Transformers & Attention

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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.

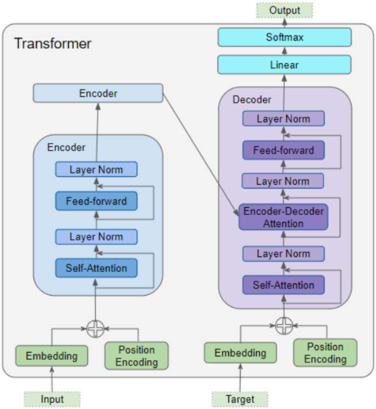
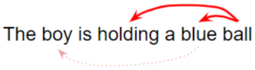


Figure: Transformer schematic, Source.

- 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.
- The Embedding layer encodes the meaning of the word.
- The Position Encoding layer represents the position of the word.

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 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.

- 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.

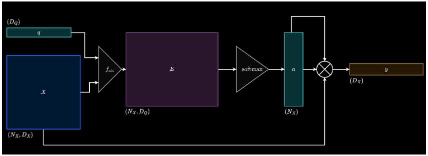
Figure: Implementation of self attention on the example, Source.

- 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, Source.

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.
  - 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.



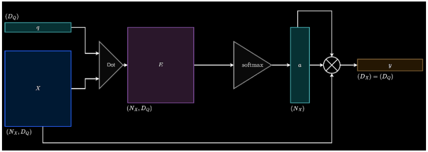
(a) Schematic of attention Version 0, Source

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

(b) Outputs Table, Source

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.



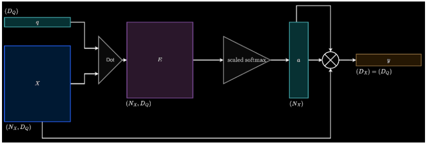
(a) Schematic of attention Version 1, Source

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

(b) Outputs Table, Source

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.



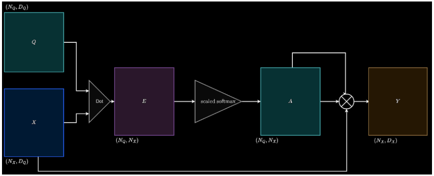
(a) Schematic of attention Version 2, Source

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

(b) Outputs Table, Source

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.



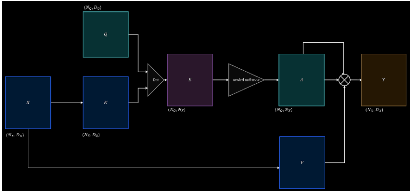
(a) Schematic of attention Version 3, Source

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

(b) Outputs Table, Source

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.



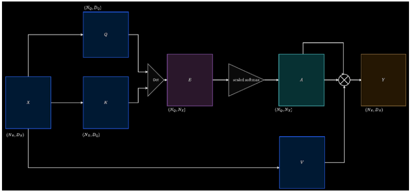
(a) Schematic of attention Version 4, Source

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

(b) Outputs Table, Source

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, Source

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

(b) Outputs Table, Source

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.

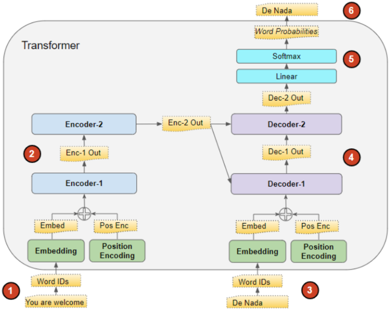


Figure: Training the transformer, Source.

Inference

- During Inference, we have only the input sequence.
- The goal of the Transformer is to produce the target sequence from the input sequence alone.

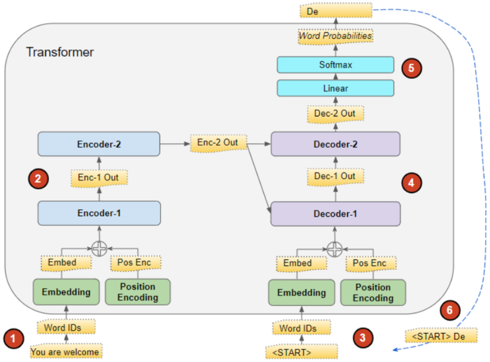


Figure: Schematic of inference process after first timestamp, Source.

Teacher Forcing

- The approach of feeding the target sequence to the Decoder during training is known as Teacher Forcing.
- During training, we could have used the same approach that is used during inference. But there are two major problem:
  - The looping cause training to take much longer.
  - The looping also makes it harder to train the model. The model would have to predict the second word based on a potentially erroneous first predicted word, and so on.
- Instead, by feeding the target sequence to the Decoder, we are giving it a hint, so to speak, just like a Teacher would.
- In addition, the Transformer is able to output all the words in parallel without looping, which greatly speeds up training.

