Deep Learning

Recurrent Neural Networks

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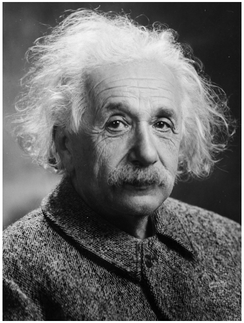


Everything should be made as simple as possible, but no simpler.

Albert Einstein

Understanding Recurrent Neural Networks requires some effort and a correct perspective. Do not expect them to be as simple as linear regression.

Static vs. Dynamic Inputs

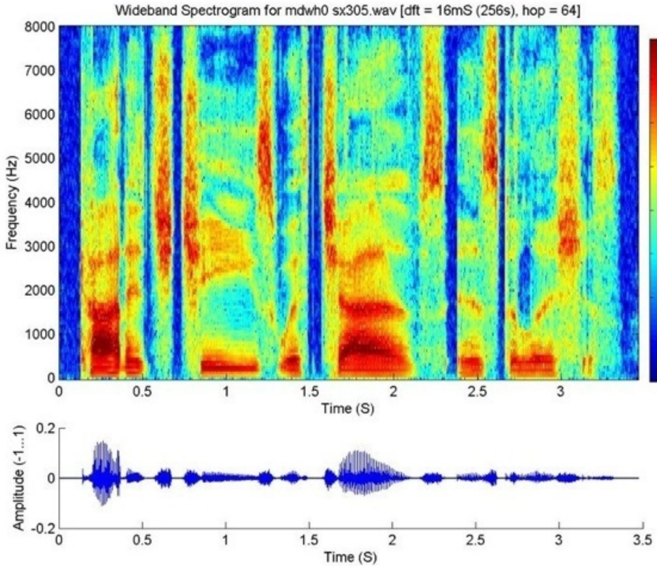
- *Static* signals, such as an image, do not change over time.
  - Ordered with respect to space.
  - Output depends on current input.
- *Dynamic* signals, such as text, audio, video or stock price change over time.
  - Ordered with respect to time.
  - Output depends on current input as well as past (or even future) inputs.
  - Also called *temporal*, *sequential* or *time-series* data.

Context in Text

The Taj ____ was commissioned by Shah Jahan in 1631, to be built in the memory of ___ wife Mumtaz Mahal, who died on 17 June that *year, giving birth to* their *14th child, Gauhara Begum.* Construction *started in 1632, and the mausoleum was completed ___ 1643.*

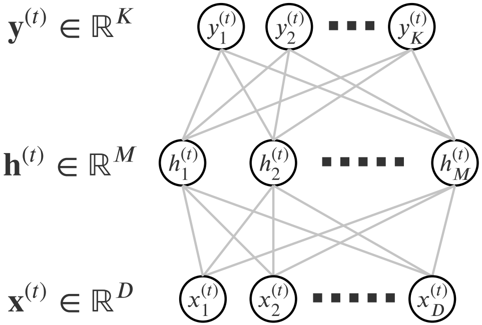
Context in Video

Context in Audio



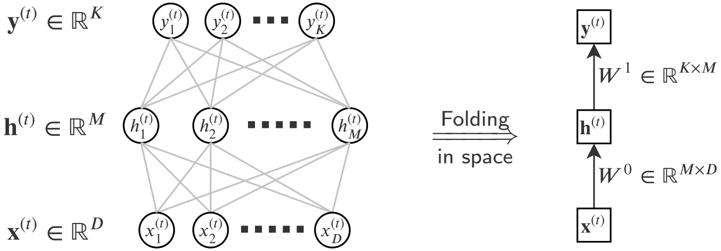
Time-series Data

- A *single* input will be a *series of vectors* $\mathbf{x}^1, \mathbf{x}^2, \ldots, \mathbf{x}^T$.


