Vanishing Gradient, Gated RNN, Seq2Seq and Transformer

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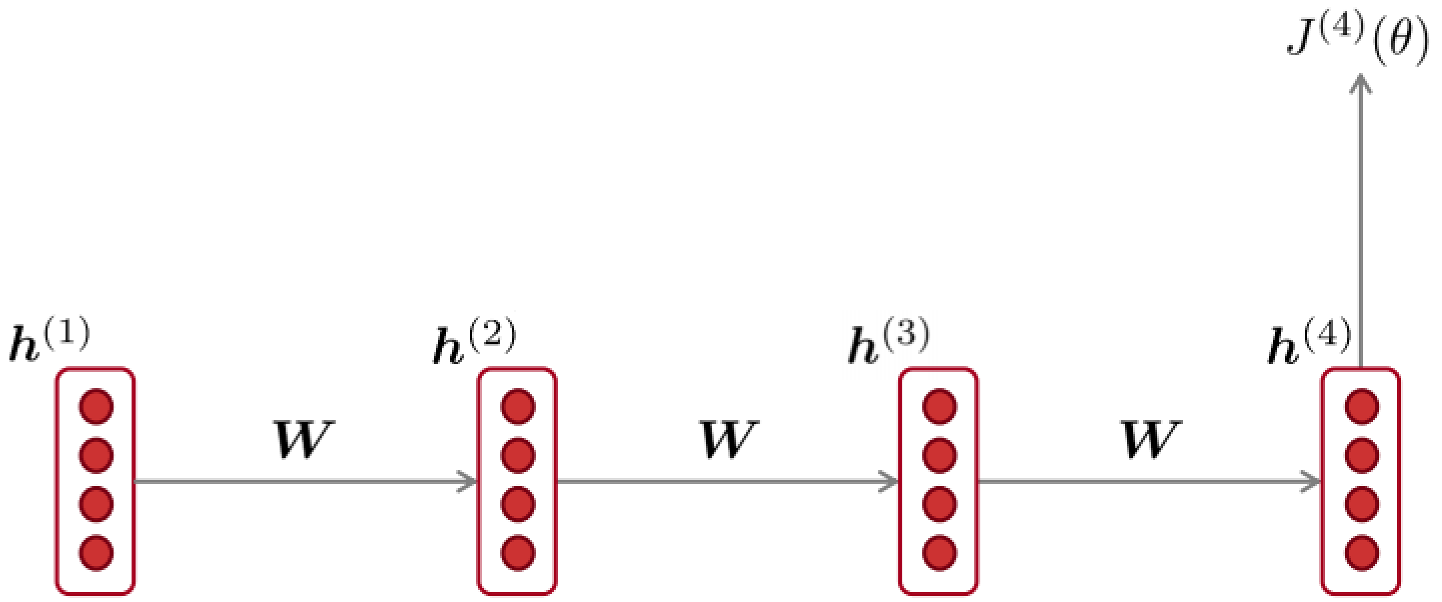
https://github.com/chiayisu/Natural-Language-Processing

Agenda

- Vanishing Gradient
- Problems of Vanishing / Exploding Gradients
- Long Short-Term Memory (LSTM)
- Gated Recurrent Unit (GRU)
- LSTM & GRU Comparison
- Neural Machine Translation (NMT)
- Attention
- Transformer

Vanishing Gradient

Vanishing Gradient Intuition



- $$\frac{\partial J^{(4)}}{\partial h^{(1)}} = \boxed{\frac{\partial h^{(2)}}{\partial h^{(1)}}} * \boxed{\frac{\partial h^{(3)}}{\partial h^{(2)}}} * \boxed{\frac{\partial h^{(4)}}{\partial h^{(3)}}} * \boxed{\frac{\partial J^{(4)}}{\partial h^{(4)}}}$$

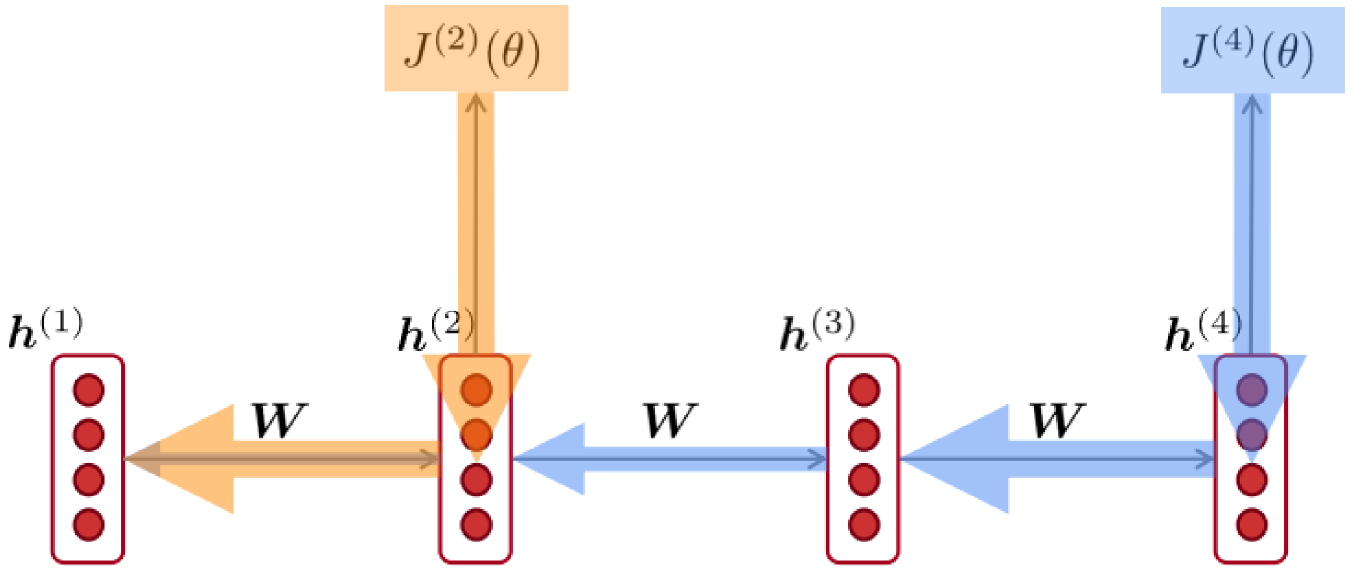
What if these values are small?

