





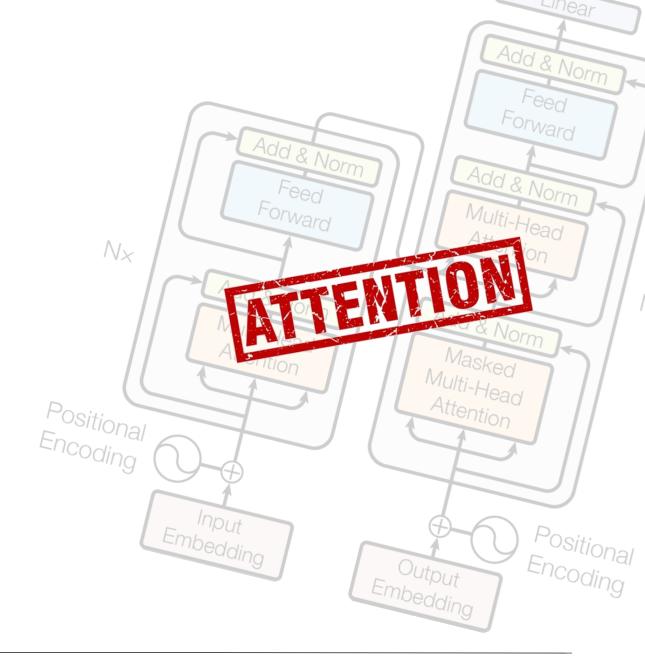
Transformers

Active Training Course "Advanced Deep Learning"





RWTH Aachen University



Current Hype: Text-to-Image Models

Text Prompt

Photography of an Astronaut wearing a green spacesuit standing in front of the Colosseum on the moon, with a bouquet of roses in his hand

Text Analysis (Typically *Transformer*)

Image Generation (Typically *Diffusion*)

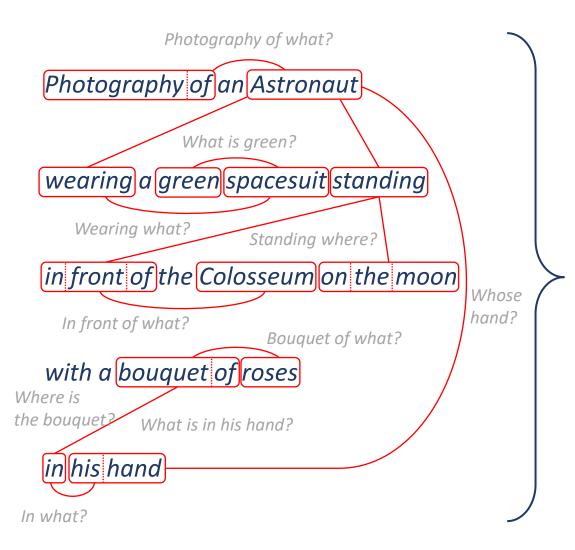
Unusual color, unusual location, **unusual** item

→ Network must understand prompt well!



https://arxiv.org/abs/2112.10752 https://github.com/CompVis/stable-diffusion

Understanding the Text Prompt



Cherry-picked examples:

Successful generations:



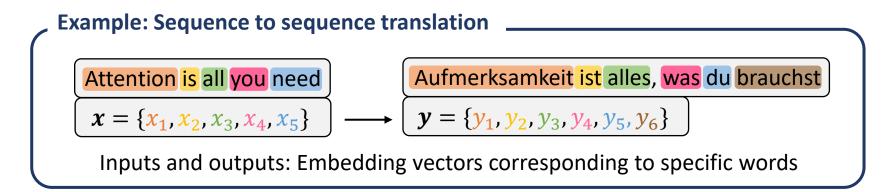
Misunderstandings:



https://github.com/CompVis/stable-diffusion

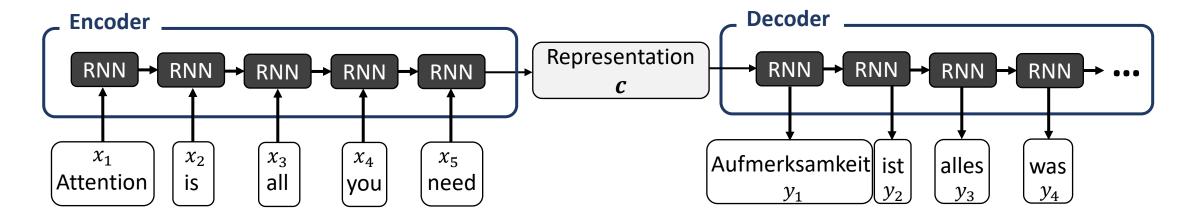
Understanding a long text is **hard**, but network (often) manages to do it \rightarrow **How does it work?**

Natural Language Processing



Before transformers: Recurrent Neural Networks ("RNNs", e.g. LSTMs)

Approach: Analyze the data **sequentially** → current step always depends on all previous steps



Sequential Data Processing

Sequential analysis is helpful to understand **context**!

I like your house, **it** is great!

I like your dog, **it** is great!

I like your cat, **it** is great!

I like your cat, **it** is great!

I like your cat, **it** is great!

I ch mag deine Hund, **er** ist toll!

Correct translations of words can depend on **previous** or **following** words

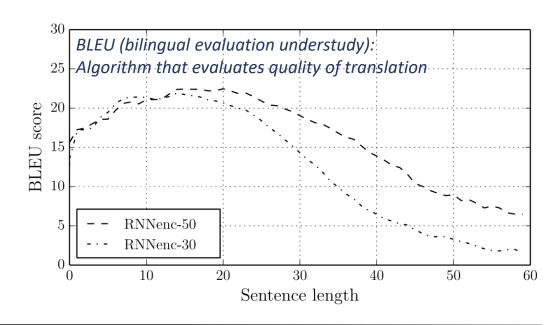
In theory: Using an RNN, current step has access to

information from all previous steps

In practice: Only works well for **small sequences**

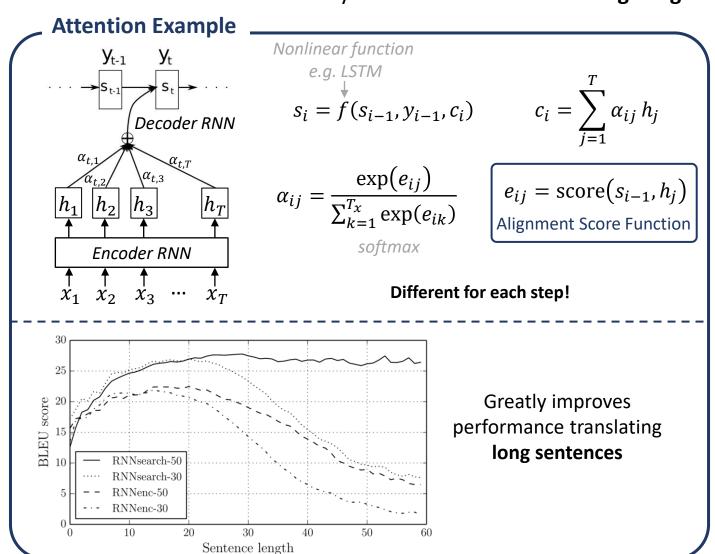
(<20 timesteps) due to too small gradients

