Using RNNs to generate Super Mario Maker levels, Adam Geitgey

COMP547

DEEP UNSUPERVISED LEARNING

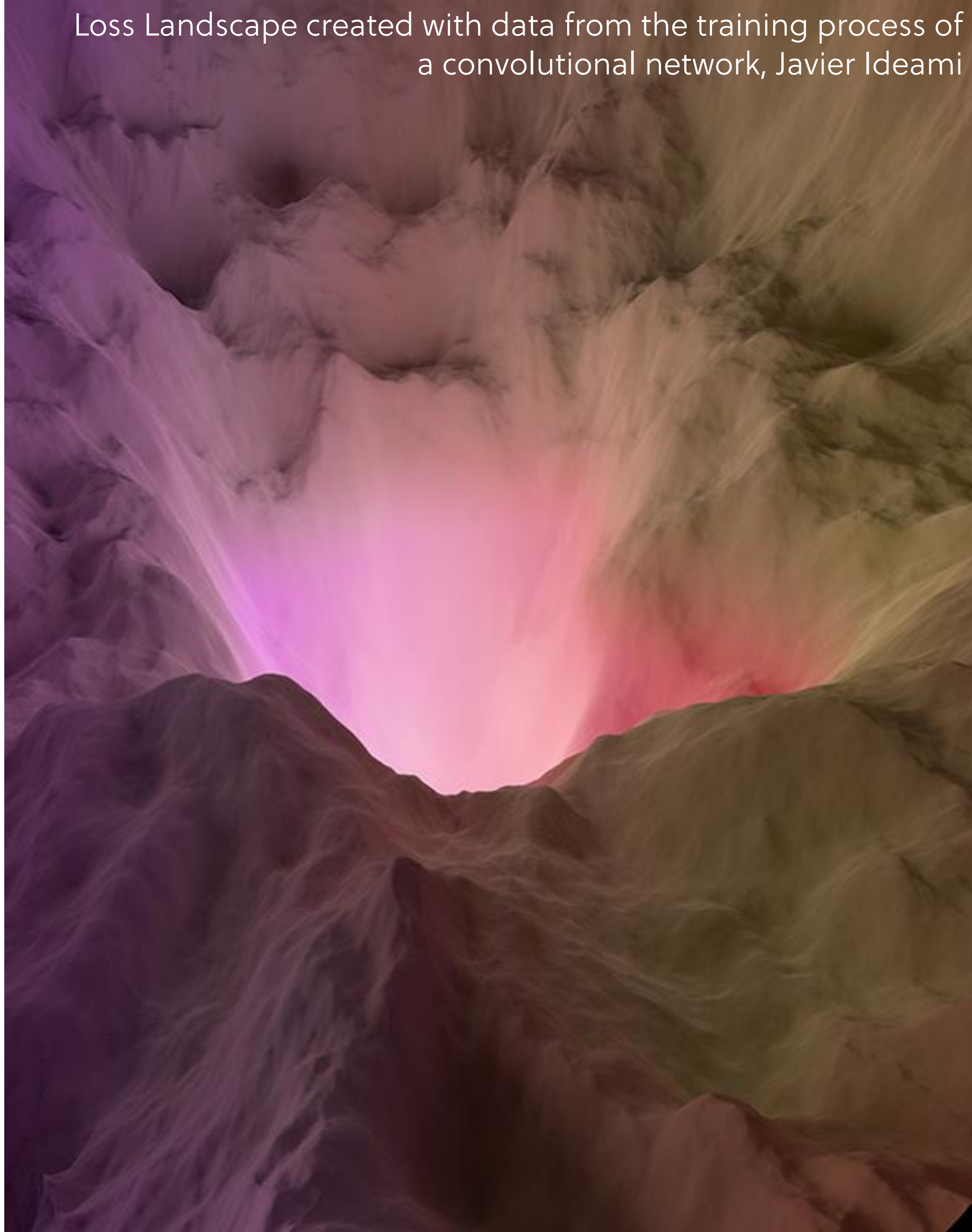
Lecture #3 – Neural Networks Basics II: Sequential Processing with NNs

KOÇ UNIVERSITY

Aykut Erdem // Koç University // Spring 2021

Previously on COMP547

- deep learning
- computation in a neural net
- optimization
- backpropagation
- training tricks
- convolutional neural networks



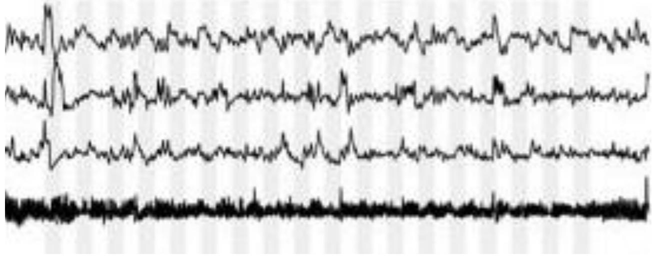
Loss Landscape created with data from the training process of a convolutional network, Javier Ideami

Lecture overview

- sequence modeling
- convolutions in time
- recurrent neural networks (RNNs)
- autoregressive generative models
- attention models
- case study: transformer model

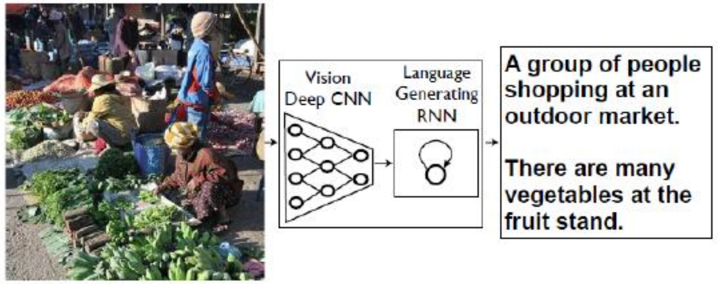
- **Disclaimer:** Much of the material and slides for this lecture were borrowed from
  —Bill Freeman, Antonio Torralba and Phillip Isola's MIT 6.869 class
  —Phil Blunsom's Oxford Deep NLP class
  —Fei-Fei Li, Andrej Karpathy and Justin Johnson's CS231n class
  —Arun Mallya's tutorial on Recurrent Neural Networks

Sequential data

- "I took the dog for a walk this morning." sentence
-  medical signals
-  speech waveform
-  video frames

Modeling sequential data

- Sample data sequences from a certain distribution $P(x_1, \ldots, x_N)$
- Generate natural sentences to describe an image $P(y_1, \ldots, y_M | I)$



- Activity recognition from a video sequence $P(y | x_1, \ldots, x_N)$

- [ ] Running
- [x] Jumping
- [ ] Dancing
- [ ] Fighting
- [ ] Eating

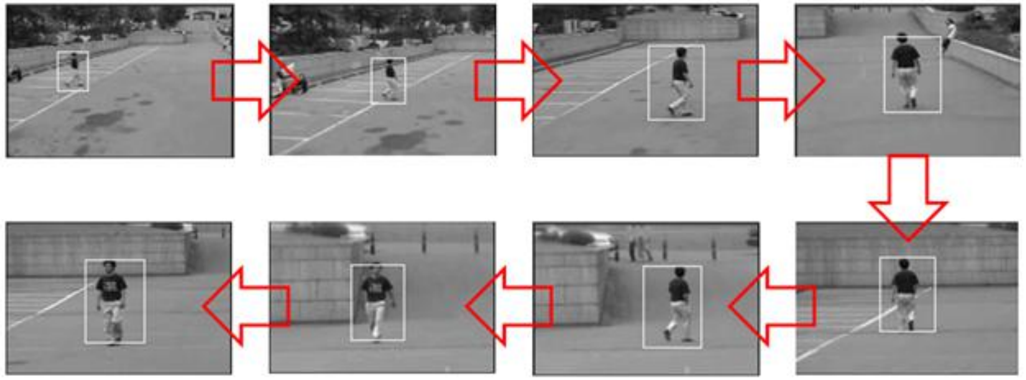
Modeling sequential data

- Speech recognition

$$P(y_1, \ldots, y_N | x_1, \ldots, x_N)$$

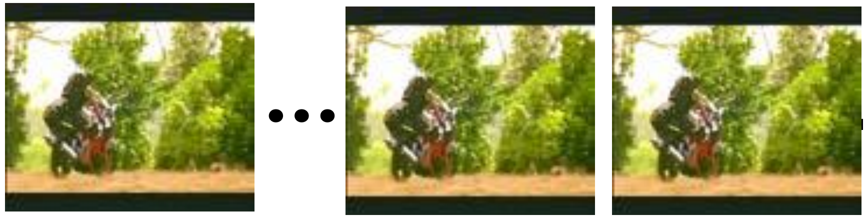
- Object tracking

$$P(y_1, \ldots, y_N | x_1, \ldots, x_N)$$



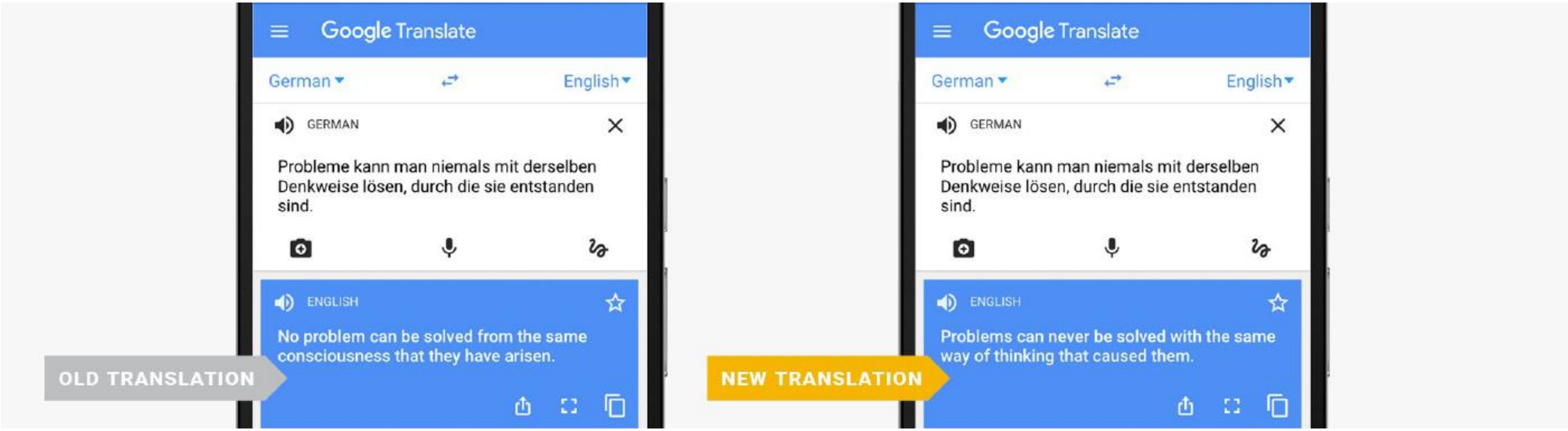
Modeling sequential data

- Generate natural sentences to describe a video $P(y_1, \dots, y_M | x_1, \dots, x_N)$

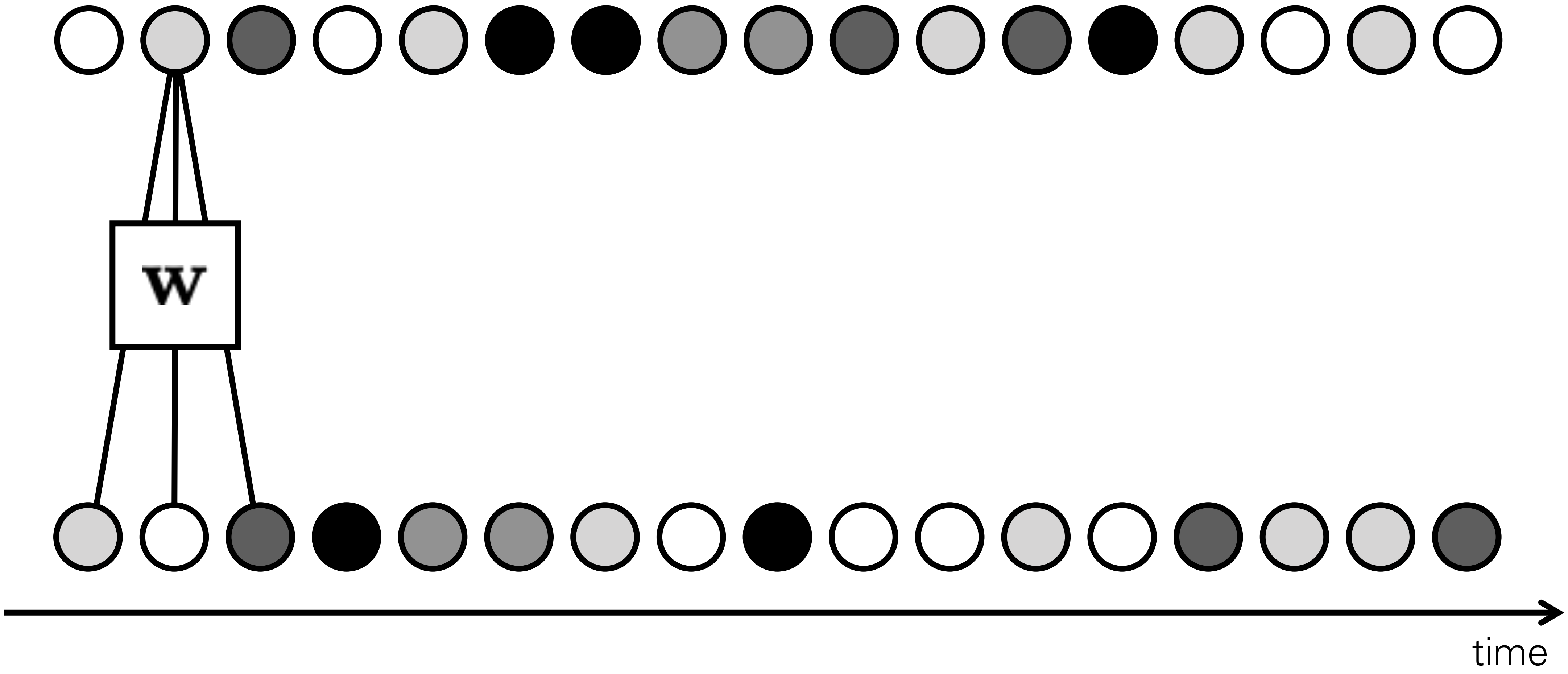


$\longrightarrow$ **A man is riding a bike**

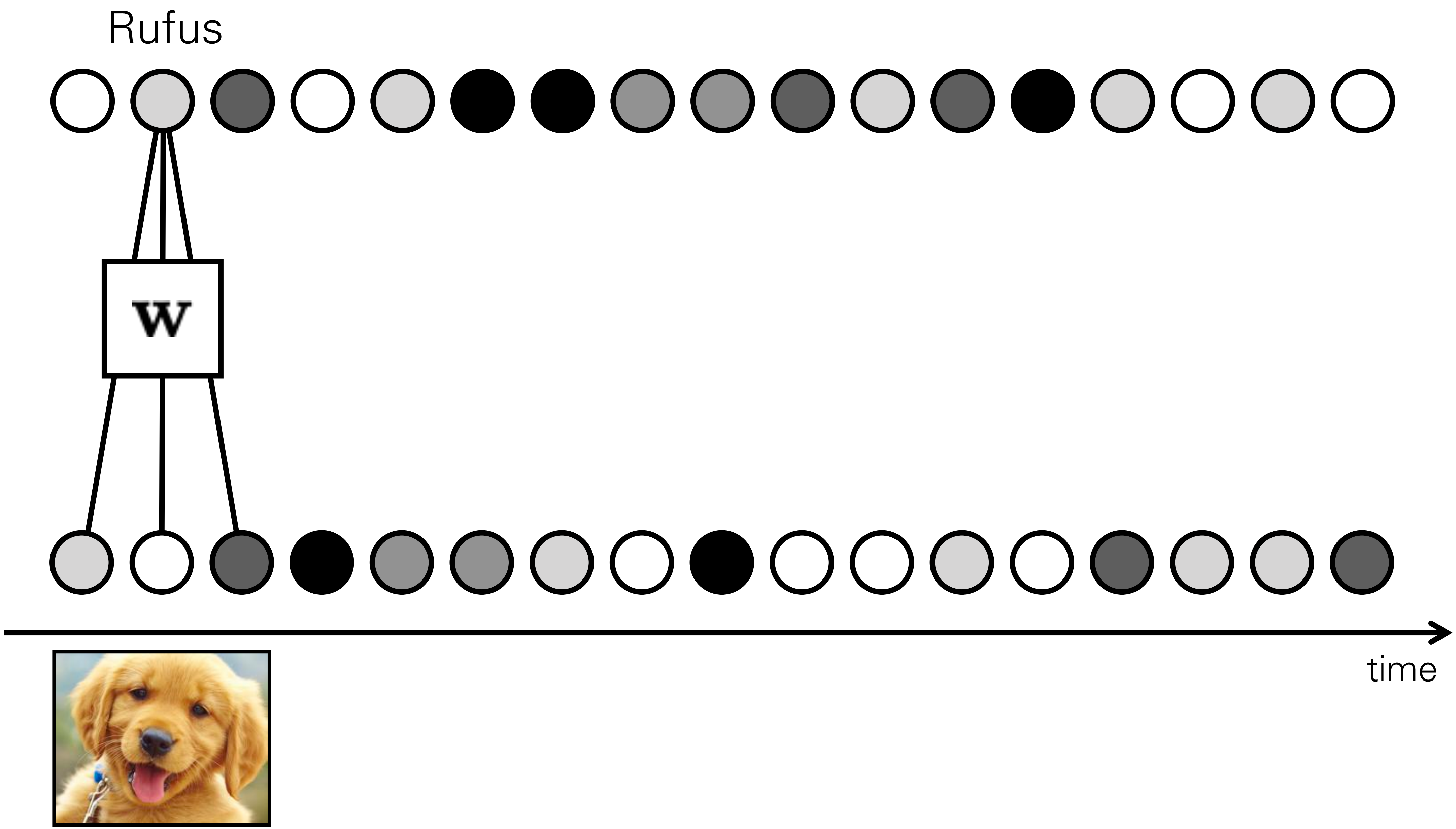
- Machine translation $P(y_1, \dots, y_M | x_1, \dots, x_N)$

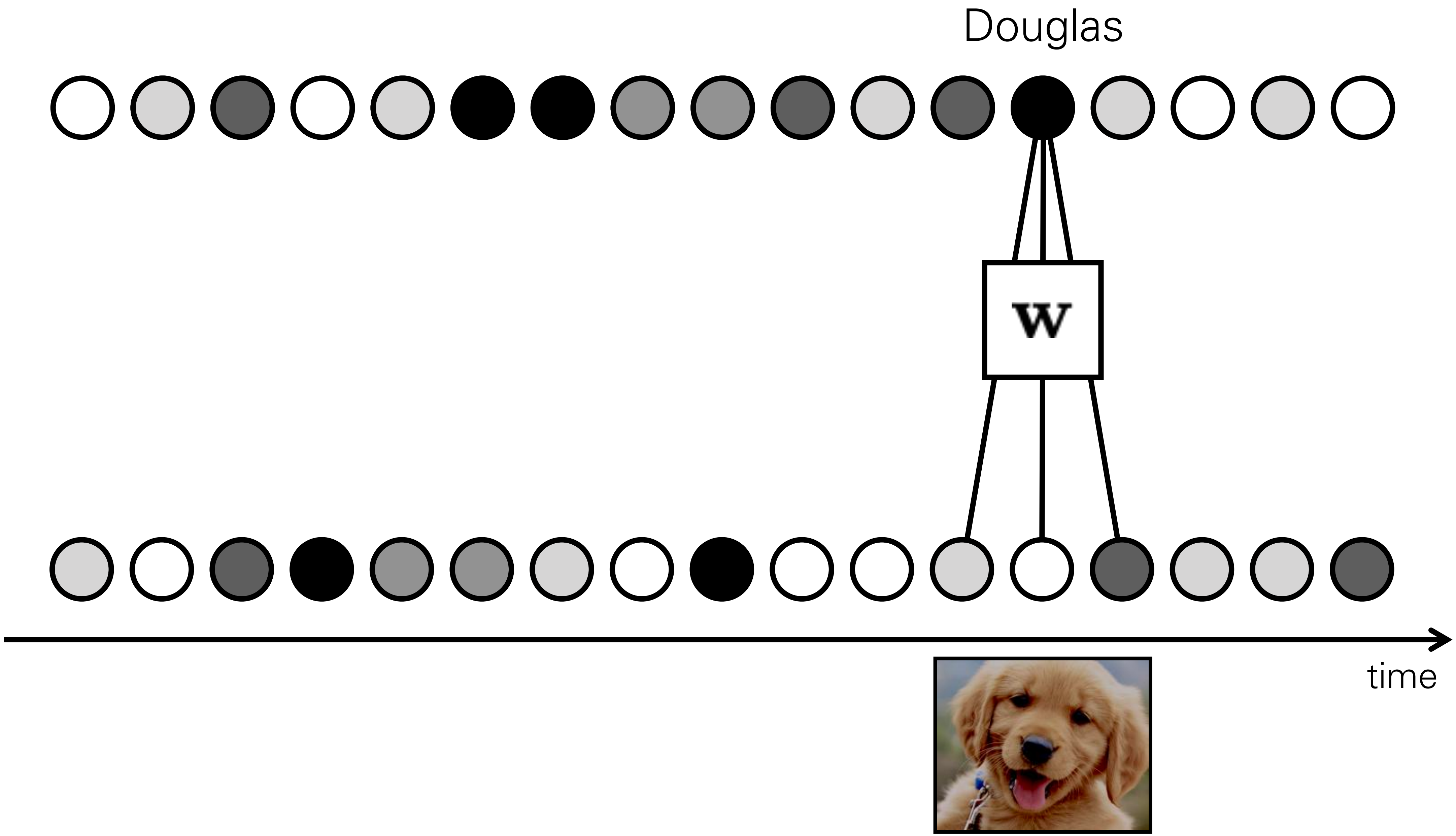


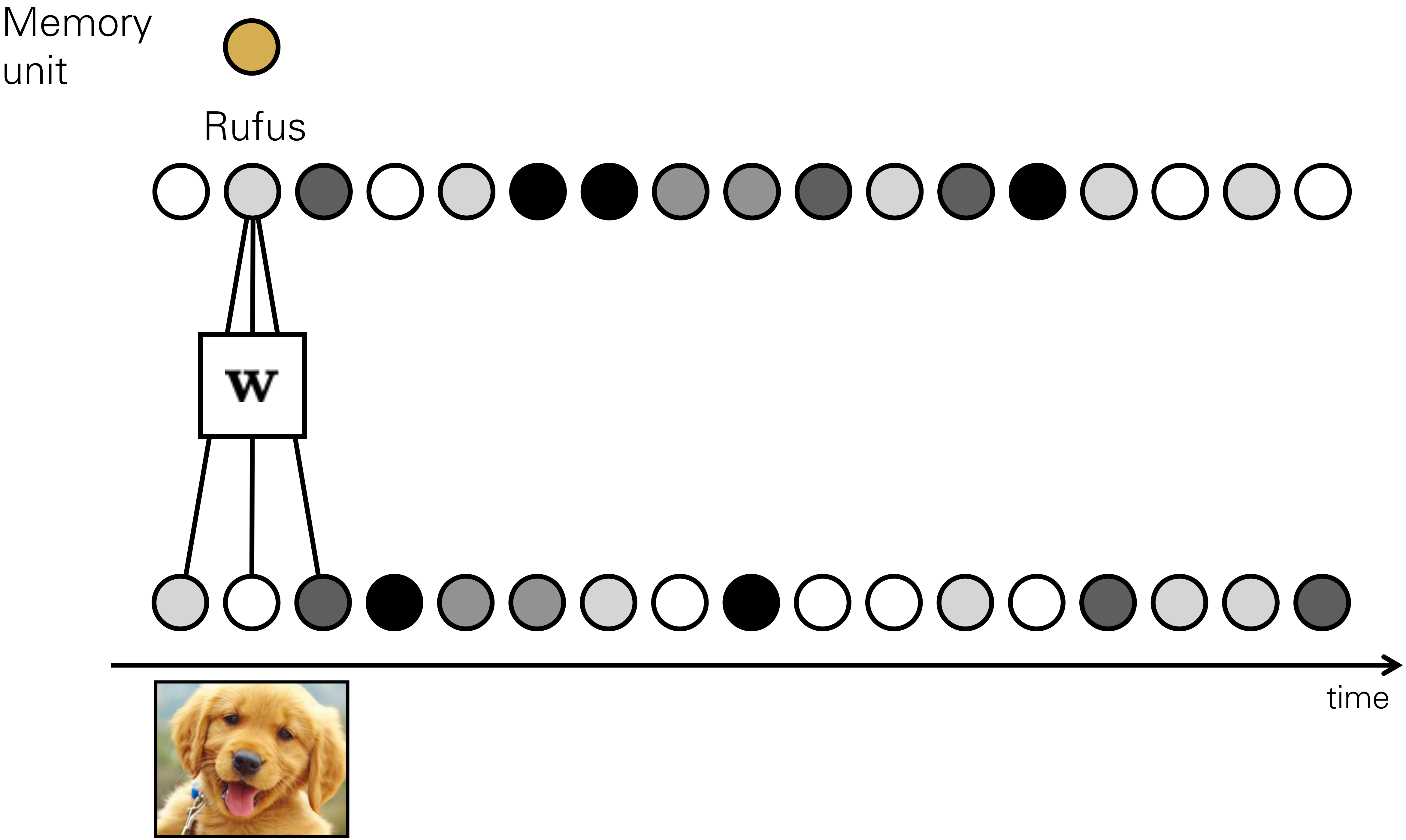
Convolutions in time

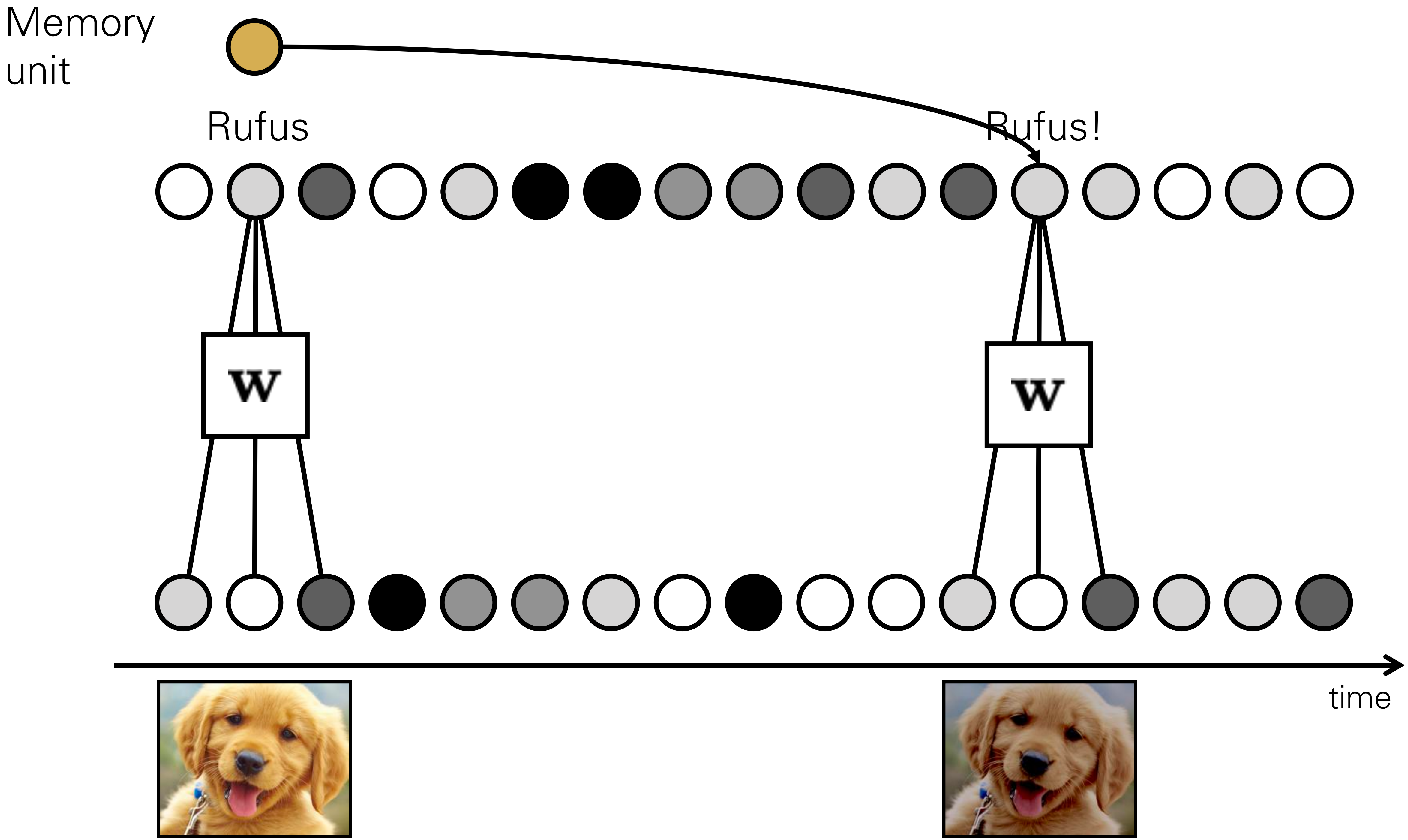


[https://www.youtube.com/watch?v=wxfGT-kKxiM

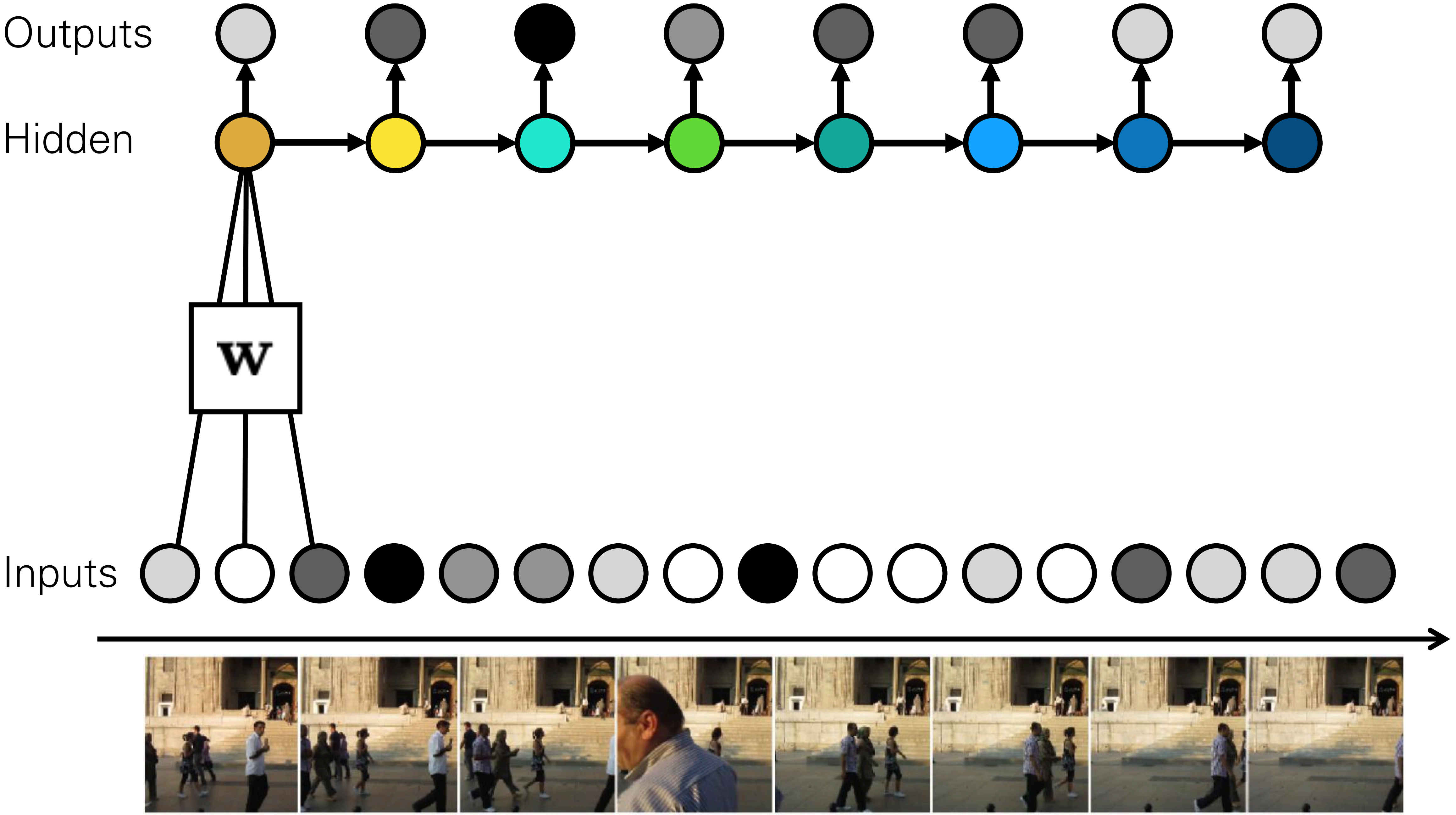

Rufus
w
time


Douglas
w
time


Memory
unit
Rufus
w
time


Memory
unit
Rufus
Rufus!
w
w
time

Recurrent Neural Networks (RNNs)

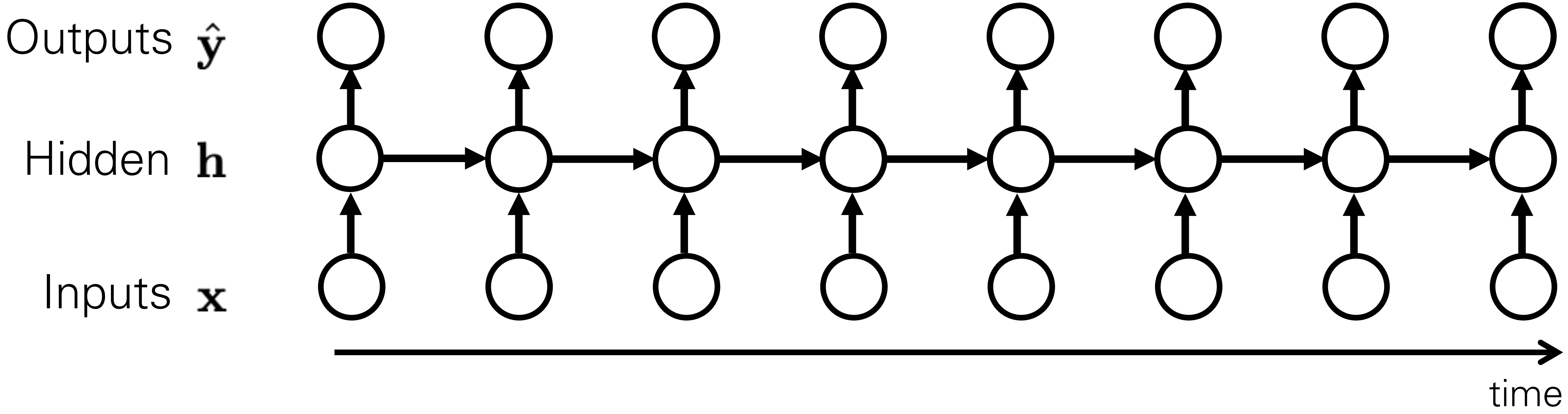


To model sequences, we need

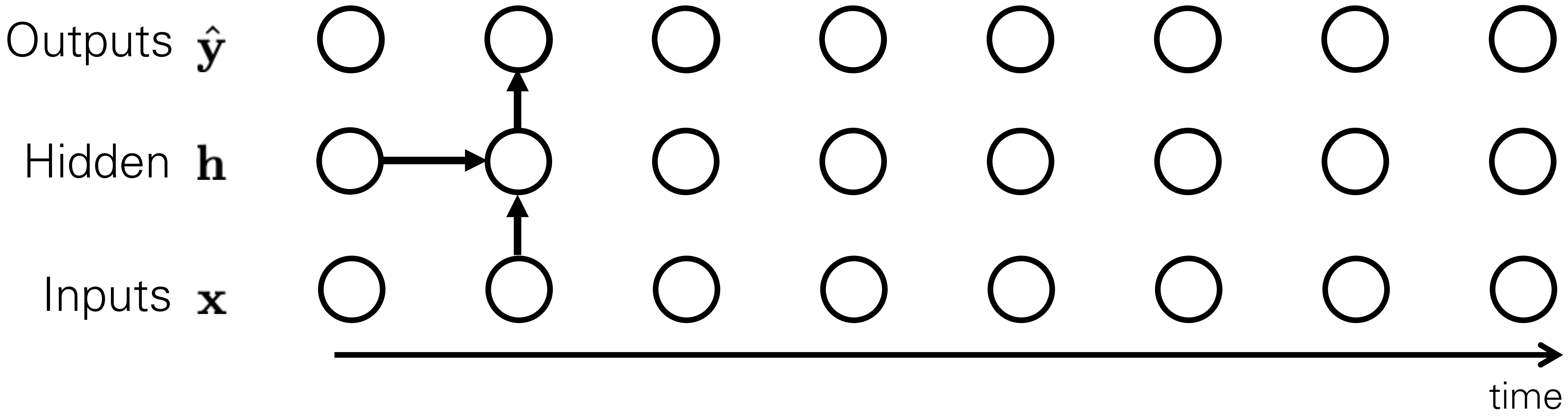
1. to deal with variable length sequences
2. to maintain sequence order
3. to keep track of long-term dependencies
4. to share parameters across the sequence

