Applied Machine Learning for Business Analytics

Lecture 3: Transformers

Lecturer: Zhao Rui

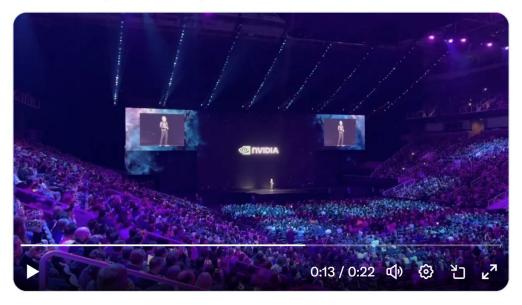
Logistics

- HW schedule has been updated.
 3 -> 2
- HW1 has been released

Fri 01/31	From Word2Vec to Transformers	Link	Form your team & Assignment I Out
Fri 02/07	LLM and its Practices I		LangChain Tutorial & Assignment I Due
Fri 02/14	LLM and its Practices II	Link	N.A.
Fri 02/21	LLM and its Practices III	Link	Build your First RAG & Assignment II Out
Sun 03/02	Recess Week	N.A.	Proposal Due
Fri 03/07	Data Preparation	Link	Assignment II Due



Jensen Huang is the new Taylor Swift



^{4:07} AM \cdot Mar 19, 2024 from San Jose, CA \cdot **511.2K** Views

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Transforming AI Panel at GTC 2024

Jensen Huang will host a panel with the authors of "*Attention Is All You Need*", a seminal research paper that introduced the Transformer neural network architecture (NeurIPS, 2017)



Jensen Huang Founder and CEO NVIDIA



Ashish Vaswani Co-Founder & CEO Essential Al



Noam Shazeer CEO and Co-Founder Character.Al



Niki Parmar Co-Founder Essential Al



Jakob Uskoreit CEO Inceptive



Llion Jones Co-Founder and CTO Sakana Al



Aidan Gomez Co-Founder and CEO Cohere



Lukasz Kaiser Member of Technical Staff OpenAl



Illia Polosukhini Co-Founder NEAR Protocol



Attention Is All You Need

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Abstract

The dominant sequence transduction models are based on complex recurrent or convolutional neural networks that include an encoder and a decoder. The best performing models also connect the encoder and decoder through an attention mechanism. We propose a new simple network architecture, the Transformer, based solely on attention mechanisms, dispensing with recurrence and convolutions entirely. Experiments on two machine translation tasks show these models to be superior in quality while being more parallelizable and requiring significantly less time to train. Our model achieves 28.4 BLEU on the WMT 2014 English-to-German translation task, improving over the existing best results, including ensembles, by over 2 BLEU. On the WMT 2014 English-to-French translation task, our model establishes a new single-model state-of-the-art BLEU score of 41.8 after training for 3.5 days on eight GPUs, a small fraction of the training costs of the best models from the literature. We show that the Transformer generalizes well to other tasks by applying it successfully to English constituency parsing both with large and limited training data.

Market Summary > NVIDIA Corp

128.86 USD

+128.82 (322,056.25%) **↑** all time

Closed: 28 Jan, 7:53 pm GMT-5 • Disclaimer After hours 127.47 -1.39 (1.08%)







What happened to NVDA this WEEK?

Nvidia (NVDA) stock dropped nearly 17% Monday, leading a sell-off across chip stocks and the broader market after a new AI model from China's DeepSeek raised questions about AI investment and the rise of more cost-efficient artificial intelligence agents.

Nvidia's decline shaved \$589 billion off the AI chipmaker's market cap, the largest single-day loss in stock market history.

Donald Trump: DeepSeek's AI should be 'wakeup call' to US tech industry

'The release of DeepSeek, AI from a Chinese company should be a wakeup call for our industries that we need to be laser-focused on competing to win'

DeepSeek is still on top of Transformer

performance comparable to opera it o or beries mouelo.

In this paper, we take the first step toward improving language model reasoning capabilities using pure reinforcement learning (RL). Our goal is to explore the potential of LLMs to develop reasoning capabilities without any supervised data, focusing on their self-evolution through a pure RL process. Specifically, we use DeepSeek-V3-Base as the base model and employ GRPO (Shao et al., 2024) as the RL framework to improve model performance in reasoning. During training, DeepSeek-R1-Zero naturally emerged with numerous powerful and interesting reasoning behaviors. After thousands of RL steps, DeepSeek-R1-Zero exhibits super performance on reasoning benchmarks. For instance, the pass@1 score on AIME 2024 increases from 15.6% to 71.0%, and with majority voting, the score further improves to 86.7%, matching the performance of OpenAI-o1-0912.

DeepSeekR1: https://arxiv.org/ab s/2501.12948

2.1 Basic Architecture

The basic architecture of DeepSeek-V3 is still within the Transformer (Vaswani et al., <u>2017</u>) framework. For efficient inference and economical training, DeepSeek-V3 also adopts MLA and DeepSeekMoE, which have been thoroughly validated by DeepSeek-V2. Compared with DeepSeek-V2, an exception is that we additionally introduce an auxiliary-loss-free load balancing strategy (Wang et al., <u>2024a</u>) for DeepSeekMoE to mitigate the performance degradation induced by the effort to ensure load balance. Figure <u>2</u> illustrates the basic architecture of DeepSeek-V3, and we will briefly review the details of MLA and DeepSeekMoE in this section.

