SPONSORED BY THE

Federal Ministry of Education and Research

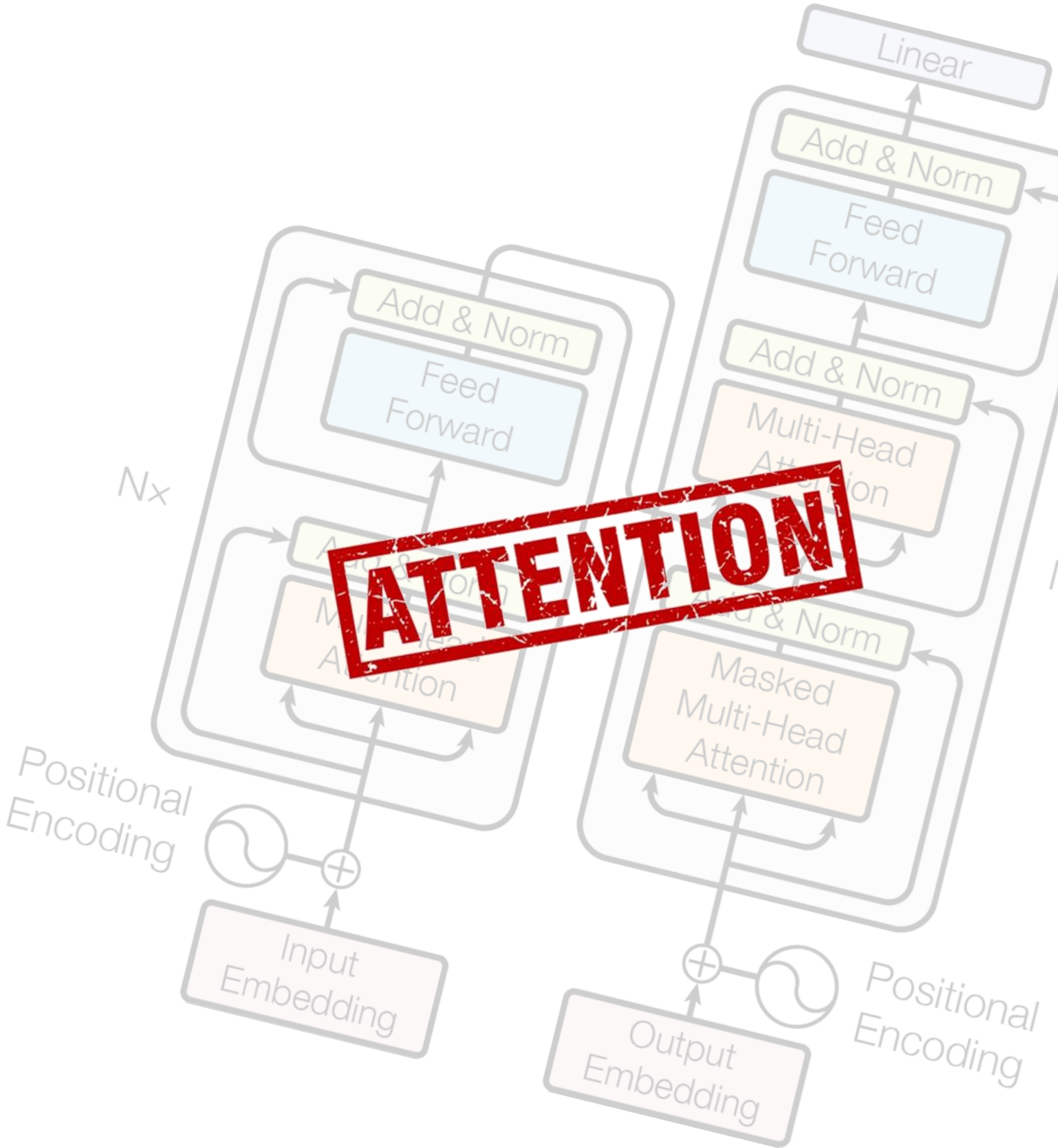
III. Physikalisches Institut A

RWTH AACHEN UNIVERSITY

Transformers

Conceptual Advances in Deep Learning for Research on Universe and Matter

ERUM DATA HUB



Niklas Langner

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!

Output Image

Generated with Stable Diffusion
https://arxiv.org/abs/2112.10752
https://github.com/CompVis/stable-diffusion

Understanding the Text Prompt

Photography of what?

Photography of an Astronaut

What is green?

wearing a green spacesuit standing

Wearing what?

Standing where?

in front of the Colosseum on the moon

Whose hand?

In front of what?

Bouquet of what?

with a bouquet of roses

Where is the bouquet?

What is in his hand?

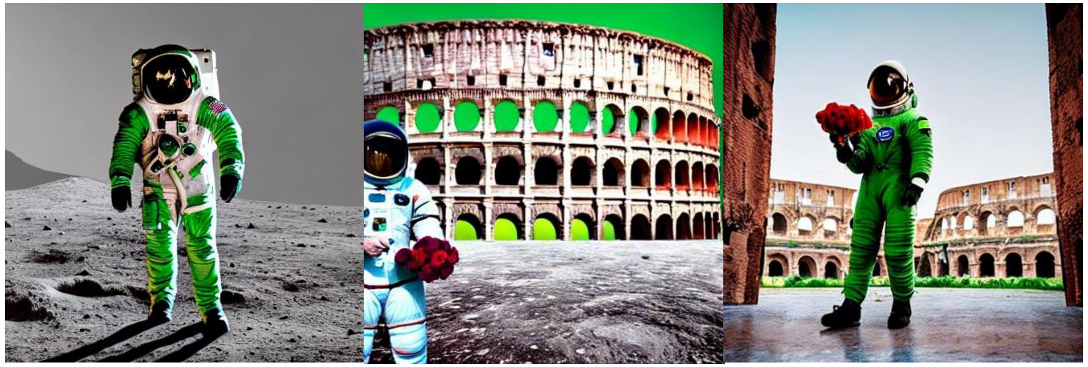
in his hand

In what?

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

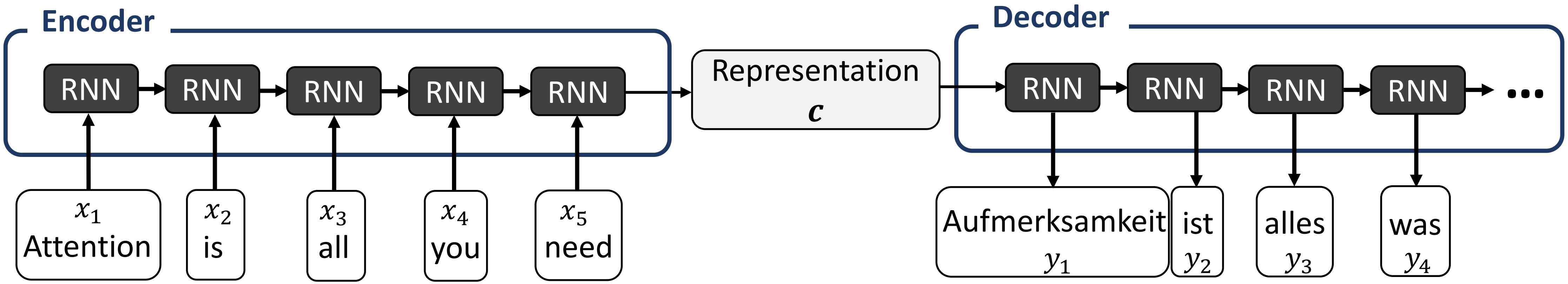
Attention is all you need → Aufmerksamkeit ist alles, was du brauchst

$\boldsymbol{x} = \{x_1, x_2, x_3, x_4, x_5\} \longrightarrow \boldsymbol{y} = \{y_1, y_2, y_3, y_4, y_5, y_6\}$

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!

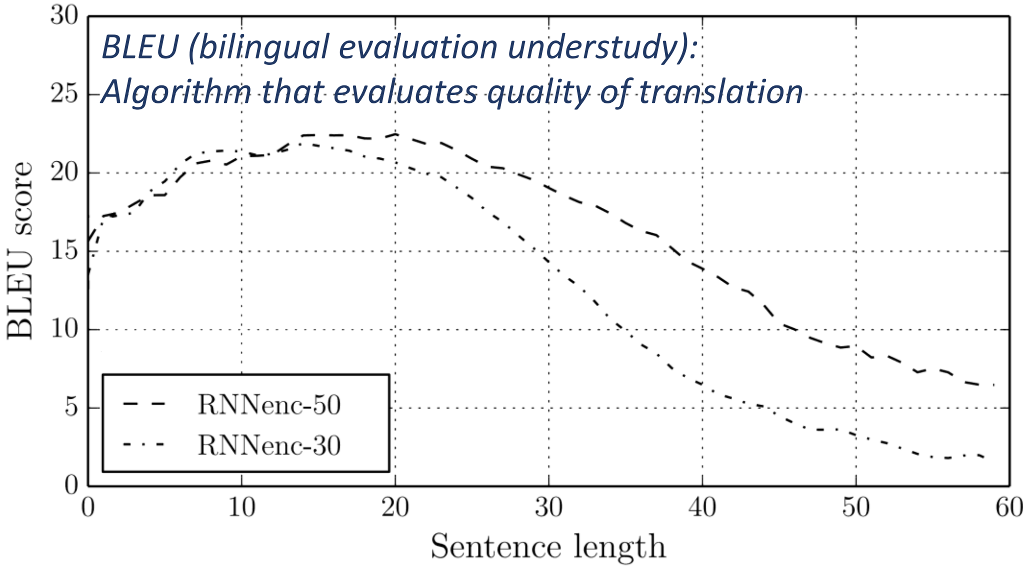
I like your dog, **it** is great! → Ich mag deinen Hund, **er** ist toll!

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

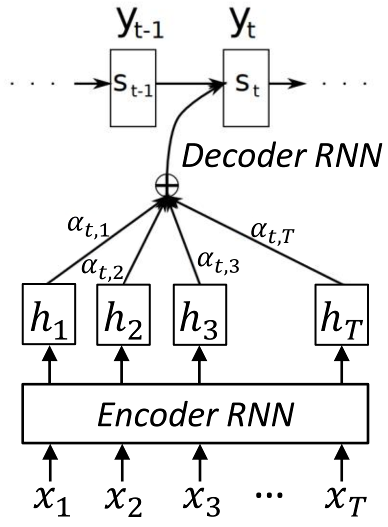


https://arxiv.org/abs/1409.0473

Solution: Attention

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

Attention Example



Nonlinear function
e.g. LSTM

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

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

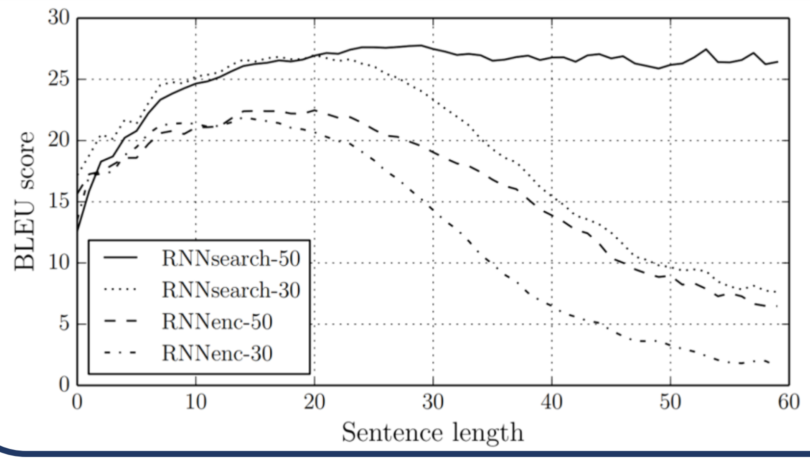
$$\alpha_{ij} = \frac{\exp(e_{ij})}{\sum_{k=1}^{T_x} \exp(e_{ik})}$$

softmax

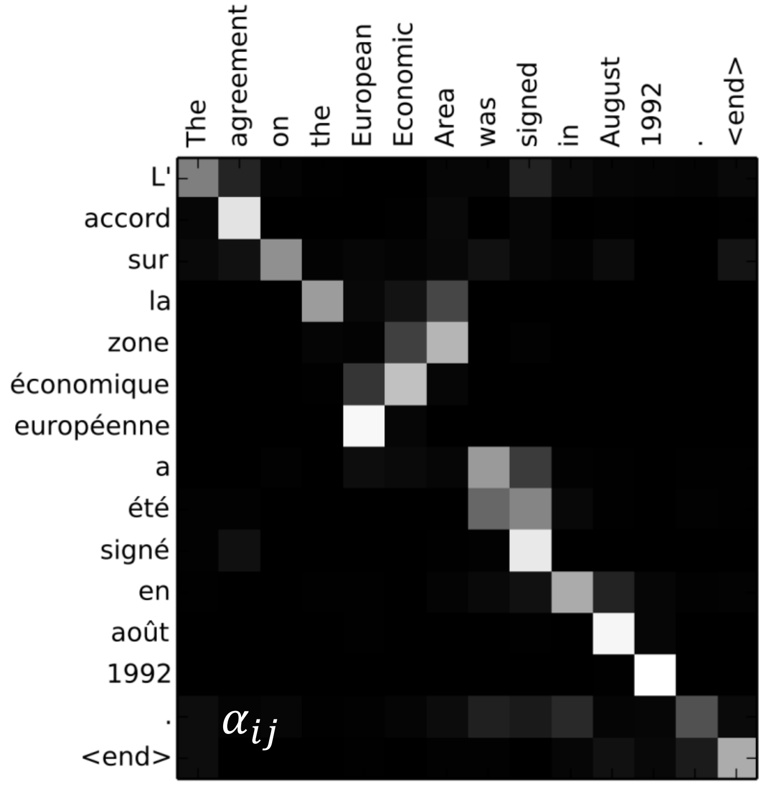
$$e_{ij} = \mathrm{score}(s_{i-1}, h_j)$$

Alignment Score Function

Different for each step!



