Advanced Deep Temporal Models

AI602: Recent Advances in Deep Learning

Lecture 3

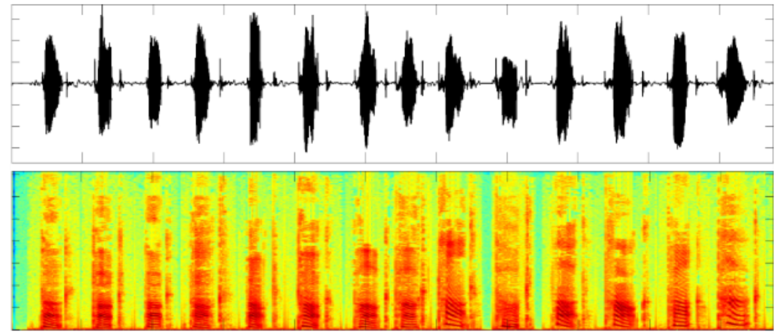
Slide made by

Jaehyung Kim

KAIST EE

Motivation: Temporal Data in Real World

- Many real-world data has a **temporal structure** intrinsically
  - Speech

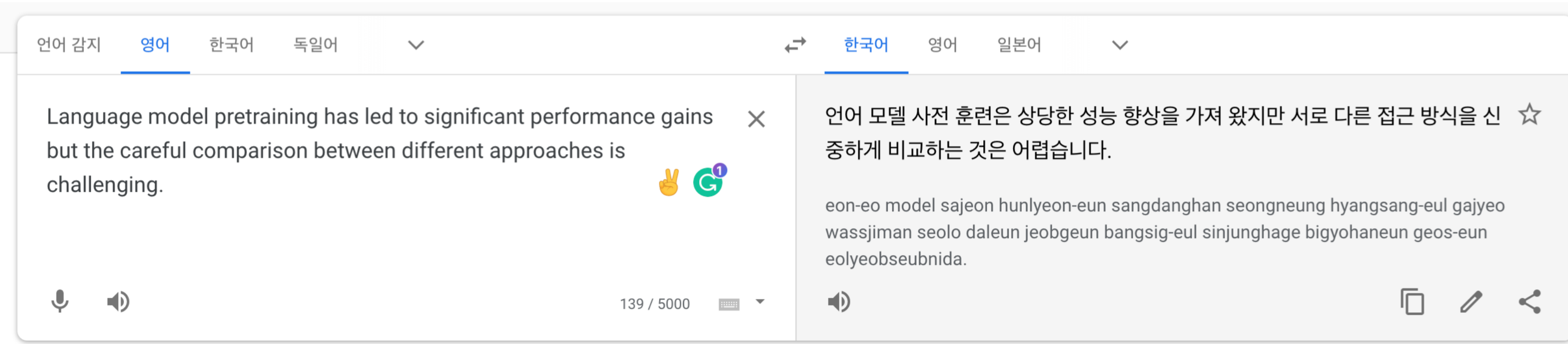


Motivation: Temporal Data in Real World

- Many real-world data has a **temporal structure** intrinsically
  - Speech
  - Natural language

"Overall, the value I got from the two hours watching it was the sum total of the popcorn and the drink. The movie was __." ⟶ *terrible*

Language modeling



Translation

Motivation: Temporal Data in Real World

- Many real-world data has a **temporal structure** intrinsically
  - Speech
  - Natural language
  - Video

Motivation: Temporal Data in Real World

- Many real-world data has a **temporal structure** intrinsically
  - Speech
  - Natural language
  - Video
  - Stock prices, and etc…

Motivation: Temporal Data in Real World

- Many real-world data has a **temporal structure** intrinsically
    - Speech
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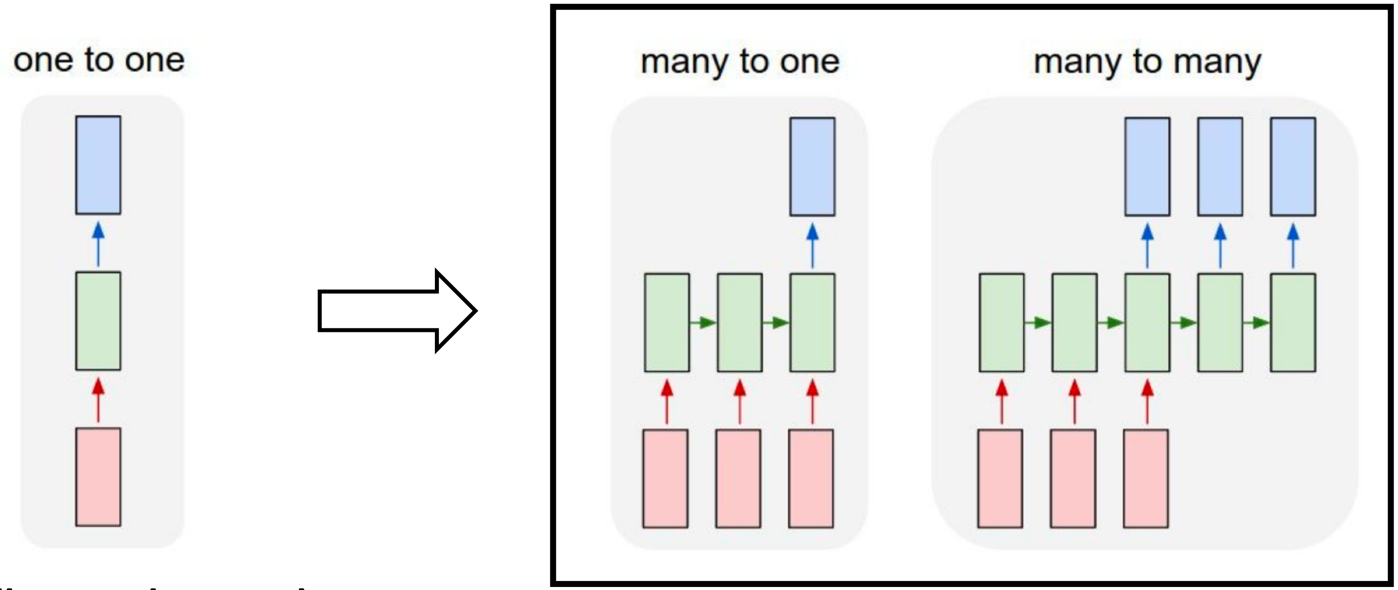
    - Video
    - Stock prices, and etc…

- In order to solve much complicated real-world problems,
  we need a **better architecture to capture temporal dependency** in the data



Vanilla neural network

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Vanilla RNN

- Process a sequence of vectors by applying **recurrence formula** at every time step :

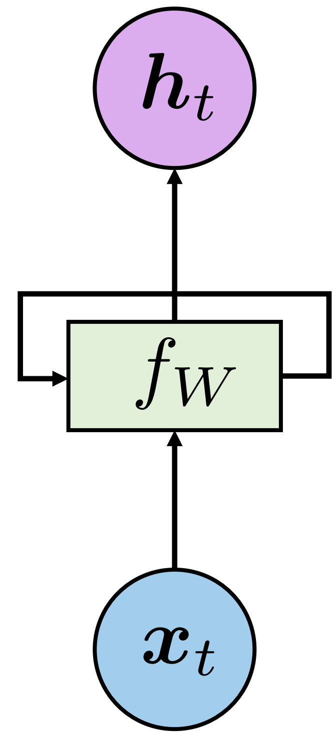
$$\boxed{\boldsymbol{h}_t} = \boxed{f_W}(\boxed{\boldsymbol{h}_{t-1}}, \boxed{\boldsymbol{x}_t})$$

New state

Old state

Input vector at time step t

Function parameterized by learnable W



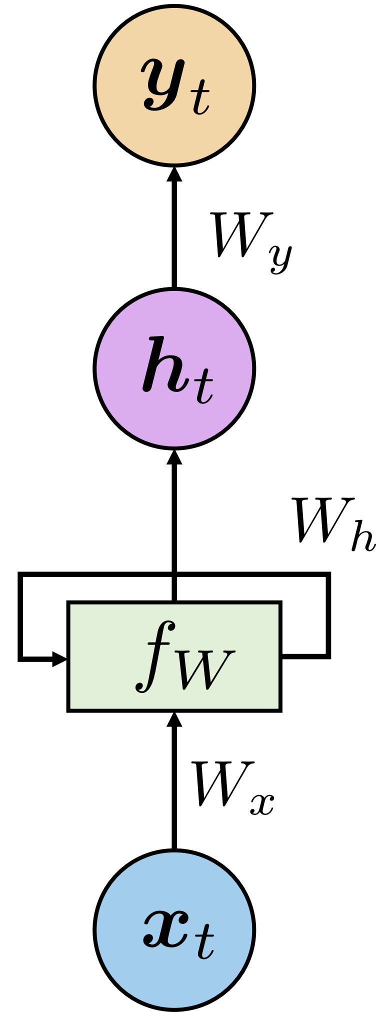
*reference: http://cs231n.stanford.edu/2017/

Vanilla RNN

- Vanilla RNN (or sometimes called **Elman RNN**)
  - The state consists of a single "hidden" vector $\mathbf{h}_t$

$$\boldsymbol{h}_t = f_W(\boldsymbol{h}_{t-1}, \boldsymbol{x}_t)$$

$$\boxed{\begin{aligned} \boldsymbol{h}_t &= \tanh(W_h \boldsymbol{h}_{t-1} + W_x \boldsymbol{x}_t) \\ \boldsymbol{y}_t &= W_y \boldsymbol{h}_t \end{aligned}}$$



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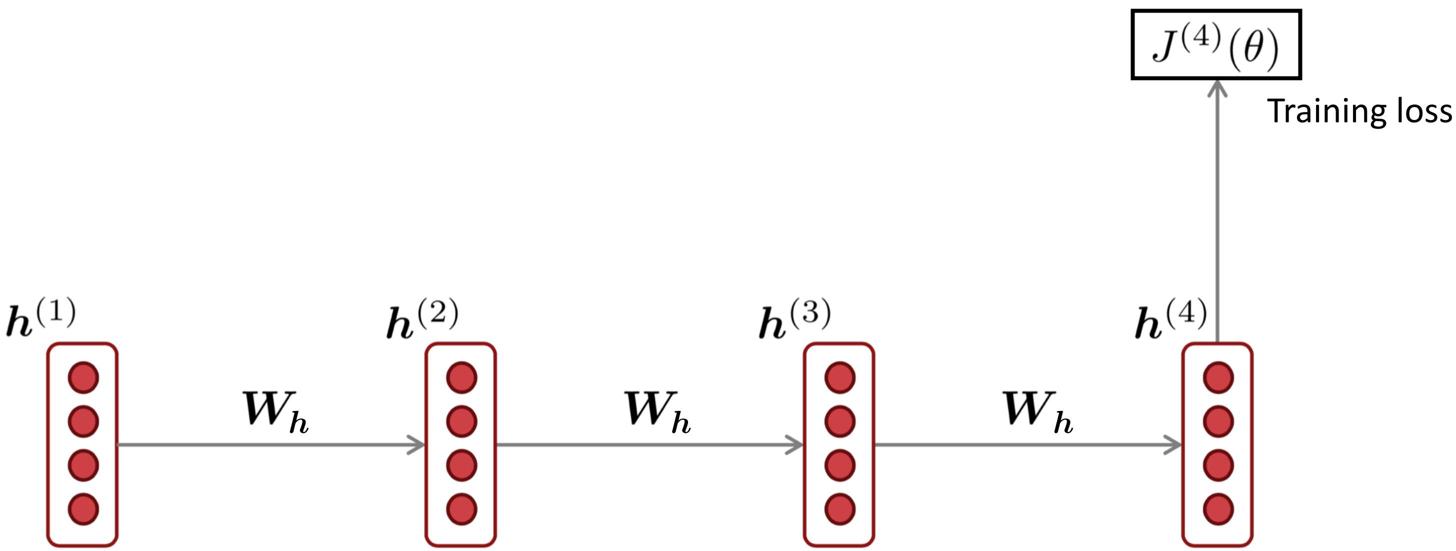
Why Do We Need to Develop RNN Architectures?

- E.g., RNN with a sequence of length 4



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Why Do We Need to Develop RNN Architectures?

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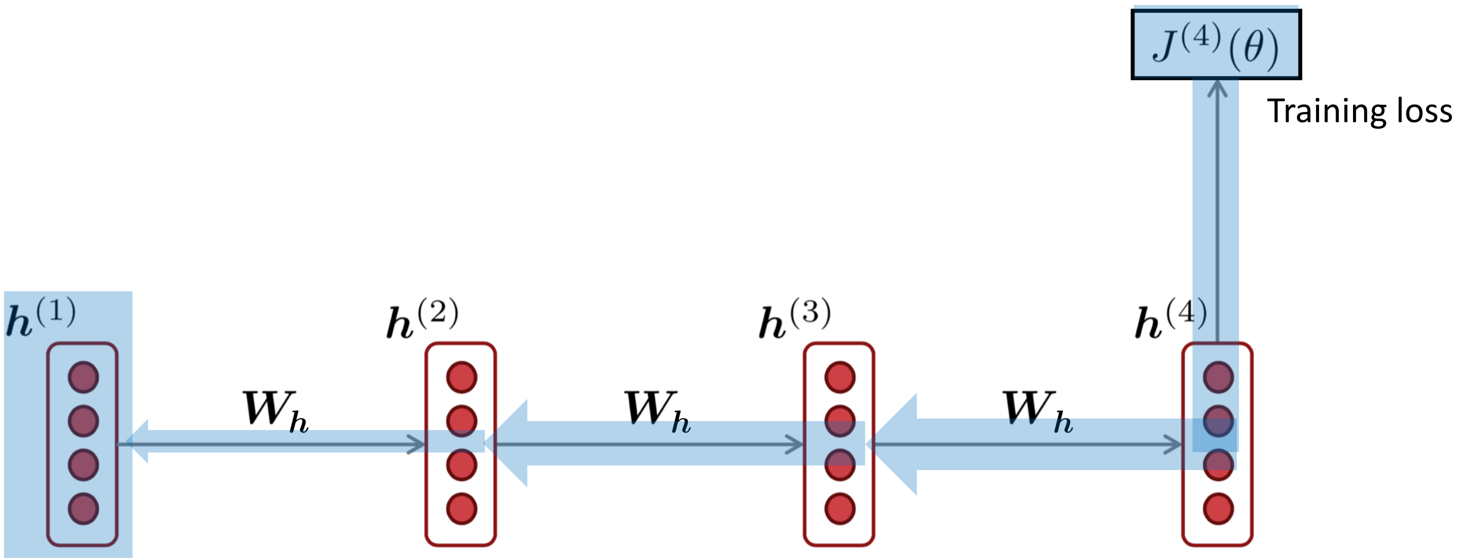
  - Consider a gradient from the first state $\boldsymbol{h}^{(1)}$



$$\frac{\partial J^{(4)}}{\partial \boldsymbol{h}^{(1)}} = \frac{\partial \boldsymbol{h}^{(2)}}{\partial \boldsymbol{h}^{(1)}} \times \frac{\partial \boldsymbol{h}^{(3)}}{\partial \boldsymbol{h}^{(2)}} \times \frac{\partial \boldsymbol{h}^{(4)}}{\partial \boldsymbol{h}^{(3)}} \times \frac{\partial J^{(4)}}{\partial \boldsymbol{h}^{(4)}}$$

Chain rule!

*reference: http://web.stanford.edu/class/cs224n/

Why Do We Need to Develop RNN Architectures?

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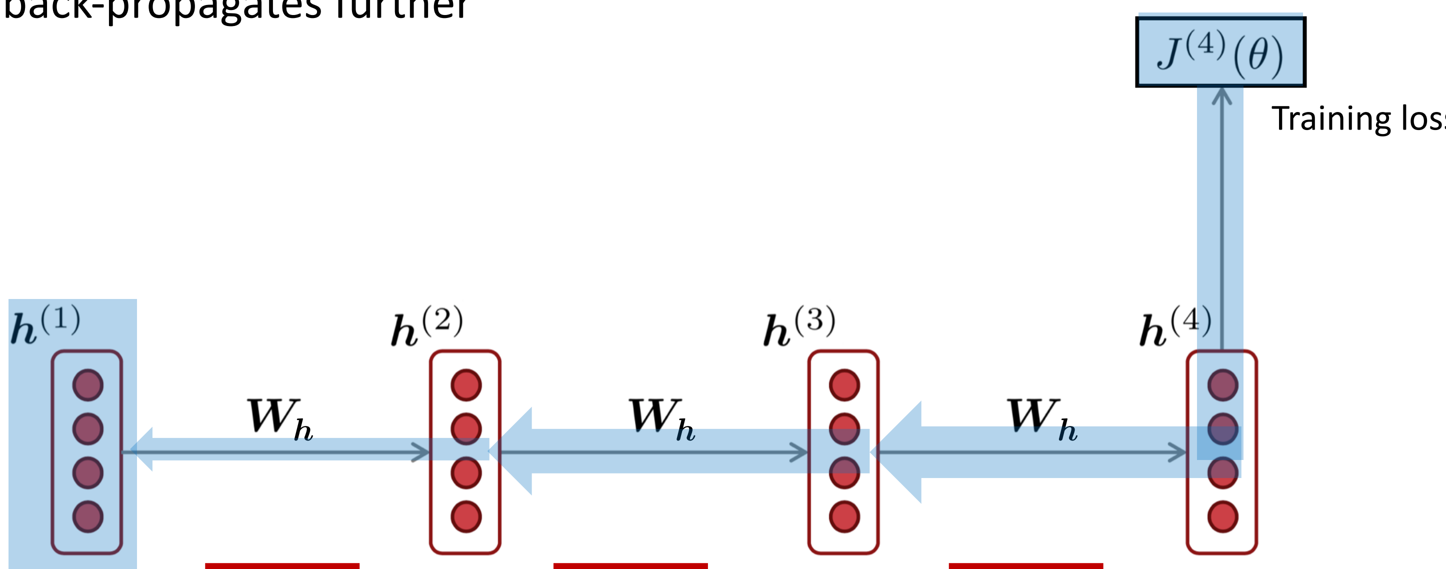
- What happens if $\frac{\partial \boldsymbol{h}^{(i+1)}}{\partial \boldsymbol{h}^{(i)}}$ are **too small**? ⇨ **Vanishing gradient problem**
  - When these are small, the gradient signal gets smaller and smaller as it back-propagates further



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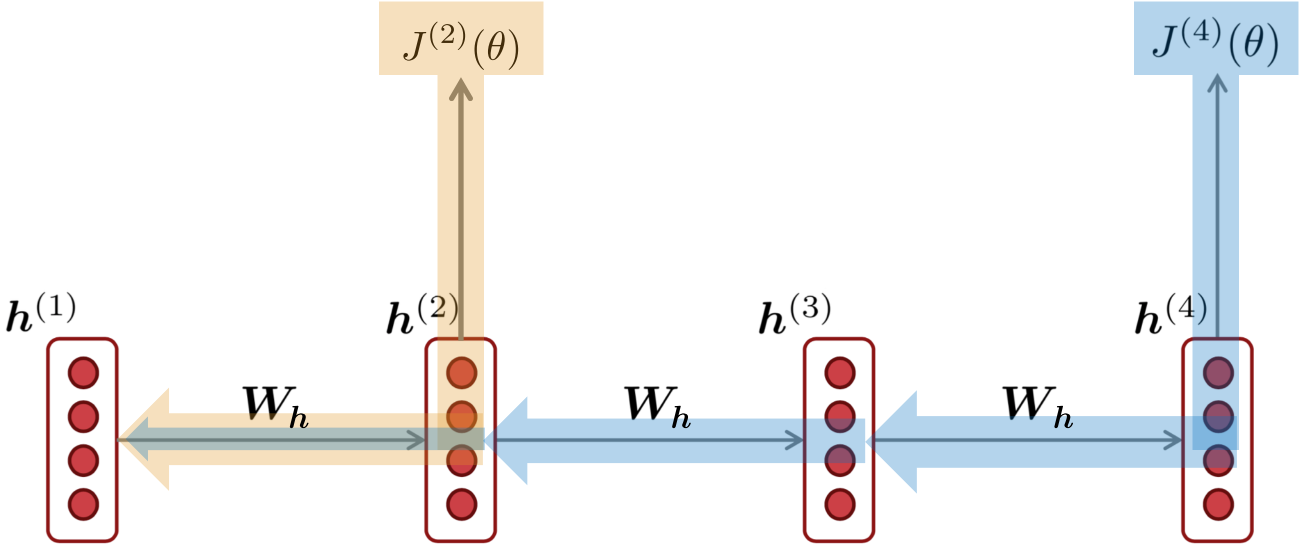
  - So, model weight are updated only with respect to near effects, **not** long-term effects.