$\mathbf{y}^{(t)} \in \mathbb{R}^K$
$y_1^{(t)}$
$y_2^{(t)}$
$y_K^{(t)}$
$\mathbf{h}^{(t)} \in \mathbb{R}^M$
$h_1^{(t)}$
$h_2^{(t)}$
$h_M^{(t)}$
$\mathbf{x}^{(t)} \in \mathbb{R}^D$
$x_1^{(t)}$
$x_2^{(t)}$
$x_D^{(t)}$

Input component at time t forward propagated through a network.

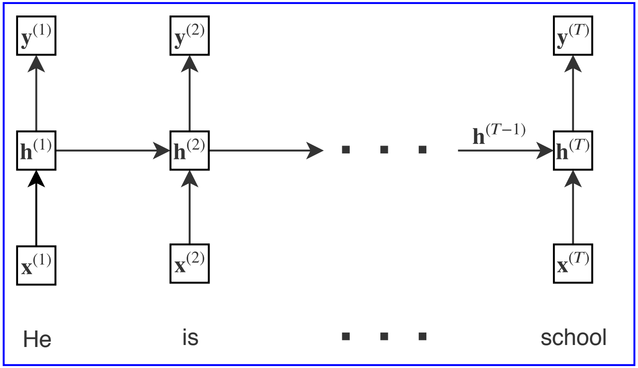
Representational Shortcut 1 – Space Folding


$\mathbf{y}^{(t)} \in \mathbb{R}^K$
$y_1^{(t)}$
$y_2^{(t)}$
$y_K^{(t)}$
$\mathbf{h}^{(t)} \in \mathbb{R}^M$
$h_1^{(t)}$
$h_2^{(t)}$
$h_M^{(t)}$
$\mathbf{x}^{(t)} \in \mathbb{R}^D$
$x_1^{(t)}$
$x_2^{(t)}$
$x_D^{(t)}$
Folding
in space
$\mathbf{y}^{(t)}$
$W^1 \in \mathbb{R}^{K\times M}$
$\mathbf{h}^{(t)}$
$W^0 \in \mathbb{R}^{M\times D}$
$\mathbf{x}^{(t)}$

Each box represents a layer of neurons.

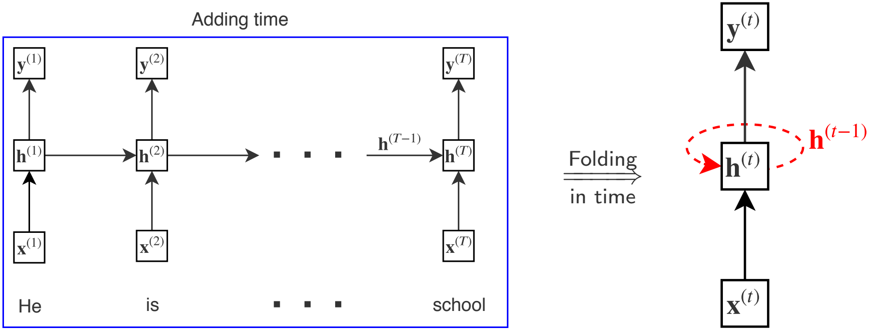
Recurrent Neural Networks

Adding time



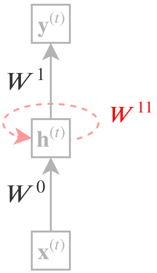
- A recurrent neural network (RNN) makes hidden state at time t directly dependent on the hidden state at time $t-1$ and therefore indirectly *on all previous times*.
- Output $\mathbf{y}_t$ depends on all that the network has already seen so far.