Greatly improves performance translating **long sentences**



https://arxiv.org/abs/1409.0473

Attention Mechanisms

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

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

Commonly used neural network approach

Alignment score: Many different options

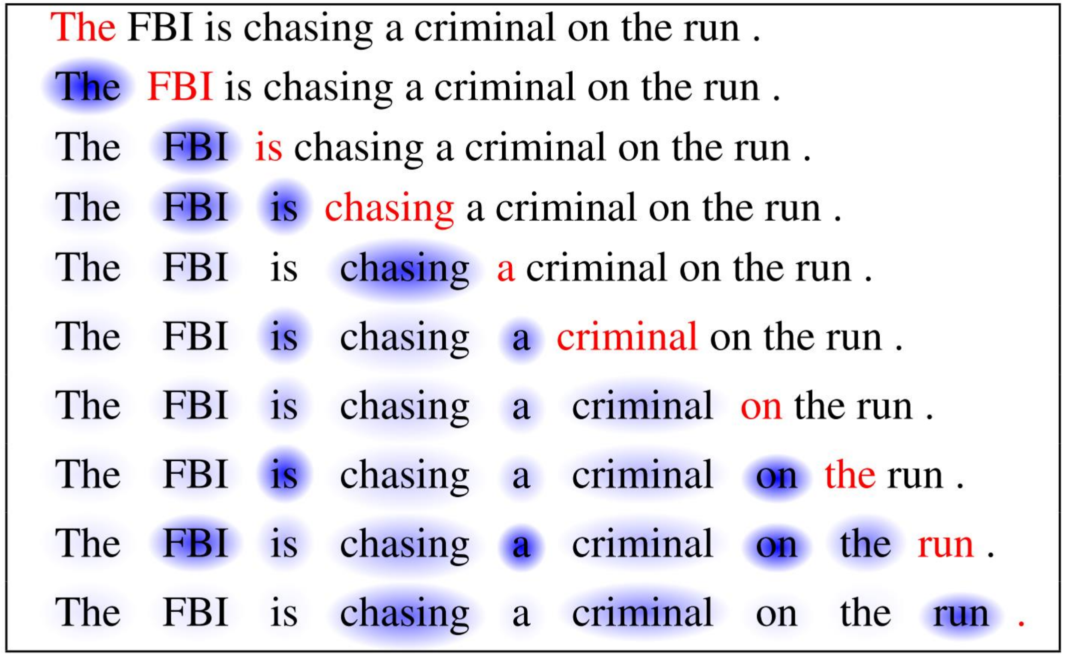
Name	Alignment score function	Citation
Content-base attention	$\mathrm{score}(s_{i-1}, h_i) = \cos(\theta)$ where θ is the angle between s_{i-1} and h_j	Graves2014
Additive	$\mathrm{score}(s_{i-1}, h_j) = v_a^{\mathrm{T}} \tanh(W_a[s_{i-1}; h_j])$	Bahdanau2015
Location-Based	$\alpha_{ij} = \mathrm{softmax}(W_a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

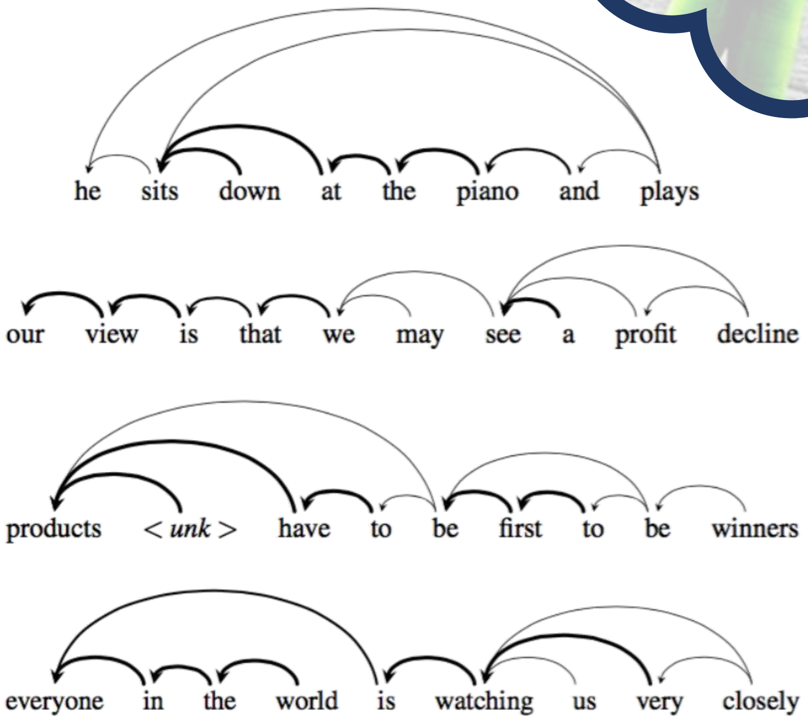
Important for Transformer

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

Self-Attention

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





Bolder line: **Higher** attention

⇒ 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

Ashish Vaswani* Google Brain avaswani@google.com

Noam Shazeer* Google Brain noam@google.com

Niki Parmar* Google Research nikip@google.com

Jakob Uszkoreit* Google Research usz@google.com

Llion Jones* Google Research llion@google.com

Aidan N. Gomez* † University of Toronto aidan@cs.toronto.edu

Łukasz Kaiser* Google Brain lukaszkaiser@google.com

Illia Polosukhin* ‡ illia.polosukhin@gmail.com

Abstract

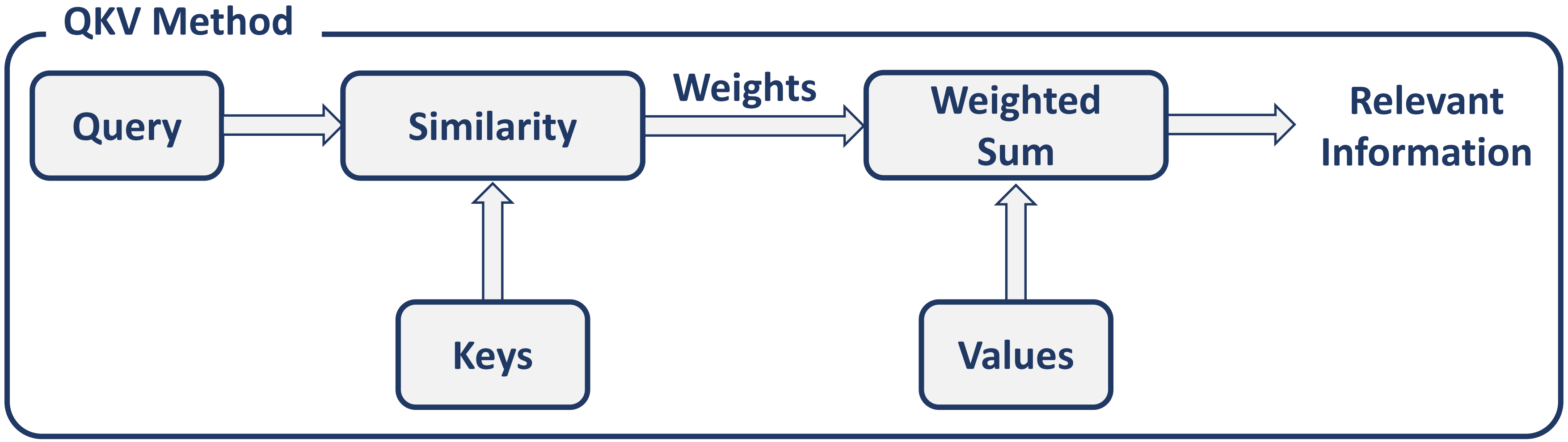
The dominant sequence transduction models are based on complex recurrent or convolutional neural networks that include an encoder and a decoder. The best performing models also connect the encoder and decoder through an attention mechanism. We propose a new simple network architecture, the Transformer,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

Introducing: The Transformer

https://arxiv.org/abs/1706.03762

Transformer: Attention Mechanism

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

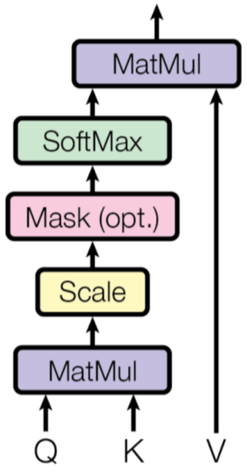


Scaled dot-product attention:

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

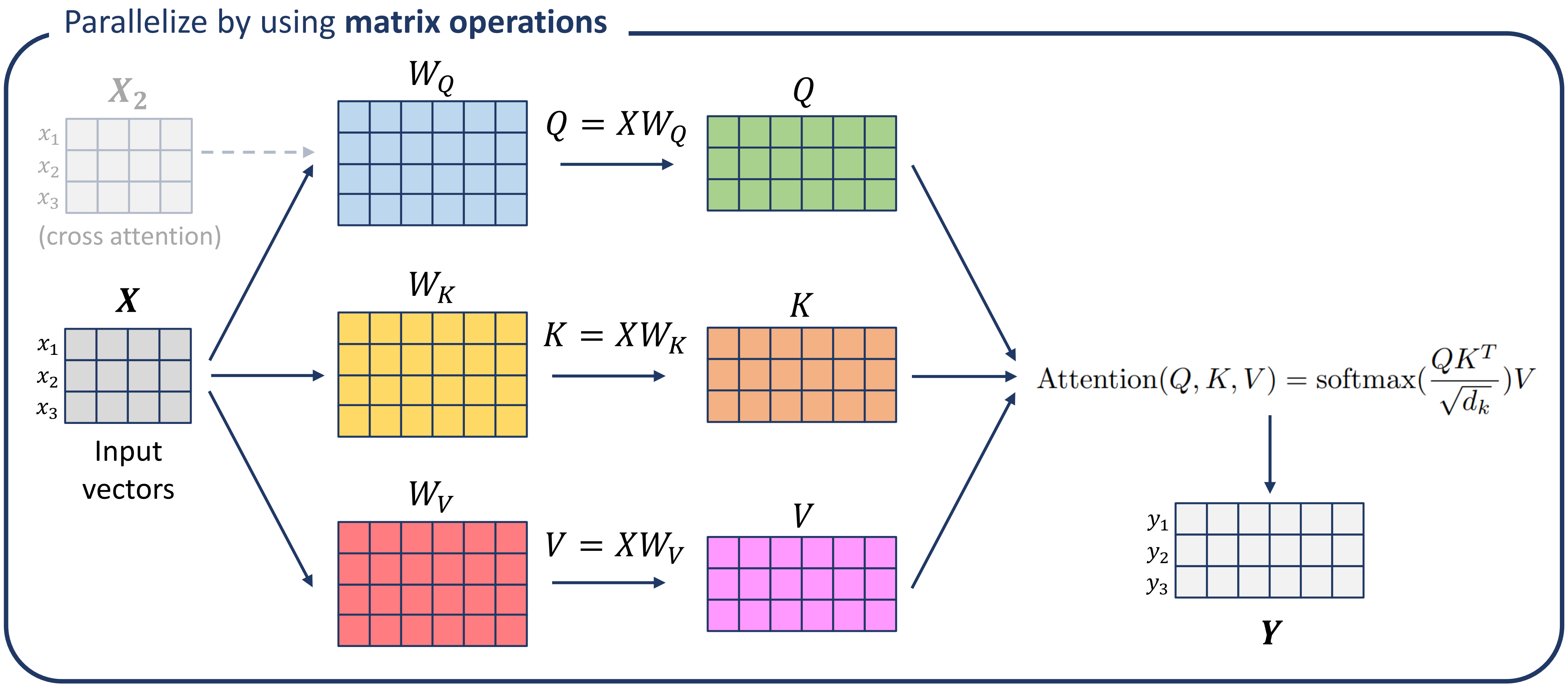
$$\text{score}(s_{i-1}, h_j) = \frac{s_{i-1}^{\mathrm{T}} h_j}{\sqrt{n}} \Rightarrow \text{Attention}(Q, K, V) = \text{softmax}\left(\frac{QK^T}{\sqrt{d_k}}\right)V$$

