Neural Networks and Deep Learning Lecture 8

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Mid-term survey

- Slides
  - Upload the final version directly
  - Use notations consistently and more graphics/examples
  - High-level overview first
- Practice
  - More sample/pseudo code
  - Tutorials
- Assignment
  - Implementation from scratch vs calling keras/tensorflow/etc.
- Consultation
  - Consultation on Saturday and after lecture

Intended learning outcomes

1. Explain the logics (intuitions) of the operations of different layers and training algorithms
2. Compare different neural network architectures in terms of their characteristics
3. Implement popular neural networks
4. Solve real problems using neural networks and deep learning techniques

Announcement

- Quiz 30%
  - March 19, 19:20-20:20
  - Closed book with one page cheat sheet
  - Scope: all materials from week 1 to week 9 (inclusive)
  - Question types: MCQ, True/False, Calculation, Explanation.
- Tutorial for Assignment 1
  - 15:00 to 17:00 on Saturday, 3/17/2018.
  - 39/COM1-B109 (46 seats)
  - Poll on IVLE by Thursday.

Recurrent Neural Networks (RNN)

Road map and goals

01

Understand the properties of RNN compared with feed-forward NN

02

Implement the BP of vanilla RNN

03

Know the problem of vanilla RNN and the properties of LSTM/GRU

04

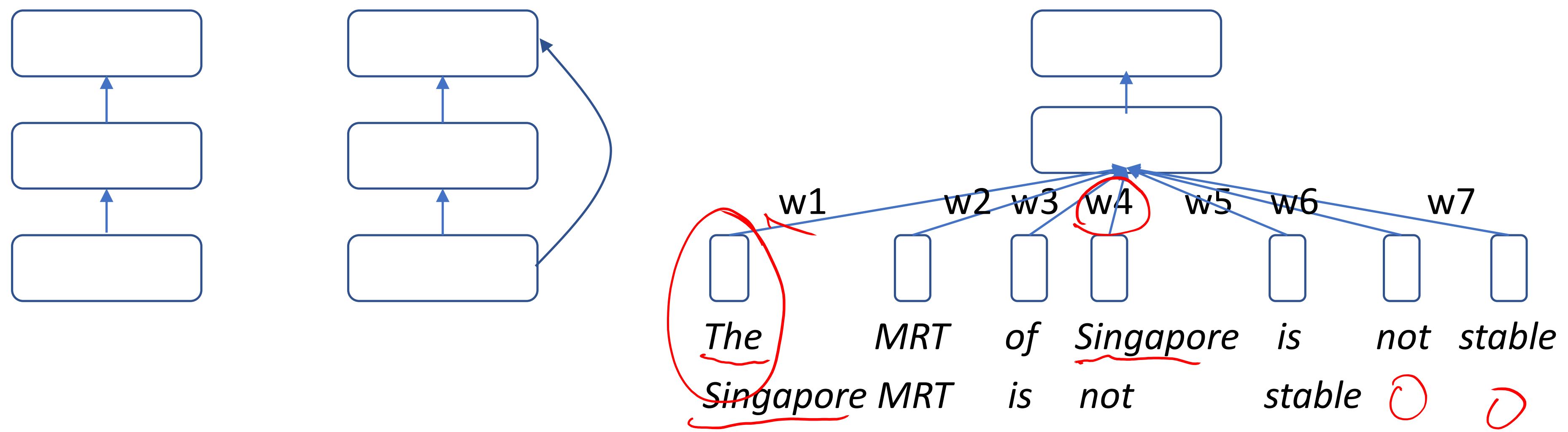
Train RNN (vanilla/LSTM/GRU) for NLP applications

Motivation

From feed-forward NN to RNN

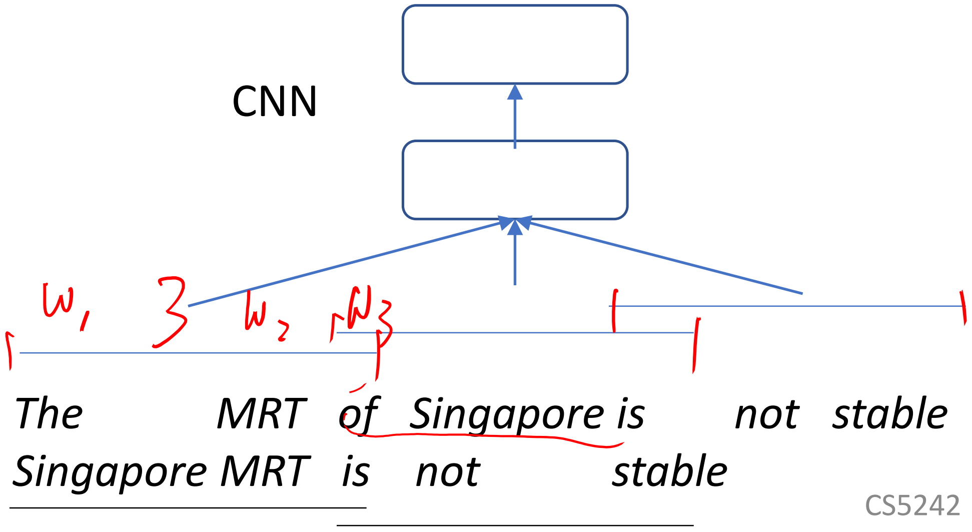
- Feed-forward NN (acyclic)
  - Accept single/static input sample, e.g. image
  - Not good at processing a sequence of data
    - E.g. a sentence of words for sentiment analysis; **how to do it using MLP or CNN?**

Feed-forward NN



From feed-forward NN to RNN

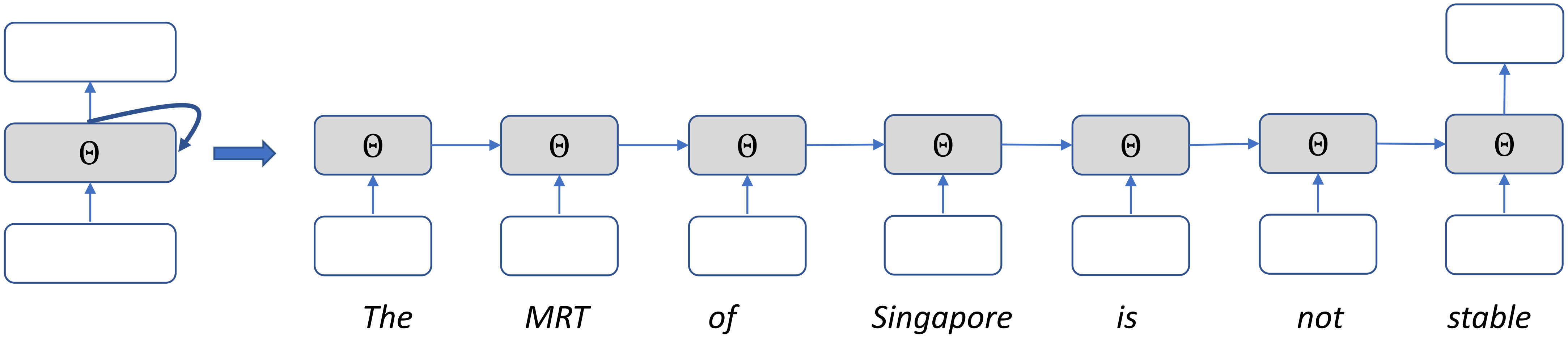
- Feed-forward NN (acyclic)
  - Accept single/static input sample, e.g. image
  - Not good at processing a sequence of data
    - CNN's receptive fields share the parameters (i.e. kernels)
    - Kernel size typically > 1 -> words within the receptive field are processed differently
      - "MRT of Singapore" != "Singapore MRT is"



http://www.wildml.com/2015/11/understanding-convolutional-neural-networks-for-nlp/

From feed-forward NN to RNN

- RNN
  - Accept dynamic/sequence data (length not fixed)
    - Words are processed in the same way recurrently
      - # unfold units = input sequence length
      - Weights （Θ） are tied/shared



RNN

- Applications
  - Language modelling
    - Predict the next words given the previous words in a sentence
  - Machine translation
    - Translate the input English sentence to French
  - Speech recognition
    - Recognize and translate spoken language into text
  - Question answering
    - Generate text answers for (simple) questions
  - Etc.