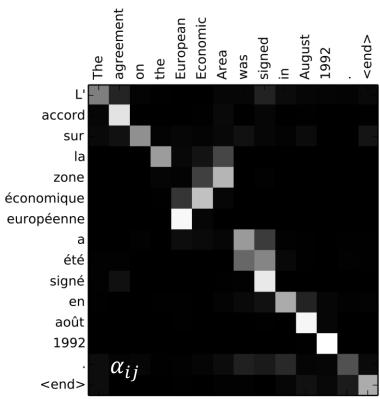
in regard to far away timesteps



Solution: Attention

Use intermediate results of RNN layers and combine them using weights α (alignment score)





https://arxiv.org/abs/1409.0473

Attention Mechanisms

$$s_i = f(s_{i-1}, y_{i-1}, c_i)$$

$$c_i = \sum_{j=1}^T \alpha_{ij} \, h_j$$

$$s_i = f(s_{i-1}, y_{i-1}, c_i)$$
 $c_i = \sum_{j=1}^{I} \alpha_{ij} h_j$ $\alpha_{ij} = \frac{\exp(e_{ij})}{\sum_{k=1}^{T_x} \exp(e_{ik})}$

$$e_{ij} = \operatorname{score}(s_{i-1}, h_j)$$

Commonly used neural network approach

Alignment score: Many different options

_			
	Name	Alignment score function	Citation
	Content-base attention	$\mathrm{score}(s_{i-1}, h_i) = \mathrm{cos}(\theta)$ where θ is the angle between s_{i-1} and h_j	Graves2014
*	Additive	$score(s_{i-1}, h_j) = v_a^{T} \tanh(W_a[s_{i-1}; h_j])$	Bahdanau2015
	Location-Based	$lpha_{ij}=\mathrm{softmax}(W_as_i)_{\mathrm{j}}$ Note: This simplifies the softmax alignment to only depend on the target position.	<u>Luong2015</u>
	General	$score(s_{i-1}, h_j) = s_{i-1}^{T} W_a h_j$ where W_a is a trainable weight matrix in the attention layer.	<u>Luong2015</u>
	Dot-Product	$score(s_{i-1}, h_j) = s_{i-1}^{T} h_j$	Luong2015
	Scaled Dot-Product	$score(s_{i-1},h_j) = \frac{s_{i-1}^T h_j}{\sqrt{n}}$ Note: very similar to the dot-product attention except for a scaling factor; where n is the dimension of the source hidden state.	<u>Vaswani2017</u>

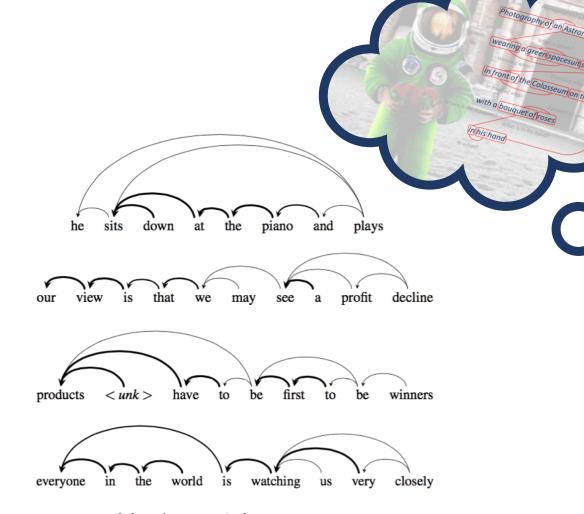
Important for Transformer

https://lilianweng.github.io/posts/2018-06-24-attention/

Self-Attention

Relate input **to itself** to determine **self-attention**:

```
The FBI is chasing a criminal on the run.
The FBI is chasing a criminal on the run.
     FBI is chasing a criminal on the run.
The
     FBI is chasing a criminal on the run.
The
              chasing a criminal on the run.
The
     FBI is
     FBI is
              chasing a criminal on the run.
The
The
     FBI
              chasing a criminal on the run.
          is
     FBI is
                          criminal on the run.
The
              chasing
              chasing a
                          criminal on
                                        the run.
              chasing a criminal
The
     FBI
                                        the run.
```



Bolder line: **Higher** attention

⇒ Adding attention mechanisms to RNNs improves the performance (especially for long sentences) and can enable interesting insights

Attention Is All You Need

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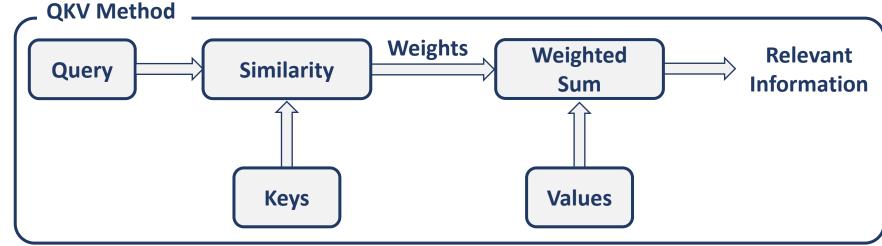
Abstract

The dominant sequence transduction models are based on complex recurrent or convolutional neural networks that include an encoder and a decoder. The best performing models also connect the encoder and decoder through an attention mechanism. We propose a new simple network architecture, the Transformer, based solely on attention mechanisms, dispensing with recurrence and convolutions entirely. Experiments on two machine translation tasks show these models to

Introducing: The Transformer

Transformer: Attention Mechanism

Interpret attention as function of query Q, keys K and values V

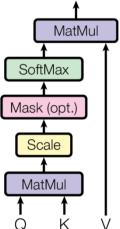


Scaled dot-product attention:

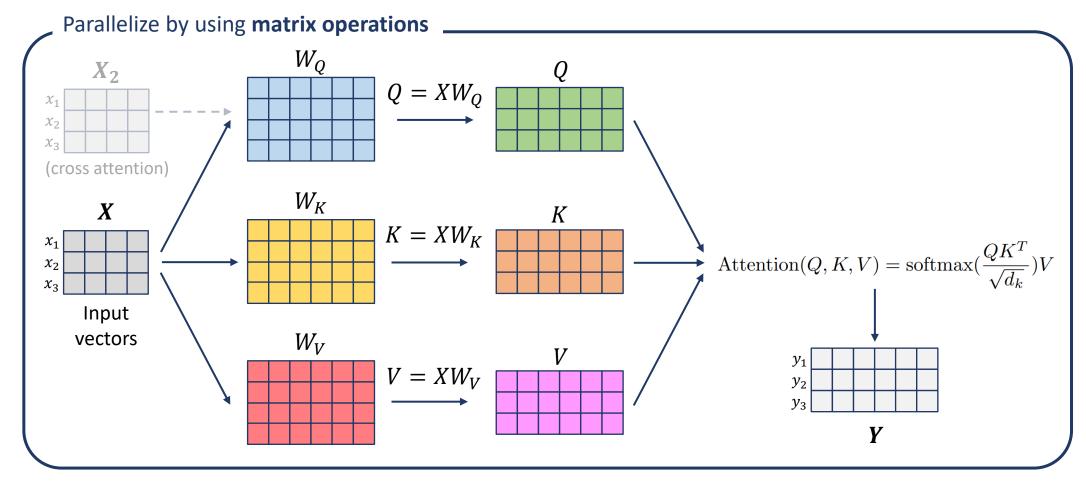
Dot-product (vector projection) as **similarity measure**