d_k: length of keys vector



https://arxiv.org/abs/1706.03762

QKV-Self-Attention Implementation

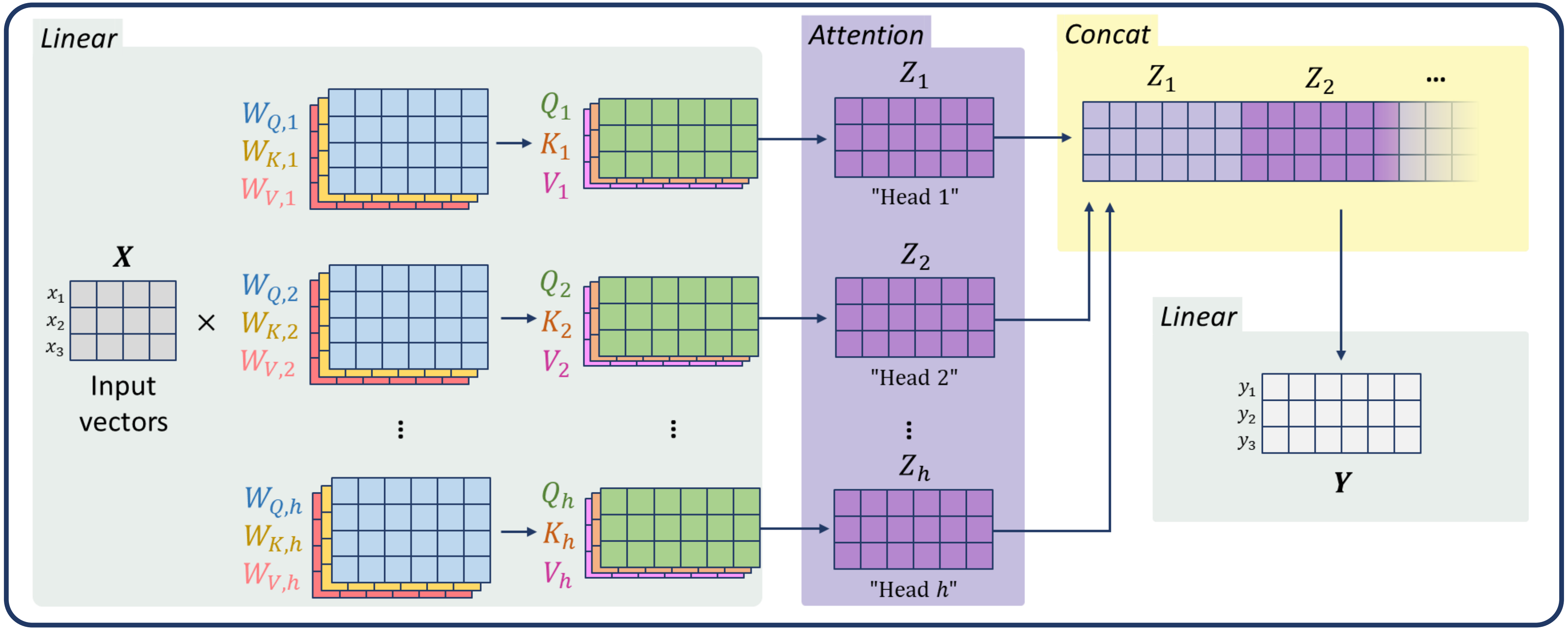


Here: Always use X → calculate **self-attention**

To **relate X** to **different input data $\mathbf{X}_2$**, use X_2 to calculate Q (**cross attention**)

https://arxiv.org/abs/1706.03762

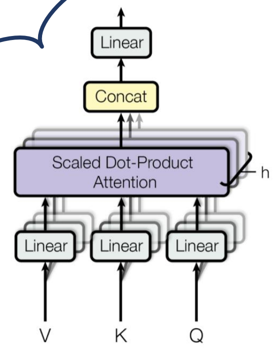
Multi-Head Attention



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 ⚡
→ Use **positional encoding**!

Building block of transformer

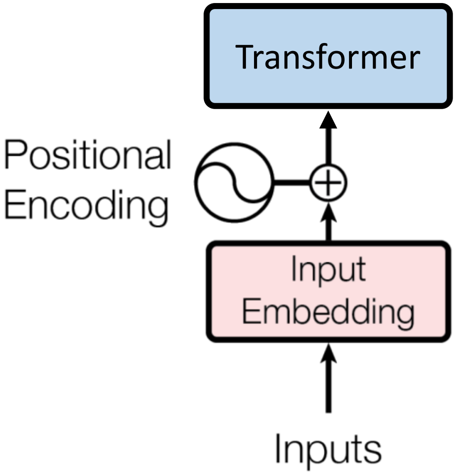


https://arxiv.org/abs/1706.03762

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**:

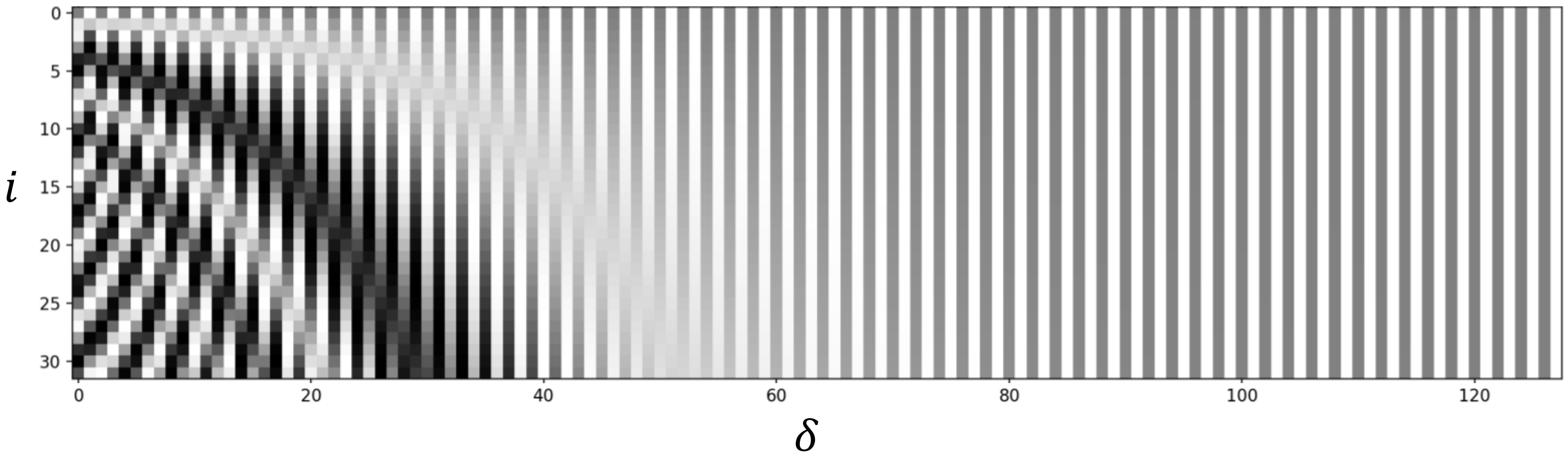


Example

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

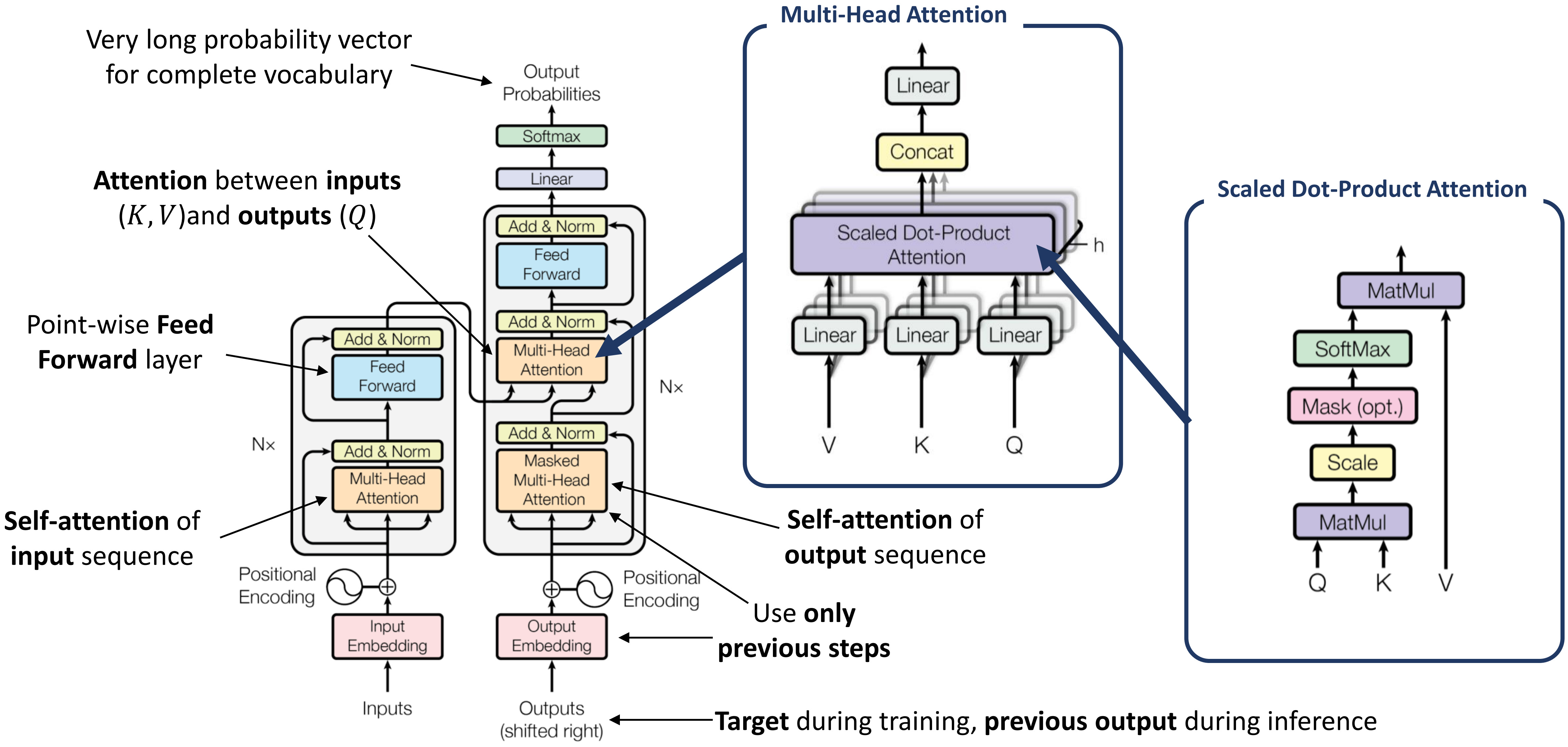
i: word position
δ: vector dimension
d: vector length in network

