Transformers

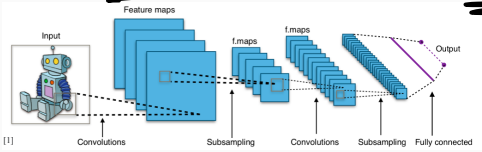
Lucas Beyer, lbeyer@google.com

The classic landscape:

One architecture per "community"

Computer Vision

Convolutional NNs (+ResNets)

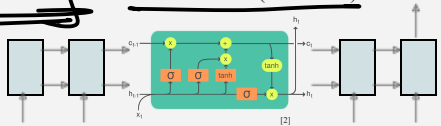


[1]

Originally

Natural Lang. Proc.

Recurrent NNs (+LSTMs)



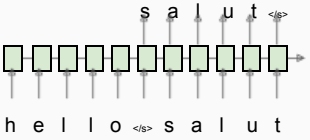
h e l l o

Speech

Deep Belief Nets (+non-DL)

Translation

Seq2Seq



RL

BC/GAIL

Algorithm 1 Generative adversarial imitation learning

1: **Input:** Expert trajectories $\tau_E \sim \pi_E$, initial policy and discriminator parameters θ_0, w_0
2: **for** $i = 0, 1, 2, \ldots$ **do**
3: Sample trajectories $\tau_i \sim \pi_{\theta_i}$
4: Update the discriminator parameters from w_i to w_{i+1} with the gradient

$$\hat{\mathbb{E}}_{\tau_i}[\nabla_w \log(D_w(s,a))] + \hat{\mathbb{E}}_{\tau_E}[\nabla_w \log(1 - D_w(s,a))] \tag{17}$$

5: Take a policy step from θ_i to θ_{i+1}, using the TRPO rule with cost function $\log(D_{w_{i+1}}(s,a))$. Specifically, take a KL-constrained natural gradient step with

$$\hat{\mathbb{E}}_{\tau_i}[\nabla_\theta \log \pi_\theta(a|s) Q(s,a)] - \lambda \nabla_\theta H(\pi_\theta), \quad \text{where } Q(\hat{s},\hat{a}) = \hat{\mathbb{E}}_{\tau_i}[\log(D_{w_{i+1}}(s,a)) \,|\, s_0 = \hat{s}, a_0 = \hat{a}] \tag{18}$$

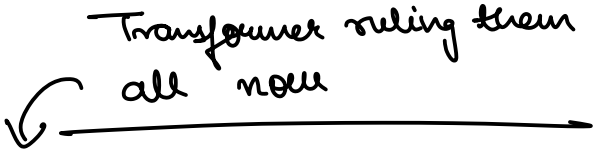
6: **end for**

[1] CNN image CC-BY-SA by Aphex34 for Wikipedia https://commons.wikimedia.org/wiki/File:Typical_cnn.png
[2] RNN image CC-BY-SA by GDbe for Wikipedia https://commons.wikimedia.org/wiki/File:The_LSTM_Cell.svg

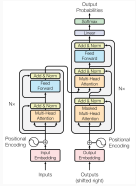
RBM trained in Autoencoder fashion layer by layer

The Transformer's takeover:

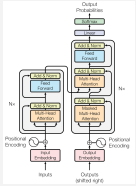
One community at a time



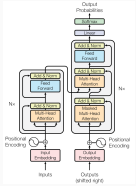
Computer Vision



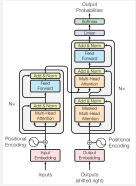
Natural Lang. Proc.



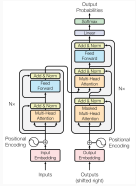
Reinf. Learning



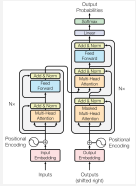
Speech



Translation



Graphs/Science



Transformer image source: "Attention Is All You Need" paper

The origins:

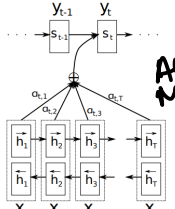
Translation, learned alignment

Neural Machine Translation by Jointly Learning to Align and Translate

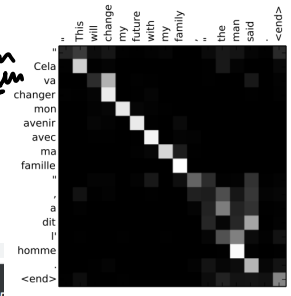
2014, Dzmitry Bahdanau, KyungHyun Cho, Yoshua Bengio

↳ First paper Attention mechanism

"Learning to Align"



Attention Mechanism



(d)

↳ Attention Map

Figure 1: The graphical illustration of the proposed model trying to generate the t-th target word y_t given a source sentence $(x_1, x_2, \ldots, x_T)$.

