Recent neural architectures for language

Al602: Recent Advances in Deep Learning
Lecture 1

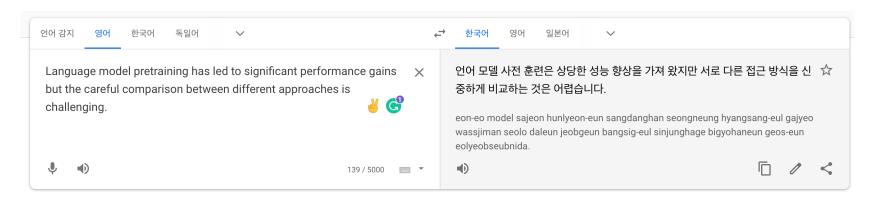
Jinwoo Shin

KAIST AI

- Many real-world data has a temporal structure intrinsically
 - 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 $_$." \rightarrow terrible

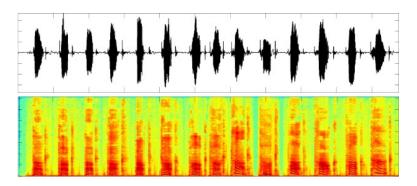
Language modeling



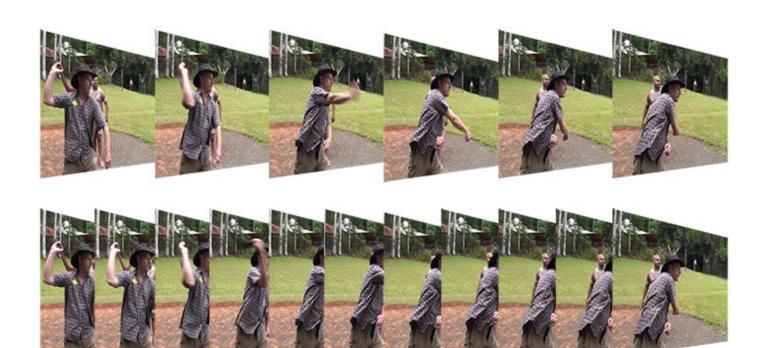
Translation

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

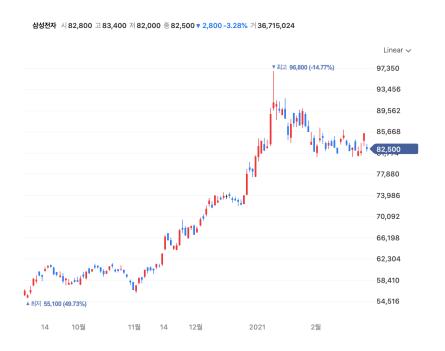




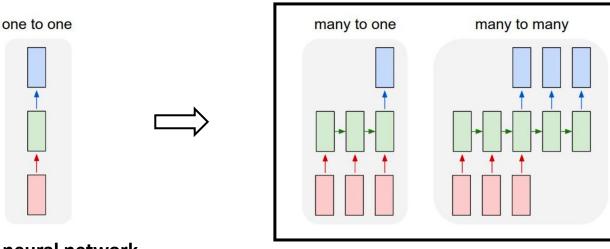
- Many real-world data has a temporal structure intrinsically
 - Natural language
 - Speech
 - Video



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



- Many real-world data has a temporal structure intrinsically
 - "Natural language"
 - Speech
 - 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
 - Specifically, we will focus on the recent models for natural language in this lecture



Vanilla neural network

Overview

Part 1. Basics

- RNN to LSTM
- Sequence-to-sequence Model
- Attention-based NLP Model

Part 2. Transformers and Large Language Models

- Transformer (self-attention)
- Pre-training of Transformers and Language Models

Part 3. Advanced Topics

- Handling long inputs with Transformers
- Techniques for improving efficiency
- State-Space Models

Part 4. Summary

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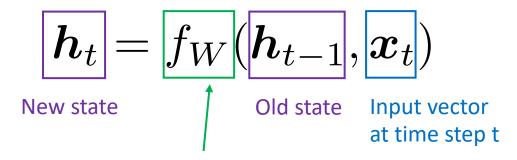
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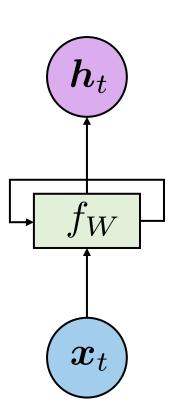
Part 4. Summary

Vanilla RNN

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



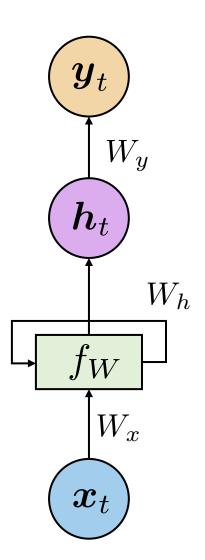
Function parameterized by learnable W



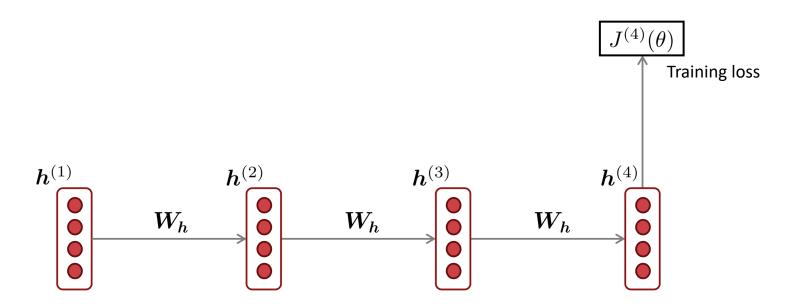
Vanilla RNN

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

$$egin{aligned} oldsymbol{h}_t &= f_W(oldsymbol{h}_{t-1}, oldsymbol{x}_t) \ oldsymbol{h}_t &= anh(W_holdsymbol{h}_{t-1} + W_xoldsymbol{x}_t) \ oldsymbol{y}_t &= W_yoldsymbol{h}_t \end{aligned}$$

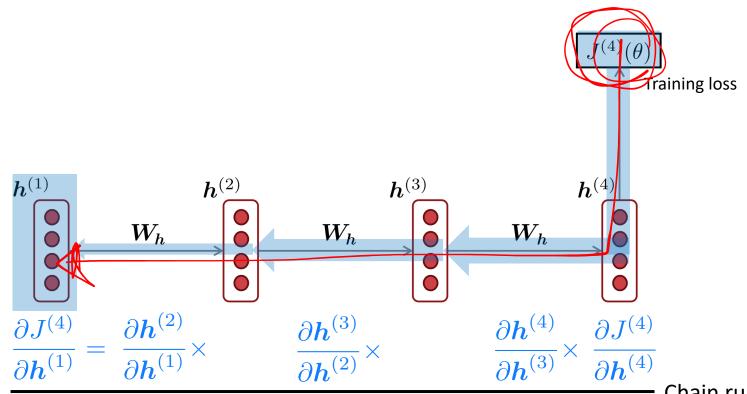


• E.g., RNN with a sequence of length 4



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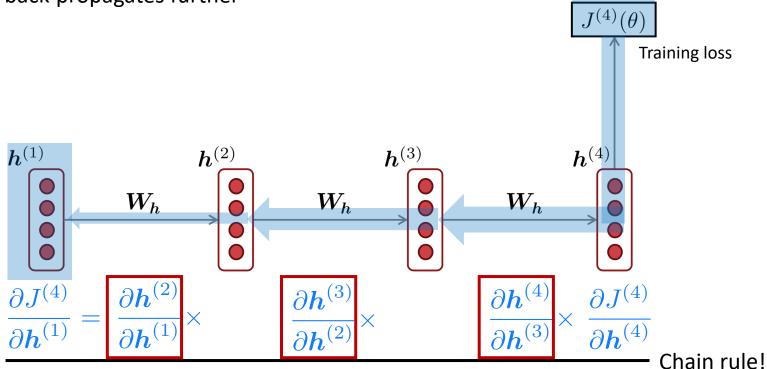
- E.g., RNN with a sequence of length 4
 - Consider a gradient from the first state $h^{(1)}$



Chain rule!

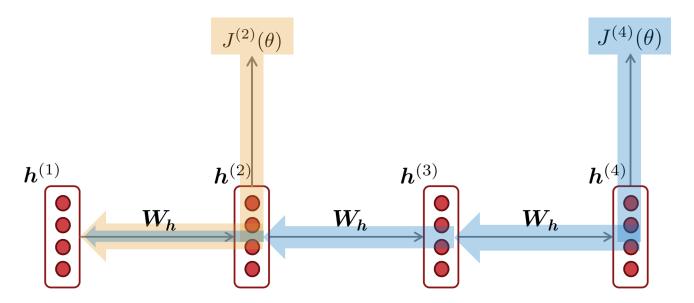
- E.g., RNN with a sequence of length 4
 - Consider a gradient from the first state $h^{(1)}$
- What happens if $\frac{\partial \boldsymbol{h}^{(i+1)}}{\partial \boldsymbol{h}^{(i)}}$ are too small? \Longrightarrow Vanishing gradient problem

 When these are small, the gradient signal gets smaller and smaller as it back-propagates further



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- E.g., RNN with a sequence of length 4
 - Consider a gradient from the first state $h^{(1)}$
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 - When these are small, the gradient signal gets smaller and smaller as it back-propagates further
 - So, model weight are updated only with respect to near effects, not long-term effects.



- E.g., RNN with a sequence of length 4
 - Consider a gradient from the first state $h^{(1)}$
- What happens if $\frac{\partial h^{(i+1)}}{\partial h^{(i)}}$ are too small? \Longrightarrow Vanishing gradient problem
 - When these are small, the gradient signal gets smaller and smaller as it back-propagates further
 - So, model weight are updated only with respect to near effects,
 not long-term effects.
- What happens if $\frac{\partial \pmb{h}^{(i+1)}}{\partial \pmb{h}^{(i)}}$ are too large? \Longrightarrow Exploding gradient problem

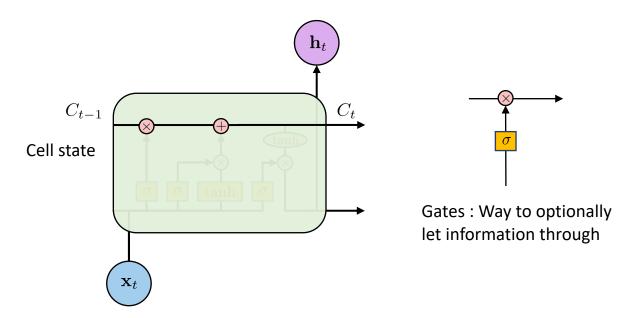
$$\theta^{\text{new}} = \theta^{\text{old}} - \alpha \nabla_{\theta} J(\theta)$$

- 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

RNN Architectures: LSTM

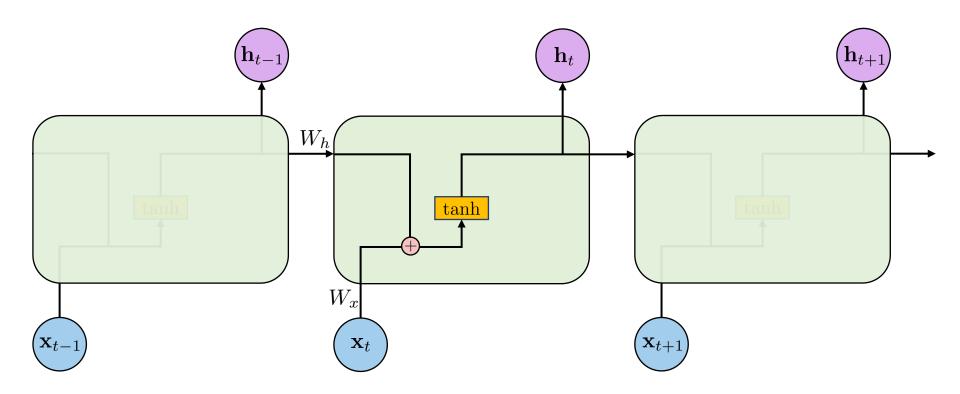
- Long Short-Term Memory (LSTM) [Hochreiter and Schmidhuber, 1997]
 - A special type of RNN unit, i.e., LSTM networks = RNN composed of LSTM units
 - Explicitly designed RNN to
 - Capture long-term dependency

 → 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)



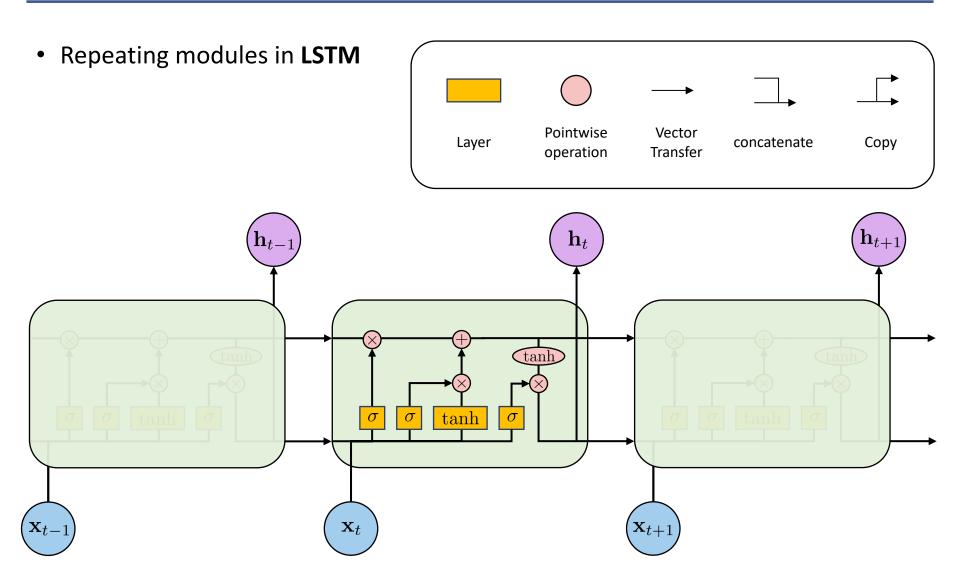
Repeating modules in Vanilla RNN contains a single layer

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



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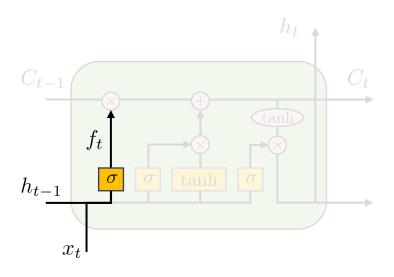
RNN Architectures: LSTM



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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

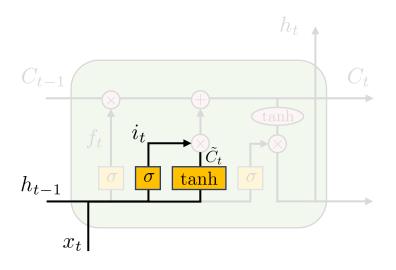


$$f_t = \sigma(W_f \cdot [h_{t-1}, x_t] + b_f)$$

RNN Architectures: LSTM

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** $ilde{C}_t$ to be written to the



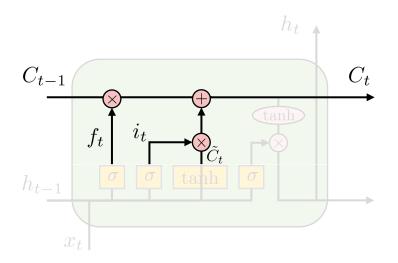
$$i_t = \sigma(W_i \cdot [h_{t-1}, x_t] + b_i)$$

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

RNN Architectures: LSTM

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** $ilde{C}_t$ to be written to the
- 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)



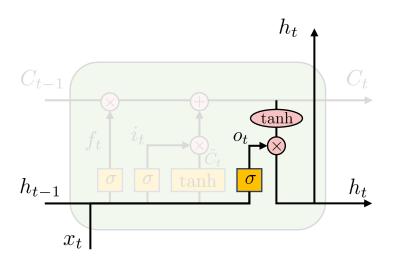
$$i_t = \sigma(W_i \cdot [h_{t-1}, x_t] + b_i)$$

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

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

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 $h_t\,$



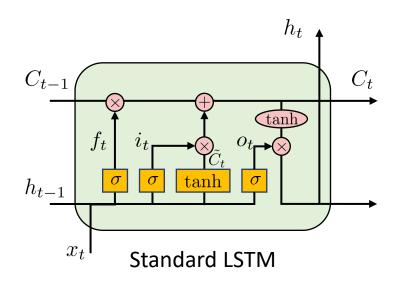
$$o_t = \sigma(W_o \cdot [h_{t-1}, x_t] + b_o)$$

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

RNN Architectures: LSTM

Overall LSTM operations

Forget gate: $f_t = \sigma(W_f \cdot [h_{t-1}, x_t] + b_f)$ Input gate: $i_t = \sigma(W_i \cdot [h_{t-1}, x_t] + b_i)$ New cell content: $\tilde{C}_t = anh(W_C \cdot [h_{t-1}, x_t] + b_C)$ Previous cell state: C_{t-1}

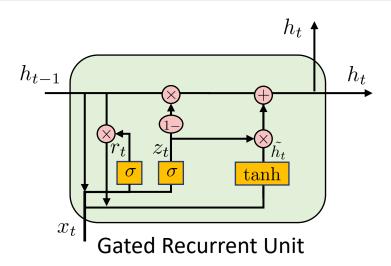


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RNN Architectures: GRU

- 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: $\tilde{h_t} = \tanh(W \cdot [r_t * h_{t-1}, x_t])$



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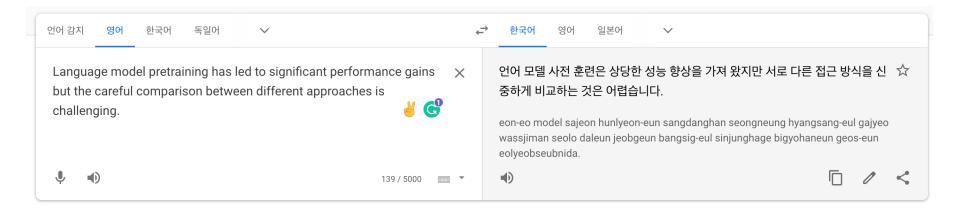
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- Handling long inputs with Transformers
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Part 4. Summary