$$score(s_{i-1}, h_j) = \frac{s_{i-1}^T h_j}{\sqrt{n}}$$
 \longrightarrow Attention $(Q, K, V) = softmax(\frac{QK^T}{\sqrt{d_k}})V$

 d_k : length of keys vector

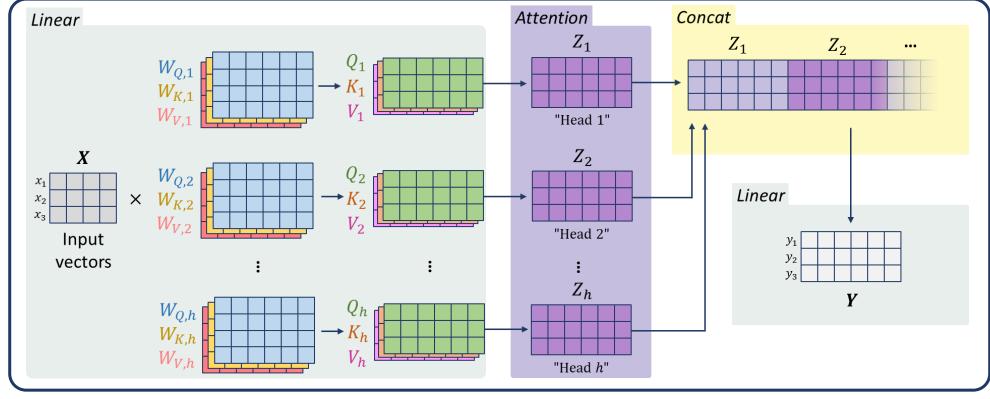


QKV-Self-Attention Implementation



Here: Always use $X \to \text{calculate self attention}$ To relate X to different input data X_2 , use X_2 to calculate Q (cross attention)

Multi-Head Attention

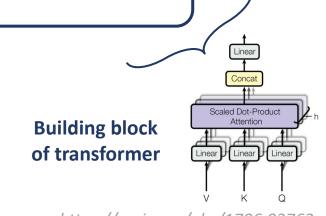


Heads are **independent** of each other!

- → Can be **trained in parallel** on multiple GPUs
- → Enables **training on huge** datasets in reasonable time

Input treated as set instead of sequence \rightarrow permutation invariant \ref{figure}

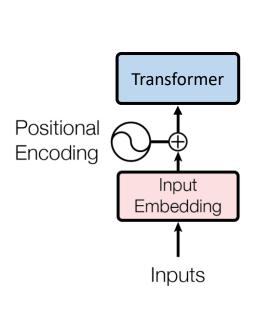
→ Use **positional encoding!**

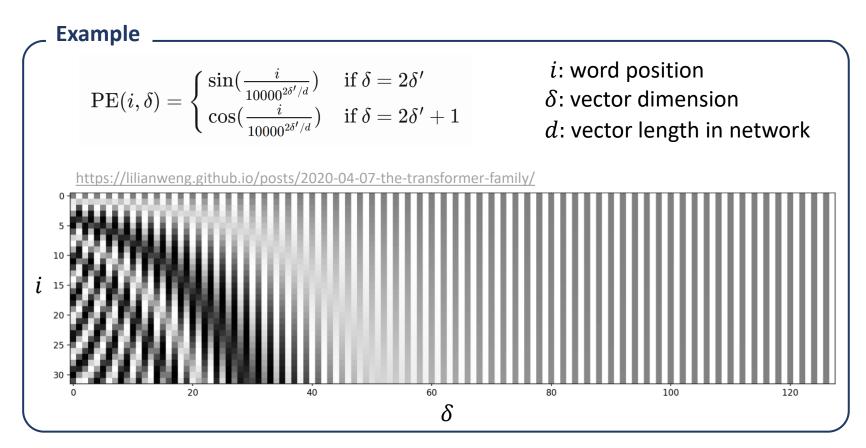


https://arxiv.org/abs/1706.03762

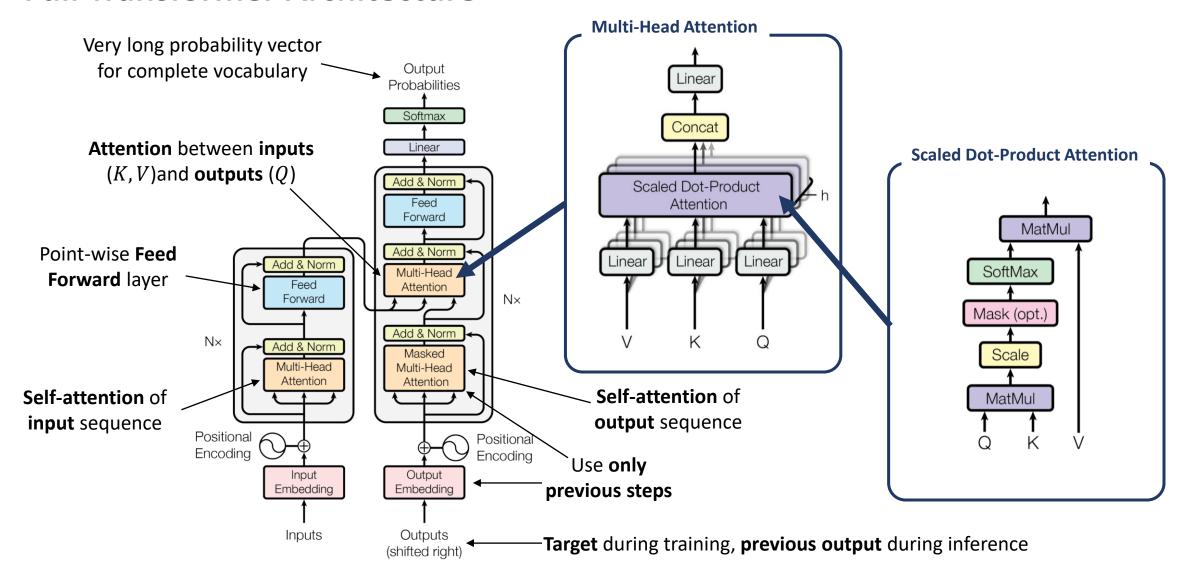
Positional Encoding

Positional Encoding PE is **added to embedded vectors from inputs** to pass positional information to transformer Many different options (both **trainable** and **fixed**), paper uses **fixed encoding**:

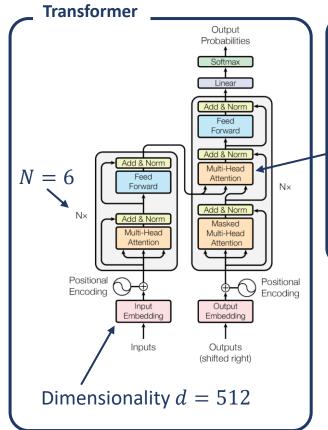


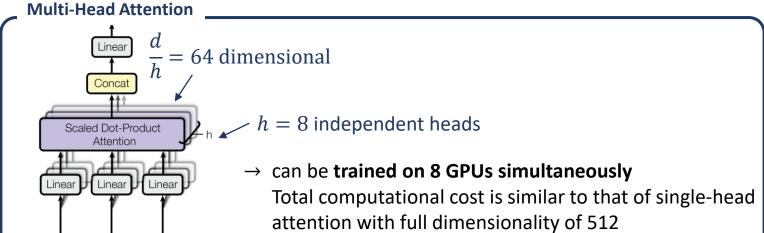


Full Transformer Architecture



Text Translation with Transformer





Model	BLEU		Training C	Training Cost (FLOPs)	
Model	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		10^{18}	
Transformer (big)	28.4	41.8	2.3 ·	10^{19}	

