DD2437 – Artificial Neural Networks and Deep Architectures (annda)

Lecture 7: **Temporal processing with ANNs: feedforward vs recurrent networks**

Pawel Herman

Computational Science and Technology (CST)

KTH Royal Institute of Technology

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Lecture overview

- Temporal processing with feedforward NNs
- Recurrent architectures for sequence modelling
- Backpropagation through time (BPTT)
- Echo state networks (ESNs)
- Long short-term memory model (LSTM)

Temporal aspects

- Time is an essential component of the description of many phenomena, observations, data structures
- Omnipotence of sequences – ordering of entities
  - numerical codes
  - language and speech
  - motor behaviour
  - signals, time series: sensor readings, market prices, biological recordings etc.
- Discrete vs continuous time
- Implicit vs explicit representation

Static MLP for handling dynamics

The use of a static MLP to account for temporal dimension

- short-term memory function
- nonlinear regression capabilities

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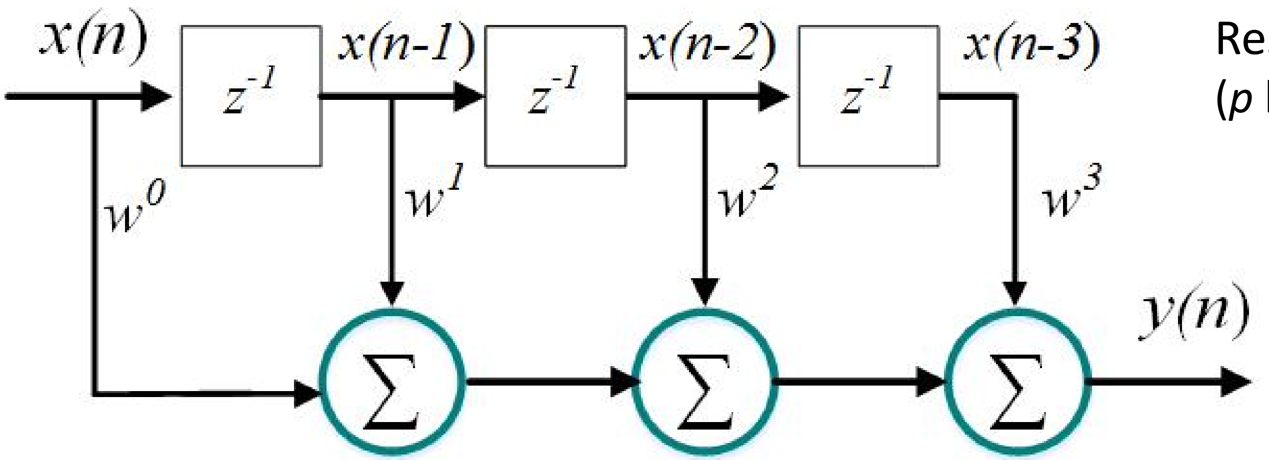
Tapped delay line memory



Memory depth = *p* (3)

Resolution = 1
(*p* lags per *p* units of time)

Static MLP for handling dynamics

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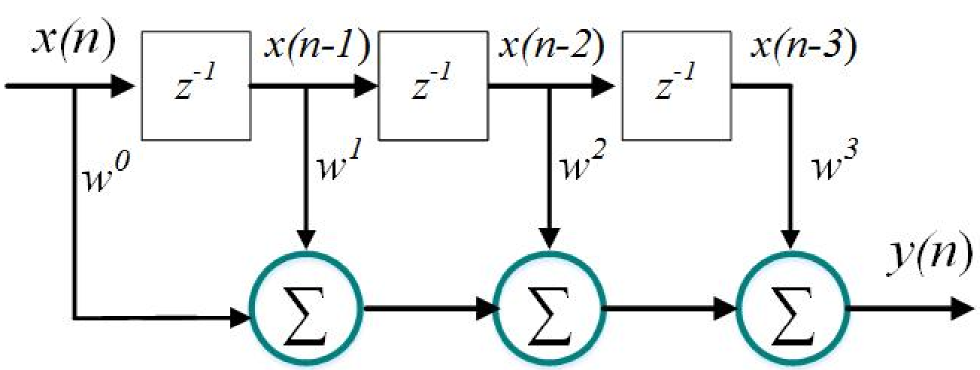
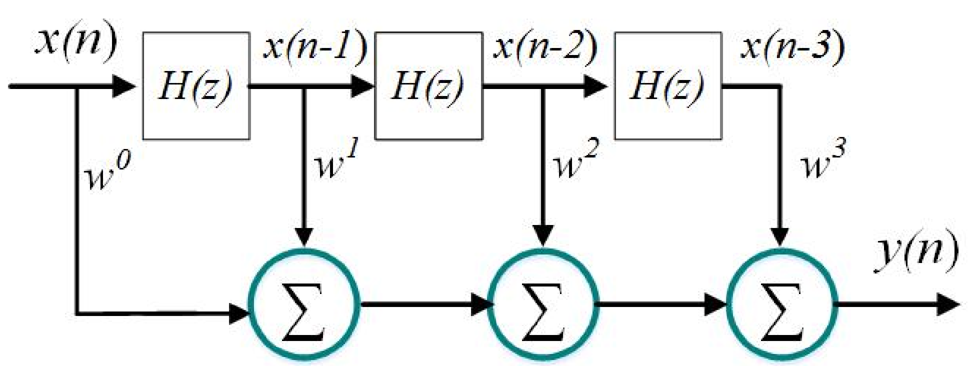
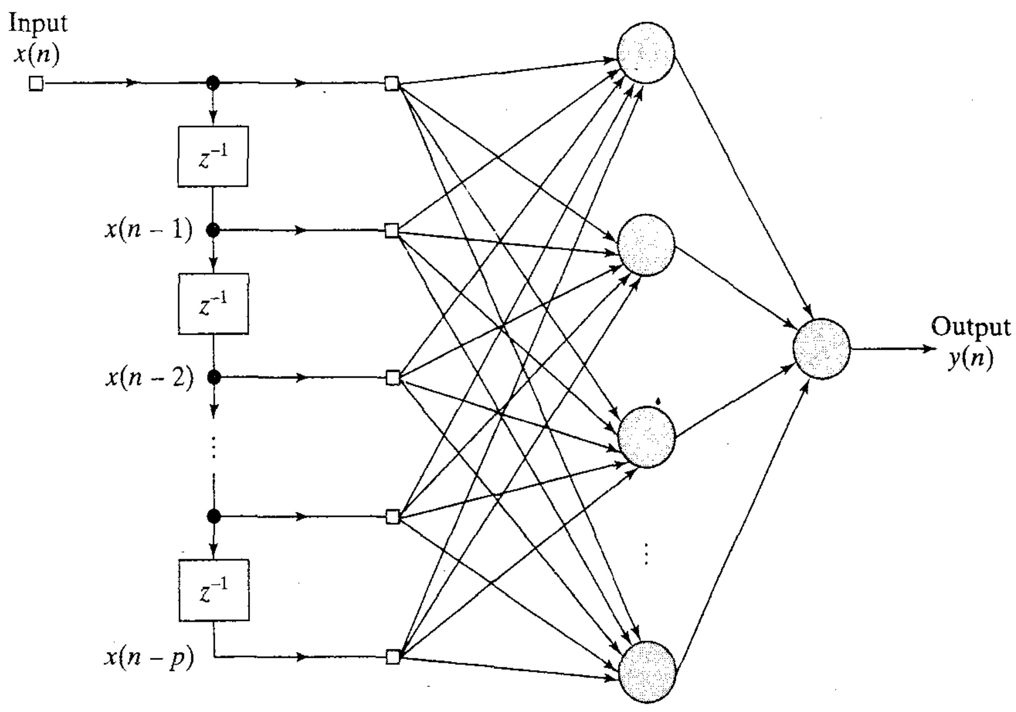


Generalized tapped delay line memory



Learning approach to TLFN

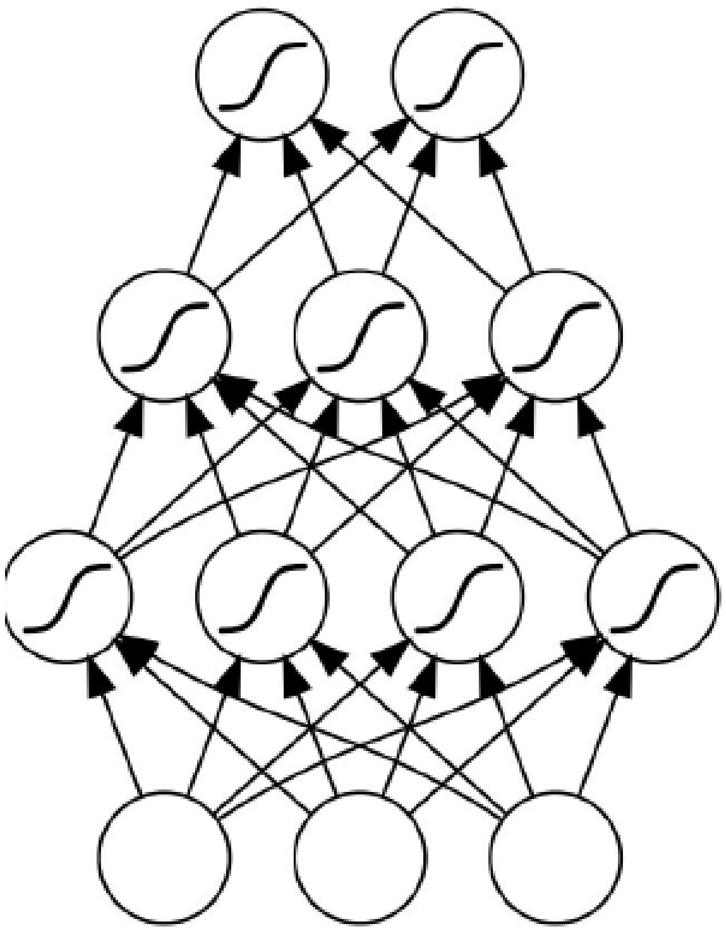


Backprop can be used with relatively simple *focused TLFNs* .

A general principle to unfold the network: form a large “static“ network, and apply backprop.

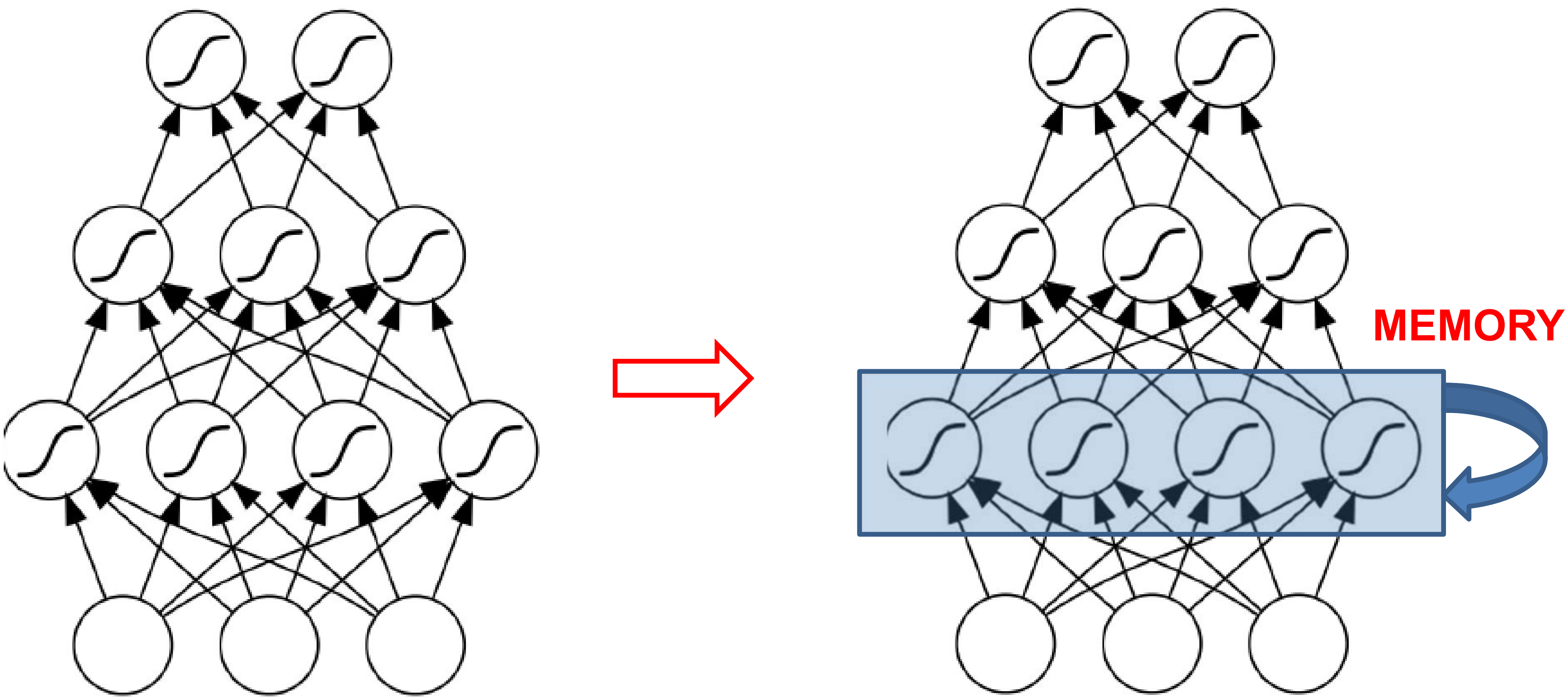
Haykin, 1999

Recurrent neural networks (RNNs)



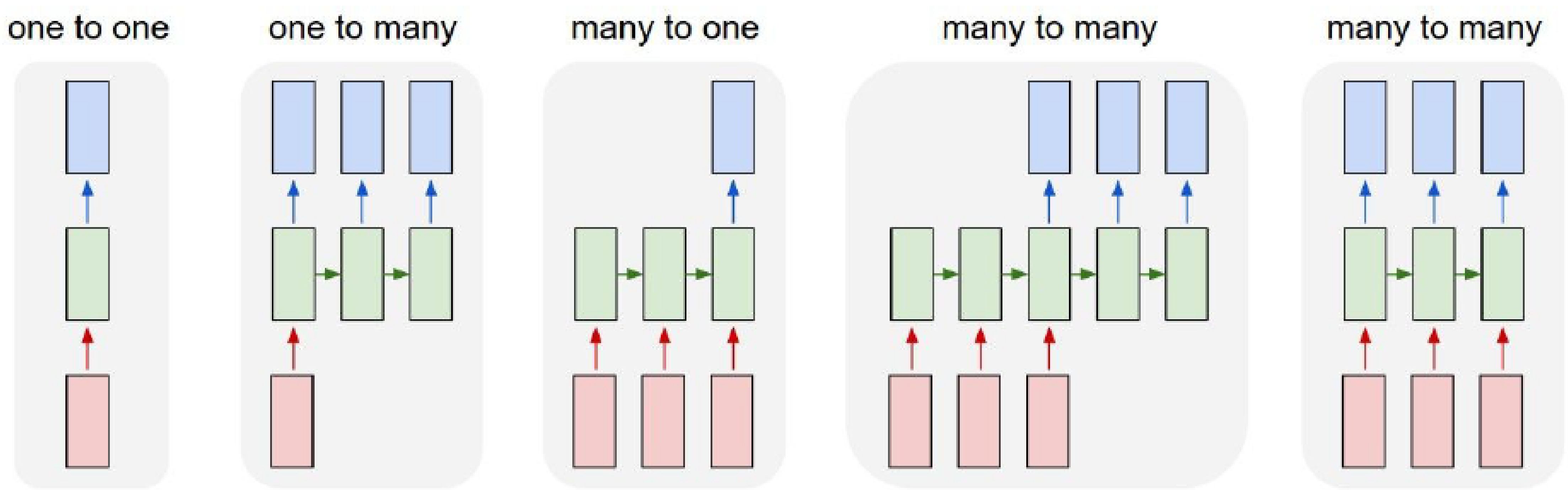
From MLP to ….