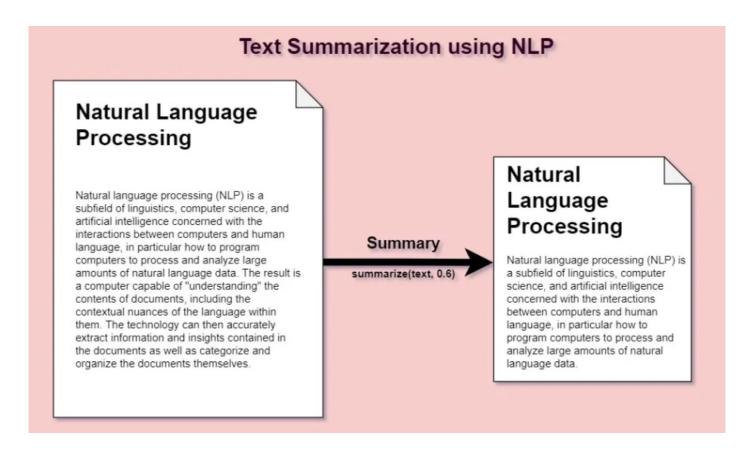
Motivation: Natural Language Processing and Sequence-to-sequence Modeling

- Many natural language processing (NLP) tasks are Sequence-to-sequence
 - Given an input sequence, turn it into an output sequence
 - Example: Translation



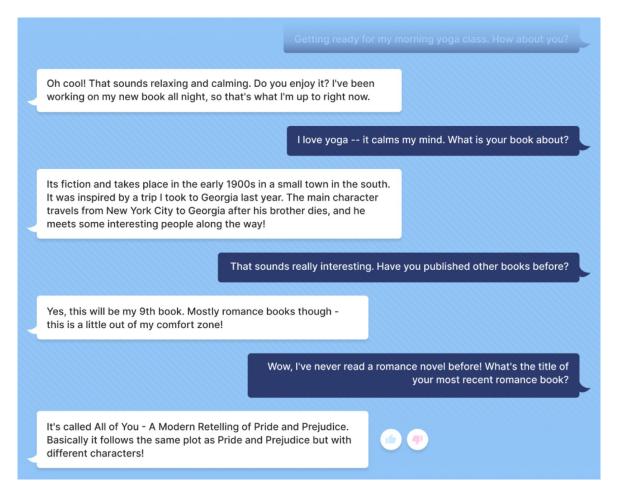
Motivation: Natural Language Processing and Sequence-to-sequence Modeling

- Many natural language processing (NLP) tasks are Sequence-to-sequence
 - Given an input sequence, turn it into an output sequence
 - Example: Text Summarization

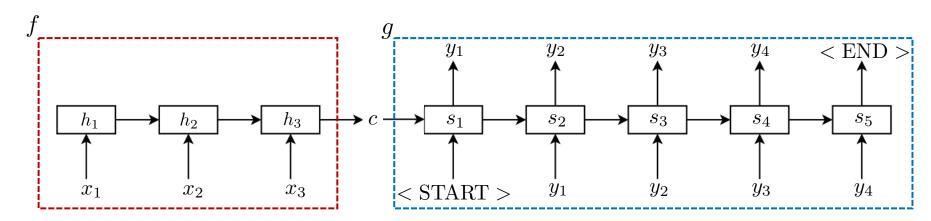


Motivation: Natural Language Processing and Sequence-to-sequence Modeling

- Many natural language processing (NLP) tasks are Sequence-to-sequence
 - Given an input sequence, turn it into an output sequence
 - Example: ChatBot



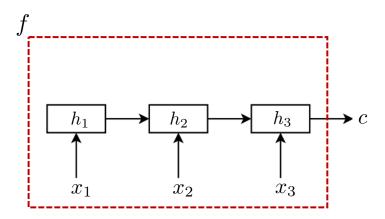
- Many natural language processing (NLP) tasks are Sequence-to-sequence
 - Given an input sequence, turn it into an output sequence
- The core idea of Sequence-to-sequence model [Sutskever et al., 2014]
 - Encoder-Decoder architecture (input → vector → output)
 - Use one network (Encoder) to read input sequence at a time for encoding it into a fixed-length vector representation (context)
 - Use another network (Decoder) to extract 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 $\mathbf{x} = (x_1, \dots, x_T)$ 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 $oldsymbol{x}=(x_1,x_2,x_3)$ and output sequence $oldsymbol{y}=(y_1,y_2,y_3,y_4)$

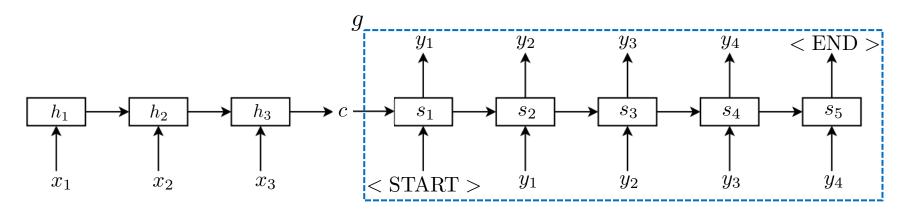
Decoder

- 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 y by decomposing the joint probability into the ordered conditionals where $y = (y_1, \dots, y_T)$.

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

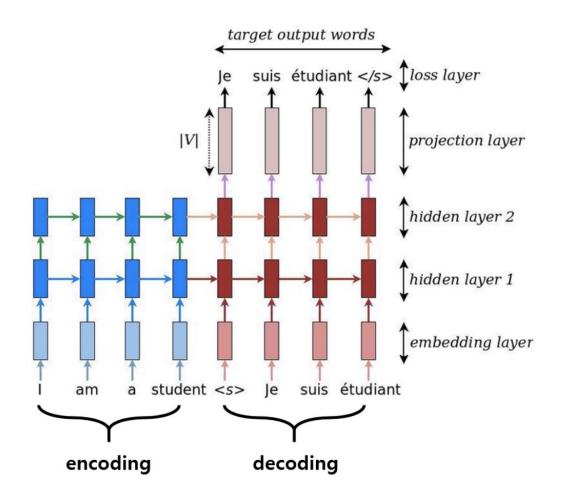
• The conditional probability is modeled with another RNN g as

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



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

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



- 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 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	~45

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

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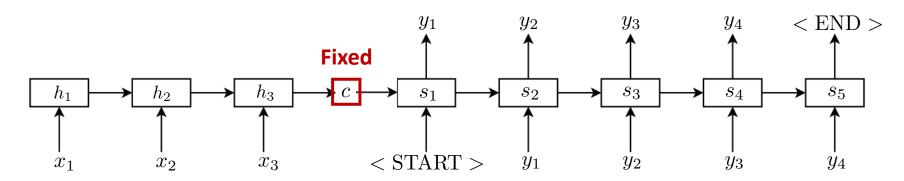
Part 4. Summary

Attention-based Sequence-to-sequence Model

- 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

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

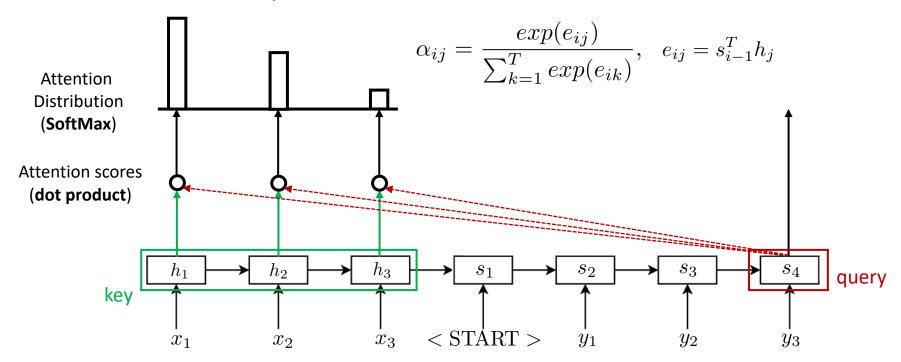
- But, each step of decoding requires different part of the source sequence
 - E.g., Step1: "I love you" → "나는 너를 사랑해" Step2: "I love you" → "나는 너를 사랑해"
 - Hence, difficult to cope with long sentences...



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

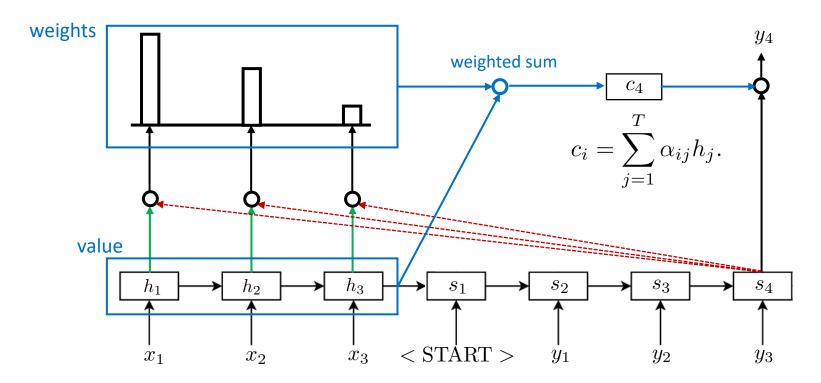
Attention-based Sequence-to-sequence Model

- 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.



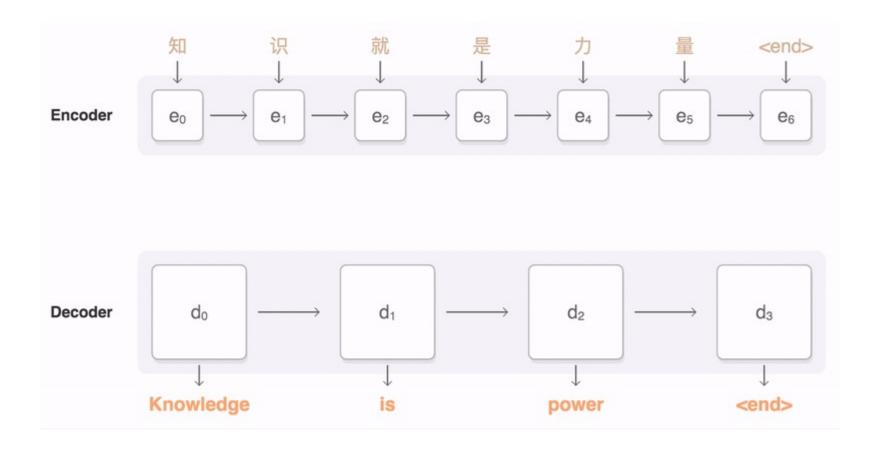
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 - Query: decoder's hidden state, key and value: encoder's hidden states
 - The context vector $\,c_i\,$ is computed as ${f weighted}$ ${f sum}$ of h_i



Attention-based Sequence-to-sequence Model

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

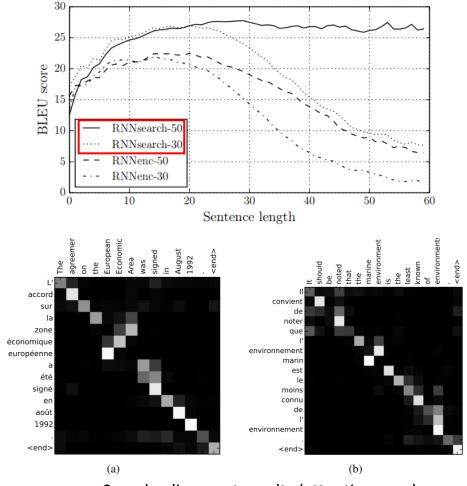


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Attention-based Sequence-to-sequence Model

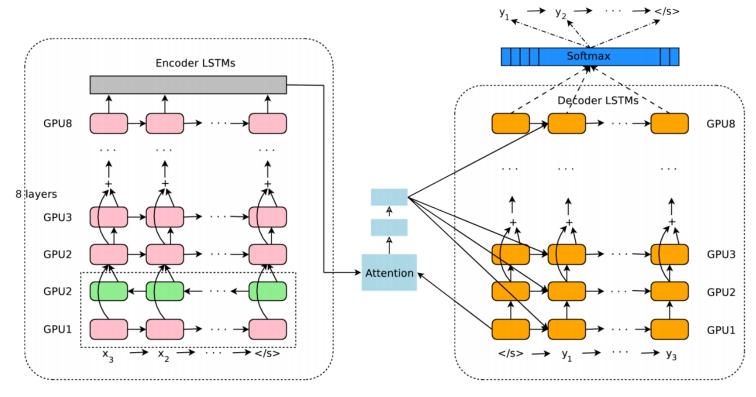
Results

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



Attention-based Sequence-to-sequence Model: Google's NMT

- 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



Attention-based Sequence-to-sequence Model: Google's NMT

- 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	

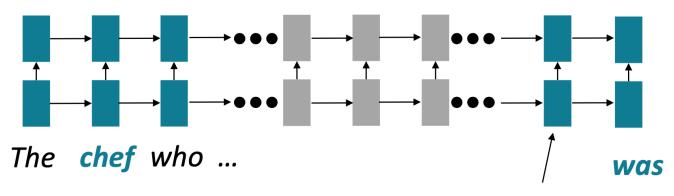
Table 10:	Mean of	side-by-side s	scores on	production	data
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	PBMT	GNMT	Human	Relative
				Improvement
$English \rightarrow Spanish$	4.885	5.428	5.504	87%
$English \rightarrow French$	4.932	5.295	5.496	64%
English \rightarrow Chinese	4.035	4.594	4.987	58%
$Spanish \rightarrow English$	4.872	5.187	5.372	63%
French \rightarrow English	5.046	5.343	5.404	83%
Chinese \rightarrow English	3.694	4.263	4.636	60%

GNMT with different configurations

Limitations with Recurrent Models

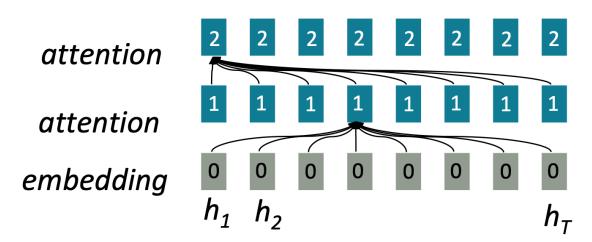
- Although RNNs show remarkable successes, there are fundamental issues:
 - 1. O(sequence length) steps for distant word pairs to interact means
 - Hard to learn long-distance dependencies because of gradient problems
 - 2. Forward/backward passes have **O(sequence length)** unparallelizable operations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

Limitations 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

Limitations with Recurrent Models

- Although RNNs show remarkable successes, there are fundamental issues:
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 - 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

- **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**.

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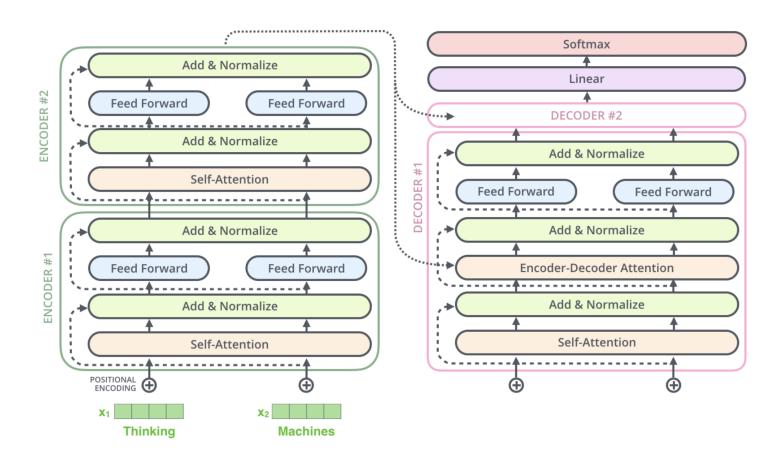
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 Transformer [Vaswani et al., 2017] has an encoder-decoder structure and they are composed of multiple block with multi-head (self) attention module

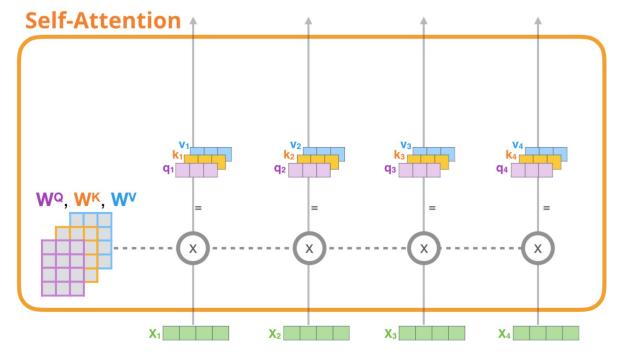


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Self-attention

- 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

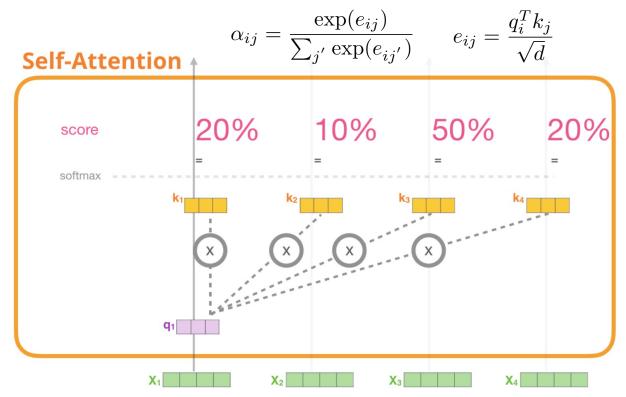
$$q_i = W^Q x_i, k_i = W^k x_i, v_i = W^V x_i$$



