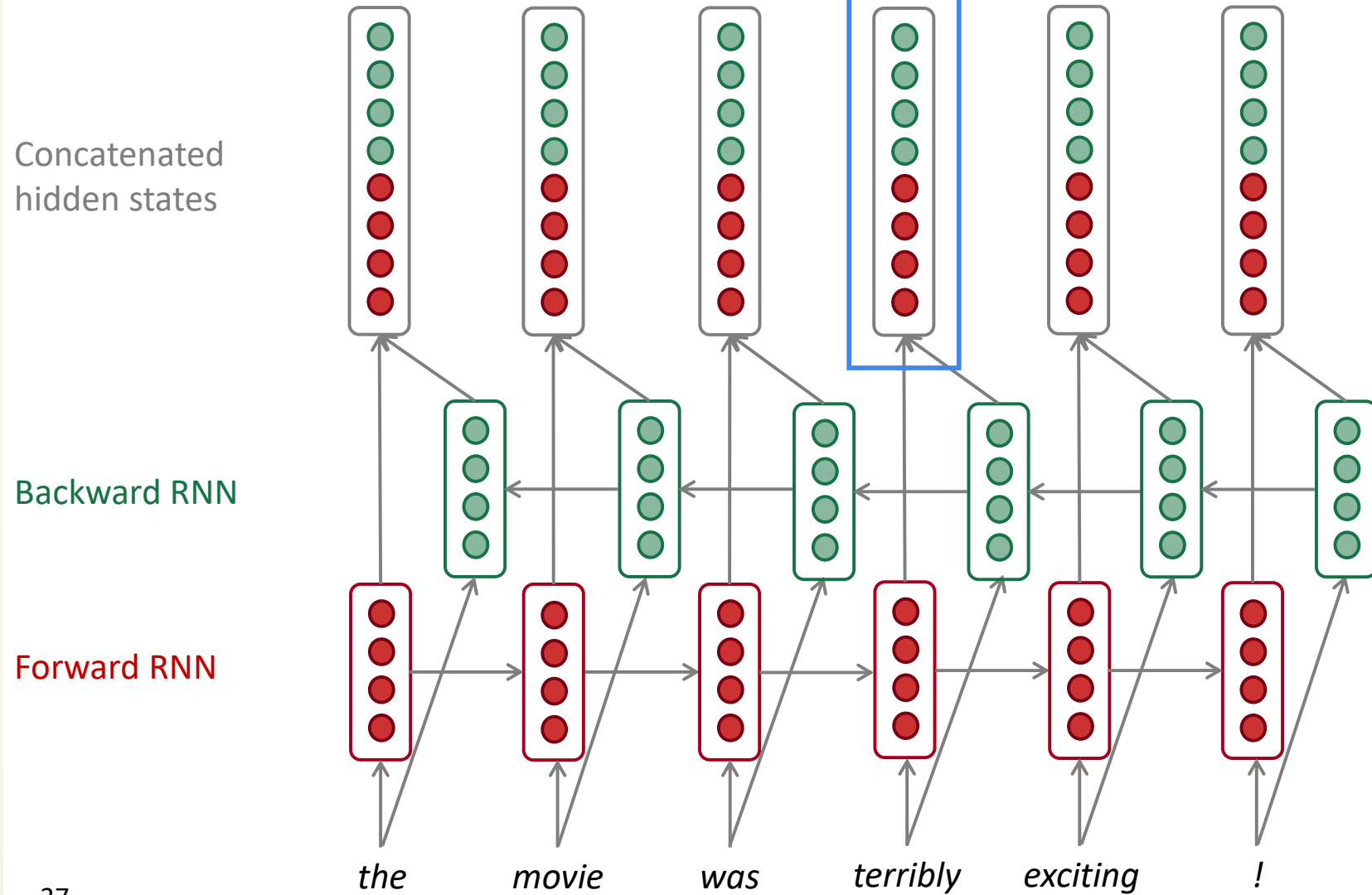
These contextual representations only contain information about the left context (e.g. "the movie was").

**What about right context?**

In this example, "exciting" is in the right context and this modifies the meaning of "terribly" (from negative to positive)

# Bidirectional RNNs

This contextual representation of "terribly" has both left and right context!



# Bidirectional RNN: simplified diagram

On timestep  $t$ :

This is a general notation to mean “compute one forward step of the RNN” – it could be a vanilla, LSTM or GRU computation.

