

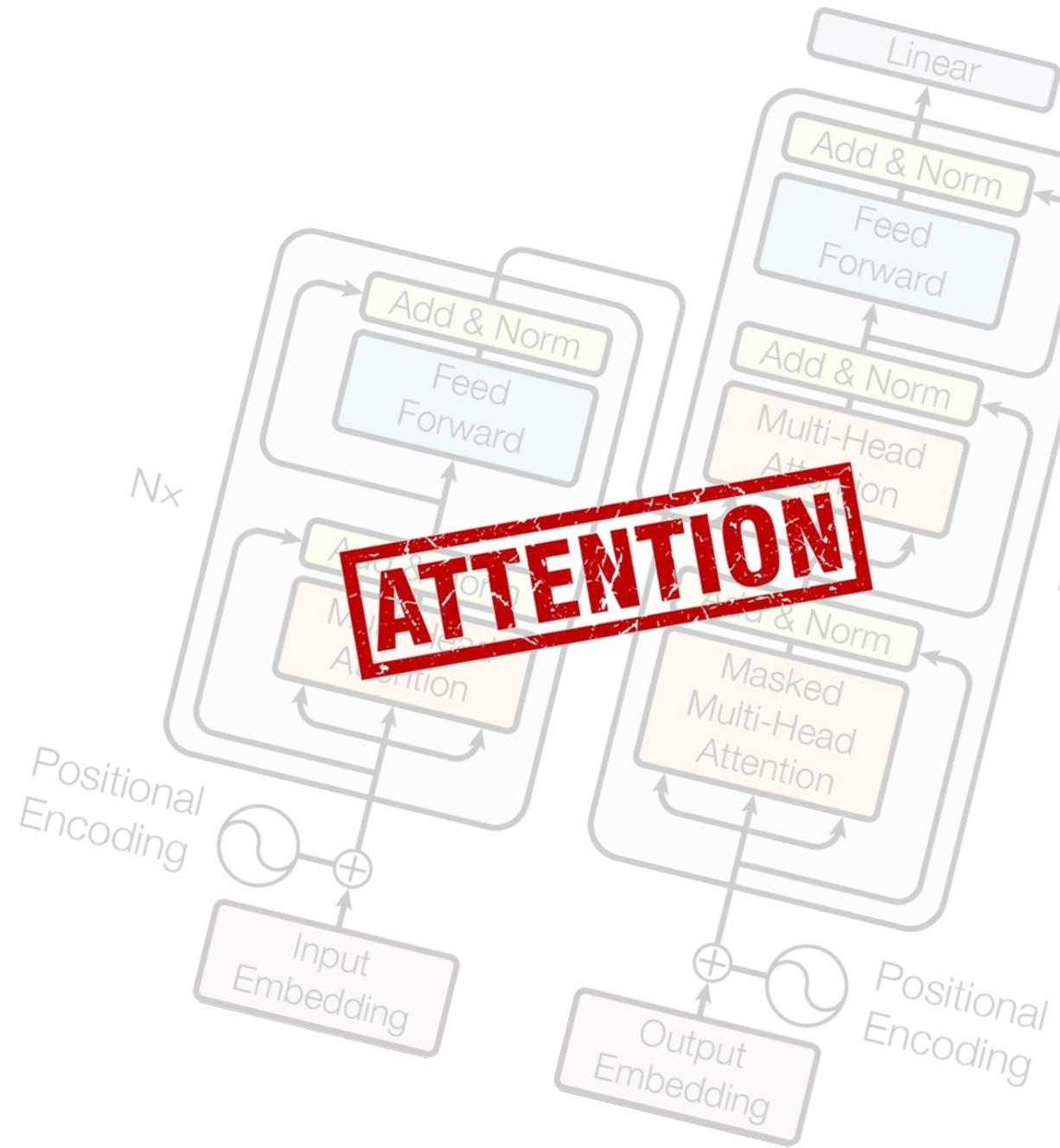


# Transformers

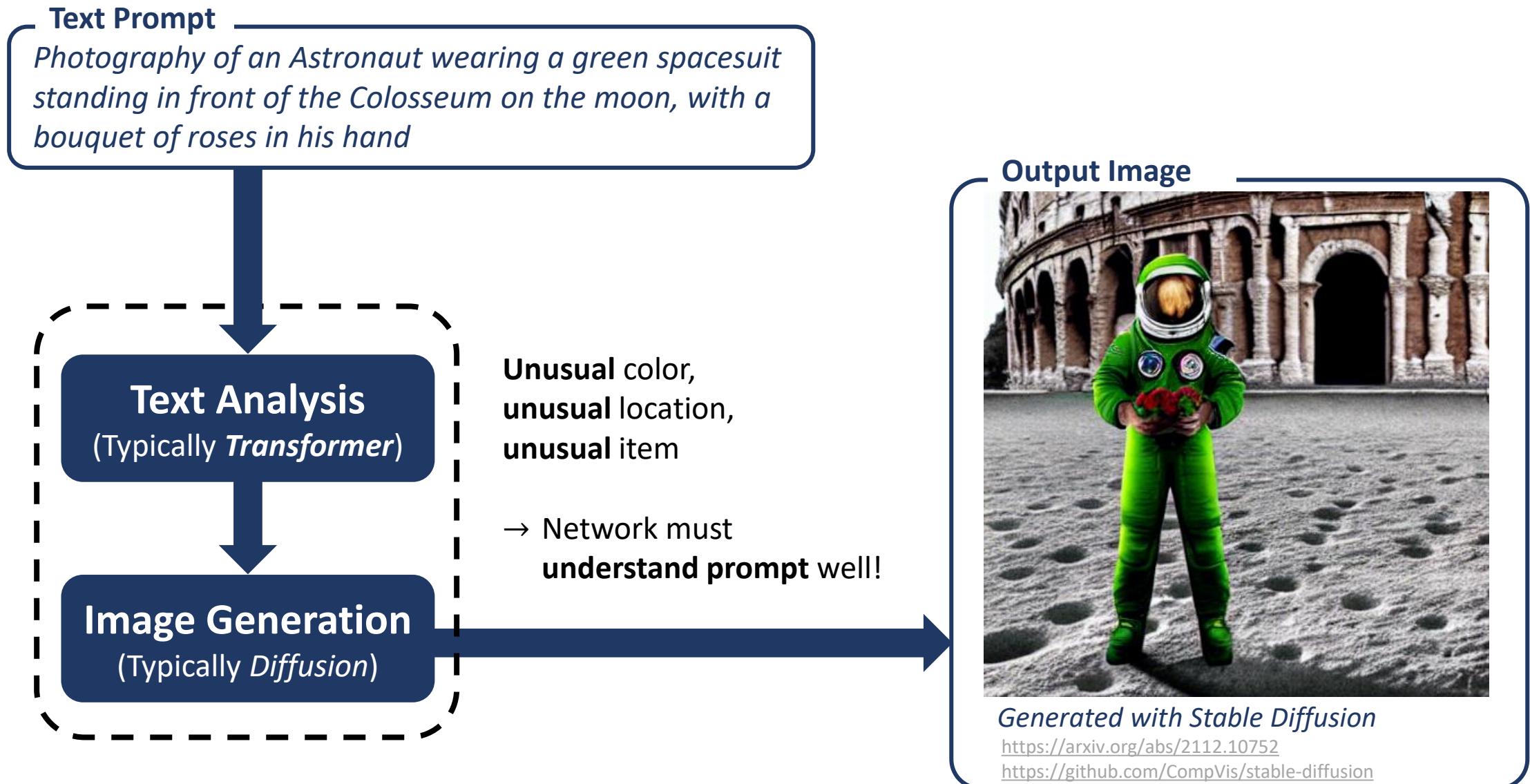
Active Training Course  
"Advanced Deep Learning"



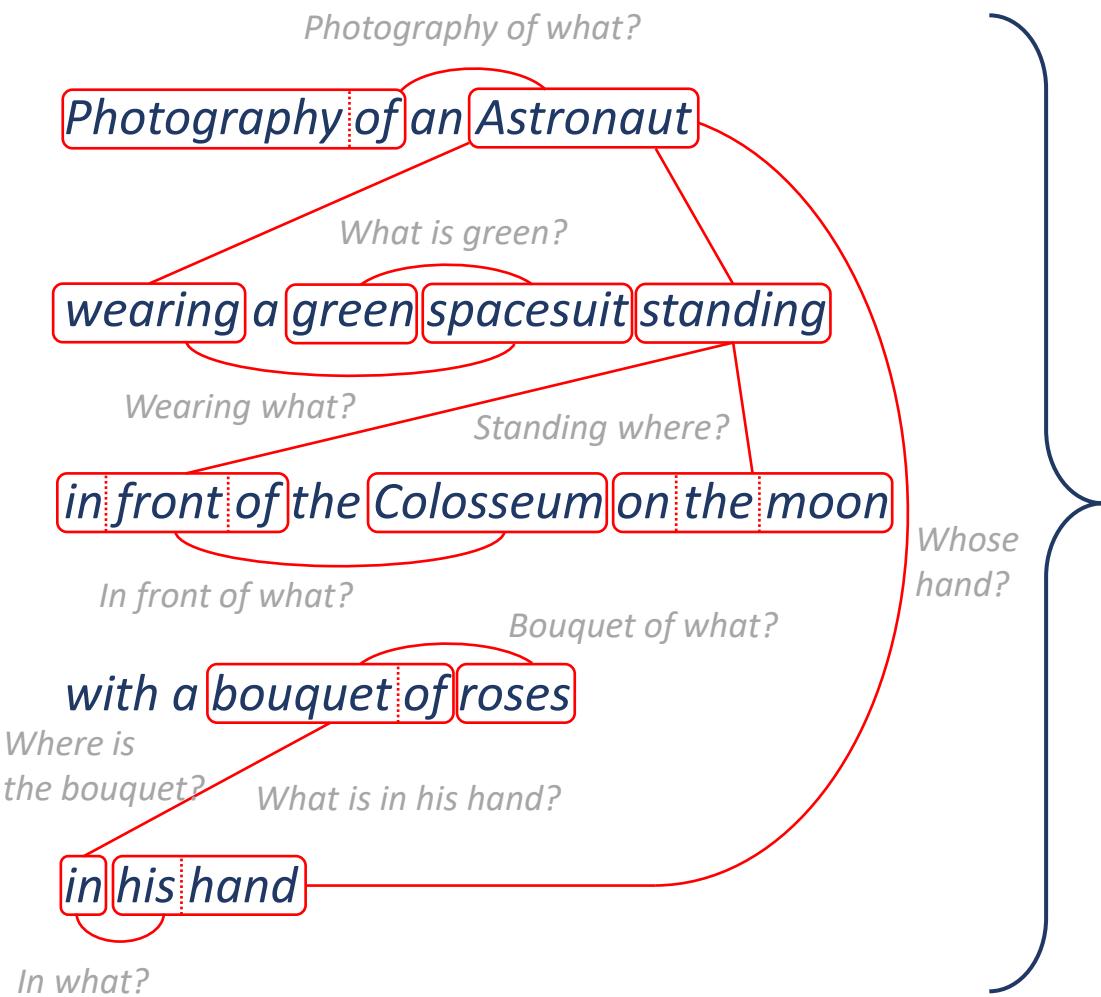
Niklas Langner  
RWTH Aachen University



# Current Hype: Text-to-Image Models



# 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 → **How does it work?**

# Natural Language Processing

## Example: Sequence to sequence translation

Attention is all you need

$$x = \{x_1, x_2, x_3, x_4, x_5\}$$

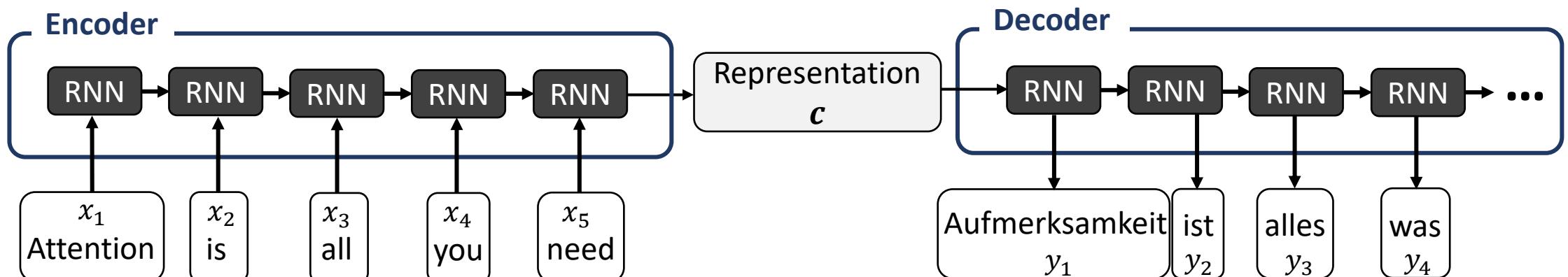
Aufmerksamkeit ist alles, was du brauchst

$$y = \{y_1, y_2, y_3, y_4, y_5, y_6\}$$

Inputs and outputs: Embedding vectors corresponding to specific words

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!