Recurrent neural networks (RNNs)



From MLP to RNN

Repertoire of recurrent architectures

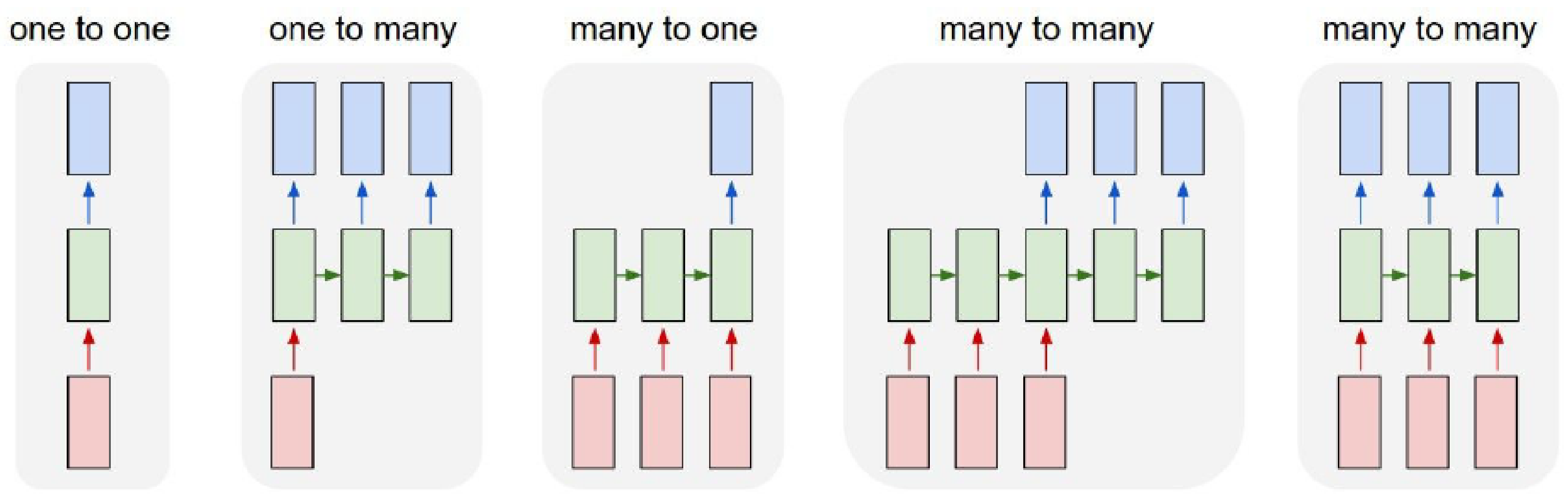


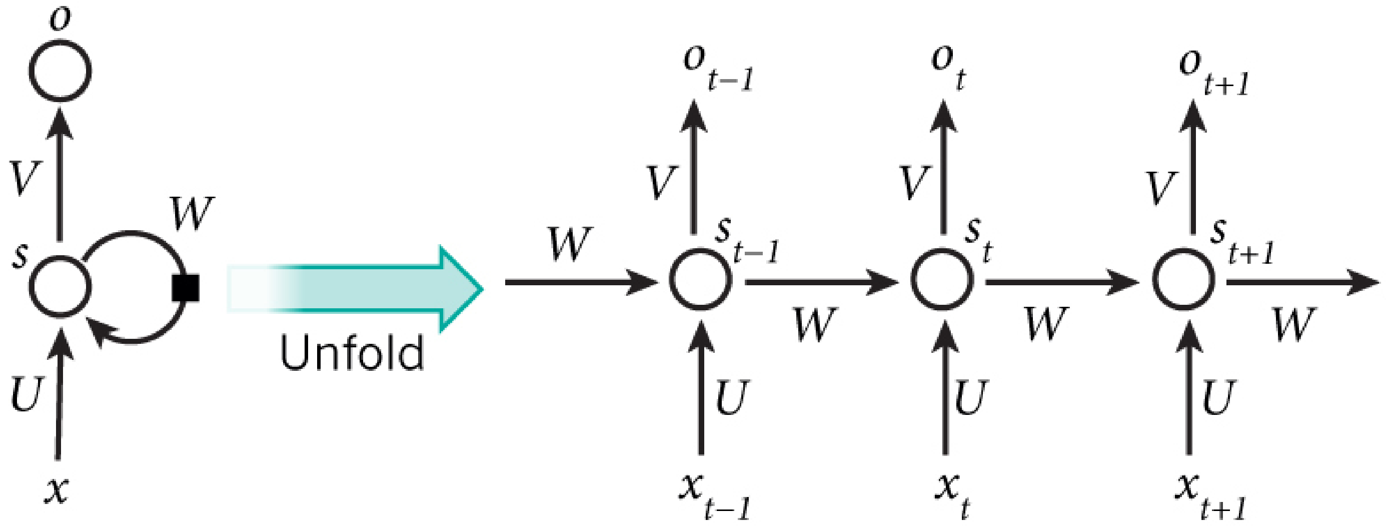
e.g. sequence generation

e.g. sentiment analysis

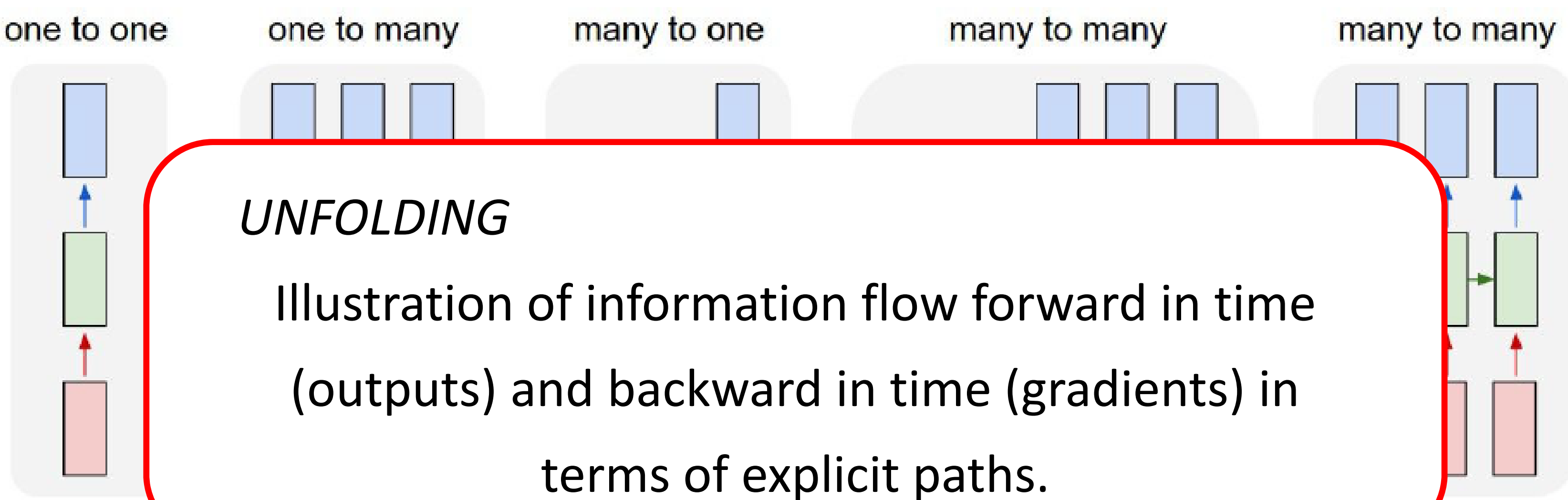
e.g. machine translation

Repertoire of recurrent architectures, unfolding



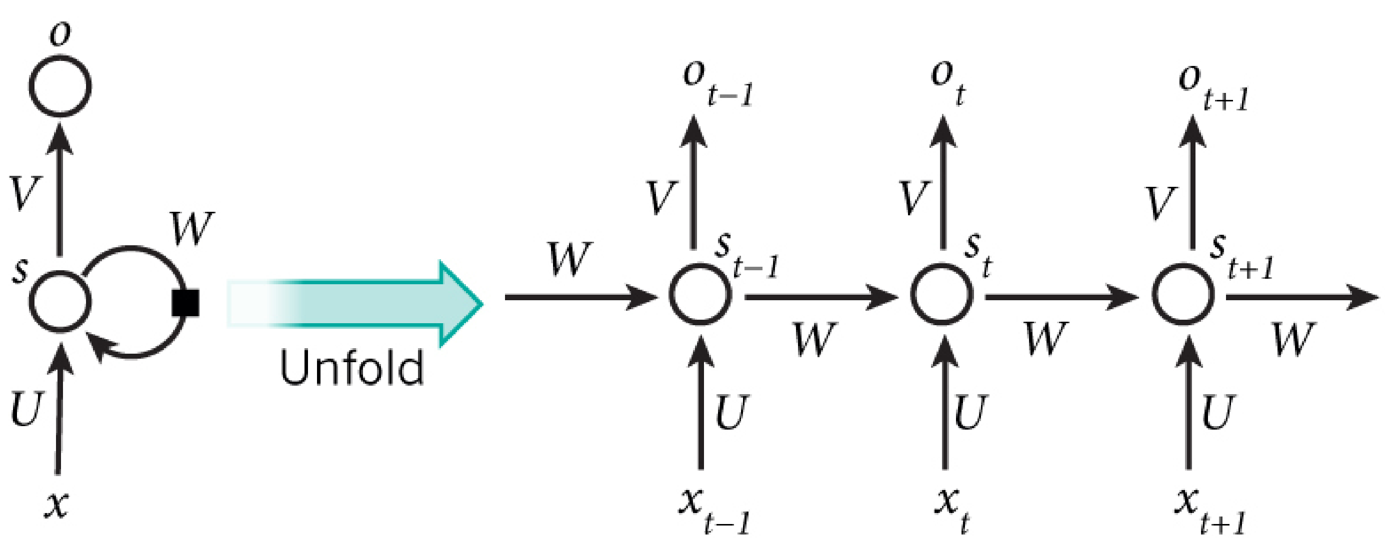


Repertoire of recurrent architectures, unfolding

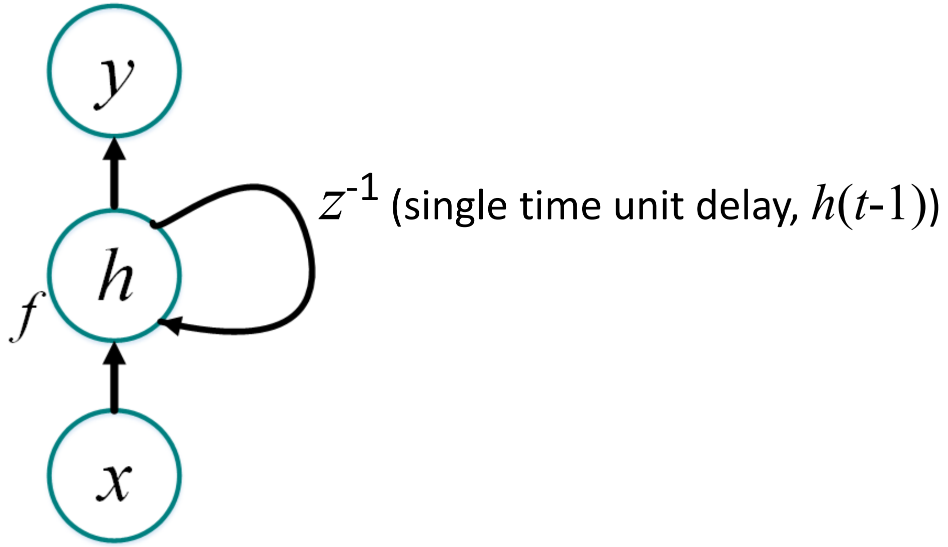


UNFOLDING

Illustration of information flow forward in time (outputs) and backward in time (gradients) in terms of explicit paths.

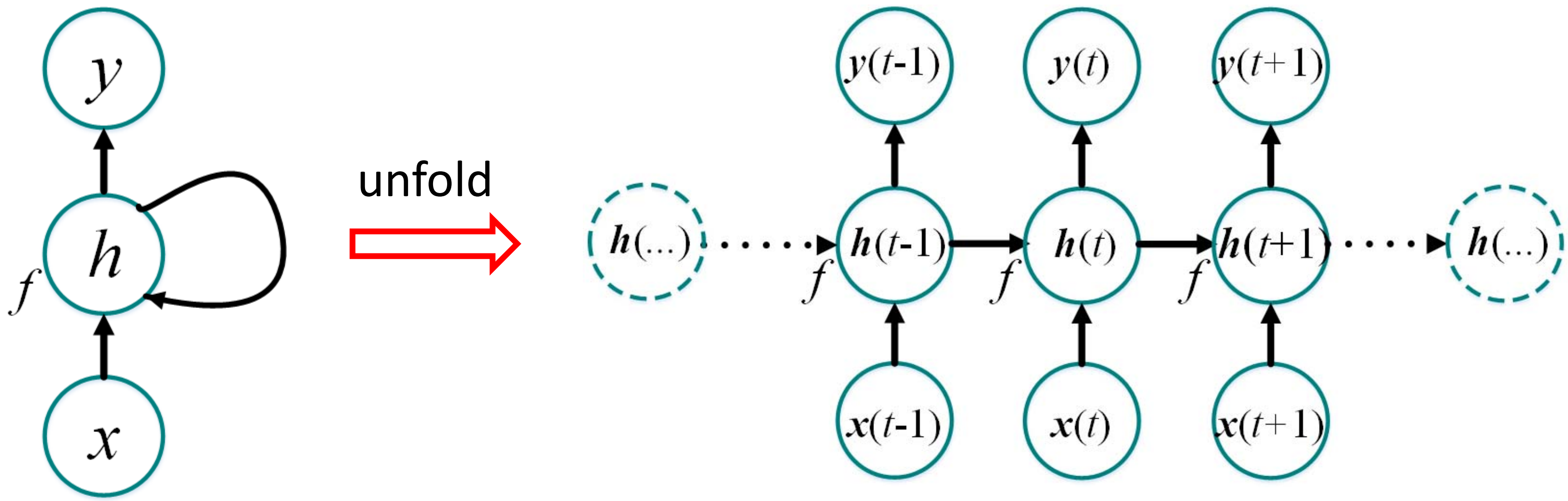


Fundamental, vanilla RNN unit



$$\boldsymbol{h}(t) = f(\boldsymbol{h}(t-1), \boldsymbol{x}(t), \boldsymbol{\theta})$$

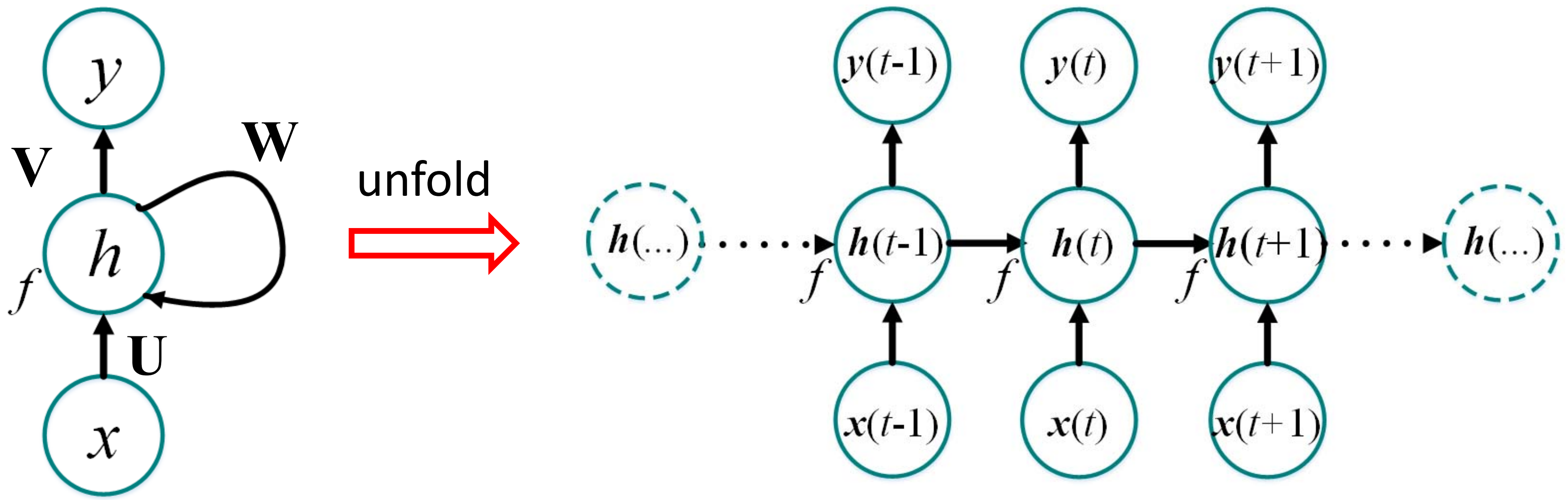
Fundamental, vanilla RNN – unfolded



$$\boldsymbol{h}(t) = f(\boldsymbol{h}(t-1), \boldsymbol{x}(t), \boldsymbol{\theta})$$

In a canonical form it allows for modelling sequences of varying length (though there are problems of technical nature).