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attention 1/3

The probability α_{ij}, or its associated energy e_{ij}, reflects the importance of the annotation h_j with respect to the previous hidden state s_{i-1} in deciding the next state s_i and generating y_i. Intuitively, this implements a mechanism of attention in the decoder. The decoder decides parts of the source sentence to pay attention to. By letting the decoder have an attention mechanism, we relieve the encoder from the burden of having to encode all information in the source sentence into a fixed-length vector. With this new approach the information can be spread throughout the sequence of annotations, which can be selectively retrieved by the decoder accordingly.

Attention Is All You Need

2017, Ashish Vaswani, Noam Shazeer, Niki Parmar, Jakob Uszkoreit, Llion Jones, Aidan N. Gomez, Łukasz Kaiser, Illia Polosukhin

Attention is a function similar to a "soft" kv dictionary lookup:

1. Attention weights a1:N are query-key similarities:

   $\hat{a}i = q \cdot ki$

   Normalized via softmax: $ai = e\hat{a}i / \sum_j e\hat{a}j$

   What we want to lookup

   How similar keys to our query.

2. Output z is attention-weighted average of values v1:N:

   $z = \sum_i \hat{a}i vi = \hat{a} \cdot v$

3. Usually, k and v are derived from the same input x:

   $k = Wk \cdot x$ $v = Wv \cdot x$

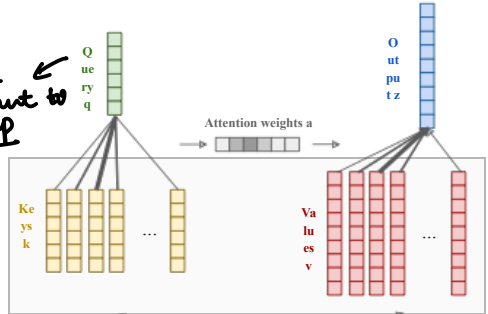
   The query q can come from a separate input y:

   $q = Wq \cdot y$

   Or from the same input x! Then we call it "self attention":

   $q = Wq \cdot x$

   Of same input for q.



Historical side-note: "non-local NNs" in computer vision and "relational NNs" in RL appeared almost at the same time and contain the same core idea!

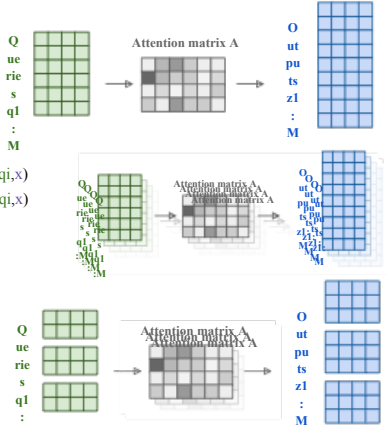
Attention Is All You Need

2017, Ashish Vaswani, Noam Shazeer, Niki Parmar, Jakob Uszkoreit, Llion Jones, Aidan N. Gomez, Łukasz Kaiser, Illia Polosukhin

But that's not actually it! There are a few more details:

1. We usually use **many queries** q1:M, not just one.
   Stacking them leads to the Attention matrix **A**1:N,1:M
   and subsequently to many outputs:

   z1:M = Attn(q1:M,x) = [Attn(q1,x) | Attn(q2,x) | ... | Attn(qM,x)]



2. We usually use **"multi-head" attention.** This means the operation is repeated K times and the results are concatenated along the feature dimension. **W**s differ.

