

RP

Deutsches Forschungszentrum für Künstliche Intelligenz German Research Center for Artificial Intelligence

TU Rheinland-Pfälzische Technische Universität Kaiserslautern Landau

TaylorShift:

Shifting the Complexity of Self-Attention from Squared to Linear (and Back) using Taylor-Softmax

ICPR 2024 - Kolkata, India

Tobias Christian Nauen Sebastian Palacio Andreas Dengel



Modern AI is largely attention-based.



Quadratic complexity prevents us from utilizing very long inputs.

Long inputs allow for:

- More context information
 - (Updated) World knowledge





al

Quadratic complexity prevents us from utilizing very long inputs.

Long inputs allow for:

- More context information
 - (Updated) World knowledge
 - High-resolution images
 - More localized information



31

Quadratic complexity prevents us from utilizing very long inputs.

Long inputs allow for:

- More context information
 - (Updated) World knowledge
 - High-resolution images
 - More localized information
- Y
- Multiple modalities
- Concatenation of information



TaylorShift is attention using the Taylor series of the exponential.



Attention

Activation



Direct-TaylorShift



TaylorShift is attention using the Taylor series of the exponential.



Direct-TaylorShift



$$\text{T-SM}^{(k)}(x) = \frac{\sum_{n=0}^{k} \frac{x^{n}}{n!}}{\left|\left|\sum_{n=0}^{k} \frac{x^{n}}{n!}\right|\right|_{1}}$$

Attention

Activation



Interaction Function $\operatorname{softmax}(x) = \frac{\exp(x)}{||\exp(x)||_1}$

TaylorShift is attention using the Taylor series of the exponential.



Direct-TaylorShift



Direct-TaylorShift

softmax(x) = $\frac{\exp(x)}{||\exp(x)||_1}$ **Function** Attention $Y = \operatorname{softmax}(QK^{\top})V$

Calculation

Activation

Interaction

Attention

TaylorShift is attention using the Taylor series of the exponential.



Attention $\exp(x) = \sum_{n=0}^{\infty} \frac{x^n}{n!}$ Activation softmax(x) = $\frac{\exp(x)}{||\exp(x)||_1}$ Interaction Function Attention $Y = \operatorname{softmax}(QK^{\top})V$ Calculation

Complexity $Q, K, V \in \mathbb{R}^{N \times d}$ $\mathcal{O}(N^2d)$

Direct-TaylorShift



$$Y = ext{T-SM}^{(k)}(QK^{+})V$$

 $extsf{Direct-TaylorShift}$
 $\mathcal{O}(N^2d)$



We can reorder calculations for efficient calculation.

$$\text{T-SM}(QK^{\top})V = \ell_1 - \text{norm}\left[\sum_{n=0}^2 \frac{(QK^{\top})^n}{n!}\right]V$$

- 1. Matrix multiplication (QK)
- 2. Activation function
- 3. Normalization
- 4. Matrix multiplication (KV) $\mathcal{O}(N^2d)$



We can reorder calculations for efficient calculation.

$$\text{T-SM}(QK^{\top})V = \ell_1 - \text{norm}\left[\sum_{n=0}^2 \frac{(QK^{\top})^n}{n!}\right]V = \text{norm}\left[\sum_{n=0}^2 \frac{(QK^{\top})^n}{n!}V \circ 1\right]$$

- 1. Matrix multiplication (QK)
- 2. Activation function
- 3. Normalization
- 4. Matrix multiplication (KV) $\mathcal{O}(N^2d)$



We can reorder calculations for efficient calculation.

$$\operatorname{T-SM}(QK^{\top})V = \ell_1 - \operatorname{norm}\left[\sum_{n=0}^2 \frac{(QK^{\top})^n}{n!}\right]V = \operatorname{norm}\left[\sum_{n=0}^2 \frac{(QK^{\top})^n}{n!}V \circ 1\right]$$

 $= \operatorname{norm}\left[\frac{1}{2}(QK^{\top})^{2}(V \circ 1) + QK^{\top}(V \circ 1) + \sum_{\operatorname{cols}}(V \circ 1)\right]$

- 1. Matrix multiplication (QK)
- 2. Activation function
- 3. Normalization
- 4. Matrix multiplication (KV) $\mathcal{O}(N^2d)$



We can reorder calculations for efficient calculation.