Vanilla RNN

Language modelling example

- Given a corpus of text (e.g. sentences), model the probability of a sentence (i.e. a sequence of words)
  - $P(x_1, x_2, \ldots, x_n)$
  - Useful for many applications involving text/sentence generation**?**
    - Machine translation, speech recognition, question answering, etc.
      - P("Singapore MRT is not **stable**") > P("Singapore MRT is not **NUS**")
      - P("Singapore **MRT is** not stable") > P("Singapore **is MRT** not stable")
  - Refer to [5] for traditional approaches for this problem

$P(x_n \mid x_1 \cdots x_{n-1})$

$\sim \dfrac{P(x_1, x_2, \cdots x_{n-1}, x_n)}{P(x_1, \cdots x_{n-1})}$

Language modelling example

- $P(x_1, x_2, \dots, x_n) = \prod_t P(x_t | x_{t-1}, x_{t-2}, \dots, x_1)$

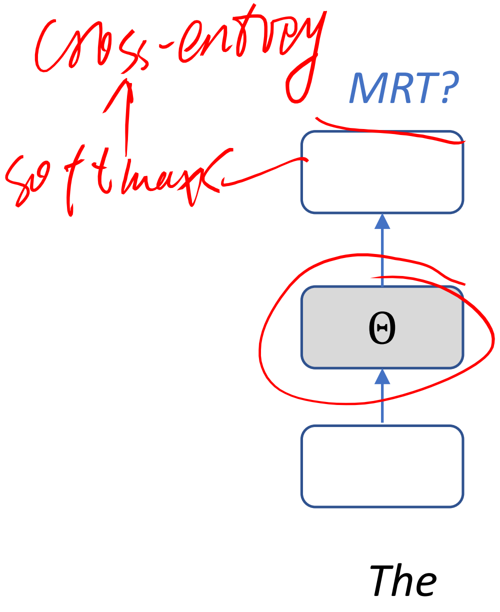
P(The, MRT, of, Singapore, is, not, stable) = *P(The)*
P(MRT | The)
P(of | The MRT)
P(Singapore | The MRT of)
P(is | The MRT of Singapore)
P(not | The MRT of Singapore is)
P(stable | The MRT of Singapore is not)

Max $logP(x_1, x_2, \dots, x_n) = \sum_t logP(x_t | x_{t-1}, x_{t-2}, \dots, x_1)$
$logP(x_t | x_{t-1}, x_{t-2}, \dots, x_1)$ **?**

cross-entropy

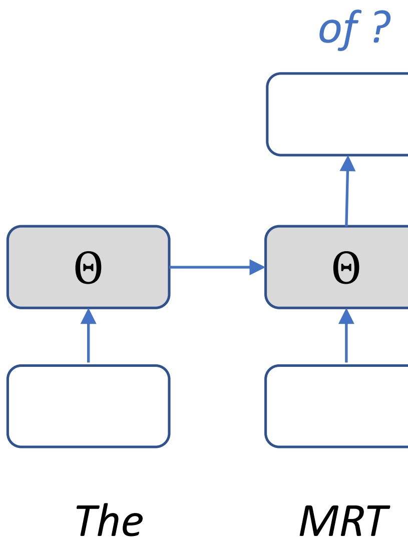
Language modelling example

- Train classifiers to predict the next word given the preceding words
- P(MRT|The)



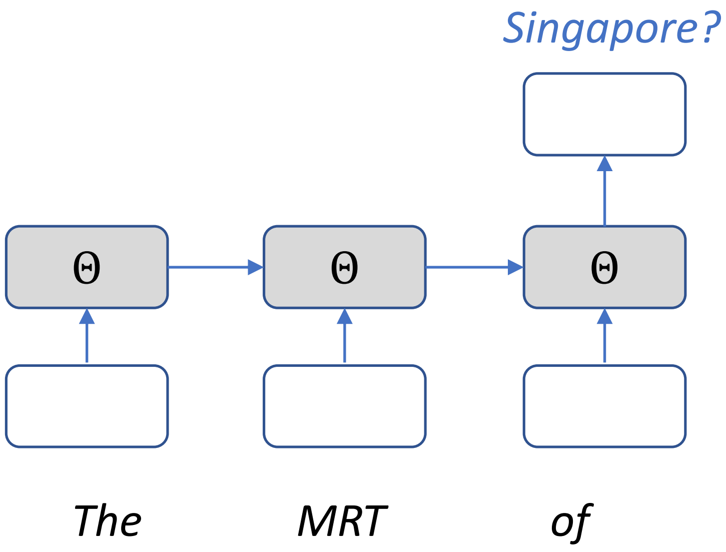
Language modelling example

- Train classifiers to predict the next word given the preceding words
- P(of|The MRT)



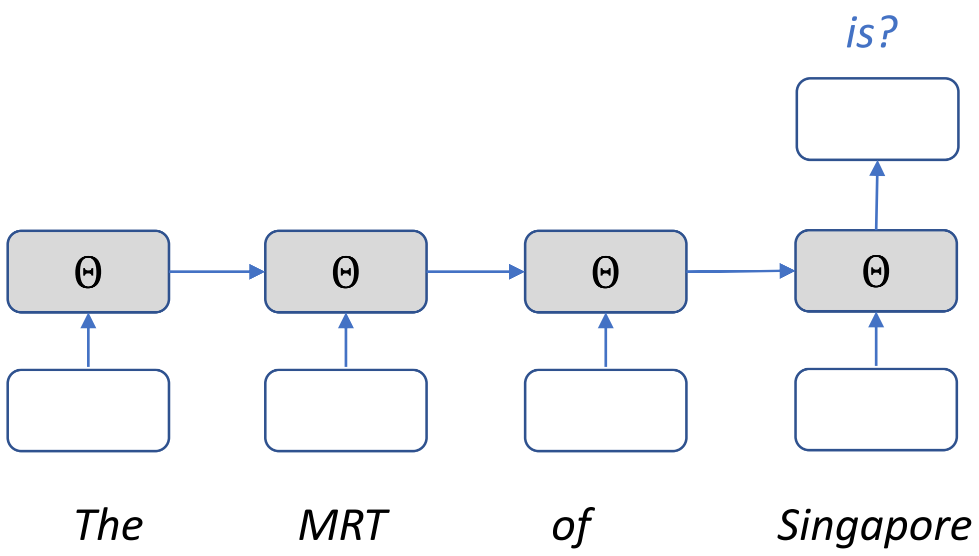
Language modelling example

- Train classifiers to predict the next word given the preceding words
- P(Singapore|The MRT of)



