Recurrent Neural Networks

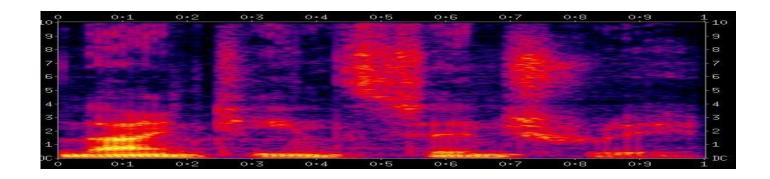
CSE 849 Deep Learning Spring 2025

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Modelling Series

- In many situations one must consider a *series* of inputs to produce an output
 - Outputs too may be a series

What did I say?



- Speech Recognition
 - Analyze a series of spectral vectors, determine what was said
- Note: Inputs are sequences of vectors. Output is a classification result

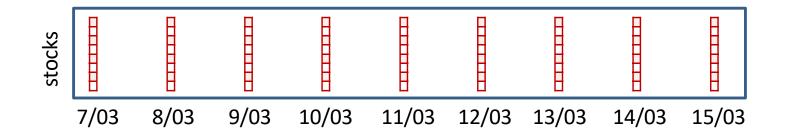
What is he talking about?

The Steelers, meanwhile, continue to struggle to make stops on defense. They've allowed, on average, 30 points a game, and have shown no signs of improving anytime soon.

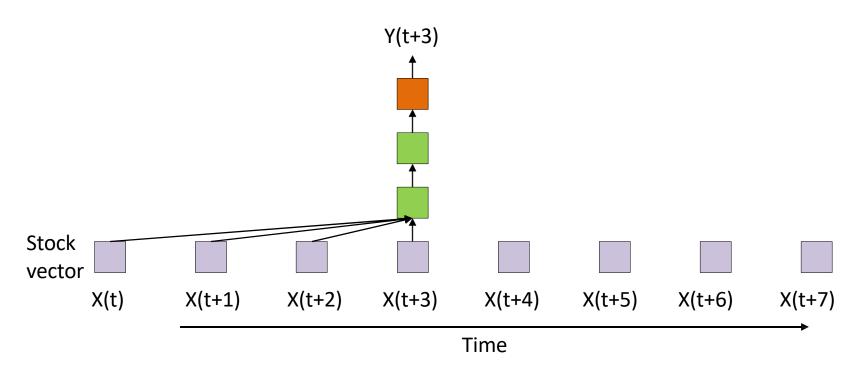
"Football" or "basketball"?

- Text analysis
 - E.g. analyze document, identify topic
 - Input series of words, output classification output
 - E.g. read English, output French
 - Input series of words, output series of words

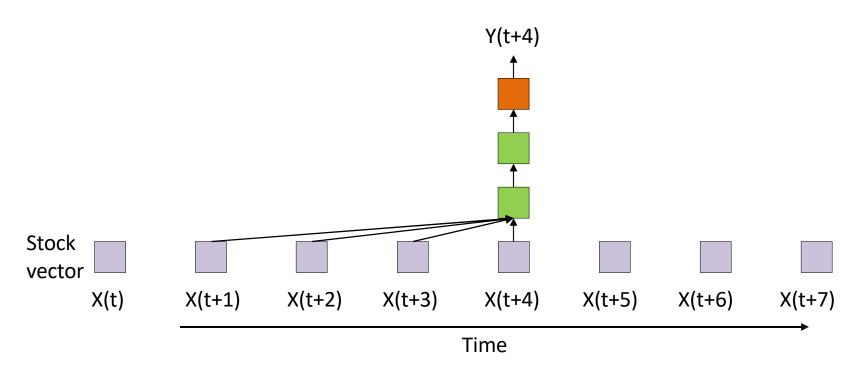
Should I invest...



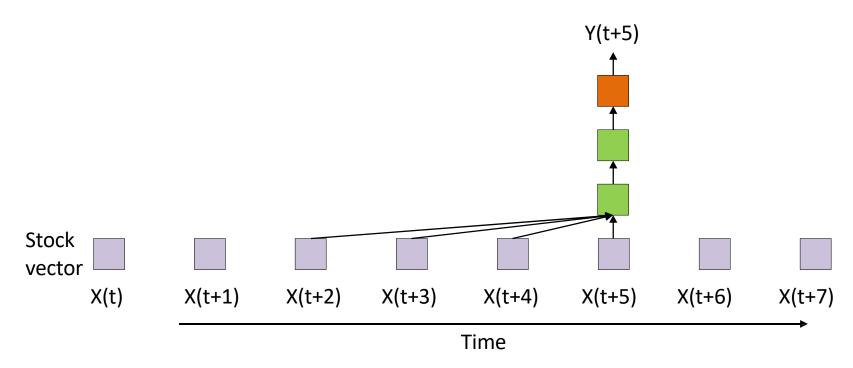
- Note: Inputs are sequences of vectors. Output may be scalar or vector
 - Should I invest, vs. should I not invest in X?
 - Decision must be taken considering how things have fared over time
- Must consider the series of stock values in the past several days to decide if it is wise to invest today



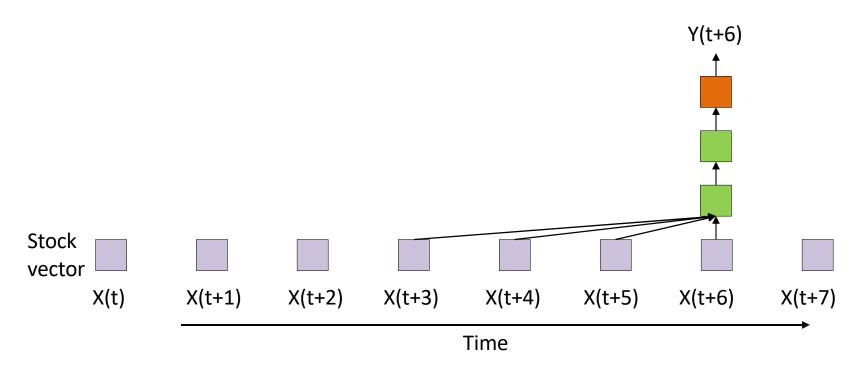
- The sliding predictor
 - Look at the last few days
 - This is just a convolutional neural net applied to series data
 - Also called a *Time-Delay neural network*



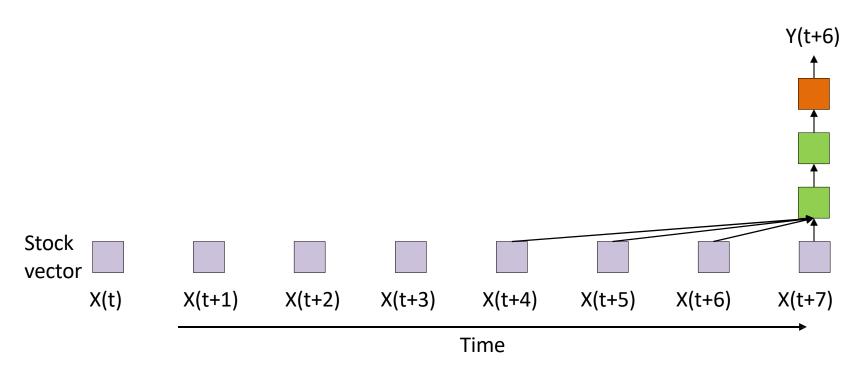
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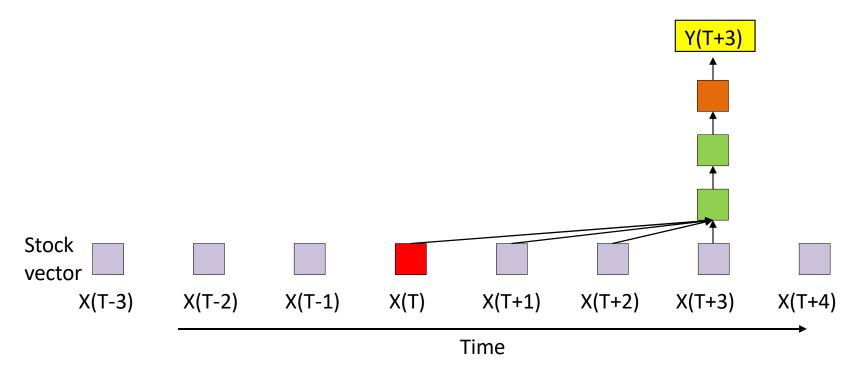
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 - This is just a convolutional neural net applied to series data
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Finite-response model

- This is a *finite response* system
 - Something that happens today only affects the output of the system for N days into the future
 - *N* is the *width* of the system

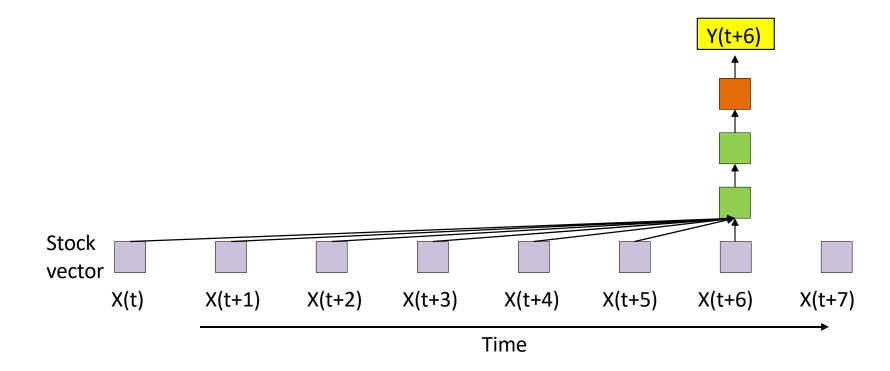
$$Y_t = f(X_t, X_{t-1}, ..., X_{t-N})$$

Finite-response model



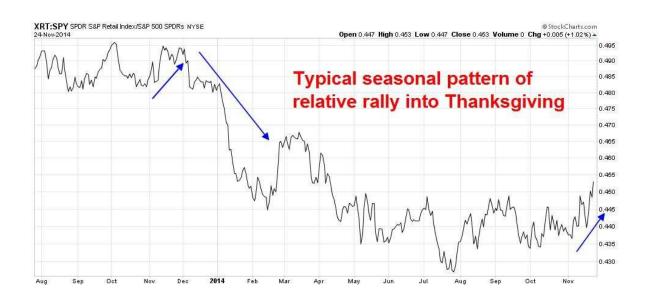
- Something that happens *today* only affects the output of the system for *N* days into the future
 - Predictions consider N days of history
- To consider more of the past to make predictions, you must increase the "history" considered by the system

