



POLITECNICO
MILANO 1863

Artificial Neural Networks and Deep Learning

- Recurrent Neural Networks-

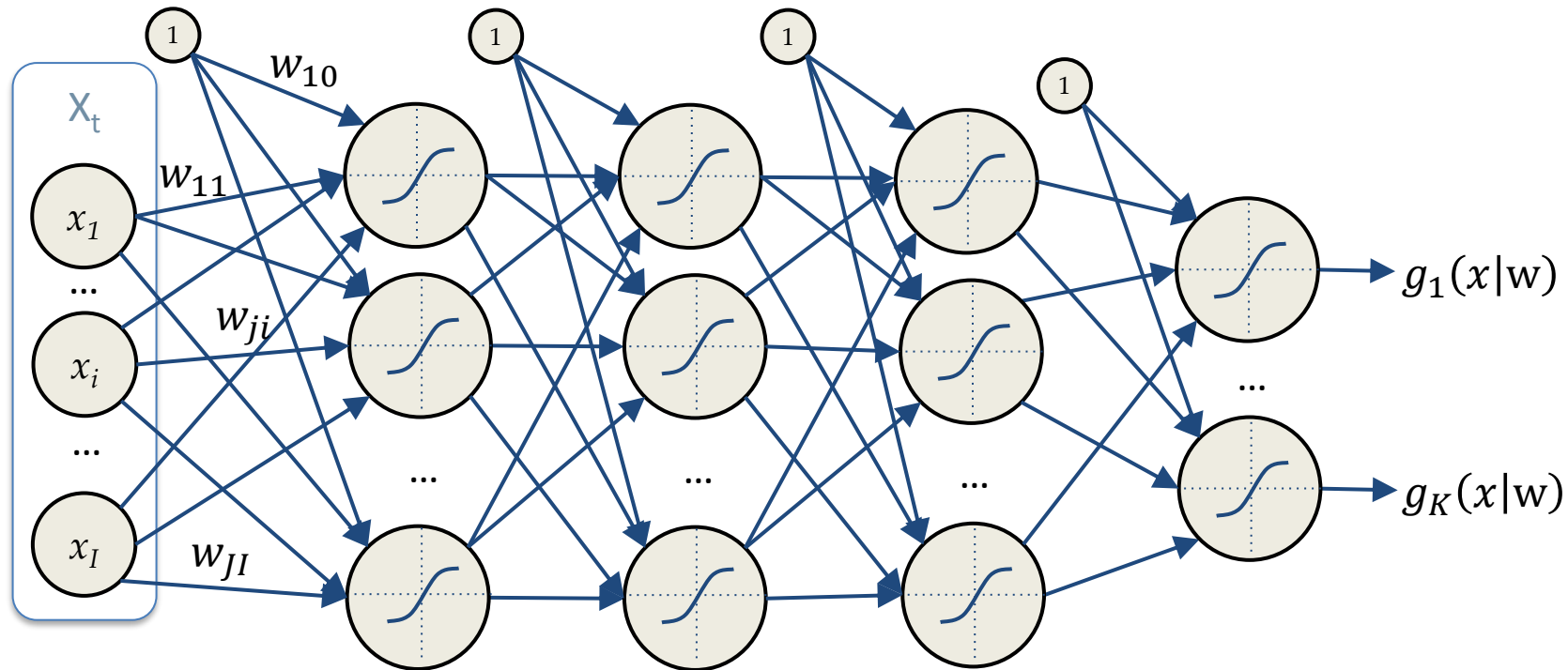
Matteo Matteucci, PhD (matteo.matteucci@polimi.it)

Artificial Intelligence and Robotics Laboratory

Politecnico di Milano

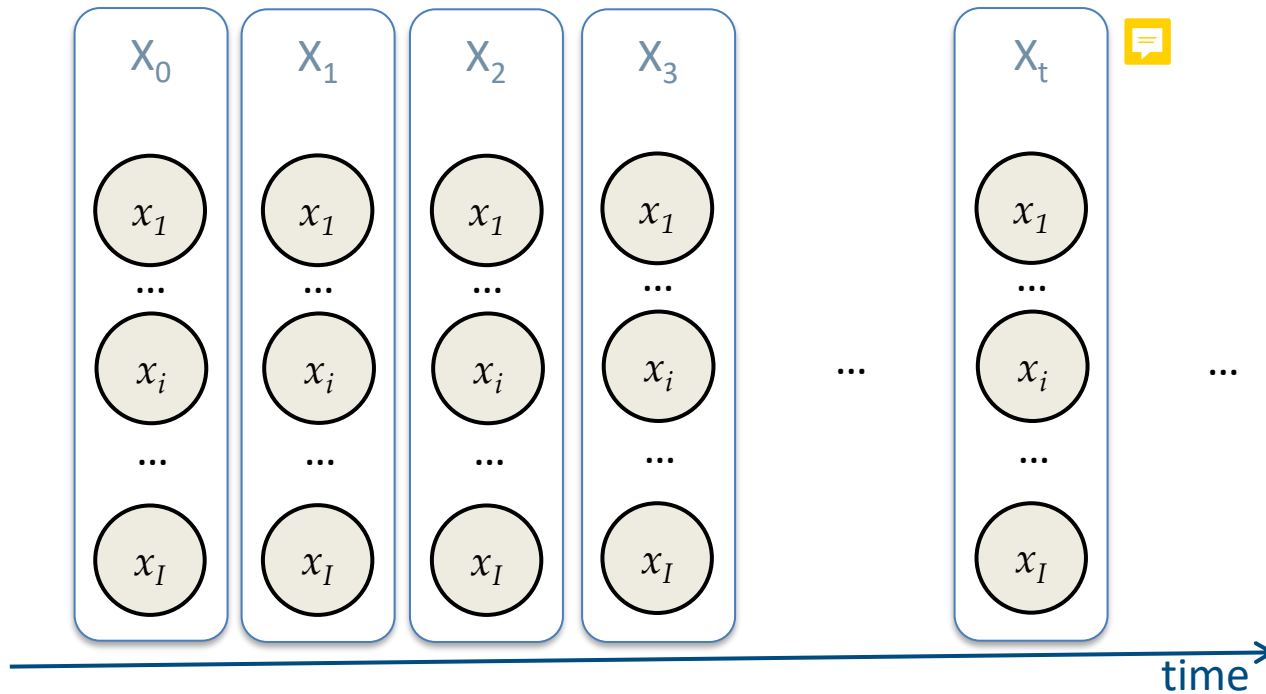
Sequence Modeling

So far we have considered only «static» datasets



Sequence Modeling

So far we have considered only «static» datasets



Sequence Modeling

Different ways to deal with «dynamic» data:

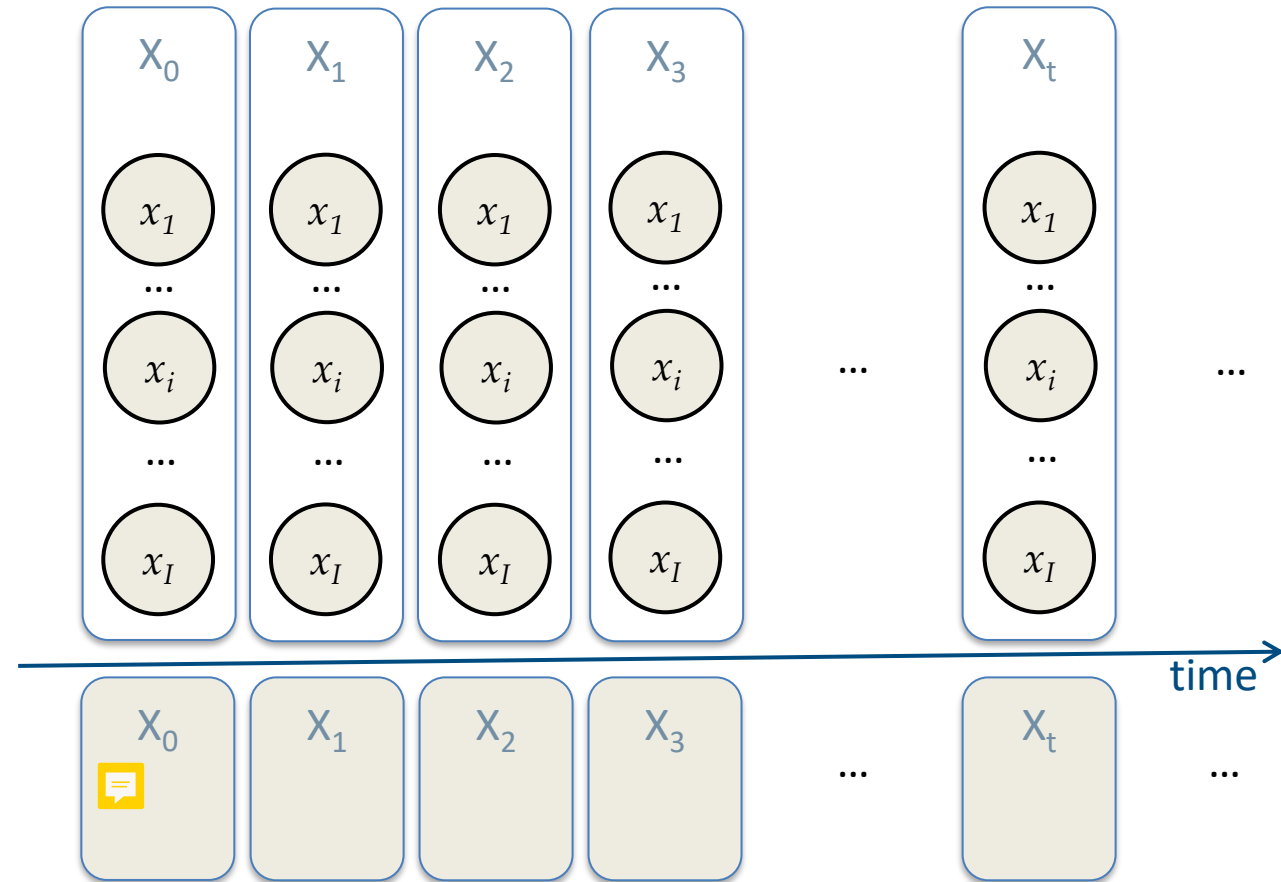
Memoryless models:

- Autoregressive models
- Feedforward neural networks



Models with memory:

- Linear dynamical systems
- Hidden Markov models
- Recurrent Neural Networks
- ...

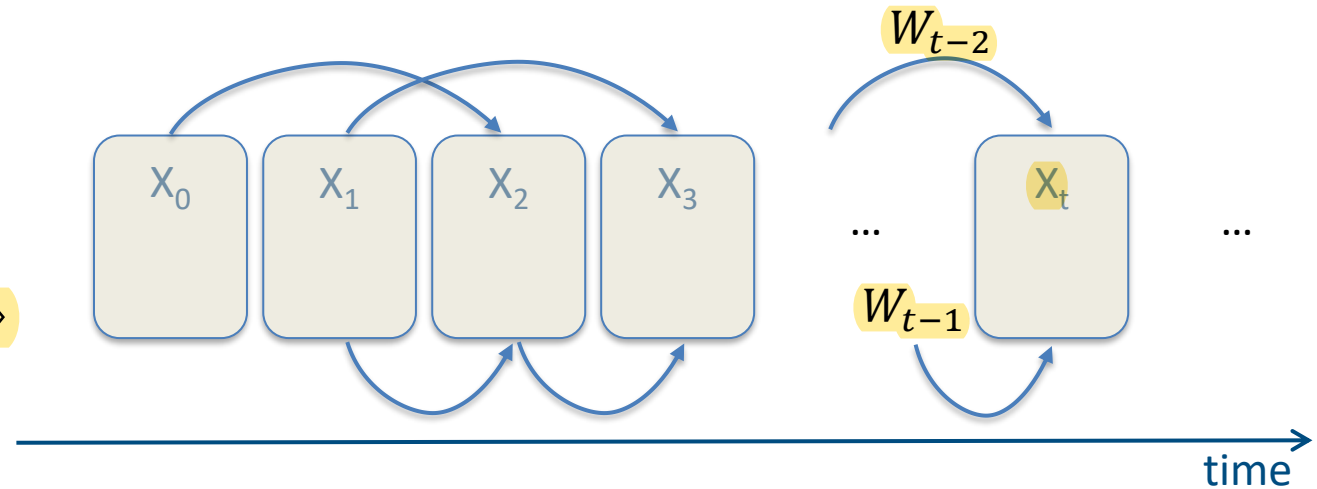


Memoryless Models for Sequences



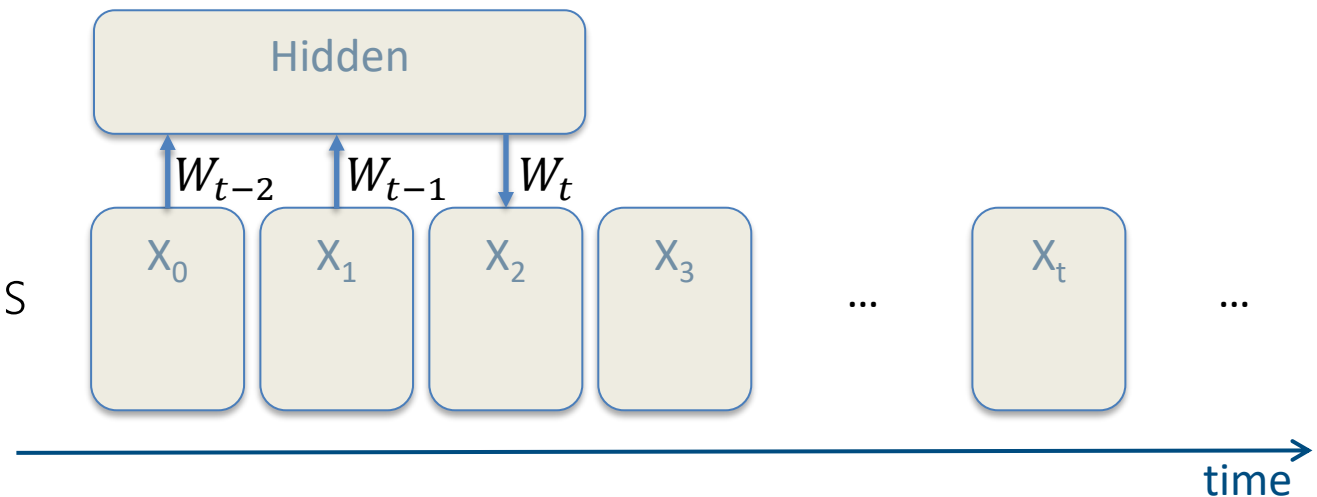
Autoregressive models

- Predict the next input from previous ones using «delay taps» 




Feed forward neural networks

- Generalize autoregressive models using non linear hidden layers





Dynamical Systems (Models with Memory)