Recurrent connections between hidden units

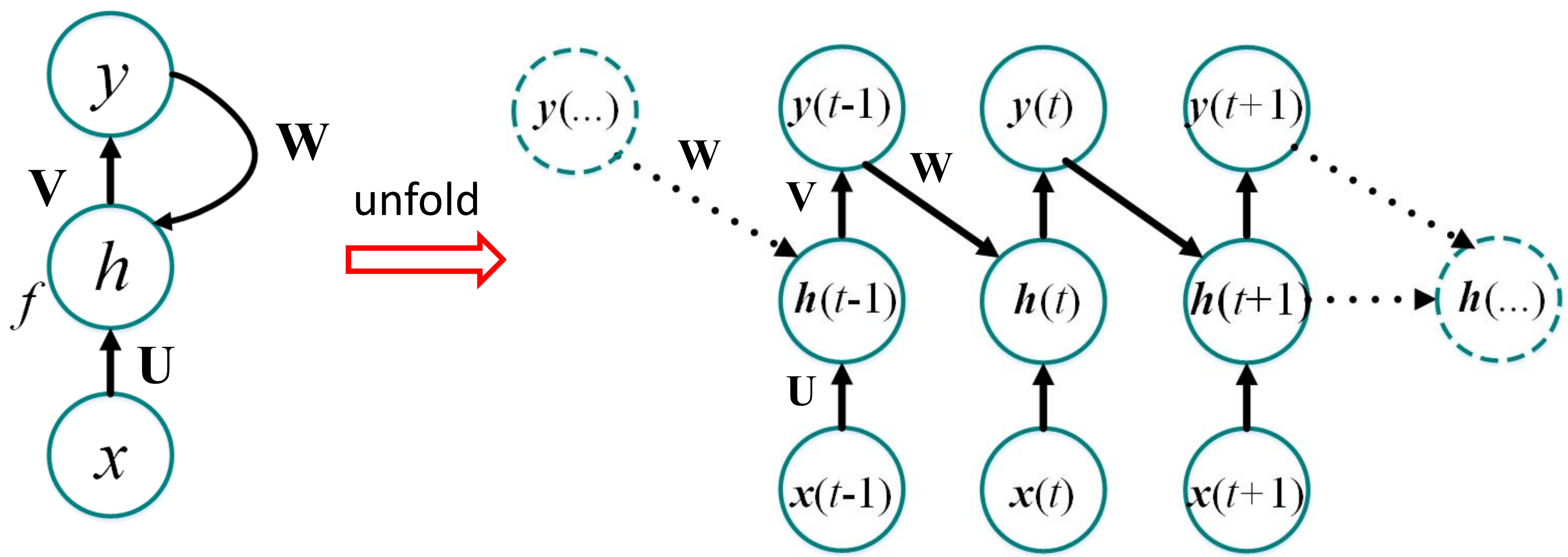


$$\boldsymbol{h}(t) = f(\mathbf{W}\boldsymbol{h}(t-1) + \mathbf{U}\boldsymbol{x}(t) + bias)$$

$$\boldsymbol{y}(t) = \mathbf{V}\boldsymbol{h}(t) + bias$$

state-space description

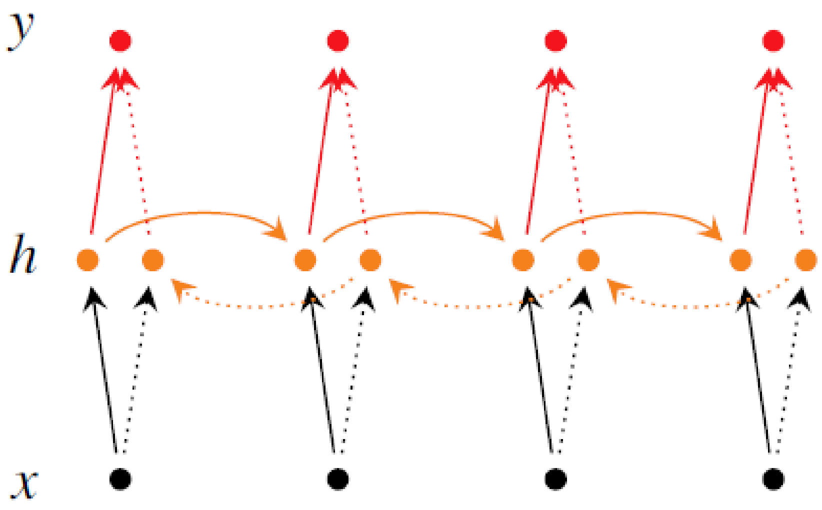
Recurrent connection from output to hidden units



$$\boldsymbol{h}(t) = f(\mathbf{W}\boldsymbol{y}(t-1) + \mathbf{U}\boldsymbol{x}(t) + bias)$$

$$\boldsymbol{y}(t) = \mathbf{V}\boldsymbol{h}(t) + bias$$

…. bidirectional neural networks



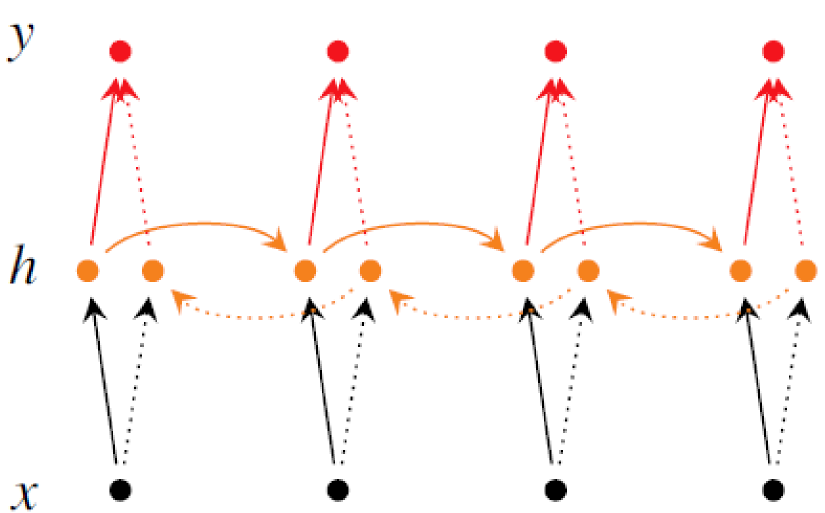
$$\overrightarrow{h}_t = f(\overrightarrow{W}x_t + \overrightarrow{V}\overrightarrow{h}_{t-1} + \overrightarrow{b})$$

$$\overleftarrow{h}_t = f(\overleftarrow{W}x_t + \overleftarrow{V}\overleftarrow{h}_{t+1} + \overleftarrow{b})$$

$$y_t = g(U[\overrightarrow{h}_t;\overleftarrow{h}_t] + c)$$

To incorporate information from words or phonemes both preceding and following, e.g. where there is clear dependency of phonemes/words on the following neighbouring phonemes/words

Shallow vs deep bidirectional neural networks



$$\vec{h}_t = f(\overrightarrow{W} x_t + \vec{V}\vec{h}_{t-1} + \vec{b})$$

$$\overleftarrow{h}_t = f(\overleftarrow{W} x_t + \overleftarrow{V}\overleftarrow{h}_{t+1} + \overleftarrow{b})$$

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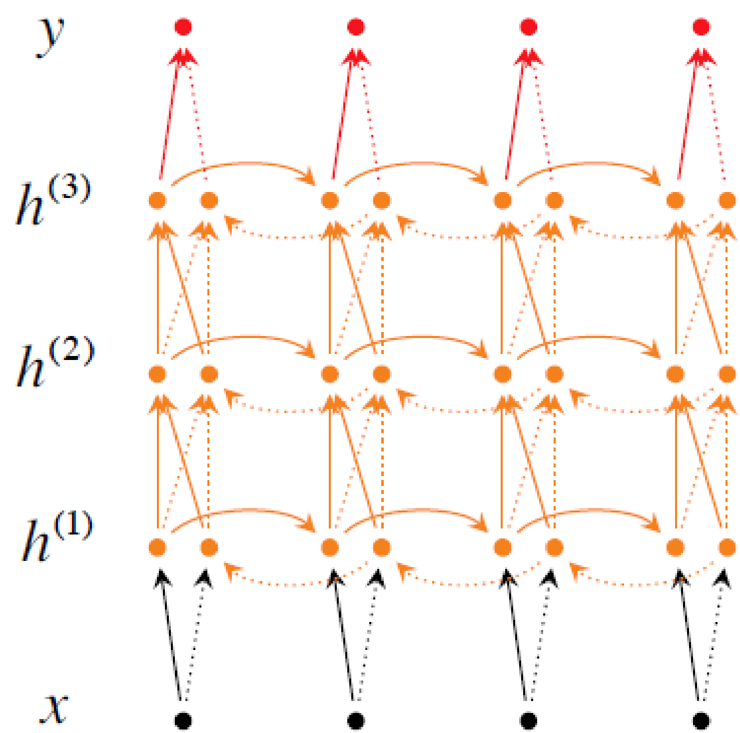


$$\vec{h}_t^{(i)} = f(\overrightarrow{W}^{(i)} h_t^{(i-1)} + \vec{V}^{(i)}\vec{h}_{t-1}^{(i)} + \vec{b}^{(i)})$$

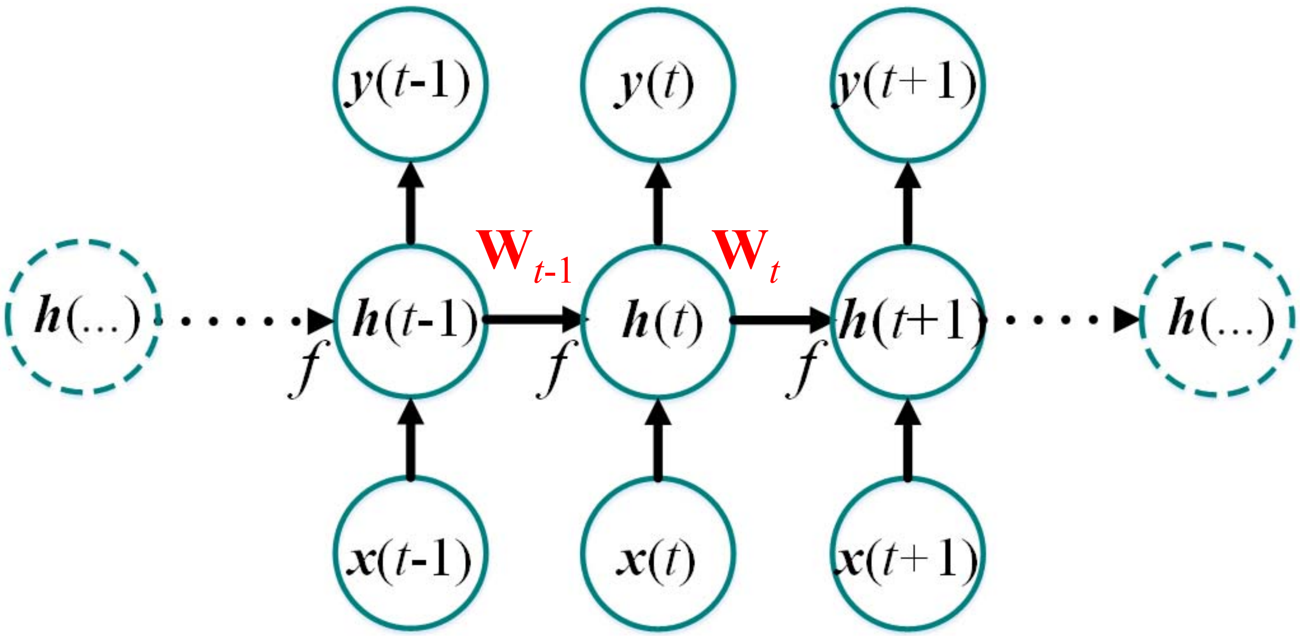
$$\overleftarrow{h}_t^{(i)} = f(\overleftarrow{W}^{(i)} h_t^{(i-1)} + \overleftarrow{V}^{(i)}\overleftarrow{h}_{t+1}^{(i)} + \overleftarrow{b}^{(i)})$$

$$y_t = g(U[\vec{h}_t^{(L)};\overleftarrow{h}_t^{(L)}] + c)$$

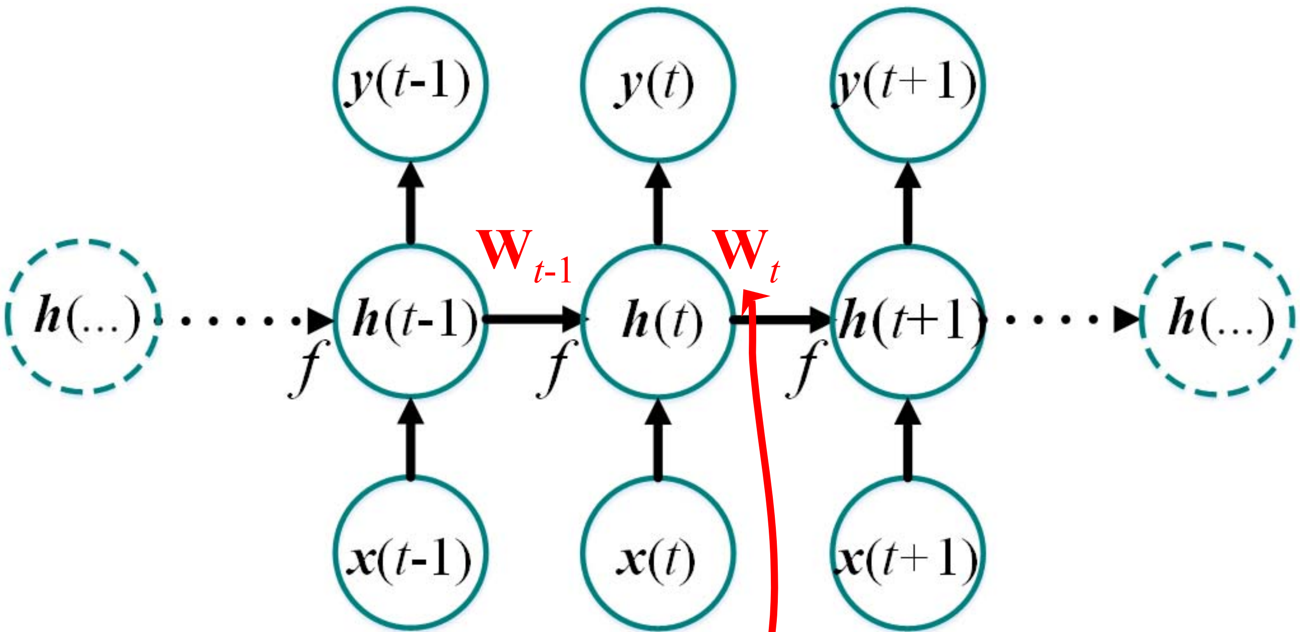
Learning algorithms for RNNs

- Epochwise vs continuous training
  - "epoch" corresponds to a data sample – a sequence
  - RNN activity reset between epochs (in epochwise training)
- Backpropagation through time (unfolding into an MLP) can be both applied epochwise and in a continuous fashion

Backpropagation through time



Backpropagation through time

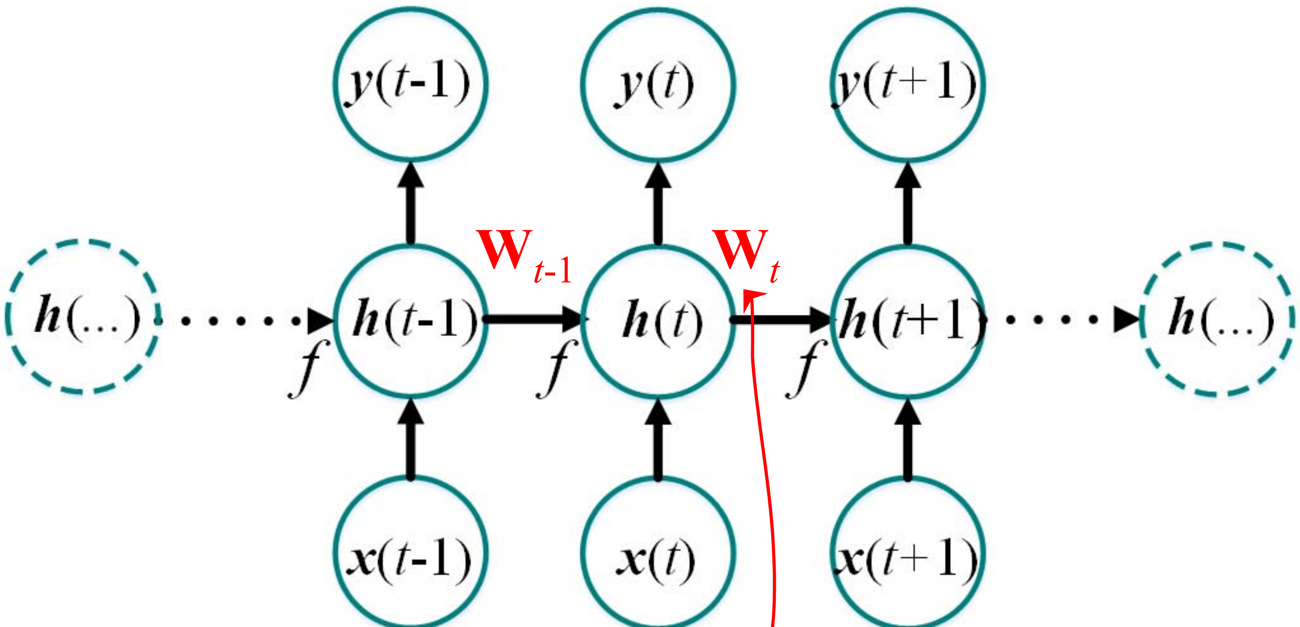


shared duplicated weights

Essentially,

$\mathbf{W}=\mathbf{W}_t$, $\mathbf{W} = \mathbf{W}_{t\text{-}1}$ etc.