Representational Shortcut 2 – Time Folding



Recurrent Neural Networks

3 sets of weights

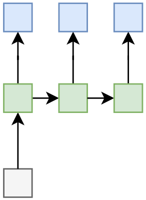


$$\mathbf{y}^{(t)} = f(\overbrace{W^1\mathbf{h}^{(t)} + \mathbf{b}_1}^{\mathbf{a}^{1(t)}})$$

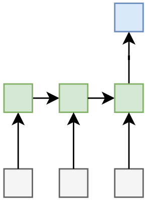
$$\mathbf{h}^{(t)} = \tanh(\underbrace{W^0\mathbf{x}^{(t)} + W^{11}\mathbf{h}^{(t-1)} + \mathbf{b}_0}_{\mathbf{a}^{0(t)}})$$

Sequence Mappings

One-to-many



Many-to-one



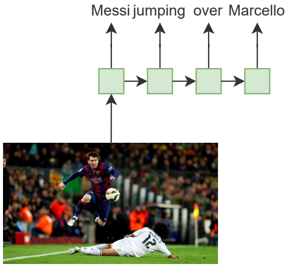
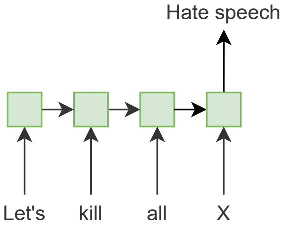
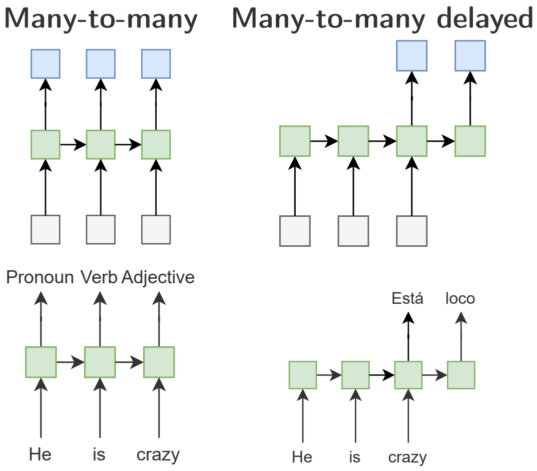


Image caption generation



Sentiment classification

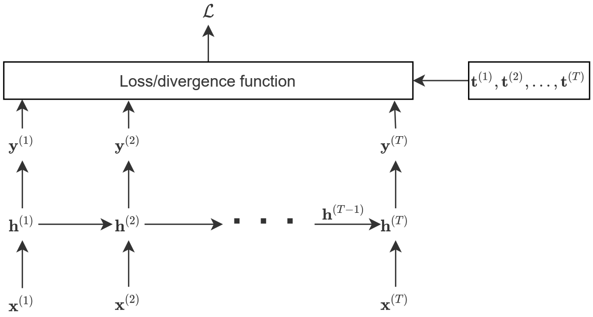
Sequence Mappings



POS tagging Language translation

Loss Functions for Sequences

- For recurrent nets, loss is between *series* of output and target vectors. That is $\mathcal{L}(\{\mathbf{y}^{(1)}, \ldots, \mathbf{y}^{(T)}\}, \{\mathbf{t}^{(1)}, \ldots, \mathbf{t}^{(}T)\})$.

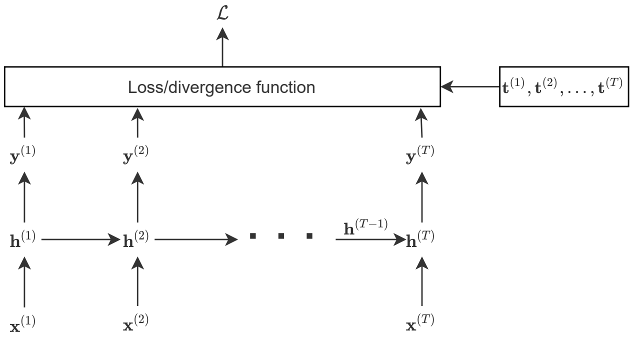


Forward propagation in an RNN unfolded in time.