Recurrent Neural Networks

Recurrent Neural Networks (RNNs)



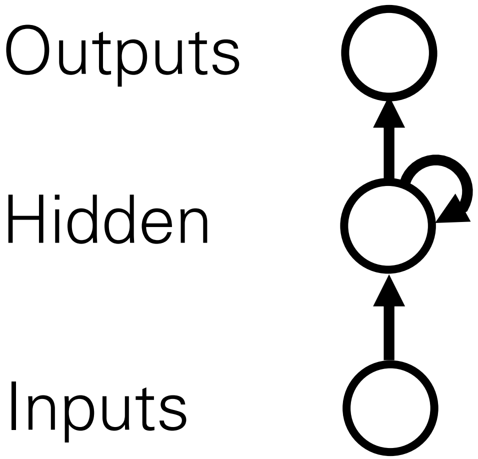
Recurrent Neural Networks (RNNs)



$$\mathbf{h}^{(t)} = f(\mathbf{h}^{(t-1)}, \mathbf{x}^{(t)})$$

$$\mathbf{y}^{(t)} = g(\mathbf{h}^{(t)})$$

Recurrent Neural Networks (RNNs)



Recurrent!

$$\mathbf{h}^{(t)} = f(\mathbf{h}^{(t-1)}, \mathbf{x}^{(t)})$$

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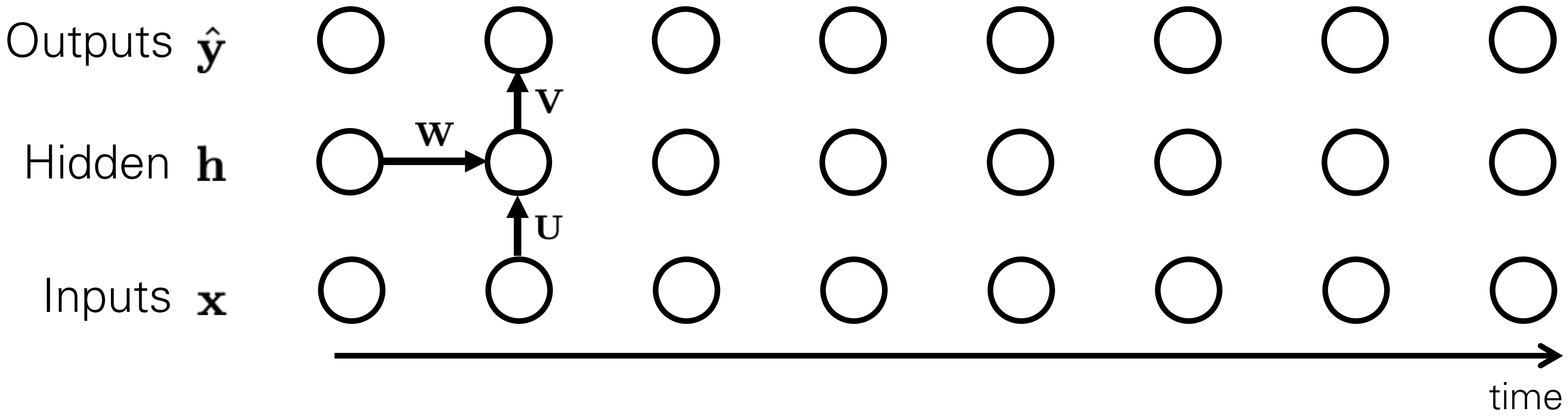
Recurrent Neural Networks (RNNs)



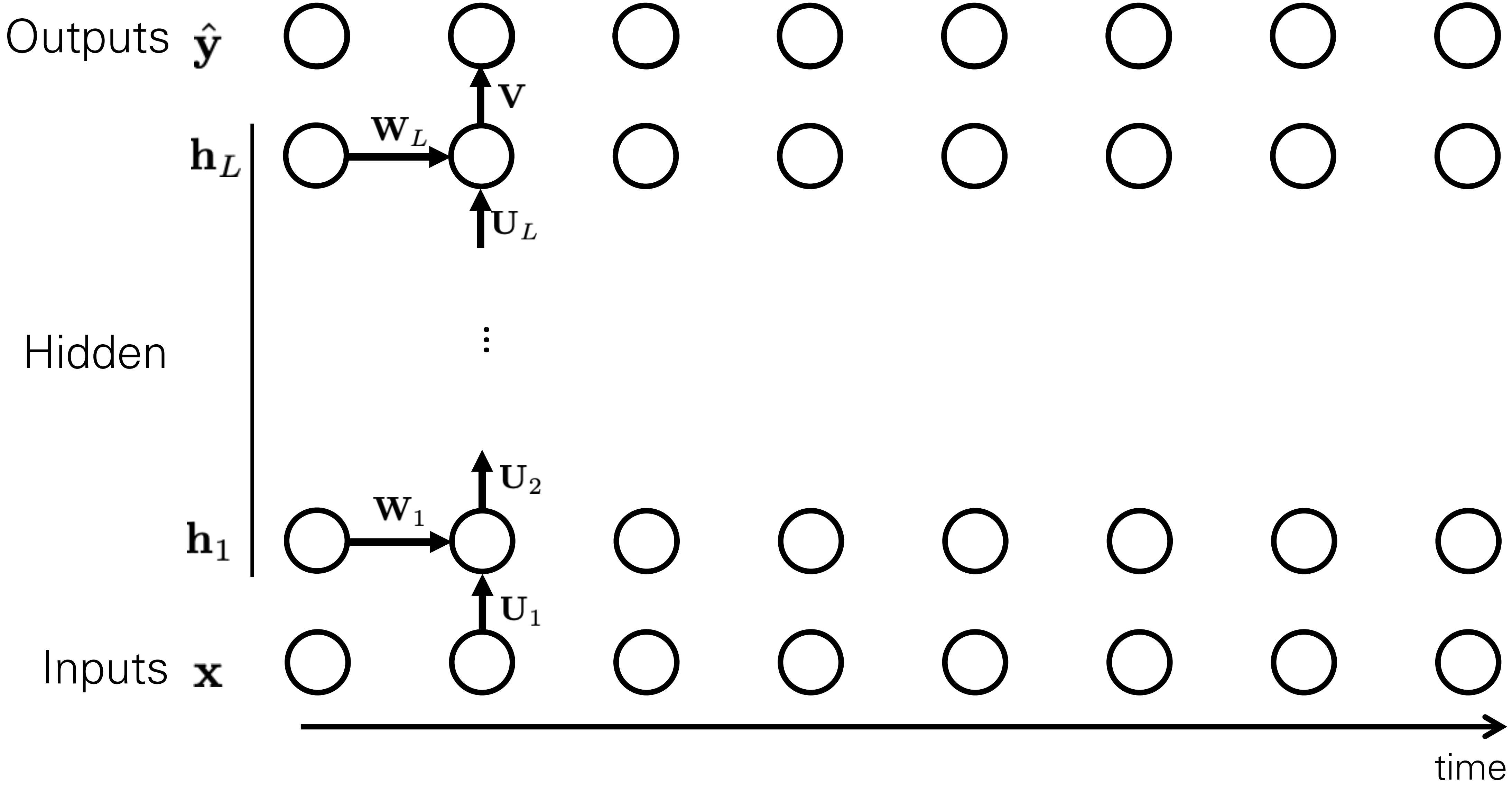
$$\mathbf{a}^{(t)} = \mathbf{W}\mathbf{h}^{(t-1)} + \mathbf{U}\mathbf{x}^{(t)} + \mathbf{b}$$

$$\mathbf{h}^{(t)} = \tanh(\mathbf{a}^{(t)})$$

$$\mathbf{o}^{(t)} = \mathbf{V}\mathbf{h}^{(t)} + \mathbf{c}$$

$$\hat{\mathbf{y}}^{(t)} = \mathtt{softmax}(\mathbf{o}^{(t)})$$

Deep Recurrent Neural Networks (RNNs)



Language Modeling

Language modeling

- Language models aim to represent the history of observed text ($w_1,\ldots,w_{t-1}$) succinctly in order to predict the next word (w_t):

all the works of shakespeare → *language model* →

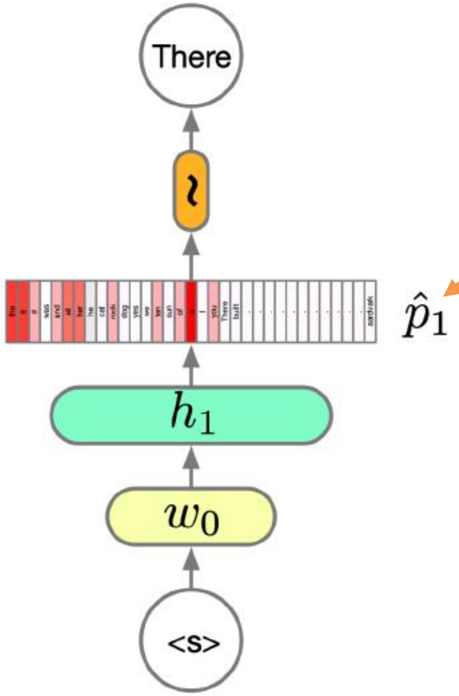
KING LEAR:
O, if you were a feeble sight,
the courtesy of your law,
Your sight and several breath,
will wear the gods
With his heads, and my hands
are wonder'd at the deeds,
So drop upon your lordship's
head, and your opinion
Shall be against your honour.

http://karpathy.github.io/2015/05/21/rnn-effectiveness/

RNN language models

$$h_n = g(V\,[x_n; h_{n-1}] + c)$$

$$\hat{y}_n = W h_n + b$$

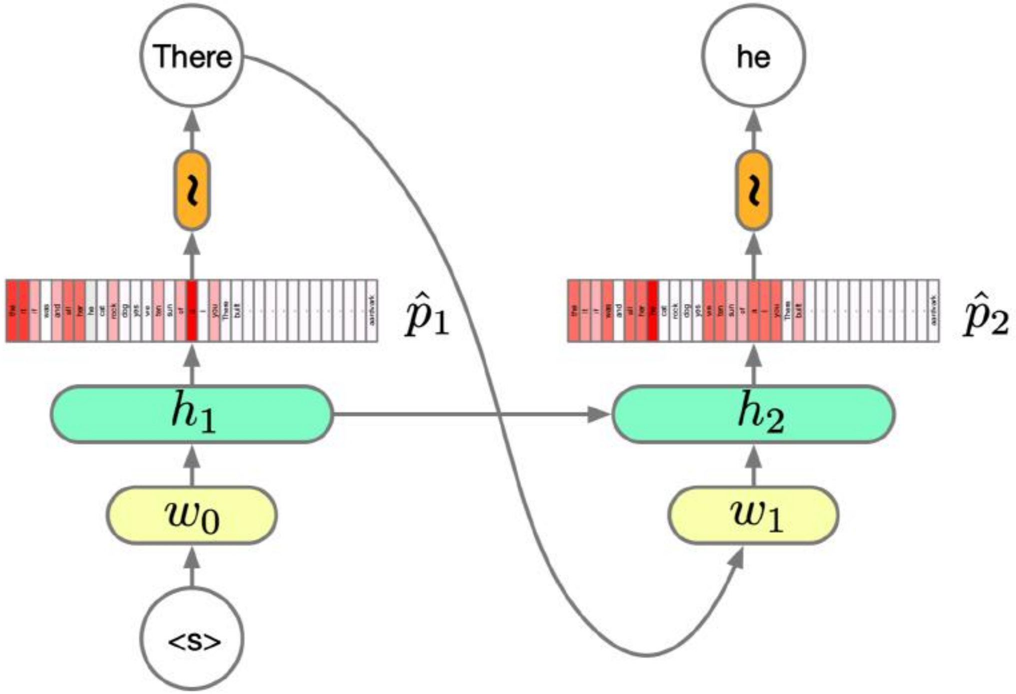


a probability distribution over possible next words, aka a softmax

RNN language models

$$h_n = g(V\,[x_n; h_{n-1}] + c)$$

$$\hat{y}_n = W h_n + b$$



RNN language models

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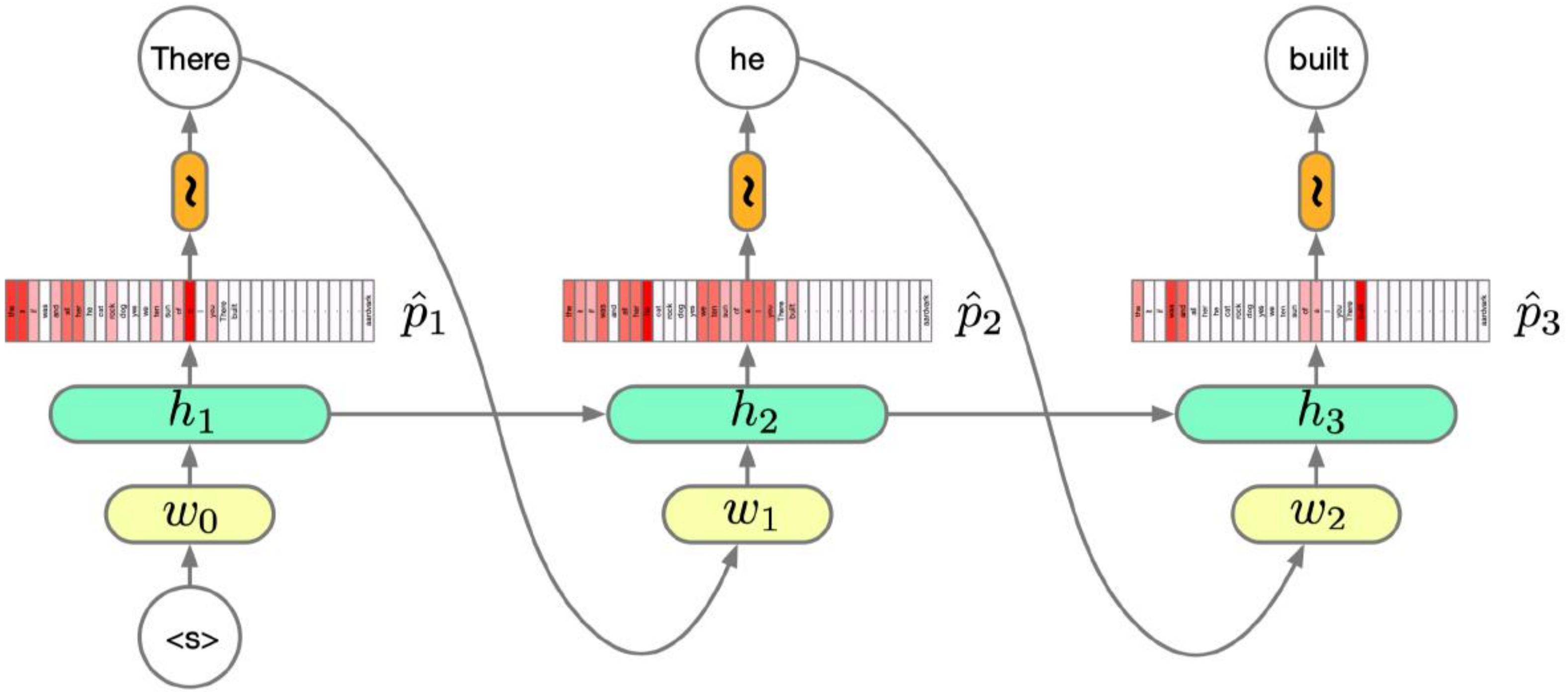

RNN language models

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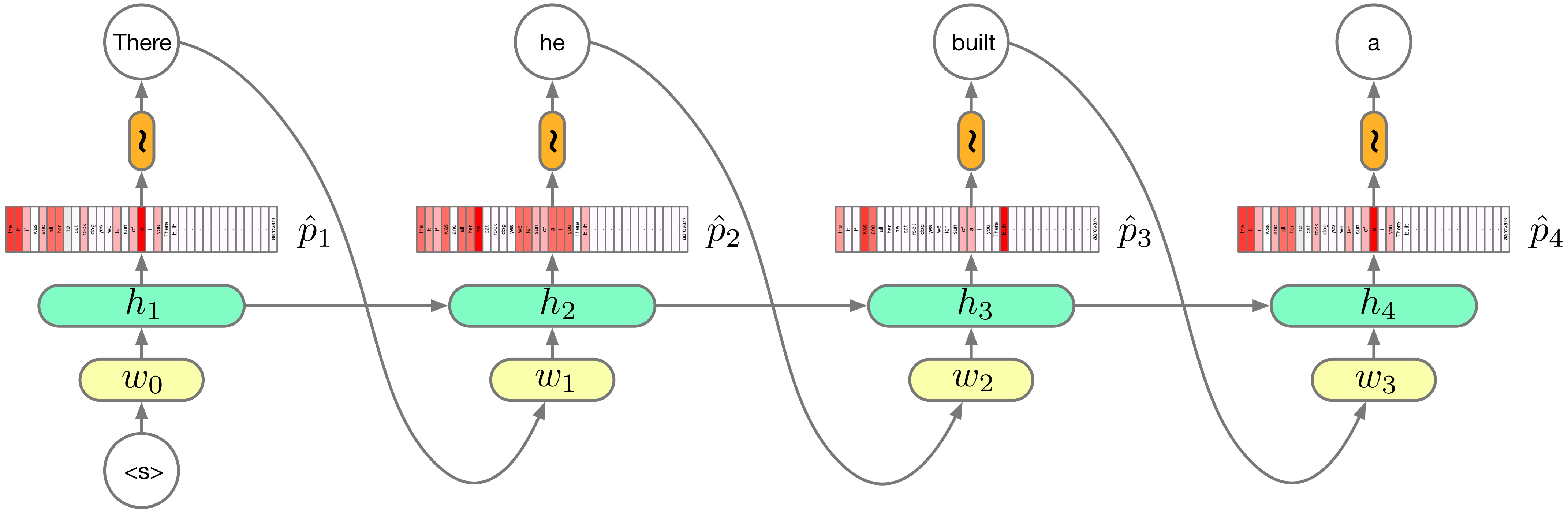
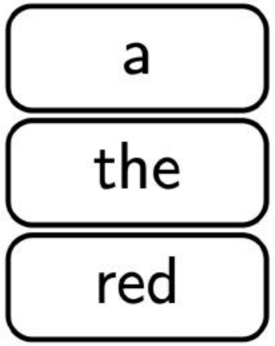


Beam Search (K = 3)



For t =1...T :

- For all k and for all possible output words w:

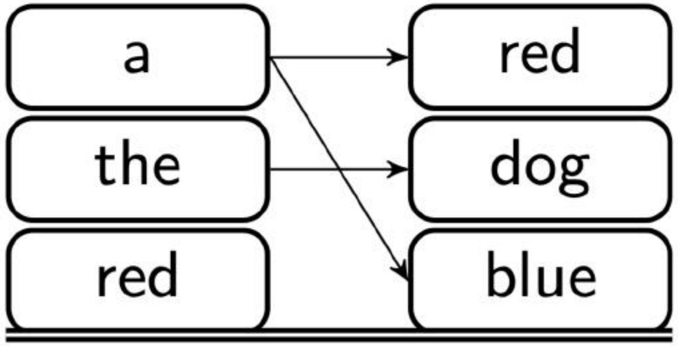
$$s(w, \hat{y}_{1:t-1}^{(k)}) \leftarrow \log p(\hat{y}_{1:t-1}^{(k)}|x) + \log p(w|\hat{y}_{1:t-1}^{(k)}, x)$$

- Update beam:

$$\hat{y}_{1:t}^{(1:K)} \leftarrow \text{K-arg max } s(w, \hat{y}_{1:t-1}^{(k)})$$

Slide credit: Alexander Rush

Beam Search (K = 3)



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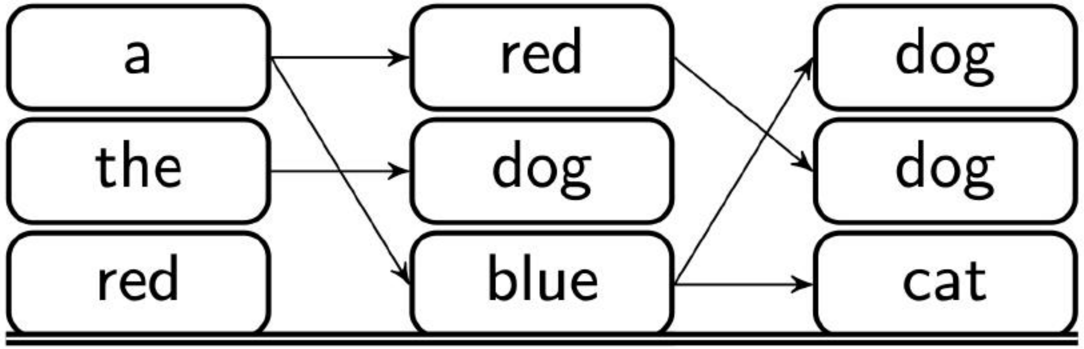

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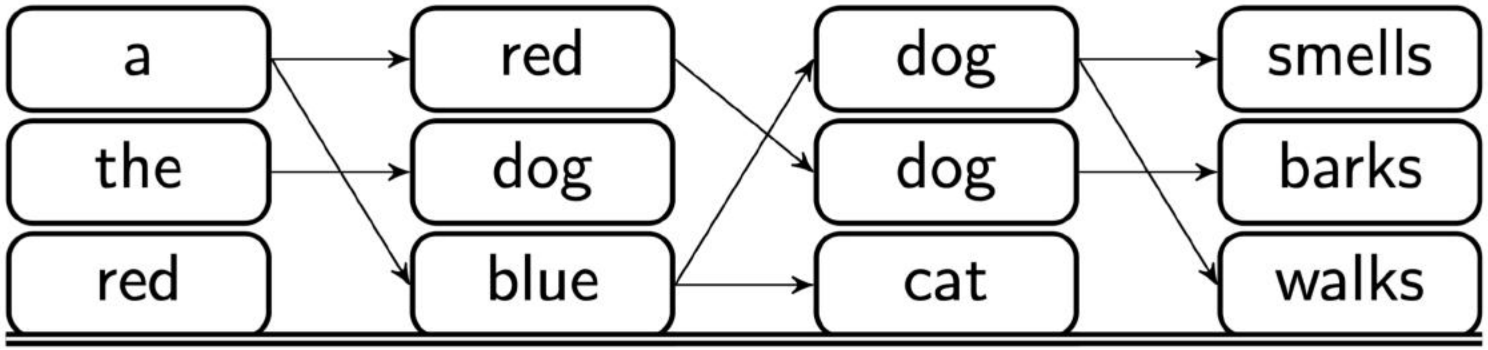

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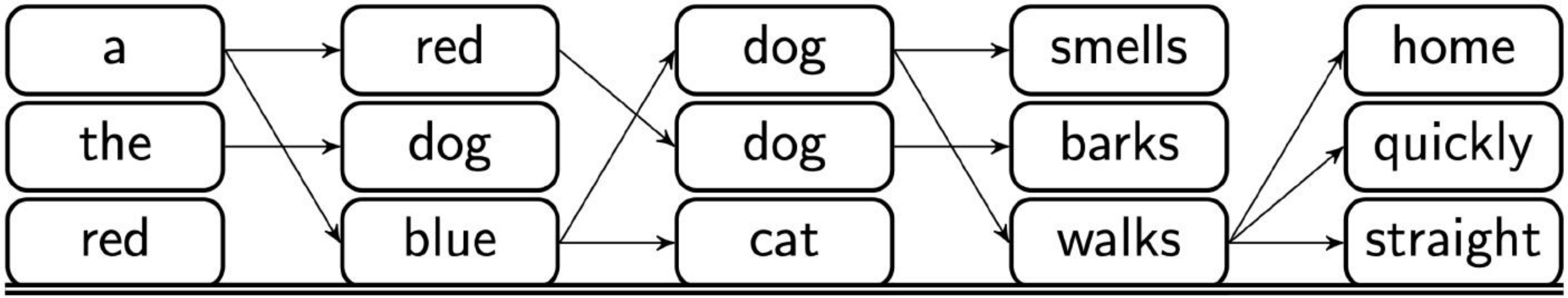

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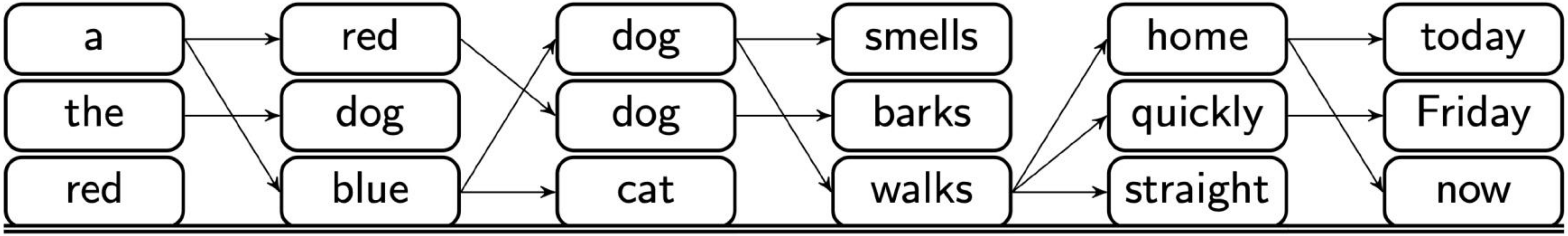
Slide credit: Alexander Rush

Beam Search ($K = 3$)



For $t = 1 \ldots T$:

- For all k and for all possible output words w:

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- Update beam:

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Slide credit: Alexander Rush

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.
```

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.
```

http://karpathy.github.io/2015/05/21/rnn-effectiveness/

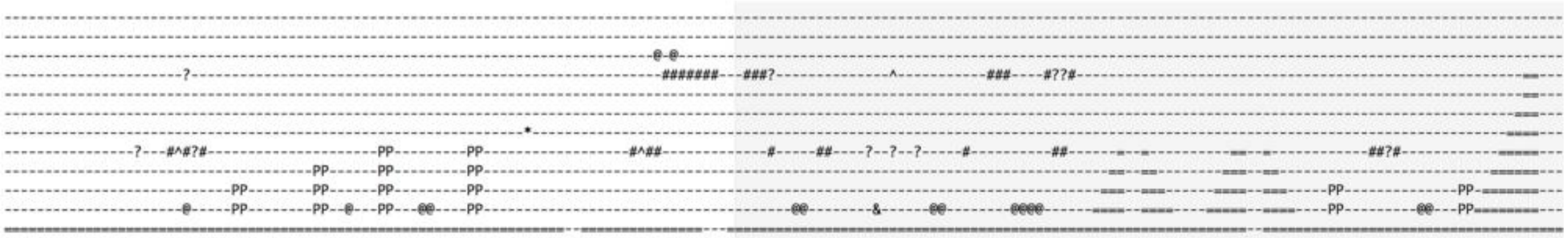
More Language Modeling Fun – DeepDrumpf

https://twitter.com/deepdrumpf

More Language Modeling Fun – Generating Super Mario Levels

Original Level:

Textual Representation:

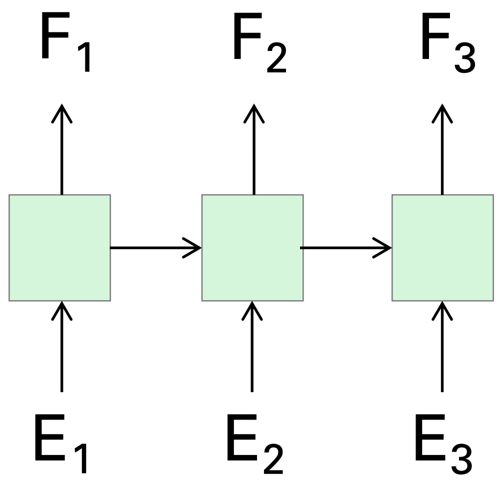


A level generated by a RNN:

https://medium.com/@ageitgey/machine-learning-is-fun-part-2-a26a10b68df3

Is this enough?

- Consider the problem of translation of English to French
- E.g. What is your name ⟶ Comment tu t'appelle
- Is the below architecture suitable for this problem?

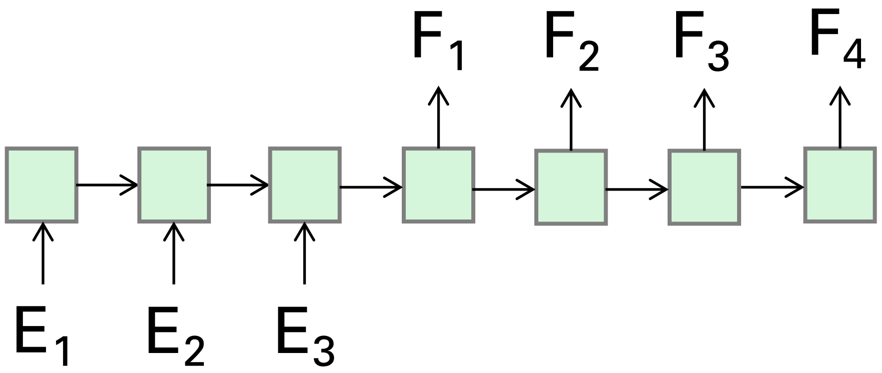


- No, sentences might be of different length and words might not align. Need to see entire sentence before translating

Adapted from http://www.cs.toronto.edu/~rgrosse/csc321/lec10.pdf

Encoder-decoder seq2seq model

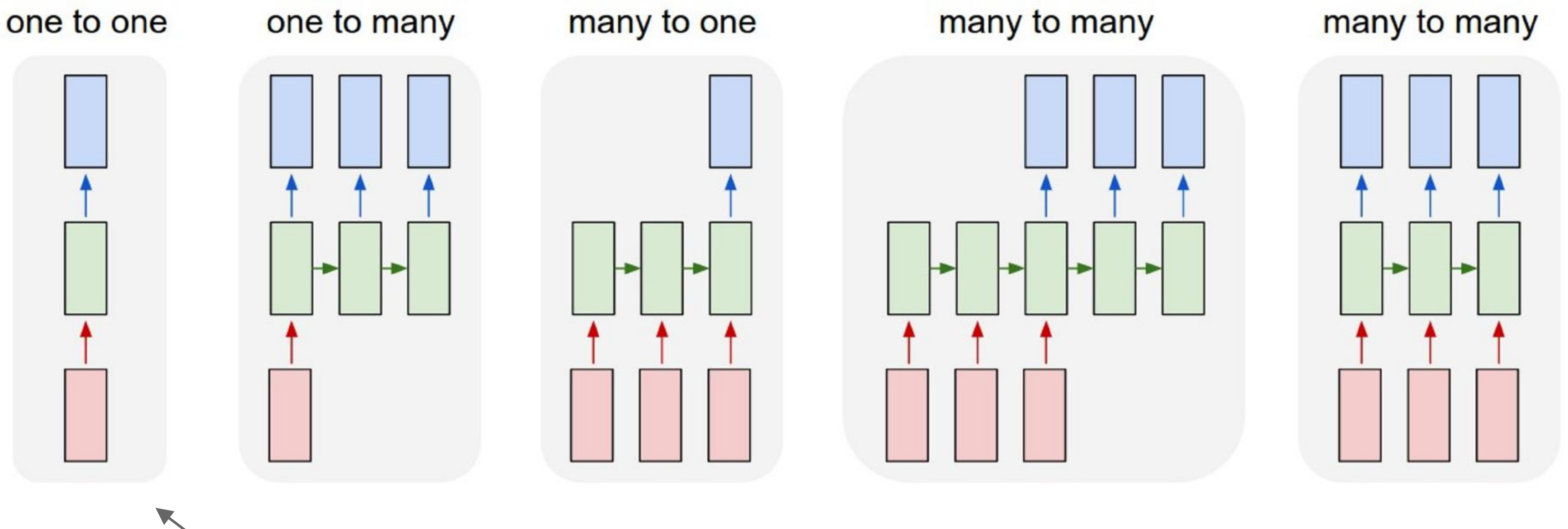
- Consider the problem of translation of English to French
- E.g. What is your name $\longrightarrow$ Comment tu t'appelle
- Sentences might be of different length and words might not align. Need to see entire sentence before translating



- Input-Output nature depends on the structure of the problem at hand

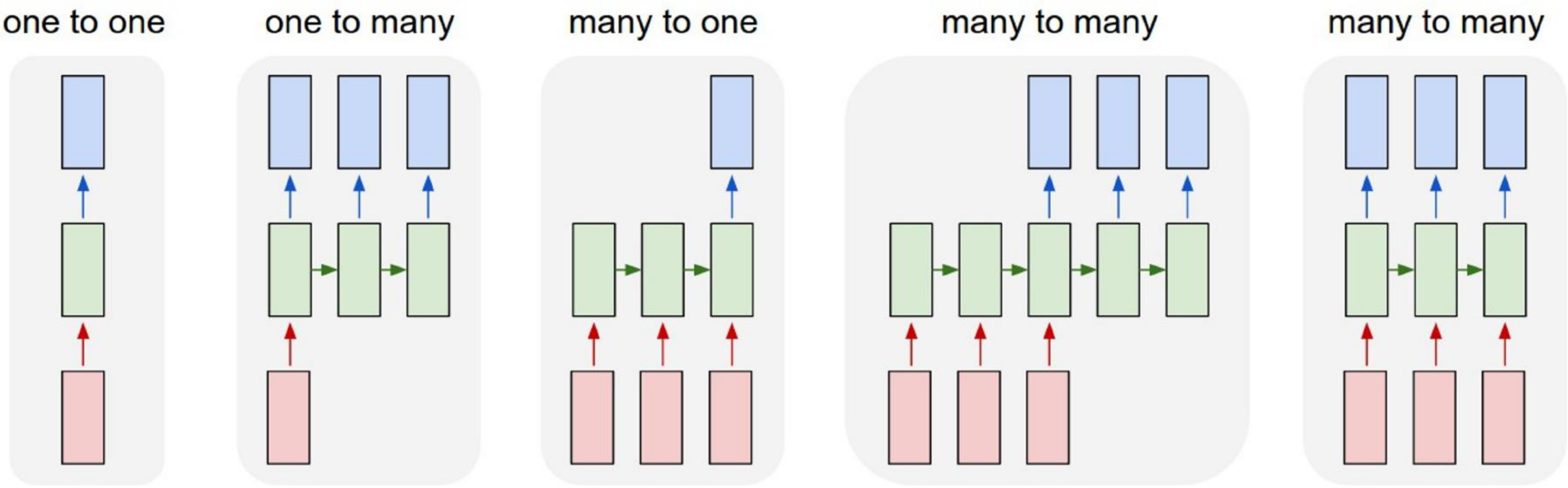
Seq2Seq Learning with Neural Networks. Sutskever et al., NIPS 2014

Recurrent Networks offer a lot of flexibility:



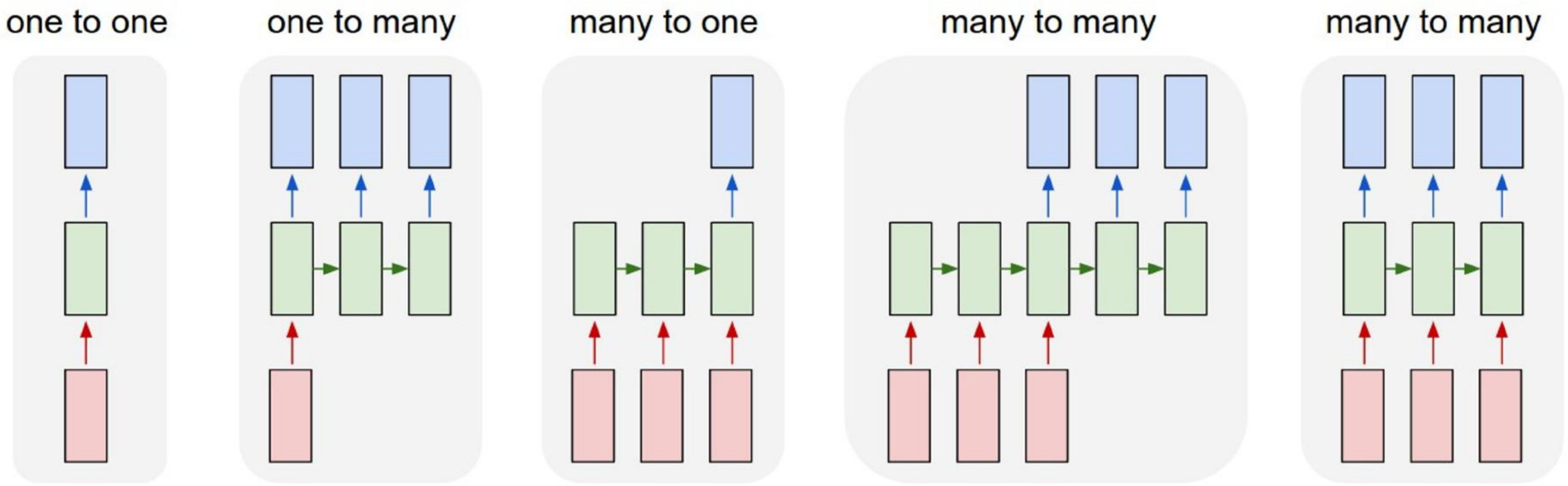
Vanilla Neural Networks

Recurrent Networks offer a lot of flexibility:



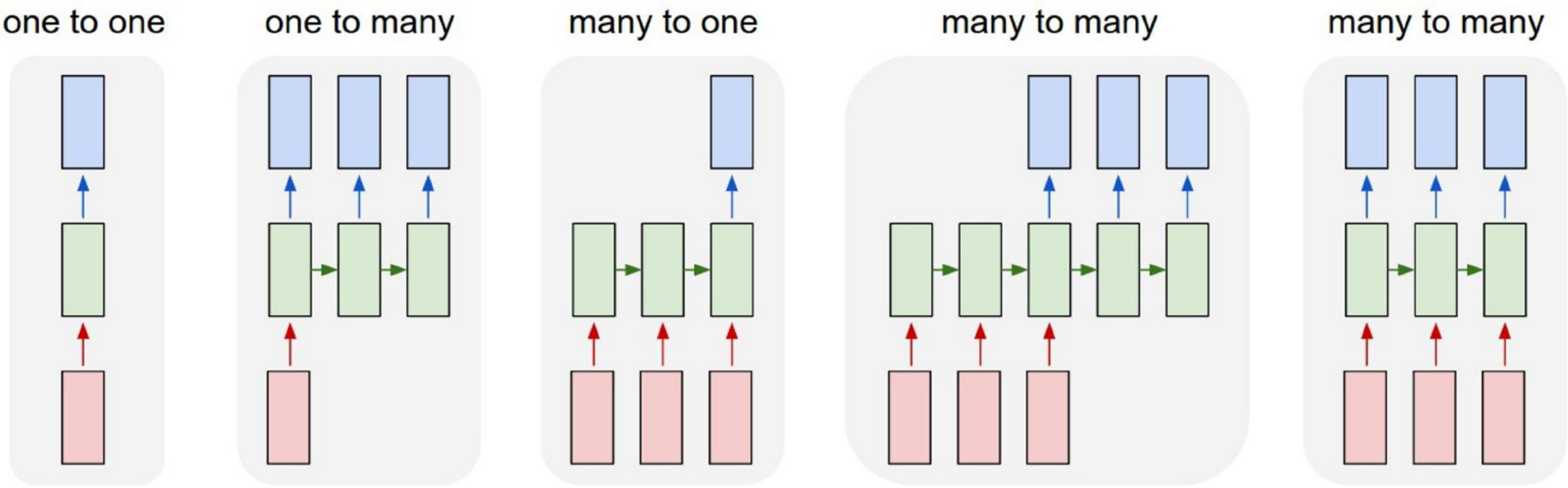
e.g. **Image Captioning**
image -> sequence of words

Recurrent Networks offer a lot of flexibility:



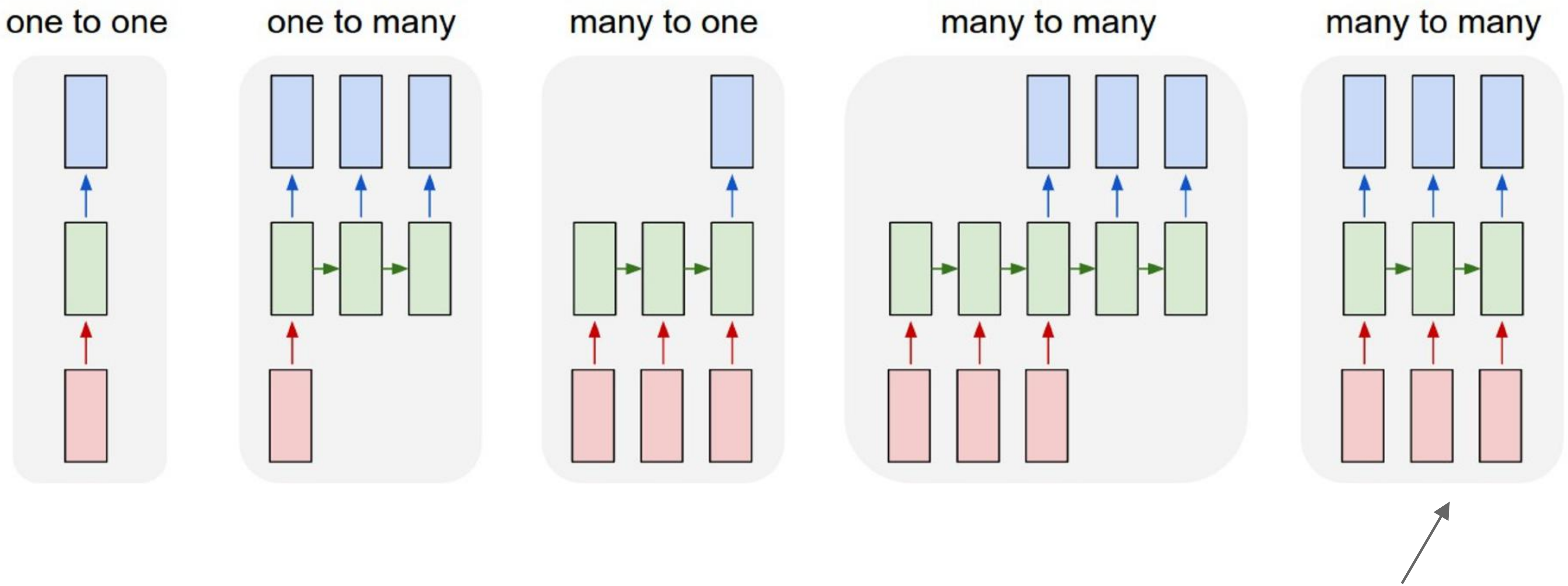
e.g. **Sentiment Classification**
sequence of words -> sentiment

Recurrent Networks offer a lot of flexibility:



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

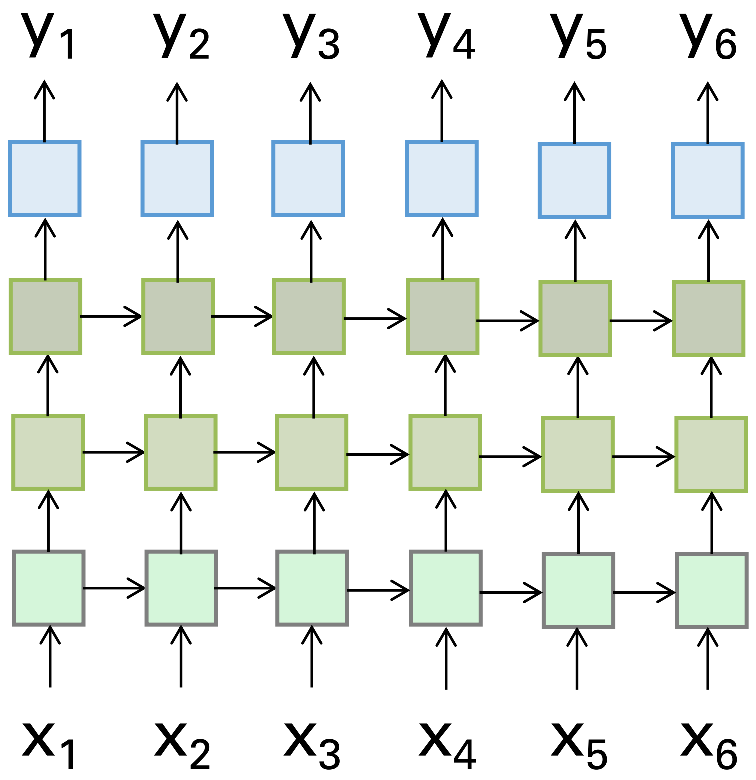
Recurrent Networks offer a lot of flexibility:



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

Multi-layer RNNs

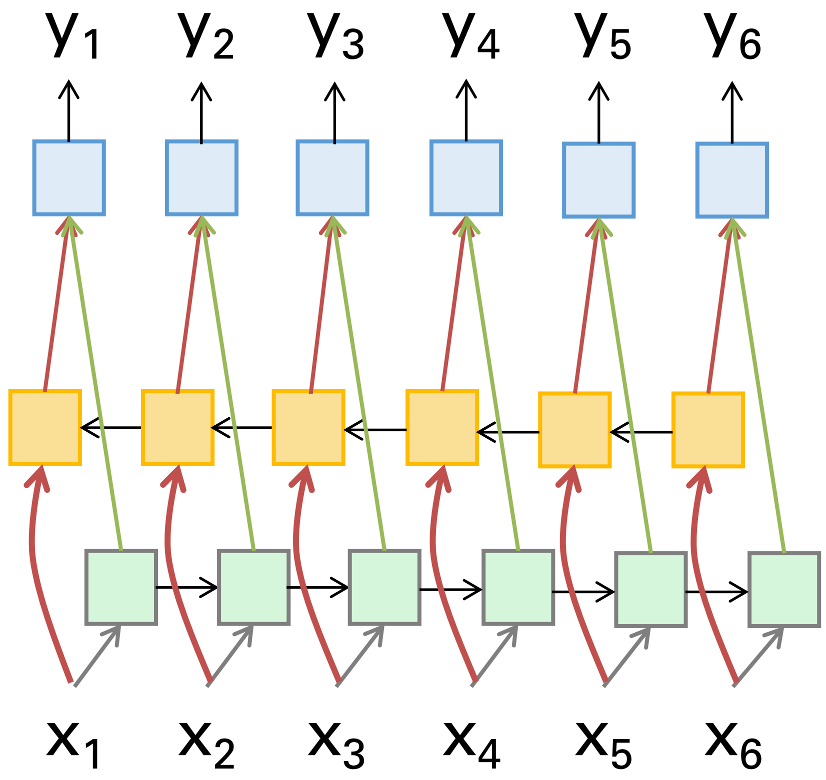
- We can of course design RNNs with multiple hidden layers



- Think exotic: Skip connections across layers, across time, …

Bi-directional RNNs

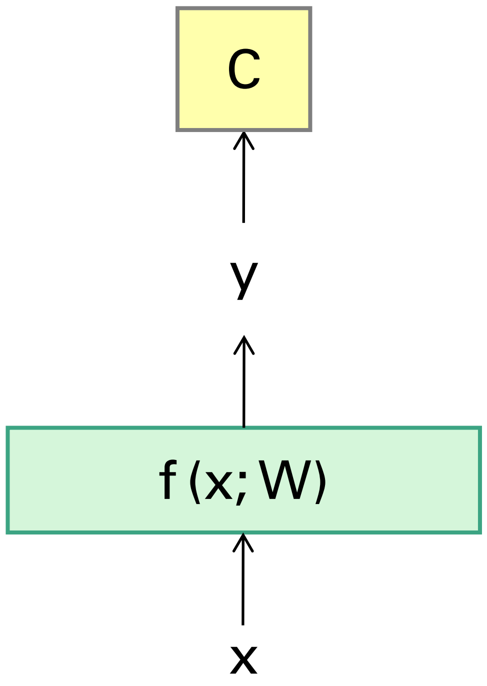
- RNNs can process the input sequence in forward and in the reverse direction



- Popular in speech recognition and machine translation

How to Train
Recurrent Neural Networks

BackPropagation Refresher



$$y = f(x;W)$$

$$C = \mathrm{Loss}(y, y_{GT})$$

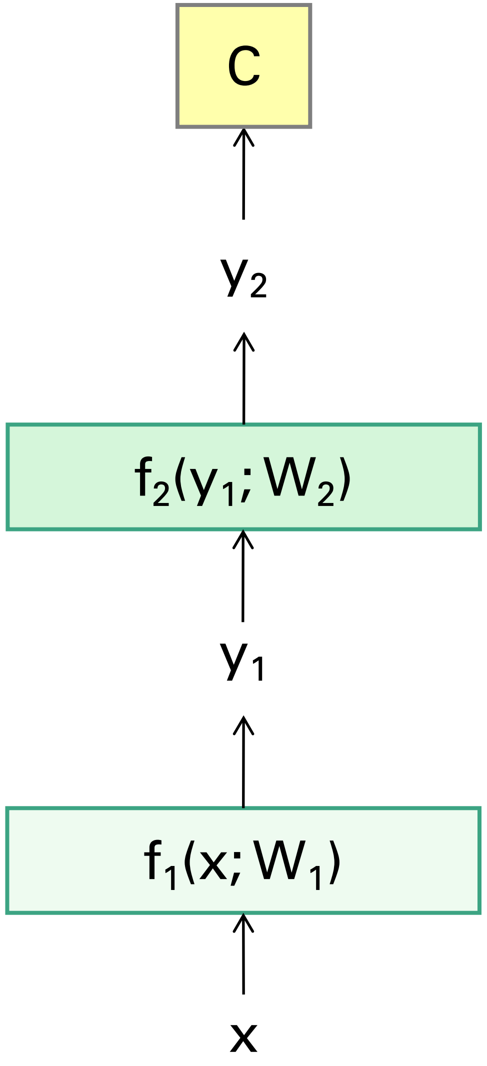
SGD Update

$$W \leftarrow W - \eta \frac{\partial C}{\partial W}$$

$$\frac{\partial C}{\partial W} = \left(\frac{\partial C}{\partial y}\right)\left(\frac{\partial y}{\partial W}\right)$$

Slide credit: Arun Mallya

Multiple Layers



$$y_1 = f_1(x; W_1)$$
$$y_2 = f_2(y_1; W_2)$$
$$C = \mathrm{Loss}(y_2, y_{GT})$$

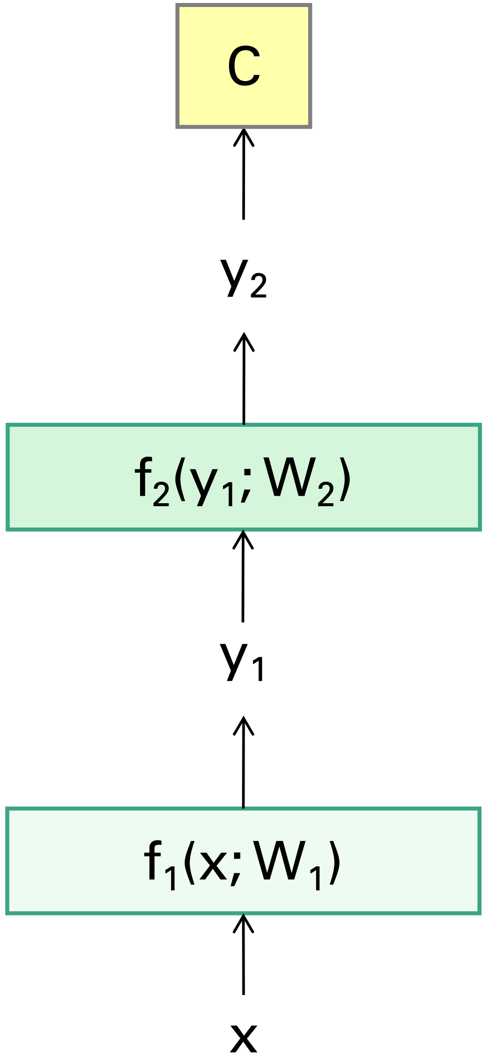
SGD Update

$$W_2 \leftarrow W_2 - \eta \frac{\partial C}{\partial W_2}$$

$$W_1 \leftarrow W_1 - \eta \frac{\partial C}{\partial W_1}$$

Slide credit: Arun Mallya

Chain Rule for Gradient Computation



$$y_1 = f_1(x; W_1)$$
$$y_2 = f_2(y_1; W_2)$$
$$C = \mathrm{Loss}(y_2, y_{GT})$$

Find $\dfrac{\partial C}{\partial W_1}, \dfrac{\partial C}{\partial W_2}$

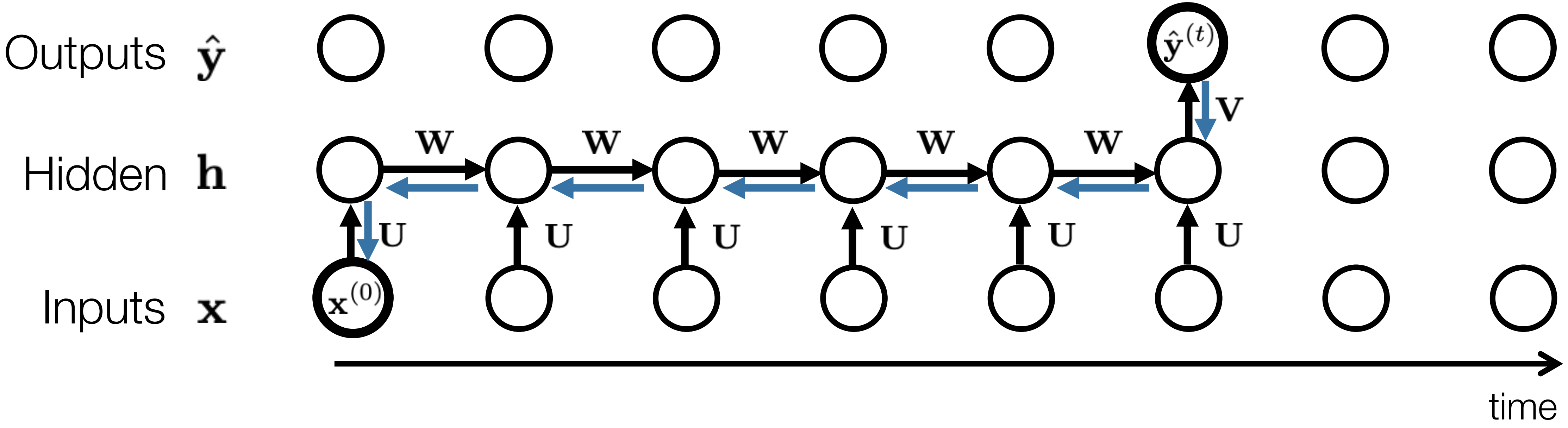
$$\frac{\partial C}{\partial W_2} = \left(\frac{\partial C}{\partial y_2}\right)\left(\frac{\partial y_2}{\partial W_2}\right)$$

$$\frac{\partial C}{\partial W_1} = \left(\frac{\partial C}{\partial y_1}\right)\left(\frac{\partial y_1}{\partial W_1}\right)$$
$$= \left(\frac{\partial C}{\partial y_2}\right)\left(\frac{\partial y_2}{\partial y_1}\right)\left(\frac{\partial y_1}{\partial W_1}\right)$$

Application of the Chain Rule

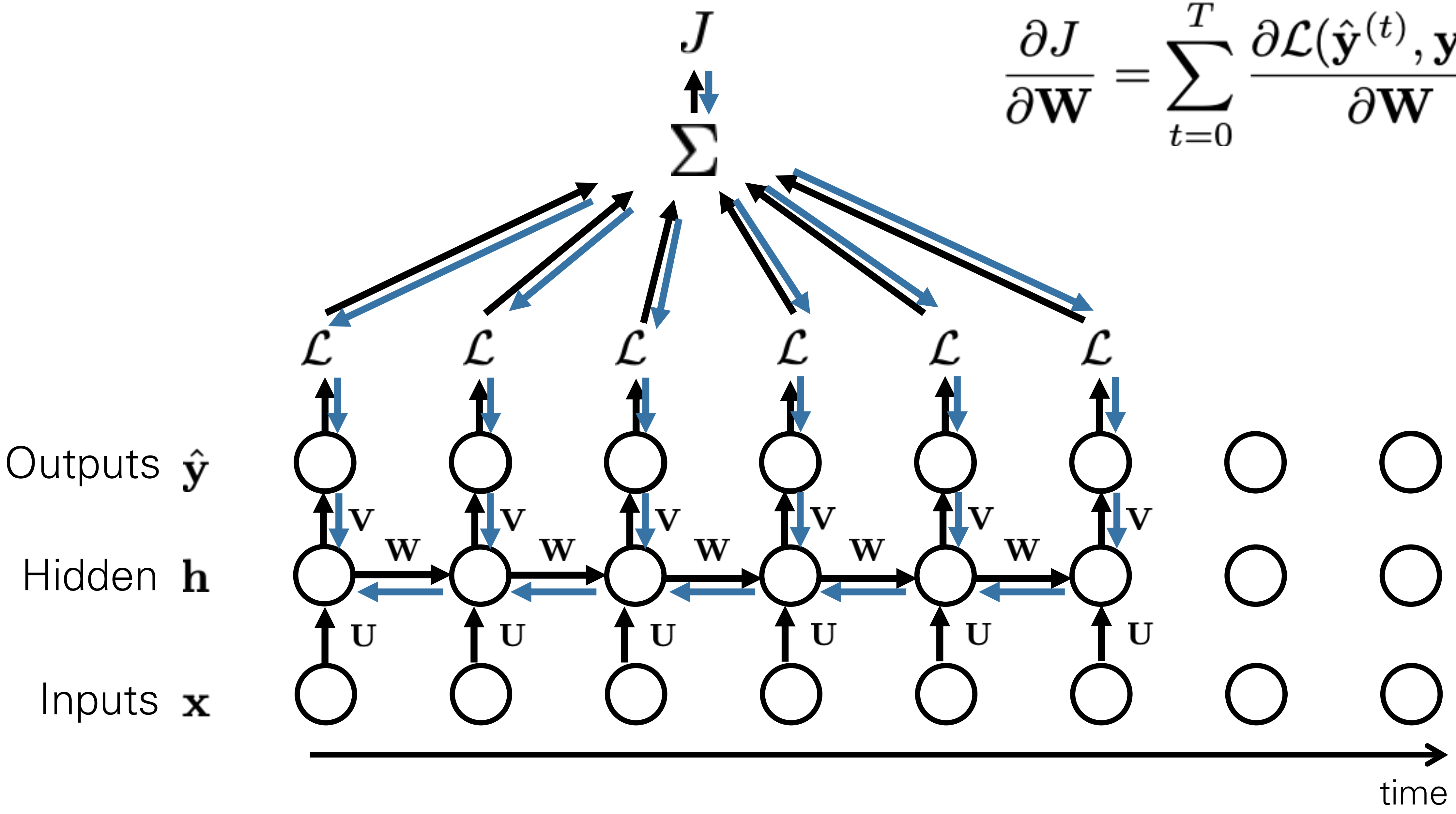
Slide credit: Arun Mallya

Backprop through time

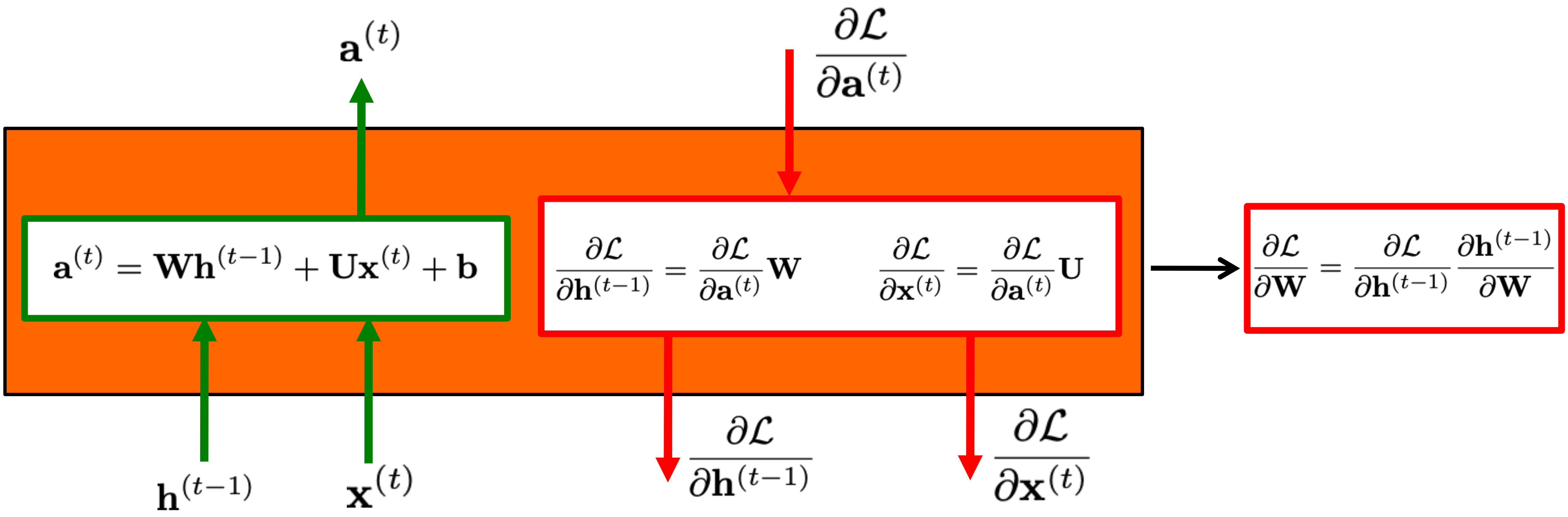


$$\frac{\partial \hat{\mathbf{y}}^{(t)}}{\partial \mathbf{x}^{(0)}} = \frac{\partial \hat{\mathbf{y}}^{(t)}}{\partial \mathbf{h}^{(t)}} \frac{\partial \mathbf{h}^{(t)}}{\partial \mathbf{h}^{(t-1)}} \cdots \frac{\partial \mathbf{h}^{(1)}}{\partial \mathbf{h}^{(0)}} \frac{\partial \mathbf{h}^{(0)}}{\partial \mathbf{x}^{(0)}}$$

$$\frac{\partial J}{\partial \mathbf{W}} = \sum_{t=0}^{T} \frac{\partial \mathcal{L}(\hat{\mathbf{y}}^{(t)}, \mathbf{y}^{(t)})}{\partial \mathbf{W}}$$



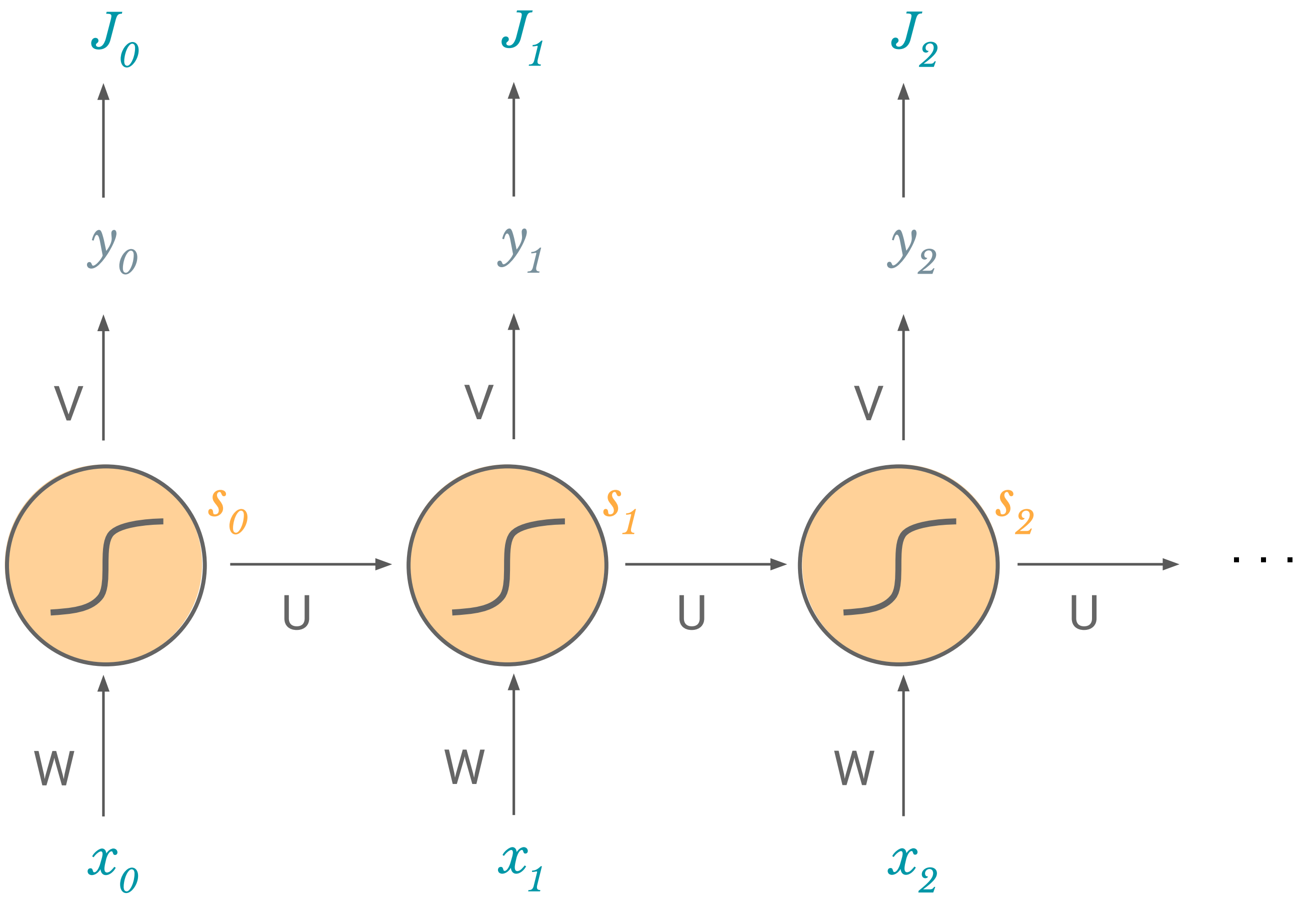
Recurrent linear layer



$$\frac{\partial J}{\partial \mathbf{W}} = \sum_{t=0}^{T} \frac{\partial \mathcal{L}(\hat{\mathbf{y}}^{(t)}, \mathbf{y}^{(t)})}{\partial \mathbf{W}}$$

We have a **loss at each timestep**:

(since we're making a prediction at each timestep)



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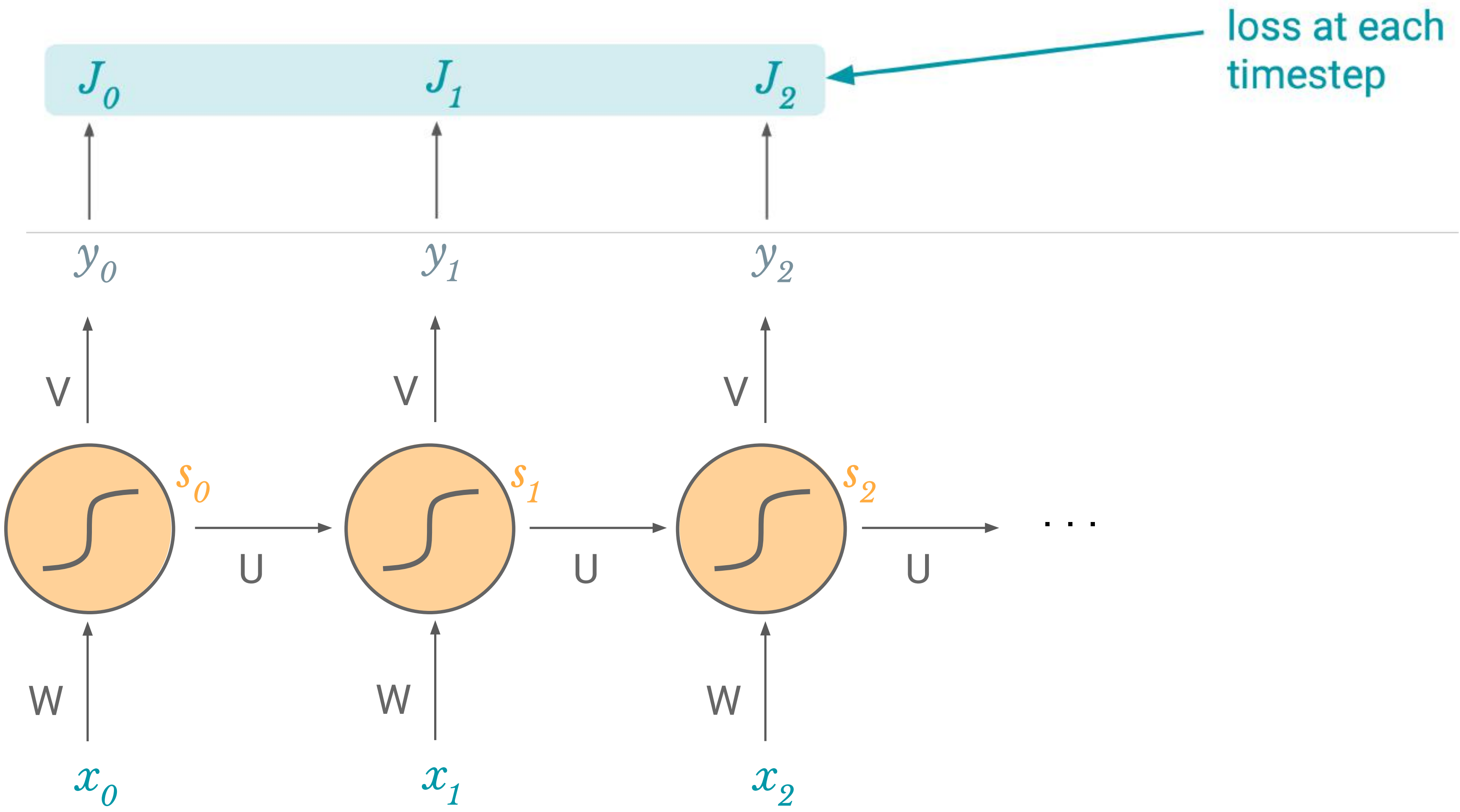
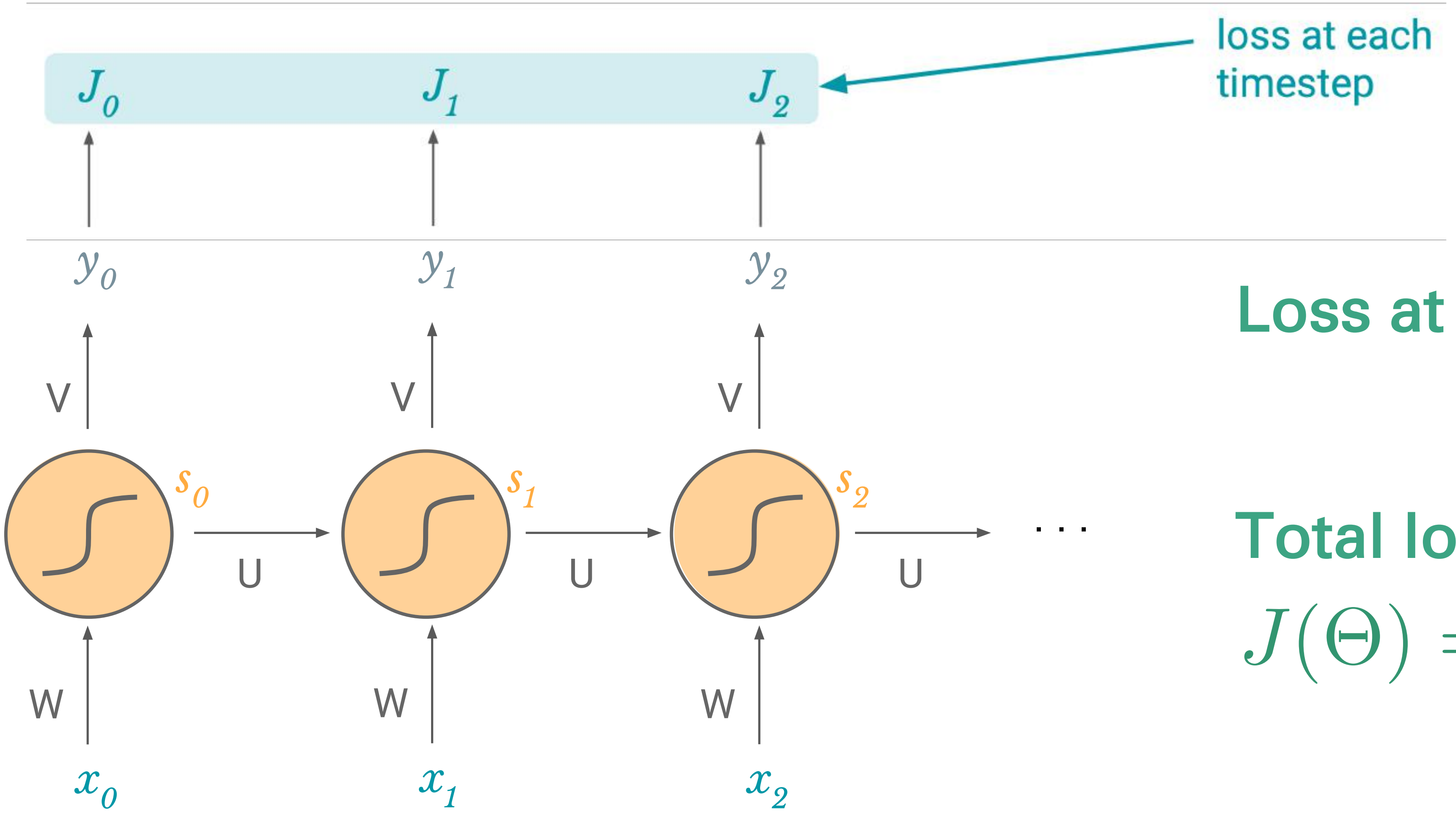
(since we're making a prediction at each timestep)