Idea: Vanishing Gradient

- 假設我們有以下三個值： 0.1, 0.01, 0.01 ，並且將它相乘
- 0.1 * 0.01 * 0.01 = 0.00001
- 因此：當我們將非常小的梯度相乘後，梯度將會越來越小

Problems of Vanishing / Exploding Gradients

梯度消失的問題



- 越接近輸出的梯度訊號將會越大
- 離輸出越遠的梯度訊號將會越小
- 模型只會考慮與輸出相近的資訊

梯度消失的問題

- 當梯度消失發生在時間t與t+n之間，我們很難知道以下資訊：
  - 時間t與t+n的依賴是否真的不存在
  - 時間t與t+n的依賴是否存在於其他不相關的參數

Vanishing Gradients : Effects on RNNLM

- **LM task:** 當她要列印票券的時候，她發現列表機沒有墨水夾。她去文具店買了非常貴的墨水夾。在她把墨水夾裝進去之後，她終於印出她的____。
- 為了要正確的預測輸出為"票券"，模型需要學習到第一個"票券"與最後一個"票券"之間的關係
- 然而：當有梯度消失問題時，將會很難學習到這些資訊
- 因此： 將會很難正確的預測出"票券"

Vanishing Gradients: Effects on RNNLM

- **LM task:** The writer of this books ___
- The writer of this books is … (Correct Answer)
- Syntactic recency : The writer of this books is - Correct
- Sequential recency : The writer of this books are – Incorrect
- According to Linzen et al., RNN is prone to make the sequential recency error because of vanishing gradients problems.

Long Short-Term Memory (LSTM)

LSTM: Introduction

- LSTM : 用來解決梯度消失的其中一種RNN模型
- 在每一個時序t都有一個隱含狀態h^t及一個細胞狀態c^t
  - 每個狀態都是一個n維的向量
  - 細胞狀態用來儲存較遠的資訊
  - LSTM可以清除、寫入以及讀取細胞狀態的資訊
- 每個輯閘控制所要清除、寫入及讀取的資訊
  - 每個輯閘都是一個n維的向量
  - 輯閘的輸出介於0到1之間
  - 輯閘會根據目前的資訊來計算

LSTM: Equations

- We have a sequence of inputs $x^{(t)}$, and a sequence of hidden states $h^{(t)}$ and cell states $c^{(t)}$ are computed.

$f^{(t)} = \sigma\left(W_f h^{(t-1)} + U_f x^{(t)} + b_f\right)$	Forget Gate
$i^{(t)} = \sigma\left(W_i h^{(t-1)} + U_i x^{(t)} + b_i\right)$	Input Gate
$o^{(t)} = \sigma\left(W_o h^{(t-1)} + U_o x^{(t)} + b_o\right)$	Output Gate
$\tilde{c}^{(t)} = tanh\left(W_c h^{(t-1)} + U_c x^{(t)} + b_c\right)$	New Cell Content
$c^{(t)} = f^{(t)} \circ c^{(t-1)} + i^{(t)} \circ \tilde{c}^{(t)}$	Cell State
$h^{(t)} = o^{(t)} \circ \tanh c^{(t)}$	Hidden State

How does LSTM solve vanishing gradients?

- 藉由採用LSTM比較容易將之前時序的資料保留
- LSTM可能還是有梯度消失的問題。然而，LSTM提供一個方法保留離輸出較遠之資訊。

LSTM: Real-World Success

- The SOTA that LSTM achieves (2013-2015)
  - Hang-writing recognition
  - Speech Recognition
  - Machine Translation
  - Parsing
  - Image Captioning
- However, other approaches (Transformer) become more dominant in 2019.
- E.g. WMT conference
- In WMT 2016, RNN related papers contain 44 times.
- In WMT 2018, RNN only appears 9 times. However, Transformer has 63 times.

Gated Recurrent Unit (GRU)

GRU: Equation

- 由 Chao et al. 提出為LSTM 的簡化版
- GRU 沒有細胞狀態。 GRU 只包含輸入狀態 $x^{(t)}$ 及隱含狀態$h^{(t)}$
- $u^{(t)} = \sigma\left(W_u h^{(t-1)} + U_u x^{(t)} + b_u\right)$ — Update Gate
- $r^{(t)} = \sigma\left(W_r h^{(t-1)} + U_r x^{(t)} + b_r\right)$ — Reset Gate
- $\tilde{h}^{(t)} = tanh\left(W_c(r^{(t)} \circ h^{(t-1)}) + U_h x^{(t)} + b_h\right)$ — New Hidden State Content
- $h^{(t)} = \left(1 - u^{(t)}\right) \circ h^{(t-1)} + u^{(t)} \circ h^{(t)}$ — Hidden State

LSTM & GRU Comparison

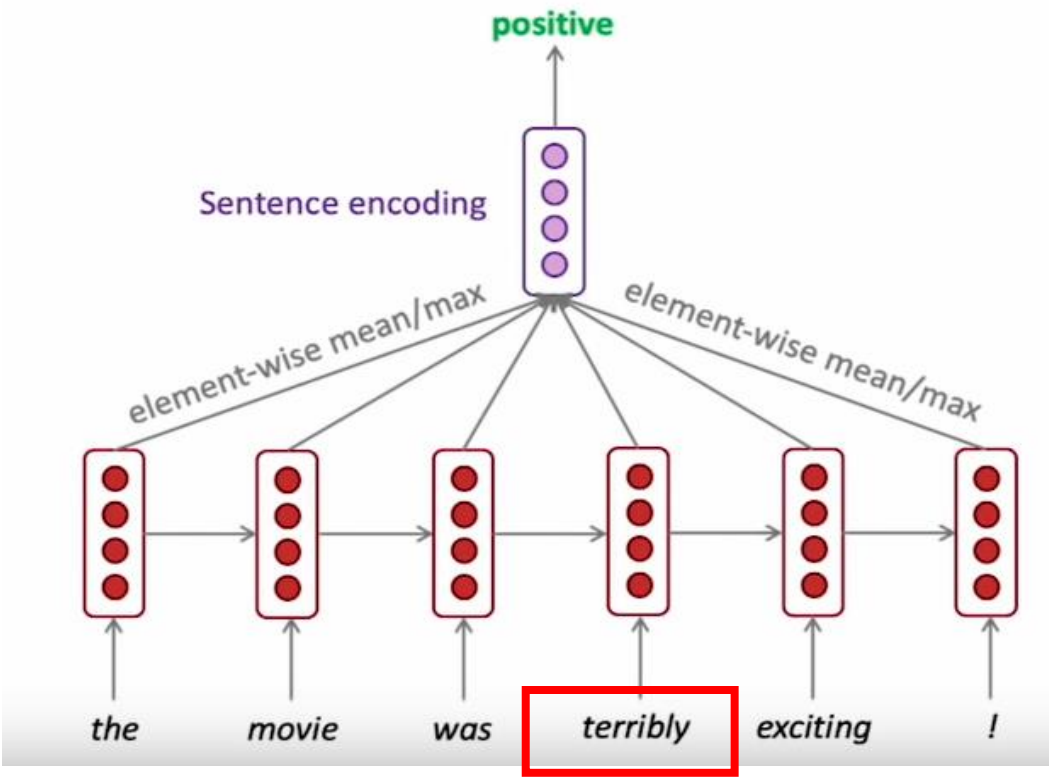
LSTM VS. GRU

- 雖然LSTM及GRU為主要被採用的架構，仍然還有許多與輯閘相關的RNN被提出
- LSTM及GRU最大的差別為其參數及運算速度
- 目前沒有任何研究顯示哪一個架構較優
- 實際經驗：一開始可以先採用LSTM，當遇到運算問題再考慮採用GRU