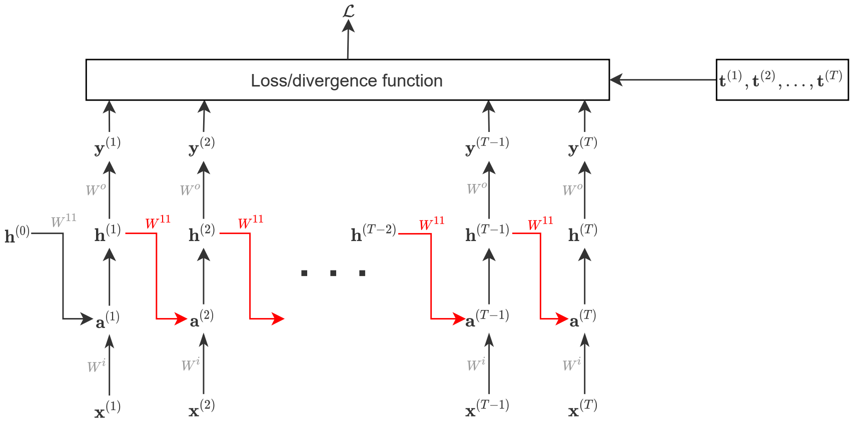
- Notice that loss $\mathcal{L}$ can be computed only after $\mathbf{y}^{(T)}$ has been computed.

Loss Functions for Sequences

- Loss is *not necessarily* decomposable.
- In the following, we will assume decomposable loss $\mathcal{L} = \sum_{t=1}^{T} \mathcal{L}(\mathbf{y}^{(t)}, \mathbf{t}^{(t)})$.
- In both cases, as long as $\frac{\partial L}{\partial \mathbf{y}^{(t)}}$ has been computed, backpropagation can proceed.

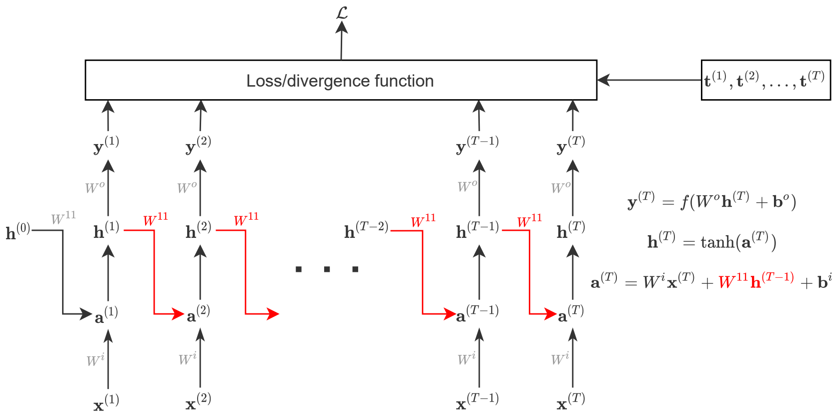


Forward Propagation Through Time



Forward propagation in an RNN unfolded in time. Recurrence between hidden states through pre-activation $\mathbf{a}^{(t)}$ is shown in red.

Forward Propagation Through Time


$\mathcal{L}$
Loss/divergence function
$\mathbf{t}^{(1)}, \mathbf{t}^{(2)}, \dots, \mathbf{t}^{(T)}$
$\mathbf{y}^{(1)}$ $\mathbf{y}^{(2)}$ $\mathbf{y}^{(T-1)}$ $\mathbf{y}^{(T)}$
W^o
$\mathbf{h}^{(0)}$ $\mathbf{h}^{(1)}$ $\mathbf{h}^{(2)}$ $\mathbf{h}^{(T-2)}$ $\mathbf{h}^{(T-1)}$ $\mathbf{h}^{(T)}$
W^{11}
$\mathbf{a}^{(1)}$ $\mathbf{a}^{(2)}$ $\mathbf{a}^{(T-1)}$ $\mathbf{a}^{(T)}$
W^i
$\mathbf{x}^{(1)}$ $\mathbf{x}^{(2)}$ $\mathbf{x}^{(T-1)}$ $\mathbf{x}^{(T)}$