   Attn1(qi,x)
   zi = ⌈Attn2(qi,x)
   \
   ....
   \
   AttnK(qi,x)⌋

   Attention is mostly MHA

3. The most commonly seen formulation:

   z = softmax(QK'/√dkey)V

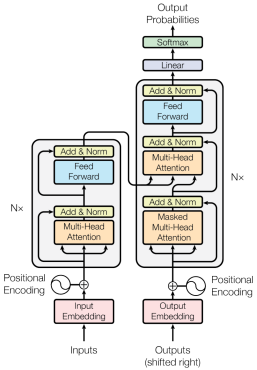
   Note that the complexity is O(N²)

(Improvable)

O(N²) complexity

Attention Is All You Need - The Transformer architecture

2017, Ashish Vaswani, Noam Shazeer, Niki Parmar, Jakob Uszkoreit, Llion Jones, Aidan N. Gomez, Łukasz Kaiser, Illia Polosukhin



Thanks to Basil Mustafa for slide inspiration

Transformer image source: "Attention Is All You Need" paper

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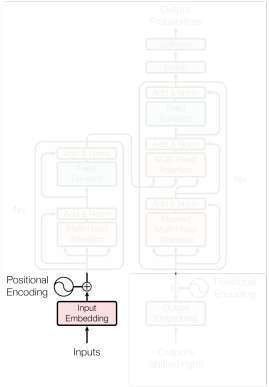


Input (Tokenization and) Embedding

Input text is first split into pieces. Can be characters, word, "tokens":

```
"The detective investigated" -> [The_] [detective_] [invest] [igat] [ed_]
```

Tokens are indices into the "vocabulary":

```
[The_] [detective_] [invest] [igat] [ed_] -> [3 721 68 1337 42]
```

Each vocab entry corresponds to a learned dmodel-dimensional vector.

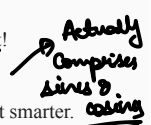
```
[3 721 68 1337 42] -> [ [0.123, -5.234, ...], [...], [...], [...], [...] ]
```

Positional Encoding

Remember attention is permutation invariant, but language is not!

Need to encode position of each word; just add something.

Think `[The_] + 10` `[detective_] + 20` `[invest] + 30` ... but smarter.



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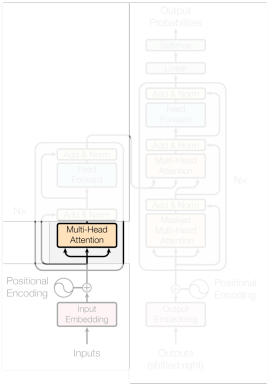


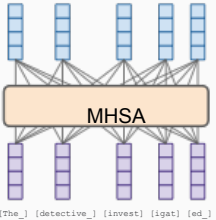
Thanks to Basil Mustafa for slide inspiration

Transformer image source: "Attention Is All You Need" paper

Multi-headed Self-Attention

Meaning the input sequence is used to create queries, keys, and values!

Each token can "look around" the whole input, and decide how to update its representation based on what it sees.



Depending on context, "invest" can now it is about investigating & not investment.

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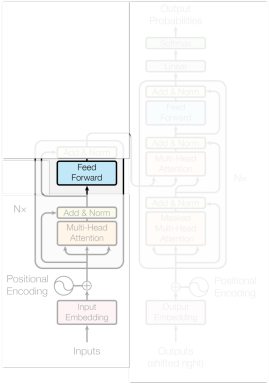


Thanks to Basil Mustafa for slide inspiration

Transformer image source: "Attention Is All You Need" paper

MLP actually stores word "knowledge" → will search for paper.

Point-wise MLP

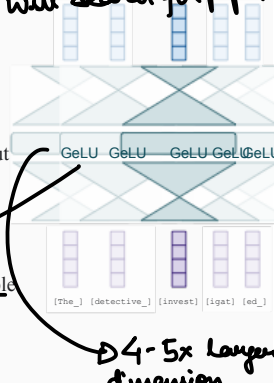
A simple MLP applied to each token individually:

$$z_i = W_2\,\mathrm{GeLU}(W_1 x + b_1) + b_2$$

Think of it as each token pondering for itself about what it has observed previously.
There's some weak evidence this is where "world knowledge" is stored, too.

It contains the bulk of the parameters. When people make giant models and sparse/moe, this is what becomes giant.

Some people like to call it 1x1 convolution.



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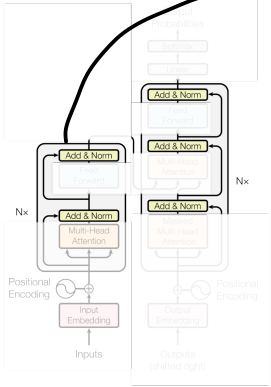

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Transformer image source: "Attention Is All You Need" paper

("Add" part)

Residual connections

Each module's output has the exact same shape as its input.

