Deep Learning

13. Recurrent Neural Networks

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So far...

1. Perceptron, MLP, Gradient Descent (Backpropagation)

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2. CNNs (visualizing and understanding)

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2. CNNs (visualizing and understanding)
3. 'Feedforward Neural networks'

Feedforward NNs: some observations

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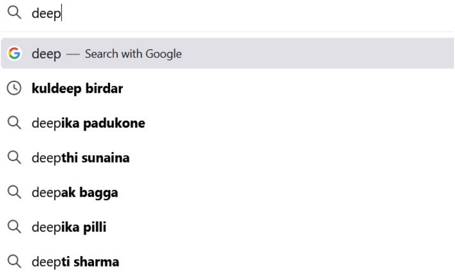
2. Successive i/p are i.i.d.
3. Processing of successive i/p is independent of each other

Consider ‘auto-completion’ task



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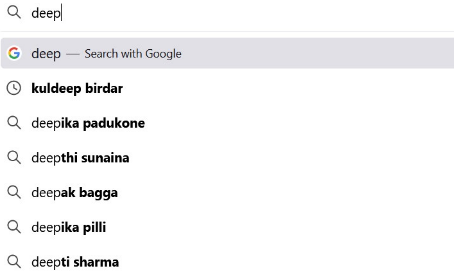

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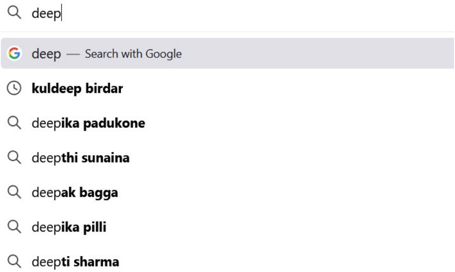

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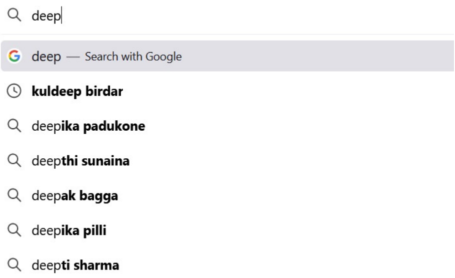

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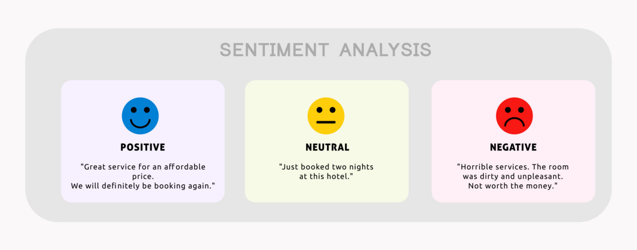
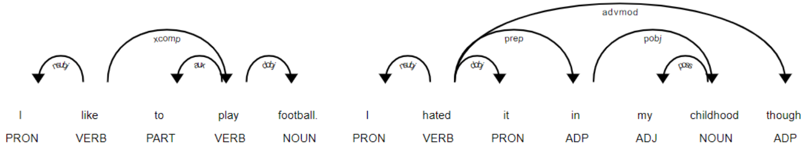
3. Same underlying task at different ‘time instances’
4. Sequence Learning Problems

Sequence Learning Tasks: Example



Sentiment Analysis (Source)

Sequence Learning Tasks: Example



POS-Tagging (Source:Kaggle)

Sequence Learning Tasks: Example

Action Recognition (Source)

Sequence Learning Tasks: Example

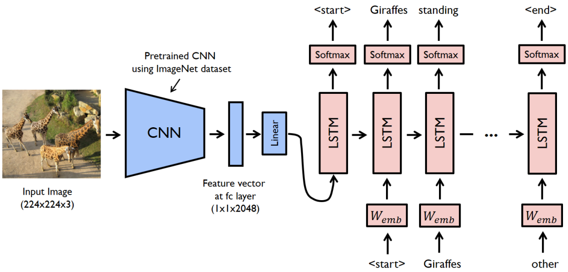
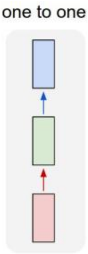


Image Captioning(Source)

Sequence Learning Tasks: Variations



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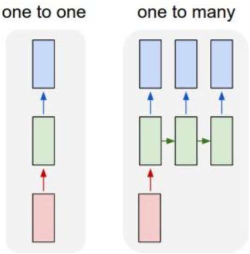

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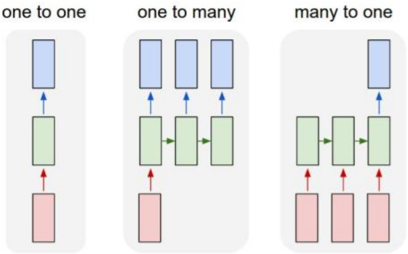

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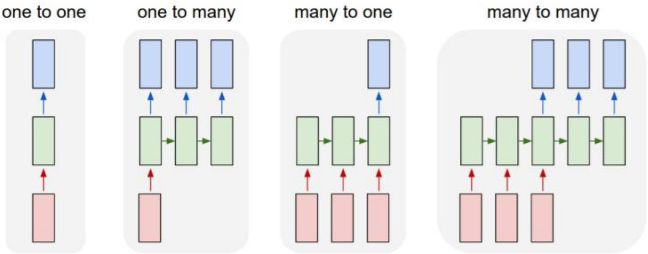