29.11.2022

Impact of Transformers – Language Processing



https://gluebenchmark.com/leaderboard

Rank Name		Model	URL S	Score
1	Microsoft Alexander v-team	Turing ULR v6	₫	91.3
2	JDExplore d-team	Vega v1		91.3
3	Microsoft Alexander v-team	Turing NLR v5		91.2
4	DIRL Team	DeBERTa + CLEVER		91.1
5	ERNIE Team - Baidu	ERNIE		91.1
6	AliceMind & DIRL	StructBERT + CLEVER		91.0
7	DeBERTa Team - Microsoft	DeBERTa / TuringNLRv4		90.8
8	HFL iFLYTEK	MacALBERT + DKM		90.7
9	PING-AN Omni-Sinitic	ALBERT + DAAF + NAS		90.6
10	T5 Team - Google	T5		90.3
11	Microsoft D365 AI & MSR AI & GATECH	MT-DNN-SMART		89.9
12	Huawei Noah's Ark Lab	NEZHA-Large		89.8
79	GLUE Baselines	BiLSTM+ELMo+Attn		70.0

All using Transformers Transformers beat LSTMs/Recurrent Neural Networks as state of the art in natural language processing!

Huge transformer models are widely-used for language processing:

- Google BERT
 (340 Million parameters)
- Google T5
 (11 billion parameters)
- OpenAl GPT-3 (175 billion parameters)
- Microsoft Megatron-Turing NLG (530 billion parameters)
- → Models using more than one **trillion** parameters are already tested

Transformer for Language Processing - Overview

- Transformers: Use attention-mechanism to analyze data → Relevance between different inputs
- Positional Encoding enables the analysis of sequences
 - → Ability to understand **long and complicated** texts
 - Transformers replaced RNNs as state-of-the-art methods for natural language processing

Enabled new applications:

Generating large texts

A robot wrote this entire article. Are you scared yet, human? *GPT-3*

We asked GPT-3, OpenAI's powerful new language generator, to write an essay for us from scratch. The assignment? To convince us robots come in peace

Writing code

Your Al pair programmer

GitHub Copilot uses the OpenAl Codex to suggest code and entire functions in real-time, right from your editor.

Understanding complex prompts



Conversational models

Hi! I am Mount Everest. What would you like to know about me?



Why do people climb you?

Some people want to show others they could do it, others enjoy the hike and the scenery, and then some people just want to see the world.



Who was the first?

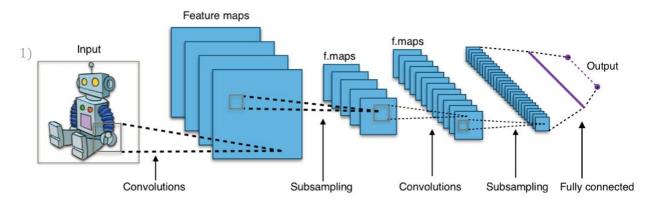
Sir Edmund Hillary and Tenzing Norgay from Nepal were the first to summit Mount Everest in May 1953. They were joined by several others at different times in the successful attempt.



...and many more

Image Recognition

Previous state of the art in image recognition: Convolutional Neural Networks



- Learned filters that are used to scan images for features
- Inherently uses the **symmetries of 2D images**, i.e. which pixels are neighbors, where does the image end, etc.
- However: Can be computationally demanding

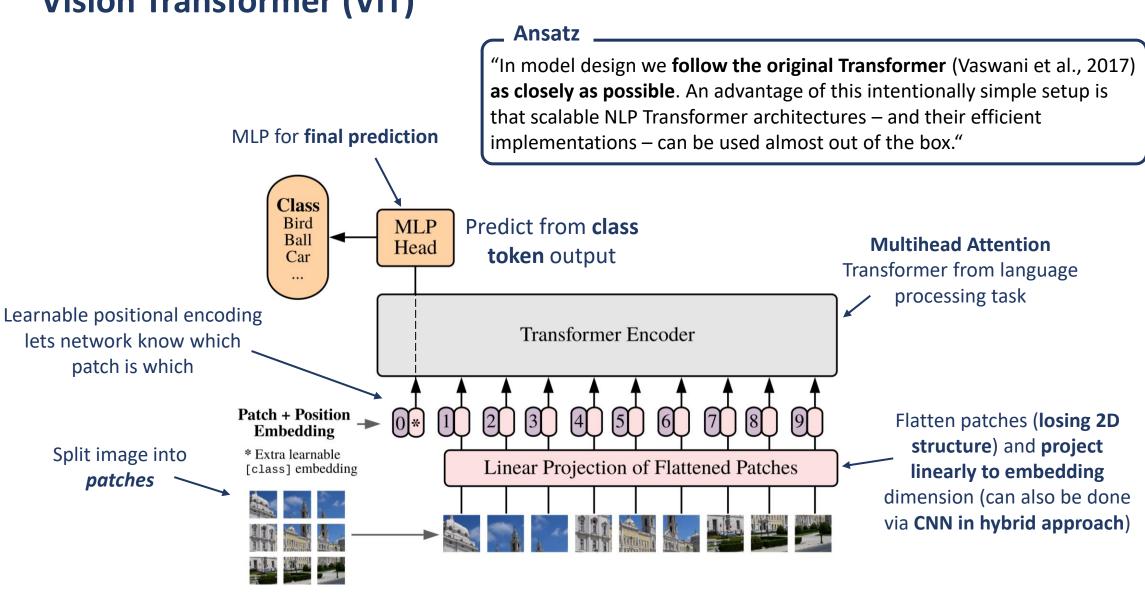
"Looking forward to the next generation of **scalable vision models**, one might ask whether this domain-specific design is necessary, or if one could successfully leverage **more domain agnostic and computationally efficient architectures** to achieve state-of-the-art results."

https://ai.googleblog.com/2020/12/transformers-for-image-recognition-at.html

⇒ Vision Transformer

https://commons.wikimedia.org/wiki/File:Typical_cnn.png

Vision Transformer (ViT)



Vision Transformer Performance

Model	Layers	${\it Hidden size } D$	MLP size	Heads	Params
ViT-Base	12	768	3072	12	86M
ViT-Large	24	1024	4096	16	307M
ViT-Huge	32	1280	5120	16	632M