We **sum the losses** across time:

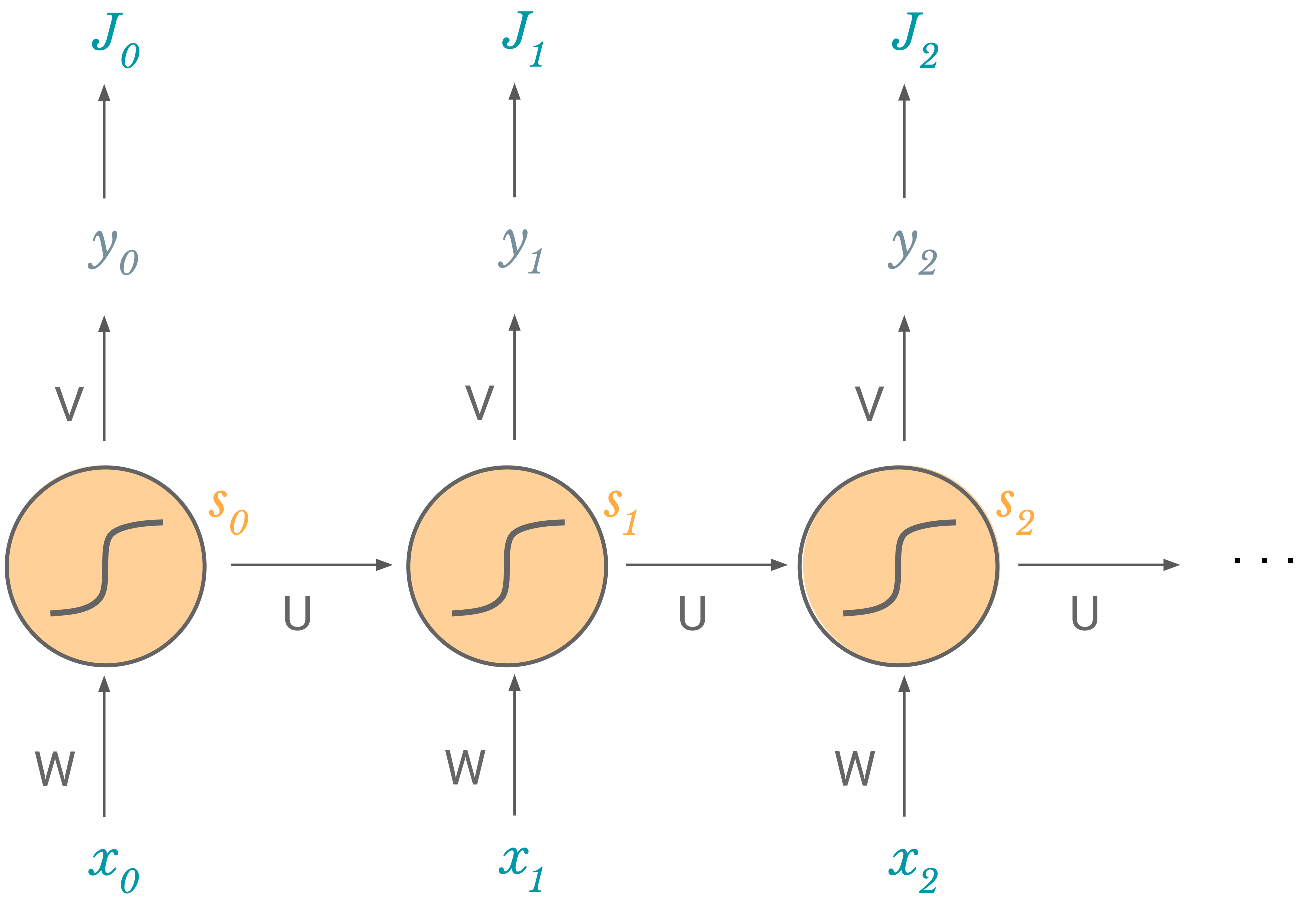


Loss at time t: $J_t(\Theta)$

Total loss:

$$J(\Theta) = \sum_t J_t(\Theta)$$

Let's try it our for W with the **chain rule:**



$$\frac{\partial J}{\partial W} = \sum_t \frac{\partial J_t}{\partial W}$$

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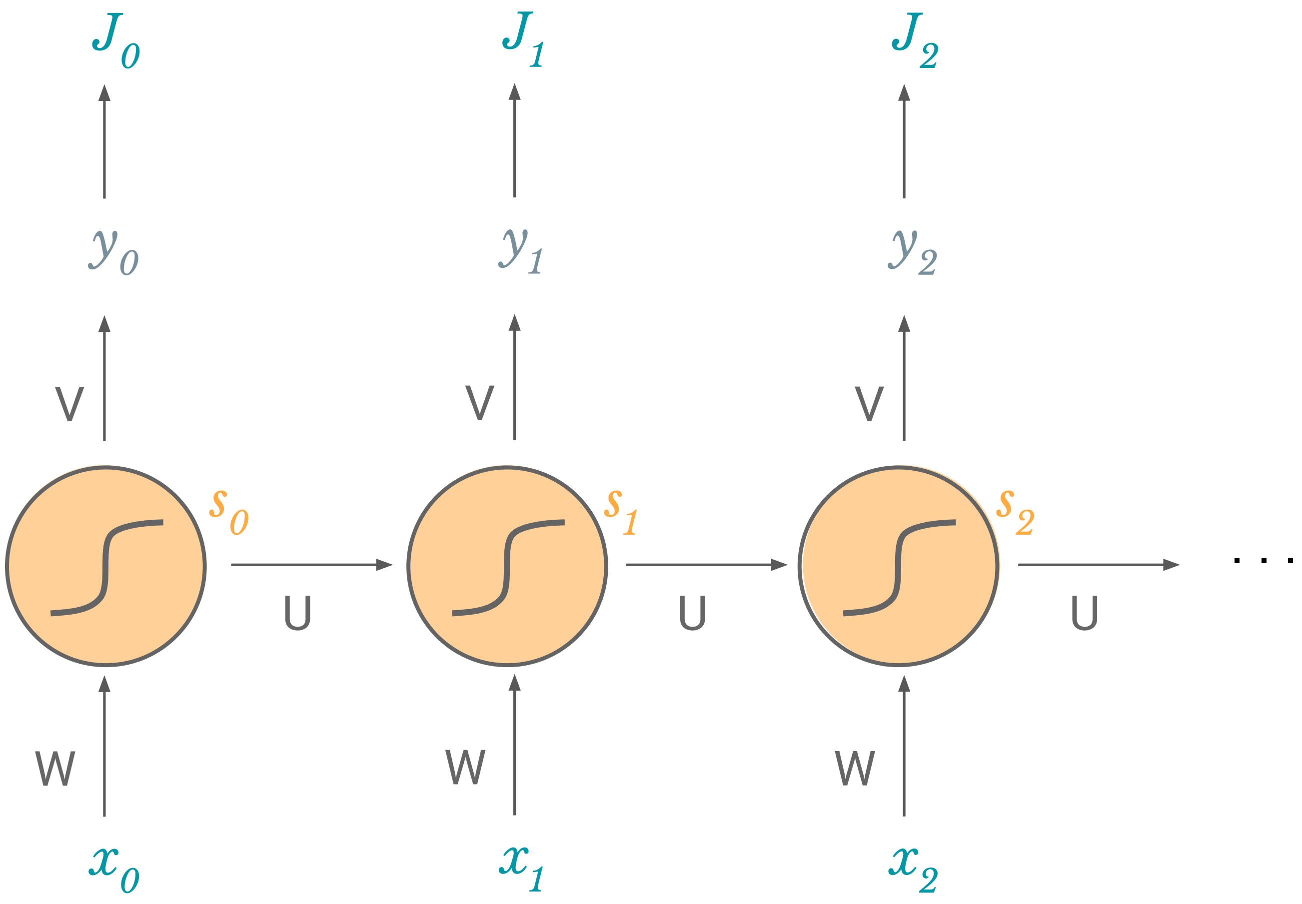

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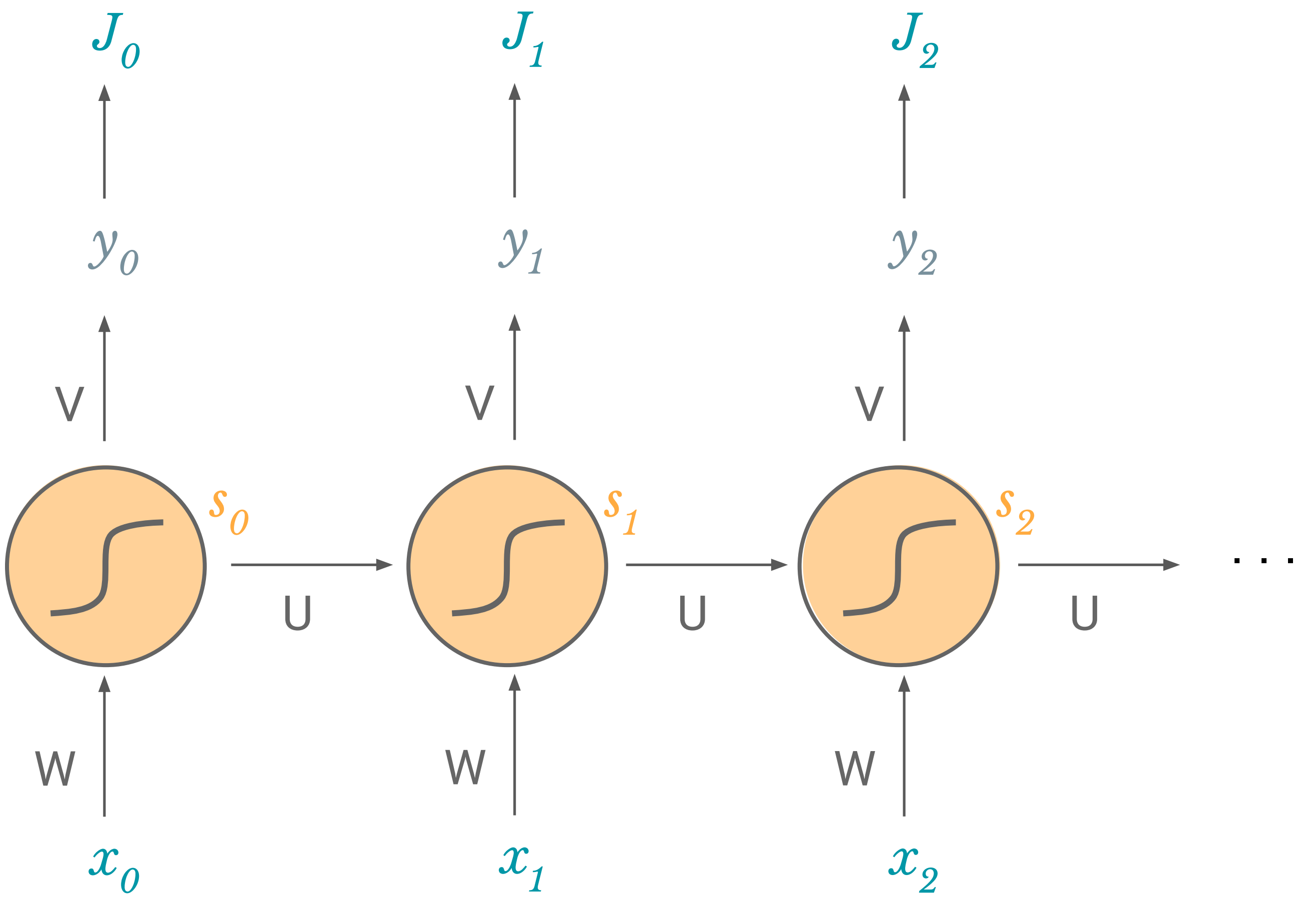
so let's take a single timestep t:

Let's try it our for W with the **chain rule:**

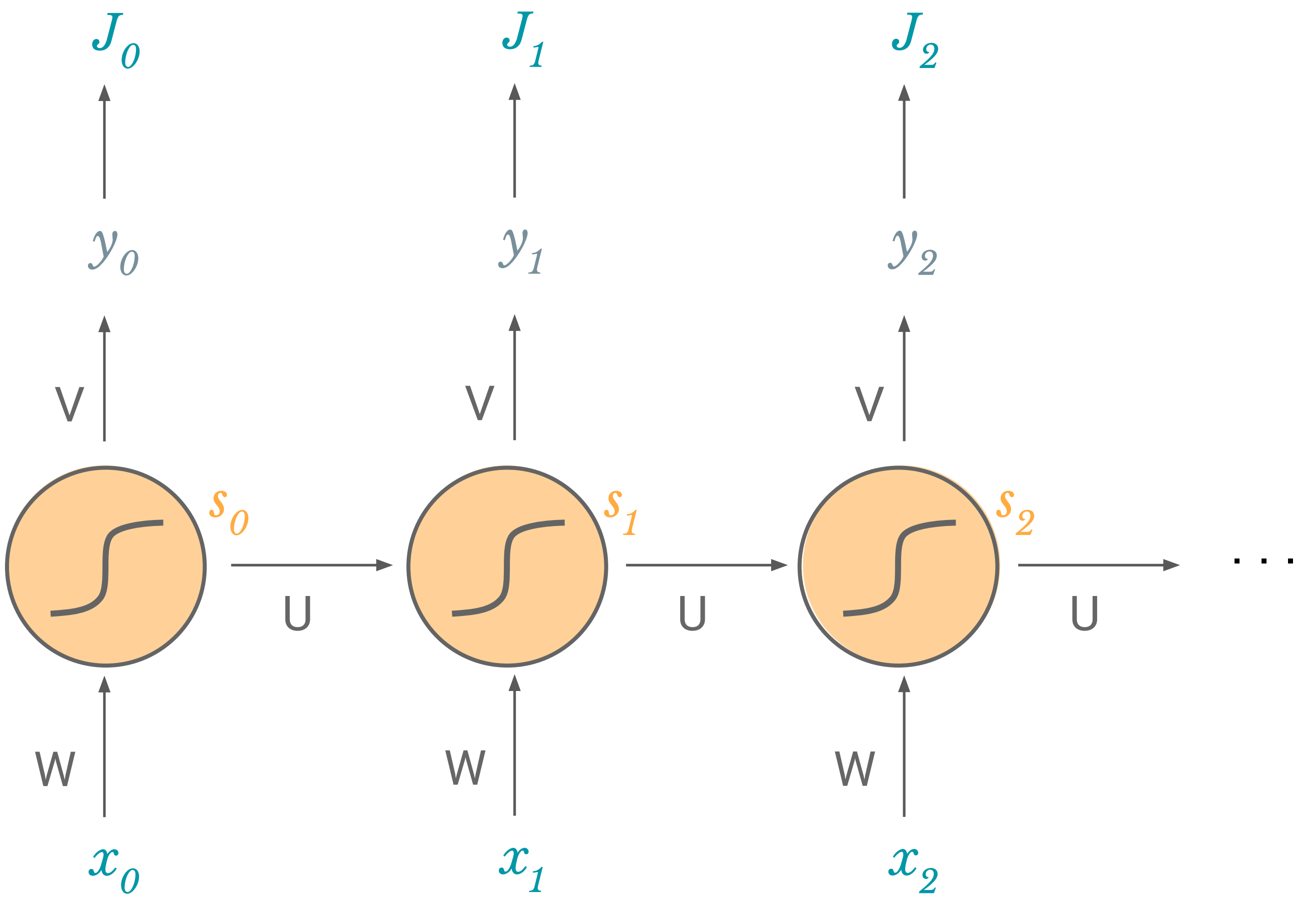


$$\frac{\partial J}{\partial W} = \sum_t \frac{\partial J_t}{\partial W}$$

so let's take a single timestep t:

$$\frac{\partial J_2}{\partial W}$$

Let's try it our for W with the **chain rule:**

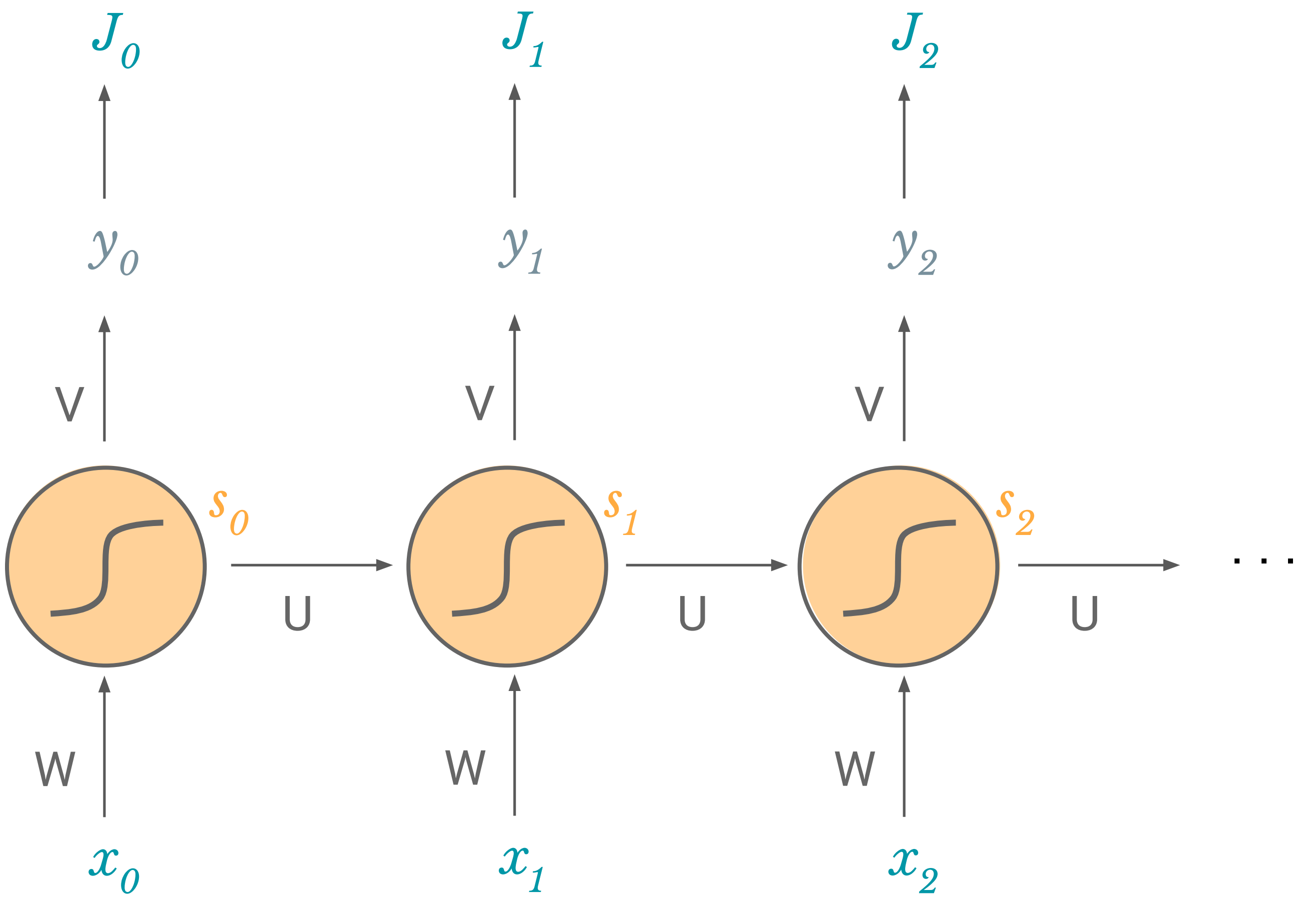


$$\frac{\partial J}{\partial W} = \sum_t \frac{\partial J_t}{\partial W}$$

so let's take a single timestep t:

$$\frac{\partial J_2}{\partial W} = \frac{\partial J_2}{\partial y2}$$

Let's try it our for W with the **chain rule:**

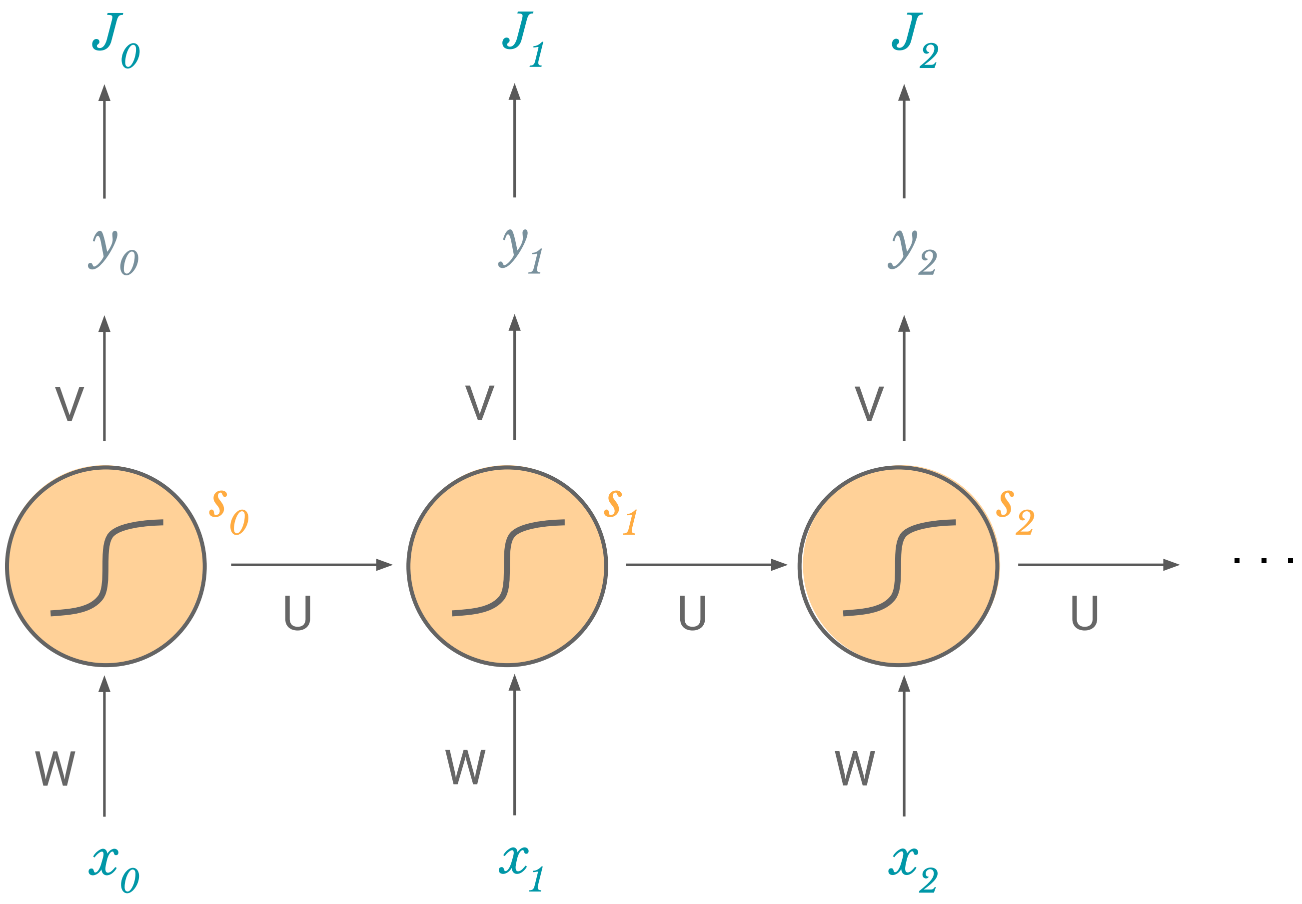


$$\frac{\partial J}{\partial W} = \sum_t \frac{\partial J_t}{\partial W}$$

so let's take a single timestep t:

$$\frac{\partial J_2}{\partial W} = \frac{\partial J_2}{\partial y2} \frac{\partial y_2}{\partial s_2}$$

Let's try it our for W with the **chain rule:**

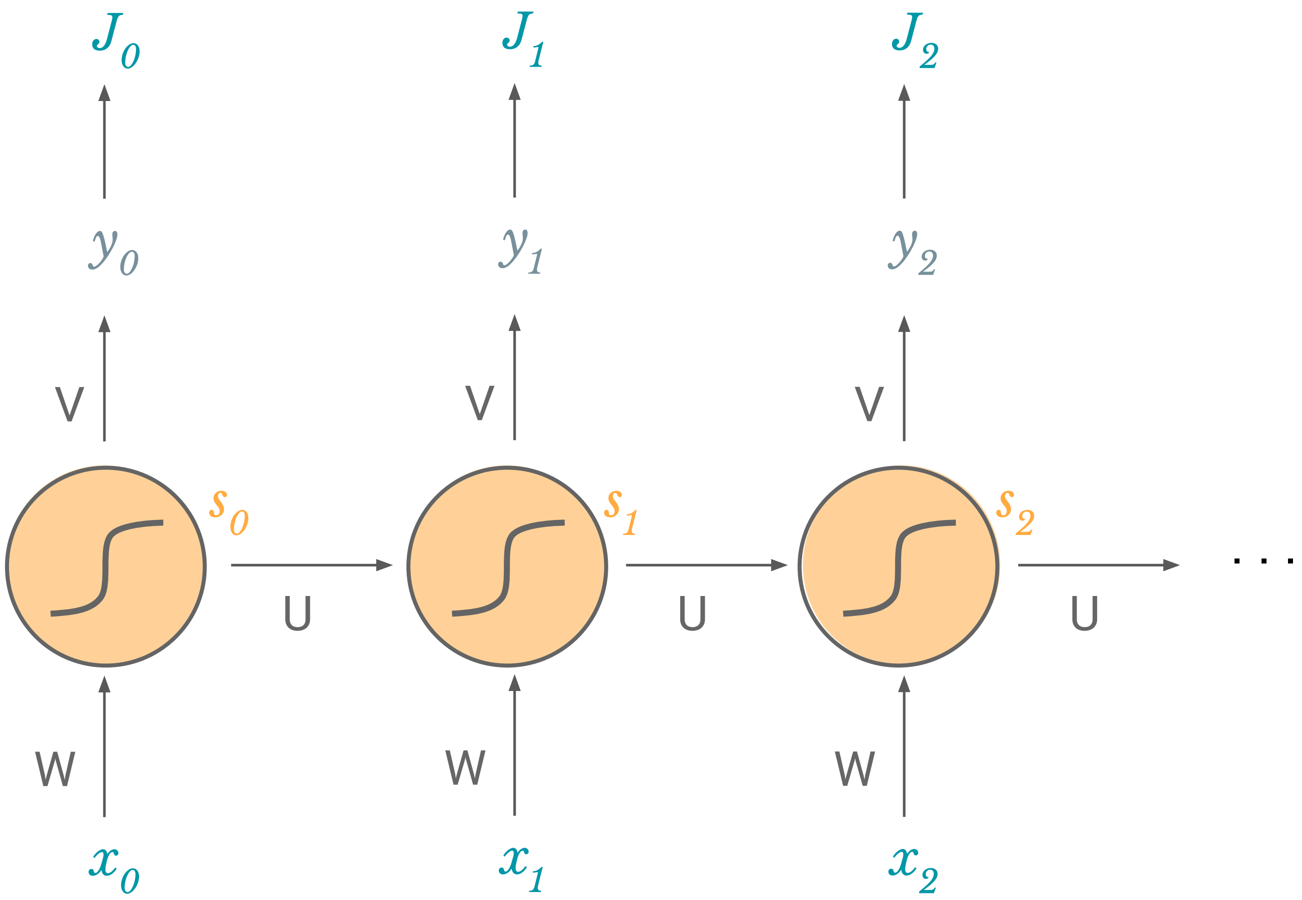


$$\frac{\partial J}{\partial W} = \sum_t \frac{\partial J_t}{\partial W}$$

so let's take a single timestep t:

$$\frac{\partial J_2}{\partial W} = \frac{\partial J_2}{\partial y2} \frac{\partial y_2}{\partial s_2} \frac{\partial s_2}{\partial W}$$

Let's try it our for W with the **chain rule:**



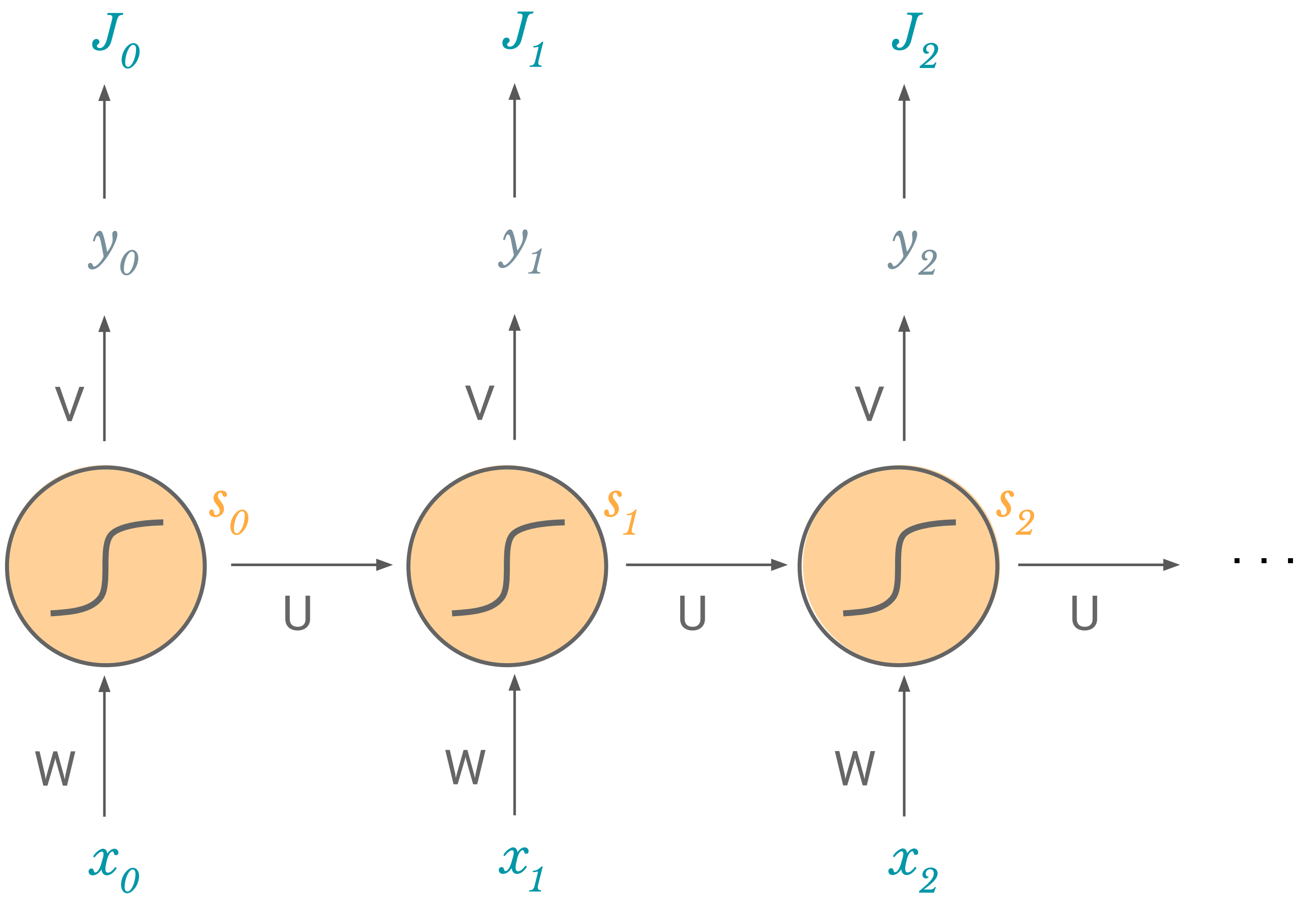
$$\frac{\partial J}{\partial W} = \sum_t \frac{\partial J_t}{\partial W}$$

so let's take a single timestep t:

$$\frac{\partial J_2}{\partial W} = \frac{\partial J_2}{\partial y2}\frac{\partial y_2}{\partial s_2}\boxed{\frac{\partial s_2}{\partial W}}$$

but wait…

Let's try it our for W with the **chain rule:**



$$\frac{\partial J}{\partial W} = \sum_t \frac{\partial J_t}{\partial W}$$

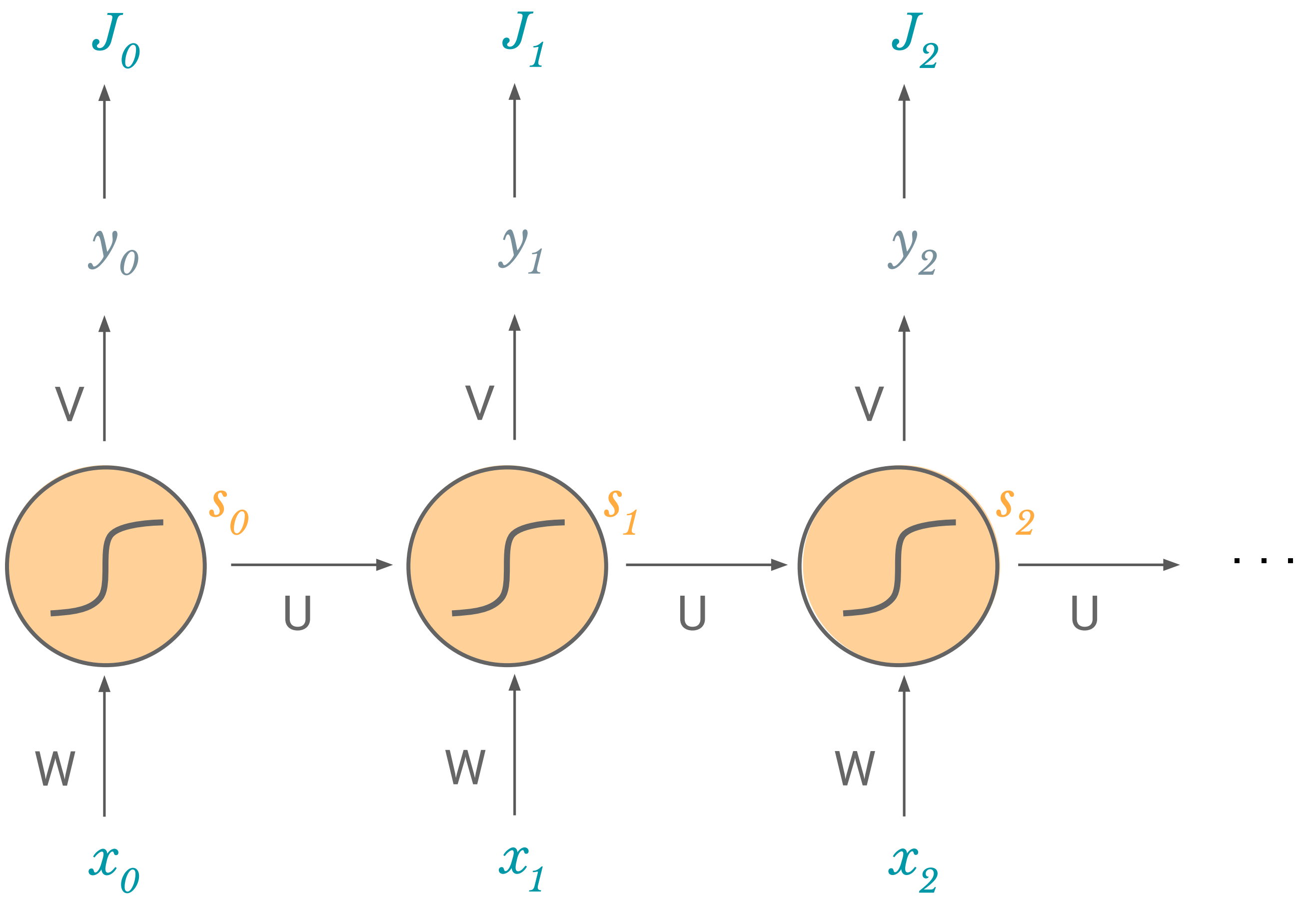
so let's take a single timestep t:

$$\frac{\partial J_2}{\partial W} = \frac{\partial J_2}{\partial y2}\frac{\partial y_2}{\partial s_2}\boxed{\frac{\partial s_2}{\partial W}}$$

but wait…

$$s_2 = tanh(Us_1 + Wx_2)$$

Let's try it our for W with the **chain rule:**



$$\frac{\partial J}{\partial W} = \sum_t \frac{\partial J_t}{\partial W}$$

so let's take a single timestep t:

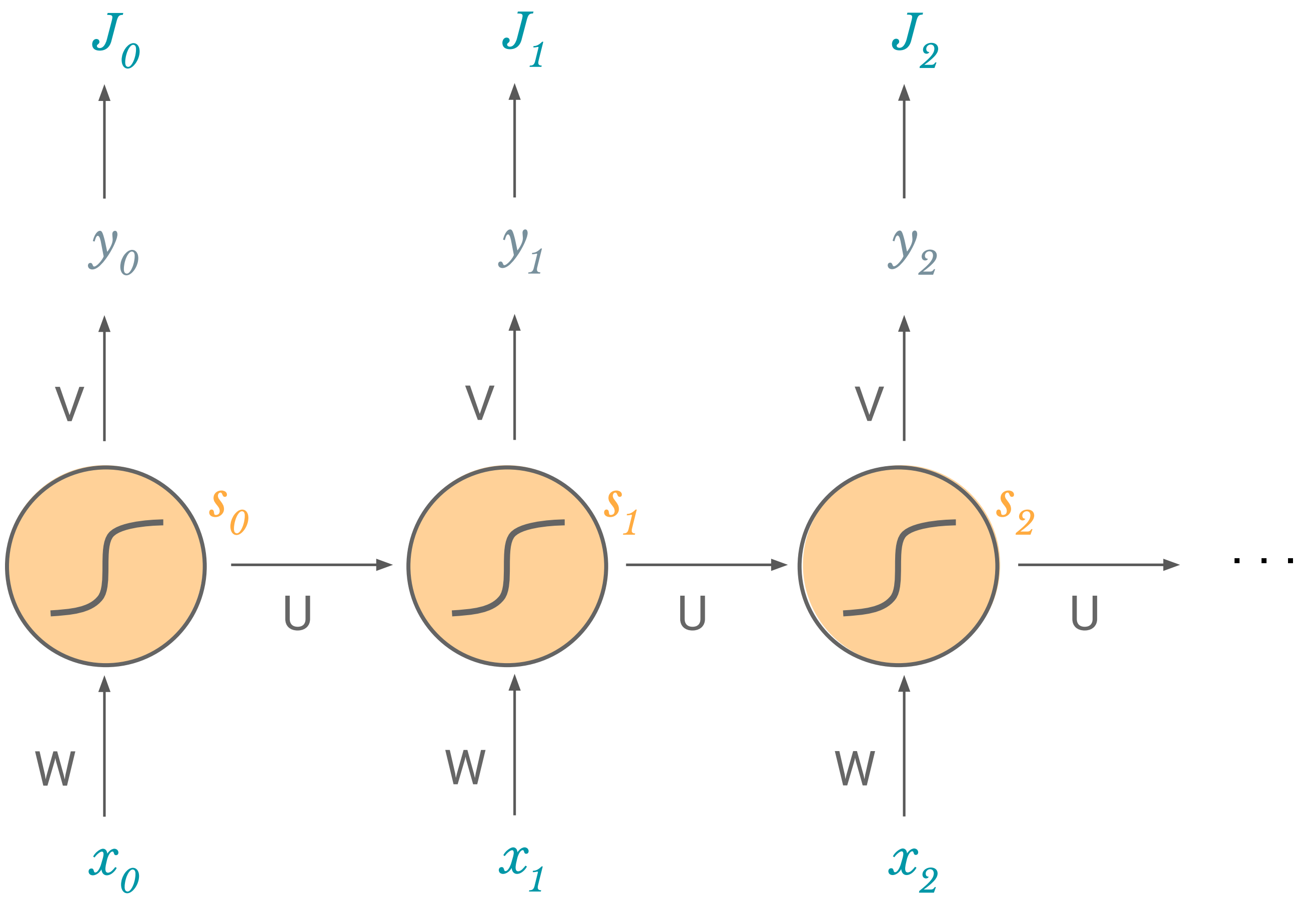
$$\frac{\partial J_2}{\partial W} = \frac{\partial J_2}{\partial y2} \frac{\partial y_2}{\partial s_2} \boxed{\frac{\partial s_2}{\partial W}}$$

but wait…

$$s_2 = tanh(U \boxed{s_1} + W x_2)$$

s_1 also depends on W so we can't just treat $\frac{\partial s_2}{\partial W}$ as a constant!

Let's try it our for W with the **chain rule:**



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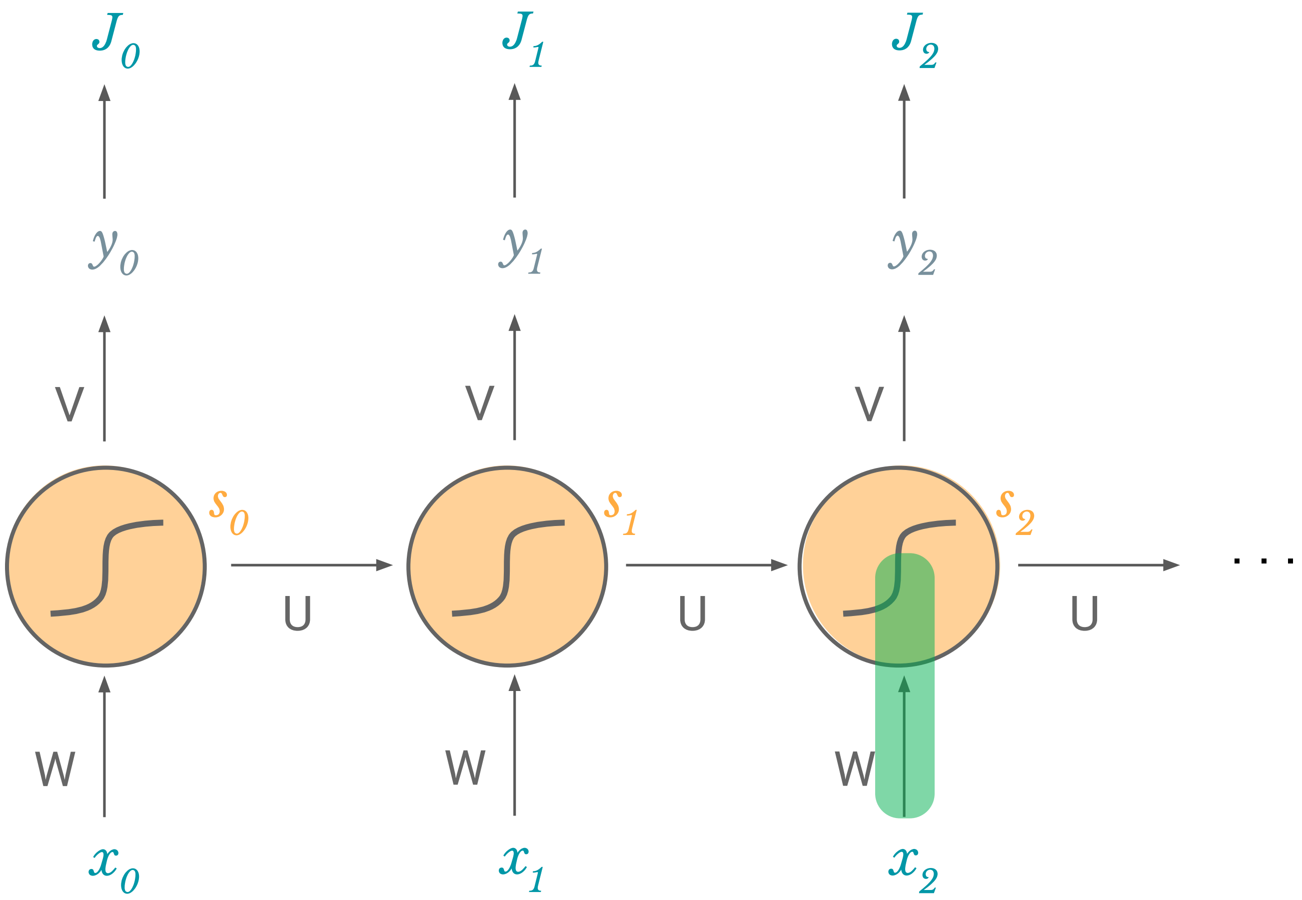
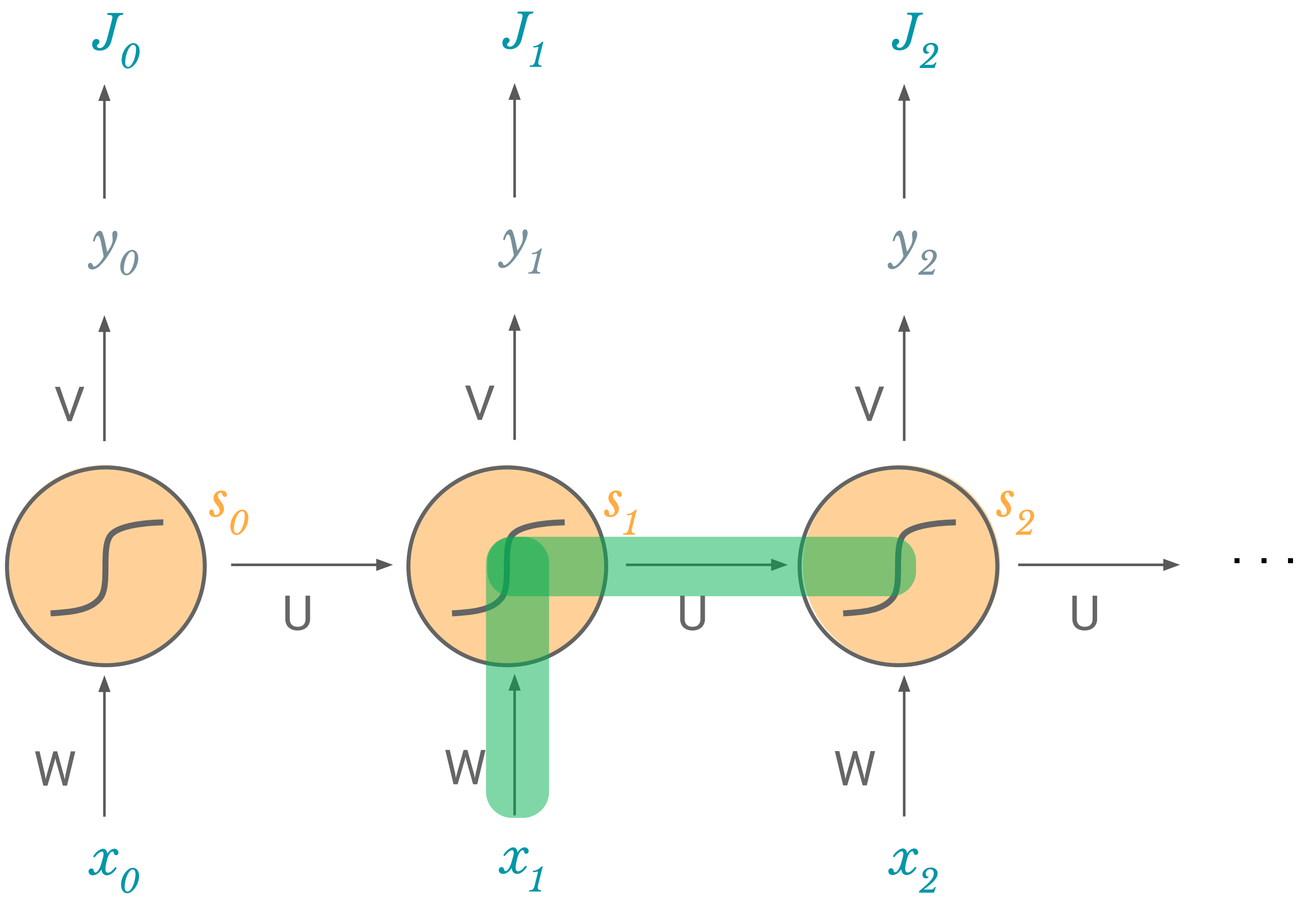


$$\frac{\partial s_2}{\partial W}$$

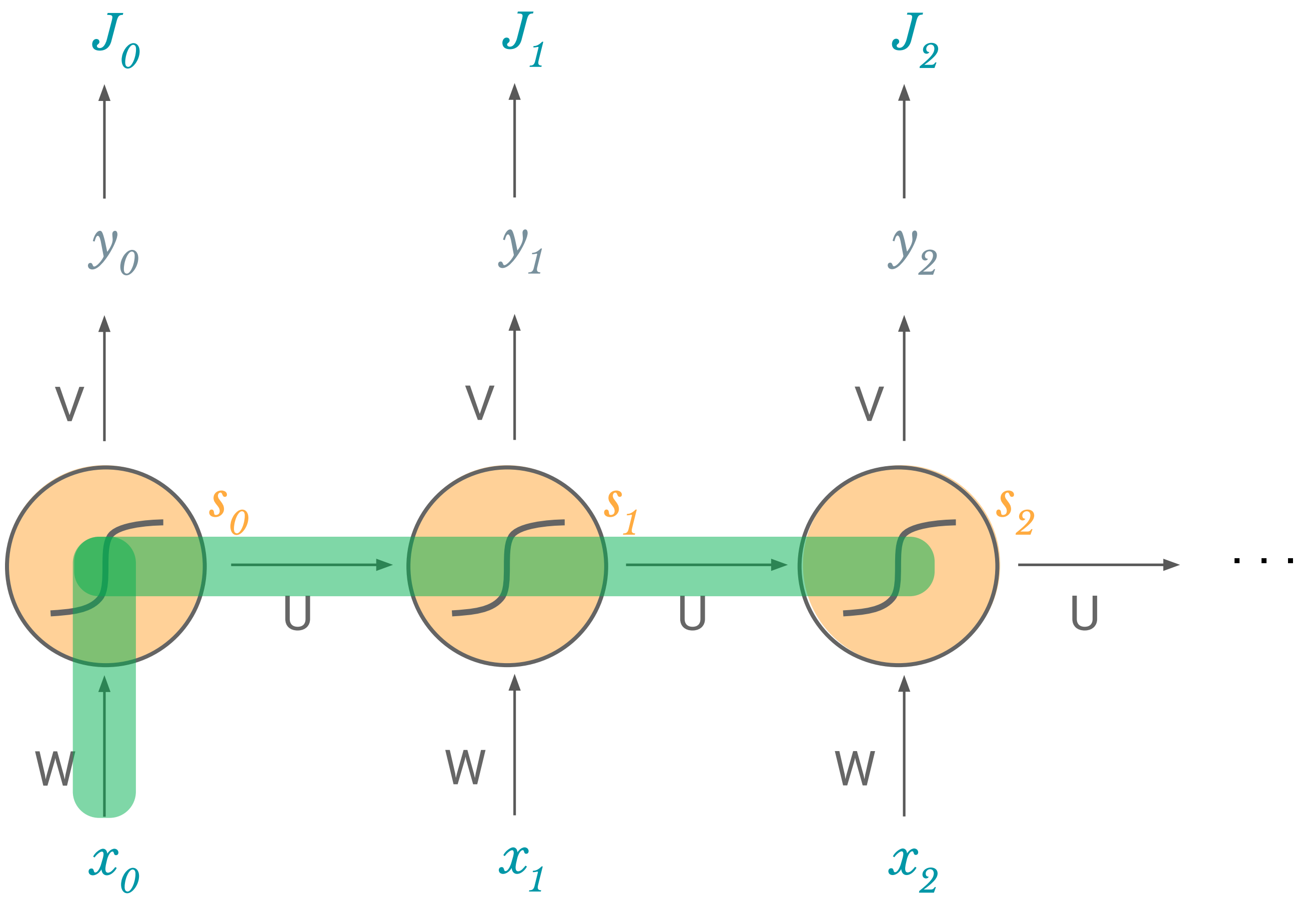
Let's try it our for W with the **chain rule:**



$$\frac{\partial s_2}{\partial W}$$

$$+\frac{\partial s_2}{\partial s_1}\frac{\partial s_1}{\partial W}$$

Let's try it our for W with the **chain rule:**



$$\frac{\partial s_2}{\partial W} + \frac{\partial s_2}{\partial s_1}\frac{\partial s_1}{\partial W} + \frac{\partial s_2}{\partial s_0}\frac{\partial s_0}{\partial W}$$

Backpropagation through time:

$$\frac{\partial J_2}{\partial W} = \sum_{k=0}^{2} \frac{\partial J_2}{\partial y_2} \frac{\partial y_2}{\partial s_2} \underbrace{\frac{\partial s_2}{\partial s_k} \frac{\partial s_k}{\partial W}}_{\substack{\text{Contributions of } W \text{ in previous} \\ \text{timesteps to the error at timestep } t}}$$

Backpropagation through time:

$$\frac{\partial J_t}{\partial W} = \sum_{k=0}^{t} \frac{\partial J_t}{\partial y_t} \frac{\partial y_t}{\partial s_t} \underbrace{\frac{\partial s_t}{\partial s_k} \frac{\partial s_k}{\partial W}}$$

Contributions of W in previous timesteps to the error at timestep t

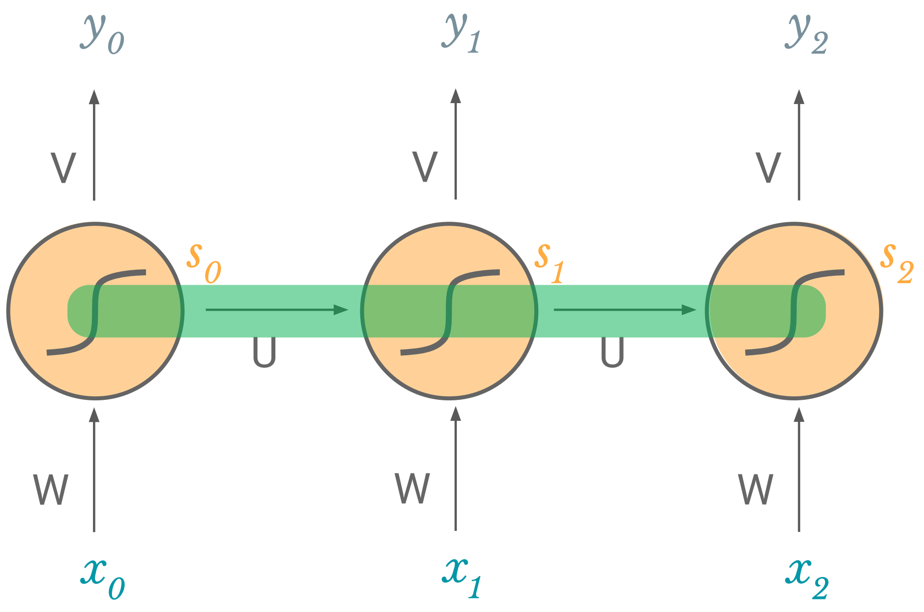
Why are RNNs hard to train?

Vanishing Gradient Problem

$$\frac{\partial J_2}{\partial W} = \sum_{k=0}^{2} \frac{\partial J_2}{\partial y_2} \frac{\partial y_2}{\partial s_2} \boxed{\frac{\partial s_2}{\partial s_k}} \frac{\partial s_k}{\partial W}$$

Vanishing Gradient Problem

$$\frac{\partial J_2}{\partial W} = \sum_{k=0}^{2} \frac{\partial J_2}{\partial y_2} \frac{\partial y_2}{\partial s_2} \boxed{\frac{\partial s_2}{\partial s_k}} \frac{\partial s_k}{\partial W}$$



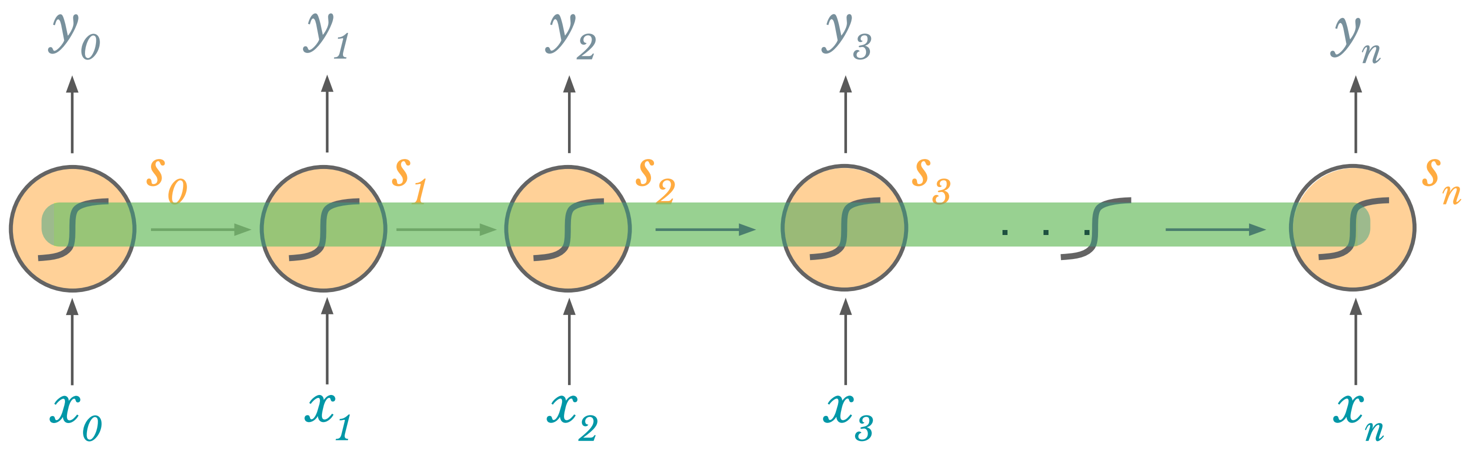
at k=0: $\boxed{\frac{\partial s_2}{\partial s_0} = \frac{\partial s_2}{\partial s_1} \frac{\partial s_1}{\partial s_0}}$

Vanishing Gradient Problem

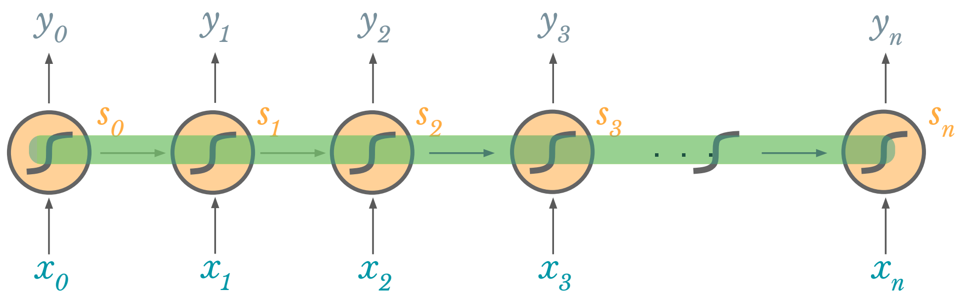
$$\frac{\partial J_n}{\partial W} = \sum_{k=0}^{n} \frac{\partial J_n}{\partial y_n} \frac{\partial y_n}{\partial s_n} \boxed{\frac{\partial s_n}{\partial s_k}} \frac{\partial s_k}{\partial W}$$

$$\boxed{\frac{\partial s_n}{\partial s_{n-1}} \frac{\partial s_{n-1}}{\partial s_{n-2}} \cdots \frac{\partial s_3}{\partial s_2} \frac{\partial s_2}{\partial s_1} \frac{\partial s_1}{\partial s_0}}$$

as the gap between timesteps gets bigger, this product gets longer and longer!



Vanishing Gradient Problem



what are each of these terms?

$$\frac{\partial s_n}{\partial s_{n-1}} \frac{\partial s_{n-1}}{\partial s_{n-2}} \cdots \frac{\partial s_3}{\partial s_2} \frac{\partial s_2}{\partial s_1} \frac{\partial s_1}{\partial s_0}$$

$$\frac{\partial s_n}{\partial s_{n-1}} = W^T diag\left[f'(W_{s_{j-1}+Ux_j})\right]$$

W = sampled from standard normal distribution = mostly < 1

f = tanh or sigmoid so f' < 1

we're multiplying a lot of **small numbers** together.

Vanishing Gradient Problem

we're multiplying a lot of **small numbers** together.

so what?

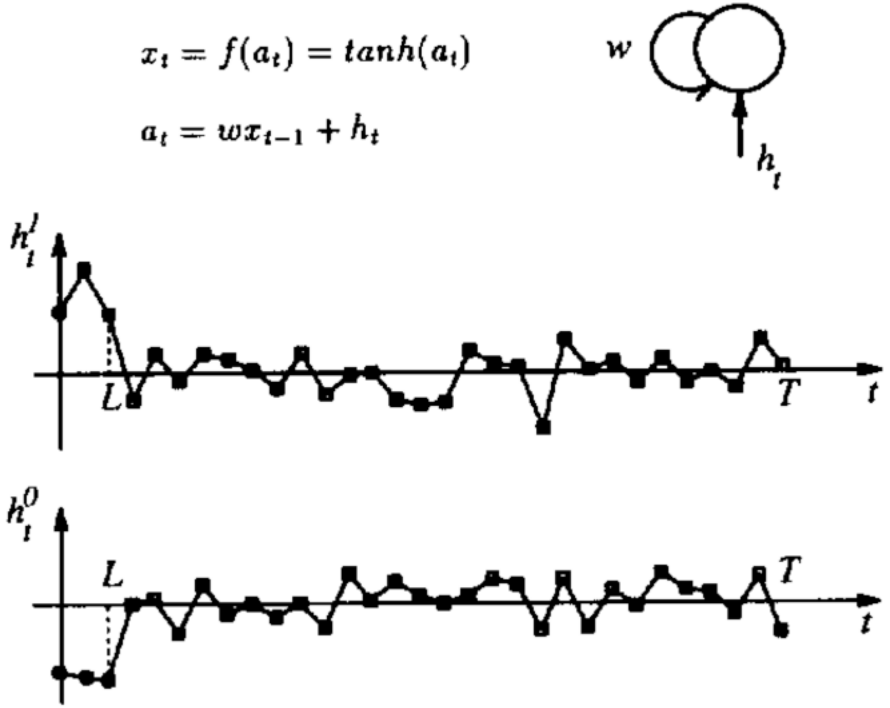
errors due to further back timesteps have increasingly **smaller gradients**.

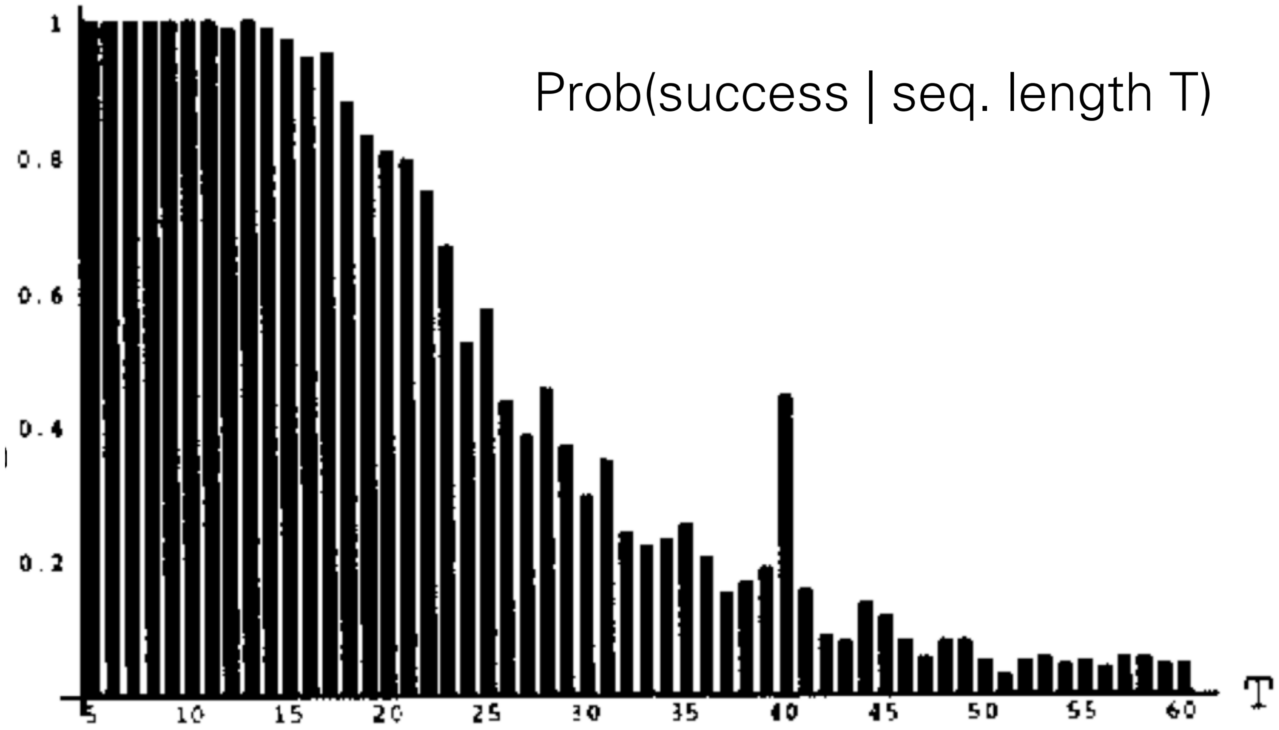
so what?

parameters become biased to **capture shorter-term** dependencies.

A Toy Example

- 2 categories of sequences
- Can the single tanh unit learn to store for T time steps 1 bit of information given by the sign of initial input?





Vanishing Gradient Problem

"In France, I had a great time and I learnt some of the _____ language."

our parameters are not trained to capture long-term dependencies, so the word we predict will mostly depend on the previous few words, not much earlier ones

Long-Term Dependencies

- The RNN gradient is a product of Jacobian matrices, each associated with a step in the forward computation. To store information robustly in a finite-dimensional state, the dynamics must be contractive [Bengio et al 1994].

$$L = L(s_T(s_{T-1}(\ldots s_{t+1}(s_t, \ldots))))$$

$$\frac{\partial L}{\partial s_t} = \frac{\partial L}{\partial s_T} \frac{\partial s_T}{\partial s_{T-1}} \cdots \frac{\partial s_{t+1}}{\partial s_t}$$

- Problems:
  - sing. values of Jacobians > 1 → **gradients explode**
  - or sing. values < → **gradients shrink & vanish**
  - or random → **variance grows exponentially**

Slide credit: Yoshua Bengio

RNN Tricks

(Pascanu et al., 2013; Bengio et al., 2013; Gal and Ghahramani, 2016;Morishita et al., 2017)

- Mini-batch creation strategies (efficient computations)
- Clipping gradients (avoid exploding gradients)
- Leaky integration (propagate long-term dependencies)
- Momentum (cheap 2nd order)
- Dropout (avoid overfitting)
- Initialization (start in right ballpark avoids exploding/vanishing)
- Sparse Gradients (symmetry breaking)
- Gradient propagation regularizer (avoid vanishing gradient)
- Gated self-loops (LSTM & GRU, reduces vanishing gradient)

Slide adapted from Yoshua Bengio

Mini-batching in RNNs

- Mini-batching makes things much faster!
- But mini-batching in RNNs is harder than in feed-forward networks
  - Each word depends on the previous word
  - Sequences are of various length
- Padding:

this	is	an	example	</s>
this	is	another	</s>	**</s>**

- If we use sentences of different lengths, too much padding and sorting can **result in decreased performance**
- To remedy this: **sort sentences** so similarly-lengthed seqs are in the same batch

Slide adapted from Graham Neubig

Mini-batching in RNNs

- Many alternatives:
  1. Shuffle the corpus randomly before creating mini-batches (with no sorting).
  2. Sort based on the source sequence length.
  3. Sort based on the target sequence length.
  4. Sort using the source sequence length, break ties by sorting by target sequence length.
  5. Sort using the target sequence length, break ties by sorting by source sequence length.