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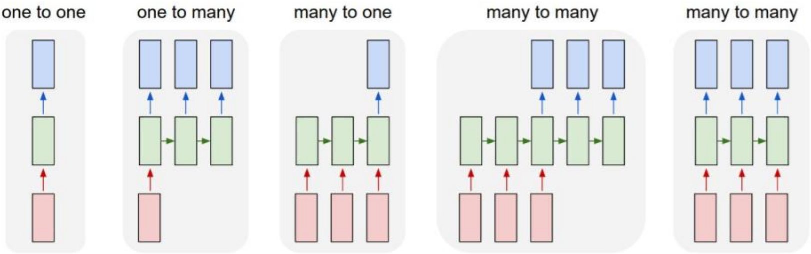

Source

Recurrent Neural Networks (RNN)

1. NNs designed to solve sequence learning tasks

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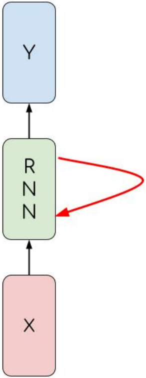
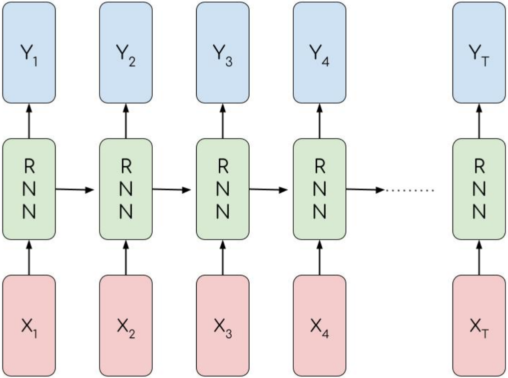
2. Characteristics
    1. Model the dependence among the i/p
    2. Handle variable length of i/p
    3. Same function applied at all time instances

RNNs: internal state



RNNs have internal state (or, memory) that gets updated with input

RNNs: unfolding



RNNs

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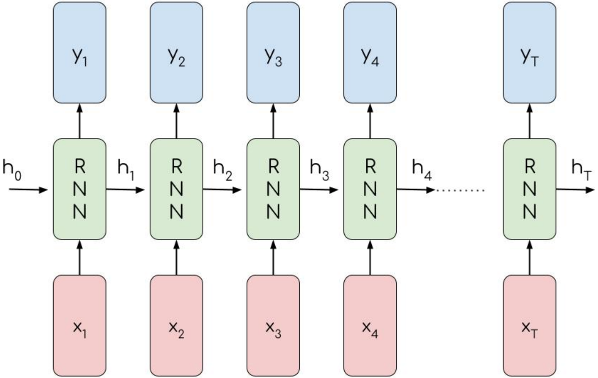
1. Apply the same transformation at every time step $\rightarrow$ 'Recurrent' NNs
2. i/p sequence $x_t \in \mathbb{R}^{\mathbb{D}}$
3. Initial recurrent state $h_0 \in \mathbb{R}^{\mathbb{Q}}$
4. RNN model computes sequence of recurrent states iteratively
   $h_t = \phi(x_t, h_{t-1}; w)$

RNNs



Elmon RNN (1990)

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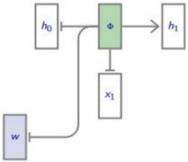
3. $y_t = softmax(W_{hy}.h_t + b_y)$

RNNs as computational graph

1. Use the same set of parameters at each time step



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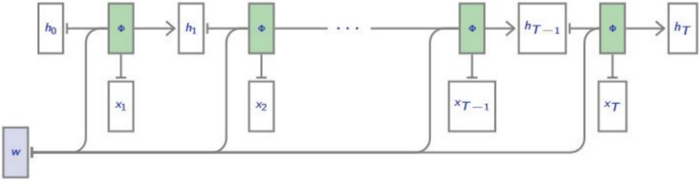

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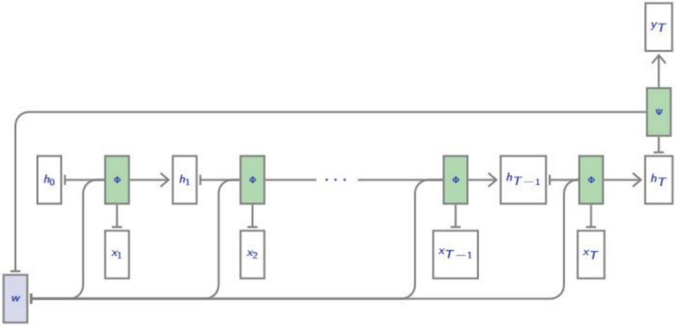
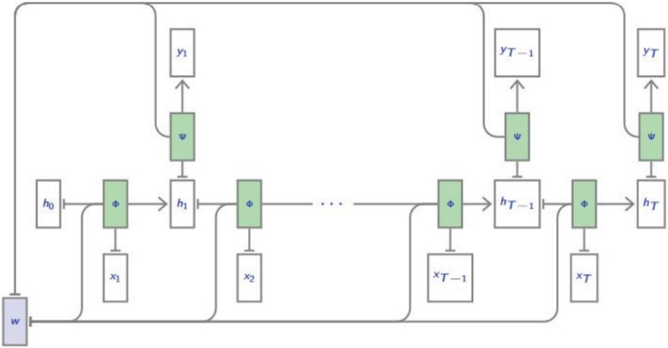