	Ours-JFT (ViT-H/14)	Ours-JFT (ViT-L/16)	Ours-I21k (ViT-L/16)	BiT-L (ResNet152x4)	Noisy Studen (EfficientNet-I	
ImageNet	88.55 ± 0.04	87.76 ± 0.03	85.30 ± 0.02	87.54 ± 0.02	88.4/88.5*	
ImageNet ReaL	90.72 ± 0.05	90.54 ± 0.03	88.62 ± 0.05	90.54	90.55	
CIFAR-10	99.50 ± 0.06	99.42 ± 0.03	99.15 ± 0.03	99.37 ± 0.06	_	
CIFAR-100	94.55 ± 0.04	93.90 ± 0.05	93.25 ± 0.05	93.51 ± 0.08	_	
Oxford-IIIT Pets	97.56 ± 0.03	97.32 ± 0.11	94.67 ± 0.15	96.62 ± 0.23	_	
Oxford Flowers-102	99.68 ± 0.02	99.74 ± 0.00	99.61 ± 0.02	99.63 ± 0.03	_	
VTAB (19 tasks)	77.63 ± 0.23	76.28 ± 0.46	72.72 ± 0.21	76.29 ± 1.70		
TPUv3-core-days	2.5k	0.68k	0.23k	9.9k	12.3k	

Transformers

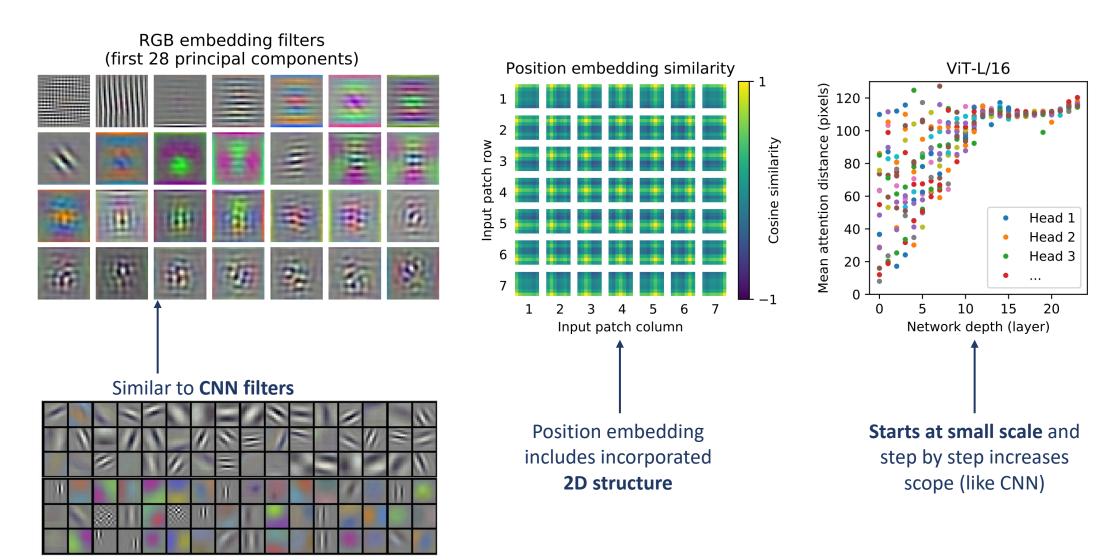
Transformer: More efficient

"ViT performs **significantly worse** than the CNN equivalent (BiT) when **trained on ImageNet** (1M images). However, on **ImageNet-21k** (14M images) performance is **comparable**, and on **JFT** (300M images), **ViT now outperforms BiT**."

⇒ Vision Transformer already outperforms (highly-optimized) CNNs, despite using architecture created for language processing

CNNs

Vision Transformer Insight



https://papers.nips.cc/paper/2012/file/c399862d3b9d6b76c8436e924a68c45b-Paper.pdf

https://arxiv.org/abs/2010.11929

Vision Transformer Insight

Input

Attention













Global self-attention, in contrast to local filters of CNN

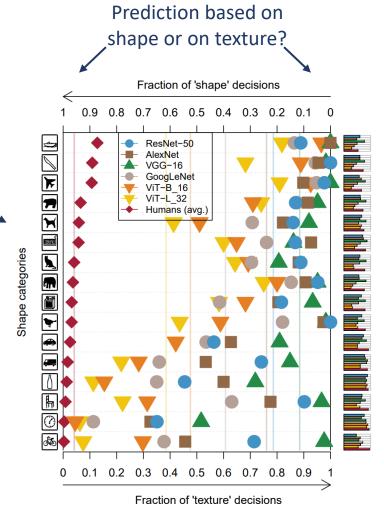
Shape = Cat, Texture = Elephant





Are Vision Transformers **more similar to human vision** than CNNs?

Ongoing research...

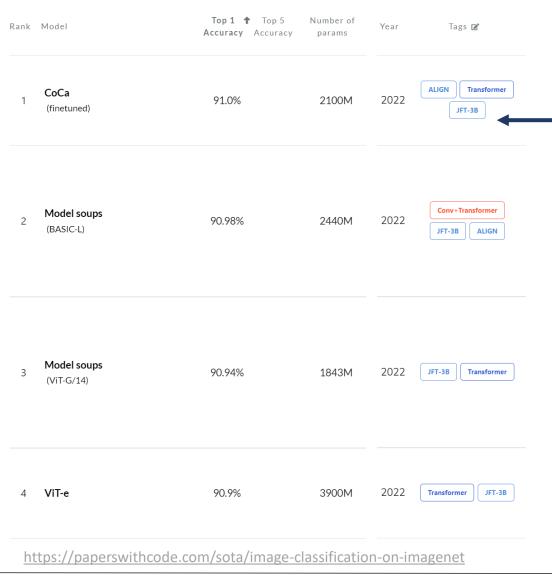


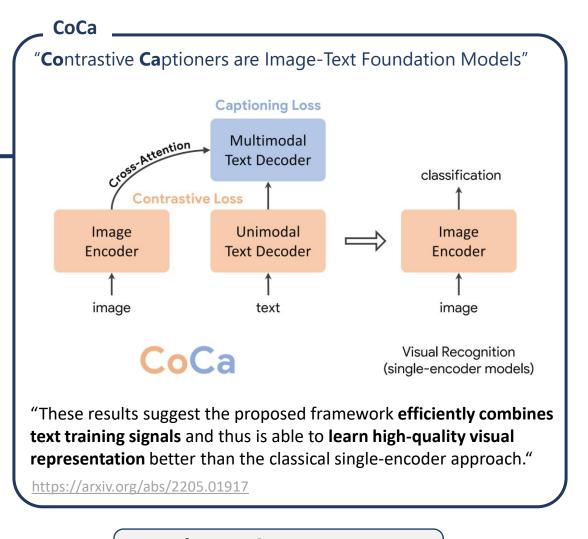
https://arxiv.org/abs/2010.11929

https://arxiv.org/abs/2105.07197

ImageNet Leaderboard

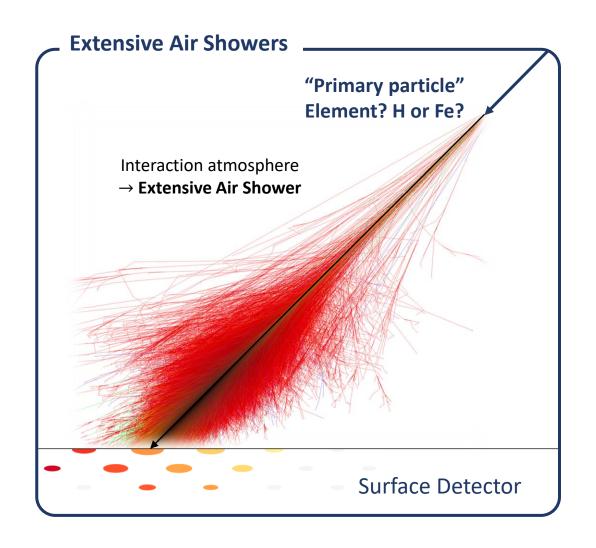
Image Classification on ImageNet:



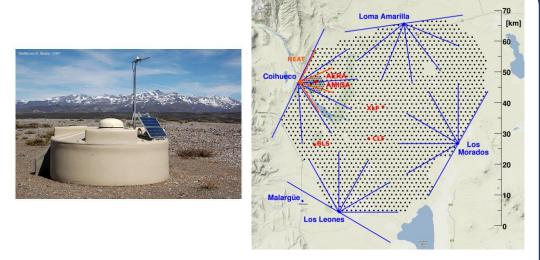


Transformers beat CNNs as state of the art in image recognition!

