LLMs: a theoretical overview of the Transformer architecture and the novel concepts of LLaMA 3, Gemma and Mixtral

Rafael Guedes July 11th, 2024

Experience





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First things first: Tokenization...

Tokenization

Tokenization is used to transform raw input text data into tokens.

SentencePiece was developed by Google and one of the most used tokenizers for LLMs.

1. Splits the words into individual characters

Imagine that the training data contains the following set of words and the frequency of each word has been determined:

```
("hug", 10), ("pug", 5), ("pun", 12), ("bun", 4), ("hugs", 5)
```

Then, if we split into individual characters we will get:

```
("h" "u" "g", 10), ("p" "u" "g", 5), ("p" "u" "n", 12), ("b" "u" "n", 4), ("h" "u" "g" "s", 5)
```

2. Iteratively merges the most frequent character pairs into subwords until a predefined vocabulary size is reached

```
("h" "u" "g", 10), ("p" "u" "g", 5), ("p" "u" "n", 12), ("b" "u" "n", 4), ("h" "u" "g" "s", 5)
```

We see that "u" followed by "g" appears 20 times, the most frequent symbol pair, therefore we merge them:

```
("h" "ug", 10), ("p" "ug", 5), ("p" "u" "n", 12), ("b" "u" "n", 4), ("h" "ug" "s", 5)
```

Repeat until it reaches a vocabulary size of 9 tokens:

```
("hug", 10), ("p" "ug", 5), ("p" "un", 12), ("b" "un", 4), ("hug" "s", 5)
```

3. When it comes to unseen data

```
("hug", 10), ("p" "ug", 5), ("p" "un", 12), ("b" "un", 4), ("hug" "s", 5)
```

If we get the word "bug" in new data, it will be tokenized as ["b", "ug"]

But, if the new word is "mug" since, we do not have "m" in the vocabulary, then it will be encoded as ["<unk>", "ug"]

4. Encoding

Finally, each subword will be encoded by assigning a token ID:

"hug" -> 1

"p" -> 2

"uq" -> 3

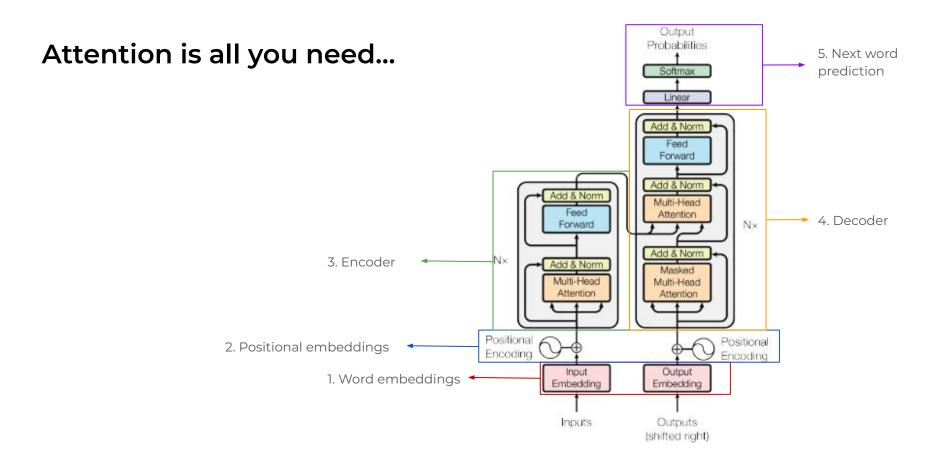
"un" -> 4

"b" -> 5

...