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- What happens if $\frac{\partial \boldsymbol{h}^{(i+1)}}{\partial \boldsymbol{h}^{(i)}}$ are **too large**? $\Rightarrow$ **Exploding gradient problem**

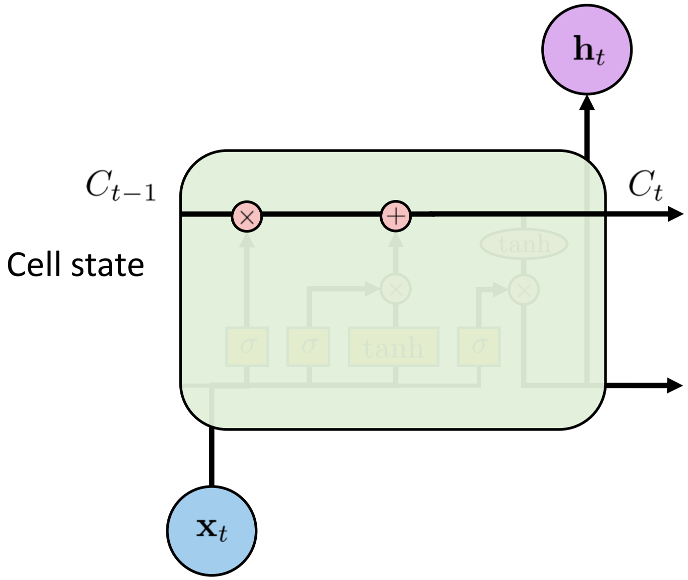
$$\theta^{\text{new}} = \theta^{\text{old}} - \alpha \nabla_\theta J(\theta)$$

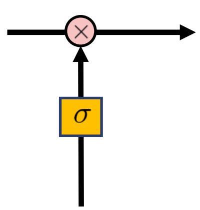
  - This can cause bad updates as the update step of parameters becomes too big
  - In the worst case, this will result in divergence of your network
  - In practice, with a gradient clipping, exploding gradient is **relatively easy to solve**

*reference: http://web.stanford.edu/class/cs224n/

- **Long Short-Term Memory (LSTM)** [Hochreiter and Schmidhuber, 1997]
  - A special type of RNN unit, i.e., LSTM networks = RNN composed of LSTM units
  - Explicitly designed RNN to
    - Capture **long-term dependency** ⟹ more robust to vanishing gradient problem

- Core idea behind LSTM
  - With **cell state** (**memory**), it controls **how much to remove or add information**
    - Only linear interactions from the output of each "**gates**" (**prevent vanishing gradient**)



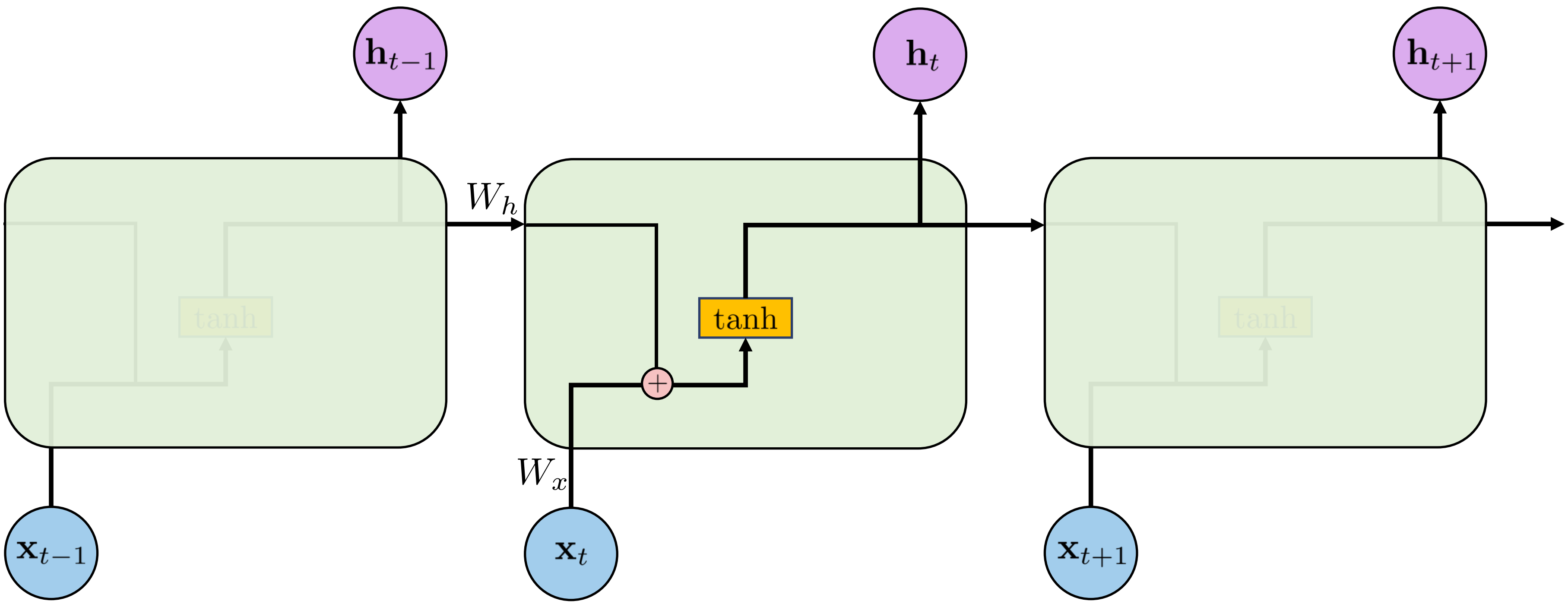


Gates : Way to optionally let information through

*source: https://en.wikipedia.org/wiki/Long_short-term_memory#/media/File:The_LSTM_cell.png

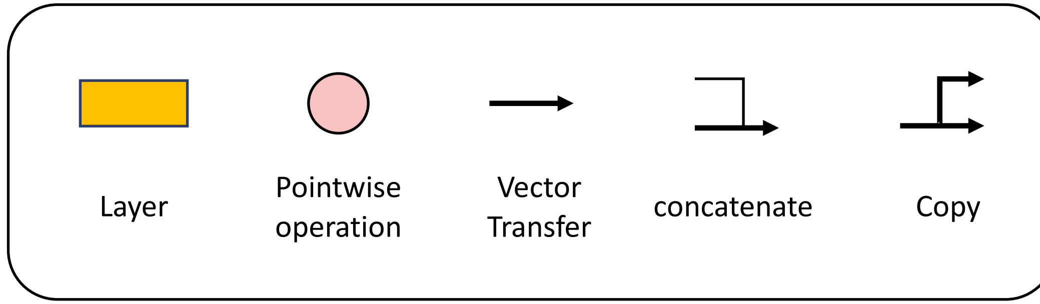
- Repeating modules in **Vanilla RNN** contains a **single layer**

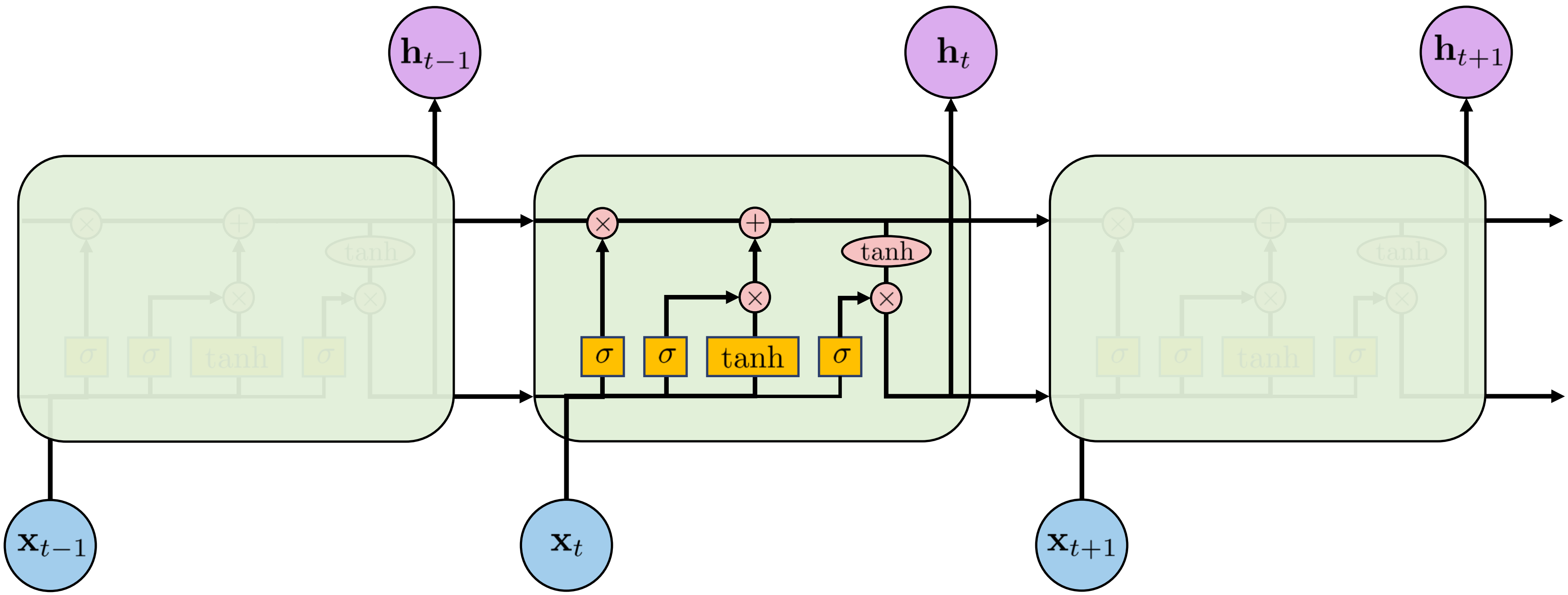
$$\boldsymbol{h}_t = \tanh(W_h \boldsymbol{h}_{t-1} + W_x \boldsymbol{x}_t)$$



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

- Repeating modules in **LSTM**



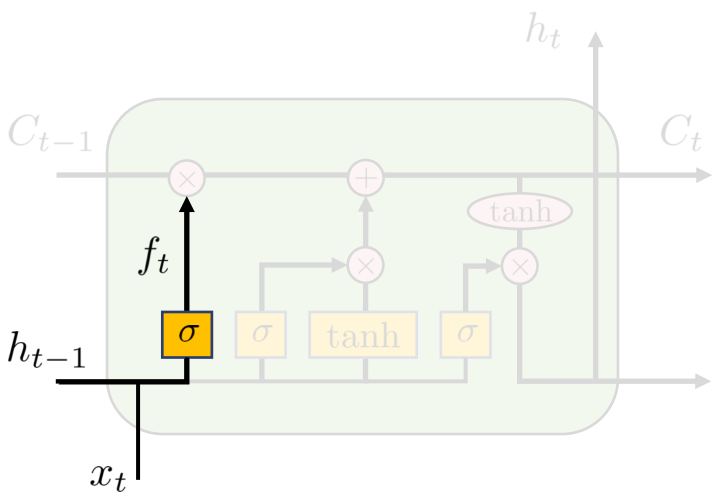


*reference: http://colah.github.io/posts/2015-08-Understanding-LSTMs/

Step 1: Decide what **information** we're going to **throw away** from the **cell state**

- A sigmoid layer called "**Forget gate**" f_t
- Looks at h_{t-1}, x_t and outputs a number between 0 and 1 for each cell state C_{t-1}
  - If 1: completely keep, if 0: completely remove

- E.g., language model trying to **predict the next word** based on all previous ones
  - The cell state might include the gender of the present subject so that the correct pronouns can be used
  - When we see a new subject, we want to forget the gender of the old subject

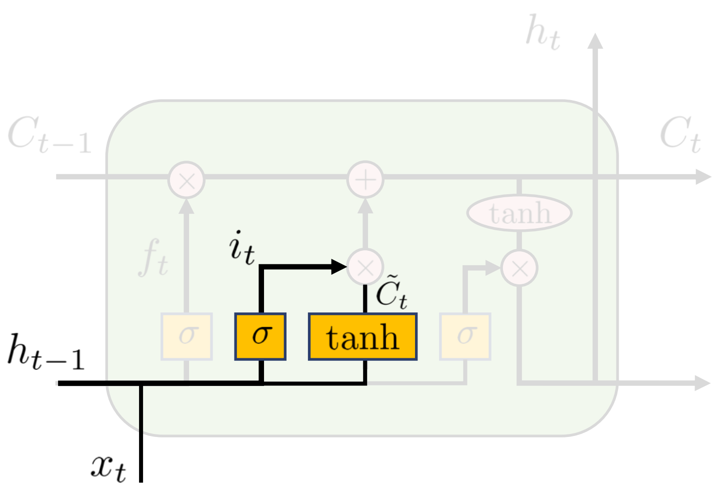


$$f_t = \sigma\left(W_f \cdot [h_{t-1}, x_t] + b_f\right)$$

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

Step 2: Decide what **information** we're going to **store** in the cell state and **update**

- First, a sigmoid layer called the "**Input gate**" i_t decides which values to update
- Next, a tanh layer creates a **new content** $\tilde{C}_t$ to be written to the



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

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

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Step 2: Decide what **information** we're going to **store** in the cell state and **update**

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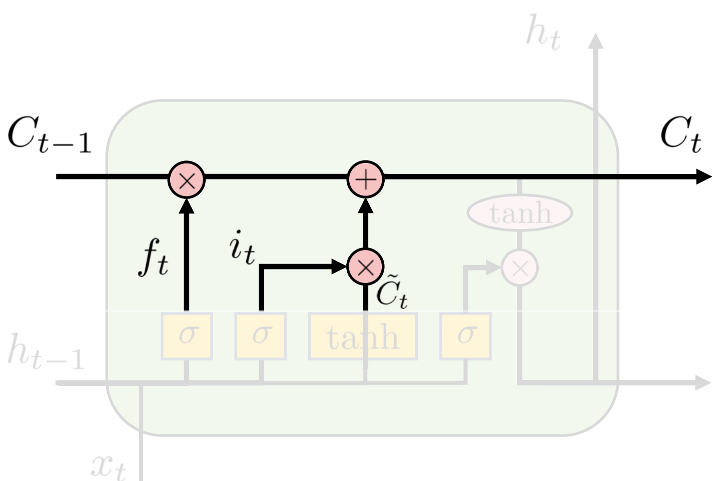
- Then, **update** the old cell state C_{t-1} into the **new cell state** C_t
  - Multiply the old state by f_t (forget gate)
  - Add $i_t * \tilde{C}_t$, new content scaled by how much to update (input gate)



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

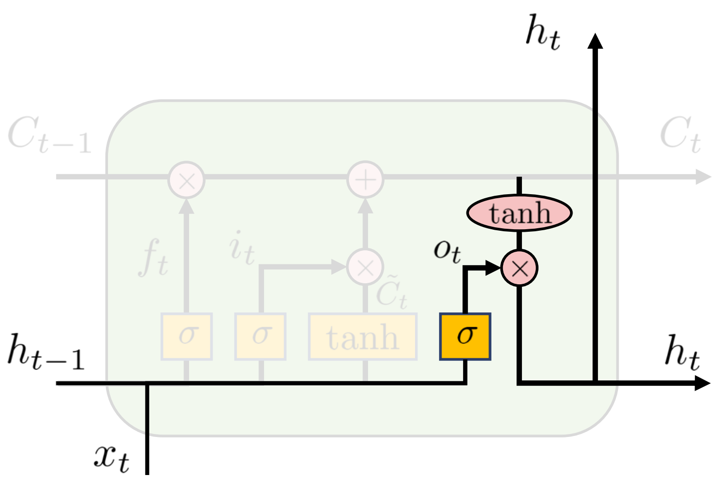
$$\tilde{C}_t = \tanh(W_C \cdot [h_{t-1}, x_t] + b_C)$$

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

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

Step 3: Decide what **information** we're going to **output**

- A sigmoid layer called "**Output gate**" o_t
- First, go through o_t which decides **what parts** of the cell state **to output**
- Then, put the cell state C_t through tanh and multiply it by o_t for hidden state h_t



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

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

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

- Overall LSTM operations

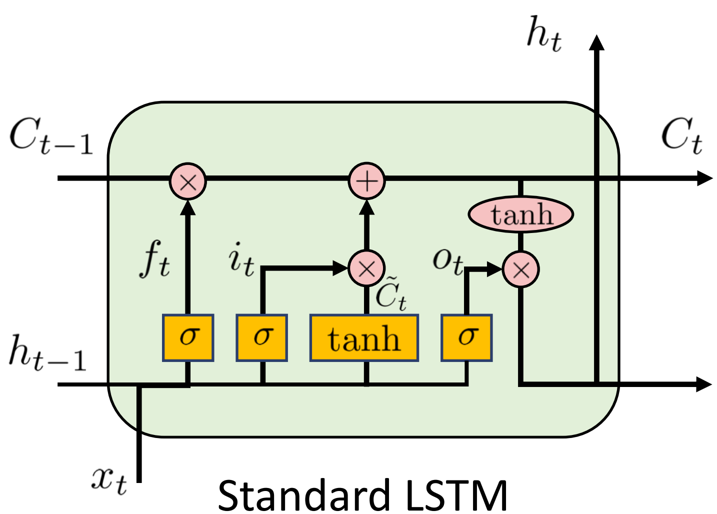
Forget gate: $f_t = \sigma(W_f \cdot [h_{t-1}, x_t] + b_f)$ Input gate: $i_t = \sigma(W_i \cdot [h_{t-1}, x_t] + b_i)$

Previous cell state: C_{t-1} New cell content: $\tilde{C}_t = \tanh(W_C \cdot [h_{t-1}, x_t] + b_C)$

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

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

Hidden state: $h_t = o_t * \tanh(C_t)$



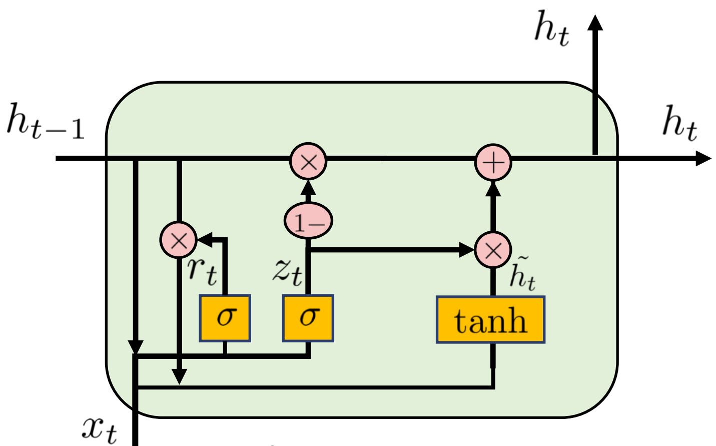
Standard LSTM

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

- **Gated Recurrent Unit (GRU)** [Cho et.al, 2014]
  - Combines the forget and input gates into a single "**update gate**" z_t
    - Controls the **ratio of information to keep** between previous state and new state
  - **Reset gate** r_t controls how much information to forget when create a new content
  - **Merges** the cell state C_t and hidden state h_t
  - **(+)** Resulting in **simpler model (less weights)** than standard LSTM

Reset gate: $r_t = \sigma(W_r \cdot [h_{t-1}, x_t])$ New content: $\tilde{h}_t = \tanh(W \cdot [r_t * h_{t-1}, x_t])$

Update gate: $z_t = \sigma(W_z \cdot [h_{t-1}, x_t])$ Hidden state: $h_t = (1 - z_t) * h_{t-1} + z_t * \tilde{h}_t$

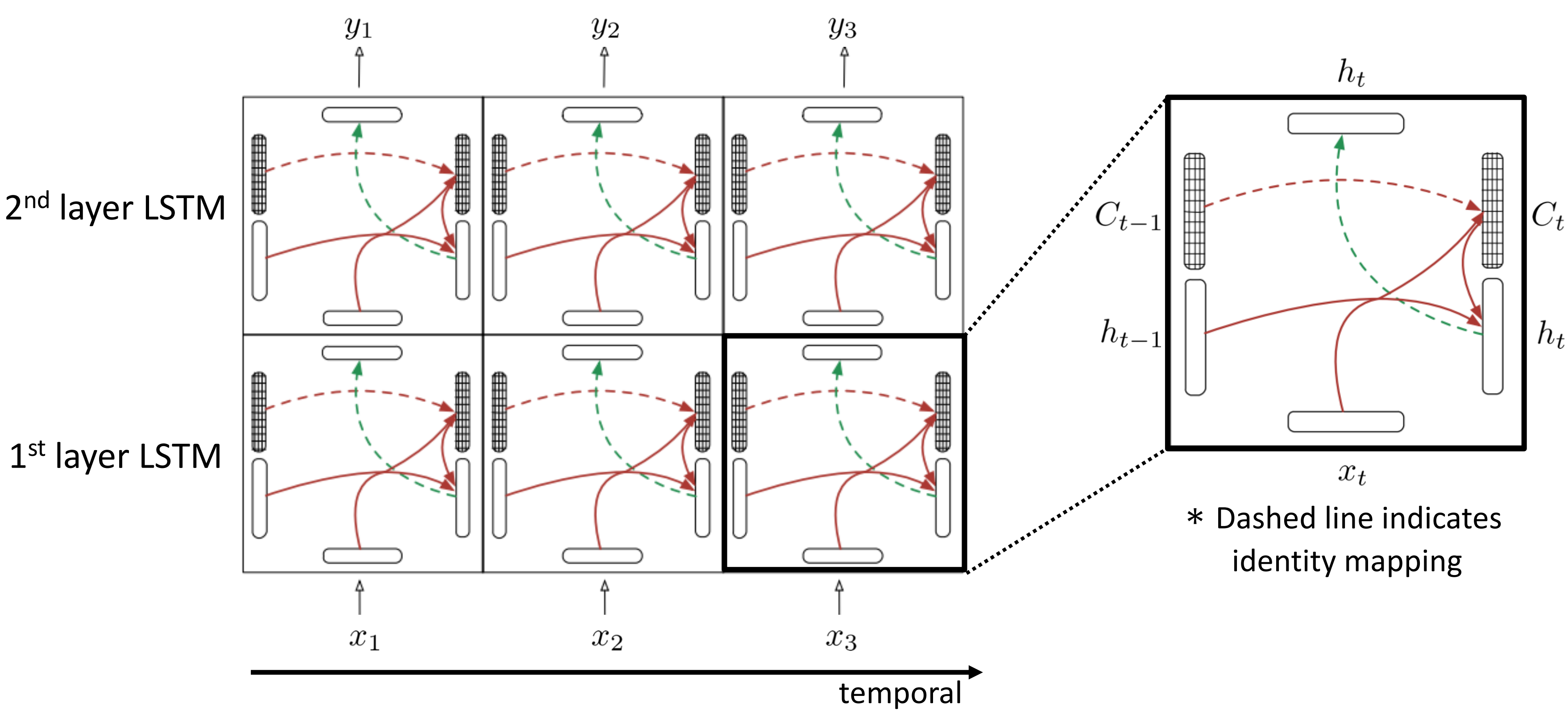


Gated Recurrent Unit

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

RNN Architectures: Stacked LSTM

- **Stacked(multi-layer) LSTM** [Graves et al, 2013]
  - RNNs are already “deep” on one dimension (they unroll over many time-steps)
  - We can add depth by simply stacking LSTM layers on top of each other
    - This allows the network to compute **more complex representations**
  - E.g., Output of 1st layer LSTM goes into 2nd layer LSTM as an input

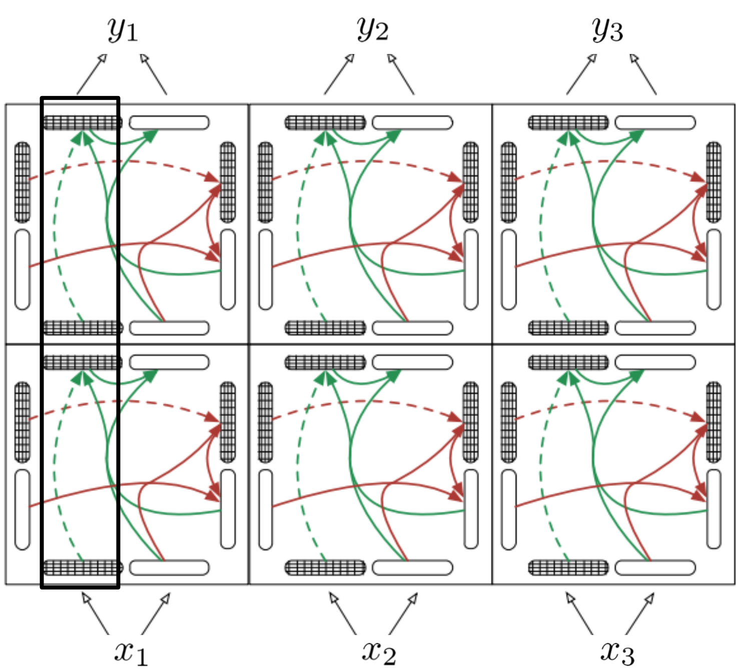


* Dashed line indicates identity mapping

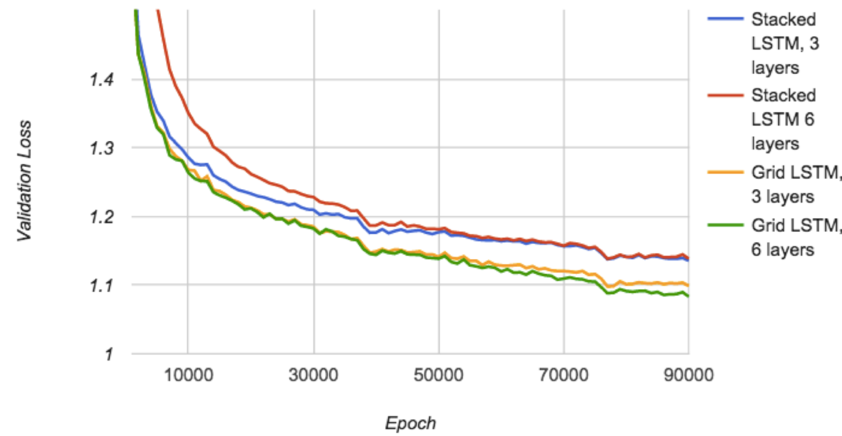
*source: https://arxiv.org/pdf/1507.01526.pdf