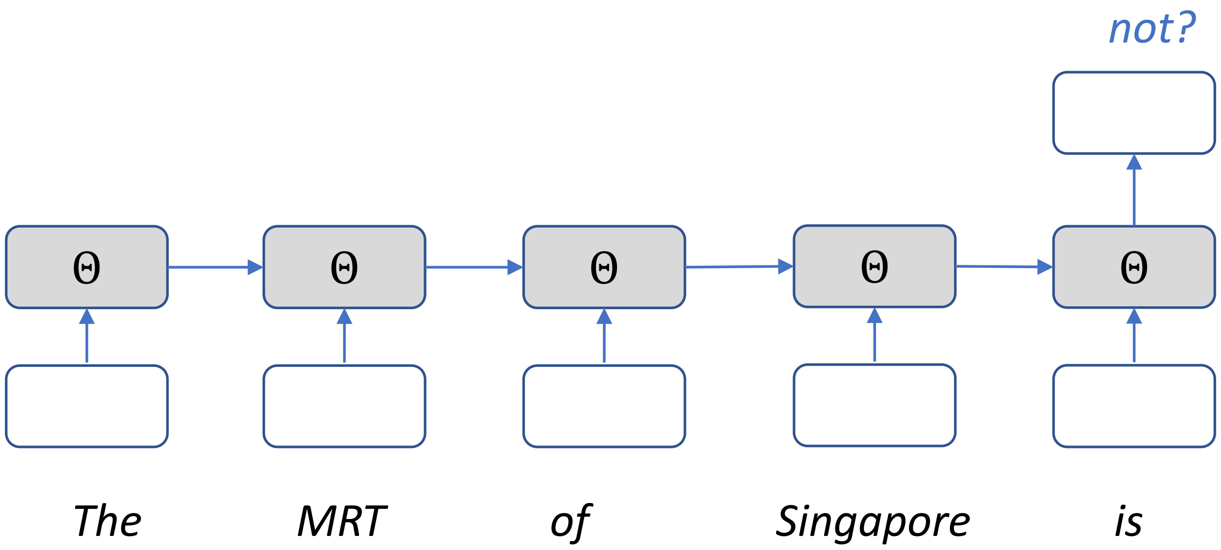
Language modelling example

- Train classifiers to predict the next word given the preceding words
- P(is|The MRT of Singapore)



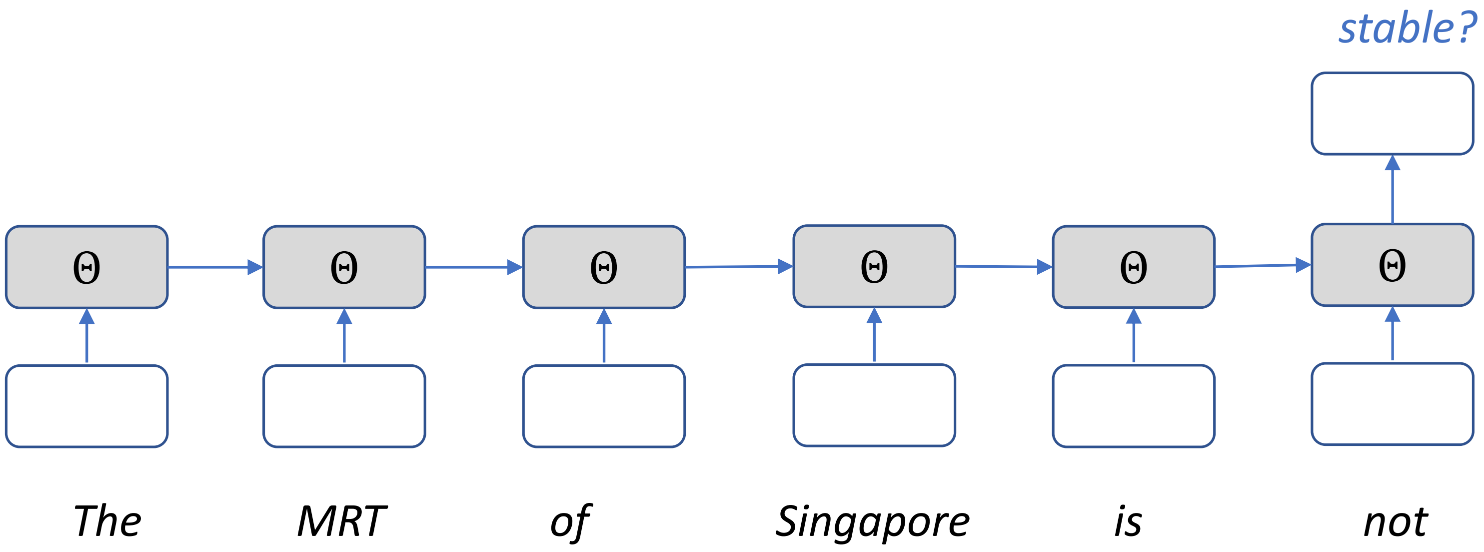
Language modelling example

- Train classifiers to predict the next word given the preceding words
- P(not|The MRT of Singapore is)



Language modelling example

- Train classifiers to predict the next word given the preceding words
- P(stable | The MRT of Singapore is not)

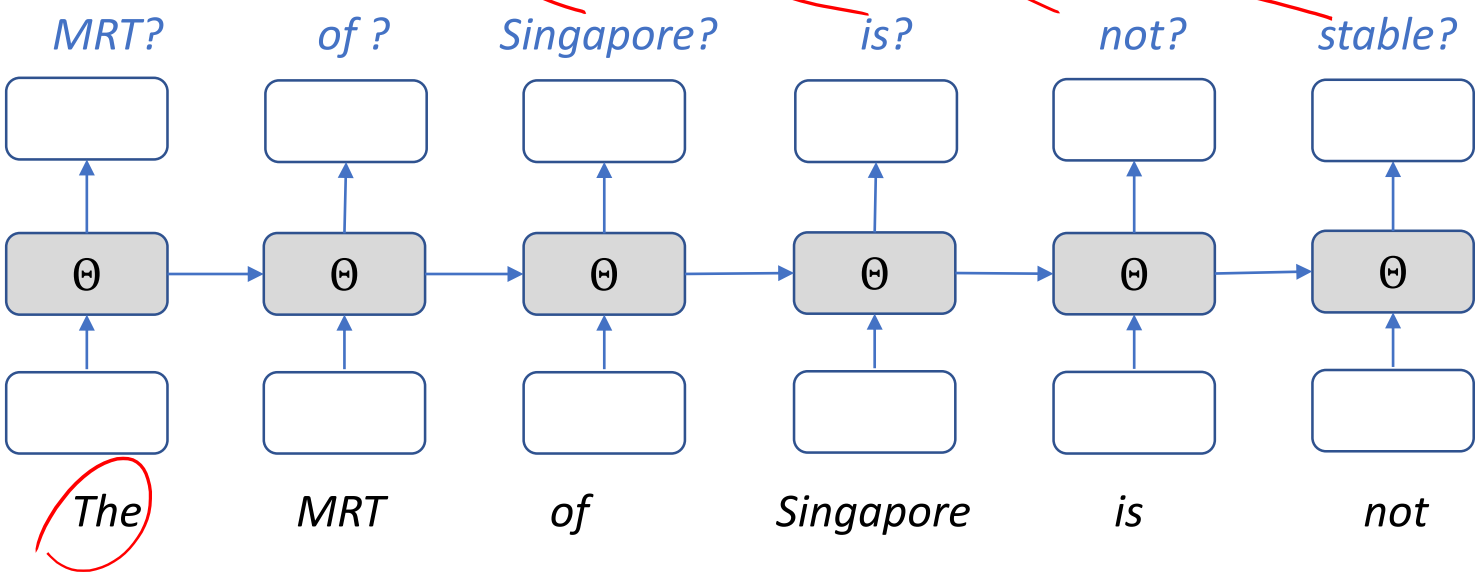


Language modelling example

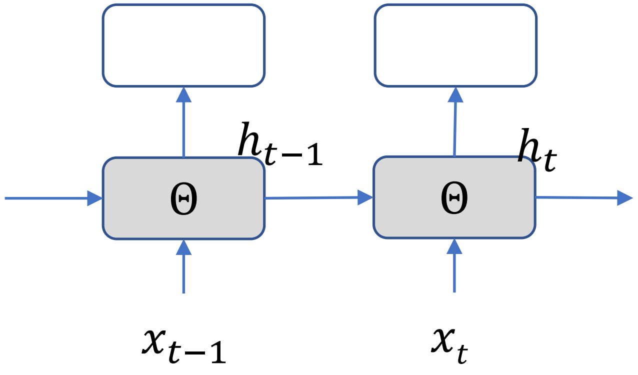
P(the)