Finite-response



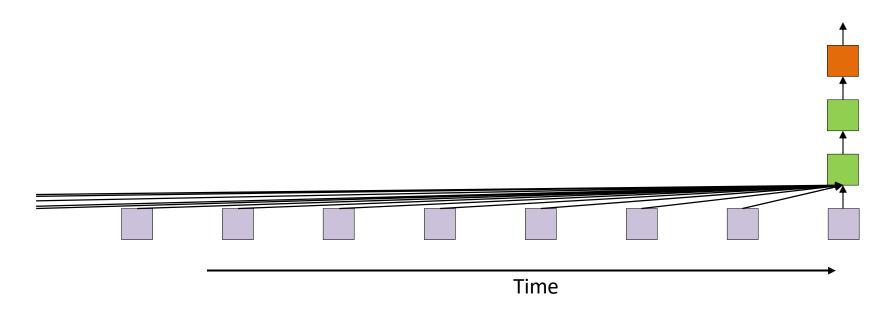
- Problem: Increasing the "history" makes the network more complex
 - -- require more computational resources

Systems often have long-term dependencies



- Longer-term trends
 - Weekly trends in the market
 - Monthly trends in the market
 - Annual trends

We want infinite memory



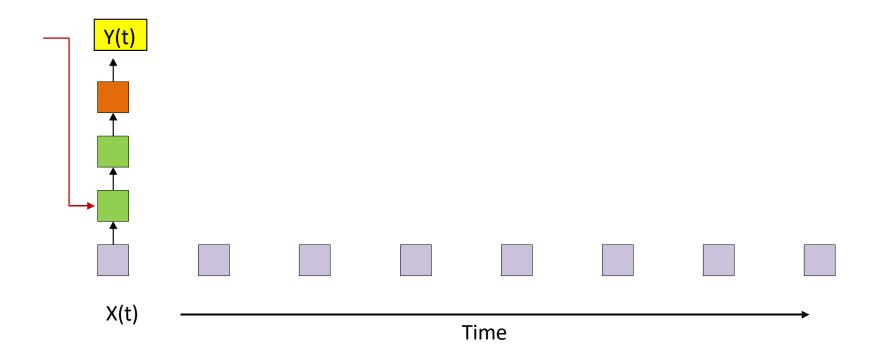
- Required: Infinite response systems
 - What happens today can continue to affect the output forever
 - Possibly with weaker and weaker influence

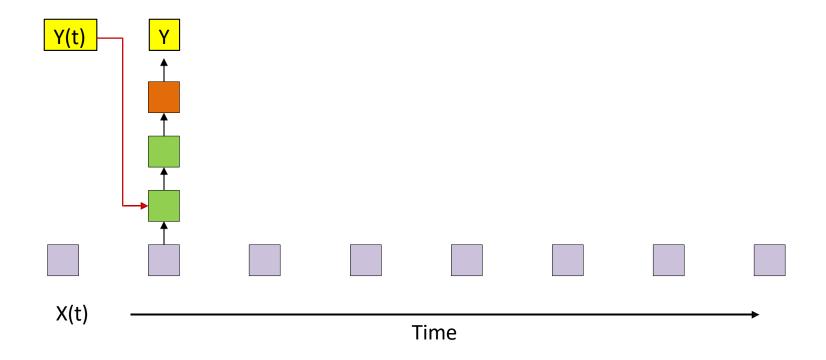
$$Y_t = f(X_t, X_{t-1}, \dots, X_{t-\infty})$$

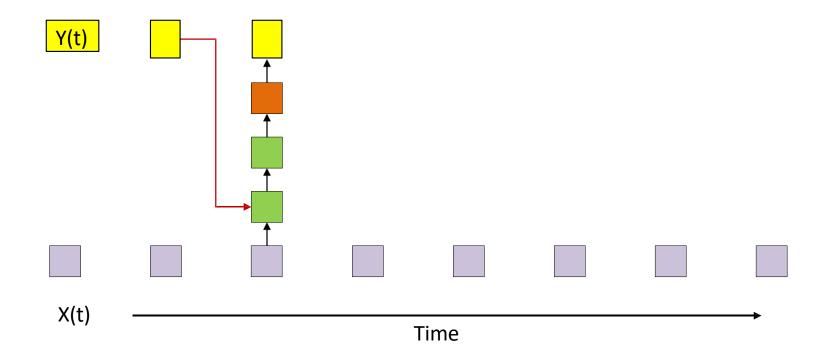
Examples of infinite response systems

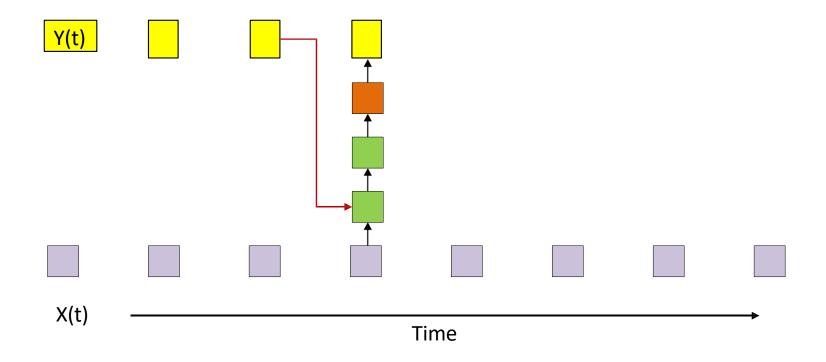
$$Y_t = f(X_t, Y_{t-1})$$

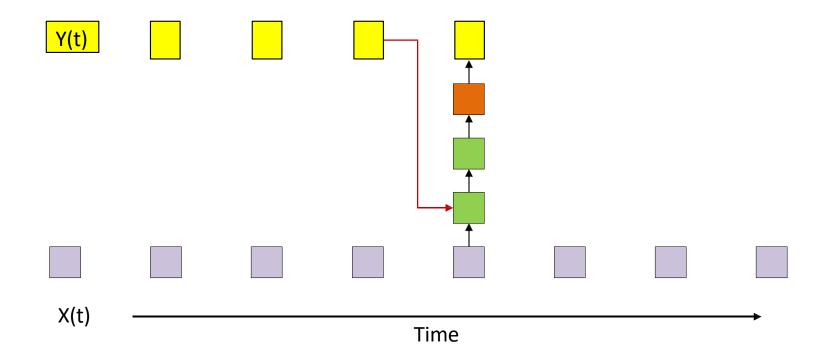
- Required: Define initial state: Y_{-1} for t = 0
- An input X_0 at t=0 produces Y_0
- Y_0 produces Y_1 which produces Y_2 and so on until Y_∞ even if $X_1 \dots X_\infty$ are 0
 - i.e. even if there are no further inputs!
- A single input influences the output for the rest of time!
- This is an instance of a NARX network
 - "nonlinear autoregressive network with exogenous inputs"
 - $Y_t = f(X_{0:t}, Y_{0:t-1})$
- Output contains information about the entire past

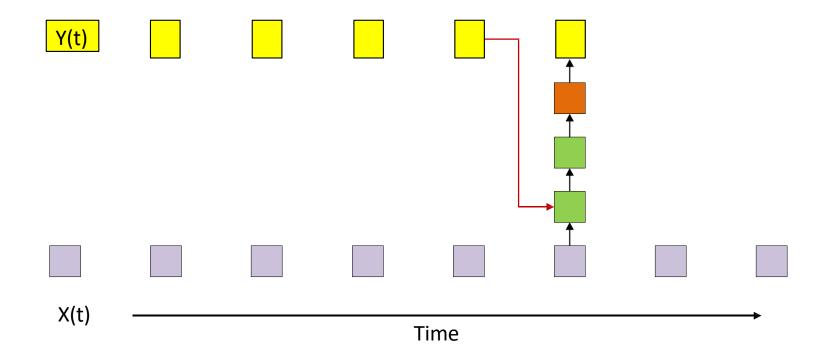


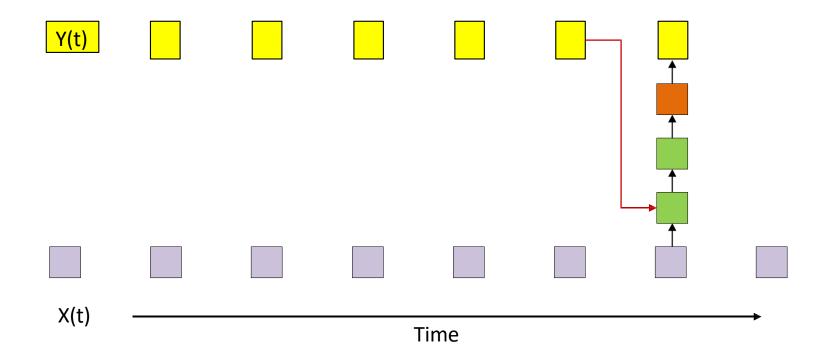


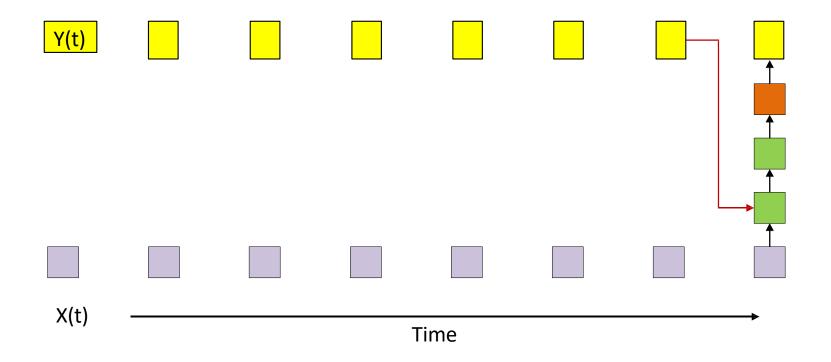




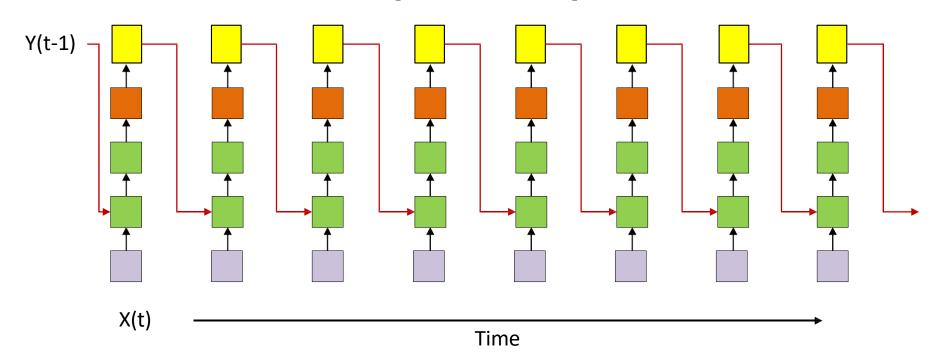








A more complete representation



- A NARX net with recursion from the output
- Showing all computations
- All columns are identical
- An input at t=0 affects outputs forever

NARX Networks

- Very popular for time-series prediction
 - Weather
 - Stock markets
 - As alternate system models in tracking systems
 - Language
- Note: here the "memory" of the past is in the output itself, and not in the network