Loss Function

- During training, we use a loss function such as cross-entropy loss to compare the generated output probability distribution to the target sequence.
- The probability distribution gives the probability of each word occurring in that position.
- As usual, the loss is used to compute gradients to train the Transformer via backpropagation .

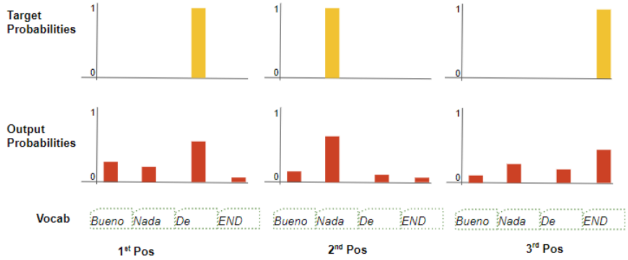


Figure: The loss function that is used for Transformers, Source.

Transformers in Practice

- Transformer Classification architecture: one of its examples is in Sentiment Analysis.

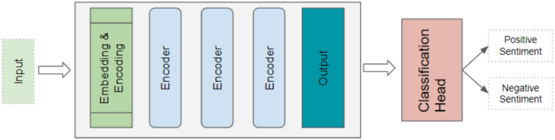


Figure: Source

- Transformer Language Model architecture: one of its examples is generating new text by predicting sentences that would follow a given text as input.

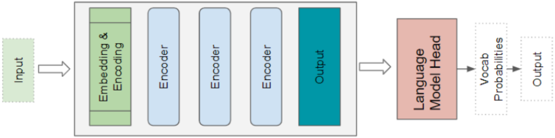


Figure: Source

Why Transformers instead of RNNs?

- RNNs and their relatives, LSTMs and GRUs had two main limitations:
  - It was challenging to deal with long-range dependencies between words that were spread far apart in a long sentence.
  - They process the input sequence sequentially one word at a time , which means that it cannot do the computation for time-step t until it has completed the computation for time-step t—1.

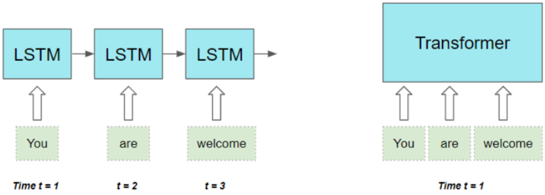


Figure: Transformers unlike LSTMs process the words in parallel, Source.

Position Encoding

- Transformers don't use RNNs and all words in a sequence are input in parallel.
- This is its major advantage over the RNN architecture, but it means that the position information is lost, and has to be added back in separately.
- The Position Encoding is computed independently of the input sequence.
- These are fixed values that depend only on the max length of the sequence. These constants are computed as follows:

$$PE_{(pos,2i)} = sin(\frac{pos}{10000^{2i/d_{model}}})$$

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

where,

- pos is the position of the word in the sequence.
- d_{model} is the length of the encoding vector
- i is the index value into this vector.

Bahdanau’s Attention

- We can think of the google translate as a perfect practice for the Bahdanau’s Attention !
- The related paper ”Neural Machine Translation by Jointly Learning to Align and Translate”, propose to build the encoder representation each time a word is decoded in the decoder.
- This dynamic representation will depend on the parts of the input sentence most relevant to the current decoded word.

Encoder for the Bahdanau's Attention:

- A RNN takes the present input x_t and the previous hidden state h_{t-1} to model the present hidden state h_t.
- For the encoder, the authors have suggested a Bidirectional RNN.
- In a Bidirectional RNN, RNN will provide two sets of hidden states, the forward $\overrightarrow{h_t}$ and the backward $\overleftarrow{h_t}$ hidden states.
- The authors suggest that concatenating the two states gives a richer and better representation $h_t = [\overrightarrow{h_t}; \overleftarrow{h_t}]$

Decoder for the Bahdanau's Attention:

- The equation below is of the conditional probability, which needs to be maximized for the decoder to translate properly.

$$P(y_i|y_{<\mathrm{i}}, c_i) = \mathrm{RNN}(y_{i-1}, s_{i-1}, c_i)$$

  where s is the hidden state for the decoder and c_i is a newly built context vector for each step.
- Each context vector depends on the relevant information from which the source sentence is attended.
- But how important is h_t for s_t? $\longrightarrow$ we need to apply a softmax on the unnormalized importance.