Algorithm 1 Create mini-batches

$\boldsymbol{C} \leftarrow$ Training corpus
$\boldsymbol{C} \leftarrow \mathrm{sort}(\boldsymbol{C})$ or $\mathrm{shuffle}(\boldsymbol{C})$ ▷ sort or shuffle the whole corpus
$\boldsymbol{B} \leftarrow \{\}$ ▷ mini-batches
$i \leftarrow 0,\ j \leftarrow 0$
while $i < \boldsymbol{C}$.size() **do**
  $\boldsymbol{B}[j] \leftarrow \boldsymbol{B}[j] + \boldsymbol{C}[i]$
  if $\boldsymbol{B}[j]$.size() $\geq$ max mini-batch size **then**
    $\boldsymbol{B}[j] \leftarrow \mathrm{padding}(\boldsymbol{B}[j])$ ▷ Padding tokens to the longest sentence in the mini-batch
    $j \leftarrow j + 1$
  end if
  $i \leftarrow i + 1$
end while
$\boldsymbol{B} \leftarrow \mathrm{shuffle}(\boldsymbol{B})$ ▷ shuffle the order of the mini-batches

M. Morishita, Y. Oda, G. Neubig, K. Yoshino, K. Sudoh, and S. Nakamura. **"An Empirical Study of Mini-Batch Creation Strategies for Neural Machine Translation"**. 1st Workshop on NMT 2017

Mini-batching in RNNs

- Many
  1. Sh
     mi
  2. So
  3. So
  4. So
     tie
  5. So
     tie

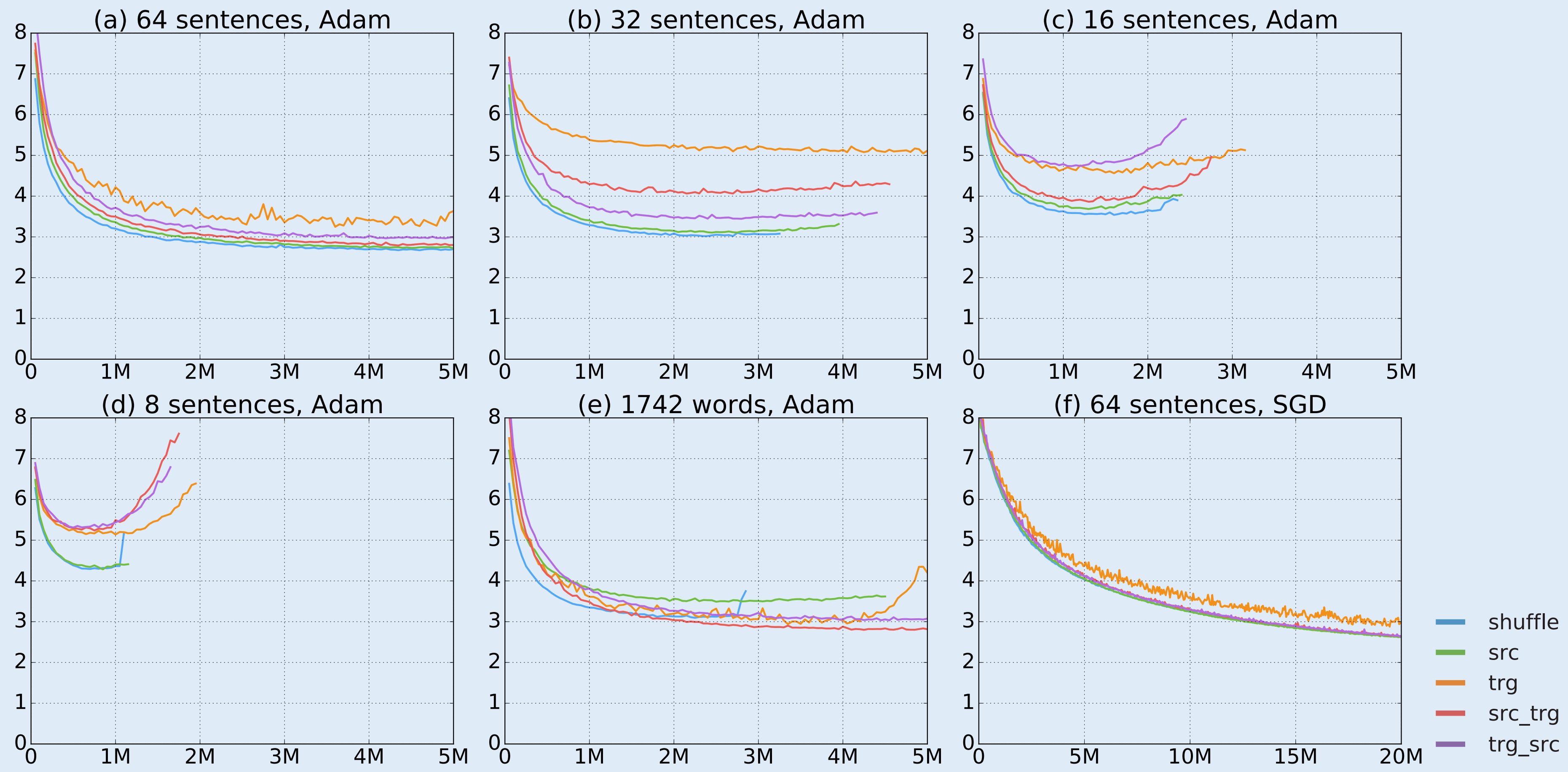
rt or shuffle

nini-batches

ch size **then** ▷

tence in the

order of the



- **May affect performance!**

M. Morishita, Y. Oda, G. Neubig, K. Yoshino, K. Sudoh, and S. Nakamura. **"An Empirical Study of Mini-Batch Creation Strategies for Neural Machine Translation"**. 1st Workshop on NMT 2017

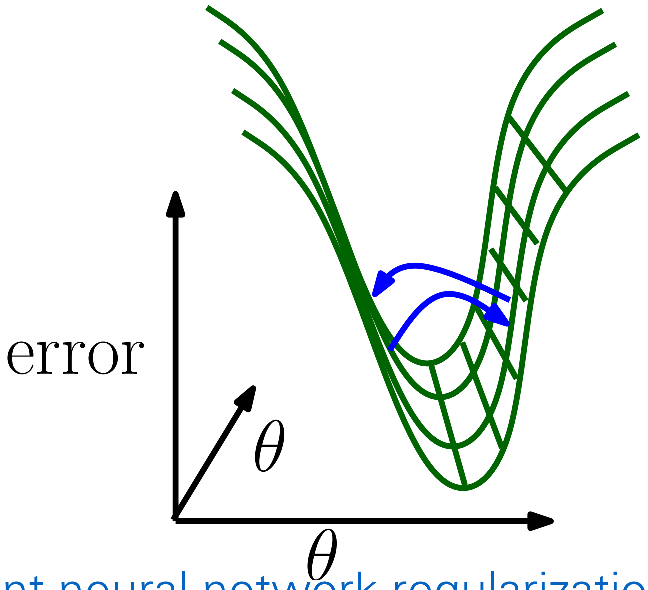
Gradient Norm Clipping

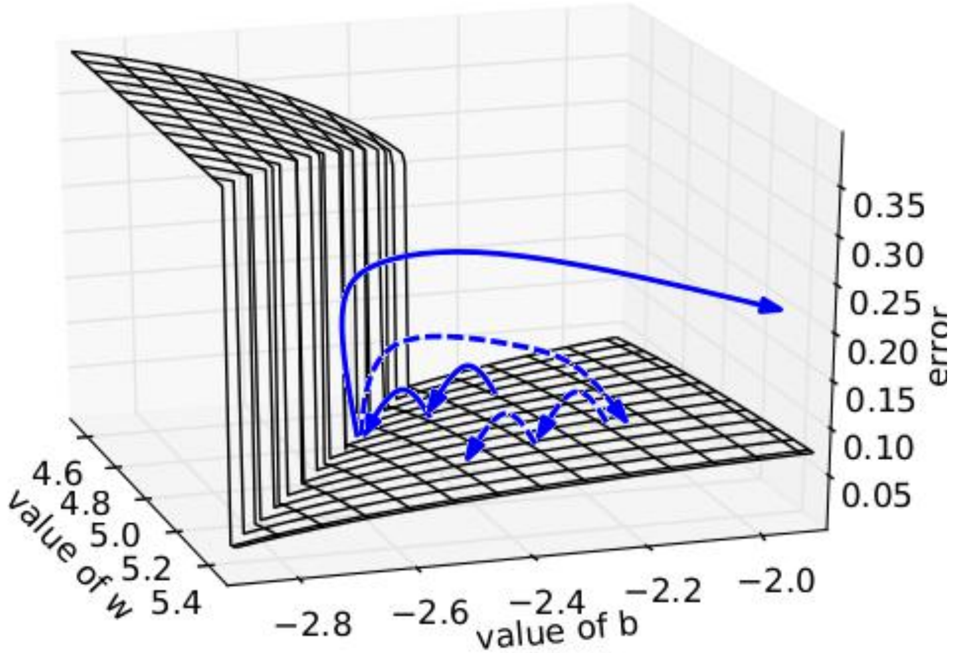
$$\hat{\mathbf{g}} \leftarrow \frac{\partial error}{\partial \theta}$$

if $\|\hat{\mathbf{g}}\| \geq threshold$ **then**

$$\quad \hat{\mathbf{g}} \leftarrow \frac{threshold}{\|\hat{\mathbf{g}}\|} \hat{\mathbf{g}}$$

end if





[Recurrent neural network regularization. Zaremba et al., arXiv 2014.]

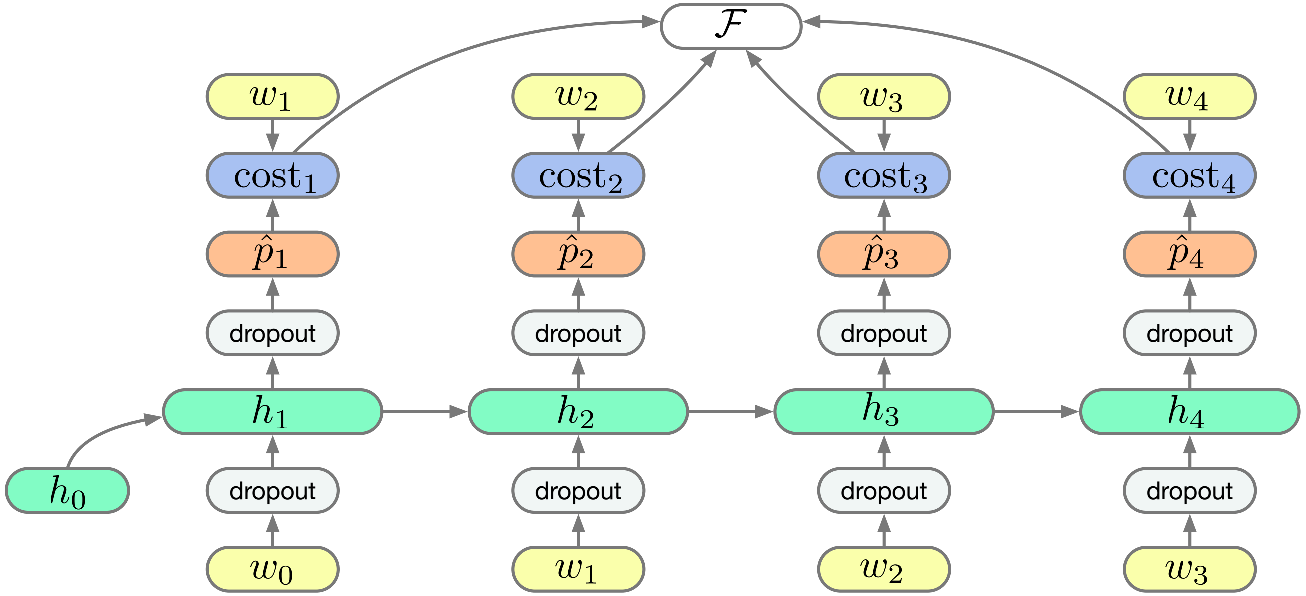
Regularization: Dropout

- Large recurrent networks often overfit their training data by memorizing the sequences observed. Such models generalize poorly to novel sequences.
- A common approach in Deep Learning is to overparametrize a model, such that it could easily memorize the training data, and then heavily regularize it to facilitate generalization.
- The regularization method of choice is often Dropout.

[Dropout: A Simple Way to Prevent Neural Networks from Overfitting. Srivastava et al. JMLR 2014.]

Regularization: Dropout

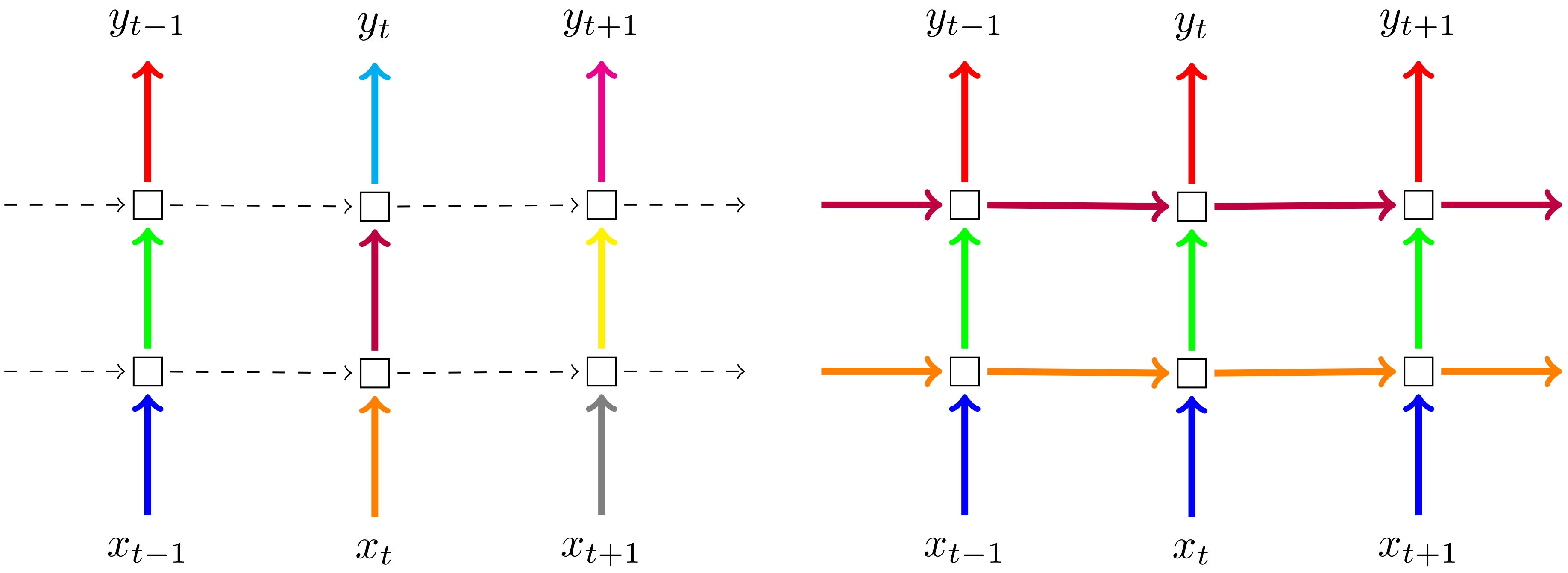
- Dropout is ineffective when applied to recurrent connections, as repeated random masks zero all hidden units in the limit.
- The most common solution is to only apply dropout to non-recurrent connections



[Recurrent neural network regularization. Zaremba et al., arXiv 2014.]

Regularization: Dropout

- **A Better Solution:** Use the same dropout mask at each time step for both inputs, outputs, and recurrent layers.



(a) Naive dropout RNN (b) Variational RNN

Each square represents an RNN unit, with horizontal arrows representing recurrent connections. Vertical arrows represent the input and output to each RNN unit. Coloured connections represent dropped-out inputs, with different colours corresponding to different dropout masks. Dashed lines correspond to standard connections with no dropout.

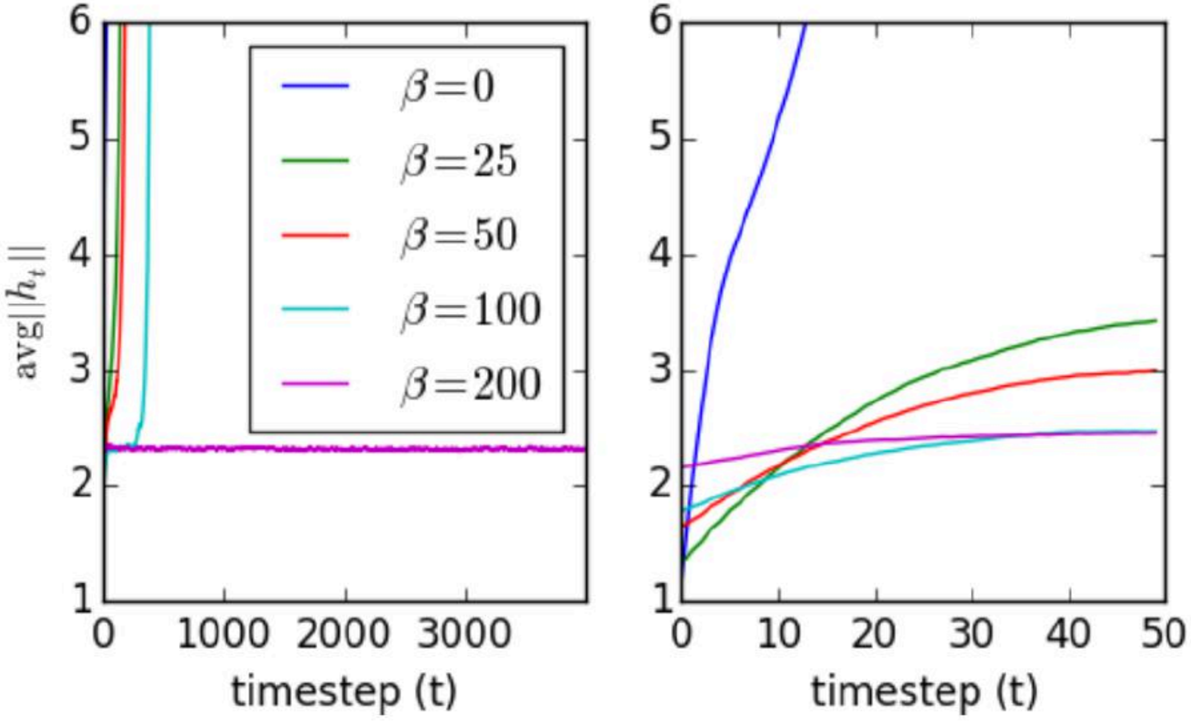
[A Theoretically Grounded Application of Dropout in Recurrent Neural Networks. Gal and Ghahramani. NIPS 2016]

Regularization: Norm-stabilizer

- Stabilize the activations of RNNs by penalizing the squared distance between successive hidden states' norms

$$\beta \frac{1}{T} \sum_{t=1}^{T} (\|h_t\|_2 - \|h_{t-1}\|_2)^2$$

- Enforce the norms of the hidden layer activations approximately constant across time



[Regularizing RNNs by Stabilizing Activations. Krueger and Memisevic, ICLR 2016]

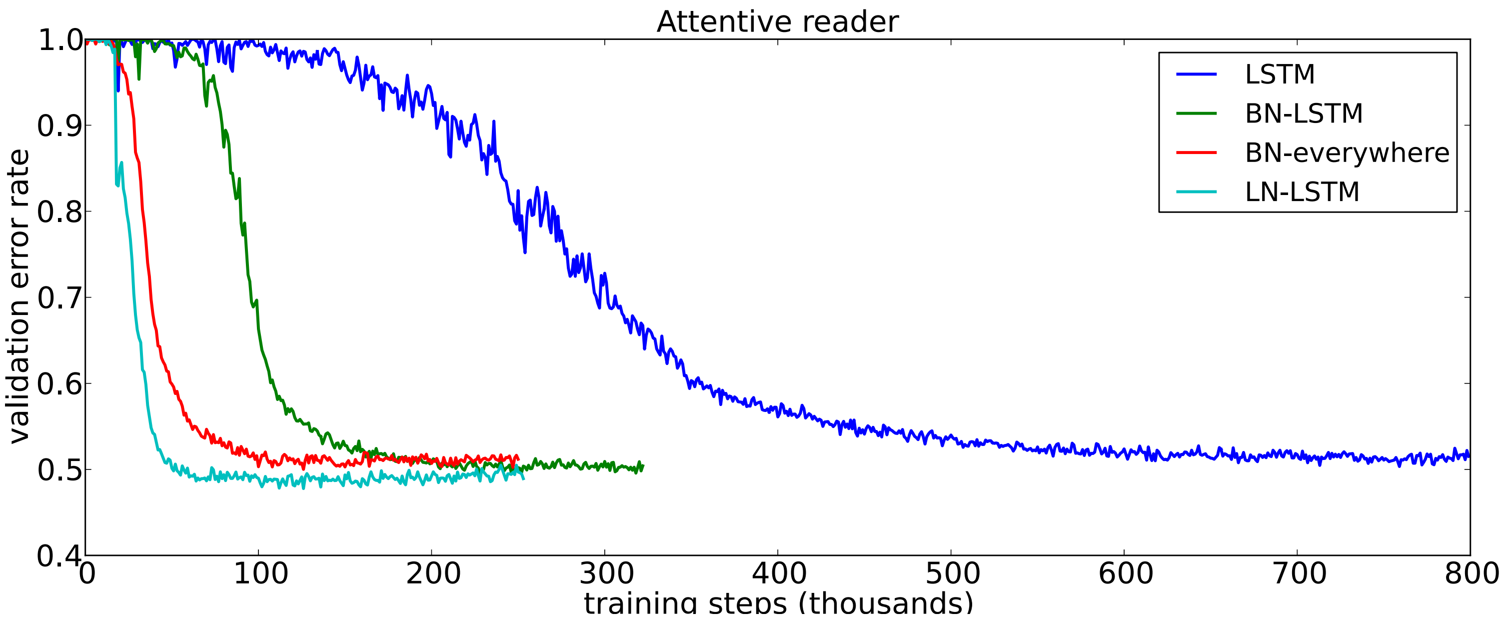
Regularization: Layer Normalization

- Similar to batch normalization
- Computes the normalization statistics separately at each time step
- Effective for stabilizing the hidden state dynamics in RNNs
- Reduces training time

$$\mathbf{h}^t = f\left[\frac{\mathbf{g}}{\sigma^t} \odot \left(\mathbf{a}^t - \mu^t\right) + \mathbf{b}\right]$$

$$\mu^t = \frac{1}{H}\sum_{i=1}^{H} a_i^t$$

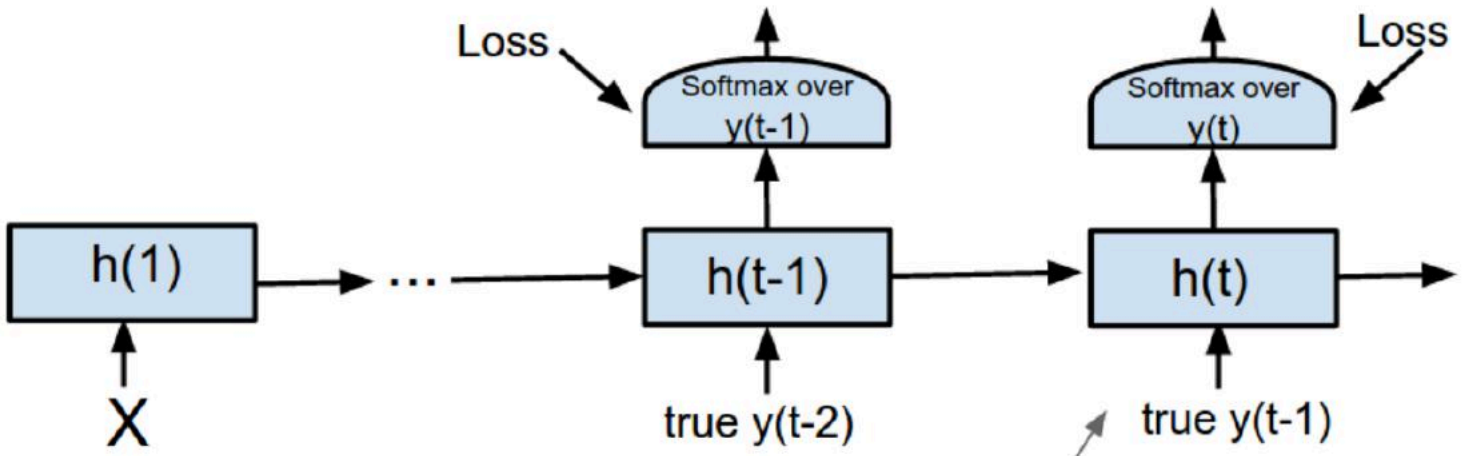
$$\sigma^t = \sqrt{\frac{1}{H}\sum_{i=1}^{H}\left(a_i^t - \mu^t\right)^2}$$



Layer Normalization [Ba, Kiros & Hinton, 2016]

Scheduled Sampling

- *"change the training process from a fully guided scheme using the true previous token, towards a less guided scheme which mostly uses the generated token instead."*

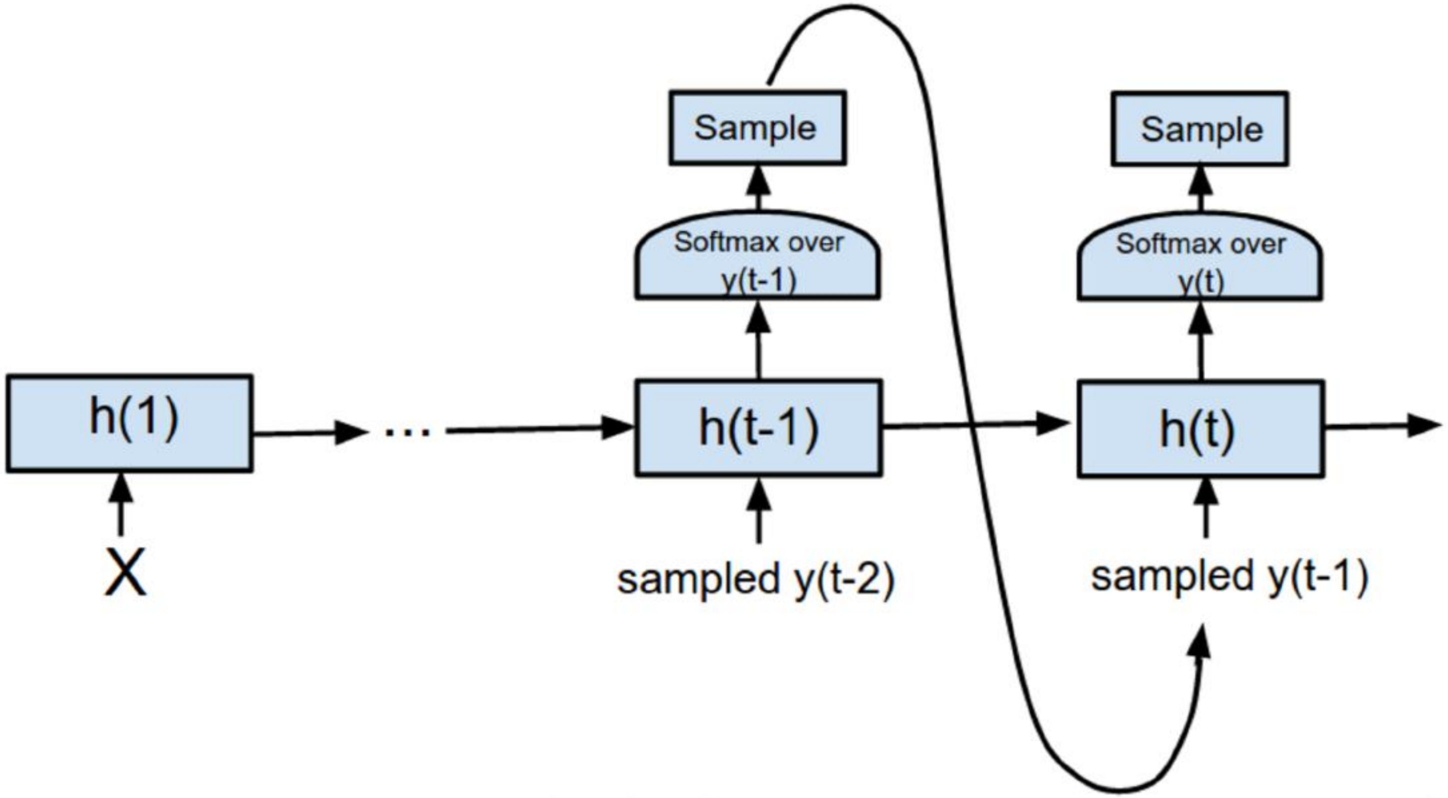


$$P(y_t|h_t) \text{ with } h_t = f(h_{t-1}, y_{t-1})$$

[Scheduled Sampling for Sequence Prediction with Recurrent Neural Networks. Bengio et al., NIPS 2015]

Scheduled Sampling

- *“change the training process from a fully guided scheme using the true previous token, towards a less guided scheme which mostly uses the generated token instead.”*
- During training, randomly replace a **conditioning** ground truth token by the model's previous prediction

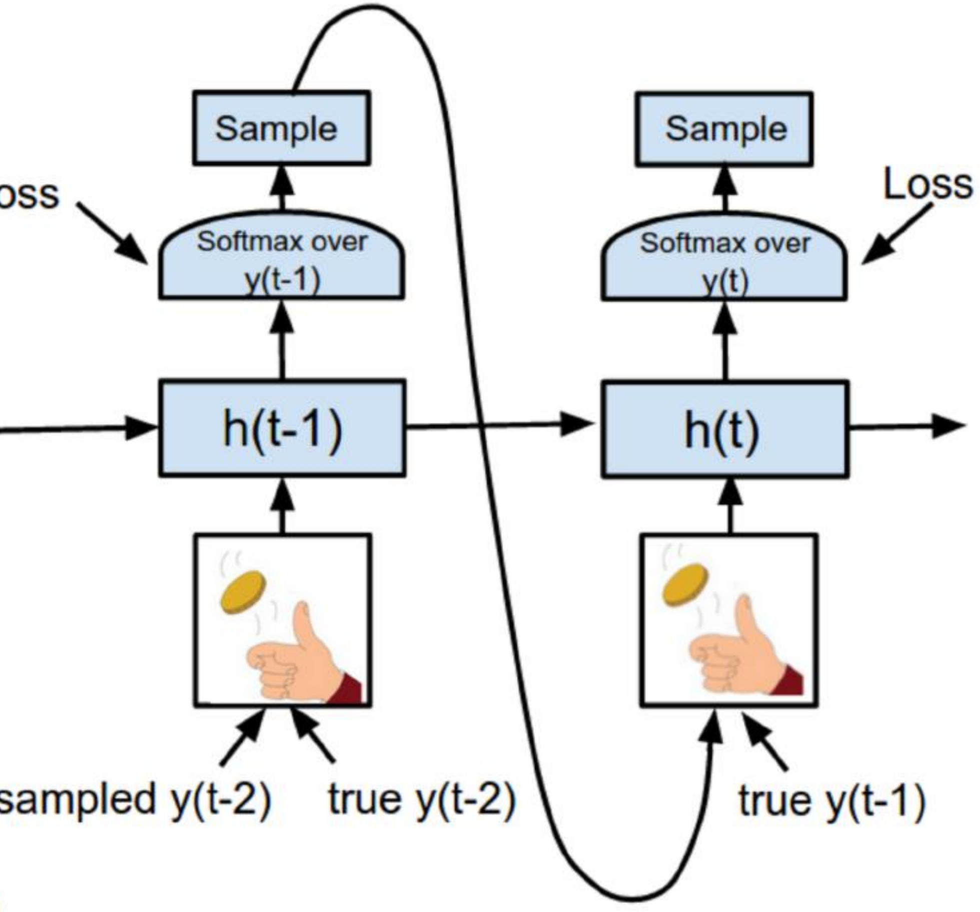


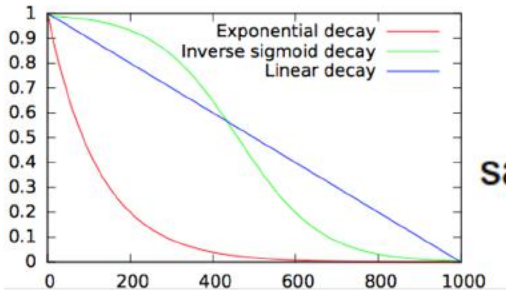
$$P(y_t|h_t) \text{ with } h_t = f(h_{t-1}, \hat{y}_{t-1})$$

[Scheduled Sampling for Sequence Prediction with Recurrent Neural Networks. Bengio et al., NIPS 2015](#)

Scheduled Sampling

- *"change the training process from a fully guided scheme using the true previous token, towards a less guided scheme which mostly uses the generated token instead."*
- During training, randomly replace a **conditioning** ground truth token by the model's previous prediction

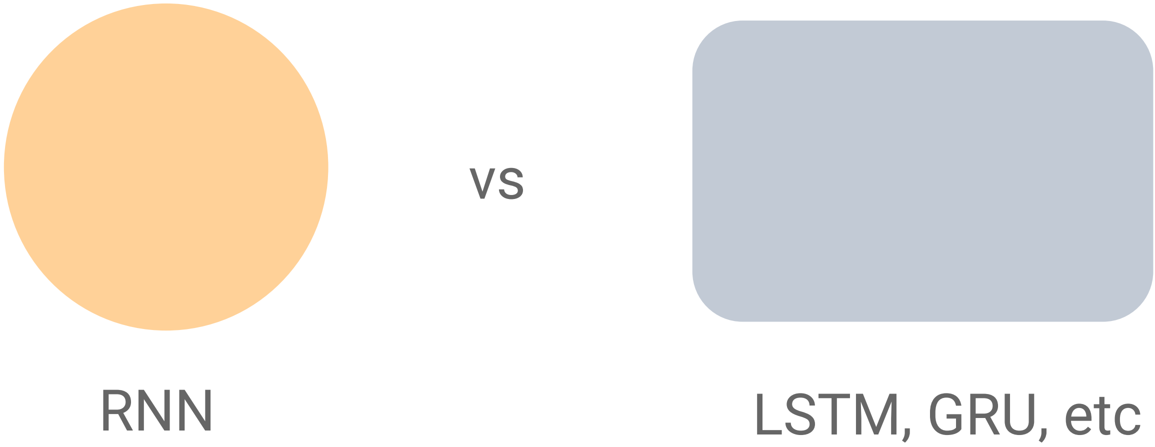




[Scheduled Sampling for Sequence Prediction with Recurrent Neural Networks. Bengio et al., NIPS 2015]

Gated Cells

- rather each node being just a simple RNN cell, make each node a more **complex unit with gates** controlling what information is passed through



Long short term memory cells are able to keep track of information throughout many timesteps.