https://lilianweng.github.io/posts/2020-04-07-the-transformer-family/



https://arxiv.org/abs/1706.03762

Full Transformer Architecture

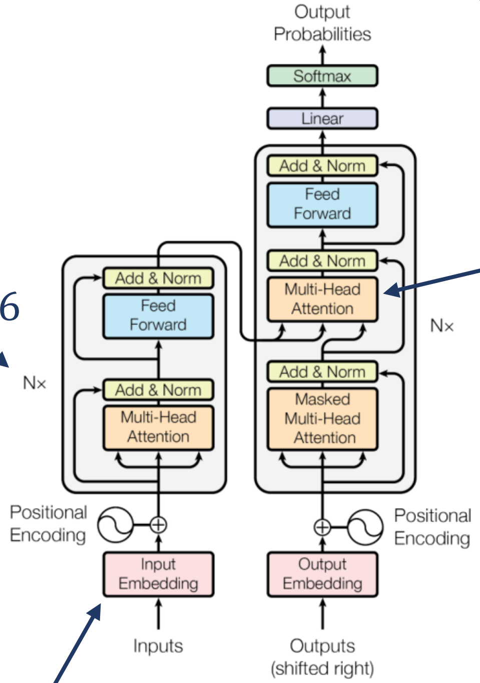


https://arxiv.org/abs/1706.03762

Text Translation with Transformer

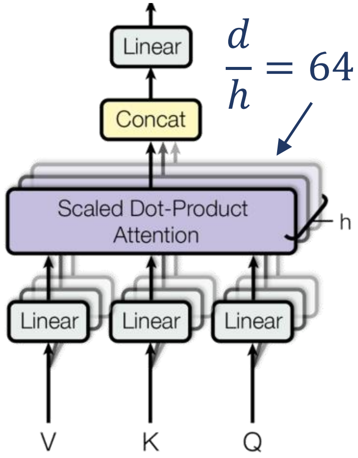
Transformer

$N = 6$



Dimensionality $d = 512$

Multi-Head Attention



$\frac{d}{h} = 64$ dimensional

$h = 8$ independent heads

→ can be **trained on 8 GPUs simultaneously**
Total computational cost is similar to that of single-head attention with full dimensionality of 512

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	$\mathbf{3.3 \cdot 10^{18}}$	
Transformer (big)	**28.4**	**41.8**	$2.3 \cdot 10^{19}$	

https://arxiv.org/abs/1706.03762

Impact of Transformers – Language Processing

GLUE https://gluebenchmark.com/leaderboard

Rank	Name	Model	URL	Score
1	JDExplore d-team	Vega v1 (Could not find architecture, but likely transformers)		91.3
2	Microsoft Alexander v-team	Turing NLR v5		91.2
3	DIRL Team	DeBERTa + CLEVER		91.1
4	ERNIE Team - Baidu	ERNIE		91.1
5	AliceMind & DIRL	StructBERT + CLEVER		91.0
6	DeBERTa Team - Microsoft	DeBERTa / TuringNLRv4		90.8
7	HFL iFLYTEK	MacALBERT + DKM		90.7
8	PING-AN Omni-Sinitic	ALBERT + DAAF + NAS		90.6
9	T5 Team - Google	T5		90.3
10	Microsoft D365 AI & MSR AI & GATECH	MT-DNN-SMART		89.9
11	Huawei Noah's Ark Lab	NEZHA-Large		89.8
12	Zihang Dai	Funnel-Transformer (Ensemble B10-10-10H1024)		89.7
⋮				
21	GLUE Human Baselines	GLUE Human Baselines		87.1
⋮				
75	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)

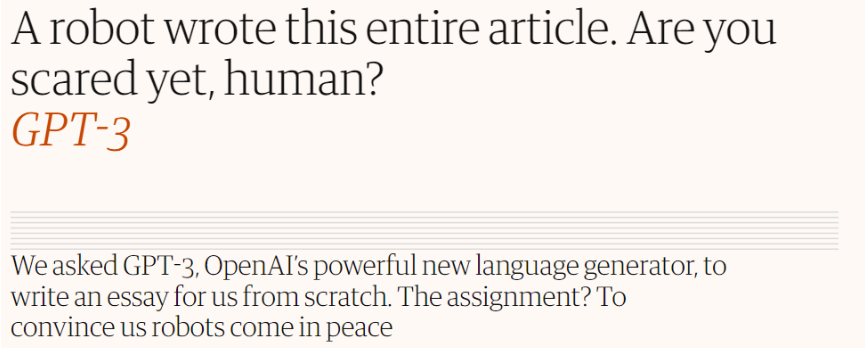
→ Models using more than one **trillion** parameters are already tested

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**

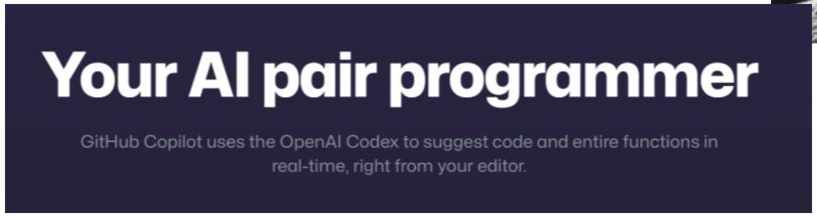
Enabled new applications:

Generating large texts


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

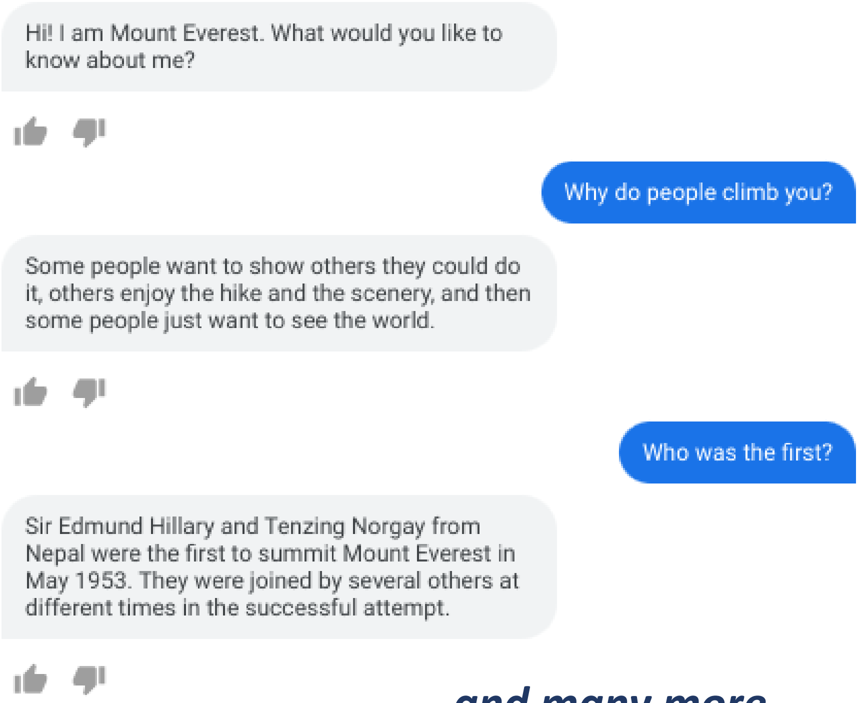
We asked GPT-3, OpenAI's powerful new language generator, to write an essay for us from scratch. The assignment? To convince us robots come in peace

Writing code



Understanding complex prompts

Conversational models

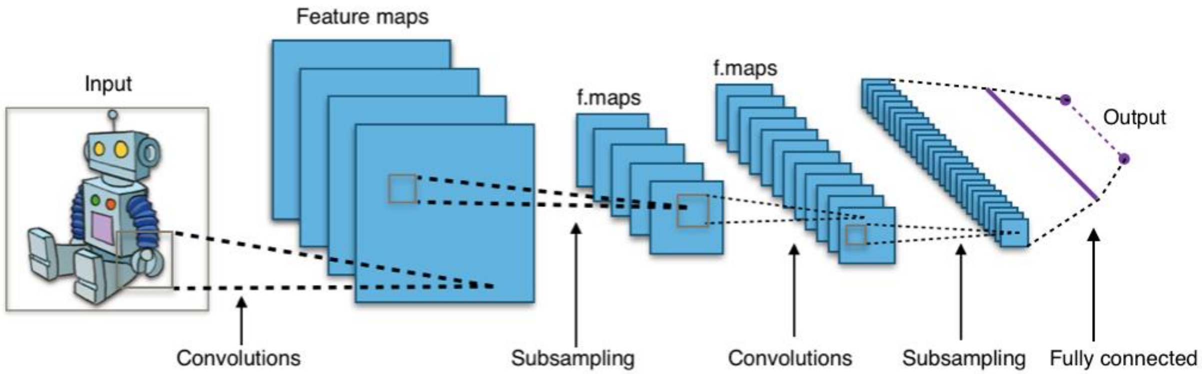


...and many more

Image Recognition

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

1)



- 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**

[1] https://commons.wikimedia.org/wiki/File:Typical_cnn.png

Vision Transformer (ViT)

Ansatz

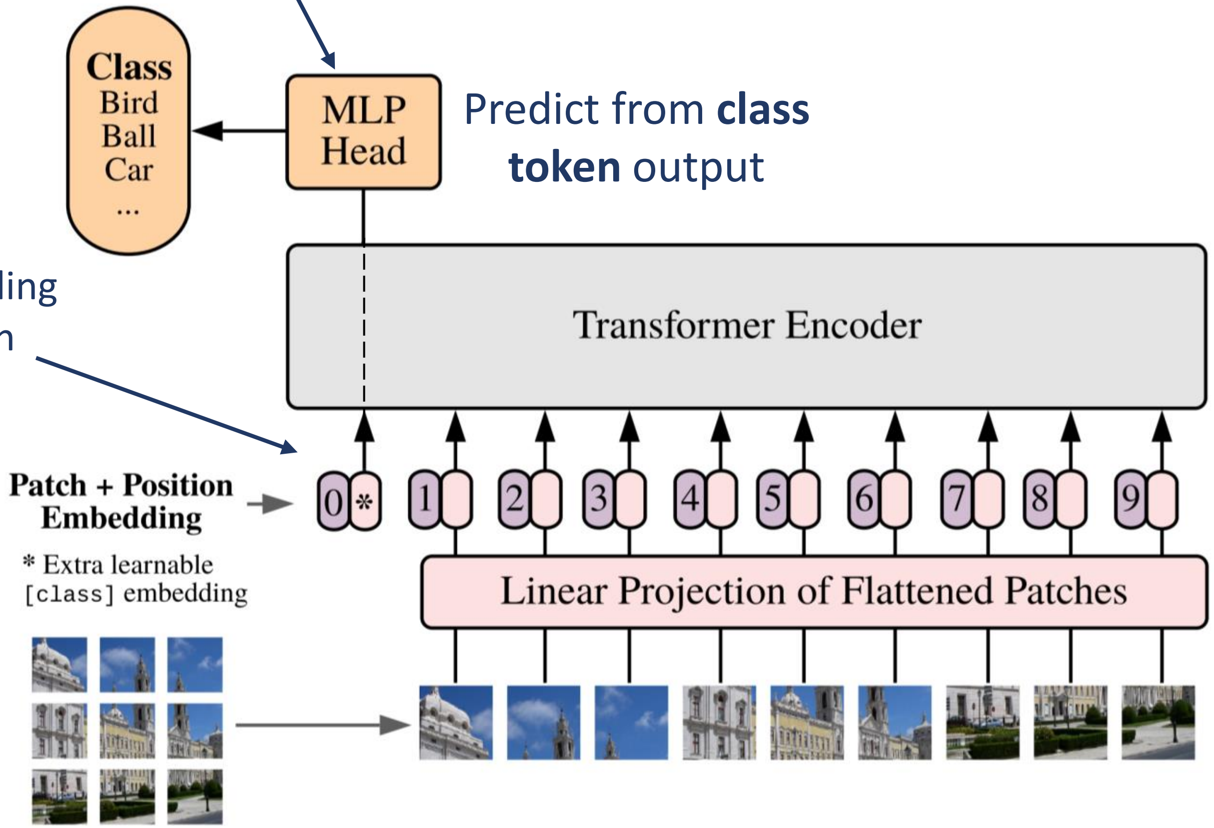
"In model design we **follow the original Transformer** (Vaswani et al., 2017) **as closely as possible**. An advantage of this intentionally simple setup is that scalable NLP Transformer architectures – and their efficient implementations – can be used almost out of the box."