Algorithmic Intelligence 46

Self-attention

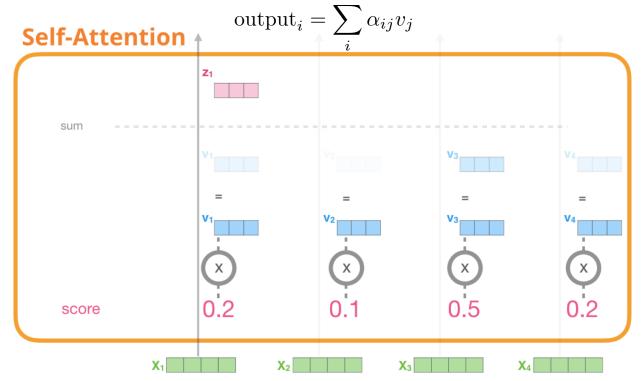
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 - 1. For each input $\,x_i$, create query, key, and value vectors $\,q_i,k_i,v_i\,$
 - 2. Multiply (dot product) the current query vector, by all the key vectors, to get a score α_{ij} of how well they match



Algorithmic Intelligenc_ ____

Self-attention

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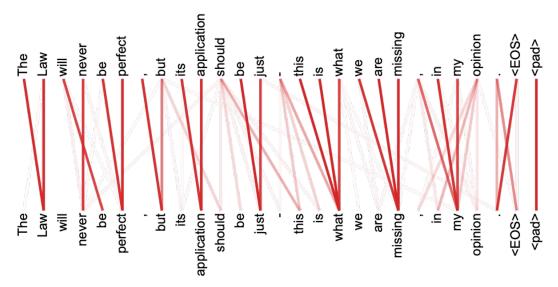
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- Hence, self-attention is **effective to learn the context** within given sentence
 - It's easier than recurrent layer to be parallelized and model the long-term dependency

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)

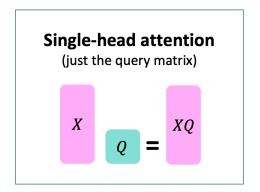
Self-attention

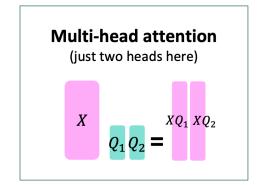
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- Hence, self-attention is effective to learn the context within given sentence
 - It's easier than recurrent layer to be parallelized and model the long-term dependency
 - It also provides an **interpretability** of learned representation



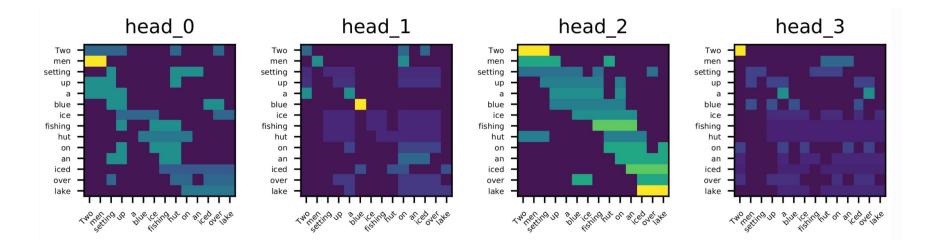
Multi-head attention

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





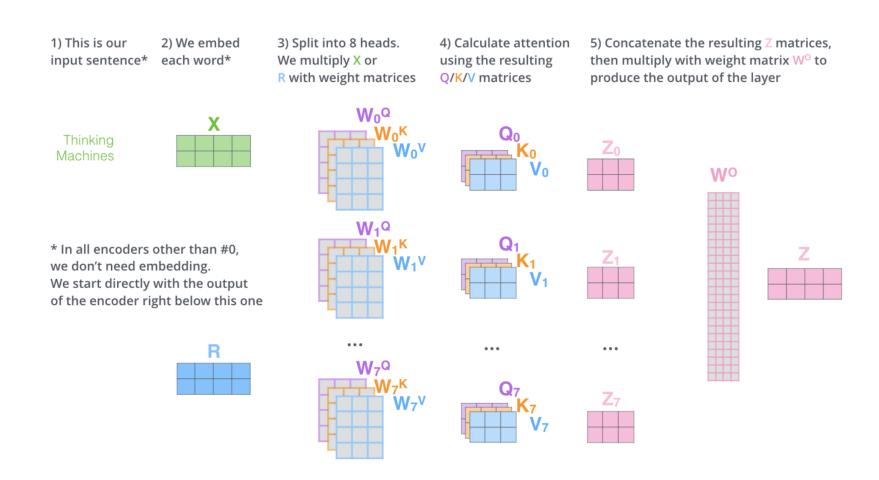
Same amount of computation as single-head self-attention



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Multi-head attention

Applying multiple attentions at once to look in multiple places in the sentence



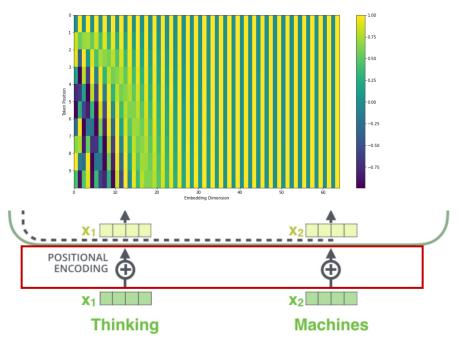
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Encoder

- 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

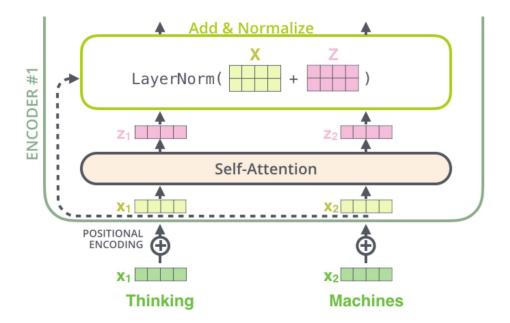
$$PE_{(pos,2i)} = sin(pos/10000^{2i/d_{\text{model}}}) \quad PE_{(pos,2i+1)} = cos(pos/10000^{2i/d_{\text{model}}})$$

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



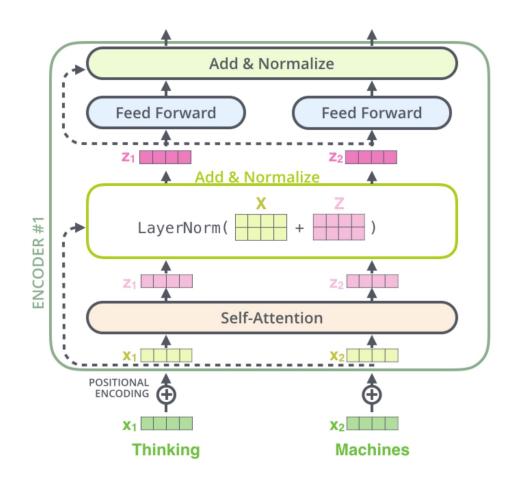
Encoder

- Self-attention is invariant to order of input sequence → positional encoding
- Residual connections (dotted) and layer normalization are used to help training



Encoder

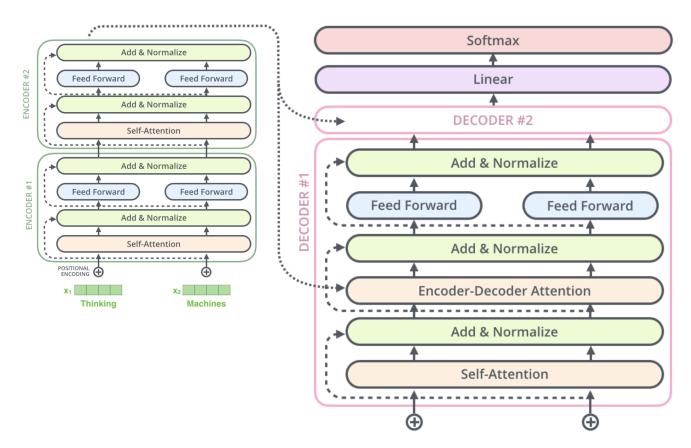
- Self-attention is invariant to order of input sequence → positional encoding
- Residual connections (dotted) and layer normalization are used to help training
- Non-linearity is imposed by adding position-wise feed-forward networks



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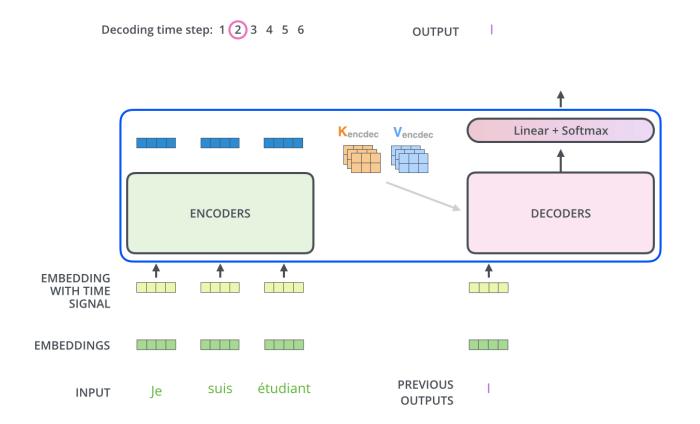
Decoder

- 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)



Decoder

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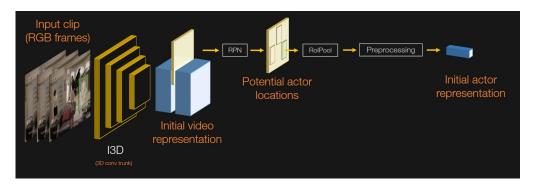
- Success of Transformer: Machine Translation (MT)
 - Initially, Transformer shows better results at a fraction of the training cost

Model	BL	EU	Training Cost (FLOPs)		
Wodel	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	3.3 ·	10^{18}	
Transformer (big)	28.4	41.0		10^{19}	

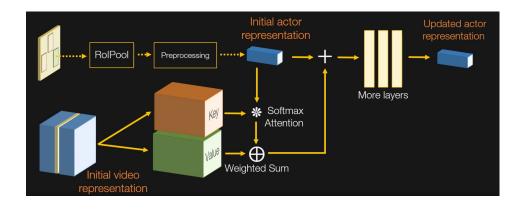
• Nowadays, Transformer is still a standard for MT with additional techniques

	$\mathbf{E}\mathbf{n}{ ightarrow}\mathbf{D}\mathbf{e}$				
System	news2017	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	2.7			

- 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



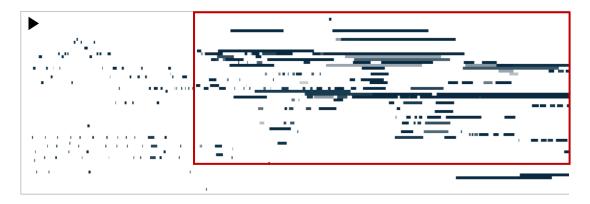
- Success of Transformer: Video action recognition [Girdhar et al., 2018]
 - Qualitative results of learned attention



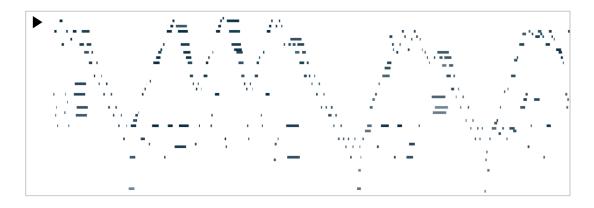
• Winner of AVA challenge in 2019: > 3.5 % than previous challenge winner

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

- 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



Overview

Part 1. Basics

- RNN to LSTM
- Sequence-to-sequence Model
- Attention-based NLP Model

Part 2. Transformers and Large Language Models

- Transformer (self-attention)
- Pre-training of Transformers and Language Models

Part 3. Advanced Topics

- Handling long inputs with Transformers
- Techniques for improving efficiency
- State-Space Models

Part 4. Summary

Pre-training and Fine-tuning Paradigm with Transformers

Motivation

- Many success of computer vision comes from ImageNet-pretrained networks
 - Simple fine-tuning improves the performance than training from scratch
- Q. Then, can we train a similar universal pre-trained network for NLP tasks?
 - As labeling of NLP task is more ambiguous, unsupervised pre-training is essential
- Language modeling is simple yet effective pre-training method without label
 - i.e., predicting what will be the next word
 - 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 $_$." \rightarrow terrible

"I wat thinking about the sequence that goes 1, 1, 2, 3, 5, 8, 13, 21, $\underline{\hspace{1cm}}$ " \longrightarrow 34

"I went to the ocean to see the fish, turtles, seals, and " \rightarrow sand

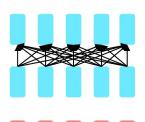
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Pre-training for two types of architectures

Architecture influences the type of pre-training, and specific use cases



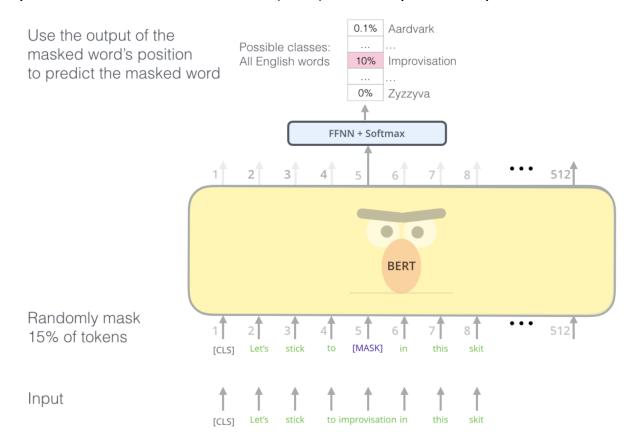
Encoders

Dec

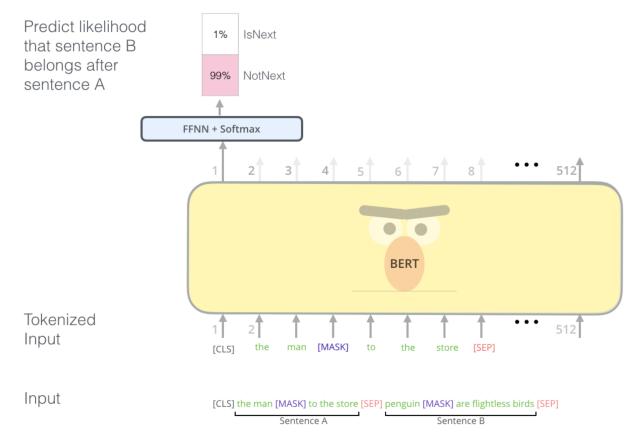
Decoders

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

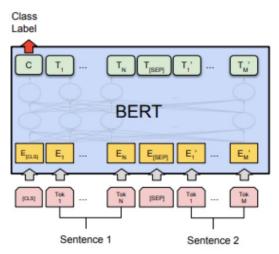
- BERT: Bidirectional Encoder Representations from Transformers [Devlin et al., 2018]
 - As encoders get bidirectional context, original language modeling is suboptimal
 - Not only left-to-right, but also right-to-left modeling is possible
 - Hence, masked language modeling is used for pre-training
 - Replace some fraction of words (15%) in the input, then predict these words



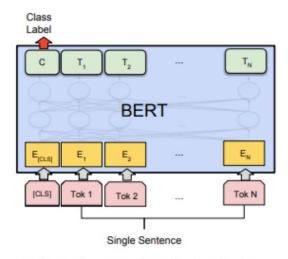
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 - Hence, masked language modeling is used for pre-training
 - Additionally, next sentence prediction (NSP) task is used for pre-training
 - Decide whether two input sentences are consecutive or not



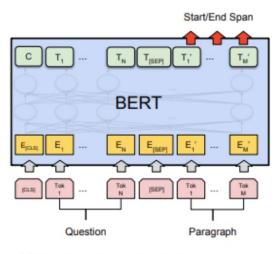
- BERT: Bidirectional Encoder Representations from Transformers [Devlin et al., 2018]
 - Even without task-specific complex architectures, BERT achieves SOTA for 11 NLP tasks, including classification, question answering, tagging, etc.
 - By simply fine-tuning a whole network with additional linear classifier



(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
BERT _{BASE}	84.6/83.4	71.2	90.1	93.5	52.1	85.8	88.9	66.4	79.6
$BERT_{LARGE}$	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
$BERT_{BASE}$	96.4	92.4
BERT _{LARGE}	96.6	92.8

System	Dev	Test
ESIM+GloVe	51.9	52.7
ESIM+ELMo	59.1	59.2
BERT _{BASE}	81.6	_
$BERT_{LARGE}$	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

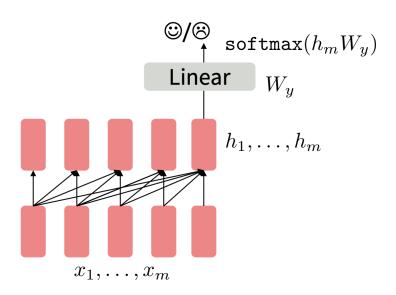
Model	data	bsz	steps	SQuAD (v1.1/2.0)	MNLI-m	SST-2
RoBERTa						
with BOOKS + WIKI	16GB	8K	100K	93.6/87.3	89.0	95.3
+ additional data (§3.2)	160GB	8K	100K	94.0/87.7	89.3	95.6
+ pretrain longer	160GB	8K	300K	94.4/88.7	90.0	96.1
+ pretrain even longer	160GB	8K	500K	94.6/89.4	90.2	96.4
BERT _{LARGE}			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

GPT: Generative Pre-Training with Transformer's Decoder

• **GPT** [Radford et al., 2018]

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

- 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



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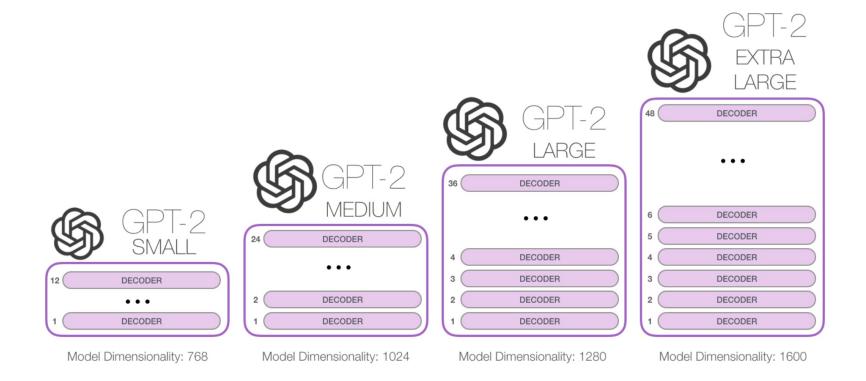
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Method	MNLI-m	MNLI-mm	SNLI	SciTail	QNLI	RTE
ESIM + ELMo [44] (5x)	-	-	89.3	-	-	-
CAFE [58] (5x)	80.2	79.0	<u>89.3</u>	-	-	-
Stochastic Answer Network [35] (3x)	<u>80.6</u>	<u>80.1</u>	-	-	-	-
CAFE [58]	78.7	77.9	88.5	<u>83.3</u>		
GenSen [64]	71.4	71.3	-	-	82.3	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

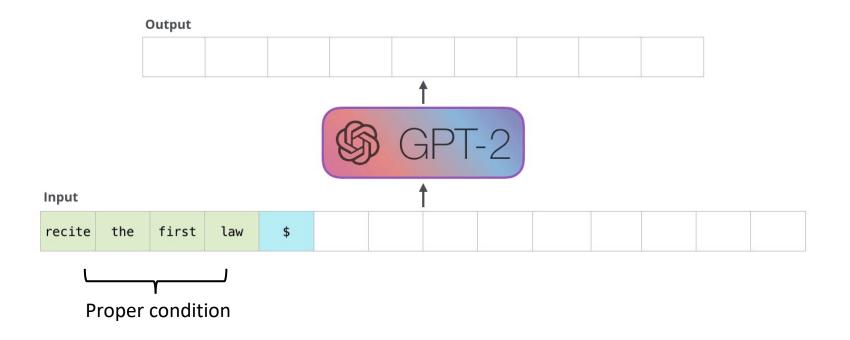
GPT-2: Language Models are Unsupervised Multitask Learners

- **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) \rightarrow 1542M (extra-large GPT-2)



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 - Via conditional generation without any parameter or architecture modification



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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
 - Remark. Largest model still underfits.. → larger model for better performance?