L = sum( )

Max $\log P(x_1, x_2, \ldots, x_n) = \sum_t \log P(x_t | x_{t-1}, x_{t-2}, \ldots, x_1)$

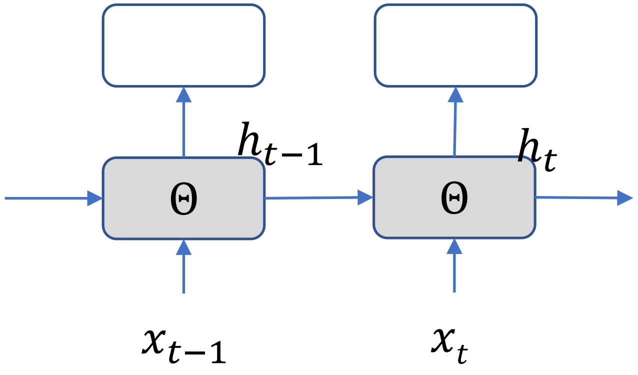


Input Layer



- How to represent word x_t (feature vector)?
    - One-hot representation
        - Denote the vocabulary of all words as V={MRT:0, Singapore:1, Stable:2, …}.
        - MRT is (1,0,0,…0), Singapore is (0,1,0,0,…0), Stable is (0,0,1,0,…0); length = |V|
        - Problem of one-hot representation?

Input Layer

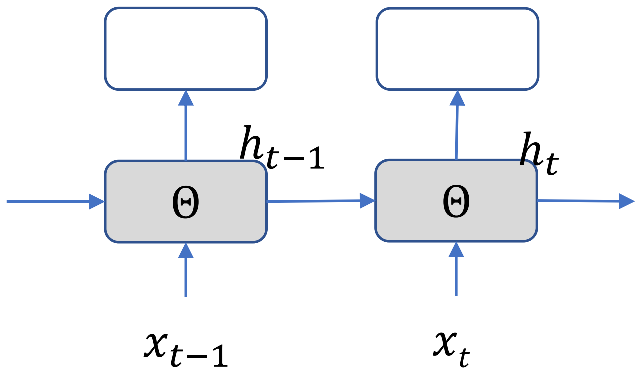


- How to represent word x_t （ feature vector)?
  - One-hot representation
  - Word vector [2,3] (demo1, demo2)
    - A dense vector for each word (user defined length, e.g 32, 64, 128)
    - Learned from a text corpus, e.g. Wikipedia
      - Initialize the dense vectors randomly, e.g. from Gaussian distribution
      - Update the vectors by max P(a|s) where a is a word in a sentence s
  - Denote $x_t \in R^d$

	x_t
One-hot	(0, 1, 0, 0, …,0)
WordVector	(0.1, -1.2, 0.5, 0.3, …,-0.1)

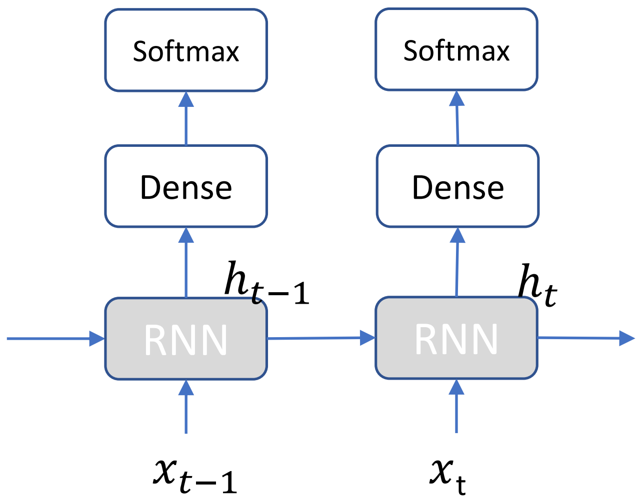
Hidden Layer

- Denote the hidden layer at position t as $h_t \in R^k$
  - k is defined by users
  - $h_t = f(h_{t-1}, x_t | \theta)$
    - $a_t = Ux_t + Wh_{t-1} + b,$
      - $\theta = \{U \in R^{k\times d}, W \in R^{k\times k}, b \in R^k\}$
    - $h_t = \tanh(a_t), h_t \in R^k$



Output

- $o_t = Vh_t + c,$
  - $V \in R^{|V| \times k}, c \in R^{|V|}, ot \in R^{|V|}$
- $y_t = softmax(o_t)$
  - If |V| is very large, the prediction layer needs special optimization [6]
  - $y_t \in R^{|V|}$, a probability vector

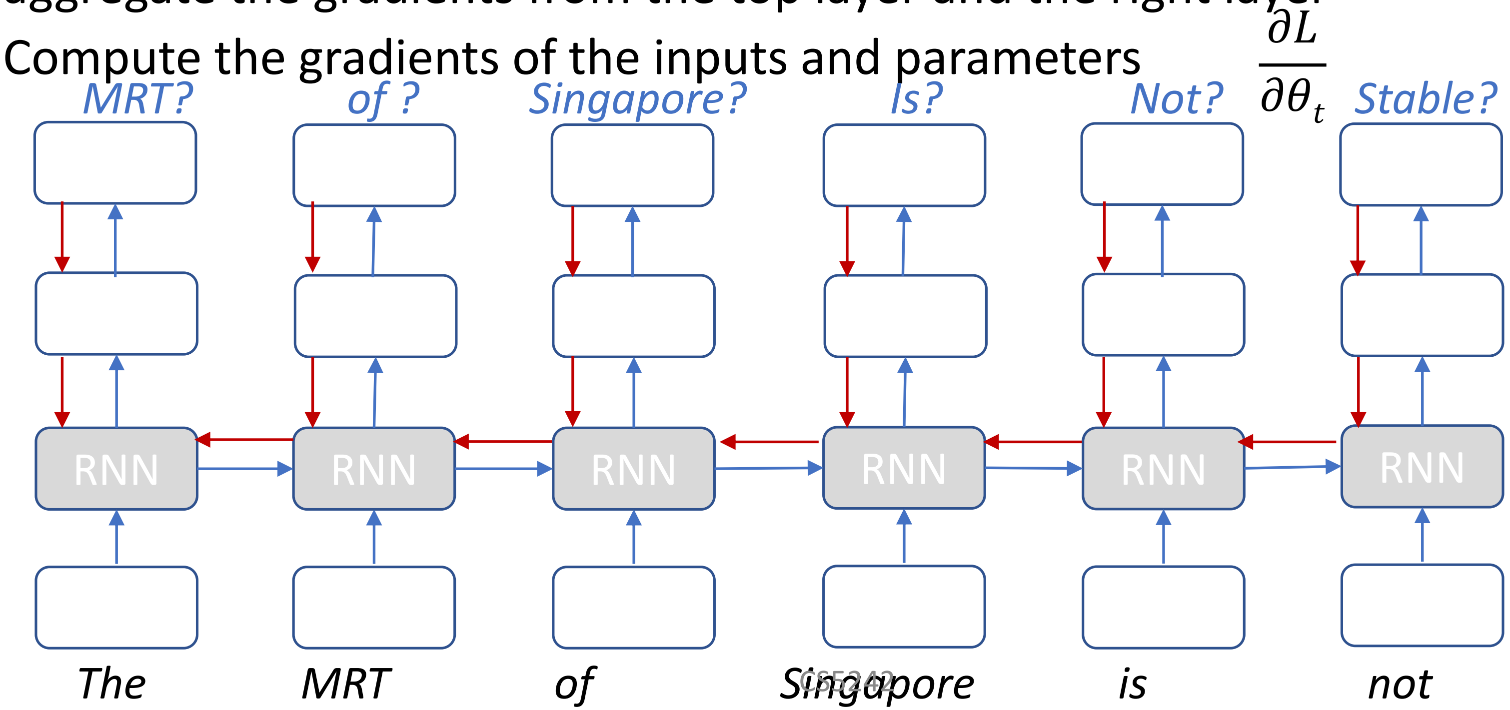


Training

- Given a corpus of text data (e.g. sentences), train the parameters of the RNN.
- Objective:
  - Maximize $logP(x_1, x_2, \ldots, x_n) = \sum_t logP(\, x_t | x_{t-1}, x_{t-2}, \ldots, x_1)$
    → minimize the cross-entropy loss at each position t, denoted as L_t
  - $L = \sum_t L_t$
- SGD
  - For each data sample (e.g. a sentence)
    - Compute the **gradients** of each parameter
    - Update the parameters by $\theta = \theta - \alpha \times \frac{\partial L}{\partial \theta}$