DeepSeekv3: https://arxiv.org/ht ml/2412.19437v1

Agenda

- 1. Transformers
- 2. Attention is all you need
 - a. Self-Attention
 - b. Positional Embeddings
- 3. Summary
- 4. Appendix
 - a. Masked Self-Attention
 - b. Encoder-Decoder Attention

1. Transformers

What is Transformer

Transformer is a sequence to sequence model (Encoder and Decoder)

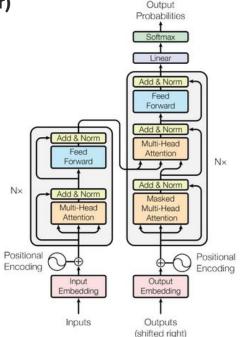
Attention Is All You Need

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Abstract

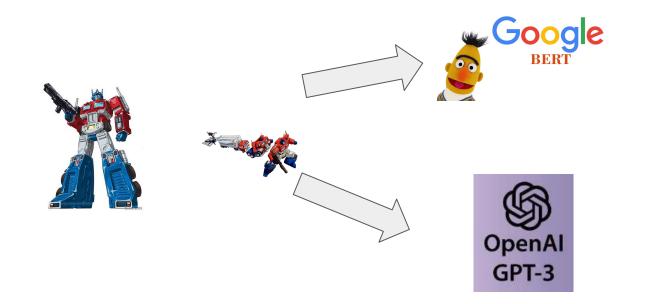
The dominant sequence transduction models are based on complex recurrent or convolutional neural networks that include an encoder and a decoder. The best performing models also connect the encoder and decoder through an attention mechanism. We propose a new simple network architecture, the Transformer, based solely on attention mechanisms, dispensing with recurrence and convolutions entirely. Experiments on two machine translation tasks show these models to be superior in quality while being more parallelizable and requiring significantly less time to train. Our model achieves 28.4 BLEU on the WMT 2014 Englishto-German translation task, improving over the existing best results, including ensembles, by your 2 BLEU. On the WMT 2014 English-to-Terruch translation tarks training for 3.5 days on eight GPUs, as small fraction of the training costs of the best models from the literature. We show that the Transformer generalizes well to other tasks by applying it successfully to English constituency parsing both with large and limited training data.





All LLMs so far use transformer architecture

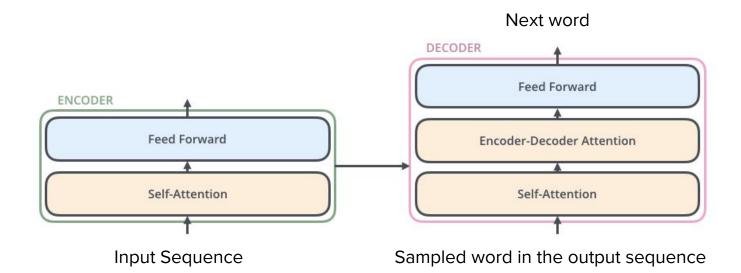
• BERT and GPT are the most representative ones



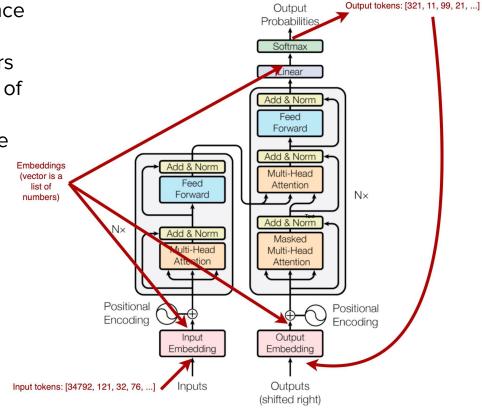
Bi-directional Encoder Representations from Transformers

Generative Pre-trained Transformers

Transformer is solving Seq2Seq

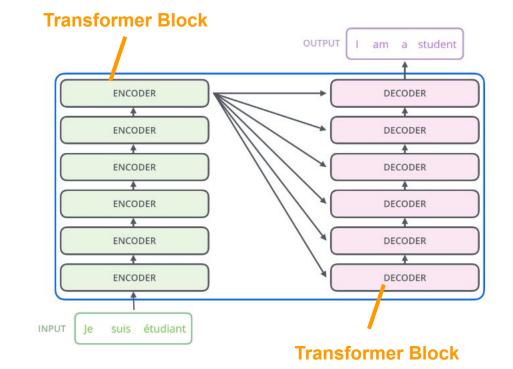


- Input text is encoded with tokenizers to sequence of integers
- Input tokens are mapped to sequence of vectors
- Output vectors can be classified to a sequence of tokens
- Output tokens can then be decoded back to the text

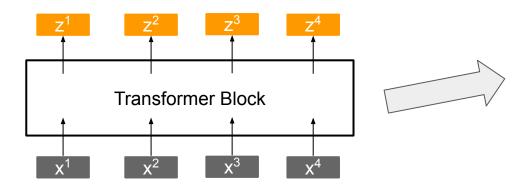


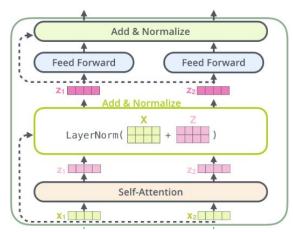
Transformer

- 1. Transformer block: operation unit
 - a. Consists of multiple computations
 - b. A sequence of embeddings in
 - c. A sequence of embeddings out
- 2. Encoder:
 - a. Stack 6 transformer blocks
 - b. Learn representations for the input sequence
- 3. Decoder:
 - a. Stack another 6 transformer blocks.
 - b. Generate output sequences conditioned on the learned representations from encoder.



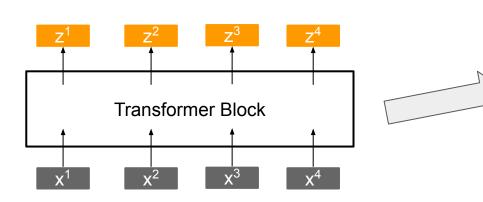
Transformer block in Encoder

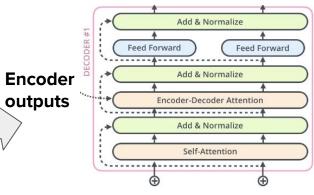




- 1. Input: A sequence of vectors
- 2. Output: A sequence of vectors
- 3. Key Components:
 - a. Self-attention Layer
 - b. Positional Embeddings
 - c. Residual and Normalization Layer
 - d. Fully-connected Layer