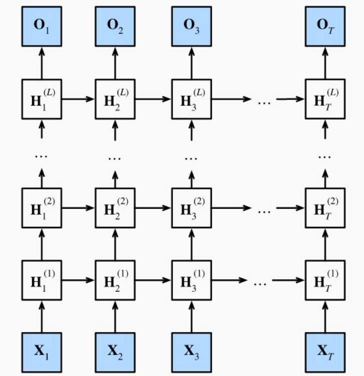
RNNs as computational graph

1. Use the same set of parameters at each time step
2. Flexible to realize different variants (with some tricks!)



Multi-layered RNNs

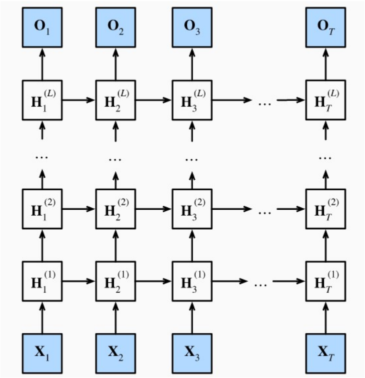
1. Stack multiple RNNs between i/p and o/p layers



Source

Multi-layered RNNs

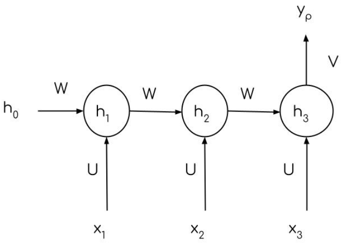
1. Stack multiple RNNs between i/p and o/p layers
2. $H_t^{(l)} = W_{xh}^{(l)} \cdot H_t^{(l-1)} + W_{hh}^{(l)} \cdot H_{t-1}^{(l)} + b_h^{(l)}$



Source

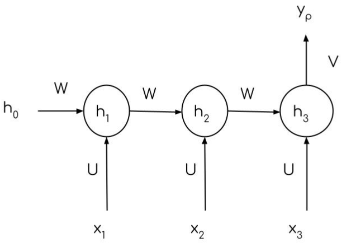
Backpropagation Through Time (BPTT)

1. Consider a many-to-one variant RNN (e.g. sentiment analysis)



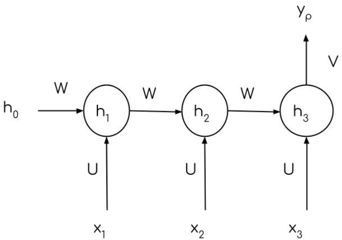
Backpropagation Through Time (BPTT)

1. Consider a many-to-one variant RNN (e.g. sentiment analysis)
2. Let's separate the parameters into U, V, and W



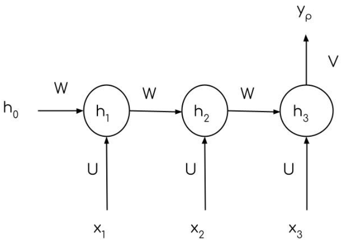
Backpropagation Through Time (BPTT)

1. Let's now perform SGD (assume loss L is formulated on y_p)



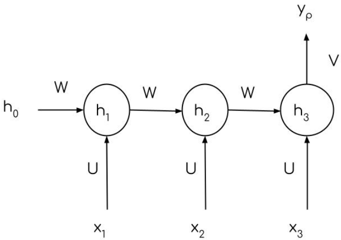
Backpropagation Through Time (BPTT)

1. Let's now perform SGD (assume loss L is formulated on y_p)
2. $\rightarrow$ we need to compute $\frac{\partial L}{\partial V}$, $\frac{\partial L}{\partial W}$, and $\frac{\partial L}{\partial U}$



Backpropagation Through Time (BPTT)

1. $\frac{\partial L}{\partial V} = \frac{\partial L}{\partial y_p} \frac{\partial y_p}{\partial V} = \frac{\partial L}{\partial y_p} \cdot \frac{\partial y_p}{\partial z_3} \cdot \frac{\partial z_3}{\partial V}$



Backpropagation Through Time (BPTT)

भारतीय प्रौद्योगिकी संस्थान हैदराबाद
Indian Institute of Technology Hyderabad

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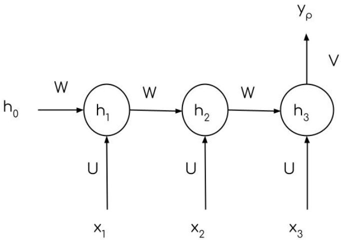
2. $y_p = softmax(z_3)$ and $z_3 = V \cdot h_3 + b_y$