Following ResNets, the module computes a "residual" instead of a new value:

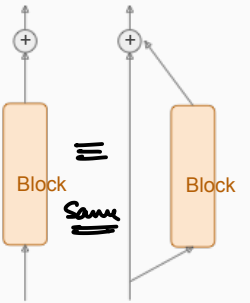
$$z_i = \text{Module}(x_i) + x_i$$

Add input back

This was shown to dramatically improve trainability.

Skip Connections

"Skip connection" "Residual block"



LayerNorm → Scales representations

Normalization also dramatically improves trainability.

There's **post-norm** (original) and **pre-norm** (modern)

$z_i = \text{LN}(\text{Module}(x_i) + x_i)$ Evidence of both performing well. $z_i = \text{Module}(\text{LN}(x_i)) + x_i$

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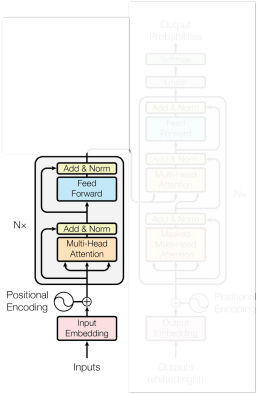

Encoding / Encoder

Since input and output shapes are identical, we can stack N such blocks.

Typically, N=6 ("base"), N=12 ("large") or more.

Encoder output is a "heavily processed" (think: "high level, contextualized") version of the input tokens, i.e. a sequence.

Output of encoder ≈ Contextualized version of inputs

This has nothing to do with the requested output yet (think: translation). That comes with the decoder.

Thanks to Basil Mustafa for slide inspiration

Transformer image source: "Attention Is All You Need" paper

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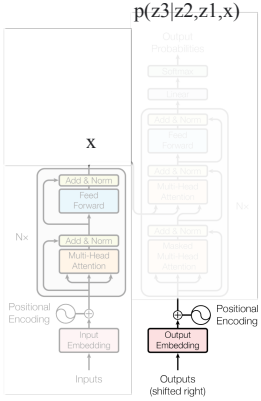

Thanks to Basil Mustafa for slide inspiration

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Decoding / the Decoder **(alternatively Generating / the Generator)**

What we want to model: p(z|x)

for example, in translation: p(z | "the detective investigated") ∀z

z → Sentence in target language.

Seems impossible at first, but we can *exactly* decompose into tokens:

p(z|x) = p(z1|x) p(z2|z1,x) p(z3|z2,z1,x)...

Meaning, we can generate the answer one token at a time.

Each p is a full pass through the model.

Decoder is "actual" probability.

For generating p(z3|z2,z1,x):

x comes from the encoder,

z1, z2 is what we have predicted so far, goes into the decoder.

Once we have p(z|x) we still need to actually sample a sentence such as "le détective a enquêté". Many strategies: greedy, beam-search, ...

↳ Decoding Strategies.

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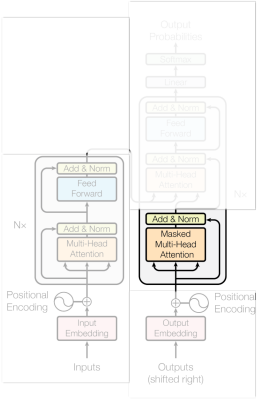

Masked self-attention

This is regular self-attention as in the encoder, to process what's been decoded so far, but with a trick...

If we had to train on one single p(z3|z2,z1,x) at a time: SLOW!

Instead, train on all p(zi|z1:i,x) simultaneously.

How? In the attention weights for zi, set all entries i:N to 0.

This way, each token only sees the already generated ones.

At generation time

There is no such trick. We need to generate one zi at a time. This is why autoregressive decoding is extremely slow.

Caching can be used

Thanks to Basil Mustafa for slide inspiration

Transformer image source: "Attention Is All You Need" paper

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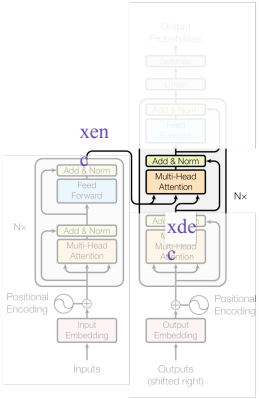
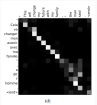


"Cross" attention

Each decoded token can "look at" the encoder's output:

Attn(q=Wqxdec, k=Wkxenc, v=Wvxenc)

Decoded part — What to look at?



This is the same as in the 2014 paper.
This is where |x in p(z3|z2,z1,x) comes from.

