Natural Language Understanding, Generation, and Machine Translation

Lecture 8: Transformers

Shay Cohen
based on slides by Frank Keller

31 January 2024 (week 3)

School of Informatics
University of Edinburgh
scohen@inf.ed.ac.uk

Overview

Reading: [Vaswani et al.2017], [Bloem2019].

The Story so Far

Encoder-Decoder Architecture

When we do MT, we encode a source sentence and then decode it into a target sentence:

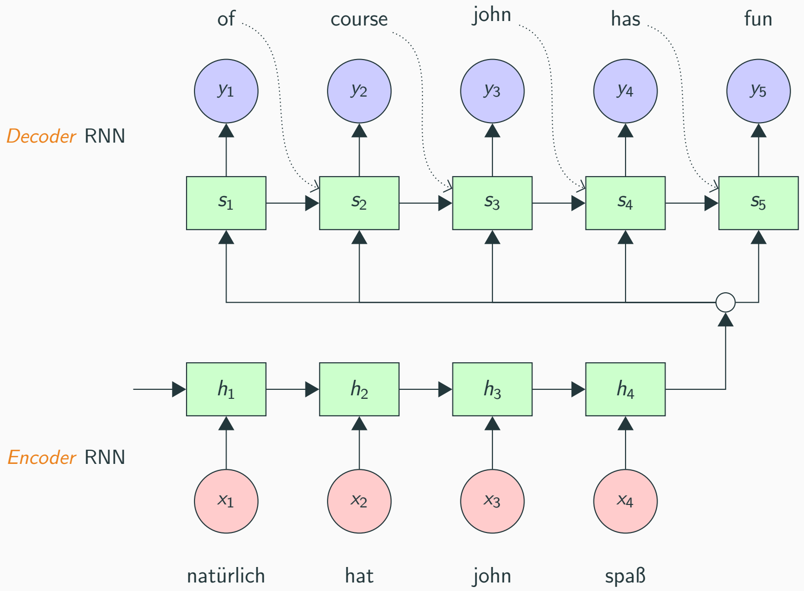
Input:	Så varför minskar inte vi våra utsläpp?
Output:	So why are we not reducing our emissions?

We can model this using an *encoder-decoder* architecture.
Sequence transduction is a common way to formulate NLP tasks:

- question answering
- syntactic and semantic parsing
- generation from a database
- image description

Often RNNs are used for both the encoder and the decoder.

Encoder-Decoder Architecture



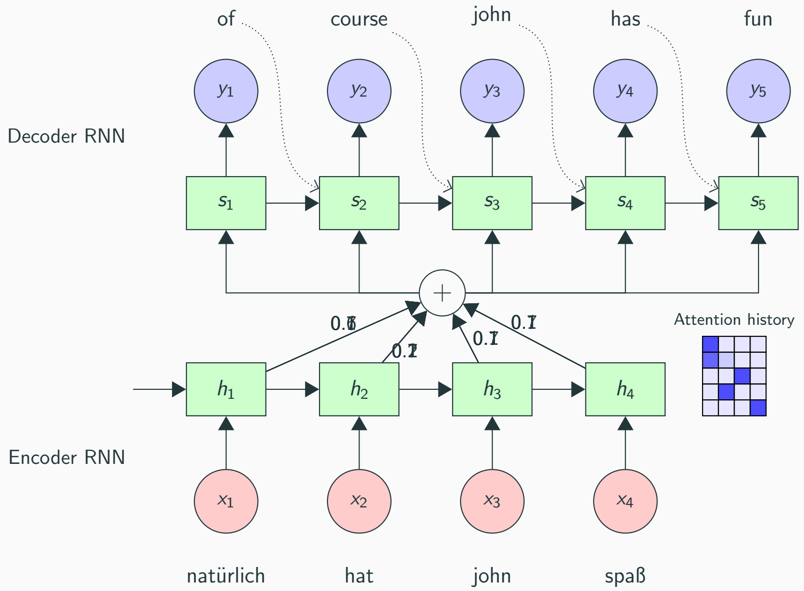
Encoder-Decoder with Attention

This works pretty well, but:

- the hidden representation is a *bottleneck:* it has to represent a sentence of any length, but its size is fixed;
- RNNs and their variants suffer from vanishing gradients;
- the encoder representation also has a *recency bias:* mostly represents final words of the input;
- target words whose corresponding source words are at the beginning therefore more difficult to generate correctly.

