Introduction to NLP

CSE5321/CSEG321

Lecture 11. Transformers (2)

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Materials are referenced from Stanford CS224n

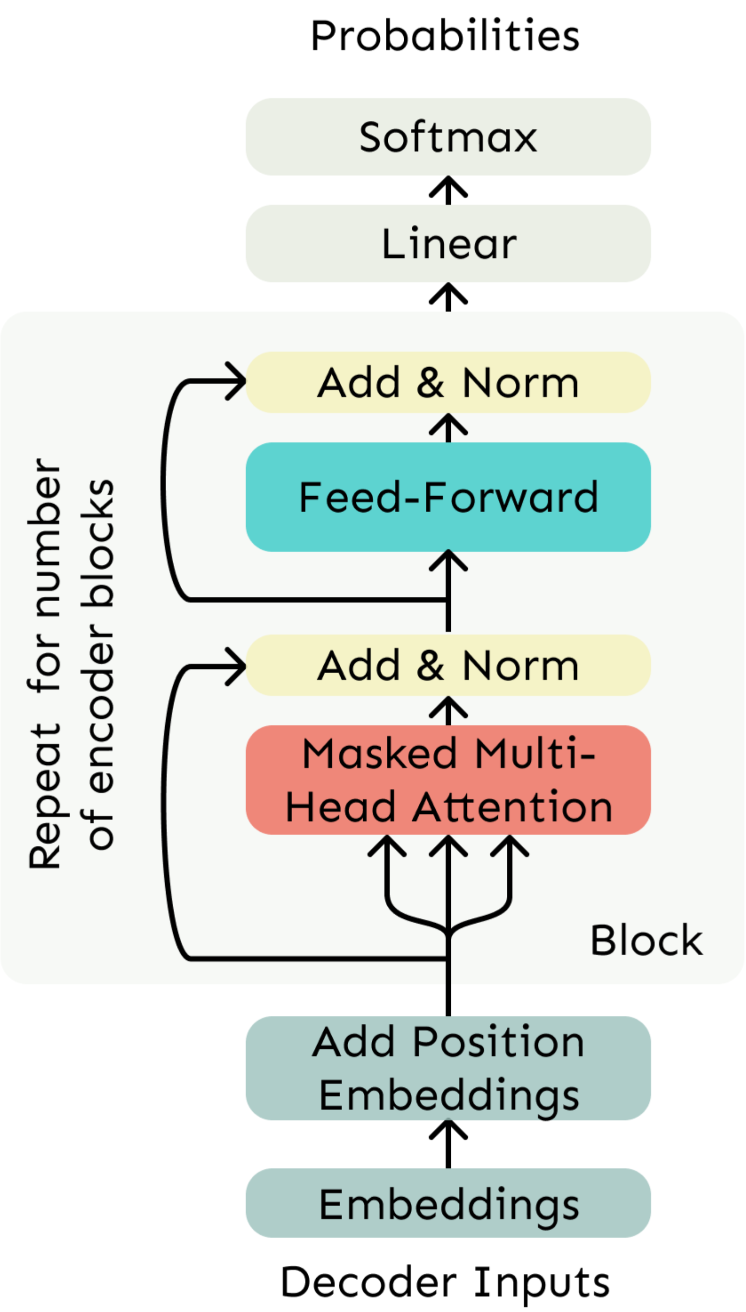
Lecture Plan

Lecture 11: Transformers

1. Notification on "Discussion in Class"
2. Recap Transformer Architectures
3. Positional Embeddings
4. Great results with Transformers
5. Drawbacks and variants of Transformers

The Transformer Decoder

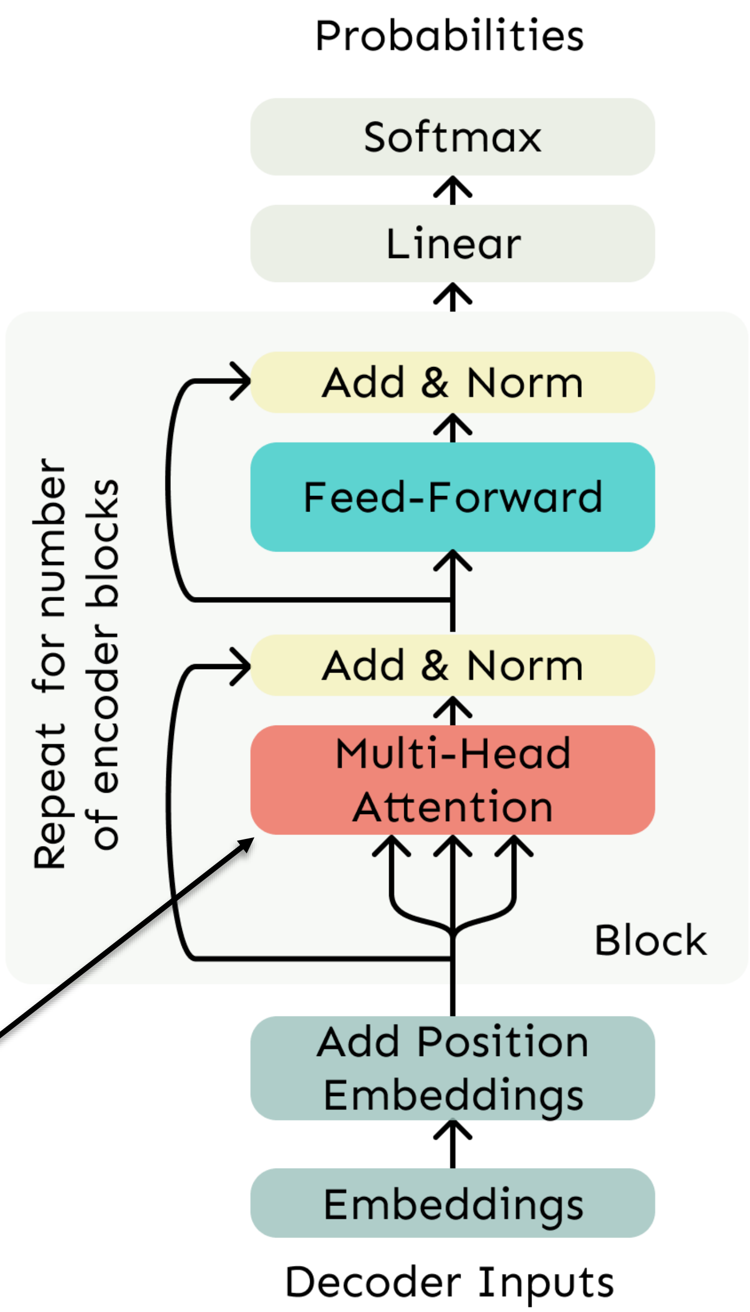
- The Transformer Decoder is a stack of Transformer Decoder **Blocks**.
- Each Block consists of:
  - Self-attention
  - Add & Norm
  - Feed-Forward
  - Add & Norm
- That's it! We've gone through the Transformer Decoder.



The Transformer Encoder

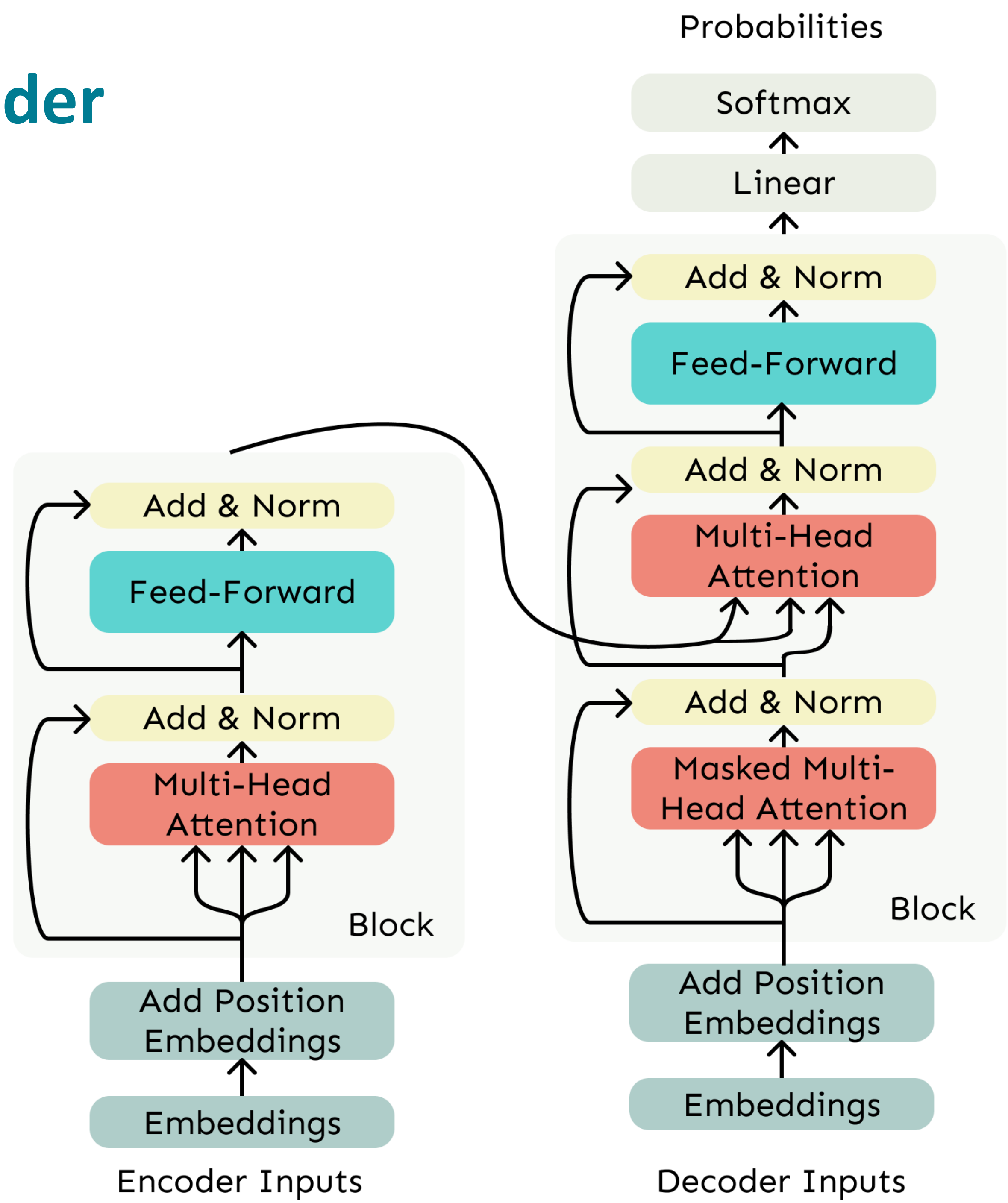
- The Transformer Decoder constrains to **unidirectional context**, as for **language models.**
- What if we want **bidirectional context**, like in a bidirectional RNN?
- This is the Transformer Encoder. The only difference is that we **remove the masking** in the self-attention.

No Masking!



The Transformer Encoder-Decoder

- Recall that in machine translation, we processed the source sentence with a **bidirectional** model and generated the target with a **unidirectional model**.
- For this kind of seq2seq format, we often use a Transformer Encoder-Decoder.
- We use a normal Transformer Encoder.
- Our Transformer Decoder is modified to perform **cross-attention** to the output of the Encoder.