Ich mag dein Haus, **es** ist toll!

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



Ich mag deinen Hund, **er** ist toll!

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

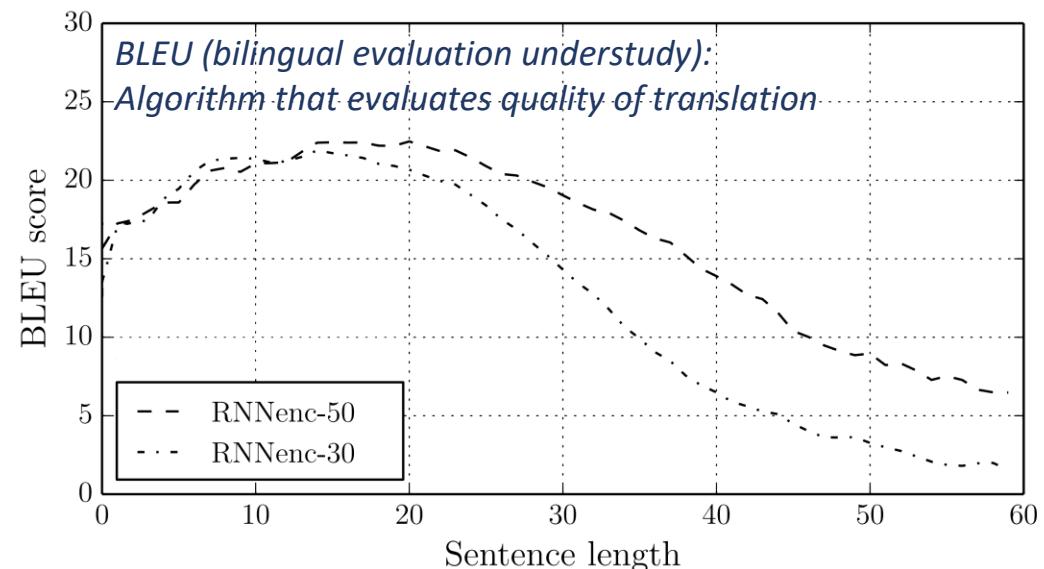


Ich mag deine Katze, **sie** ist toll!

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**

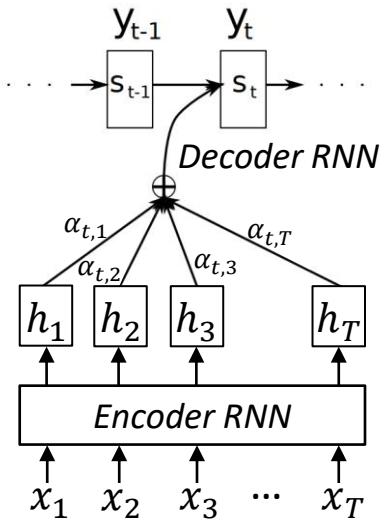
**In practice:** Only works well for **small sequences** (<20 timesteps) due to too small gradients in regard to far away timesteps



# Solution: Attention

Use intermediate results of RNN layers and **combine them using weights  $\alpha$  (alignment score)**

## Attention Example

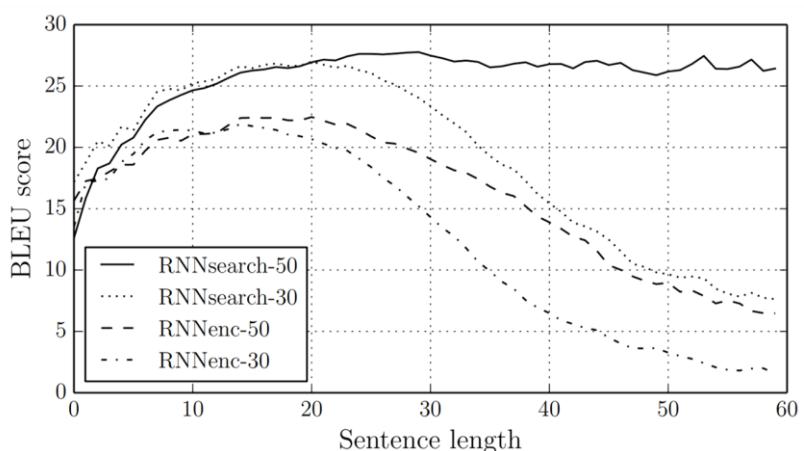


$$s_i = f(s_{t-1}, y_{i-1}, c_i)$$
$$\alpha_{ij} = \frac{\exp(e_{ij})}{\sum_{k=1}^{T_x} \exp(e_{ik})}$$

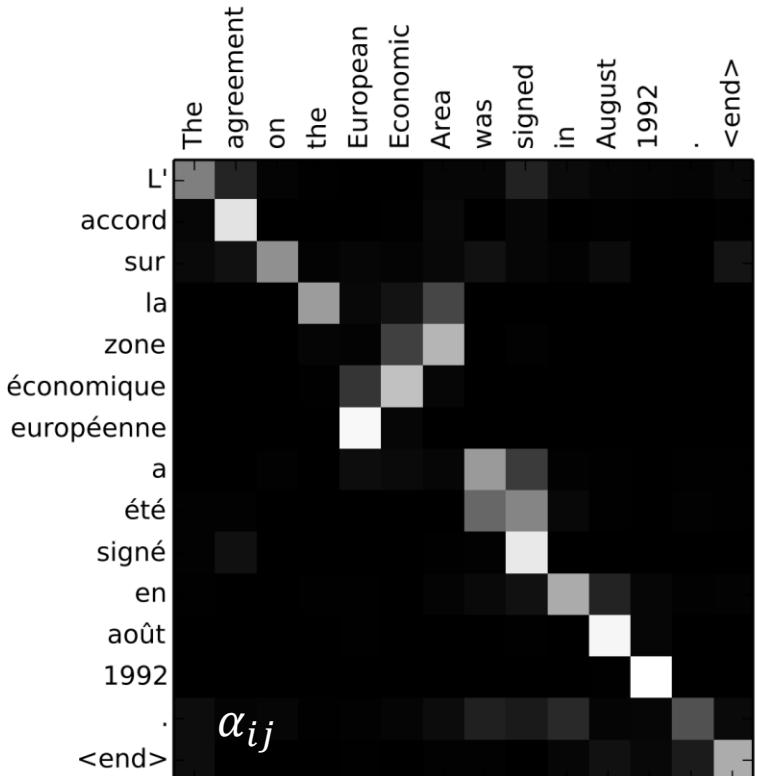
softmax

$e_{ij} = \text{score}(s_{t-1}, h_j)$   
Alignment Score Function

Different for each step!



Greatly improves  
performance translating  
long sentences



<https://arxiv.org/abs/1409.0473>

# Attention Mechanisms

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

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

*Commonly used  
neural network approach*

**Alignment score:**  
Many different options

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

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



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

<https://arxiv.org/abs/1601.06733>

# Attention Is All You Need

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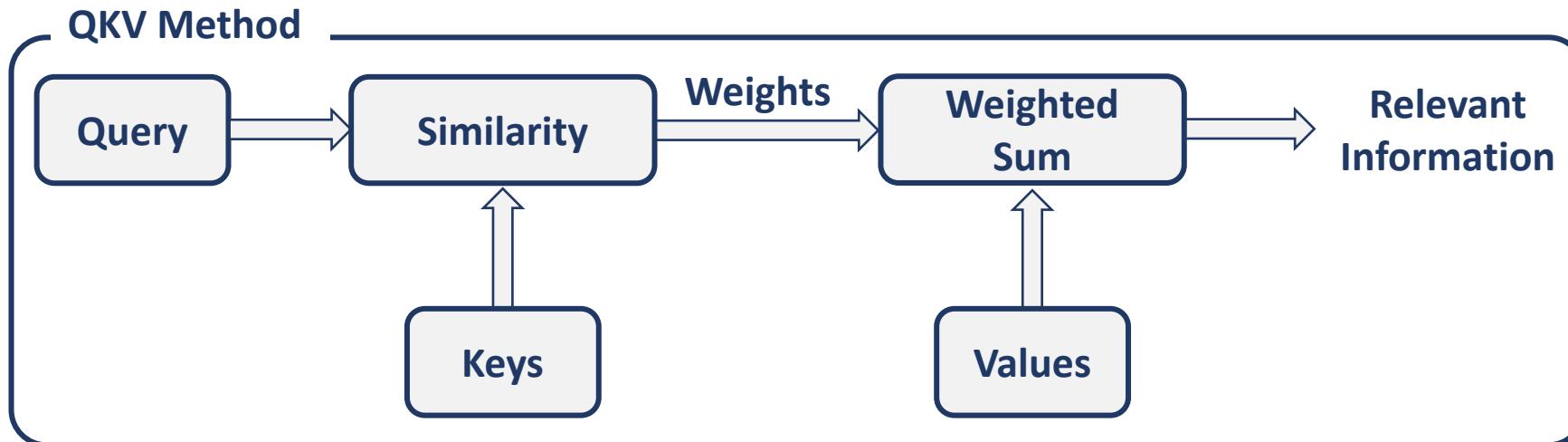
## Abstract

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:**

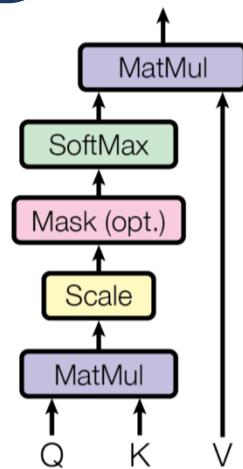
$$\text{score}(s_{i-1}, h_j) = \frac{s_{i-1}^T h_j}{\sqrt{n}}$$