9

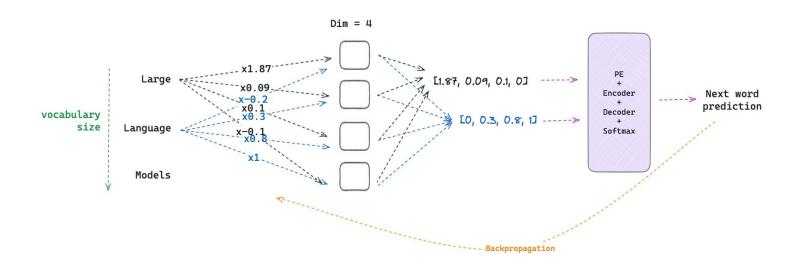
Transformer Architecture





1. Word Embeddings

First layer in a Transformer is the word embedding that converts each token input into a d-dimensional vector. Let's consider each word as token:



Positional Encoding Input Embedding Inputs

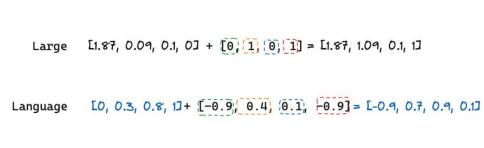
2. Positional Embedding

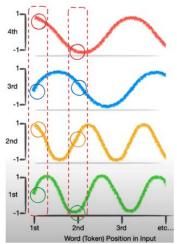
Second step in a Transformer is the positional embedding that helps Transformers keep track of order since they are order invariant.

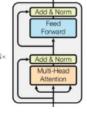
If positional embeddings did not exist the sentences: 'LLaMA is better than Gemma' and

'Gemma is better than LLaMA' would mean the same.

Sine and Cosine functions with different frequencies

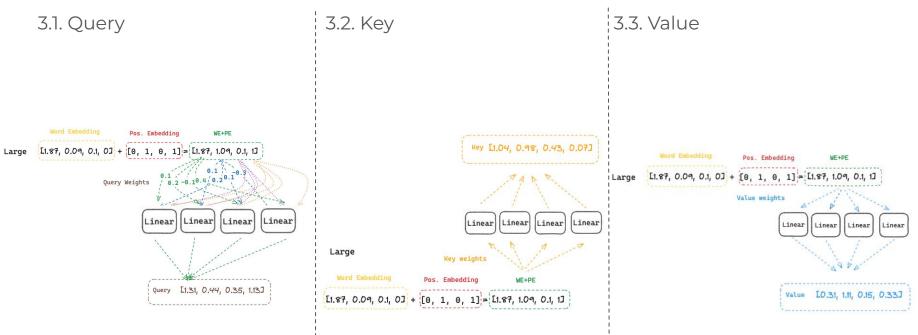






3. Encoder - Self-Attention

Self-attention calculates how similar each word is to all of the words in a sentence, including itself in order to determine how the Transformer will encode each word.



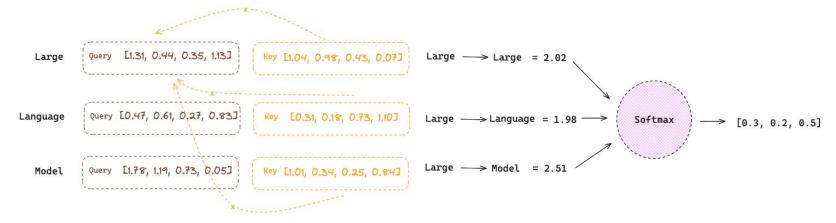
Add & Norm Feed Forward Add & Norm Multi-Head Attention

3. Encoder - Self-Attention

3.4. Calculate similarity between words based on query and keys.

For example, the similarity between the word 'Large' and all words will be the dot product between the Query of the word 'Large' and all the keys.

After that, the values go through a softmax activation function so that they sum up to 1 and we consider this the weight that each word has in the encoding of 'Large'.