Fixing the first self-attention problem: **sequence order**

- Since self-attention doesn't build in order information, we need to encode the order of the sentence in our keys, queries, and values.
- Consider representing each **sequence index** as a **vector**

$$\boldsymbol{p}_i \in \mathbb{R}^d, \text{ for } i \in \{1,2,\dots,n\} \text{ are position vectors}$$

- Don't worry about what the p_i are made of yet!
- Easy to incorporate this info into our self-attention block: just add the $\boldsymbol{p}_i$ to our inputs!
- Recall that $\boldsymbol{x}_i$ is the embedding of the word at index i. The positioned embedding is:

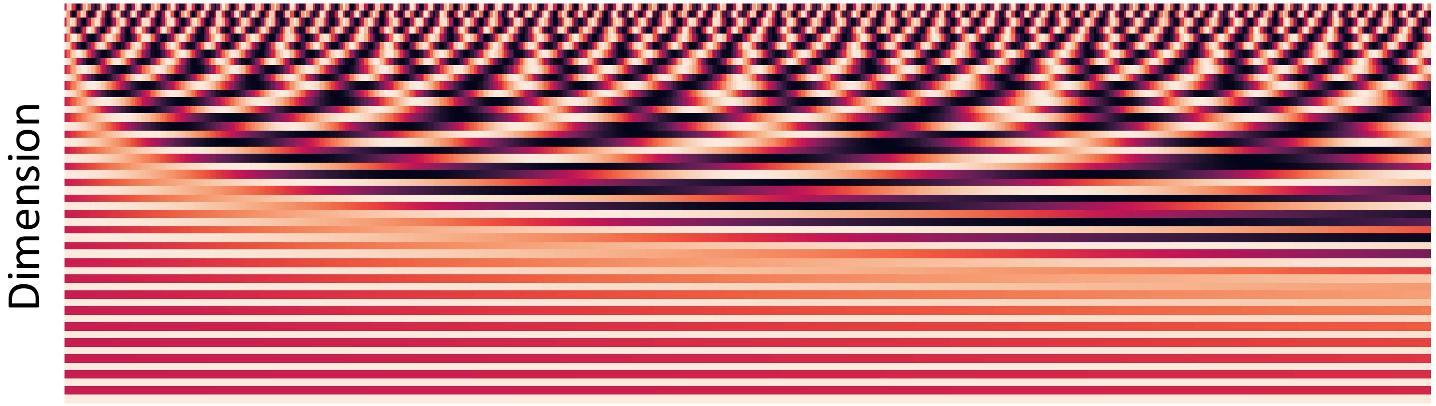
$$\tilde{\boldsymbol{x}}_i = \boldsymbol{x}_i + \boldsymbol{p}_i$$

In deep self-attention networks, we do this at the first layer! You could concatenate them as well, but people mostly just add…

Position representation vectors through sinusoids

- **Sinusoidal position representations:** concatenate sinusoidal functions of varying periods:

$$
\boldsymbol{p}_i = \begin{pmatrix} \sin(i/10000^{2*1/d}) \\ \cos(i/10000^{2*1/d}) \\ \vdots \\ \sin(i/10000^{2*\frac{d}{2}/d}) \\ \cos(i/10000^{2*\frac{d}{2}/d}) \end{pmatrix}
$$



- Pros:
  - Periodicity indicates that maybe “absolute position” isn’t as important
  - Maybe can extrapolate to longer sequences as periods restart!
- Cons:
  - Not learnable; also the extrapolation doesn’t really work!

Image: https://timodenk.com/blog/linear-relationships-in-the-transformers-positional-encoding/

Position representation vectors learned from scratch

- **Learned absolute position representations:** Let all p_i be learnable parameters!
  Learn a matrix $\boldsymbol{p} \in \mathbb{R}^{d \times n}$, *and let each* $\boldsymbol{p}_i$ *be a column of that matrix!*

- Pros:
  - Flexibility: each position gets to be learned to fit the data
- Cons:
  - Definitely can't extrapolate to indices outside $1, \dots, n$.
- Most systems use this!

- Sometimes people try more flexible representations of position:
  - Relative linear position attention [Shaw et al., 2018]
  - Dependency syntax-based position [Wang et al., 2019]

Positional Embeddings

- Motivating Example:

  - The **dog** chased another **dog**

  - -> Without any positional information, the output is *identical* for the same token in different positions.

https://huggingface.co/blog/designing-positional-encoding

Positional Embeddings

- Motivating Example:

  - The **dog** chased another **dog**

  - -> Without any positional information, the output is *identical* for the same token in different positions.

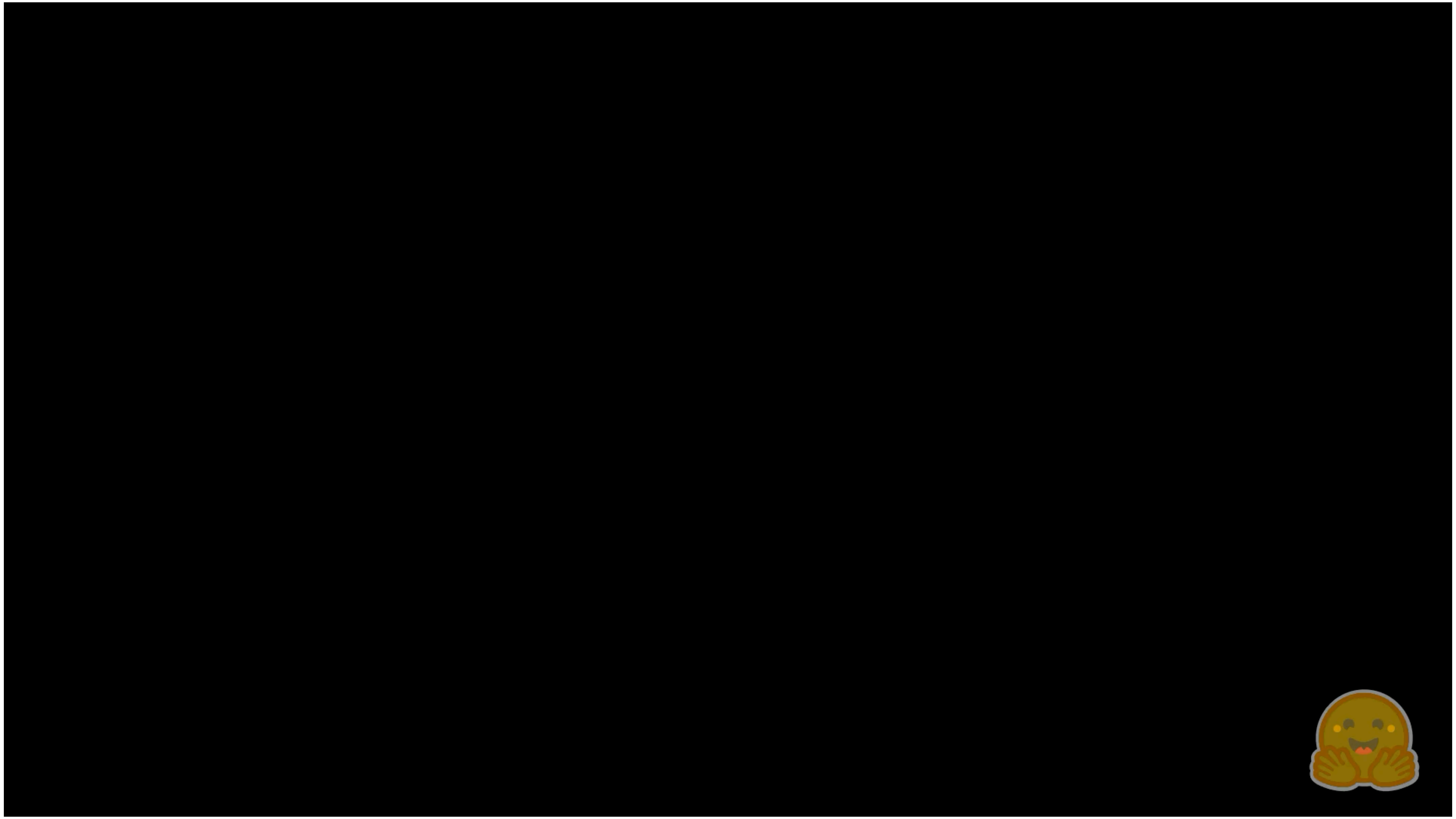
```python
import torch
import torch.nn as nn
from transformers import AutoTokenizer, AutoModel

model_id = "meta-llama/Llama-3.2-1B"
tok = AutoTokenizer.from_pretrained(model_id)
model = AutoModel.from_pretrained(model_id)

text = "The dog chased another dog"
tokens = tok(text, return_tensors="pt")["input_ids"]
embeddings = model.embed_tokens(tokens)
hdim = embeddings.shape[-1]

W_q = nn.Linear(hdim, hdim, bias=False)
W_k = nn.Linear(hdim, hdim, bias=False)
W_v = nn.Linear(hdim, hdim, bias=False)
mha = nn.MultiheadAttention(embed_dim=hdim, num_heads=4, batch_first=True)

with torch.no_grad():
    for param in mha.parameters():
        nn.init.normal_(param, std=0.1) # Initialize weights to be non-negligible

output, _ = mha(W_q(embeddings), W_k(embeddings), W_v(embeddings))

dog1_out = output[0, 2]
dog2_out = output[0, 5]
print(f"Dog output identical?: {torch.allclose(dog1_out, dog2_out, atol=1e-6)}")
```

https://huggingface.co/blog/designing-positional-encoding

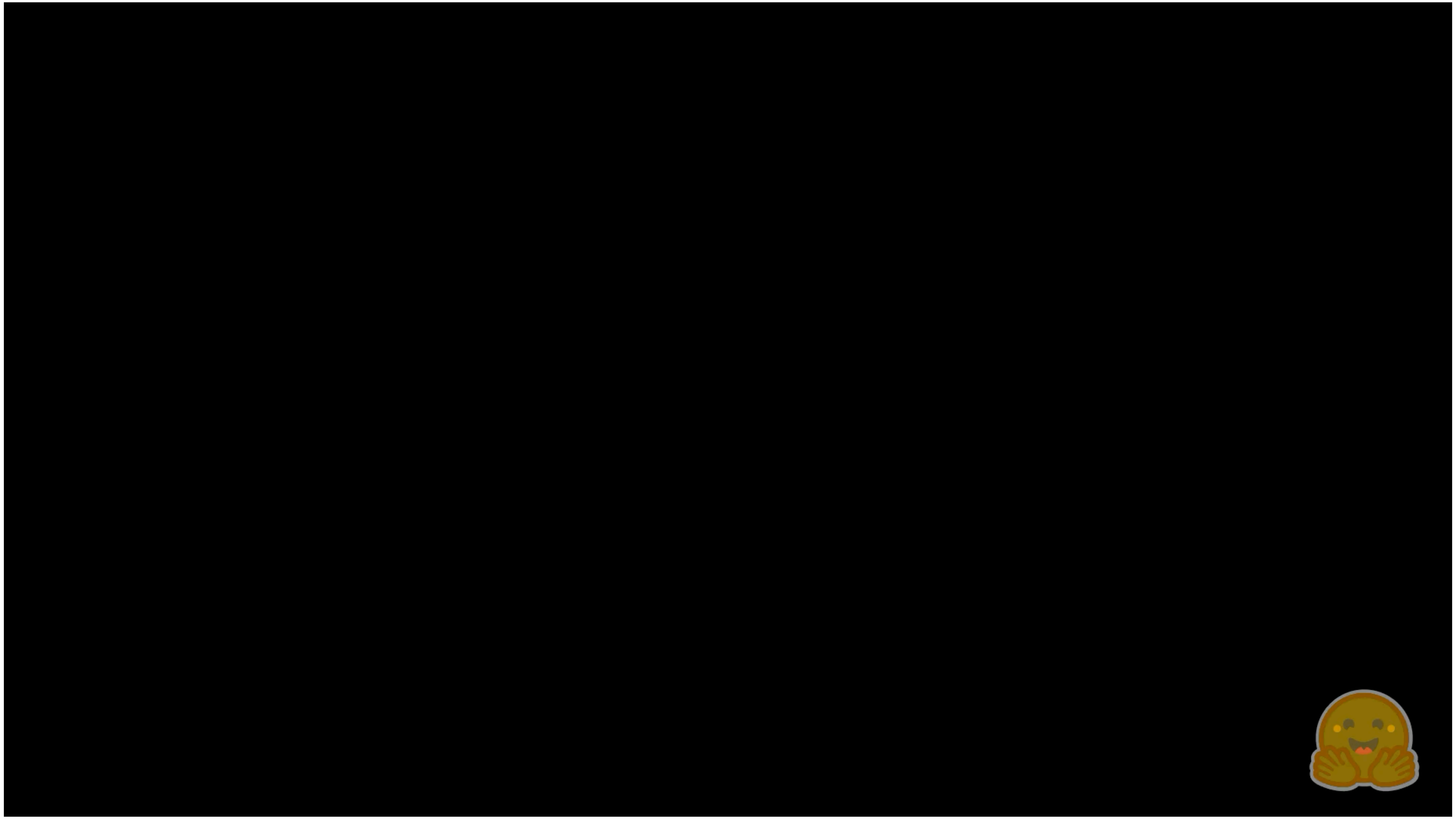
Positional Embeddings

- Desirable Properties
  - Property 1 - Unique encoding for each position (across sequences)
  - Property 2 - Linear relation between two encoded positions
  - Property 3 - Generalizes to longer sequences than those encountered in training
  - Property 4 - Generated by a deterministic process the model can learn
  - Property 5 - Extensible to multiple dimensions