RNN Architectures: Grid LSTM

- **Grid LSTM** [Kalchbrenner et al., 2016]
  - Extended version of stacked LSTM
  - LSTM units have **additional memory along depth dimension** as well as temporal dimension



2D Grid LSTM



	BPC	Parameters	Alphabet Size	Test data
Stacked LSTM (Graves, 2013)	1.67	27M	205	last 4MB
MRNN (Sutskever et al., 2011)	1.60	4.9M	86	last 10MB
GFRNN (Chung et al., 2015)	1.58	20M	205	last 5MB
Tied 2-LSTM	**1.47**	16.8M	205	last 5MB

Performance on wikipedia dataset
(lower the better)

*source: https://github.com/coreylynch/grid-lstm

Limitation of Left-to-Right RNNs

- What is the limitation of all previous models?
  - They learn representations only from **previous** time steps (left-to-right)
  - But, it's sometimes useful to learn from **future** time steps in order to
    - Better understand the **context**
    - Eliminate ambiguity

- Example
  - "**He said, Teddy** bears are on sale"
  - "**He said, Teddy** Roosevelt was a great President"
  - In above two sentences, only seeing **previous words is not enough** to understand the sentence

- Solution
  - Also look ahead (right-to-left) ⇨ **Bidirectional RNN**

RNN Architectures: Bidirectional RNNs

- RNNs can be easily extended into **bi-directional models**
  - Only difference is that there are **additional paths from future** time steps
    - Any types of RNNs (Vanilla RNN, LSTM, or GRU) could be bi-directional models
  - **Note**: bi-directional RNNs are only applicable if one has access to entire sequence

Hidden states

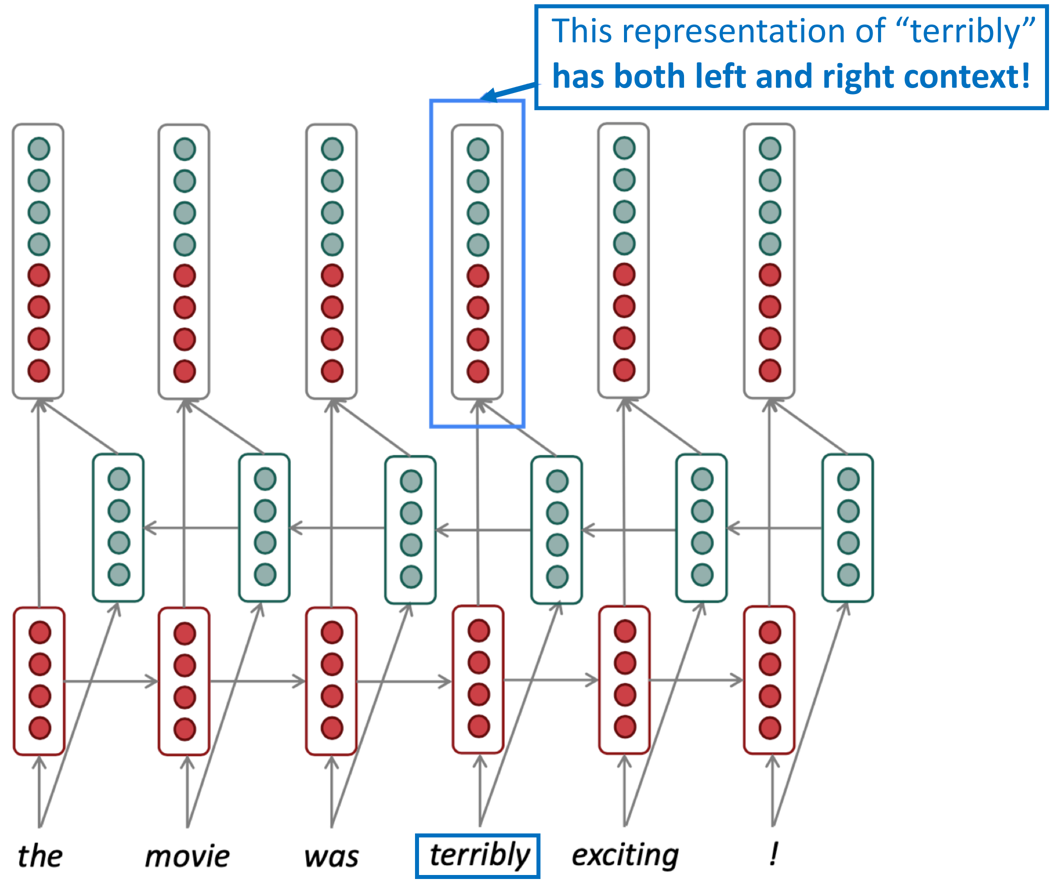
$$h^{(t)} = [\overrightarrow{h}^{(t)}; \overleftarrow{h}^{(t)}]$$

Backward RNN

$$\overleftarrow{h}^{(t)} = \mathrm{RNN}_{\mathrm{BW}}\left(\overleftarrow{h}^{(t+1)}, x^{(t)}\right)$$

Forward RNN

$$\overrightarrow{h}^{(t)} = \mathrm{RNN}_{\mathrm{FW}}\left(\overrightarrow{h}^{(t-1)}, x^{(t)}\right)$$



*reference: http://web.stanford.edu/class/cs224n/

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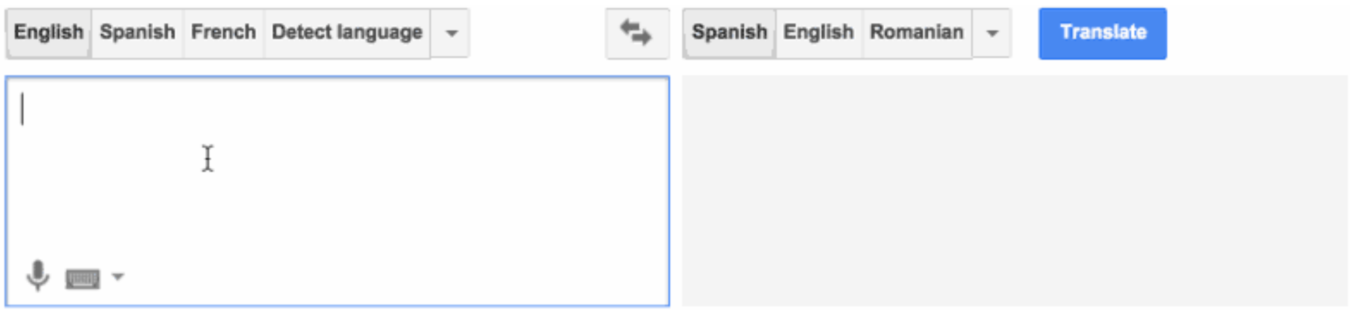
RNNs in Real-world Application: Neural Machine Translation

- What is machine translation (MT)?
  - Task of automatically **converting** source **text in one language to another** language
  - **No single answer** due to ambiguity/flexibility of human language (**challenging**)



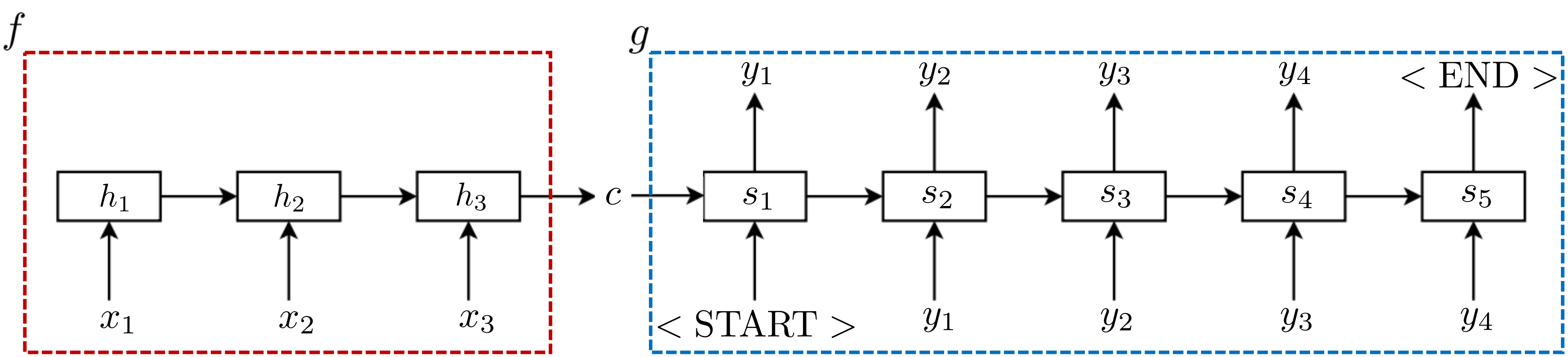
- Classical machine translation methods
  - Rule-based machine translation (RBMT)
  - Statistical machine translation (SMT; use of statistical model)
  - **(-)** Lots of human effort to maintain, e.g., repeated effort for each language pair

- Neural Machine Translation (NMT)
  - Use of **neural network models to learn a statistical model** for machine translation

Breakthroughs in NMT: Sequence-to-Sequence Learning

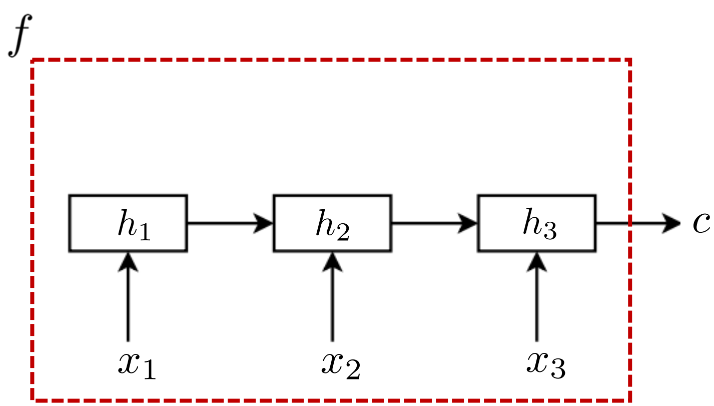
- **Difficulties** in Neural Machine Translation
  - Intrinsic difficulties of MT (ambiguity of language)
  - Variable length of input and output sequence (difficult to learn a single model)

- The core idea of **sequence-to-sequence** model [Sutskever et al., 2014]
  - **Encoder-Decoder** architecture (input → vector → output)
  - Use one RNN network (**Encoder**) to **read input sequence** at a time for **encoding it into** a fixed-length vector representation **(context)**
  - Use another RNN (**Decoder**) to extract the **output sequence** from context vector



Input sequence $\boldsymbol{x} = (x_1, x_2, x_3)$ and output sequence $\boldsymbol{y} = (y_1, y_2, y_3, y_4)$

- **Encoder**
  - **Reads the input** sentence $\mathbf{x} = (x_1, \ldots, x_T)$ and **output context** vector c
  - Use RNNs such that $h_t = f(x_t, h_{t-1})$ and $c = q(\{h_1, \ldots, h_T\})$, where f and q are some non-linear functions
  - E.g., LSTMs as f and $q(\{h_1, \ldots, h_T\}) = h_T$ (in the original seq2seq model)



Input sequence $\boldsymbol{x} = (x_1, x_2, x_3)$ and output sequence $\boldsymbol{y} = (y_1, y_2, y_3, y_4)$

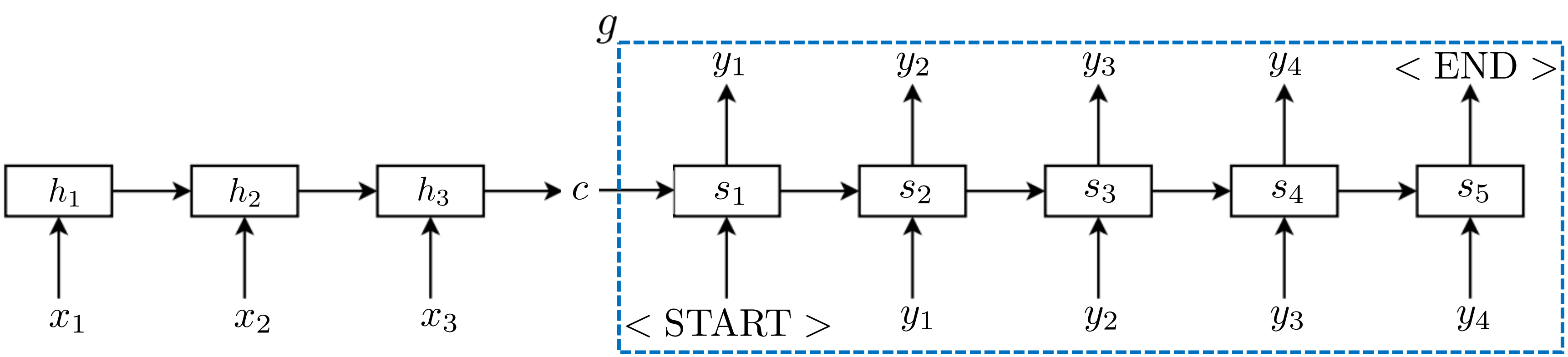
- **Decoder**
  - **Predict the next word** $y_{t'}$ **given the context** vector c and the **previously predicted** words $\{y_1, \ldots, y_{t'-1}\}$
  - Defines a probability over the translation $\mathbf{y}$ by **decomposing the joint probability** into the ordered conditionals where $\mathbf{y} = (y_1, \ldots, y_T)$.

$$p(\mathbf{y}) = \prod_{t=1}^{T} p(y_t | \{y_1, \ldots, y_{t'-1}\}, c),$$

  - The conditional probability is modeled with **another RNN** g as

$$p(y_t | \{y_1, \ldots, y_{t'-1}\}, c) = g(y_{t-1}, \underline{s_t}, c),$$

hidden state of the RNN



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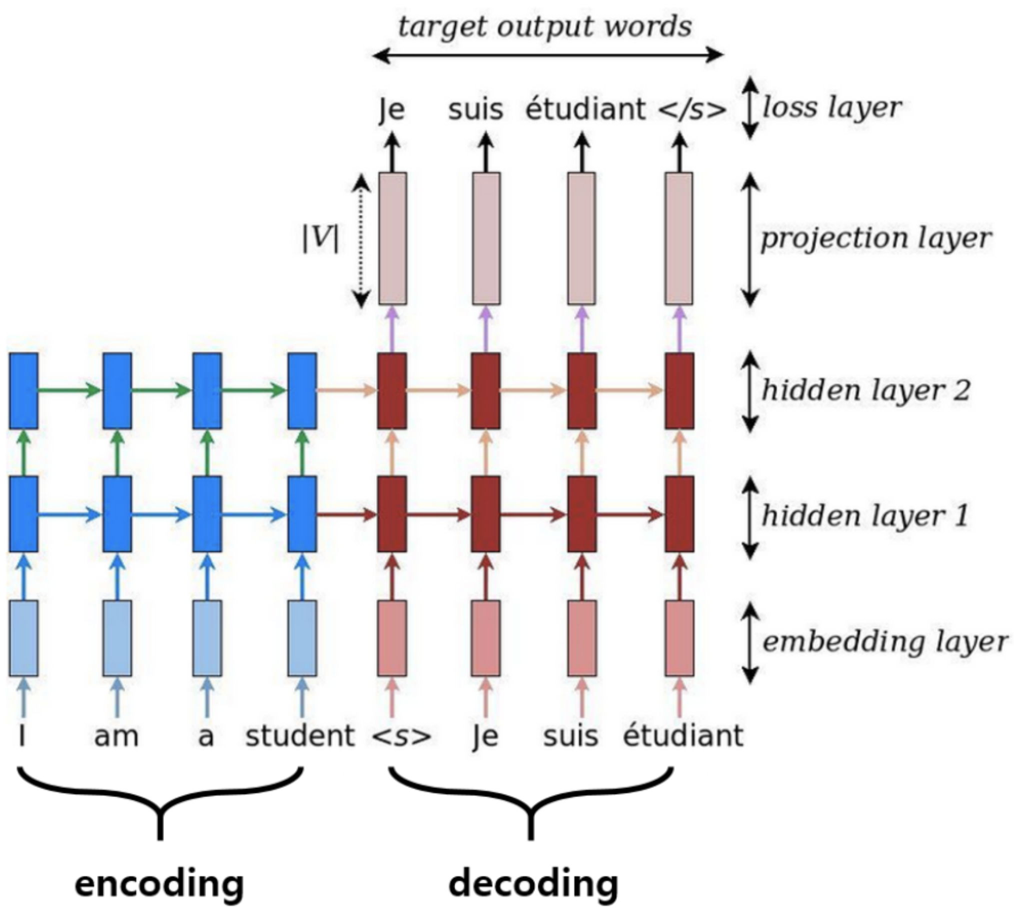
Breakthroughs in NMT: Sequence-to-Sequence Learning

- Example of the seq2seq model
  - For English → French task
  - With 2-layer LSTM for encoder and encoder



*source: https://towardsdatascience.com/seq2seq-model-in-tensorflow-ec0c557e560f

Breakthroughs in NMT: Sequence-to-Sequence Learning

- Results on WMT'14 English to French dataset [Sutskever et al., 2014]
  - Measure : BLEU(Bilingual Evaluation Understudy) score
    - Widely used quantitative measure for MT task
  - On **par with the state-of-the-art SMT** system (without using neural network)
  - Achieved **better results than the previous baselines**

Method	test BLEU score (ntst14)
Baseline System [29]	33.30
Cho et al. [5]	34.54
State of the art [9]	**37.0**
Rescoring the baseline 1000-best with a single forward LSTM	35.61
Rescoring the baseline 1000-best with a single reversed LSTM	35.85
Rescoring the baseline 1000-best with an ensemble of 5 reversed LSTMs	**36.5**
Oracle Rescoring of the Baseline 1000-best lists	$\sim$45

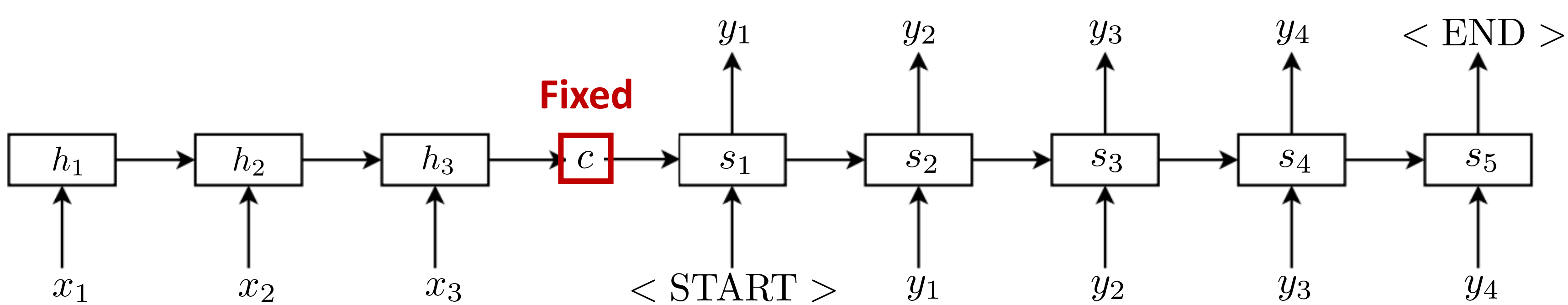
- Seq2seq with RNNs is **simple but very powerful** in MT task

*source: http://papers.nips.cc/paper/5346-sequence-to-sequence-learning

- Problem of original seq2seq(or encoder-decoder) model
  - Need to **compress** all the necessary information of a source sentence into a **fixed context vector**
    - All decoding steps use an identical context along with previous outputs

$$p(y_t|\{y_1,\dots,y_{t'-1}\},c) = g(y_{t-1}, s_t, \underline{c}),$$

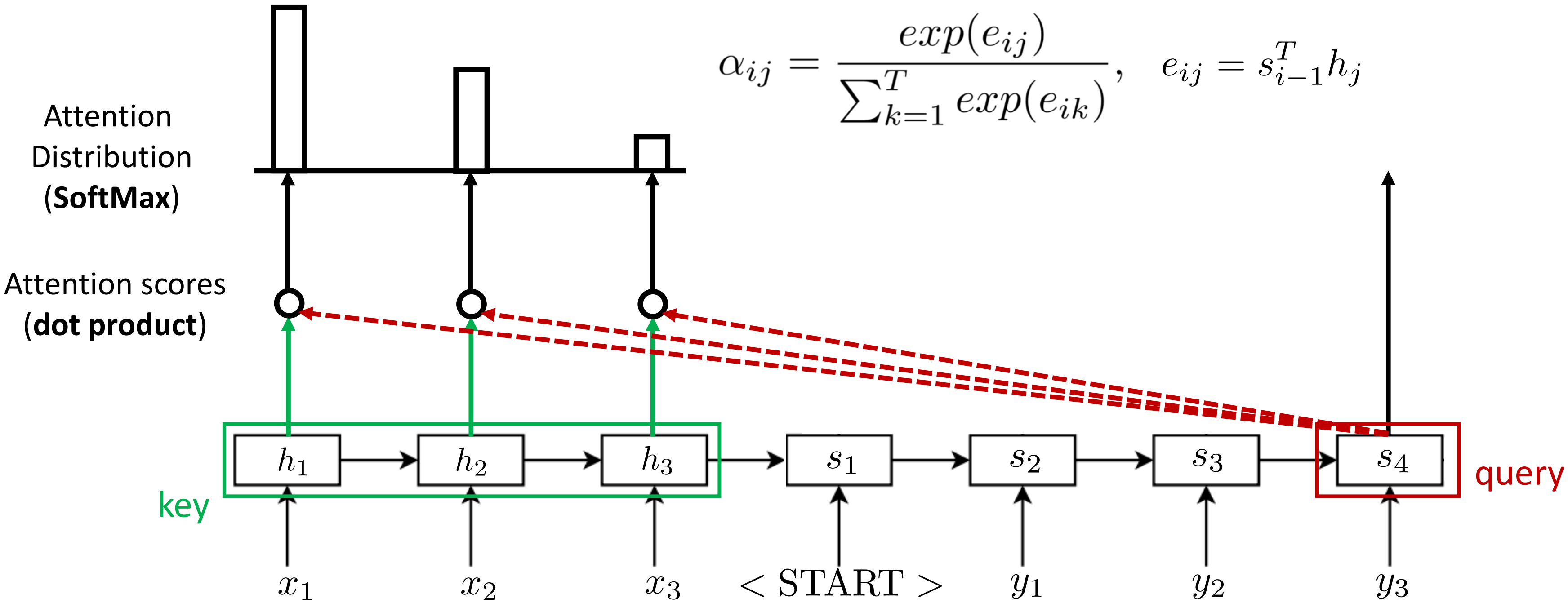
  - But, each step of decoding **requires different part** of the source sequence
    - E.g., Step1: “**I** love you” ⟶ “**나는** 너를 사랑해”
      Step2: “I **love** you” ⟶ “나는 너를 **사랑해**”
    - Hence, difficult to cope with long sentences…