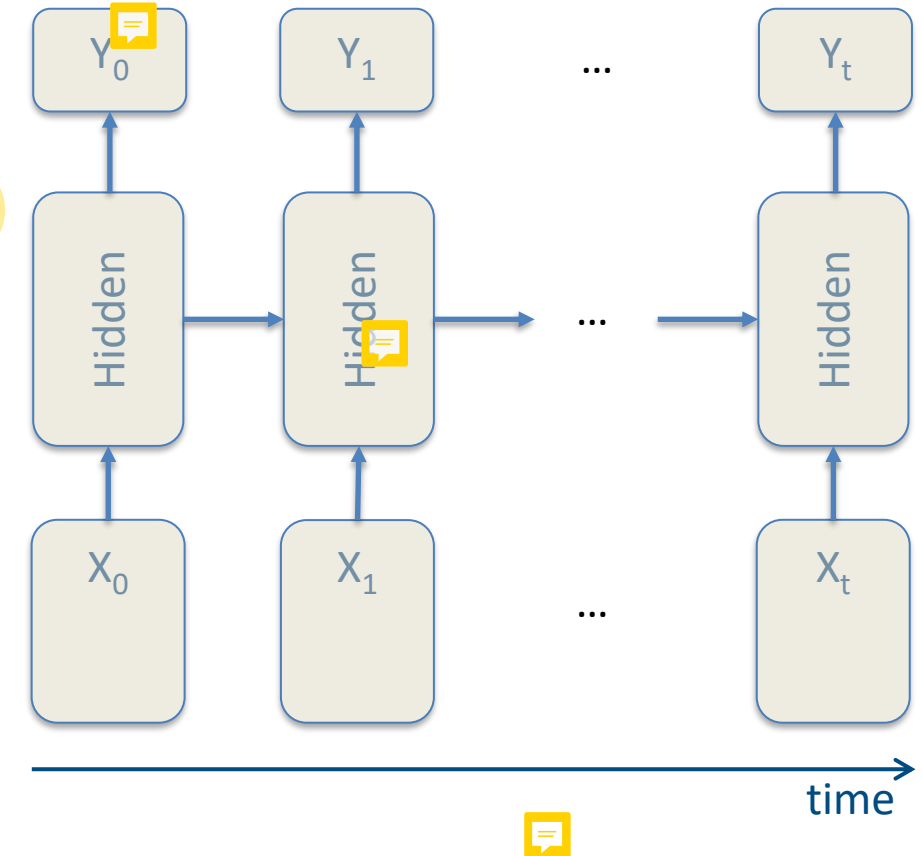
Stochastic systems ...

Generative models with a  hidden state which cannot be observed directly

- The hidden state has some dynamics possibly affected by noise and produces the output
- To compute the output need to infer hidden state
- Input are treated as driving inputs

In linear dynamical systems this becomes:

-  • State continuous with Gaussian uncertainty
- Transformations are assumed to be linear
- State can be estimated using *Kalman filtering* 

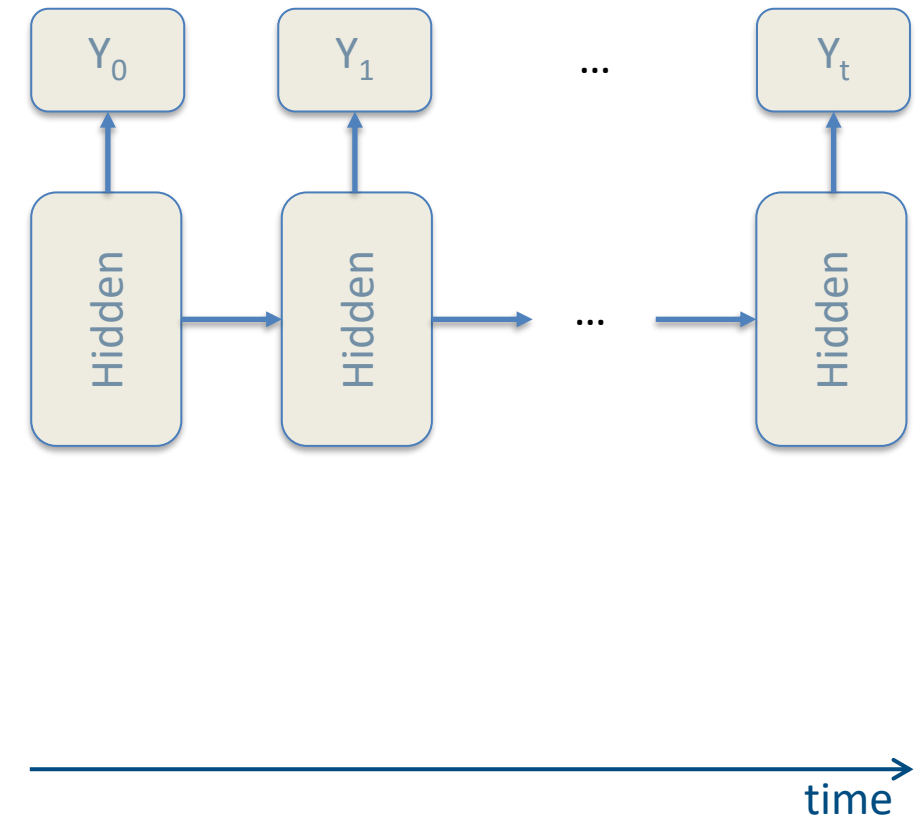


Dynamical Systems (Models with Memory)

Stochastic systems ...

Generative models with a hidden state which cannot be observed directly

- The hidden state has some dynamics possibly affected by noise and produces the output
- To compute the output need to infer hidden state
- Input are treated as driving inputs



In hidden Markov models this becomes:

- State assumed to be discrete, state transitions are stochastic (transition matrix)
- Output is a stochastic function of hidden states
- State can be estimated via *Viterbi algorithm*.

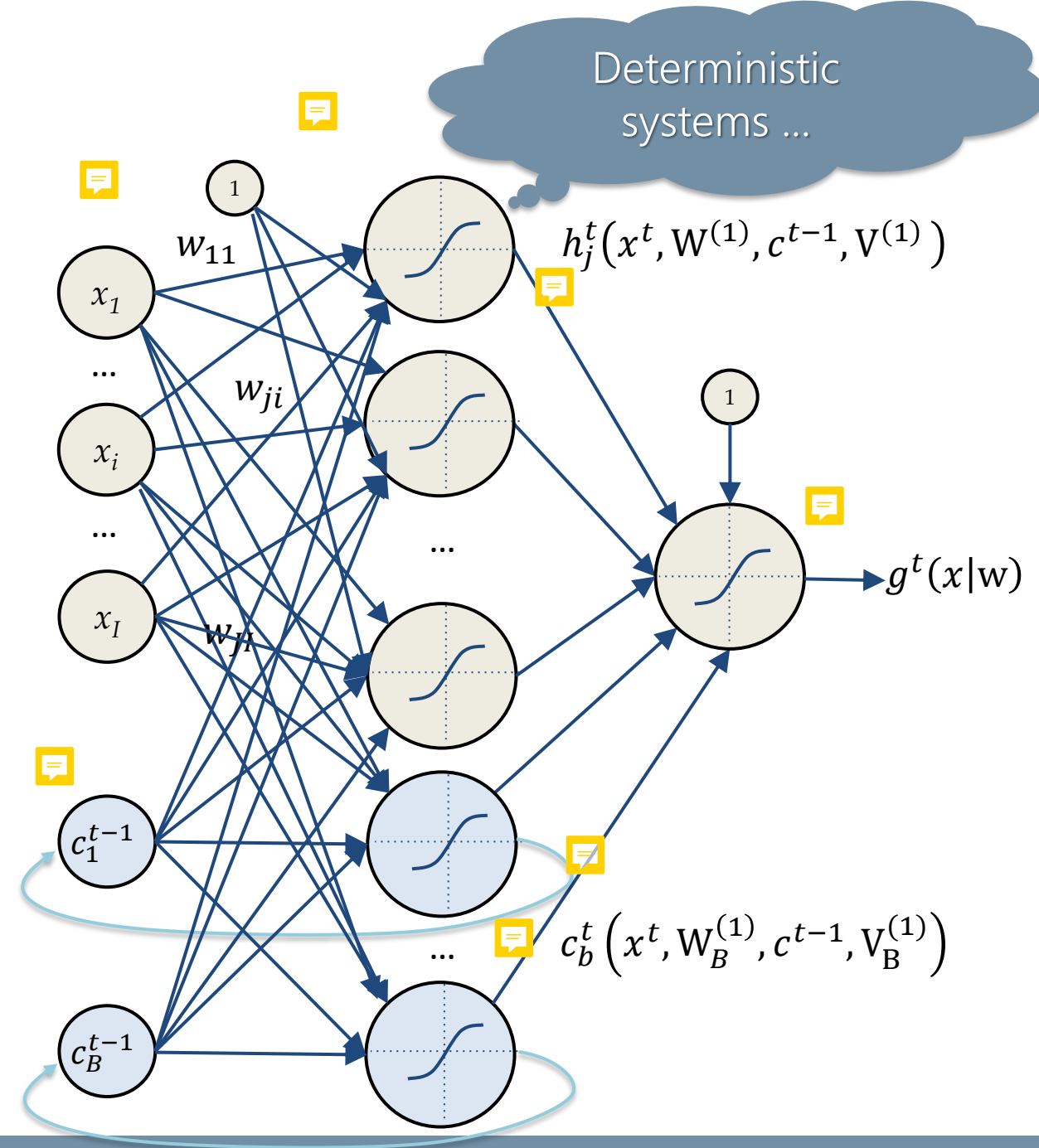
Recurrent Neural networks

Memory via recurrent connections:

- Distributed hidden state allows to store information efficiently
- Non-linear dynamics allows complex hidden state updates

“With enough neurons and time, RNNs can compute anything that can be computed by a computer.”

(Computation Beyond the Turing Limit
Hava T. Siegelmann, 1995)



Recurrent Neural networks

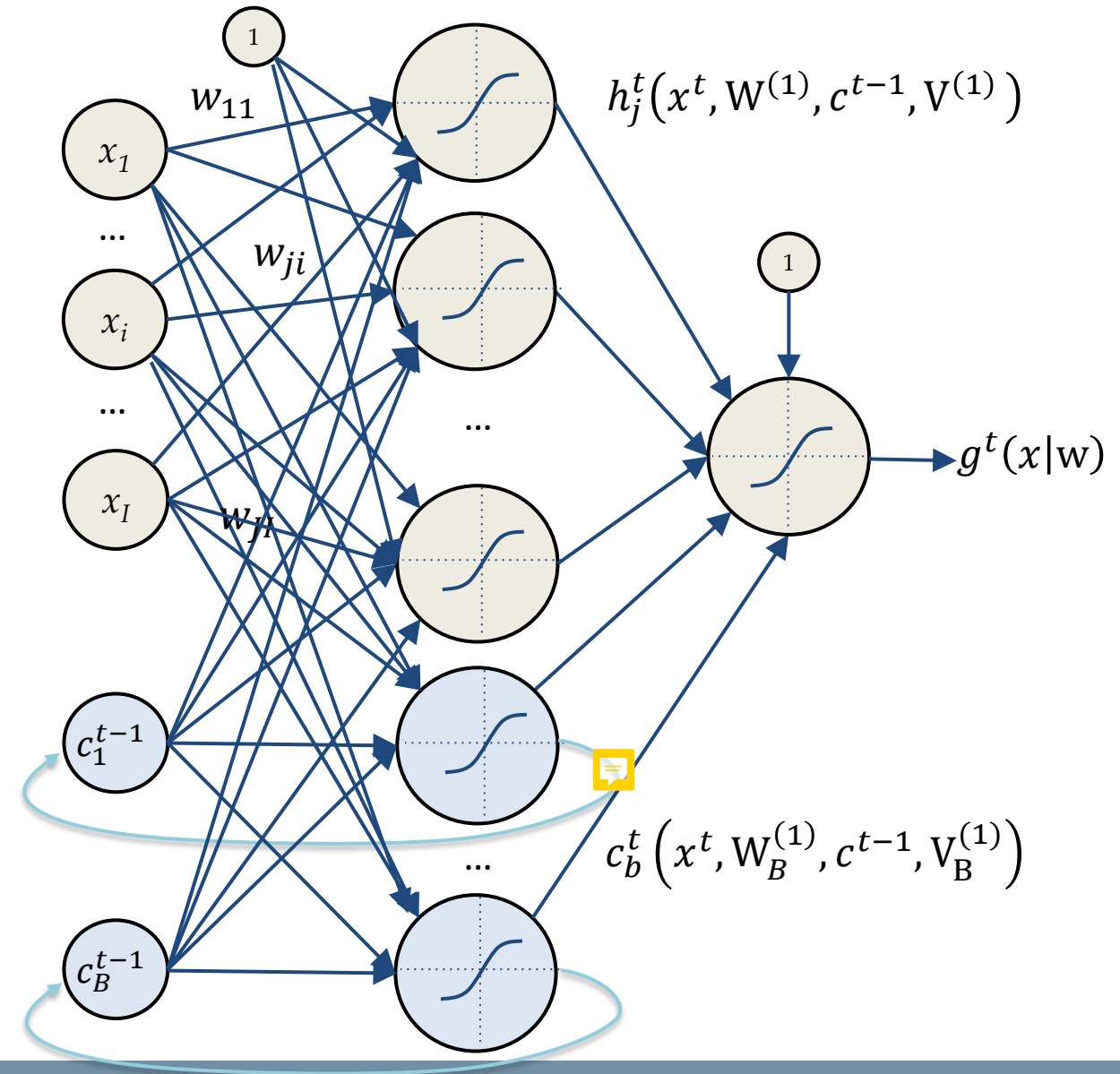
Memory via recurrent connections:

- Distributed hidden state allows to store information efficiently
- Non-linear dynamics allows complex hidden state updates