Transformer block in Decoder

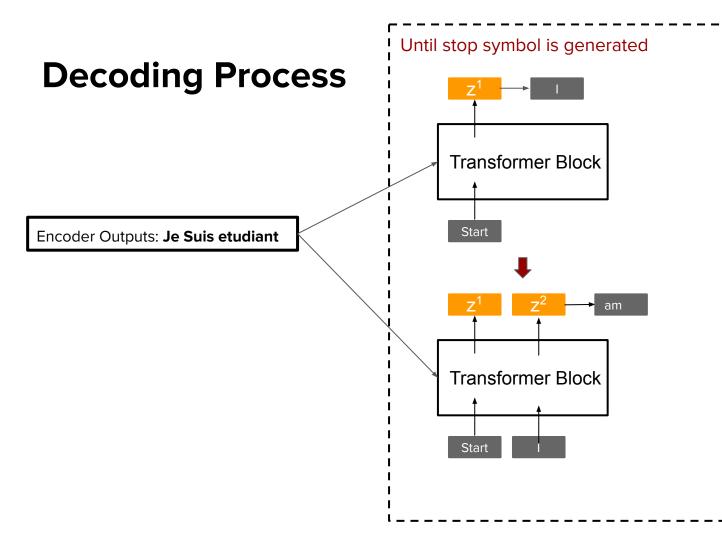




- 1. Input: A sequence of vectors
- 2. Output: A sequence of vectors
- 3. Key Components:
 - a. Masked Self-attention Layer
 - b. Positional Embeddings
 - c. Encoder-Decoder Attention
 - d. Residual and Normalization Layer
 - e. Fully-connected Layer

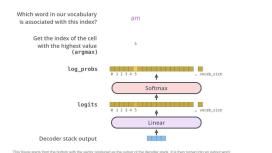
Decoding Process

- The decoder is **autoregressive**
 - Begins with a start token
 - Before the stop token is generated, repeat
 - Take the list of previous outputs with the encoder outputs that contain the attention information from the input
 - Generate the current output

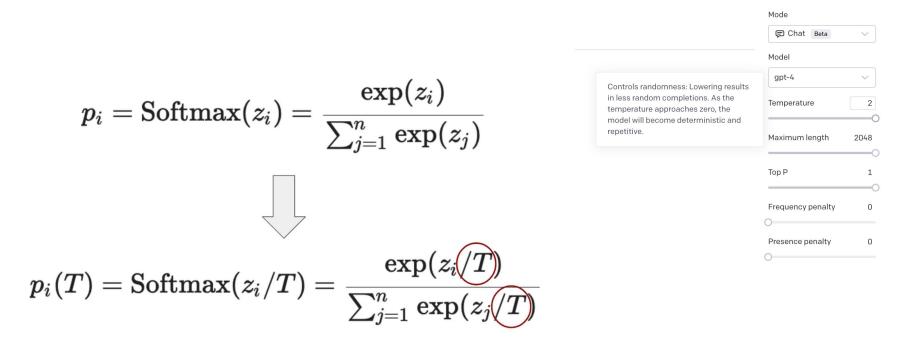


Decoding Process

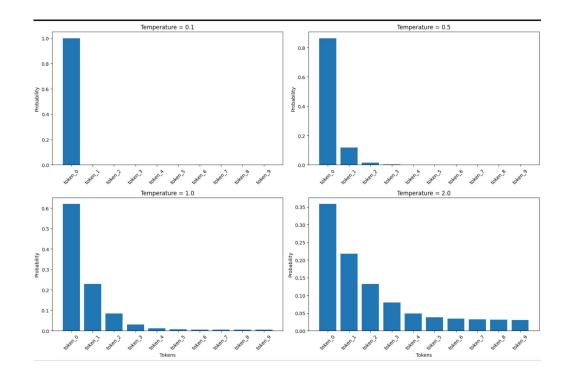
- Linear Classifier with Final softmax for output probabilities
 - The output of the classifier would be the size of vocabulary
 - After softmax, probability scores between 0 and 1 will be generated
 - Decoding Strategies:
 - Greedy search: the index of the highest probability score would be taken to predict the current word
 - Beam search: takes into account the N most likely tokens
 - Other advanced sampling: <u>https://deci.ai/blog/from-top-k-to-beam-search-IIm-decoding-strategies/</u>



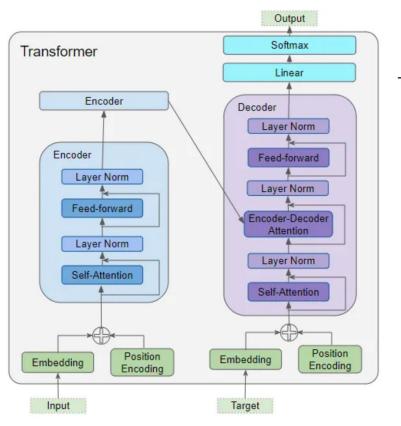
Temperature Sampling



Temperature Sampling



Encoder-Decoder



Three kinds of attention in transformers:

- Self-attention
 - Input sequence <> Input sequence
- Masked self-attention
 - Previous steps in output sequence <> current steps in output sequence
- Encoder-Decoder attention
 - Input sequence <> Output sequence

Source:

https://towardsdatascience.com/transformers-explainedvisually-part-2-how-it-works-step-by-step-b49fa4a64f34

2. Attention

Word Embeddings

- Apple in two sentences:
 - Sentence 1: My favorite fruit is apple
 - Sentence 2: Solution: My favorite brand is **apple**



One embedding has multiple senses

Contextualized Word Embeddings

• Telling context in words

- Sentence 1: My favorite fruit is apple1
- Sentence 2: Solution: My favorite brand is apple2

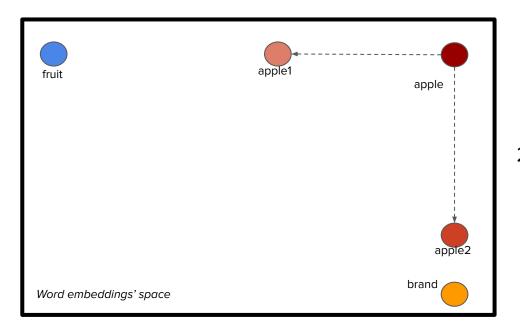


From nearby words, we can guess two different meanings of this word (i.e., food and brand)