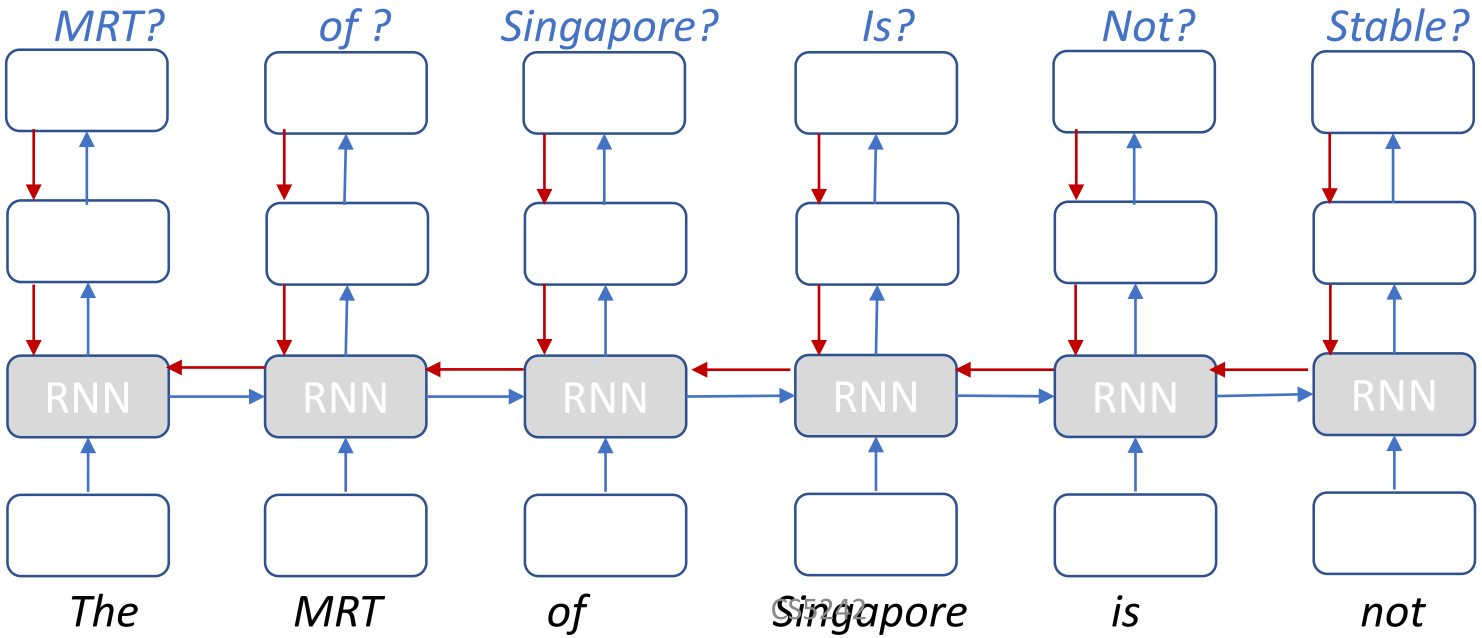
Back-propagation through time (BPTT)

- Back-propagation for each position as normal
  - From the cross-entropy to the RNN layer
  - For each RNN layer/timestep
    - aggregate the gradients from the top layer and the right layer
    - Compute the gradients of the inputs and parameters



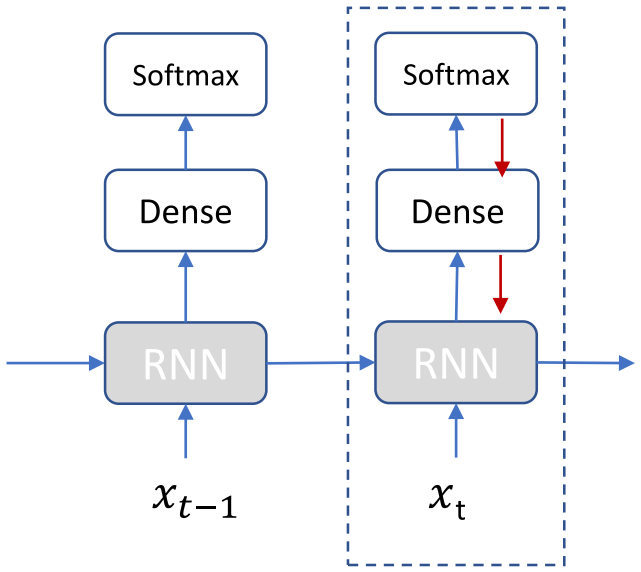
Back-propagation through time (BPTT)

- Back-propagation for each position as normal
  - From the cross-entropy to the RNN layer
  - For each RNN layer
  - For each parameter, aggregate the gradient across all positions $\frac{\partial L}{\partial \theta} = \sum_t \frac{\partial L}{\partial \theta_t}$



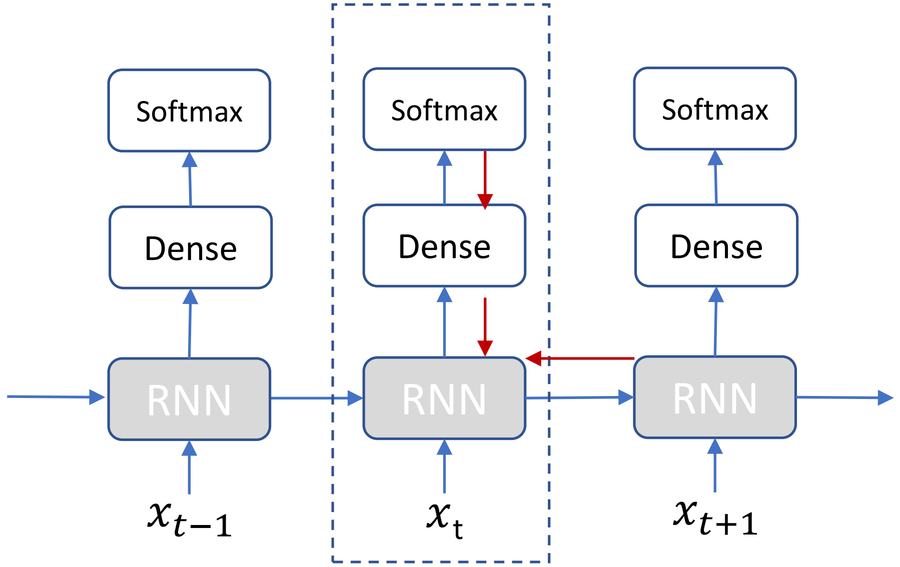
Back-propagation through time (BPTT)

- Forward
  - $a_t = Ux_t + Wh_{t-1} + b,$
  - $h_t = \tanh(a_t)$
  - $o_t = Vh_t + c, y_t = softmax(o_t)$
- Softmax+cross-entropy
  - $\frac{\partial L_t}{\partial o_t} = y_t - l_t, l_t \in \{0,1\}^{|V|}$, the ground truth vector
- Dense
  - $\frac{\partial L_t}{\partial h_t} = V^T \frac{\partial L_t}{\partial o_t}$
  - $\frac{\partial L_t}{\partial V_t} = \left(\frac{\partial L_t}{o_t}\right)(h_t)^T, \frac{\partial L_t}{\partial c_t} = \frac{\partial L_t}{\partial o_t},$ gradients of V and c from t-th position