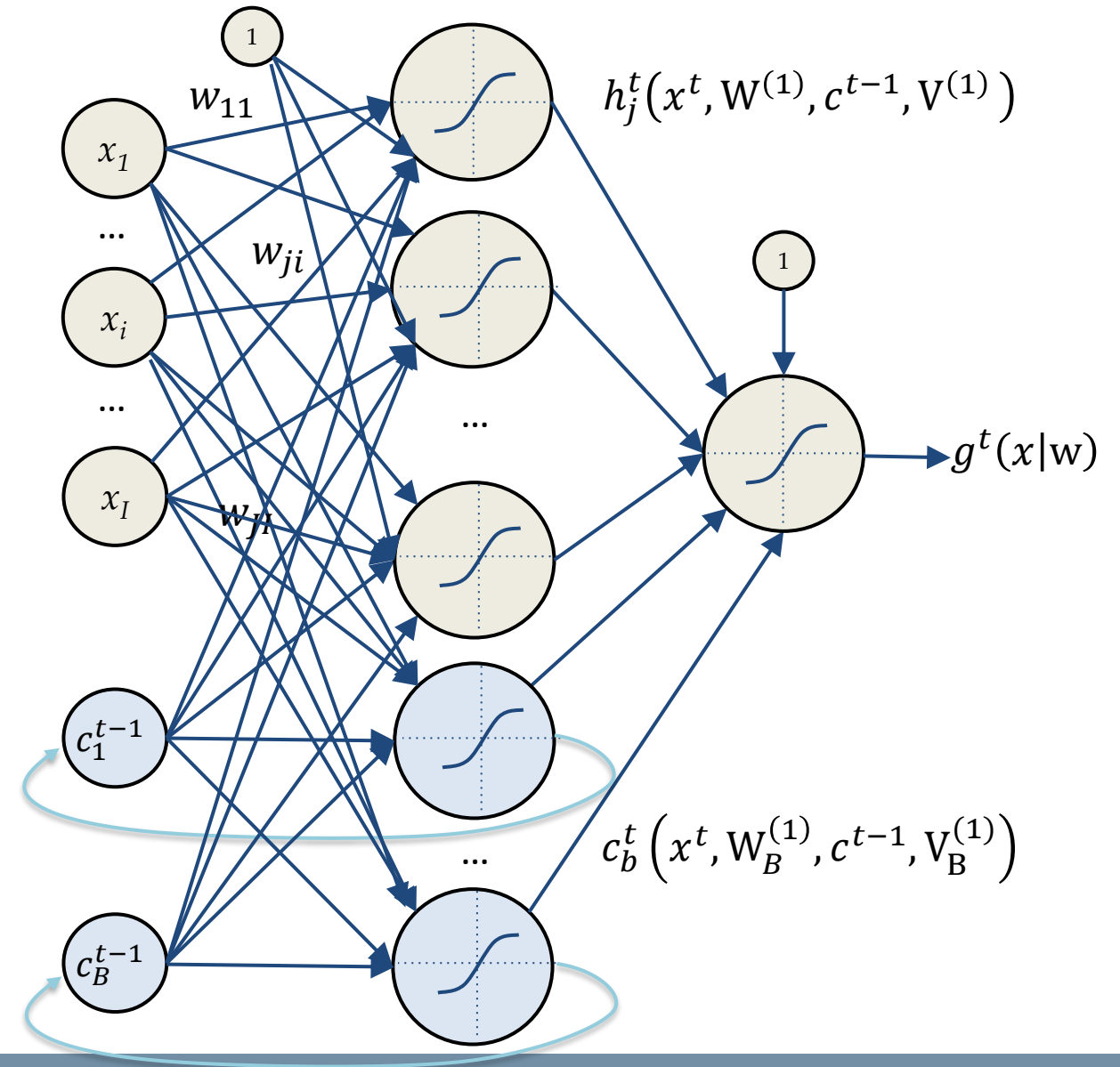
$$g^t(x_n|w) = g \left(\sum_{j=0}^J w_{1j}^{(2)} \cdot h_j^t(\cdot) + \sum_{b=0}^B v_{1b}^{(2)} \cdot c_b^t(\cdot) \right)$$

$$h_j^t(\cdot) = h_j \left(\sum_{i=0}^J w_{ji}^{(1)} \cdot x_{i,n}^t + \sum_{b=0}^B v_{jb}^{(1)} \cdot c_b^{t-1} \right)$$

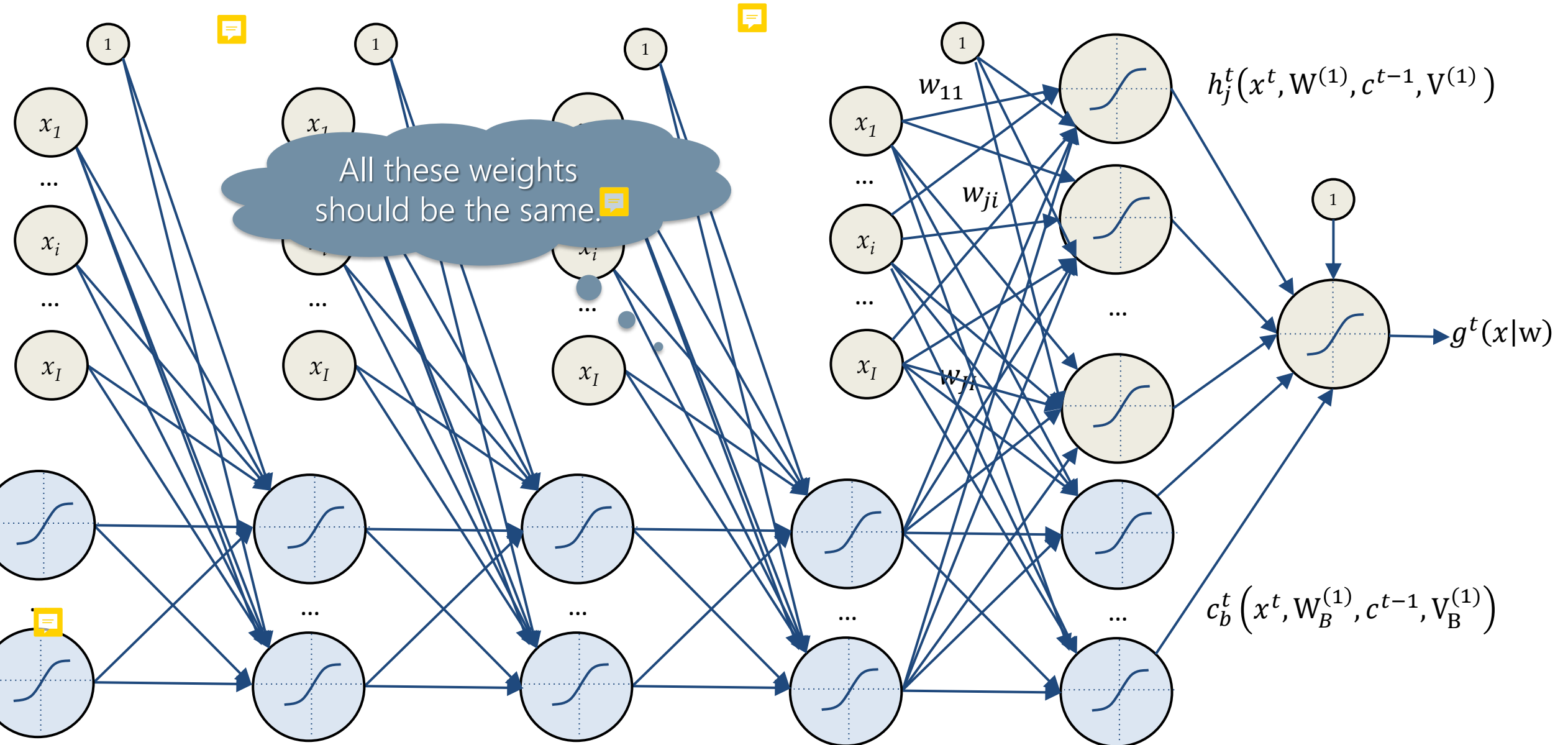
$$c_b^t(\cdot) = c_b \left(\sum_{i=0}^J w_{bi}^{(1)} \cdot x_{i,n}^t + \sum_{b'=0}^B v_{bb'}^{(1)} \cdot c_{b'}^{t-1} \right)$$



Backpropagation Through Time



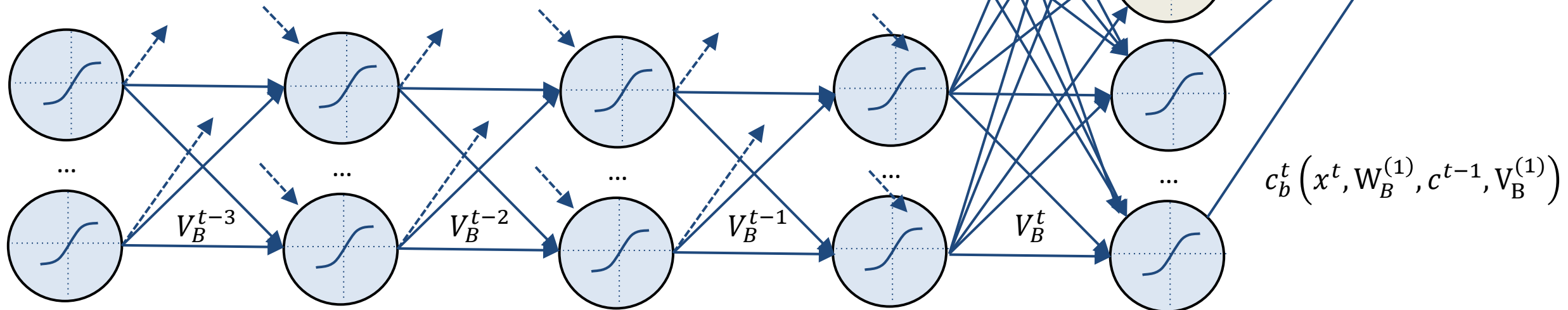
Backpropagation Through Time



Backpropagation Through Time

- Perform network unroll for U steps
- Initialize W_B, V_B replicas to be the same
- Compute gradients and update replicas with the average of their gradients

$$W_B = W_B - \eta \cdot \frac{1}{U} \sum_{u=0}^{U-1} \frac{\partial E}{\partial W_B^{t-u}} \quad V_B = V_B - \eta \cdot \frac{1}{U} \sum_{u=0}^{U-1} \frac{\partial E^t}{\partial V_B^{t-u}}$$

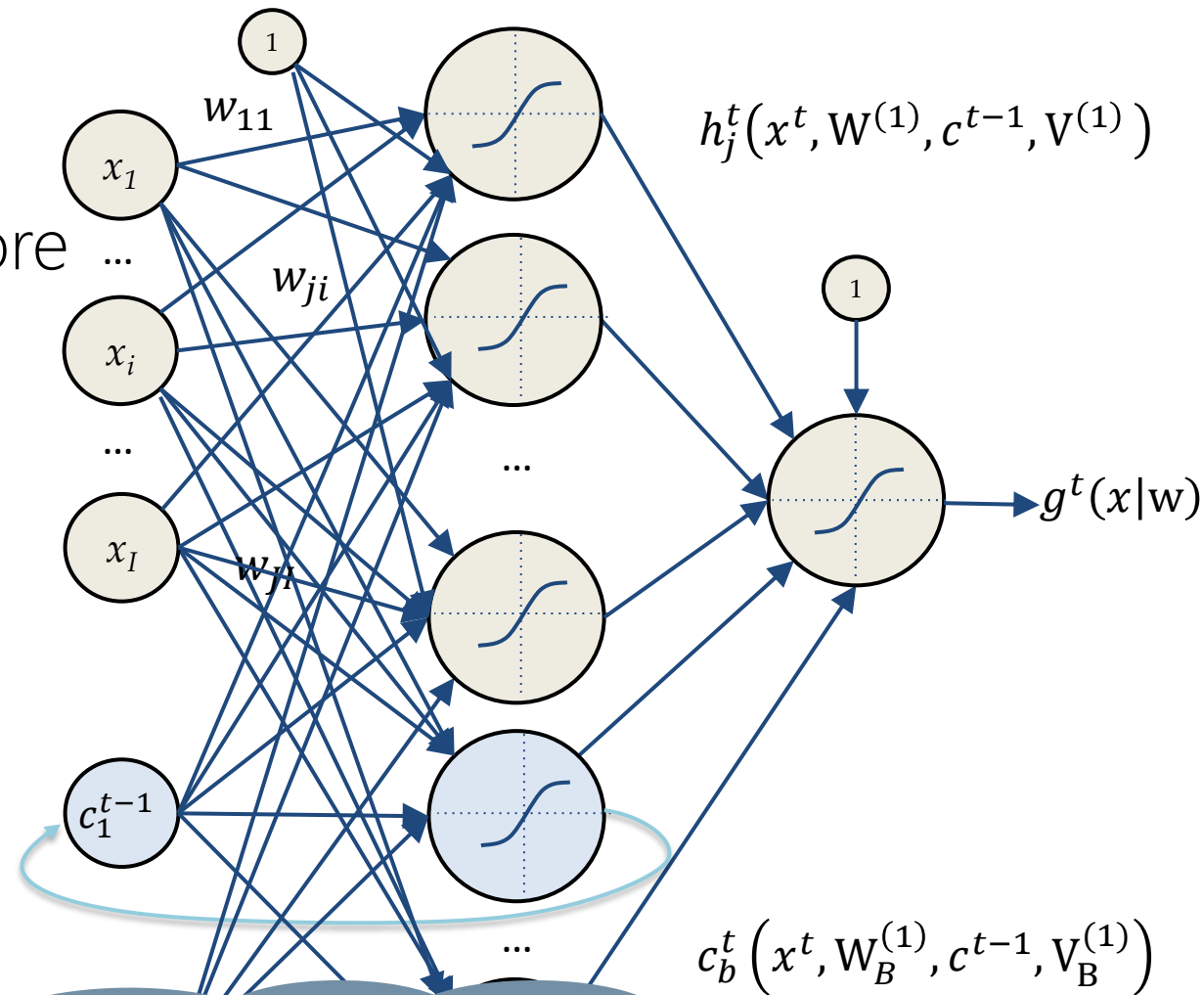


How much should we go back in time?

Sometime output might be related to some input happened quite long before

Jane walked into the room. John walked in too.
It was late in the day. Jane said hi to <???

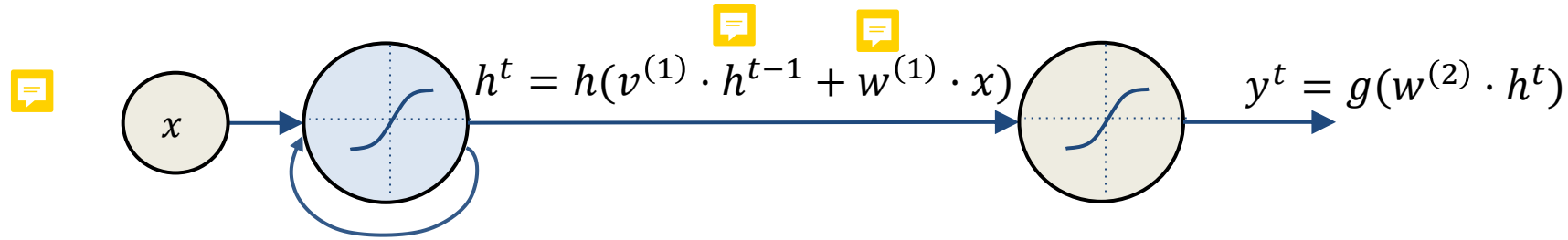
However backpropagation through time was not able to train recurrent neural networks significantly back in time ...



Was due to not being able to backprop through many layers ...

How much can we go back in time?