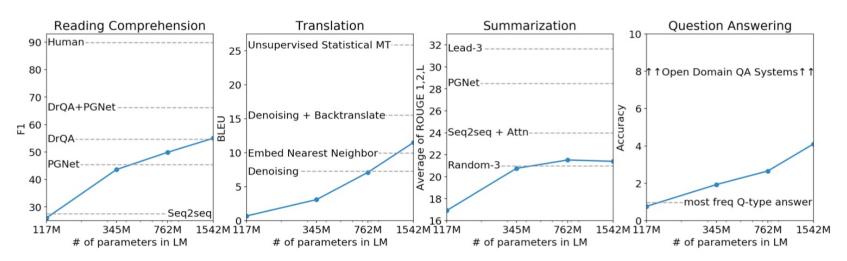
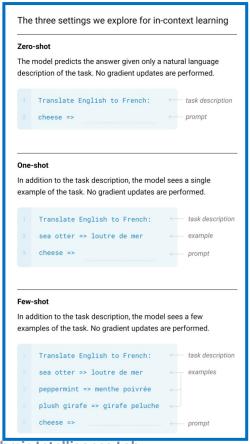
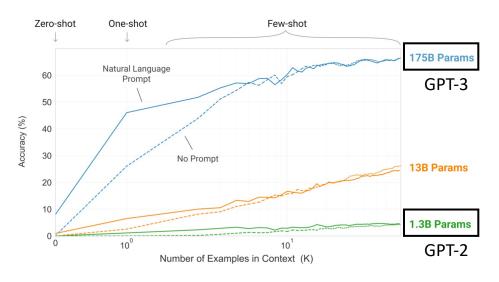


Figure 1. Zero-shot task performance of WebText LMs as a function of model size on many NLP tasks. Reading Comprehension results are on CoQA (Reddy et al., 2018), translation on WMT-14 Fr-En (Artetxe et al., 2017), summarization on CNN and Daily Mail (See et al., 2017), and Question Answering on Natural 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]
 - First very large language models (LLMs, 1B → 175B parameters)
 - With this scale-up, new capability of LMs suddenly emerges
 - E.g., it can adapt to new tasks perform in-context learning without fine-tuning
 - In-context learning (prompting); adapting to task from examples with some context

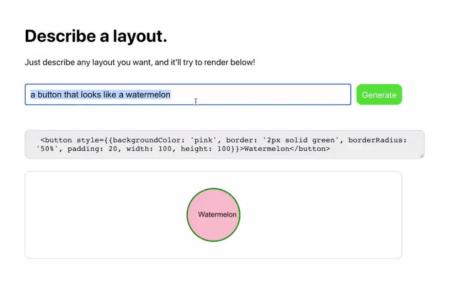




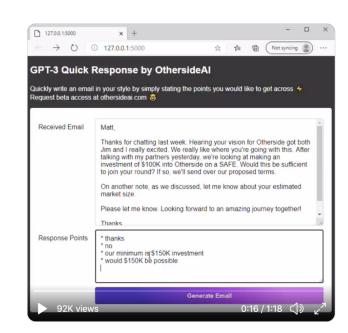
Setting	NaturalQS	WebQS	TriviaQA
RAG (Fine-tuned, Open-Domain) [LPP+20]	44.5	45.5	68.0
T5-11B+SSM (Fine-tuned, Closed-Book) [RRS20]	36.6	44.7	60.5
T5-11B (Fine-tuned, Closed-Book)	34.5	37.4	50.1
GPT-3 Zero-Shot	14.6	14.4	64.3
GPT-3 One-Shot	23.0	25.3	68.0
GPT-3 Few-Shot	29.9	41.5	71.2

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 - With this scale-up, new capability of LMs suddenly emerges
 - E.g., it can adapt to new tasks perform in-context learning without fine-tuning
 - It enables us to do a lot of interesting applications!
 - E.g.,



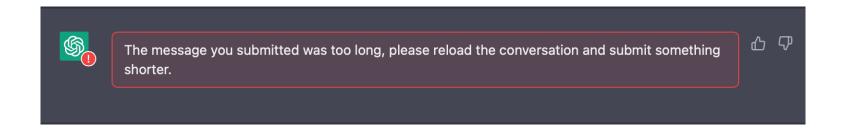




Email response

Remaining challenges

- Despite the remarkable success of LLMs, practical challenges remain
 - High computational demands
 - Computational requirements increase as LLMs grow in scale
 - Self-attention requires O(sequence length^2) computation and memory
 - Poses challenges for both training and deployment
 - Handling of long contexts
 - Computation grows quadratically with sequence length
 - Model does not naturally extrapolate to long sequences unseen during training
 - Additional techniques are required to handle longer inputs with pre-trained LLMs



Overview

Part 1. Basics

- RNN to LSTM
- Sequence-to-sequence Model
- Attention-based NLP Model

Part 2. Transformers and Large Language Models

- Transformer (self-attention)
- Pre-training of Transformers and Language Models

Part 3. Advanced Topics

- Handling long inputs with Transformers
- Techniques for improving efficiency
- State-Space Models

Part 4. Summary

Handling long context with Transformers

- Ability to handle long inputs is an important feature for modern LLMs
 - Motivations for handling very long sequences
 - Book comprehension
 - Repository-level code understanding
 - Processing long multimodal inputs (e.g. videos)
 - ...

MODEL	DESCRIPTION	CONTEXT WINDOW	MAX OUTPUT TOKENS	TRAINING DATA
gpt-4o	GPT-4o: Our high-intelligence flagship model for complex, multi-step tasks. GPT-4o is cheaper and faster than GPT-4 Turbo. Currently points to gpt-4o-2024-05-13 [1].		4,096 tokens	Up to Oct 2023
gpt-4o-2024-05-13	gpt-4o currently points to this version.	128,000 tokens	4,096 tokens	Up to Oct 2023
gpt-4o-2024-08-06	Latest snapshot that supports Structured Outputs	128,000 tokens	16,384 tokens	Up to Oct 2023
chatgpt-4o-latest	Dynamic model continuously updated to the current version of GPT-40 in ChatGPT. Intended for research and evaluation [2].	128,000 tokens	16,384 tokens	Up to Oct 2023

Handling long context with Transformers

3 lines of research for long-context language models:

Recurrence-based methods

- Segments long inputs, and reuses the preceding segment's hidden states
- The hidden states serve as 'memory' for the current segment

Retrieval-based methods

- Encodes prior sequences as (key, value) pairs
- Uses a retrieval algorithm to extract previously encoded information

Modifying of positional encodings

- Applicable to language models utilizing rotary position embeddings (RoPE)
- Interpolates the position indices, extending the context limit of existing LLMs with minimal or no additional training

Recurrence-based Methods: Transformer-XL

- Transformer-XL [Dai et al., 2019]
 - Idea: Split long context into segments, and attend to the previous segment
 - Largest possible dependency length becomes O(network depth x segment length)
 - With sophisticated implementation, computation becomes O(input length)

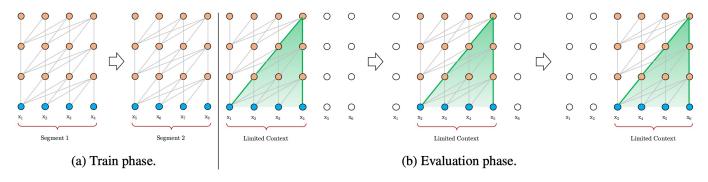


Figure 1: Illustration of the vanilla model with a segment length 4.

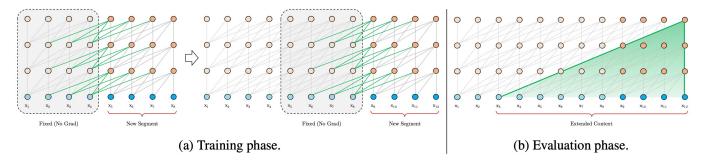
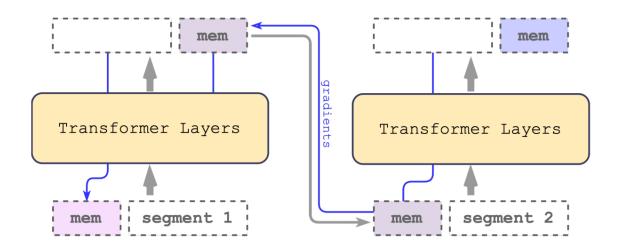
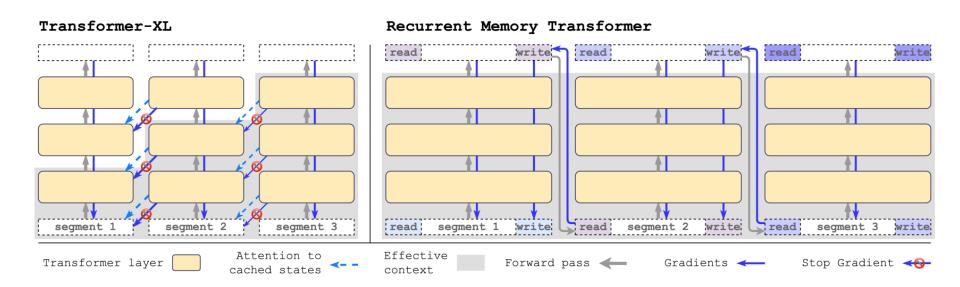


Figure 2: Illustration of the Transformer-XL model with a segment length 4.

- Recurrent Memory Transformer (RMT) [Bulatov et al., 2022]
 - Idea: Transformer with token-level memory storage & segment-level recurrence
 - Recurrently compress information in **tokens**, instead of external memory
 - Naturally, computation increases linearly with the input length
 - Like RNNs, RMT is trained with BPTT (backpropagation through time)



- Recurrent Memory Transformer (RMT) [Bulatov et al., 2022]
 - Idea: Transformer with token-level memory storage & segment-level recurrence
 - Comparison to Transformer-XL
 - **Unlimited** effective context length
 - No memory overhead for maintaining state cache



- Recurrent Memory Transformer (RMT) [Bulatov et al., 2022]
 - RMT outperforms Transformer-XL in algorithmic tasks and language modeling
 - Algorithmic tasks:
 - Copy/Reverse: Replicating & reversing the input sequence
 - Associative retrieval: Key-value retrieval task

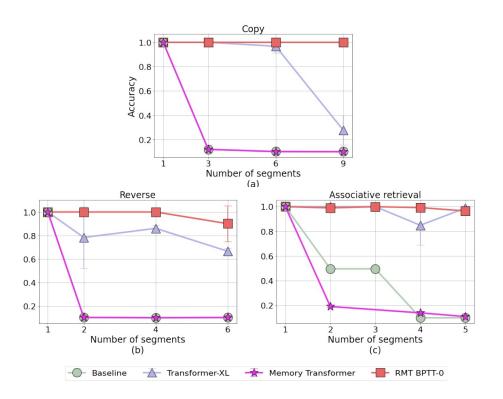
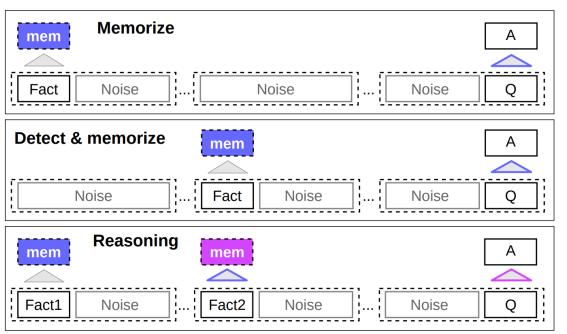


Table 2: Language modeling on WikiText-103. Average perplexity for the best performed variations of RMT models reported (see full results in Appendix A.5). Underlined values show Tr-XL and RMT models with close results. RMT models with smaller memory sizes achieve similar scores to Tr-XL models with larger memory. Combination of cache with recurrent memory (Tr-XL + RMT) shows the best performance.

Model	MEMORY	SEGMENT LEN	$\mathtt{PPL}_{\pm\mathtt{STD}}$
TR-XL (PAPER)	150	150	24.0
BASELINE MEMTR TR-XL (OURS)	0 10 150	150 150 150	$\begin{array}{c} 29.95 \pm 0.15 \\ 29.63 \pm 0.06 \\ 24.12 \pm 0.05 \end{array}$
TR-XL TR-XL RMT BPTT-3 RMT BPTT-2 TR-XL + RMT TR-XL + RMT	25 75 10 25 75+5 150+10	150 150 150 150 150 150	$\begin{array}{c} 25.57 \pm 0.02 \\ \underline{24.68} \pm 0.01 \\ 25.04 \pm 0.07 \\ \underline{24.85} \pm 0.31 \\ \underline{24.47} \pm 0.05 \\ 23.99 \pm 0.09 \end{array}$
BASELINE TR-XL TR-XL TR-XL TR-XL RMT BPTT-1 RMT BPTT-3	0 100 50 25 10 1	50 50 50 50 50 50 50	39.05 ± 0.01 25.66 ± 0.01 26.54 ± 0.01 27.57 ± 0.09 28.98 ± 0.11 28.71 ± 0.03 26.37 ± 0.01

- Recurrent Memory Transformer (RMT) [Bulatov et al., 2022]
 - BERT finetuned with RMT can extrapolate to long inputs over 1M tokens
 - Evaluated with synthetic, memory-intensive tasks
 - Construct long input, with a given fact hidden inside irrelevant text
 - Ask question at the end of the input (6-way classification task)



Fact: Daniel went back to the hallway.

Question: Where is Daniel?

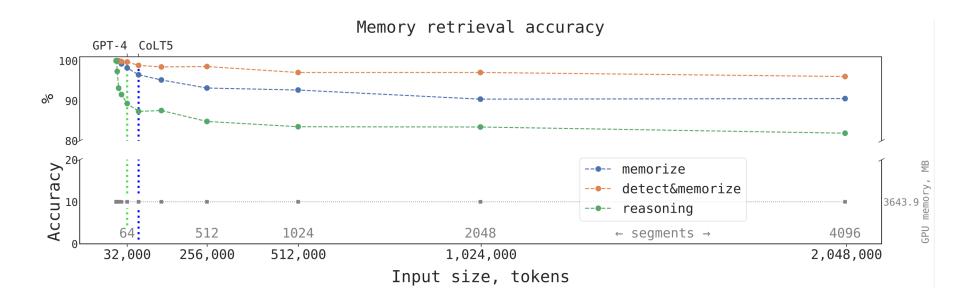
Answer: hallway

Fact1: The hallway is east of the bathroom. Fact2: The bedroom is west of the bathroom.

Question: What is the bathroom east of?