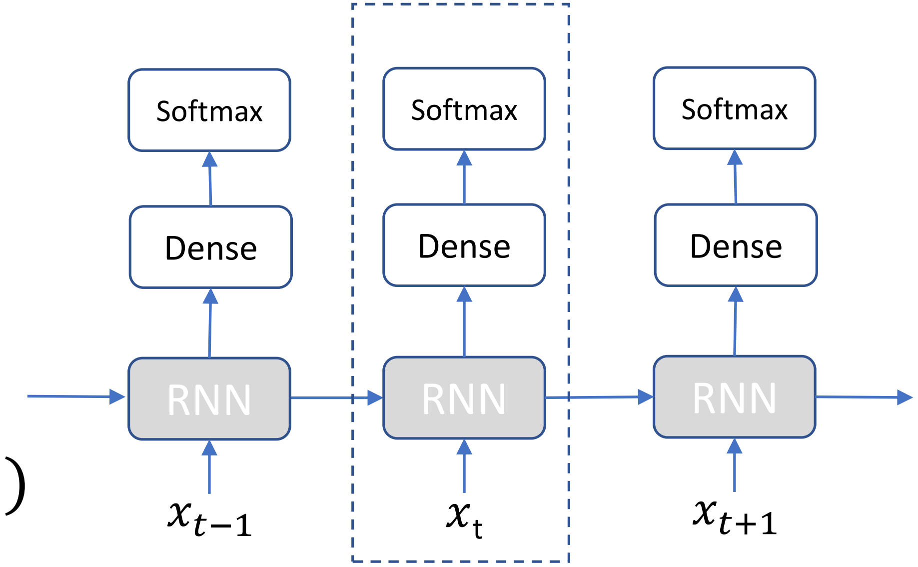
Back-propagation through time (BPTT)

- Forward
  - $a_t = Ux_t + Wh_{t-1} + b,$
  - $h_t = \tanh(a_t)$
  - $o_t = Vh_t + c$
- RNN layer
  - $\frac{\partial L}{\partial h_t} = \frac{\partial L_t}{\partial h_t} + \boxed{\frac{\partial L_{t+1}}{\partial h_t} + \cdots + \frac{\partial L_n}{\partial h_t}} = \frac{\partial L_t}{\partial h_t} + \frac{\partial L_{t+}}{\partial h_t}$
  - $\frac{\partial L}{\partial a_t} = \frac{\partial L}{\partial h_t} \times (1 - h_t^2)$
  - $\frac{\partial L}{\partial U_t} = \frac{\partial L}{\partial a_t} x_t^T, \frac{\partial L}{\partial W_t} = \frac{\partial L}{\partial a_t} h_{t-1}^T, \frac{\partial L}{\partial b_t} = \frac{\partial L}{\partial a_t},$ gradients of U, W, b from position t
  - $\frac{\partial L_{(t-1)+}}{\partial h_{t-1}} = W^T \frac{\partial L}{\partial a_t}$
- $\frac{\partial L}{\partial \theta} = \sum_t \frac{\partial L}{\partial \theta_t}$



Back-propagation through time (BPTT)

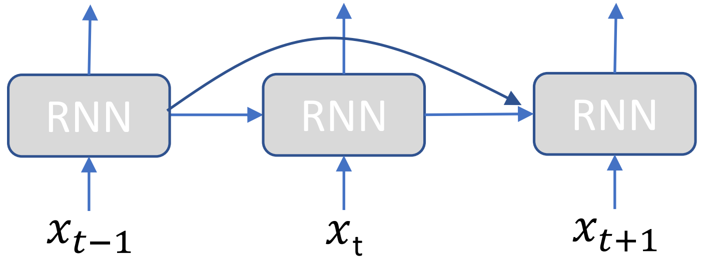
- Gradient vanishing/exploding
  - $\frac{\partial L}{\partial h_t} = \frac{\partial L_t}{\partial h_t} + \frac{\partial L_{t+1}}{\partial h_t} + \cdots + \frac{\partial L_n}{\partial h_t} = \frac{\partial L_t}{\partial h_t} + \frac{\partial L_{t+}}{\partial h_t}$
  - $\frac{\partial L}{\partial a_t} = \frac{\partial L}{\partial h_t} \times (1 - h_t^2)$
  - $\rightarrow \frac{\partial L_{(t-1)+}}{\partial h_{t-1}} = W^T \frac{\partial L}{\partial a_t} = W^T \frac{\partial L}{\partial h_t} \times (1 - h_t^2)$
  - $= W^T (\frac{\partial L_t}{\partial h_t} + \frac{\partial L_{t+}}{\partial h_t}) \times (1 - h_t^2)$
  - $\rightarrow \frac{\partial L_{(t-1)+}}{\partial h_{t-1}} \leftarrow W^T \frac{\partial L_{t+}}{\partial h_t} \ldots \leftarrow (W^T)^k \frac{\partial L_{(t+k)+}}{\partial h_t}$



Gradients from right most positions vanish when back-propagated to the left-most positions

Back-propagation through time (BPTT)

- $\frac{\partial L_{(t-1)+}}{\partial h_{t-1}} \leftarrow W^T \frac{\partial L_{t+}}{\partial h_t} \dots \leftarrow (W^T)^k \frac{\partial L_{(t+k)+}}{\partial h_t}$
  - If |W| is small, gradient vanishing
    - The losses after position t+k have little influence for the RNN layer at t-1 if k is large
    - Cannot capture long-term relationship
      - "The **red line** went down last night, which is why there are many tweets about __ "(red line).
  - If |W| is large, gradient exploding
- Solutions
  - Gradient vanishing?
    - Careful initialization
      - Identity matrix with ReLU as the activation function[7]
    - Skip-connections
    - leaky units-> LSTM and GRU
      - $h_t = \gamma h_{t-1} + (1-\gamma)\tanh(Uxt + Wh_{t-1} + b)$
  - Gradient exploding?
    - Gradient clipping



Gradient Clipping

- $W = W - \alpha \times \frac{\partial L}{\partial W}$
- Hard clipping
  - For each value of $\frac{\partial L}{\partial W}$, if it is larger than a threshold μ, set it to be μ
- Normalization (L2)
  - g= $\frac{\partial L}{\partial W}$
  - If |g|> μ, $\mathrm{g} = \frac{\mu}{|g|} g$

Mini-batch SGD

- SGD uses a single sample per iteration
- Mini-batch SGD uses multiple samples per iteration
  - To accelerate the processing by matrix (batch) operations
  - Different sentences have different lengths, e.g.

