TRANSFORMER

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Motivation

The transformer architecture, introduced in ”Attention is All You Need” [15], aimed to overcome limitations of existing sequence-to-sequence models based on recurrent neural networks and convolutional neural networks. These models struggled with capturing long-range dependencies, processing long sequences, and efficiently utilizing parallel computation.

In order to overcome these challenges, the team [15] proposed a new architecture relying on attention mechanisms, to capture global dependencies between input and output elements. This design allows for more effectively attending long-range dependencies, and is the reason behind the transformers huge success in performing tasks related to natural language processing, among other things.

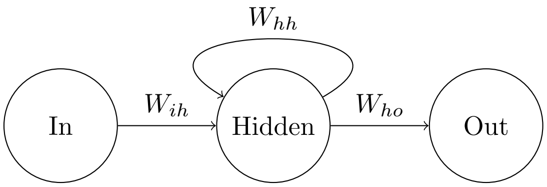
Traditional sequence based deep learning

Recurrent neural networks (RNNs) are a type of neural network designed for sequence-based data. Unlike traditional feedforward neural networks, RNNs have connections that loop back within the network, providing a way to maintain an internal state (*i.e.*, its memory).

BASIC STRUCTURE

A basic RNN has an input layer (In), a hidden recurrent layer (Hidden), and an output layer (Out). The recurrent layer processes sequences of data by looping its output back into its input, allowing it to learn from past information.

$$h_t = f_{\text{activation}}(W_{hh}h_{t-1} + W_{ih}x_t + b_h)$$
$$o_t = f_{\text{activation}}(W_{ho}h_t + b_o)$$



Where t represents the position in the sequence (*e.g.*, time), o the output, i the input and b the bias. h_{t-1} therefore represents the hidden output for the previous time-step, and h_t the current hidden output. $f_{\text{activation}}$ for the hidden and output layers may differ, and represent their activation functions.

LONG SHORT-TERM MEMORY

A Long Short-Term Memory (LSTM) model is a special type of RNN that can better learn long-term dependencies in the data compared to a simple RNN. It has a more complex internal structure involving gates that control the flow of information.

The LSTM structure consists of four gates, which combine or remove information. The operations done are linear, being

$$\oplus \text{ Element-wise addition. } \begin{bmatrix}0.8\\0.8\\0.8\end{bmatrix} \oplus \begin{bmatrix}1.0\\0.5\\0.0\end{bmatrix} = \begin{bmatrix}0.8+1.0\\0.8+0.5\\0.8+0.0\end{bmatrix} = \begin{bmatrix}1.8\\1.3\\0.8\end{bmatrix}$$

$$\otimes \text{ Element-wise multiplication. } \begin{bmatrix}0.8\\0.8\\0.8\end{bmatrix} \otimes \begin{bmatrix}1.0\\0.5\\0.0\end{bmatrix} = \begin{bmatrix}0.8\cdot 1.0\\0.8\cdot 0.5\\0.8\cdot 0.0\end{bmatrix} = \begin{bmatrix}0.8\\0.4\\0.0\end{bmatrix}$$

By inspecting these operations, we can see that gates using $\otimes$ is able to either block or allow information to pass through (respectively through values of 0.0 or 1.0), or something in-between. This means, that the network can learn previous state values, and take these into account when filtering values of new inputs.

An LSTM network has a *cell state* C, which acts as the memory of the network. This state is being transferred across the time-steps, thus allowing for previous inputted information to be retained in future time-steps.

Γ_f **FORGET GATE LAYER**

The first step in an LSTM is the *forget gate* layer. This is a neural network which takes in the previous output along with current input. This layer has a sigmoid activation function, $\sigma(\cdot)$, where inputs resulting in 0's lead to variables being left out of the cell state C.

$$\Gamma_f = \sigma(W_f \cdot [h_{t-1}, x_t] + b_f) \qquad\qquad C_t^* = \Gamma_f \otimes C_{t-1}$$

Γ_u **UPDATE/INPUT GATE LAYER**

The next step is to decide what new information to store in the cell state.

