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Coláiste na Tríonóide, Baile Átha Cliath

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## 09 - Attention Mechanism and Transformer Model

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The [Attention Mechanism](#) (2015) and the [Transformer model](#) (2017), which builds on it, have revolutionised the field of natural language processing (NLP) and have been widely adopted in all Deep Learning applications.

In this handout, we'll be looking in detail at the Attention Mechanism and the Transformer model that is based on it.

As these architectures have mainly originated from NLP, we'll introduce them in the context of text processing.

# The Attention Mechanism

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## The Problem with RNNs

To give a bit of context, let's look back at RNNs. Recurrent Neural Networks (LSTM/GRU) are the model of choice when working with variable-length inputs and are thus a natural fit to operate on text processing.

...but:

- the sequential nature of RNNs prohibits parallelisation,
- the context is computed from past only,
- there is no explicit distinction between short and long range dependencies (everything is dealt with via the context),
- training is tricky,
- how can we do you do efficiently transfer learning?

## The Problem with CNNs

On the other hand, Convolution can

- operate on both time-series (1D convolution), and images,
- be massively parallelised,
- exploit local dependencies (within the kernel) and long range dependencies (using multiple layers),

...but:

- we can't deal with variable-size inputs,
- the position of these dependencies is fixed (see next slide).

## The Problem with Relative and Fixed Positions of Dependencies

Take a simple 1D convolution on a sequence of feature vectors  $\mathbf{x}_i$  with a kernel size of 5. To simplify the argument, we are going to ignore cross-channels interactions:

$$\text{output}_i = w_{-2}\mathbf{x}_{i-2} + w_{-1}\mathbf{x}_{i-1} + w_0\mathbf{x}_i + w_1\mathbf{x}_{i+1} + w_{+2}\mathbf{x}_{i+2} + b,$$

The weight  $w_{-1}$  is always associated to the dependence relationship between the current and previous context sample (ie. distance = 1 away in past).

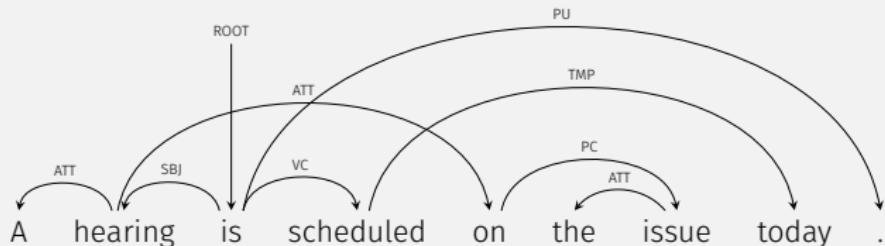
Now, take a dense layer (again ignoring cross-channels interactions):

$$\text{output}_i = \sum_{j=1}^L w_{i,j}\mathbf{x}_j + b,$$

we have same issue that all the relationships are defined according to fixed positions between words, eg. the relationship between the first and third words is assumed to be the same in all sentences.

## But in Text Processing, Relationships Positions Can Vary.

But look at an actual dependency graph in a sentence:



Distances between relations are not set in stone.

e.g. the verb is not always the next word after the subject.

Convolutional and Dense layers are not well equipped to deal with such relationships.

## So, We Have a Problem

So, what is the problem? Can't we just make the network bigger?

Yes, the Universal Approximation Theorem tells us that you can always throw more filters at the problem, and basically train the neural net to learn all possible dependency graphs, ...but it's clearly not optimal.

The [Attention Mechanism](#) comes to the rescue.

## Attention Mechanism

The idea of the Attention Mechanism was originally motivated by how different regions of an image or correlate words in one sentence in image captioning applications [1]. This idea was then quickly adapted to explain the relationship between words in sentences [2,3].

The idea of the Attention Mechanism has since then been iterated through many papers, and has taken many forms (eg. Bahdanau-Attention, Luong-Attention, etc.). We will look here at the *Dot-Product Attention Mechanism* as presented in Transformers, as it is arguably the most popular.

[1] Show, Attend and Tell: Neural Image Caption Generation with Visual Attention  
Xu et al., 2015 [<https://arxiv.org/abs/1502.03044>]

[2] Neural Machine Translation by jointly learning to align and translate  
Bahdanau et al., 2015 [<https://arxiv.org/abs/1409.0473>]

[3] Effective Approaches to Attention-based Neural Machine Translation  
Luong et al., 2015 [<https://arxiv.org/abs/1508.04025>]

## Attention Mechanism (Motivation)

Consider again our Dense layer formulation:

$$\text{output}_i = \sum_{j=1}^L w_{i,j} \mathbf{x}_j + b,$$

The core idea of Attention is that, instead of learning all possible weights  $w_{i,j}$ , we could try to learn a recipe to generate these weights. For instance, something like this:

$$\text{output}_i = \sum_{j=1}^L f(\mathbf{x}_i, \mathbf{x}_j) \mathbf{x}_j,$$

where  $f$  would be a formula that computes the weights.