Input sequence $\boldsymbol{x} = (x_1, x_2, x_3)$ and output sequence $\boldsymbol{y} = (y_1, y_2, y_3, y_4)$

- Extension of seq2seq model with **attention** mechanism [Bahdanau et al., 2015]
  - **Core idea**: on each step of the decoder, **focus on a particular part** of the source sequence using a **direct connection (attention)** to the encoder states
  - Dependent on the query with key, **attention** is a technique to compute a weighted sum of the values
    - Query: decoder's hidden state, key and value: encoder's hidden states
    - α_{ij} is a **relative importance** which means how well the inputs around position i and the output position j match.

$$\alpha_{ij} = \frac{exp(e_{ij})}{\sum_{k=1}^{T} exp(e_{ik})}, \quad e_{ij} = s_{i-1}^{T} h_j$$



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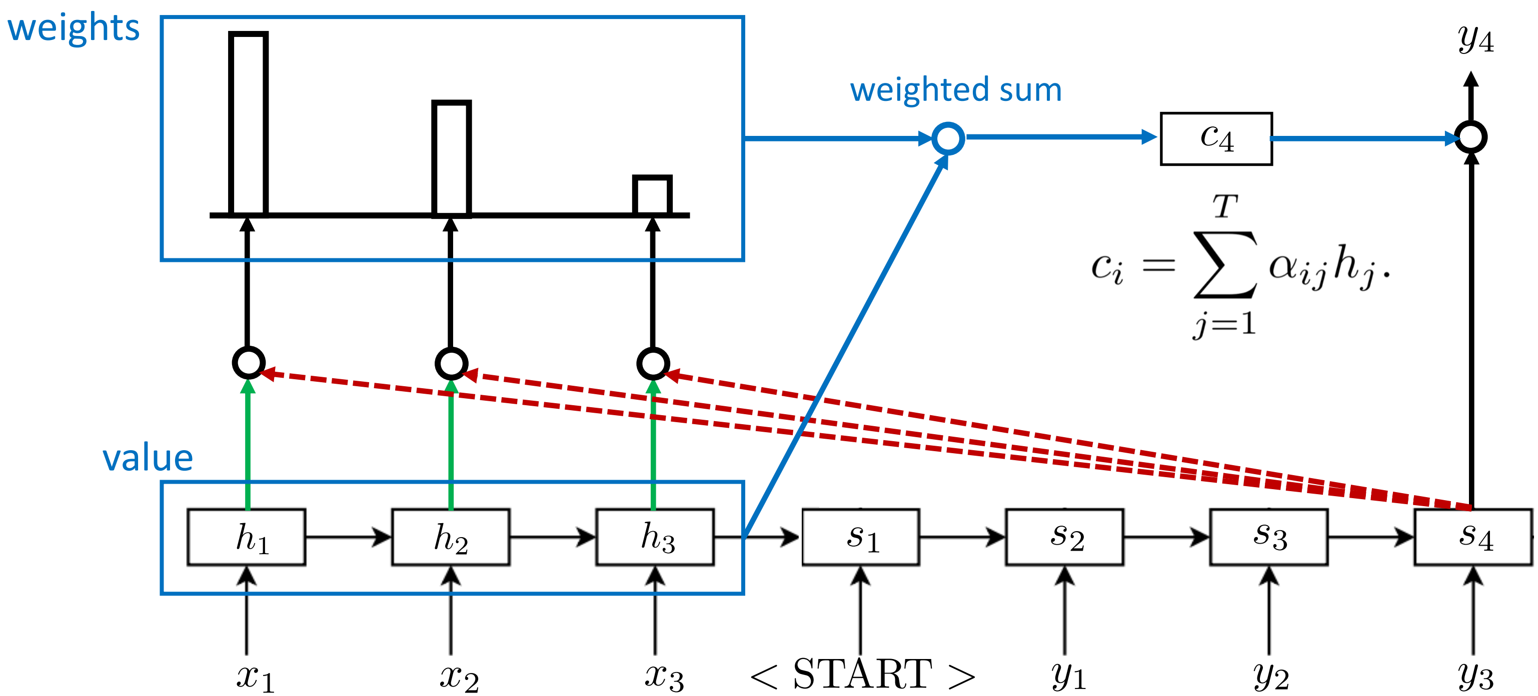
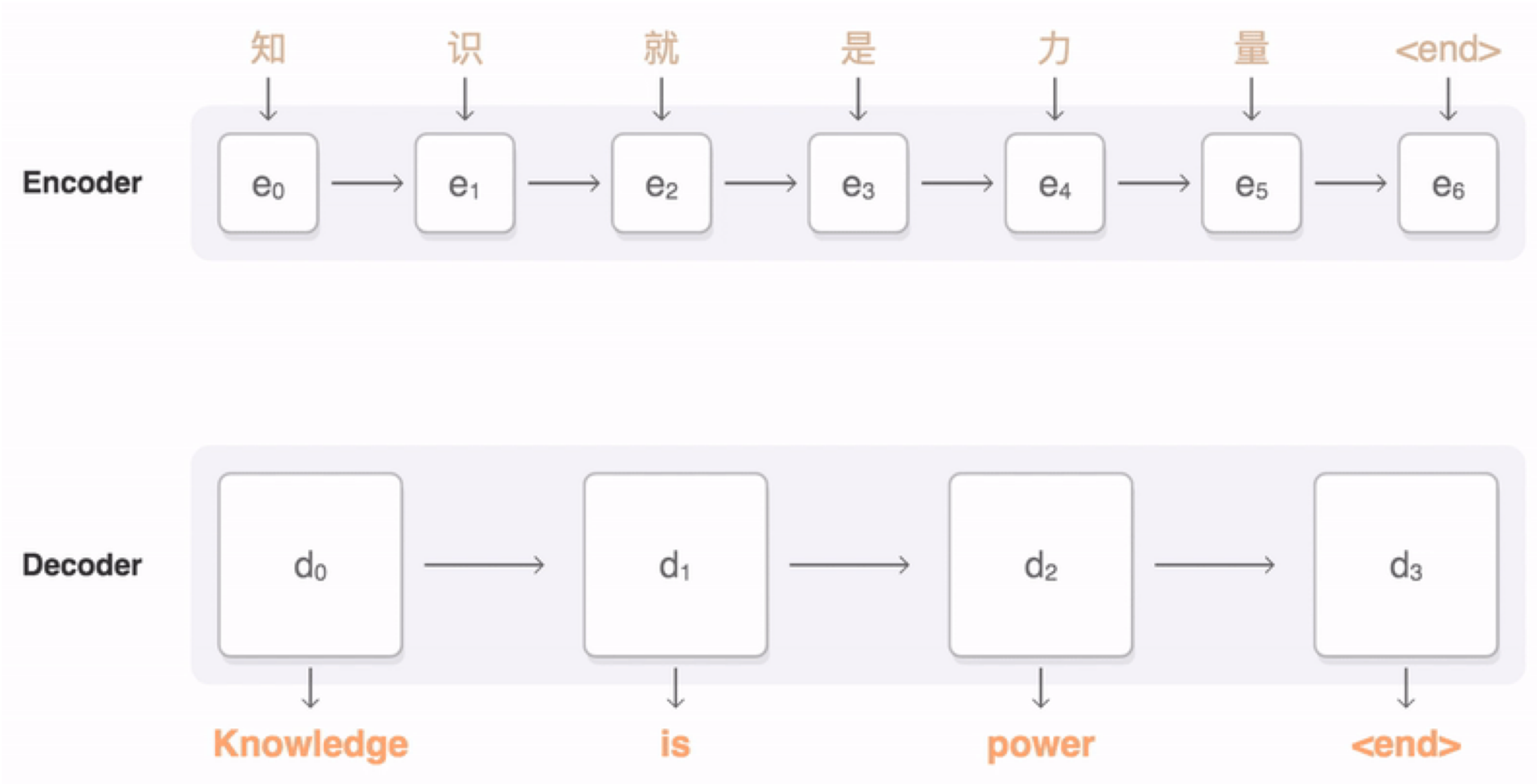
  - Dependent on the query with key, **attention** is a technique to compute a weighted sum of the values
    - Query: decoder's hidden state, key and value: encoder's hidden states
    - The context vector c_i is computed as **weighted sum** of h_i



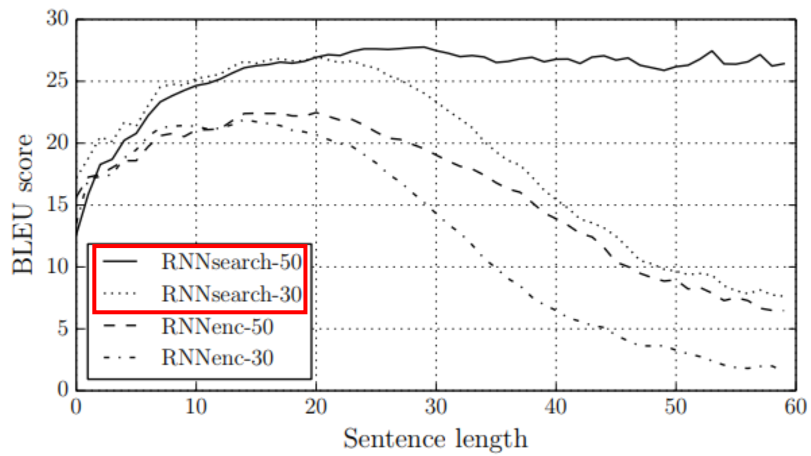
Breakthroughs in NMT: Sequence-to-Sequence Model with Attention

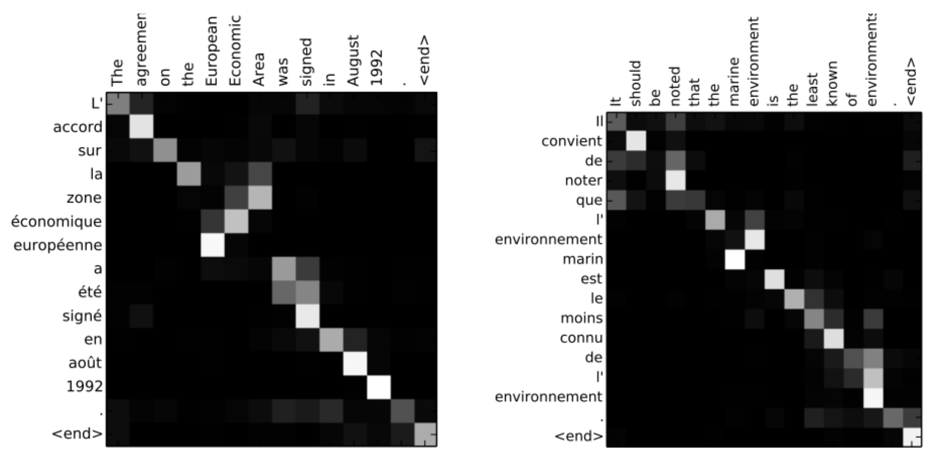
- **Graphical illustration** of seq2seq with **attention**
  - E.g., Chinese to English



*source: https://google.github.io/seq2seq/

- **Results**
  - RNNsearch (with attention) is better than RNNenc (vanilla seq2seq)
  - RNNsearch-50: model trained with sentences of length up to 50 words



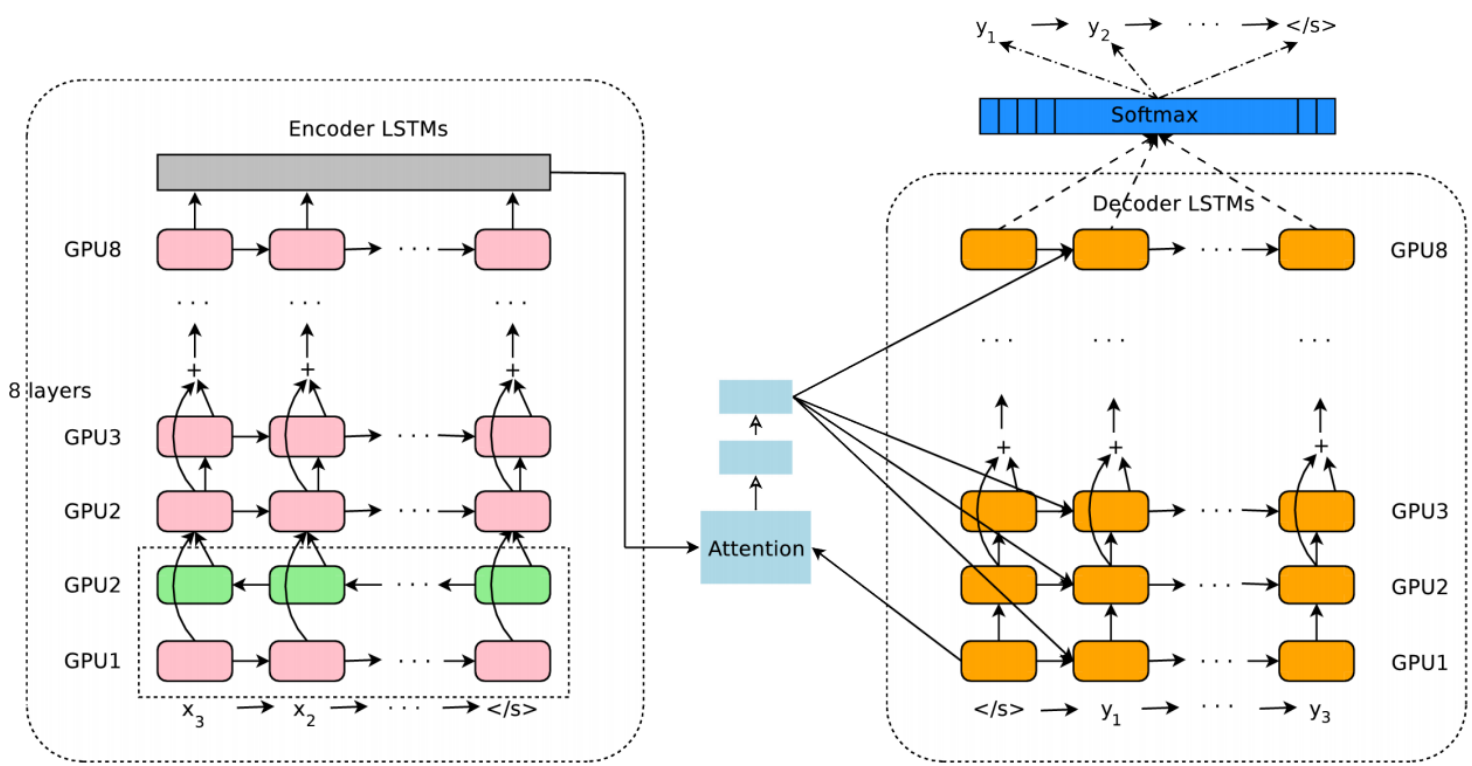


(a) (b)

Sample alignment results (attention map)

Google's Neural Machine Translation (GNMT)

- **Google's NMT** [Wu et al., 2016]
  - Improves over previous NMT systems on **accuracy** and **speed**
  - **8-layer LSTMS** for encoder/decoder with **attention**
    - Achieve **model parallelism** by assigning each LSTM layer into different GPUs
    - Add **residual connections in standard LSTM**
    - … and lots of domain-specific details to apply it to production model



Google's Neural Machine Translation (GNMT)

- **Google's NMT** [Wu et al., 2016]
  - Improves over previous NMT systems on **accuracy** and **speed**
  - **8-layer LSTMS** for encoder/decoder with **attention**
  - State-of-the-art results on various MT datasets and comparable with Human expert

Table 5: Single model results on WMT En→De (newstest2014)

Model	BLEU	CPU decoding time per sentence (s)
Word	23.12	0.2972
Character (512 nodes)	22.62	0.8011
WPM-8K	23.50	0.2079
WPM-16K	24.36	0.1931
WPM-32K	24.61	0.1882
Mixed Word/Character	24.17	0.3268
PBMT [6]	20.7	
RNNSearch [37]	16.5	
RNNSearch-LV [37]	16.9	
RNNSearch-LV [37]	16.9	
Deep-Att [45]	20.6	

Table 10: Mean of side-by-side scores on production data

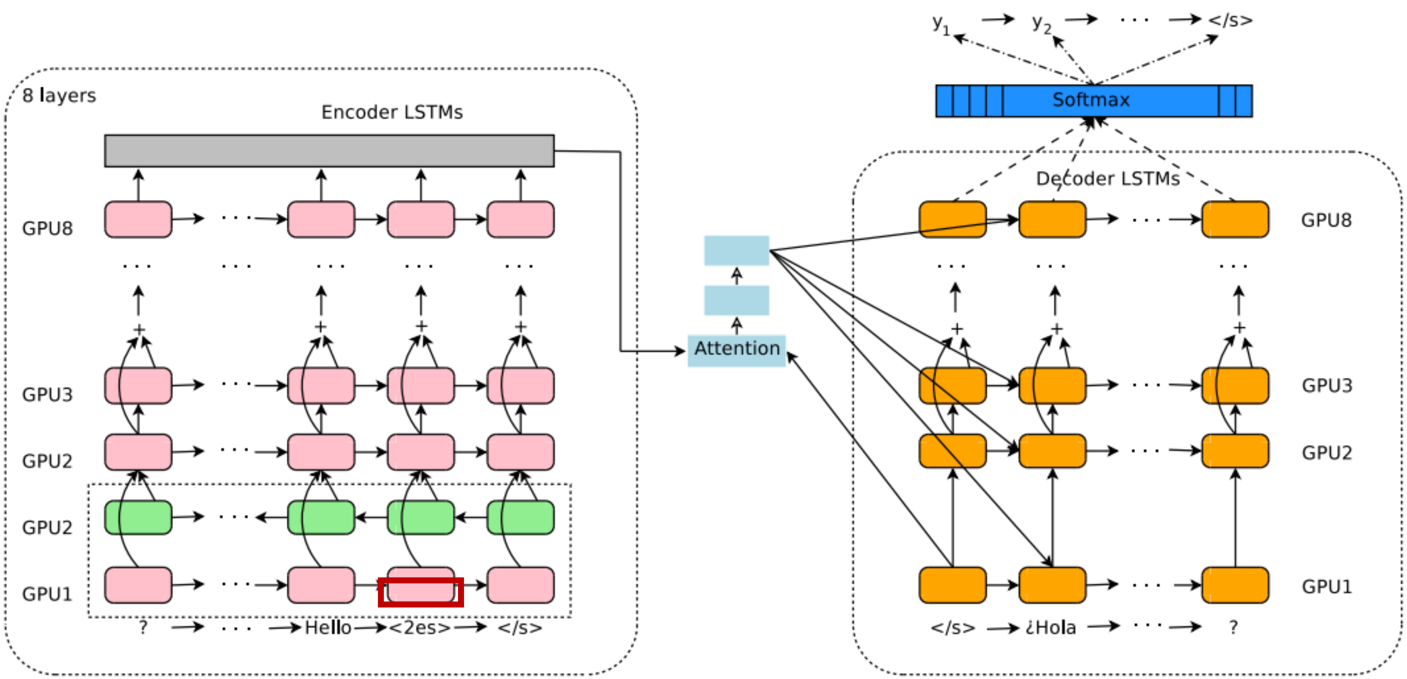
	PBMT	GNMT	Human	Relative Improvement
English → Spanish	4.885	5.428	5.504	87%
English → French	4.932	5.295	5.496	64%
English → Chinese	4.035	4.594	4.987	58%
Spanish → English	4.872	5.187	5.372	63%
French → English	5.046	5.343	5.404	83%
Chinese → English	3.694	4.263	4.636	60%

GNMT with different configurations

Google's Multilingual Neural Machine Translation (Multilingual GNMT)

- Google's NMT is further improved in [Johnson et al., 2016]

- Extensions to make this model to be **Multilingual NMT** system by adding **artificial token** to indicate the required **target language**
  - E.g., the token "<2es>" indicates that the target sentence is in Spanish
  - Can do multilingual NMT using a **single model w/o increasing the parameters**



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  - E.g., the token "<2es>" indicates that the target sentence is in Spanish
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- **Summary**
  - **2014**: First seq2seq paper published
  - **2016**: Google Translate switches from SMT to NMT – and by **2018 everyone has**
  - **Remark**. **SMT** systems, built by hundreds of engineers over many years, outperformed by **NMT** systems trained by a small group of engineers in a few months

*reference: http://web.stanford.edu/class/cs224n/

Google's Multilingual Neural Machine Translation (Multilingual GNMT)

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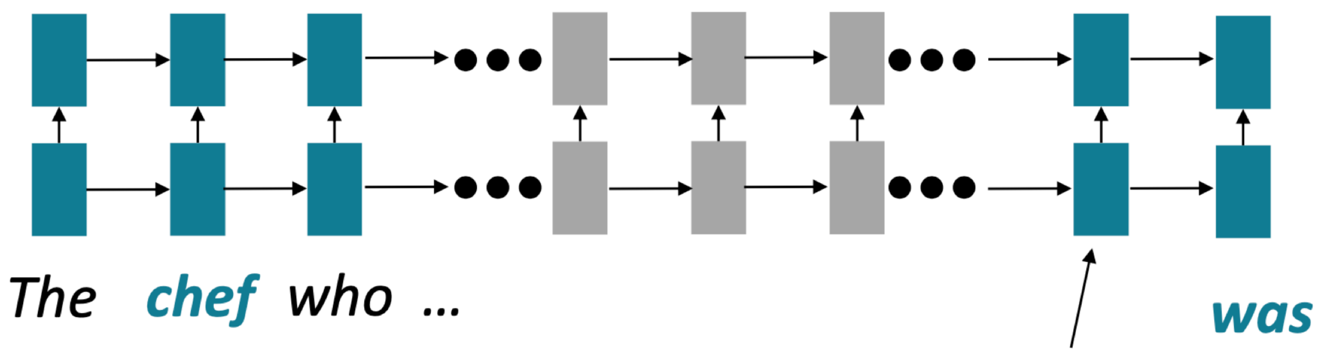
- Extensions to make this model to be **Multilingual NMT** system by adding **artificial token** to indicate the required **target language**
  - E.g., the token "<2es>" indicates that the target sentence is in Spanish
  - Can do multilingual NMT using a **single model w/o increasing the parameters**
- **Next**
  - **Now (2021)**, other approaches have become dominant for many tasks
  - For example, in **WMT** (a Machine Translation conference + competition):
    - In WMT **2016**, the summary report contains "**RNN**" **44** times
    - In WMT **2019**: "RNN" 7 times, "**Transformer**" **105** times

Next, Transformer (self-attention)

Table of Contents

Issue with Recurrent Models

- Although RNNs show remarkable successes, there are **fundamental issues**:
  1. **O(sequence length)** steps for distant word pairs to interact means
     - Hard to learn long-distance dependencies because of gradient problems
  2. Forward/backward passes have **O(sequence length)** unparallelizable operations
     - Future RNN hidden states can't be computed before past states have been computed
     - This aspect inhibits training on the very large datasets