$$\Gamma_u = \sigma(W_u \cdot [h_{t-1}, x_t] + b_u) \qquad\qquad \tilde{C}_t = \texttt{tanh}(W_C \cdot [h_{t-1}, x_t] + b_C)$$

These two are then pairwise multiplied together, and added to the forgotten state.

$$\begin{aligned} \textbf{CELL STATE} \qquad C_t &= C^*_{t-1} \oplus (\Gamma_u \otimes \tilde{C}_t) \\ &= (\Gamma_f \otimes C_{t-1}) \oplus (\Gamma_u \otimes \tilde{C}_t) \end{aligned}$$

Γ_o **OUTPUT GATE LAYER**

The output of the model is then calculated based on both the cell state and previous ouput as well as input.

$$\begin{aligned} \Gamma_o &= \sigma(W_o \cdot [h_{t-1}, x_t] + b_o) \\ \textbf{OUTPUT} \qquad h_t &= \Gamma_o \otimes \texttt{tanh}(C_t) \end{aligned}$$

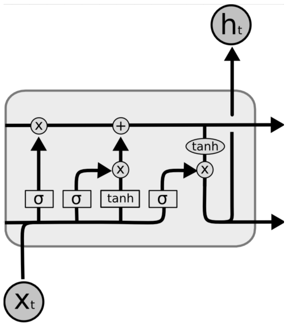


Figure 1: LSTM block.

Although models like the mentioned Recurrent Neural Network (RNN) and Long Short-Term Memory (LSTM) enable the retention of some prior information, they inherently struggle with handling long sequences. For example, when an LSTM cell state, C, is presented with an input sequence of length L, it is unable to maintain information from all previous steps when evaluating step l. This is because the cell state progressively becomes more abstract as it processes each step in the sequence, making it challenging to retain information from the distant past.

Attention

Skrive at attention er det ”viktige” hos transformers.

As artificial intelligence models continuously try to mimic its biological counterpart, the concept of attention is also based on biological neuronal networks. Arguably, the most important core function of information processing in the brain is to selectively attend important impressions [12]. For instance, when reading a document, much of its content is redundant. Here, the human brain is able to attend to the important parts and their connection – and disregard most of the redundant information. Likewise, modern artificial intelligence models tries (to some extent) to mimic the human brain when processing information.

Attention mechanisms used in transformers can in simple terms be thought of as scalars that enhance or diminish some input, like the **forget gate** in the LSTM which use **element wise multiplication**. However, in order to capture more intricate connections in the input-sequence, a few tricks are applied.

When calculating the attention based on some input, it is important to note that the ”input” consists of the full sequence. A practical example would be when predicting the next word based on the sentence;

`At my dairy farm we always get our milk from ___,`

where the model would need the full context in order to properly complete the sentence.

ORIGIN OF ATTENTION IN DEEP LEARNING

> When trying to solve problems related to machine translation, Bahdanau *et al.* [2] began experimenting with how the context of a given sentence may be used when predicting an output. In the paper [2], they came up with a method where, for any given word i in the sequence, its context is composed of a weighed sum of the other words in the sequence.
>
> While recent methods has optimized this approach by using matrices [15] instead of a neural network [2], the theory remains the same.
>
> While it is possible to obtain the (additive) attention through a separate neural network, it is deemed more computational efficient to use (multiplicative attention through) optimized matrix multiplication algorithms [15].

QUERY, KEY AND VALUE

> When calculating what to attend based on some input, $\mathbf{X}$, three new quantities, query, key and value, are introduced, respectively;
>
> $$\begin{aligned} \mathbf{Q} &= \mathbf{X}\mathbf{W}_Q \\ \mathbf{K} &= \mathbf{X}\mathbf{W}_K, \\ \mathbf{V} &= \mathbf{X}\mathbf{W}_V \end{aligned} \tag{1}$$
>
> along with their respective sets of weights, $\mathbf{W}_i$. Here, $\mathbf{X}$ is typically a lower-triangular representation of the inputs (for unidirectional attention) [14, 10, 16], such that the first row of the matrix only contains the first element, the second the two first, and so on until the full sequence length is reached;

$$\mathbf{X} = \begin{bmatrix} \mathbf{x}_{11} & \dots & 0 \\ \vdots & \ddots & \vdots \\ \mathbf{x}_{N1} & \dots & \mathbf{x}_{NN} \end{bmatrix}. \tag{2}$$

It is worth noting that the inputs, $\mathbf{X}$, typically consists of vector representations of its elements. That is, if the input is a sentence, the elements of the first column, $\mathbf{x}_{i1}$ are all equal and equal to the **embedding** of the word.