## Attention Mechanism (Motivation)

Taking our previous NLP example, the word ‘is’ is clearly a verb and ‘hearing’ is a subject, hence we could imagine that the weight  $w_{\text{is}, \text{hearing}}$  could be defined, just based on the semantics of  $\mathbf{x}_{\text{is}}$  and  $\mathbf{x}_{\text{hearing}}$  alone, regardless of their actual positions in the sentence:

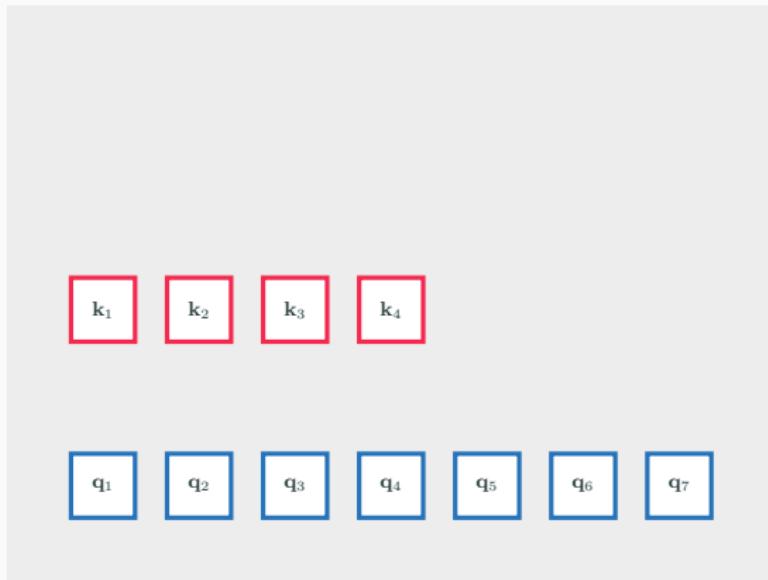
$$w_{\text{is}, \text{hearing}} = f(\mathbf{x}_{\text{is}}, \mathbf{x}_{\text{hearing}}).$$

Now, this is the idea, let’s see how it is actually done.

## Attention Mechanism

To make things more generic we'll consider two sequences of vectors  $\mathbf{q}_1, \dots, \mathbf{q}_{L_q}$  (the *queries*) and another sequence  $\mathbf{k}_1, \dots, \mathbf{k}_{L_k}$  (the *keys*).

(yes there is a link to dictionaries as you will see)



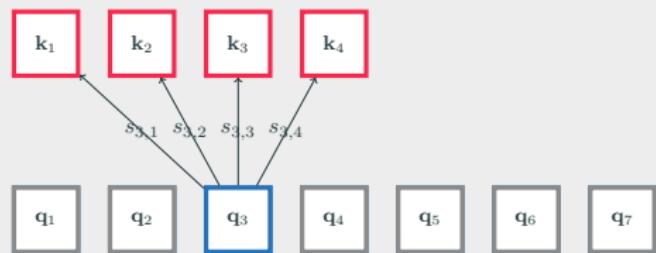
## Attention Mechanism

Let's consider a single element of the original sequence, e.g.  $\mathbf{q}_3$ :



## Attention Mechanism

The Attention layer will compute an alignment/similarity score  $s$  between each of the keys  $\mathbf{k}_1, \dots, \mathbf{k}_4$  and the query  $\mathbf{q}_3$ :

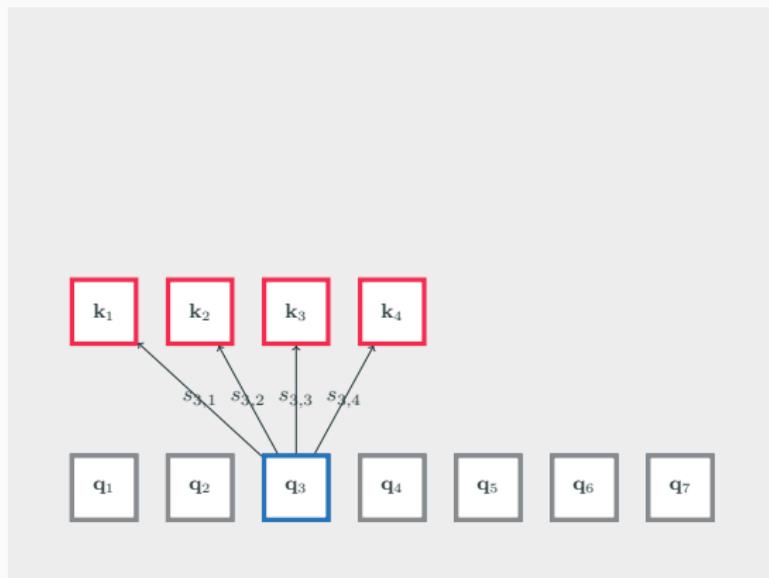


# Attention Mechanism

Many formulas for the alignment score exist. The formula in the Transformer paper is based on the feature vectors scalar product:

$$s_{i,j} = \mathbf{q}_j^\top \mathbf{k}_i / \sqrt{d_k}$$

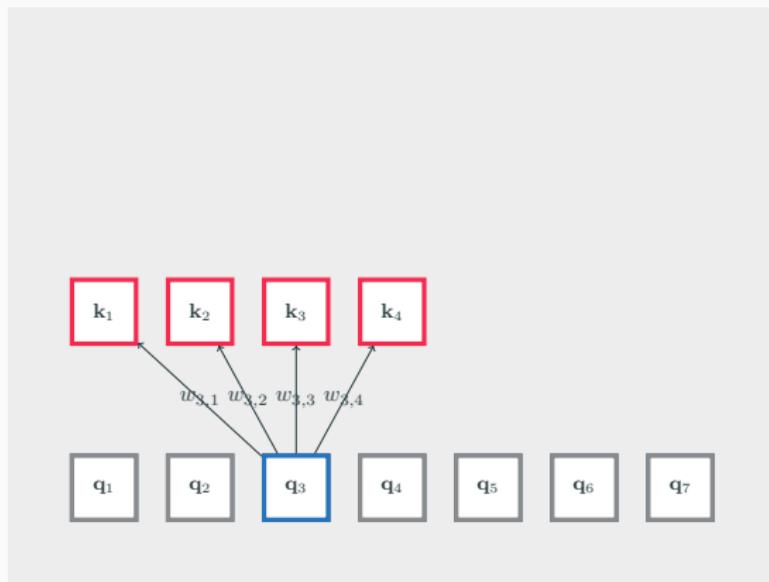
(note: the normalisation with vector dimension  $d_k$  is optional, but was found to help in training)



## Attention Mechanism

The scores  $s$  are a bit like our logits ( $s \gg 0$  means  $\mathbf{q}$  and  $\mathbf{k}$  are very related). Softmax can normalise these to weights that sum up to 1:

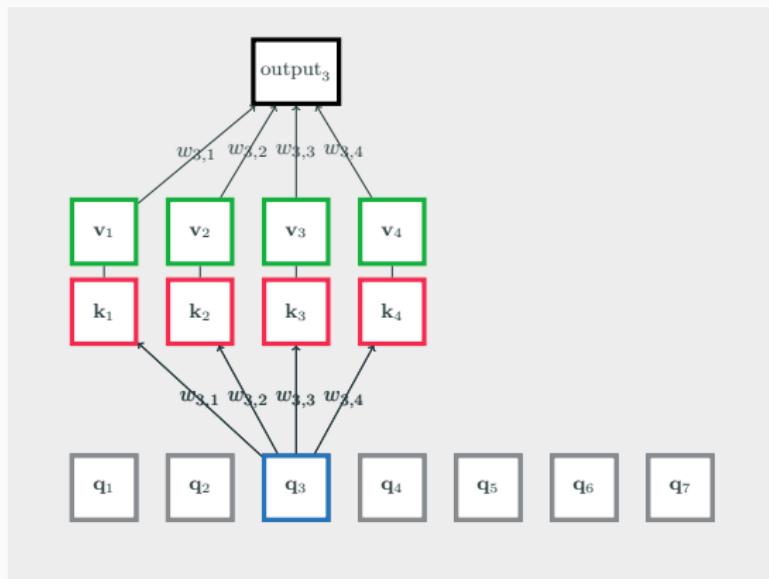
$$[w_{3,1}; w_{3,2}; w_{3,3}; w_{3,4}] = \text{softmax}([s_{3,1}; s_{3,2}; s_{3,3}; s_{3,4}])$$



# Attention Mechanism

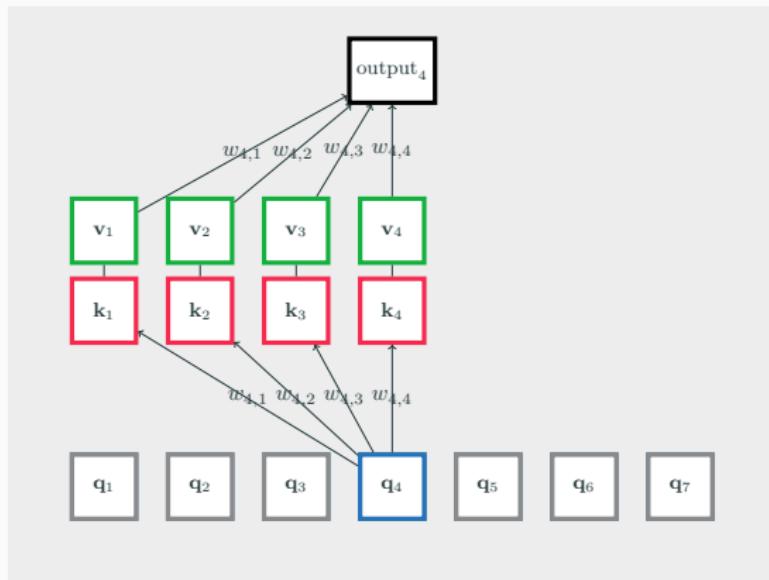
Instead of combining the keys, we combine associated *value* vectors  $\mathbf{v}_1, \dots, \mathbf{v}_{L_k}$ :

$$\text{output}_3 = w_{3,1}\mathbf{v}_1 + w_{3,2}\mathbf{v}_2 + w_{3,3}\mathbf{v}_3 + w_{3,4}\mathbf{v}_4$$