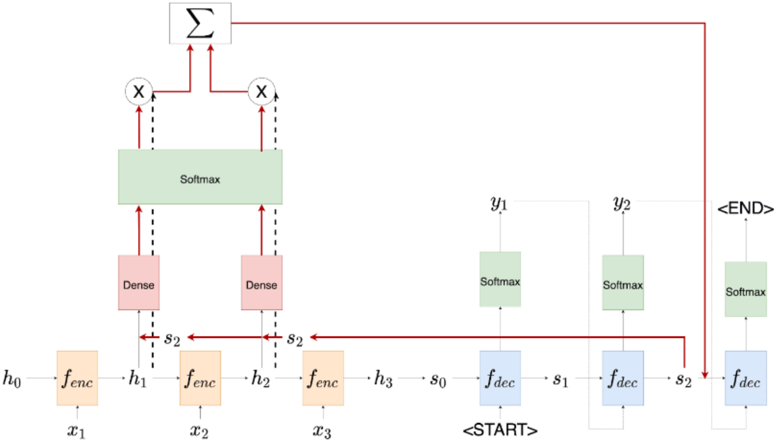


Figure: Neural machine translation with Bahdanau's attention, Source.

Luong's Attention

- In the related paper "Effective Approaches to Attention-Based Neural Machine Translation", Luong et al. provide more effective approaches to building attention.
- The basic intuition behind attention is still the same as before.
- Luong et al. suggested subtle changes to Bahdanau et al. work to break through the limitations of the old architecture.

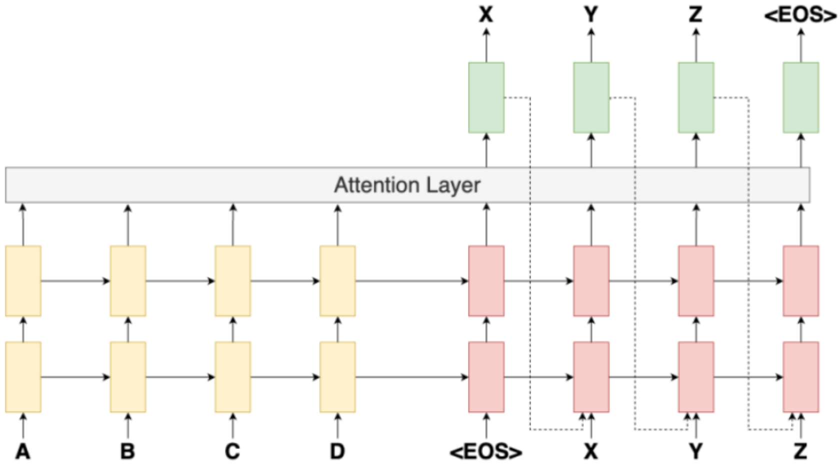


Figure: Diagram of the Luong attention architecture, Source.

Encoder for the Luong's Attention:

- In this model, authors opt for a unidirectional (instead of bidirectional as in Bahdanau's implementation) Recurrent Neural architecture for the encoder.
- Unidirectional RNNs speed up the computation.

Decoder for the Luong's Attention:

- given the target hidden state, s_t, and the source-side context vector, c_t, they employ a simple concatenation layer as follows:

$$\widetilde{s}_t = tanh(W_c[c_t; s_t])$$

- The attention vector, $\tilde{s}_t$, is then fed through the softmax layer to produce the probability of the next decoder word.

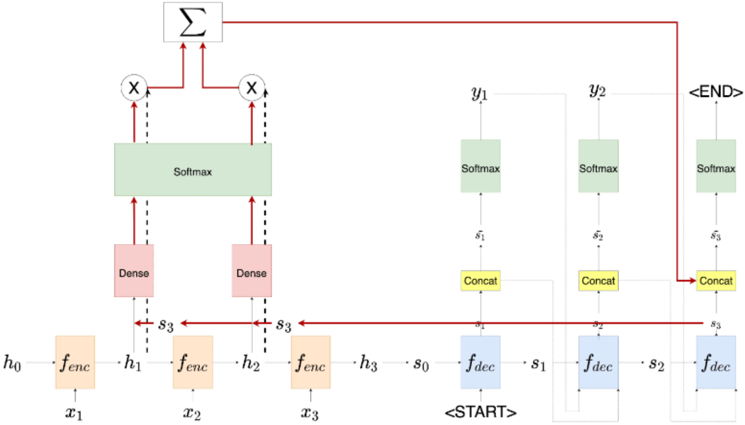


Figure: Neural machine translation with Luong's attention, Source.

Thank You!

Any Question?