Yandex

SCHOOL OF DATA ANALYSIS

Recurrent Neural Networks

RNN, biRNN, BPTT, LSTM, RecNN

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Sequence modelling

Recurrent neural network
- Defenition
- Training

Gated architectures

RNN generators

Bonus I: seq2seq

Bonus II: RecNN

Sequence modelling

Sequential data

1. Time series
   - Financial data analysis: stock market, commodities, Forex
   - Healthcare: pulse rate, sugar level (from medical equipment and wearables)
2. Text and speech: speech understanding, text generation
3. Spatiotemporal data
   - Self-driving and object tracking
   - Plate tectonic activity
4. Physics: jet identification
5. etc.

Sequence modelling I

Sequence labelling

1. $\boldsymbol{x} = x_1, x_2, \ldots, x_n$, $x_i \in V$, - objects
2. $\boldsymbol{y} = y_1, y_2, \ldots, y_n$, $y_i \in \{1, \ldots, L\}$ - labels
3. $\{(\boldsymbol{x}^{(1)}, \boldsymbol{y}^{(1)}), (\boldsymbol{x}^{(2)}, \boldsymbol{y}^{(2)}), \ldots, (\boldsymbol{x}^{(m)}, \boldsymbol{y}^{(m)})\}$ — training data
4. exponential number of possible solutions : if $\texttt{length}(x) = n$, there are L^n possible solutions

Classification problem: $\gamma : \boldsymbol{x} \to \boldsymbol{y}$

1. Speech recognition: x — spoken words, y — transcription
2. Genome annotation: x — DNA, y — genes

Sequence modelling II

Sequence classification

1. $\boldsymbol{x} = x_1, x_2, \ldots, x_n$, $x_i \in V$, - objects
2. $y \in \{1, \ldots, L\}$ - labels
3. $\{(\boldsymbol{x}^{(1)}, y_1), (\boldsymbol{x}^{(2)}, y_2), \ldots, (\boldsymbol{x}^{(m)}, y_m)\}$ — training data

Classification problem: $\gamma : \boldsymbol{x} \to y$

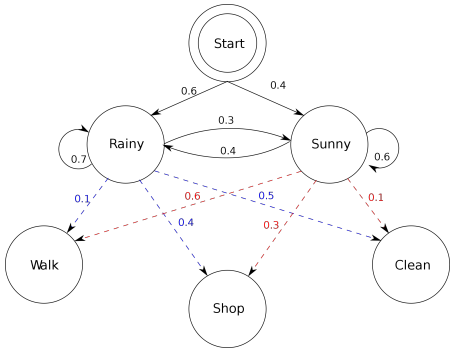
1. Activity recognition: x — pulse rate, y — activity (walking, running, peace)
2. Opinion mining: x — sentence, y — sentiment (positive, negative)
3. Trading: x — stock market, y — action (sell, buy, do nothing)

Traditional ML approaches to sequence modelling

- Hidden Markov Models (HMM)
- Conditional Random Fields (CRF)
- Local classifier: for each x define features, based on x_{-1}, x_{+1}, etc, and perform classification n times

Problems:

1. Markov assumption: fixed length history
2. Computation complexity



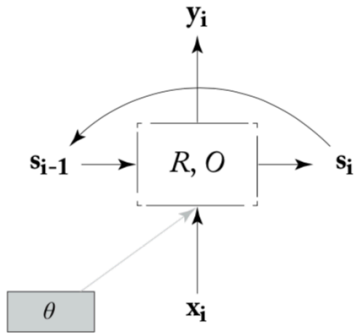
Recurrent neural network

Recurrent neural network

Defenition

Recurrent neural network

- Input: sequence of vectors
- $x_{1:n} = x_1, x_2, \ldots, x_n, x_i \in \mathbb{R}^{d_{in}}$
- Output: a single vector
  $y_n = RNN(x_{1:n}), y_n \in \mathbb{R}^{d_{out}}$
- For each prefix $x_{i:j}$ define an output vector y_i:
  $y_i = RNN(x_{1:i})$
- RNN^* is a function returning this sequence for input sequence $x_{1:n}$:
  $y_{1:n} = RNN^*(x_{1:n}), y_i \in \mathbb{R}^{d_{out}}$



Sequence modelling with RNN

1. Sequence labelling
   Produce an output y_i for each input RNN reads in. Put a dense layer on top of each output to predict the desired class of the input