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

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

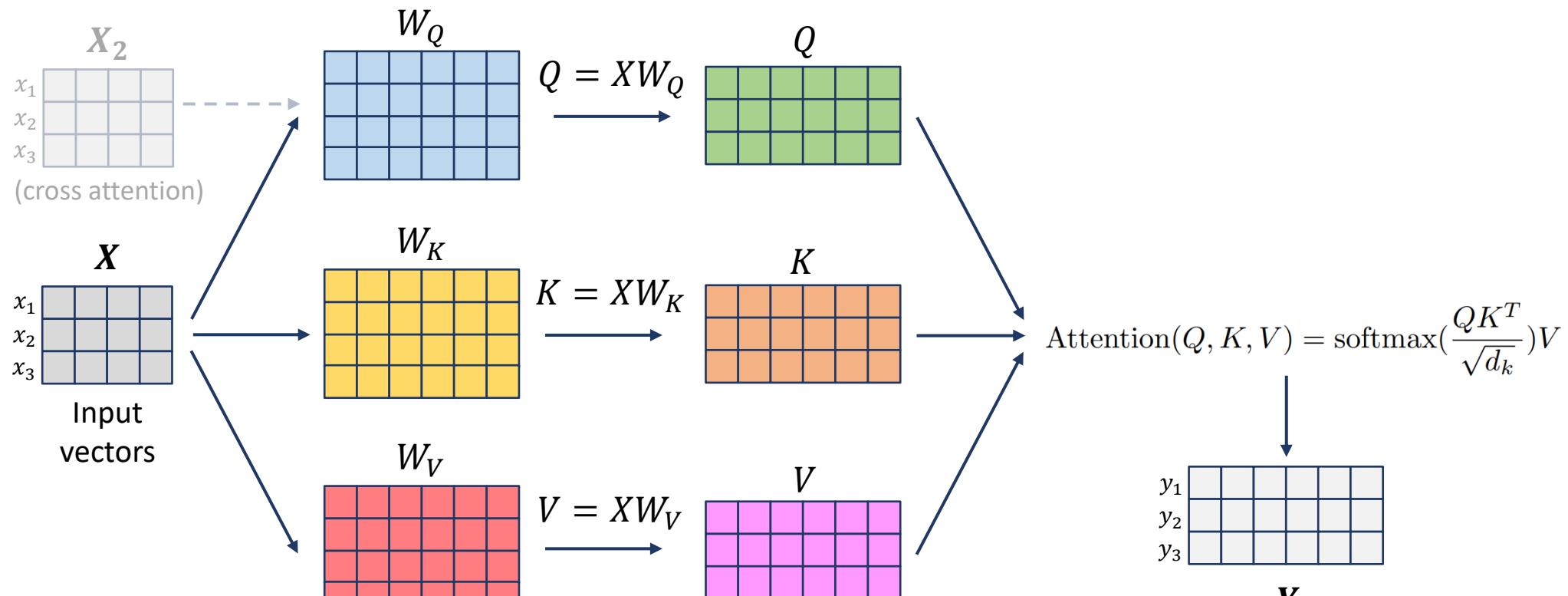
$d_k$ : length of keys vector



<https://arxiv.org/abs/1706.03762>

# QKV-Self-Attention Implementation

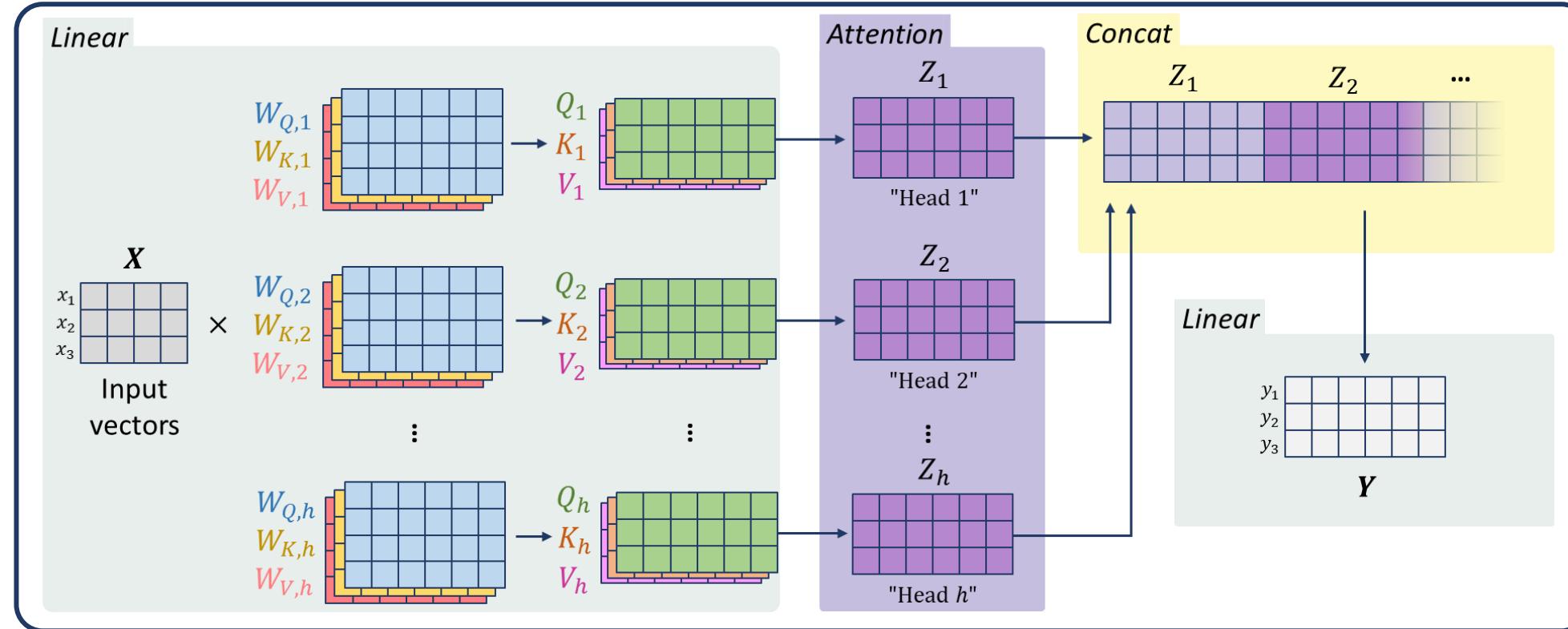
Parallelize by using **matrix operations**



**Here:** Always use  $X \rightarrow$  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!

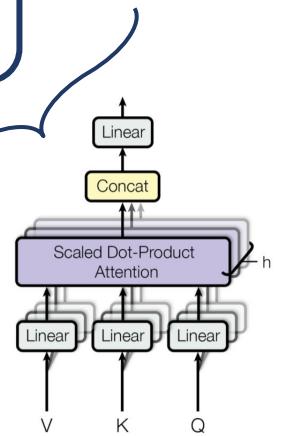
→ Can be **trained in parallel** on multiple GPUs

→ Enables **training on huge** datasets in reasonable time

Input treated as set instead of sequence → permutation invariant  $\lightning$

→ Use **positional encoding**!

**Building block  
of transformer**

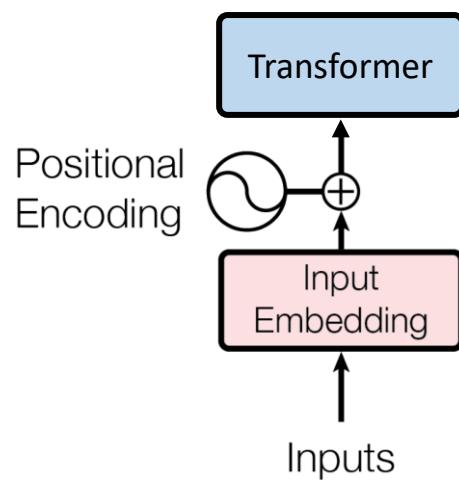


<https://arxiv.org/abs/1706.03762>

# 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**:



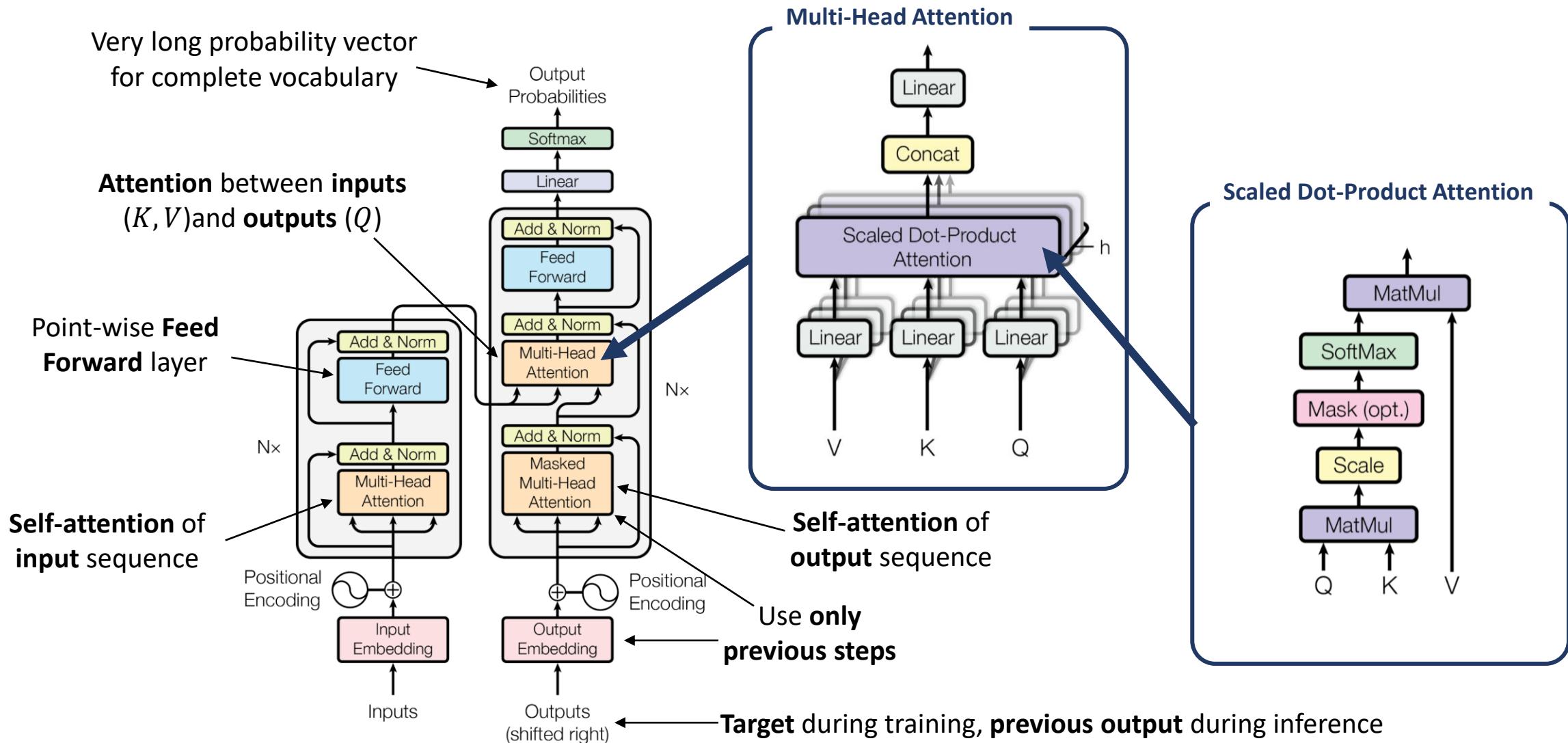
## Example

$$PE(i, \delta) = \begin{cases} \sin\left(\frac{i}{10000^{2\delta'/d}}\right) & \text{if } \delta = 2\delta' \\ \cos\left(\frac{i}{10000^{2\delta'/d}}\right) & \text{if } \delta = 2\delta' + 1 \end{cases}$$

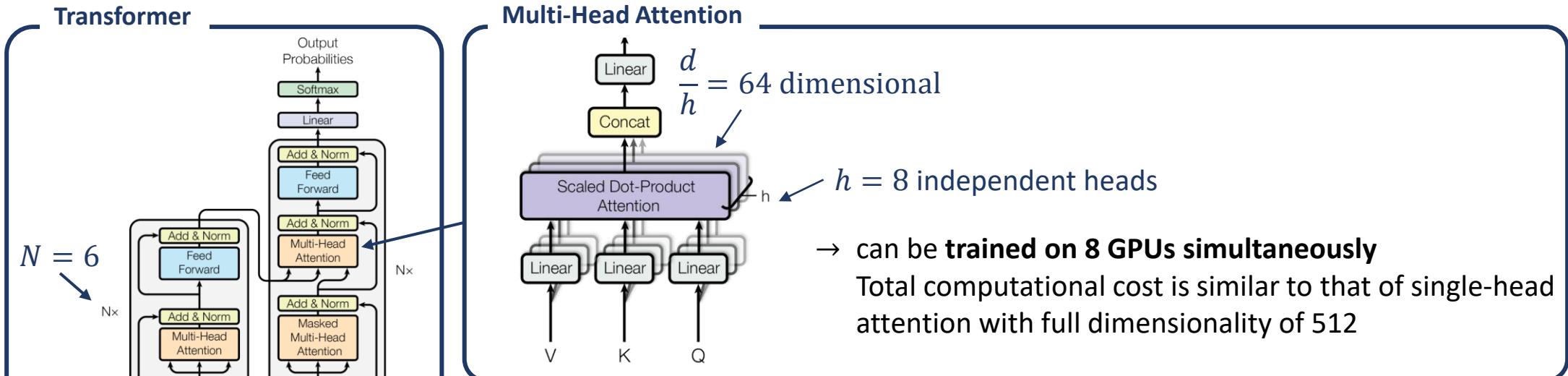
$i$ : word position  
 $\delta$ : vector dimension  
 $d$ : vector length in network



# Full Transformer Architecture



# Text Translation with Transformer



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	<b>41.29</b>	$7.7 \cdot 10^{19}$	$1.2 \cdot 10^{21}$
Transformer (base model)	27.3	38.1	<b><math>3.3 \cdot 10^{18}</math></b>	
Transformer (big)	<b>28.4</b>	<b>41.8</b>	$2.3 \cdot 10^{19}$	

<https://arxiv.org/abs/1706.03762>

# Impact of Transformers – Language Processing

 <https://gluebenchmark.com/leaderboard>

Rank	Name	Model	URL 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-Sinic	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)
  - **OpenAI 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 AI pair programmer

GitHub Copilot uses the OpenAI 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?

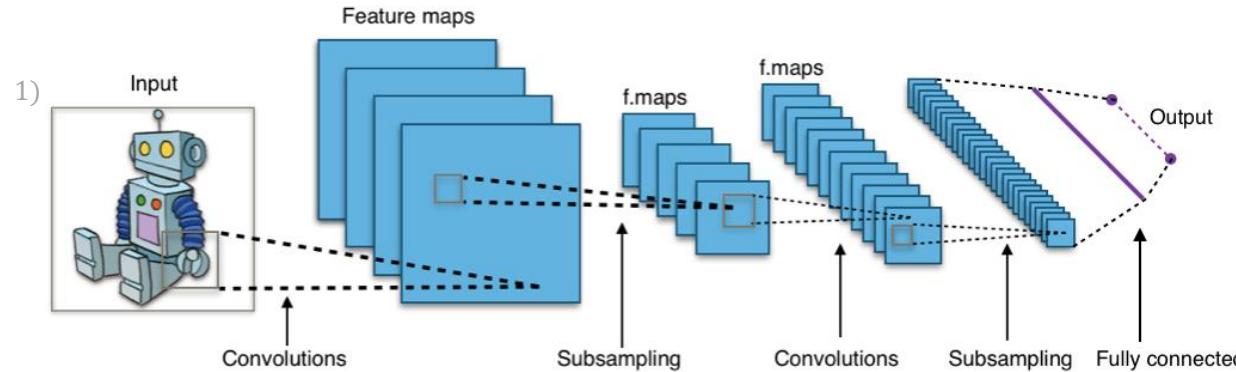
Sir Edmund Hillary and Tenzing Norgay from Nepal were the first to summit Mount Everest in May 1953. They were joined by several others at different times in the successful attempt.