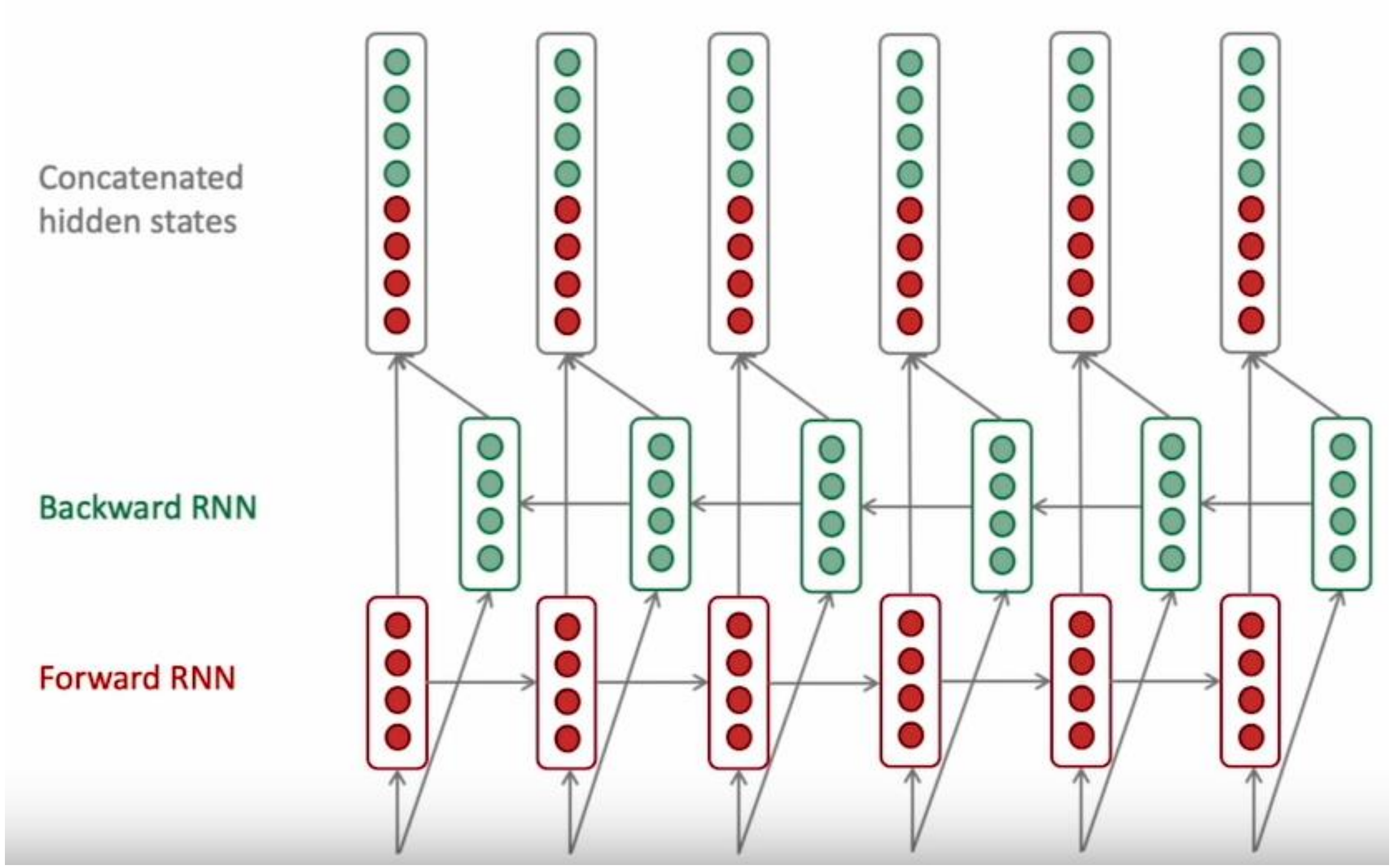
Bidirectional RNN

Bidirectional RNNs: Motivation

- Terribly can have two kinds of meaning.



Bidirectional RNN



Bidirectional RNN

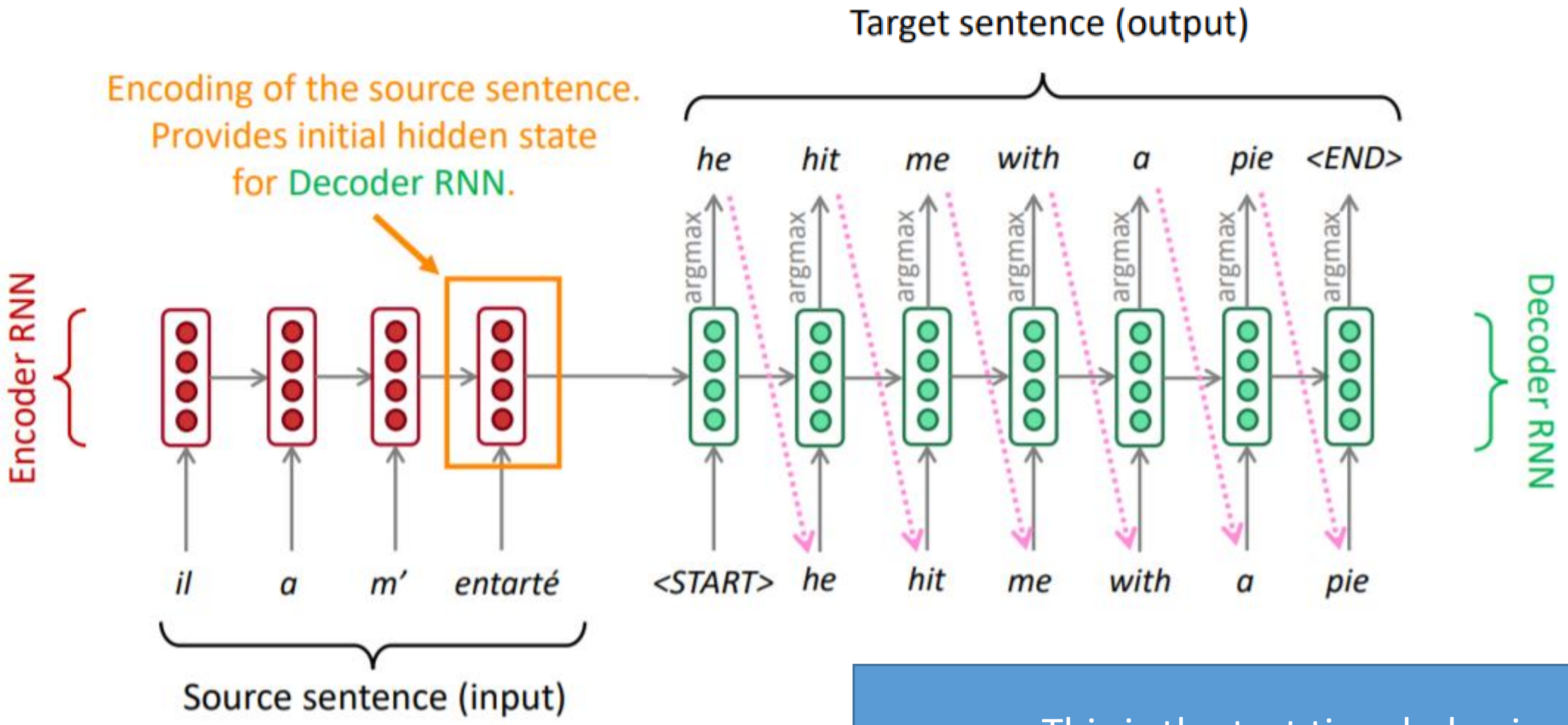
- On time t
- Forward RNN : $\overrightarrow{h}^{(t)} = RNN_{FW}\left(\overrightarrow{h}^{(t-1)}, x^{(t)}\right)$
- Backward RNN : $\overleftarrow{h}^{(t)} = RNN_{BW}\left(\overleftarrow{h}^{(t+1)}, x^{(t)}\right)$
- Concatenated hidden state : $h^{(t)} = \left[\overrightarrow{h}^{(t)}, \overleftarrow{h}^{(t)}\right]$