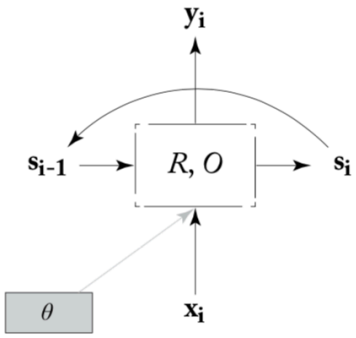
$$p(l_j|\boldsymbol{x}_j) = \texttt{softmax}(RNN(\boldsymbol{x}_{1:j}) \times W + b)_{[j]}$$

2. Sequence classification
   Put a dense layer on top of RNN to predict the desired class of the sequence after the whole sequence is processed

$$p(l_j|\boldsymbol{x}_{1:n}) = \texttt{softmax}(RNN(\boldsymbol{x}_{1:n}) \times W + b)_{[j]}$$

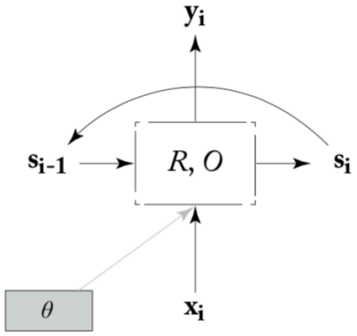
More details on RNN

- $RNN^*(x_{1:n}, s_0) = y_{1:n}$
- $y_i = O(s_i)$ — simple activation function
- $s_i = R(s_{i-1,x_i})$, where R is a recursive function, s_i is a state vector
- s_0 is initialized randomly or is a zero vector
- $x_i \in \mathbb{R}^{d_{in}}$, $y_i \in \mathbb{R}^{d_{out}}$, $s_i \in \mathbb{R}^{f(d_{out})}$
- θ — shared weights

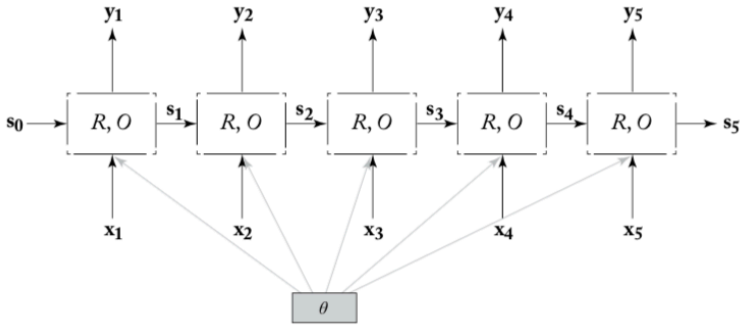


More details on RNN

- $s_i = R(x_i, s_{i-1}) = g(s_{i-1}W^s + x_iW^x + b)$
- $y_i = O(s_i) = s_i$
- $y_i, s_i, b \in \mathbb{R}^{d_{out}}, x_i \in \mathbb{R}^{d_{in}}$
- $W^x \in \mathbb{R}^{d_{in} \times d_{out}}, W^s \in \mathbb{R}^{d_{out} \times d_{out}}$



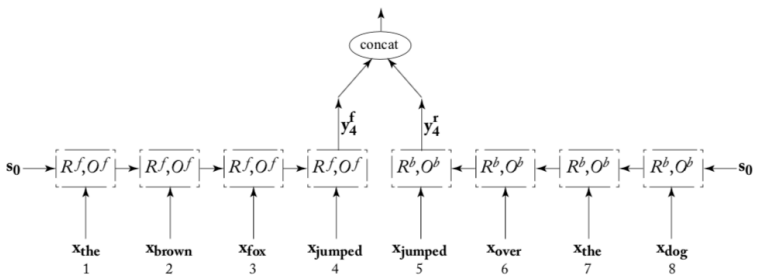
RNN unrolled



$$s_4 = R(s_3, x_4) = R(R(s_2, x_3), x_4) = R(R(R(s_1, x_2), x_3), x_4) =$$
$$= R(R(R(R(s_0, x1), x_2), x_3), x_4)$$