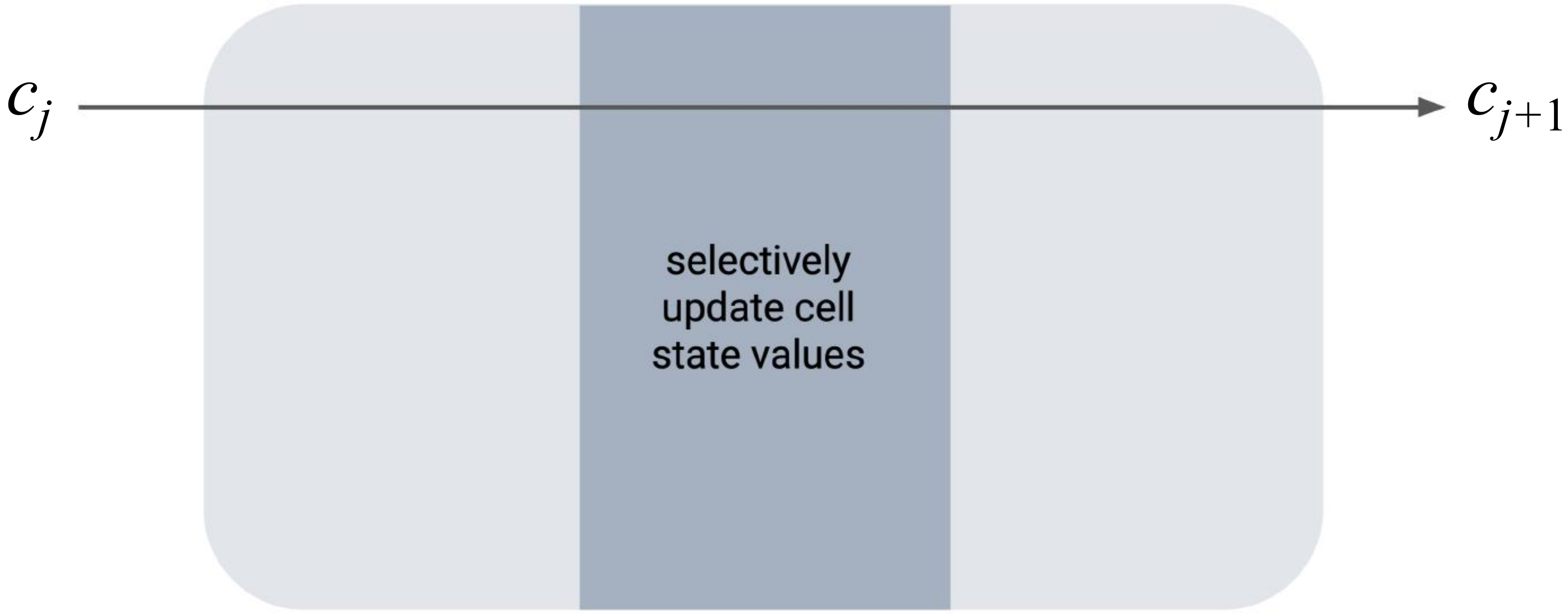
Long Short-Term Memory (LSTM)

[Long Short-Term Memory [Hochreiter et al., 1997]]

Long Short-Term Memory (LSTM)

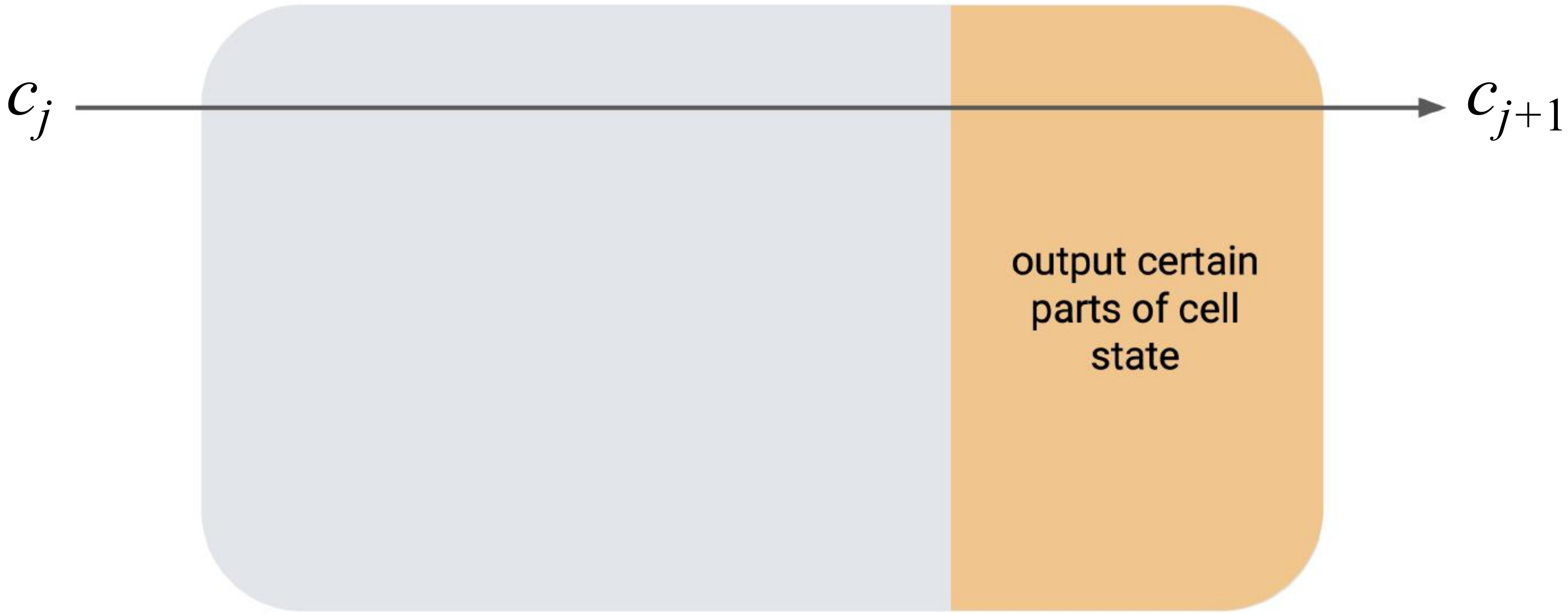
[Long Short-Term Memory [Hochreiter et al., 1997]]

Long Short-Term Memory (LSTM)



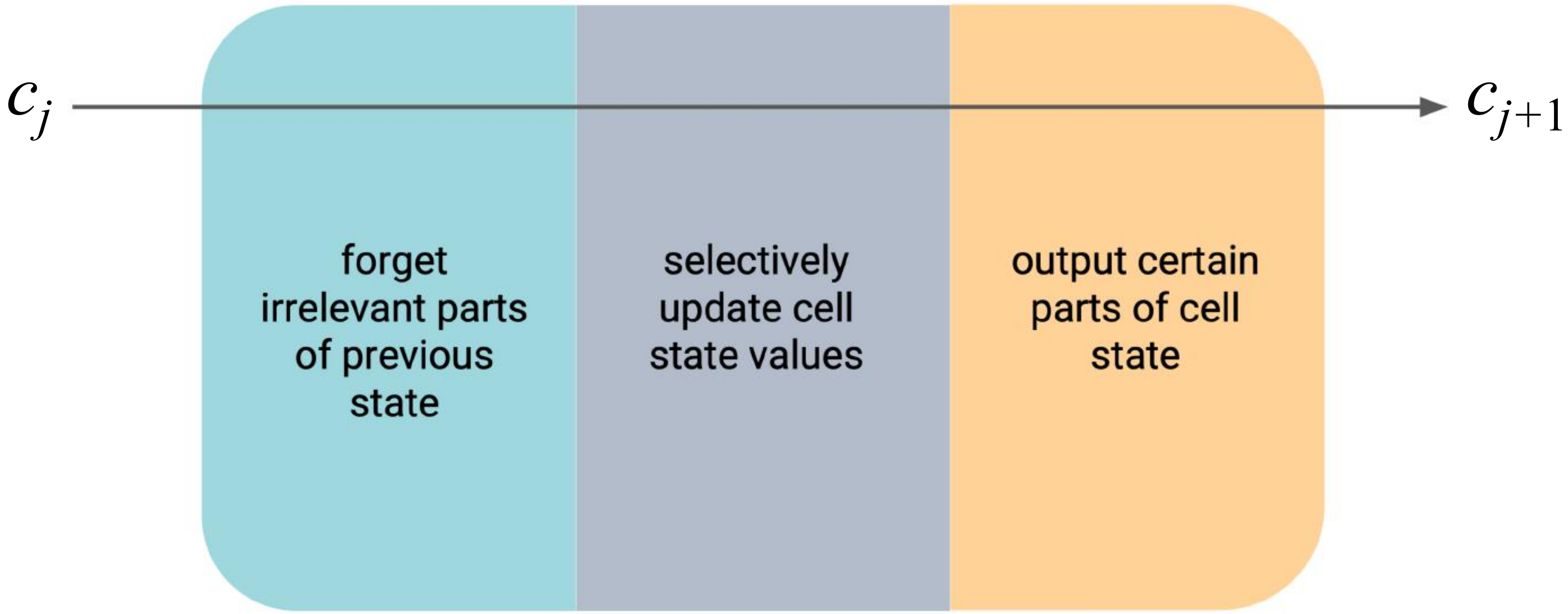
Long Short-Term Memory [Hochreiter et al., 1997]

Long Short-Term Memory (LSTM)



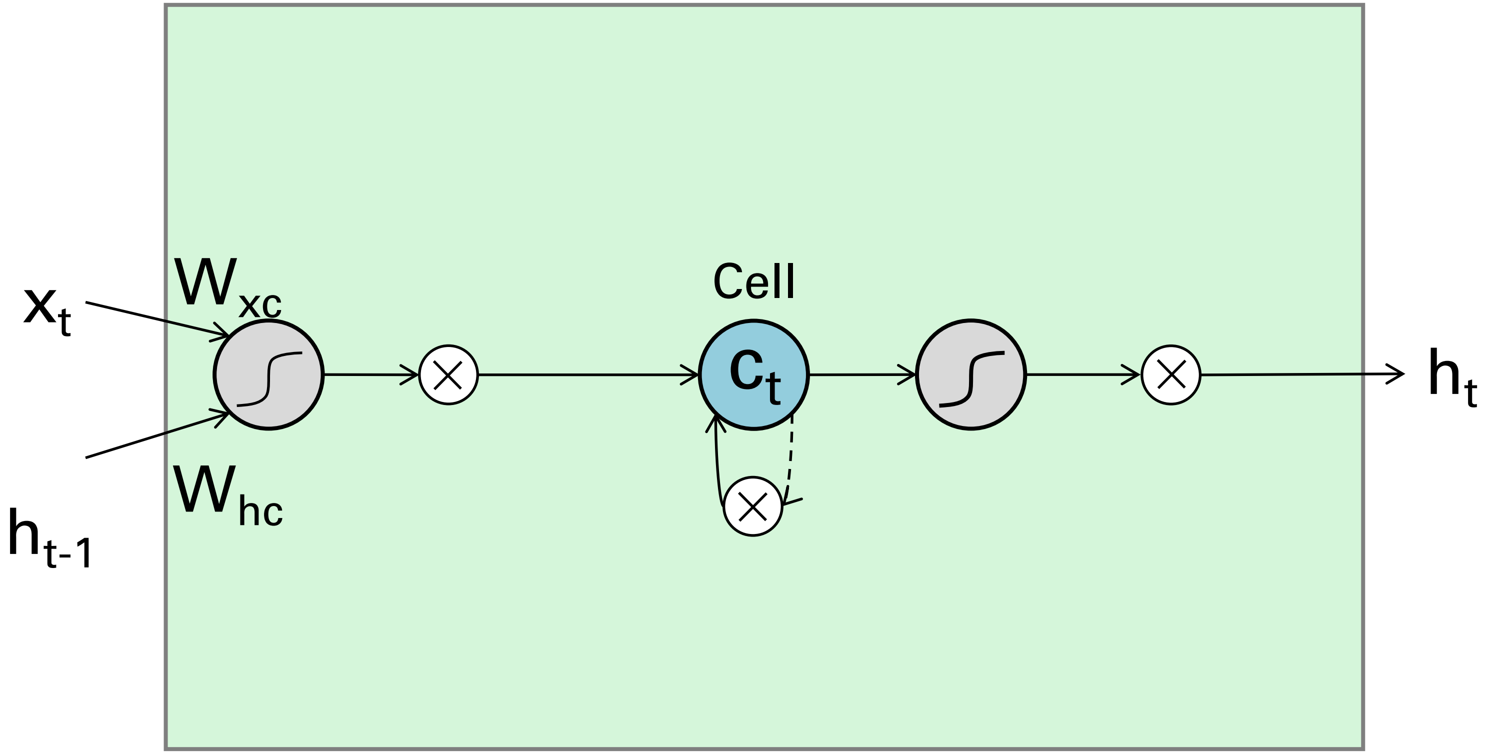
[Long Short-Term Memory [Hochreiter et al., 1997]]

Long Short-Term Memory (LSTM)



[Long Short-Term Memory [Hochreiter et al., 1997]]

The LSTM Idea

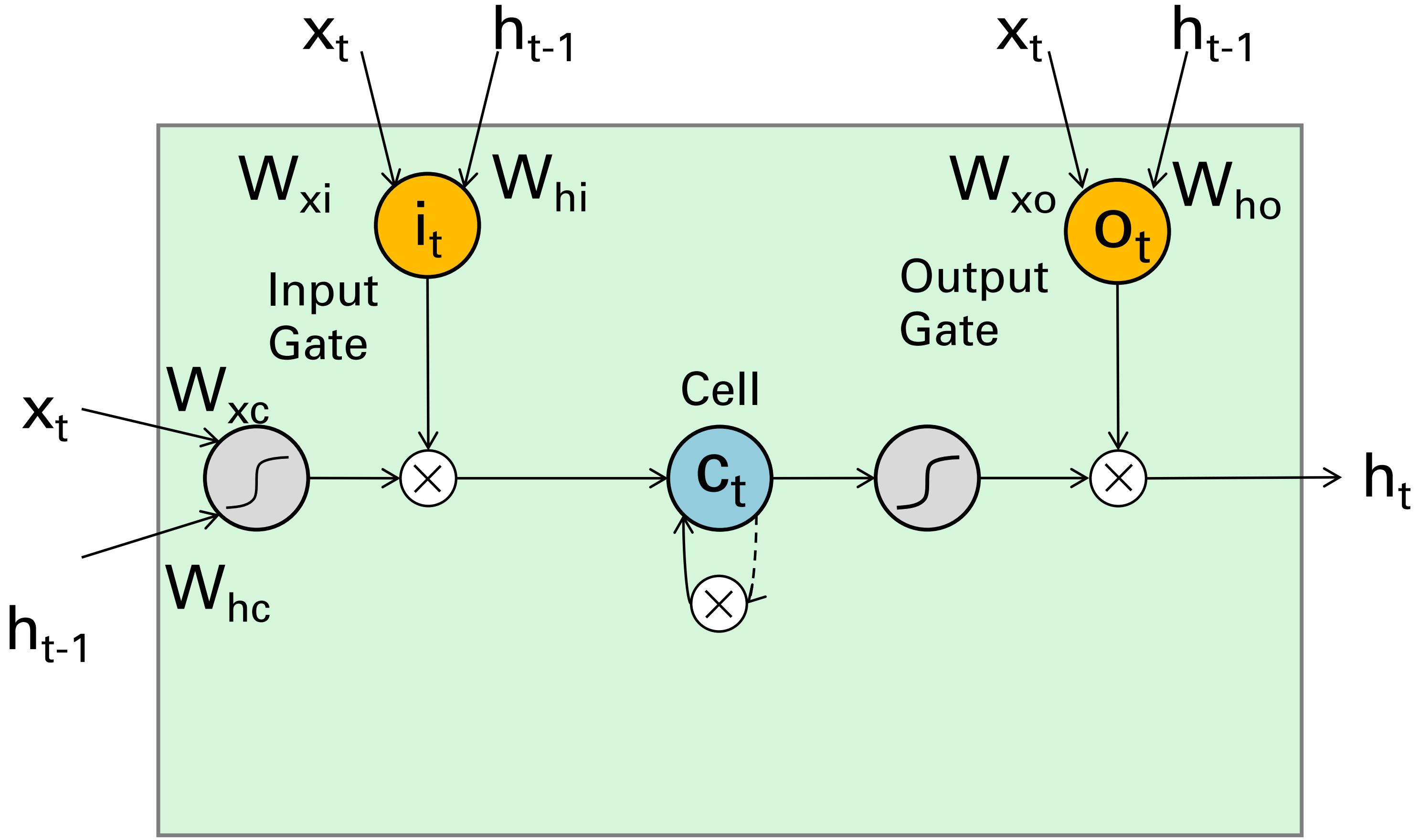


$$c_t = c_{t-1} + \tanh W \begin{pmatrix} x_t \\ h_{t-1} \end{pmatrix}$$

$$h_t = \tanh c_t$$

* Dashed line indicates time-lag

The Original LSTM Cell



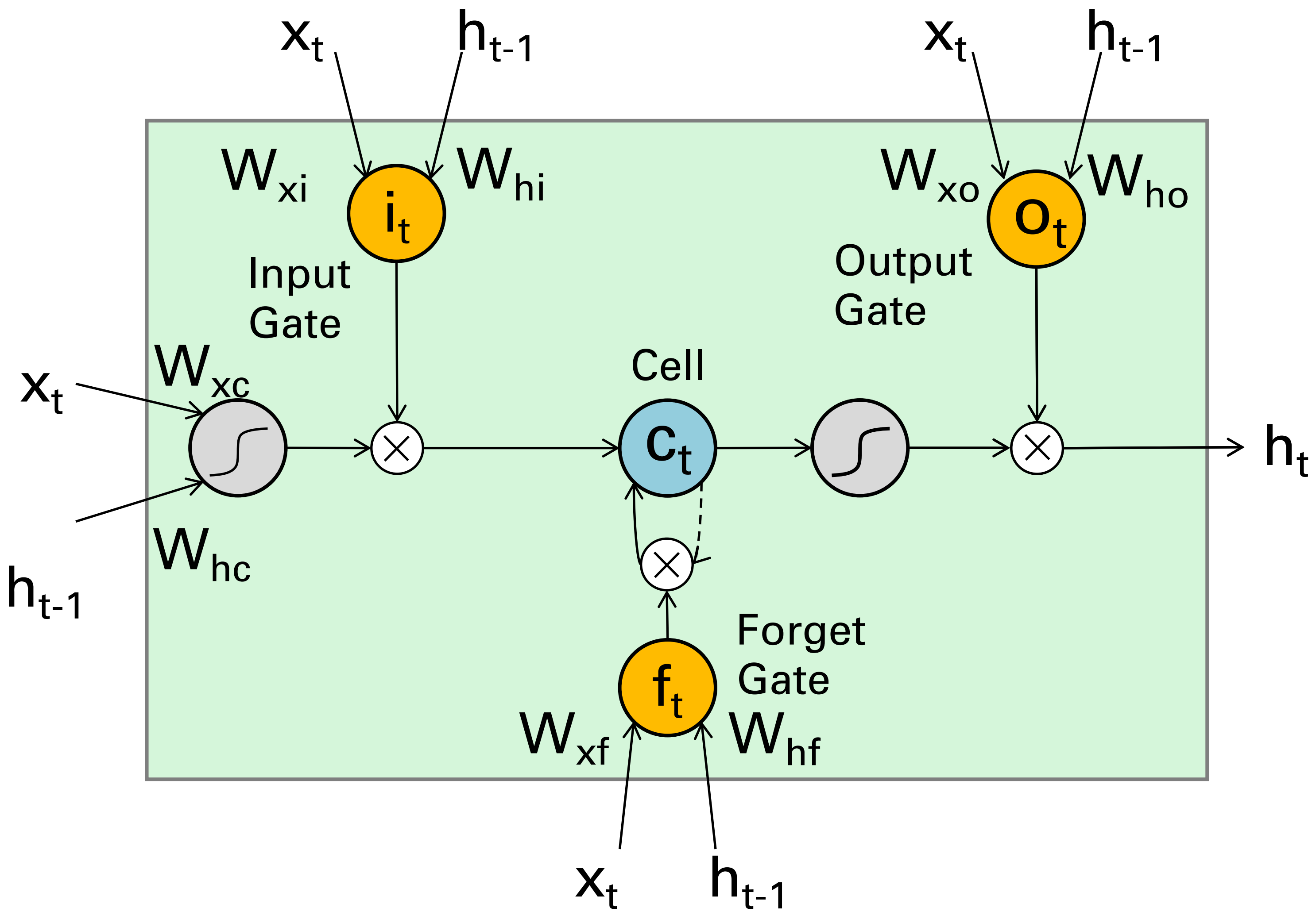
$$c_t = c_{t-1} + i_t \otimes \tanh W \begin{pmatrix} x_t \\ h_{t-1} \end{pmatrix}$$

$$h_t = o_t \otimes \tanh c_t$$

$$i_t = \sigma \left(W_i \begin{pmatrix} x_t \\ h_{t-1} \end{pmatrix} + b_i \right)$$

Similarly for o_t

The Popular LSTM Cell



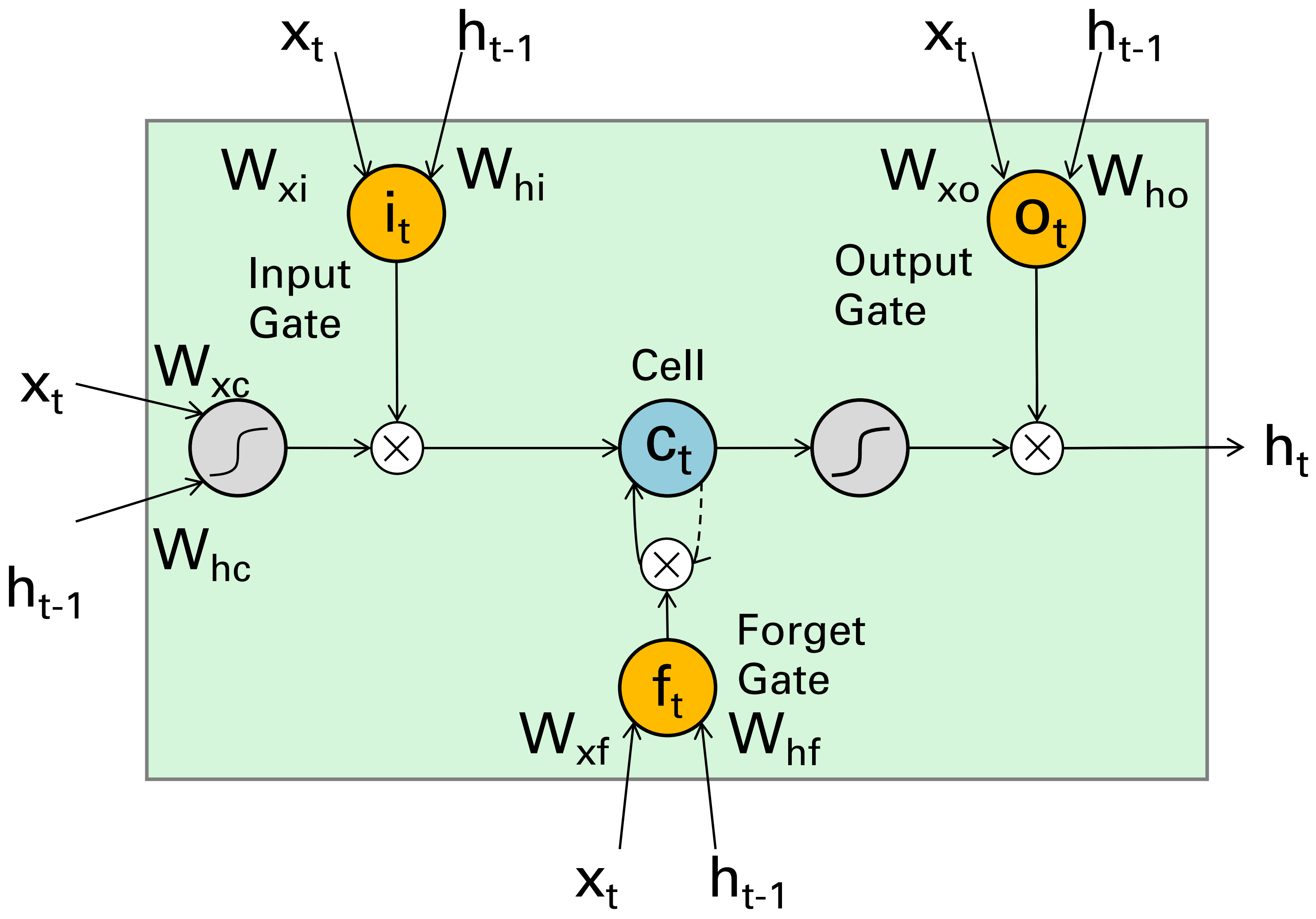
$$i_t = \sigma\left(W_i\begin{pmatrix}x_t\\h_{t-1}\end{pmatrix}+b_i\right)$$

$$c_t = f_t \otimes c_{t-1} + i_t \otimes \tanh W\begin{pmatrix}x_t\\h_{t-1}\end{pmatrix}$$

$$f_t = \sigma\left(W_f\begin{pmatrix}x_t\\h_{t-1}\end{pmatrix}+b_f\right)$$

$$h_t = o_t \otimes \tanh c_t$$

The Popular LSTM Cell



$$i_t = \sigma\left(W_i \begin{pmatrix} x_t \\ h_{t-1} \end{pmatrix} + b_i\right)$$

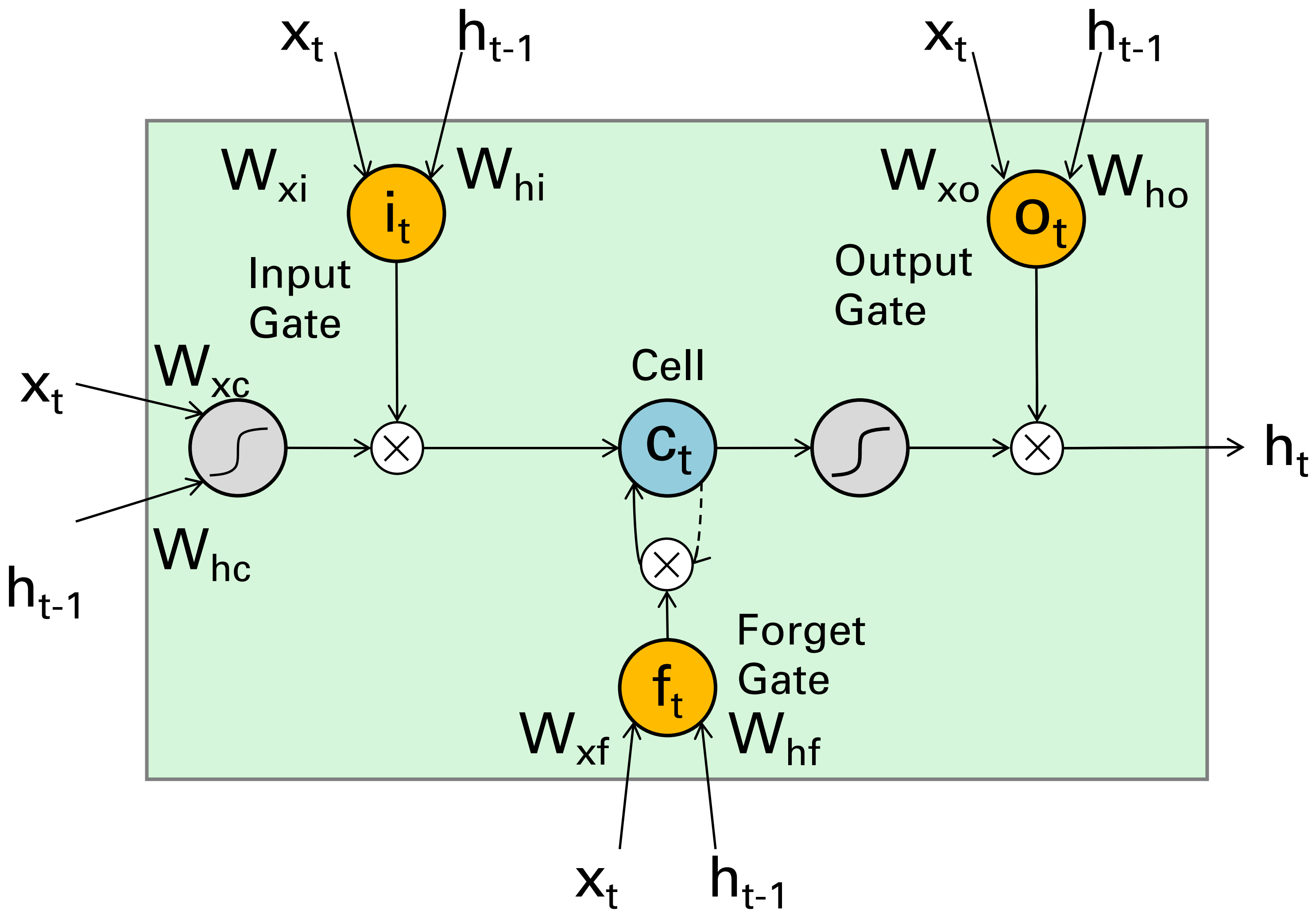
$$c_t = f_t \otimes c_{t-1} + i_t \otimes \tanh W \begin{pmatrix} x_t \\ h_{t-1} \end{pmatrix}$$

$$\boxed{f_t = \sigma\left(W_f \begin{pmatrix} x_t \\ h_{t-1} \end{pmatrix} + b_f\right)}$$

$$h_t = o_t \otimes \tanh c_t$$

forget gate decides what information is going to be thrown away from the cell state

The Popular LSTM Cell



$$\boxed{i_t = \sigma\left(W_i \begin{pmatrix} x_t \\ h_{t-1} \end{pmatrix} + b_i \right)}$$

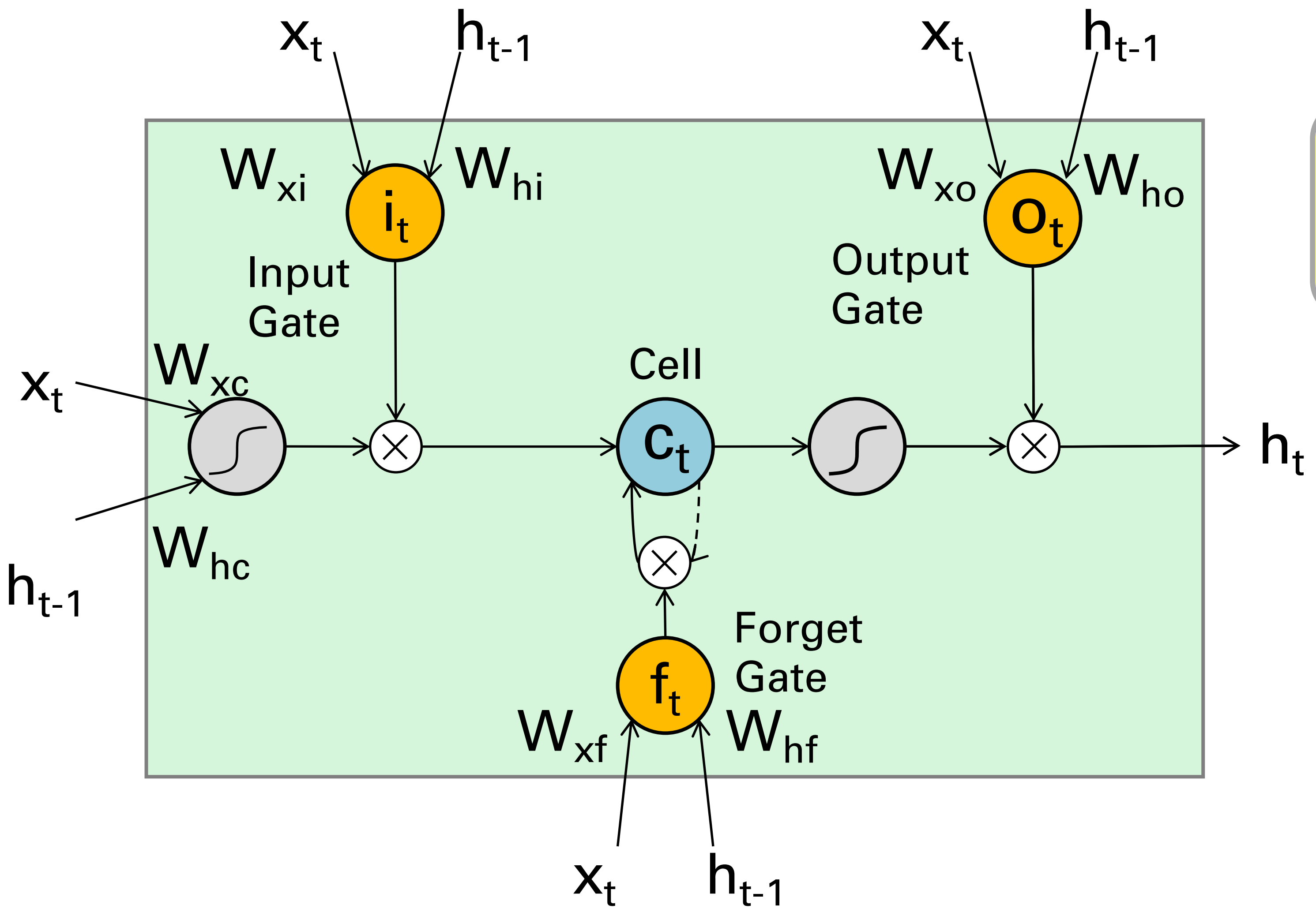
$$c_t = f_t \otimes c_{t-1} + \boxed{i_t \otimes \tanh W \begin{pmatrix} x_t \\ h_{t-1} \end{pmatrix}}$$

$$f_t = \sigma\left(W_f \begin{pmatrix} x_t \\ h_{t-1} \end{pmatrix} + b_f \right)$$

$$h_t = o_t \otimes \tanh c_t$$

input gate and **a tanh layer** decides what information is going to be stored in the cell state

The Popular LSTM Cell



$$i_t = \sigma\left(W_i \begin{pmatrix} x_t \\ h_{t-1} \end{pmatrix} + b_i\right)$$

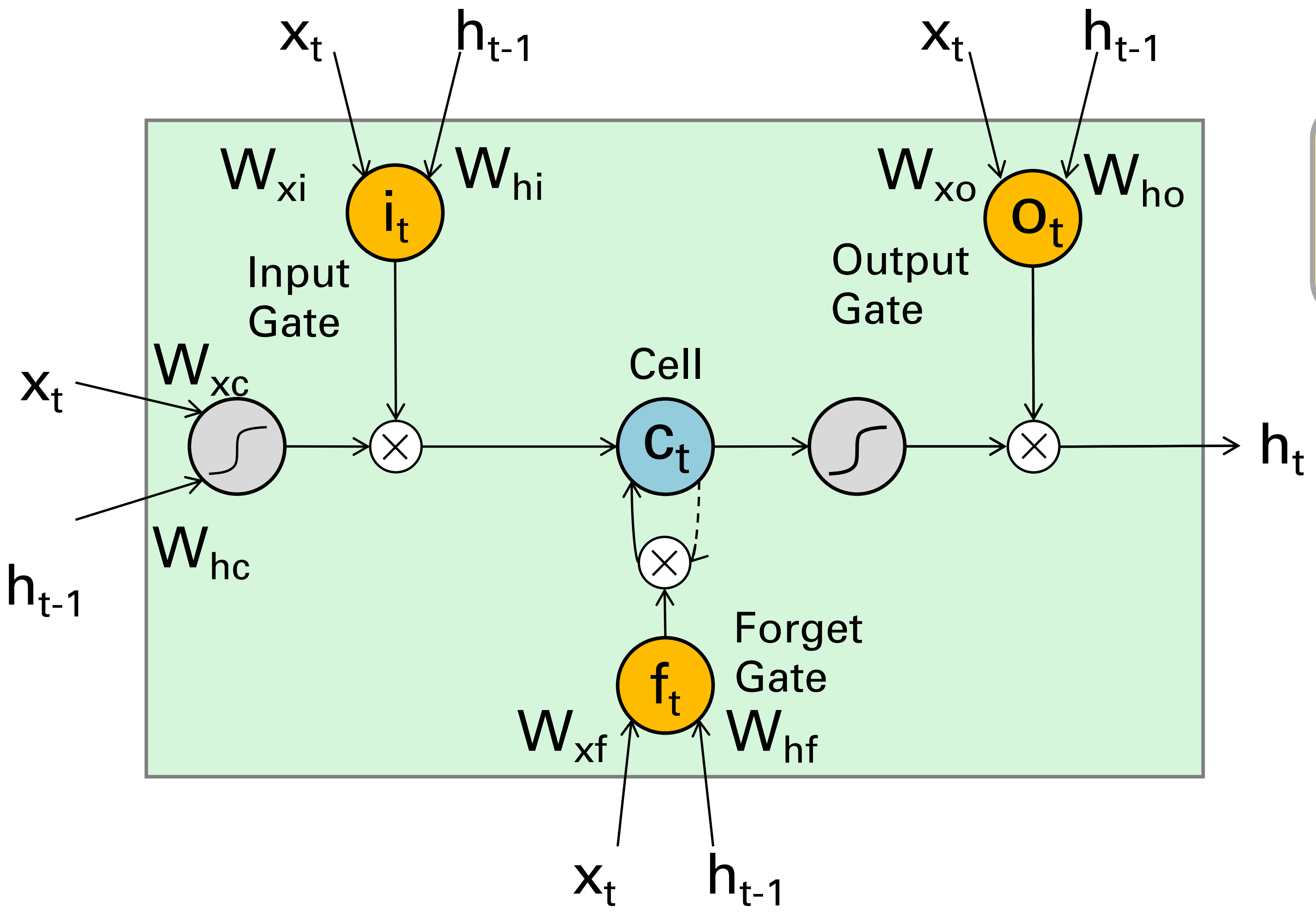
$$\boxed{c_t = f_t \otimes c_{t-1} + i_t \otimes \tanh W \begin{pmatrix} x_t \\ h_{t-1} \end{pmatrix}}$$

$$f_t = \sigma\left(W_f \begin{pmatrix} x_t \\ h_{t-1} \end{pmatrix} + b_f\right)$$

$$h_t = o_t \otimes \tanh c_t$$

Update the old cell state with the new one.