Singapore MRT is not stable
Chicken rice is very popular in Singapore
It is hot

Word to index →

0 2 1 5 6
7 8 1 4 8 9 0
10 1 11

Mini-batch SGD

- Solution?
  - Truncate the sentences into the same fixed length

3 2 1 5 6
7 8 1 4 8 9 3
10 1 11

Max len = 3 →

3 2 1 ~~5 6~~
7 8 1 ~~4 8 9 3~~
10 1 11

Mini-batch SGD

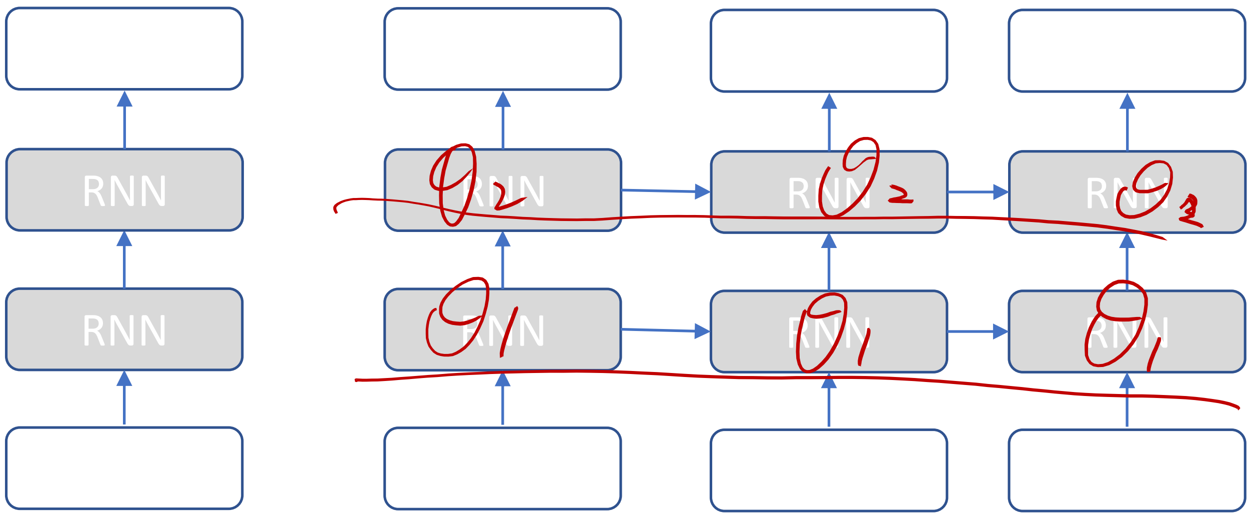
- Solution
  - Truncate the sentences into the same fixed length
  - Padding
    - E.g. [PyTorch]

      pack = torch.nn.utils.rnn.pack_padded_sequence(batch_in, seq_lengths, batch_first=True)
    - Index 0 is for a special 'PAD' symbol. Index of words in the vocabulary starts from 1.

3 2 1 5 6	Sort based on length in descending order c		**Padded**								**Length**			
7 8 1 4 8 9 3	b		7	8	1	4	8	9	3		7			x[1] . . . x[6]
10 1 11	a		3	2	1	5	6	*0*	*0*		*5*			y[1] . . . y[6].
			10	1	11	*0*	*0*	*0*	*0*		*3*			z[0] - . . . z[6]
			0	1	2	3	4	5	6					

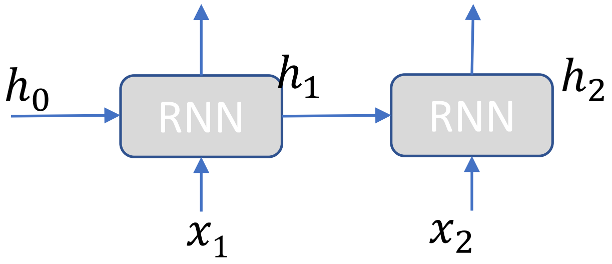
Other tricks for training

- Adaptive learning rate
  - E.g. Adam, RMSProp
- Normalizing the losses
  - $L = \sum_t L_t$ -> $L = \frac{1}{n \sum_t L_t}$
- Use gated RNN units
  - LSTM or GRU (not introduced yet)
- Stack multiple RNN layers
  - As shown by the right figure
- Layer normalization [8, 10]
  - Applied before activation function
- Recurrent Dropout [9, 10]



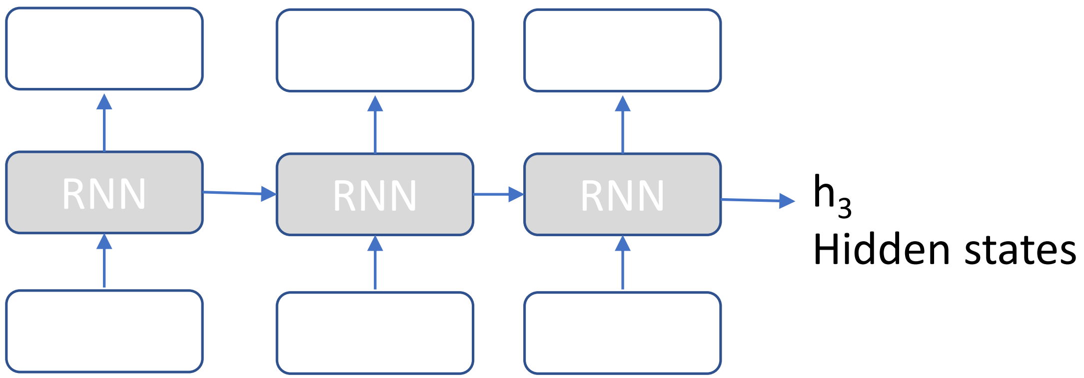
Other tricks for training

- Learn the initial state h_0 [11]
  - Typically, we set h0 to be a all 0 vector
  - It can also be learned like a bias vector
    - computing the gradient $\frac{\partial L}{\partial h_0}$ and then apply SGD update
- Trunked BPTT
  - Some sentences are very long, e.g. > 1000 positions.
  - Split the sentence into shorter sub-sentences, e.g. 200
    - Each sub-sentence is a new training sample
    - Use the last hidden vector (h_n) of the previous sub-sentence as the initial state h_0 for the next sub-sentence



Truncated BPTT

- Truncated BPTT for very long sequence
  - Gradient vanishing
  - Efficiency (less memory for intermediate results)
    - The memory for storing the hidden states will be erased after training each sub-sentence



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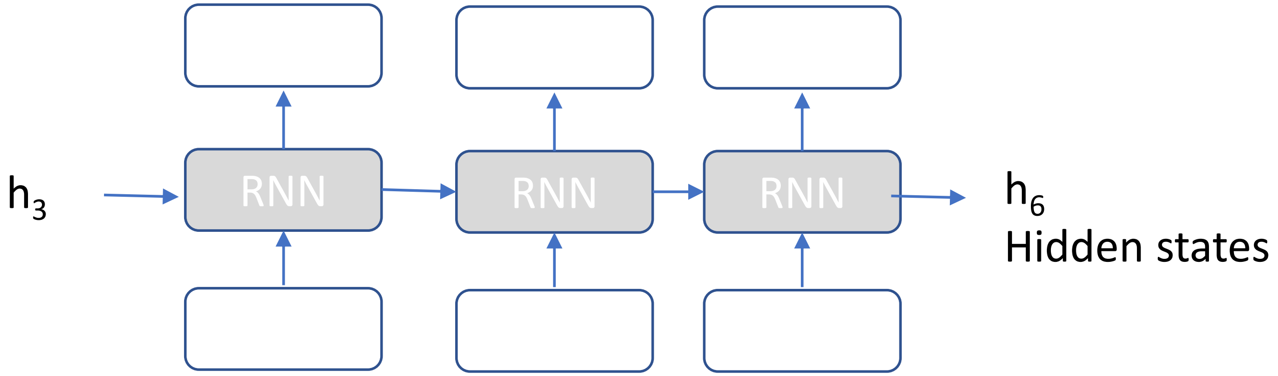