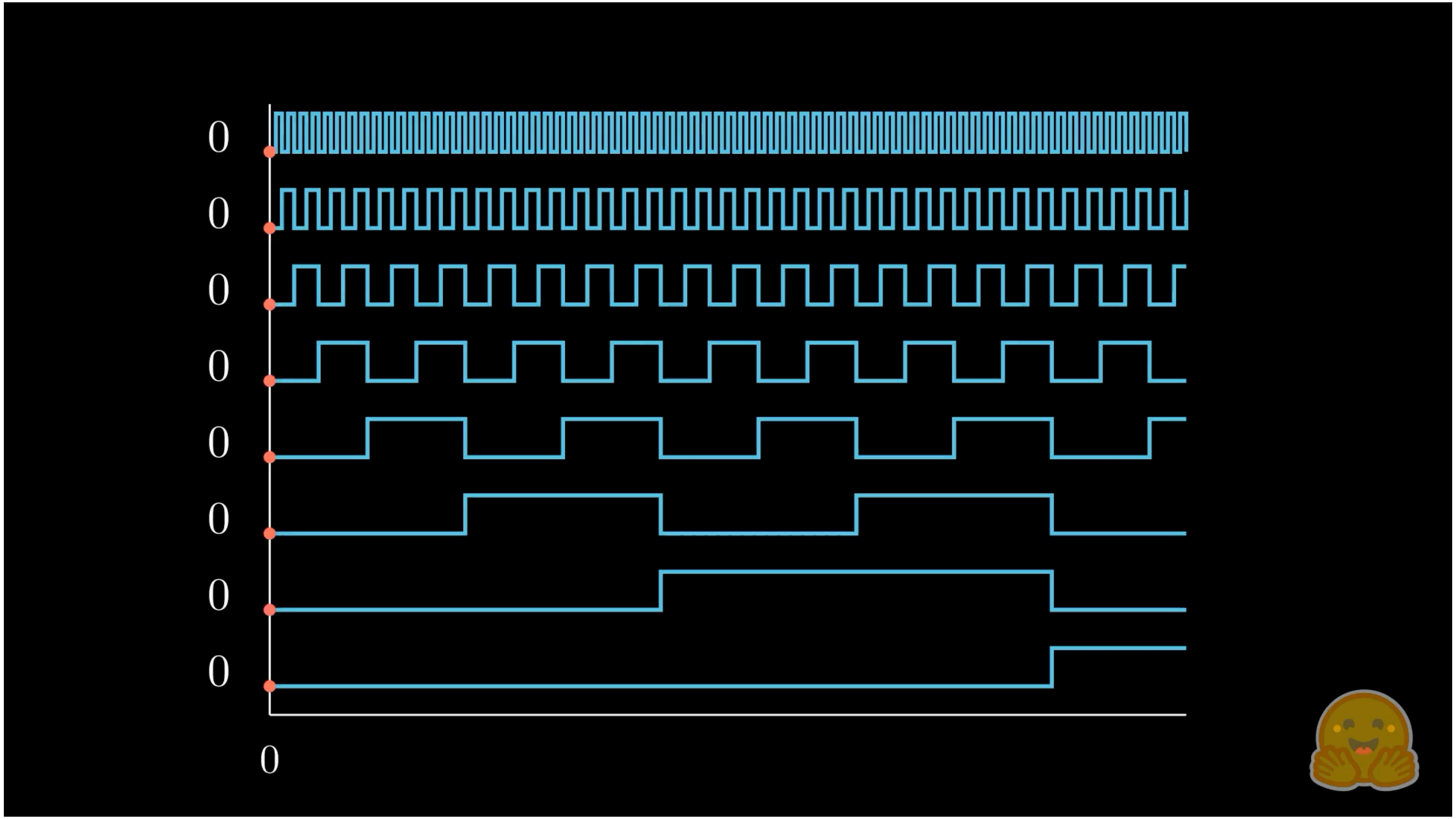
Positional Embeddings: Integer Position Encoding



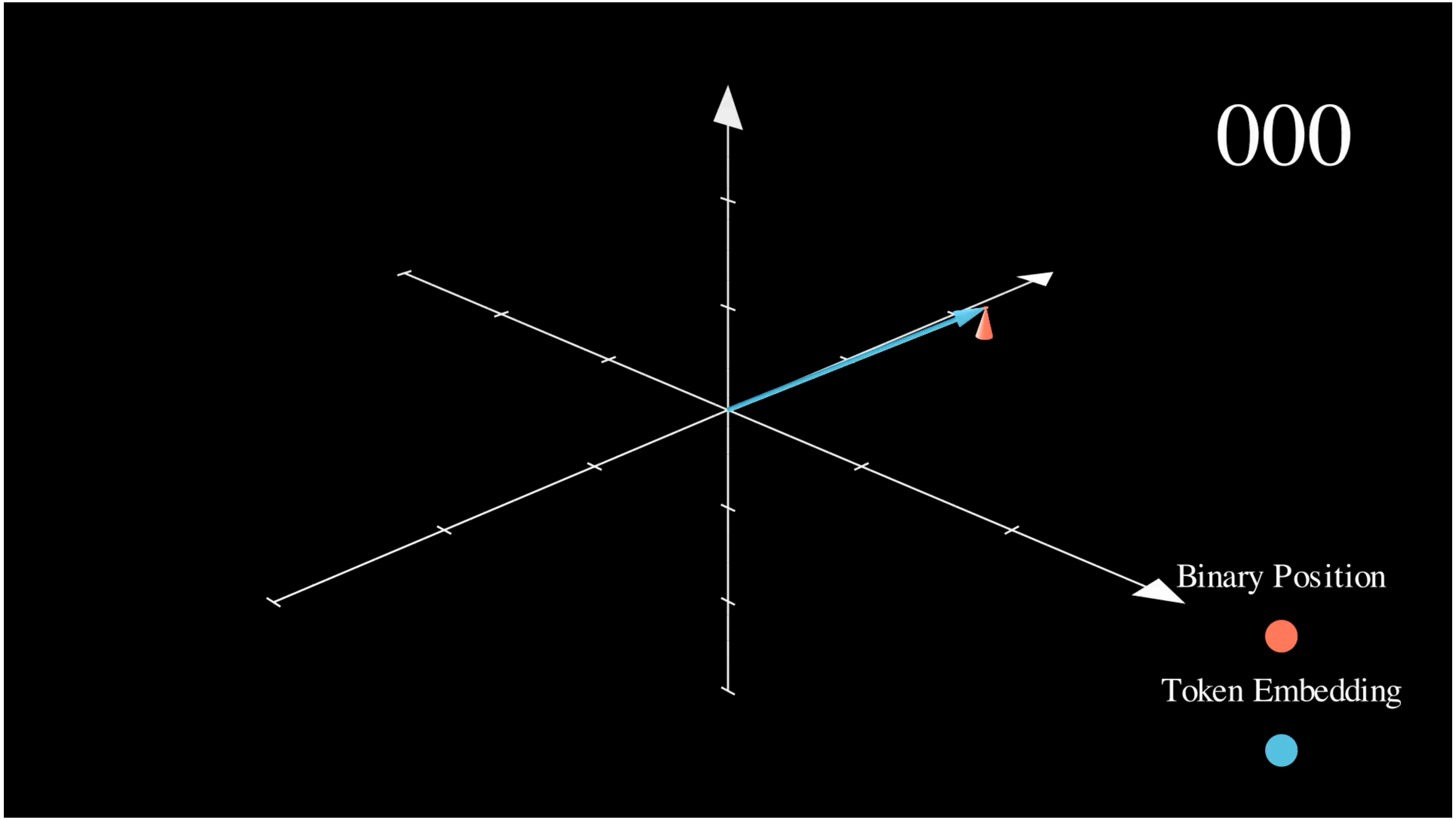
Positional Embeddings: Binary Position Encoding



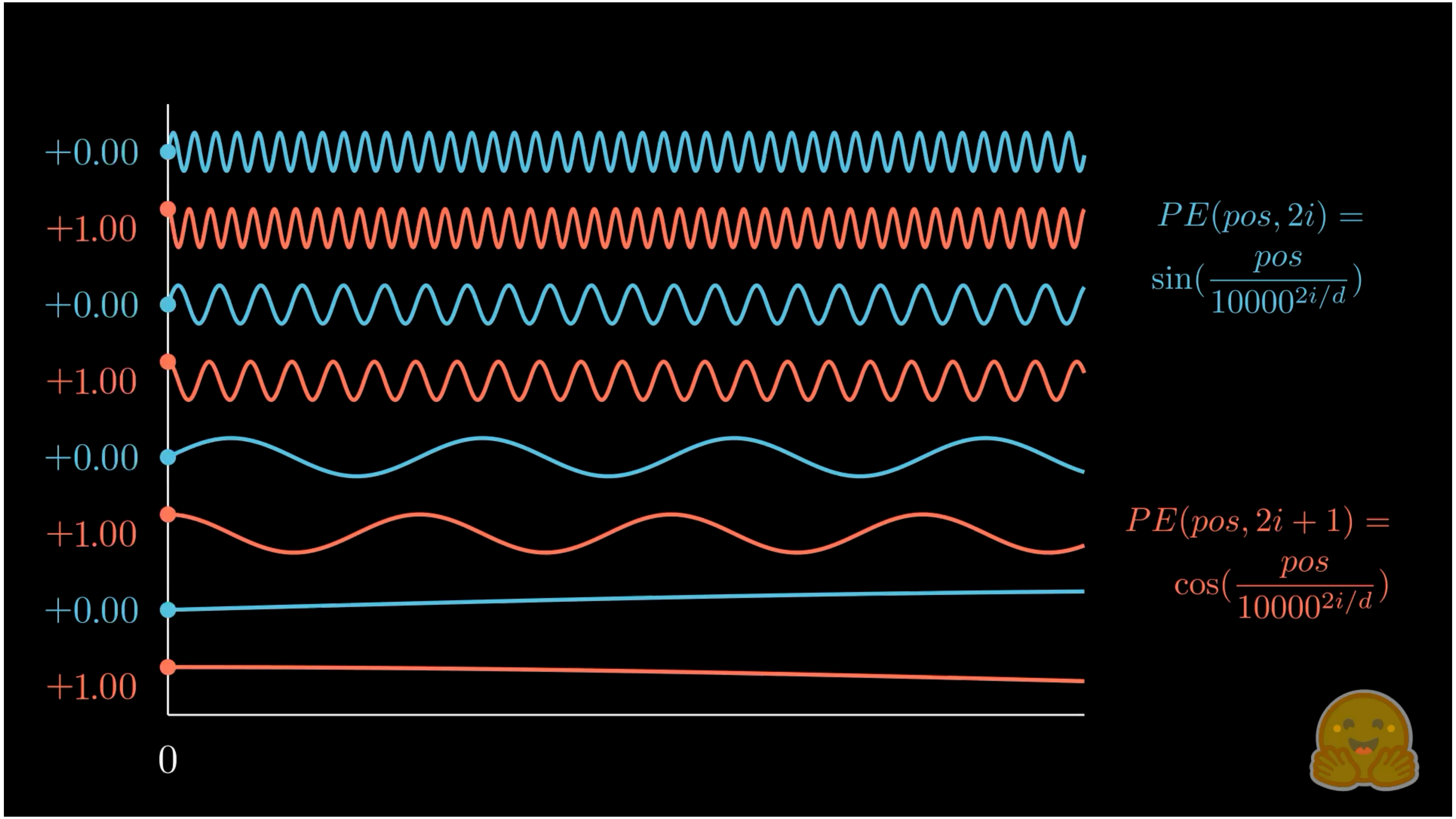
Positional Embeddings: Binary Position Encoding



Positional Embeddings: Binary Position Encoding



Positional Embeddings: Sinusoidal Positional Encoding



Common, modern position embeddings - RoPE

High level thought process: a *relative* position embedding should be some $f(x, i)$ s.t.

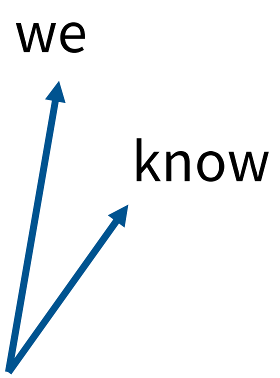
$$\langle f(x, i), f(y, j) \rangle = g(x, y, i - j)$$

That is, the attention function *only* gets to depend on the relative position (i-j). How do existing embeddings not fulfill this goal?