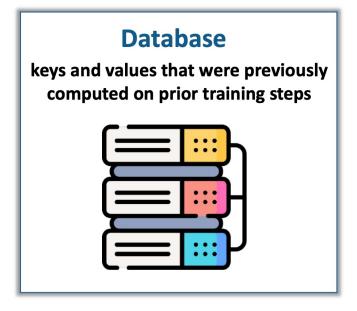
Answer: bedroom

- Recurrent Memory Transformer (RMT) [Bulatov et al., 2022]
 - BERT finetuned with RMT can extrapolate to long inputs over 1M tokens
 - Evaluated with synthetic, memory-intensive tasks
 - Construct long input, with a given fact hidden inside irrelevant text
 - Ask question at the end of the input (6-way classification task)

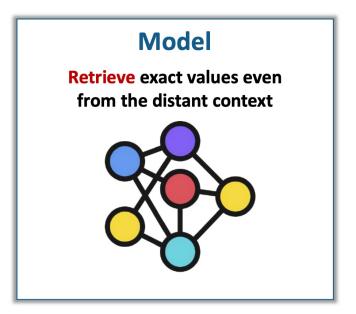


Retrieval-based Methods

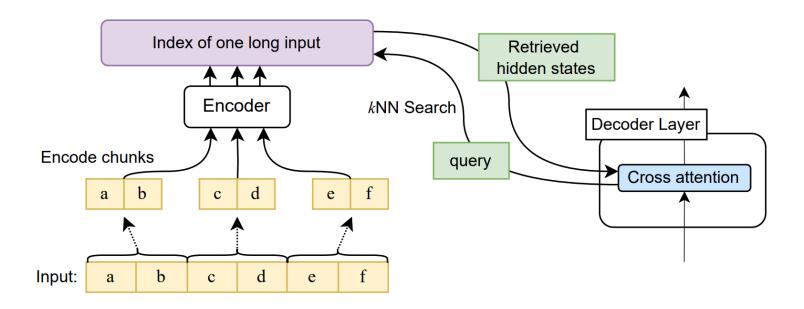
- Instead of using the preceding segment's hidden states, store all previous states
- When processing the current segment, retrieve the relevant information
- Enables random access to previous inputs



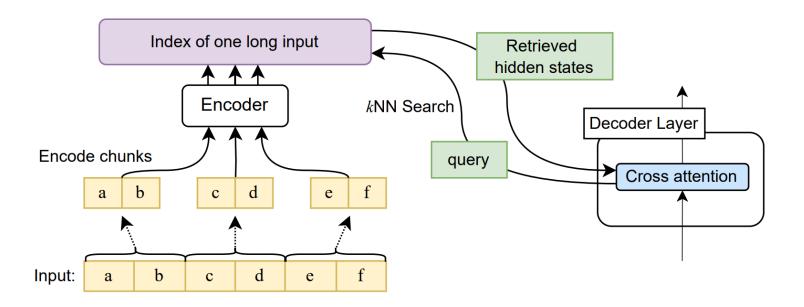




- Unlimiformer [Bertsch et al., 2024]
 - TL;DR: Retrieval-based language model that does not require fine-tuning
 - Basic approach is similar to Memory Transformers
 - Separately encode multiple segments, and store the hidden states in external memory
 - Use kNN search to retrieve relevant tokens



- Unlimiformer [Bertsch et al., 2024]
 - Unlimiformer applies knn retrieval on cross-attention
 - Retrieved tokens serve as usual encoder outputs
 - Memory fusion does not require gating, thus introducing no additional parameter
 - This allows Unlimiformer to work without fine-tuning



- Unlimiformer [Bertsch et al., 2024]
 - Attention reformulation
 - Originally, attention keys & values have to be stored for every layer/attention head
 - Memory requirement is further reduced through attention reformulation
 - Only a single vector has to be stored for every token
 - This allows memory retrieval to take place at every layer
 - Note: Memory Transformers apply retrieval on a single layer

$$egin{aligned} QK^T &= \left(oldsymbol{h}_d W_q
ight) \left(oldsymbol{h}_e W_k
ight)^{ op} \ &= \left(oldsymbol{h}_d W_q
ight) W_k^{ op} oldsymbol{h}_e^{ op} \ &= \left(oldsymbol{h}_d W_q W_k^{ op}
ight) oldsymbol{h}_e^{ op} \end{aligned}$$

Q/K: Query/key vector

Wq/Wk: layer- & head-specific linear layers

he: encoder hidden statehd: decoder hidden state

- Unlimiformer [Bertsch et al., 2024]
 - Unlimiformer extends the context limit without fine-tuning
 - Evaluated on summarization benchmarks

Base model	Training method	ROUGE 1 / 2 / L / BERTScore				
		GovReport	SummScreen			
BARTbase	Standard finetuning	48.7 / 19.2 / 22.8 / 64.3	29.7 / 6.2 / 17.7 / 56.3			
$BART_{base}$	+test SLED (Ivgi et al., 2022)	45.8 / 16.1 / 20.2 / 62.7	27.5 / 5.5 / 16.7 / 55.9			
$BART_{base}$	+test Unlimiformer	49.7 / 19.6 / 22.0 / 64.8	30.9 / 6.5 / 18.2 / 57.5			
$BART_{\texttt{base}}$	+early stop w/ Unlimiformer	51.0 / 20.5 / 21.5 / 65.1	32.1 / 6.8 / 18.6 / 57.6			

Performance is further improved with fine-tuning

20 X 10 X			
BART _{base}	Train chunked +test Unlimiformer		28.1 / 5.6 / 17.0 / 55.6 29.3 / 6.6 / 17.6 / 57.0
DANIbase	rtest Chimmonner	55.47 22.57 22.57 00.0	27.57 0.07 17.07 57.0
PRIMERA PRIMERA	Standard finetuning +test Unlimiformer	55.1 / 23.9 / 25.9 / 67.0 56.5 / 24.8 / 26.3 / 67.7	

- Unlimiformer [Bertsch et al., 2024]
 - Unlimiformer can handle extremely long (book-level) context
 - Evaluated on BookSum (average input length ~143k tokens)

Base model	Training method	ROUGE 1/2/L	EntMent
BART _{base}	Hierarchical (Kryściński et al., 2021)	30.0 / 6.0 / 11.0	-
$BART_{base}$	Standard finetuning	36.4 / 7.6 / 15.3	10.0
$BART_{base}$	+test Unlimiformer	35.5 / 7.7 / 15.4	21.9
$BART_{base}$	+early stop w/ Unlimiformer	35.5 / 7.7 / 15.4	21.9
$BART_{base}$	Memorizing Transformers	35.6 / 6.4 / 14.6	10.1
$BART_{base}$	Unlimiformer (random-encoded training)	37.3 / 6.7 / 15.2	20.8
$BART_{base}$	Unlimiformer (alternating training)	36.7 / 7.3 / 15.5	20.3
PRIMERA	Standard finetuning	38.6 / 7.2 / 15.6	11.6
PRIMERA	+test Unlimiformer	38.3 / 7.5 / 15.9	18.9
PRIMERA	+early stop w/ Unlimiformer	39.5 / 7.3 / 15.8	22.2
PRIMERA	Unlimiformer (retrieval training)	37.9 / 8.2 / 16.3	25.5
PRIMERA	Unlimiformer (random-encoded training)	39.5 / 7.1 / 15.9	19.7

Handling long context with Transformers

• 3 lines of research for long-context language models:

Recurrence-based methods

- Segments long inputs, and reuses the preceding segment's hidden states
- The hidden states serve as 'memory' for the current segment

Retrieval-based methods

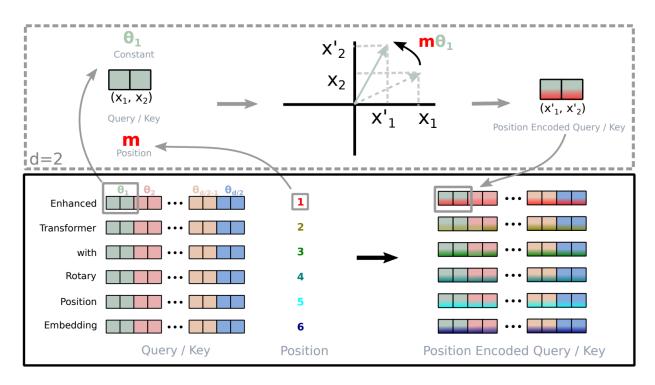
- Encodes prior sequences as (key, value) pairs
- Uses a retrieval algorithm to extract previously encoded information

RoPE scaling methods

- Applicable to language models utilizing rotary position embeddings (RoPE)
- Interpolates the position indices, extending the context limit of existing LLMs with minimal or no additional training

RoPE Scaling Methods

- Rotary Position Embeddings (RoPE) [Su et al., 2021]
 - Idea: Rotate the hidden states according to the token's position
 - View a pair of hidden state values as a complex number
 - ullet Rotate each pair by a different frequency $heta_i$
 - Captures the relative positional information between each token
 - One of the most widely-used positional embeddings for modern LLMs
 - Including Llama, GPT-NeoX, and PaLM



RoPE Scaling Methods

- Rotary Position Embeddings (RoPE) [Su et al., 2021]
 - Idea: Rotate the hidden states according to the token's position
 - Mathematical formulation of RoPE is given as follows
 - **m**: position id
 - W: linear projection matrix (query, key)
 - xm: hidden states
 - d: hidden state dimension

$$f_{\mathbf{W}}(\mathbf{x}_m, m, \theta_i) = \begin{pmatrix} \cos m\theta_1 & -\sin m\theta_1 & 0 & 0 & \cdots & 0 & 0\\ \sin m\theta_1 & \cos m\theta_1 & 0 & 0 & \cdots & 0 & 0\\ 0 & 0 & \cos m\theta_2 & -\sin m\theta_2 & \cdots & 0 & 0\\ 0 & 0 & \sin m\theta_2 & \cos m\theta_2 & \cdots & 0 & 0\\ 0 & 0 & 0 & 0 & \cdots & \cos m\theta_{d/2} & -\sin m\theta_{d/2}\\ 0 & 0 & 0 & 0 & \cdots & \sin m\theta_{d/2} & \cos m\theta_{d/2} \end{pmatrix} \mathbf{W} \mathbf{x}_m$$

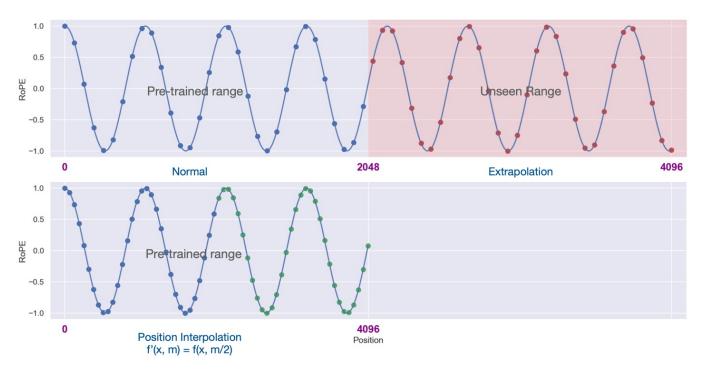
$$\theta_i = 10000^{-2(i-1)/d}, i \in [1, 2, \dots, d/2]$$

Algorithmic Intelligence Lab

RoPE Scaling Methods: Linear Interpolation

- Positional Interpolation (i.e. linear interpolation) [Chen et al., 2023]
 - Motivation: Naïvely finetuning LLMs for longer context shows limited success
 - Primarily due to introduction of new position ids, unseen while training
 - Idea: Instead of extrapolating, interpolate the position ids
 - L: Original context length, L': Extended context length

$$f'_{\mathbf{W}}(\mathbf{x}_m, m, \theta_i) = f_{\mathbf{W}}(\mathbf{x}_m, \frac{L}{L'}m, \theta_i)$$



RoPE Scaling Methods: Linear Interpolation

- Positional Interpolation (i.e. linear interpolation) [Chen et al., 2023]
 - Interpolation effectively extends Llama context length with minimal training
 - Fine-tuning possible with ~1000 steps

	Model		E	valuation	Context V	Window S	Size
Size	Context Window	Method	2048	4096	8192	16384	32768
7B	2048	None	7.20	$> 10^3$	$> 10^{3}$	$> 10^3$	$> 10^3$
7B	8192	FT	7.21	7.34	7.69	-	-
7B	8192	PI	7.13	6.96	6.95	-	-
7B	16384	PΙ	7.11	6.93	6.82	6.83	-
7B	32768	PI	7.23	7.04	6.91	6.80	6.77
13B	2048	None	6.59	-	-	-	-
13B	8192	FT	6.56	6.57	6.69	-	-
13B	8192	PI	6.55	6.42	6.42	-	-
13B	16384	PΙ	6.56	6.42	6.31	6.32	-
13B	32768	PI	6.54	6.40	6.28	6.18	6.09
33B	2048	None	5.82	-	-	-	-
33B	8192	FT	5.88	5.99	6.21	-	-
33B	8192	PI	5.82	5.69	5.71	-	-
33B	16384	PI	5.87	5.74	5.67	5.68	-
65B	2048	None	5.49	-	-	-	-
65B	8192	PI	5.42	5.32	5.37	-	-

RoPE Scaling Methods: NTK-aware Scaling

- NTK-aware Scaling [bloc97, 2023]
 - Motivation: Linear interpolation sacrifices high-frequency information
 - Position embeddings of adjacent tokens become indistinguishable
 - Such inspiration comes from the neural tangent kernel (NTK) theory
 - A simple solution is to scale each dimension differently
 - Position interpolation scales every dimension uniformly by a factor s (=L/L')
 - Scale high frequencies more, and low frequencies less
 - This work uses a simple base scaling to implement this

$$\theta_i = 10000^{-2(i-1)/d}, i \in [1, 2, \cdots, d/2]$$

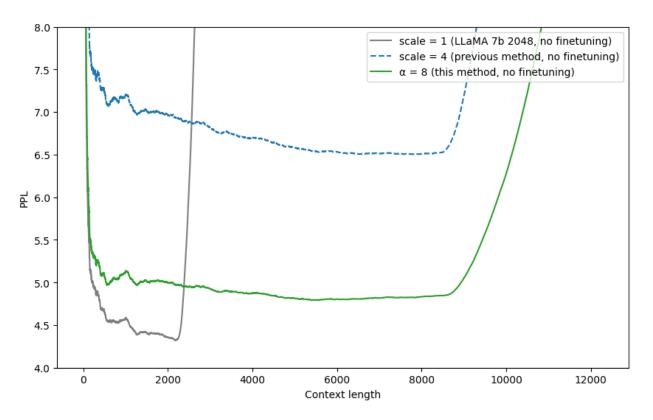


$$\theta'_i = \left(10000 \times s^{\frac{d}{d-2}}\right)^{-2(i-1)/d}, i \in [1, 2, \cdots, d/2]$$

base is scaled according to the scaling factor **s**

RoPE Scaling Methods: NTK-aware Scaling

- NTK-aware Scaling [bloc97, 2023]
 - NTK-aware scaling extends the context limit without any finetuning
 - Llama-7b model maintains low perplexity for longer context
 - This scaling method was used for training Code Llama, which has 100k context limit



previous method: linear scaling this method: NTK-aware scaling

- NTK-by-parts Scaling [bloc97, 2023]
 - Investigates deeper into the different characteristics of each dimension
 - Key idea is to consider the RoPE embedding wavelength
 - The **number of tokens** needed for the RoPE embedding to perform a **full rotation** (2π) .
 - Wavelength for dimension i is defined as follows

$$\lambda_i = \frac{2\pi}{\theta_i} = 2\pi \times 10000^{2(i-1)/d}$$

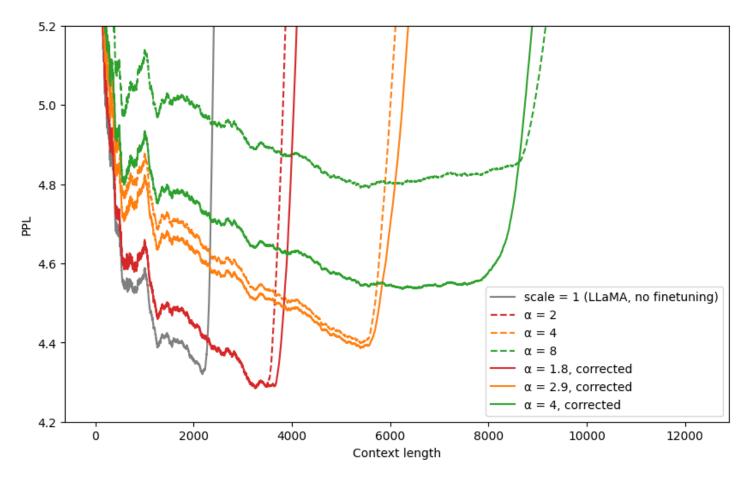
- NTK-by-parts Scaling [bloc97, 2023]
 - Investigates deeper into the different characteristics of each dimension
 - Dimensions with λ > L (L: model's original context limit)
 - The embedding does not perform a full rotation
 - Position embeddings are unique
 - Intuition: The absolute positional information remains intact
 - Dimensions with λ << L
 - The embedding rotates multiple times within the context limit
 - Position embeddings are not unique
 - Intuition: Only relative positional information can be modeled

- NTK-by-parts Scaling [bloc97, 2023]
 - Idea: Interpolate only the dimensions with long wavelengths
 - L: Original context length, L': Extended context length
 - α , β are hyperparameters

No interpolation
$$\theta_i' = (1 - \gamma_i) \frac{L}{L'} \theta_i + \gamma_i \theta_i \qquad \gamma_i = \begin{cases} 0, & \text{if } L/\lambda_i < \alpha \\ 1, & \text{if } L/\lambda_i > \beta \\ \frac{L/\lambda_i - \alpha}{\beta - \alpha}, & \text{otherwise} \end{cases}$$
 Linear interpolation

- Dimensions with λ > L
 - These dimensions model the **global** position information
 - Use linear interpolation
- Dimensions with λ << L
 - These dimensions model the **relative** position information
 - Use no interpolation
- Dimensions in between
 - Use a bit of both methods, by mixing them with a ramp function

- NTK-by-parts Scaling [bloc97, 2023]
 - The 'by-parts' modification further improves NTK-based scaling



'corrected' denotes NTK-by-parts

Algorithmic Intelligence Lab

RoPE Scaling Methods: YaRN

- YaRN (Yet another RoPE ExtensioN method) [Peng et al., 2024]
 - TL;DR: NTK-by-parts with temperature scaling
 - Remark: NTK and NTK-by-parts scaling were also formally introduced in this paper
 - NTK-by-parts scaling empirically smooths the attention weights
 - Scaling the attention weights by a factor of t helps, making the weights 'spikier'

softmax
$$\left(\frac{oldsymbol{q}_m^T oldsymbol{k}_n}{t\sqrt{|D|}} \right)$$

Empirically, the following formula works well for Llama and Llama-2 models

$$\sqrt{\frac{1}{t}} = 0.1\ln(s) + 1$$

RoPE Scaling Methods: YaRN

- YaRN (Yet another RoPE ExtensioN method) [Peng et al., 2024]
 - Fine-tuning with YaRN is efficient and effective
 - Training data consists of 400M tokens (0.1% of original training corpus)
 - Training done with only 400 steps
 - YaRN extends the context limit of Llama-2 to 64k/128k tokens
 - Original model has a limit of 4k tokens