Backpropagation through time



shared duplicated weights

Essentially,

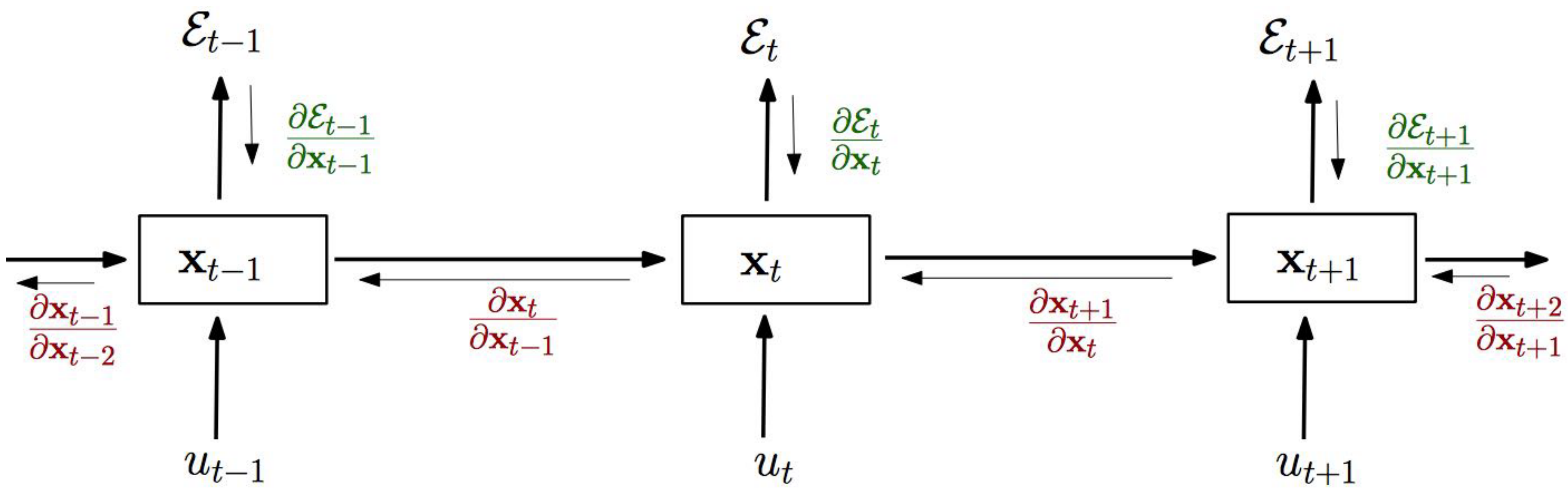
$\mathbf{W}=\mathbf{W}_t$, $\mathbf{W} = \mathbf{W}_{t\text{-}1}$ etc.

So: $$\underbrace{\frac{\partial E}{\mathrm{W}} = \frac{\partial E}{\mathrm{W}_t} + \frac{\partial E}{\mathrm{W}_{t-1}} + \ldots.}_{\#\text{time steps in a training sample}}$$

Backpropagation through time

For each pair of input-output sequences, the error is defined and n refers to the index over the duration of sequences (not the number of samples):

$$E = \sum_{n=1}^{T} (d(n) - y(n))^2 = \sum_{n=1}^{T} \varepsilon_n^2$$



<u>Please note:</u> According to our earlier notation, $\boldsymbol{x}$ should be $\boldsymbol{h}$ and u should be x.

Backpropagation through time

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We can also think of this training algorithm in the time domain (*Hinton, 2013*):

- FORWARD PASS: a stack of the activities of all the units at each time step.
- BACKWARD PASS: activities are peeled off the stack to compute the error derivatives at each time step.
- THEN we add together the derivatives at all the different times for each weight.

Backpropagation through time

For each pair of input-output sequences, the error is defined and n refers to the index over the duration of sequences (not the number of samples):

$$E = \sum_{n=1}^{T} (d(n) - y(n))^2 = \sum_{n=1}^{T} \varepsilon_n^2$$

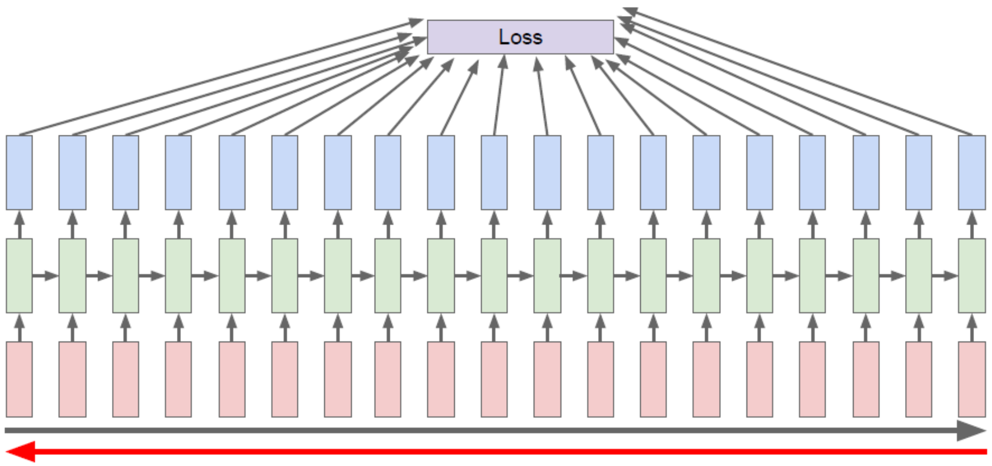
Comments:

- epoch refers here to a single pair of input-output sequences
- if there are backprojections from the output to hidden layer, teacher output $d(n)$ can be used in the computation of activations in layer n+1 in the forward pass
  - o teacher forcing is likely to speed the convergence
  - o if it is exploited for the trained network however it may exhibit instability
- BPTT does not scale too well and may not converge even to the local minimum
- BPTT may result in instability

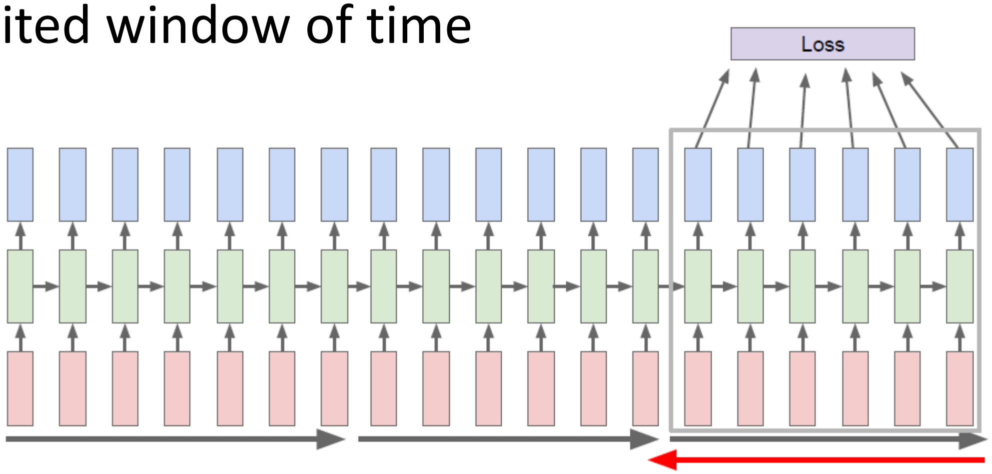
Backpropagation through time – online with truncation

Truncated BPTT for “online” learning

- if there are no batches and the network is supposed to work continuously, the number of recursive steps for weight updates has to be finite
- beyond the truncation there is no memory effect



with *truncation* backpropagate loss within a limited window of time



For more details, please see Haykin and Goodfellow et al.

Other learning algorithms for RNNs

- Real-time recurrent learning (Williams & Zipser, 1989)
  - the exact gradients are calculated and the synaptic updates are made at every step during network's processing stage
  - very high computational cost
- Kalman filters (*optimal filtering*)
  - solid theory formulated in the state-space concepts
  - rather than instantaneously estimate gradients, the network state is recursively estimated based on input data
  - the network has to be linearised
- Extended Kalman filter (*decoupled*)

Long-term dependencies problem

Vanishing (more rarely exploding) gradients for recurrent networks

$$\boldsymbol{h}(t) = \mathbf{W}^{\mathrm{T}}\boldsymbol{h}(t-1) \Rightarrow \boldsymbol{h}(t) = (\mathbf{W}^{t})^{\mathrm{T}}\boldsymbol{h}(0)$$

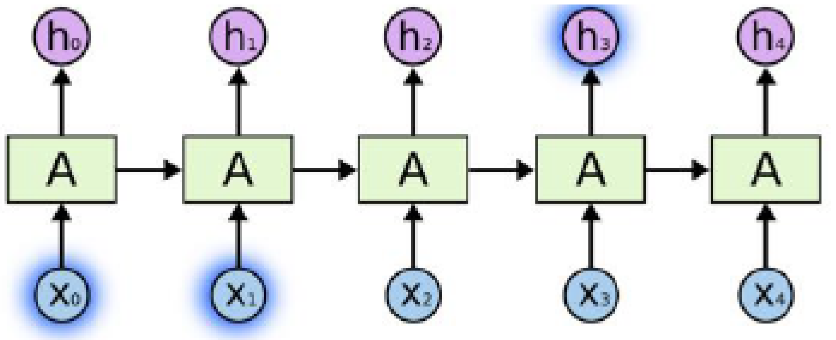
$$\mathbf{W} = \mathbf{Q}\boldsymbol{\Lambda}\mathbf{Q}^{\mathrm{T}} \Rightarrow \boldsymbol{h}(t) = \mathbf{Q}^{\mathrm{T}}\boldsymbol{\Lambda}^{t}\mathbf{Q}\,\boldsymbol{h}(0)$$

Eigenvalues are usually less than 1

Long-term dependencies problem

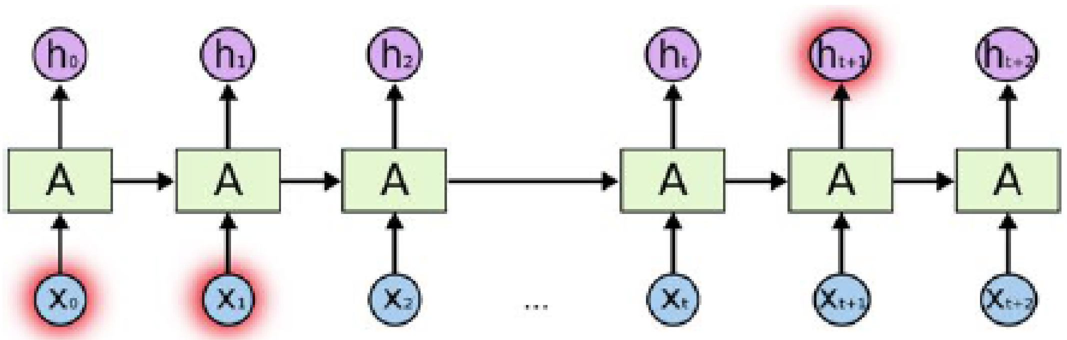
Handling (predicting) close words:

"The *clouds* are in the *sky*."



Problem with the need for wider context:

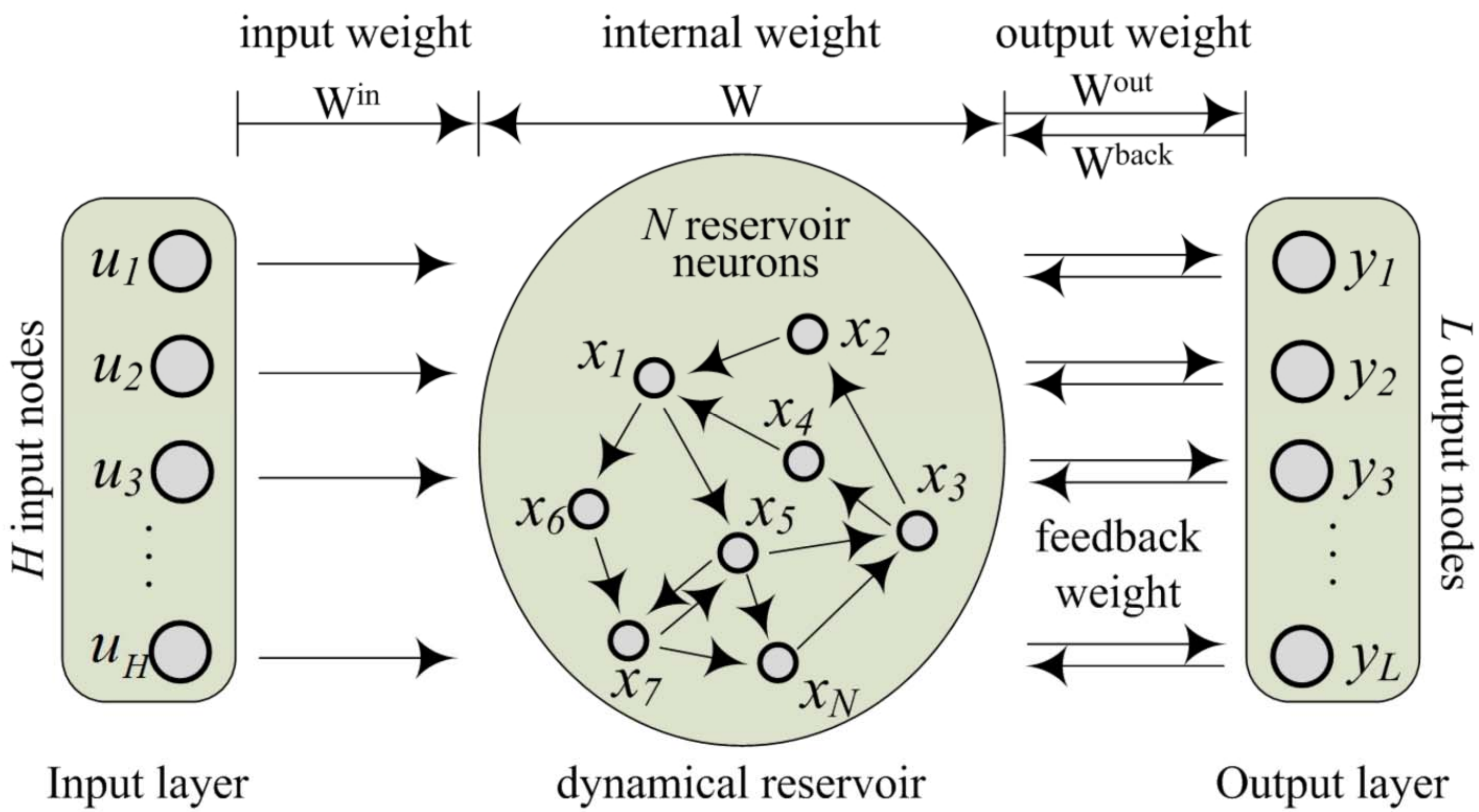
"I grew up in *France*… I speak fluent *French*."