*...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**

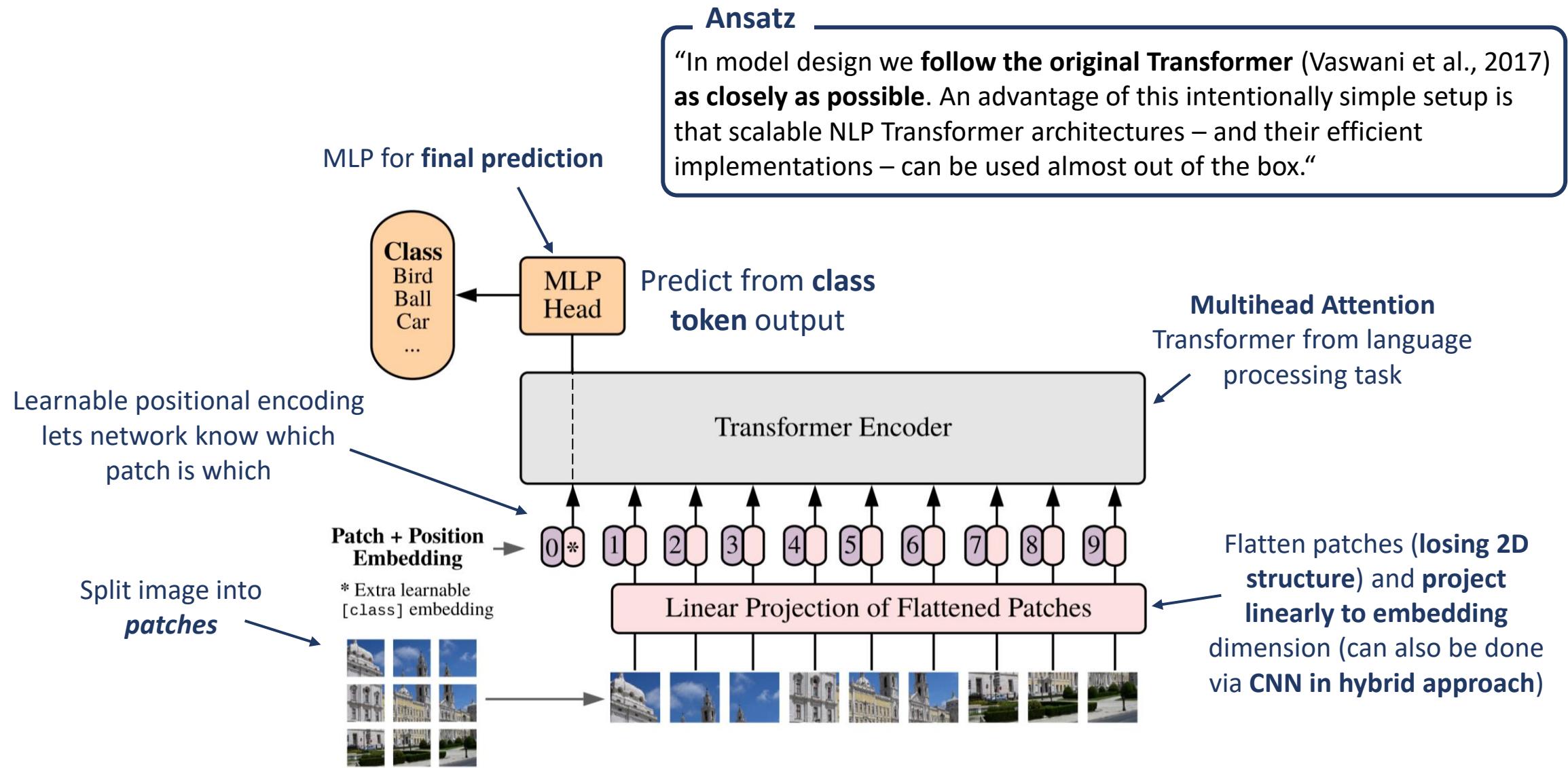
*“Looking forward to the next generation of **scalable vision models**, one might ask whether this domain-specific design is necessary, or if one could successfully leverage **more domain agnostic and computationally efficient architectures** to achieve state-of-the-art results.”*

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

⇒ **Vision Transformer**

<sup>1)</sup> [https://commons.wikimedia.org/wiki/File:Typical\\_cnn.png](https://commons.wikimedia.org/wiki/File:Typical_cnn.png)

# Vision Transformer (ViT)



<https://arxiv.org/abs/2010.11929>

# Vision Transformer Performance

Model	Layers	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

	Transformers			CNNs	
	Ours-JFT (ViT-H/14)	Ours-JFT (ViT-L/16)	Ours-I21k (ViT-L/16)	BiT-L (ResNet152x4)	Noisy Student (EfficientNet-L2)
ImageNet	<b>88.55</b> ± 0.04	87.76 ± 0.03	85.30 ± 0.02	87.54 ± 0.02	88.4/88.5*
ImageNet ReaL	<b>90.72</b> ± 0.05	90.54 ± 0.03	88.62 ± 0.05	90.54	90.55
CIFAR-10	<b>99.50</b> ± 0.06	99.42 ± 0.03	99.15 ± 0.03	99.37 ± 0.06	—
CIFAR-100	<b>94.55</b> ± 0.04	93.90 ± 0.05	93.25 ± 0.05	93.51 ± 0.08	—
Oxford-IIIT Pets	<b>97.56</b> ± 0.03	97.32 ± 0.11	94.67 ± 0.15	96.62 ± 0.23	—
Oxford Flowers-102	99.68 ± 0.02	<b>99.74</b> ± 0.00	99.61 ± 0.02	99.63 ± 0.03	—
VTAB (19 tasks)	<b>77.63</b> ± 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

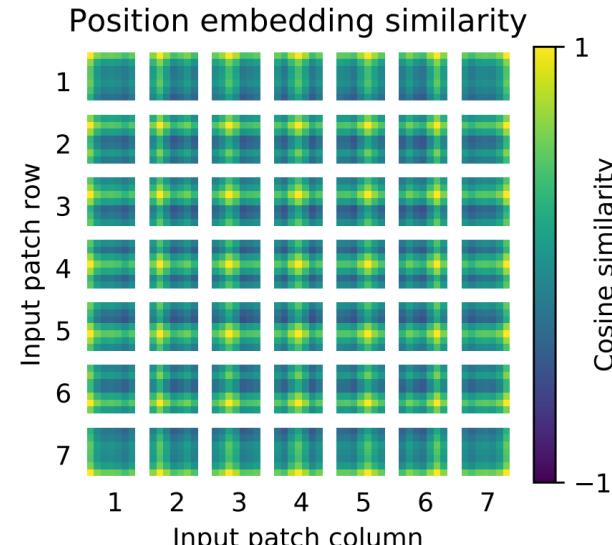
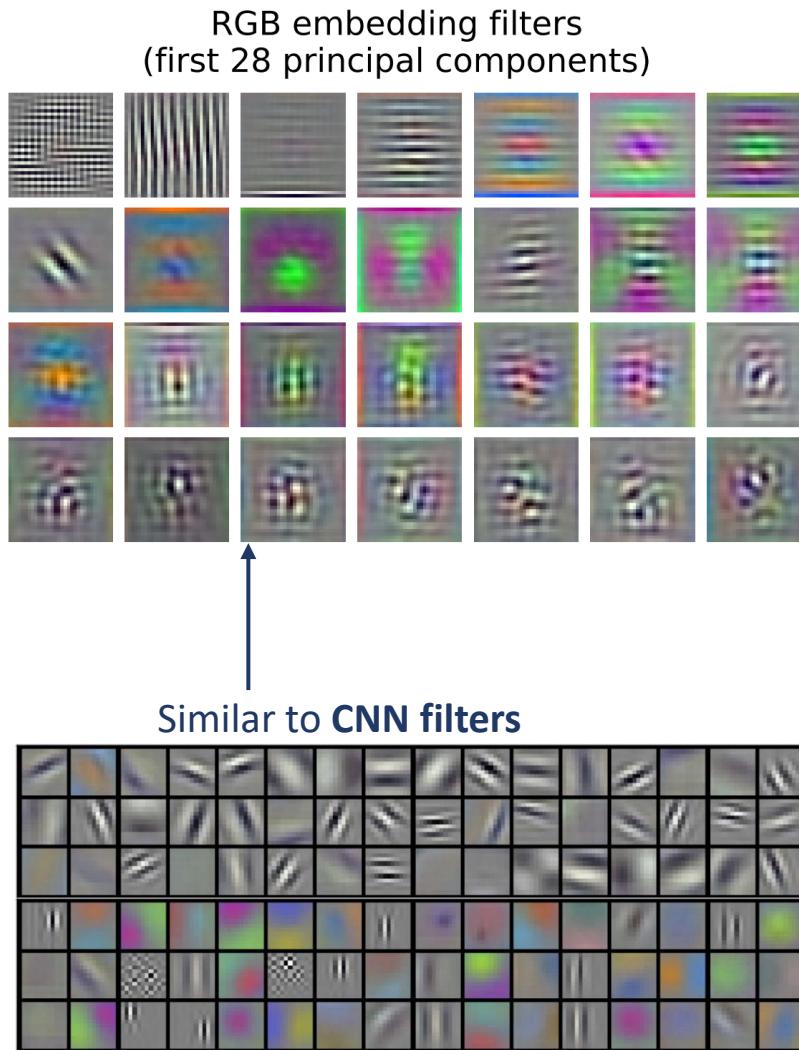
Transformer: More efficient

“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**.”

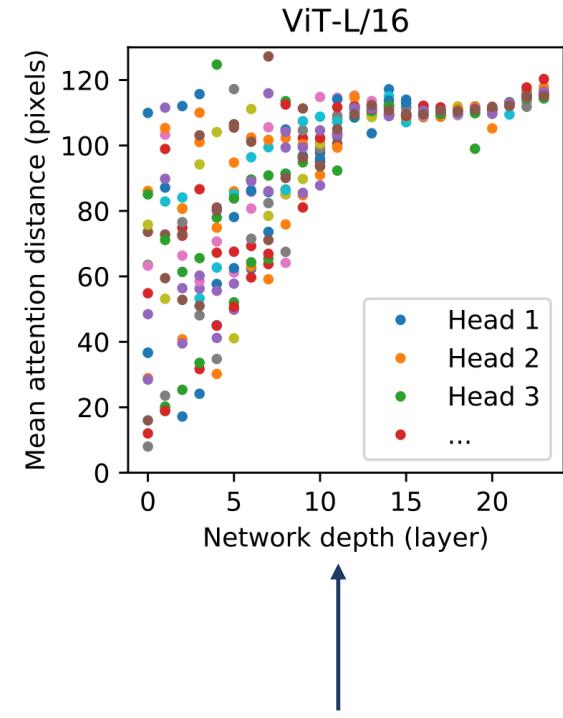
- ⇒ **Vision Transformer** already **outperforms (highly-optimized) CNNs**, despite using architecture created for language processing