Let's make memory more explicit

- Task is to "remember" the past
- Introduce an explicit memory variable whose job it is to remember

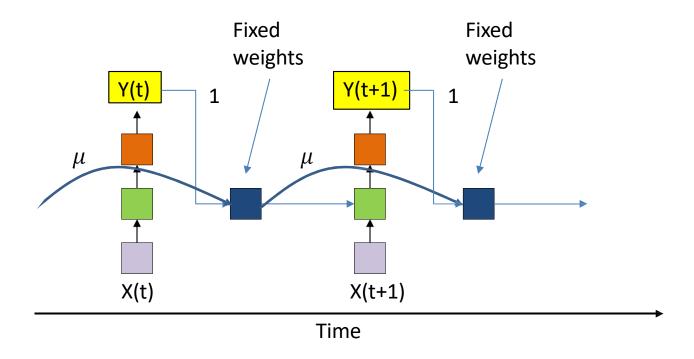
$$m_t = r(y_{t-1}, h_{t-1}, m_{t-1})$$

$$h_t = f(x_t, m_t)$$

$$y_t = g(h_t)$$

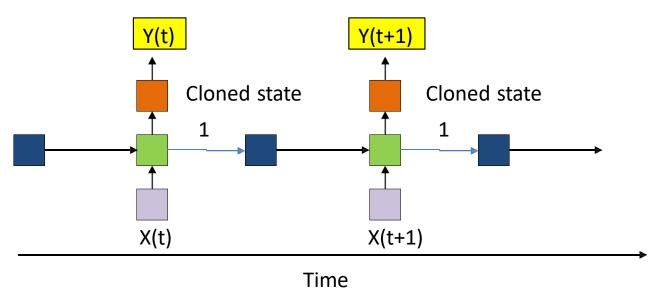
- m_t is a "memory" variable
 - Generally stored in a "memory" unit
 - Used to "remember" the past

Jordan Network



- Memory unit simply retains a running average of past outputs
 - "Serial order: A parallel distributed processing approach", M.I.Jordan, 1986
 - Memory has fixed structure; does not "learn" to remember
 - The running average of outputs considers entire past, rather than immediate past

Elman Networks



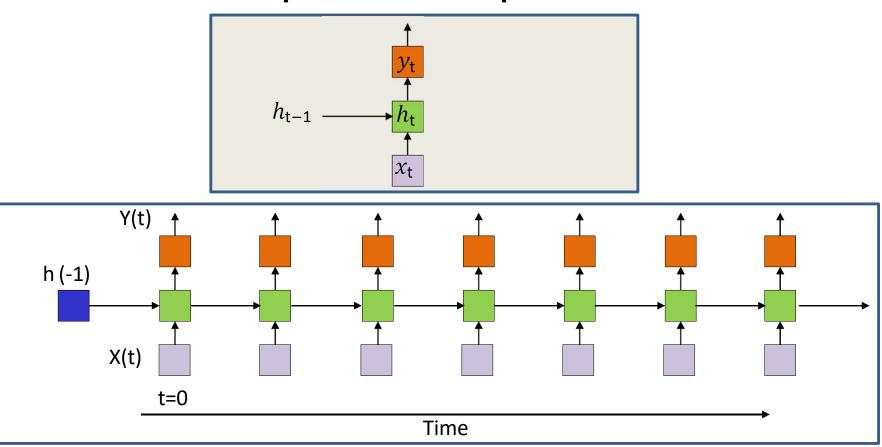
- Separate memory state from output
 - "Context" units that carry historical state
 - "Finding structure in time", Jeffrey Elman, Cognitive Science, 1990
- Only the weight from the memory unit to the hidden unit is learned
 - But during training no gradient is backpropagated over the "1" link

An alternate model for infinite response systems: the state-space model

$$h_t = f(x_t, h_{t-1})$$
$$y_t = g(h_t)$$

- h_t is the *state* of the network
 - State summarizes information about the entire past
 - Model directly embeds the memory in the state
- Need to define initial state h_{-1}
- This is a *recurrent* neural network

The simple state-space model



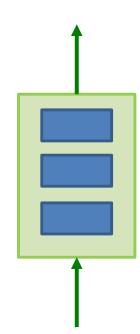
- The state (green) at any time is determined by the input at that time, and the state at the previous time
- An input at t=0 affects outputs forever
- Also known as a recurrent neural net

An alternate model for infinite response systems: the state-space model

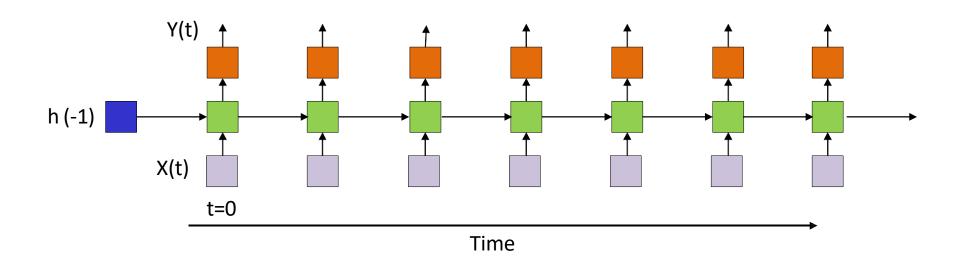
$$h_t = f(x_t, h_{t-1})$$
$$y_t = g(h_t)$$

- h_t is the *state* of the network
- Need to define initial state h_{-1}

• The state can be *arbitrarily complex*

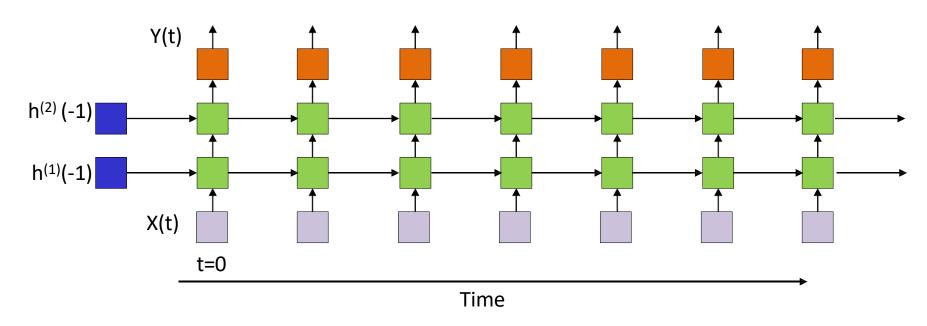


Single hidden layer RNN



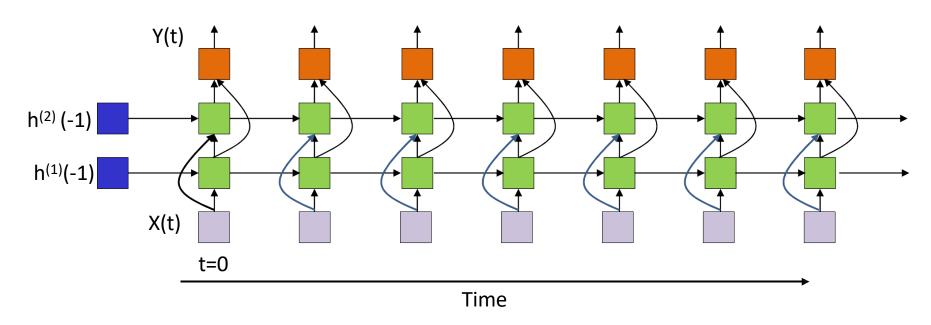
- Recurrent neural network
- All columns are identical
- An input at t=0 affects outputs forever

Multiple recurrent layer RNN



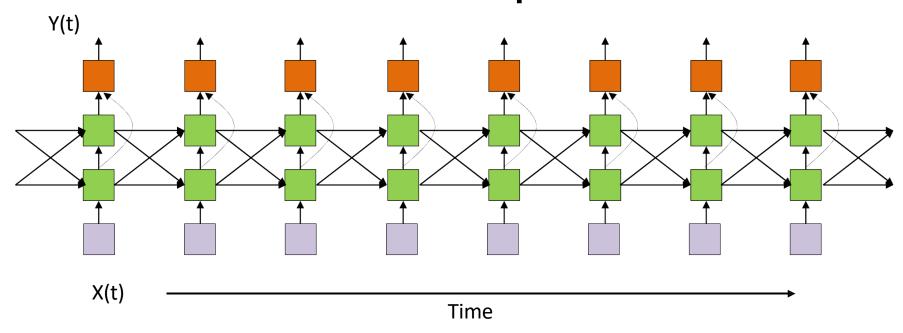
- Recurrent neural network
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Multiple recurrent layer RNN



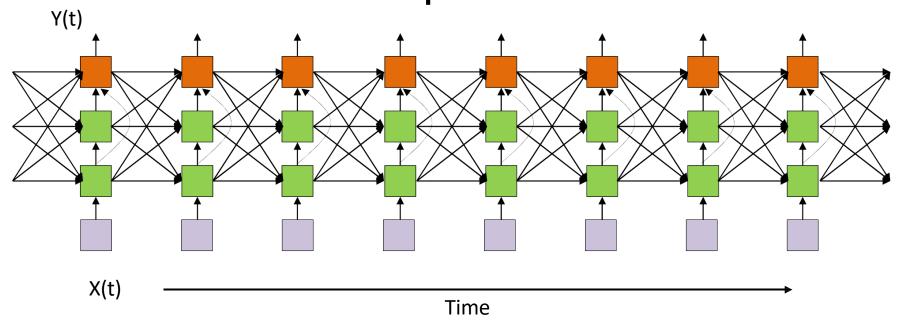
• We can also have skips..