To better understand why it was not working consider a simplified case:



Backpropagation over an entire sequence S is computed as

$$\frac{\partial E}{\partial w} = \sum_{t=1}^S \frac{\partial E^t}{\partial w} \rightarrow \frac{\partial E^t}{\partial w} = \sum_{t=1}^t \frac{\partial E^t}{\partial y^t} \frac{\partial y^t}{\partial h^t} \frac{\partial h^t}{\partial h^k} \frac{\partial h^k}{\partial w} \rightarrow \frac{\partial h^t}{\partial h^k} = \prod_{i=k+1}^t \frac{\partial h_i}{\partial h_{i-1}} = \prod_{i=k+1}^t v^{(1)} h'(v^{(1)} \cdot h^{i-1} + w^{(1)} \cdot x)$$

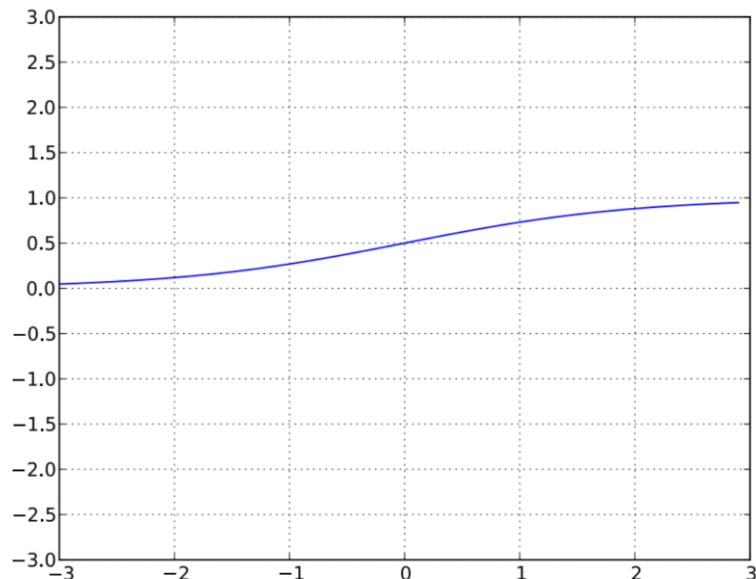
If we consider the norm of these terms

$$\left\| \frac{\partial h_i}{\partial h_{i-1}} \right\| \leq \|v^{(1)}\| \|h'(\cdot)\| \rightarrow \left\| \frac{\partial h^t}{\partial h^k} \right\| \leq (\gamma_v \cdot \gamma_{h'})^{t-k}$$

If $(\gamma_v \cdot \gamma_{h'}) < 1$ this converges to 0 ...

With Sigmoids and Tanh we have vanishing gradients

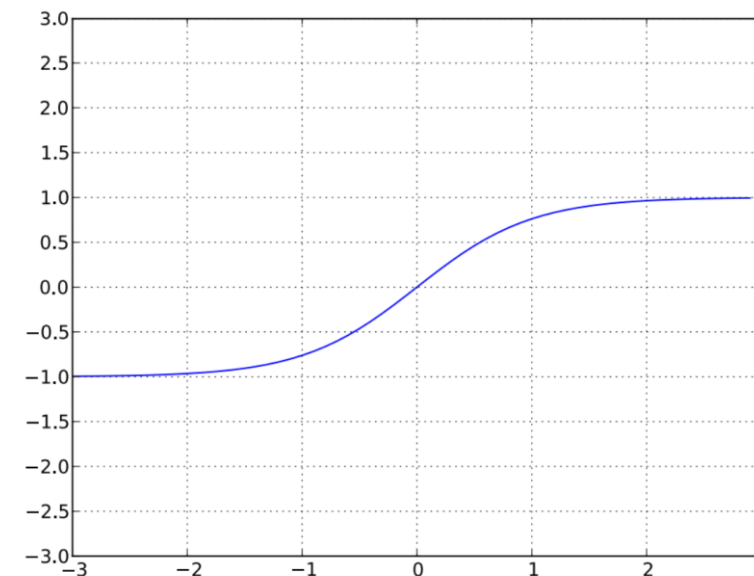
Which Activation Function?



Sigmoid activation function

$$g(a) = \frac{1}{1 + \exp(-a)}$$
$$g'(a) = g(a)(1 - g(a))$$

$$g'(0) = g(0)(1 - g(0)) = \frac{1}{1 + \exp(0)} \cdot \frac{\exp(0)}{1 + \exp(0)} = 0.25$$



Tanh activation function

$$g(a) = \frac{\exp(a) - \exp(-a)}{\exp(a) + \exp(-a)}$$
$$g'(a) = 1 - g(a)^2$$

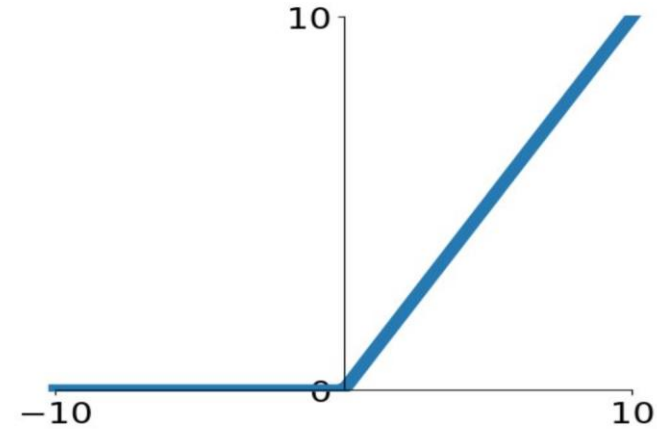
$$g'(0) = 1 - g(0)^2 = 1 - \left(\frac{\exp(0) - \exp(0)}{\exp(0) + \exp(0)}\right)^2 = 1$$

Dealing with Vanishing Gradient

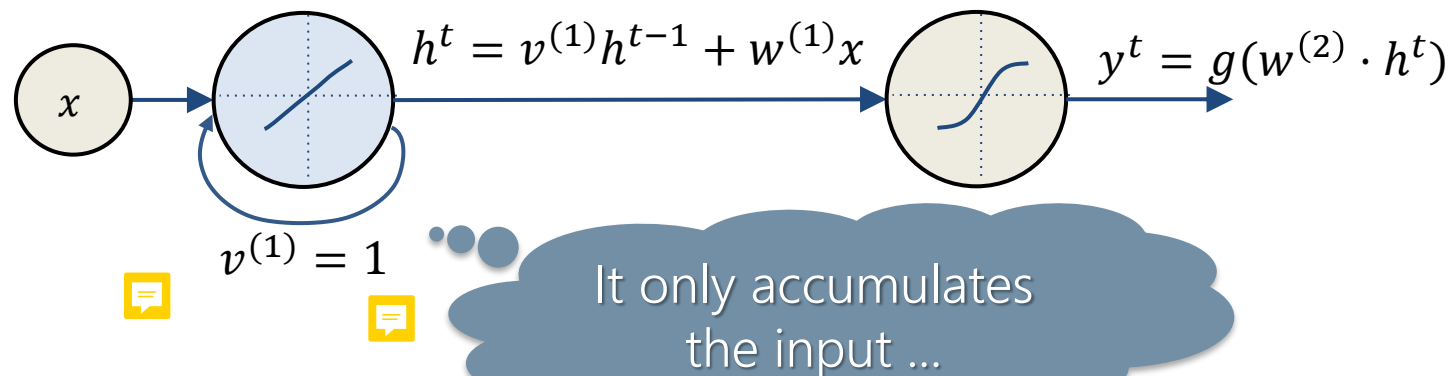
Force all gradients to be either 0 or 1

$$g(a) = \text{ReLu}(a) = \max(0, a)$$

$$g'(a) = 1_{a>0}$$



Build Recurrent Neural Networks using small modules that are designed to remember values for a long time.



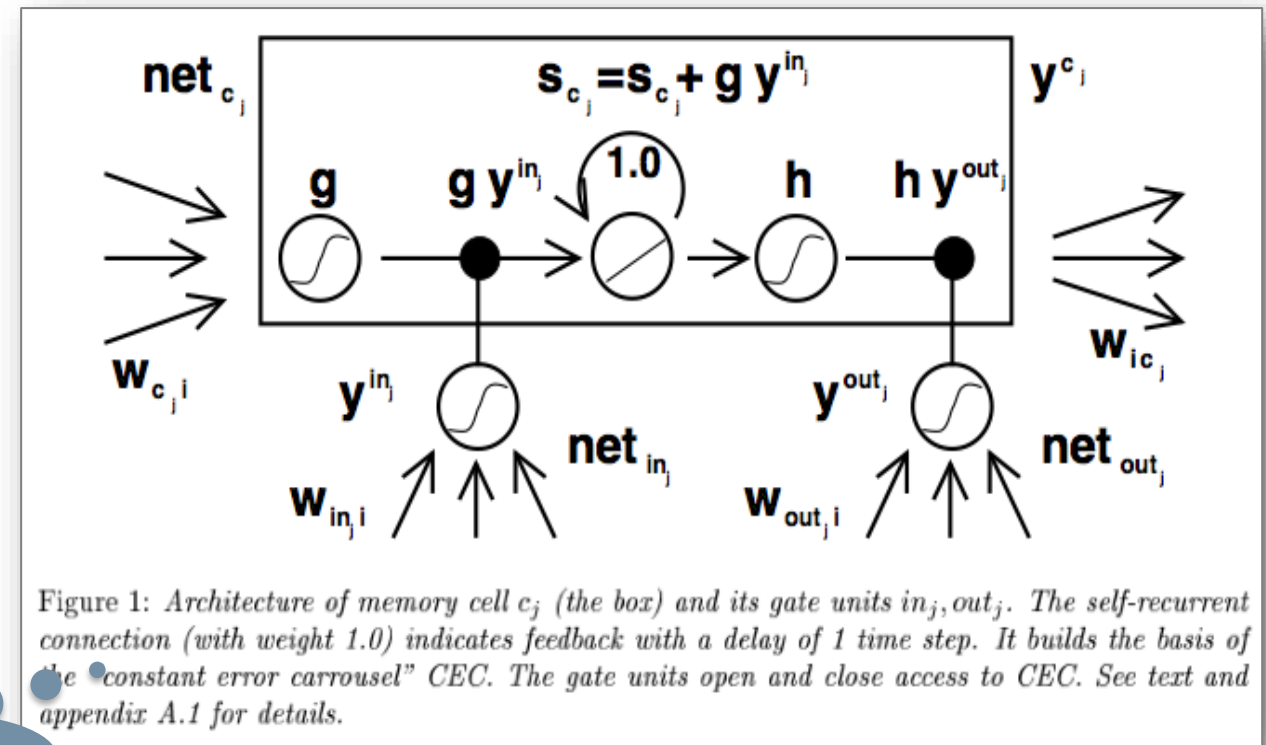
Long Short-Term Memories (LSTM)



Hochreiter & Schmidhuber (1997) solved the problem of vanishing gradient designing a memory cell using logistic and linear units with multiplicative interactions:

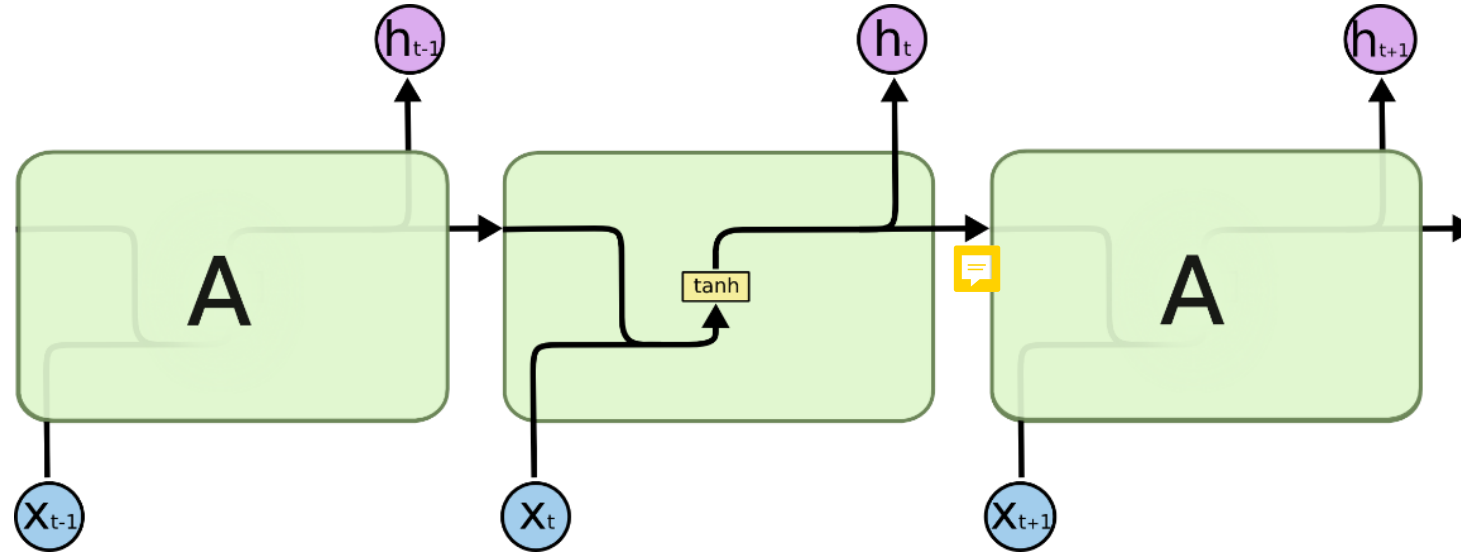
- Information gets into the cell whenever its "write" gate is on.
- The information stays in the cell so long as its "keep" gate is on.
- Information is read from the cell by turning on its "read" gate.

Can backpropagate through this since the loop has fixed weight.