Solution: learn which input words are important for the decoder.

Encoder-Decoder with Attention



Encoder-Decoder with Attention

In the decoder softmax, the *context* is now a *weighted average* of source hidden state vectors:

$$P(y_i \mid y_1, \ldots, y_{i-1}, x_1, \ldots, x_{|x|}) = \mathrm{softmax}(\mathbf{W}\, \mathrm{concat}(\mathbf{s}_i, \mathbf{c}_i) + \mathbf{b})$$

$$\mathbf{c}_i = \sum_{j=1}^{|x|} \alpha_{ij} \mathbf{h}_j$$

$\boldsymbol{\alpha}_i$ is a *distribution* over elements of x. In its simplest form, we can compute it as *dot product attention:*

$$a_{ij} = \mathbf{s}_i \cdot \mathbf{h}_j$$

$$\boldsymbol{\alpha}_i = \mathrm{softmax}(\mathbf{a}_i)$$

Encoder-Decoder with Attention

Observation:

- Attention is a powerful mechanism; maybe we can use it simplify the encoder and the decoder?
- Removing the RNNs would make our model a lot more efficient and scalable (larger models, more data).

But first, we need to make attention more complicated:

- We use two types of attention: *self-attention* and *multihead attention.*
- We split up the attention computation into *key, value,* and *query* vectors.

Self-attention

Self-attention

The original [Vaswani et al.2017] paper is a bit impenetrable. We will instead follow the tutorial by [Bloem2019].

Self-attention is what we get when compute attention over the input sequence. Let $\mathbf{x}_1, \ldots, \mathbf{x}_t$ be the input vectors and $\mathbf{y}_1, \ldots, \mathbf{y}_t$ be the output vectors:

$$\mathbf{y}_i = \sum_j w_{ij} \mathbf{x}_j$$

We now compute the attention weight as the dot-product of each input token with every other token.

$$w'_{ij} = \mathbf{x}_i \cdot \mathbf{x}_j$$
$$\mathbf{w}_i = \text{softmax}(\mathbf{w}'_i)$$

Note that the attention weight is now called $\mathbf{w}'$ and the attention distribution $\mathbf{w}$ (rather than $\mathbf{a}$ and α).

Self-attention

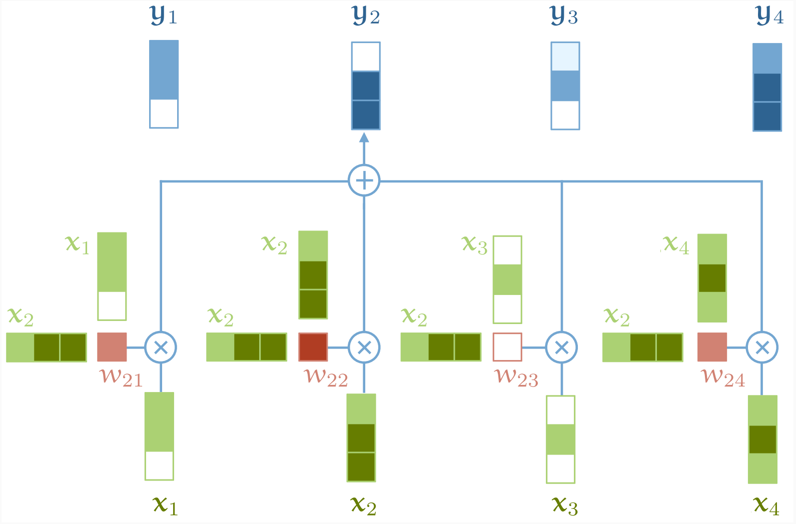


Figure from [Bloem2019].

Self-attention

Why is self-attention useful?