Contextualized Word Embeddings

• Telling context in words

- Sentence 1: My favorite fruit is apple1
- Sentence 2: Solution: My favorite brand is apple2

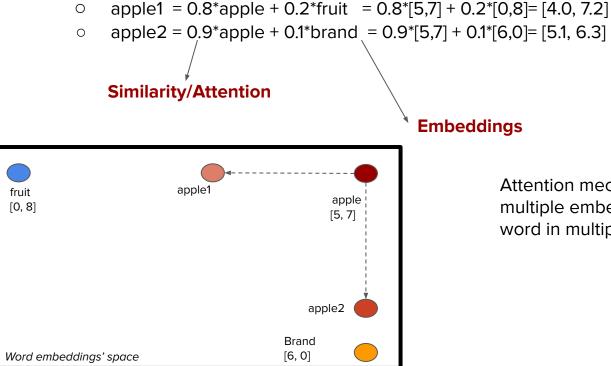


- In sentence 1, move the word embedding of apple towards the word "fruit"
- In sentence 2, move the word embedding of apple toward the word "brand"

This is how attention will work

How to move one word closer to another one

• Average two words



Attention mechanism is able to learn multiple embeddings for the same word in multiple sentences

- Apple in two sentences:
 - Sentence 1: My favorite fruit is **apple**
 - Sentence 2: My favorite brand is apple
- Why we move apple to fruit in sentence 1? Instead of other words as "my" and "is"
- It is based on the similarity!
- Assume every word has its own base vector (as word2vec), the contextualized word embedding of **apple** in the sentence: my favorite fruit is **apple**

⁼ Attention(apple, my)*base_vec(my) + Attention(apple, favorite)*base_vec(favorite) + Attention(apple, fruit)*base_vec(fruit) + Attention(apple, is)*base_vec(is) + Attention(apple, apple)*base_vec(apple)

• Via embeddings, the similarity between two irrelevant words would be zero, while the similarity between the related pair would be high

	my	favourite	fruit	is	apple
my	1	0	0	0	0
favourite	0	1	0	0	0
fruit	0	0	1	0	0.25
is	0	0	0	1	0
apple	0	0	0.25	0	1

	my	favourite	brand	is	apple
my	1	0	0	0	0
favourite	0	1	0	0	0
brand	0	0	1	0	0.11
is	0	0	0	1	0
apple	0	0	0.11	0	1

- The diagonal entries are all 1
- The similarity between any irrelevant words is 0 (for simplicity)
- The similarity between apple and fruit is 0.25 while the one between apple and brand is 0.11 considering apple is used more often in the same context as fruit

	my	favourite	fruit	is	apple
my	1	0	0	0	0
favourite	0	1	0	0	0
fruit	0	0	1	0	0.25
is	0	0	0	1	0
apple	0	0	0.25	0	1

	my	favourite	brand	is	apple	
my	1	0	0	0	0	
favourite	0	1	0	0	0	
brand	0	0	1	0	0.11	
is	0	0	0	1	0	
apple	0	0	0.11	0	1	31

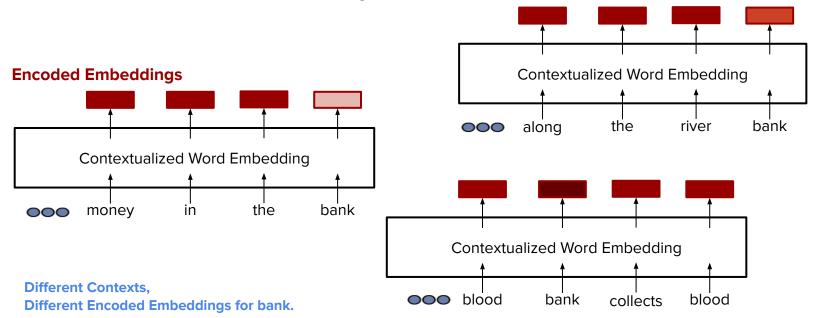
- Contextualized Target Word = The sum of a product between the similarity between target word and context word * context word embeddings
- We should also normalize the similarity along the sentence (softmax)
- Therefore
 - my (in the sentence 1) = my
 - apple (in the sentence 1) = 0.2 * fruit + 0.8 * apple
 - \circ apple (in the sentence 2) = ?

	my	favourite	fruit	is	apple	
my	1	0	0	0	0	
favourite	0	1	0	0	0	
fruit	0	0	0.8	0	0.2	Normalized
is	0	0	0	1	0	
apple	0	0	0.2	0	0.8	

	my	favourite	brand	is	apple	
my	1	0	0	0	0	
favourite	0	1	0	0	0	
brand	0	0	0.9	0	0.9	
is	0	0	0	1	0	
apple	0	0	0.1	0	0.1	32

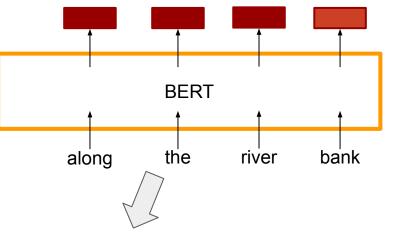
Contextualized Word Embeddings

- Transformers is proposed to learn better feature for NLP data
- The core layer is self-attention layer which can map a sequence of word embeddings to another sequence of word embeddings which is contextualized

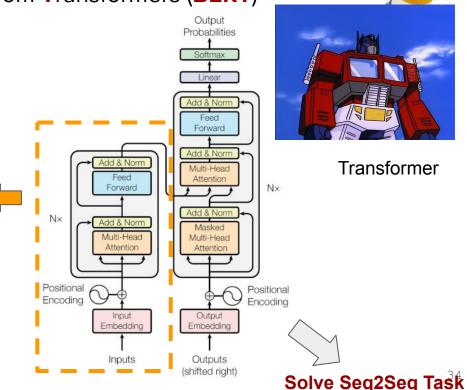


What is **BERT**

- Bidirectional Encoder Representations from Transformers (BERT)
- BERT: Encoder of Transformer,