The Popular LSTM Cell

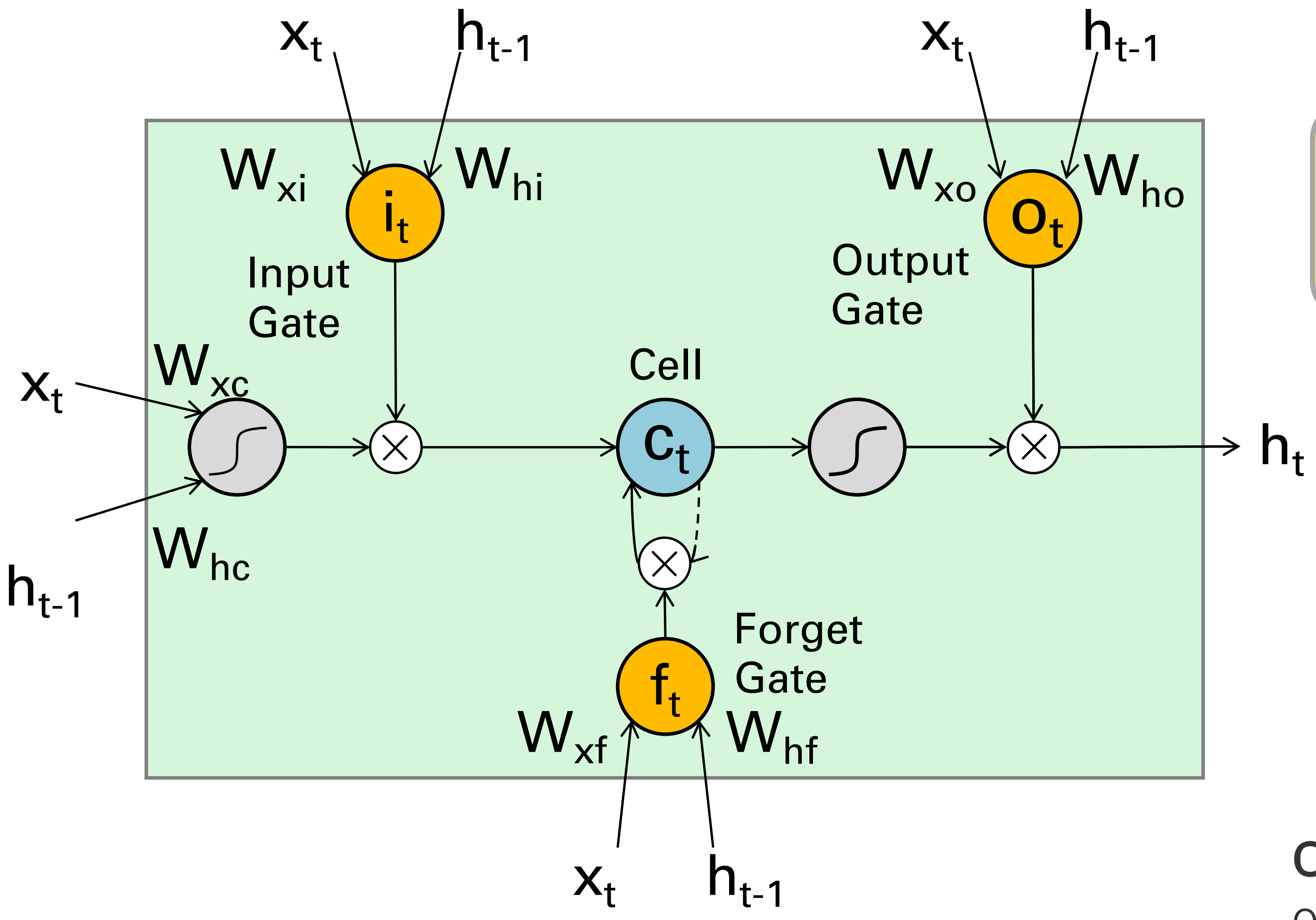


$$i_t = \sigma\left(W_i \begin{pmatrix} x_t \\ h_{t-1} \end{pmatrix} + b_i \right)$$

$$c_t = f_t \otimes c_{t-1} + i_t \otimes \tanh W \begin{pmatrix} x_t \\ h_{t-1} \end{pmatrix}$$

input gate	forget gate	behavior
0	1	remember the previous value
1	1	add to the previous value
0	0	erase the value
1	0	overwrite the value

The Popular LSTM Cell



$$i_t = \sigma\left(W_i\begin{pmatrix}x_t\\h_{t-1}\end{pmatrix}+b_i\right)$$

$$\boxed{c_t = f_t \otimes c_{t-1} + i_t \otimes \tanh W\begin{pmatrix}x_t\\h_{t-1}\end{pmatrix}}$$

$$f_t = \sigma\left(W_f\begin{pmatrix}x_t\\h_{t-1}\end{pmatrix}+b_f\right)$$

$$h_t = o_t \otimes \tanh c_t$$

$$o_i = \sigma\left(W_o\begin{pmatrix}x_t\\h_{t-1}\end{pmatrix}+b_o\right)$$

Output gate decides what is going to be outputted. The final output is based on cell state and output of sigmoid gate.

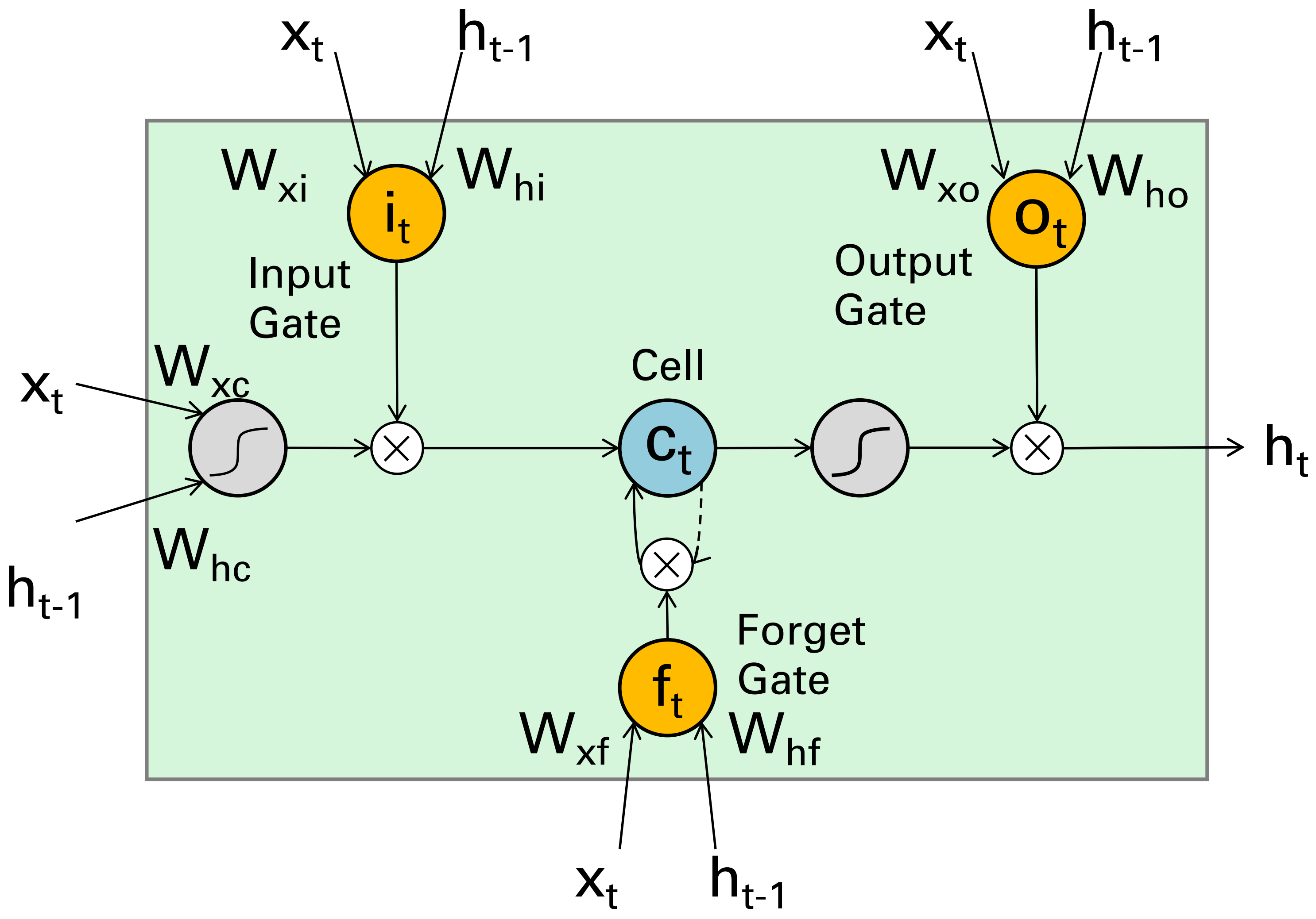
LSTM – Forward/Backward

[Illustrated LSTM Forward and Backward Pass](http://arunmallya.github.io/writeups/nn/lstm/index.html)

http://arunmallya.github.io/writeups/nn/lstm/index.html

LSTM variants

The Popular LSTM Cell



$$f_t = \sigma\left(W_f \begin{pmatrix} x_t \\ h_{t-1} \end{pmatrix} + b_f \right)$$

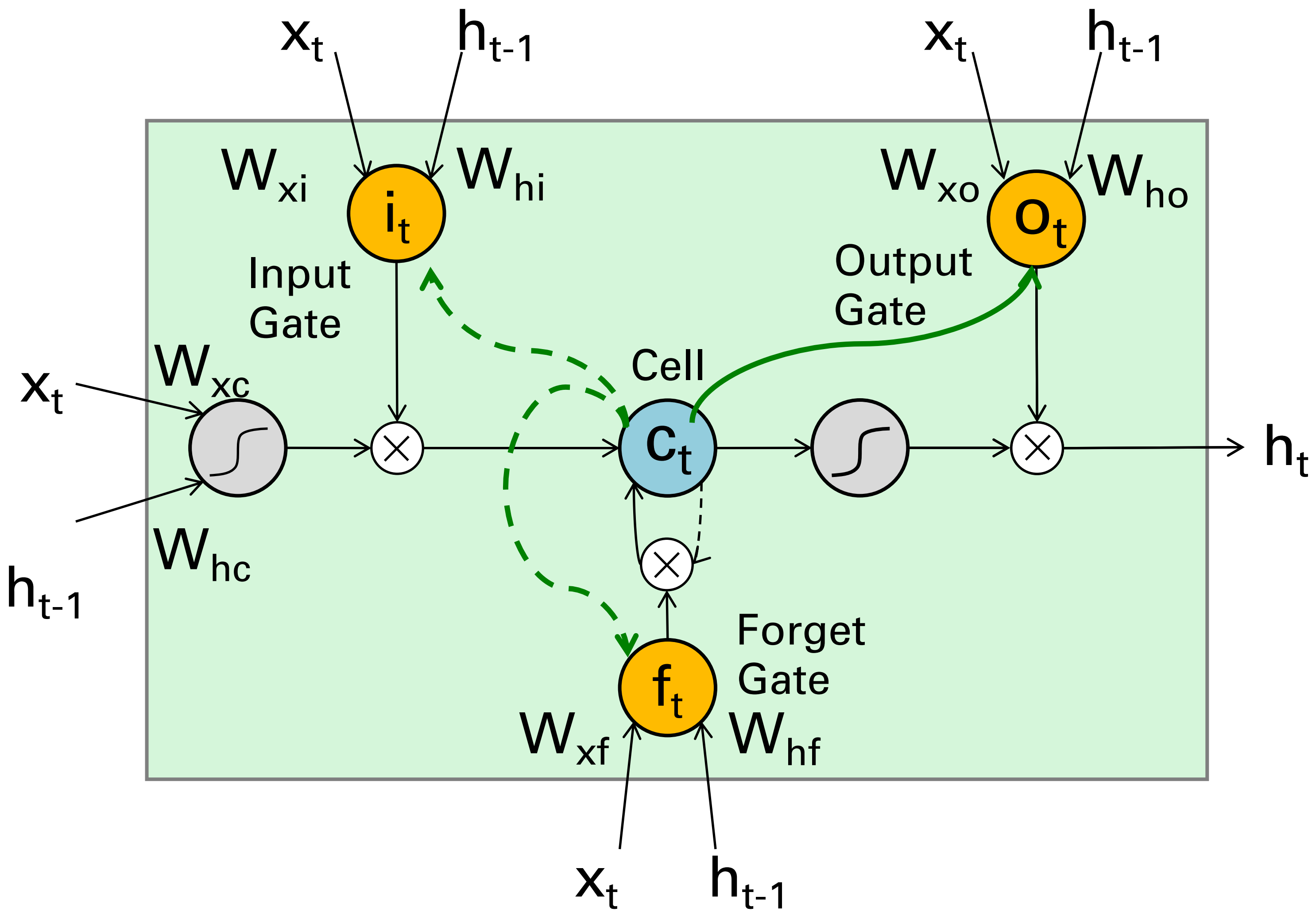
Similarly for i_t, o_t

$$c_t = f_t \otimes c_{t-1} + i_t \otimes \tanh W \begin{pmatrix} x_t \\ h_{t-1} \end{pmatrix}$$

$$h_t = o_t \otimes \tanh c_t$$

* Dashed line indicates time-lag

Extension I: Peephole LSTM



$$f_t = \sigma\left(W_f \begin{pmatrix} x_t \\ h_{t-1} \\ c_{t-1} \end{pmatrix} + b_f \right)$$

Similarly for i_t, o_t (uses c_t)

$$c_t = f_t \otimes c_{t-1} + i_t \otimes \tanh W \begin{pmatrix} x_t \\ h_{t-1} \end{pmatrix}$$

$$h_t = o_t \otimes \tanh c_t$$

- Add **peephole connections**.
- All gate layers look at the cell state!

* Dashed line indicates time-lag

Other minor variants

- Coupled Input and Forget Gate $f_t = 1 - i_t$

- Full Gate Recurrence

$$f_t = \sigma\left(W_f \begin{pmatrix} x_t \\ h_{t-1} \\ c_{t-1} \\ i_{t-1} \\ f_{t-1} \\ o_{t-1} \end{pmatrix} + b_f \right)$$

LSTM: A Search Space Odyssey

- Tested the following variants, using Peephole LSTM as standard:
  1. No Input Gate (NIG)
  2. No Forget Gate (NFG)
  3. No Output Gate (NOG)
  4. No Input Activation Function (NIAF)
  5. No Output Activation Function (NOAF)
  6. No Peepholes (NP)
  7. Coupled Input and Forget Gate (CIFG)
  8. Full Gate Recurrence (FGR)

- On the tasks of:
  – Timit Speech Recognition: Audio frame to 1 of 61 phonemes
  – IAM Online Handwriting Recognition: Sketch to characters
  – JSB Chorales: Next-step music frame prediction

LSTM: A Search Space Odyssey [Greff et al., 2015]

LSTM: A Search Space Odyssey

- The standard LSTM performed reasonably well on multiple datasets and none of the modifications significantly improved the performance
- Coupling gates and removing peephole connections simplified the LSTM without hurting performance much
- The forget gate and output activation are crucial

- Found interaction between learning rate and network size to be minimal – indicates calibration can be done using a small network first

LSTM: A Search Space Odyssey [Greff et al., 2015]

Gated Recurrent Unit

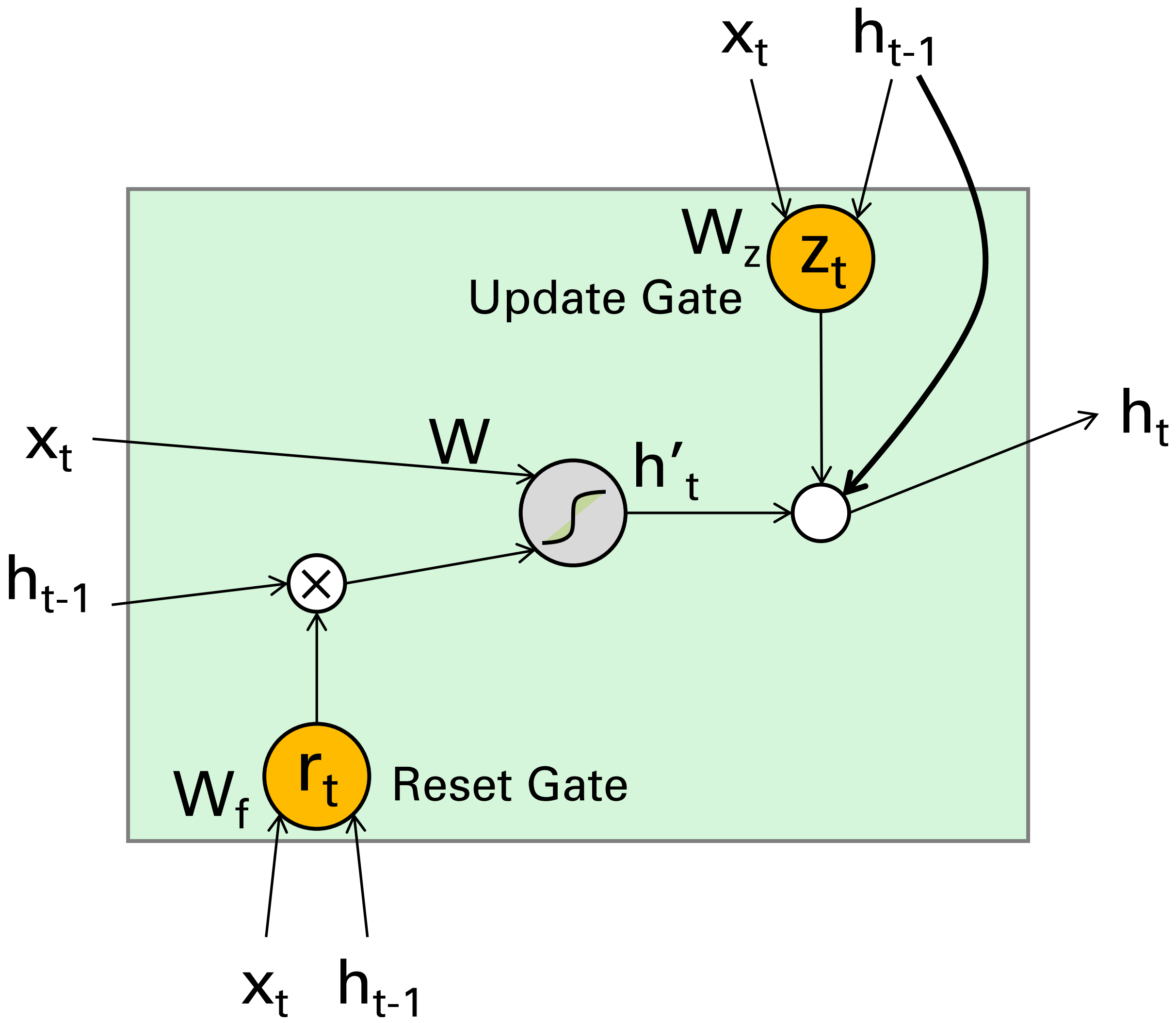
Gated Recurrent Unit (GRU)

- A very simplified version of the LSTM
  - Merges forget and input gate into a single ‘update’ gate
  - Merges cell and hidden state

- Has fewer parameters than an LSTM and has been shown to outperform LSTM on some tasks

Learning Phrase Representations using RNN Encoder-Decoder for Statistical Machine Translation [Cho et al.,14]

GRU



$$r_t = \sigma\left(W_r\begin{pmatrix}x_t\\h_{t-1}\end{pmatrix} + b_f\right)$$

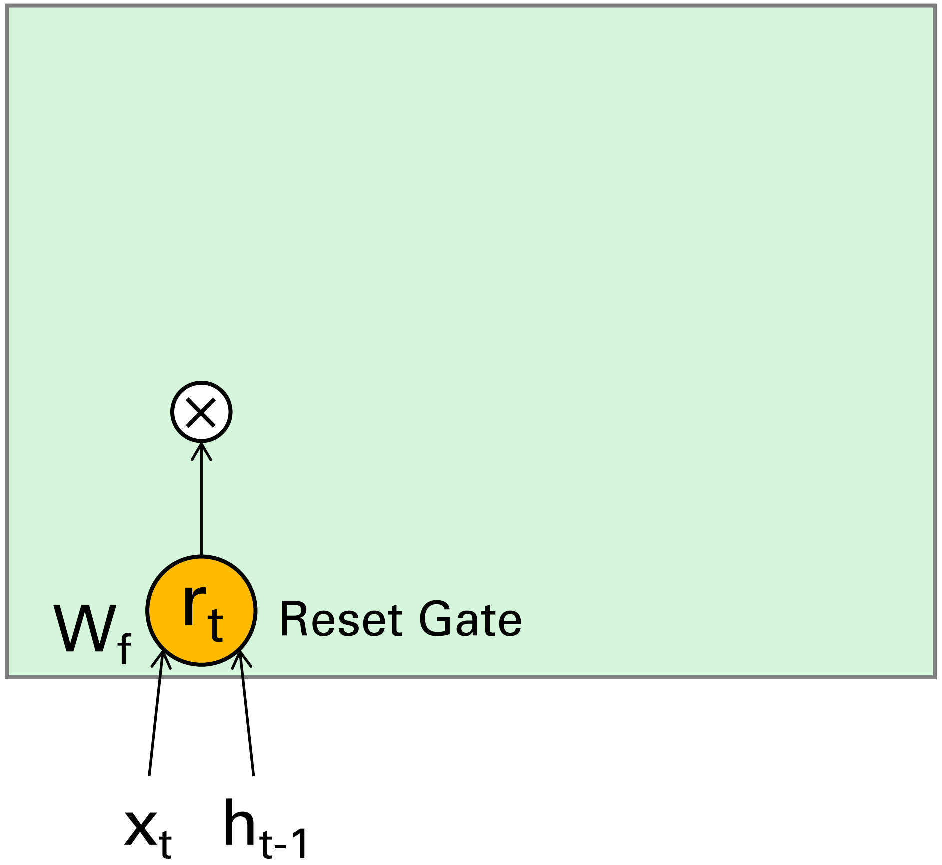
$$h'_t = \tanh W\begin{pmatrix}x_t\\r_t \otimes h_{t-1}\end{pmatrix}$$

$$z_t = \sigma\left(W_z\begin{pmatrix}x_t\\h_{t-1}\end{pmatrix} + b_f\right)$$

$$h_t = (1 - z_t) \otimes h_{t-1} + z_t \otimes h'_t$$

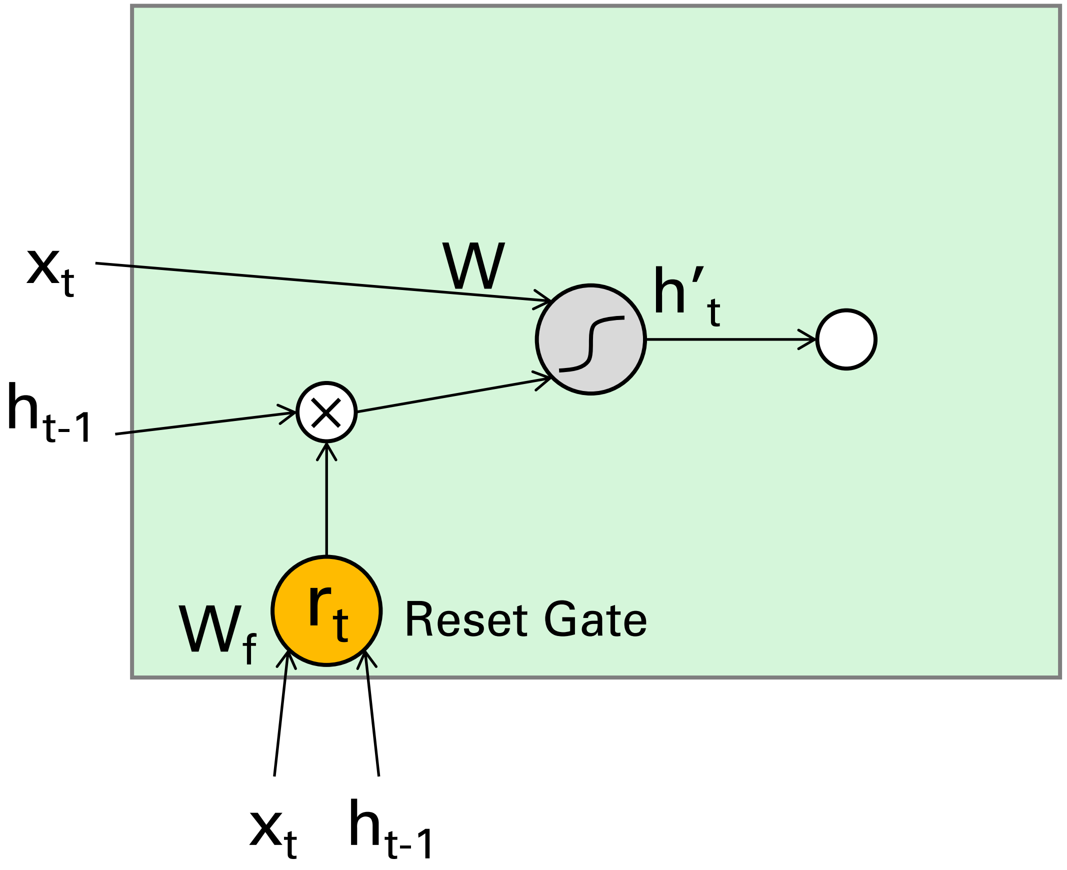
GRU

$$r_t = \sigma\left(W_r \begin{pmatrix} x_t \\ h_{t-1} \end{pmatrix} + b_f \right)$$



computes a **reset gate** based on current input and hidden state

GRU



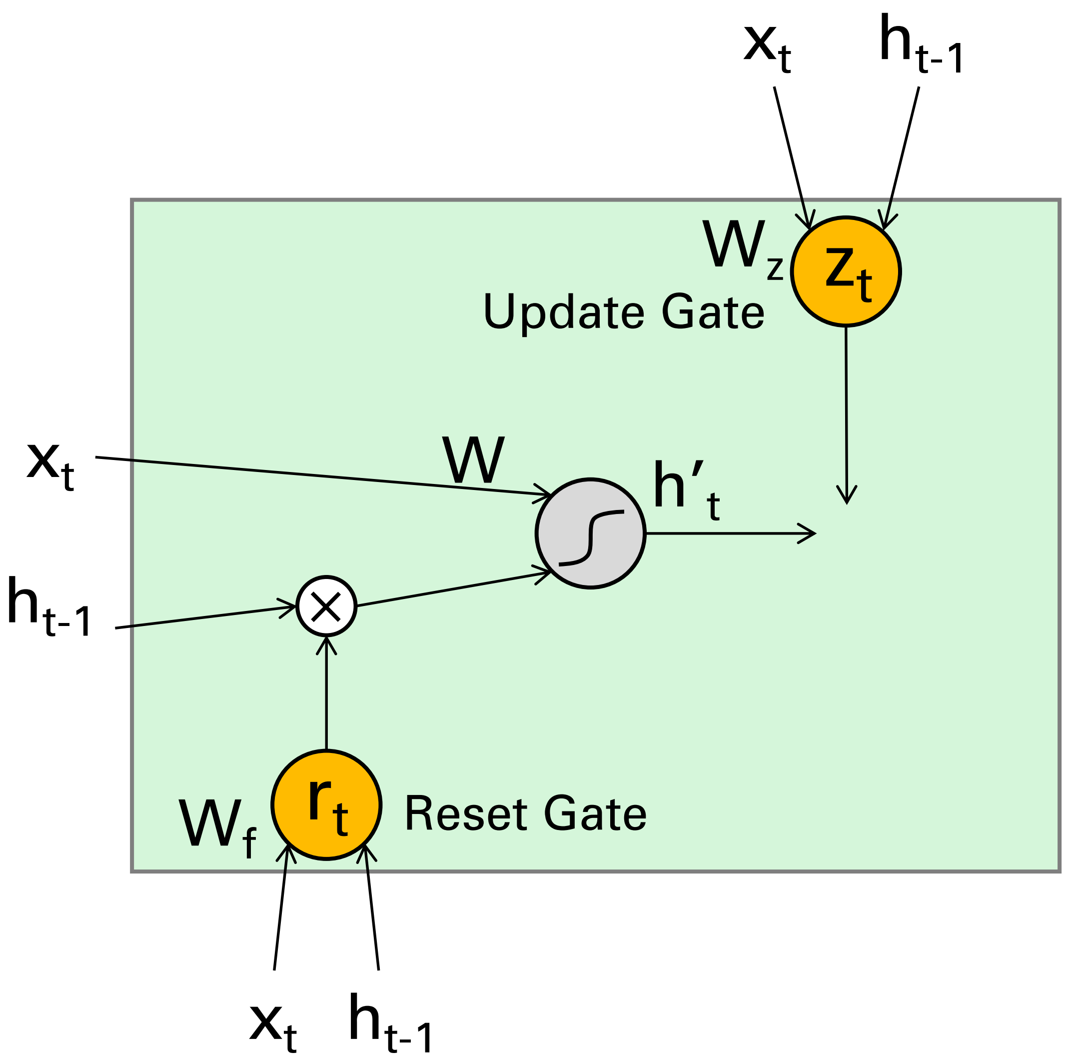
$$r_t = \sigma\left(W_r \begin{pmatrix} x_t \\ h_{t-1} \end{pmatrix} + b_f \right)$$

$$h'_t = \tanh W \begin{pmatrix} x_t \\ r_t \otimes h_{t-1} \end{pmatrix}$$

computes the **hidden state** based on current input and hidden state

if reset gate unit is ~0, then this ignores previous memory and only stores the new input information

GRU



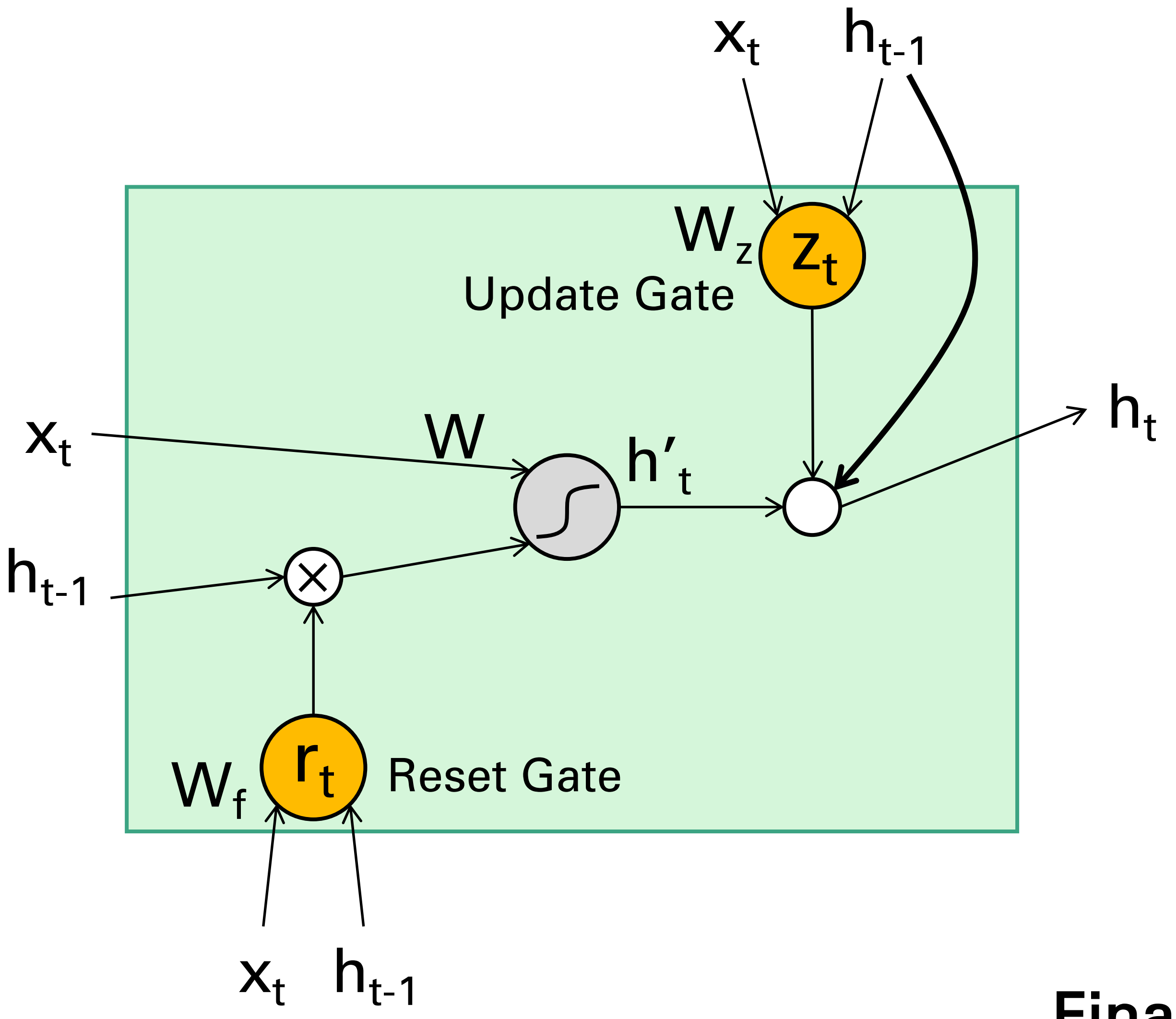
$$r_t = \sigma\left(W_r\begin{pmatrix}x_t\\h_{t-1}\end{pmatrix}+b_f\right)$$

$$h'_t = \tanh W\begin{pmatrix}x_t\\r_t \otimes h_{t-1}\end{pmatrix}$$

$$z_t = \sigma\left(W_z\begin{pmatrix}x_t\\h_{t-1}\end{pmatrix}+b_f\right)$$

computes an **update gate** again based on current input and hidden state

GRU



$$r_t = \sigma\left(W_r\begin{pmatrix}x_t\\h_{t-1}\end{pmatrix}+b_f\right)$$

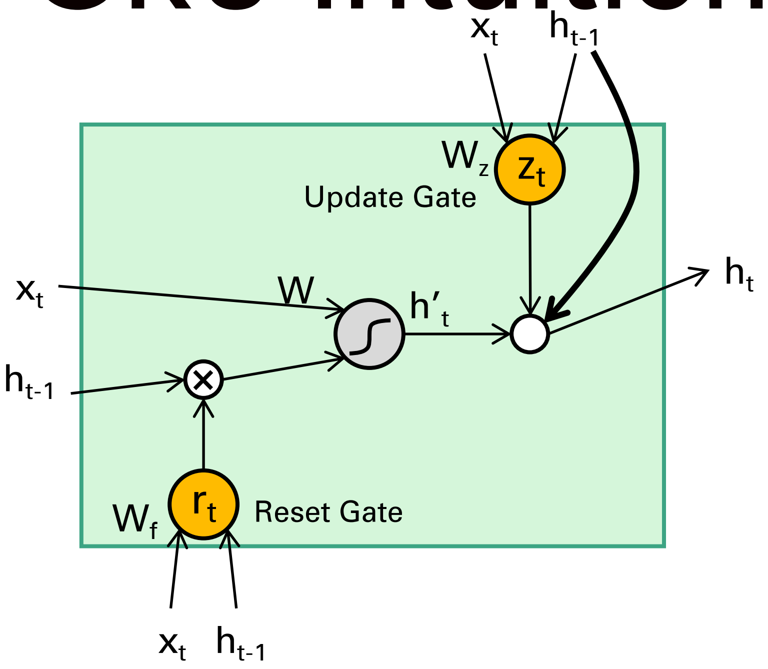
$$h'_t = \tanh W\begin{pmatrix}x_t\\r_t\otimes h_{t-1}\end{pmatrix}$$

$$z_t = \sigma\left(W_z\begin{pmatrix}x_t\\h_{t-1}\end{pmatrix}+b_f\right)$$

$$h_t = (1-z_t)\otimes h_{t-1} + z_t\otimes h'_t$$

Final memory at timestep t combines both current and previous timesteps

GRU Intuition



$$r_t = \sigma\left(W_r\begin{pmatrix}x_t\\ h_{t-1}\end{pmatrix} + b_f\right)$$

$$h'_t = \tanh W\begin{pmatrix}x_t\\ r_t \otimes h_{t-1}\end{pmatrix}$$

$$z_t = \sigma\left(W_z\begin{pmatrix}x_t\\ h_{t-1}\end{pmatrix} + b_f\right)$$

$$h_t = (1 - z_t) \otimes h_{t-1} + z_t \otimes h'_t$$

- If reset is close to 0, ignore previous hidden state
  - ➢ Allows model to drop information that is irrelevant in the future
- Update gate z controls how much of past state should matter now.
  - – If z close to 1, then we can copy information in that unit through many time steps! **Less vanishing gradient!**
- Units with short-term dependencies often have reset gates very active

Slide credit: Richard Socher

LSTMs and GRUs

Good

- Careful initialization and optimization of vanilla RNNs can enable them to learn long(ish) dependencies, but gated additive cells, like the LSTM and GRU, often just work.

Bad

- LSTMs and GRUs have considerably more parameters and computation per memory cell than a vanilla RNN, as such they have less memory capacity per parameter*

Next Lecture:
Attention and Transformers