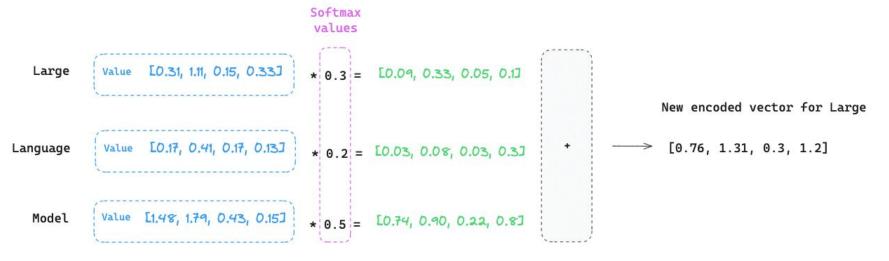


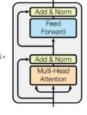
Add & Norm Feed Forward Add & Norm Multi-Head Attention

3. Encoder - Self-Attention

3.5. Create values to represent each word in the sentence (same process as queries and keys).

Calculate the new encoded vector of each word based on the Value of each word and the its weight. This way we embed context into the word vector representation.

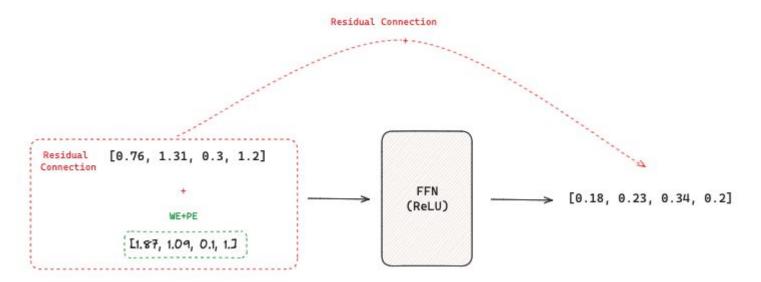




3. Encoder - Feed Forward Network

3.6. There is a residual connection in the end that adds the new word embedding to the initial word embedding with positional encoding.

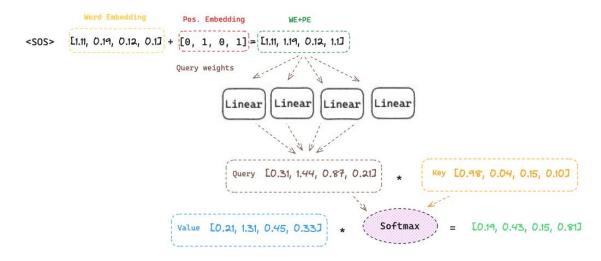
This new vector is fed into a Feed Forward Neural Network with ReLU activation function.



4. Decoder

The Decoder is responsible for generating the vector used in the next word prediction component based on the output of the encoder and all the tokens in the current sequence.

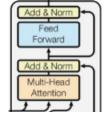
4.1. First token to be processed in <SOS> which means start of sentence. Just like before, this token will be encoded through word embedding + positional encoding + self-attention



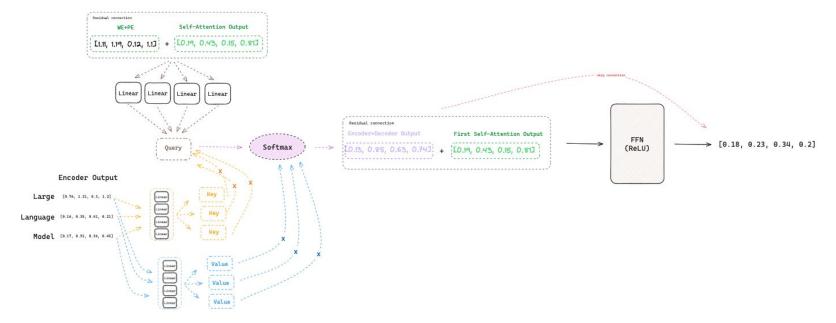
Encodina

Embedding

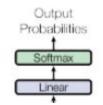




4.2. There is a residual connection that will add to the new word representation the old word representation and the positional encoding. This final vector together with the encoder output go through a new self-attention layer, followed by a skip connection and a FNN.