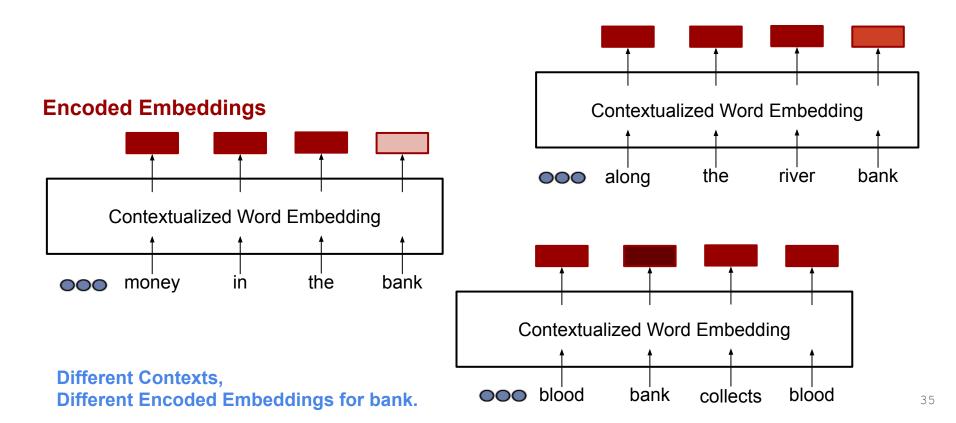


Given a sequence of words, generate a sequence of vectors and then can be used for various NLP tasks





Contextualized Word Embeddings



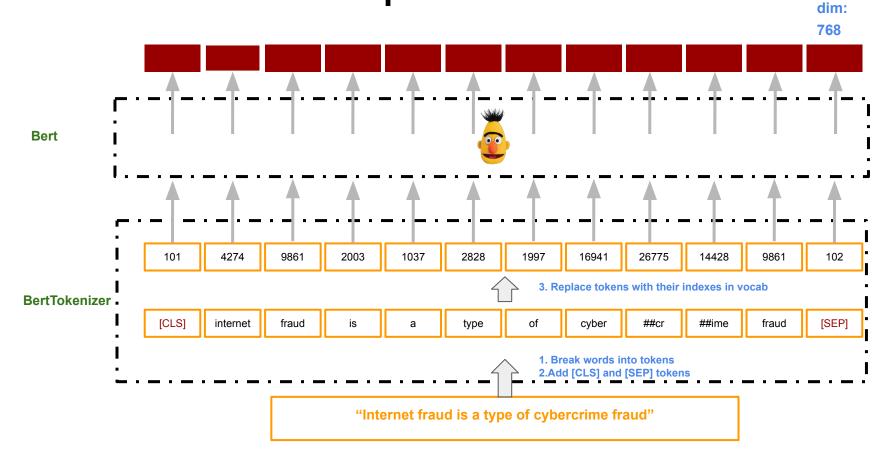
Embeddings generated from BERT

10 0.53 0.48 0.74 0.5 An apple is sweet in taste. 1 0.8 0.71 0.51 0.48 0.74 0.47 We can make juice and jam from apple. - 0.6 0.46 0.71 0.42 0.44 An apple a day keeps the doctor away. 0.53 0.51 0.46 0.82 1 Investors in Apple have a love-hate relationship with the iPhone. - 0.4 0.48 0.48 0.42 0.82 0.72 Both Apple and Huawei have wireless charging features. - 0.2 0.47 0.72 0.5 0.44 1 Steve Jobs returned to Apple in 1196. 0.0 36

in different context

Cos-similarities among vectors of "apple"

How does BERT compute



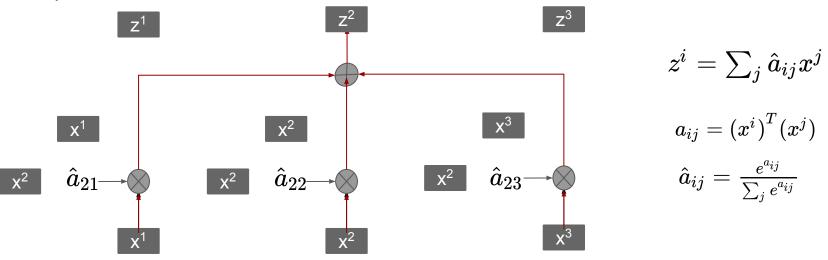
In the case of ChatGPT the generated numbers are probabilities. ChatGPT has a limited vocabulary, and the probabilities indicate how likely each vocabulary word is based on the input word sequence. ChatGPT has a limited reading range, and the input sequence has a maximum length of about 3000 words, broken into 4000 sub-word tokens. Once ChatGPT generates a word, it adds that word to the input sequence, and generates a new word. This process continues until it produces a special word called a "stop" token, or it hits a preset word limit.

Why is the reading range limited?

2.1 Self-Attention

Basic Self-Attention

- A sequence-to-sequence operation taking a sequence of vectors in and generate a sequence of vectors out
 - \circ [x1, x2, x3] -> [z1, z2, z3]
- Relating different positions of the input sequence in order to compute the representation



Basic Self-Attention

Sentence i: My favourite fruit is apple

	my	favourite	fruit	is	apple
my	1	0	0	0	0
favourite	0	1	0	0	0
fruit	0	0	1	0	0.25
is	0	0	0	1	0
apple	0	0	0.25	0	1

New Word Index	Attention Step
my_i	my
favourite_i	favourite
fruit_i	0.8*fruit+0.2*apple
is_i	is
apple_i	0.2*fruit+0.8*apple

Basic Self-Attention

- There are no model parameters. It is totally determined by the embedding layer
 - Solution: introduce model parameters -> using three sets of embeddings to get contextualized embeddings
- Self attention is permutation equivariant. It ignores the order information.
 - Solution: add positional embeddings

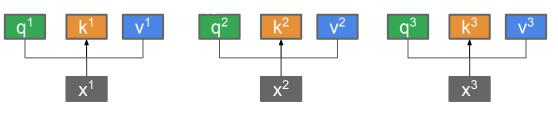
Step 1: Generate query, key, and value vector for the input vector at each time step.