Extension	Trained	Context		luation (Size
Method	Tokens	Window	2048	4096	6144	8192	10240
PI(s=2)	1B	8k	3.92	3.51	3.51	3.34	8.07
NTK ($\theta = 20$ k)	1B	8k	4.20	3.75	3.74	3.59	6.24
YaRN $(s=2)$	400M	8k	3.91	3.50	3.51	3.35	6.04

Model Size	Model Name	Context Window	Extension Method	Evaluation Context Window Size 8192 32768 65536 98304 131072				
7B 7B 7B 7B	Together Code Llama YaRN $(s = 16)$ YaRN $(s = 32)$	32k 100k 64k 128k	PI NTK YaRN YaRN	3.50 3.71 3.51 3.56	2.64 2.74 2.65 2.70	$> 10^2$ 2.55 2.42 2.45	$> 10^3$ 2.54 $> 10^1$ 2.36	$> 10^4$ 2.71 $> 10^1$ 2.37
13B 13B 13B	Code Llama YaRN $(s = 16)$ YaRN $(s = 32)$	100k 64k 128k	NTK YaRN YaRN	3.54 3.25 3.29	2.63 2.50 2.53	2.41 2.29 2.31	2.37 $> 10^{1}$ 2.23	2.54 $> 10^{1}$ 2.24

RoPE Scaling Methods: YaRN

- YaRN (Yet another RoPE ExtensioN method) [Peng et al., 2024]
 - YaRN-finetuned models show minimal performance degradation on short inputs

Model Size	Model Name	Context Window	Extension Method	ARC-c	Hellaswag	MMLU	TruthfulQA
7B	Llama 2	4k	None	53.1	77.8	43.8	39.0
7B 7B 7B 7B	Together Code Llama YaRN $(s = 16)$ YaRN $(s = 32)$	32k 100k 64k 128k	PI NTK YaRN YaRN	47.6 39.9 52.3 52.1	76.1 60.8 78.8 78.4	43.3 31.1 42.5 41.7	39.2 37.8 38.2 37.3
13B	Llama 2	4k	None	59.4	82.1	55.8	37.4
13B 13B 13B	Code Llama YaRN $(s = 16)$ YaRN $(s = 32)$	100k 64k 128k	NTK YaRN YaRN	40.9 58.1 58.0	63.4 82.3 82.2	32.8 52.8 51.9	43.8 37.8 37.3

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Part 3. Advanced Topics

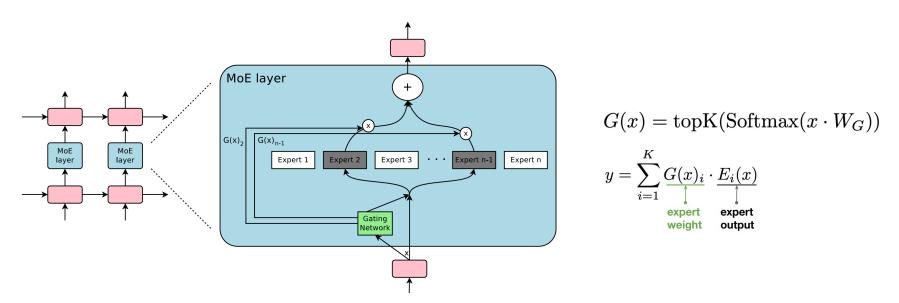
- Handling long inputs with Transformers
- Techniques for improving efficiency
- State-Space Models

Part 4. Summary

Towards efficient LLMs

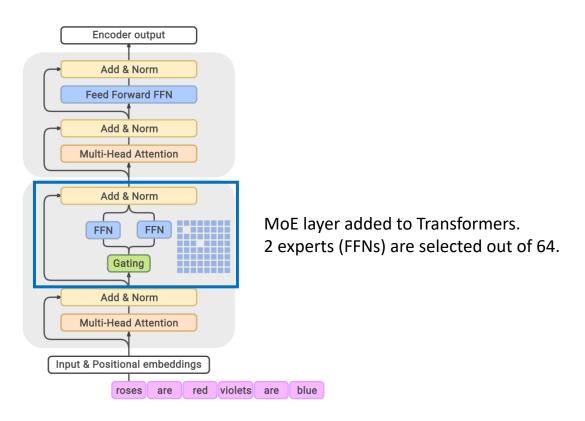
- Scaling has been the key for the success of modern LLMs
 - However, large computation poses a significant bottleneck
 - Improving computational efficiency is critical for further scaling
- Possible solutions include:
 - Architectures that enable scaling without severely increasing computation
 - Further computation optimization for the current architecture

- GLaM (Generalist Language Model) [Du et al., 2022]
 - Intuition: Can we decouple the computation cost from the model size?
 - The key idea is to introduce Mixture-of-Experts (MoE) layers
 - Consists of multiple experts (simple feed-forward network) and a gating network
 - Gating network selects the K 'best' experts for a given input
 - Final output is the weighted sum of each expert's output



MoE layer [Shazeer et al., 2017] applied on LSTM

- GLaM (Generalist Language Model) [Du et al., 2022]
 - Intuition: Can we decouple the computation cost from the model size?
 - The key idea is to introduce **Mixture-of-Experts (MoE)** layers
 - In this work, MoE layer is applied to the FFN layer of Transformers
 - 2 experts are selected, providing O(number of experts^2) combination of FFN layers, providing more flexibility



- GLaM (Generalist Language Model) [Du et al., 2022]
 - Enables efficient scaling, while keeping the computation small
 - Largest GLaM model (64B/64E) has 1.2T parameters
 - However, only 96.6B are activated per prediction

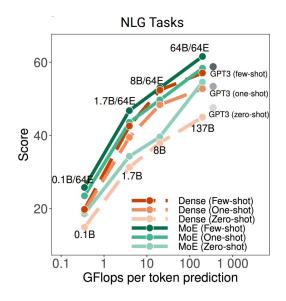
GLaM Model	Type	$n_{ m params}$	$n_{ m act ext{-}params}$
0.1B	Dense	130M	130M
0.1B/64E	MoE	1.9B	145M
1.7B	Dense	1.7B	1.700B
1.7B/32E	MoE	20B	1.878B
1.7B/64E	MoE	27B	1.879B
1.7B/128E	MoE	53B	1.881B
1.7B/256E	MoE	105B	1.886B
8B	Dense	8.7B	8.7B
8B/64E	MoE	143B	9.8B
137B	Dense	137B	137B
64B/64E	MoE	1.2T	96.6B

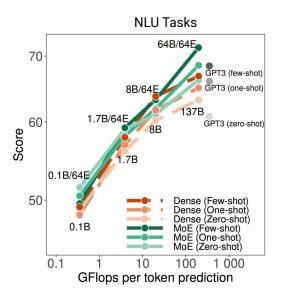
Number of total parameters and activated parameters for each GLaM model (base dense size / number of experts)

- GLaM (Generalist Language Model) [Du et al., 2022]
 - GLaM outperforms GPT-3 while requiring less computation

		GPT-3	GLaM	relative
cost	FLOPs / token (G) Train energy (MWh)	350 1287	180 456	-48.6% -64.6%
accuracy on average	Zero-shot One-shot Few-shot	56.9 61.6 65.2	62.7 65.5 68.1	+10.2% +6.3% +4.4%

- Models trained with mixture-of-experts successfully scale
 - Achieves higher performance using similar FLOPs per token prediction





- Multi-head Latent Attention [Liu, Aixin, et al., 2024]
 - Motivation: Reduce KV cache memory and computation costs while maintaining performance for efficient inference.
 - KV cache: Previously computed key and value tensors in attention mechanisms.



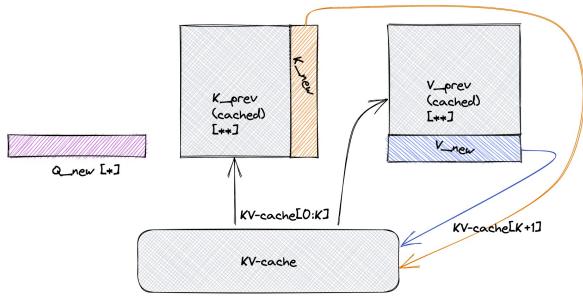
Notes:

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^{*} When processing token[K], we only need the K'th row of Q

^{**} When processing token [K], we require the full K & V tensors, but we can mostly reuse the cached values (This enables skipping the computation of K & V

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- Multi-head Latent Attention [Liu, Aixin, et al., 2024]
 - **Idea**: Jointly compress key and value tensors into a low-rank latent representation and reconstruct them when needed.
 - Standard Multi-Head Attention:
 - Let d be the embedding dim., n_h be the number of heads, d_h be the dim. per head.
 - $q_t = W^Q h_t$, $k_t = W^K h_t$, $v_t = W^V h_t$, where W^Q , W^K , $W^V \in \mathbb{R}^{d_h n_h \times d}$
 - Latent compression:
 - $c_t^{KV} = W^{DKV} h_t$, where $W^{DKV} \in \mathbb{R}^{d_c \times d}$
 - Compress the hidden state h_t into a compressed latent vector c_t^{KV} .
 - Key-value reconstruction:
 - $k_t^C = W^{UK} c_t^{KV}$, $v_t^C = W^{UV} c_t^{KV}$, where W^{UK} , $W^{UV} \in \mathbb{R}^{d_h n_h \times d_C}$
 - Reconstruct the key and value vector from the compressed latent vector.
 - No need to compute Keys and Values during inference:
 - Attention Computation:
 - Attention_i = Softmax $\left(\frac{h^T W^{QT} W^K h}{\sqrt{d}}\right) W^V h$ = Softmax $\left(\frac{h^T W^{QT} W^{UK} c^{KV}}{\sqrt{d}}\right) W^{UV} c^{KV}$
 - Output = W^{O} [Attention_{1:n_h}], where [] is concatenation
 - W^{UK} can be absorbed to W^Q
 - W^{UV} can be absorbed to W^O , where W^O is the output projection matrix

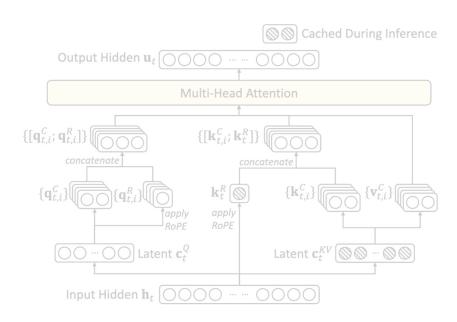
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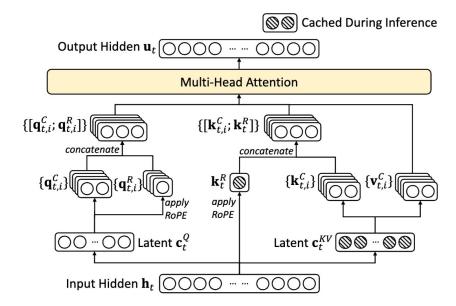
- Multi-head Latent Attention [Liu, Aixin, et al., 2024]
 - However, RoPE is not compatible with matrix absorption.
 - W^{UK} cannot be absorbed into W^Q anymore during the inference.
 - Since the RoPE matrix will lie between W^{UK} and W^Q , and RoPE weight will vary for all tokens.

• Attention_i = Softmax
$$\left(\frac{RoPE(h^TW^Q)^TRoPE(W^{UK}c^{KV})}{\sqrt{d}}\right)W^{UV}c^{KV}$$

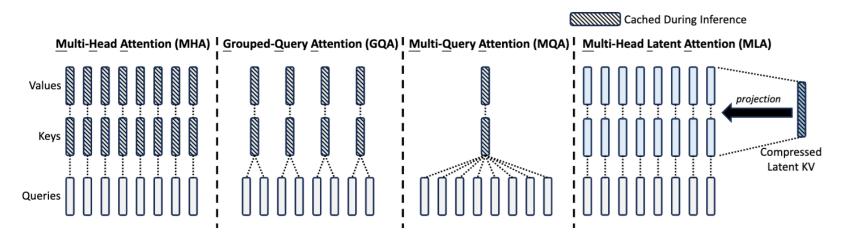
• Thus, we must **recompute the keys for all tokens** during inference.



- Multi-head Latent Attention [Liu, Aixin, et al., 2024]
 - Decoupled Rotary Position Embedding (RoPE)
 - Idea: 1. Partially apply the PE for the query and keys
 2. Share the key carrying PE across the heads
 - Additional multi-head queries and shared key carrying RoPE:
 - $q_t^R = RoPE(W^{QR}c_t^Q)$, $k_t^R = RoPE(W^{KR}h_t)$, $W^{QR} \in \mathbb{R}^{d_h^R n_h \times d_c'}$, $W^{KR} \in \mathbb{R}^{d_h^R \times d_c}$ where d_h^R is the per-head dim. of the decoupled q and k
 - Then, concatenate with query and keys:
 - $q_{t,i} = [q_{t,i}^C; q_{t,i}^R], k_{t,i} = [k_{t,i}^C; k_t^R]$



- Multi-head Latent Attention [Liu, Aixin, et al., 2024]
 - Comparing with existing methods
 - MLA can significantly reduce the memory requirement compared to MHA, and GQA.



Simplified illustration of MHA, GQA, MQA, and MLA

Attention Mechanism	KV Cache per Token (# Element)
Multi-Head Attention (MHA)	$2n_hd_hl$
Grouped-Query Attention (GQA)	$2n_gd_hl$
Multi-Query Attention (MQA)	$2d_h l$
MLA (Ours)	$(d_c + d_h^R)l \approx \frac{9}{2}d_h l$

KV cache per Token

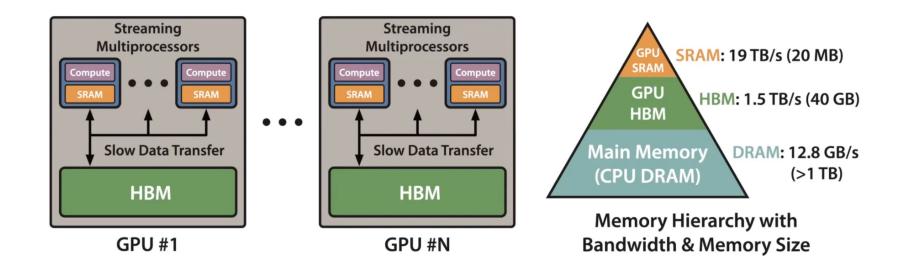
- Multi-head Latent Attention [Liu, Aixin, et al., 2024]
 - Comparing with existing methods
 - Both MQA, and GQA underperforms MHA in all benchmarks
 - However, MLA surpasses MHA on most benchmarks with different model sizes.
 - While requiring significantly smaller amount of KV cache

Benchmark (Metric)	# Shots	Dense 7B w/ MQA	Dense 7B w/ GQA (8 Groups)	Dense 7B w/ MHA
# Params	-	7.1B	6.9B	6.9B
BBH (EM)	3-shot	33.2	35.6	37.0
MMLU (Acc.)	5-shot	37.9	41.2	45.2
C-Eval (Acc.)	5-shot	30.0	37.7	42.9
CMMLU (Acc.)	5-shot	34.6	38.4	43.5

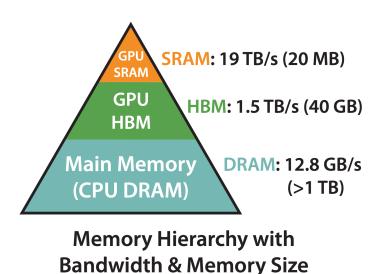
Comparing MQA, GQA, and MHA

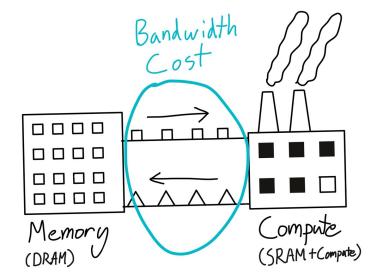
Benchmark (Metric)	# Shots	Small MoE w/ MHA	Small MoE w/ MLA	Large MoE w/ MHA	Large MoE w/ MLA
# Activated Params	-	2.5B	2.4B	25.0B	21.5B
# Total Params	-	15.8B	15.7B	250.8B	247.4B
KV Cache per Token (# Element)	-	110.6K	15.6K	860.2K	34.6K
BBH (EM)	3-shot	37.9	39.0	46.6	50.7
MMLU (Acc.)	5-shot	48.7	50.0	57.5	59.0
C-Eval (Acc.)	5-shot	51.6	50.9	57.9	59.2
CMMLU (Acc.)	5-shot	52.3	53.4	60.7	62.5

- FlashAttention [Dao et al., 2022]
 - Motivation: HBM access is the bottleneck in self-attention operation
 - Memory hierarchy
 - GPU memory hierarchy comprises multiple forms of memory of different size and speed
 - On-chip SRAM is much smaller, but faster than high bandwidth memory (HBM)

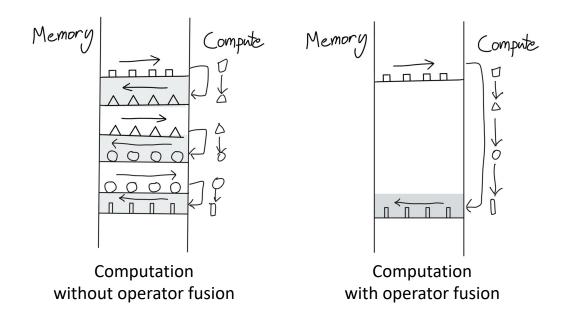


- FlashAttention [Dao et al., 2022]
 - Motivation: HBM access is the bottleneck in self-attention operation
 - Typical GPU operation
 - Load inputs from HBM to registers and SRAM
 - 2. Compute
 - Write outputs to HBM
 - Turns out: Most operations in self-attention are memory-bounded
 - More time is spent on IO to HBM, not the compute itself