MLP for **final prediction**

Predict from **class token** output

Multihead Attention
Transformer from language processing task

Learnable positional encoding lets network know which patch is which



Split image into ***patches***

Flatten patches (**losing 2D structure**) and **project linearly to embedding** dimension (can also be done via **CNN in hybrid approach**)

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	**88.55** $\pm$ 0.04	87.76 $\pm$ 0.03	85.30 $\pm$ 0.02	87.54 $\pm$ 0.02	88.4/88.5*
ImageNet ReaL	**90.72** $\pm$ 0.05	90.54 $\pm$ 0.03	88.62 $\pm$ 0.05	90.54	90.55
CIFAR-10	**99.50** $\pm$ 0.06	99.42 $\pm$ 0.03	99.15 $\pm$ 0.03	99.37 $\pm$ 0.06	–
CIFAR-100	**94.55** $\pm$ 0.04	93.90 $\pm$ 0.05	93.25 $\pm$ 0.05	93.51 $\pm$ 0.08	–
Oxford-IIIT Pets	**97.56** $\pm$ 0.03	97.32 $\pm$ 0.11	94.67 $\pm$ 0.15	96.62 $\pm$ 0.23	–
Oxford Flowers-102	99.68 $\pm$ 0.02	**99.74** $\pm$ 0.00	99.61 $\pm$ 0.02	99.63 $\pm$ 0.03	–
VTAB (19 tasks)	**77.63** $\pm$ 0.23	76.28 $\pm$ 0.46	72.72 $\pm$ 0.21	76.29 $\pm$ 1.70	–
TPUv3-core-days	2.5k	0.68k	0.23k	9.9k	12.3k

Transformer: More efficient

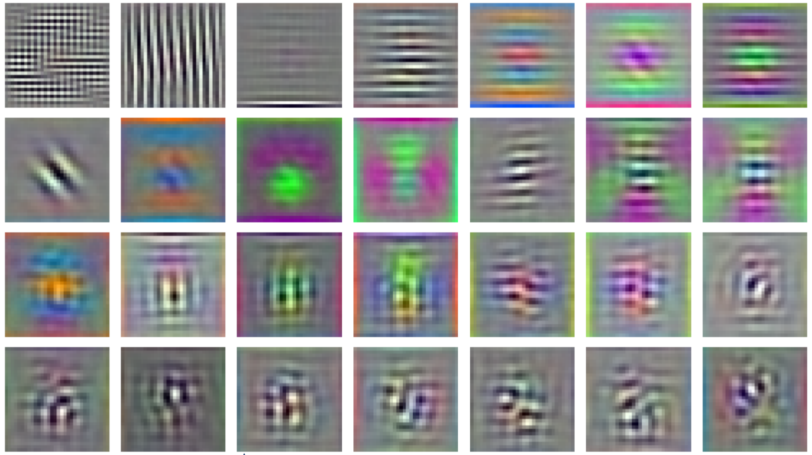
"ViT performs **significantly worse** than the CNN equivalent (BiT) when **trained on ImageNet** (1M images). However, on **ImageNet-21k** (14M images) performance is **comparable**, and on **JFT** (300M images), **ViT now outperforms BiT**."

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

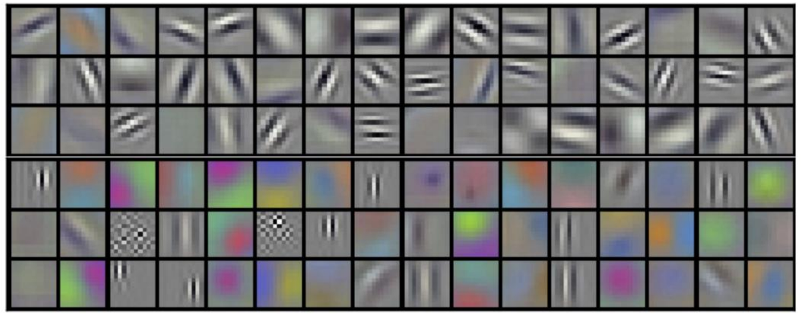
https://arxiv.org/abs/2010.11929

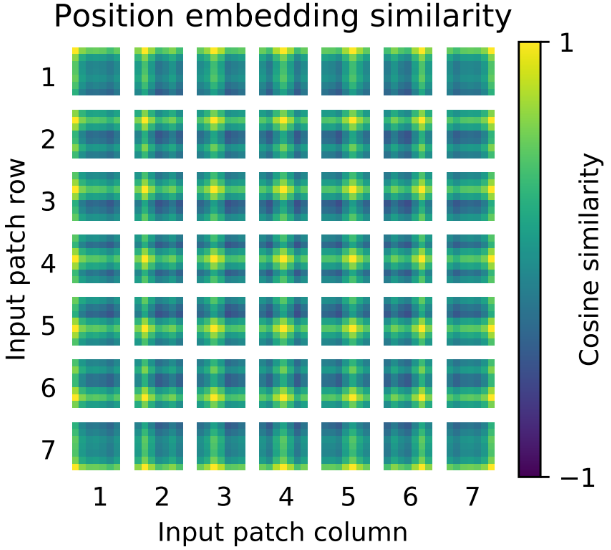
Vision Transformer Insight

RGB embedding filters
(first 28 principal components)

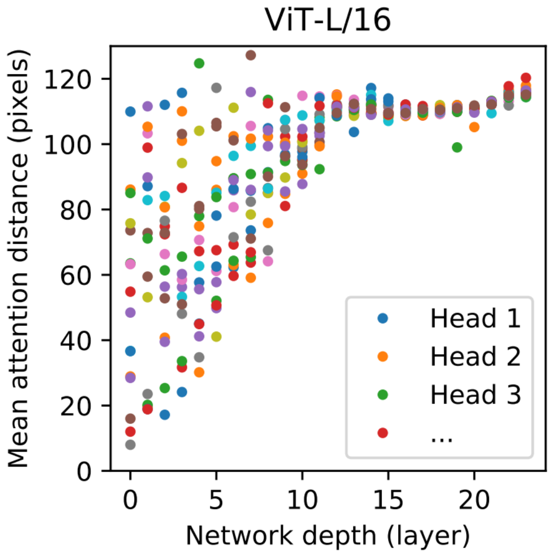


Similar to **CNN filters**





Position embedding includes incorporated **2D structure**

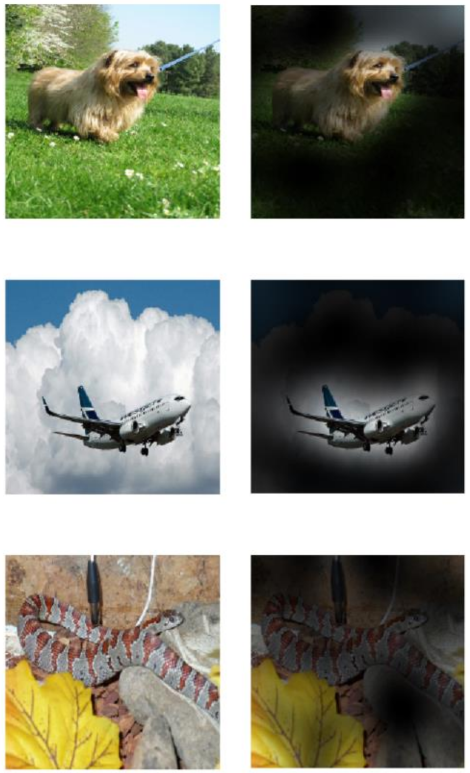


Starts at small scale and step by step increases scope (like CNN)

https://arxiv.org/abs/2010.11929

Vision Transformer Insight

Input Attention



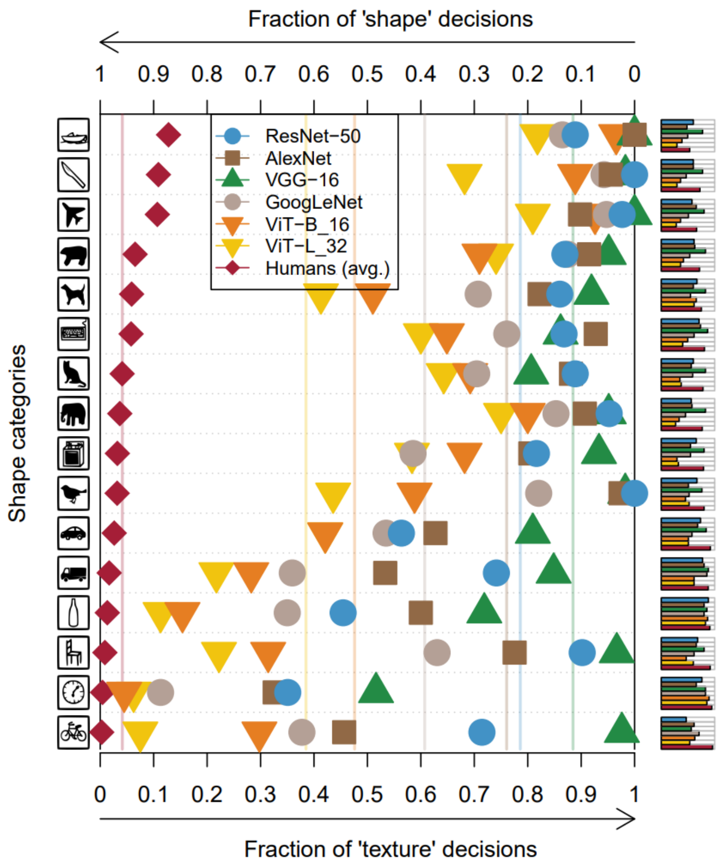
Global self-attention, in contrast to local filters of CNN

Shape = Cat, Texture = Elephant

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

Ongoing research…

Prediction based on shape or on texture?



https://arxiv.org/abs/2010.11929

https://arxiv.org/abs/2105.07197

ImageNet Leaderboard

Image Classification on ImageNet:

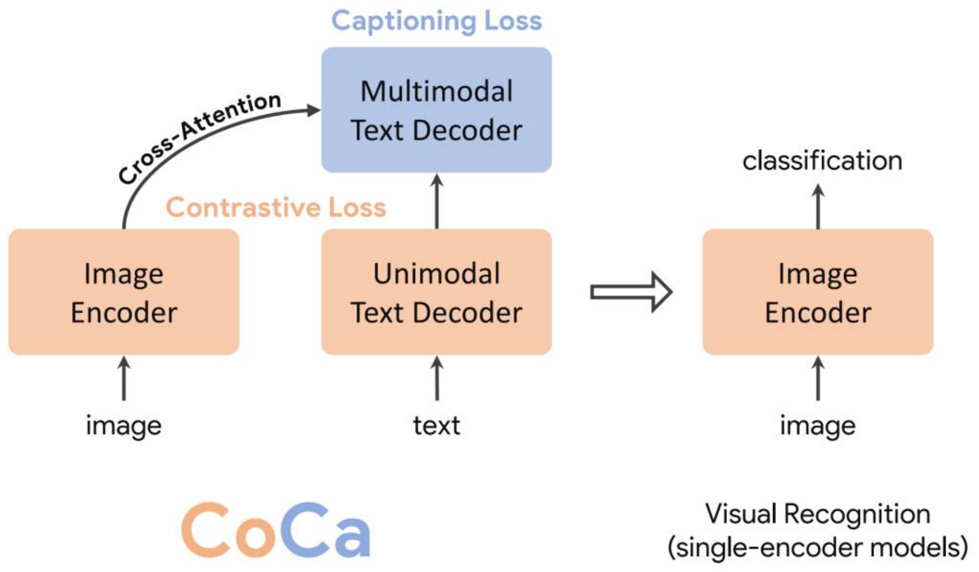
Rank	Model	Top 1 Accuracy	Year	Tags
1	CoCa (finetuned)	91.0%	2022	Transformer, JFT-3B, ALIGN
2	Model soups (BASIC-L)	90.98%	2022	Conv+Transformer, JFT-3B, ALIGN
3	Model soups (ViT-G/14)	90.94%	2022	Transformer, JFT-3B
4	CoAtNet-7	90.88%	2021	Conv+Transformer, JFT-3B

...