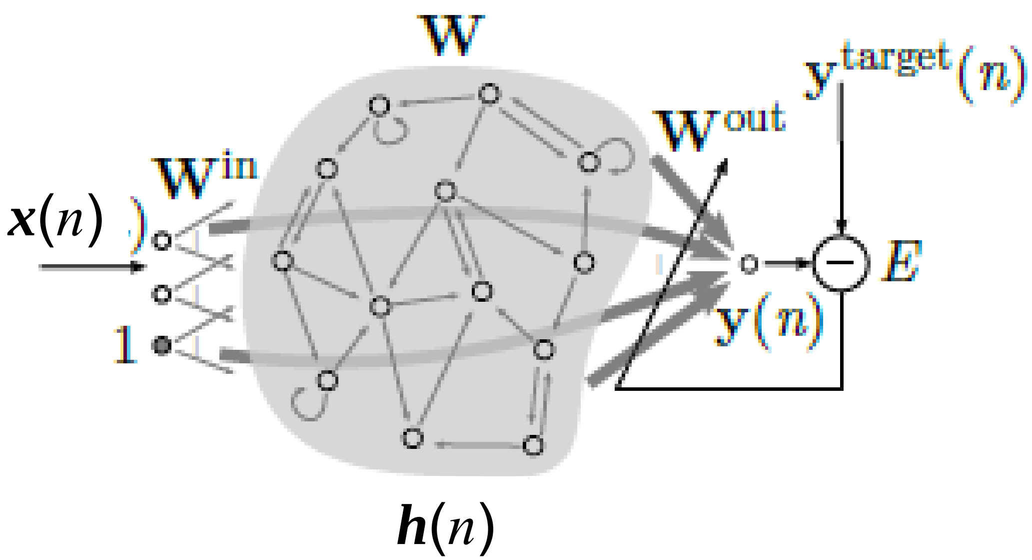
Reservoir computing

Echo state network

(non-spiking version of liquid state machine)



Reservoir computing – fundamentals



biases

$$\boldsymbol{y}(n) = \mathbf{W}^{out}\left[1; \boldsymbol{h}(n); \boldsymbol{x}(n)\right]$$

$$\tilde{\boldsymbol{h}}(n) = \tanh(\mathbf{W}_{in}\left[1; \boldsymbol{x}(n)\right] + \mathbf{W}\boldsymbol{h}(n-1))$$

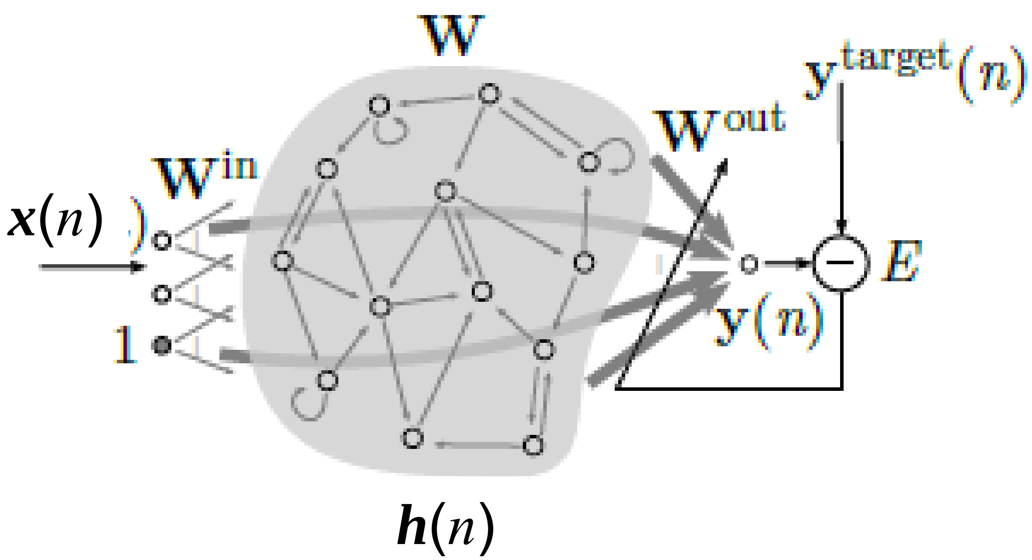
$$\boldsymbol{h}(n) = (1-\alpha)\boldsymbol{h}(n-1) + \alpha\tilde{\boldsymbol{h}}(n)$$

$$\mathbf{W} \in \mathbb{R}^{N_x \times N_x}$$

$$\mathbf{W}_{in} \in \mathbb{R}^{N_x \times (1+N_u)}$$

$$\mathbf{W}^{out} \in \mathbb{R}^{N_y \times (1+N_h+N_x)}$$

Reservoir computing – fundamentals



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extra *feedback* projections from the output to the hidden layer

$$\mathbf{W} \in \mathbb{R}^{N_x \times N_x}$$

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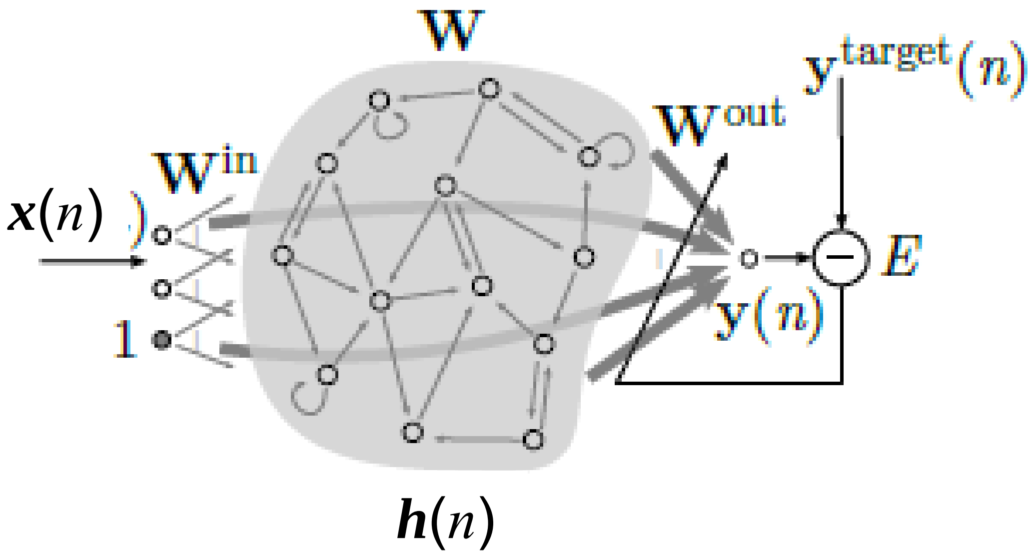

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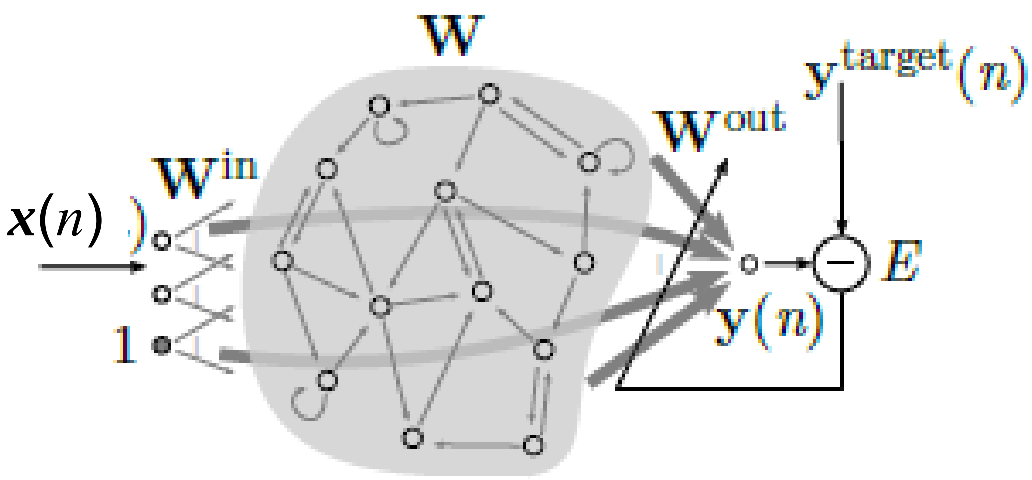
Could be used for providing feedback for training – *teacher forcing*:

$$y(n) = y^{\text{target}}(n)$$

extra *feedback* projections from the output to the hidden layer

Reservoir computing – fundamentals



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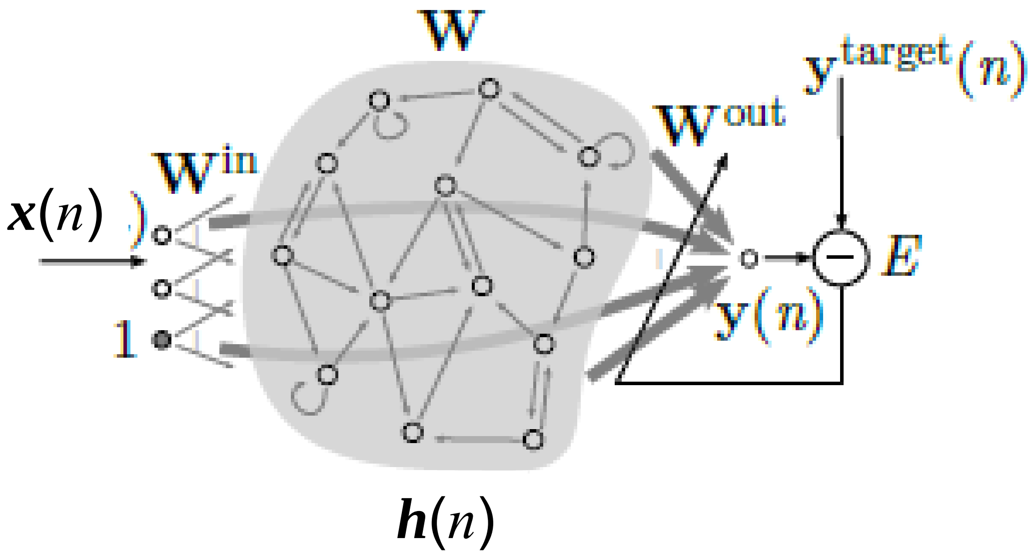
$$\boldsymbol{h}(n) = (1-\alpha)\boldsymbol{h}(n-1) + \alpha\tilde{\boldsymbol{h}}(n)$$

HOWEVER, in on-line learning the use of $y(n)$ for feedback is preferred for the stability.

extra *feedback* projections from the output to the hidden layer

Reservoir properties

Reservoir serves as a memory (temporal context) and a nonlinear expansion



Key parameters: .

- size (N_x) (the bigger the better, even in the order of 10k)

- sparsity (2-20%) and the distribution of nonzero elements (uniform distribution)

- spectral radius, ρ (less than 1 to be near the edge of stability)

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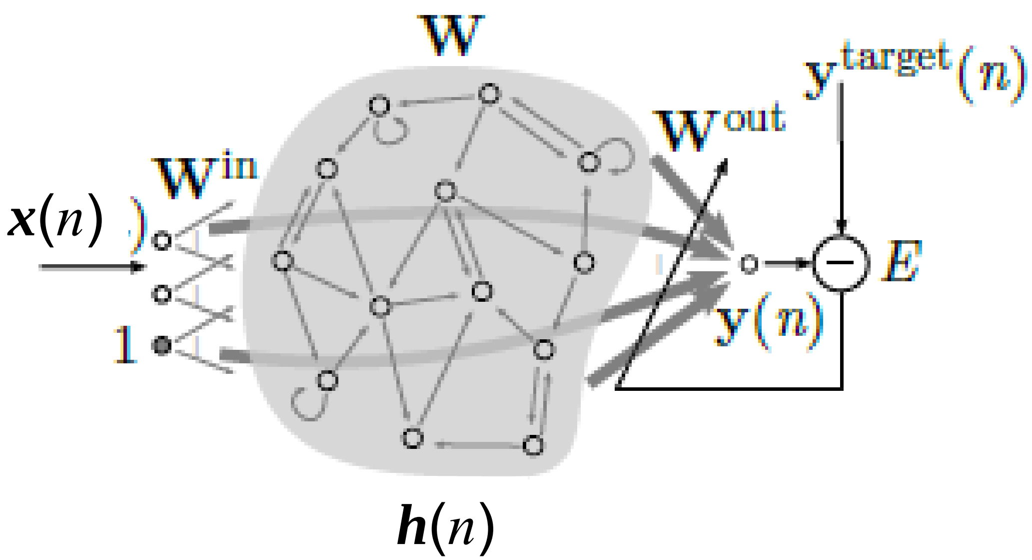

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- spectral radius, ρ (less than 1 to be near the edge of stability)

For nonlinear networks, the system can still be contractive and stable for ρ >1.
So, commonly in practice, $\rho \approx 3$.

Reservoir properties

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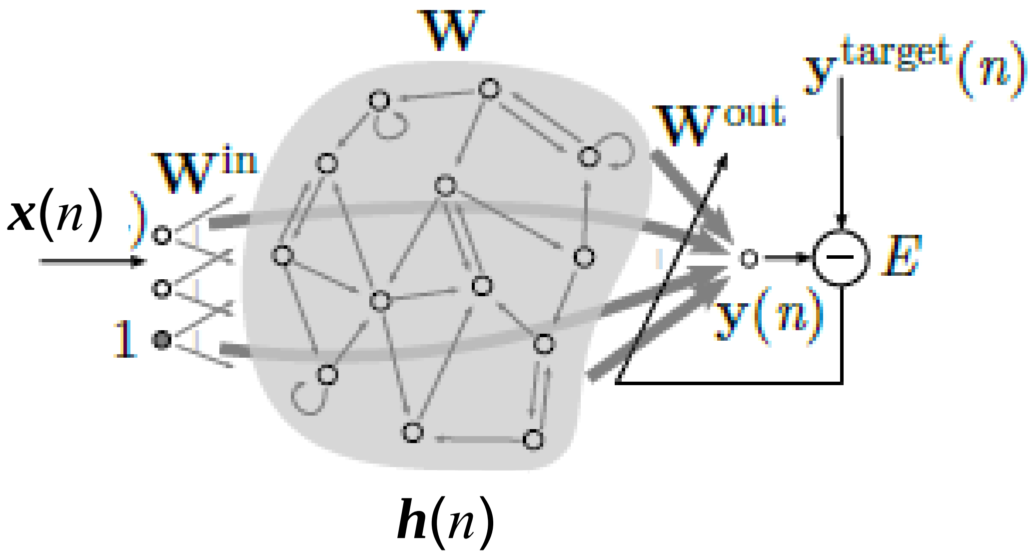
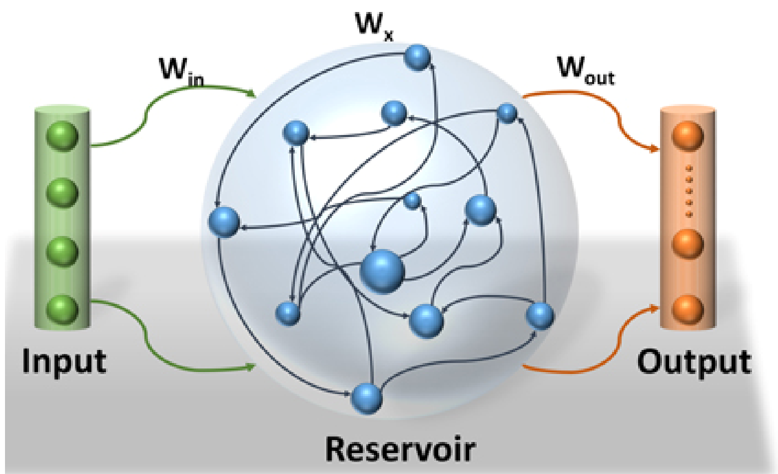


Sparse, random and fixed connections in the reservoir…



Key parameters: .

- size (N_x)
- sparsity (2-20%)
- spectral radius, ρ

….with "leaky" units

Leak modulated by α

$$h(t) = \alpha h(t-1) + (1-\alpha)x(t)$$

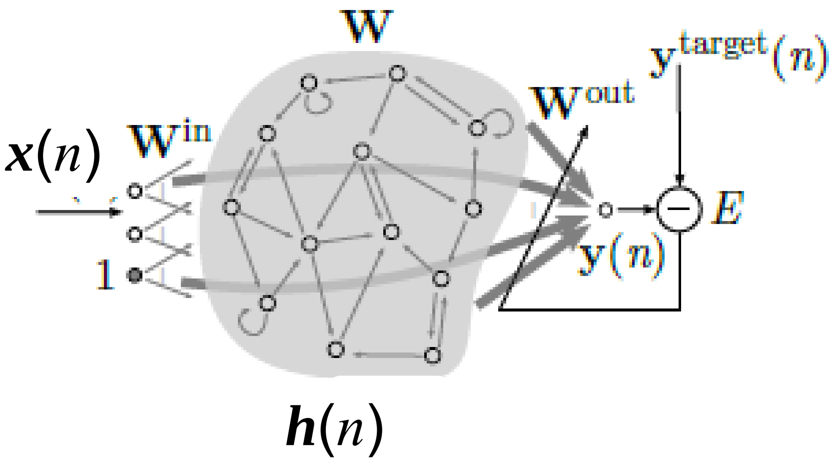
Training readouts

- One-shot learning with least mean square (LMS) error approaches
  - the design matrix is usually overdetermined -> ridge regression (regularization):

$$\mathbf{Y}^{target} = \mathbf{W}^{out}\mathbf{H} \quad \rightarrow \quad \underline{\mathbf{W}^{out} = \mathbf{Y}^{target}\mathbf{H}^{\mathrm{T}}\left(\mathbf{H}\mathbf{H}^{\mathrm{T}} + \beta\mathbf{I}\right)^{-1}}$$

  - be careful with extremely large values in **W** as they may indicate problems with stability
- Online learning with, for example, *recursive* LMS
- The need to deal with initial transients, esp. for long sequences
- Possible use of teacher forcing (forcing output data through backprojections)

Reservoir computing – overall recipe



Recipe

1. Generation of the dynamic reservoir ($\boldsymbol{W}_{in}$, $\mathbf{W}$)
2. Application of inputs, $\boldsymbol{x}(n)$, and collecting the corresponding activation states, $\boldsymbol{h}(n)$.
3. Computation of the linear output weights from the reservoir with a linear regression approach (MSE error to be minimised).
4. Use of the RNN for new data – predictions.

