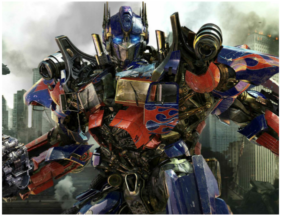

TRANSFORMERS

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INTRODUCTION

Why ?

- Transformers have revolutionized NLP
- Emerged as a powerful paradigm for computer vision applications, imaging or multi-modal datasets.

Key points

- Attention mechanism
- Self attention

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Basic form of self attention

Self attention philosophy

Convert one set of input embeddings to a set of output embeddings.

Input sequence: T vectors $\mathbf{x}_1 \cdots \mathbf{x}_T$ of size $d_e \to \mathbf{X} \in \mathcal{M}_{T,d_e}(\mathbb{R})$

$$\mathbf{x}_i = \begin{cases} \text{timeseries} \\ \text{flattened part of an image} \\ \text{tokens representing words (LLM)} \\ \dots \end{cases}$$

Embedding: related inputs are represented by similar vectors

Self-attention mechanism transforms $\mathbf{x}_1 \cdots \mathbf{x}_T$ to $\mathbf{y}_1 \cdots \mathbf{y}_T$ where $\mathbf{y}_i = \sum_{j=1}^{T} W_{ij}\mathbf{x}_j$

Goal

Create context-aware output vectors, i.e. output vectors that account for the pair-wise relationships between input vectors

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EXAMPLE

"The Queen died on September 8^{th} 2022"

"He uses the Queen to beat his opponent in the match"

$\mathbf{x}_i = "Queen"$

$\Rightarrow$ The transformation $\mathbf{y}_i = \sum_{j=1}^{T} W_{ij}\mathbf{x}_j$ aims to create representations that are aware of the surrounding words, and thus the context the word is used in

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WEIGHT MATRIX

Weights

- The weight matrix is derived from the inputs
- High weight to those inputs that have a high similarity to $\mathbf{x}_i$.
- Example= $w_{ij} = \mathbf{x}_i^T \mathbf{x}_j$

We want positive weights summing up to one $\Rightarrow$ softmax

$\rightarrow$ $w_{ij} = exp(w_{ij})$

$\rightarrow$ $W_{ij} = \dfrac{w_{ij}}{\sum_j w_{ij}}$

$\mathbf{x}_1 \cdots \mathbf{x}_T$ have been transformed into weighted combinations of all the other vectors, with weights being larger for input vectors that are more similar (it "attends" more to them).

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Learnable weights

For the moment, weights are not learnable $\Rightarrow$ the model cannot be optimized for a specific task.

$$\mathbf{y}_i = \sum_j softmax(\mathbf{x}_i^T \mathbf{x}_j)\mathbf{x}_j$$

$\mathbf{x}_i$ is used three times in three different roles
$\Rightarrow$ modify each occurrence of $\mathbf{x}_i$ by multiplying it with a different matrix containing learnable weights.

Query, Key, and Value

$$\mathbf{q}_i = \mathbf{x}_i \mathbf{W_Q}$$
$$\mathbf{k}_i = \mathbf{x}_i \mathbf{W_K}$$
$$\mathbf{v}_i = \mathbf{x}_i \mathbf{W_V}$$

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Query, Key, and Value??

- Suppose you want to find a YouTube video on how to build a house.
- You write on the search tab "How to build a house" $\rightarrow$ **Query**
- Every YouTube video has some keywords related to its contents $\rightarrow$ **Key**
- The similarity of the Query to the Keys of each video is computed
- Videos with the highest similarity scores are returned at the top of the search.
- The content of these top-ranked videos contains the **Value** (information) that best answers the initial question (Query)

Attention mechanism

Each input vector acts as a Query that is compared to every other vector (Keys) to find those combinations with the highest similarity (W_{ij}).
The output is a linear combination of the input, dominated by those input vectors (Values) with the highest attention scores.