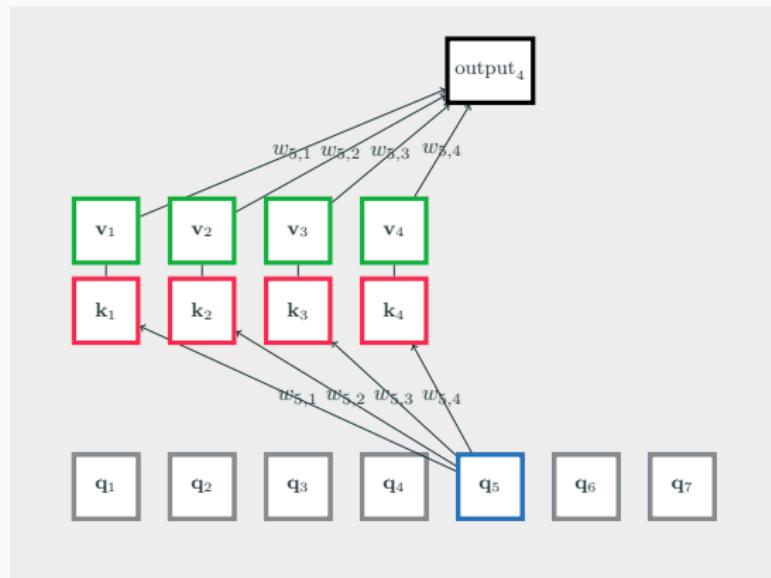
# Attention Mechanism

We can repeat this operation for other query vectors.



# Attention Mechanism

We can repeat this operation for other query vectors.



## Attention Mechanism

Thus Attention takes as an input three tensors.

$\mathbf{Q} = [\mathbf{q}_1, \dots, \mathbf{q}_{L_q}]^T$ , is a tensor of queries. It is of size  $L_q \times d_q$ , where  $L_q$  is the length of the sequence of queries and  $d_q$  the dimension of the queries feature vectors.

$\mathbf{K} = [\mathbf{k}_1, \dots, \mathbf{k}_{L_k}]^T$  and  $\mathbf{V} = [\mathbf{v}_1, \dots, \mathbf{v}_{L_k}]^T$  are the tensor containing the keys and values. They are of size  $L_k \times d_q$  and  $L_k \times d_v$ , where  $L_k$  is the number of keys,  $d_k = d_q$ , and  $d_v$  the dimension of the value feature vectors.

The *values* correspond to your typical context vectors associated with each word, as you would have in RNNs. The *keys* and *queries* are versions/representations of your current word  $i$  under a certain relationship.

## Attention Mechanism

From  $[\mathbf{q}_1, \dots, \mathbf{q}_{L_q}]^T$ ,  $[\mathbf{k}_1, \dots, \mathbf{k}_{L_k}]^T$ ,  $[\mathbf{v}_1, \dots, \mathbf{v}_{L_k}]^T$ , the Attention layer returns a new tensor made of weighted average *value* vectors:

$$\text{output}_i = \sum_{j=1}^{L_k} w_{i,j} \mathbf{v}_j$$

as we have seen, on the face of it, this looks like a dense layer (each output vector is obtained as a linear combination of the *value* vectors). The difference is that we have a formula to **dynamically** compute the weights  $w_{i,j}$  as a function of a score of how aligned  $\mathbf{q}_i$  and  $\mathbf{k}_j$  are:

$$s_{i,j} = \mathbf{q}_j^\top \mathbf{k}_i / \sqrt{d_k}$$

which are then normalised through a softmax layer:

$$w_{i,j} = \frac{\exp(s_{i,j})}{\sum_{j=1}^{L_k} \exp(s_{i,j})} \quad \text{so as to have } \sum_j w_{i,j} = 1 \text{ and } 0 \leq w_{i,j} \leq 1.$$

## Attention Mechanism

In other words, for each entry  $i$ :

1. We evaluate the alignment/similarity between the current *query* vector  $\mathbf{q}_i$  and all the other *keys*  $\mathbf{k}_j$ :

$$s_{i,j} = \mathbf{q}_i^\top \mathbf{k}_j / \sqrt{d_k}$$

2. The scores are then normalised across the *keys* using softmax:

$$w_{i,j} = \frac{\exp(s_{i,j})}{\sum_{j=1}^{L_k} \exp(s_{i,j})}$$

3. We return a new context vector that is the corresponding weighted average of the *value/context* vectors  $\mathbf{v}_j$ :

$$\text{output}_i = \sum_{j=1}^{L_k} w_{i,j} \mathbf{v}_j$$

## Attention Mechanism (Complexity)

As we loop through the queries and keys, the number of similarities to compute is thus  $L_q \times L_k$ . Each similarity measure takes  $\mathcal{O}(d_k)$  multiplications/add so the overall computation complexity is  $\mathcal{O}(L_q \times L_k \times d_k)$ .