$$\mathbf{y}^{(T)} = f(W^o \mathbf{h}^{(T)} + \mathbf{b}^o)$$

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

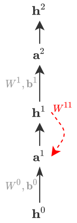
$$\mathbf{a}^{(T)} = W^i \mathbf{x}^{(T)} + W^{11} \mathbf{h}^{(T-1)} + \mathbf{b}^i$$

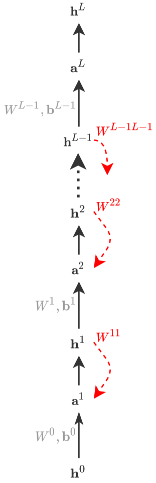
Forward propagation in an RNN unfolded in time. Recurrence between hidden states through pre-activation $\mathbf{a}^{(t)}$ is shown in red.

Notational Clarity

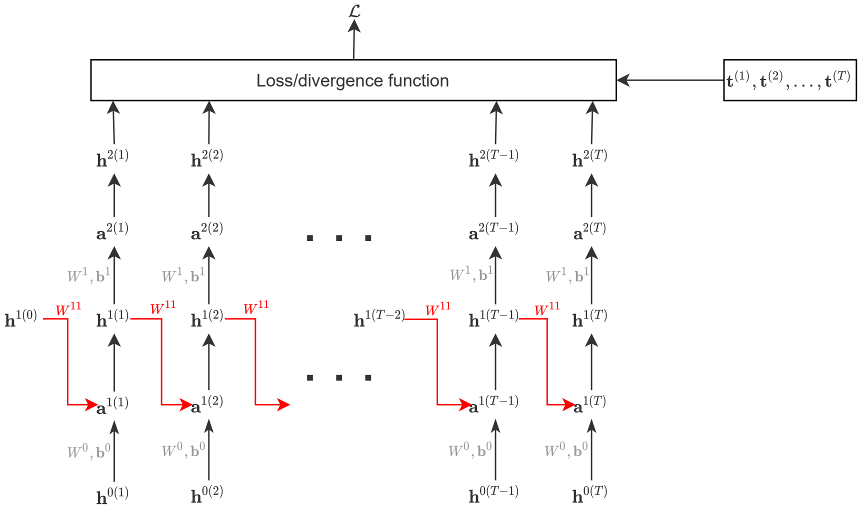
- At layer l, we will denote the pre-activation by $\mathbf{a}^l$ and activation by $\mathbf{h}^l$.
- So output layer $\mathbf{y}$ will be denoted by $\mathbf{h}^L$ in an L-layer network.
- Input will be denoted by $\mathbf{h}^0$.
- So forward propagation entails $\mathbf{h}^0 \rightarrow \underbrace{\mathbf{a}^1 \rightarrow \mathbf{h}^1}_{\text{layer } 1} \cdots \rightarrow \underbrace{\mathbf{a}^{L-1} \rightarrow \mathbf{h}^{L-1}}_{\text{layer } L-1} \rightarrow \underbrace{\mathbf{a}^L \rightarrow \mathbf{h}^L}_{\text{layer } L}$.
- For 2 layer network

$$\mathbf{h}^{2,T} = f(\mathbf{a}^{2,T})$$
$$\mathbf{a}^{2,T} = W^1\mathbf{h}^{1,T} + \mathbf{b}^1$$
$$\mathbf{h}^{1,T} = \tanh(\mathbf{a}^{1,T})$$
$$\mathbf{a}^{1,T} = W^0\mathbf{h}^{0,T} + W^{11}\mathbf{h}^{1,T-1} + \mathbf{b}^0$$