Reservoir computing

- set spectral radius ρ, large value means slow forgetting, e.g. storage of long time scales
- input scaling, small input means reservoir nodes operate on linear regime, large means binary operation
- output feedback weights if autonomous pattern generation needed (attractor property)
- connectivity structure: small world, distribution of loop lengths, fixed number of inputs to each node
- propagation delay on a fraction of connections

Long short-term memory (LSTM)

Main motivation behind LSTMs

- vanishing gradients when using backprop through time for RNNs
- poor capacity to handle long-term dependencies

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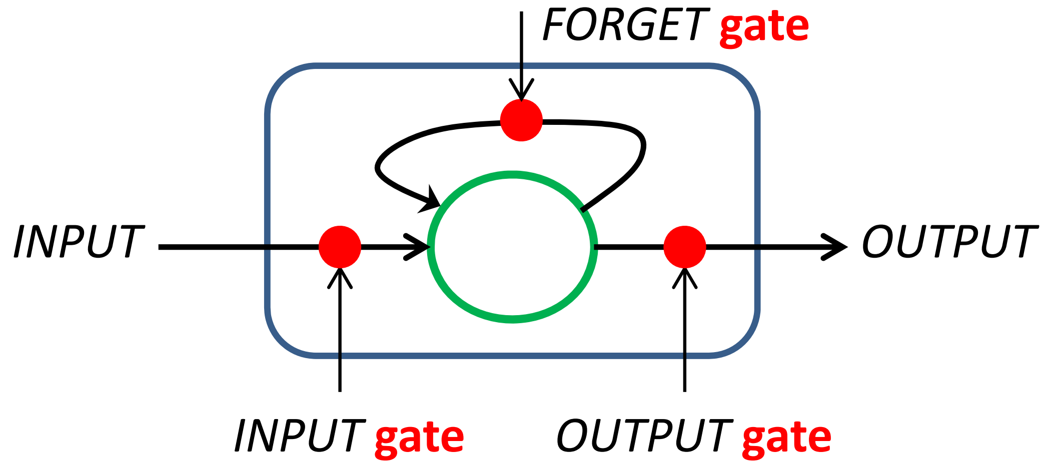

The key idea is to have a “memory cell” capable of keeping the state over time

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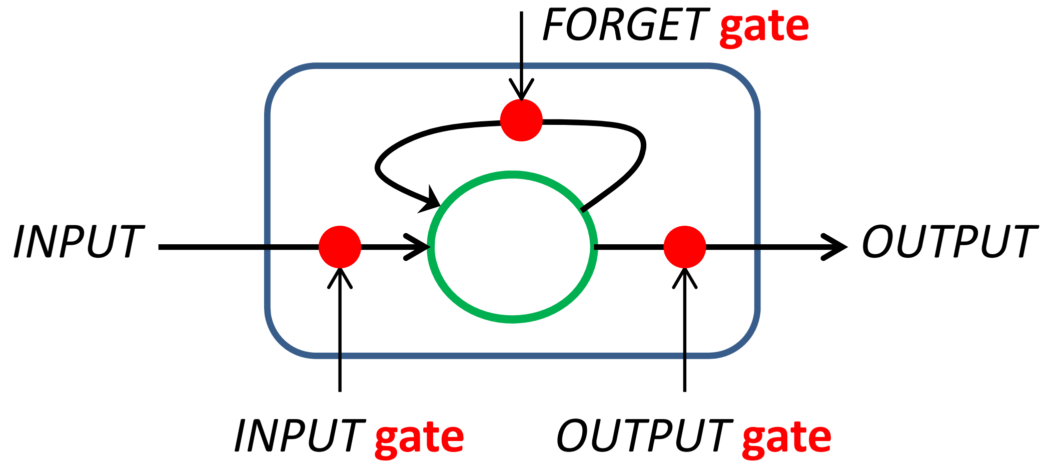


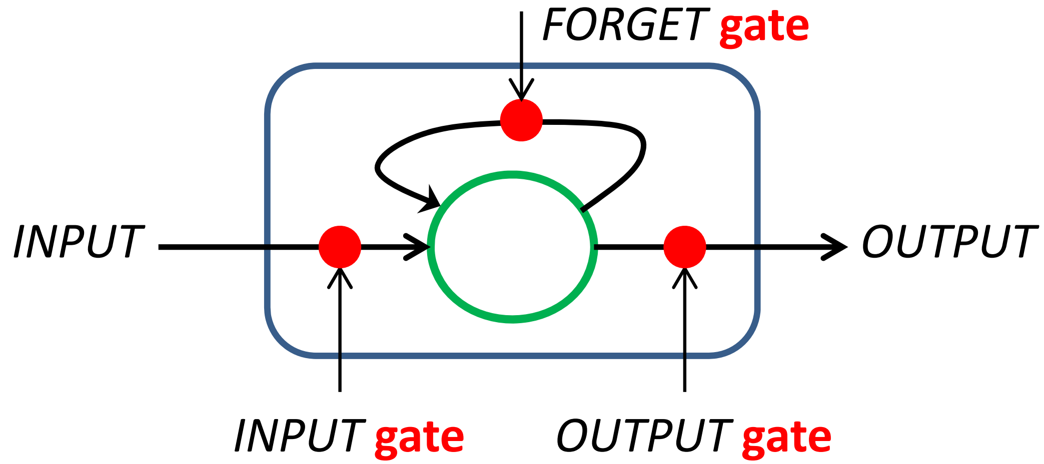
The key idea is to have a “memory cell” capable of keeping the state over time

forget gate acts like a “leak” with tuneable gain $h(t) = \alpha h(t-1) + (1-\alpha)x(t)$

Long short-term memory (LSTM)

Main motivation behind LSTMs

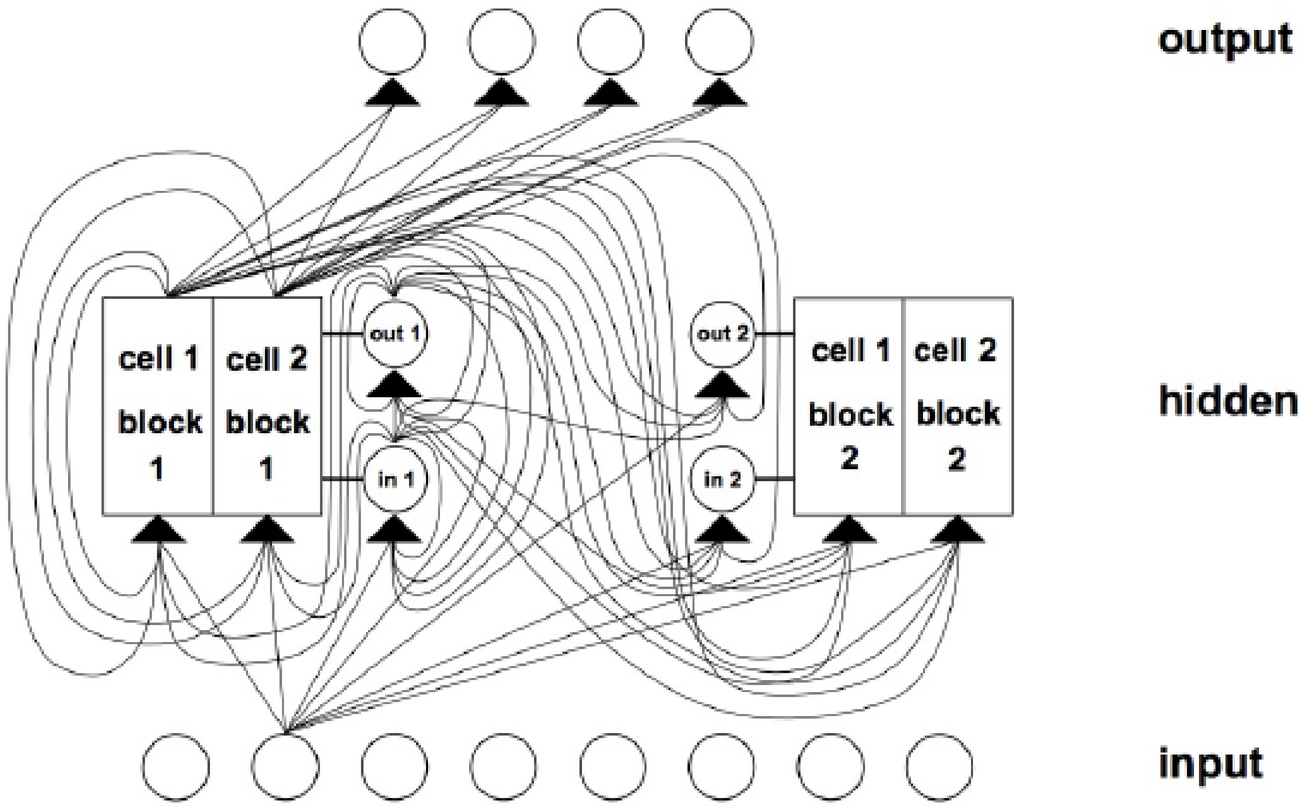
- vanishing gradients when using backprop through time for RNNs
- poor capacity to handle long-term dependencies



The key idea is to have a "memory cell" capable of keeping the state over time

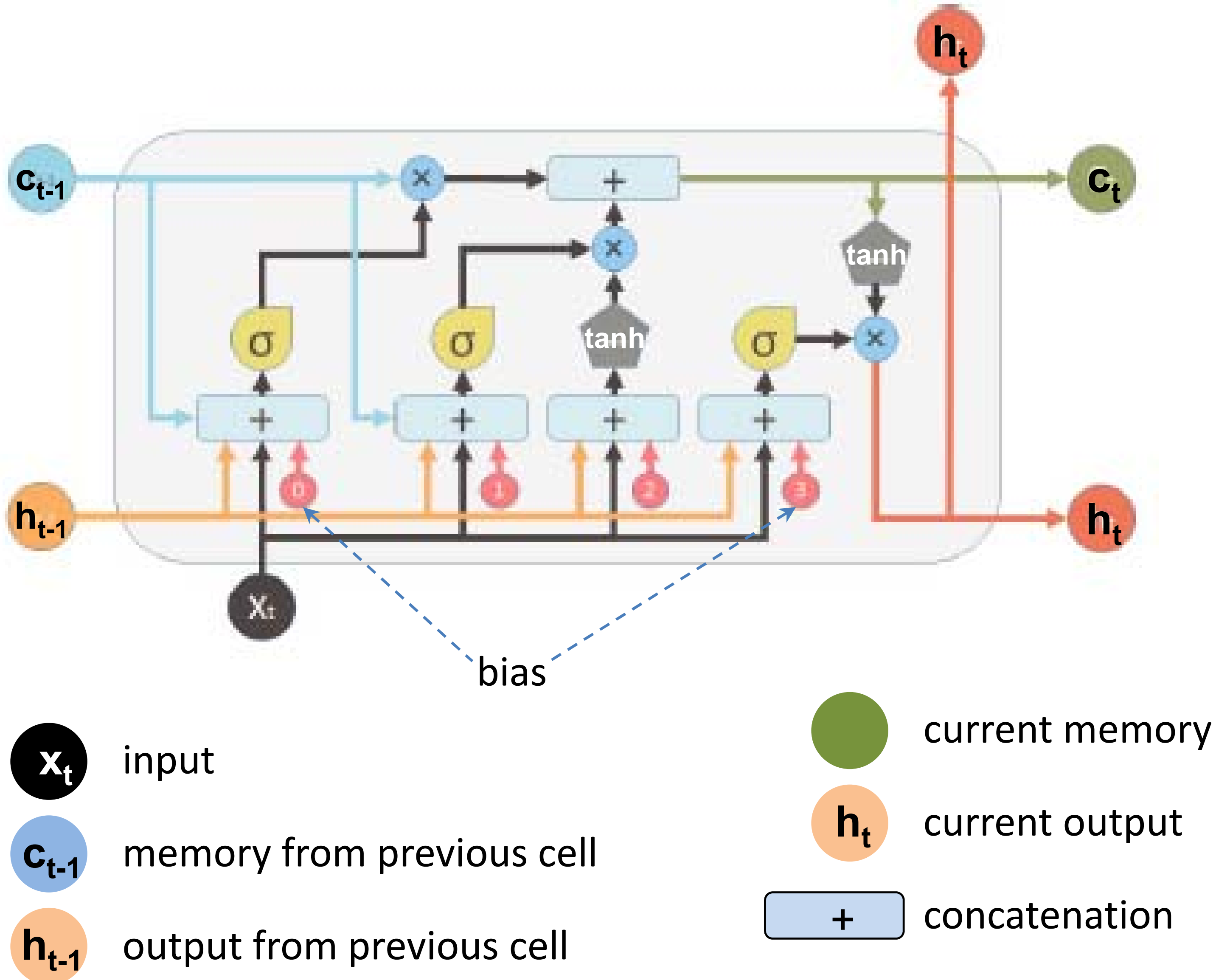
- explicit memory – **cell state vector** (on top of the *hidden* state)
- regulatory mechanism for information flow in and out – **gating unit**

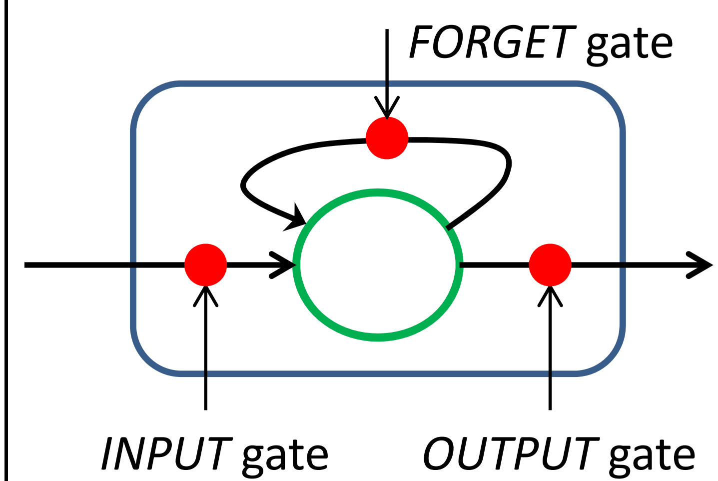
Long short-term memory (LSTM) network



Hochreiter S, Schmidhuber J. Long short-term memory. *Neural computation*. 1997 Nov 15;9(8):1735-80.