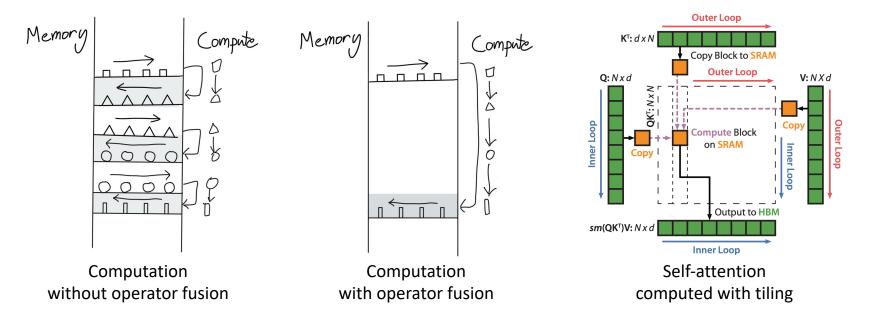




- FlashAttention [Dao et al., 2022]
 - Idea: Utilize kernel fusion to reduce HBM access
 - Access HBM only once, and perform multiple operations in a row



- FlashAttention [Dao et al., 2022]
 - Idea: Utilize kernel fusion to reduce HBM access
 - Access HBM only once, and perform multiple operations in a row
 - However, SRAM memory is much smaller than HBM
 - The full attention matrix does not fit in SRAM
 - Key intuition: compute self-attention by parts, without materializing the large attention matrix (Tiling)
 - This introduces a few challenges in the context of model training



- FlashAttention [Dao et al., 2022]
 - Challenge 1: Computing softmax without full input access
 - Solution: Decompose large softmax into smaller ones by scaling
 - With scaling, exact softmax results can be obtained after computing each block independently

$$\operatorname{softmax}([A_1, A_2]) = [\alpha \operatorname{softmax}(A_1), \beta \operatorname{softmax}(A_2)]$$

$$\operatorname{softmax}([A_1, A_2]) \ \begin{bmatrix} V_1 \\ V_2 \end{bmatrix} = \alpha \ \operatorname{softmax}(A_1) \ V_1 + \beta \ \operatorname{softmax}(A_2) \ V_2$$

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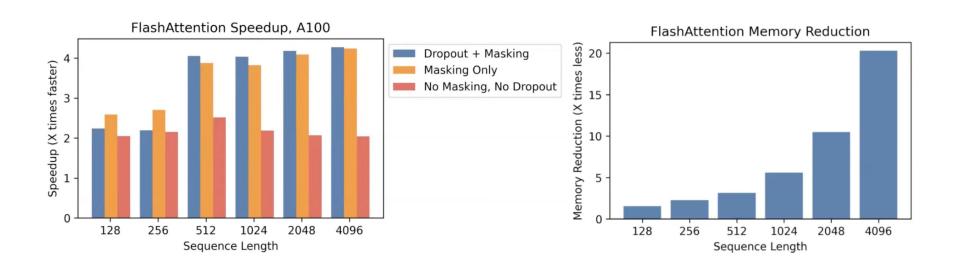
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- Challenge 2: Backward pass requires intermediate values
 - The attention matrix have to be saved, requiring extensive HBM access
 - Solution: Recompute the attention matrix during the backward pass
 - This approach is faster despite requiring more FLOPs, thanks to reduced HBM access

Attention	Standard	FLASHATTENTION
GFLOPs	66.6	75.2
HBM R/W (GB)	40.3	4.4
Runtime (ms)	41.7	7.3

- FlashAttention [Dao et al., 2022]
 - FlashAttention provides actual wall-clock speedup of 2-4x
 - Note: Many previous approximation-based approaches focus on reducing FLOPs, and do not display wall-clock speedup
 - Memory requirement becomes linear in sequence length
 - Naïve attention requires quadratic memory
 - FlashAttention makes training & inference with longer inputs feasible

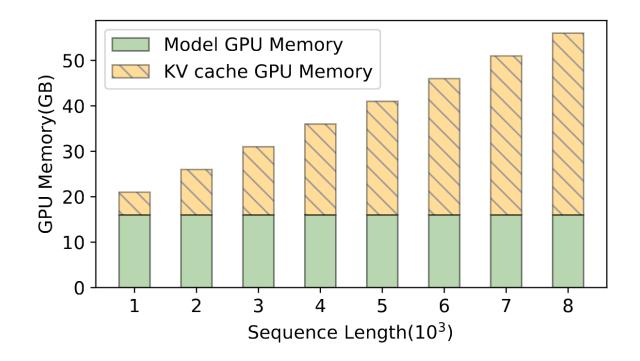


- FlashAttention [Dao et al., 2022]
 - FlashAttention also enables faster end-to-end training
 - BERT training is 3.2x faster than Huggingface
 - GPT-2 training is 2.0-3.5x faster

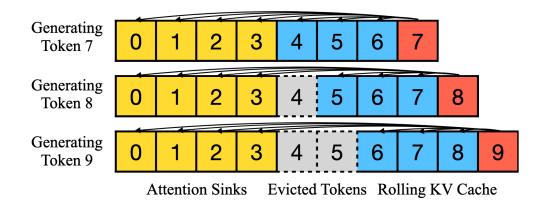
BERT Implementation	Training time (minutes)
Huggingface [91]	55.6 ± 3.9
Nvidia MLPerf 1.1 [63]	20.0 ± 1.5
FLASHATTENTION (ours)	17.4 ± 1.4

Model implementations	OpenWebText (ppl)	Training time (speedup)
GPT-2 small - Huggingface [84]	18.2	9.5 days (1.0×)
GPT-2 small - Megatron-LM [74]	18.2	$4.7 \text{ days } (2.0 \times)$
GPT-2 small - FlashAttention	18.2	$2.7 ext{ days } (3.5 \times)$
GPT-2 medium - Huggingface [84]	14.2	$21.0 \text{ days } (1.0 \times)$
GPT-2 medium - Megatron-LM [74]	14.3	$11.5 \text{ days } (1.8 \times)$
GPT-2 medium - FLASHATTENTION	14.3	$6.9 ext{ days } (3.0 \times)$

- Memory Bottleneck in Long-context Processing
 - Key-Value (KV) cache grows linearly with respect to the sequence length
 - With large models and long inputs, large KV cache introduces a memory bottleneck
 - Large GPU memory is required to store the cache
 - Recent works propose to compress the KV cache at inference-time by evicting less important tokens from the cache
 - Such approach also provides decoding speedup, thanks to the smaller cache



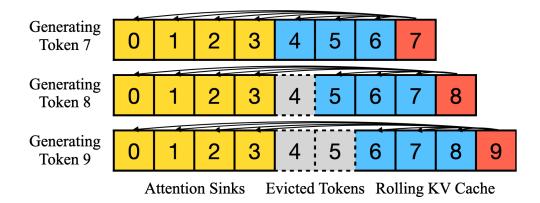
- StreamingLLM [Xiao et al., 2024]
 - Idea: Only keep the initial tokens ('attention sinks') and the recent tokens
 - Initial tokens typically take up significant attention scores
 - Therefore, preserving the initial tokens is important for reducing distribution shifts introduced by the compression
 - Position id reassignment
 - Positional encodings are applied according to the relative position within the cache rather than those in the original context
 - Position ids are reassigned after each eviction operation



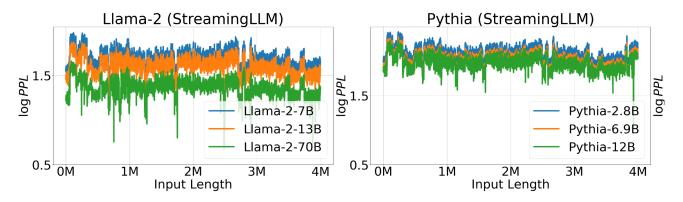
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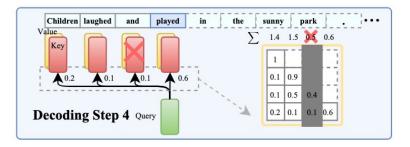
- StreamingLLM [Xiao et al., 2024]
 - StreamingLLM shows stable perplexity at extremely long sequences while using a fixed-sized KV cache

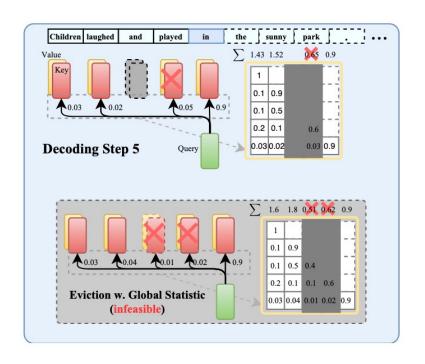


- However, it shows limited performance at long-context benchmarks
 - Information at the middle of the prompt is lost due to token eviction
 - StreamingLLM shows comparable performance with input truncation

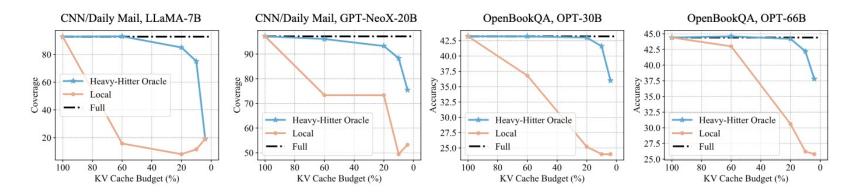
Llama2-7B-chat	Single-Docur	ingle-Document QA Multi-Document QA		cument QA	Summarization	
Liailiaz-/D-cliat	NarrativeQA	Qasper	HotpotQA	2WikiMQA	GovReport	MultiNews
Truncation 1750+1750	18.7	19.2	25.4	32.8	27.3	25.8
StreamingLLM 4+3496	11.6	16.9	21.6	28.2	23.9	25.5
StreamingLLM 1750+1750	18.2	19.7	24.9	32.0	26.3	25.9

- H2O (Heavy-Hitter Oracle) [Zhang et al., 2023]
 - Idea: Keep the heavy-hitters (i.e., tokens that receive high attention scores) as well as the recent tokens
 - Intuition: keep the 'important' tokens in the cache to minimize information loss
 - By preserving the tokens based on the accumulated attention scores, H2O has minimal impact on attention computation despite using token eviction





- H2O (Heavy-Hitter Oracle) [Zhang et al., 2023]
 - H2O shows robust performance under small KV cache budgets



H2O also enables high-throughput inference thanks to the reduced KV cache

Seq. length	512+32		512+512		512+1024	
Model size	6.7B	30B	6.7B	30B	6.7B	30B
Accelerate DeepSpeed FlexGen	20.4 (2, G) 10.2 (16, C) 20.2 (2, G)	0.6 (8, C) 0.6 (4, C) 8.1 (144, C)	15.5 (1, G) 9.6 (16, C) 16.8 (1, G)	0.6 (8, C) 0.6 (4, C) 8.5 (80, C)	5.6 (16, C) 10.1 (16, C) 16.9 (1, G)	0.6 (8, C) 0.6 (4, C) 7.1 (48, C)
H ₂ O (20%)	35.1 (4, G)	12.7 (728, C)	51.7 (4, G)	18.83 (416, C)	52.1 (4, G)	13.82 (264, C)

Generation Throughput Comparison

Overview

Part 1. Basics

- RNN to LSTM
- Sequence-to-sequence Model
- Attention-based NLP Model

Part 2. Transformers and Large Language Models

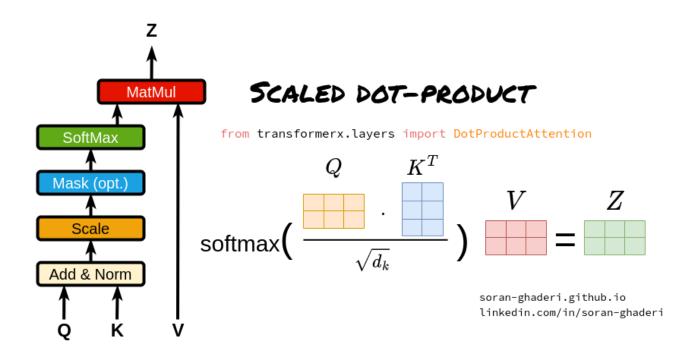
- Transformer (self-attention)
- Pre-training of Transformers and Language Models

Part 3. Advanced Topics

- Handling long inputs with Transformers
- Techniques for improving efficiency
- State-Space Models

Part 4. Summary

Transformers are "Heavy" and "Slow"



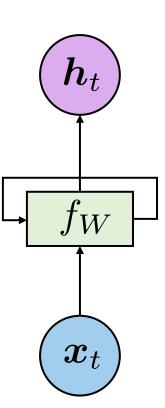
 $O(N^2)$ for both inference **memory** and **time** where N is the sequence length

Need to save all the previous tokens in the memory (i.e., KV-cache)

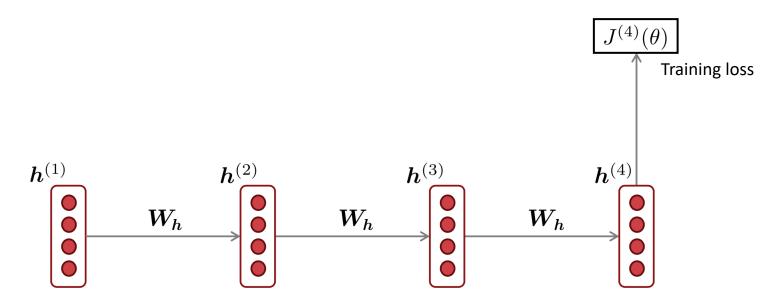
- Revisit RNNs Efficient inference
 - Only requires saving the previous hidden state
 - \rightarrow Constant memory usage O(1)
 - \rightarrow Linear time inference speed O(N)

$$oldsymbol{h}_t = f_W(oldsymbol{h}_{t-1}, oldsymbol{x}_t)$$
New state Old state Input vector at time step t

Function parameterized by learnable W

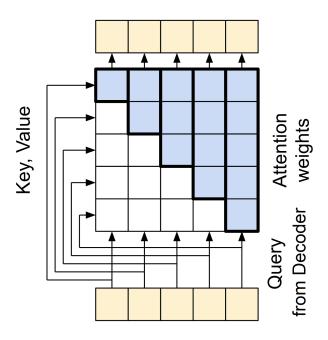


- Revisit RNNs Efficient inference but inefficient training
 - Only requires saving the previous hidden state
 - But the bottleneck is the training: Not able to parallelize



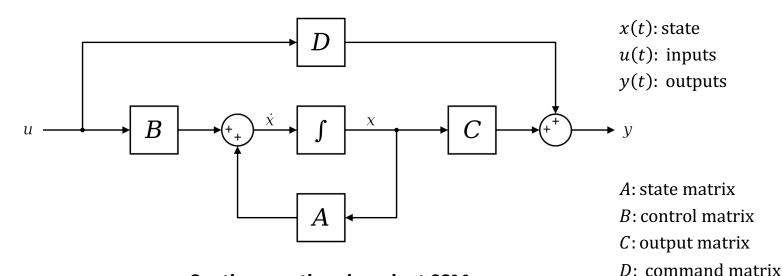
Need to wait for the previous hidden states...

- Revisit RNNs Efficient inference but inefficient training
 - Only requires saving the previous hidden state
 - But the bottleneck is the training: Not able to parallelize
 - Not for Attention: Training is super efficient as on can parallelize the forward pass.



Forward all tokens at ones, and use causal attention mask for autoregressive learning

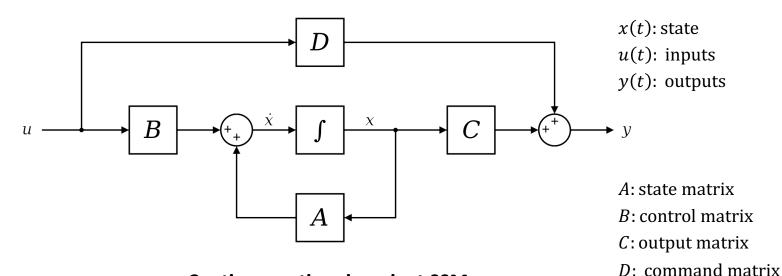
- What is the state space model (SSM)?
 - In the context of deep learning, "Linear invariant (or stationary) systems".



Continuous, time-invariant SSM

$$x'(t) = Ax(t) + Bu(t)$$
$$y(t) = Cx(t) + Du(t)$$

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 - In the context of deep learning, "Linear invariant (or stationary) systems".

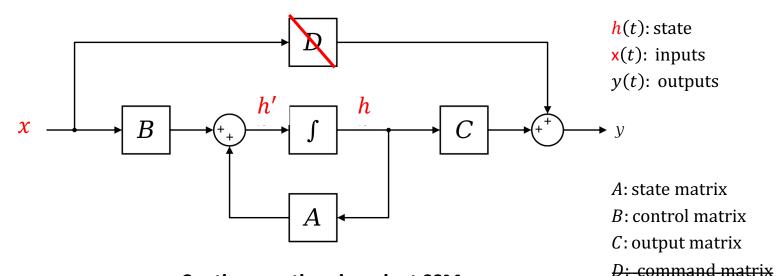


Continuous, time-invariant SSM

$$x' = Ax + Bu$$
$$y = Cx$$

We can simplify the SSM in this form of system.

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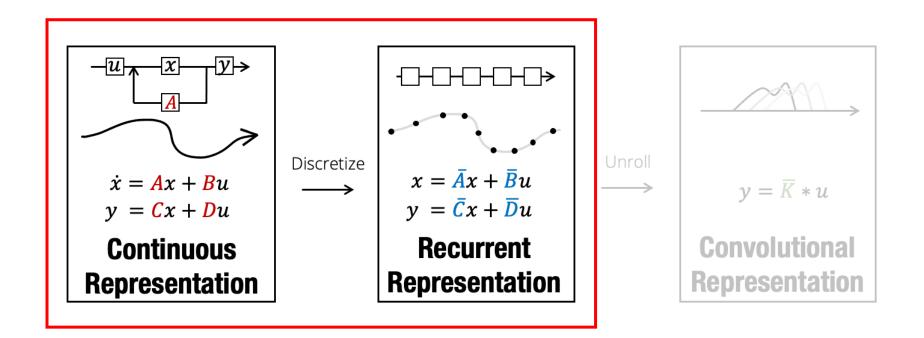


Continuous, time-invariant SSM

$$h' = Ah + Bx$$
$$y = Ch$$

We can simplify the SSM in this form of system.