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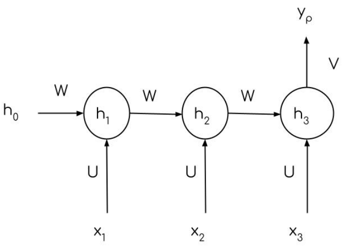
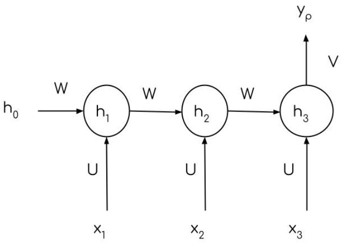
2. $y_p = softmax(z_3)$ and $z_3 = V \cdot h_3 + b_y$
3. Since we know that h_3, b_y are independent of V, we can compute $\frac{\partial L}{\partial V}$ in a single step



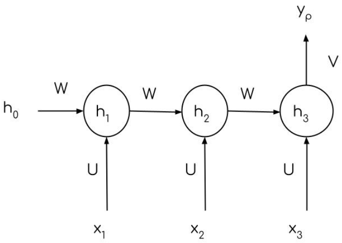
Backpropagation Through Time (BPTT)

1. Let's now consider $\frac{\partial L}{\partial W}$



Backpropagation Through Time (BPTT)

1. Let's now consider $\frac{\partial L}{\partial W}$
2. There are multiple 'W's in the computational graph!



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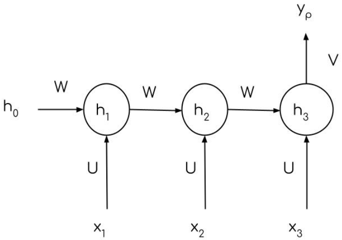
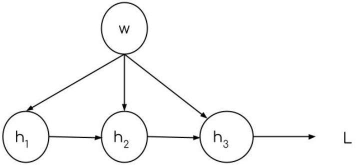
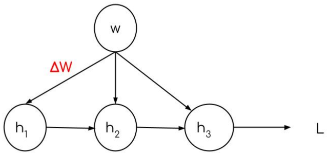


1. For ease of understanding



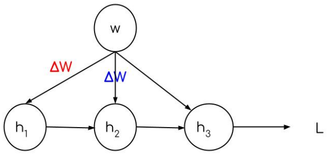
Backpropagation Through Time (BPTT)

1. $\color{red}{\Delta w}$ change in W$\rightarrow$ $\left(\frac{\partial h_1}{\partial W} \cdot \Delta w\right)$ change in h_1



Backpropagation Through Time (BPTT)

1. Δw change in W$\rightarrow$
   $\left(\frac{\partial h_1}{\partial W} \cdot \Delta w\right)$ change in h_1
2. Δw change in W $\rightarrow$
   $\left(\frac{\partial h_2}{\partial W} \cdot \Delta w\right)$ change in h_2



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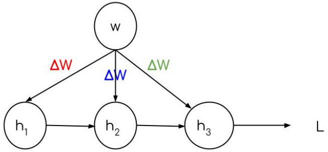
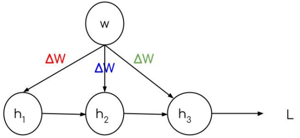


Backpropagation Through Time (BPTT)

1. $\Delta L = \frac{\partial L}{\partial h_1} \cdot \Delta h_1 + \frac{\partial L}{\partial h_2} \cdot \Delta h_2 + \frac{\partial L}{\partial h_3} \cdot \Delta h_3$



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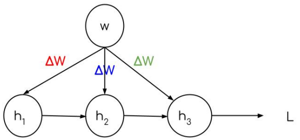

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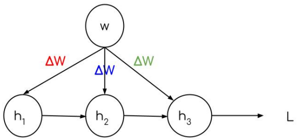

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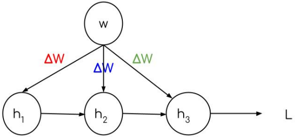
4. $\frac{\partial L}{\partial h_2} = ?$



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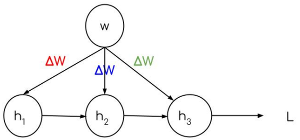

Backpropagation Through Time (BPTT)

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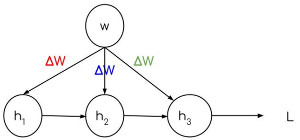

Backpropagation Through Time (BPTT)

1. $$\frac{\partial L}{\partial W} = \frac{\partial L}{\partial h_1}\frac{\partial h_1}{\partial W} + \frac{\partial L}{\partial h_2}\frac{\partial h_2}{\partial W} + \frac{\partial L}{\partial h_3}\frac{\partial h_3}{\partial W}$$
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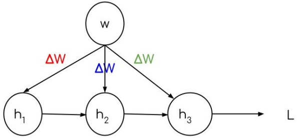

Backpropagation Through Time (BPTT)

1. $$\frac{\partial L}{\partial W} = \frac{\partial L}{\partial h_1}\frac{\partial h_1}{\partial W} + \frac{\partial L}{\partial h_2}\frac{\partial h_2}{\partial W} + \frac{\partial L}{\partial h_3}\frac{\partial h_3}{\partial W}$$
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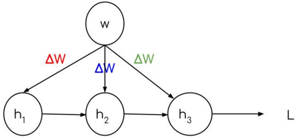
4. $$\frac{\partial L}{\partial W} = \frac{\partial L}{\partial h_3}\frac{\partial h_3}{\partial h_2}\frac{\partial h_2}{\partial h_1}\frac{\partial h_1}{\partial W} + \frac{\partial L}{\partial h_3}\frac{\partial h_3}{\partial h_2}\frac{\partial h_2}{\partial W} + \frac{\partial L}{\partial h_3}\frac{\partial h_3}{\partial W}$$