Bidirectional RNN

- 雙向RNN的假設
  - 需要有完整的句子
  - 並不適合用在語言模型 (沒有完整句子)
- 由於雙向RNN可以學習到雙向的資訊，因此雙向RNN是一個不錯的預設網路。

Neural Machine Translation (NMT)

NMT: Sequence-to-Sequence Model



This is the test time behavior.

Seq2Seq is versatile!!

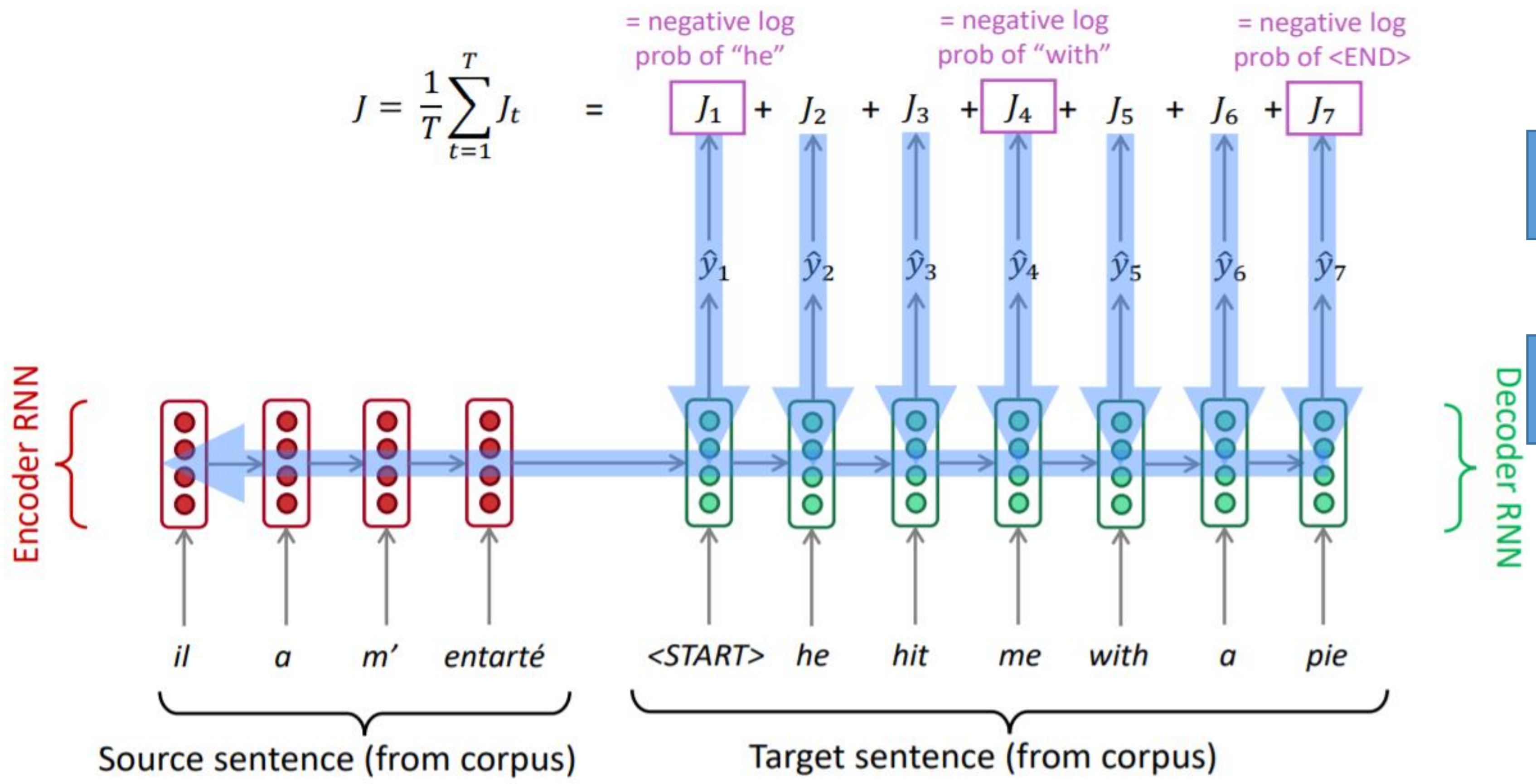
- 其他Seq2Seq模型可以運用的任務
  - 文本總結 (long text -> short text)
  - 對話系統 (previous utterance -> next utterance)
  - 文本描述影像(input image -> description of the image)
  - 文本分析 (input text -> output parse as sequence)

NMT: Sequence-to-Sequence Model

- Seq2Seq 為一個條件式語言模型的例子：
  - 語言模型： 預測下一個所會出現的語詞
  - 條件式語言模型：根據輸入的句子預測下一個語詞
- Seq2Seq 會計算p(y|x):

$$\mathrm{p(y|x)} = \mathrm{p}(y_1|\mathrm{x})\mathrm{p}(y_2|y_1, \mathrm{x}) \ldots \mathrm{p}(y_T|y_1 \ldots y_{T-1}, \mathrm{x})$$

NMT: Training Steps

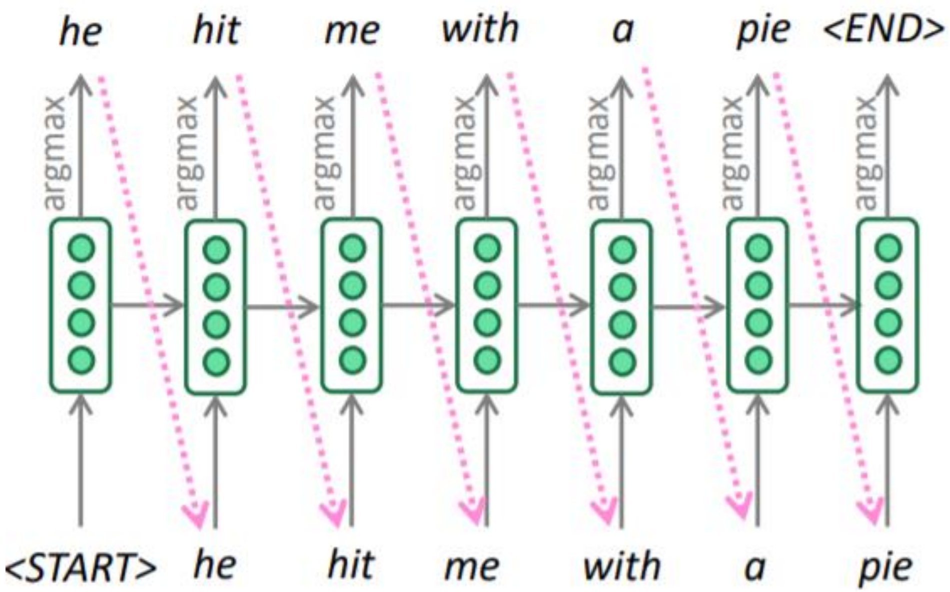


Seq2seq is optimized as a single system.