This is thus very similar complexity to a dense layer (expect that we don't try to have cross-channel weights).

Importantly, as we have a formula to compute the weights, **Attention does not have any trainable parameter**. This is something that is apparent when we write down the full mathematical formula:

$$\text{Attention}(\mathbf{Q}, \mathbf{K}, \mathbf{V}) = \text{softmax}\left(\frac{\mathbf{Q}\mathbf{K}^T}{\sqrt{d_k}}\right)\mathbf{V}$$

where softmax denotes a *row-wise* softmax normalisation function.

## Self-Attention

Self-Attention is a particular use-case of Attention, where the tensors  $\mathbf{Q}$  and  $\mathbf{K}, \mathbf{V}$  are all derived from a single input tensor  $\mathbf{X} = [\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_L]^T$  of size  $L \times d$ , by means of 3 simple linear feature transforms:

$$\mathbf{q}_i = \mathbf{W}_Q^\top \mathbf{x}_i,$$

$$\mathbf{k}_i = \mathbf{W}_K^\top \mathbf{x}_i,$$

$$\mathbf{v}_i = \mathbf{W}_V^\top \mathbf{x}_i.$$

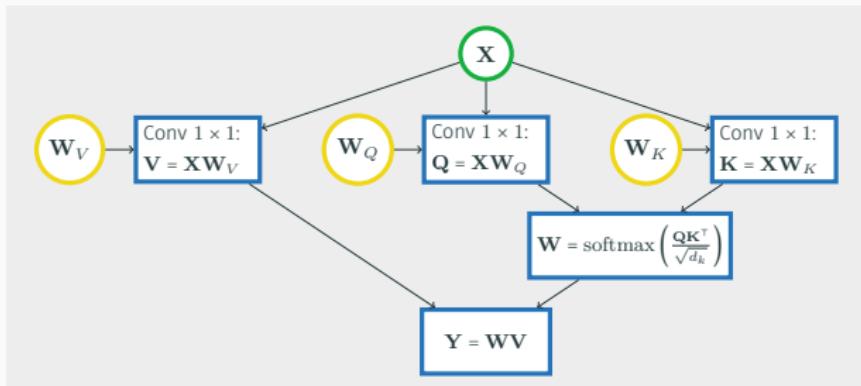
Self-Attention is thus simply given by:

$$\text{Self-Attention}(\mathbf{X}, \mathbf{W}_q, \mathbf{W}_k, \mathbf{W}_v) = \text{Attention}(\mathbf{X}\mathbf{W}_V, \mathbf{X}\mathbf{W}_Q, \mathbf{X}\mathbf{W}_K)$$

## Self-Attention

If we want to put all that in a single equation we have:

$$\text{Self-Attention}(\mathbf{X}, \mathbf{W}_q, \mathbf{W}_k, \mathbf{W}_v) = \text{softmax}\left(\frac{\mathbf{X}\mathbf{W}_q\mathbf{W}_k^\top\mathbf{X}^\top}{\sqrt{d_k}}\right)\mathbf{X}\mathbf{W}_v$$



The only trainable parameters are contained in the  $d \times d_k$  matrices  $\mathbf{W}_K$  and  $\mathbf{W}_Q$  and in the  $d \times d_v$  matrix  $\mathbf{W}_V$ . These are relatively small matrices, and they can operate on sequences of any length.

# Example of Self-Attention in Numpy

```
def softmax(x):
    return(np.exp(x)/np.exp(x).sum())

# encoder representations of four different words
word_1 = np.array([1, 0, 0]); word_2 = np.array([0, 1, 0]);
word_3 = np.array([1, 1, 0]); word_4 = np.array([0, 0, 1])

# initialisation of the weight matrices
W_Q = np.random.randn(3, 2) # d=3, dK=dQ=2, needs to be trained
W_K = np.random.randn(3, 2) # d=3, dK=dQ=2, needs to be trained
W_V = np.random.randn(3, 2) # d=3, dV=2,      needs to be trained

# generating the queries, keys and values
query_1 = word_1 @ W_Q; key_1 = word_1 @ W_K; value_1 = word_1 @ W_V
query_2 = word_2 @ W_Q; key_2 = word_2 @ W_K; value_2 = word_2 @ W_V
query_3 = word_3 @ W_Q; key_3 = word_3 @ W_K; value_3 = word_3 @ W_V
query_4 = word_4 @ W_Q; key_4 = word_4 @ W_K; value_4 = word_4 @ W_V

# scoring the first query vector against all key vectors
scores_1 = array([dot(query_1, key_1), dot(query_1, key_2),
                  dot(query_1, key_3), dot(query_1, key_4)])

# computing the weights by a softmax operation
weights_1 = softmax(scores_1 / key_1.shape[0] ** 0.5)

# computing first attention vector
attention_1 = weights_1[0]*value_1 + weights_1[1]*value_2 + weights_1[2]*value_3 + weights_1[3]*value_4

print(attention_1)
```

## Computational Complexity: Quadratic in the Input Dimension $L$

Since each feature vector is compared to all the other feature vectors of the sequence, the computational complexity is, similarly to a dense layer, **quadratic** in the input sequence dimension  $L$ .