A more complex state



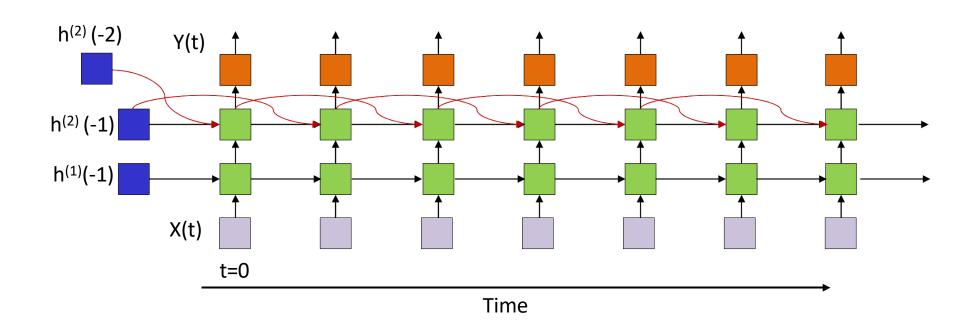
- All columns are identical
- An input at t=0 affects outputs forever

Or the network may be even more complicated



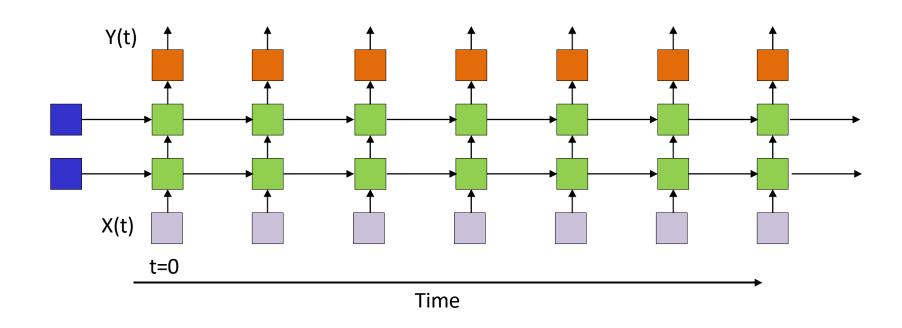
- All columns are identical
- An input at t=0 affects outputs forever

Generalization with other recurrences



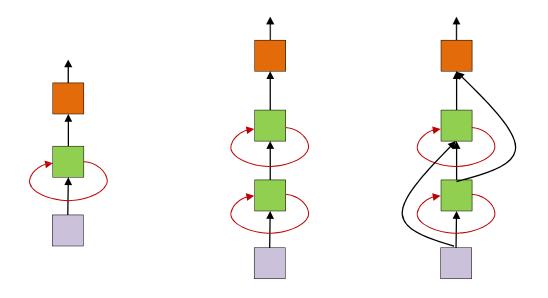
All columns (including incoming edges) are identical

The simplest structures are most popular



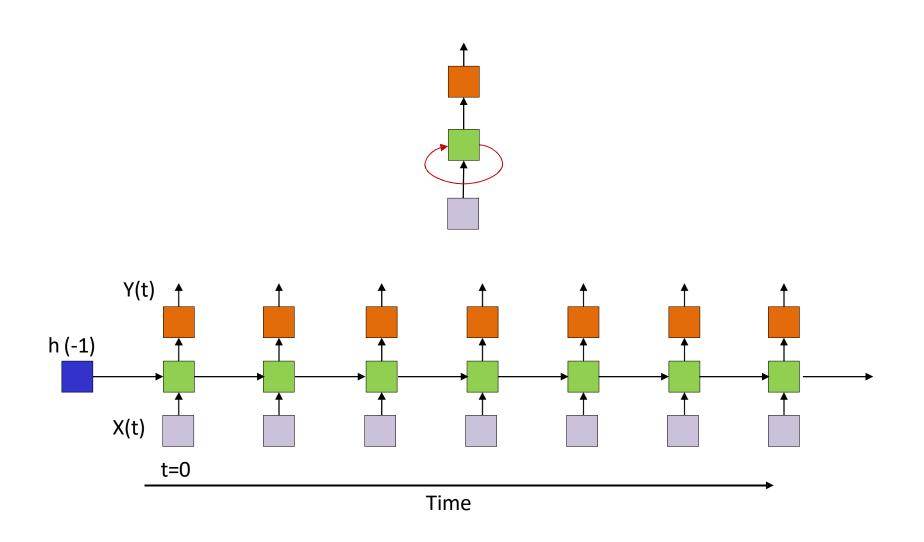
- Recurrent neural network
- All columns are identical
- An input at t=0 affects outputs forever

A Recurrent Neural Network

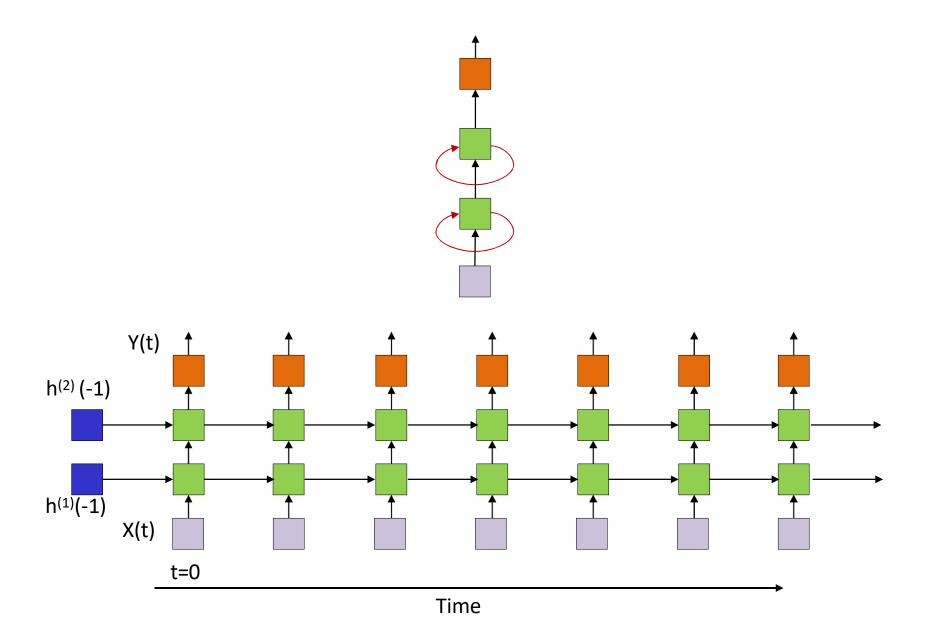


- Simplified models often drawn
- The loops imply recurrence

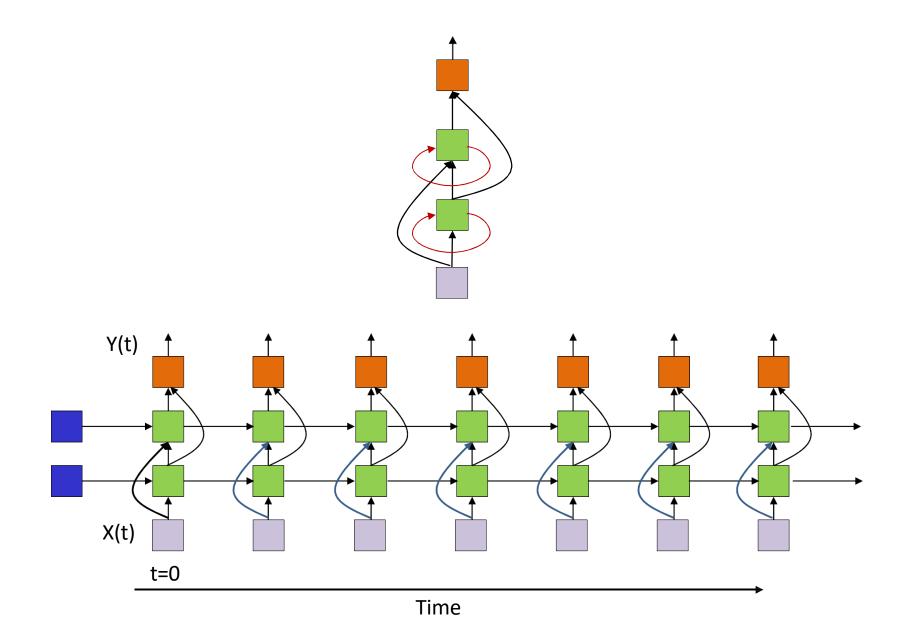
The detailed version of the simplified representation

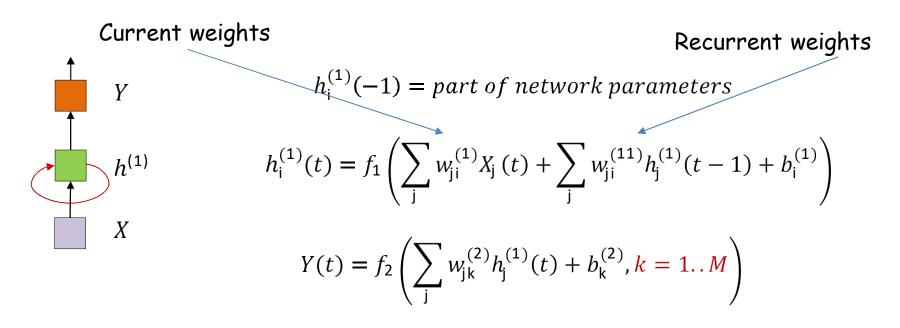


Multiple recurrent layer RNN

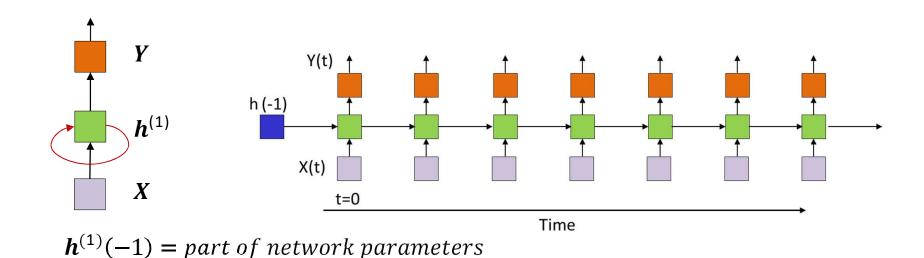


Multiple recurrent layer RNN





- Note superscript in indexing, which indicates layer of network from which inputs are obtained
- Assuming vector function at output, e.g. softmax
- The *state* node activation, f_1 () is typically tanh()
- Every neuron also has a bias input

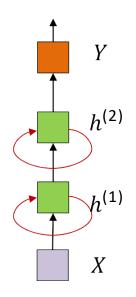


Computation:

$$h^{(1)}(t) = f_1 (W^{(1)}X(t) + W^{(11)}h^{(1)}(t-1) + b^{(1)})$$

$$Y(t) = f_2 (W^{(2)}h^{(1)}(t) + b^{(2)})$$

• The recurrent state activation f_1 () is typically tanh()



$$h_i^{(1)}(-1) = part \ of \ network \ parameters$$

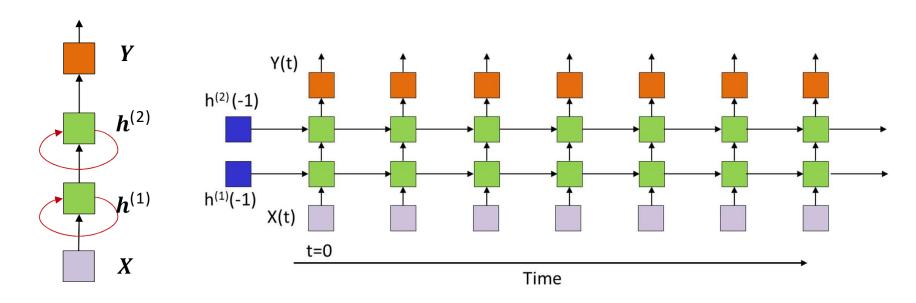
 $h_i^{(2)}(-1) = part \ of \ network \ parameters$

$$h_{i}^{(1)}(t) = f_{1}\left(\sum_{j} w_{ji}^{(1)} X_{j}(t) + \sum_{j} w_{ji}^{(11)} h_{j}^{(1)}(t-1) + b_{i}^{(1)}\right)$$

$$h_{i}^{(2)}(t) = f_{2} \left(\sum_{j} w_{ji}^{(2)} h_{j}^{(1)}(t) + \sum_{j} w_{ji}^{(22)} h_{j}^{(2)}(t-1) + b_{i}^{(2)} \right)$$

$$Y(t) = f_3 \left(\sum_{j} w_{jk}^{(3)} h_j^{(2)}(t) + b_k^{(3)}, k = 1...M \right)$$