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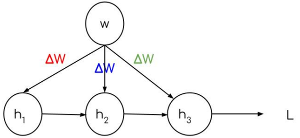

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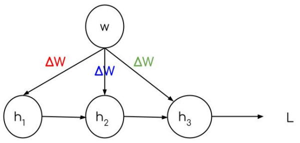
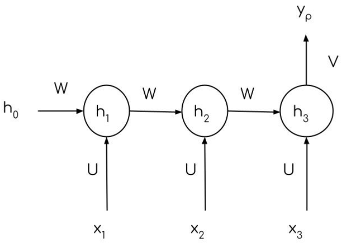


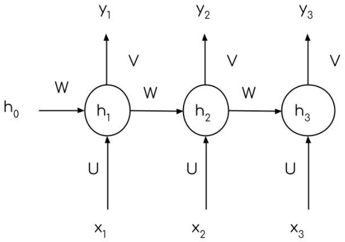
Backpropagation Through Time (BPTT)

1. Similarly $\frac{\partial L}{\partial U}$



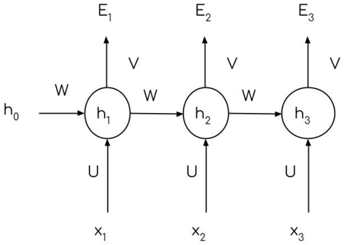
Backpropagation Through Time (BPTT)

1. Consider a many-to-many variant RNN (e.g. PoS tagging)



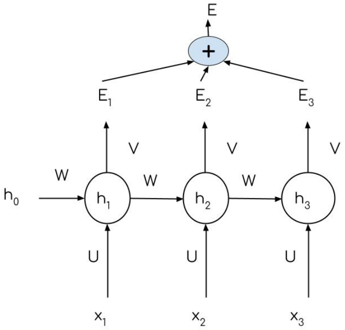
Backpropagation Through Time (BPTT)

1. Consider a many-to-many variant RNN (e.g. PoS tagging)
2. Full sequence is one training example (although there is an error computed at each time step)



Backpropagation Through Time (BPTT)

1. Consider a many-to-many variant RNN (e.g. PoS tagging)
2. Total error is the sum of errors at each time step



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4. Leads to Vanishing Gradient problem!
5. No impact of earlier time steps at later times (difficult to learn long-term dependencies!)

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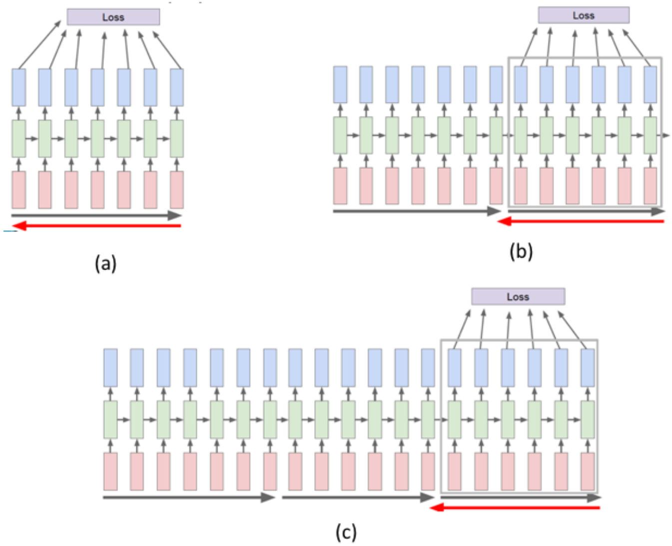
4. Better initialization, Regularization, short time sequences (Truncation)

Backpropagation Through Time (BPTT)



Truncated BPTT (CS231n)

Handling long-term dependencies

1. Architectural modifications to RNNs

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   - LSTM (1997 by Sepp Hochreiter and Jürgen Schmidhuber; Improved by Gers et al. in 2000)

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    - LSTM (1997 by Sepp Hochreiter and Jürgen Schmidhuber; Improved by Gers et al. in 2000)
    - GRU (Cho et al. 2014)

LSTM

1. Long Short-Term Memory

LSTM

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2. At a time ‘t’, **hidden state** $h^{(t)}$ and **cell state** $c^{(t)}$

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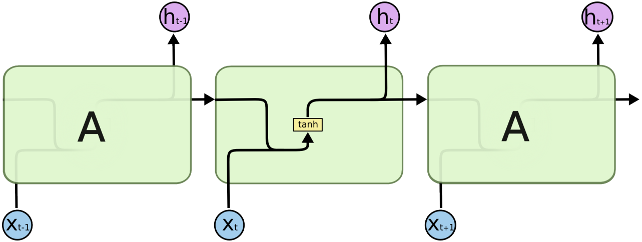
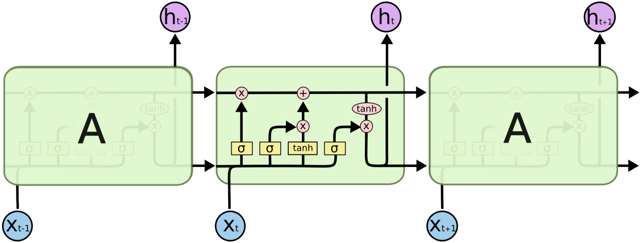
3. What to erase/write/read is controltted by corresponding **gates**
   - At time t, elements of the gates can be 0 (closed), 1 (open), or in-between
   - Gates are dynamically computed based on the context