Application Example: Cosmic-Ray Element Reconstruction at Pierre Auger Observatory

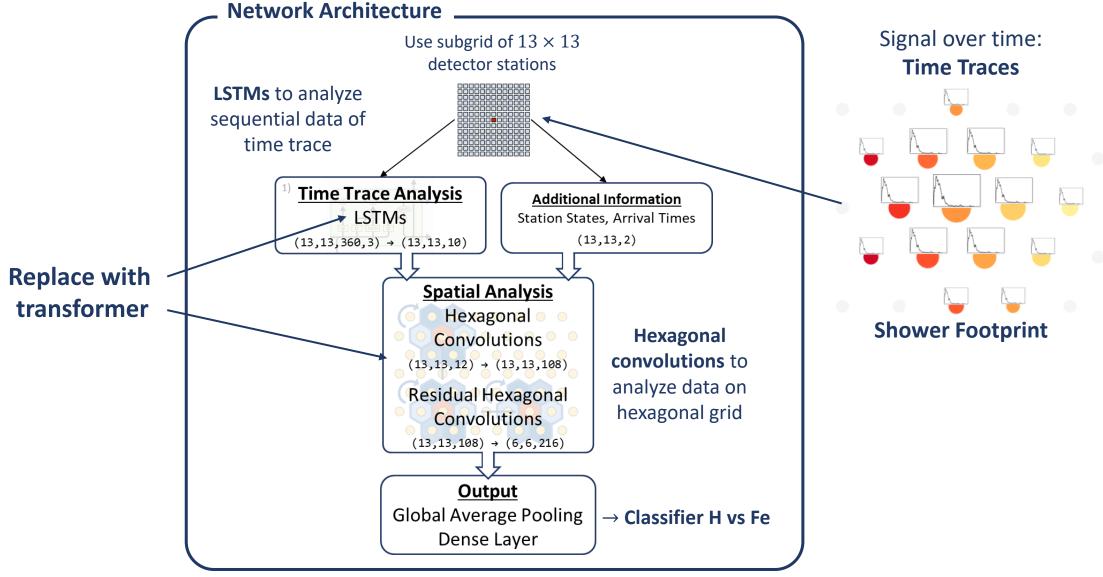


Pierre Auger Observatory Surface Detector

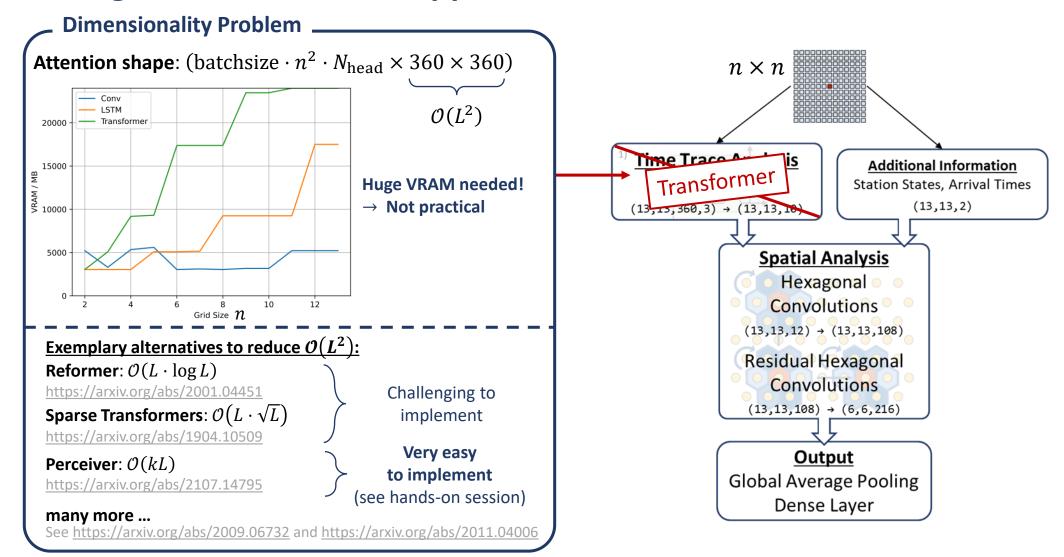


- Located in the *Pampa Amarilla* near Malargüe, Argentina
- Covers an area of roughly 3000 km²
- Hexagonal grid of 1660 water-Cherenkov stations
- Sample air shower footprint

Cosmic-Ray Mass Reconstruction Neural Network

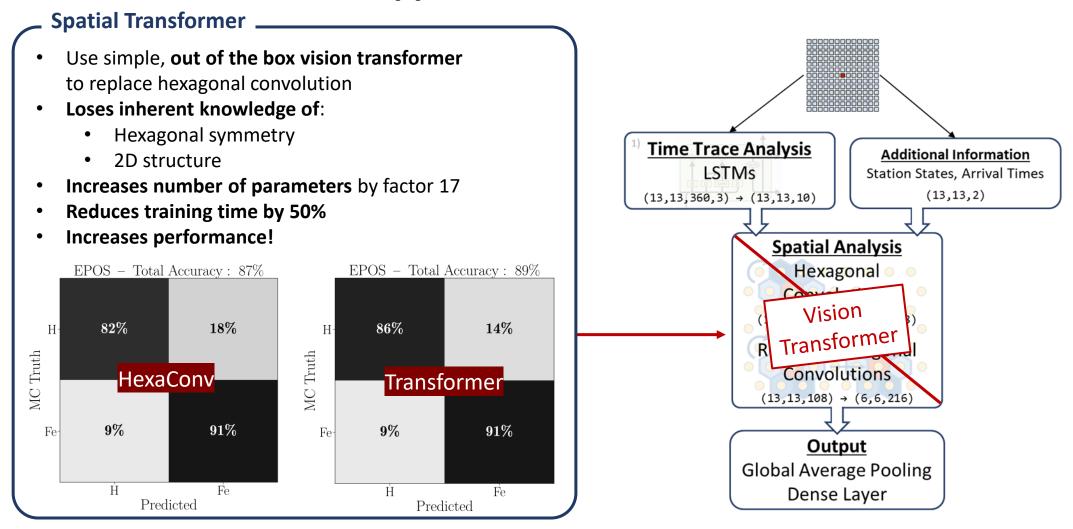


Challenges of Transformer Application



⇒ **Default attention quickly needs very large amounts of VRAM** if data structure is too large, **alternatives exist**