- Assuming vector function at output, e.g. softmax f_3 ()
- The state node activations, $f_k()$ are typically tanh()
- Every neuron also has a bias input



 $\mathbf{h}^{(1)}(-1)$ and $\mathbf{h}^{(2)}(-1) = part\ of\ network\ parameters$

• Computation:

$$h^{(1)}(t) = f_1 (W^{(1)}X(t) + W^{(11)}h^{(1)}(t-1) + b^{(1)})$$

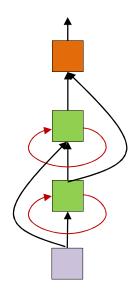
$$h^{(2)}(t) = f_2 (W^{(2)}h^{(1)}(t) + W^{(22)}h^{(2)}(t-1) + b^{(2)})$$

$$Y(t) = f_3 (W^{(3)}h^{(2)}(t) + b^{(3)})$$

The recurrent state activation is typically tanh()

$$\mathbf{h}^{(1)}(-1) = part\ of\ network\ parameters$$

$$\mathbf{h}^{(2)}(-1) = part\ of\ network\ parameters$$

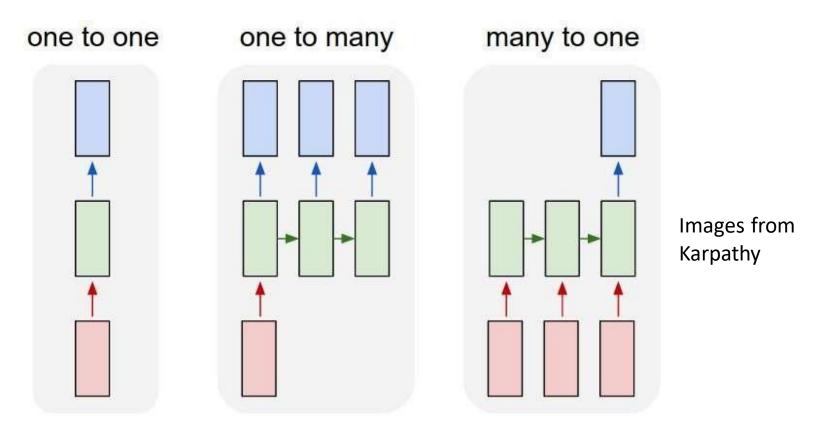


$$\mathbf{h}^{(1)}(t) = f_1 (\mathbf{W}^{(01)} \mathbf{X}(t) + \mathbf{W}^{(11)} \mathbf{h}^{(1)}(t-1) + \mathbf{b}^{(1)})$$

$$\boldsymbol{h}^{(2)}(t) = f_2 (\boldsymbol{W}^{(12)} \boldsymbol{h}^{(1)}(t) + \boldsymbol{W}^{(02)} \boldsymbol{X}(t) + \boldsymbol{W}^{(22)} \boldsymbol{h}^{(2)}(t-1) + \boldsymbol{b}^{(2)})$$

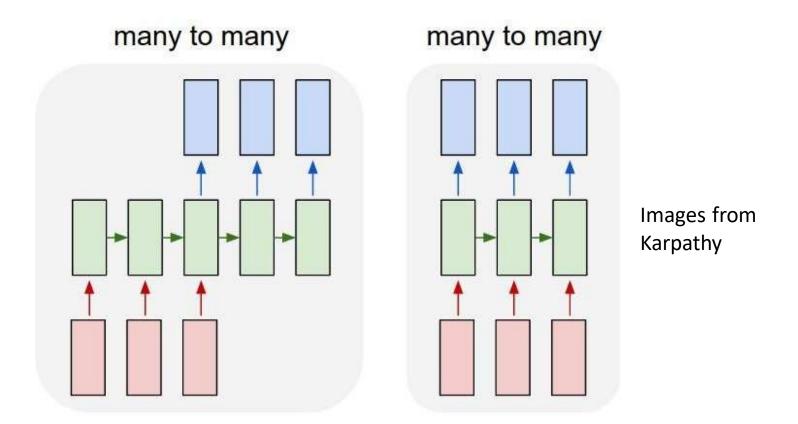
$$Y(t) = f_3 (W^{(23)}h^{(2)}(t) + W^{(13)}h^{(1)}(t) + b^{(3)})$$

Variants on recurrent nets



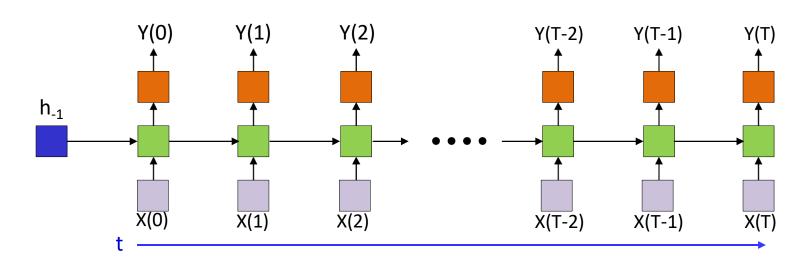
- 1: Conventional MLP
- 2: Sequence *generation*, e.g. image to caption
- 3: Sequence based *prediction or classification*, e.g. Speech recognition, text classification

Variants



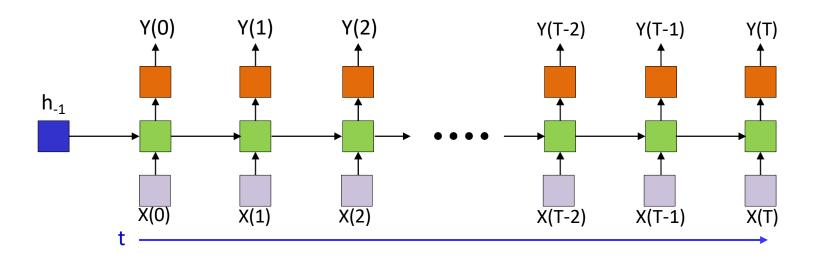
- 1: Delayed sequence to sequence, e.g. machine translation
- 2: Sequence to sequence, e.g. stock problem, label prediction
- Etc...

How do we *train* the network



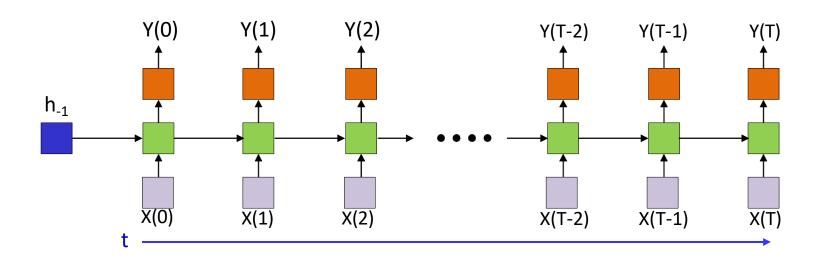
- Back propagation through time (BPTT)
- Given a collection of *sequence* inputs
 - $(\mathbf{X}_{\mathsf{i}}, \mathbf{D}_{\mathsf{i}})$
 - $X_i = X_{i,0}, ..., X_{i,T}$
 - $\mathbf{D}_{i} = D_{i,0}, ..., D_{i,T}$
- Train network parameters to minimize the error between the output of the network $\mathbf{Y}_i = Y_{i,0}, ..., Y_{i,T}$ and the desired outputs
 - This is the most generic setting.

Training the RNN



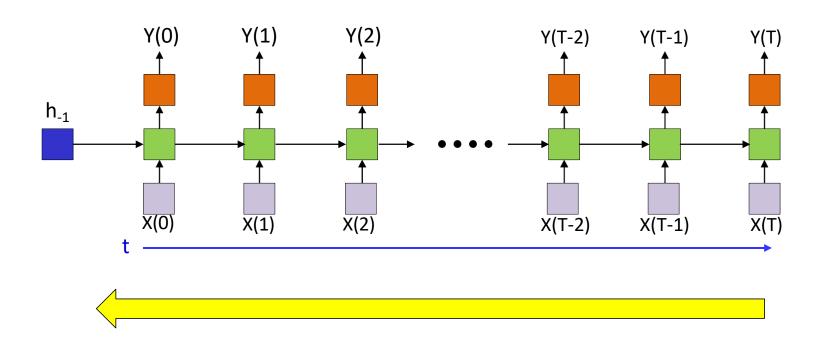
- The "unrolled" computation is just a giant shared-parameter neural network
 - All columns are identical and share parameters
- Network parameters can be trained via gradient-descent (or its variants) using shared-parameter gradient descent rules
 - Gradient computation requires a forward pass, back propagation, and pooling of gradients (for parameter sharing)

Training: Forward pass

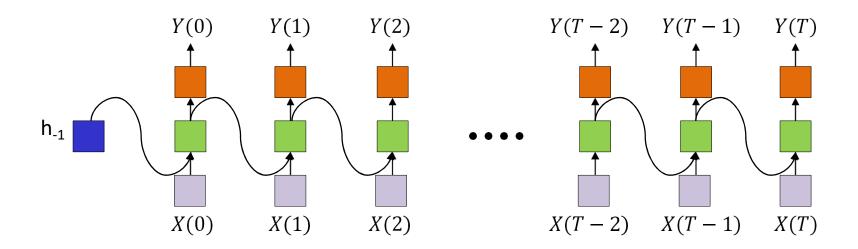


- For each training input:
- Forward pass: pass the entire data sequence through the network, generate outputs

Training: Computing gradients

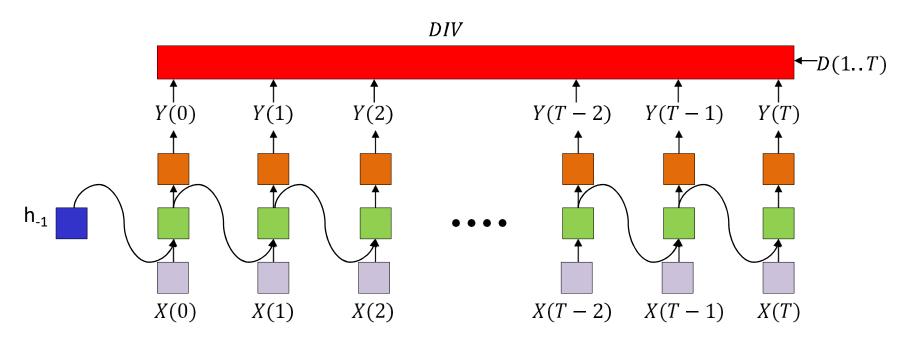


- For each training input:
- Backward pass: Compute gradients via backpropagation
 - Back Propagation Through Time