Гэ

$$T-SM(QK^{\top})V = \ell_{1} - \operatorname{norm}\left[\sum_{n=0}^{2} \frac{(QK^{\top})^{n}}{n!}\right]V = \operatorname{norm}\left[\sum_{n=0}^{2} \frac{(QK^{\top})^{n}}{n!}V \circ 1\right]$$
$$= \operatorname{norm}\left[\frac{1}{2}(QK^{\top})^{2}(V \circ 1) + QK^{\top}(V \circ 1) + \sum_{\operatorname{cols}}(V \circ 1)\right]$$
$$= \operatorname{norm}\left[\frac{1}{2}Q^{\boxtimes 2}(K^{\boxtimes 2})^{\top}(V \circ 1) + QK(V \circ 1) + \sum_{\operatorname{cols}}(V \circ 1)\right]$$
Efficient-TaylorShift

Га

- 1. Matrix multiplication (QK)
- 2. Activation function
- 3. Normalization

Ъ

4. Matrix multiplication (KV) $O(N^2d)$





We can reorder calculations for efficient calculation.

$$T-SM(QK^{\top})V = \ell_{1} - norm \left[\sum_{n=0}^{2} \frac{(QK^{\top})^{n}}{n!}\right]V = norm \left[\sum_{n=0}^{2} \frac{(QK^{\top})^{n}}{n!}V \circ 1\right]$$

$$= norm \left[\frac{1}{2}(QK^{\top})^{2}(V \circ 1) + QK^{\top}(V \circ 1) + \sum_{cols}(V \circ 1)\right]$$

$$= norm \left[\frac{1}{2}Q^{\boxtimes 2}(K^{\boxtimes 2})^{\top}(V \circ 1) + QK(V \circ 1) + \sum_{cols}(V \circ 1)\right]$$

$$= norm \left[\frac{1}{2}Q^{\boxtimes 2}(K^{\boxtimes 2})^{\top}(V \circ 1) + QK(V \circ 1) + \sum_{cols}(V \circ 1)\right]$$

$$= norm \left[\frac{1}{2}Q^{\boxtimes 2}(K^{\boxtimes 2})^{\top}(V \circ 1) + QK(V \circ 1) + \sum_{cols}(V \circ 1)\right]$$

$$= norm \left[\frac{1}{2}Q^{\boxtimes 2}(K^{\boxtimes 2})^{\top}(V \circ 1) + QK(V \circ 1) + \sum_{cols}(V \circ 1)\right]$$

$$= norm \left[\frac{1}{2}Q^{\boxtimes 2}(K^{\boxtimes 2})^{\top}(V \circ 1) + QK(V \circ 1) + \sum_{cols}(V \circ 1)\right]$$

$$= norm \left[\frac{1}{2}Q^{\boxtimes 2}(K^{\boxtimes 2})^{\top}(V \circ 1) + QK(V \circ 1) + \sum_{cols}(V \circ 1)\right]$$

$$= norm \left[\frac{1}{2}Q^{\boxtimes 2}(K^{\boxtimes 2})^{\top}(V \circ 1) + QK(V \circ 1) + \sum_{cols}(V \circ 1)\right]$$

$$= norm \left[\frac{1}{2}Q^{\boxtimes 2}(K^{\boxtimes 2})^{\top}(V \circ 1) + QK(V \circ 1) + \sum_{cols}(V \circ 1)\right]$$

- 1. Matrix multiplication (QK)
- ctivation function
- Iormalization
- 1atrix multiplication (KV) $_{\mathcal{O}(N^2d)}$

4

 $\mathcal{O}(Nd^3)$





We counteract numerical instabilities by introducing multiple normalizations.

Normalization at the end

 \Rightarrow large intermediate results

 \Rightarrow numerical instability

Expr.	$(K^{\boxtimes 2})^\top V = A_{\text{mod}}$	$(QK^T)^2 V$	$QK^{\top}V$	Y_{denom}	Y
Size	$\frac{N+1}{\sqrt{d}}$	$rac{N}{d}$	$\sqrt{N}\frac{4d+1}{4d}$	$N\frac{d+2}{2d}$	$\sqrt{\frac{d}{N}}$

Normalization at the end 1. Normalize queries and keys, ⇒ large intermediate results use attention temperature ⇒ numerical instability

 $(K^{\boxtimes 2})^\top V = A_{\text{mod}} \quad (QK^T)^2 V$

Expr.

Size

 $\frac{N}{d}$

 $QK^{+}V$

 $\sqrt{N}\frac{4d+1}{4d} \quad N\frac{d+2}{2d}$

 Y_{denom}

Y

We counteract numerical instabilities by introducing multiple normalizations.