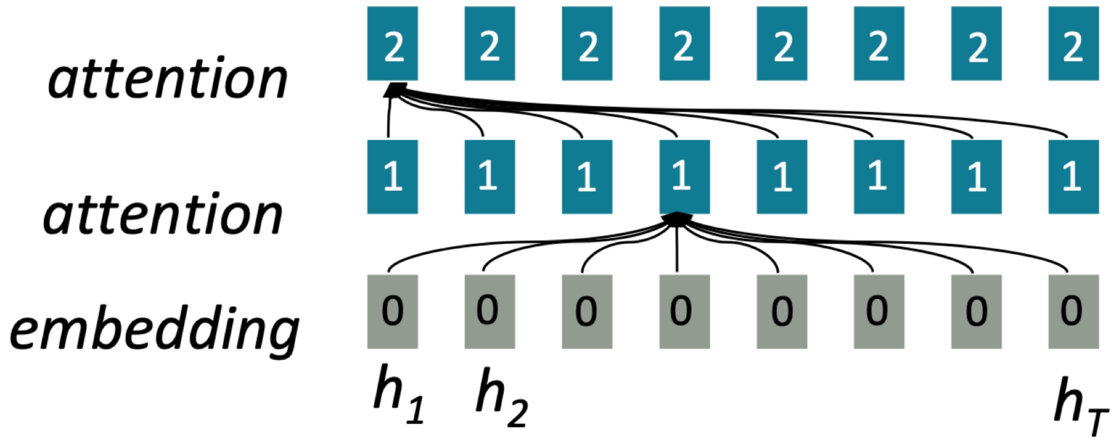


Info of **chef** has gone through **O(sequence length)** many layers

Issue with Recurrent Models

- Although RNNs show remarkable successes, there are **fundamental issues**:
  1. **O(sequence length)** steps for distant word pairs to interact means
  2. Forward/backward passes have **O(sequence length)** unparallelizable operations

- In contrast, **attention has some advantages** in these aspects:
  1. Maximum interaction distance: **O(1)**
     - Since all words interact at each layer
  2. Number of unparallelizable operations does **not increase with respect to length**



All words can attend to all words in previous layer

Issue with Recurrent Models

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  1. **O(sequence length)** steps for distant word pairs to interact means
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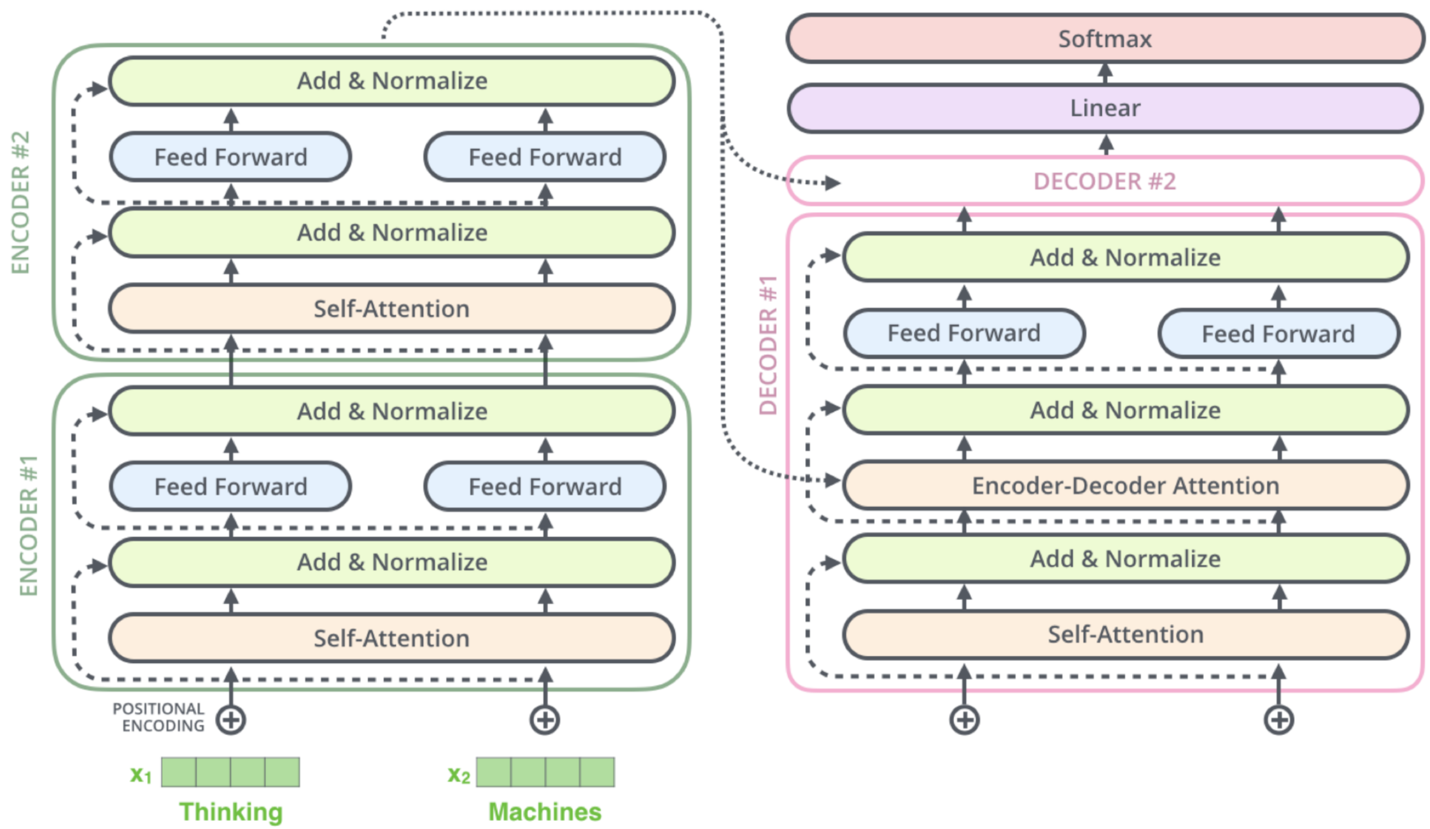
  2. Number of unparallelizable operations does **not increase with respect to length**

Q. Then, can we design an architecture **only using attention** modules?
- Remark. We saw attention from the **decoder to the encoder**; but here, we'll think about attention **within a single sentence**.

Transformer (Self-attention)

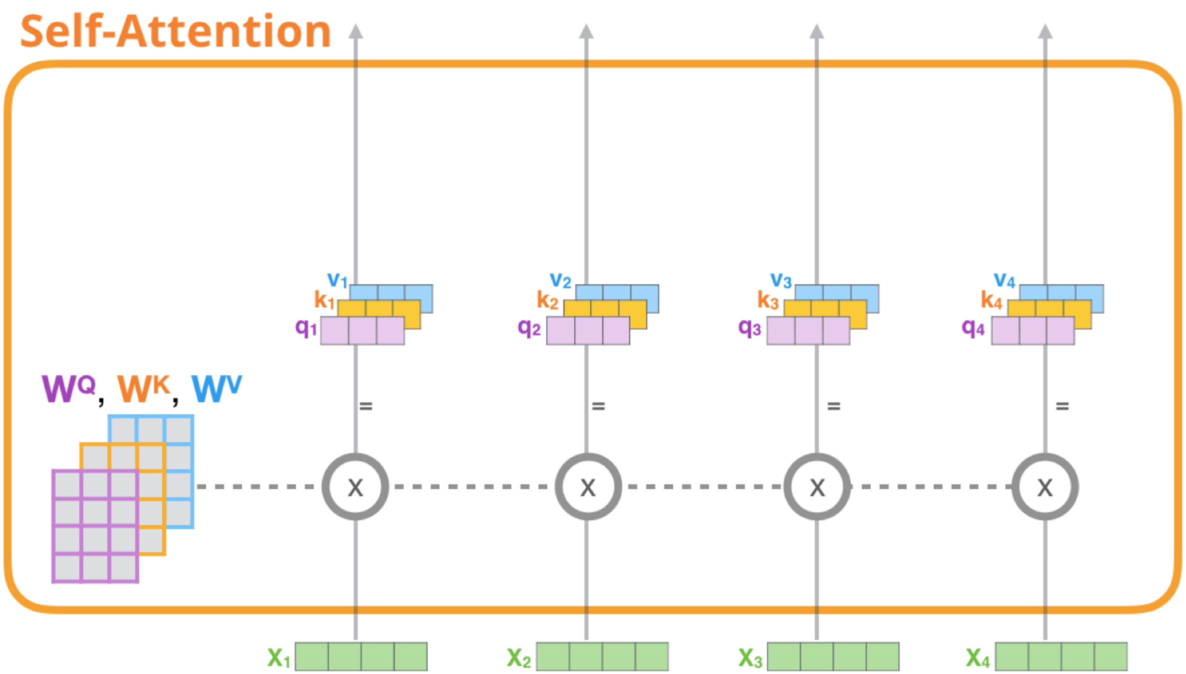
- Transformer [Vaswani et al., 2017] has an **encoder-decoder** structure and they are composed of multiple block with **multi-head (self) attention** module



*reference: http:// http://jalammar.github.io/illustrated-transformer

- **Self-attention**
  - **Recall**: Attention operates on query, key, and value
    - Query is decoder's hidden state, key and value are encoder's hidden states in seq2seq
  - In self-attention, the query, key, and value are drawn from the **same source**
    1. For each input x_i , create query, key, and value vectors q_i, k_i, v_i by multiplying **learnable** weight matrices

$$q_i = W^Q x_i, k_i = W^k x_i, v_i = W^V x_i$$



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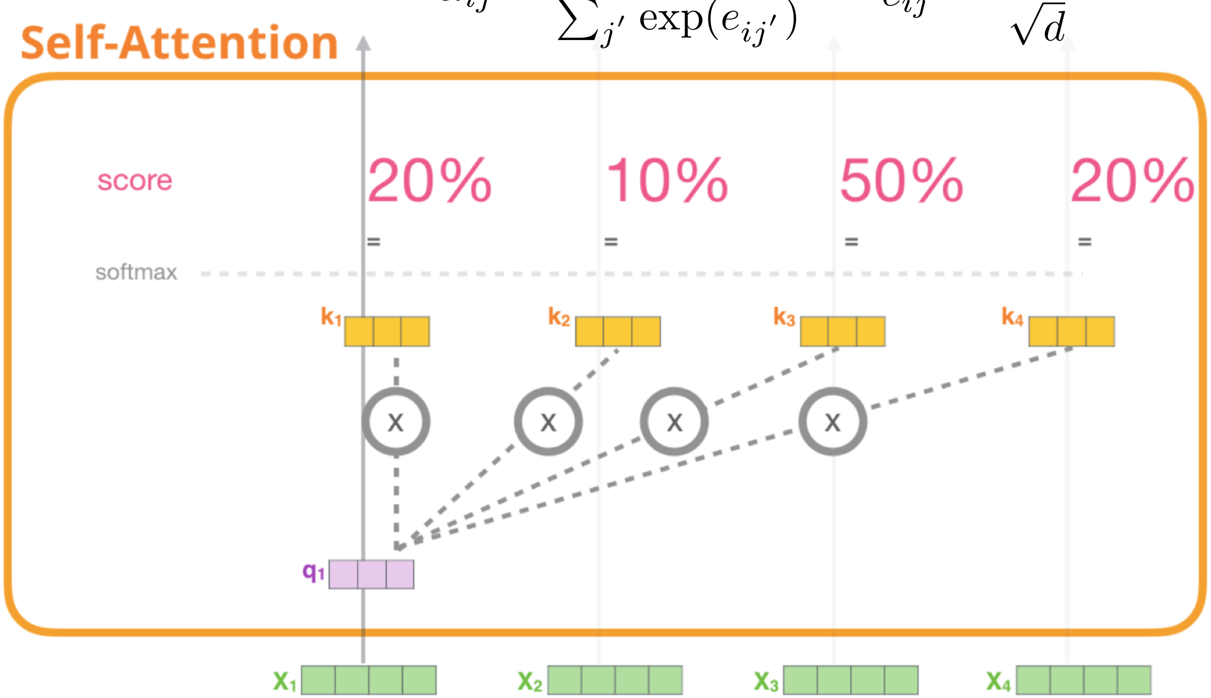
    1. For each input x_i , create query, key, and value vectors q_i, k_i, v_i
    2. Multiply (**dot product**) the current query vector, by all the key vectors, to get a **score** α_{ij} of **how well they match**

$$\alpha_{ij} = \frac{\exp(e_{ij})}{\sum_{j'} \exp(e_{ij'})} \qquad e_{ij} = \frac{q_i^T k_j}{\sqrt{d}}$$



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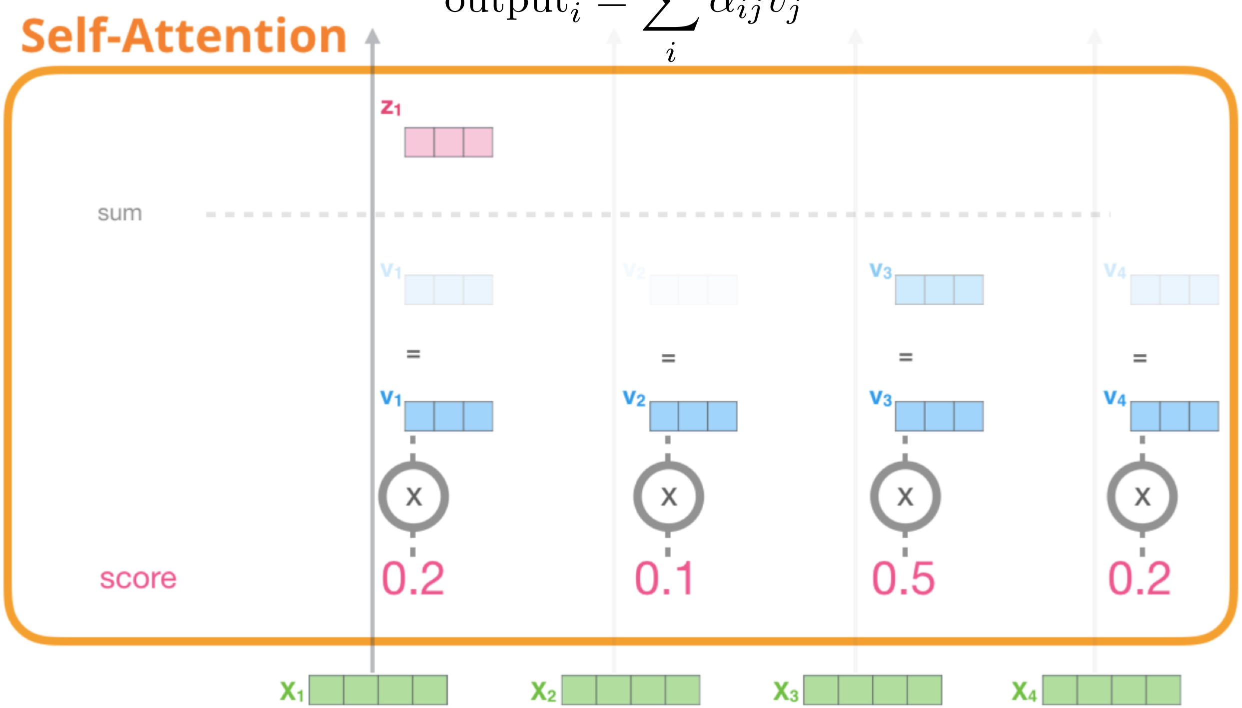
    2. Multiply (**dot product**) the current query vector, by all the key vectors, to get a **score** α_{ij}
    3. Multiply the value vectors by the scores, then **sum up**

$$\text{output}_i = \sum_i \alpha_{ij} v_j$$



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  - Hence, self-attention is **effective to learn the context** within given sentence
    - It's easier than recurrent layer to be parallelized and model the long-term dependency

Layer Type	Complexity per Layer	Sequential Operations	Maximum Path Length
Self-Attention	$O(n^2 \cdot d)$	$O(1)$	$O(1)$
Recurrent	$O(n \cdot d^2)$	$O(n)$	$O(n)$
Convolutional	$O(k \cdot n \cdot d^2)$	$O(1)$	$O(log_k(n))$
Self-Attention (restricted)	$O(r \cdot n \cdot d)$	$O(1)$	$O(n/r)$

*reference: http:// http://jalammar.github.io/illustrated-gpt2

Transformer (Self-attention)

- **Self-attention**
  - **Recall**: Attention operates on query, key, and value
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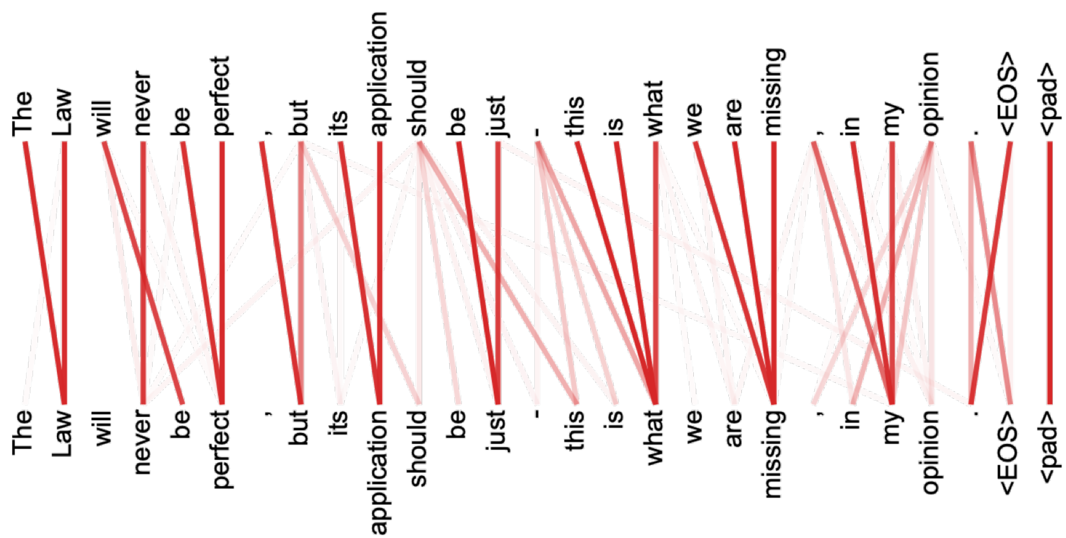
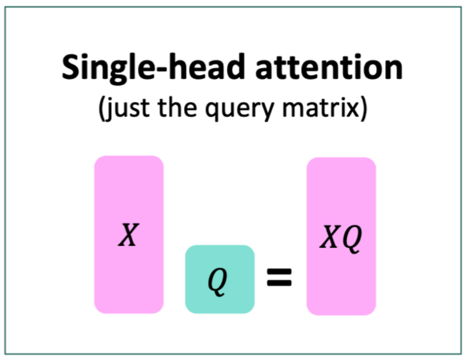
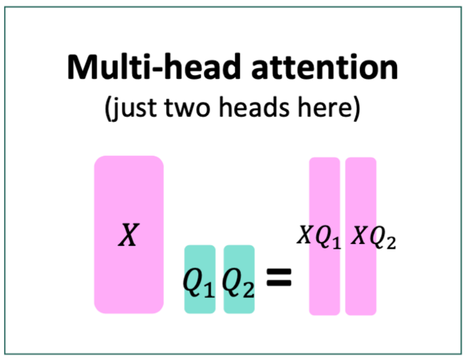
    3. Multiply the value vectors by the scores, then **sum up**
  - Hence, self-attention is **effective to learn the context** within given sentence
    - It's easier than recurrent layer to be parallelized and model the long-term dependency
    - It also provides an **interpretability** of learned representation



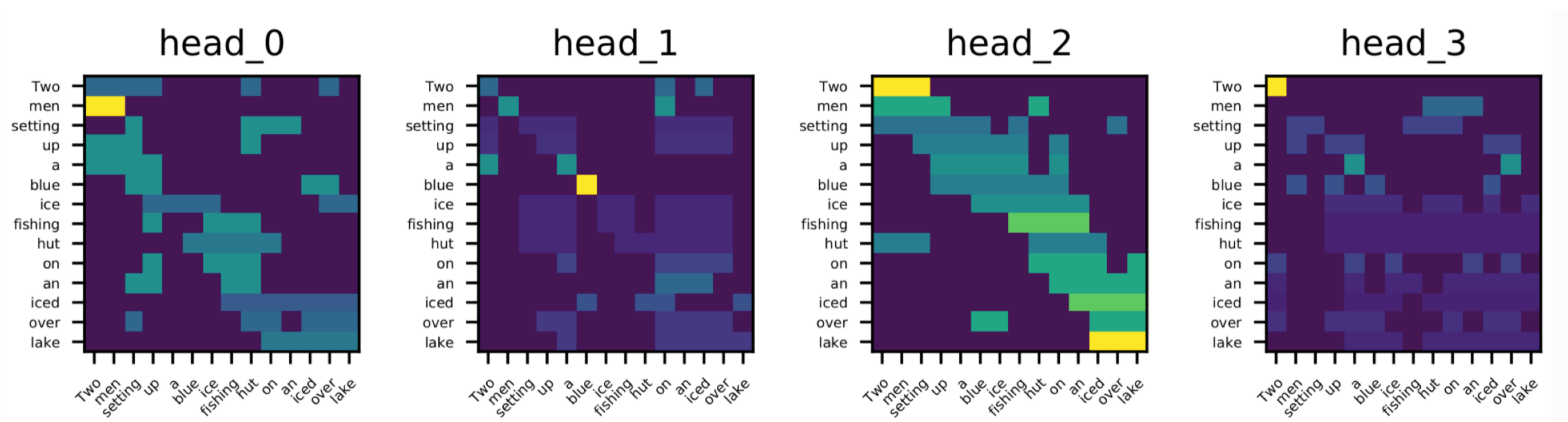
*reference: http:// http://jalammar.github.io/illustrated-gpt2

- **Multi-head attention**
  - Applying **multiple attentions at once** to look in multiple places in the sentence
    - To prevent the increase of computation, original attentions weights are **divided**