Query (to match others): qⁱ=W^qxⁱ

Key (to be matched): kⁱ=W^kxⁱ

Value (representation): $v^{i}=W^{v}x^{i}$



Model parameters are introduced here.

In practice, bias vectors may be added to the product of matrix multiplication

Word embeddings



The key/value/query formulation of attention is from the paper Attention Is All You Need.

How should one understand the queries, keys, and values

The key/value/query concept is analogous to retrieval systems. For example, when you search for videos on Youtube, the search engine will map your **query** (text in the search bar) against a set of **keys** (video title, description, etc.) associated with candidate videos in their database, then present you the best matched videos (**values**).



The attention operation can be thought of as a retrieval process as well.

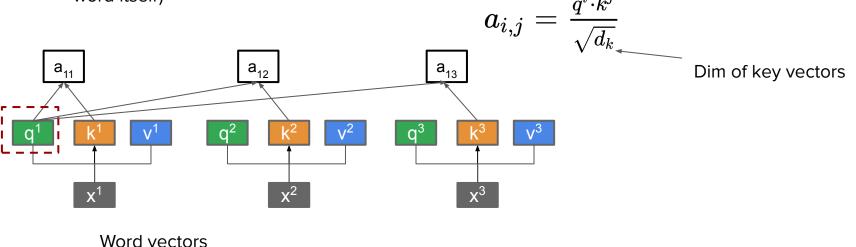
As mentioned in the paper you referenced (<u>Neural Machine Translation by Jointly Learning to</u> <u>Align and Translate</u>), attention by definition is just a weighted average of values,

$$c=\sum_j \alpha_j h_j$$

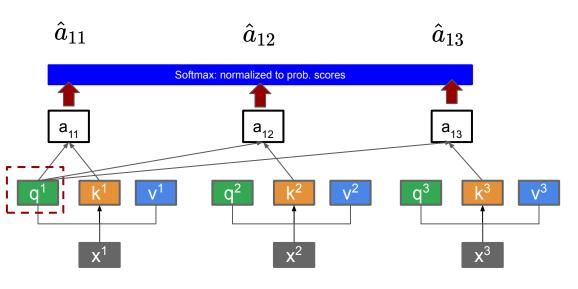
Step 2: Compute attention scores using query vectors and key vectors

To encode the i-th word in the sequence, we need to compute the attention scores between this i-th word and all the words in the sequence.

- 1. Pick the query vector from the i-th word: qⁱ
- 2. Attention score computation between q^i and all key vectors of the nearby words (including the target word itself) $a^i \cdot k^j$



Step 3: Fed unscaled attention scores into softmax layers $\hat{a}_{1i}=rac{e^{a_{1i}}}{\sum_{i}e^{a_{1j}}}$

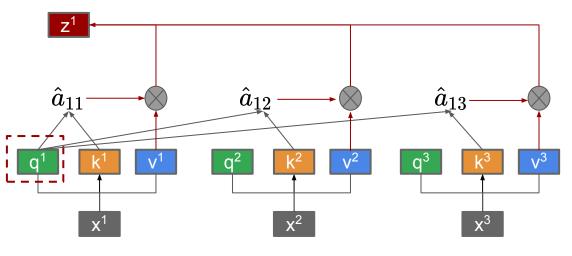


Word vectors

Step 4: Take the sum of all the value vectors weighted by the attention scores.

Encoded vector for z^1 the first element

$$\hat{v} = \sum_i \hat{a}_{1i} v^i$$

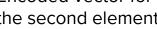


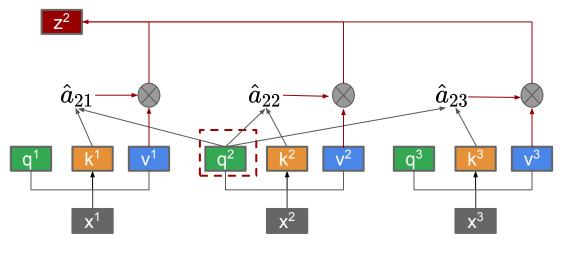
Word vectors

Step 5: All elements in input sequence xⁱ will be encoded into new vectors zⁱ

Encoded vector for the second element

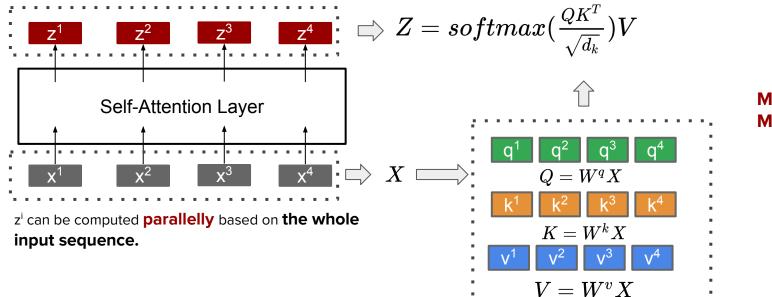
$$z^2 = \sum_i \hat{a}_{2i} v^i$$





Word vectors

Matrix formulation



Matrix Multiplication

Multi-head Self-Attention

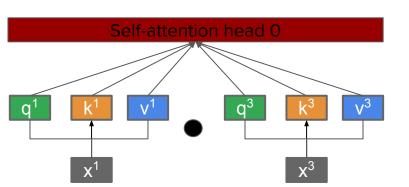
- Model parameters: W^k, W^q, W^v specific one kind of attention
- We can have multiple set of W^k, W^q, W^v