LSTM



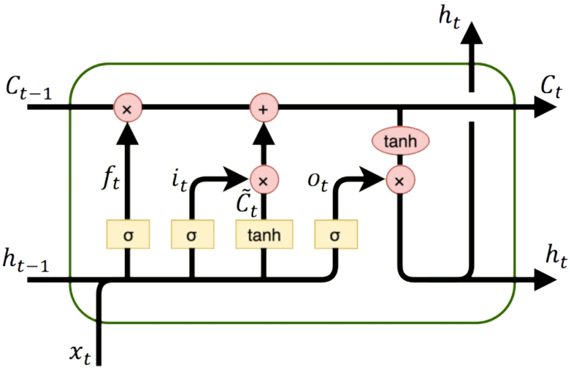
RNNs are chain of repeating moduels. Basic RNN (Colah's blog)

LSTM



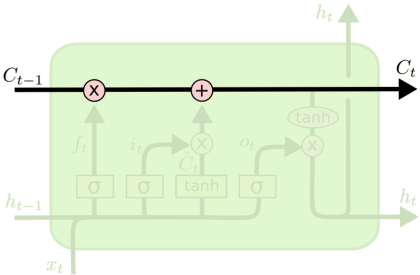
RNNs are chain of repeating moduels. LSTM (Colah's blog)

LSTM



The LSTM node. (Colah's blog)

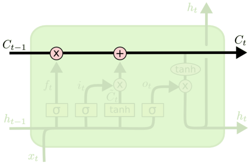
LSTM: The cell state



Cell state in LSTM (Colah's blog)

LSTM: The cell state

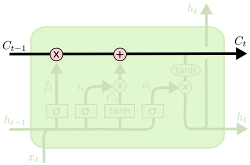
1. Info. can flow through unchanged



Cell state in LSTM (Colah's blog)

LSTM: The cell state

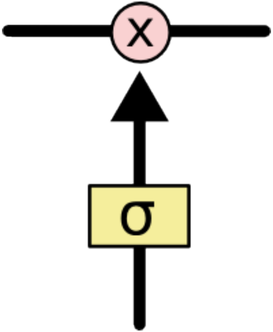
1. Info. can flow through unchanged
2. Gates can add/remove information to cell state



Cell state in LSTM (Colah's blog)

LSTM: The gates

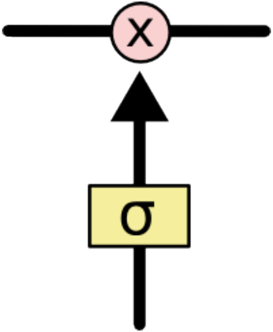
1. Sigmoid neural nets (o/p numbers in [0, 1])



Cell state in LSTM (Colah's blog)

LSTM: The gates

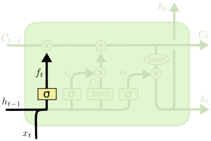
1. Sigmoid neural nets (o/p numbers in [0, 1])
2. Point-wise multiplication operation



Cell state in LSTM (Colah's blog)

LSTM: The forget gate

1. Decides what to throw away from cell state (e.g. forgetting the gender of old subject in light of a new one)

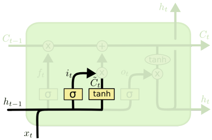


$$f_t = \sigma\left(W_f \cdot [h_{t-1}, x_t] \; + \; b_f\right)$$

Forget gate in LSTM (Colah's blog)

LSTM: The input gate

1. Next is to decide what new to store in cell state (e.g. add the gender of a new subject)

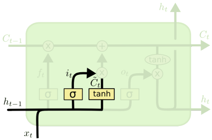


$$i_t = \sigma\left(W_i \cdot [h_{t-1}, x_t] + b_i\right)$$
$$\tilde{C}_t = \tanh(W_C \cdot [h_{t-1}, x_t] + b_C)$$

Input gate in LSTM (Colah's blog)

LSTM: The input gate

1. Next is to decide what new to store in cell state (e.g. add the gender of a new subject)
2. Done in two steps
   - input gate decides what to update
   - A tanh layer creates a candidate cell state



$$i_t = \sigma\left(W_i \cdot [h_{t-1}, x_t] \ + \ b_i\right)$$
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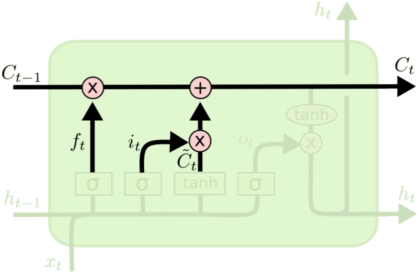
Input gate in LSTM (Colah's blog)

