Transformers & Attention

ML Instruction Team, Fall 2022

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Overview

- There has been an array of Transformer based architectures such as BERT, SpanBERT, Transformer-XL, XLNet, GPT-2, etc getting released frequently for the past couple of years.
- The OpenAI's GPT-3 had taken the internet by storm with its ability to perform extremely well on tasks such as QA, Comprehension, even Programming
- But all of this started with a research paper released back in 2017 "Attention is all you need".

What is a Transformer

- They take a text sequence as input and produce another text sequence as output. eg. to translate an input English sentence to Spanish.
- At its core, it contains a stack of Encoder layers and Decoder layers.

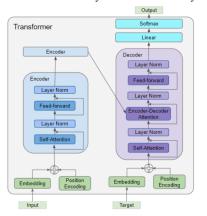


Figure: Transformer schematic consists of Encoder and Decoder.

- As we can observe in the above figure:
 - ➤ The Encoder contains the all-important Self-attention layer that computes the relationship between different words in the sequence, as well as a Feed-forward layer.
 - ▶ The Decoder contains the Self-attention layer and the Feed-forward layer, as well as a second Encoder-Decoder attention layer.
 - ► Each Encoder and Decoder has its own set of weights.

What Does Attention Do?

- The key to the Transformer's ground-breaking performance is its use of Attention.
- While processing a word, Attention enables the model to focus on other words in the input that are closely related to that word.
- eg. 'Ball' is closely related to 'blue' and 'holding'. On the other hand, 'blue' is not related to 'boy'.

The boy is holding a blue ball

- The Transformer architecture uses self-attention by relating every word in the input sequence to every other word. eg. Consider two sentences:
 - ▶ The cat drank the milk because it was hungry.
 - ▶ The cat drank the milk because it was sweet.

Introduction

When the model processes the word 'it', self-attention gives the model more information about its meaning so that it can associate 'it' with the correct word.

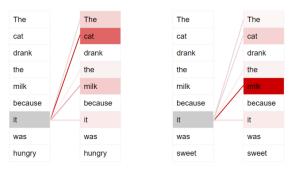


Figure: Implementation of self attention on the example (Dark colors represent higher attention).

To enable it to handle more nuances about the intent and semantics of the sentence, Transformers include multiple attention scores for each word. For instance:

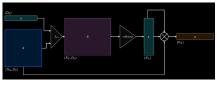


Figure: Including multiple attention scores for the same example.

Evolution of Attention

Version 0

- To understand the intuition of attention, we start with an **input** and a **query**.
- In terms of computation, **attention is given** to parts of the input matrix which is **similar** to the query vector.
- $igwedge f_{att}$ which is a "feed-forward network". The feed-forward network takes the query and input, and projects both of them to dimension D_E .



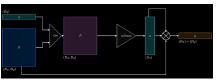
- (a	Schematic	of attention	Version	0

	Notation	Equation	Shape
Similarity Score	e	$e_i = f_{att}(X_i, q)$	(N_X,D_E)
Attention Weights	a	a = softmax (e)	(N_X)
Output Vector	y	$y = \sum_i a_i X_i$	(D_X)

(b) Outputs Table

Version 1

- ► The first change we make to the mechanism is swapping out the feed-forward network with a **dot product operation**.
- Turns out that this is **highly efficient** with reasonably good results.



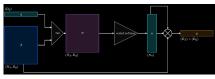
(0)	Sahamatia	of attention	Varcion

	Notation	Equation	Shape
Similarity Score	e	$e_i=q.X_i$	(N_X,D_Q)
Attention Weights	a	$a = \operatorname{softmax}(e)$	(N_X)
Output Vector	y	$y = \sum_i a_i X_i$	(D_X)

(b) Outputs Table

Version 2

- ➤ This version is a very important concept realized in the original paper. The authors propose **scaled dot product** instead of **normal dot product** as the similarity function.
- ► This little change can solve many challenges such as Vanishing Gradient Problem and Unnormalized softmax.



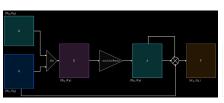
(a)	Schematic	of attention	Version	2

	Notation	Equation	Shape
Similarity Score	e	$e_i = rac{q.X_i}{\sqrt{D_Q}}$	(N_X,D_Q)
Attention Weights	a	$a = \operatorname{softmax}(e)$	(N_X)
Output Vector	y	$y = \sum_i a_i X_i$	(D_X)

(b) Outputs Table

Version 3

- Previously we looked at a single query vector. Here we scale this implementation to multiple query vectors.
- ▶ We calculate the similarities of the input matrix with all the query vectors (query matrix) we have.



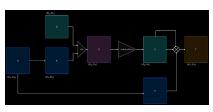
	Notation	Equation	Shape
Similarity Score	E	$E=rac{QX^T}{\sqrt{D_Q}}$	(N_Q,N_X)
Attention Weights	A	$A = \operatorname{softmax}(E)$	(N_Q,N_X)
Output Vector	Y	Y = AX	(N_X,D_X)

(a) Schematic of attention Version 3

(b) Outputs Table

■ Version 4 (Cross-Attention)

- ➤ To build cross-attention, we make some changes. The changes are specific to the input matrix. As we already know, attention needs an input matrix and a query matrix.
- ▶ Suppose we projected the input matrix into a pair of matrices, namely the **key** and **value** matrices.
- ▶ This is done to **decouple** the complexity. The input matrix can now have a better projection that takes care of building attention weights and better output matrices as well.



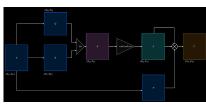
	Notation	Equation	Shape
Similarity Score	E	$E=rac{QK^T}{\sqrt{D_Q}}$	(N_Q,N_X)
Attention Weights	A	$A = \operatorname{softmax}(E)$	(N_Q,N_X)
Output Vector	Y	Y = AX	(N_X,D_X)

(a) Schematic of attention Version 4

(b) Outputs Table

Version 5 (Self-Attention)

- ▶ Like the Version 4 that the key and value matrix are projected versions of the input matrix. What if the query matrix also was projected from the input?
- ▶ Here the main motivation is to build a richer implementation of self with respect to self. This sounds funny, but it is highly important and forms the basis of the Transformer architecture.



(a) Schematic	of attention	Version	5

	Notation	Equation	Shape
Similarity Score	E	$E=rac{QK^T}{\sqrt{D_Q}}$	(N_Q,N_X)
Attention Weights	A	$A = \operatorname{softmax}(E)$	(N_Q,N_X)
Output Vector	Y	Y = AX	(N_X, D_X)

(b) Outputs Table

Training the Transformer

- Training data consists of two parts:
 - ▶ The source or input sequence (eg. "You are welcome" in English, for a translation problem).
 - ▶ The destination or target sequence (eg. "De nada" in Spanish).
- The Transformer's goal is to learn how to output the target sequence, by using both the input and target sequence.

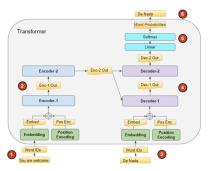


Figure: Training the transformer.