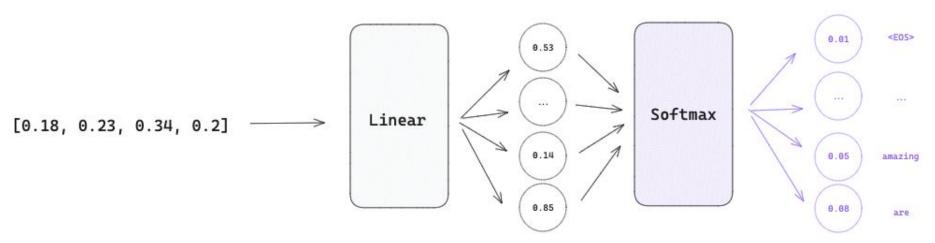




The final output of the decoder goes through a simple neural network that will convert this vector into a new one with the same dimension as the vocabulary size.

After that, a Softmax function is applied to determine which word should come next. The process stops when a <EOS> token (end of sentence) is predicted.

1 value for each word in the vocabulary



Final remarks about Self-Attention:

- Query, Keys and Values are calculated in parallel, i.e., Q, K and V are calculated at the same time for each word.
- We can have several Self-Attention Cells to train different weights and capture different relationships between words (the original had 8 cells that are combined through concatenation followed by a linear layer).
- There are multiple stacked layers (N=6) of self-attention cells + FFN which means the second layer input is the output of the first layer, the third layer input is the second layer output and so on and so forth.
- After each self-attention cell and FFN block, a normalization step is applied.

LLaMA 3, Mixtral and Gemma: what's new?

Overview

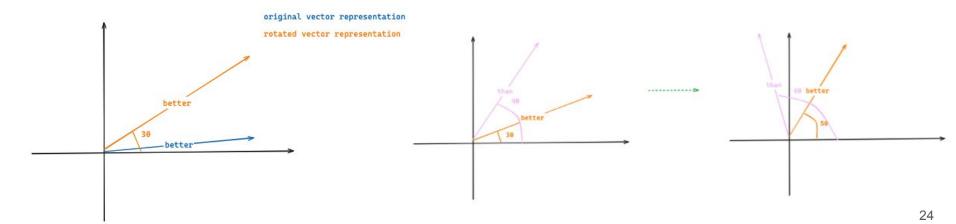
	Original	Gemma	Mixtral	LLaMA 3
Vocab. Size	32k	256k	32k	128k
Context Length	512	8192	4096	8192

Positional Embeddings

LLaMA 3 and Gemma use Rotary Positional Embedding (RoPE) instead of the original version. This approach brings benefits such as modelling the relative position between tokens which means that the tokens in position 1 and 2 will be more similar than the tokens in position 1 and 500.

Let's consider the sentence 'Gemma is better than LLaMA' and a 2D word embedding.

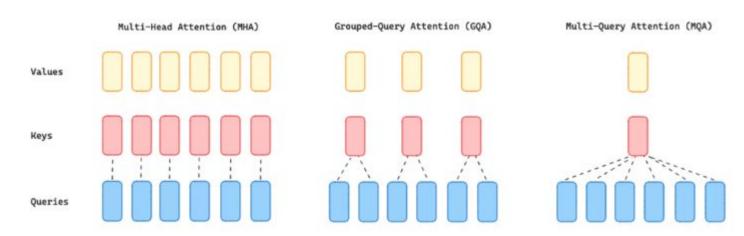
The positional embedding of the word better will be given by a rotation of the vector based on position 3 and a constant θ . If two new words are added to the sentence, then the angle between 'better' and 'than' will keep the same.



Grouped Query Attention instead of Multi Head Attention

LLaMA 3, Gemma and Mixtral replaced the traditional Multi Head Attention with Grouped Query Attention for faster decoding, hence, faster inference.

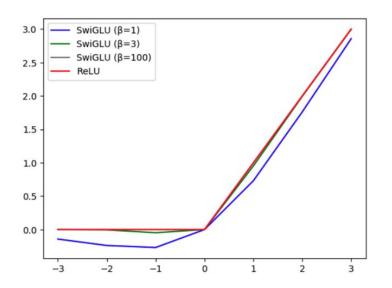
GQA-G divides query values into G groups that share a single key and value head (GQA-1 = MQA while a GQA-H = MHA). This approach reduces the number of keys and values heads into a single key and value per query group, accelerating the inference speed and reducing the memory requirements during decoding with a quality closer to MHA.