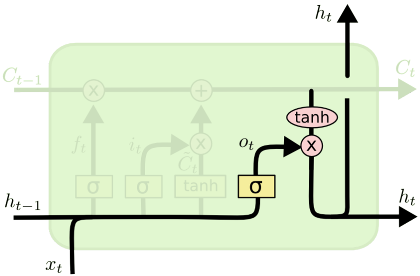
LSTM: The cell state update



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

Cell state update in LSTM (Colah's blog)

LSTM: The output



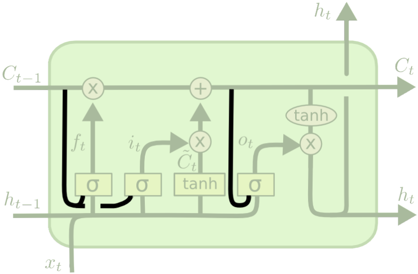
$$o_t = \sigma\left(W_o\ [h_{t-1}, x_t]\ +\ b_o\right)$$

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

Output computation in LSTM (Colah's blog)
e.g. may be a verb that is coming next in case of a language model

LSTM variant: Peephole connections

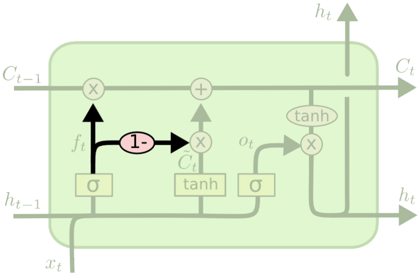
भारतीय प्रौद्योगिकी संस्थान हैदराबाद
Indian Institute of Technology Hyderabad



$$f_t = \sigma\left(W_f \cdot [\boldsymbol{C_{t-1}}, h_{t-1}, x_t] \; + \; b_f\right)$$
$$i_t = \sigma\left(W_i \cdot [\boldsymbol{C_{t-1}}, h_{t-1}, x_t] \; + \; b_i\right)$$
$$o_t = \sigma\left(W_o \cdot [\boldsymbol{C_t}, h_{t-1}, x_t] \; + \; b_o\right)$$

Variant with gates looking into the Cell state in LSTM by Ger et al. (Colah's blog)

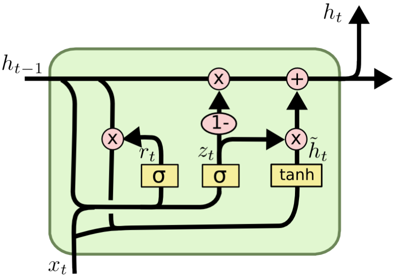
LSTM variant: Coupled i/p and forget gates



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

Variant with coupled input and forget gates. (Colah's blog)

LSTM → GRU



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

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

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

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

Gated Recurrent Unit (Colah's blog)

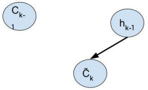
LSTM: handling the vanishing gradients

1. Via the gates!

LSTM: handling the vanishing gradients

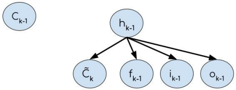
1. Computational graph at time $k-1$

LSTM: handling the vanishing gradients



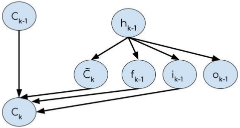
1. $\tilde{C}_k = \tanh(W_c[h_{t-1}, x_t] + b_c)$

LSTM: handling the vanishing gradients



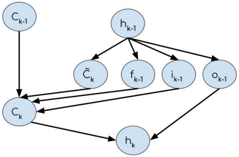
1. All the gates

LSTM: handling the vanishing gradients



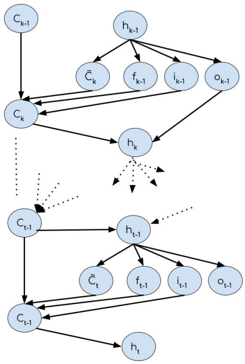
1. Next cell state

LSTM: handling the vanishing gradients



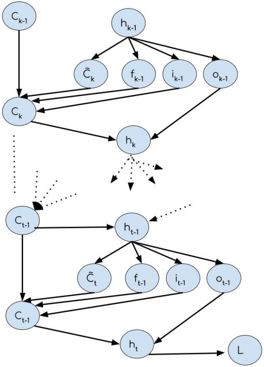
1. Next hidden state

LSTM: handling the vanishing gradients



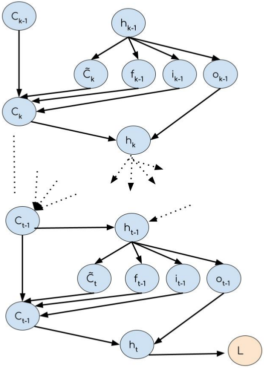
1. Running till time step 't'

LSTM: handling the vanishing gradients



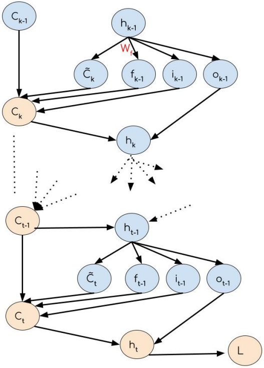
1. Consider loss computation

LSTM: handling the vanishing gradients



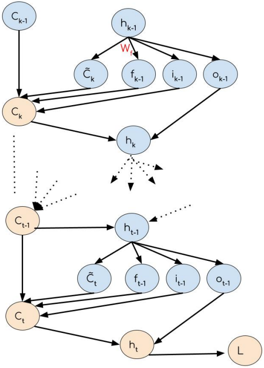
1. Let's know if the gradient flows to an arbitrary time step 'k'