The matrices containing the queries, keys and values can thus be seen as three different representations of the inputs which is used to enhance or diminish certain aspects of the context, when predicting the next element of the sequence.

While *Geometry of Deep Learning* tries to provide a biological analogy as to what the query and key represents, its actual representation in terms of the transformer is rather abstracted [17, 1]. It is however worth noting that all three of them is some form of embedding of the input, and is used to process the context of said input.

In practice, these three matrices are obtained by a single fully-connected layer which takes the inputs, $\mathbf{X}$, and outputs $\texttt{concat}(\mathbf{Q}, \mathbf{K}, \mathbf{V})$.

SIMILARITY SCORE

The score of an arbitrary query vector, $\mathbf{q}_i$ contained as a column in $\mathbf{Q}$, and the key vectors $\mathbf{k}_j$ $\texttt{ for }$ $\mathbf{k}_j \in \mathbf{K}$, is found by taking the dot product between them

$$\texttt{score}_{ij} = \mathbf{q}_i \cdot \mathbf{k}_j \qquad \texttt{for } j = 1, \cdots, d_k, \tag{3}$$

where d_k is the dimension of $\mathbf{k}$. Here, we get a score for each key element in the sequence $\mathbf{k}_j$ and the chosen query element, $\mathbf{q}_i$. The intuition behind the dot product is to find the importance of the other elements contained in the sequence with respect to the current element.

These scores are then (typically) scaled by the root of their dimension, d_k, and normalized using the softmax function such that a probabilistic representation is obtained;

$$\texttt{weighting}_{ij} = \texttt{softmax}\left(\frac{\mathbf{q}_i \cdot \mathbf{k}_j}{\sqrt{d_k}}\right) \qquad \texttt{for } j = 1, \cdots, d_k. \tag{4}$$

SIMILARITY FUNCTIONS

While the mentioned approach using the scaled dot product is the most common [17, 14, 1, 10], other functions for calculating the score may be used.

Other such functions include the non-scaled dot product, $\mathbf{q}_i \cdot \mathbf{k}_j$, and the cosine similarity, $\frac{\mathbf{q}_i \cdot \mathbf{k}_j}{||\mathbf{q}_i|| ||\mathbf{k}_j||}$, as presented in *Geometry of Deep Learning* [17].

When the softmax score has been calculated, it is multiplied with the value representation of the input, $\mathbf{V}$, much like the **forget gate** in the LSTM which enhance or diminish the focus on certain elements of the sequence. The output of the attention layer for element i is then the sum of all j products. That is;

$$\begin{aligned}\texttt{attention}_i &= \sum_{j=1}^{N} \texttt{weighting}_{ij} \mathbf{v}_j \\ &= \sum_{j=1}^{N} \texttt{softmax}\left(\frac{\mathbf{q}_i \cdot \mathbf{k}_j}{\sqrt{d_k}}\right) \mathbf{v}_j \qquad \texttt{for } j = 1, \cdots, d_k.\end{aligned} \tag{5}$$

Which can be rewritten in terms of matrix notation [15]:

$$\texttt{attention} = \texttt{softmax}\left(\frac{\mathbf{QK}^T}{\sqrt{d_k}}\right)\mathbf{V}. \tag{6}$$

This allows the transformer model to selectively focus on different parts of the input sequence when generating each output element, improving its ability to capture long-range dependencies and context compared to just transferring the cell state C as is done in LSTMs.

PARALLELIZATION

Unlike recurrent neural networks, which process input tokens one at a time, the attention mechanism calculates the weighted sum of value vectors for each input by considering all key and value vectors at once, enabling parallel computation, as seen in **Equation** (6).