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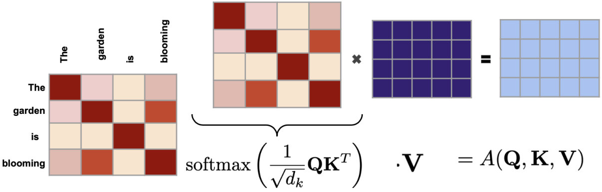
Query, Key, and Value

Query, Key, and Value

$\mathbf{q}_i = \mathbf{x}_i \mathbf{W_Q}, \mathbf{W_Q} \in \mathcal{M}_{d_e, d_q}(\mathbb{R})$
$\mathbf{k}_i = \mathbf{x}_i \mathbf{W_K}, \mathbf{W_K} \in \mathcal{M}_{d_e, d_k}(\mathbb{R})$
$\mathbf{v}_i = \mathbf{x}_i \mathbf{W_V}, \mathbf{W_V} \in \mathcal{M}_{d_e, d_v}(\mathbb{R})$
$\mathbf{W_Q}, \mathbf{W_K}, \mathbf{W_V}$: projection matrices on lower dimensional spaces

$$W_{ij} = softmax\left(\frac{\mathbf{q}_i \mathbf{k}_j^T}{\sqrt{d_k}}\right)$$

$$\mathbf{y}_i = \sum_{j=1}^{T} W_{ij} \mathbf{v}_j \rightarrow Attention(\mathbf{Q}, \mathbf{K}, \mathbf{V}) = softmax\left(\frac{1}{\sqrt{d_k}} \mathbf{Q}\mathbf{K}^T\right) \mathbf{V}$$



Summary

Up to now

- the similarity matrix $\mathbf{QK}^T$ is used to create the attention weights that capture the relevance of the combination of inputs
- these attention weight matrices multiply the matrix of value vectors to extract important features that are subsequently passed to the next stage of the network.
- $\mathbf{W_Q}, \mathbf{W_K}, \mathbf{W_V}$: attention head.

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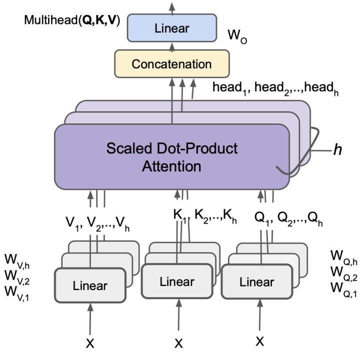
Multi-head attention

Multi-head attention

- ▶ CNN: multiple kernels
- ≈ multiple $\mathbf{W_Q}, \mathbf{W_K}, \mathbf{W_V}$: capture different relationships between the input embeddings.
- ▶ h attention heads in parallel
- ▶ $\mathbf{W}^O$: linear projection matrix used in order to project the concatenated vector to the output model space



$$MultiHead(\mathbf{Q}, \mathbf{K}, \mathbf{V}) = Concat(h_1, \cdots h_h)\mathbf{W}^O, \; h_i = Attention(\mathbf{Q}_i, \mathbf{K}_i, \mathbf{V}_i)$$

The $T \times d_e$ input is transformed into $T \times d_O$

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Positional encoding

As described for now, the self-attention mechanism is oblivious to the position of the inputs.
$\Rightarrow$ Architecture invariant under permutations.

The position is important (image, words,...)

Positional encoding: $\mathbf{p}_i \in \mathbb{R}^{d_e}$

$$\mathbf{x}_i \leftarrow \mathbf{x}_i + \mathbf{p}_i$$

i: position in the sequence.

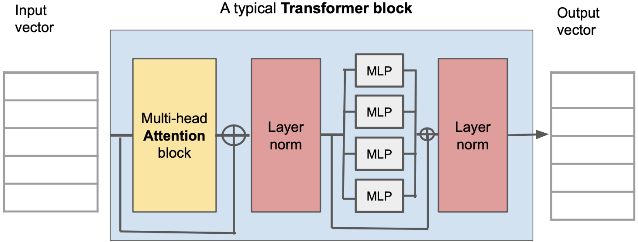
- learnable $\mathbf{p}_i$: positional embedding
- specific form $\mathbf{p}_i$: encodes the position

Example (seminal work)

$$\left\{ \begin{array}{ccc} \mathbf{p}_i(2j+1) & = & cos\left(\frac{1}{10000^{2j/d_e}}\right) \\ \mathbf{p}_i(2j) & = & sin\left(\frac{1}{10000^{2j/d_e}}\right) \end{array} \right.$$

The transformer block

Transformer: any architecture that has a transformer block as a basic building element.



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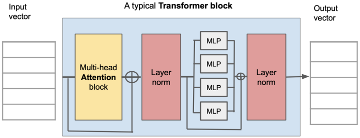
The transformer block

Multi-head attention

- Skip connections: $\mathbf{X}' = MultiHead(\mathbf{Q}, \mathbf{K}, \mathbf{V}) + X$
- Layer norm: normalize w.r.t. mean and standard deviations of the hidden units of the layer
- MLP: Increase the capability of the model without increasing its computational complexity (MLP acts on each position independently, the attention mechanism having already learned the correlations across positions)



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