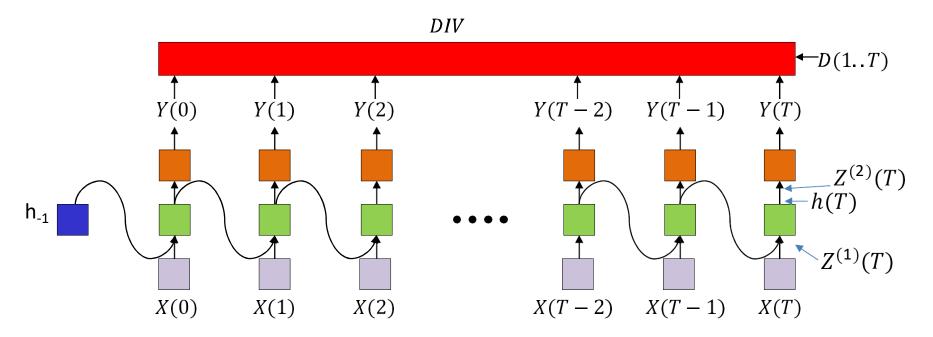
Will only focus on *one* training instance

All subscripts represent *components* and not training instance index



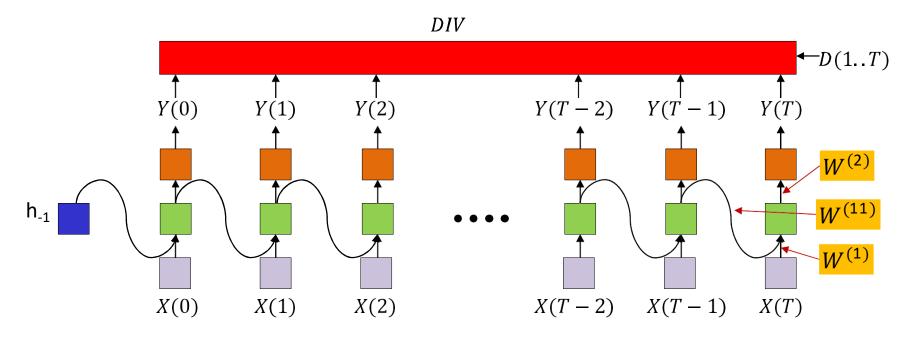
- The divergence computed is between the *sequence of outputs* by the network and the *desired sequence of outputs*
 - DIV is a scalar function of a series of vectors!
- This is not just the sum of the divergences at individual times
 - Unless we explicitly define it that way

Notation

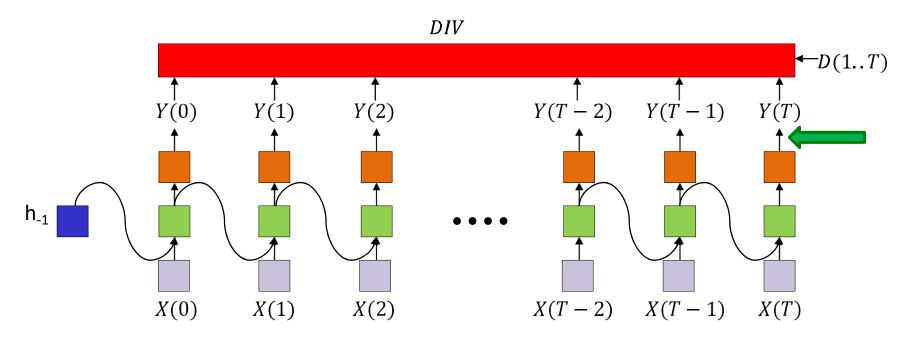


- *Y*(*t*) is the output at time *t*
 - $-Y_{i}(t)$ is the ith output
- $Z^{(2)}(t)$ is the pre-activation value of the neurons at the output layer at time t
- h(t) is the output of the hidden layer at time t
 - Assuming only one hidden layer in this example
- $Z^{(1)}(t)$ is the pre-activation value of the hidden layer at time t

Notation



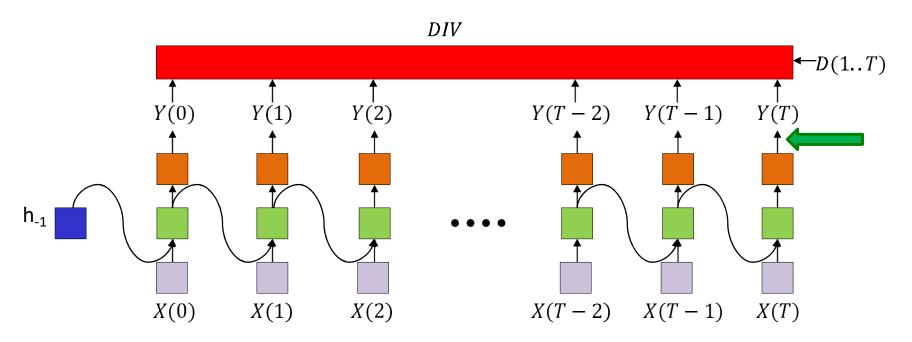
- $W^{(1)} [w_{ij}^{(1)}]$ is the matrix of *current* weights from the input to the hidden layer.
- $W^{(2)} \left[w_{ij}^{(2)}\right]$ is the matrix of *current* weights from the hidden layer to the output layer
- $W^{(11)} [w_{ij}^{(11)}]$ is the matrix of *recurrent* weights from the hidden layer to itself



First step of backprop: Compute $\nabla_{Y(T)} DIV$ (Compute $\frac{dDIV}{dY_i(T)}$ for all i)

Note: DIV is a function of all outputs Y(0) ... Y(T)

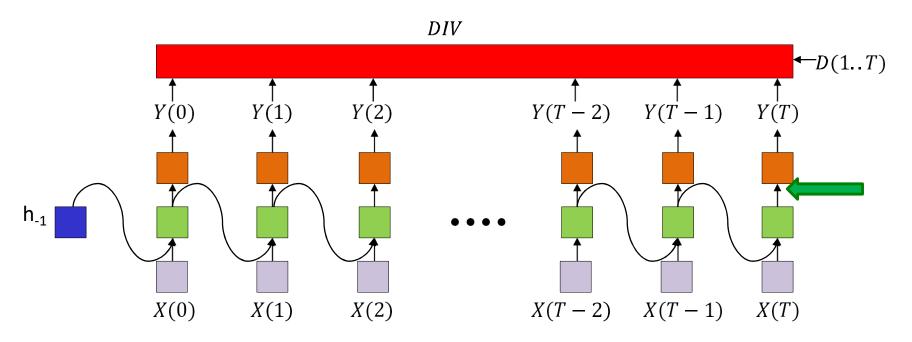
In general we will be required to compute $\frac{dDIV}{dY_i(t)}$ for all i and t. This can be a source of significant difficulty in many scenarios.



Special case, when the overall divergence is a simple sum of local divergences at each time: $DIV = \sum_t Div(t)$

Will get
$$\nabla_{Y(t)}Div(t)$$

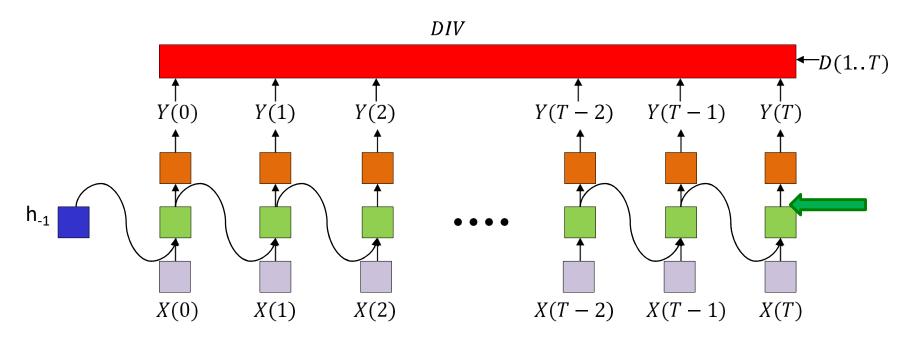
$$\frac{\partial DIV}{\partial Y_{i}(t)} = \frac{\partial Div(t)}{\partial Y_{i}(t)}$$



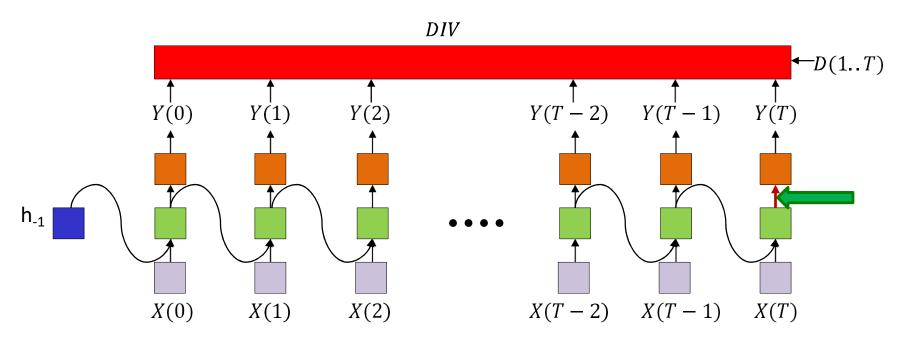
$$\nabla_{\mathsf{Z}^{(2)}(\mathsf{T})} \ DIV = \nabla_{\mathsf{Y}(\mathsf{T})} \ DIV \nabla_{\mathsf{Z}^{(2)}(\mathsf{T})} \ Y(T)$$

Vector output activation

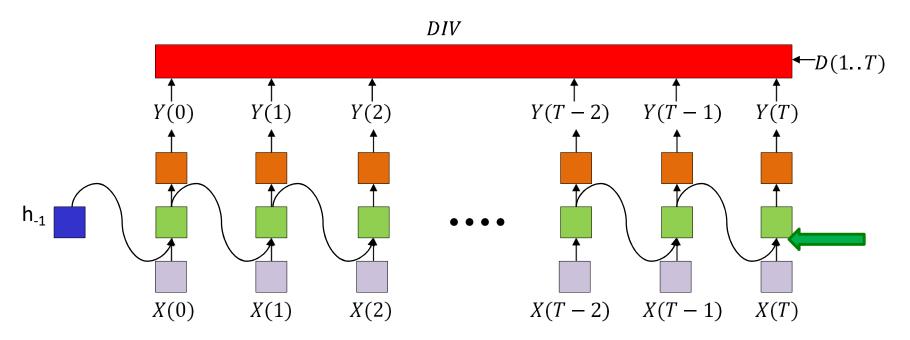
$$\frac{dDIV}{dZ_{i}^{(2)}(T)} = \frac{dDIV}{dY_{i}(T)} \frac{dY_{i}(T)}{dZ_{i}^{(2)}(T)} \text{ or } \frac{dDIV}{dZ_{i}^{(2)}(T)} = \sum_{j} \frac{dDIV}{dY_{j}(T)} \frac{dY_{j}(T)}{dZ_{i}^{(2)}(T)}$$