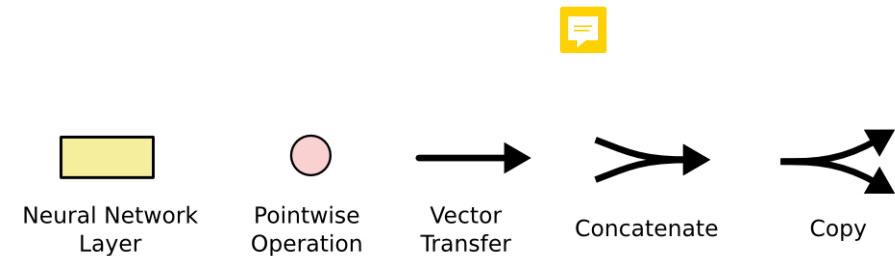
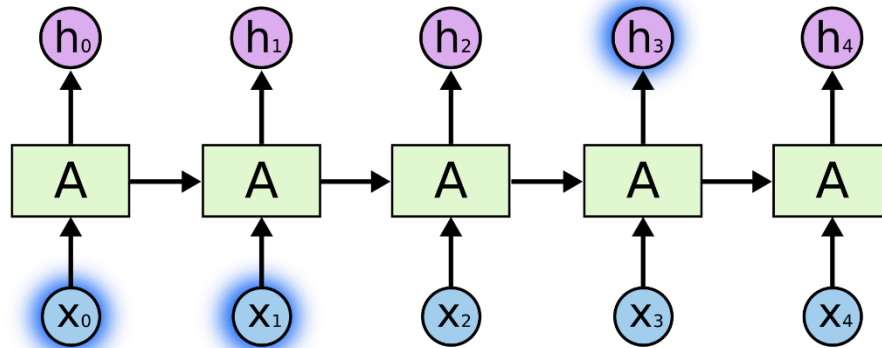
RNN vs. LSTM

RNN



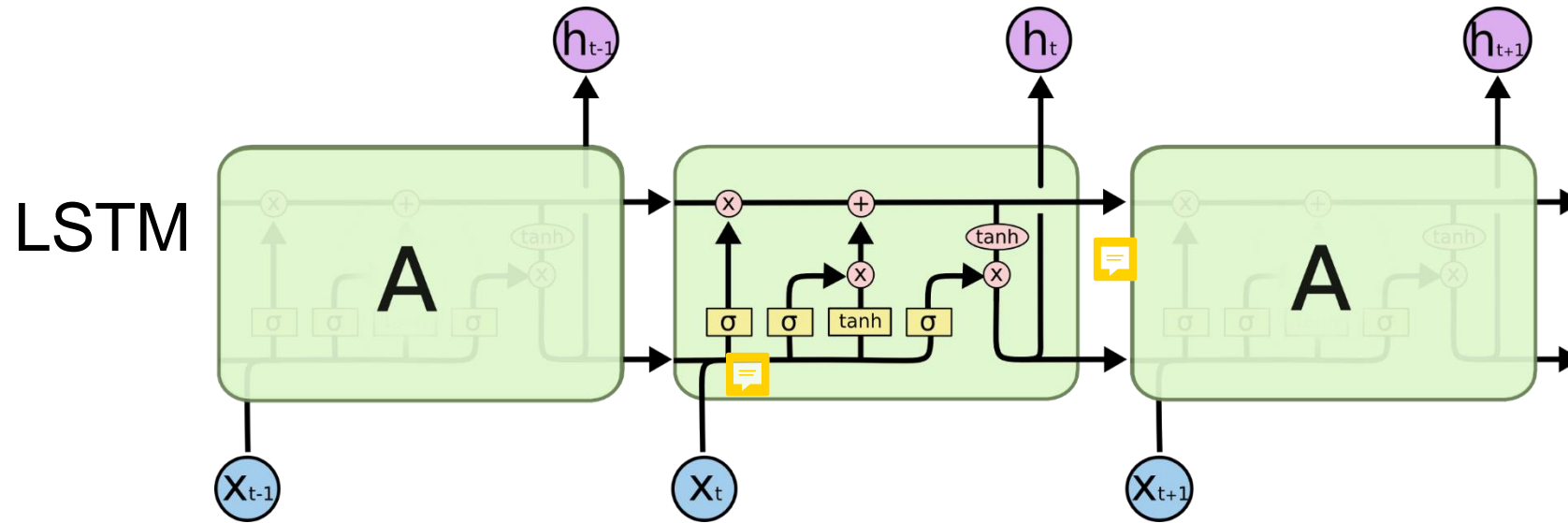
$$a_h^t = \sum_{i=1}^I w_{ih} x_i^t + \sum_{h'=1}^H w_{h'h} b_{h'}^{t-1}$$

$$b_h^t = \theta_h(a_h^t)$$



LSTM Images from: <https://colah.github.io/posts/2015-08-Understanding-LSTMs/>

Long Short-Term Memory



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

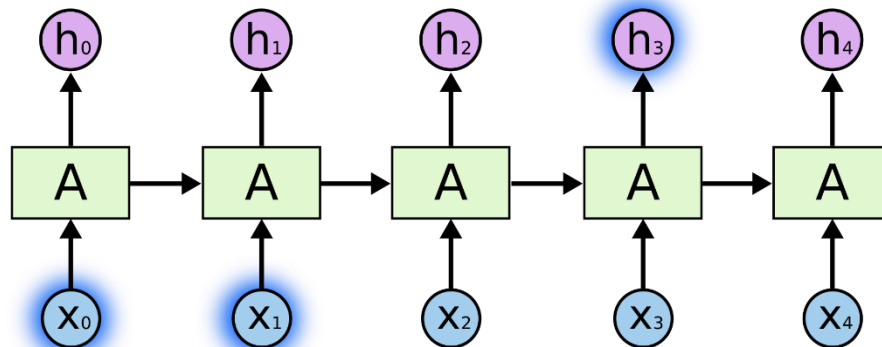
$$\tilde{C}_t = \tanh(W_C \cdot [h_{t-1}, x_t] + b_C)$$

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

$$C_t = f_t * C_{t-1} + i_t * \tilde{C}_t$$

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

$$h_t = o_t * \tanh(C_t)$$



Neural Network Layer

Pointwise Operation

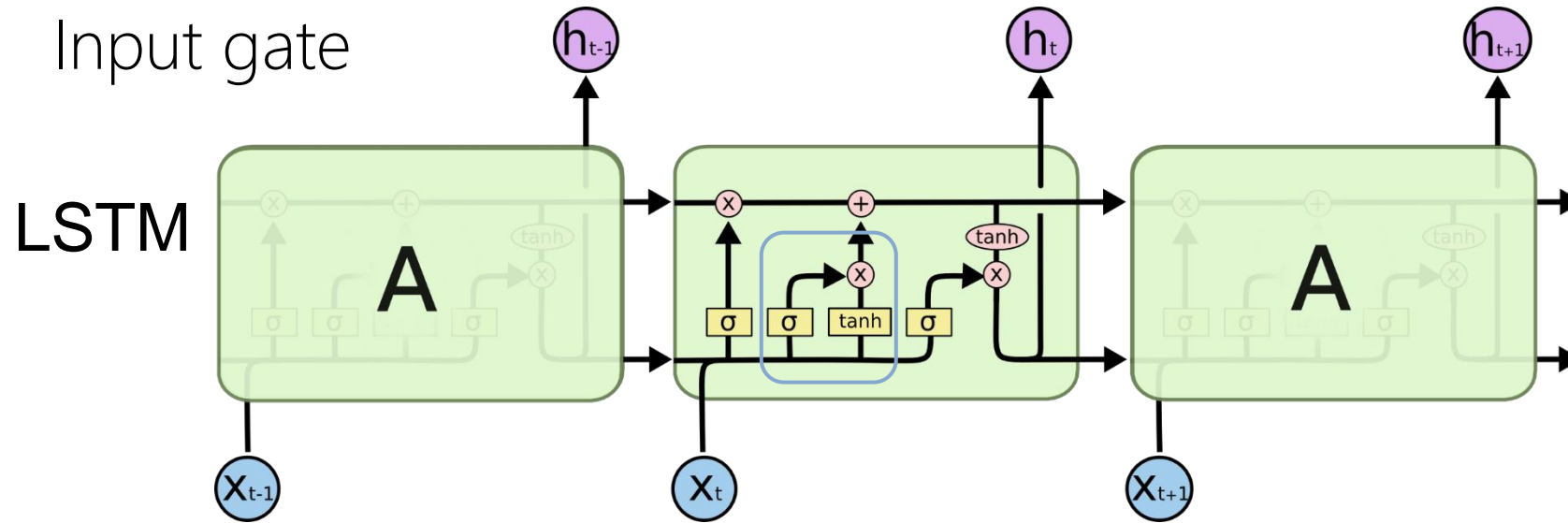
Vector Transfer

Concatenate

Copy

LSTM Images from: <https://colah.github.io/posts/2015-08-Understanding-LSTMs/>

Long Short-Term Memory



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

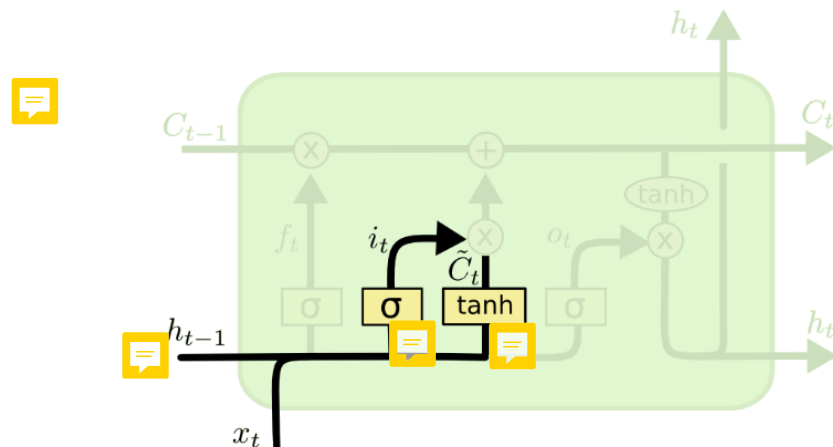
$$\tilde{C}_t = \tanh(W_C \cdot [h_{t-1}, x_t] + b_C)$$

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

$$C_t = f_t * C_{t-1} + i_t * \tilde{C}_t$$

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

$$h_t = o_t * \tanh(C_t)$$

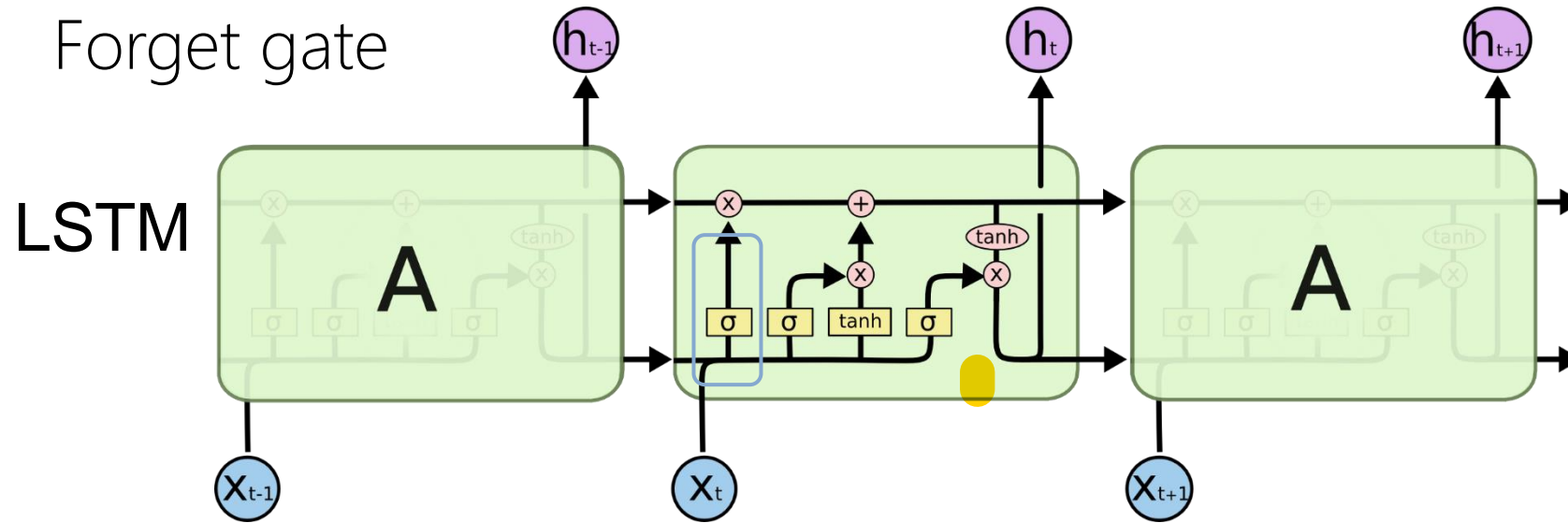


$$i_t = \sigma(W_i \cdot [h_{t-1}, x_t] + b_i)$$

$$\tilde{C}_t = \tanh(W_C \cdot [h_{t-1}, x_t] + b_C)$$

LSTM Images from: <https://colah.github.io/posts/2015-08-Understanding-LSTMs/>

Long Short-Term Memory



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

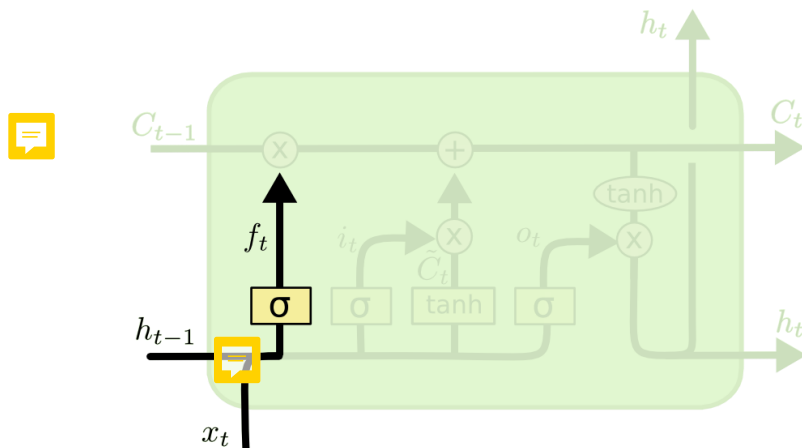
$$\tilde{C}_t = \tanh(W_C \cdot [h_{t-1}, x_t] + b_C)$$