MULTI-HEAD ATTENTION

Multi-head attention is an extension of attention that allows the model to attend to multiple positions in the sequence simultaneously. This is achieved by linearly projecting the input tokens into multiple attention heads, computing the attention scores for each head independently, and then concatenating the results. This process enables the model to capture a diverse range of contextual information and improve its overall understanding of the input sequence. [15]

Natural language processing

TOKENIZATION

Tokenization, in terms of language processing, involves breaking down text into smaller pieces called tokens. Said tokens vary between methods, and could include words, phrases, or even single characters.

As state-of-the-art artificial intelligence language models rely on numerical input, tokenization methods are used to preprocess the inputted text. [9]

BYTE-PAIR ENCODING

Byte-Pair Encoding (BPE) is a type of tokenization that is commonly used in state-of-the-art language models [16]. It works by initially representing text as a sequence of characters, and then iteratively replacing the most frequent pair of bytes with a single, new byte. This process continues until the desired vocabulary size is reached. The result is a set of tokens that represent common sequences of characters, which can be more efficient and effective for language modeling than word-based tokenization. [4, 9, 13]

BPE is commonly used because it strikes a balance between character-level and word-level tokenization. It can handle out-of-vocabulary words and rare words more effectively than word-level tokenization, while still capturing meaningful linguistic units. [4, 13]

REGULAR EXPRESSION

In order to simplify the vocabulary creation, regular expressions are useful. The regular expressions are increasingly complex [13], but help filter out redundant characters. The regular expression below is used for GPT-4 when tokenizing inputs (according to Karpathy [9]) [13]. This regular expression is extremely complex, and a description of its components are found in **Table 1**.

```
'(?i:[sdmt]|ll|ve|re)|[^\r\n\p{L}\p{N}]?+\p{L}+|\p{N}{1,3}| ?[^\s\p{L}\p{N
    }]++[\r\n]*|\s*[\r\n]|\s+(?!\S)|\s+
```

<table>
<tr><th>COMPONENT</th><th>DESCRIPTION</th></tr>
<tr><td>’(?i:[sdmt]|ll|ve|re)</td><td>Uses a case-insensitive inline modifier (?i:...) to match common abbreviations and contractions in English text (’). Matches either a single character that is one of s, d, m, or t, or the two-letter sequences ll, ve, or re.</td></tr>
<tr><td>[^\r\n\p{L}\p{N}]?+\p{L}+</td><td>Uses a possessive quantifier ?+ to match one or more Unicode letters (\p{L}) that are preceded by zero or more characters that are not (^) Unicode letters, line breaks (\r\n), or Unicode numbers (\p{N}). Matches words that start with non-letter characters, such as hyphenated words.</td></tr>
<tr><td>\p{N}{1,3}</td><td>Matches up to three Unicode numbers (\p{N}). Matches numbers in the text.</td></tr>
<tr><td>␣?[^\s\p{L}\p{N}]++[\r\n]*</td><td>Matches zero or one space character (␣), followed by one or more characters that are not (^) whitespace (\s), Unicode letters (\p{L}), or Unicode numbers (\p{N}), followed by zero or more line breaks ([\r\n]*). The ? at the beginning of the pattern makes the preceding space optional. Matches punctuation and symbols that are not part of words or numbers.</td></tr>
<tr><td>\s*[\r\n]</td><td>Matches zero or more whitespace characters (\s*) followed by a line break ([\r\n]). Matches line breaks in the text.</td></tr>
<tr><td>\s+(?!\S)</td><td>Matches one or more whitespace characters (\s+) that are not followed by a non-whitespace character ((?!\S)). Matches whitespace at the end of lines.</td></tr>
<tr><td>\s+</td><td>Matches one or more whitespace characters, <i>i.e.</i>, spaces between words.</td></tr>
</table>

EMBEDDING

| Fyll inn her!

Architecture

The transformer architecture consists of two primary components: the encoder and the decoder, both of which contain multiple identical layers stacked upon each other. The sub-layers of the encoder and decoder can be seen in the left and right part of **Figure 2**, respectively.
As the transformer architecture processes the entire input sequence simultaneously, its computational efficiency is far greater compared to traditional **RNNs** or **LSTMs**, as explained in the original paper by Vaswani *et al.* [15].
While the architecture displayed in **Figure 2** is the originally presented transformer [15, 8], variations of the core architecture which aim at overcoming certain disadvantages can be found throughout the literature (like [6, 7, 3, 5, 11]).