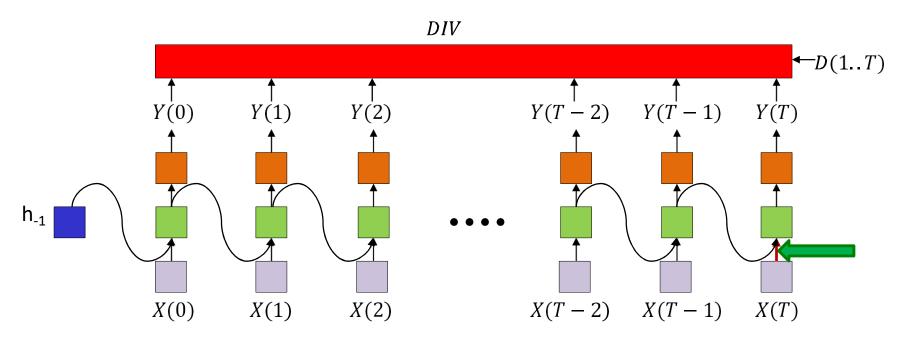
$$\frac{dDIV}{dh_{i}(T)} = \sum_{j} \frac{dDIV}{dZ_{j}^{(2)}(T)} \frac{dZ_{j}^{(2)}(T)}{dh_{i}(T)} = \sum_{j} w_{ij}^{(2)} \frac{dDIV}{dZ_{j}^{(2)}(T)}$$



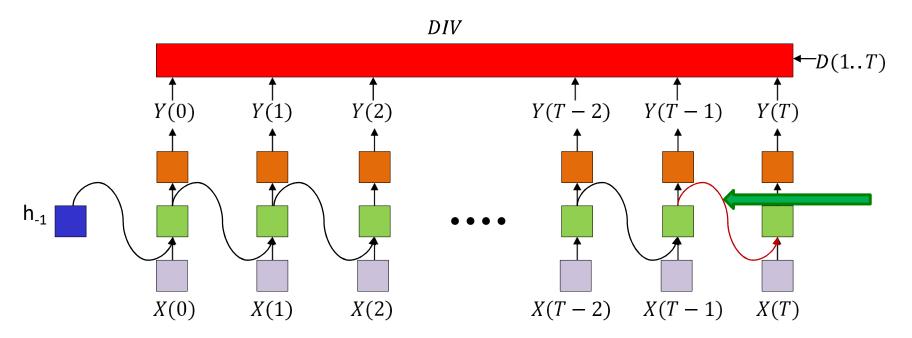
$$\frac{dDIV}{dw_{ij}^{(2)}} = \frac{dDIV}{dZ_{j}^{(2)}(T)} h_{i}(T)$$



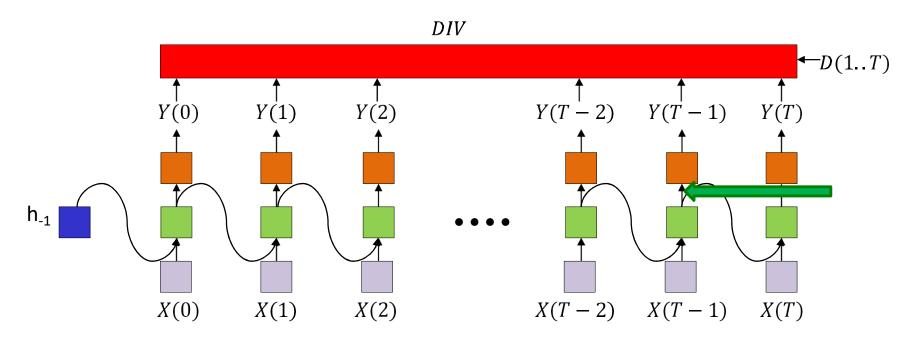
$$\frac{dDIV}{dZ_{i}^{(1)}(T)} = \frac{dDIV}{dh_{i}(T)} \frac{dh_{i}(T)}{dZ_{i}^{(1)}(T)}$$



$$\frac{dDIV}{dw_{ij}^{(1)}} = \frac{dDIV}{dZ_{j}^{(1)}(T)} X_{i}(T)$$

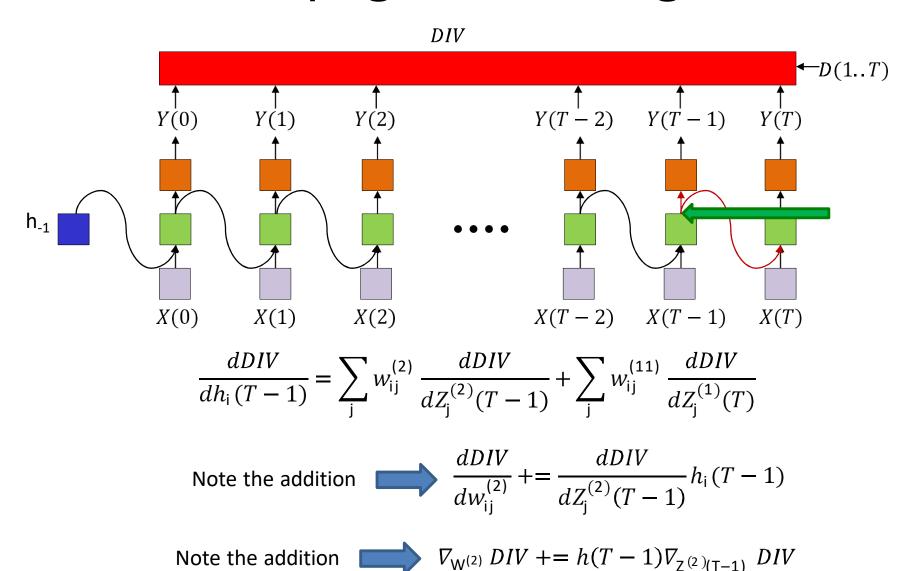


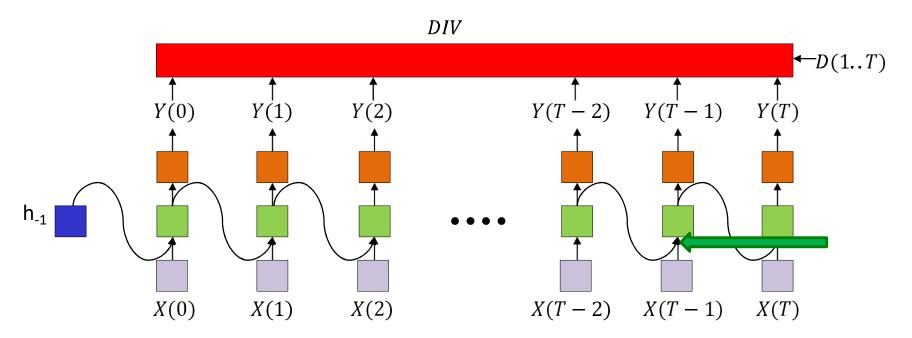
$$\frac{dDIV}{dw_{ij}^{(11)}} = \frac{dDIV}{dZ_{j}^{(1)}(T)} h_{i}(T-1)$$



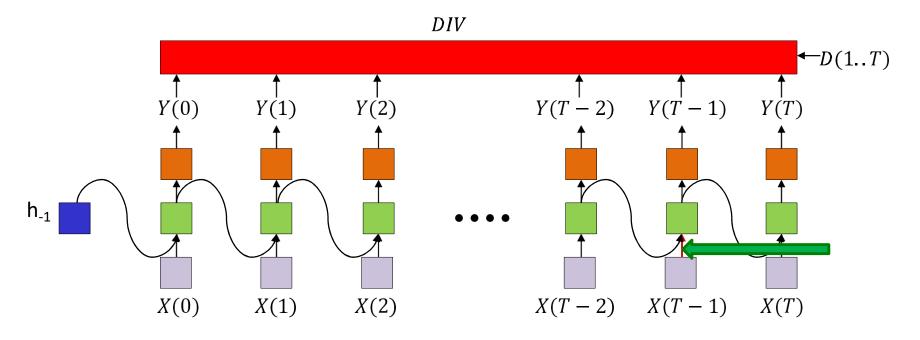
Vector output activation

$$\frac{dDIV}{dZ_{i}^{(2)}(T-1)} = \frac{dDIV}{dY_{i}(T-1)} \frac{dY_{i}(T-1)}{dZ_{i}^{(2)}(T-1)} \text{ OR } \frac{dDIV}{dZ_{i}^{(2)}(T-1)} = \sum_{j} \frac{dDIV}{dY_{j}(T-1)} \frac{dY_{j}(T-1)}{dZ_{i}^{(2)}(T-1)}$$





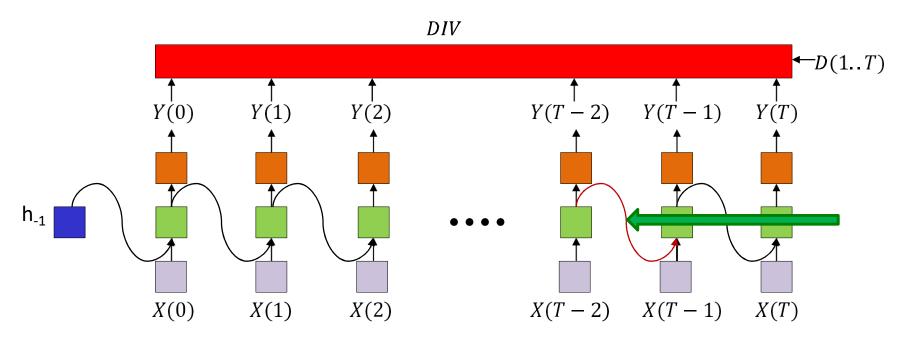
$$\frac{dDIV}{dZ_{i}^{(1)}(T-1)} = \frac{dDIV}{dh_{i}(T-1)} \frac{dh_{i}(T-1)}{dZ_{i}^{(1)}(T-1)}$$