Expr. $(K^{\boxtimes 2})^{\top}V = A_{\text{mod}} \quad (QK^T)^2V \quad QK^{\top}V$

We counteract numerical instabilities by

 $\frac{1}{d}$

introducing multiple r	normalizations.
Normalization at the end	1. Normalize que

 $\frac{N+1}{N}\frac{1}{\sqrt{d}}$

 \Rightarrow large intermediate results \Rightarrow numerical instability

Size

1. Normalize queries and keys, use attention temperature 2. $(V \circ 1) \leftarrow \frac{1}{N}(V \circ 1)$

 Y_{denom}

 $\frac{d+2}{2d}$

 $\frac{1}{\sqrt{N}}\frac{4d+1}{4d}$

Y

 $\frac{d}{N}$



3. $Q, K \leftarrow \sqrt[4]{d}Q, \sqrt[4]{d}K$, adjust factors accordingly

We counteract numerical instabilities by introducing multiple normalizations.

 \Rightarrow large intermediate results \Rightarrow numerical instability

Size

- Normalization at the end
 - 1. Normalize queries and keys,
 - use attention temperature **2.** $(V \circ 1) \leftarrow \frac{1}{N} (V \circ 1)$

Expr. $(K^{\boxtimes 2})^{\top}V = A_{\text{mod}} \quad (QK^T)^2V$ $QK^{\top}V$ Y_{denom} Y $\frac{\sqrt{d}}{\sqrt{N}} + \frac{1}{4\sqrt{Nd}} \qquad \frac{d+2}{2d}$ $\frac{d}{N}$ $\frac{N+1}{N}$ 1



nerical instability **2.** $(V \circ 1) \leftarrow \frac{1}{N}(V \circ 1)$ **3.** $Q, K \leftarrow \sqrt[4]{d}Q, \sqrt[4]{d}K$, adjust factors accordingly

We counteract numerical instabilities by

introducing multiple normalizations.

 \Rightarrow large intermediate results \Rightarrow numerical instability

Normalization at the end

Expr. $(K^{\boxtimes 2})^{\top}V = A_{\text{mod}} \quad (QK^T)^2 V \quad QK^{\top}V \quad Y_{denom} \quad Y$ Size $\frac{N+1}{N} \quad 1 \quad \frac{\sqrt{d}}{\sqrt{N}} + \frac{1}{4\sqrt{Nd}} \quad \frac{d+2}{2d} \quad 1$

4. $Y \leftarrow \sqrt{\frac{N}{d}}Y$

1. Normalize queries and keys,

use attention temperature





TaylorShift calculates token-to-token interactions in linear time.



- 1. Softmax \rightarrow Taylor-Softmax
- 2. Reorder operations for efficient calculation
- 3. Normalize intermediate results



TaylorShift is efficient for long sequences, depending on $d\,.$



Speed

Proxy Metric

FLOPs



TaylorShift is efficient for long sequences, depending on $d\,.$



Speed

Proxy Metric

FLOPs

Direct-TaylorShift

 $\mathrm{ops}_{\mathrm{dir}} = 4N^2d + 6N^2$

Efficient-TaylorShift

 $ops_{eff} = N(4d^3 + 10d^2 + 9d + 4)$



TaylorShift is efficient for long sequences, depending on $d\,.$



Speed

FLOPs

Proxy Metric

 $ops_{dir} = 4N^2d + 6N^2$

Efficient-TaylorShift

Direct-TaylorShift

 $ops_{eff} = N(4d^3 + 10d^2 + 9d + 4)$

Intersection length

 $s_{eff} = N(4a + 10a + 9a + 10a)$

 $N_0 \le d^2 + d + 1$

TaylorShift – Tobias Christian Nauen – ICPR 2024 – Kolkata, India





	When is O(N d ³) actually better than O(N ² d)?			
	Speed	Memory		
Proxy Metric	# FLOPs	# Entries in intermediate results		
Direct-TaylorShift	$\mathrm{ops}_{\mathrm{dir}} = 4N^2d + 6N^2$	$\operatorname{entr}_{\operatorname{dir}} = Nd + 2N^2$		
Efficient-TaylorShift	$ops_{eff} = N(4d^3 + 10d^2 + 9d + 4)$	$entr_{eff} = d^2(d+1) + 2Nd + N(d+1) + Nd^2$		
Intersection length	$N_0 \le d^2 + d + 1$			



TaylorShift is efficient for long sequences, depending on d.



