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10 - Attention Mechanism and Transformer Model

François Pitié

Assistant Professor in Media Signal Processing
Department of Electronic & Electrical Engineering, Trinity College Dublin
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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 since then been widely adopted across many areas of Deep Learning.

In this handout, we will be looking in detail at the Attention Mechanism and only briefly introduce the Transformer model. The objective is to present you with enough material to digest recent papers on the topic.

As these architectures have mainly originated from NLP, we'll introduce them in the context of text processing, ie. with tensors of 1D sequences. But keep in mind that, like convolution, these architectures can be extended to any dimensions.

The Attention Mechanism

The Problem with RNNs

To have a bit of context, we need to 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.

However, …

- 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 Positional Dependencies

Take a simple 1D convolution (1 channel) with a kernel size of 5:

$$\text{output}_i = w_{-2}x_{i-2} + w_{-1}x_{i-1} + w_0 x_i + w_1 x_{i+1} + w_{+2}x_{i+2} + b$$

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

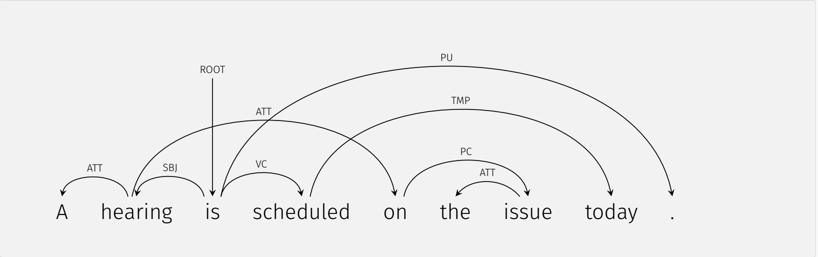
Take a dense layer:

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

and we have the similar issue that all the relationships are fixed, ie. that $w_{i,j}$ is defined as function of the sole positions (i, j).

But in Text Processing, the Positions of Relationships Can Vary.

Look at an actual dependency graph in a sentence:



Distances between relationships are not set in stone, eg. the verb is not always the next word after the subject.

Convolutions are not well equipped to deal with such relationships that have varying positions.

So, We Have a Problem

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.

Here comes the Attention Mechanism to the rescue.

Attention Mechanism

The concept of Attention first appeared in image captioning as a tool to investigate how various elements of an image connect to the words that are formed in a generated sentence [1]. This idea was then quickly adapted to explain relationships 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 adopt here 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

Attention takes as an input three tensors.

$\mathbf{Q} = [\mathbf{q_1}, \dots, \mathbf{q_{L_q}}]^\top$, 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.

$\mathbf{K} = [\mathbf{k_1}, \dots, \mathbf{k_{L_k}}]^\top$ and $\mathbf{V} = [\mathbf{v_1}, \dots, \mathbf{v_{L_k}}]^\top$ 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, eg. subject-verb relationship (this will become clearer in the next few slides).

Attention Mechanism

From $[\mathbf{q_1}, \dots, \mathbf{q_{L_q}}]^\top$, $[\mathbf{k_1}, \dots, \mathbf{k_{L_k}}]^\top$, $[\mathbf{v_1}, \dots, \mathbf{v_{L_k}}]^\top$, the Attention layer returns a new tensor made of weighted average *value* vectors:

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

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 key difference is that we have a formula to **dymanically** compute the weights $w_{i,j}$ as a function of a <u>score</u> of how aligned $\mathbf{q}_i$ and $\mathbf{k}_j$ are. This alignment/affinity score is typically computed as a dot product, eg.:

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

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:

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

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

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:

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

where $\mathrm{softmax}$ 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 $\mathbf{X} = [\mathbf{x}_1, \mathbf{x}_2, \cdots, \mathbf{x}_L]^\top$ of size $L \times d$, by means of 3 simple linear feature transforms:

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

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

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

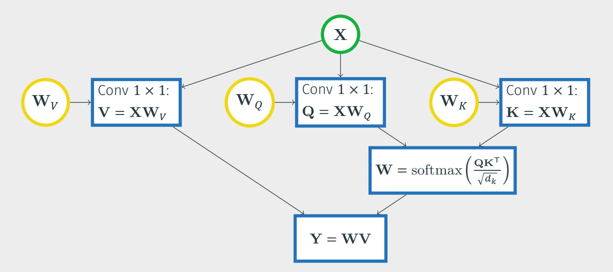
Self-Attention is thus simply given by:

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

Self-Attention

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

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



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])

# generating the weight matrices
np.random.seed(42) # to allow us to reproduce the same attention values
W_Q = np.random.randn(3, 2) # d=3, dK=dQ=2
W_K = np.random.randn(3, 2) # d=3, dK=dQ=2
W_V = np.random.randn(3, 2) # d=3, dV=2

# 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

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

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

Note that we typically choose d_k to be much smaller than d, so the computational complexity is reduced, but is still quadratic in the input dimension L.

As with the convolution, we are allowed to restrict the length of the sequence L by restricting the attention window to a local neighbourhood. We can also constrain the input tensor to be of a fixed size.

The Attention Mechanism Requires Few Parameters

As the Attention function does not contain any trainable parameters, the number of parameters is 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

The Attention Mechanism is a versatile tool. We have some flexibility about how to design the three input tensors $(\mathbf{Q}, \mathbf{K}, \mathbf{V})$. In self-attention, we chose $\mathbf{Q} = \mathbf{X}\mathbf{W}_q$, etc., but we can find other uses. For instance, the Attention mechanism is very well suited for combining multi-modal inputs, eg. tensors derived from text and audio inputs:

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

Note that the sources do not need to be perfectly synchronised (ie. text vector i doesn't have to align with audio vector i — see exercise below), and, in fact, the sources don't even need to be of the same length (ie. $L_q \neq L_k$).

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:

$$\text{Attention}([\mathbf{q}_1, \dots, \mathbf{q}_L], [\mathbf{k}_1, \mathbf{k}_2, \dots, \mathbf{k}_L], [\mathbf{v}_1, \mathbf{v}_2, \dots, \mathbf{v}_L]) =$$
$$\text{Attention}([\mathbf{q}_1, \dots, \mathbf{q}_L], [\mathbf{k}_L, \mathbf{k}_{L-1}, \dots, \mathbf{k}_1], [\mathbf{v}_L, \mathbf{v}_{L-1}, \dots, \mathbf{v}_1])$$

Transformers

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. 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).

Think of Attention model as a replacement for convolution layers.

You can then chain multiple Attention layers, in a similar way to what you would do with convolutional layers.

One set of (W_Q, W_K, W_V) matrices is called an attention head.

A multi-head attention layer is simply a layer made of multiple attention layers. This is the same as convolutional layer defining multiple filters.

Take Away (1/2)

RNNs don't parallelise well and Convolutions assume fixed positional relationships, when a verb is not always just after its subject.

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 corresponding *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.

Self-Attention and Attention are well suited to work with text processing and multiple modalities (eg. audio, video, images, text) as they are agnostic to the position of the keys/values and thus can deal with any potential synchronisation issues.

Take Away (2/2)

The Transformer model is an encoder-decoder architecture, that is solely based on Attention, Self-Attention layers blocks (in the block, the attention layers are combined with batch-norm, residual blocks and fully connected layers).