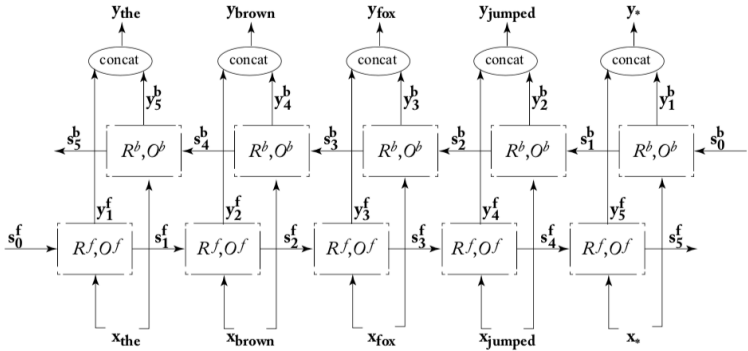
Bidirectional RNN (Bi-RNN)

The input sequence can be read from left to right and from right to left. Which direction is better?



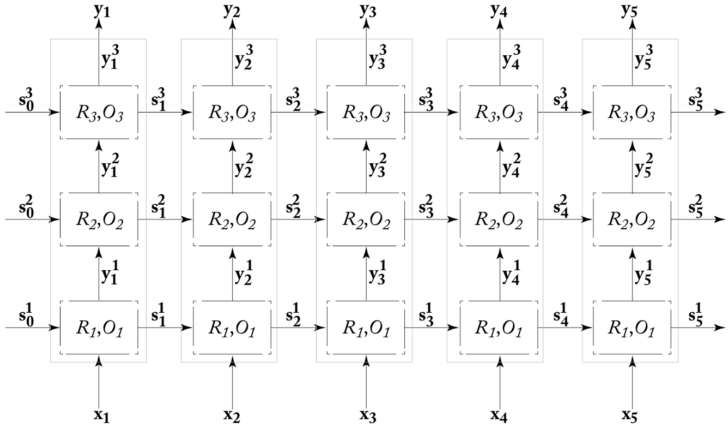
$$biRNN(x_{1:n}, i) = y_i = [RNN^f(x_{1:i}); RNN^r(x_{n:i})]$$

Bi-RNN



$$biRNN^*(x_{1:n}, i) = y_{1:n} = biRNN(x_{1:n}, 1) \dots biRNN(x_{1:n}, n)$$

Multilayer RNN



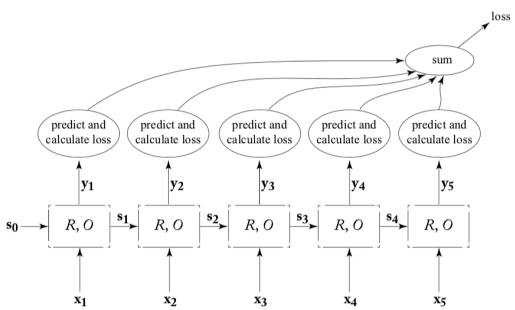
Connections between different layers are possible too: $y_1^2 = \texttt{concat}(x_1, y_1^1)$

Recurrent neural network

Training

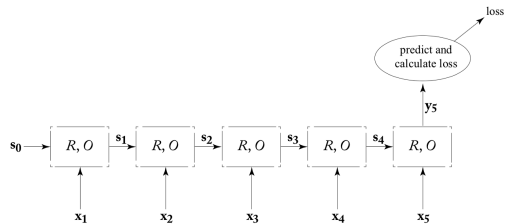
Sequence labelling

- Output $\hat{t_i}$ for each input $x_{1,i}$
- Local loss: $L_{local}(\hat{t_i}, t_i)$
- Global loss: $L(\hat{t_n}, t_n) = \sum_i L_{local}(\hat{t_i}, t_i)$
- L can take any form: cross entropy, hinge, margin, etc.

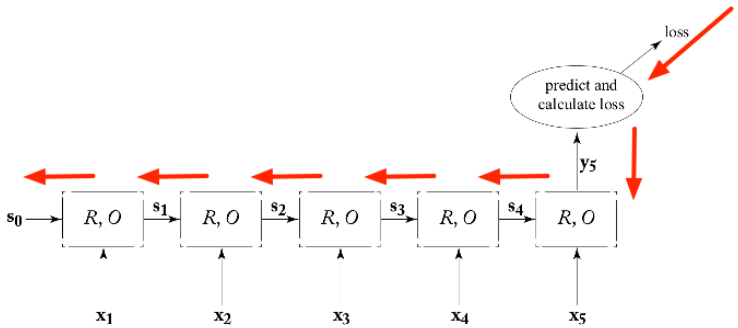


Sequence classification

- $\hat{y_n} = O(s_n)$
- `prediction` $= MLP(\hat{y_n})$
- Loss: $L(\hat{y_n}, y_n)$
- L can take any form: cross entropy, hinge, margin, etc.