- The dot product returns large values when the two vectors are similar. The softmax normalizes the resulting vectors.
- The output $\mathbf{y}_i$ is the weighted sum of all input vectors, weighted by their similarity with input $\mathbf{x}_i$.
- We have no trainable parameters! We're relying on the input vectors $\mathbf{x}_j$ being good representations for our task.
- The input is a *position invariant,* i.e., we have no way to represent word order (unlike in an RNN).

Example: represent words as embeddings:

word sequence:	the, cat, walks, on, the, street
input (embeddings):	$\mathbf{x}_{the}, \mathbf{x}_{cat}, \mathbf{x}_{walks}, \mathbf{x}_{on}, \mathbf{x}_{the}, \mathbf{x}_{street}$
output:	$\mathbf{y}_{the}, \mathbf{y}_{cat}, \mathbf{y}_{walks}, \mathbf{y}_{on}, \mathbf{y}_{the}, \mathbf{y}_{street}$

More Advanced Self-attention

Every input vector $\mathbf{x}_i$ is used in three ways in self-attention:

- *Query:* compare $\mathbf{x}_i$ to every other vector to compute attention weights for its own output $\mathbf{y}_i$.
- *Key:* compare $\mathbf{x}_i$ to every other vector to compute attention weights for the other outputs $\mathbf{y}_j$.
- *Value:* use $\mathbf{x}_i$ in the weighted sum to compute every output vector based on these weights.

We can make attention more flexible by assuming separate, trainable weights for each of these roles: the $k \times k$ weight matrices W_q, W_k, and W_v (k: dimensionality of $\mathbf{x}$ and $\mathbf{y}$).

More Advanced Self-attention

Now we compute attention as follows:

$$\mathbf{q}_i = W_q \mathbf{x}_i \quad \mathbf{k}_i = W_k \mathbf{x}_i \quad \mathbf{v}_i = W_v \mathbf{x}_i$$

$$w'_{ij} = \mathbf{q}_i \cdot \mathbf{k}_j$$

$$\mathbf{w}_i = \mathrm{softmax}(\mathbf{w}'_i)$$

$$\mathbf{y}_i = \sum_j w_{ij} \mathbf{v}_j$$

Now the self-attention layer has parameters that allow it to modify the incoming vectors to suit the three roles they must play.

More Advanced Self-attention

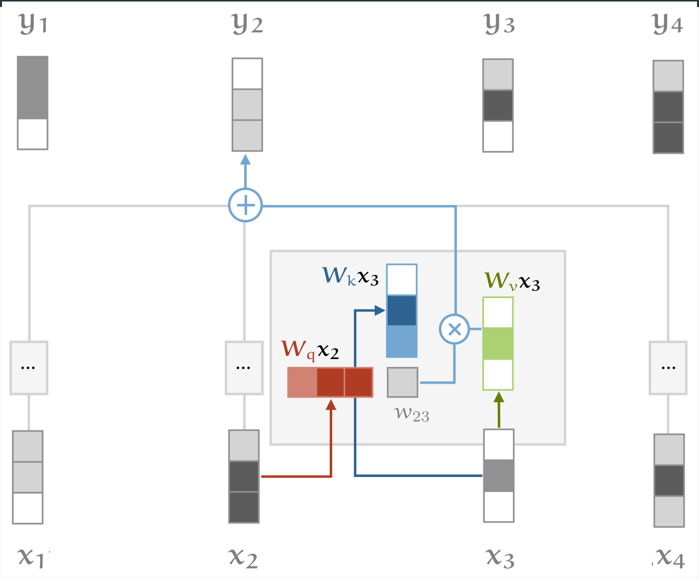


Figure from [Bloem2019].

Scaling the Dot Product

- The softmax function can be sensitive to very large input values;
- this kills the gradient and can slow down learning or cause it to stop;
- it helps to scale the dot product back to stop the inputs to the softmax function from growing too large:

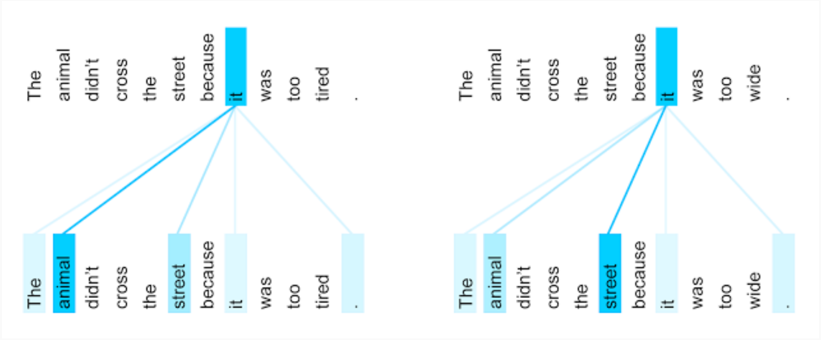
$$w'_{ij} = \frac{\mathbf{q}_i \cdot \mathbf{k}_j}{\sqrt{k}}$$

Multi-head Attention

Multi-head Attention

Multi-head attention is able to jointly attend to different parts of the input. If we just have a single head, have to average.

For example, one head could attend to the subject of a verb, another one to its object. Or different heads could attend to different referents of a pronoun.


The animal didn't cross the street because it was too tired .
The animal didn't cross the street because it was too tired .
The animal didn't cross the street because it was too wide .
The animal didn't cross the street because it was too wide .

Multi-head Attention

We use separate weight matrices for each head: W_q^r, W_k^r, W_v^r, where r is an index over heads.

For the input $\mathbf{x}_i$, each attention head now produces a different output $\mathbf{y}_i^r$. We concatenate them and pass them through a linear transformation to reduce the dimensions to k. Two variants:

- *Narrow self-attention:* cut the input into chunks of size k/h (h: number of heads), use weight matrices of size $k/h \times k/h$.
- *Wide self-attention:* use weight matrices that cover the whole input for each head, i.e., of size $k \times k$.

The Transformer

The Transformer

The multi-head self attention mechanism needs to be integrated into a larger architecture to be useful:

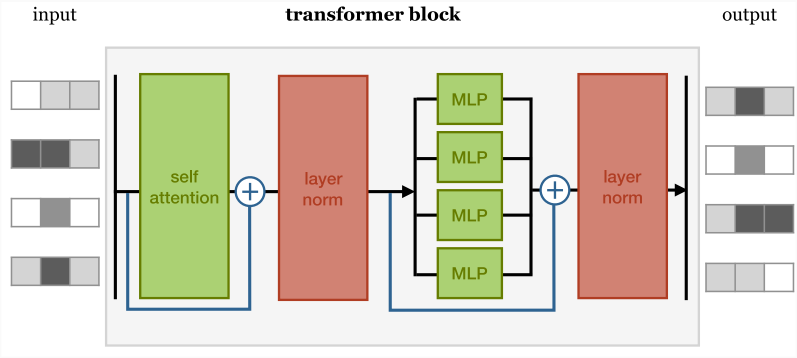


Figure from [Bloem2019].

The Transformer

- The blue connections are residual connections. They prevent the gradients from getting too large or small.
- Layer normalization makes training faster.
- The feedforward layer applies a single MLP independently to each input vector.

Example: Movie Classification

Transformer to classify a movie review as positive or negative:

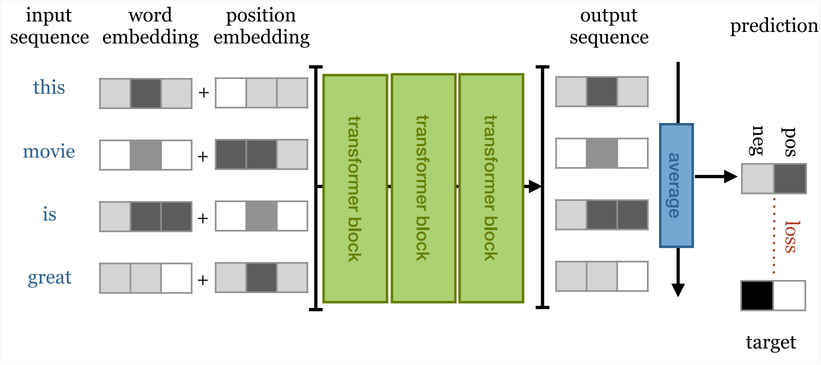


Figure from [Bloem2019].