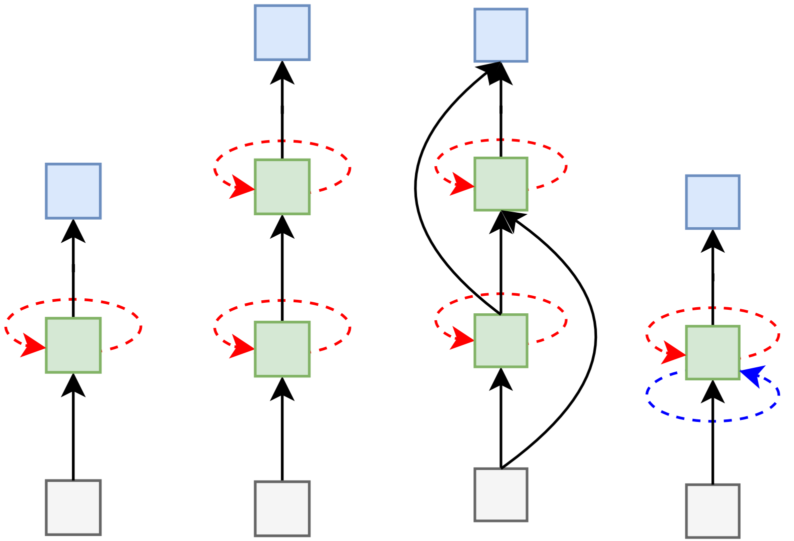




Notational Clarity



RNN Variations



1 hidden state 2 hidden states Skip connections Bidirectional

Bidirectional RNN

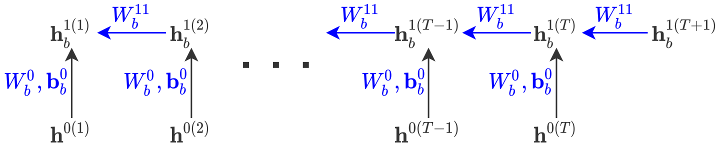
Step 1: Forward propagation into the future

$$\begin{tikzcd}
\mathbf{h}_f^{1(0)} \arrow[r, "W_f^{11}"] & \mathbf{h}_f^{1(1)} \arrow[r, "W_f^{11}"] & \mathbf{h}_f^{1(2)} & \cdots \arrow[r, "W_f^{11}"] & \mathbf{h}_f^{1(T-1)} \arrow[r, "W_f^{11}"] & \mathbf{h}_f^{1(T)} \\
& \mathbf{h}^{0(1)} \arrow[u, "{W_f^0, \mathbf{b}_f^0}"] & \mathbf{h}^{0(2)} \arrow[u, "{W_f^0, \mathbf{b}_f^0}"] & & \mathbf{h}^{0(T-1)} \arrow[u, "{W_f^0, \mathbf{b}_f^0}"] & \mathbf{h}^{0(T)} \arrow[u, "{W_f^0, \mathbf{b}_f^0}"]
\end{tikzcd}$$

$$\boxed{fprop\left(\underbrace{\mathbf{h}^0(1), \mathbf{h}^0(2), \ldots, \mathbf{h}^0(T)}_{\text{input sequence}}; \underbrace{\mathbf{h}_f^1(0)}_{\text{init}}, \underbrace{W_f^0, \mathbf{b}_f^0, W_f^{11}, W_f^1, \mathbf{b}_f^1}_{\text{parameters}}\right)}$$

Bidirectional RNN

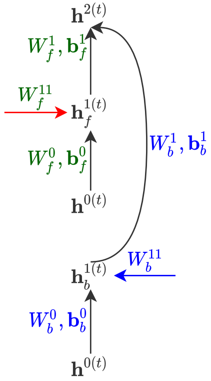
Step 2: Forward propagation into the past



$$\boxed{fprop\left(\underbrace{\mathbf{h}^0(T), \mathbf{h}^0(T-1), \ldots, \mathbf{h}^0(1)}_{\text{input sequence}}; \underbrace{\mathbf{h}_b^1(T+1)}_{\text{init}}, \underbrace{W_b^0, \mathbf{b}_b^0, W_b^{11}, W_b^1, \mathbf{b}_b^1}_{\text{parameters}}\right)}$$