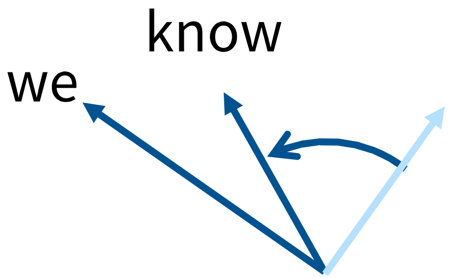
RoPE – Embedding via rotation

How can we solve this problem?

- We want our embeddings to be invariant to absolute position
- We know that inner products are invariant to arbitrary rotation.

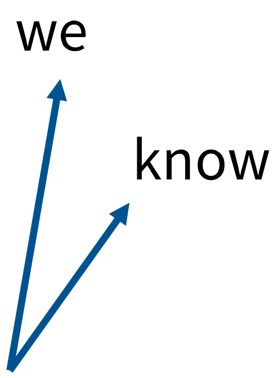


Position independent embedding



Embedding
“of course we know”

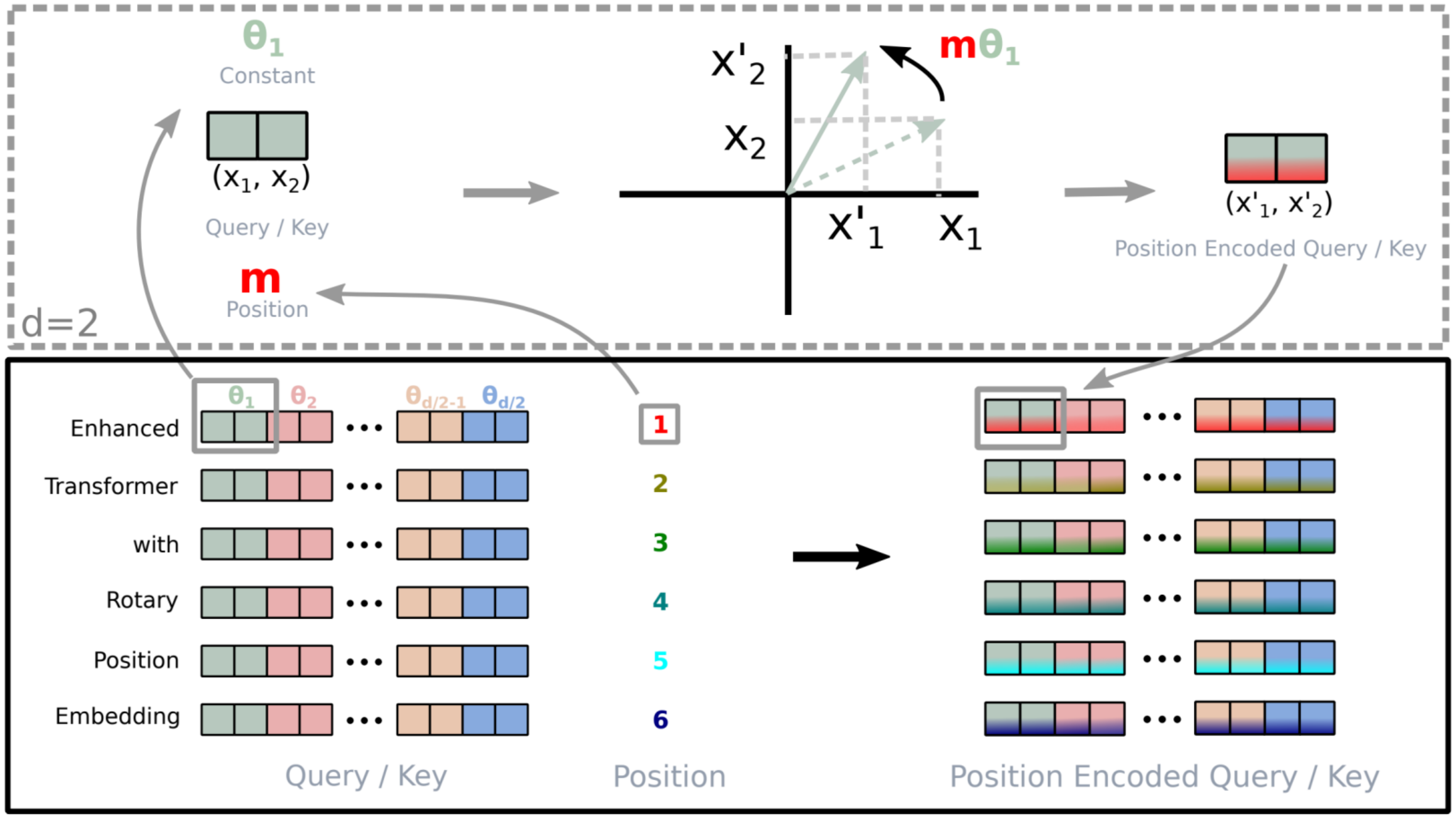
Rotate by ‘2 positions’



Embedding
“we know that”

Rotate by ‘0 positions’

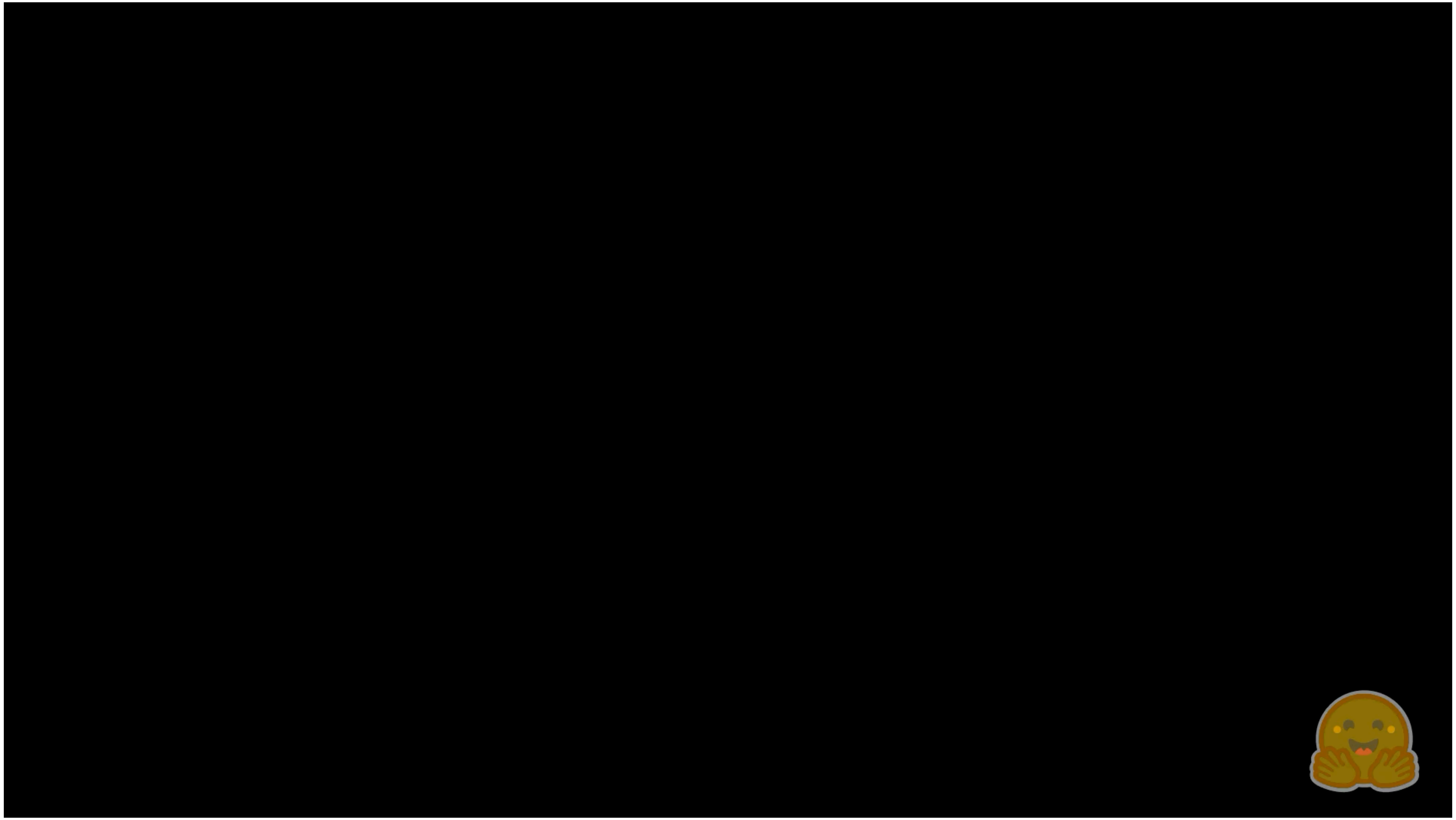
RoPE – From 2 to many dimensions



[Su et al 2021]

Just pair up the coordinates and rotate them in 2d (motivation: complex numbers)

Positional Embeddings: RoPE



Great Results with Transformers

First, Machine Translation from the original Transformers paper!

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

 [Test sets: WMT 2014 English-German and English-French]

[Vaswani et al., 2017]

Great Results with Transformers

Next, document generation!

Model	Test perplexity	ROUGE-L
seq2seq-attention, $L = 500$	5.04952	12.7
Transformer-ED, $L = 500$	2.46645	34.2
Transformer-D, $L = 4000$	2.22216	33.6
Transformer-DMCA, no MoE-layer, $L = 11000$	2.05159	36.2
Transformer-DMCA, MoE-128, $L = 11000$	1.92871	37.9
Transformer-DMCA, MoE-256, $L = 7500$	1.90325	38.8

The old standard

Transformers all the way down.

[Liu et al., 2018]; WikiSum dataset

Great Results with Transformers

Before too long, most Transformers results also included **pretraining**, a method we'll go over next.

Transformers' parallelizability allows for efficient pretraining, and have made them the de-facto standard.

On this popular aggregate benchmark, for example:

GLUE

All top models are Transformer (and pretraining)-based.

	Rank	Name	Model	URL	Score
	1	DeBERTa Team - Microsoft	DeBERTa / TuringNLRv4	↗	90.8
	2	HFL iFLYTEK	MacALBERT + DKM		90.7
+	3	Alibaba DAMO NLP	StructBERT + TAPT	↗	90.6
+	4	PING-AN Omni-Sinitic	ALBERT + DAAF + NAS		90.6
	5	ERNIE Team - Baidu	ERNIE	↗	90.4
	6	T5 Team - Google	T5	↗	90.3

[Liu et al., 2018]

Outline

1. From recurrence (RNN) to attention-based NLP models
2. Introducing the Transformer model
3. Great results with Transformers
4. Drawbacks and variants of Transformers

What would we like to fix about the Transformer?

- **Training instabilities (Pre vs Post norm)**

- **Quadratic compute in self-attention** :
  - Computing all pairs of interactions means our computation grows **quadratically** with the sequence length!
  - For recurrent models, it only grew linearly!