Backpropagation operates end-to-end

Greedy Decoding

- 目前為止，Decoder主要將有最大機率的語詞輸出



- 這方法稱作Greedy Decoding

NMT: the Biggest Success Story of NLP Deep Learning

- 2014年前： NMT為較少研究的主題
- 2014年：Seq2Seq的論文被發表
- 2016年: Google翻譯從SMT轉乘NMT
- 雖然SMT已經被許多研究員維護多年，但是NMT的表現仍然超越了SMT的表現

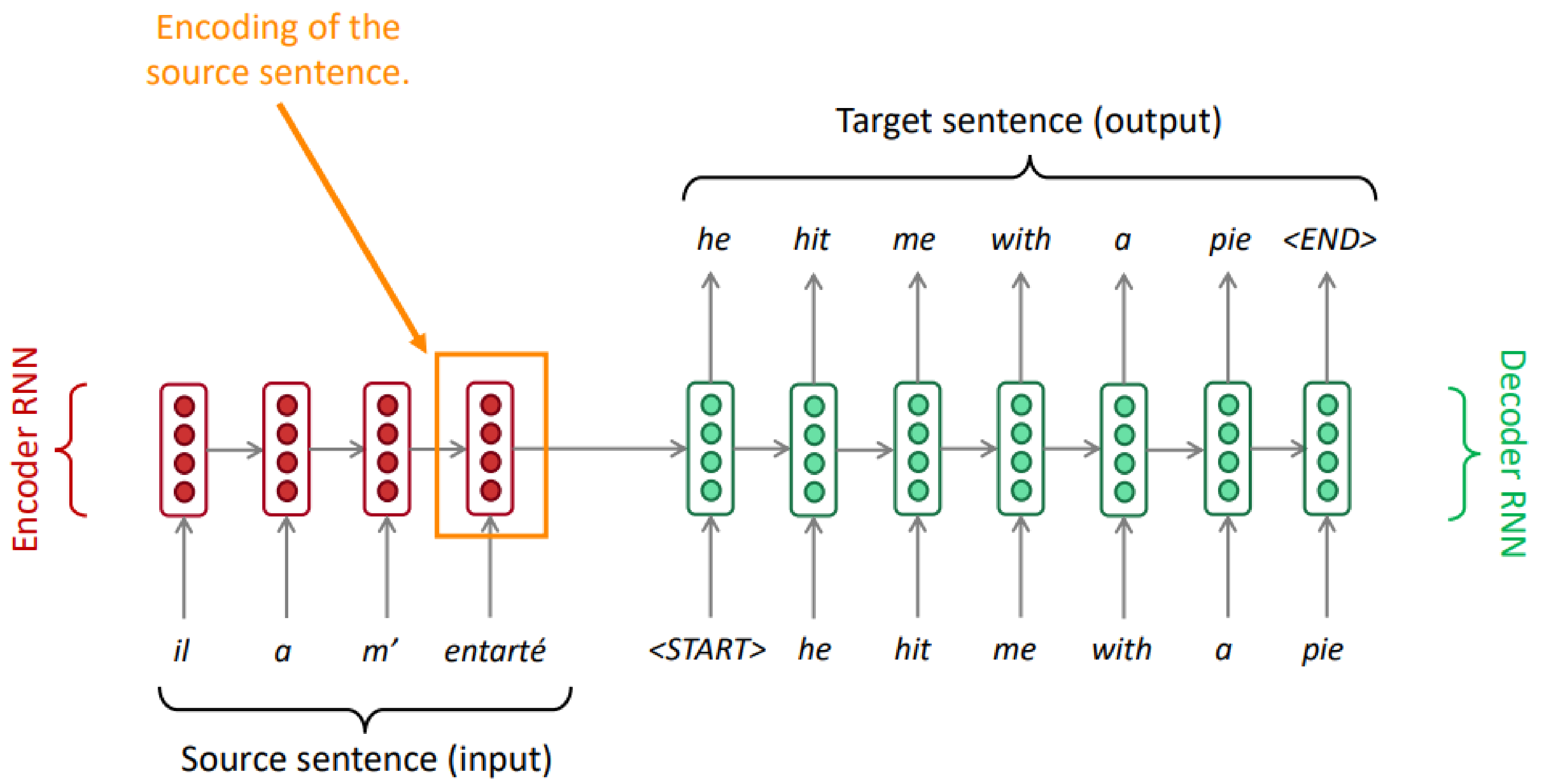
Attention

NMT Research Continues

- NMT在自然語言處理為一標記性的任務。
- NMT也促使了許多自然語言與深度學習的研究。
- 2019年： NMT 的研究仍然繼續進展
  - Seq2Seq也有了許多的演進
  - 然而：最核心的演進為