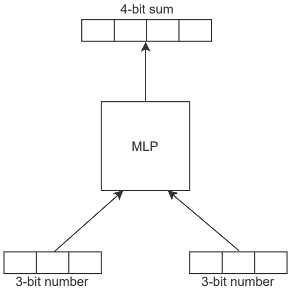
Bidirectional RNN

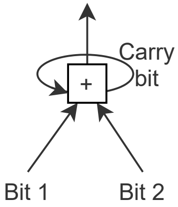
Step 3: Fusion of forward and backward hidden states



$$\mathbf{h}^{2(t)} = \tanh(\mathbf{a}^{2(t)})$$
$$\mathbf{a}^{2(t)} = W_f^1 \mathbf{h}_f^{1(t)} + \mathbf{b}_f^1 + W_b^1 \mathbf{h}_b^{1(t)} + \mathbf{b}_b^1$$

Benefit of Recurrent Architectures
n-bit addition

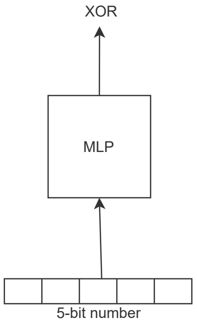




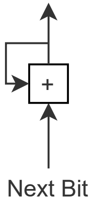
- Only for n-bit numbers
- Training set exponential in n
- Training errors

- Iterative application to numbers of arbitrary size
- Exact answers

Benefit of Recurrent Architectures
n-bit XOR



- Only for *n*-bit numbers
- Training set exponential in *n*
- Training errors



- Iterative application to numbers of arbitrary size
- Exact answer
- Will be 1 for odd number of ones in input.

Stability issues

- Even a 1-hidden layer RNN is a very deep network.
- Viewed in time, an RNN is as deep as the number of time steps.
- Suffers from vanishing gradients.
- Also suffers from *exploding gradients*.

Exploding Gradients

- Consider input $\mathbf{x}^{(1)}$ at time 1 and *assume linear* hidden layer.
- At time t, the RNN carries a term of the form

$$W^{11} \dots W^{11} W^{0} \mathbf{x}^{(1)} = \left(W^{11}\right)^{t-1} W^{0} \mathbf{x}^{(1)}$$

  which is an M-dimensional vector.
- Magnitude of this vector depends on largest eigenvalue λ_{max} of W^{11}.
  - $\lambda_{\text{max}} > 1 \implies$ magnitude of $\left(W^{11}\right)^{t-1} W^{0} \mathbf{x}^{(1)}$ keeps increasing.
  - $\lambda_{\text{max}} < 1 \implies$ magnitude of $\left(W^{11}\right)^{t-1} W^{0} \mathbf{x}^{(1)}$ keeps decreasing.

Exploding Gradients

- Even during forward propagation, depending on the largest eigenvalue of the recurrent weight matrix W^{11}, input at time t
  - is either forgotten very soon,
  - or explodes to very large values.
- Similar case for backpropagation.
- Notice that this has nothing to do with the choice of activation function.
- *Information will explode or vanish through time*.
- Similar behaviour for non-linear neurons.
- So, in practice, RNNs do not have long-term memory. Solution: LSTM.

Summary

- Dynamic signals that change over time can be modeled by RNNs.
- RNNs can represent mappings of one-to-many, many-to-one, many-to-many, and many-to-many delayed sequences.
- Previous hidden layer output influences subsequent output.
- Forward propagation is through space as well as time.
- Forward propagation can be into the future and/or into the past.
- Recurrent connection implies really deep network.
- Information can vanish or even explode through time.