Forward RNN  $\vec{h}^{(t)} = \text{RNN}_{\text{FW}}(\vec{h}^{(t-1)}, \mathbf{x}^{(t)})$

Backward RNN  $\overleftarrow{h}^{(t)} = \text{RNN}_{\text{BW}}(\overleftarrow{h}^{(t+1)}, \mathbf{x}^{(t)})$

Generally, these two RNNs have separate weights

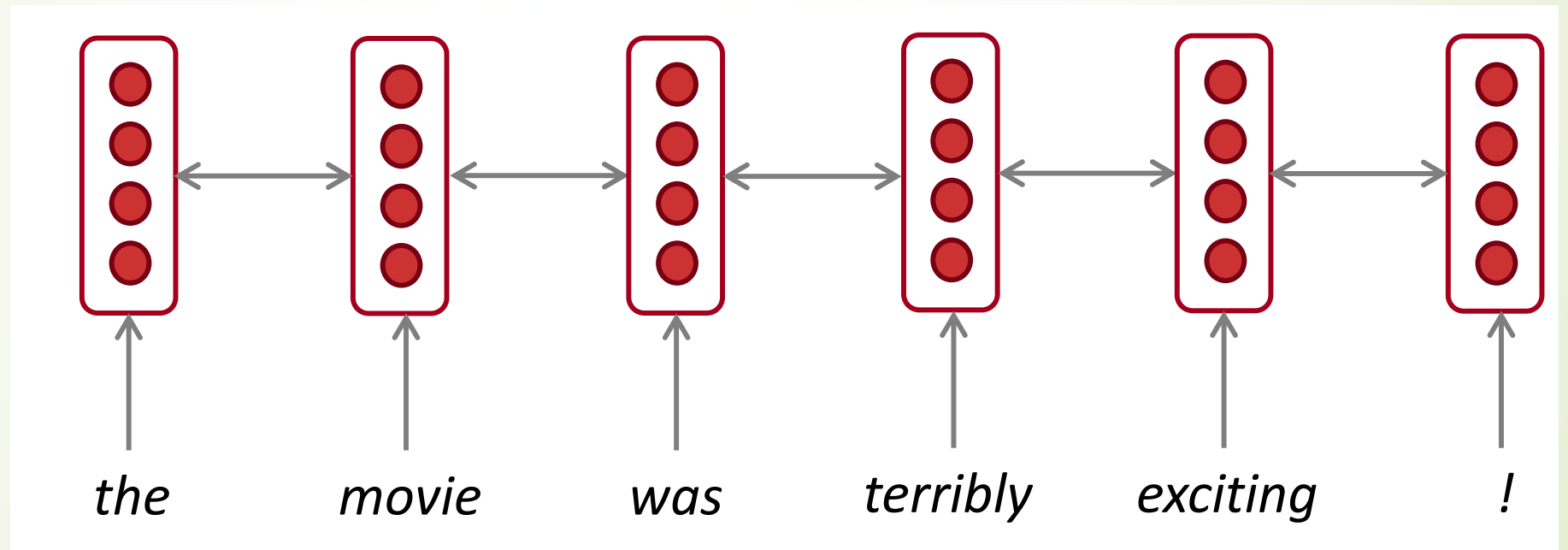
Concatenated hidden states  $\mathbf{h}^{(t)} = [\vec{h}^{(t)}; \overleftarrow{h}^{(t)}]$

We regard this as “the hidden state” of a bidirectional RNN. This is what we pass on to the next parts of the network.



# Bidirectional RNN: simplified diagram

- ▶ The two-way arrows indicate bidirectionality and the depicted hidden states are assumed to be the concatenated forwards+backwards states.





# Bidirectional RNNs

- ▶ Note: bidirectional RNNs are only applicable if you have access to the **entire input sequence**.
  - ▶ They are **not** applicable to Language Modeling, because in LM you *only* have left context available.
- ▶ If you do have entire input sequence (e.g. any kind of encoding), bidirectionality is powerful (you should use it by default).
- ▶ For example, **BERT** (**Bidirectional** Encoder Representations from Transformers) is a powerful pretrained contextual representation system built on bidirectionality.

# History note

- ▶ In 2013-2015, LSTMs started achieving state-of-the-art results
  - ▶ Successful tasks include: handwriting recognition, speech recognition, machine translation, parsing, image captioning
  - ▶ LSTM became the dominant approach
- ▶ Now (2019), other approaches (e.g. Transformers) have become more dominant for certain tasks.
  - ▶ For example in **WMT** (a MT conference + competition):
  - ▶ In WMT 2016, the summary report contains "RNN" 44 times
  - ▶ In WMT 2018, the report contains "RNN" 9 times and "**Transformer**" 63 times
  - ▶ **Source:** "Findings of the 2016 Conference on Machine Translation (WMT16)", Bojar et al. 2016, <http://www.statmt.org/wmt16/pdf/W16-2301.pdf>
  - ▶ **Source:** "Findings of the 2018 Conference on Machine Translation (WMT18)", Bojar et al. 2018, <http://www.statmt.org/wmt18/pdf/WMT028.pdf>

Thank you!