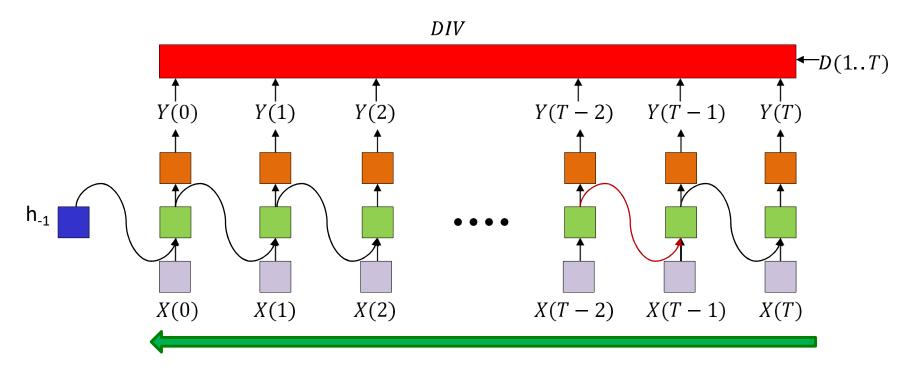
$$\frac{dDIV}{dZ_{i}^{(1)}(T-1)} = \frac{dDIV}{dh_{i}(T-1)} \frac{dh_{i}(T-1)}{dZ_{i}^{(1)}(T-1)}$$

$$\frac{dDIV}{dw_{ij}^{(1)}} + = \frac{dDIV}{dZ_{j}^{(1)}(T-1)}X_{i}(T-1)$$

Note the addition

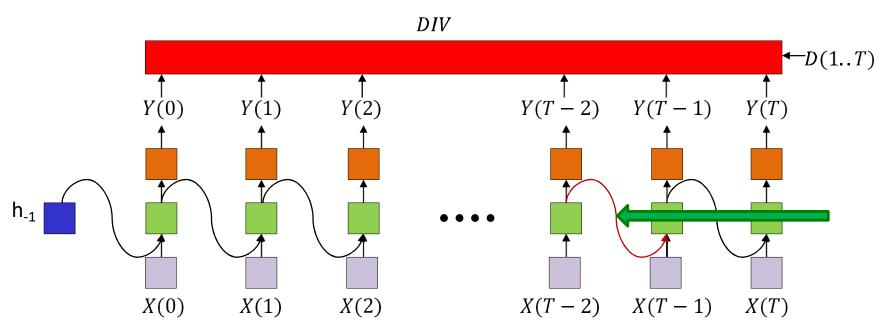


Note the addition
$$\frac{dDIV}{dw_{ij}^{(11)}} + = \frac{dDIV}{dZ_j^{(1)}(T-1)} h_i (T-2)$$



Continue computing derivatives going backward through time until..

$$\frac{dDIV}{dh_i(-1)} = \sum_{j} w_{ij}^{(11)} \frac{dDIV}{dZ_j^{(1)}(0)}$$



Initialize all derivatives to 0

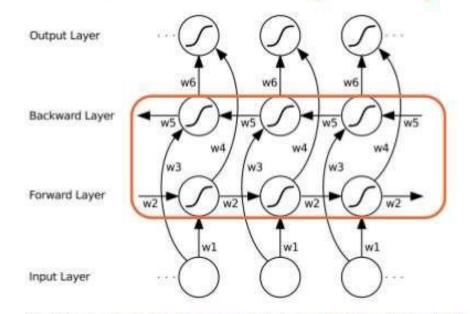
For t = T downto 0

$$\begin{aligned} & \nabla_{\mathsf{Z}^{(2)}(\mathsf{t})} \; DIV = \nabla_{\mathsf{F}(\mathsf{t})} \; DIV \; \nabla_{\mathsf{Z}^{(2)}(\mathsf{t})} Y(t) \\ & \nabla_{\mathsf{h}(\mathsf{t})} \; DIV = \nabla_{\mathsf{Z}^{(2)}(\mathsf{t})} \; DIV \; W^{(2)} \; + \nabla_{\mathsf{Z}^{(1)}(\mathsf{t}+1)} \; DIV \; W^{(11)} \\ & \nabla_{\mathsf{Z}^{(1)}(\mathsf{t})} \; DIV = \nabla_{\mathsf{h}(\mathsf{t})} \; DIV \; \nabla_{\mathsf{Z}^{(1)}(\mathsf{t})} h(t) \end{aligned}$$

$$\nabla_{W^{(2)}} DIV += h(t) \nabla_{Z^{(2)}(t)} DIV
\nabla_{W^{(11)}} DIV += h(t-1) \nabla_{Z^{(1)}(t)} DIV
\nabla_{W^{(1)}} DIV += X(t) \nabla_{Z^{(1)}(t)} DIV
\nabla_{h_{-1}} DIV = \nabla_{Z^{(1)}(0)} DIVW^{(11)_{9}}$$

Extensions to the RNN: Bidirectional RNN

Bidirectional RNN (BRNN)



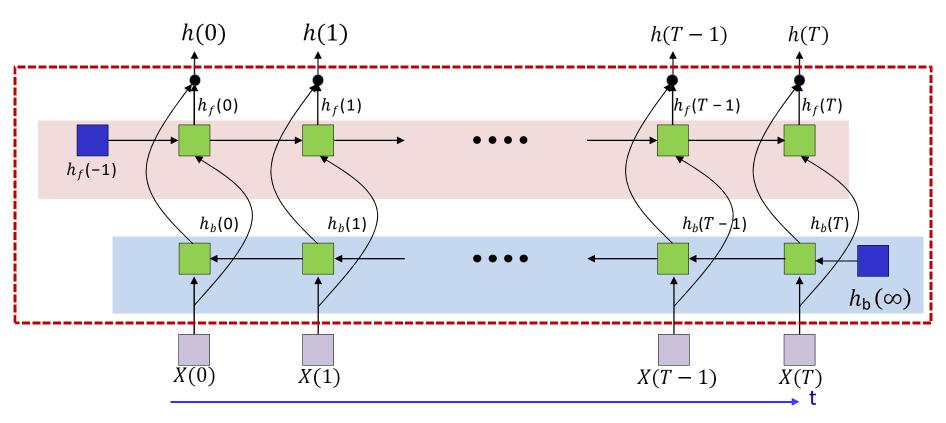
Must learn weights w2, w3, w4 & w5; in addition to w1 & w6.

Proposed by Schuster and Paliwal 1997

Alex Graves, "Supervised Sequence Labelling with Recurrent Neural Networks"

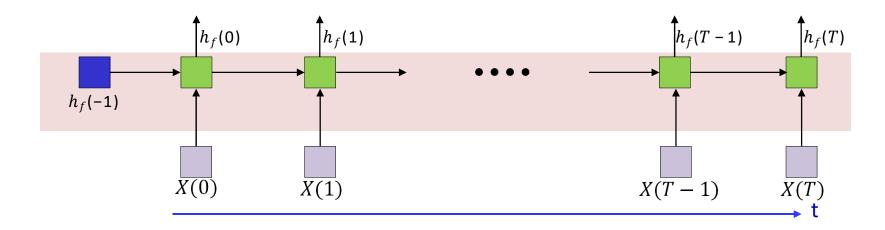
- In problems where the entire input sequence is available, RNNs can be bidirectional
- RNN with both forward and backward recursion
- Explicitly models the fact that just as the future can be predicted from the past, the past can be deduced from the future

Bidirectional RNN



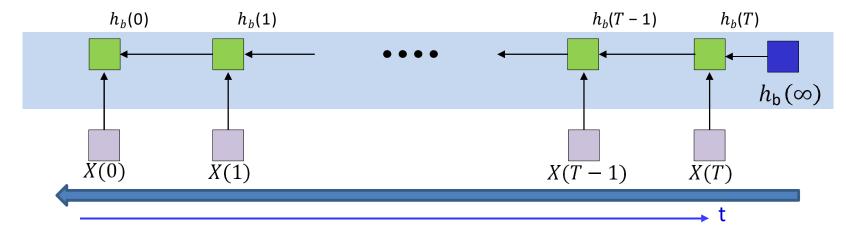
- "Block" performs bidirectional inference on input
 - "Input" could be input series X(0)...X(T) or the output of a previous layer (or block)
- The Block has two components
 - A forward net process the data from t=0 to t=T
 - A backward net processes it backward from t=T down to t=0

Bidirectional RNN block



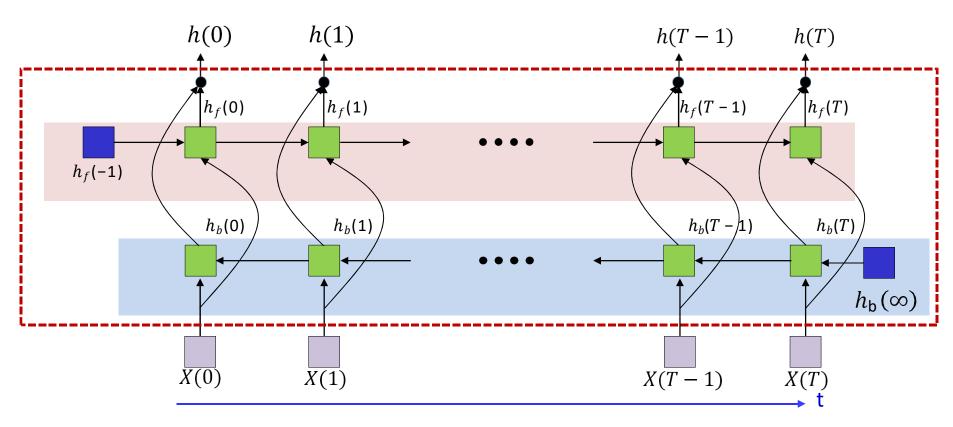
- The forward net process the data from t=0 to t=T
 - Only computing the hidden state values.

Bidirectional RNN block



- The backward nets processes the input data in reverse time, end to beginning
 - Initially only the hidden state values are computed
 - Clearly, this is not an online process and requires the entire input data
 - Note: This is not the backward pass of backprop.

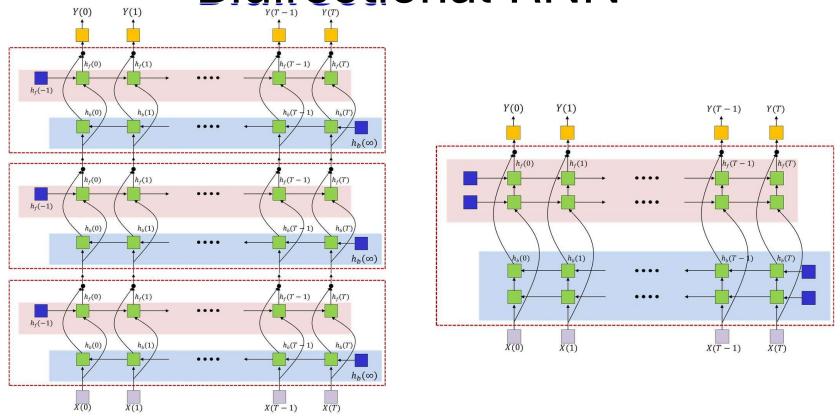
Bidirectional RNN block



- The computed states of both networks are combined to give you the output of the bidirectional block
 - Typically just concatenate them

$$h(t) = [h_f(t); h_b(t)]$$

Bidirectional RNN



- Actual network may be formed by stacking many independent bidirectional blocks followed by an output layer
 - Forward and backward nets in each block are a single layer
- Or by a single bidirectional block followed by an output layer
 - The forward and backward nets may have several layers
- In either case, it's sufficient to understand forward inference and backprop rules for a single block
 - Full forward or backprop computation simply requires repeated application of these rules