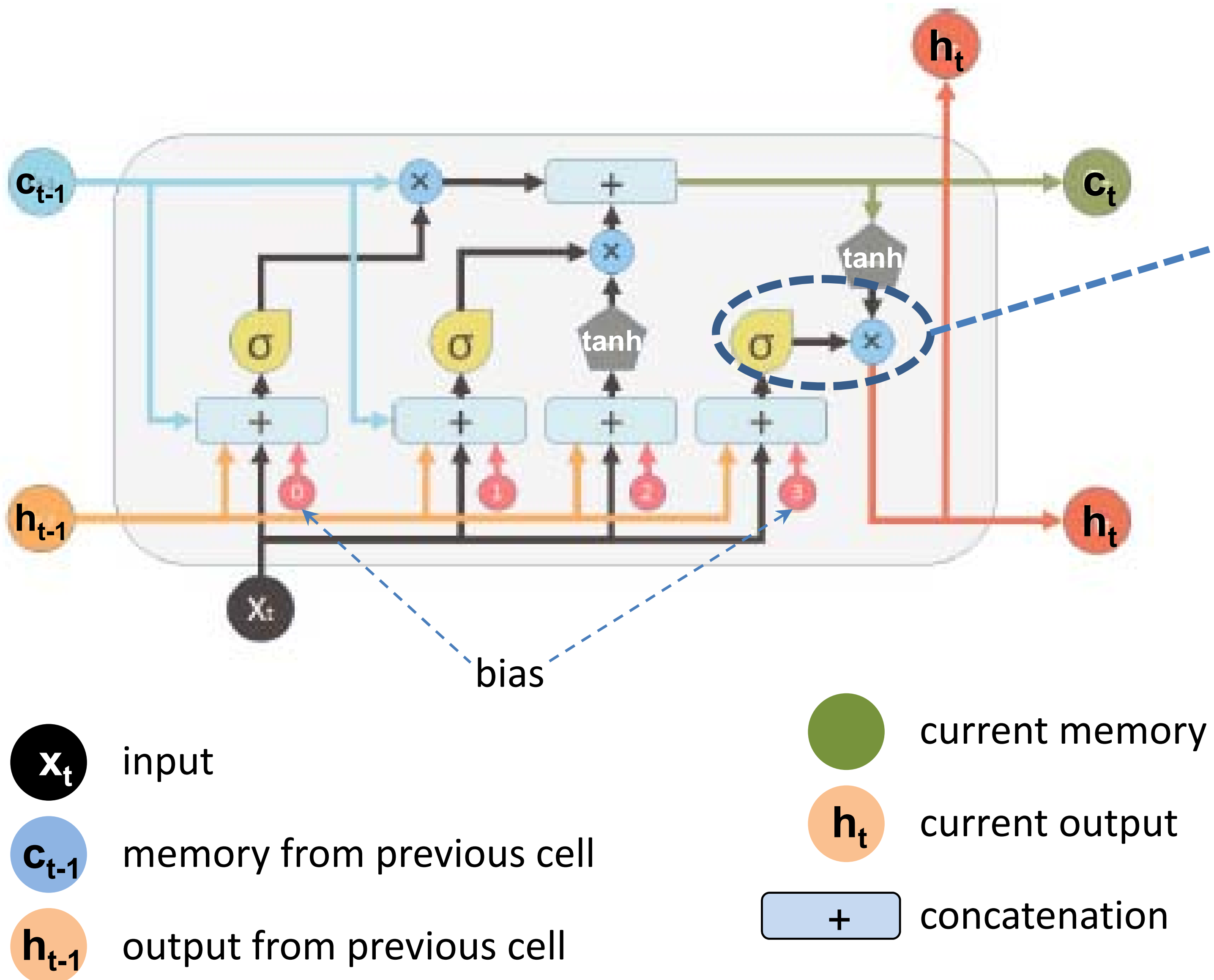
Long short-term memory (LSTM) cell

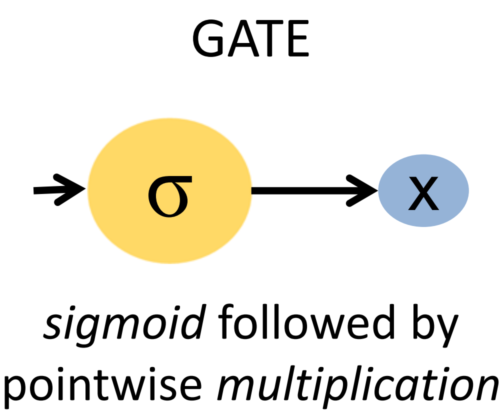


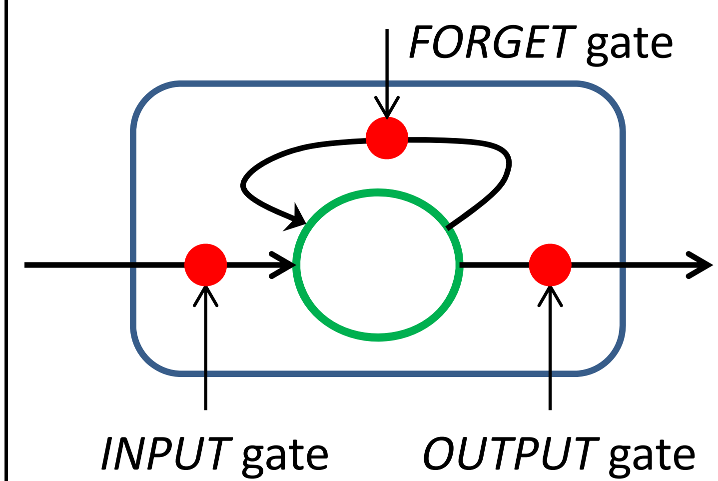


adapted from A. Sood and colah's blog

Long short-term memory (LSTM) cell

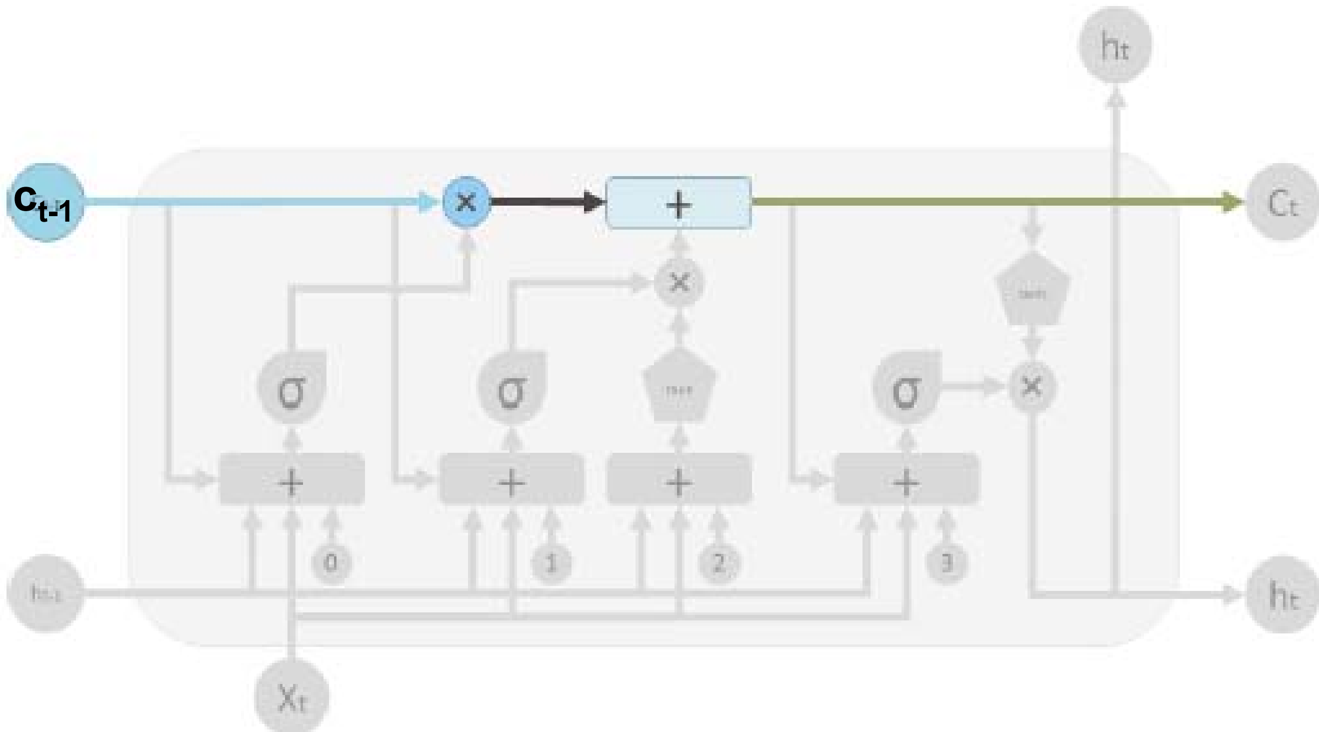




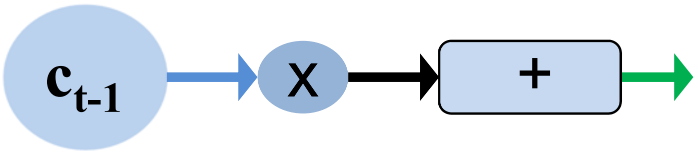


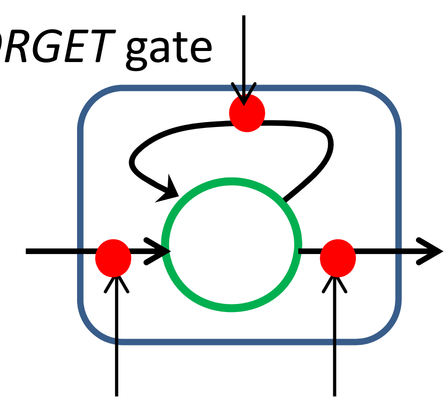
adapted from A. Sood and colah's blog

Memory cell components – cell state vector



CELL STATE vector



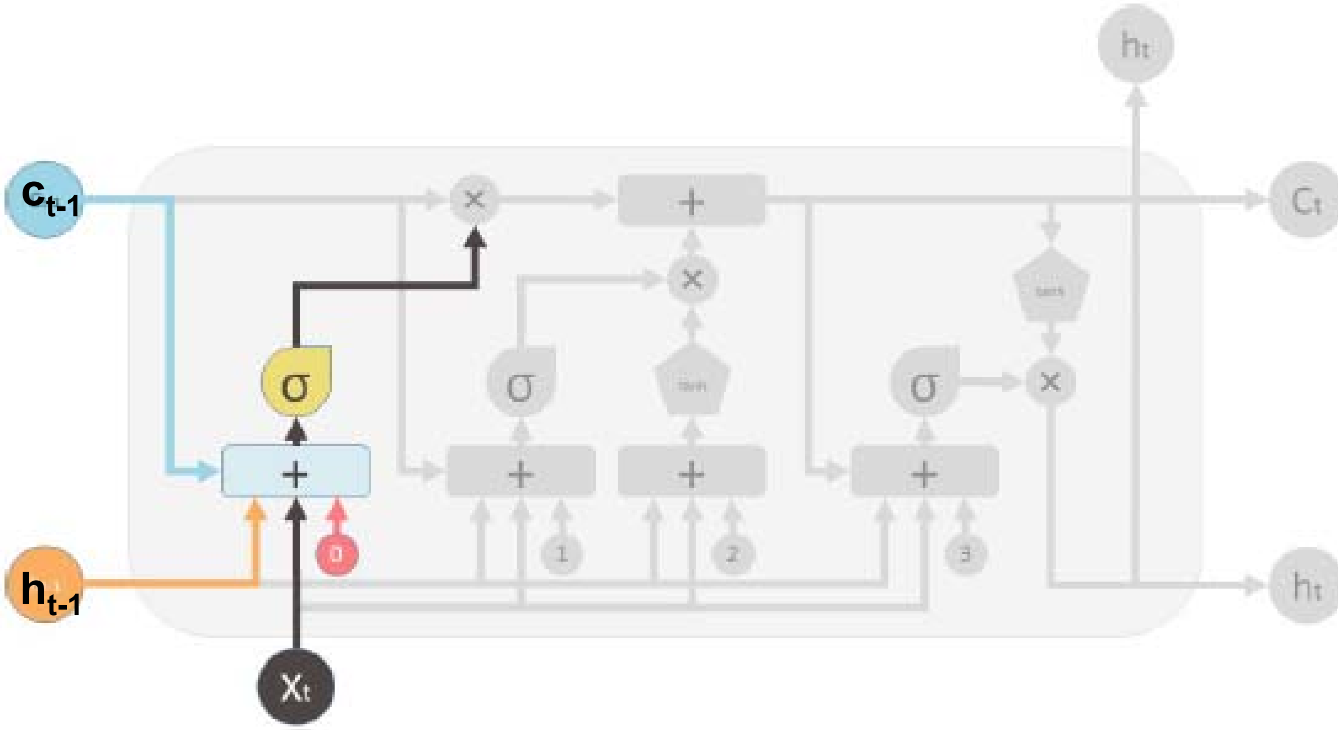


adapted from A. Sood and colah's blog

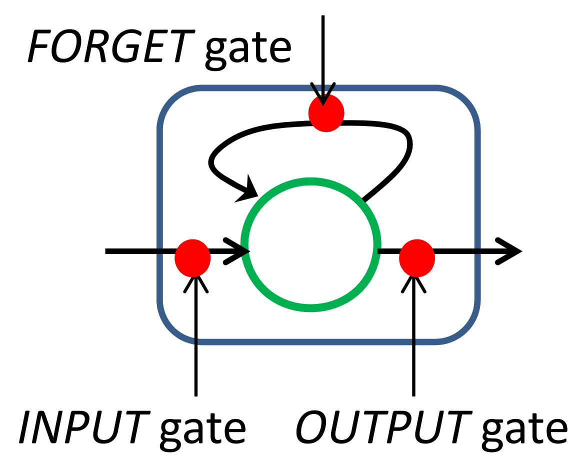
Cell state vector

- represents memory
- it is changing as a result of new information (input gate) and forgetting (forget gate)

Memory cell components – forget gate



$$f(t) = \sigma\left(\mathbf{W}_f\,[h(t-1), x(t)] + b_f\right)$$

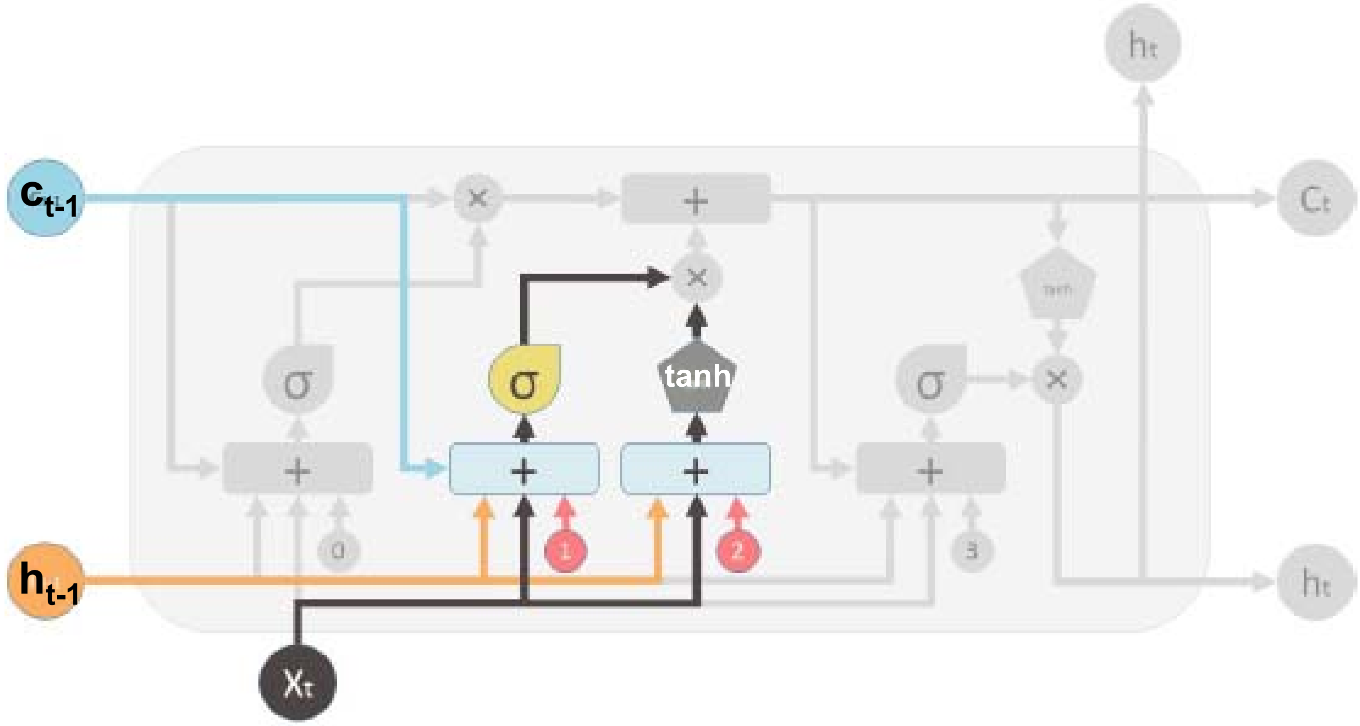


adapted from A. Sood and colah's blog

Forget gate

- controls what information should be forgotten (removed from memory)