	Speed	Memory		
Proxy Metric	# FLOPs	# Entries in intermediate results		
Direct-TaylorShift	$\mathrm{ops}_{\mathrm{dir}} = 4N^2d + 6N^2$	$entr_{dir} = Nd + 2N^2$		
Efficient-TaylorShift	$ops_{eff} = N(4d^3 + 10d^2 + 9d + 4)$	$entr_{eff} = d^2(d+1) + 2Nd + N(d+1) + Nd$		
Intersection length	$N_0 \le d^2 + d + 1$	$N_1 \le rac{1}{2}d^2 + 2d + rac{1}{2}$		

TaylorShift is efficient for long sequences, depending on \boldsymbol{d} .



When is $O(N d^3)$ actually better than $O(N^2 d)$? Speed Memory **Proxy Metric** # FLOPs # Entries in intermediate results $ops_{dir} = 4N^2d + 6N^2$ $entr_{dir} = Nd + 2N^2$ Direct-TaylorShift $entr_{eff} = d^2(d+1) + 2Nd + N(d+1) + Nd^2$ $ops_{eff} = N(4d^3 + 10d^2 + 9d + 4)$ Efficient-TaylorShift $N_1 \le \frac{1}{2}d^2 + 2d + \frac{1}{2}$ $N_0 \le d^2 + d + 1$ Intersection length d8 163264 128 N_0 732731057416116513

TaylorShift – Tobias Christian Nauen – ICPR 2024 – Kolkata, India

47

159

574

2174

8446

 N_1



Reducing the dimension d makes TaylorShift more efficient.



GI



- lacksim D Reducing the dimension d makes TaylorShift more efficient.
 - Reduces the representational capacity of the model.
 - $\hat{\Sigma}$ Change the number of attention-heads instead.





Reducing the dimension d makes TaylorShift more efficient.

Reduces the representational capacity of the model.

 $\dot{\Sigma}$ Change the number of attention-heads instead.

$$d = \frac{d_{\text{embed}}}{h} \qquad \qquad h \times \text{ops}_{\text{eff}} \qquad \qquad h \times \text{entr}_{\text{eff}}$$

$$h \nearrow \qquad \qquad \searrow \qquad \qquad \searrow$$

⇒ Increase efficiency without decreasing overall capacity by increasing the number of heads



RPTU

TaylorShift is efficient for long sequences, as predicted.

Speed:

- Direct-TaylorShift outperforms attention
- Intersection point is larger than predicted
- Slow memory reads on current hardware







TaylorShift is efficient for long sequences, as predicted.

Speed:

- Direct-TaylorShift outperforms attention
- Intersection point is larger than predicted
- Slow memory reads on current hardware

Memory:

 Almost exactly like predicted theoretically al

TaylorShift outperforms standard attention in 4/5 tasks.

al **RPTU**

TaylorShift outperforms the other models, including the baseline Transformer encoder, in (at least) 4/5 tasks.

Model	CIFAR (Pixel)	IMDB (Byte)	ListOps	ImageNet (Ti)	ImageNet (S)	Average
Linformer	29.2	58.1	-	64.3	76.3	(57.0)
RFA	44.9	65.8	-	-	-	(55.4)
Performer	34.2^{\star}	65.6^{\star}	35.4^{\star}	62.0^{\star}	67.1^{\star}	52.9
Reformer	44.8	63.9	47.6	73.6	76.2^{\star}	61.2
Nystromformer	49.4	65.6	44.5	75.0	78.3^{\star}	62.6
EVA	46.1	64.0	45.3	73.4	78.2	61.4
Transformer	44.7	65.8	46.0	75.6	79.1	62.2
Ours	47.6	66.2	46.1	75.0	79.3	62.8



Increasing the number of heads speeds up TaylorShift and can increase accuracy.

Q

Increasing the number of heads:

- Reduces memory consumption
- Increases speed
- Sometimes increases accuracy

1 1		Acc [%]	direct		efficient		
n a	$TP \ [ims/s]$		Mem [MiB@16]	$TP \ [ims/s]$	Mem [MiB@16]		
4	64	47.1	12060	596	2975	840	
8	32	47.5	7657	1 1 1 1	5749	585	
16	16	47.3	4341	2135	9713	459	
32	8	46.9	2528	4187	14087	397	
64	4	45.9	1235	8291	13480	125	

Accuracy, throughput and VRAM usage of TaylorShift on the CIFAR Pixel task with increased number of attention heads with:

$$l_{\text{embed}} = d \times h = 256$$
 $N = 1024$



TaylorShift:



Shifting the Complexity of Self-Attention from Squared to Linear (and Back) using Taylor-Softmax