Attention

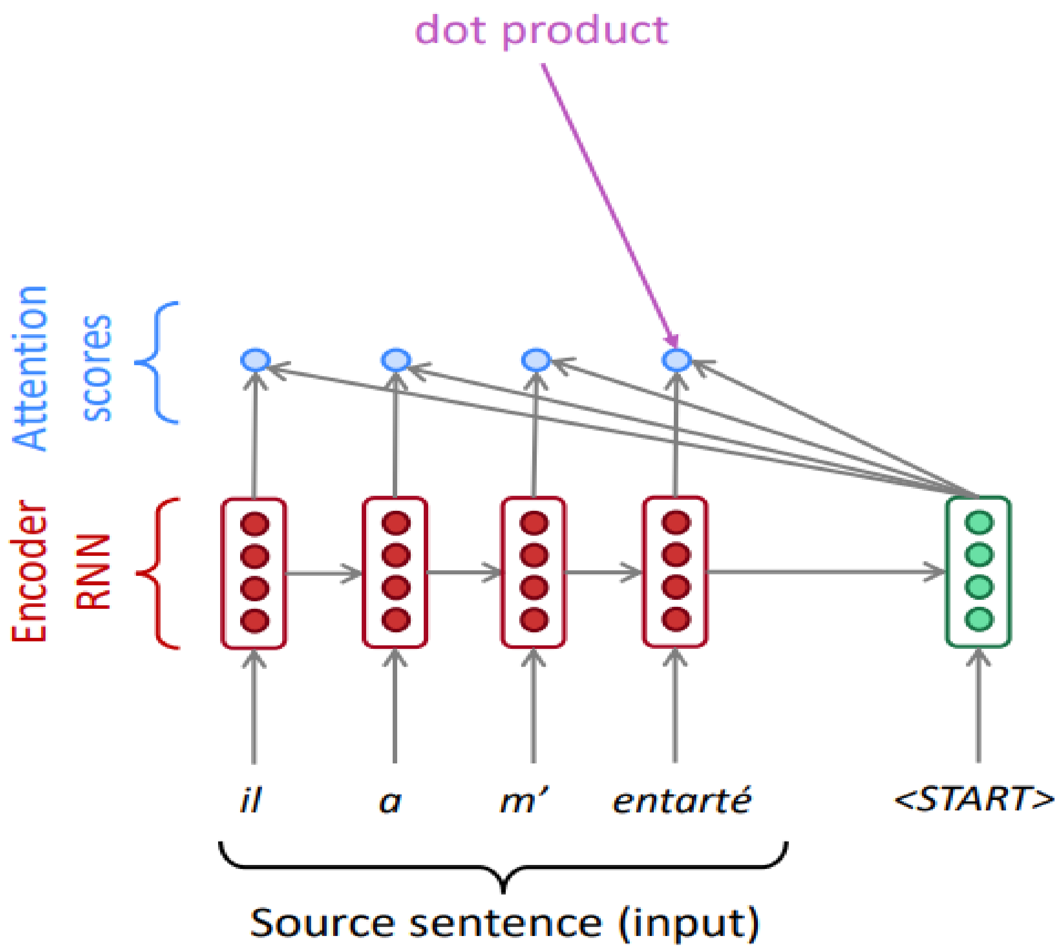
Seq2Seq: the Bottleneck Problem



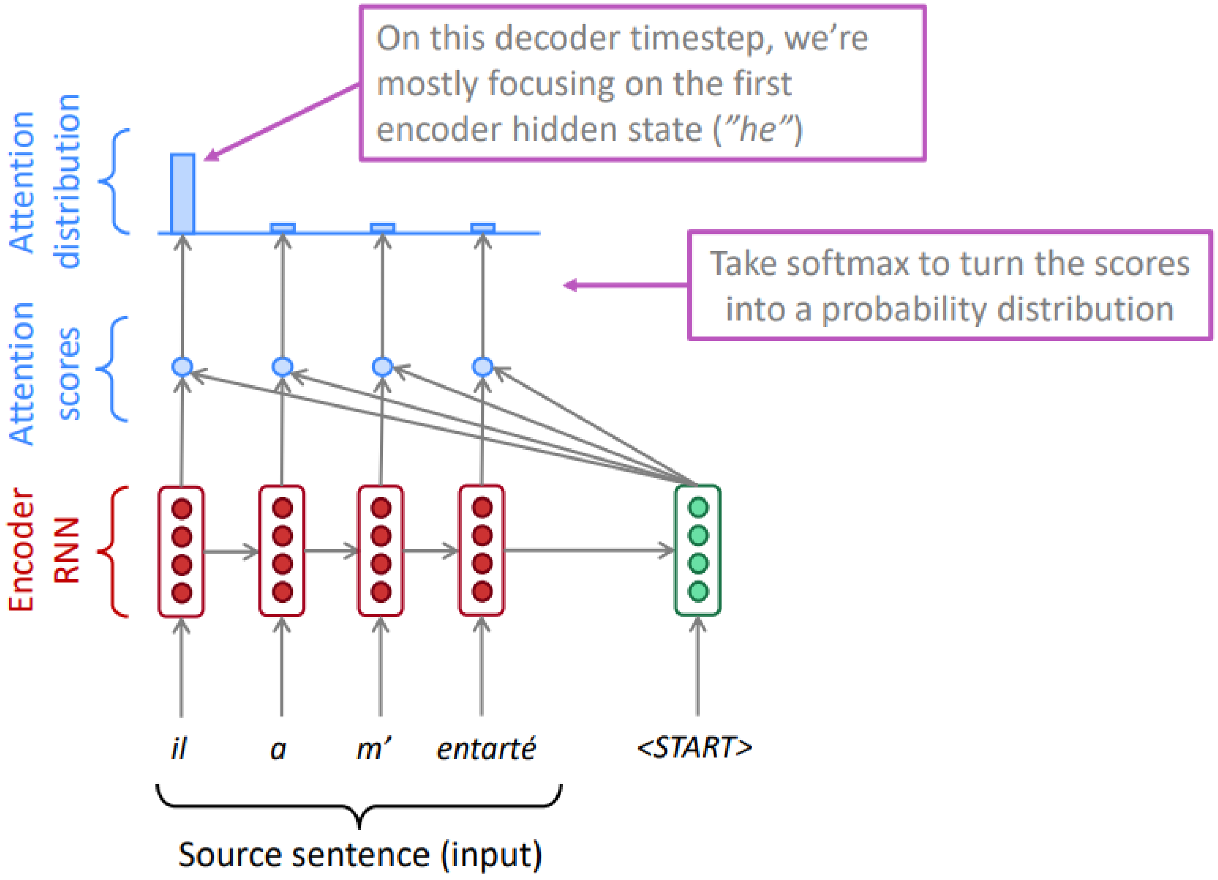
Attention

- Attention 解決了原本Seq2Seq訓練時所會遇到的問題
- 想法：將解碼的隱含狀態注意到每一個編碼的隱含狀態

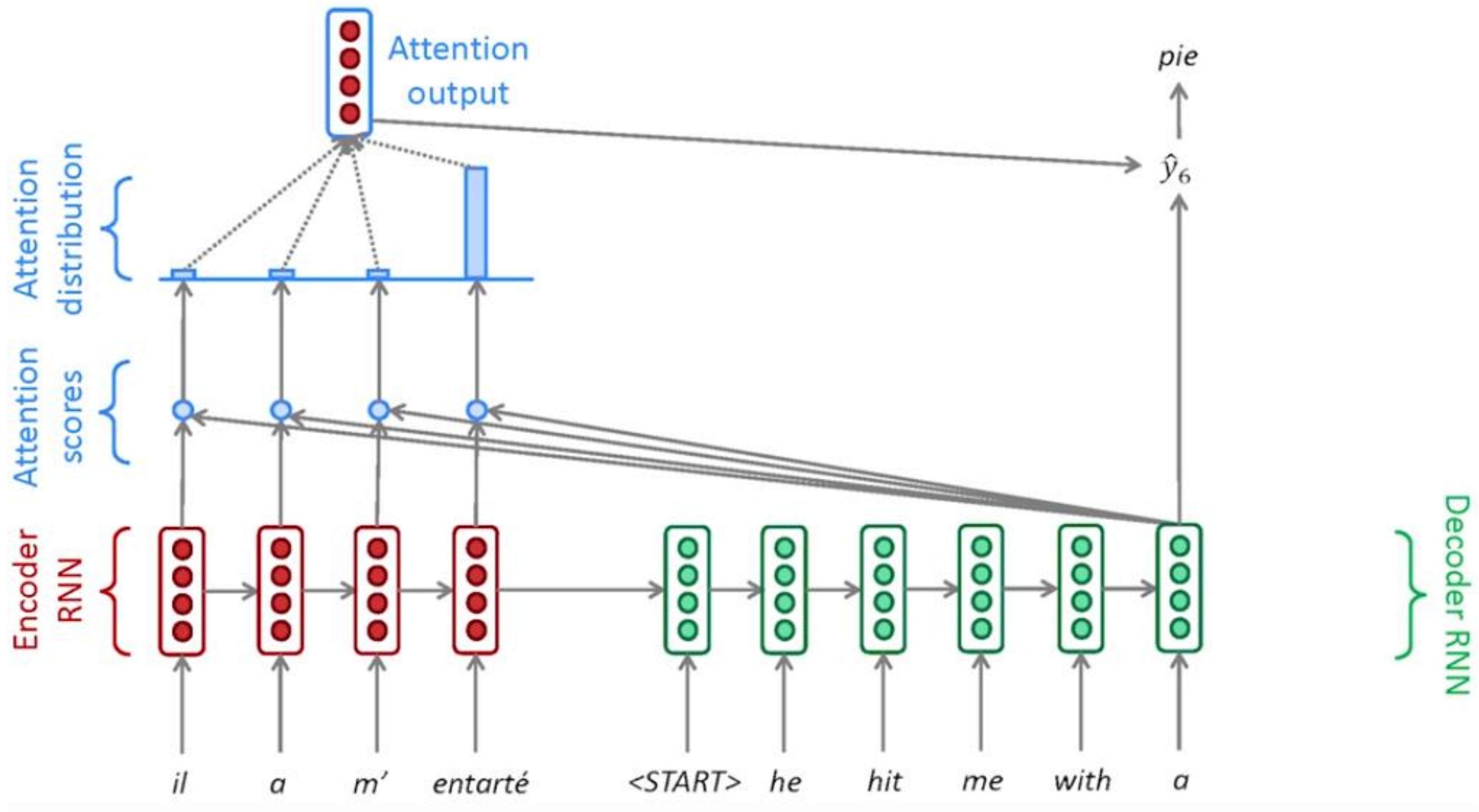
Seq2Seq with Attention



Seq2Seq with Attention



Seq2Seq with Attention



Attention: Equations

- 假設編碼器的隱含狀態如下：$h_1, \dots, h_N \in \mathbb{R}^h$
- 假設時序t的解碼器隱含狀態為 $s_t \in \mathbb{R}^h$
- 時序t的注意力分數為e^t：

$$e^t = [S_t^T h_1, \dots, S_t^T h_N] \in \mathbb{R}^N$$

- 運用Softmax函數將時序t的注意力分數轉成機率分布 $\propto^t$

$$\propto^t = softmax(e^t) \in \mathbb{R}^N$$