<https://arxiv.org/abs/2010.11929>

# Vision Transformer Insight

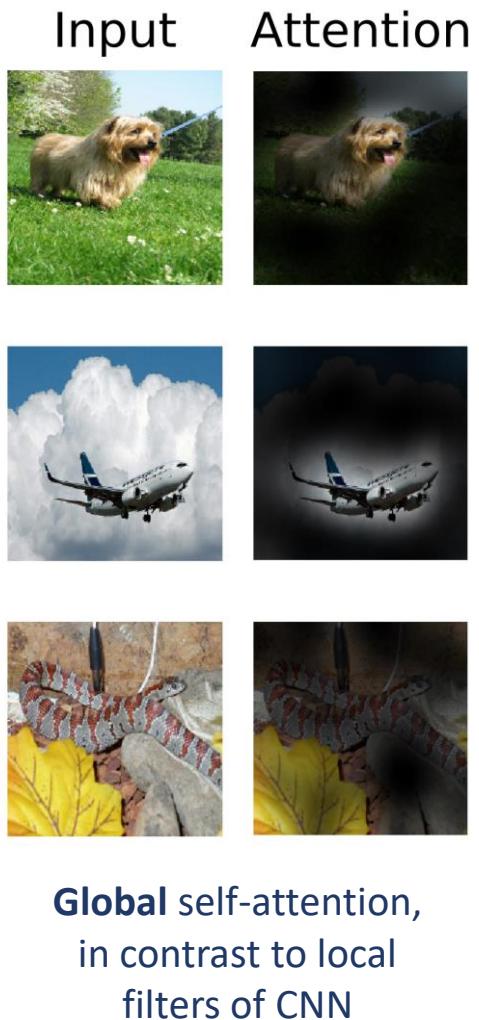


Position embedding includes incorporated  
**2D structure**



**Starts at small scale and**  
**step by step increases**  
**scope (like CNN)**

# Vision Transformer Insight

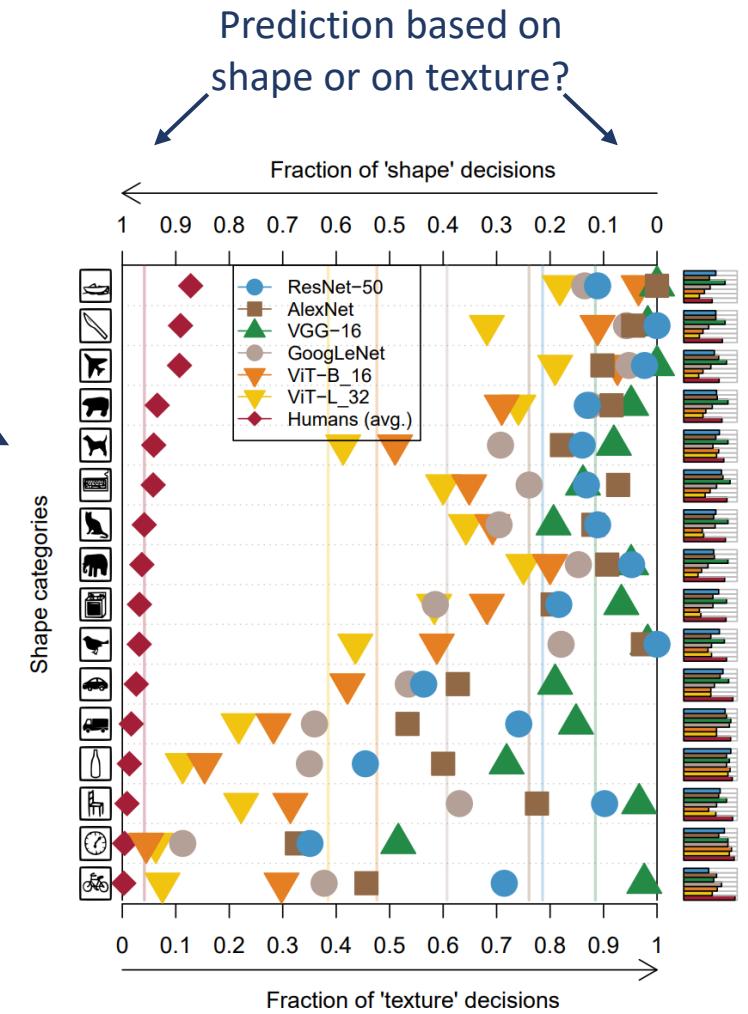


Shape = Cat, Texture = Elephant



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

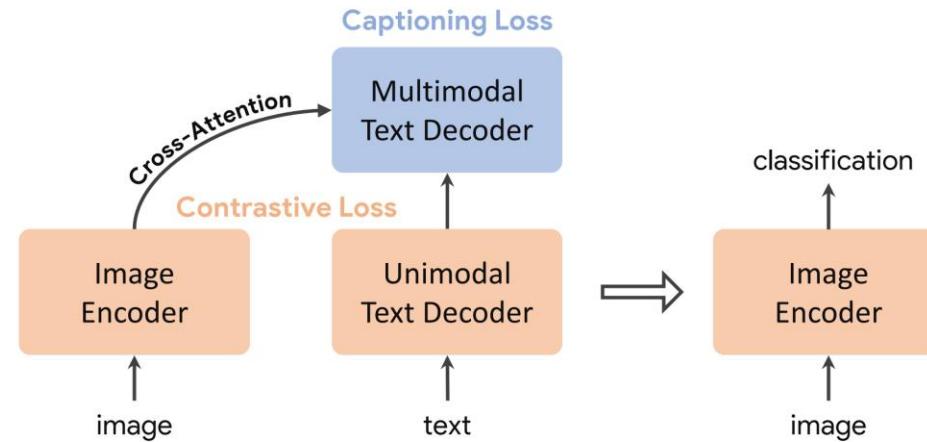
Image Classification on ImageNet:

Rank	Model	Top 1 Accuracy	Top 5 Accuracy	Number of params	Year	Tags
1	CoCa (finetuned)	91.0%		2100M	2022	ALIGN, Transformer, JFT-3B
2	Model soups (BASIC-L)	90.98%		2440M	2022	Conv+Transformer, JFT-3B, ALIGN
3	Model soups (ViT-G/14)	90.94%		1843M	2022	JFT-3B, Transformer
4	ViT-e	90.9%		3900M	2022	Transformer, JFT-3B

<https://paperswithcode.com/sota/image-classification-on-imagenet>

CoCa

"Contrastive Captioners are Image-Text Foundation Models"



CoCa

Visual Recognition  
(single-encoder models)

"These results suggest the proposed framework **efficiently combines text training signals** and thus is able to **learn high-quality visual representation** better than the classical single-encoder approach."

<https://arxiv.org/abs/2205.01917>

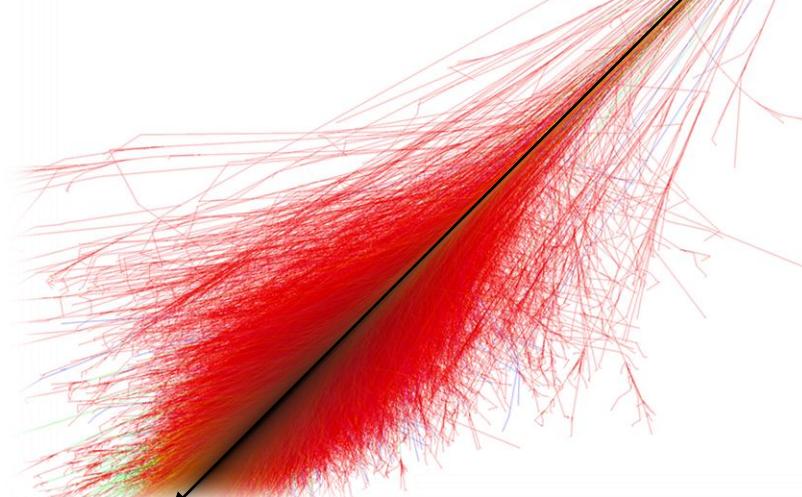
Transformers beat CNNs as state of the art in image recognition!

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

## Extensive Air Showers

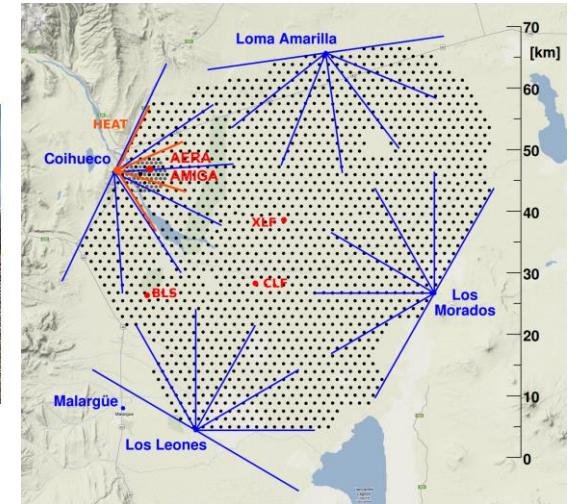
“Primary particle”  
Element? H or Fe?

Interaction atmosphere  
→ Extensive Air Shower



Surface Detector

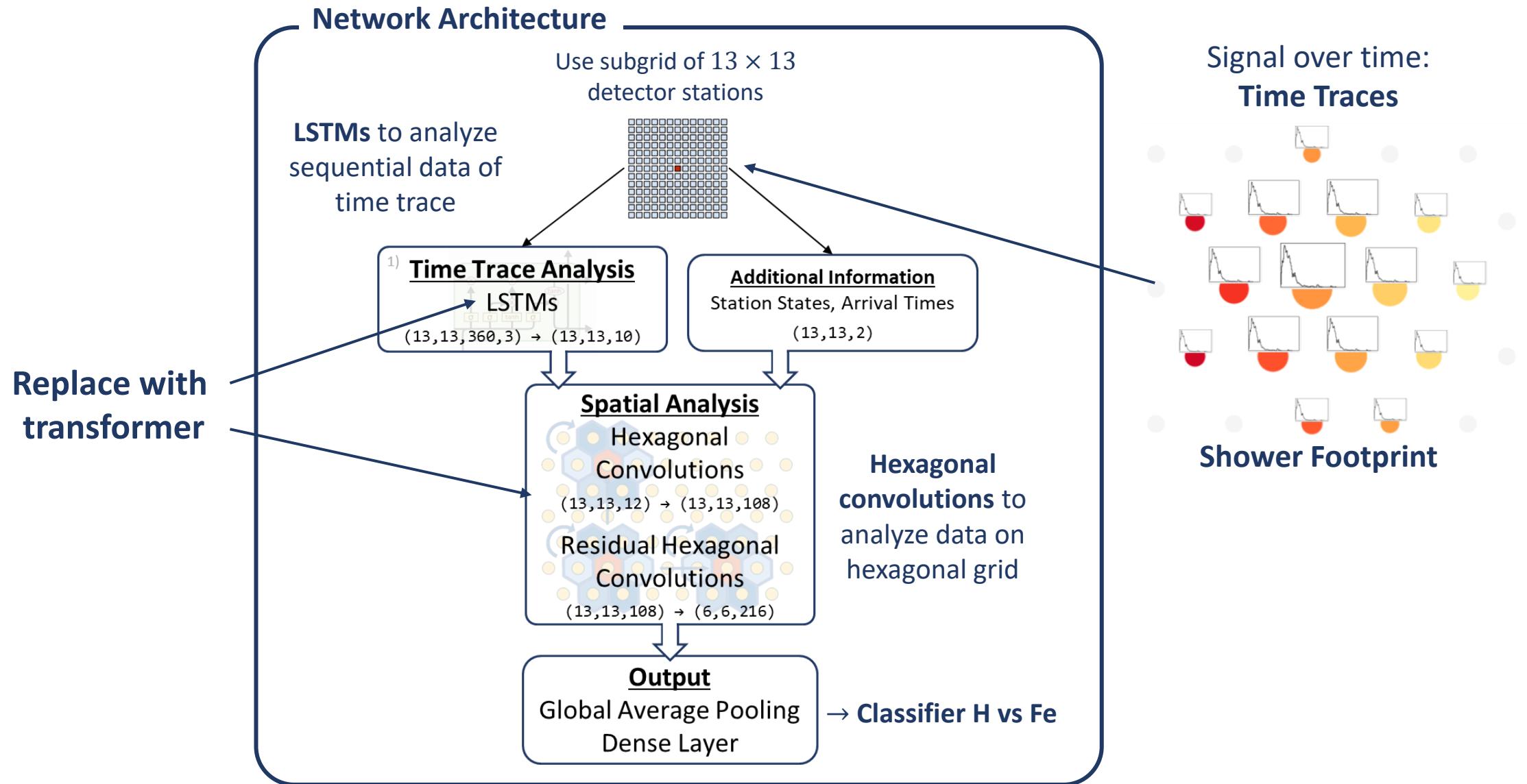
## Pierre Auger Observatory Surface Detector



- Located in the *Pampa Amarilla* near Malargüe, Argentina
- Covers an area of roughly  $3000 \text{ km}^2$
- **Hexagonal grid** of 1660 water-Cherenkov stations
- Sample air shower footprint

Shower Image Credit: <https://www-zeuthen.desy.de/~jknapp/fs/proton-showers.html>

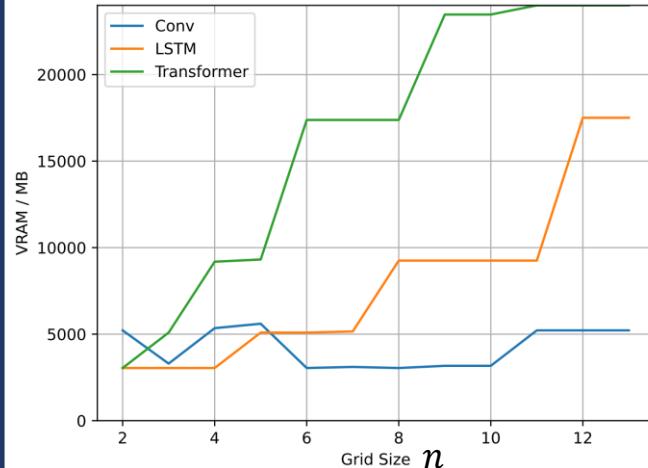
# Cosmic-Ray Mass Reconstruction Neural Network