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

$$C_t = f_t * C_{t-1} + i_t * \tilde{C}_t$$

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

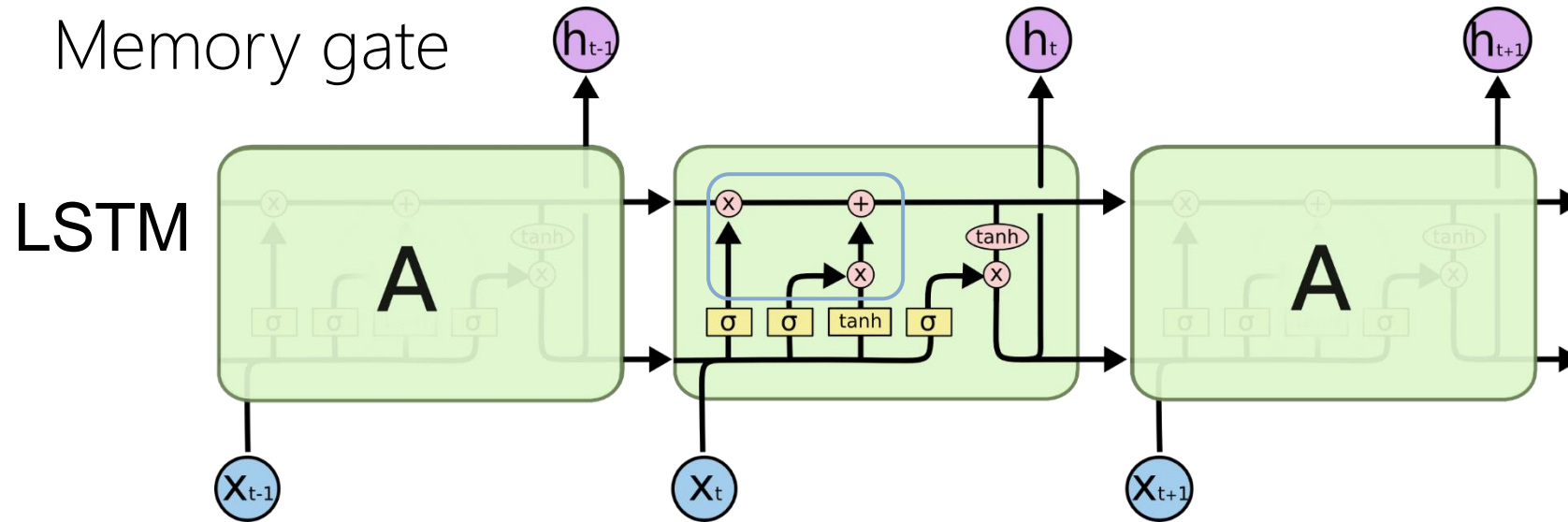
$$h_t = o_t * \tanh(C_t)$$



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

LSTM Images from: <https://colah.github.io/posts/2015-08-Understanding-LSTMs/>

Long Short-Term Memory



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

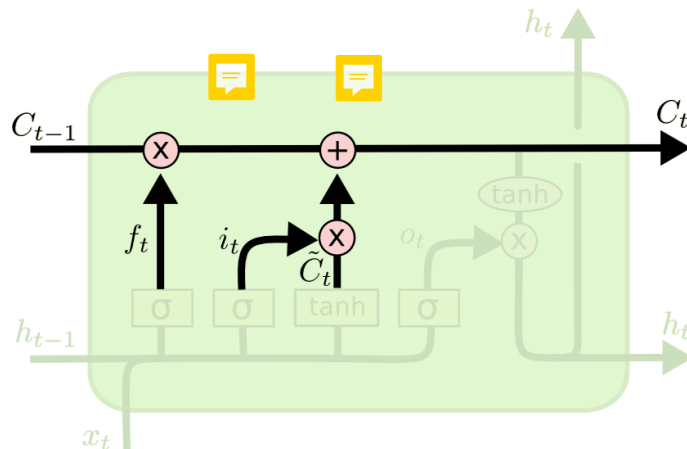
$$\tilde{C}_t = \tanh(W_C \cdot [h_{t-1}, x_t] + b_C)$$

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

$$C_t = f_t * C_{t-1} + i_t * \tilde{C}_t$$

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

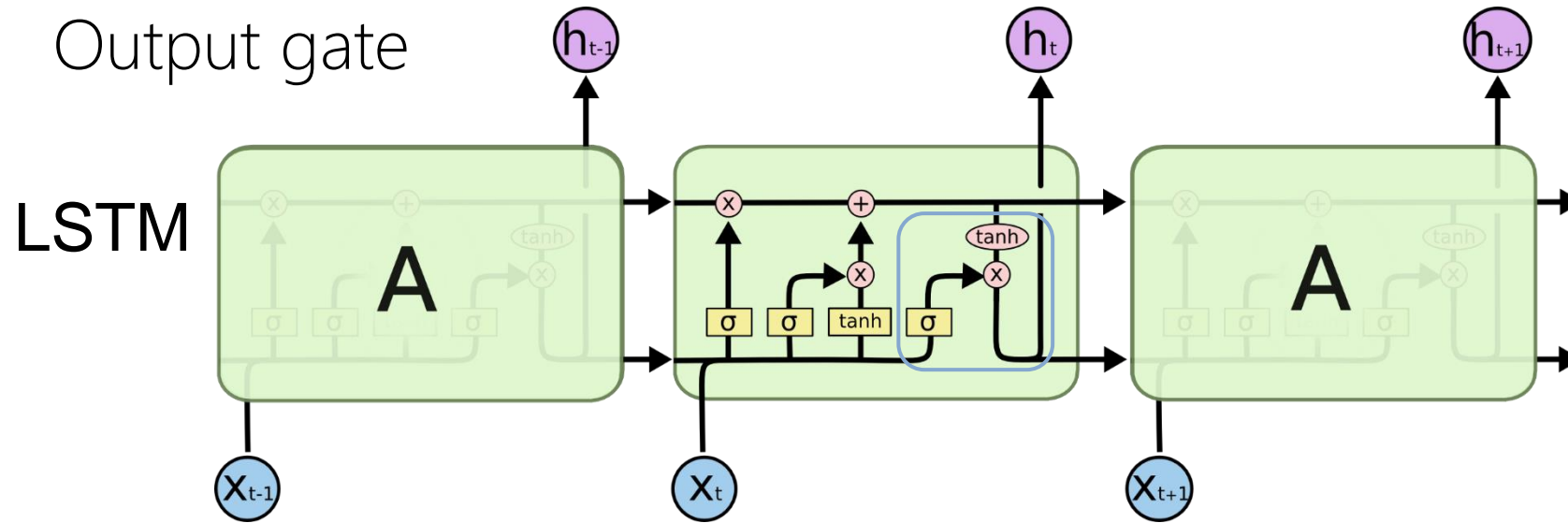
$$h_t = o_t * \tanh(C_t)$$



$$C_t = f_t * C_{t-1} + i_t * \tilde{C}_t$$

LSTM Images from: <https://colah.github.io/posts/2015-08-Understanding-LSTMs/>

Long Short-Term Memory



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

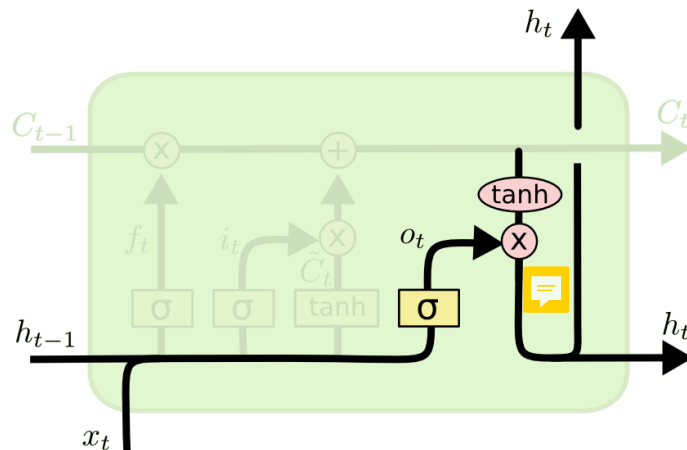
$$\tilde{C}_t = \tanh(W_C \cdot [h_{t-1}, x_t] + b_C)$$

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

$$C_t = f_t * C_{t-1} + i_t * \tilde{C}_t$$

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

$$h_t = o_t * \tanh(C_t)$$



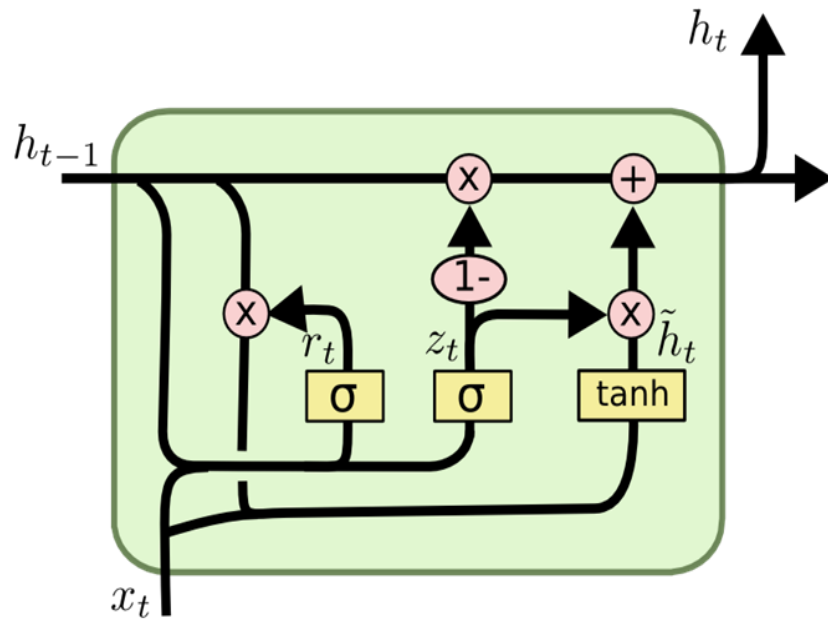
$$o_t = \sigma(W_o [h_{t-1}, x_t] + b_o)$$

$$h_t = o_t * \tanh(C_t)$$

LSTM Images from: <https://colah.github.io/posts/2015-08-Understanding-LSTMs/>

Gated Recurrent Unit (GRU)

It combines the forget and input gates into a single “update gate.” It also merges the cell state and hidden state, and makes some other changes.



$$z_t = \sigma (W_z \cdot [h_{t-1}, x_t])$$

$$r_t = \sigma (W_r \cdot [h_{t-1}, x_t])$$

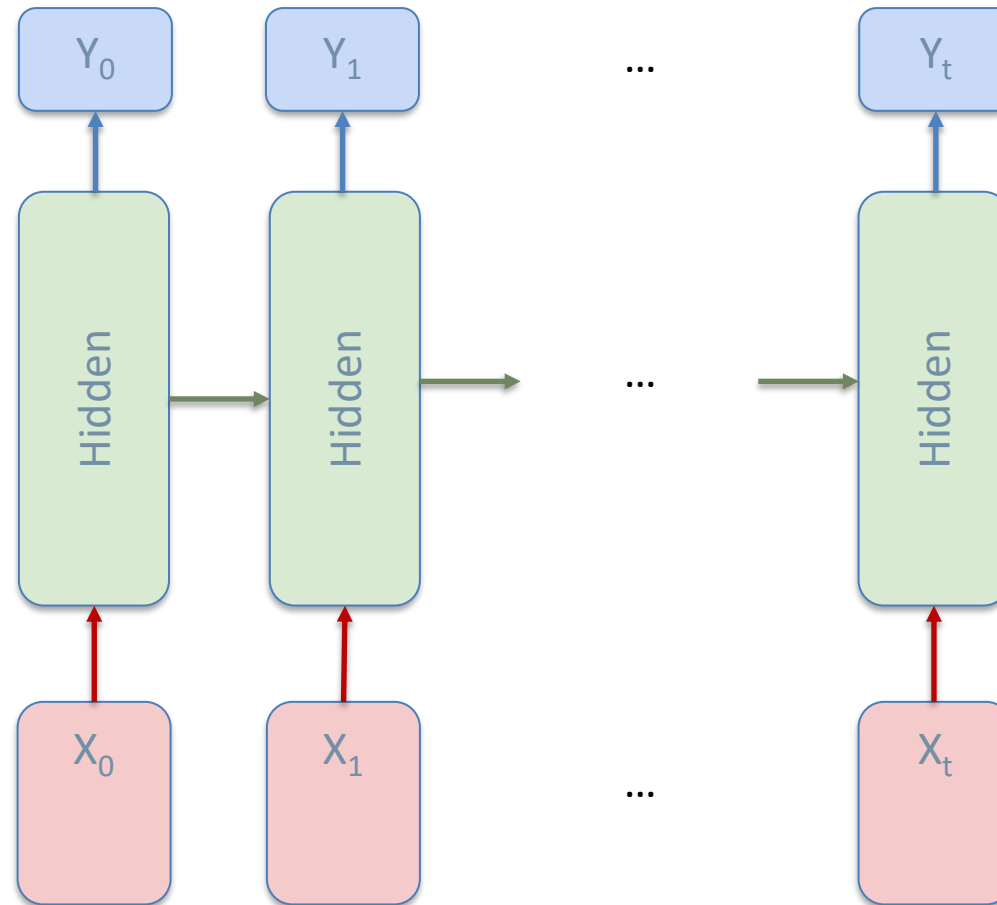
$$\tilde{h}_t = \tanh (W \cdot [r_t * h_{t-1}, x_t])$$

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

LSTM Images from: <https://colah.github.io/posts/2015-08-Understanding-LSTMs/>

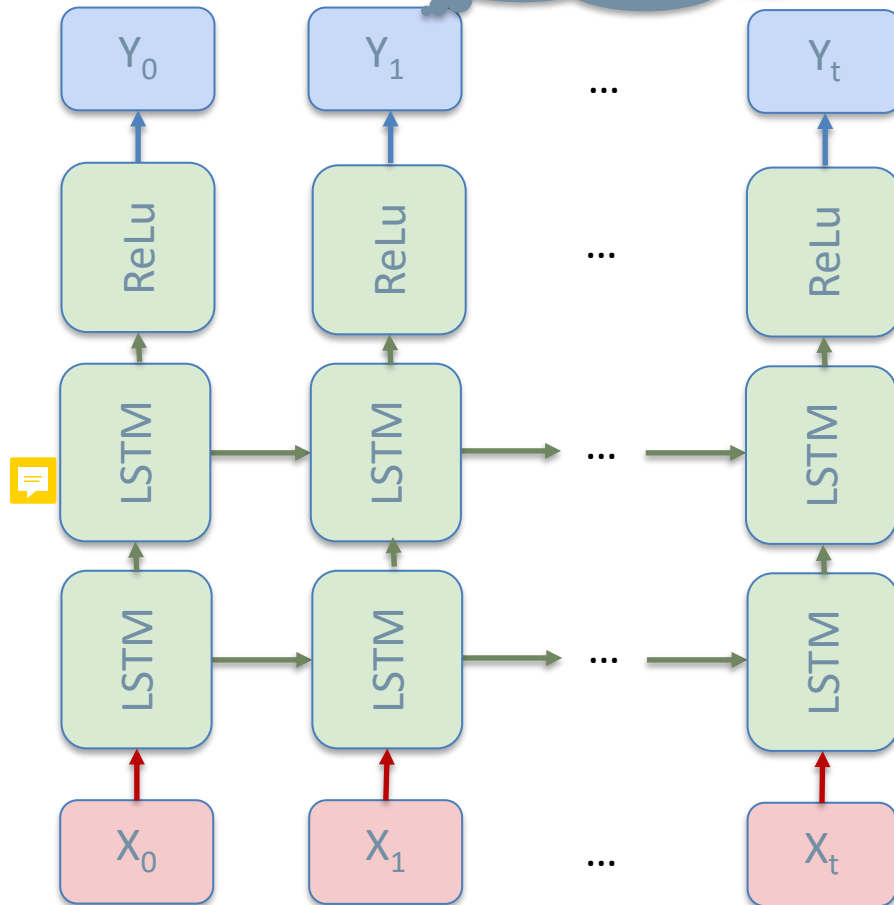
LSTM Networks

You can build a computation graph with continuous transformations.



Multiple Layers and Bidirectional LSTM Networks

A computational graph with continuous transformations.