- Discretizing the SSMs.
 - Since continuous representation is significantly slow for both training and inference,
 - We discretize the SSM to view the system in the recurrent representation.



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- Discretizing the SSMs.

 - Discretize matrices (we are introducing the ZOH discretization method here).

State Space Representation

$$h'(t) = Ah(t) + Bx(t)$$

$$y(t) = Ch(t)$$



Discretized State Space Model

$$h_t = \bar{A}h_{t-1} + \bar{B}x_t$$
$$y_t = \bar{C}h_t$$

$$y_t = \bar{C}h_t$$

ZOH discretization where Δ is a steps size

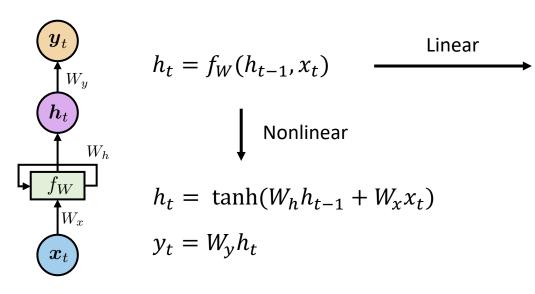
$$\bar{A} = \exp(\Delta A)$$

 $\bar{B} = (\Delta A)^{-1}(\exp \Delta A - I) \cdot \Delta B$
 $\bar{C} = C$

- Discretizing the SSMs.
 - Since continuous representation is significantly slow for both training and inference,
 - We discretize the SSM to view the system in the recurrent representation.
 - Connection with recurrent neural networks (RNNs)?
 - Generally, SSMs are Linear RNNs.

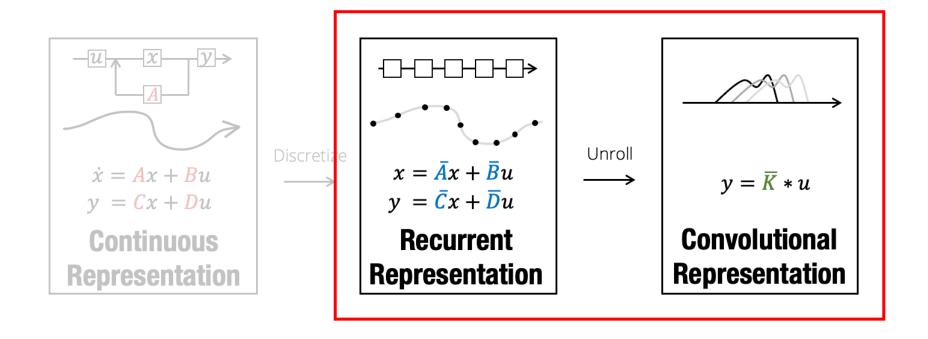
Recap. Recurrent Neural Net

Discretized State Space Model



$$h_t = \bar{A}h_{t-1} + \bar{B}x_t$$
$$y_t = \bar{C}h_t$$

- Parallelizing the SSM training.
 - The sequential nature of RNN is the primary cause of slow training.
 - Several approaches have been suggested to tackle this problem.
 - We will first look at the convolutional representation of SSM.



- Parallelizing the SSM training.
 - The sequential nature of RNN is the primary cause of slow training.
 - Linearity is the key: Convolutional representation.

Discretized State Space Model (Linear RNN)

$$h_t = \bar{A}h_{t-1} + \bar{B}x_t$$
$$y_t = \bar{C}h_t$$

Assuming the initial state $h_{t-1} = 0$, then ...

$$h_0 = \overline{B}x_0 \qquad h_1 = \overline{AB}x_0 + \overline{B}x_1 \qquad h_2 = \overline{A^2B}x_0 + \overline{AB}x_1 + \overline{B}x_2$$
$$y_0 = \overline{CB}x_0 \qquad y_1 = \overline{CAB}x_0 + \overline{CB}x_1 \qquad y_2 = \overline{CA^2B}x_0 + \overline{CAB}x_1 + \overline{CB}x_2$$

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$$y_t = \overline{CA^tB}x_0 + \overline{CA^{t-1}B}x_1 + \dots + \overline{CAB}x_{t-1} + \overline{CB}x_t$$

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$$y_t = \overline{CA^tB}x_0 + \overline{CA^{t-1}B}x_1 + \dots + \overline{CAB}x_{t-1} + \overline{CB}x_t$$

$$\rightarrow y = \overline{K} * x$$
. where $\overline{K} = (\overline{CB}, \overline{CAB}, ..., \overline{CA^TB})$

Able to parallelize: Forward all input tokens at once and perform convolution

- We've discussed SSM's efficiency (Faster decoding, Parallelizing the training...).
- The next thing we will discuss is how to make SSM effective.
 - How to define the state matrix: Hippo^[Gu et al., 2020].
 - How to make the state computation efficient: S4^[Gu et al., 2022a], and S4D^[Gu et al., 2022b]

- How to define the state matrix.
 - A well-defined (initialized) state matrix is the key to success.
 - Hippo: High-order Polynomial Projection Operators^[Gu et al., 2020]
 - Suggests a way of initializing the state matrix A so that it enjoys long-term dependencies.

$$A_{nk} = \begin{cases} (2n+1)^{1/2} (2k+1)^{1/2} & \text{if } n > k \\ n+1 & \text{if } n = k \text{ ,} \quad B_n = (2n+1)^{1/2} \\ 0 & \text{if } n < k \end{cases}$$

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However, such a matrix is inefficient while using the convolutional kernel

$$y_{t} = \overline{CA^{t}B}x_{0} + \overline{CA^{t-1}B}x_{1} + \dots + \overline{CAB}x_{t-1} + \overline{CB}x_{t}$$

$$y = \overline{K} * x. \text{ where } \overline{K} = (\overline{CB}, \overline{CAB}, \dots, \overline{CA^{T}B})$$

- How to make the state computation efficient.
 - \$4 [Gu et al., 2022a]: State matrix can be decomposed as Normal Plus Low-rank (NPLR).

$$A = V\Lambda V^* - PQ^T = V(\Lambda - (V^*P)(V^*Q)^*)V^*$$

for unitary $V \in \mathbb{C}^{N \times N}$, diagonal Λ , and low—rank factorization $P, Q \in \mathbb{R}^{N \times r}$.

• S4D [Gu et al., 2022b]: State matrix can be expressed with a diagonal matrix.

(S4D-Inv)
$$A_n = -\frac{1}{2} + i\frac{N}{\pi} \left(\frac{N}{2n+1} - 1 \right)$$
 (S4D-Lin) $A_n = -\frac{1}{2} + i\pi n$

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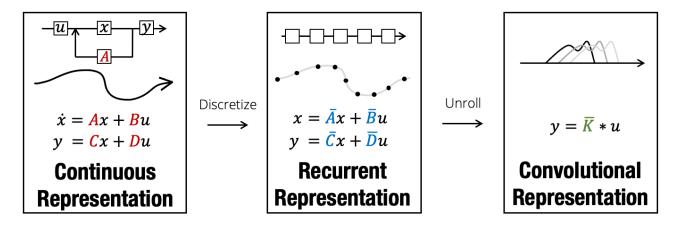
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Now the convolution kernel $\overline{K}=(\overline{CB},\overline{CAB},...,\overline{CA^TB})$ is super efficient to compute

- Summary of the SSM overview.
 - Discretizing and unrolling to do parallel training.
 - Well-defining the state matrix for both efficiency and effectiveness.

Three different views of state space models



S4D^[Gu et al., 2022b]: Diagonal state matrix for efficient computation

(S4D-Inv)
$$A_n = -\frac{1}{2} + i\frac{N}{\pi} \left(\frac{N}{2n+1} - 1 \right)$$
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- Mamba: Selective State-Space Models [Gu et al., 2024]
 - Motivation: SSM lacks content-based reasoning abilities
 - The state update is done independently with the input
 - Which tasks require content-based reasoning?
 - Summarization, retrieval, basically all NLP tasks





Albert Gu @_albertgu · Dec 5, 2023

Quadratic attention has been indispensable for information-dense modalities such as language... until now.

Announcing Mamba: a new SSM arch. that has linear-time scaling, ultra long context, and most importantly—outperforms Transformers everywhere we've tried.

Algorithmic Intelligence Lab

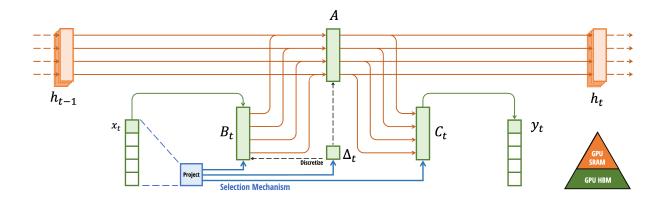
- Mamba: Selective State-Space Models [Gu et al., 2024]
 - **Key idea**: Define input-dependent (content-aware) state matrices
 - Define Δ, B, C as input-dependent factors
 - Denote such SSM as a Selective SSM

Algorithm 1 SSM (S4)	Algorithm 2 SSM + Selection (S6)				
Input: $x:(B,L,D)$	Input: $x : (B, L, D)$				
Output: $y:(B,L,D)$	Output: $y:(B,L,D)$				
1: $A : (D, N) \leftarrow Parameter$	1: $A:(D,N) \leftarrow Parameter$				
▶ Represents structured $N \times N$ matrix	▶ Represents structured $N \times N$ matrix				
2: $\mathbf{B}: (D, N) \leftarrow Parameter$	$2: B: (B, L, N) \leftarrow s_B(x)$				
$S: C: (D, N) \leftarrow Parameter$	3: $C: (B, L, N) \leftarrow s_C(x)$				
4: $\Delta: (D) \leftarrow \tau_{\Delta}(Parameter)$	4: $\Delta : (B, L, D) \leftarrow \tau_{\Delta}(Parameter + s_{\Delta}(x))$				
5: $\overline{A}, \overline{B} : (D, N) \leftarrow \text{discretize}(\Delta, A, B)$	5: $\overline{A}, \overline{B} : (B, L, D, N) \leftarrow \text{discretize}(\Delta, A, B)$				
6: $y \leftarrow SSM(\overline{A}, \overline{B}, C)(x)$	6: $y \leftarrow SSM(\overline{A}, \overline{B}, C)(x)$				
▶ Time-invariant: recurrence or convolution	▶ Time-varying: recurrence (scan) only				
7: return <i>y</i>	7: return y				

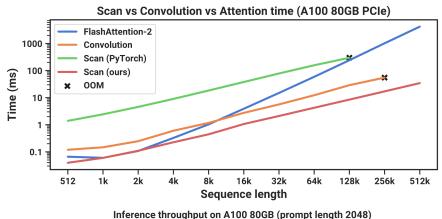
- Mamba: Selective State-Space Models [Gu et al., 2024]
 - Problem of selective SSM: It is not an LTI system
 - Cannot use convolution because Δ , B, C are input-dependent now

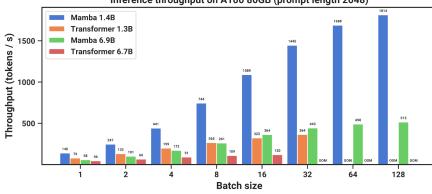
$$y_t = \overline{CA^tB}x_0 + \overline{CA^{t-1}B}x_1 + \dots + \overline{CAB}x_{t-1} + \overline{CB}x_t$$
$$y = \overline{K} * x. \text{ where } \overline{K} = (\overline{CB}, \overline{CAB}, \dots, \overline{CA^TB})$$

- Another option for computing linear recurrence is associative parallel scan
 - \$5 [Smith et al., 2023] shows that linear recurrence operation is associative
 - Mamba provides efficient, hardware-aware implementation of associative scan



- Mamba: Selective State-Space Models [Gu et al., 2024]
 - Overall, the inference time significantly reduces
 - Faster then Flash Attention 2, especially with longer sequence lengths
 - Provides up to 5x higher throughput





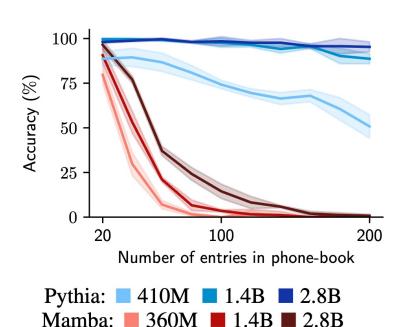
- Mamba: Selective State-Space Models [Gu et al., 2024]
 - Mamba shows high zero-shot performance on various NLP tasks

Table 3: (**Zero-shot Evaluations**.) Best results for each size in bold. We compare against open source LMs with various tokenizers, trained for up to 300B tokens. Pile refers to the validation split, comparing only against models trained on the same dataset and tokenizer (GPT-NeoX-20B). For each model size, Mamba is best-in-class on every single evaluation result, and generally matches baselines at twice the model size.

Model	Token.	Pile ppl↓	LAMBADA ppl↓	LAMBADA acc ↑	HellaSwag acc ↑	PIQA acc↑	Arc-E acc ↑	Arc-C acc↑	WinoGrande acc ↑	Average acc ↑
Hybrid H3-130M	GPT2	_	89.48	25.77	31.7	64.2	44.4	24.2	50.6	40.1
Pythia-160M	NeoX	29.64	38.10	33.0	30.2	61.4	43.2	24.1	51.9	40.6
Mamba-130M	NeoX	10.56	16.07	44.3	35.3	64.5	48.0	24.3	51.9	44.7
Hybrid H3-360M	GPT2	_	12.58	48.0	41.5	68.1	51.4	24.7	54.1	48.0
Pythia-410M	NeoX	9.95	10.84	51.4	40.6	66.9	52.1	24.6	53.8	48.2
Mamba-370M	NeoX	8.28	8.14	55.6	46.5	69.5	55.1	28.0	55.3	50.0
Pythia-1B	NeoX	7.82	7.92	56.1	47.2	70.7	57.0	27.1	53.5	51.9
Mamba-790M	NeoX	7.33	6.02	62.7	55.1	72.1	61.2	29.5	56.1	57.1
GPT-Neo 1.3B	GPT2	_	7.50	57.2	48.9	71.1	56.2	25.9	54.9	52.4
Hybrid H3-1.3B	GPT2	_	11.25	49.6	52.6	71.3	59.2	28.1	56.9	53.0
OPT-1.3B	OPT	_	6.64	58.0	53.7	72.4	56.7	29.6	59.5	55.0
Pythia-1.4B	NeoX	7.51	6.08	61.7	52.1	71.0	60.5	28.5	57.2	55.2
RWKV-1.5B	NeoX	7.70	7.04	56.4	52.5	72.4	60.5	29.4	54.6	54.3
Mamba-1.4B	NeoX	6.80	5.04	64.9	59.1	74.2	65.5	32.8	61.5	59.7
GPT-Neo 2.7B	GPT2	_	5.63	62.2	55.8	72.1	61.1	30.2	57.6	56.5
Hybrid H3-2.7B	GPT2	_	7.92	55.7	59.7	73.3	65.6	32.3	61.4	58.0
OPT-2.7B	OPT	_	5.12	63.6	60.6	74.8	60.8	31.3	61.0	58.7
Pythia-2.8B	NeoX	6.73	5.04	64.7	59.3	74.0	64.1	32.9	59.7	59.1
RWKV-3B	NeoX	7.00	5.24	63.9	59.6	73.7	67.8	33.1	59.6	59.6
Mamba-2.8B	NeoX	6.22	4.23	69.2	66.1	75.2	69.7	36.3	63.5	63.3
GPT-J-6B	GPT2	_	4.10	68.3	66.3	75.4	67.0	36.6	64.1	63.0
OPT-6.7B	OPT	-	4.25	67.7	67.2	76.3	65.6	34.9	65.5	62.9
Pythia-6.9B	NeoX	6.51	4.45	67.1	64.0	75.2	67.3	35.5	61.3	61.7
RWKV-7.4B	NeoX	6.31	4.38	67.2	65.5	76.1	67.8	37.5	61.0	62.5

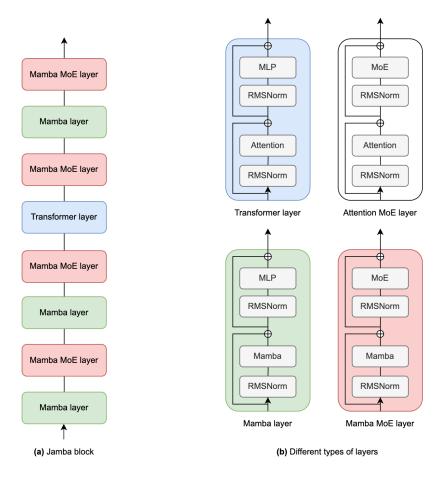
Hybrid architectures

- SSMs are known to show bad performance in certain scenarios
 - E.g., Mamba shows low accuracy in phone-book retrieval task
- This is due to SSM's limited random-access capability
 - All information have to be compressed into a single SSM state
 - Random-access is the key advantage of attention mechanism (Transformer)



Hybrid architectures

- Recent architectures leverage both attention layers and SSM layers together
 - E.g. Jamba [Lieber et al., 2024] and Griffin [De et al., 2024]
- Hybrid approach provides both efficiency and random-access capability



Overview

Part 1. Basics

- RNN to LSTM
- Sequence-to-sequence Model
- Attention-based NLP Model

Part 2. Transformers and Large Language Models

- Transformer (self-attention)
- Pre-training of Transformers and Language Models

Part 3. Advanced Topics

- Handling long inputs with Transformers
- Techniques for improving efficiency
- State-space models

Part 4. Summary

Summary

- For language, specified model which can capture temporal dependency is a key
- Previously, 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 → Transformer
- Transformer significantly improves the performance on many sequential tasks
 - 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)
- Various techniques are emerging to address the remaining practical challenges
 - Improving efficiency in training and deployment
 - Extending the language models to handle longer inputs
 - State-space models enable efficient long context handling

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