Concatenating all heads

 z^1 \bullet z^3





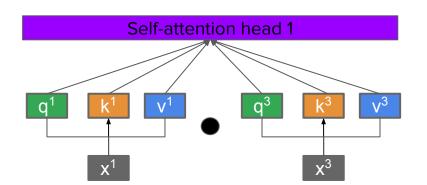
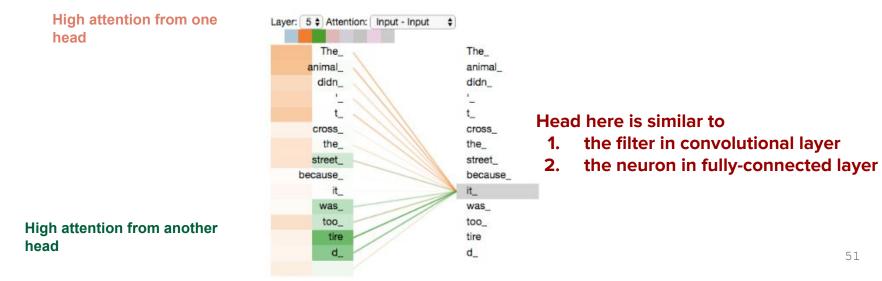


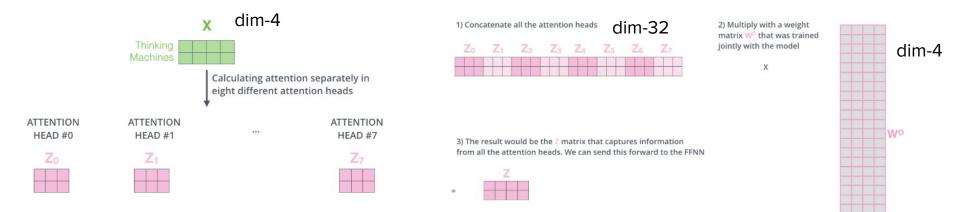
Illustration of Self-Attention

- Multi-head means separate W^k, W^q, W^v matrices
 - Expands the model's ability to focus on different positions
 - Gives the attention layer multiple "representation subspaces"
 - For example, two-head self-attention

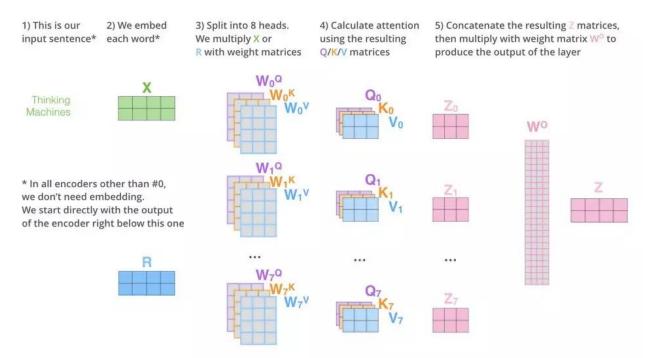


Multi-head Self-Attention

- If the layer has k heads, the output would be k sets of embeddings
- We need to reduce the dimensionality by concatenating and projection into the low dimensional
 - For example, as below: 4->32->4



That's pretty much all there is to multi-headed self-attention. It's quite a handful of matrices, I realize. Let me try to put them all in one visual so we can look at them in one place



MultiHeadAttention in Keras

import tensorflow as tf
from tensorflow import keras
from tensorflow.keras.layers import MultiHeadAttention

```
target = tf.keras.Input(shape=[6, 16])
```

```
# assume it is a sentence of 6 words. Then, each word has a
```

layer = MultiHeadAttention(num_heads=1, key_dim=2)
output_tensor, attention_scores = layer(target, target, return_attention_scores=True)
print(output_tensor.shape)
print(attention_scores.shape)

(None, 6, 16) (None, 1, 6, 6)

<pre>for matrix in layer.weights: print(matrix.shape)</pre>		
(16, 1, 2) (1, 2) (16, 1, 2) (1, 2) (16, 1, 2) (16, 1, 2) (1, 2) (1, 2, 16) (16,)		

MultiHeadAttention in Keras

```
layer = MultiHeadAttention(num_heads=3, key_dim=2)
 target = tf.keras.Input(shape=[6, 16])
 output_tensor, attention_scores = layer(target, target, return_attention_scores=True)
 print(output_tensor.shape)
 print(attention_scores.shape)
 (None, 6, 16)
 (None, 3, 6, 6)
for matrix in layer.weights:
     print(matrix.shape)
 (16, 3, 2)
 (3, 2)
 (16, 3, 2)
 (3, 2)
 (16, 3, 2)
 (3, 2)
 (3, 2, 16)
 (16,)
```

MultiHeadAttention in Keras

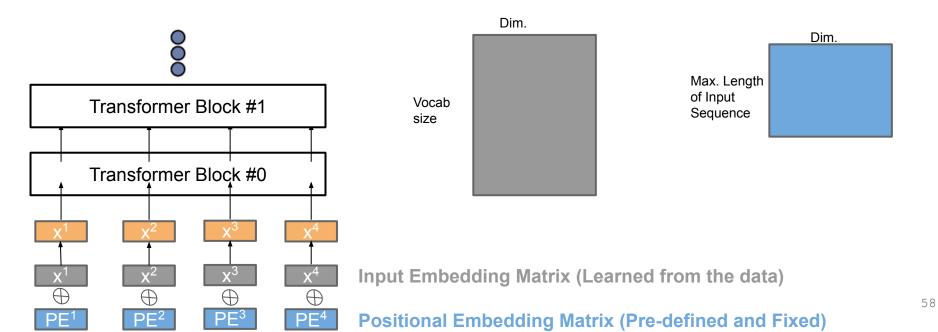
If we change the key_dim from 2 to 5?

```
layer = MultiHeadAttention(num_heads=3, key_dim=2)
 target = tf.keras.Input(shape=[6, 16])
 output_tensor, attention_scores = layer(target, target, return_attention_scores=True)
 print(output_tensor.shape)
 print(attention_scores.shape)
  (None, 6, 16)
  (None, 3, 6, 6)
for matrix in layer.weights:
     print(matrix.shape)
  (16, 3, 2)
 (3, 2)
 (16, 3, 2)
  (3, 2)
  (16, 3, 2)
  (3, 2)
  (3, 2, 16)
  (16,)
```

2.2 Position Embedding

Positional embeddings

- No position information in self-attention
- Positional Embeddings: each position has a unique positional vector PE(pos)
 - Add this vector to each input embeddings
 - Expands the model's ability to focus on different positions.