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

CoCa

"**Co**ntrastive **Ca**ptioners are Image-Text Foundation 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

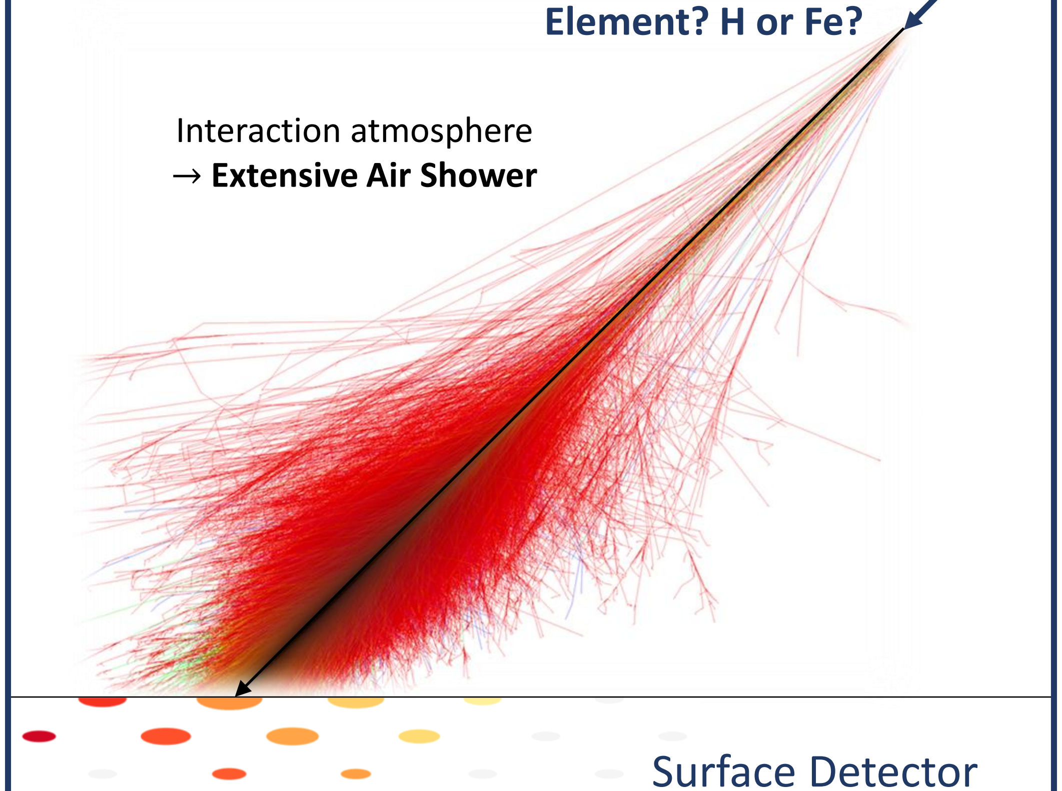
Transformers beat CNNs as state of the art in image recognition!

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

Extensive Air Showers

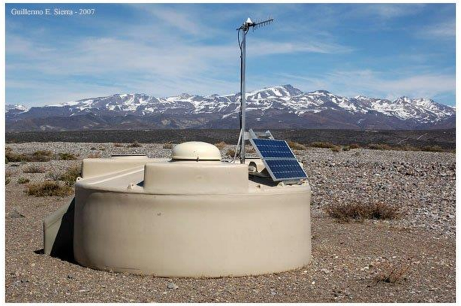
“Primary particle”
Element? H or Fe?

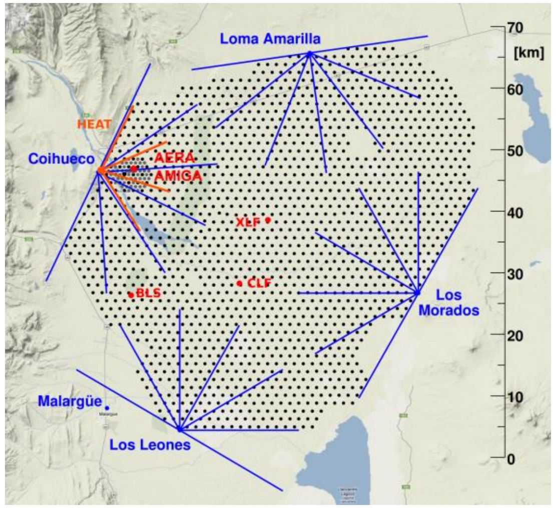
Interaction atmosphere
→ **Extensive Air Shower**



Surface Detector

Pierre Auger Observatory Surface Detector

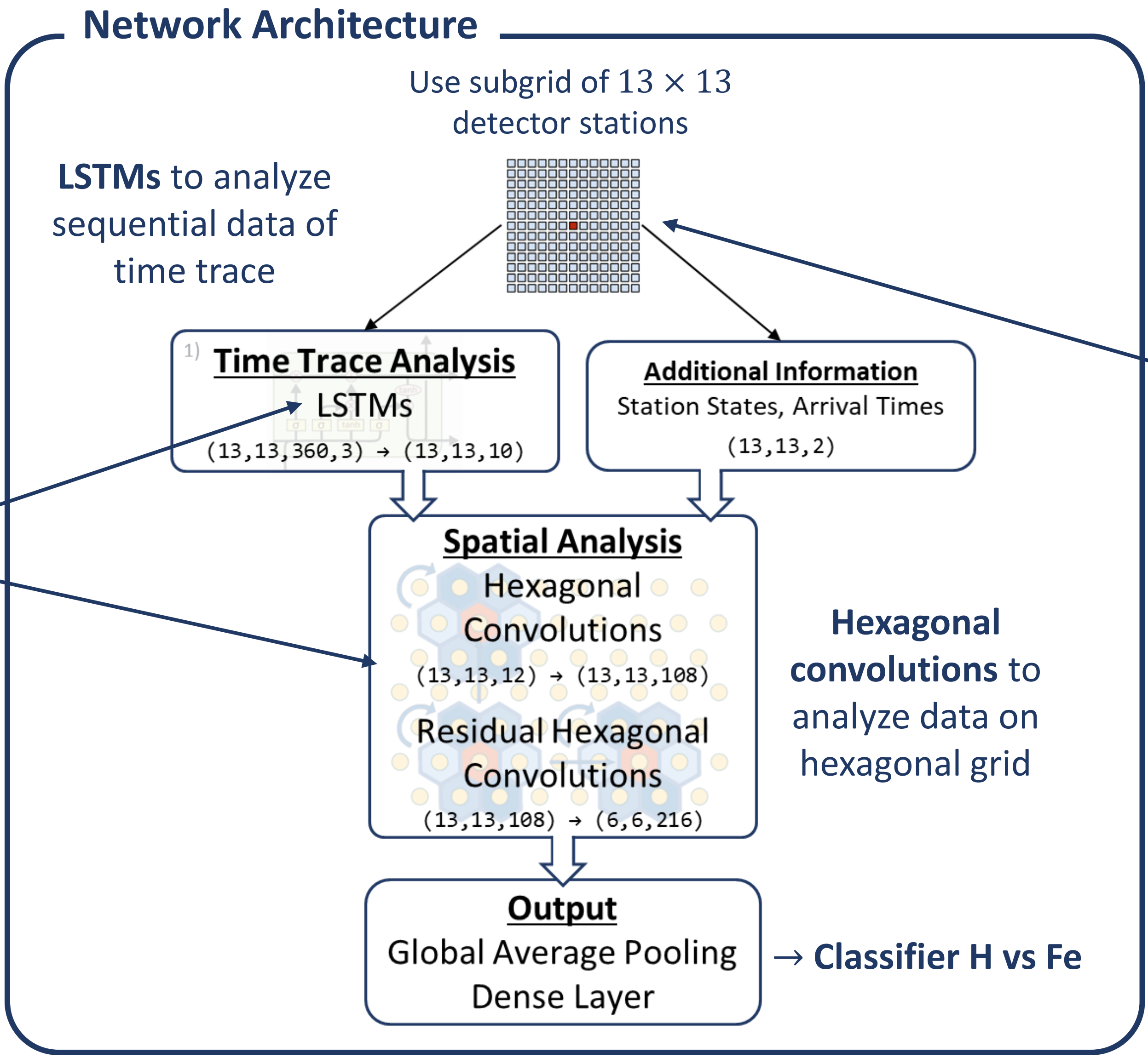




- Located in the *Pampa Amarilla* near Malargüe, Argentina
- Covers an area of roughly $3000\ \mathrm{km}^2$
- **Hexagonal grid** of 1660 water-Cherenkov stations
- Sample air shower footprint

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

Cosmic-Ray Mass Reconstruction Neural Network



Replace with transformer

Signal over time:
Time Traces

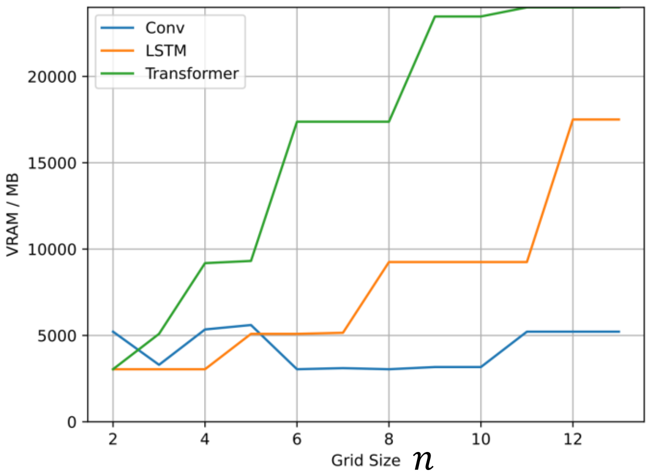
Shower Footprint

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

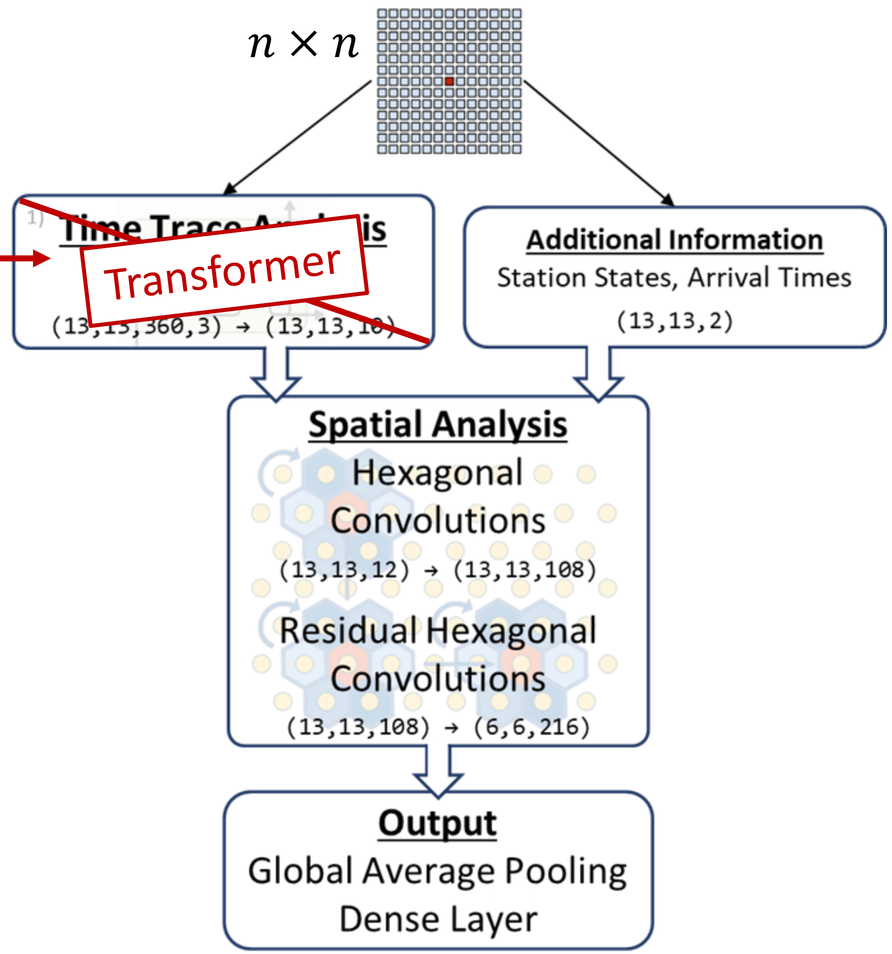
Challenges of Transformer Application

Dimensionality Problem

Attention shape: $(\text{batchsize} \cdot n^2 \cdot N_{\text{head}} \times \underbrace{360 \times 360}_{\mathcal{O}(L^2)})$