# Challenges of Transformer Application

## Dimensionality Problem

Attention shape:  $(\text{batchsize} \cdot n^2 \cdot N_{\text{head}} \times 360 \times 360)$



$$\mathcal{O}(L^2)$$

Huge VRAM needed!  
→ Not practical

Exemplary alternatives to reduce  $\mathcal{O}(L^2)$ :

**Reformer:**  $\mathcal{O}(L \cdot \log L)$

<https://arxiv.org/abs/2001.04451>

**Sparse Transformers:**  $\mathcal{O}(L \cdot \sqrt{L})$

<https://arxiv.org/abs/1904.10509>

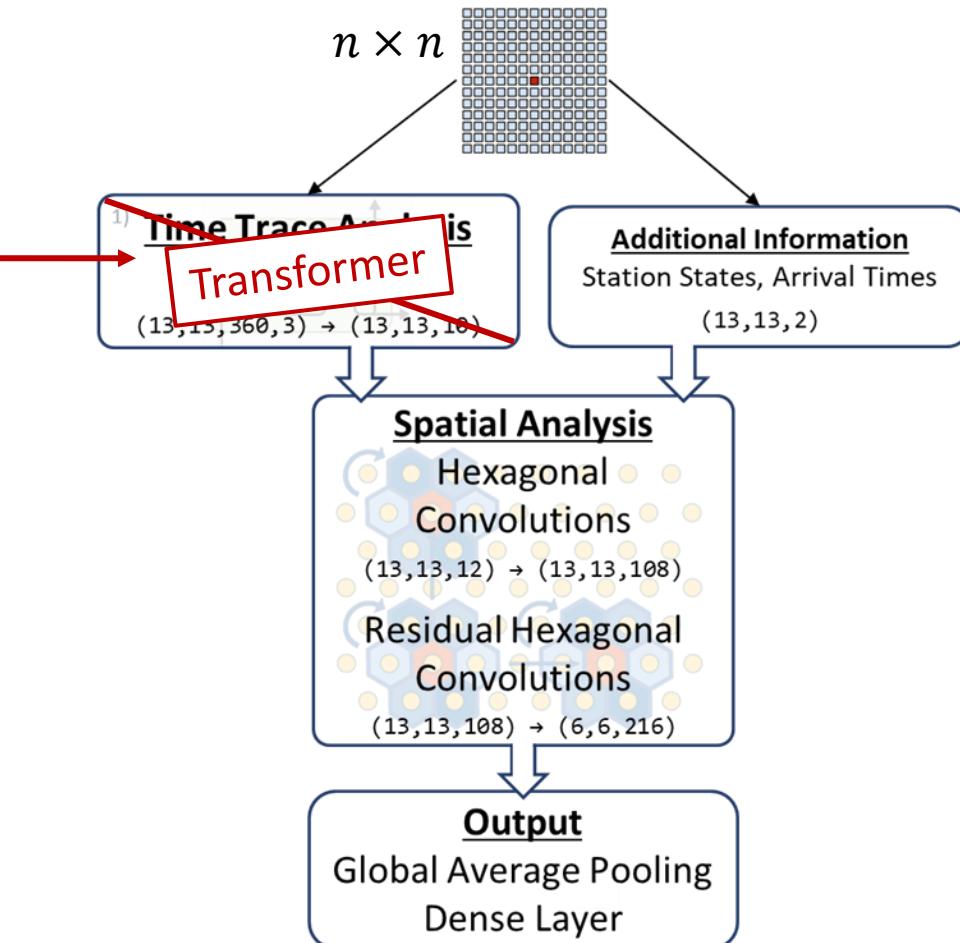
**Perceiver:**  $\mathcal{O}(kL)$

<https://arxiv.org/abs/2107.14795>

many more ...

See <https://arxiv.org/abs/2009.06732> and <https://arxiv.org/abs/2011.04006>

Challenging to implement  
**Very easy to implement**  
(see hands-on session)



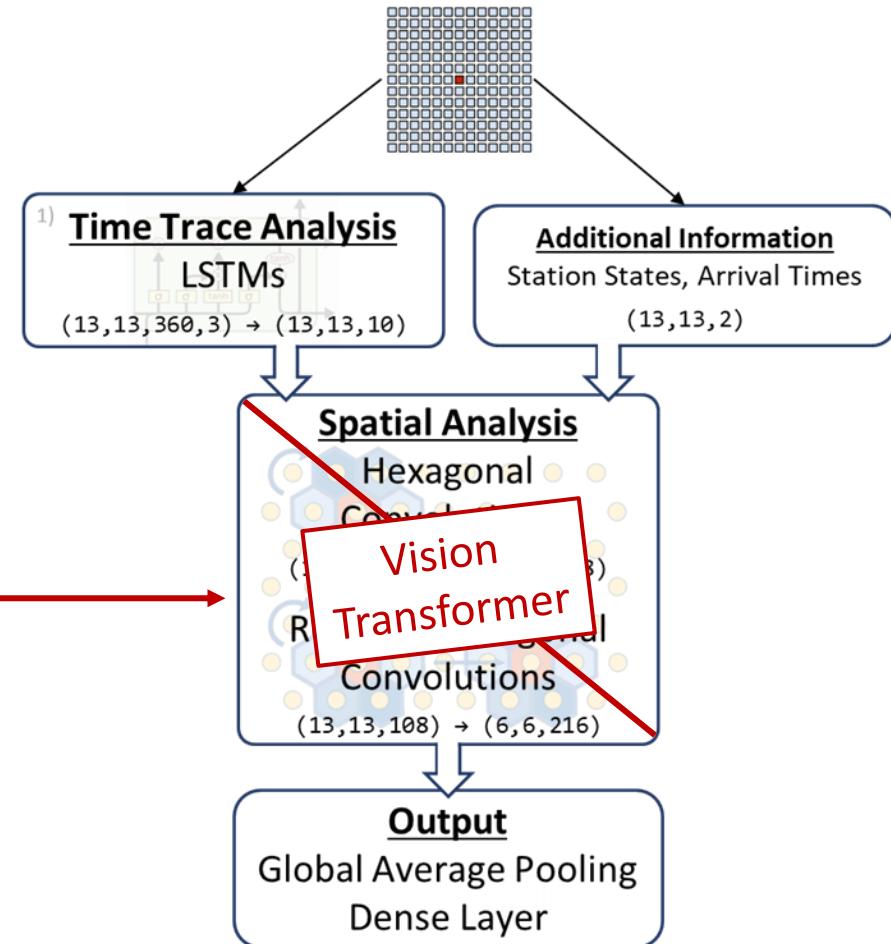
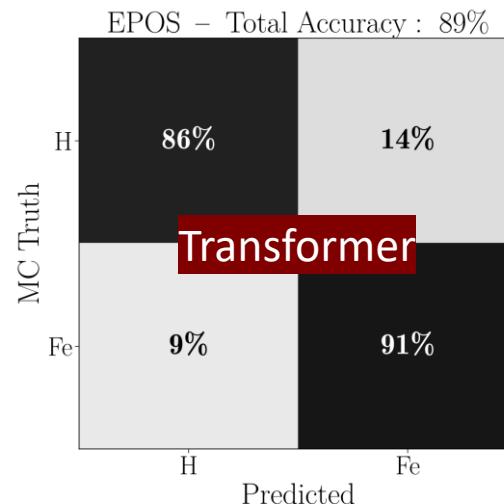
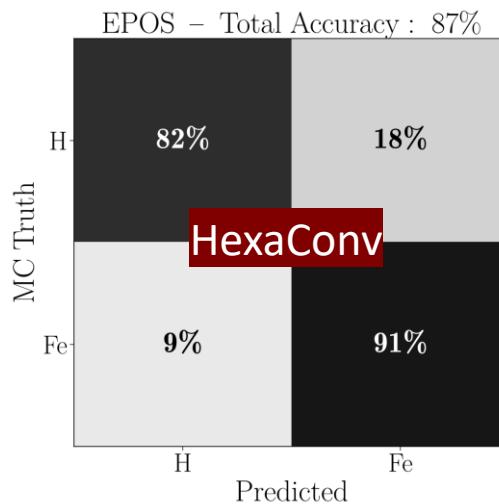
⇒ Default attention quickly needs very large amounts of VRAM if data structure is too large, alternatives exist

1) Image Credit: <https://colah.github.io/posts/2015-08-Understanding-LSTMs/>

# Chances of Transformer Application

## Spatial Transformer

- Use simple, **out of the box vision transformer** to replace hexagonal convolution
- **Loses inherent knowledge of:**
  - Hexagonal symmetry
  - 2D structure
- **Increases number of parameters by factor 17**
- **Reduces training time by 50%**
- **Increases performance!**

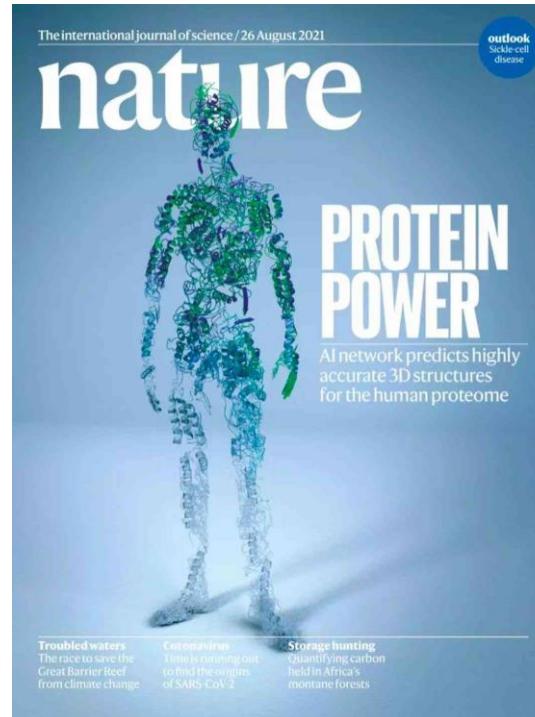
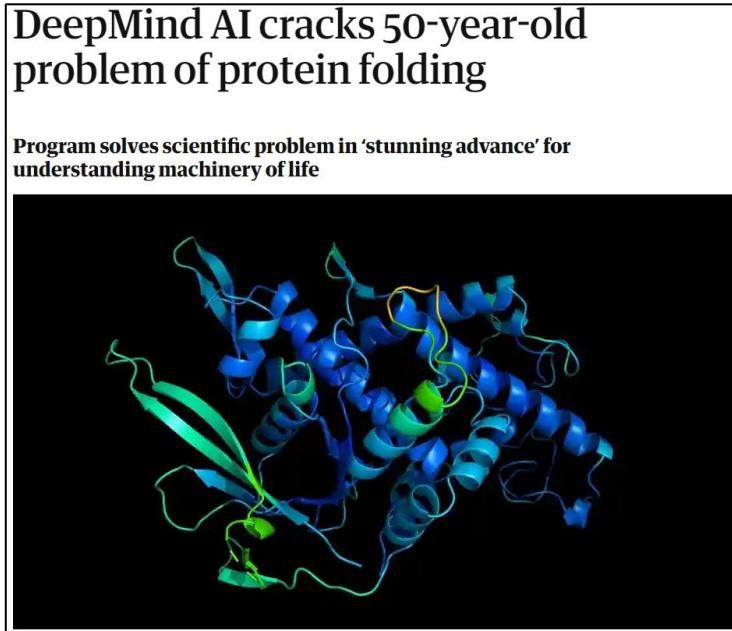


⇒ **Domain agnostic transformer** can be trained quickly, and **outperforms approach focused on data symmetry** (similar to Vision Transformer on images)

1) Image Credit: <https://colah.github.io/posts/2015-08-Understanding-LSTMs/>

# Transformers in Science

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



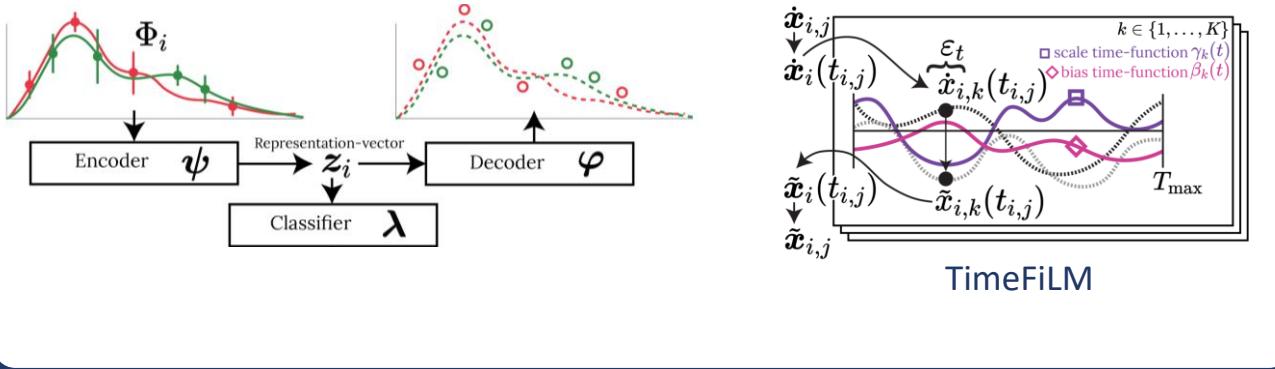
**Famous science application:  
Protein unfolding**