Backpropogation through time



$$s_i = R(x_i, s_{i-1}) = g(s_{i-1}W^s + x_i W^x + b)$$

Chain rule: $\frac{\partial L}{\partial w} = \frac{\partial L}{\partial p(\hat{y_5})} \frac{\partial p(\hat{y_5})}{\partial s_4} (\frac{\partial s_4}{\partial w} + \frac{\partial s_4}{\partial s_3}\frac{\partial s_3}{\partial w} + \frac{\partial s_4}{\partial s_3}\frac{\partial s_3}{\partial s_2}\frac{\partial s_2}{\partial s_w} + \dots)$

Vanishing gradient problem

Chain rule: $\frac{\partial L}{\partial w} = \frac{\partial L}{\partial p(\hat{y_5})} \frac{\partial p(\hat{y_5})}{\partial s_4} (\frac{\partial s_4}{\partial w} + \frac{\partial s_4}{\partial s_3} \frac{\partial s_3}{\partial w} + \frac{\partial s_4}{\partial s_3} \frac{\partial s_3}{\partial s_2} \frac{\partial s_2}{\partial s_w} + \dots)$
g — sigmoid

1. Many sigmoids near 0 and 1
   - Gradients $\to 0$
   - Not training for long term dependencies
2. Many sigmoids > 1
   - Gradients $\to +\inf$
   - Not training again

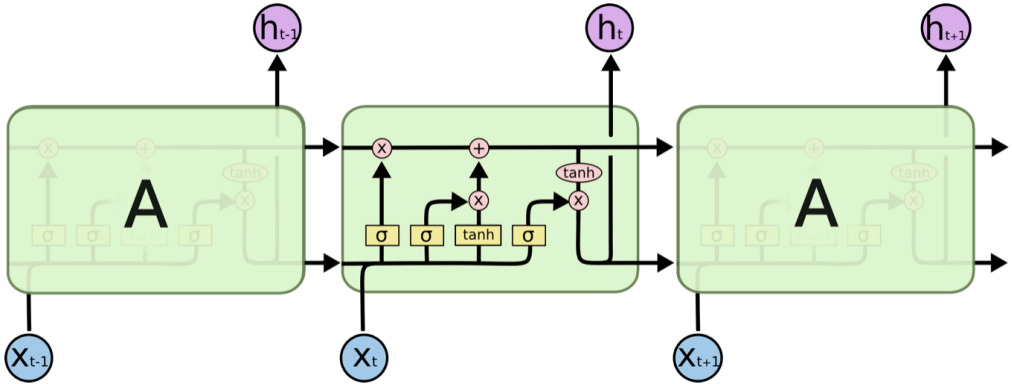
Solution: gated architectures (LSTM and GRU)

Gated architectures

Controlled memory access

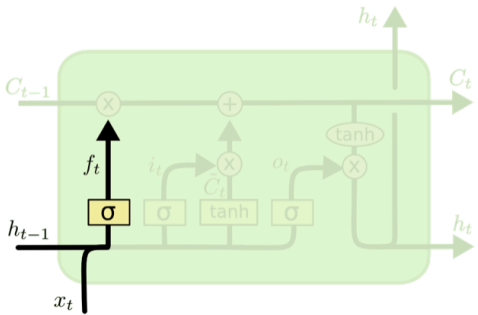
- Entire memory vector is changed: $s_{i+1} = R(x_i, s_i)$
- Controlled memory access: $s_{i+1} = g \odot R(x_i, s_i) + (1 - g)s_i$
  $g \in [0, 1]^d, s, x \in \mathbb{R}^d$
- Differential gates: $\sigma(g), g' \in \mathbb{R}^d$
- This controllable gating mechanism is the basis of the LSTM and the GRU architectures