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

} Challenging to implement

Perceiver: $\mathcal{O}(kL)$
https://arxiv.org/abs/2107.14795

} **Very easy to implement** (see hackathon)

many more …
See https://arxiv.org/abs/2009.06732 and https://arxiv.org/abs/2011.04006

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

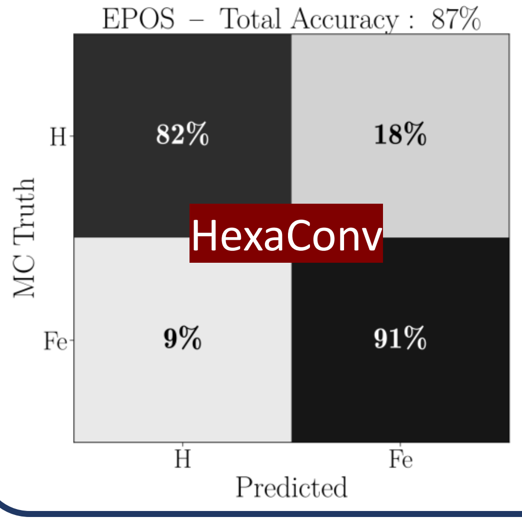
1) Image Credit: https://colah.github.io/posts/2015-08-Understanding-LSTMs/

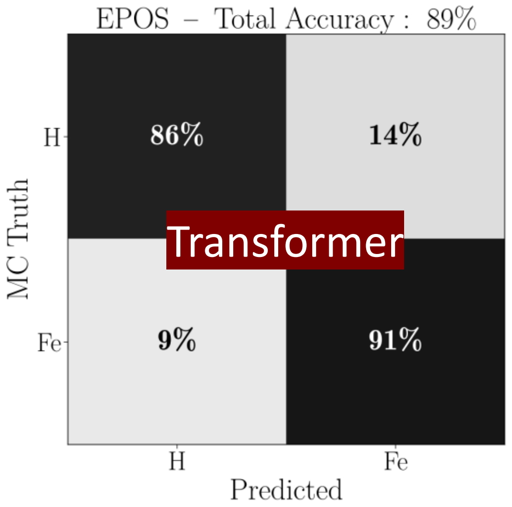
niklas.langner@rwth-aachen.de

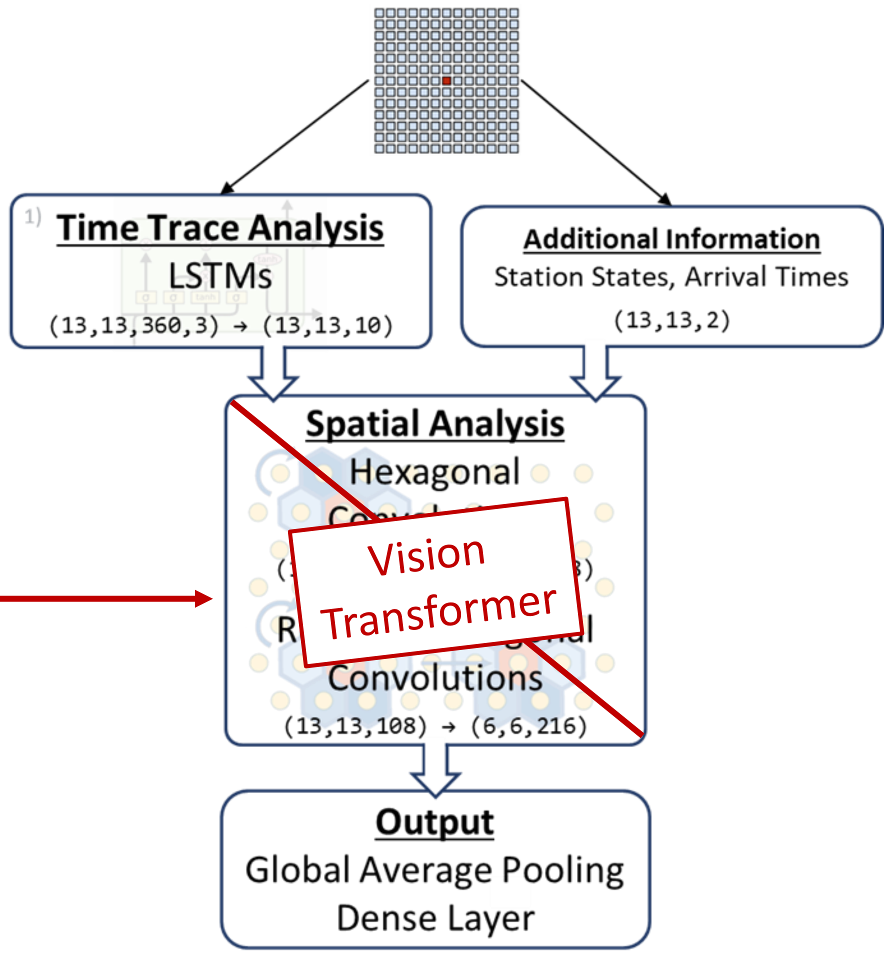
Chances of Transformer Application

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!**





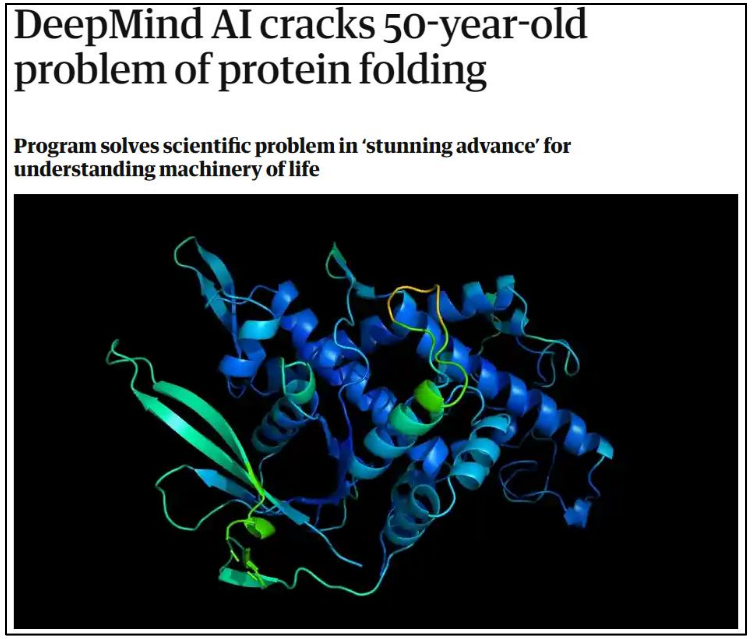


⇒ **Domain agnostic transformer** can be trained quickly, and **outperforms approach focused on data symmetry** (similar to Vision Transformer on images)

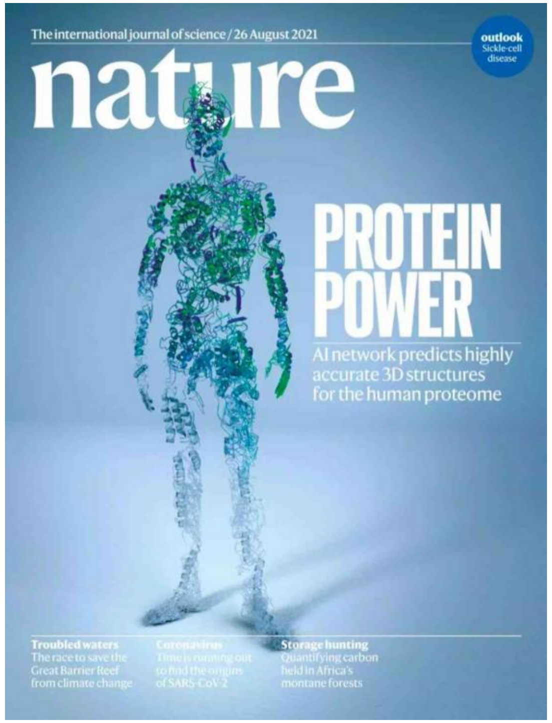
1) Image Credit: https://colah.github.io/posts/2015-08-Understanding-LSTMs/

Transformers in Science

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


DeepMind AI cracks 50-year-old problem of protein folding

Program solves scientific problem in 'stunning advance' for understanding machinery of life



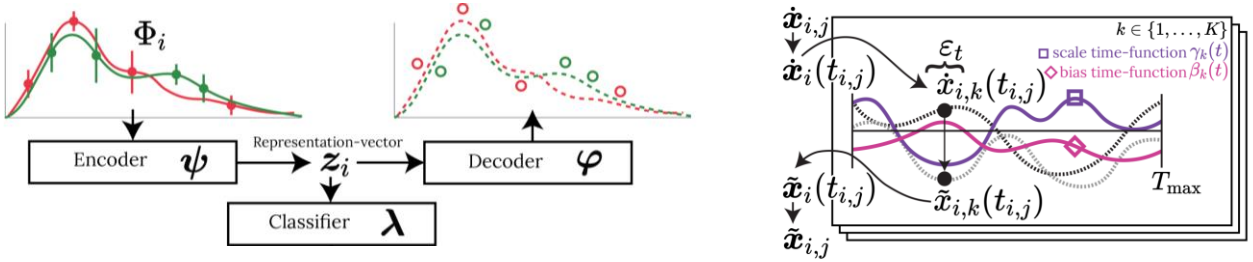
Famous science application: Protein unfolding

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

Time Sequence Analyses

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

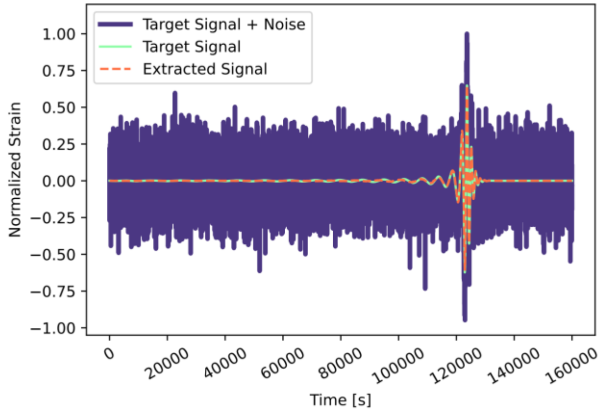
Deep Attention-Based Supernovae Classification of Multi-Band Light-Curves



TimeFiLM
(See hackathon)