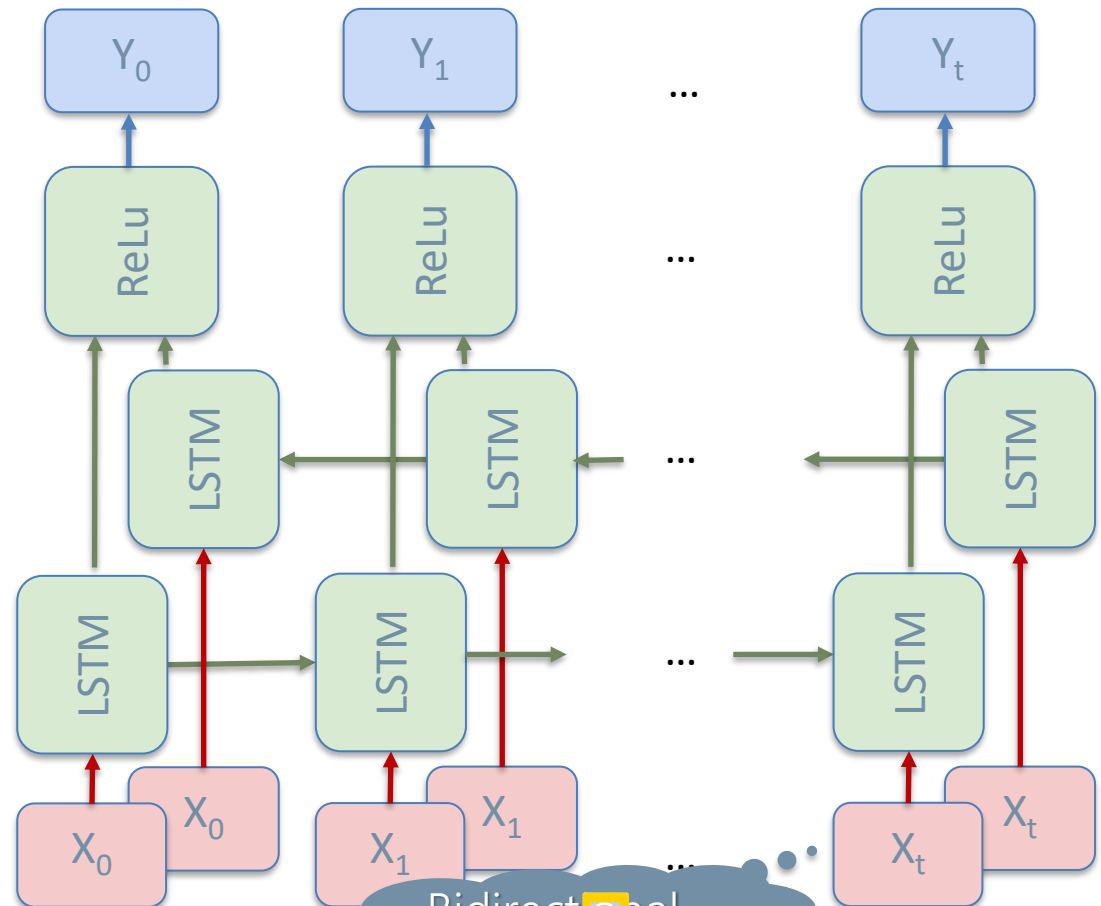
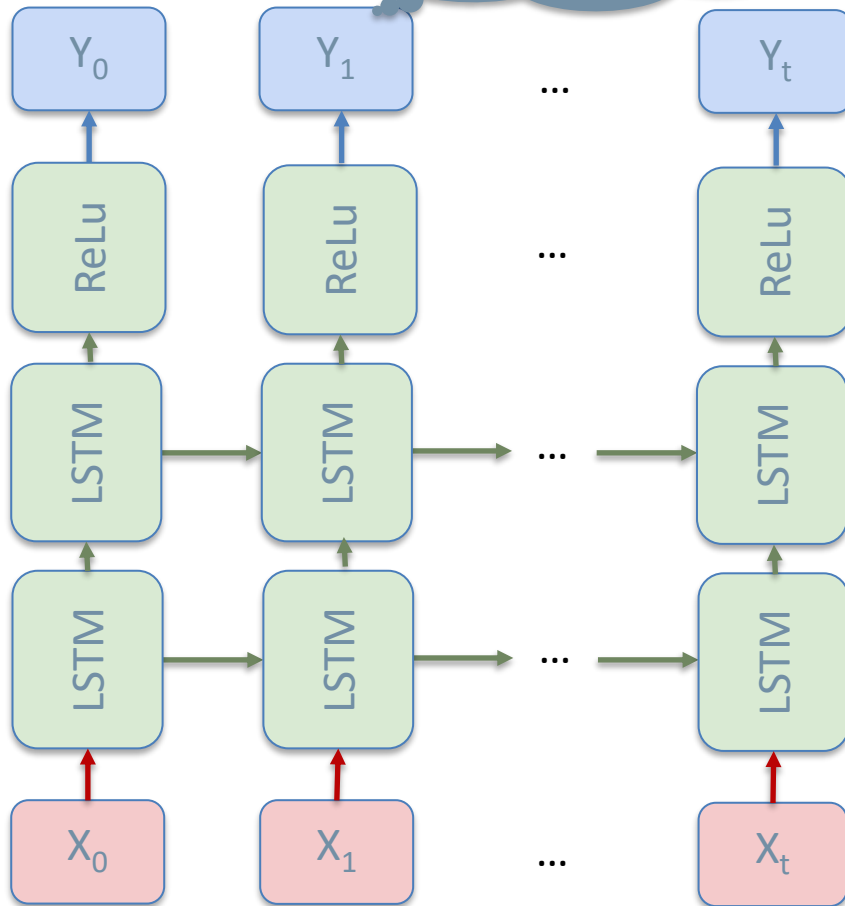
Tips & Tricks

When conditioning on full input sequence Bidirectional RNNs exploit it:

- Have one RNNs traverse the sequence left-to-right
- Have another RNN traverse the sequence right-to-left
- Use concatenation of hidden layers as feature representation

Multiple Layers and Bidirectional LSTM Networks

A computational graph with continuous transformations.



Tips & Tricks

When conditioning on full input sequence Bidirectional RNNs exploit it:

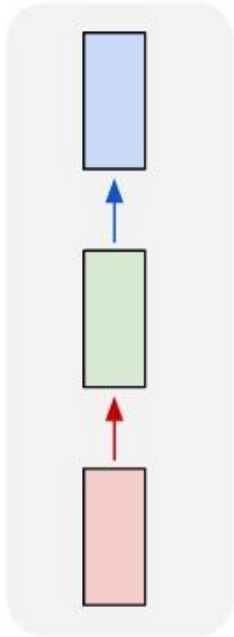
- Have one RNNs traverse the sequence left-to-right
- Have another RNN traverse the sequence right-to-left
- Use concatenation of hidden layers as feature representation


When initializing RNN we need to specify the initial state

- Could initialize them to a fixed value (such as 0)
- Better to treat the initial state as learned parameters
 - Start off with random guesses of the initial state values
 - Backpropagate the prediction error through time all the way to the initial state values and compute the gradient of the error with respect to these
 - Update these parameters by gradient descent

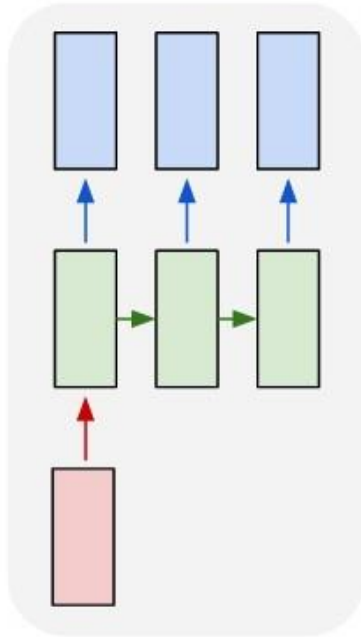
Sequential Data Problems

one to one



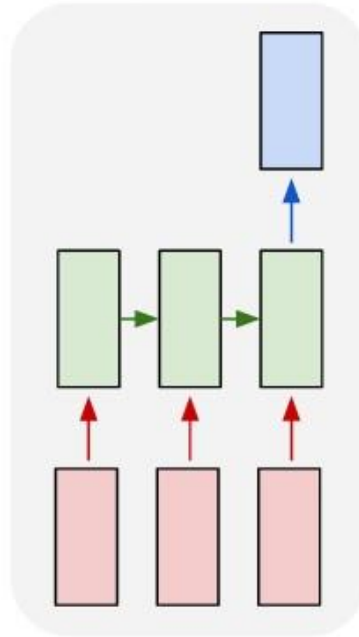
Fixed-sized input to fixed-sized output 
(e.g. image classification)

one to many



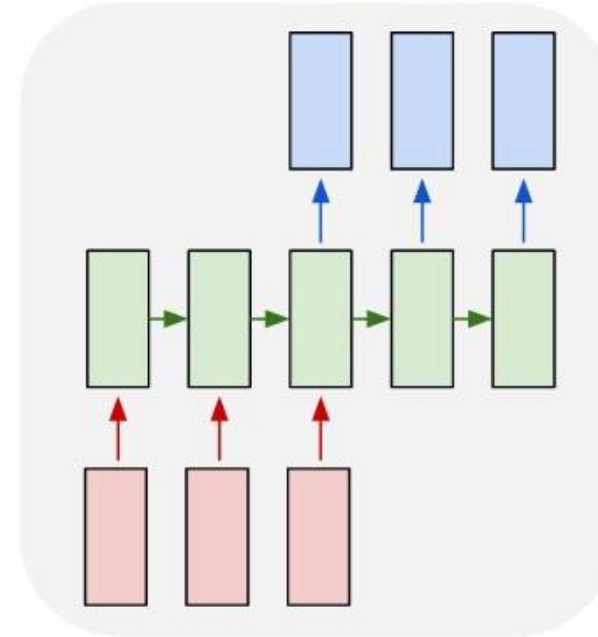
Sequence output
(e.g. image captioning takes an image and outputs a sentence of words).

many to one



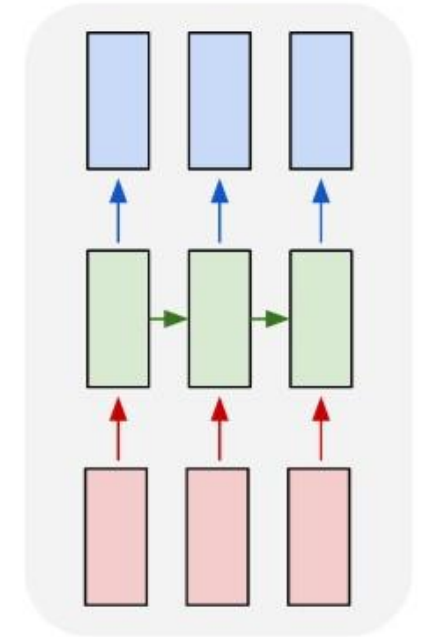
Sequence input (e.g. sentiment analysis where a given sentence is classified as expressing positive or negative sentiment).

many to many



Sequence input and sequence output (e.g. Machine Translation: an RNN reads a sentence in English and then outputs a sentence in French)

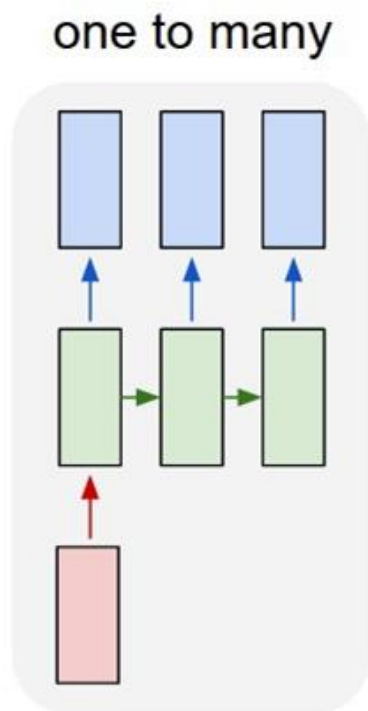
many to many



Synced sequence input and output (e.g. video classification where we wish to label each frame of the video)

Sequence to Sequence Learning Examples (1/3)

Image Captioning: input a single image and get a series or sequence of words as output which describe it. The image has a fixed size, but the output has varying length.



A person riding a motorcycle on a dirt road.



Two dogs play in the grass.



A group of young people playing a game of frisbee.

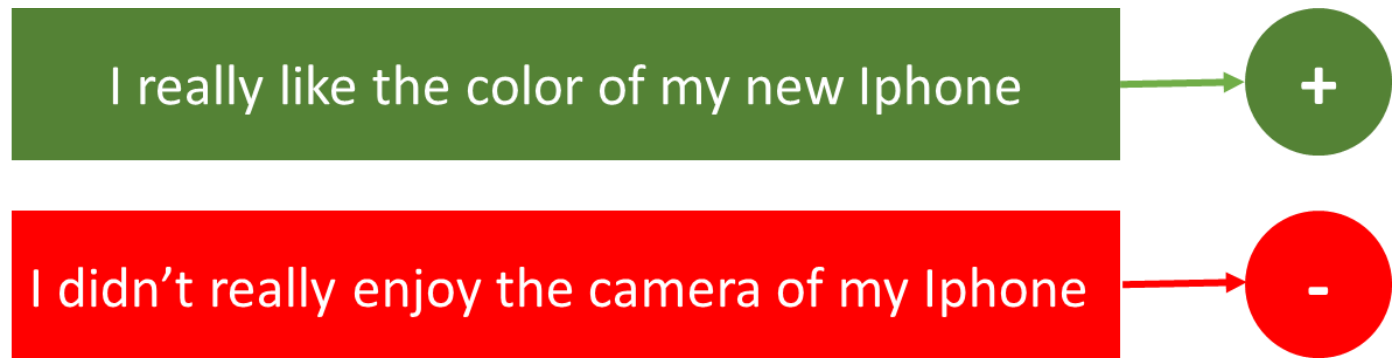
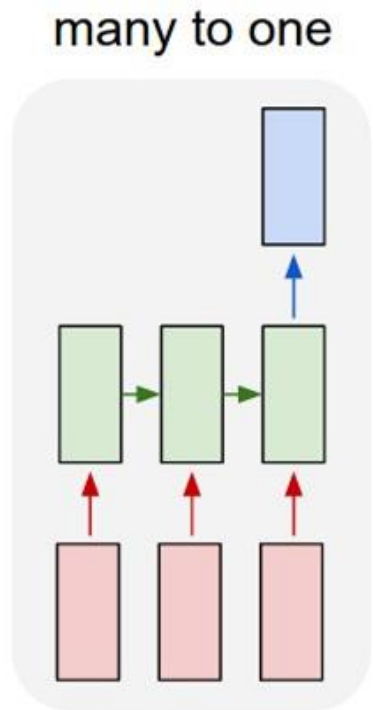


Two hockey players are fighting over the puck.