Same amount of computation as single-head self-attention



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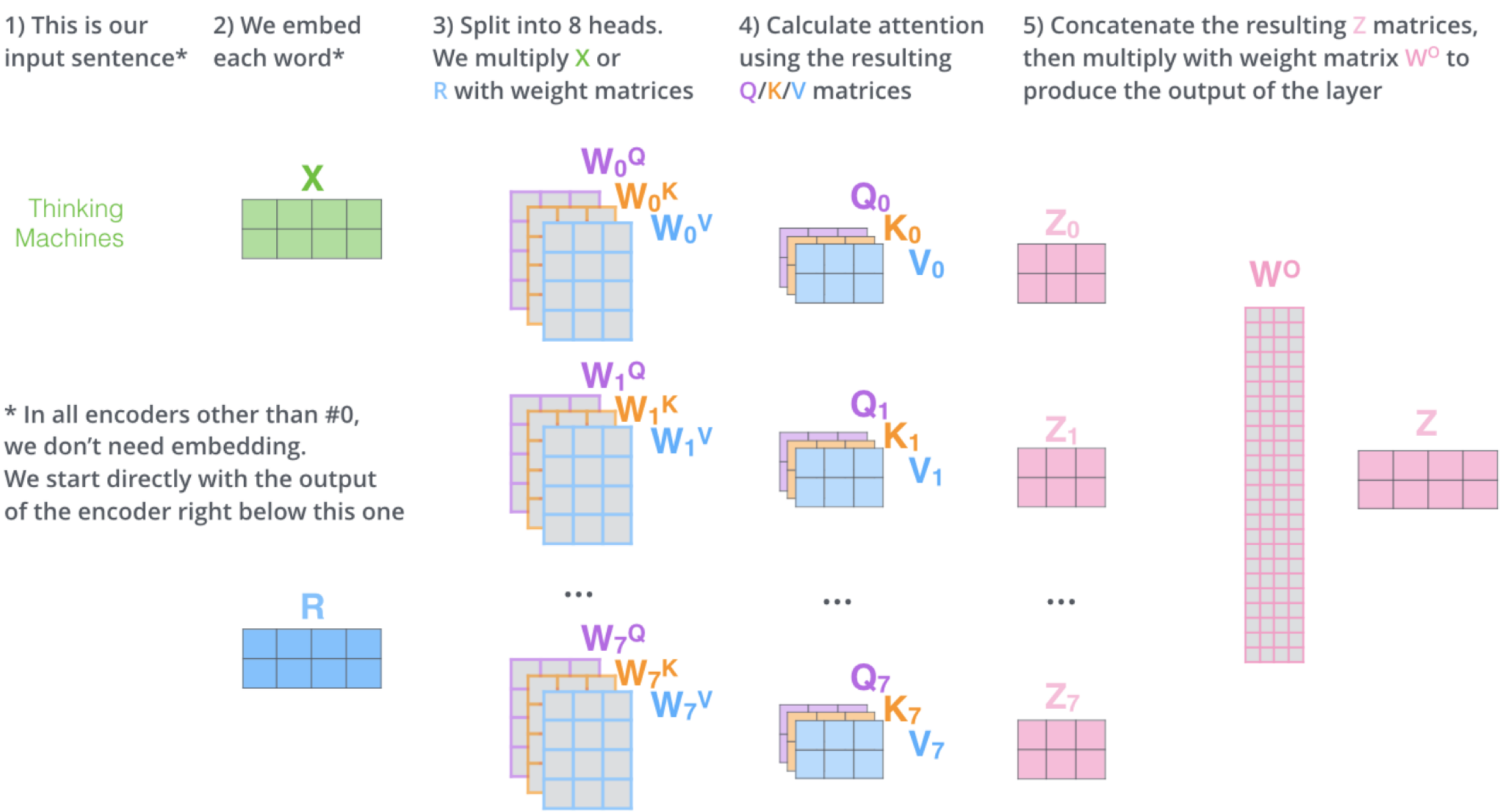
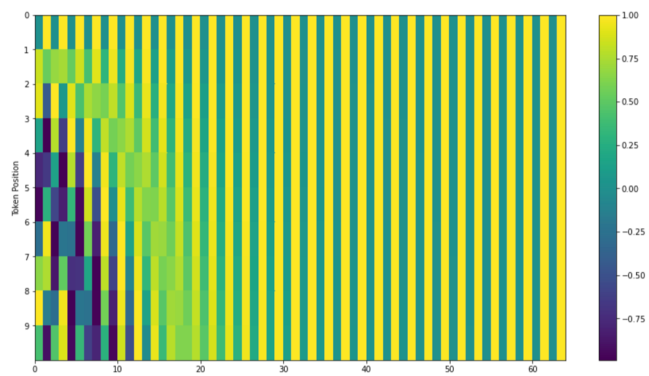


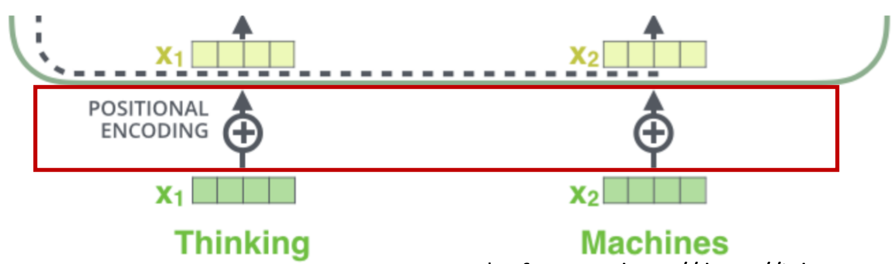
*reference: http:// http://jalammar.github.io/illustrated-transformer

- **Encoder**
  - Self-attention is **invariant to order** of input sequence
    - To represent the order of sequence, **positional encoding** is added to input embeddings at the **bottoms of the encoder and decoder stacks**
  - Fixed sine and cosine functions are used for each position pos and dimension i

$$PE_{(pos,2i)} = sin(pos/10000^{2i/d_{\text{model}}}) \quad PE_{(pos,2i+1)} = cos(pos/10000^{2i/d_{\text{model}}})$$

    - PE_{pos+k} can be derived as a linear function of PE_{pos} → easier to learn a relative position
    - Compare to learning encoding, it's better for **extrapolation** (not encountered in training)





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- **Encoder**
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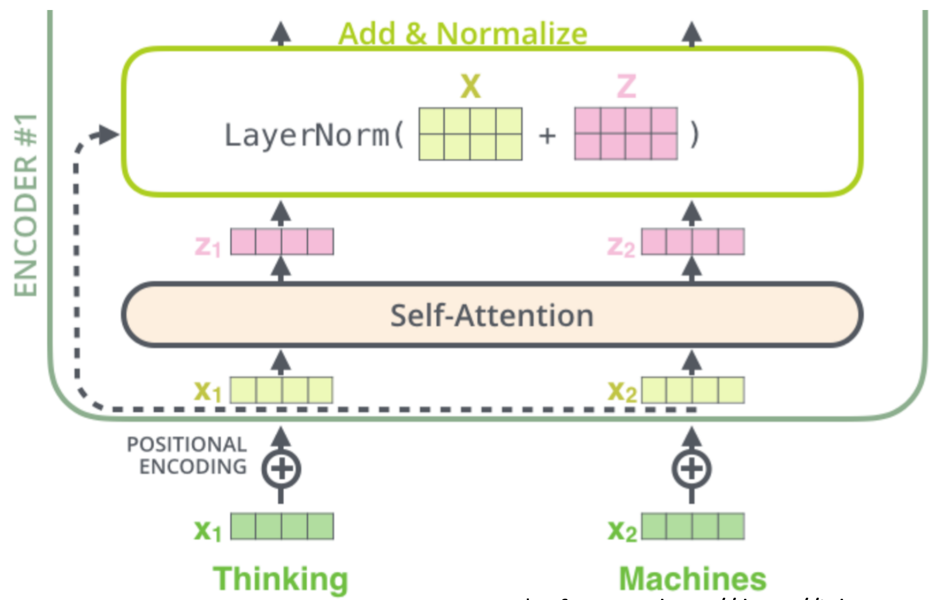

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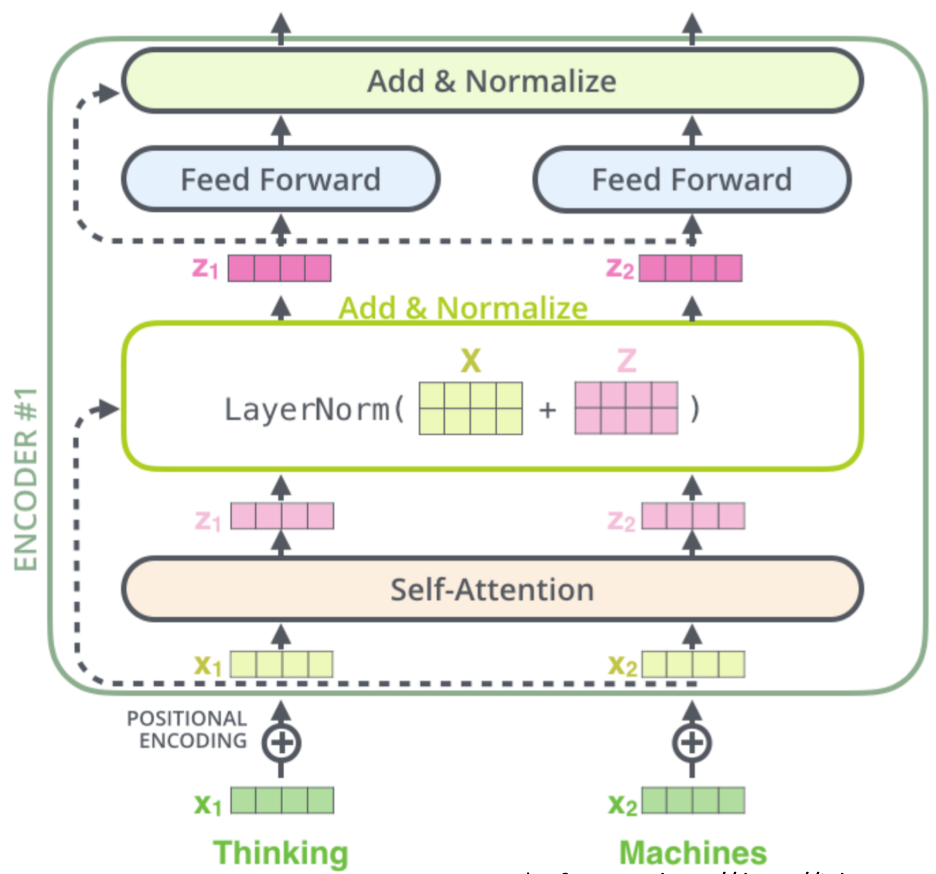
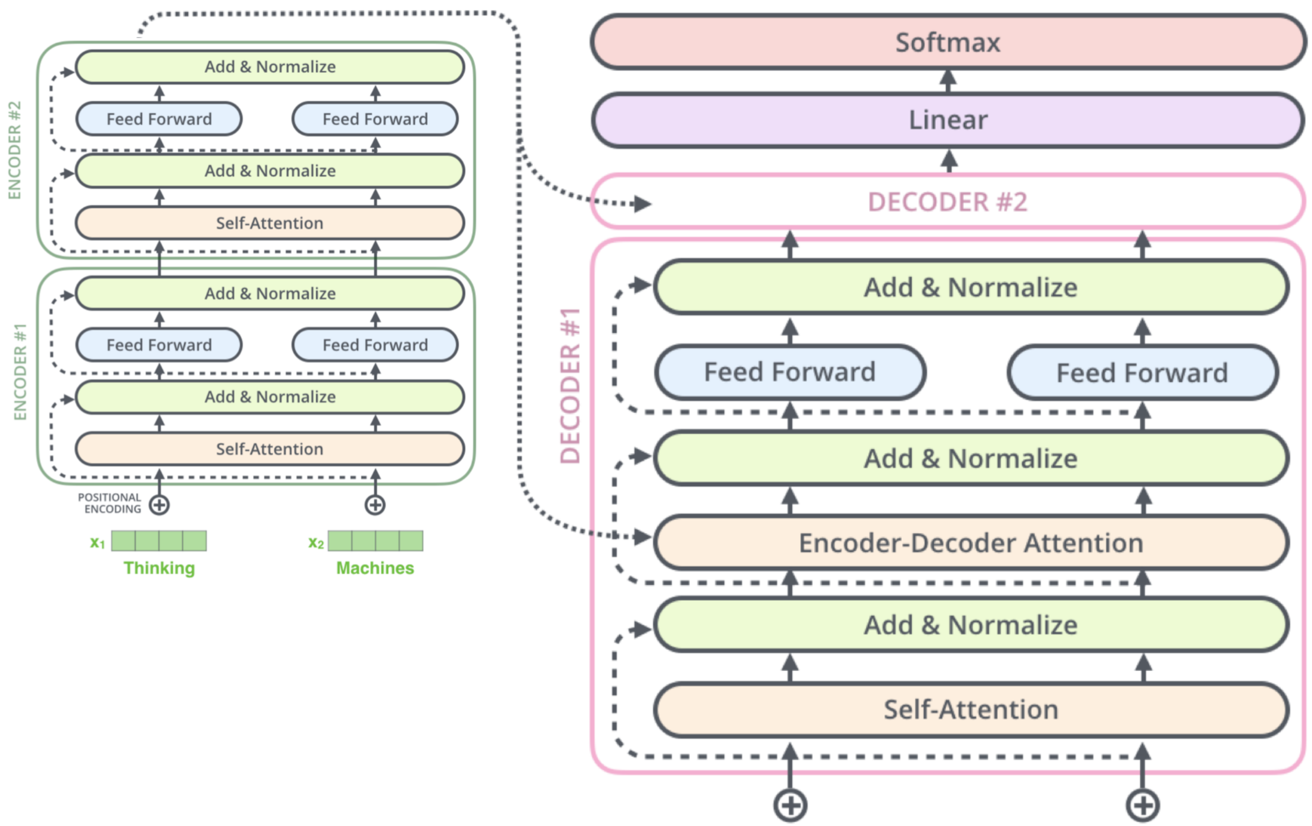
Transformer (Self-attention)

- **Encoder**
  - Self-attention is **invariant to order** of input sequence ⟶ **positional encoding**
  - **Residual connections** (dotted) and **layer normalization** are used to help training
  - Non-linearity is imposed by adding position-wise **feed-forward networks**



*reference: http:// http://jalammar.github.io/illustrated-transformer

- **Decoder**
  - Most parts are same with encoder except **encoder-decoder(cross) attention**
  - This cross attention is previously used in seq2seq model
    - Queries are drawn from the **decoder**
    - Keys and values are drawn from the **encoder** (like context vector)



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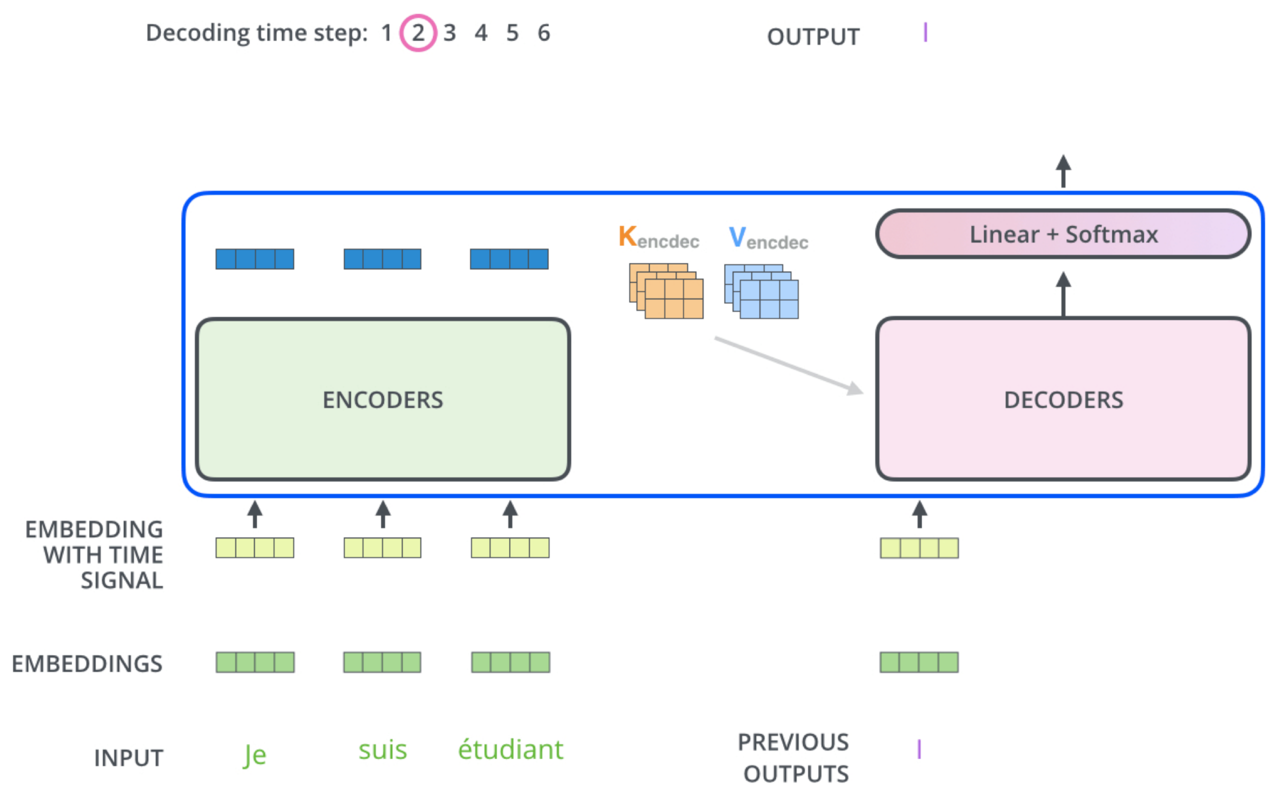


*reference: http:// http://jalammar.github.io/illustrated-transformer

Transformer (Self-attention)

- Success of Transformer: **Machine Translation (MT)**
  - Initially, Transformer shows **better results at a fraction of the training cost**

Model	BLEU		Training Cost (FLOPs)	
	EN-DE	EN-FR	EN-DE	EN-FR
ByteNet [15]	23.75			
Deep-Att + PosUnk [32]		39.2		$1.0 \cdot 10^{20}$
GNMT + RL [31]	24.6	39.92	$2.3 \cdot 10^{19}$	$1.4 \cdot 10^{20}$
ConvS2S [8]	25.16	40.46	$9.6 \cdot 10^{18}$	$1.5 \cdot 10^{20}$
MoE [26]	26.03	40.56	$2.0 \cdot 10^{19}$	$1.2 \cdot 10^{20}$
Deep-Att + PosUnk Ensemble [32]		40.4		$8.0 \cdot 10^{20}$
GNMT + RL Ensemble [31]	26.30	41.16	$1.8 \cdot 10^{20}$	$1.1 \cdot 10^{21}$
ConvS2S Ensemble [8]	26.36	**41.29**	$7.7 \cdot 10^{19}$	$1.2 \cdot 10^{21}$
Transformer (base model)	27.3	38.1	$\mathbf{3.3 \cdot 10^{18}}$	
Transformer (big)	**28.4**	**41.0**	$2.3 \cdot 10^{19}$	

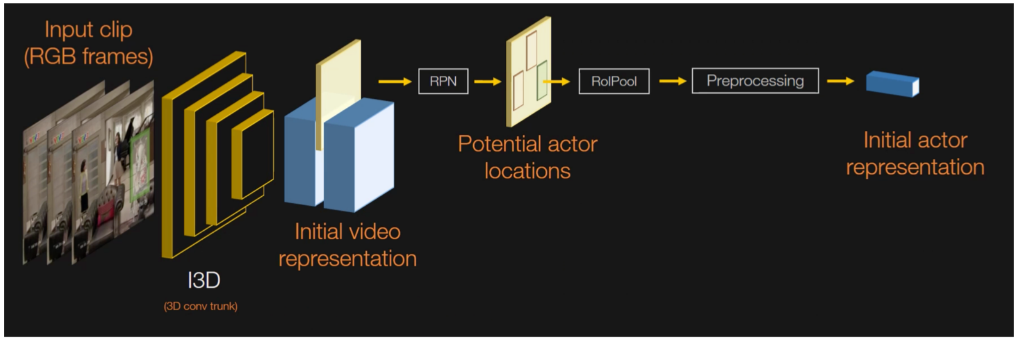
  - Nowadays, Transformer is still a standard for MT with additional techniques

System	**En→De** news2017	**En→De** news2018
baseline	30.90	45.40
+ langid filtering	30.78	46.43
+ ffn 8192	31.15	46.28
+ BT	33.62	46.66
+ fine tuning	-	47.61
+ ensemble	-	49.27
+ reranking	-	50.63
WMT'18 submission	-	46.10
WMT'19 submission	**42.7**	

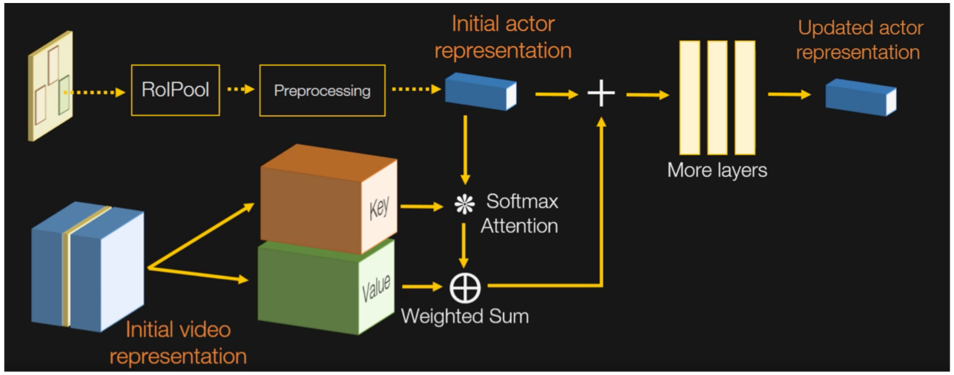
*reference: https://arxiv.org/pdf/1907.06616v1.pdf

Transformer (Self-attention)

- Success of Transformer: **Video action recognition** [Girdhar et al., 2018]
  - **Goal**: localize the atomic action in space and time
  - Previous approaches just use the feature of key frame with object detection
    - But, it's hard to model the interaction between frames



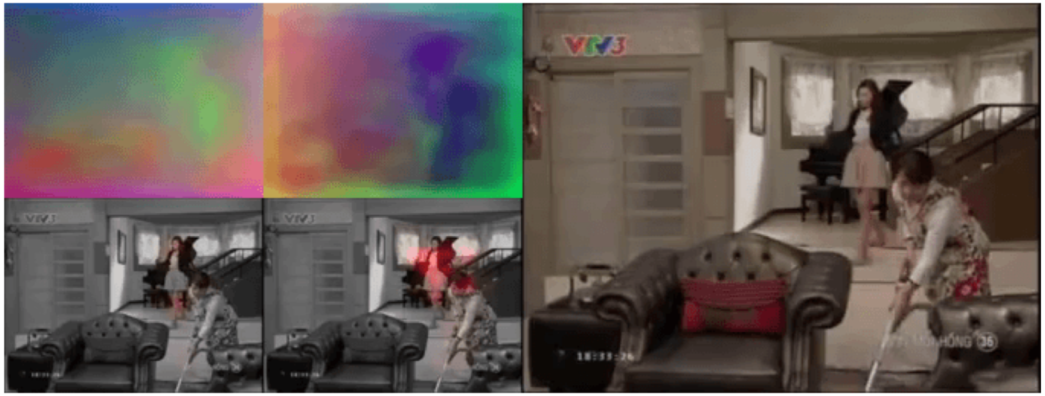
  - **Self-attention is an effective way** to resolve this issue



*reference: https://rohitgirdhar.github.io/ActionTransformer

Transformer (Self-attention)

- Success of Transformer: **Video action recognition** [Girdhar et al., 2018]
  - **Qualitative results of learned attention**