Because self-attention is so widely used, people have started just calling it "attention".
Hence, we now often need to explicitly call this "cross attention".

Thanks to Basil Mustafa for slide inspiration

Transformer image source: "Attention Is All You Need" paper ; heatmap image source: "Neural Machine Translation by Jointly Learning to Align and Translate" paper

Attention Is All You Need - The Transformer architecture

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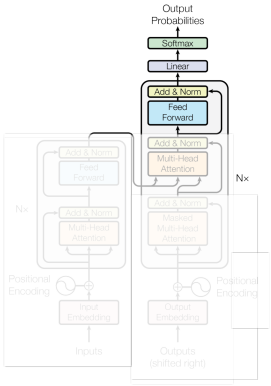

Feedforward and stack layers.

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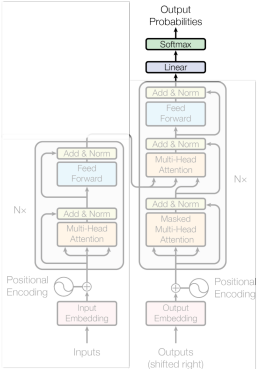
Attention Is All You Need - The Transformer architecture

2017, Ashish Vaswani, Noam Shazeer, Niki Parmar, Jakob Uszkoreit, Llion Jones, Aidan N. Gomez, Łukasz Kaiser, Illia Polosukhin



Thanks to Basil Mustafa for slide inspiration

Transformer image source: "Attention Is All You Need" paper

Output layer

Assume we have already generated K tokens, generate the next one.

The decoder was used to gather all information necessary to predict a probability distribution for the next token (K), over the whole vocab.

Simple:

- linear projection of token K
- SoftMax normalization

Attention Is All You Need - Summary and results

2017, Ashish Vaswani, Noam Shazeer, Niki Parmar, Jakob Uszkoreit, Llion Jones, Aidan N. Gomez, Łukasz Kaiser, Illia Polosukhin

Q, K, V, same initialization.
Nothing special

Table 2: The Transformer achieves better BLEU scores than previous state-of-the-art models on the English-to-German and English-to-French newstest2014 tests at a fraction of the training cost.

Model	BLEU		Training Cost (FLOPs)	
	EN-DE	EN-FR	EN-DE	EN-FR
ByteNet [18]	23.75			
Deep-Att + PosUnk [39]		39.2		$1.0 \cdot 10^{20}$
GNMT + RL [38]	24.6	39.92	$2.3 \cdot 10^{19}$	$1.4 \cdot 10^{20}$
ConvS2S [9]	25.16	40.46	$9.6 \cdot 10^{18}$	$1.5 \cdot 10^{20}$
MoE [32]	26.03	40.56	$2.0 \cdot 10^{19}$	$1.2 \cdot 10^{20}$
Deep-Att + PosUnk Ensemble [39]		40.4		$8.0 \cdot 10^{20}$
GNMT + RL Ensemble [38]	26.30	41.16	$1.8 \cdot 10^{20}$	$1.1 \cdot 10^{21}$
ConvS2S Ensemble [9]	26.36	**41.29**	$7.7 \cdot 10^{19}$	$1.2 \cdot 10^{21}$
Transformer (base model)	27.3	38.1	**$3.3 \cdot 10^{18}$**	
Transformer (big)	**28.4**	**41.8**	$2.3 \cdot 10^{19}$	

Refer this (good animation)

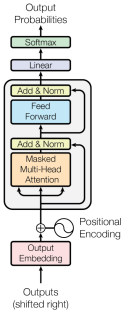
Animation source: https://ai.googleblog.com/2017/08/transformer-novel-neural-network.html
Table source: "Attention Is All You Need" paper

The first (1.5th) big takeover:

Language Modeling / NLP

Decoder-only
GPT

[sat_]



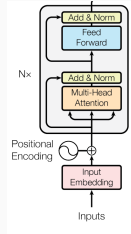
No Cross-Attention

[START] [The_] [cat_]

Encoder-only
BERT

MLM

[*] [*] [sat_] [*] [the_] [*]



[The_] [cat_] **[MASK]** [on_] **[MASK]** [mat_]

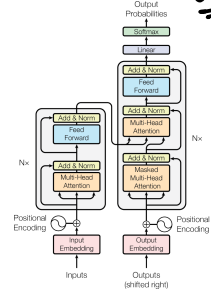
Enc-Dec
T5

Das ist gut.