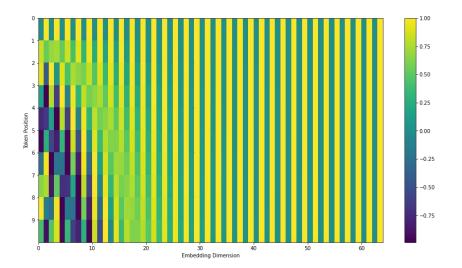


Positional embeddings

• The equation in the original paper:

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

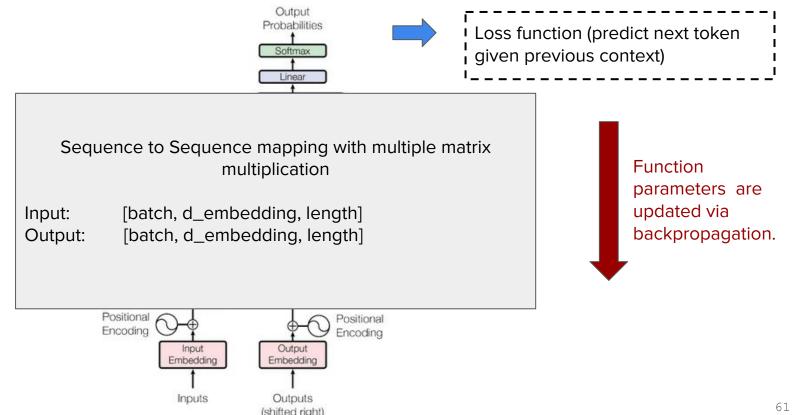
Core idea: using fixed weights which encode information related to a specific position of a token in a sentence



More details: <u>https://kazemnejad.com/blog/transformer_architecture_positional_encoding/</u>

3. Summary

A "functional" viewpoint on Transformer



Transformers is replacing RNN and CNN

- Compared to Transformers, RNN
 - can not be trained in parallel
 - suffers from long dependency issues
- Compared to Transformers, CNN
 - is unable to capture all possible combinations of words (filter size is predefined)
- Compared to the previous NN, Transformers
 - Non sequential: the input sequence are processed as a whole
 - Self Attention: contextualized word embeddings
 - **Positional embeddings**: a better way than recurrence to capture order information
- Podcast about transformers
 - <u>https://www.youtube.com/watch?v=9uw3F6rndnA</u>

BLOG >

Transformer: A Novel Neural Network Architecture for Language Understanding

THURSDAY, AUGUST 31, 2017 Posted by Jakob Uszkoreit, Software Engineer, Natural Language Understanding

Source: https://blog.research.google/2017/08/tra nsformer-novel-neural-network.html

Must Read !!

The illustrated transformer (the source of the awesome visualizations)



Implementations of Transformers

- Build Transformer from Scratch
- We can import it from huggingface

Next Class: LLM I

Appendix

Masked Self-Attention

Masked Self-Attention

- This is the attention layer used to compute the dependency among the target words
- Since the sequence is generated word by word, we need to prevent it from conditioning to the future tokens
- For example:
 - to generate "a", we should not have access to "student"

I am a stud ent

	I	am	а	stud ent
I	0.7	0.1 🗶	0.1 🗶	0.1 🗶
am	0.1	0.6	0.2 🗶	0.1 🗶
а	0.1	0.3	0.6	0.1 🗶
stud ent	0.1	0.3	0.3	0.3

Look-ahead Bias

	I	am	а	stud ent
I	0	-inf	-inf	-inf
am	0	0	-inf	-inf
а	0	0	0	-inf
stud ent	0	0	0	0

Masked Self Attention Score

	I	am	а	stud ent
I	0.7	-inf	-inf	-inf
am	0.1	0.6	-inf	-inf
а	0.1	0.3	0.6	-inf
stud ent	0.1	0.3	0.3	0.3

Masked Self-Attention

- Add look-ahead mask matrix
- Apply softmax to get the probabilistic scores
 - The negative infinities would become zero after softmax
 - For example, the attention score for "a"
 - has values for itself and all words before it
 - Zero for the word "student"

	I	am	а	student	
I	0.7	-inf	-inf	-inf	
am	0.1	0.6	-inf	-inf	
а	0.1	0.3	0.6	-inf	
student	0.1	0.3	0.3	0.3	

Masked Self Attention Score



Normalized Masked Self-Attention Scores

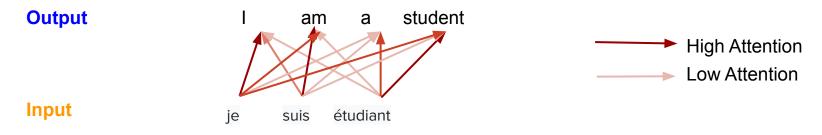
	I	am	а	student
I	1	0	0	0
am	0.37	0.62	0	0
а	0.26	0.3	0.43	0
student	0.21	0.26	0.26	0.26

Encoder-decoder Attention

Encoder-decoder attention

Attention in decoder layer:

1. Attention vectors: a vector of importance weights (measure the interaction between each target word with each input word)



2. The target is approximated by the sum of their input values weighted by the attention scores.

Encoder-Decoder attention layer

Different from Self attention layer

- 1. Generate query vector for the generated output sequence (from itself: Decoder)
- 2. Generate key and value vector for the input sequence at each time step (from Encoder)

Self Attention Score n

	je	suis	eludient
je			
suis			
eludient			

Encoder-decoder Attention Score

	I	am	a	student
je				
suis				
eludient				

Matrix formulation