Pre vs Post norm

The one thing *everyone* agrees on (in 2024)

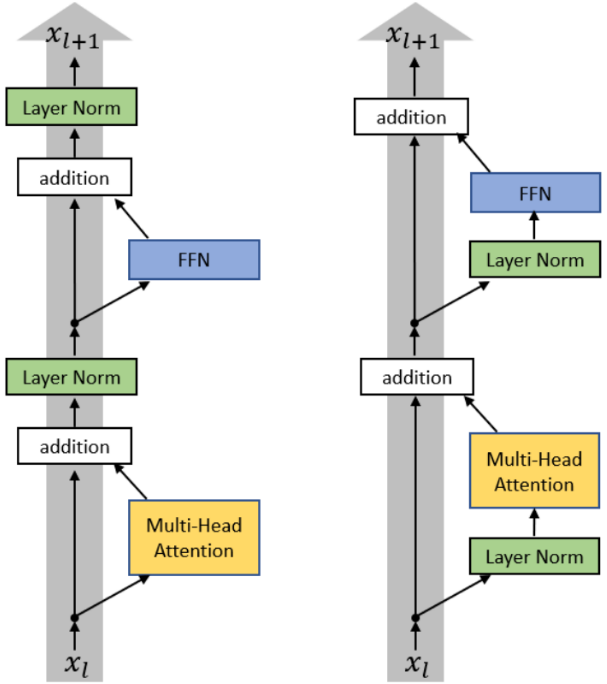


Figure from Xiong 2020

Post-LN Transformer	Pre-LN Transformer
$x^{post,1}_{l,i} = \text{MultiHeadAtt}(x^{post}_{l,i}, [x^{post}_{l,1}, \cdots, x^{post}_{l,n}])$	$x^{pre,1}_{l,i} = \text{LayerNorm}(x^{pre}_{l,i})$
$x^{post,2}_{l,i} = x^{post}_{l,i} + x^{post,1}_{l,i}$	$x^{pre,2}_{l,i} = \text{MultiHeadAtt}(x^{pre,1}_{l,i}, [x^{pre,1}_{l,1}, \cdots, x^{pre,1}_{l,n}])$
$x^{post,3}_{l,i} = \text{LayerNorm}(x^{post,2}_{l,i})$	$x^{pre,3}_{l,i} = x^{pre}_{l,i} + x^{pre,2}_{l,i}$
$x^{post,4}_{l,i} = \text{ReLU}(x^{post,3}_{l,i} W^{1,l} + b^{1,l}) W^{2,l} + b^{2,l}$	$x^{pre,4}_{l,i} = \text{LayerNorm}(x^{pre,3}_{l,i})$
$x^{post,5}_{l,i} = x^{post,3}_{l,i} + x^{post,4}_{l,i}$	$x^{pre,5}_{l,i} = \text{ReLU}(x^{pre,4}_{l,i} W^{1,l} + b^{1,l}) W^{2,l} + b^{2,l}$
$x^{post}_{l+1,i} = \text{LayerNorm}(x^{post,5}_{l,i})$	$x^{pre}_{l+1,i} = x^{pre,5}_{l,i} + x^{pre,3}_{l,i}$
	Final LayerNorm: $x^{pre}_{Final,i} \leftarrow \text{LayerNorm}(x^{pre}_{L+1,i})$

Set up LayerNorm so that it doesn't affect the main residual signal path (on the left)

Almost all modern LMs use pre-norm (but BERT was post-norm)

(One somewhat funny exception – OPT350M. I don't know why this is post-norm)

Quadratic computation as a function of sequence length

- One of the benefits of self-attention over recurrence was that it's highly parallelizable.
- However, its total number of operations grows as $O(n^2 d)$, where n is the sequence length, and d is the dimensionality.

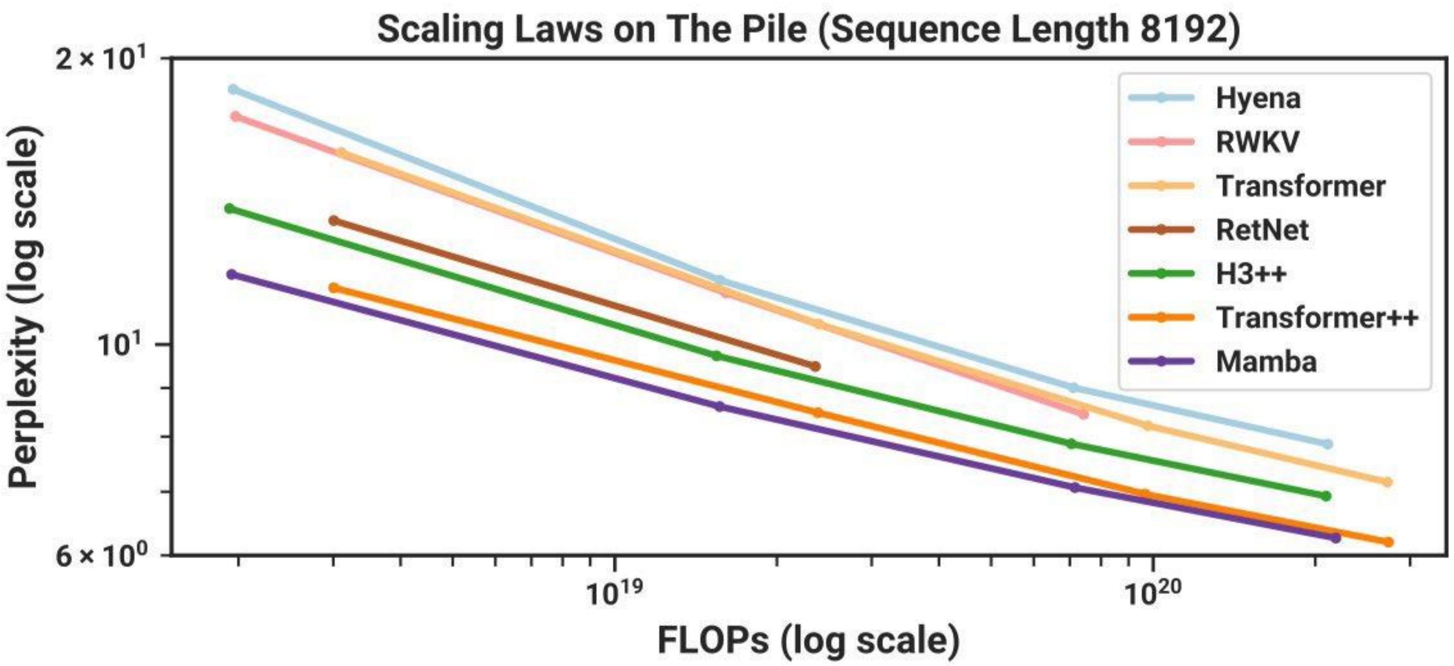
$$XQ \quad K^\top X^\top = XQK^\top X^\top \in \mathbb{R}^{n\times n}$$

Need to compute all pairs of interactions! $O(n^2 d)$

- Think of d as around $\mathbf{1,000}$ (though for large language models it's much larger!).
  - So, for a single (shortish) sentence, $n \le 30$; $n^2 \le \mathbf{900}$.
  - In practice, we set a bound like $n = 512$.
  - **But what if we'd like $\boldsymbol{n} \ge \mathbf{50,000}$?** For example, to work on long documents?

Back to the future – RNNs are back!

RNNs only require $O(nd^2)$ computations!



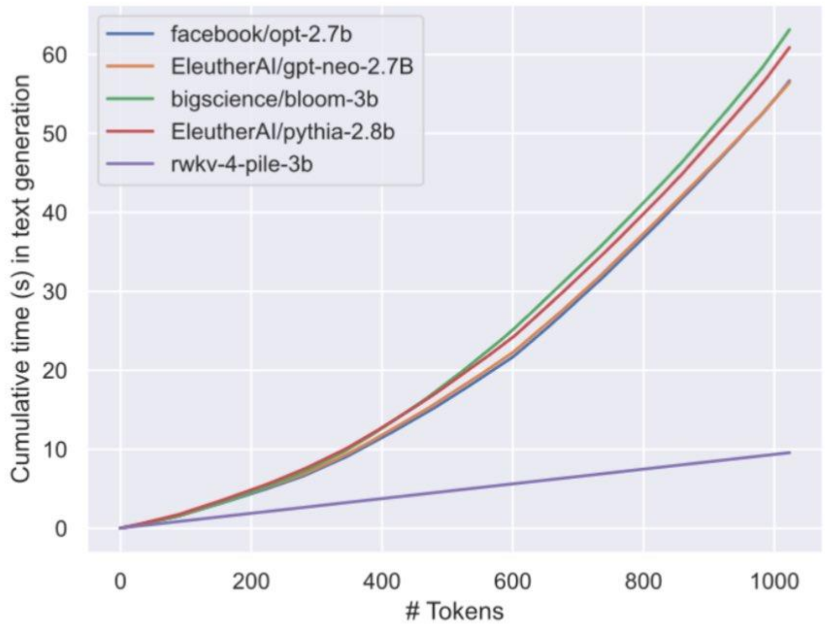
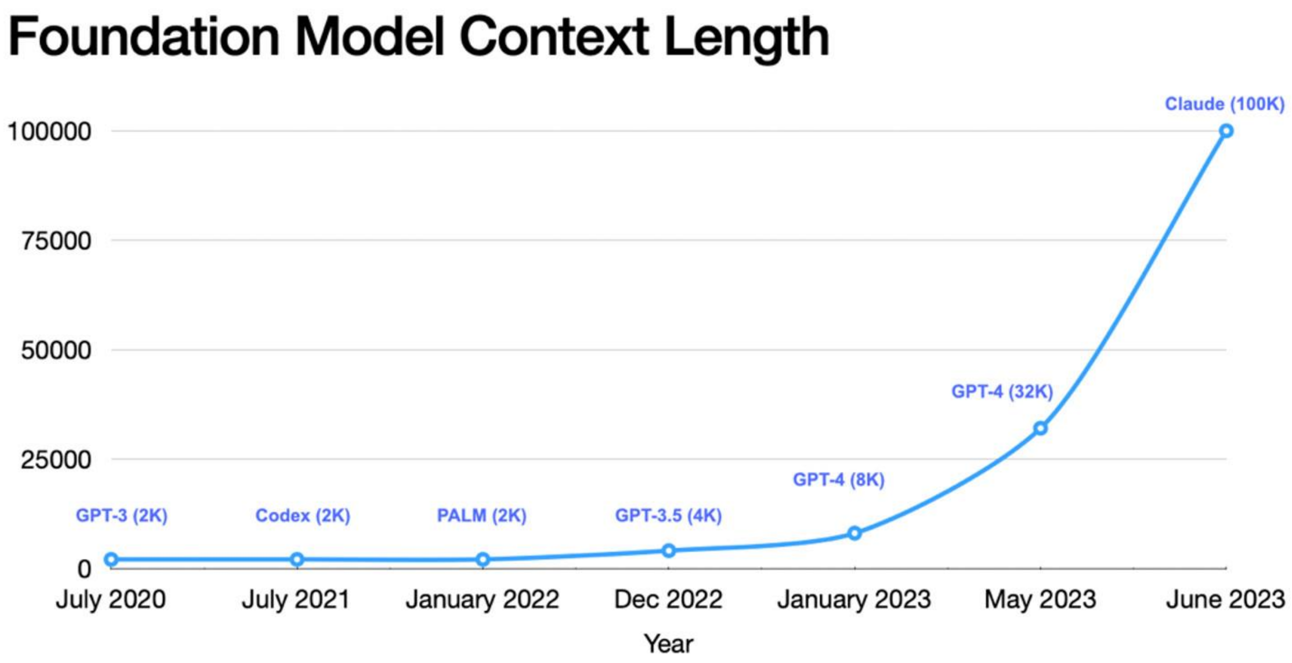


Figure 7: Cumulative time on text generation for LLM
Unlike transformers, RWKV exhibits linear scaling.

If you want *really* long context, RNNs provide this (linear complexity).
Modern RNNs (RWKV, Mamba, etc) are getting better!

Do we even need to remove the quadratic cost of attention?

- As Transformers grow larger, a larger and larger percent of compute is **outside** the self-attention portion, despite the quadratic cost.
- In practice, **production Transformer language models use quadratic cost attention**
  - The cheaper methods tend not to work as well at scale.
  - Systems optimizations work well (Flash attention – Jun 2022)



Do Transformer Modifications Transfer?

- "Surprisingly, we find that most modifications do not meaningfully improve performance."