A storm in Attala caused 6 victims.

This is not toxic.

Can diff. tasks as translation



Translate EN-DE: This is good.

Summarize: state authorities dispatched…

Is this toxic: You look beautiful today!

Transformer image source: "Attention Is All You Need" paper

The second big takeover:

Computer Vision

An Image is Worth 16x16 Words: Transformers for Image Recognition at Scale

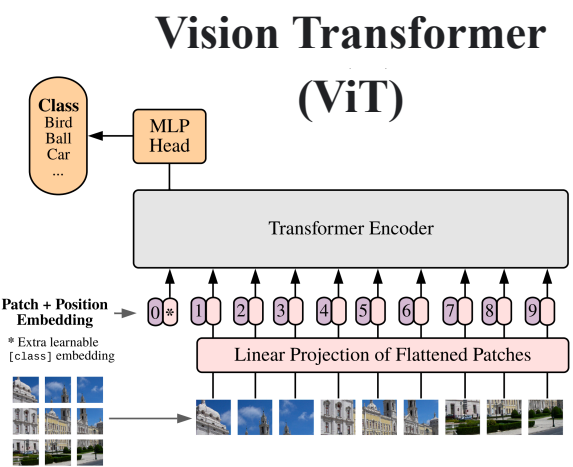
2020, A Dosovitskiy, L Beyer, A Kolesnikov, D Weissenborn, X Zhai, T Unterthiner, M Dehghani, M Minderer, G Heigold, S Gelly, J Uszkoreit, N Houlsby

Many prior works attempted to introduce self-attention at the pixel level.

For 224px², that's 50k sequence length, too much!

Thus, most works restrict attention to local pixel neighborhoods, or as high-level mechanism on top of detections.

The **key breakthrough** in using the full Transformer architecture, standalone, was to **"tokenize" the image** by **cutting it into patches** of 16px², and treating each patch as a token, e.g. embedding it into input space.



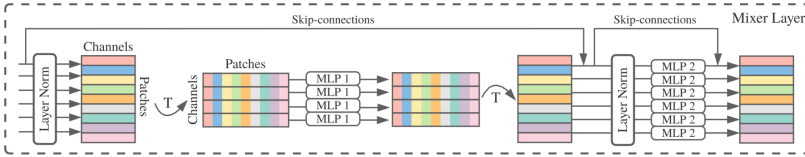
Side-note: MLP-Mixer

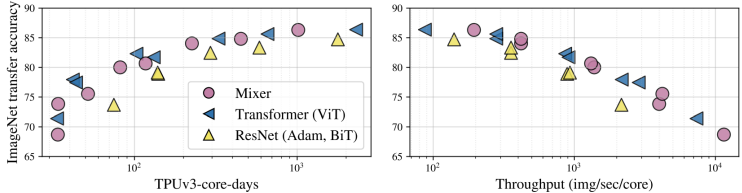
2020, I Tolstikhin, N Houlsby, A Kolesnikov, L Beyer, X Zhai, T Unterthiner, J Yung, A Steiner, D Keysers, J Uszkoreit, M Lucic, A Dosovitskiy

After ViT answered the question "Are convolutions really needed to process images?" with NO...
We wondered if self-attention is really needed?

The role of self-attention is to "mix" information across tokens.
Another simple way to achieve this, is to "transpose" tokens and run that through an MLP:

Simply transpose + MLP = Self Attention





The third big takeover:

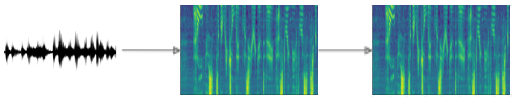
Speech

Conformer: Convolution-augmented Transformer for Speech Recognition

2020, A Gulati, J Qin, C-C Chiu, N Parmar, Y Zhang, J Yu, W Han, S Wang, Z Zhang, Y Wu, R Pang

[igat]

Largely the same story as in computer vision.
But with spectrograms instead of images.

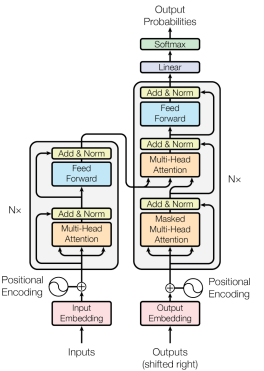


Conformer

Add a third type of block using convolutions, and slightly reorder blocks, but overall very transformer-like.