ENCODER

> The encoder takes a sequence of (*e.g.*, tokenized word) positional **embeddings** as input, processes all elements of the sequence simultaneously using **attention**, and outputs a new sequence of vectors that represent the input sequence with the added context of the full sequence.
> In order to achieve this, both a multi-head **attention** mechanism and a position-wise feed-forward network is used, the latter being a fully connected neural network applied independently to each position in the sequence [15], as seen in **Figure 2**.

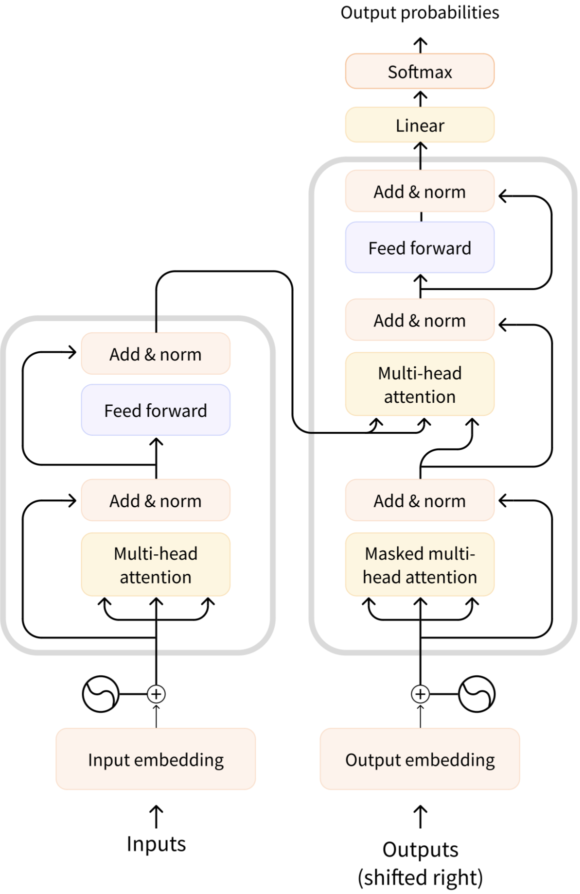


Figure 2: Transformer architecture (from Huggingface [8]).

DECODER

> The decoder take the output of the encoder and generate an output sequence (*e.g.*, a translated sentence). The decoder does this by using several layers, each of which contains three sub-layers: a masked multi-head attention mechanism, an encoder-decoder attention mechanism, and a position-wise feed-forward network.
>
> #### MASKED MULTI-HEAD ATTENTION
>
> > This mechanism is similar to the multi-head attention mechanism in the encoder, but with one key difference: it uses a mask to ensure that the predictions for position `i` are only dependent on positions before `i`. This is necessary during training to prevent the model from "cheating" by looking at the target sequence in its entirety. The mask ensures that the model only attends to previous positions when generating each token in the output sequence. [15] Intuitively, this masking has no effect when generating new text, but is important during training (where the output is known).

ENCODER-DECODER ATTENTION

This mechanism allows the decoder to focus on different parts of the input sequence when generating each token in the output sequence. It does this by taking the output of the encoder and the output of the masked multi-head attention mechanism as input, and computing a weighted sum of the encoder output based on the attention weights. This allows the decoder to take into account the entire input sequence when generating each token in the output sequence.

Forstå dette bedre.

Each of these sub-layers also includes a residual connection (or skip connection) around it, followed by layer normalization. [15]

The decoder's output is a sequence of vectors, each of which represents a token in the output sequence. The final linear layer and softmax function are then applied to each vector to produce a probability distribution over the target vocabulary, which is used to generate the output sequence.

POSITIONAL ENCODING

Since the Transformer does not inherently consider the position or order of input tokens, positional encodings are added to provide this information. These encodings can be learned or fixed and are added to the input embeddings before being passed through the model. [15] Positional encodings allow the model to maintain a sense of sequence order, which is crucial for understanding the context and relationships between tokens in the input data.

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Source code

The source code behind this report can be found here.