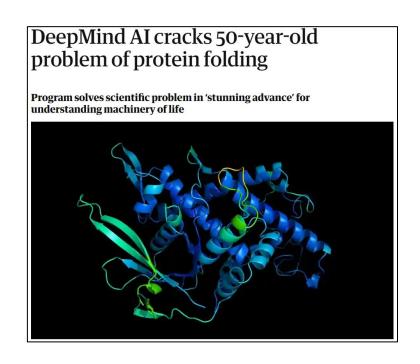
Chances of Transformer Application

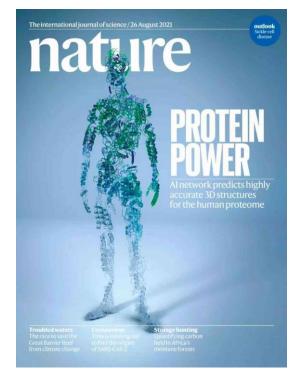


⇒ **Domain agnostic transformer** can be trained quickly, and **outperforms approach focused on data symmetry** (similar to Vision Transformer on images)

Transformers in Science

Similar to other fields, transformers are used **instead of LSTMs or CNNs**, as well as for **new applications**:



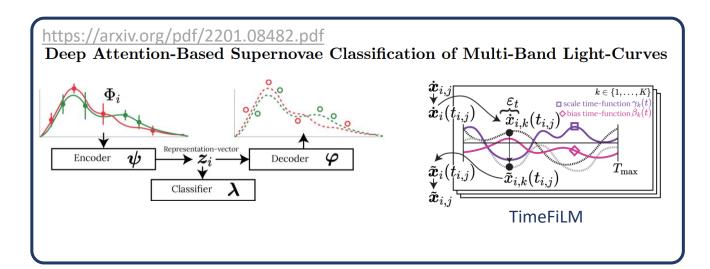


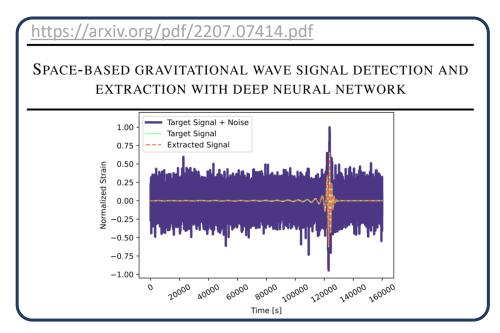
Famous science application: Protein unfolding

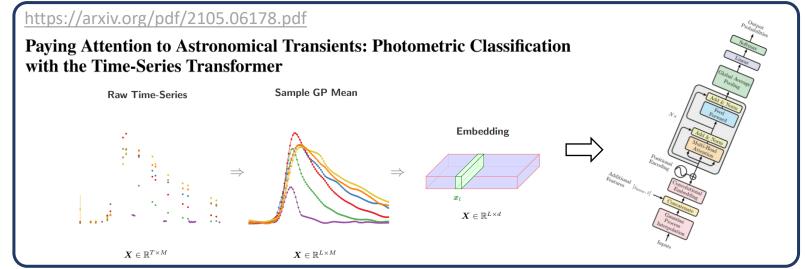
Applications in Astro- and Particle Physics are becoming more common:

(The following list contains some of the results from arXiv and is not extensive)

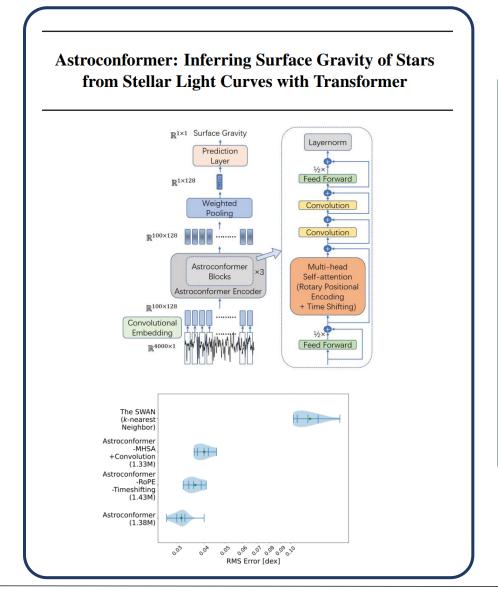
Time Sequence Analyses

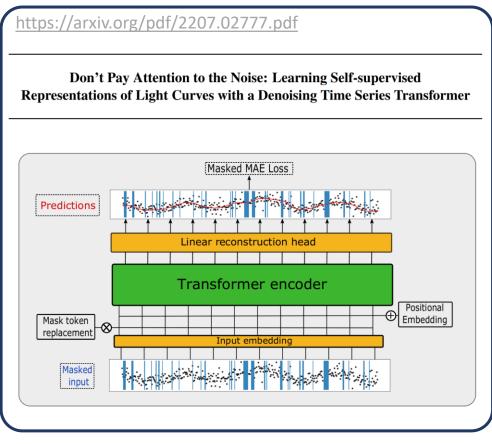




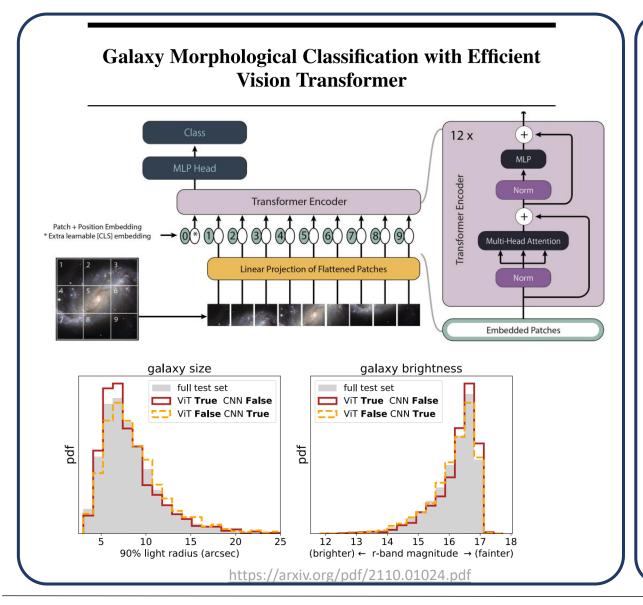


Time Sequence Analyses

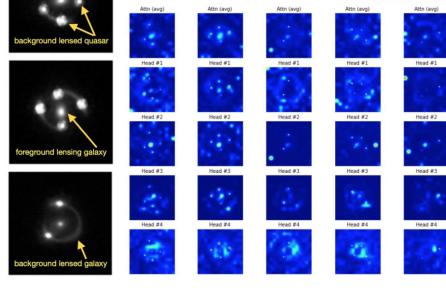




Vision Transformer Applications

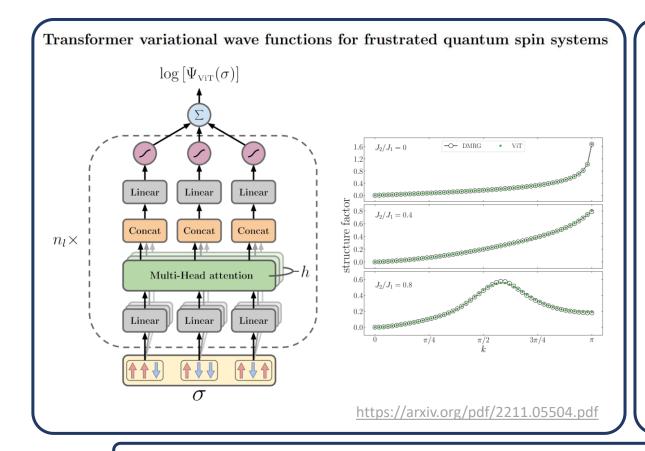


Strong Gravitational Lensing Parameter Estimation with Vision Transformer Attn (avg) Attn (avg) Attn (avg) Attn (avg) Head #1 Head #1 Head #1 Head #1 Head #1 Head #1 Head #1