Example: Movie Classification

- At the core is a chain for transformer blocks.
- *Input:* represent words as embeddings; these are then combined with position encodings.
- Recall that attention is position invariant, i.e., the transformer cannot directly represent word order.
- *Output:* apply average pooling to the final output sequence, map the result to a softmaxed class vector.

Position Encodings

We choose a function $f : \mathbb{N} \to \mathbb{R}^k$ that maps positions to real valued vectors, and let the network learn how to interpret these.

The choice of encoding function is a hyperparameter.
[Vaswani et al.2017] use:

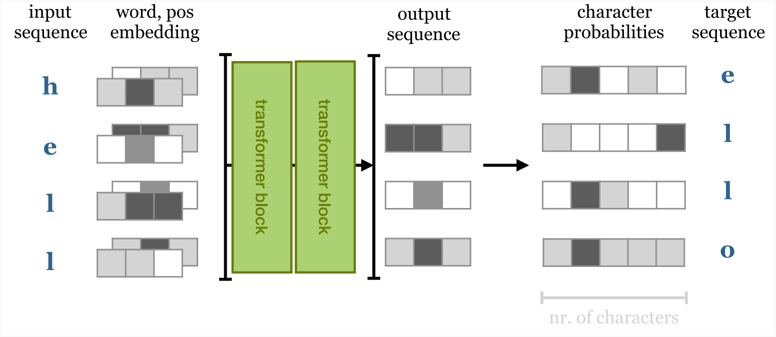
$$
\begin{aligned}
PE_{(pos,2i)} &= \sin(pos/10000^{2i/k}) \\
PE_{(pos,2i+1)} &= \cos(pos/10000^{2i/k})
\end{aligned}
$$

where *pos* is the position and *i* is an index over dimensions.

The positions encoding is then added to the input embedding (both are of dimensionality k).

Masking

What if we want to *generate text* as an output? Then we need an *autoregressive* model:



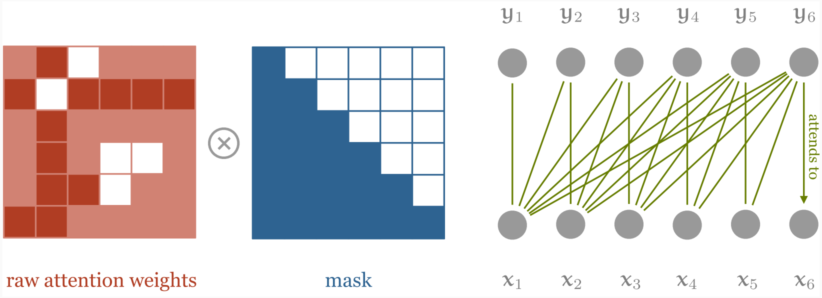
For this, we need to ensure that the transformer cannot look forward in the input when generating the output.

Else it would just generate a copy of the input! *We need masking.*

Figure from [Bloem2019].

Masking

We apply a mask to the matrix of dot products, before the softmax is applied. This disables all elements above the diagonal:



y_1 y_2 y_3 y_4 y_5 y_6
attends to
raw attention weights
$\otimes$
mask
x_1 x_2 x_3 x_4 x_5 x_6

The model can no longer look forward and just copy the upcoming input; it behaves like an RNN!

Figure from [Bloem2019].

Summary

- The transformer overcomes the problem with recurrent connections (serial bottleneck).
- It can model long-range dependencies using self-attention.
- Position encodings are needed to capture word order.
- Transformer blocks can be stacked to make models more powerful; only limited by compute and memory.
- The transformer has only two sources of non-linearity: the feedforward layer and the softmax in the self-attention.
- Masking makes it possible to use transformers in an autoregressive way for sequence-to-sequence tasks.

Now we have covered most of the key modeling ideas in the course!

Next class: Word embeddings with and without transformers.

References

Peter Bloem.
2019.
Transformers from Scratch.
http://www.peterbloem.nl/blog/transformers.

Ashish Vaswani, Noam Shazeer, Niki Parmar, Jakob Uszkoreit, Llion Jones, Aidan N Gomez, Łukasz Kaiser, and Illia Polosukhin.
2017.
Attention is all you need.
Advances in neural information processing systems, 30.