Model	Params	Ops	Step/s	Early loss	Final loss	SGLUE	XSum	WebQ	WMT EnDe
Vanilla Transformer	223M	11.1T	3.50	2.182 ± 0.005	1.838	71.66	17.78	23.02	26.62
GeLU	223M	11.1T	3.58	2.179 ± 0.003	1.838	**75.79**	**17.86**	**25.13**	26.47
Swish	223M	11.1T	3.62	2.186 ± 0.003	1.847	**73.77**	17.74	**24.34**	**26.75**
ELU	223M	11.1T	3.56	2.270 ± 0.007	1.932	67.83	16.73	23.02	26.08
GLU	223M	11.1T	3.59	2.174 ± 0.003	**1.814**	**74.20**	**17.42**	24.34	**27.12**
GeGLU	223M	11.1T	3.55	2.130 ± 0.006	**1.792**	**75.96**	**18.27**	**24.87**	**26.87**
ReGLU	223M	11.1T	3.57	2.145 ± 0.004	**1.803**	**76.17**	**18.36**	**24.87**	**27.02**
SeLU	223M	11.1T	3.55	2.315 ± 0.004	1.948	68.76	16.76	22.75	25.99
SwiGLU	223M	11.1T	3.53	2.127 ± 0.003	**1.789**	**76.00**	**18.20**	**24.34**	**27.02**
LiGLU	223M	11.1T	3.59	2.149 ± 0.005	**1.798**	**75.34**	**17.97**	**24.34**	26.53
Sigmoid	223M	11.1T	3.63	2.291 ± 0.019	1.867	**74.31**	17.51	23.02	26.30
Softplus	223M	11.1T	3.47	2.207 ± 0.011	1.850	**72.45**	17.65	**24.34**	**26.89**
RMS Norm	223M	11.1T	3.68	2.167 ± 0.008	**1.821**	**75.45**	**17.94**	**24.07**	**27.14**
Rezero	223M	11.1T	3.51	2.262 ± 0.003	1.939	61.69	15.64	20.90	26.37
Rezero + LayerNorm	223M	11.1T	3.26	2.223 ± 0.006	1.858	70.42	17.58	23.02	26.29
Rezero + RMS Norm	223M	11.1T	3.34	2.221 ± 0.009	1.875	70.33	17.32	23.02	26.19
Fixup	223M	11.1T	2.95	2.382 ± 0.012	2.067	58.56	14.42	23.02	26.31
24 layers, $d_{ff} = 1536$, $H = 6$	224M	11.1T	3.33	2.200 ± 0.007	1.843	**74.89**	17.75	**25.13**	**26.89**
18 layers, $d_{ff} = 2048$, $H = 8$	223M	11.1T	3.38	2.185 ± 0.005	**1.831**	**76.45**	16.83	**24.34**	**27.10**
8 layers, $d_{ff} = 4608$, $H = 18$	223M	11.1T	3.69	2.190 ± 0.005	1.847	**74.58**	17.69	**23.28**	**26.85**
6 layers, $d_{ff} = 6144$, $H = 24$	223M	11.1T	3.70	2.201 ± 0.010	1.857	**73.55**	17.59	**24.60**	**26.66**
Block sharing	65M	11.1T	3.91	2.497 ± 0.037	2.164	64.50	14.53	21.96	25.48
+ Factorized embeddings	45M	9.4T	4.21	2.631 ± 0.305	2.183	60.84	14.00	19.84	25.27
+ Factorized & shared embeddings	20M	9.1T	4.37	2.907 ± 0.313	2.385	53.95	11.37	19.84	25.19
Encoder only block sharing	170M	11.1T	3.68	2.298 ± 0.023	1.929	69.60	16.23	23.02	26.23
Decoder only block sharing	144M	11.1T	3.70	2.352 ± 0.029	2.082	67.93	16.13	**23.81**	26.08
Factorized Embedding	227M	9.4T	3.80	2.208 ± 0.006	1.855	70.41	15.92	22.75	26.50
Factorized & shared embeddings	202M	9.1T	3.92	2.320 ± 0.010	1.952	68.69	16.33	22.22	26.44
Tied encoder/decoder input embeddings	248M	11.1T	3.55	2.192 ± 0.002	1.840	**71.70**	17.72	**24.34**	26.49
Tied decoder input and output embeddings	248M	11.1T	3.57	2.187 ± 0.007	**1.827**	**74.86**	17.74	**24.87**	**26.67**
Untied embeddings	273M	11.1T	3.53	2.195 ± 0.005	**1.834**	**72.99**	17.58	**23.28**	26.48
Adaptive input embeddings	204M	9.2T	3.55	2.250 ± 0.002	1.899	66.57	16.21	**24.07**	**26.66**
Adaptive softmax	204M	9.2T	3.60	2.364 ± 0.005	1.982	**72.91**	16.67	21.16	25.56
Adaptive softmax without projection	223M	10.8T	3.43	2.229 ± 0.009	1.914	**71.82**	17.10	23.02	25.72
Mixture of softmaxes	232M	16.3T	2.24	2.227 ± 0.017	**1.821**	**76.77**	17.62	22.75	**26.82**
Transparent attention	223M	11.1T	3.33	2.181 ± 0.014	1.874	54.31	10.40	21.16	**26.80**
Dynamic convolution	257M	11.8T	2.65	2.403 ± 0.009	2.047	58.30	12.67	21.16	17.03
Lightweight convolution	224M	10.4T	4.07	2.370 ± 0.010	1.989	63.07	14.86	23.02	24.73
Evolved Transformer	217M	9.9T	3.09	2.220 ± 0.003	1.863	**73.67**	10.76	**24.07**	26.58
Synthesizer (dense)	224M	11.4T	3.47	2.334 ± 0.021	1.962	61.03	14.27	16.14	**26.63**
Synthesizer (dense plus)	243M	12.6T	3.22	2.191 ± 0.010	1.840	**73.98**	16.96	**23.81**	**26.71**
Synthesizer (dense plus alpha)	243M	12.6T	3.01	2.180 ± 0.007	**1.828**	**74.25**	17.02	**23.28**	26.61
Synthesizer (factorized)	207M	10.1T	3.94	2.341 ± 0.017	1.968	62.78	15.39	**23.55**	26.42
Synthesizer (random)	254M	10.1T	4.08	2.326 ± 0.012	2.009	54.27	10.35	19.56	26.44
Synthesizer (random plus)	292M	12.0T	3.63	2.189 ± 0.004	1.842	**73.32**	17.04	**24.87**	26.43
Synthesizer (random plus alpha)	292M	12.0T	3.42	2.186 ± 0.007	**1.828**	**75.24**	17.08	**24.08**	26.39
Universal Transformer	84M	40.0T	0.88	2.406 ± 0.036	2.053	70.13	14.09	19.05	23.91
Mixture of experts	648M	11.7T	3.20	2.148 ± 0.006	**1.785**	**74.55**	**18.13**	**24.08**	**26.94**
Switch Transformer	1100M	11.7T	3.18	2.135 ± 0.007	**1.758**	**75.38**	**18.02**	**26.19**	**26.81**
Funnel Transformer	223M	1.9T	4.30	2.288 ± 0.008	1.918	67.34	16.26	22.75	23.20
Weighted Transformer	280M	71.0T	0.59	2.378 ± 0.021	1.989	69.04	16.98	23.02	26.30
Product key memory	421M	386.6T	0.25	2.155 ± 0.003	**1.798**	**75.16**	17.04	**23.55**	**26.73**

Do Transformer Modifications Transfer Across Implementations and Applications?

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Transformer

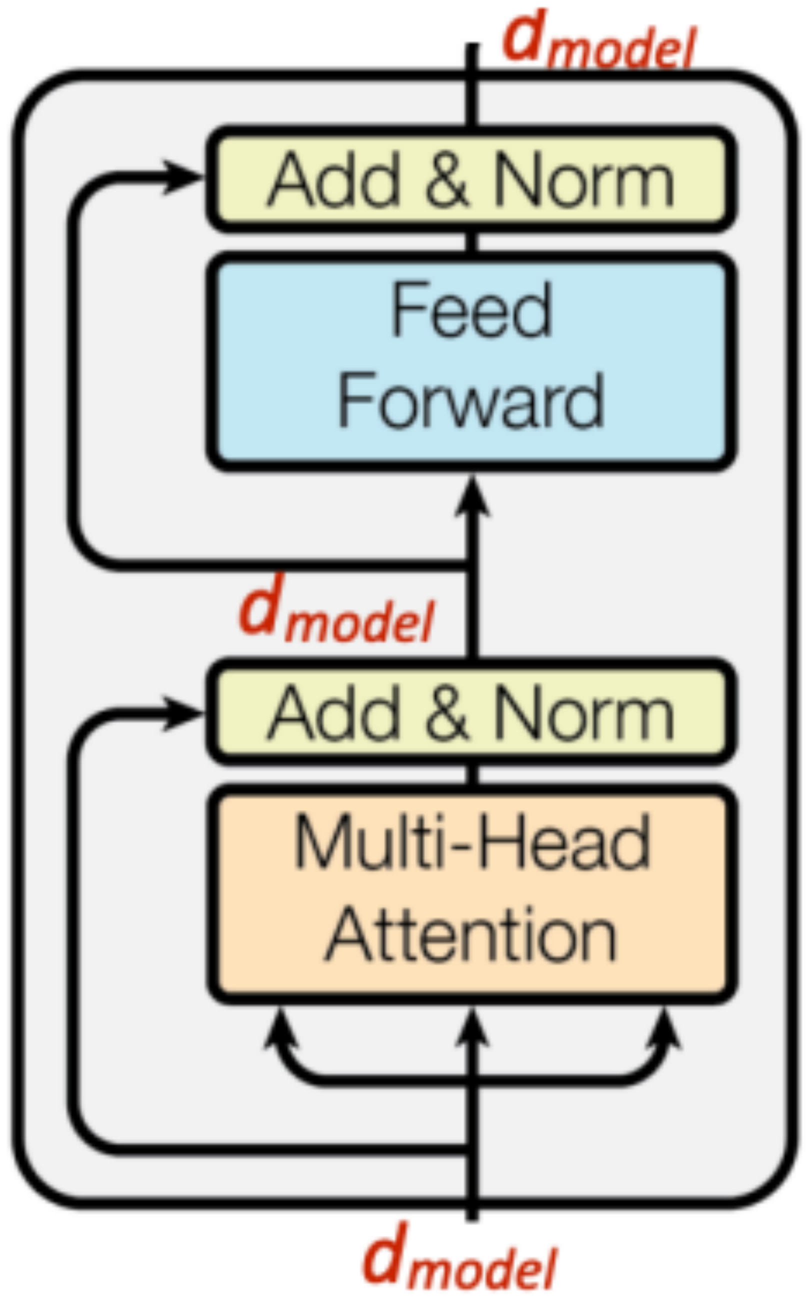
- Transformer architecture specifications

	N	d_{model}	d_{ff}	h	d_k	d_v
base	6	512	2048	8	64	64

  - From Vaswani et al.

Model Name	n_{params}	n_{layers}	d_{model}	n_{heads}	d_{head}
GPT-3 Small	125M	12	768	12	64
GPT-3 Medium	350M	24	1024	16	64
GPT-3 Large	760M	24	1536	16	96
GPT-3 XL	1.3B	24	2048	24	128
GPT-3 2.7B	2.7B	32	2560	32	80
GPT-3 6.7B	6.7B	32	4096	32	128
GPT-3 13B	13.0B	40	5140	40	128
GPT-3 175B or "GPT-3"	175.0B	96	12288	96	128