Memory cell components – input gate

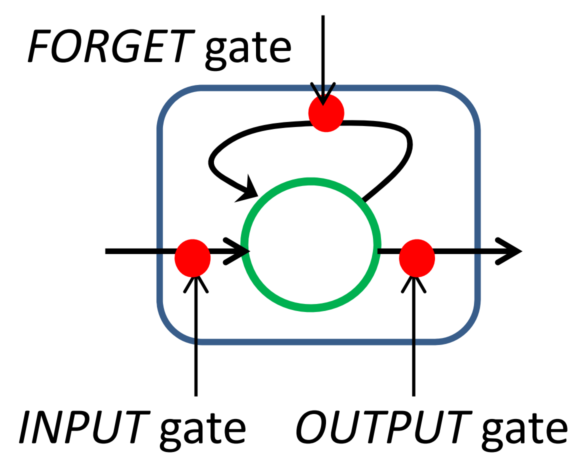


$$i(t) = \sigma\left(\mathbf{W}_i\left[h(t-1), x(t)\right] + b_i\right)$$

$$\tilde{C}(t) = \tanh\left(\mathbf{W}_C\left[h(t-1), x(t)\right] + b_C\right)$$

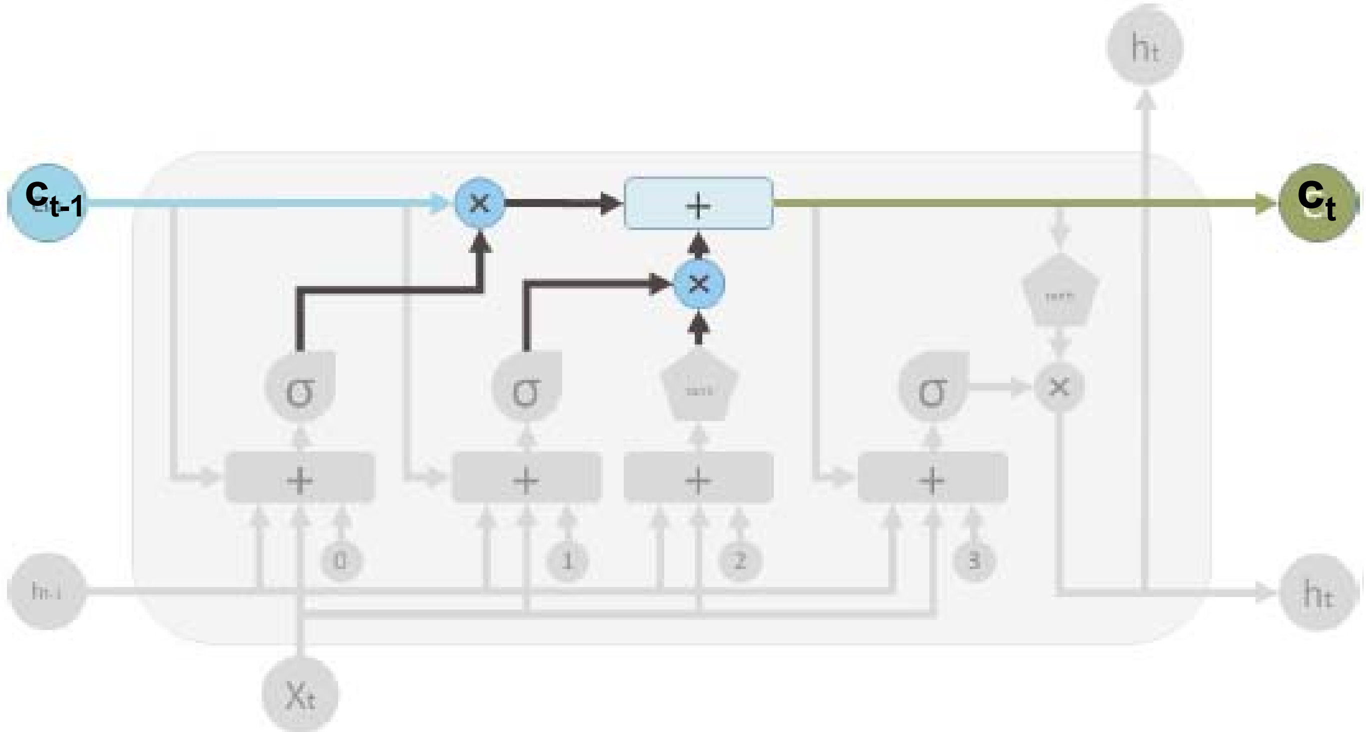
Input gate

- controls what information should be added to cell state from the current input



adapted from A. Sood and colah's blog

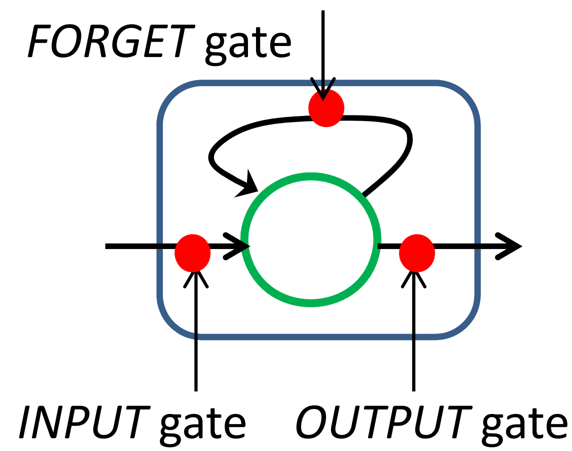
Memory update



Updating memory

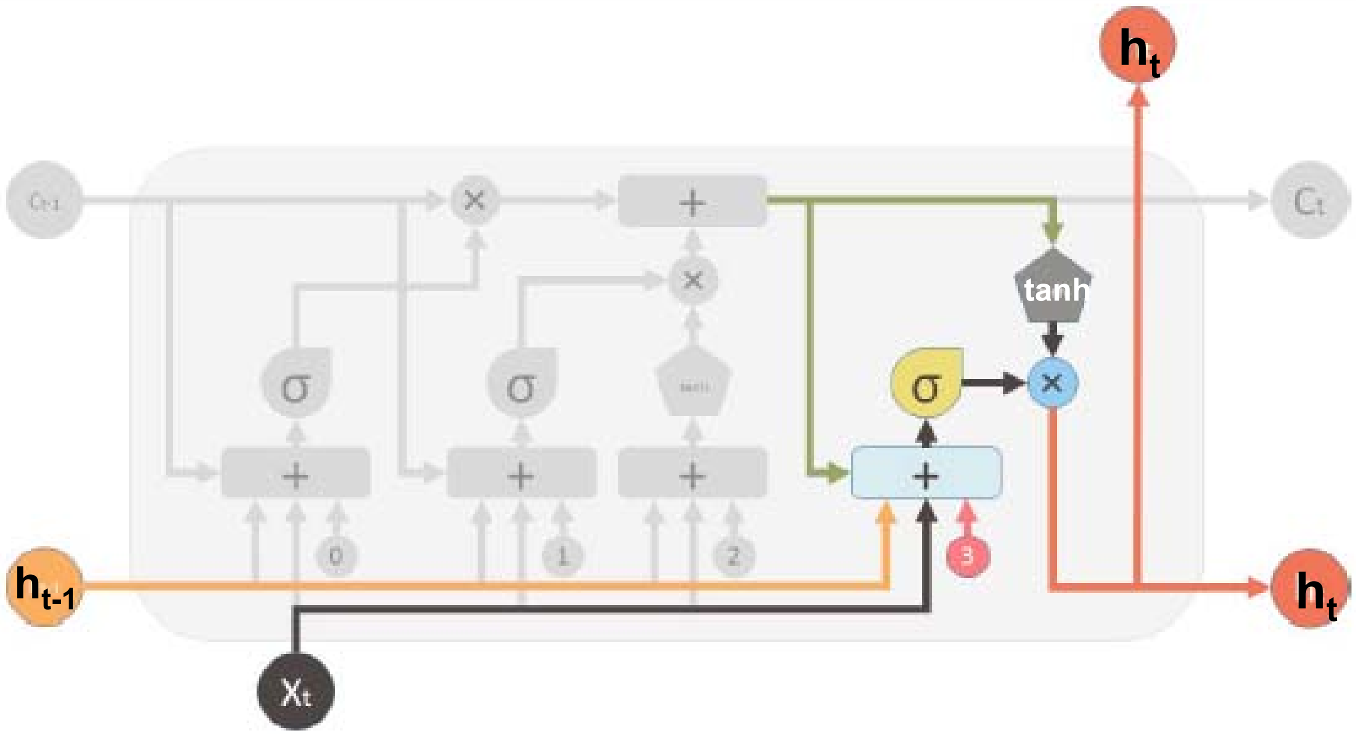
- cell state vector aggregates old memory, gated by forget gate, and a new memory, filtered by the input gate

$$C(t) = f(t) \odot C(t-1) + i(t) \odot \tilde{C}(t)$$



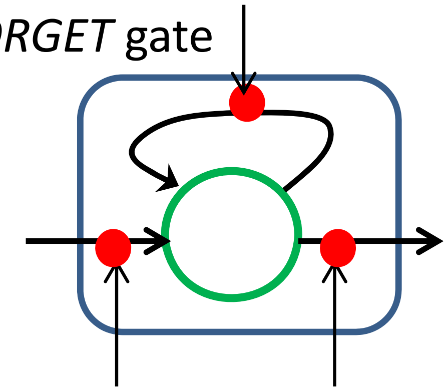
adapted from A. Sood and colah's blog

Memory cell components – output gate



$$o(t) = \sigma\left(\mathbf{W}_o\left[h(t-1), x(t)\right] + b_o\right)$$

$$h(t) = o(t) \odot \tanh\left(C(t)\right)$$

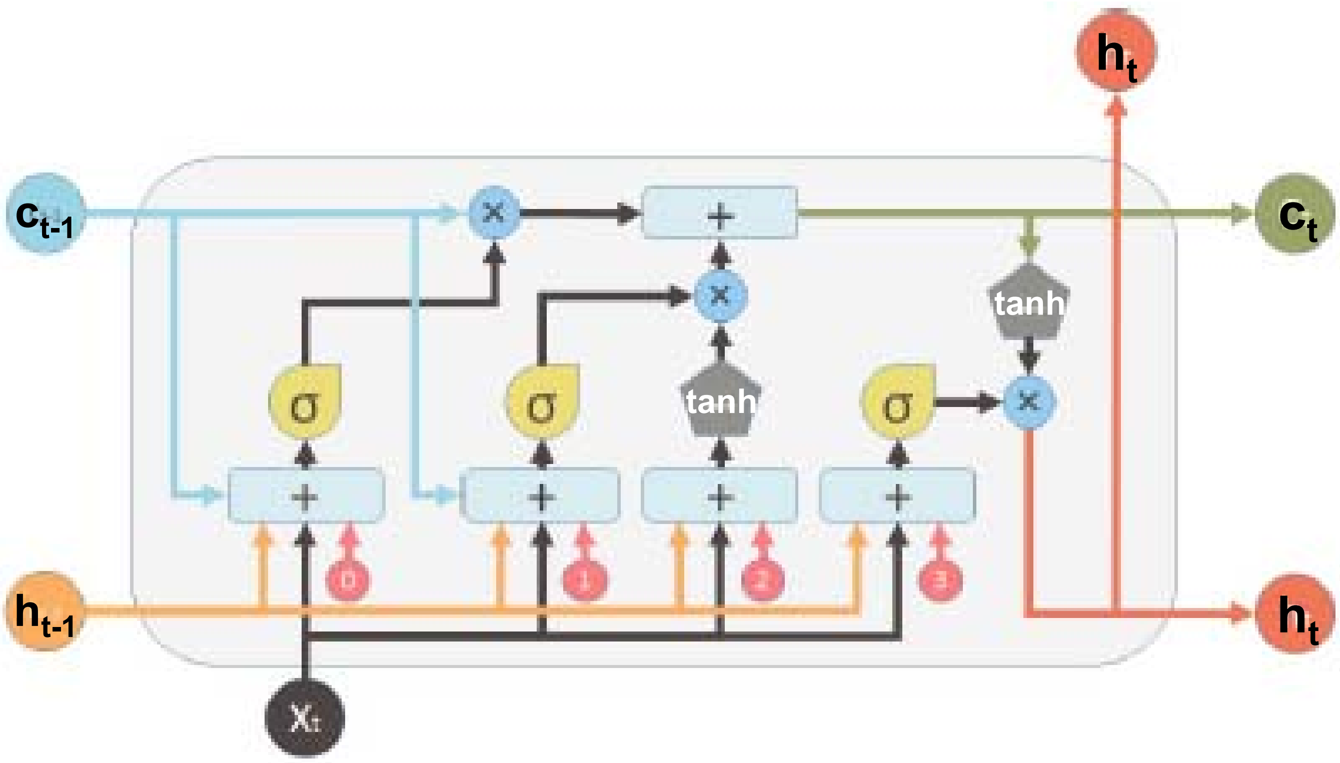


adapted from A. Sood and colah's blog

Output gate

- controls what information is sent to the output

LSTM memory cell summary



$$f(t) = \sigma\left(\mathbf{W}_f\left[h(t-1), x(t)\right] + b_f\right)$$

$$i(t) = \sigma\left(\mathbf{W}_i\left[h(t-1), x(t)\right] + b_i\right)$$

$$o(t) = \sigma\left(\mathbf{W}_o\left[h(t-1), x(t)\right] + b_o\right)$$

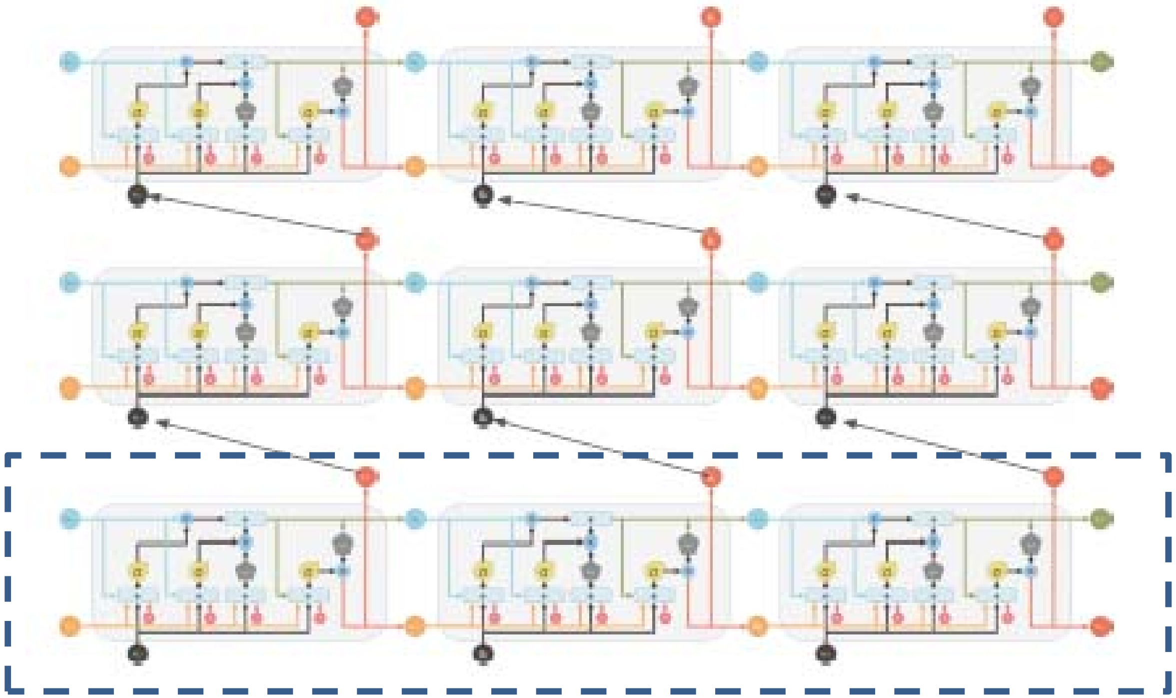
$$\tilde{C}(t) = \tanh\left(\mathbf{W}_C\left[h(t-1), x(t)\right] + b_C\right)$$

$$C(t) = f(t) \odot C(t-1) + i(t) \odot \tilde{C}(t)$$

$$h(t) = o(t) \odot \tanh\left(C(t)\right)$$

Deep LSTM

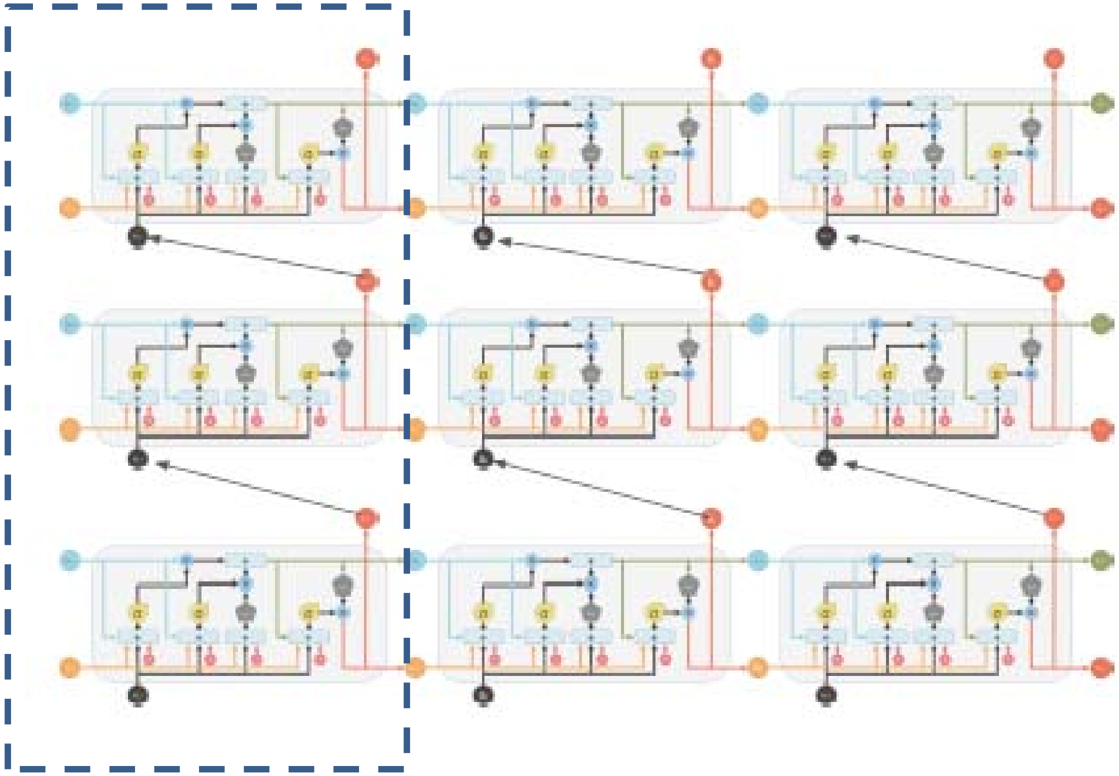
temporal unfolding



Deep LSTM

deep stacking

output sequence of one layer constitutes the input sequence to another layer



Why do we go deep?

- has the potential to perform better at handling temporal information at wide varying scales
- requires however many more parameters to be learnt

adapted from A. Sood

Video example of text understanding with LSTM

https://youtu.be/mLxsbWAYIpw