### Computational Complexity:

Self-Attention:  $\mathcal{O}(L^2 \times d_k)$

RNN/LSTM/GRU:  $\mathcal{O}(L \times d \times d_v)$

Convolution:  $\mathcal{O}(L \times \text{kernel\_size} \times d \times d_v)$

Dense Layer:  $\mathcal{O}(L^2 \times d \times d_v)$

## Computational Complexity: Quadratic in the Input Dimension $L$

Note that we typically choose  $d_k$  to be much smaller than  $d$  (eg.  $d_k = d/8$ ), so the computational complexity is reduced (but is still quadratic in the input dimension  $L$ ). The idea is that we are only looking at one aspect of the problem, eg. what is the relationship under verb-subject in the sentence?

As with Dense Layers and Convolution, Attention can be easily parallelised.

As with the convolution, we could restrict the length of the sequence  $L$  by limiting the attention window to a local neighbourhood. We could also constrain the input tensor to be of a limited fixed size.

## The Attention Mechanism Requires Few Parameters

As the Attention mechanism does not contain any trainable parameters, the trainable parameters in self-attention are only defined through the input matrices and is thus much smaller than in a dense layer or even a convolution layer.

### Number of Trainable Parameters:

Self-Attention:  $\mathcal{O}(d \times d_k + d \times d_k + d \times d_v)$

Convolution:  $\mathcal{O}(\text{kernel\_size} \times d \times d_v)$

RNN:  $\mathcal{O}(d \times d_v + d_v \times d_v)$

Dense Layer:  $\mathcal{O}(L \times d \times d_v)$

# A Perfect Tool for Multi-Modal Processing

Attention is a versatile tool that allows some flexibility about how to design the input tensors  $\mathbf{Q}$  and  $\mathbf{K}, \mathbf{V}$ . For instance, if we have one tensor derived from text and one from audio inputs, we fuse/combine both tensors using [cross-Attention](#):

$$\mathbf{V}_{\text{audio/text}} = \text{Attention}(\mathbf{Q}_{\text{audio}}, \mathbf{K}_{\text{text}}, \mathbf{V}_{\text{text}})$$

The sources do not need to be perfectly synchronised (*i.e.* text vector keys and values don't have to align with query audio vector — see exercise below), and, in fact, the sources don't even need to be of the same length (*i.e.*  $L_q \neq L_k$ ). For these reasons Attention is very well suited for combining multi-modal inputs.

## Exercise:

Show that the output of the Attention layer is the same if the entries of the keys and values tensor are shifted or shuffled, *e.g.*:

$$\text{Attention}([\mathbf{q}_1, \dots, \mathbf{q}_{L_q}], [\mathbf{k}_1, \mathbf{k}_2, \dots, \mathbf{k}_{L_k}], [\mathbf{v}_1, \mathbf{v}_2, \dots, \mathbf{v}_{L_k}]) =$$

$$\text{Attention}([\mathbf{q}_1, \dots, \mathbf{q}_{L_q}], [\mathbf{k}_{L_k}, \mathbf{k}_{L_k-1}, \dots, \mathbf{k}_1], [\mathbf{v}_{L_k}, \mathbf{v}_{L_k-1}, \dots, \mathbf{v}_1])$$

## The Multi-Head Attention Layer

You can think of Attention as a replacement for convolution layers. You can chain multiple Attention layers, in a similar way to what you would do with convolutional layers.

In Transformers, a set of  $(W_Q, W_K, W_V)$  matrices is called an [attention head](#) and [multi-head attention](#) layer is simply a layer that concatenates the output of multiple attention layers.

The number of heads loosely corresponds to your number of filters in a convolutional layer.

Below is an example in PyTorch of a self-attention layer with two heads:

```
mha = nn.MultiheadAttention(embed_dim=4, num_heads=2, batch_first=True)
y, attn = mha(query=x, key=x, value=x) # y: [B, T, 4]
```

## Takeaways (Attention Mechanism) 1/2

RNNs don't parallelise well and Convolutions assume fixed positional relationships, which is not the case in text.

The [Attention Mechanism](#) resolves these issues by defining a formula to dynamically compute the weights between any two positions  $i$  and  $j$ , based on the alignment (dot-product) between a *query* feature vector for  $i$  and a *key* feature vector for  $j$ .

With [Self-Attention](#), feature transformation matrices allow to produce the *queries*, *keys*, and *value* vectors from a single input tensor.