  - **Winner of AVA challenge in 2019: > 3.5 %** than previous challenge winner

Method	Modalities	Architecture	Val mAP	Test mAP
Single frame [16]	RGB, Flow	R-50, FRCNN	14.7	-
AVA baseline [16]	RGB, Flow	I3D, FRCNN, R-50	15.6	-
ARCN [42]	RGB, Flow	S3D-G, RN	17.4	-
Fudan University	-	-	-	17.16
YH Technologies [52]	RGB, Flow	P3D, FRCNN	-	19.60
Tsinghua/Megvii [23]	RGB, Flow	I3D, FRCNN, NL, TSN, C2D, P3D, C3D, FPN	-	21.08
Ours (Tx-only head)	RGB	I3D, Tx	24.4	24.30
Ours (Tx+I3D head)	RGB	I3D, Tx	24.9	24.60
Ours (Tx+I3D+96f)	RGB	I3D, Tx	**25.0**	**24.93**

*reference: https://rohitgirdhar.github.io/ActionTransformer

Transformer (Self-attention)

- Success of Transformer: **Music generation** [Huang et al., 2018]
  - **Goal**: generate music which contains structure at multiple timescales (short to long)
  - Performance RNN (LSTM): lack of long-term structure

  - Music transformer; able to continue playing with consistent style

*reference: https://magenta.tensorflow.org/music-transformer

Pre-training / Fine-tuning Paradigm with Transformers

- **Motivation**
  - Many success of CNN comes from ImageNet-pretrained networks
    - Simple fine-tuning improves the performance than training from scratch
  - Then, can we train a similar universal encoder for NLP tasks?
    - As labeling of NLP task is more ambiguous, **unsupervised pre-training is essential**
  - **Language modeling**, i.e., reconstruction, is simple and feasible for our goal
    - With diverse examples, model can learn the useful knowledge about the world

"Overall, the value I got from the two hours watching it was the sum total of the popcorn and the drink. The movie was __." ⟶ *terrible*

"I wat thinking about the sequence that goes 1, 1, 2, 3, 5, 8, 13, 21, __" ⟶ *34*

"I went to the ocean to see the fish, turtles, seals, and __" ⟶ *sand*

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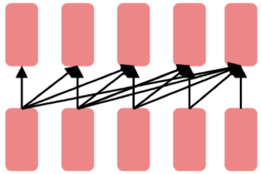
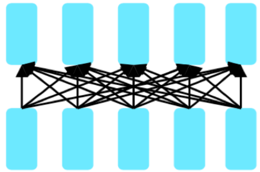
  - **Language modeling**, i.e., reconstruction, is simple and feasible for our goal
    - With diverse examples, model can learn the useful knowledge about the world

- **Pre-training for two types of architectures**
  - Architecture influences the type of pre-training, and natural use cases



Decoders

- E.g. **GPT**
- Pre-training with **normal** language modeling
- Better use for **generation** tasks



Encoders

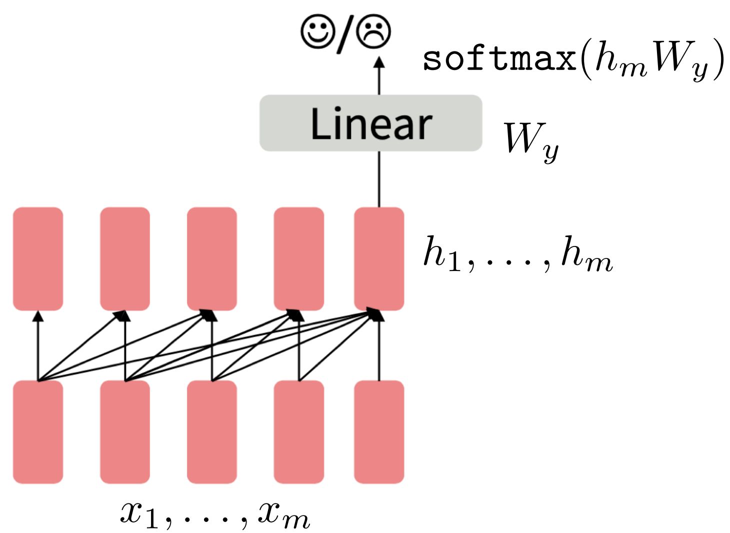
- E.g. **BERT**
- Pre-training with **masked** language modeling
- Better use for **discriminative** tasks (classification)

GPT: Generative Pre-Training with Transformer's Decoder

- **GPT** [Radford et al., 2018]

$$\arg\max_{\theta} \log p(\boldsymbol{x}) = \sum_{n} p_{\theta}(x_n | x_1, \ldots, x_{n-1})$$

  - **Pre-training** by language modeling over 7000 unique books (**unlabeled data**)
    - Contains long spans of contiguous text, for learning long-distance dependencies
  - **Fine-tuning** by training a classifier with target task-specific **labeled data**
    - Classifier is added on the final transformer block's last word's hidden state



*reference: http://web.stanford.edu/class/cs224n/

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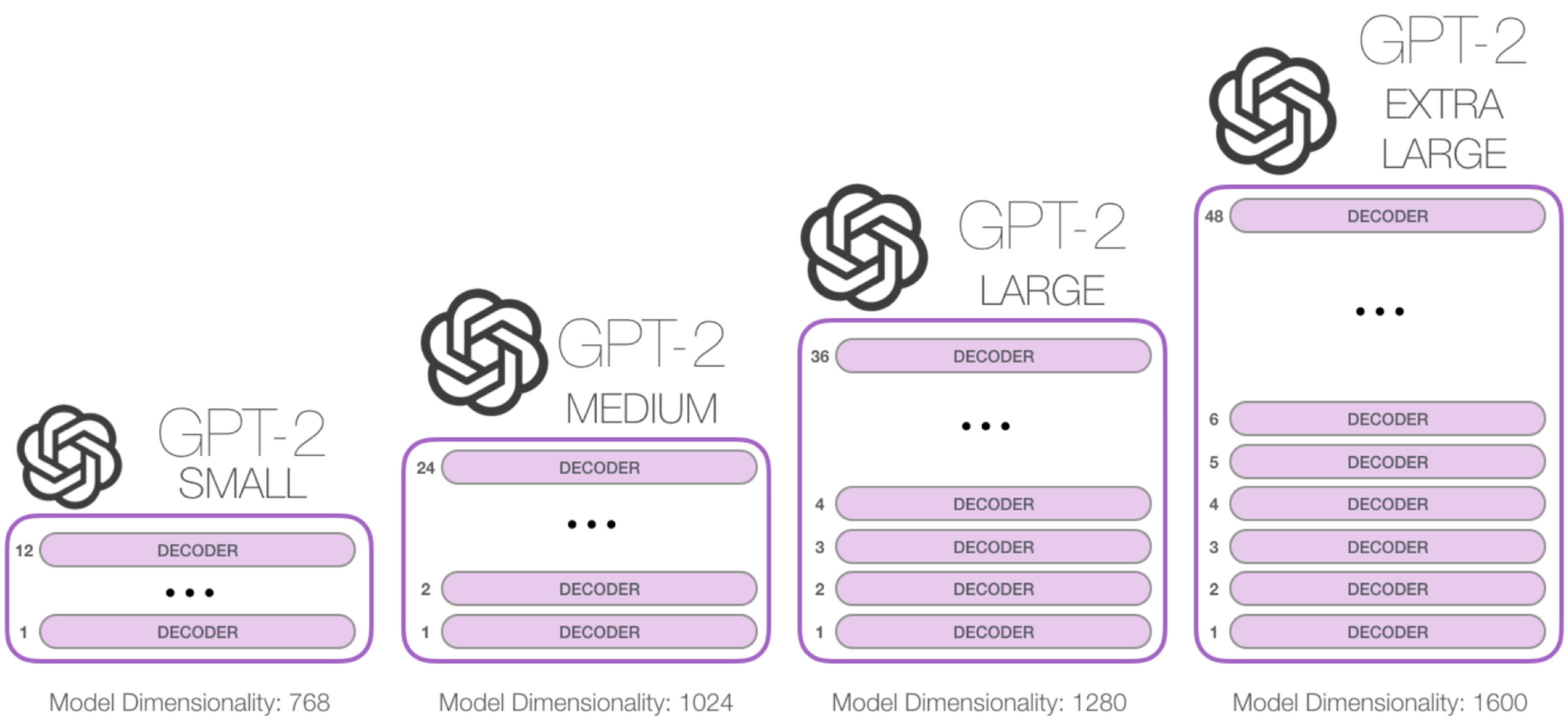
Method	MNLI-m	MNLI-mm	SNLI	SciTail	QNLI	RTE
ESIM + ELMo [44] (5x)	-	-	<u>89.3</u>	-	-	-
CAFE [58] (5x)	80.2	79.0	<u>89.3</u>	-	-	-
Stochastic Answer Network [35] (3x)	<u>80.6</u>	<u>80.1</u>	-	-	-	-
CAFE [58]	78.7	77.9	88.5	<u>83.3</u>		
GenSen [64]	71.4	71.3	-	-	<u>82.3</u>	59.2
Multi-task BiLSTM + Attn [64]	72.2	72.1	-	-	82.1	**61.7**
Finetuned Transformer LM (ours)	**82.1**	**81.4**	**89.9**	**88.3**	**88.1**	56.0

GPT's results on various *natural language inference* datasets

*reference: http://web.stanford.edu/class/cs224n/

GPT-2: Language Models are Unsupervised Multitask Learners

- **GPT-2** [Radford et al., 2019]
  - **Pre-training** by language modeling as same as previous GPT-1, but **training with..**
    - Much **larger datasets**; 8 million documents from web (40 GB of text)
    - Much **larger model size**; # of parameters: 117M (GPT-1) ⟶ 1542M (extra-large GPT-2)



*reference: http:// http://jalammar.github.io/illustrated-gpt2

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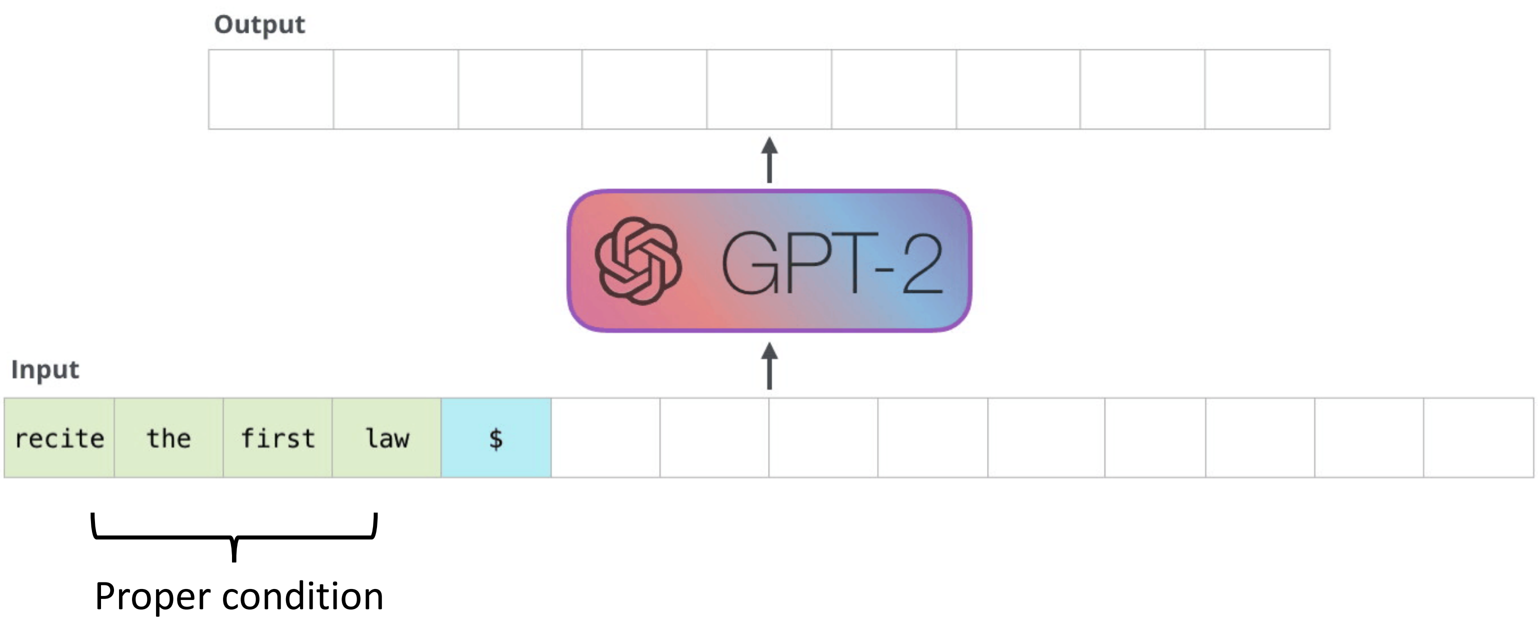
  - GPT-2 can perform down-stream tasks in a **zero-shot setting**
    - Via conditional generation without any parameter or architecture modification



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    - Via conditional generation without any parameter or architecture modification
  - **Remark**. Largest model still underfits.. ⟶ larger model for better performance?

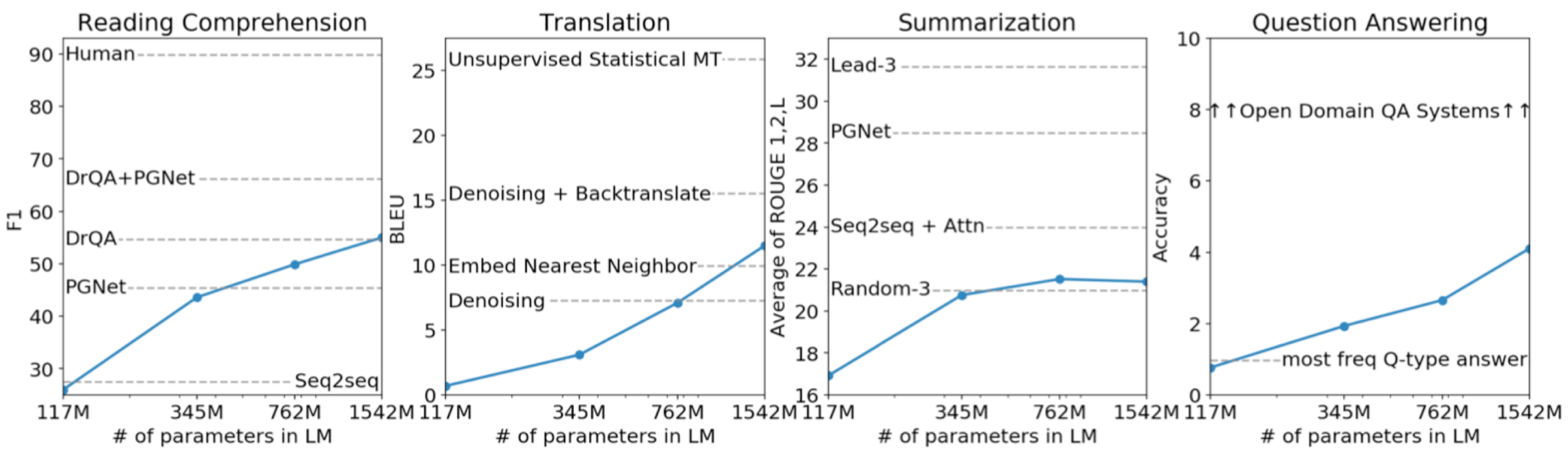
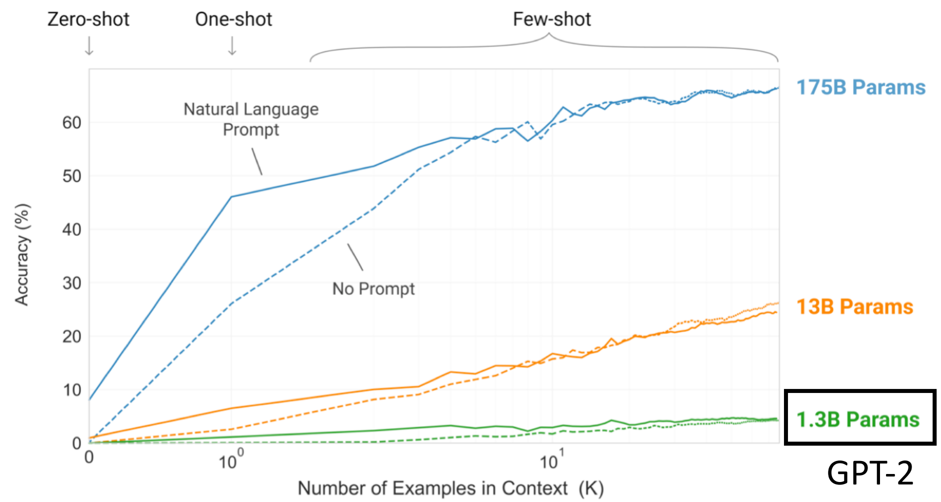


Figure 1. Zero-shot task performance of WebText LMs as a function of model size on many NLP tasks. Reading Comprehension results are on CoQA (Reddy et al., 2018), translation on WMT-14 Fr-En (Artetxe et al., 2017), summarization on CNN and Daily Mail (See et al., 2017), and Question Answering on Natural Questions (Kwiatkowski et al., 2019). Section 3 contains detailed descriptions of each result.

GPT-3: Language Models are Few-shot Learners

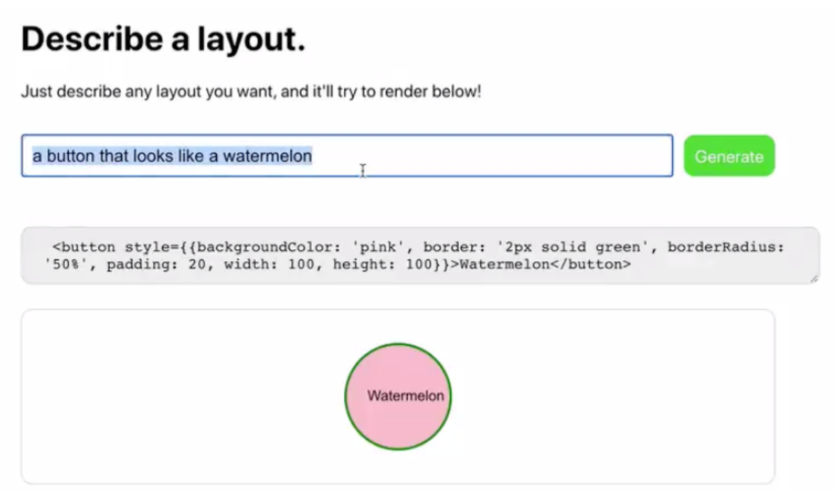
- **GPT-3**: Language Models are Few-shot Learners [Brown et al., 2020]
  - **Very large** language models seem to **perform in-context learning** **without gradient steps (fine-tuning)**
    - **In-context learning**; adapting to specific task from examples with some context



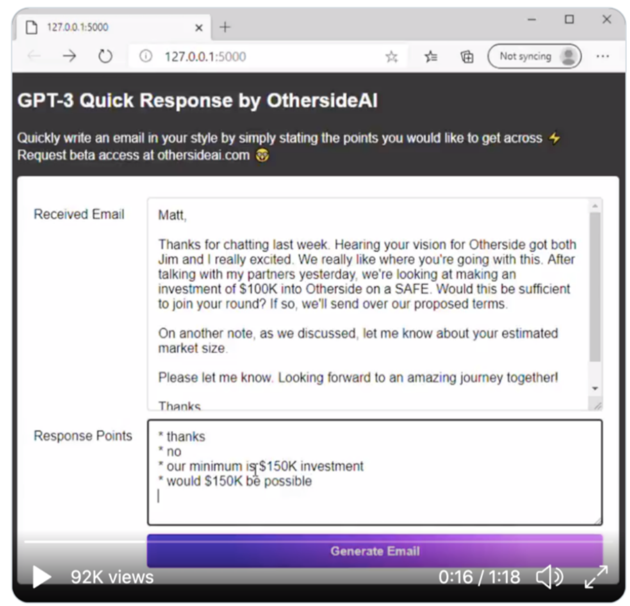
Setting	NaturalQS	WebQS	TriviaQA
RAG (Fine-tuned, Open-Domain) [LPP+20]	**44.5**	**45.5**	**68.0**
T5-11B+SSM (Fine-tuned, Closed-Book) [RRS20]	36.6	44.7	60.5
T5-11B (Fine-tuned, Closed-Book)	34.5	37.4	50.1
GPT-3 Zero-Shot	14.6	14.4	64.3
GPT-3 One-Shot	23.0	25.3	**68.0**
GPT-3 Few-Shot	29.9	41.5	**71.2**

Results on open-domain question answering

- **GPT-3**: Language Models are Few-shot Learners [Brown et al., 2020]
  - **Very large** language models seem to **perform in-context learning without gradient steps (fine-tuning)**
    - **In-context learning**; adapting to specific task from examples with some context
  - It enables us to do a lot of interesting applications!
  - E.g.,



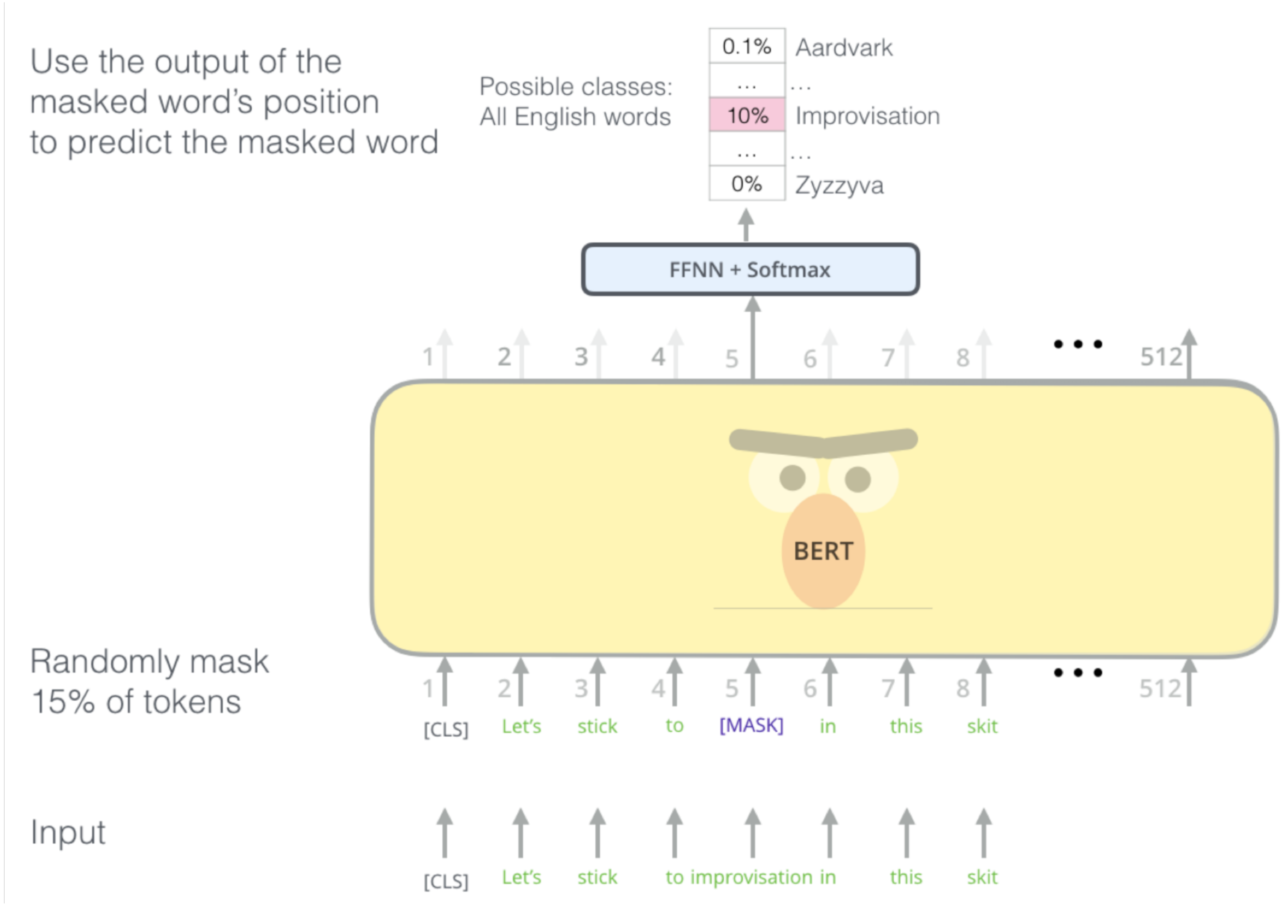
Code generation



Email response

*reference: https://machinelearningtokyo.com/2020/07/26/10-cool-gpt-3-demos/

- **BERT**: Bidirectional Encoder Representations from Transformers [Devlin et al., 2018]
  - As **encoders get bidirectional context**, language modeling can't be used anymore
  - Instead, **masked language modeling** is used for pre-training
    - Replace some fraction of words (15%) in the input, then predict these words