  - From GPT-3; d_{head} is our d_k

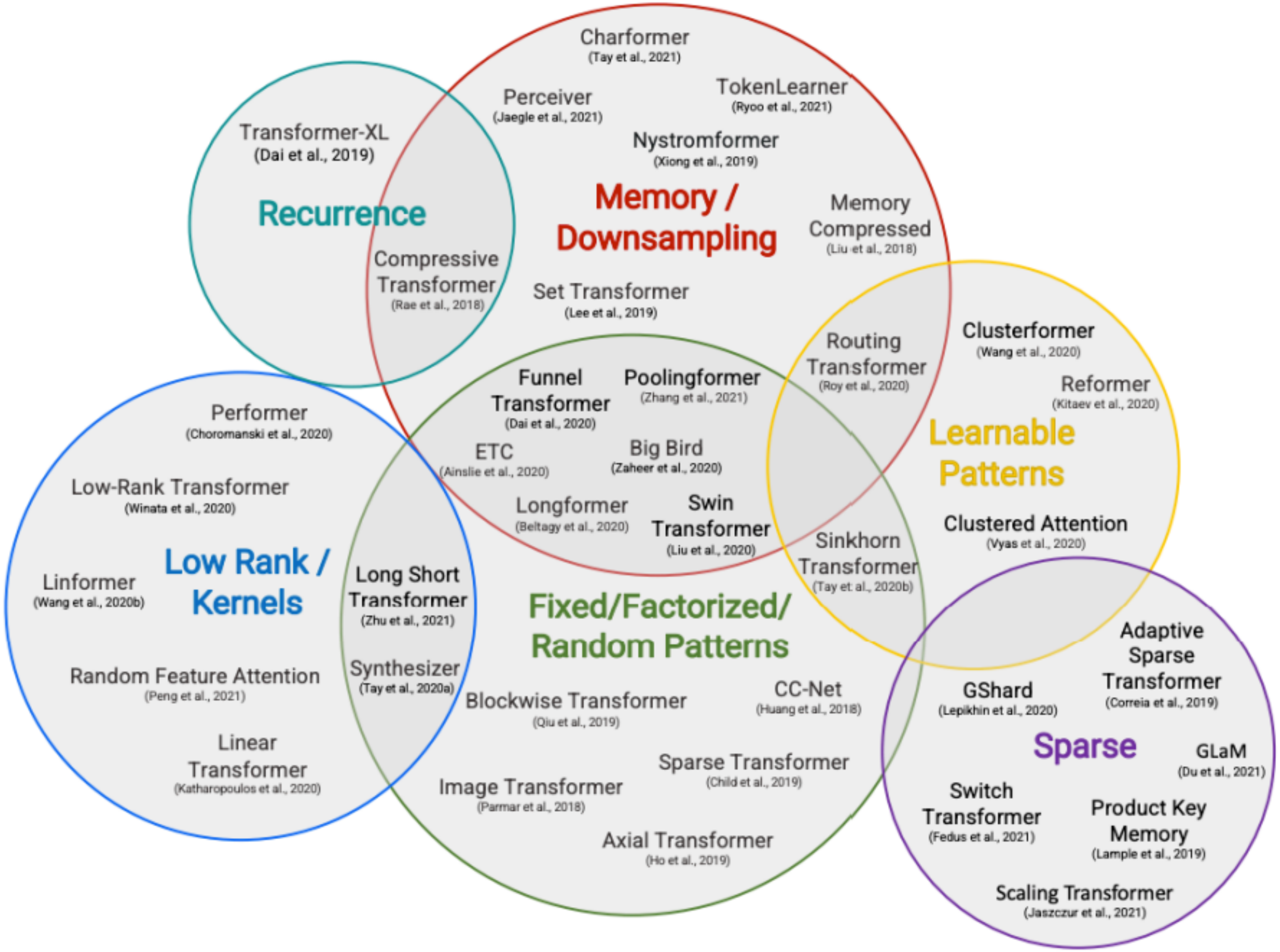


Transformer

- Advantages
  - Easier to capture long-range dependencies: we draw attention between every pair of word
  - Easier to parallelize
- Drawbacks
  - Are positional encodings enough to capture positional information?
    - Otherwise self-attention is an un unordered function of its input
  - Quadratic computation in self-attention
    - Can become very slow when the sequence length is large

Transformer

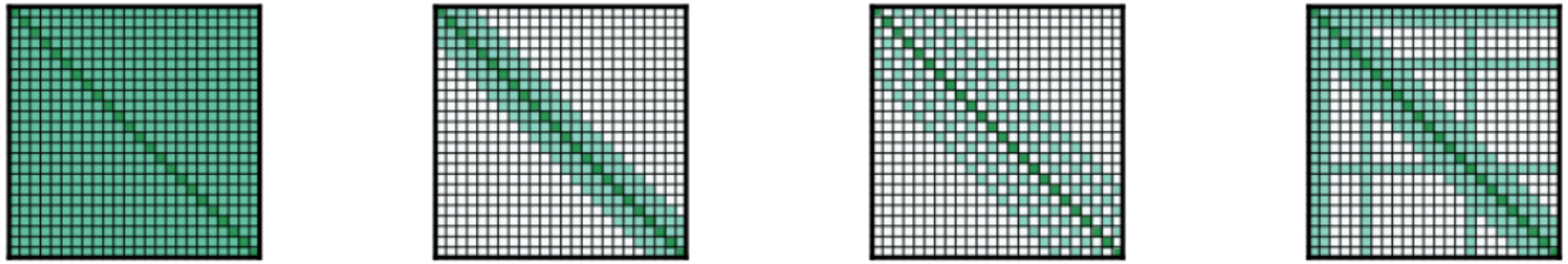
- Efficient Transformers



Transformer

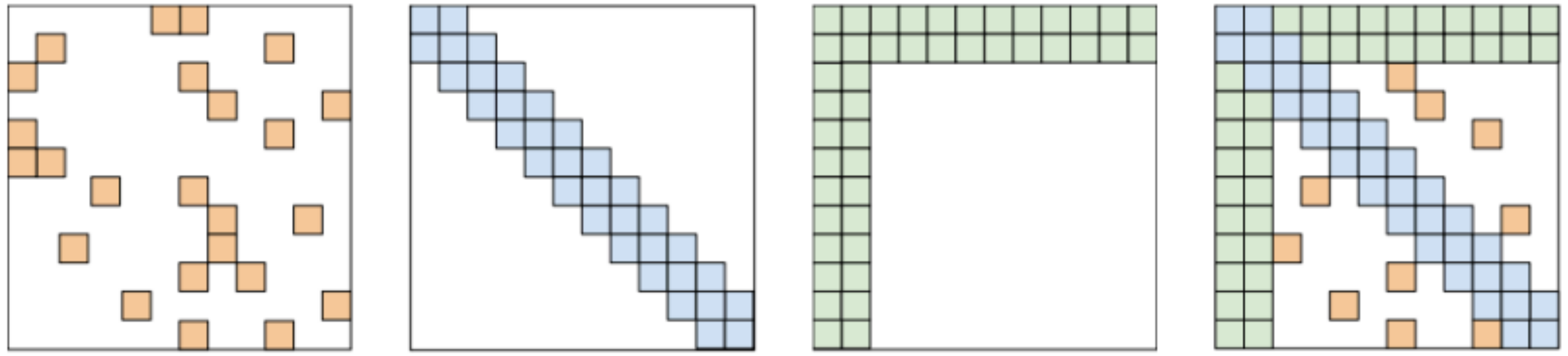
- Longformer / Big Bird

Key idea: use sparse attention patterns!



(a) Full n^2 attention (b) Sliding window attention (c) Dilated sliding window (d) Global+sliding window

(Beltagy et al., 2020): Longformer: The Long-Document Transformer



(a) Random attention (b) Window attention (c) Global Attention (d) BigBird

(Zaheer et al., 2021): Big Bird: Transformers for Longer Sequences

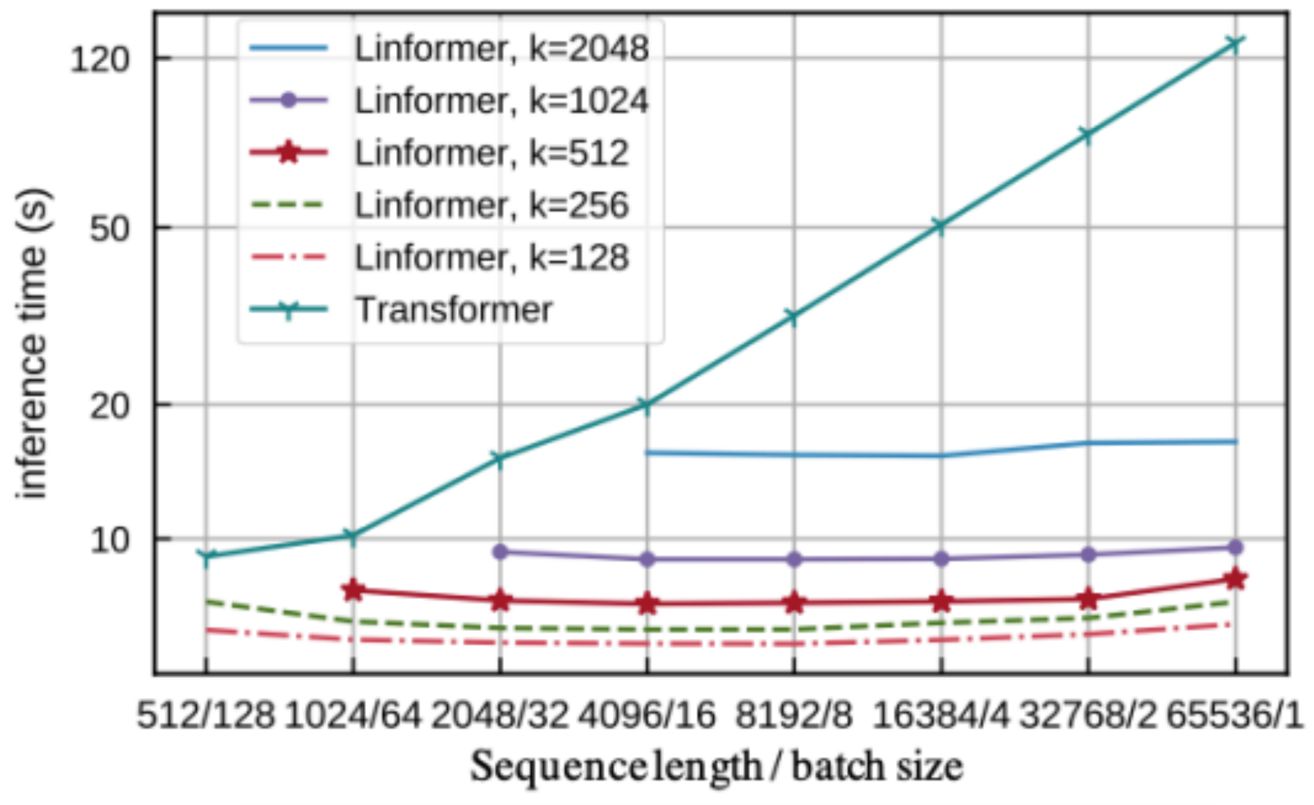
Transformer

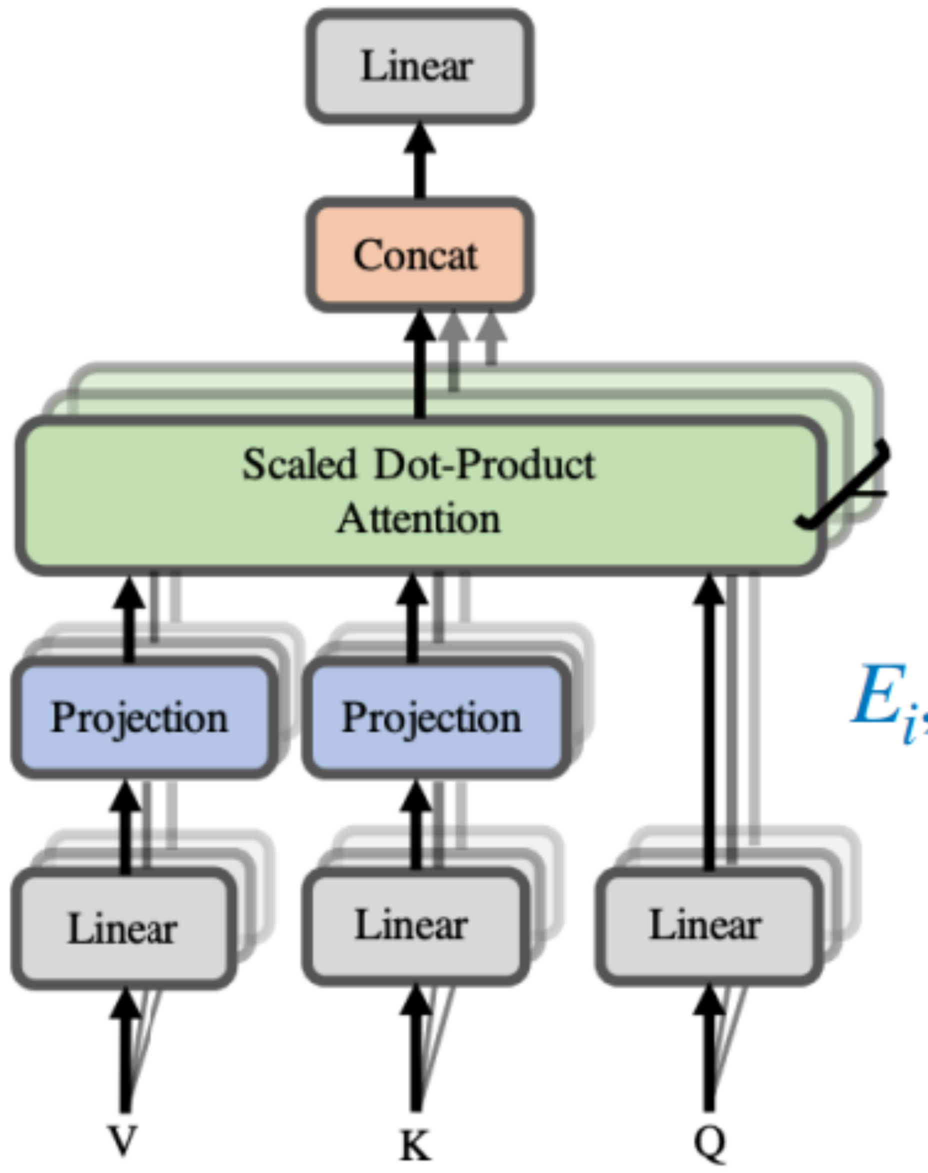
- Linformer

Key idea: The attention matrix $e_{i,j}$ can be approximated by a low-rank matrix