The computational complexity of *Attention* is quadratic in the input tensor dimension (as with Dense Layers). *Attention* does not have any trainable parameters, *Self-Attention* needs  $W_q$ ,  $W_k$  and  $W_v$ .

## Takeaways (Attention Mechanism) 2/2

Self-Attention and Attention are well suited to work with text processing as the semantics of the words takes precedence over their absolute or relative positions.

Cross-Attention allows you to work with multiple modalities (eg. audio, video, images, text) as it is agnostic to the position of the keys/-values and thus can deal with any potential synchronisation issues.

# Transformers

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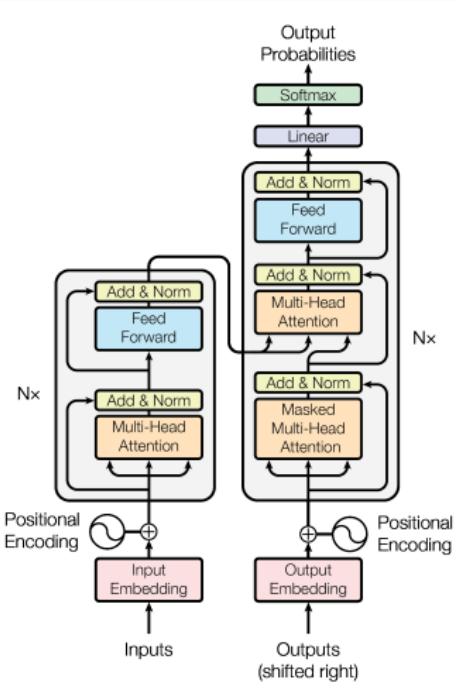
In 2017, Vaswani et al. proposed the Transformer architecture, which is a (relatively!) simple network architecture solely based on attention mechanisms.

This architecture has fundamentally impacted text processing, but also the rest of the deep learning fields.

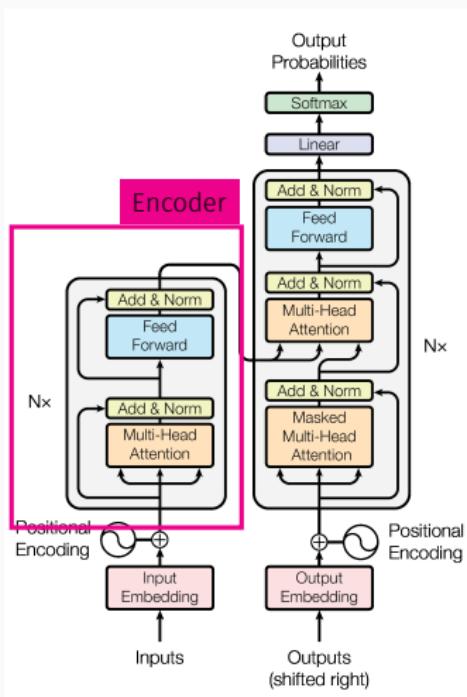
A. Vaswani, N. Shazeer, N. Parmar, J. Uszkoreit, L. Jones, A. Gomez, Kaiser, and I. Polosukhin. Attention Is All You Need. In Advances in Neural Information Processing Systems, page 5998–6008. (2017)  
[<https://arxiv.org/abs/1706.03762>]

The original publication has generated 57,463 citations as of 2022 (for reference, a paper is doing very well when it has 100+ citations).

The Transformer architecture, as described in the original paper:



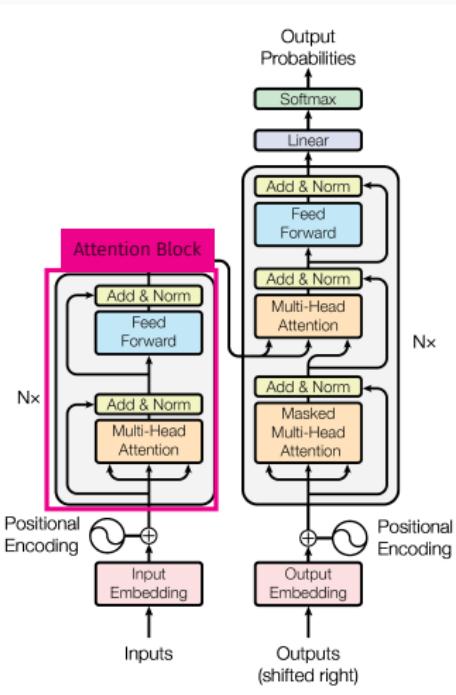
The Transformer architecture, as described in the original paper:



The First part of the network is an encoder, ie. a sub-network that transforms the input into a meaningful, compact, tensor representation.

Think of it as the VGG network that transforms an image into a compact  $4096 \times 1$  feature vector. And as for VGG, the idea is that this encoder could be re-used with transfer learning.