Exists as encoder-decoder variant, or as encoder-only variant with CTC loss.

Whisper
ConNeu



[The_] [detective_] [invest]

Transformer image source: "Attention Is All You Need" paper

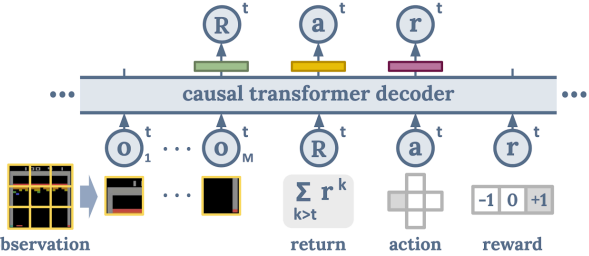
The fourth big takeover:

Reinforcement Learning

Decision Transformer: Reinforcement Learning via Sequence Modeling

2021, L Chen, K Lu, A Rajeswaran, K Lee, A Grover, M Laskin, P Abbeel, A Srinivas, I Mordatch

Cast the (supervised/offline) RL problem into a sequence ("language") modeling task:



Cut observation into parts.

Language Modelling on trajectories.

Generate reward, actions

Can generate/decode sequences of actions with desired return (eg skill)

The trick is prompting: `"The following is a trajectory of an expert player: [obs] ..."`

Proper training through replay buffers.

Slide credit: Igor Mordatch

"Let's think step by step" comes kinda from this

The Transformer's

Unification of communities

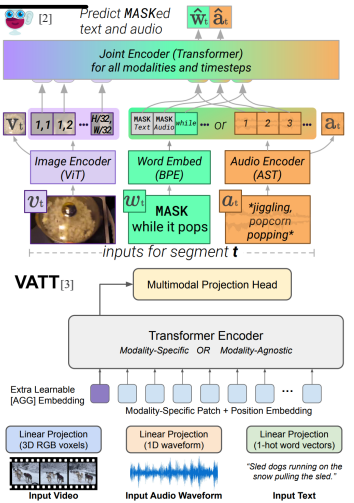
Anything you can tokenize, you can feed to Transformer

ca 2021 and onwards

Tokenize different modalities each in their own way (some kind of "patching"), and send them all jointly into a Transformer...

Seems to just work...
Currently an explosion of works doing this!

[1]



Images from:
[1] LIMoE by B Mustafa, C Riquelme, J Puigcerver, R Jenatton, N Houlsby
[2] MERLOT Reserve by R Zellers, J Lu, X Lu, Y Yu, Y Zhao, M Salehi, A Kusupati, J Hessel, A Farhadi, Y Choi
[3] VATT by H Akbari, L Yuan, R Qian, W-H Chuang, S-F Chang, Y Cui, B Gong

A note on
Efficient Transformers

A note on Efficient Transformers

The self-attention operation complexity is $O(N^2)$ for sequence length N.

We'd like to use large N:

- Whole articles or books
- Full video movies
- High resolution images

Many O(N) approximations to the full self-attention have been proposed in the past two years.

Unfortunately, none provides a clear improvement.
They always trade-off between speed and quality.

Vanilla Transformer still very good.
Speed pays in performance.

Long Range Arena Benchmark

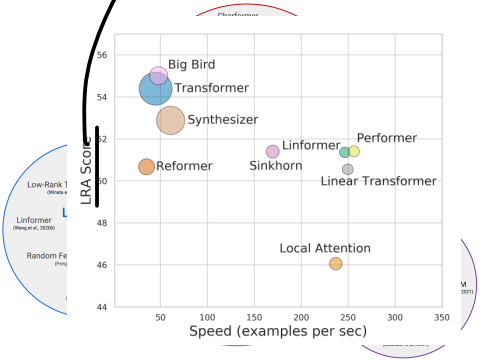


Figure 2: Taxonomy of Efficient Transformer Architectures.

Based on "Efficient Transformers: A Survey" by Yi Tay, Mostafa Dehghani, Dara Bahri, Donald Metzler
and "Long Range Arena: A Benchmark for Efficient Transformers" by Y Tay, M Dehghani, S Abnar, Y Shen, D Bahri, P Pham, J Rao, L Yang, S Ruder, D Metzler

Limitation (also advantage)

Very Flexible

So need more data

So this is also a challenge

Decoder implementation complexity high / difficult.

(Will need to review more.)

Thanks for your...

Attention

Transformer image source: "Attention Is All You Need" paper