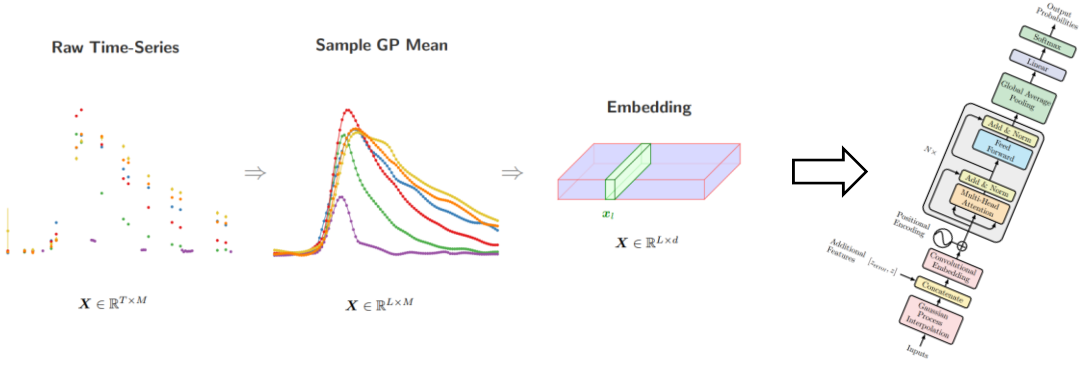
https://arxiv.org/pdf/2207.07414.pdf

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



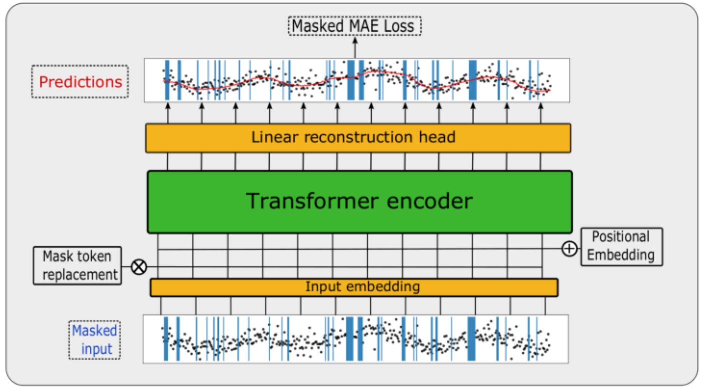
https://arxiv.org/pdf/2105.06178.pdf

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



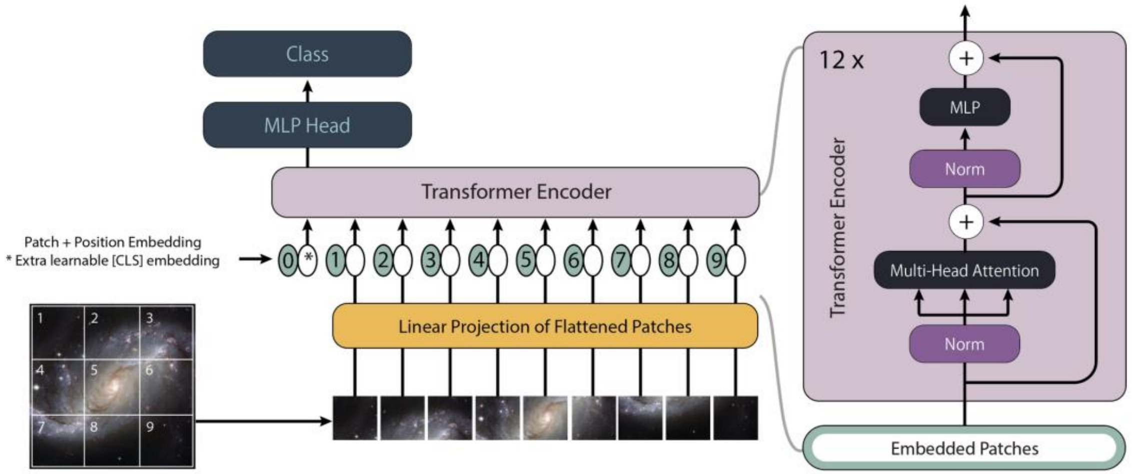
https://arxiv.org/pdf/2207.02777.pdf

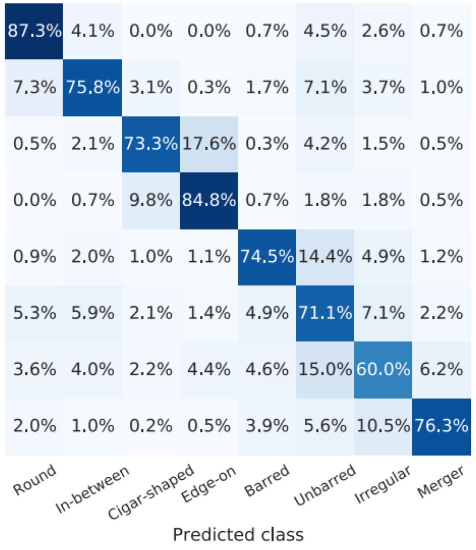
Don't Pay Attention to the Noise: Learning Self-supervised Representations of Light Curves with a Denoising Time Series Transformer

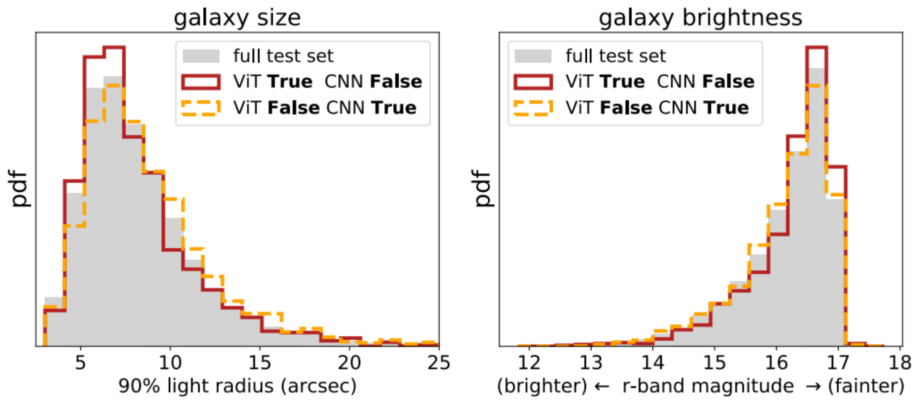


Vision Transformer Application

Galaxy Morphological Classification with Efficient Vision Transformer





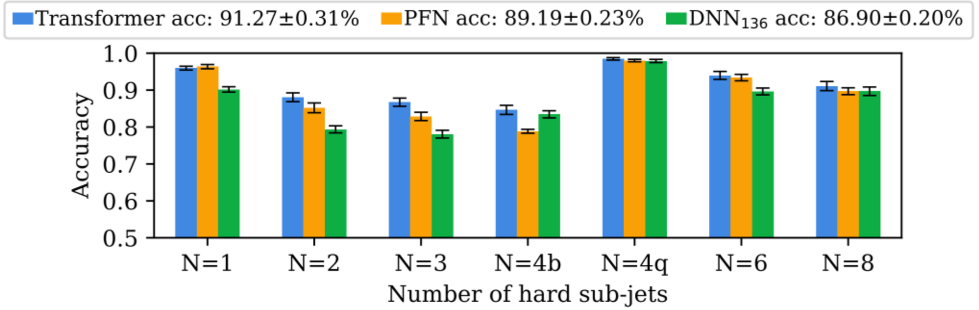


https://arxiv.org/pdf/2110.01024.pdf

Particle Physics

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

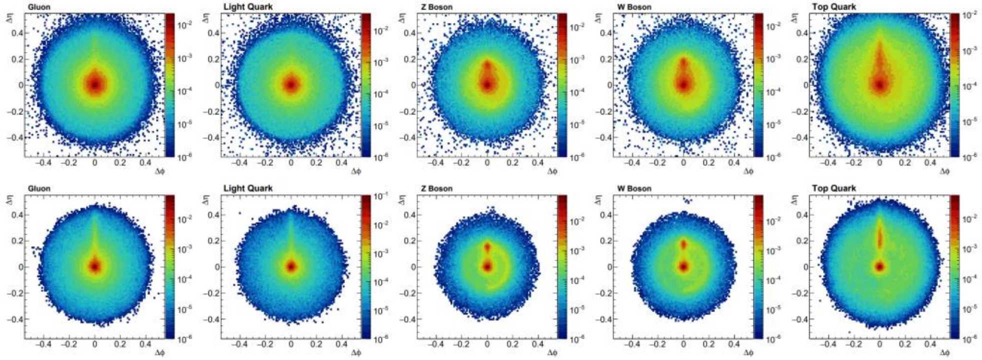
Resolving Extreme Jet Substructure



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

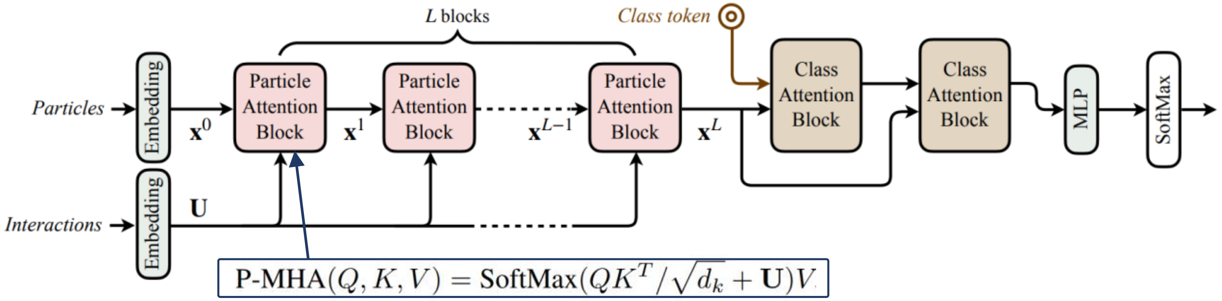
Point Cloud Transformers applied to Collider Physics

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 ***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 M	340 M
ParT (plain)	0.849	2.13 M	260 M

Top-Tagging

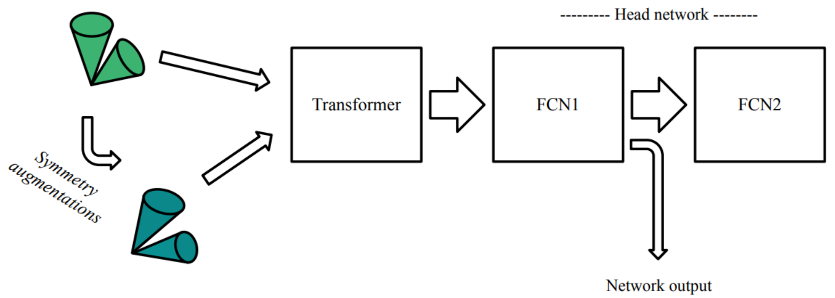
	Accuracy
P-CNN	0.930
PFN	—
ParticleNet	0.940
JEDI-net (w/ $\sum O$)	0.930
PCT	0.940
LGN	0.929
rPCN	—
LorentzNet	0.942
ParT	0.940
ParticleNet-f.t.	0.942
ParT-f.t.	**0.944**

(Also best in quark-gluon tagging)

Particle Physics

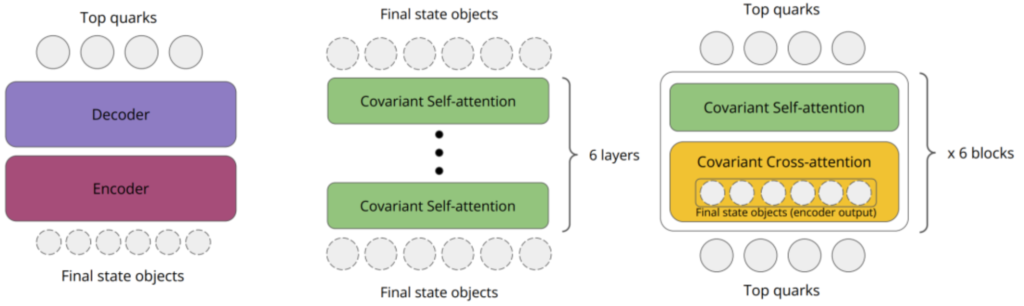
https://arxiv.org/pdf/2205.10380.pdf

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



(a) CPT (b) Encoder (c) Decoder

Contrastive Learning

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

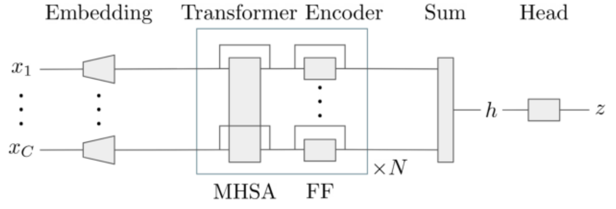
Symmetries, Safety, and Self-Supervision

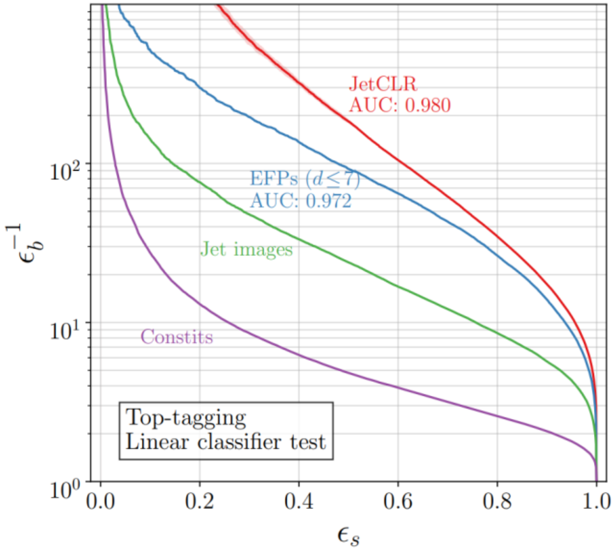
The goal of our network is to define a mapping between the jet constituents and a representation space,

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

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**