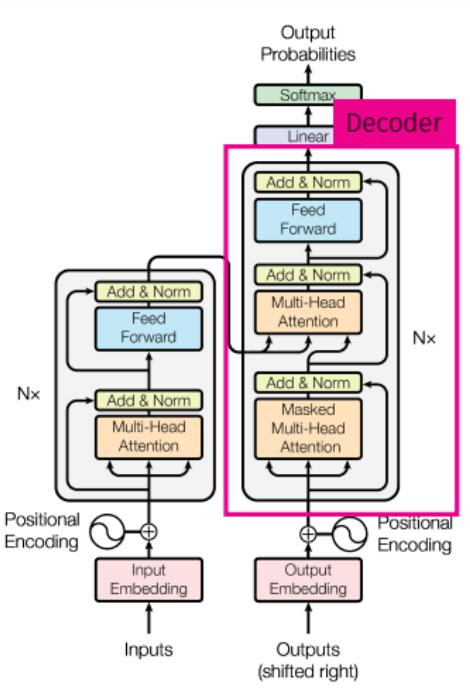
The Transformer architecture, as described in the original paper:



The Encoder itself is made of a sequence of blocks.

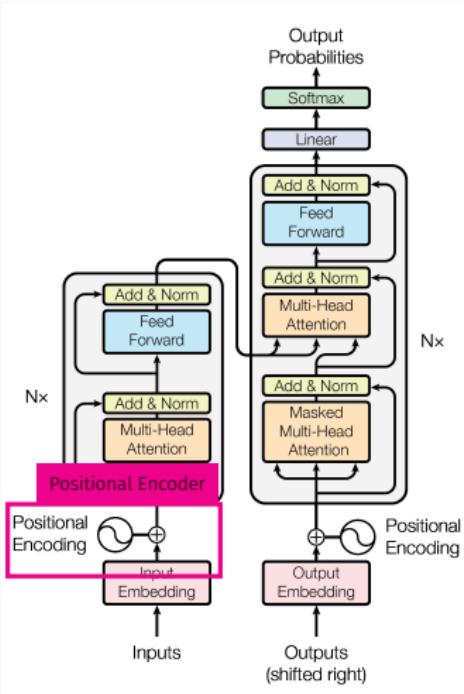
At the core of each of these blocks is a Multi-Head Attention layer followed by a FeedForward layer (or  $1 \times 1$  Conv2D layer)

The Transformer architecture, as described in the original paper:



The Decoder is also made of a sequence of Blocks with Multi-Head Attention layers.

The Transformer architecture, as described in the original paper:



Note the presence of a *Positional Encoder*. As Attention strips away any positional information, Transformers propose to encode the position as extra features in the input vector (see original paper for more details about this).

## Positional Encoding (1/3)

The positional encoder is an embedding  $i \mapsto \phi(i)$  that is appended as additional features to the feature vector, ie.  $\mathbf{x}'_i = [\mathbf{x}_i; \phi(i)]$ .

Why do we need an encoder for this? Why not simply add the position as a simple additional number? ie.  $\phi(i) = [i]$ ?

This is because the similarity measure still needs to make sense. Here we use the dot product, thus the similarity between positions  $i$  and  $j$  would simply be  $i \times j$ . But we would like  $\phi(i)^\top \phi(j)$  to be  $\gg 0$  if  $i \approx j$  and  $\ll 0$ , or at least  $\approx 0$ , if they are far away, but this is not the case.

What would work is an embedding that achieves something like this:

$$\phi(i)^\top \phi(j) = \exp(-\lambda(i - j)^2).$$

Such an embedding exists, we talked about it in the case of SVMs with RBF kernels. The embedding is the (infinite) Fourier series basis function.

## Positional Encoding (2/3)

As we can't afford the luxury of an infinite embedding, we need to truncate the series. This is what was proposed in the original Transformers paper. Assuming a positional encoding of dimension  $d_{pos}$ , they propose:

$$i \mapsto \phi(i) = \begin{bmatrix} \sin(\omega_1 i) \\ \cos(\omega_1 i) \\ \sin(\omega_2 i) \\ \cos(\omega_2 i) \\ \vdots \\ \sin(\omega_{d_{pos}/2} i) \\ \cos(\omega_{d_{pos}/2} i) \end{bmatrix} \quad \text{where } \omega_k = 1/10000^{2k/d_{pos}}$$

## Positional Encoding (3/3)

The advantage of using a positional encoding vs. hard-coding relationships, as in convolution, is that the position is treated as another piece of information, that can be transformed, combined with other features, or simply ignored. The point is it is up to training to learn what to do with it.

There is obviously a lot more to know about Transformers but we have covered here the main idea: it is an encoder/decoder network that is solely based on sequences of Attention layers.

## Take Away (Transformers)

The [Transformer model](#) is an encoder-decoder architecture based on Attention layers blocks.

The positional information, which is lost in the attention mechanism, can be embedded in the input vector as extra features.

Transformers benefit from the efficiency of the Attention Mechanism and require fewer parameters and can be easily be parallelised.

Transformers are the backbone of modern NLP networks such as Chat-GPT. They are also the backbone of any method that handles multiple modalities (eg. text, image, speech, etc.)