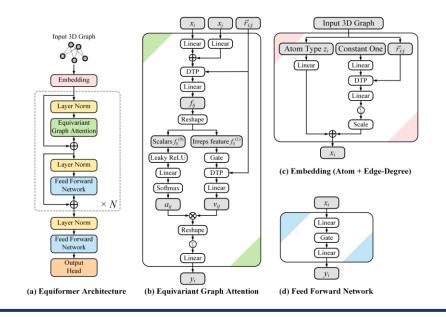


https://arxiv.org/pdf/2210.04143.pdf

Other Applications



Equiformer: Equivariant Graph Attention Transformer for 3D Atomistic Graphs

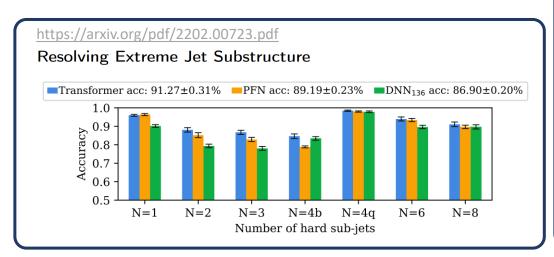


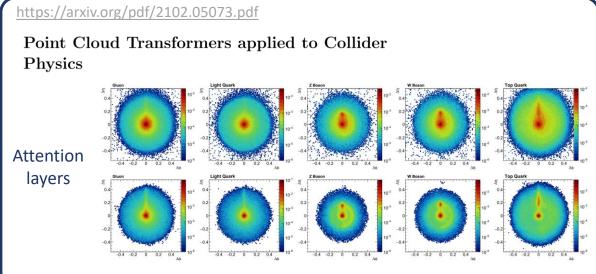
Fine-tuning Vision Transformers for the Prediction of State Variables in Ising Models

https://arxiv.org/pdf/2109.13925.pdf

System/Boundary Conditions	ViT	ResNet-18	ResNet-50
Periodic (Ferromagnetic)	$\textbf{0.934} \pm .008$	$0.865\pm.034$	$0.907\pm.021$
Periodic (Anti-ferromagnetic)	$\boldsymbol{0.935 \pm .012}$	$0.906 \pm .016$	$0.899 \pm .026$
Skewed (Ferromagnetic)	$\boldsymbol{0.931 \pm .021}$	$.886 \pm .019$	$0.917 \pm .009$
Anti-Periodic (Ferromagnetic)	$\boldsymbol{0.921 \pm .013}$	$0.91\pm.021$	$0.917 \pm .008$

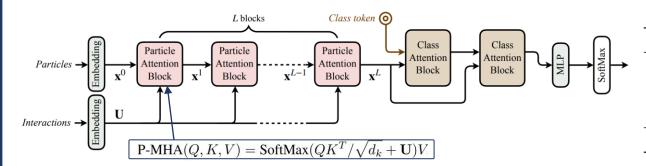
Particle Physics





https://arxiv.org/pdf/2202.03772.pdf

Particle Transformer for Jet Tagging



 $\mbox{\it "P-MHA},$ an augmented version that can also exploit the pairwise particle interactions directly [...]

Essentially, we add the interaction matrix \boldsymbol{U} [...]. This allows P-MHA to incorporate particle interaction features designed from physics principles ..."

JetClass Classification

	Accuracy	# params	FLOPs
PFN	0.772	86.1 k	4.62 M
P-CNN	0.809	354 k	15.5 M
ParticleNet	0.844	370 k	540 M
ParT	0.861	$2.14\mathrm{M}$	$340\mathrm{M}$
ParT (plain)	0.849	2.13 M	260 M

Top-Tagging

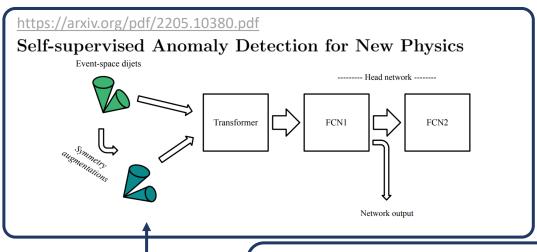
	Accuracy
P-CNN	0.930
PFN	_
ParticleNet	0.940
JEDI-net (w/ $\sum O$)	0.930
PCT	0.940
LGN	0.929
rPCN	_
LorentzNet	0.942
ParT	0.940
ParticleNet-f.t.	0.942
ParT-f.t.	0.944

(Also best in quark-gluon tagging)

Particle Physics

Contrastive

Learning



https://arxiv.org/pdf/2203.05687.pdf A Holistic Approach to Predicting Top Quark Kinematic Properties with the Covariant Particle Transformer Top quarks Final state objects Top quarks Covariant Self-attention Covariant Self-attention Decoder 6 layers x 6 blocks Covariant Cross-attention Encoder Covariant Self-attention Final state objects Final state objects

(b) Encoder

https://arxiv.org/pdf/2108.04253.pdf

Symmetries, Safety, and Self-Supervision

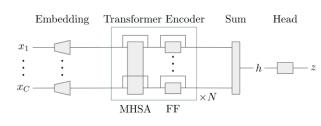
The goal of our network is to define a mapping between the jet constituents and a representation space,

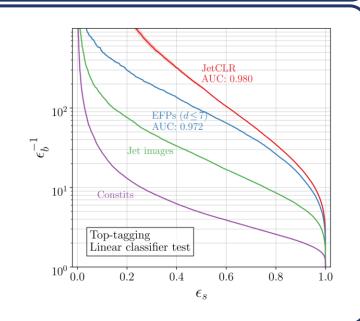
$$f: \mathcal{J} \to \mathcal{R}$$
, (1)

(a) CPT

which is, both,

- 1. invariant to symmetries and theory-driven augmentations, and
- 2. discriminative within the dataset it is optimized on.





(c) Decoder

Summary

- Transformer: Based on attention mechanism
- New State-of-the art in many fields
 - Natural language processing
 - Image recognition
 - •
- Large amounts of VRAM needed to analyze long sequences
 - Alternatives (Reformer, Sparse Transformer, Perceiver) exist, but some are less accessible
- Easily applicable to many different tasks, due to being domain agnostic
 - Quickly spreading to more branches of machine learning
 - Usage of transformers in physics at an early stage with promising results