LSTM: handling the vanishing gradients



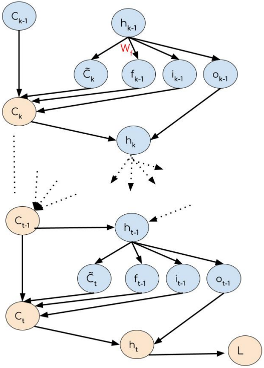
1. Specifically, let's consider if gradient flows to W_f through C_k

LSTM: handling the vanishing gradients



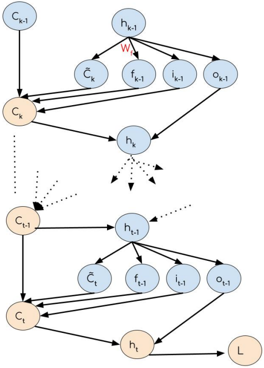
1. Specifically, let's consider if gradient flows to W_f through C_k
2. Note that there are multiple paths between L and C_k (but, consider one such path as highlighted)

LSTM: handling the vanishing gradients



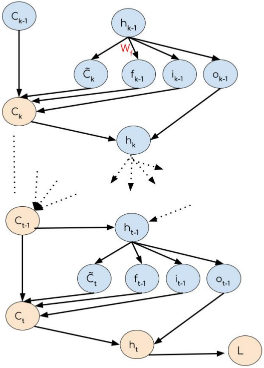
1. Grad $=$
$$\frac{\partial L}{\partial h_t} \frac{\partial h_t}{\partial C_t} \frac{\partial C_t}{\partial C_{t-1}} \cdots \frac{\partial C_{k+1}}{\partial C_k}$$

LSTM: handling the vanishing gradients



1. Grad $= \frac{\partial L}{\partial h_t} \frac{\partial h_t}{\partial C_t} \frac{\partial C_t}{\partial C_{t-1}} \cdots \frac{\partial C_{k+1}}{\partial C_k}$
2. $\frac{\partial L}{\partial h_t}$ doesn't vanish (no intermediate nodes)

LTSM: handling the vanishing gradients



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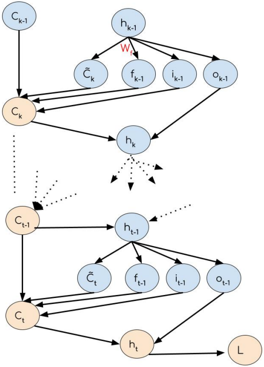

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2. $\frac{\partial L}{\partial h_t}$ doesn't vanish (no intermediate nodes)
3. $h_t = o_t \odot \sigma(C_t)$
4. $\rightarrow \frac{\partial h_t}{\partial C_t} = \mathbb{D}(o_t \odot \sigma'(C_t))$ (diagonal matrix)

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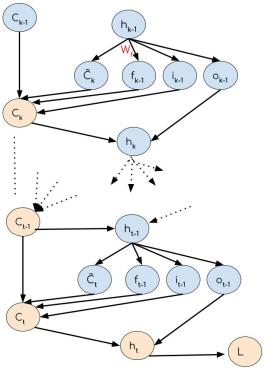

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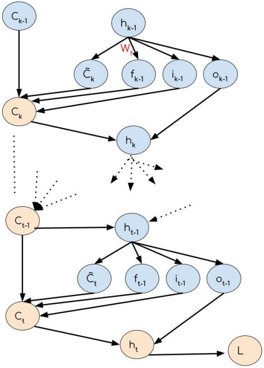

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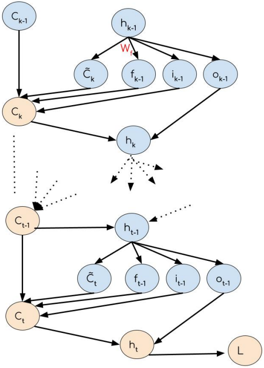

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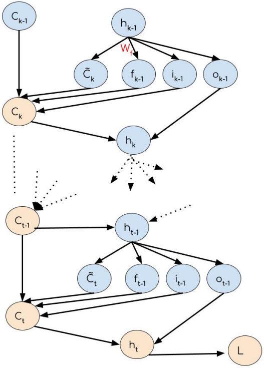

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2. Note that $\tilde{C}_t$ depends on C_{t-1}, and for simplicity assume the gradient from that term vanishes
3. Grad $=$ $\frac{\partial L}{\partial h_t} \frac{\partial h_t}{\partial C_t} \frac{\partial C_t}{\partial C_{t-1}} \cdots \frac{\partial C_{k+1}}{\partial C_k}$
4. Grad $=$ $\mathbb{L}' \cdot \mathbb{D}(o_t \odot \sigma'(C_t))\mathbb{D}(f_t) \cdot \mathbb{D}(f_{t-1}) \ldots \mathbb{D}(f_{k+1})$

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4. Gates do the same regulation in backward pass as they do in the forward

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3. Attention and Transformers are becoming more popular lately