- 利用注意力的機率分布與時序t之解碼器隱含狀態計算計算總合a_t

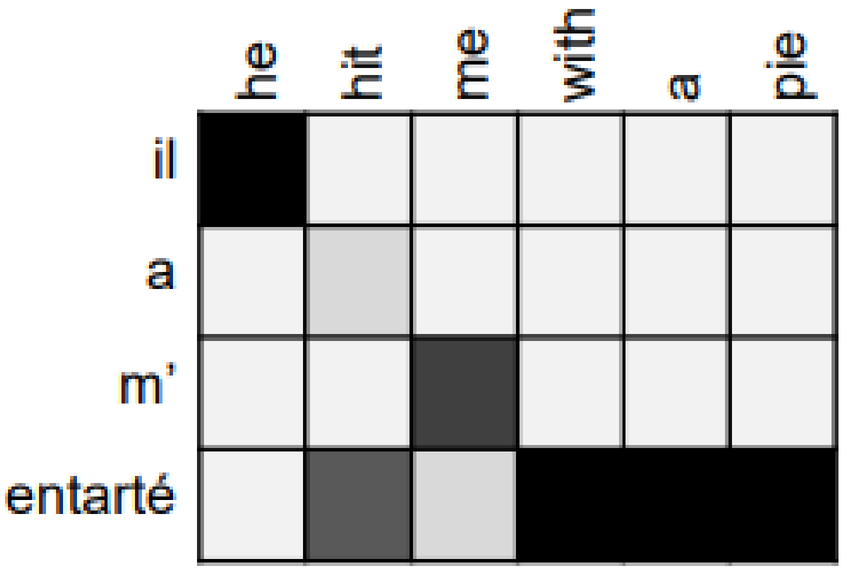
$$a_t = \sum_{i=1}^{N} \propto_i^t h_i \in \mathbb{R}^h$$

- 最後將a_t與解碼器隱含狀態做Concate

$$[a_t, s_t] \in \mathbb{R}^{2h}$$

Attention is Great

- Attention
  - 改進了NMT的表現
  - 解決了訓練Seq2Seq模型所會遇到的問題
  - 幫忙解決梯度消失的問題
  - 讓我們更容易理解模型的狀態
    - 藉由注意力分布來了解解碼的所注意的位置



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Transformer

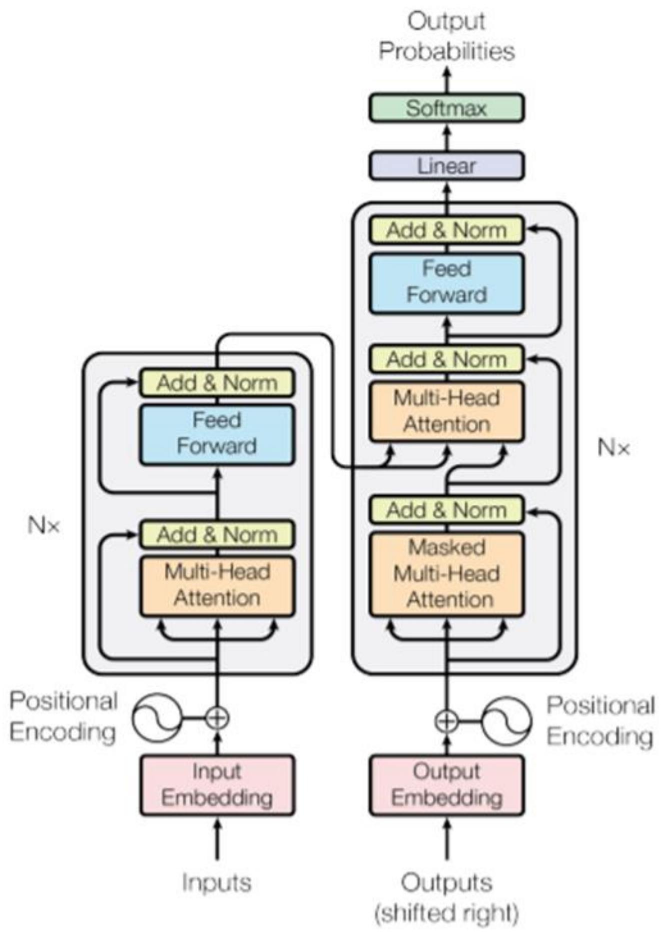
Transformer Models

All of these models are Transformer architecture models … so maybe we had better learn about Transformers?