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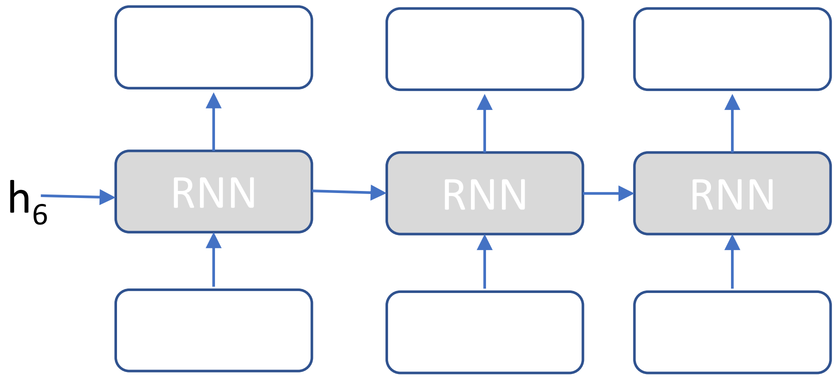
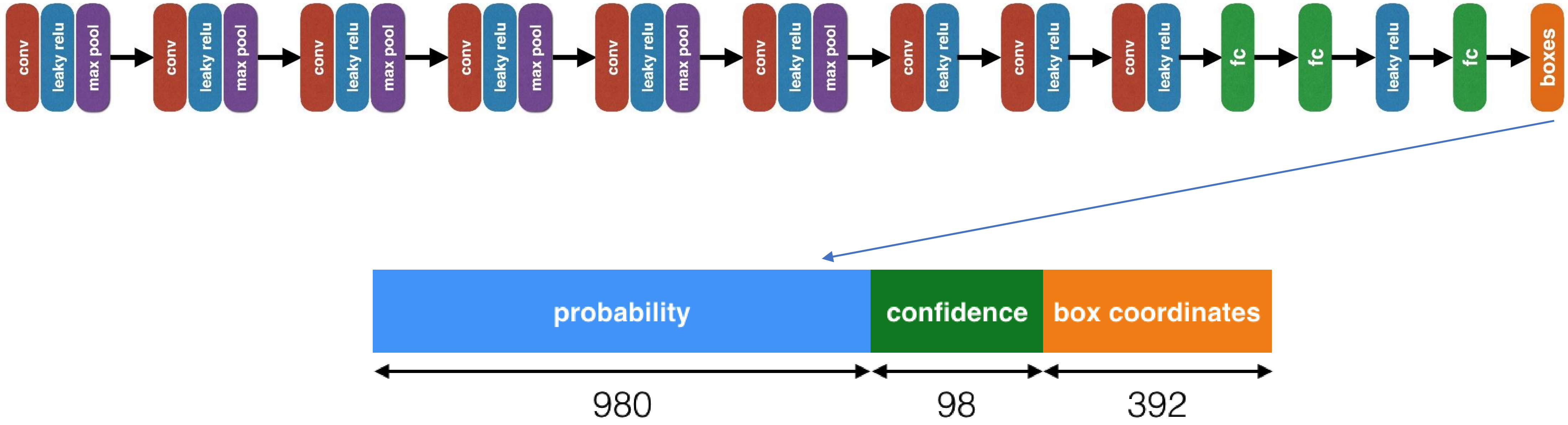


Reference

- [1] https://www.quora.com/What-are-differences-between-recurrent-neural-network-language-model-hidden-markov-model-and-n-gram-language-model
- [2] https://code.google.com/archive/p/word2vec/
- [3] https://nlp.stanford.edu/projects/glove/
- [4] Klaus Greff, Rupesh Kumar Srivastava, Jan Koutník, Bas R. Steunebrink, Jürgen Schmidhuber. LSTM: A Search Space Odyssey. https://arxiv.org/abs/1503.04069
- [5] http://web.stanford.edu/class/cs224n/lectures/cs224n-2017-lecture8.pdf
- [6] http://www.deeplearningbook.org/contents/applications.html (12.4.3)
- [7] Quoc V. Le, Navdeep Jaitly, Geoffrey E. Hinton. A Simple Way to Initialize Recurrent Networks of Rectified Linear Units. 2015. arxiv.org/abs/1504.00941v2
- [8] “Layer Normalization" Jimmy Lei Ba, Jamie Ryan Kiros, Geoffrey E. Hinton. https://arxiv.org/abs/1607.06450.
- [9] “Recurrent Dropout without Memory Loss" Stanislau Semeniuta, Aliaksei Severyn, Erhardt Barth. https://arxiv.org/abs/1603.05118
- [10] https://www.tensorflow.org/api_docs/python/tf/contrib/rnn/LayerNormBasicLSTMCell
- [11] https://r2rt.com/non-zero-initial-states-for-recurrent-neural-networks.html
- [12] LSTM: A Search Space Odyssey. Klaus Greff, Rupesh Kumar Srivastava, Jan Koutník, Bas R. Steunebrink, Jürgen Schmidhuber. https://arxiv.org/abs/1503.04069
- [13] https://github.com/karpathy/char-rnn/issues/138#issuecomment-162763435
- https://research.googleblog.com/2016/05/announcing-syntaxnet-worlds-most.html
- https://danijar.com/tips-for-training-recurrent-neural-networks/

YOLO



7x7x20

20 labels for each cell;
7x7=49 cells

7x7x2x1

7x7x2x4

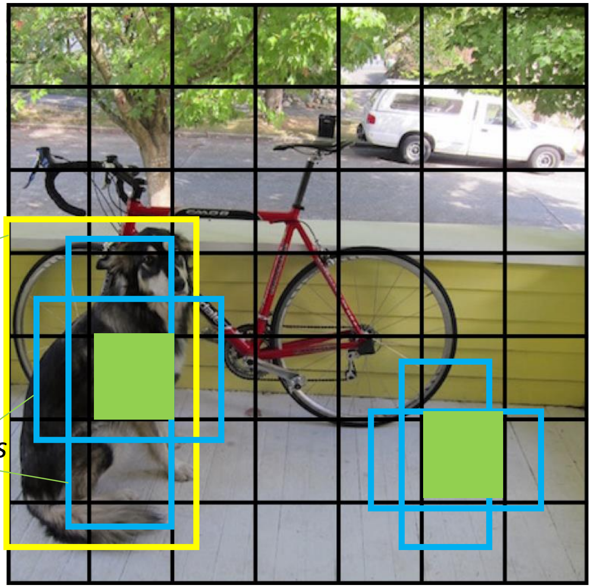
2 boxes for each cell;
one confidence score and 4 coordinates for each box

Images from: https://github.com/xslittlegrass/CarND-Vehicle-Detection

Training loss

Each cell has 30 values:

- 2 bounding boxes
  - 4 coordinates x,y,w,h
  - 1 confidence score C
- 20 label probabilities $p(c)$



L_{coord}

$$\lambda_{\mathbf{coord}} \sum_{i=0}^{S^2} \sum_{j=0}^{B} \mathbb{1}_{ij}^{\text{obj}} \left[(x_i - \hat{x}_i)^2 + (y_i - \hat{y}_i)^2 \right]$$

$$+ \lambda_{\mathbf{coord}} \sum_{i=0}^{S^2} \sum_{j=0}^{B} \mathbb{1}_{ij}^{\text{obj}} \left[\left(\sqrt{w_i} - \sqrt{\hat{w}_i} \right)^2 + \left(\sqrt{h_i} - \sqrt{\hat{h}_i} \right)^2 \right]$$

L_{obj}

$$+ \sum_{i=0}^{S^2} \sum_{j=0}^{B} \mathbb{1}_{ij}^{\text{obj}} \left(C_i - \hat{C}_i \right)^2$$

L_{noobj}

$$+ \lambda_{\text{noobj}} \sum_{i=0}^{S^2} \sum_{j=0}^{B} \mathbb{1}_{ij}^{\text{noobj}} \left(C_i - \hat{C}_i \right)^2$$

L_{class}

$$+ \sum_{i=0}^{S^2} \mathbb{1}_{i}^{\text{obj}} \sum_{c \in \text{classes}} (p_i(c) - \hat{p}_i(c))^2$$

The predicted bounding boxes have enough overlap with the ground truth box→
This cell has contribution in L_{class}

The vertical predicted box has larger overlap with the ground truth box→
Vertical box contribute in L_{coord}, L_{obj}

The other predicted box has smaller overlap with the truth box → it only contributes to L_{obj}

None of the two bounding boxes overlap enough with any ground truth bounding boxes→
This cell only contributes in L_{noobj}

Image from:https://docs.google.com/presentation/d/1kAa7NOamBt4calBU9iHgT8a86RRHz9Yz2oh4-GTdX6M/edit#slide=id.g15092aa245_0_411