Sequence to Sequence Learning Examples (2/3)

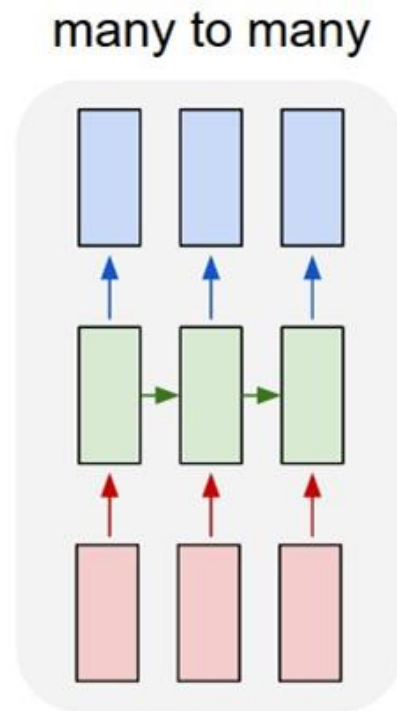
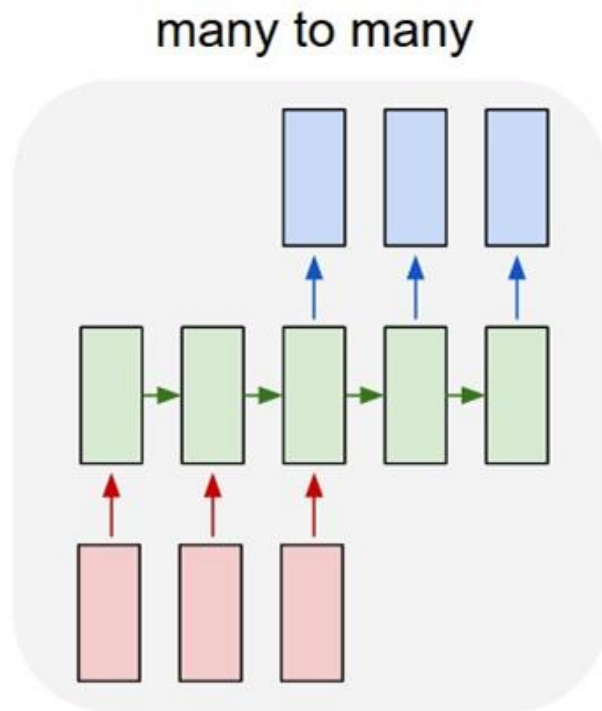


Sentiment Classification/Analysis: input a sequence of characters or words, e.g., a tweet, and classify the sequence into positive or negative sentiment. Input has varying lengths; output is of a fixed type and size.



Sequence to Sequence Learning Examples (3/3)

Language Translation: having some text in a particular language, e.g., English, we wish to translate it in another, e.g., French. Each language has its own semantics and it has varying lengths for the same sentence.



French was the official language of the colony of French Indochina, comprising modern-day Vietnam, Laos, and Cambodia. It continues to be an administrative language in Laos and Cambodia, although its influence has waned in recent years.

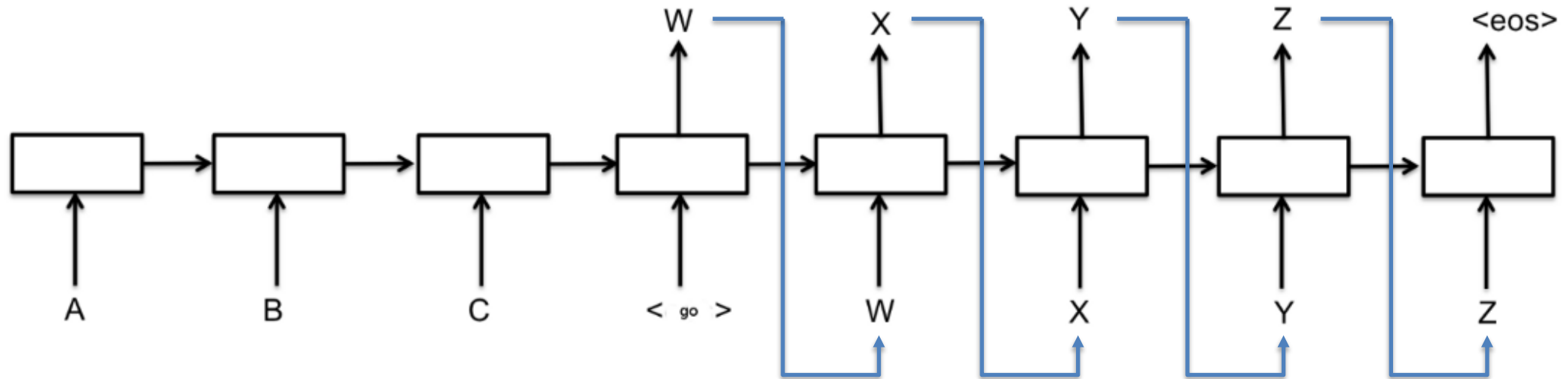


Le français était la langue officielle de la colonie de l'Indochine française, comprenant le Vietnam d'aujourd'hui, le Laos et le Cambodge. Il continue d'être une langue administrative au Laos et au Cambodge, bien que son influence a décliné au cours des dernières années.

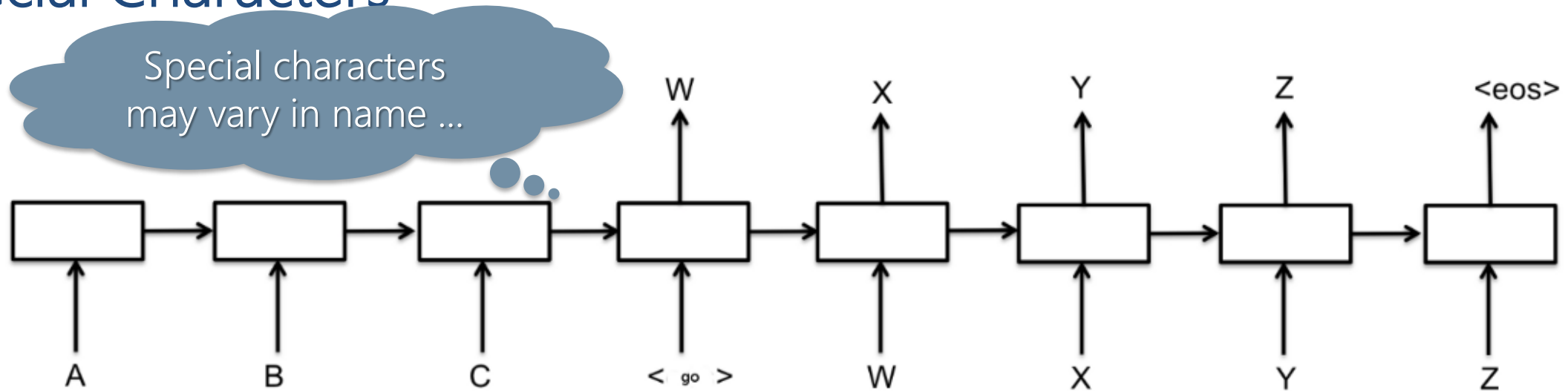
Seq2Seq Model

The Seq2Seq model follows the classical encoder decoder architecture

- At training time the decoder **does not** feed the output of each time step to the next; the input to the decoder time steps are the target from the training
- At inference time the decoder feeds the output of each time step as an input to the next one



Special Characters



<PAD>: During training, examples are fed to the network in batches. The inputs in these batches need to be the same width. This is used to pad shorter inputs to the same width of the batch

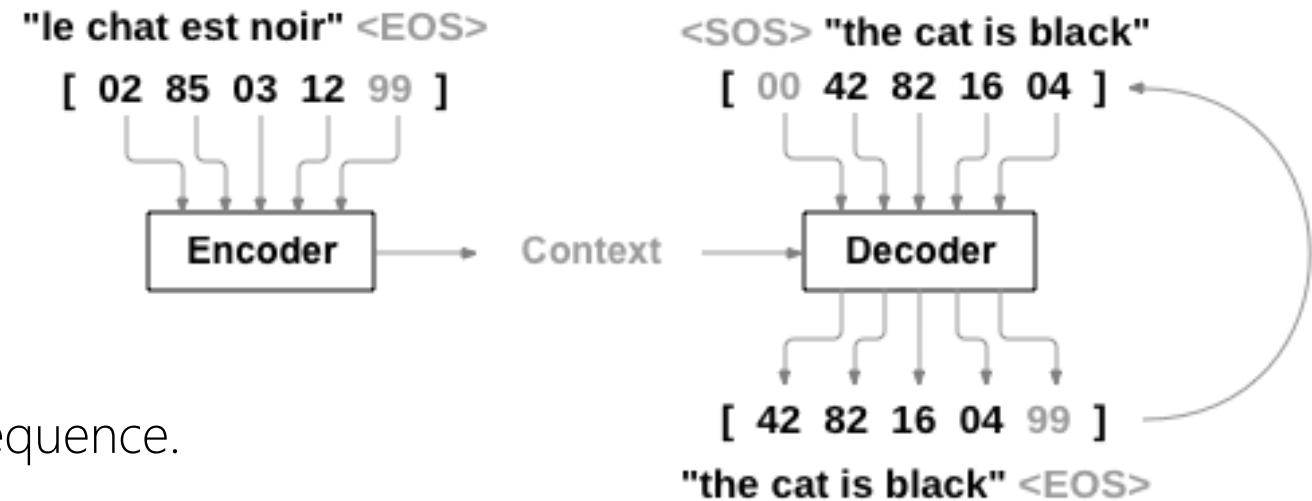
<EOS>: Needed for batching on the decoder side. It tells the decoder where a sentence ends, and it allows the decoder to indicate the same thing in its outputs as well.

<UNK>: On real data, it can vastly improve the resource efficiency to ignore words that do not show up often enough in your vocabulary by replace those with this character.

<SOS>/<GO>: This is the input to the first time step of the decoder to let the decoder know when to start generating output.

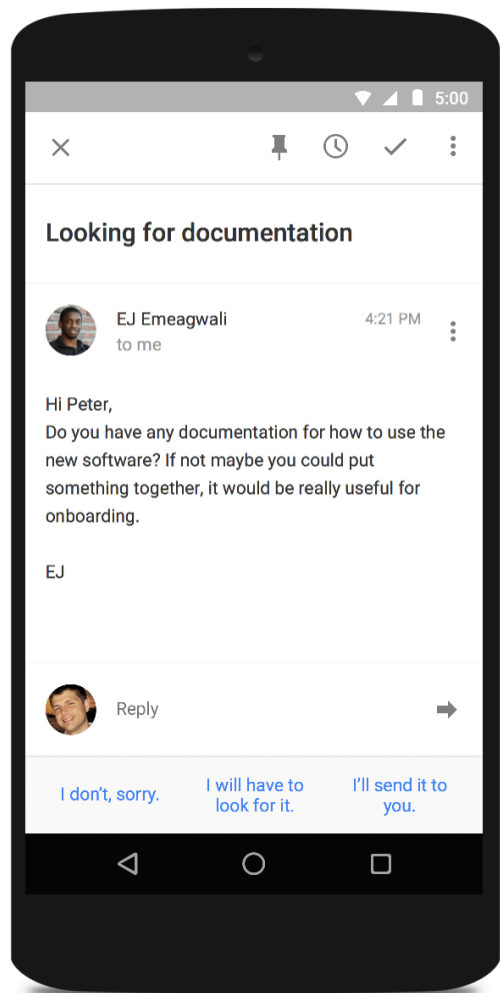
Dataset Batch Preparation

1. Sample `batch_size` pairs of (`source_sequence`, `target_sequence`).
2. Append `<EOS>` to the `source_sequence`
3. Prepend `<SOS>` to the `target_sequence` to obtain the `target_input_sequence` and append `<EOS>` to obtain `target_output_sequence`.
4. Pad up to the `max_input_length` (`max_target_length`) within the batch using the `<PAD>` token.
5. Encode tokens based of vocabulary (or embedding)
6. Replace out of vocabulary (OOV) tokens with `<UNK>`.
Compute the length of each input and target sequence in the batch.

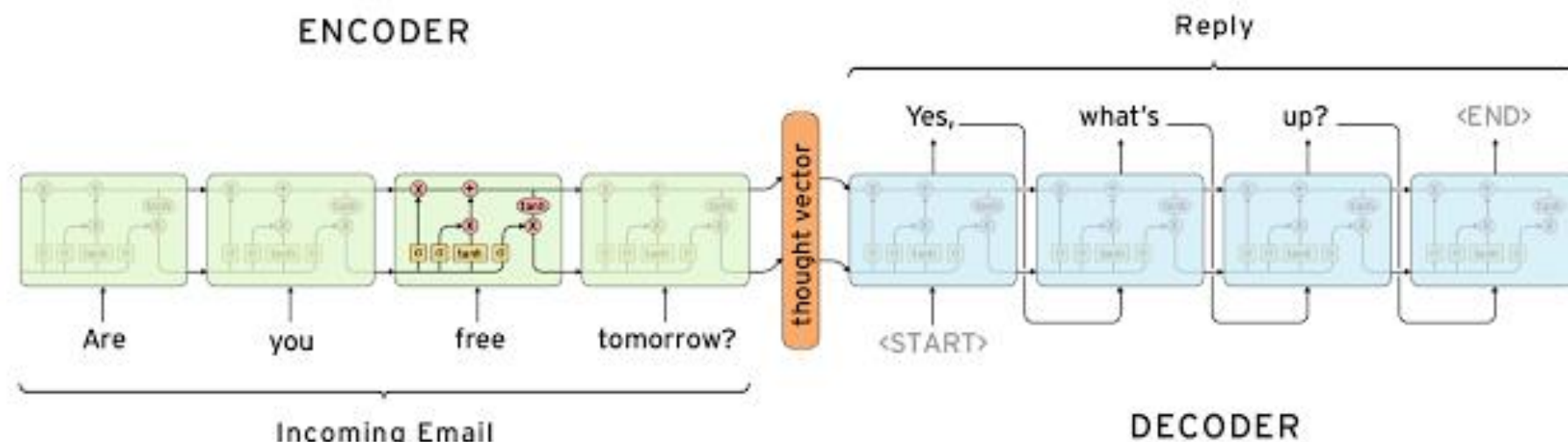


```
vocabulary = { "<SOS>": 00,  
               "<EOS>": 99,  
               "<UNK>": 01,  
               "<PAD>": 03,  
               "the": 42,  
               "is": 16,  
               ...   }
```

Sequence to Sequence Modeling



Given $\langle S, T \rangle$ pairs, read S , and output T' that best matches T



$$p(y_1, \dots, y_{T'} | x_1, \dots, x_T) = \prod_{t=1}^{T'} p(y_t | v, y_1, \dots, y_{t-1})$$

$$\frac{1}{|\mathcal{S}|} \sum_{(T,S) \in \mathcal{S}} \log p(T|S)$$

LSTM Images Credits: Andrej Karpathy