





Recurrent Neural Networks

RNN, biRNN, BPTT, LSTM, RecNN

Fourth Machine Learning in High Energy Physics Summer School, MLHEP 2018, August 6-12

Ekaterina Chernyak

National Research University Higher School of Economics

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

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

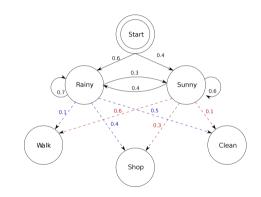
- 1. Activity recognition: x pulse rate, y activity (walking, running, peace)
- 2. Opinion mining: x sentence, y sentiment (positive, negative)
- 3. Trading: x stock market, y action (sell, buy, do nothing)

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:

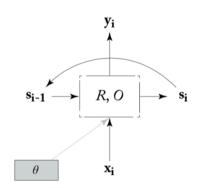
- 1. Markov assumption: fixed length history
- 2. Computation complexity



Defenition

- > Input: sequence of vectors
- $x_{1:n} = x_1, x_2, \dots, x_n, x_i \in \mathbb{R}^{d_{in}}$
- > 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

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

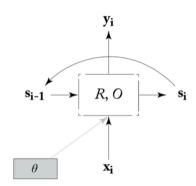
2. Sequence classification

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

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

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
- $\rightarrow s_0$ is initialized randomly or is a zero vector
- $x_i \in \mathbb{R}^{d_{in}}, y_i \in \mathbb{R}^{d_{out}}, s_i \in \mathbb{R}^{f(d_{out})}$
- $\rightarrow \theta$ shared weights



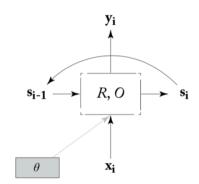
More details on RNN

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

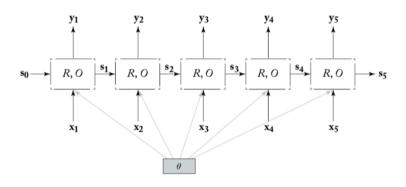
$$y_i = O(s_i) = s_i$$

$$y_i, s_i, b \in \mathbb{R}^{d_{out}}, x_i \in \mathbb{R}^{d_{in}}$$

$$W^x \in \mathbb{R}^{d_{in} \times d_{out}}, W^s \in \mathbb{R}^{d_{out} \times d_{out}}$$



RNN unrolled

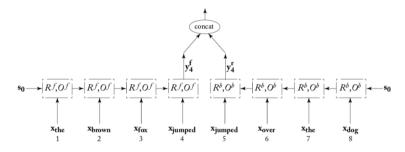


$$s_4 = R(s_3, x_4) = R(R(s_2, x_3), x_4) = R(R(R(s_1, x_2), x_3), x_4) =$$

= $R(R(R(s_0, x_1), x_2), x_3), x_4)$

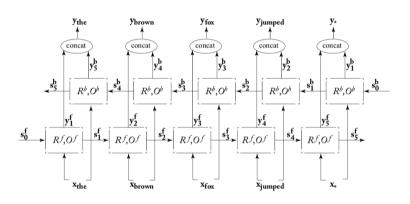
Bidirectional RNN (Bi-RNN)

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



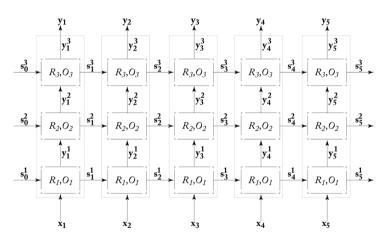
$$biRNN(x_{1:n}, i) = y_i = [RNN^f(x_{1:i}); RNN^r(x_{n:i})]$$

Bi-RNN



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

Multilayer RNN



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

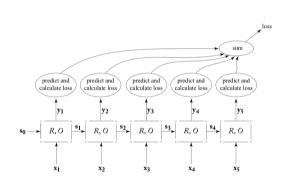
Training

Sequence labelling

- \rightarrow Output $\hat{t_i}$ for each input $x_{1,i}$
- \rightarrow Local loss: $L_{local}(\hat{t_i}, t_i)$
- > Global loss:

$$L(\hat{t_n}, t_n) = \sum_i L_{local}(\hat{t_i}, t_i)$$

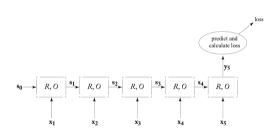
> L can take any form: cross entropy, hinge, margin, etc.



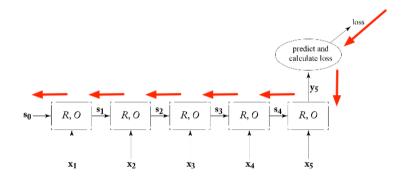
Sequence classification

$$\hat{y_n} = O(s_n)$$

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



Backpropogation through time



$$\begin{split} s_i &= R(x_i, s_{i-1}) = g(s_{i-1}W^s + x_iW^x + b) \\ \text{Chain rule: } \frac{\partial L}{\partial w} &= \frac{\partial L}{\partial p(\hat{y_5})} \frac{\partial p(\hat{y_5})}{\partial s_4} (\frac{\partial s_4}{\partial w} + \frac{\partial s_4}{\partial s_3} \frac{\partial s_3}{\partial w} + \frac{\partial s_4}{\partial s_3} \frac{\partial s_3}{\partial s_2} \frac{\partial s_2}{\partial s_w} + \ldots) \end{split}$$