ULMfit	GPT	BERT	GPT-2
Jan 2018	June 2018	Oct 2018	Feb 2019
Training:	Training	Training	Training
1 GPU day	240 GPU days	256 TPU days ~320–560 GPU days	~2048 TPU v3 days according to a reddit thread
fast.ai	OpenAI	Google AI	OpenAI

Transformer Overview

- Non-Recurrent sequence-to-sequence encoder-to-decoder model.
- Task : Machine Translation with parallel corpus
- Predict each translated word
- Loss Function
  - Cross-Entropy loss on top of the softmax classifier



Dot-Product Attention

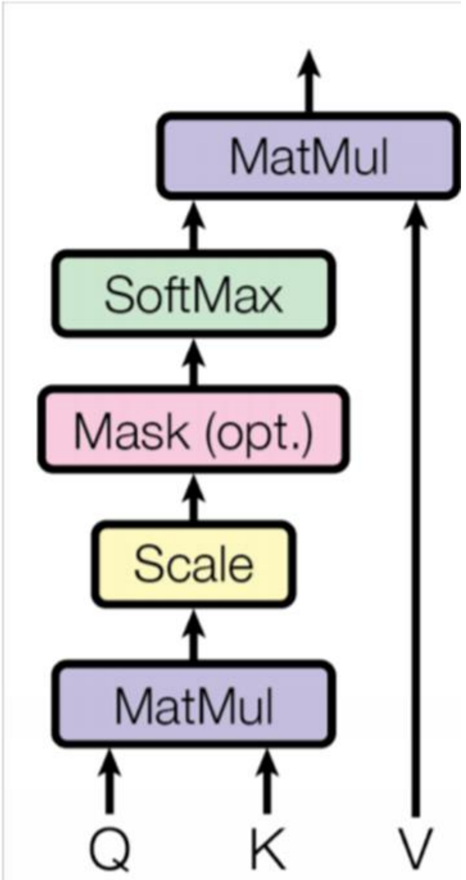
- Inputs: a query q, and a set of key-value (k-v), where
    - q, k, and v are vector.
- Output is a weighted sum of values, where
    - Dimension of queries and key are the same which are d_k
    - Dimension of values are d_v

$$A(Q, K, V) = softmax(Q^T K)\mathrm{V}$$

Scaled Dot-Product Attention

- Problem: As d_k gets large, the variance of $q^T k$ increases -> some values inside Softmax increases -> Softmax becomes very peaked -> As a result, Gradient becomes smaller
- Solution : Scaled by $1 / \sqrt{d_k}$

$$A(Q, K, V) = softmax\left(\frac{Q^T K}{\sqrt{d_k}}\right)V$$

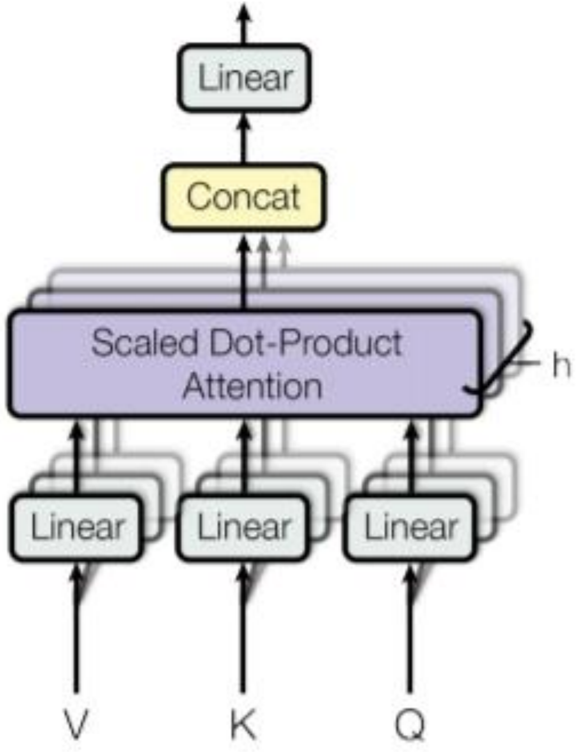


Multi-head attention

- Problems with simple attention:
  - Cannot have multiple attention
- Solution: Multi-head attention

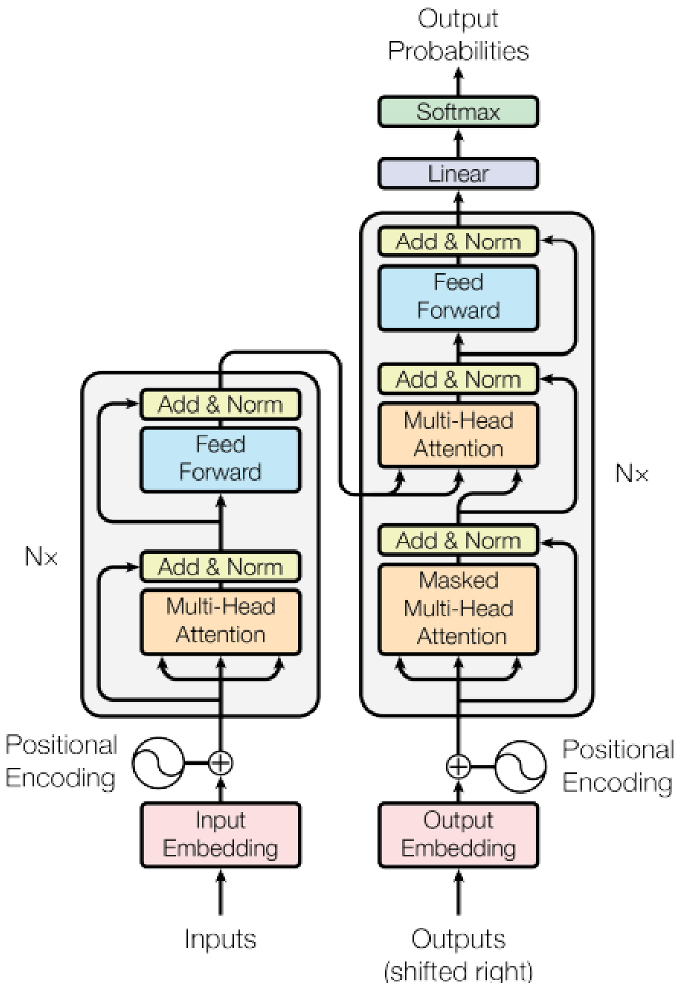
1. Feed Q, K and V into linear projection layer
2. Apply attention
3. Concatenate output
4. Pipe through linear layer

$$
\begin{aligned}
\mathrm{MultiHead}(Q, K, V) &= \mathrm{Concat}(\mathrm{head_1}, ..., \mathrm{head_h})W^O \\
\text{where } \mathrm{head_i} &= \mathrm{Attention}(QW_i^Q, KW_i^K, VW_i^V)
\end{aligned}
$$



Transformer: Complete Encoder and Decoder

- Blocks are repeated.
- Encoder: 6 layers
- Decoder: 6 layers



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