Long short term memory



http://colah.github.io/posts/2015-08-Understanding-LSTMs/

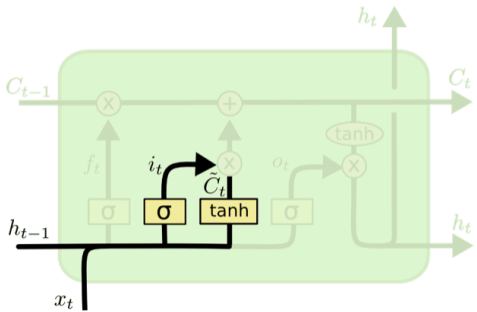
Long short term memory



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

http://colah.github.io/posts/2015-08-Understanding-LSTMs/

Long short term memory

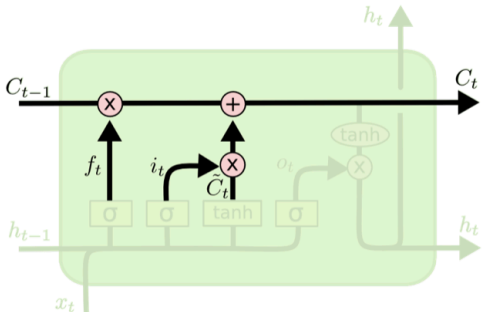


$$i_t = \sigma\left(W_i \cdot [h_{t-1}, x_t] \; + \; b_i\right)$$

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

http://colah.github.io/posts/2015-08-Understanding-LSTMs/

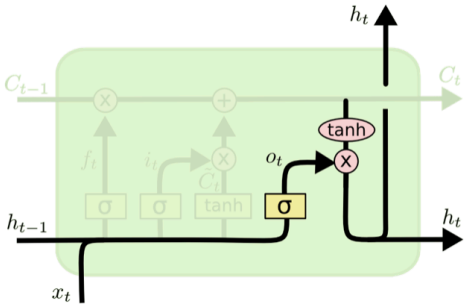
Long short term memory



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

http://colah.github.io/posts/2015-08-Understanding-LSTMs/

Long short term memory

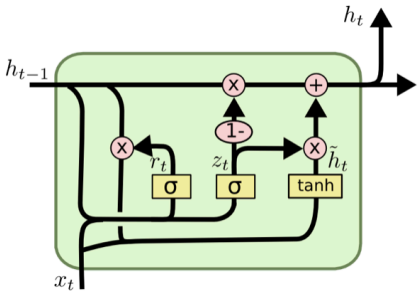


$$o_t = \sigma\left(W_o\ [h_{t-1}, x_t]\ +\ b_o\right)$$

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

http://colah.github.io/posts/2015-08-Understanding-LSTMs/

Gated recurrent unit



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

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

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

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

http://colah.github.io/posts/2015-08-Understanding-LSTMs/

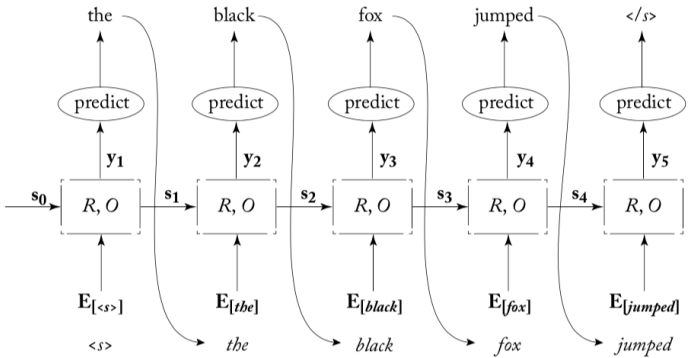
RNN generators

Sequence generation

Teacher forcing: $x :=< s > x, y := x < /s?$

$x :< s > x_1 x_2 \ldots x_n$

$y : x_1 x_2 \ldots x_n < /s >$



Sequence generation

- Examples of generated texts: `http://karpathy.github.io/2015/05/21/rnn-effectiveness/`
- Examples of generated MIDI music: `https://towardsdatascience.com/how-to-generate-music-using-a-lstm-neural-network-in-keras-6878`

Conclusion

Topics covered:

1. RNN is a powerful tool for sequence modeling
2. RNN usage scenarios: sequence labelling, sequence classification, sequence generation
3. RNN layers can be reversed $\rightarrow$ bidirectional RNN
4. RNN layers can be stacked $\rightarrow$ deep RNN
5. RNN suffers from gradient vanishing problem $\rightarrow$ LSTM, GRU

Topics not covered:

1. seq2seq models
2. Attention mechanism in RNN
3. Recursive neural networks

Bonus I: seq2seq

Bonus II: RecNN