**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

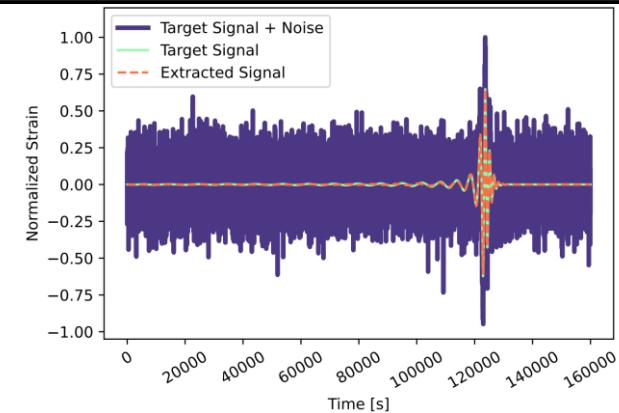
<https://arxiv.org/pdf/2201.08482.pdf>

## Deep Attention-Based Supernovae Classification of Multi-Band Light-Curves



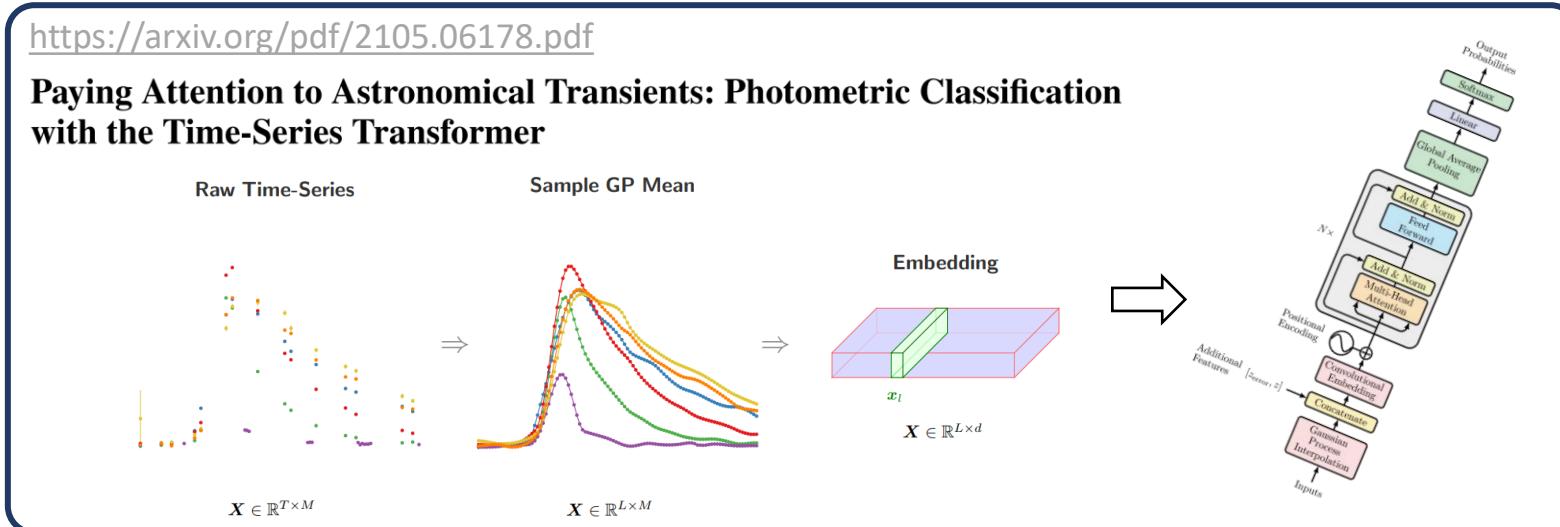
<https://arxiv.org/pdf/2207.07414.pdf>

## SPACE-BASED GRAVITATIONAL WAVE SIGNAL DETECTION AND EXTRACTION WITH DEEP NEURAL NETWORK



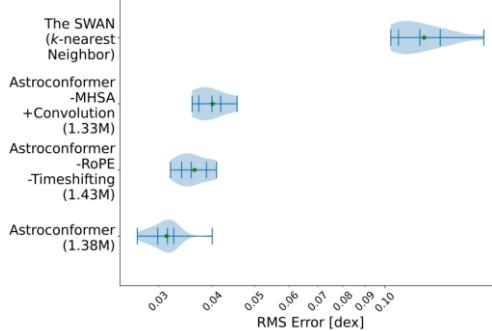
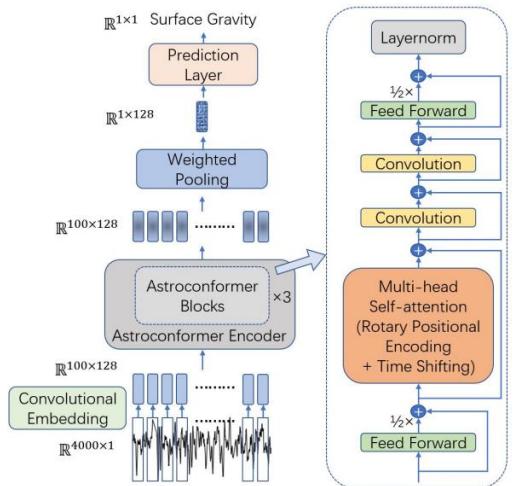
<https://arxiv.org/pdf/2105.06178.pdf>

## Paying Attention to Astronomical Transients: Photometric Classification with the Time-Series Transformer



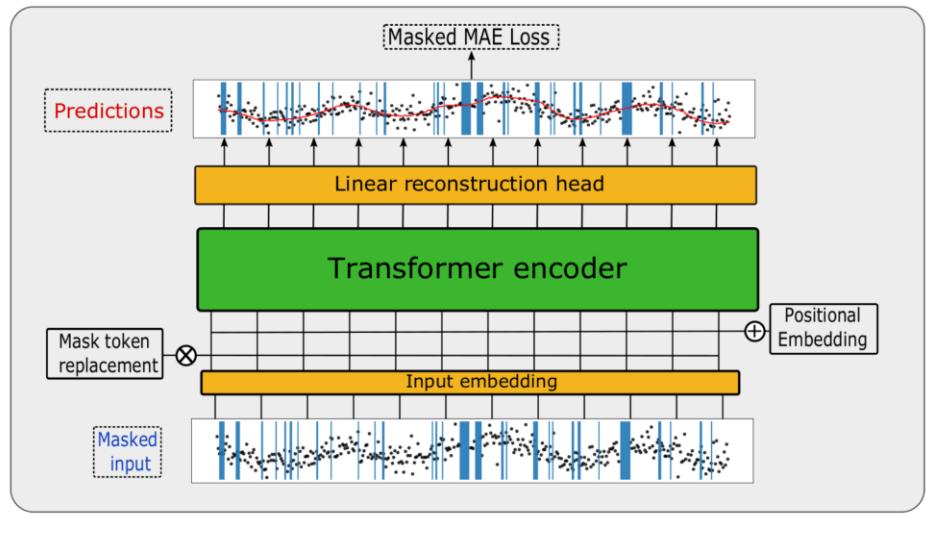
# Time Sequence Analyses

## Astroconformer: Inferring Surface Gravity of Stars from Stellar Light Curves with Transformer



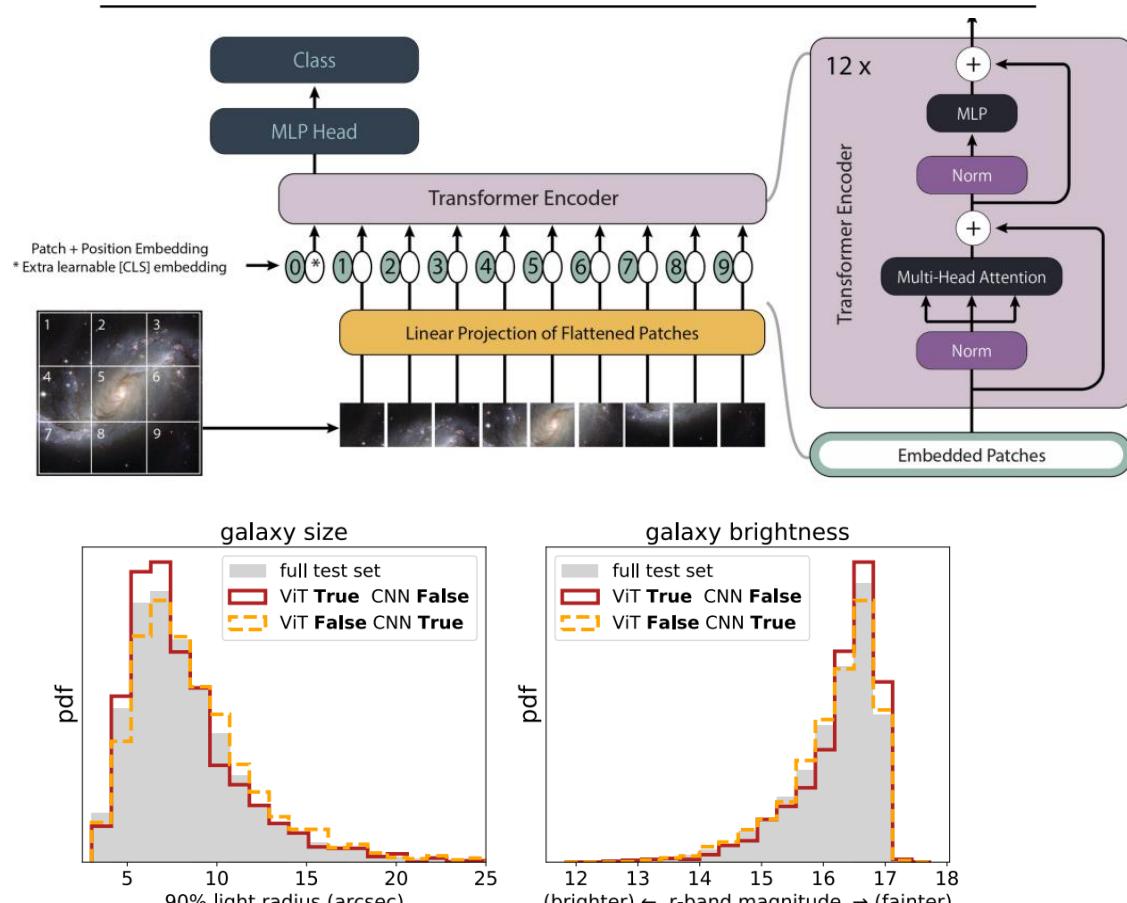
<https://arxiv.org/pdf/2207.02777.pdf>

## Don't Pay Attention to the Noise: Learning Self-supervised Representations of Light Curves with a Denoising Time Series Transformer