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

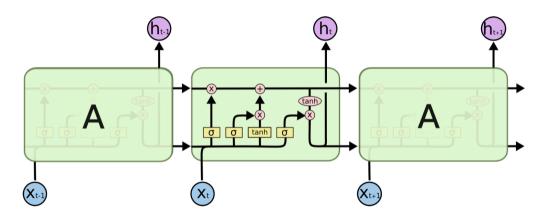
- 1. Many sigmoids near 0 and 1
 - \rightarrow Gradients \rightarrow 0
 - > Not training for long term dependencies
- 2. Many sigmoids > 1
 - \rightarrow Gradients $\rightarrow + \inf$
 - > Not training again

Solution: gated architectures (LSTM and GRU)

Gated architectures

Controlled memory access

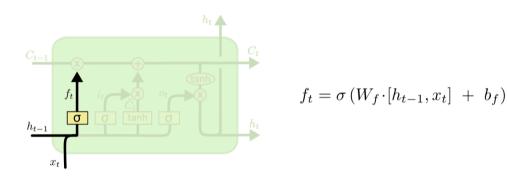
- > Entire memory vector is changed: $s_{i+1} = R(x_i, s_i)$
- > Controlled memory access: $s_{i+1} = g \odot R(x_i, s_i) + (1-g)s_i$ $g \in [0, 1]^d, s, x \in \mathbb{R}^d$
- \rightarrow Differential gates: $\sigma(g), g' \in \mathbb{R}^d$
- This controllable gating mechanism is the basis of the LSTM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



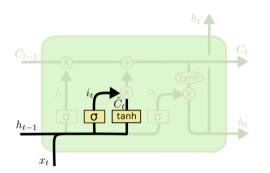
http://colah.github.io/posts/2015-08-Understanding-LSTMs/

Ekaterina Chernyak

25

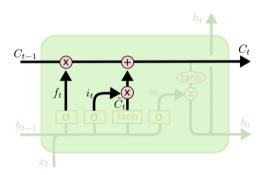


http://colah.github.io/posts/2015-08-Understanding-LSTMs/



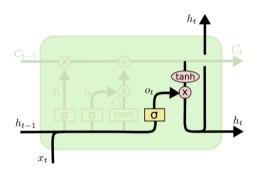
$$\begin{split} i_t &= \sigma\left(W_i \cdot [h_{t-1}, x_t] + b_i\right) \\ \tilde{C}_t &= \tanh(W_C \cdot [h_{t-1}, x_t] + b_C) \end{split}$$

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



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

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

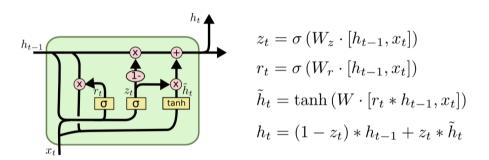


$$o_t = \sigma (W_o [h_{t-1}, x_t] + b_o)$$

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

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

Gated recurrent unit



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

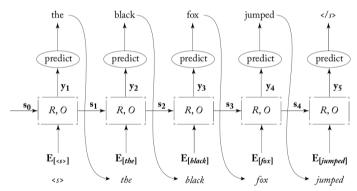
RNN generators

Sequence generation

Teacher forcing: $x := \langle s \rangle x, y := x \langle /s?$

 $x : \langle s \rangle x_1 x_2 \dots x_n$

 $y: x_1x_2 \dots x_n < /s >$



Sequence generation

> Examples of generated texts:

- http://karpathy.github.io/2015/05/21/rnn-effectiveness/
 > Examples of generated MIDI music: https://towardsdatascience.com/
- > 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:

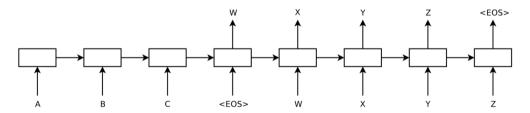
- 1. seq2seq models
- 2. Attention mechanism in RNN
- 3. Recursive neural networks

Bonus I: seq2seq

Sequence 2 sequence learning

Encoder-decoder model for:

- 1. Machine translation
- 2. Chit-chat bots



Bonus II: RecNN

Modeling trees with Recursive NN

- > Input: $x_1, x_2, ..., x_n$
- A binary tree T can be represented as a unique set of triplets (i, k, j), s.t. i < k < j, $x_{i:j}$ is parent of $x_{i:k}$, $i_{k+1,j}$
- > RecNN takes as an input a binary tree and returns as output a corresponding set of inside state vectors $s_{i:i}^A \in \mathbb{R}^d$
- > Each state vector $s_{i:j}^A$ represents the corresponding tree node $q_{i:j}^A$ and encodes the entire structure rooted at that node

RecNN

- \rightarrow Input: x_1, x_2, \dots, x_n and a binary tree T
- $\rightarrow RecNN(x_1, x_2, \dots, x_n, T) = \{ s_{i:j}^A \in \mathbb{R}^d | q_{i:j}^A \in T \}$
- $> s_{i:i}^A = v(x_i)$
- $> s_{i:j}^{A} = R(A, B, C, s_{i:k}^{B}, s_{k+1:j}^{C}), q_{i:k}^{B} \in T, q_{k+1:j}^{C} \in T$
- $ho \ R(A,B,C, s_{i:k}^{B}, s_{k+1:j}^{C}) = g([s_{i:k}^{B}, s_{k+1:j}^{C}]W)$