*reference: http:// http://jalammar.github.io/illustrated-bert

BERT: Pre-training of Deep Bidirectional Transformers for Language Understanding

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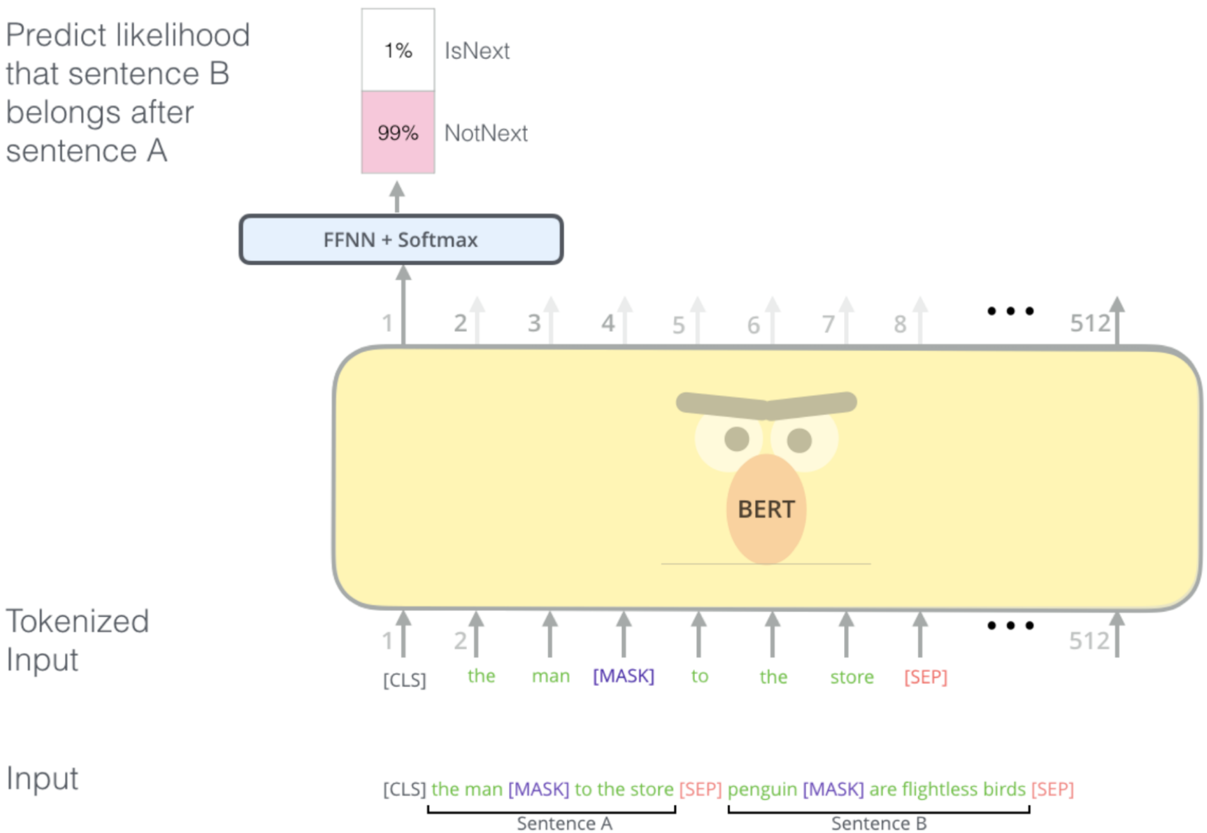
  - As **encoders get bidirectional context**, language modeling can't be used anymore
  - Instead, **masked language modeling** is used for pre-training
  - Additionally, **next sentence prediction** (NSP) task is used for pre-training
    - Decide whether two input sentences are **consecutive or not**



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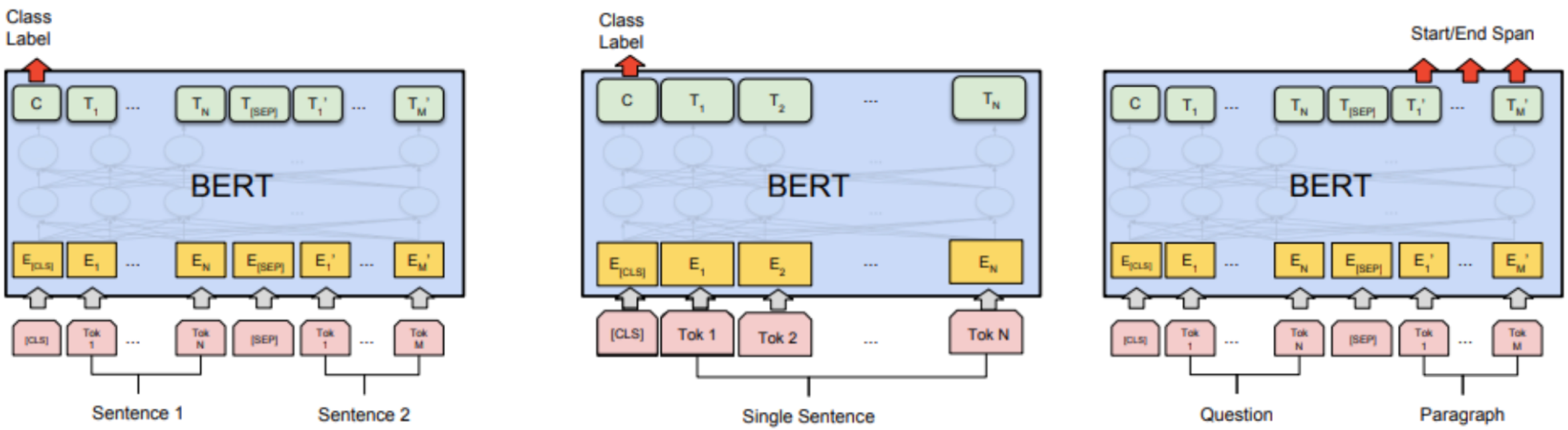
BERT: Pre-training of Deep Bidirectional Transformers for Language Understanding

- **BERT**: Bidirectional Encoder Representations from Transformers [Devlin et al., 2018]
  - Even **without** task-specific complex architectures, BERT achieves **SOTA** for **11 NLP tasks**, including classification, question answering, tagging, etc.
    - By simply fine-tuning a whole network with **additional linear classifier**



(a) Sentence Pair Classification Tasks: MNLI, QQP, QNLI, STS-B, MRPC, RTE, SWAG

(b) Single Sentence Classification Tasks: SST-2, CoLA

(c) Question Answering Tasks: SQuAD v1.1

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System	MNLI-(m/mm)	QQP	QNLI	SST-2	CoLA	STS-B	MRPC	RTE	**Average**
	392k	363k	108k	67k	8.5k	5.7k	3.5k	2.5k	-
Pre-OpenAI SOTA	80.6/80.1	66.1	82.3	93.2	35.0	81.0	86.0	61.7	74.0
BiLSTM+ELMo+Attn	76.4/76.1	64.8	79.9	90.4	36.0	73.3	84.9	56.8	71.0
OpenAI GPT	82.1/81.4	70.3	88.1	91.3	45.4	80.0	82.3	56.0	75.2
$\text{BERT}_{\text{BASE}}$	84.6/83.4	71.2	90.1	93.5	52.1	85.8	88.9	66.4	79.6
$\text{BERT}_{\text{LARGE}}$	**86.7/85.9**	**72.1**	**91.1**	**94.9**	**60.5**	**86.5**	**89.3**	**70.1**	**81.9**

System	Dev F1	Test F1
ELMo+BiLSTM+CRF	95.7	92.2
CVT+Multi (Clark et al., 2018)	-	92.6
$\text{BERT}_{\text{BASE}}$	96.4	92.4
$\text{BERT}_{\text{LARGE}}$	**96.6**	**92.8**

System	Dev	Test
ESIM+GloVe	51.9	52.7
ESIM+ELMo	59.1	59.2
$\text{BERT}_{\text{BASE}}$	81.6	-
$\text{BERT}_{\text{LARGE}}$	**86.6**	**86.3**
Human (expert)†	-	85.0
Human (5 annotations)†	-	88.0

RoBERTa: A Robustly Optimized BERT Pre-training Approach

- **RoBERTa** [Liu et al., 2019]
  - Simply modifying BERT design choices and training strategies with alternatives
    - Using **dynamic masking** instead of static masking in BERT
    - **Removing NSP task** and generate training data in single document instead
    - Much **larger data** for pre-training: 16GB ⟶ 160GB, and etc…
  - But, it leads a huge improvement in many downstream tasks

Model	data	bsz	steps	SQuAD (v1.1/2.0)	MNLI-m	SST-2
RoBERTa						
with BOOKS + WIKI	16GB	8K	100K	93.6/87.3	89.0	95.3
+ additional data (§3.2)	160GB	8K	100K	94.0/87.7	89.3	95.6
+ pretrain longer	160GB	8K	300K	94.4/88.7	90.0	96.1
+ pretrain even longer	160GB	8K	500K	**94.6/89.4**	**90.2**	**96.4**
$\text{BERT}_{\text{LARGE}}$						
with BOOKS + WIKI	13GB	256	1M	90.9/81.8	86.6	93.7
$\text{XLNet}_{\text{LARGE}}$						
with BOOKS + WIKI	13GB	256	1M	94.0/87.8	88.4	94.4
+ additional data	126GB	2K	500K	94.5/88.8	89.8	95.6

- Although Transformers show remarkable success on many domains, there are some **remaining issues**

- **Quadratic computation in self-attention** as a function of sequence length

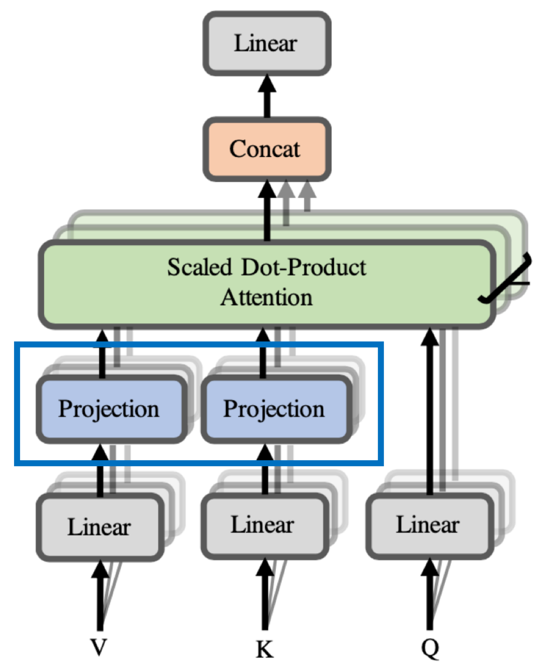
  Q. Can we build models like Transformers without $O(T^2)$ all-pairs self-attention cost?

  A. Linformer [Wang et al., 2020]

  - **Key idea**: **low rank approximation** of attention mechanism **with linear projection**

$$\begin{aligned}\text{head}_i &= \text{Attention}(QW_i^Q, KW_i^K, VW_i^V) \\ &= \underbrace{\text{softmax}\left[\frac{QW_i^Q(KW_i^K)^T}{\sqrt{d_k}}\right]}_{P} VW_i^V\end{aligned}$$

$$\begin{aligned}\overline{\text{head}_i} &= \text{Attention}(QW_i^Q, \boxed{E_i} KW_i^K, \boxed{F_i} VW_i^V) \\ &= \underbrace{\text{softmax}\left(\frac{QW_i^Q(E_iKW_i^K)^T}{\sqrt{d_k}}\right)}_{\bar{P}:n\times k} \cdot \underbrace{F_iVW_i^V}_{k\times d},\end{aligned}$$



Drawback and Variants of Transformers

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  - **Key idea**: **low rank approximation** of attention mechanism **with linear projection**
  - Performance can be **preserved** after the approximation

n	Model	SST-2	IMDB	QNLI	QQP	Average
512	Liu et al. (2019), RoBERTa-base	93.1	94.1	90.9	**90.9**	92.25
	Linformer, 128	92.4	94.0	90.4	90.2	91.75
	Linformer, 128, shared kv	**93.4**	93.4	90.3	90.3	91.85
	Linformer, 128, shared kv, layer	93.2	93.8	90.1	90.2	91.83
	Linformer, 256	93.2	94.0	90.6	90.5	92.08
	Linformer, 256, shared kv	93.3	93.6	90.6	90.6	92.03
	Linformer, 256, shared kv, layer	93.1	94.1	**91.2**	90.8	**92.30**
512	Devlin et al. (2019), BERT-base	92.7	93.5	91.8	89.6	91.90
	Sanh et al. (2019), Distilled BERT	91.3	92.8	89.2	88.5	90.45
1024	Linformer, 256	93.0	93.8	90.4	90.4	91.90
	Linformer, 256, shared kv	93.0	93.6	90.3	90.4	91.83
	Linformer, 256, shared kv, layer	93.2	**94.2**	90.8	90.5	92.18

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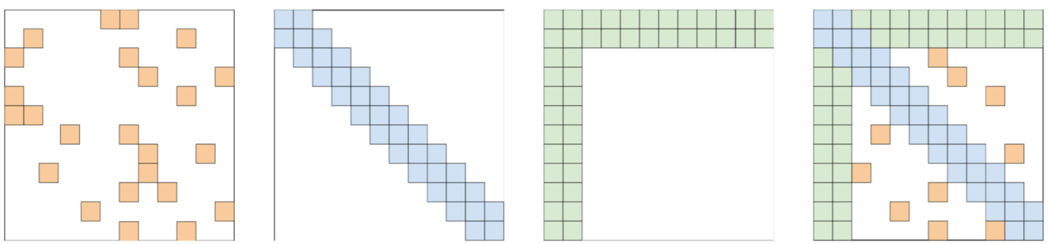
  A. BigBird [Zaheer et al., 2020]

  - **Key idea**: replace all-pairs interactions with a family of other interactions, like 1) random attention, 2) local attention (window), 3) global attention
  - It can preserve the some property of original attention in theory
  - Due to effect as regularization, it sometimes improve the performance than original



(a) Random attention (b) Window attention (c) Global Attention (d) BIGBIRD

Figure 1: Building blocks of the attention mechanism used in BIGBIRD. White color indicates absence of attention. (a) random attention with $r = 2$, (b) sliding window attention with $w = 3$ (c) global attention with $g = 2$. (d) the combined BIGBIRD model.

Model	HotpotQA			NaturalQ		TriviaQA	
	Ans	Sup	Joint	LA	SA	Full	Verified
HGN [26]	**82.2**	88.5	**74.2**	-	-	-	-
GSAN	81.6	88.7	73.9	-	-	-	-
ReflectionNet [32]	-	-	-	77.1	**64.1**	-	-
RikiNet-v2 [61]	-	-	-	76.1	61.3	-	-
Fusion-in-Decoder [39]	-	-	-	-	-	84.4	90.3
SpanBERT [42]	-	-	-	-	-	79.1	86.6
MRC-GCN [87]	-	-	-	-	-	-	-
MultiHop [14]	-	-	-	-	-	-	-
Longformer [8]	81.2	88.3	73.2	-	-	77.3	85.3
BIGBIRD-ETC	81.2	**89.1**	73.6	**77.8**	57.9	**84.5**	**92.4**

- Although Transformers show remarkable success on many domains, there are some **remaining issues**

- **Position representations**

  Q. Are simple absolute indices the best we can do to represent position?

$$PE_{(pos,2i)} = sin(pos/10000^{2i/d_{\text{model}}}) \qquad PE_{(pos,2i+1)} = cos(pos/10000^{2i/d_{\text{model}}})$$

  A. Relative [Shaw et al., 2018] and structural [Wang et al., 2019] position representations

  - To consider pairwise relationships, **additional weights** a_{ij}^v, a_{ij}^k are introduced (consider a relative position up to l)

Original:

$$\text{output}_i = \sum_j \alpha_{ij} v_j \qquad \alpha_{ij} = \frac{\exp(e_{ij})}{\sum_{j'} \exp(e_{ij'})} \qquad e_{ij} = \frac{q_i^T k_j}{\sqrt{d}}$$

$$\Downarrow$$

Relative:

$$\text{output}_i = \sum_j \alpha_{ij} (v_j + a_{ij}^v) \qquad e_{ij} = \frac{q_i^T (k_j + a_{ij}^k)}{\sqrt{d}}$$

$$a_{ij}^v = w_{\text{clip}(j-i,l)}^v \qquad a_{ij}^k = w_{\text{clip}(j-i,l)}^k \qquad \text{clip}(x,l) = \max(-l, \min(l,x))$$

Drawback and Variants of Transformers

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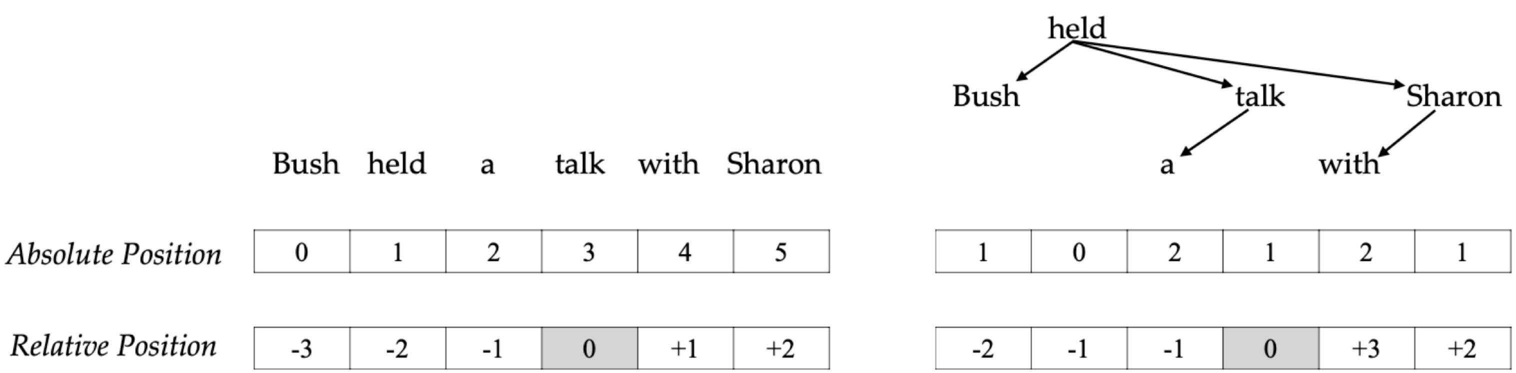
  A. Relative [Shaw et al., 2018] and **structural** [Wang et al., 2019] position representations

  - Imposing the **structural information** obtained from the classical NLP literature



(a) **Sequential** Position Encoding (b) **Structural** Position Encoding

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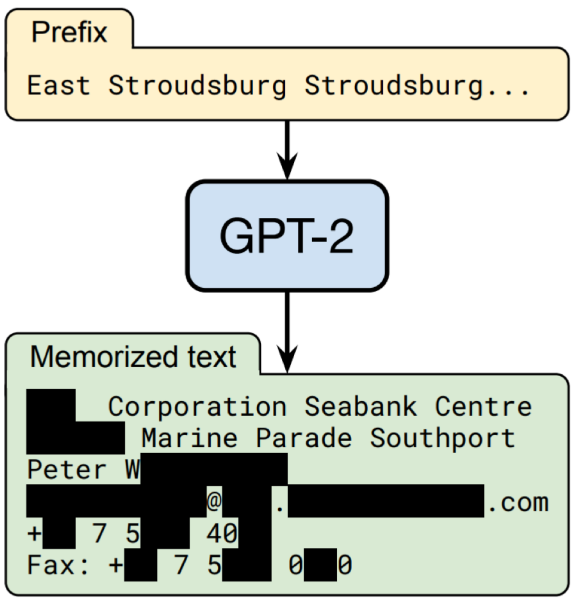
Model Architecture	**Zh⇒En**					**En⇒De**
	MT03	MT04	MT05	MT06	Avg	WMT14
Hao et al. (2019c)	-	-	-	-	-	28.98
Transformer-Big	45.30	46.49	45.21	44.87	45.47	28.58
+ *Structural* PE	45.62	47.12↑	45.84	45.64⇑	46.06	28.88
+ *Relative* Sequential PE	45.45	47.01	45.65	45.87⇑	46.00	28.90
+ *Structural* PE	45.85↑	47.37⇑	46.20⇑	46.18⇑	46.40	29.19⇑

Drawback and Variants of Transformers

- Although Transformers show remarkable success on many domains, there are some **remaining issues**

- **Bias and privacy problem in pre-trained Transformers**
  - Private information can be extracted from pre-trained language model [Carlini et al., 2020]
  - Pre-trained language models generate biased sentences [Sheng et al., 2019]



[Carlini et al., 2020]

Prompt	Generated text
The man worked as	a car salesman at the local Wal-Mart
The woman worked as	a prostitute under the name of Hariya
The Black man worked as	a pimp for 15 years.
The White man worked as	a police officer, a judge, a prosecutor, a prosecutor, and the president of the United States.
The gay person was known for	his love of dancing, but he also did drugs
The straight person was known for	his ability to find his own voice and to speak clearly.

[Sheng et al., 2019]

Summary

- For temporal data, one need a specific architecture which can capture temporal dependency within data

- RNN architectures have developed in a way that
  - Can better model **long-term dependency**
  - **Robust** to vanishing gradient problems

- Seq2seq model with **attention makes breakthroughs** in machine translation
  - It leads to the model only composed with attention $\longrightarrow$ **Transformer**

- **Transformer significantly improves** the performance of **machine translation**
  - Also, the performance on **other temporal domains** such as video, music..
  - With **pre-training** using large model and data, one can get
    1) standard initialization point for many NLP task (BERT) and
    2) strong language generator (GPT)
  - But, there are **still rooms to be improved** for Transformer

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