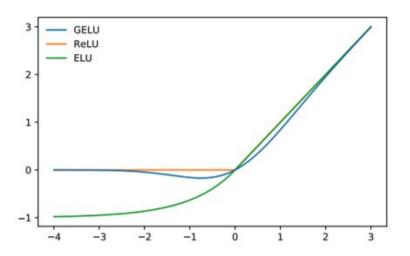


Activation function

LLaMA 3 and Gemma replaced the traditional ReLU activation function in the FFN block with SwiGLU and GeGLU, respectively.

These functions, unlike ReLU that converts all negative values to 0, have a parameter that smooths this conversion where the probability of setting negative values to 0 increases as these values are closer to 0.





SMoE: Sparse Mixture of Experts

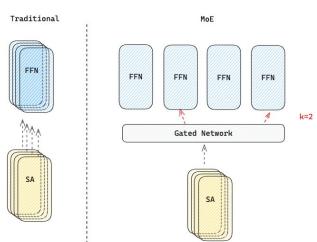
Mixtral differs from the other architectures by using Mixture of Experts rather than stacking a FFN on top of the different attention cells.

Each Expert is responsible for processing a type of token, for example, one can be a punctuation expert, a visual description expert, or a number expert.

The Expert(s) that is going to process the token is chosen by a Gated Network trained to perform this allocation.

Advantages:

- More efficiency by activating less model parameters;
- More accurate prediction because each expert is focused on a specific task



LLaMA 3 8B vs Gemma 7B vs Mistral 7B

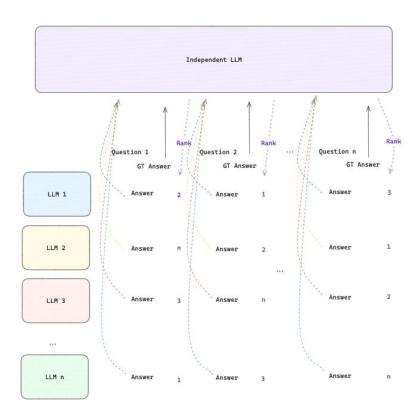
Use Case: Simple RAG system with 100 questions, contexts and ground truth answers.

Metrics:

- Words produced per second
- Answer Length
- RAQ (Relative Answer Quality) based on a rank provided by GPT 3.5.

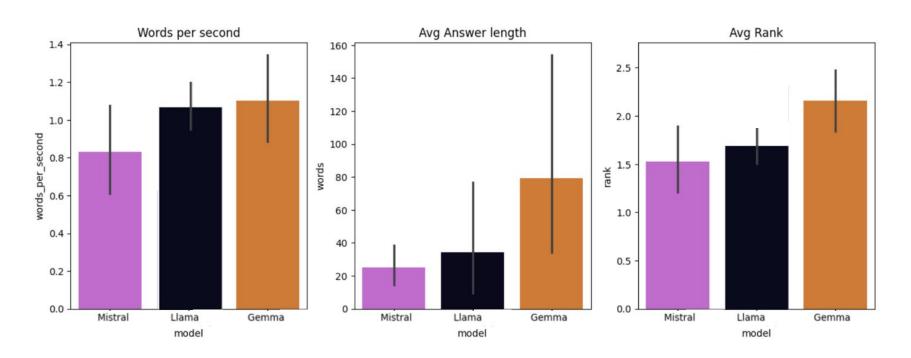
Prompt:

```
Based on the correct answer: {Ground Truth Answer}, rank the IDs of the following answers from the most to the least correct one:
ID: 1 Answer: {LLM 1 Answer}
ID: 2 Answer: {LLM 2 Answer}
ID: 3 Answer: {LLM 3 Answer}
```



LLaMA 3 8B vs Gemma 7B vs Mistral 7B

Gemma is the fastest and with the one producing more words per answer. But, **Mistral** produces better answers according to GPT 3.5.



Hands-on with DSPy