Map the sequence length dimension to a lower-dimensional space for values, keys

$$\overline{\mathrm{head}_i} = \mathrm{Attention}(QW_i^Q, E_iKW_i^K, F_iVW_i^V)$$
$$= \underbrace{\mathrm{softmax}\left(\frac{QW_i^Q(E_iKW_i^K)^T}{\sqrt{d_k}}\right)}_{\bar{P}:n\times k} \cdot \underbrace{F_iVW_i^V}_{k\times d},$$



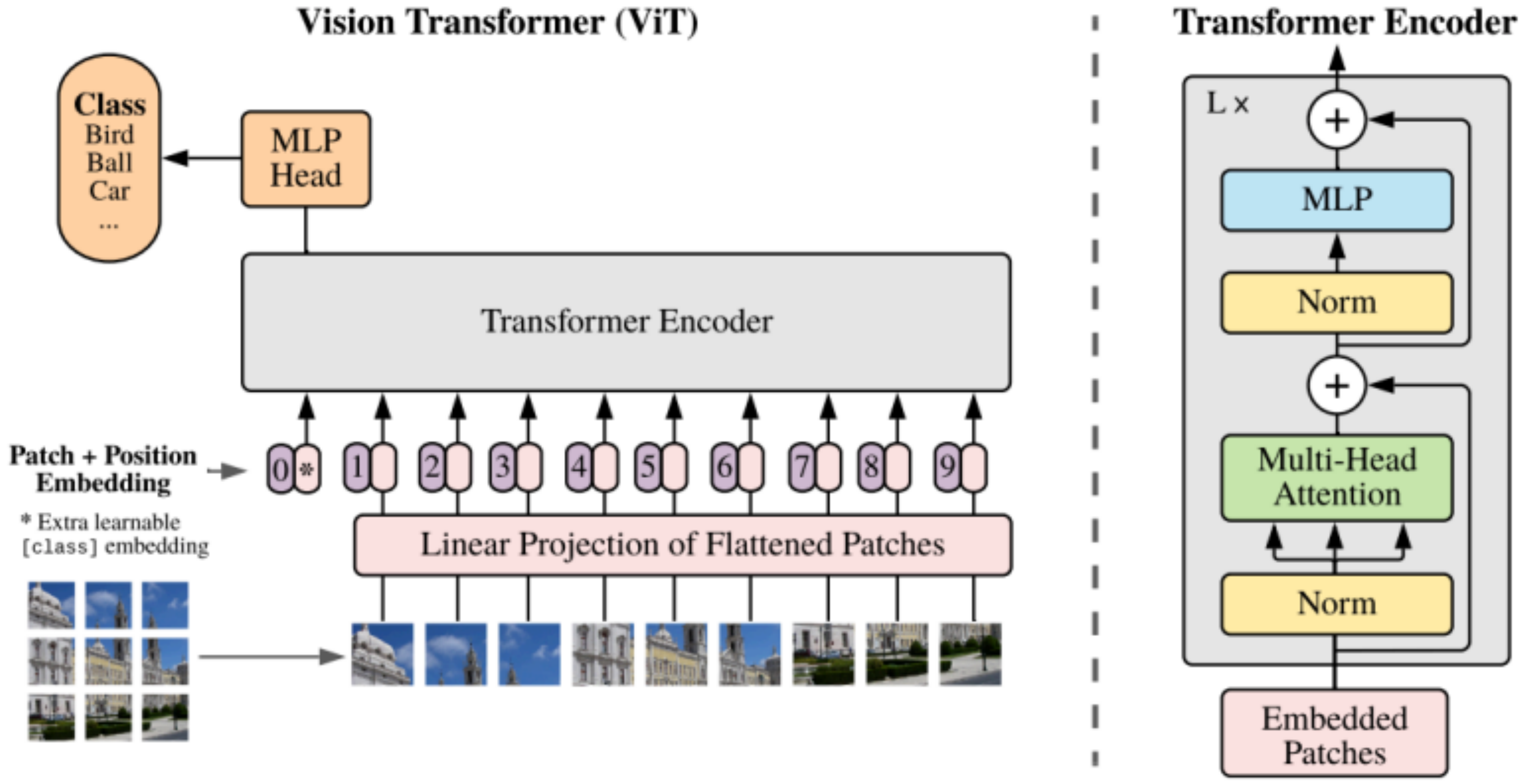


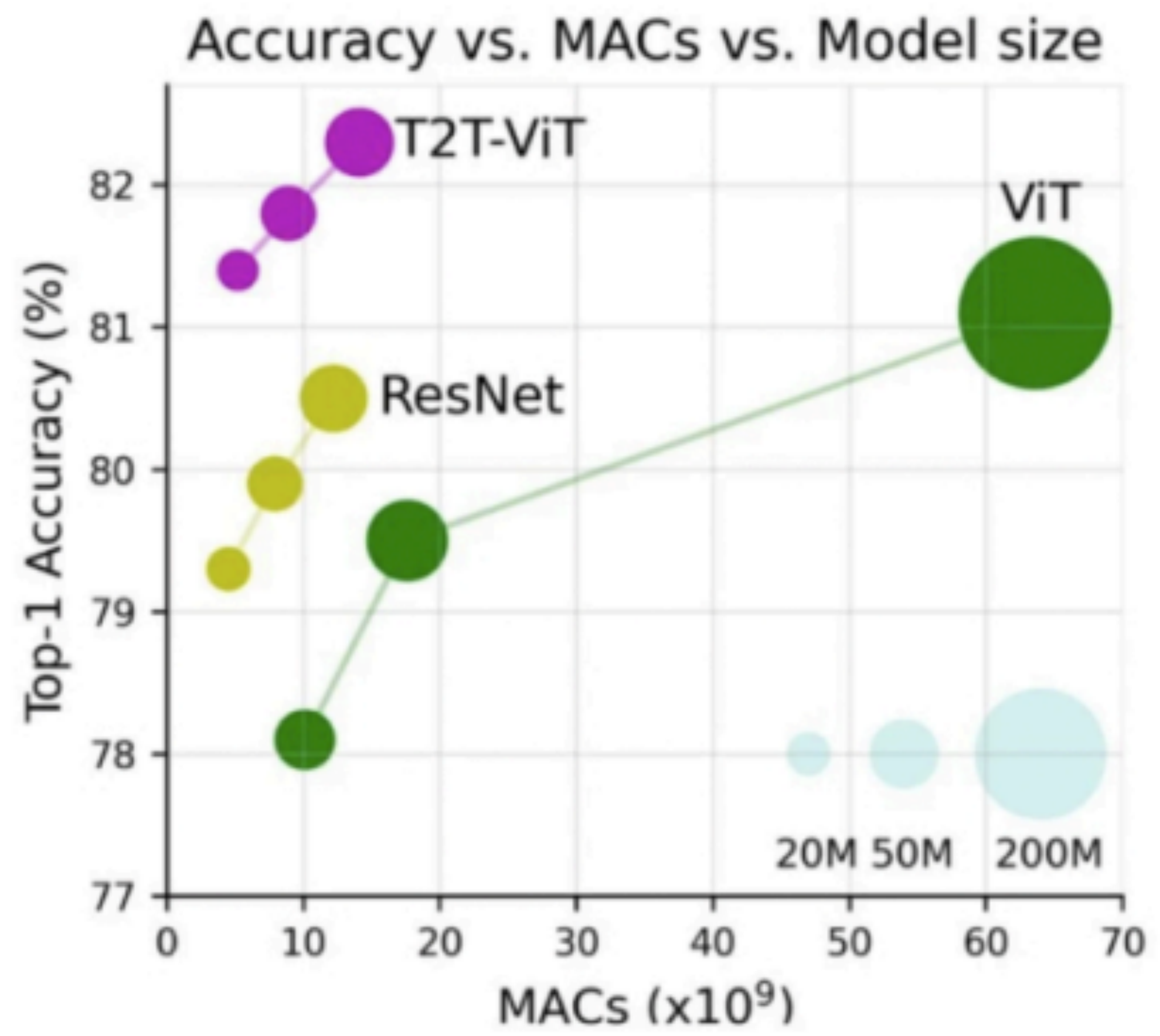
$E_i, F_i \in \mathbb{R}^{k\times n}$

(Wang et al., 2020): Linformer: Self-Attention with Linear Complexity

Transformer

- Vision Transformer (ViT)

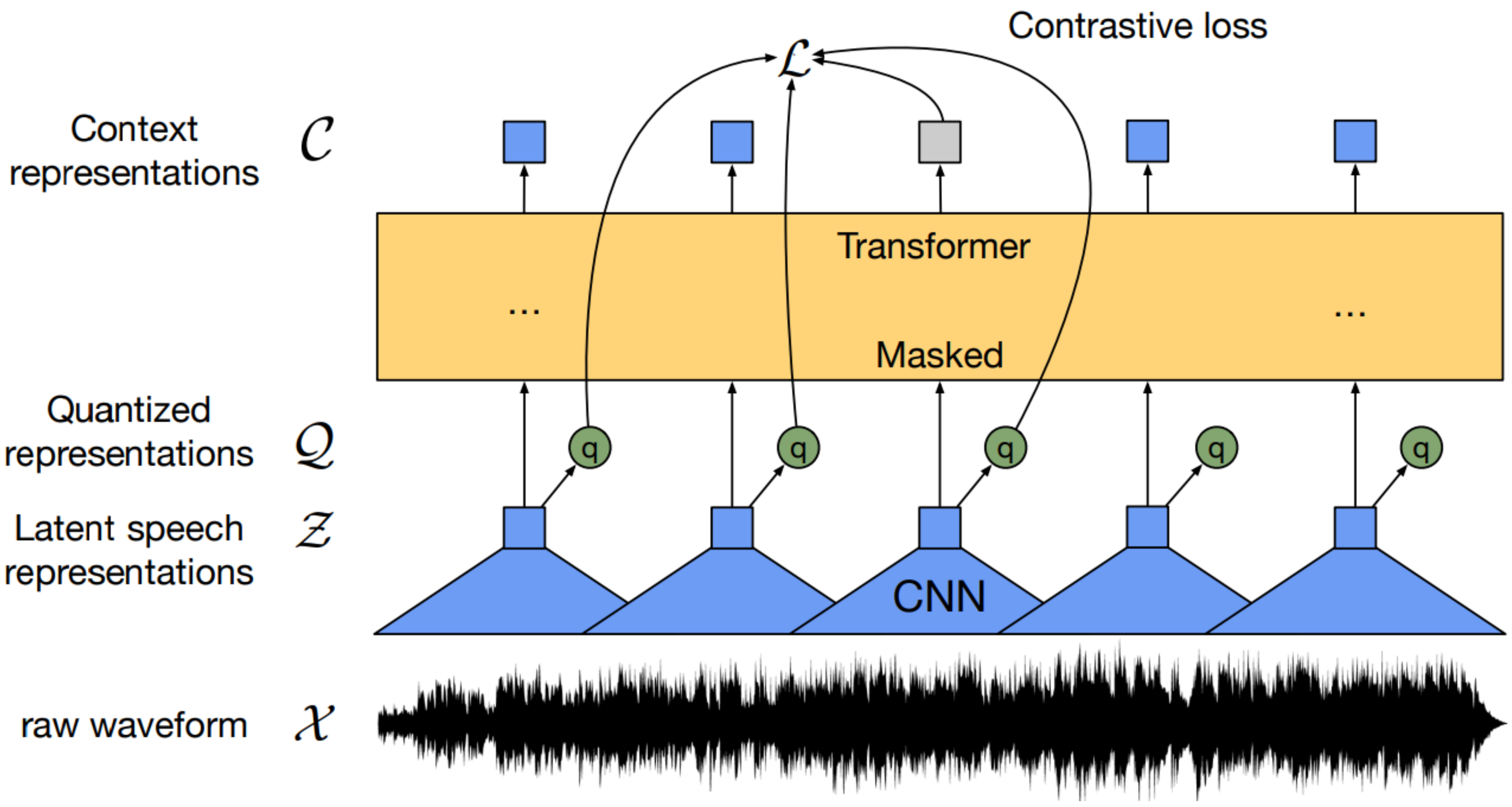




(Dosovitskiy et al., 2021): An Image is Worth 16x16 Words: Transformers for Image Recognition at Scale

Transformer

- Wav2vec 2.0



(Baevski et al., 2020): wav2vec 2.0: A Framework for Self-Supervised Learning of Speech Representations