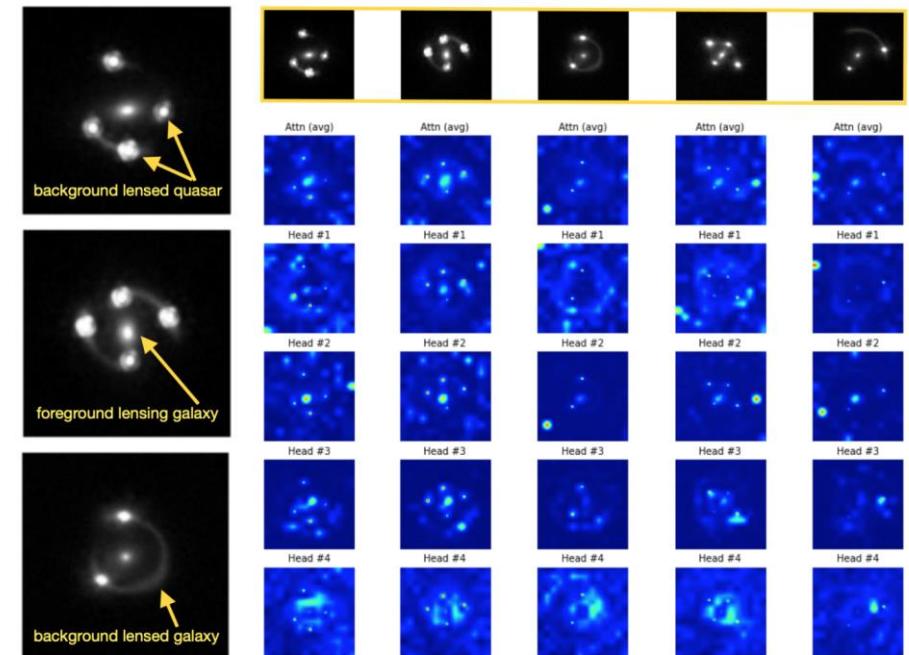
# Vision Transformer Applications

## Galaxy Morphological Classification with Efficient Vision Transformer



<https://arxiv.org/pdf/2110.01024.pdf>

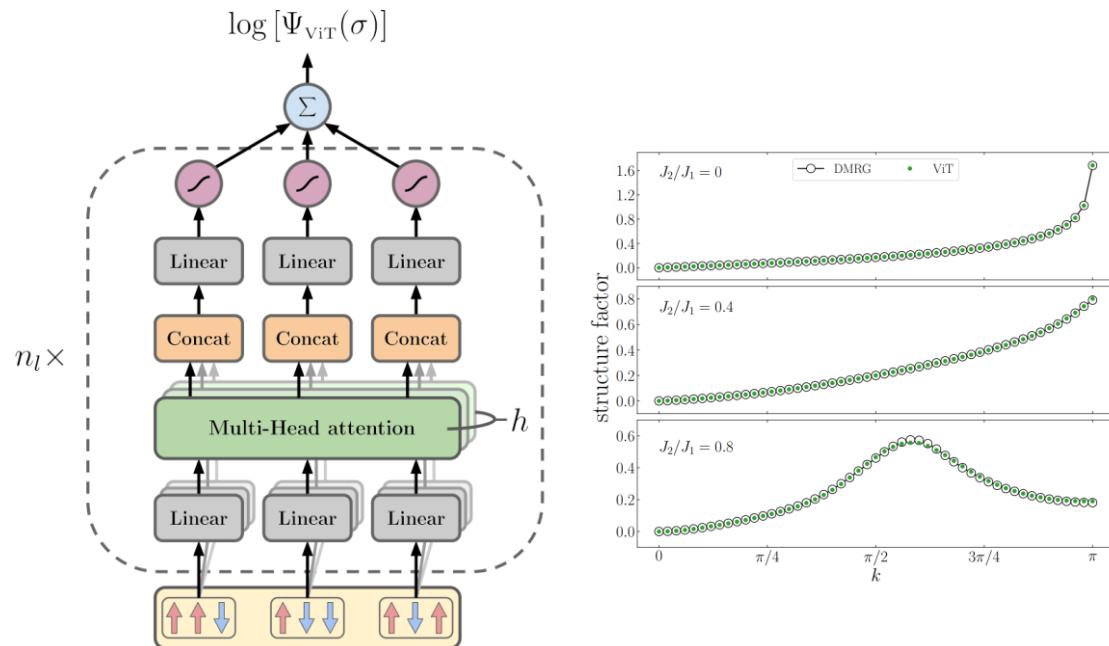
## Strong Gravitational Lensing Parameter Estimation with Vision Transformer



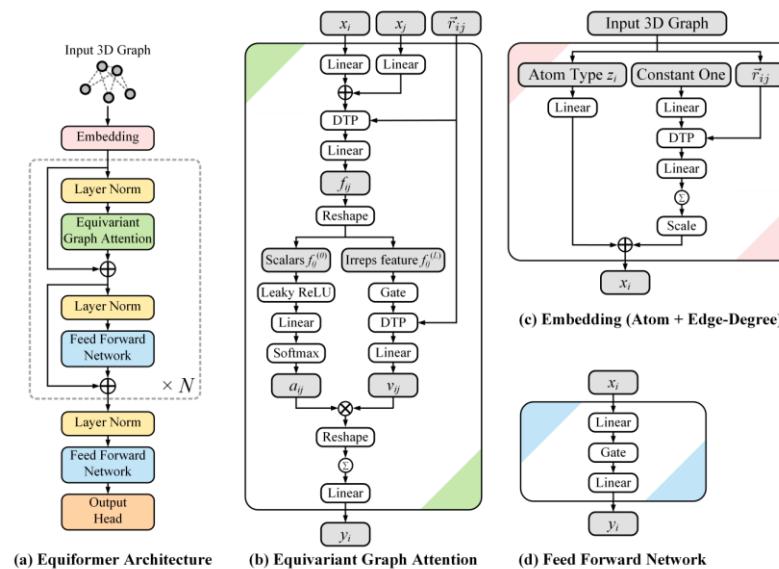
<https://arxiv.org/pdf/2210.04143.pdf>

# Other Applications

Transformer variational wave functions for frustrated quantum spin systems



## Equiformer: Equivariant Graph Attention Transformer for 3D Atomistic Graphs



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

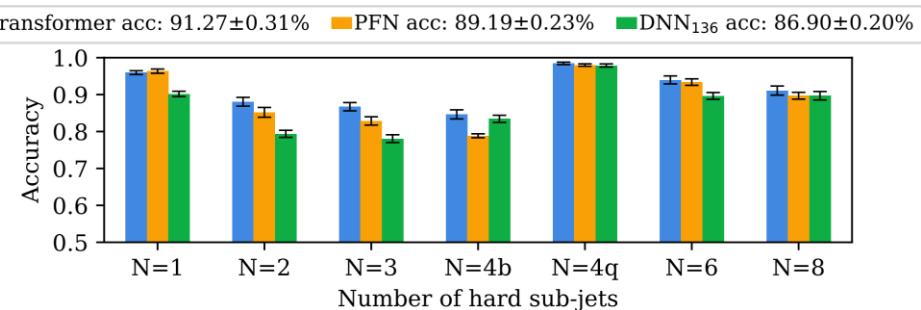
<https://arxiv.org/pdf/2109.13925.pdf>

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

# Particle Physics

<https://arxiv.org/pdf/2202.00723.pdf>

## Resolving Extreme Jet Substructure

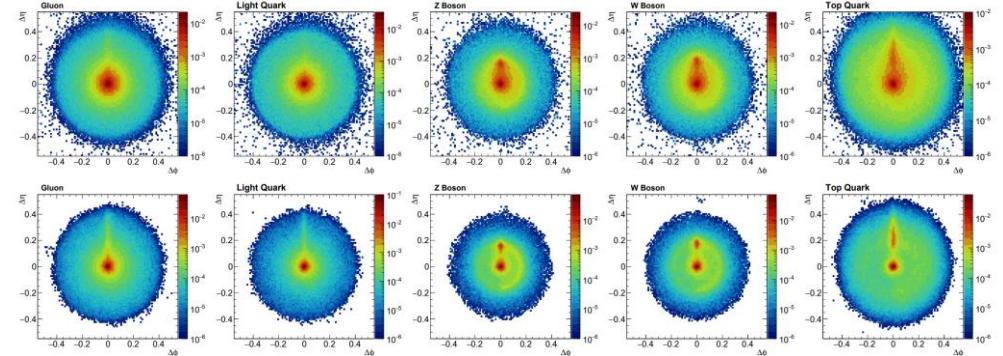


<https://arxiv.org/pdf/2102.05073.pdf>

## Point Cloud Transformers applied to Collider Physics

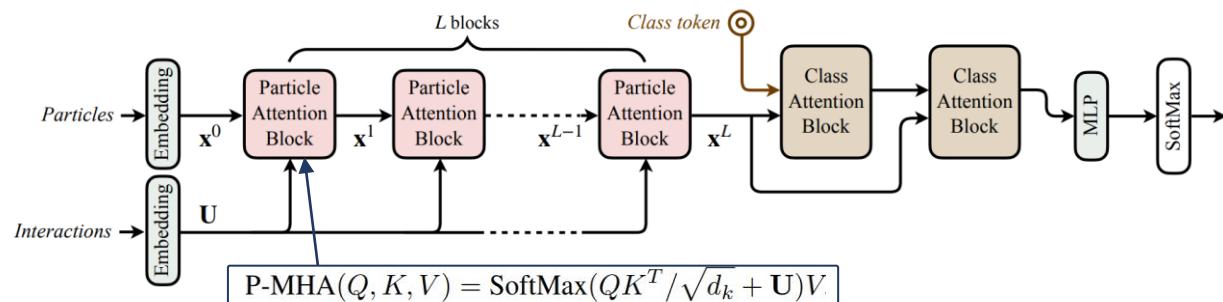
<https://arxiv.org/pdf/2102.05073.pdf>

### Attention layers



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

## Particle Transformer for Jet Tagging



"P-MHA, an augmented version that can also exploit the pairwise particle interactions directly [...]

Essentially, we add the interaction matrix  $\mathbf{U}$  [...]. 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
<b>ParT</b>	<b>0.861</b>	2.14 M	340 M
ParT (plain)	0.849	2.13 M	260 M

## Top-Tagging

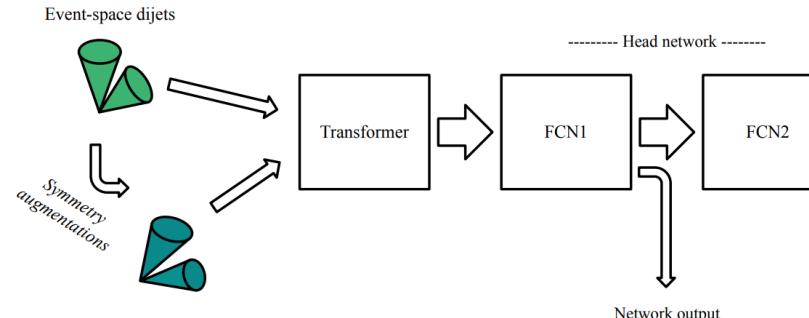
	Accuracy
P-CNN	0.930
PFN	—
ParticleNet	0.940
JEDI-net (w/ $\sum O$ )	0.930
PCT	0.940
LGN	0.929
rPCN	—
LorentzNet	0.942
ParT	0.940
ParticleNet-f.t.	0.942
<b>ParT-f.t.</b>	<b>0.944</b>

(Also best in quark-gluon tagging)

# Particle Physics

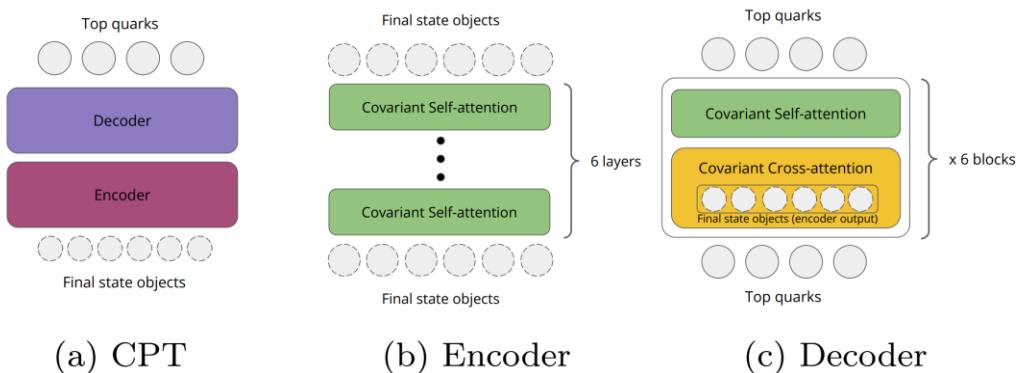
<https://arxiv.org/pdf/2205.10380.pdf>

## Self-supervised Anomaly Detection for New Physics



<https://arxiv.org/pdf/2203.05687.pdf>

## A Holistic Approach to Predicting Top Quark Kinematic Properties with the Covariant Particle Transformer



## Contrastive Learning

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

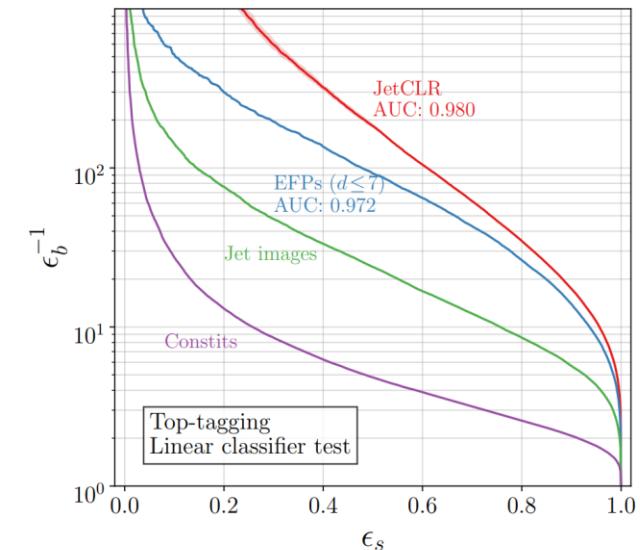
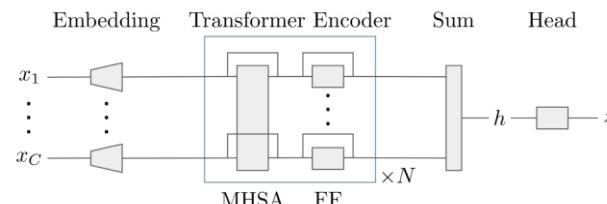
## Symmetries, Safety, and Self-Supervision

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

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

which is, both,

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



# 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**

