SAMformer: Unlocking the Potential of Transformers in Time Series Forecasting

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paris-saclay	_

Outline



- Introduction
- 2 Failure of Transformers
- SAMformer
- 4 Experiments
- **5** Take Home Message

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Time Series Data



In many applications, data are gathered sequentially.











 $\underline{\mathsf{Goal}} \to \mathsf{Analysing}$ time series data to predict future trends.

- Forecast of ECG recording to predict cardiac arrhythmia,
- Electricity consumption forecasting to match future demand,
- Predicting stock market prices.

Challenges

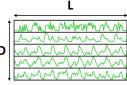
- Long-term temporal dependencies,
- Highly correlated features.



D-dimensional time series of length $L \to \text{predict next } H$ values.

- Training set of N observations $(\{\mathbf{X}^{(i)}\}_{i=0}^N, \{\mathbf{Y}^{(i)}\}_{i=0}^N)$,
- Find predictor $f_{\omega} \colon \mathbb{R}^{D \times L} \to \mathbb{R}^{D \times H}$ that minimizes the MSE

$$\mathcal{L}_{\text{train}}(\boldsymbol{\omega}) = \frac{1}{ND} \sum_{i=0}^{N} \|\mathbf{Y}^{(i)} - f_{\boldsymbol{\omega}}(\mathbf{X}^{(i)})\|_{\text{F}}^{2}.$$

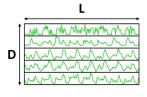




D-dimensional time series of length $L \to \text{predict next } H$ values.

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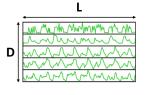




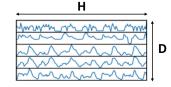
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$$\mathcal{L}_{\text{train}}(\boldsymbol{\omega}) = \frac{1}{ND} \sum_{i=0}^{N} ||\mathbf{Y}^{(i)} - f_{\boldsymbol{\omega}}(\mathbf{X}^{(i)})||_{\text{F}}^{2}.$$









Standard methods:

- AR models (ARIMA)
- Seasonal naive

Deep learning methods

- RNN, CNN
- Transformer-based models

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Transformers for Time Series Forecasting



Motivation

- Transformers tailored to deal with sequential data,
- Impressive results in NLP and Computer Vision.

Main challenges

- Quadratic computation of self-attention,
- **2** Complex long-term dependencies.

Transformers for Time Series Forecasting



Main challenges

- 1 Quadratic computation of self-attention,
- 2 Complex long-term dependencies.

Transformers for Time Series Forecasting



Main challenges

- Quadratic complexity of self-attention
 - Sparse attention: LogTrans [5], Informer [13]
 - Modified attention: Pyraformer [6]
- 2 Complex long-term dependencies
 - Decomposition scheme: Autoformer [10], Pyraformer [6]
 - Fourier domain: FEDformer [14]

It leads to a wide range of Anything-formers with heavy and complex implementation and many parameters.

Failure of Transformers



[11] showed that linear models outperform SOTA Anything-former.

Transformers in Computer Vision and NLP



Commander of the Armies of GPT, General of the Gemini Legions, loyal servant to Claude, Llama3, Mixtral

Transformers in Time Series Forecasting



Please help, I just got beaten by a linear model

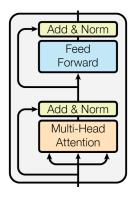
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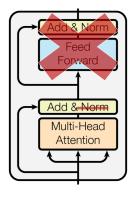


- ullet Generate toy data according to $\mathbf{Y} = \mathbf{X}\mathbf{W}_{\mathrm{toy}} + oldsymbol{arepsilon}$,
- Designing the simplest Transformer possible.





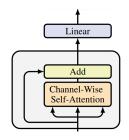
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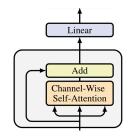
$$\begin{aligned} \mathbf{A}(\mathbf{X}) &= \mathtt{softmax}\bigg(\frac{\mathbf{X}\mathbf{W}_{\mathbf{Q}}\mathbf{W}_{\mathbf{K}}^{\top}\mathbf{X}^{\top}}{\sqrt{d_{\mathrm{m}}}}\bigg) \\ f(\mathbf{X}) &= [\mathbf{X} + \mathbf{A}(\mathbf{X})\mathbf{X}\mathbf{W}_{V}\mathbf{W}_{O}]\mathbf{W} \end{aligned}$$





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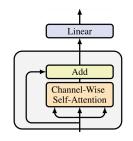
Theorem (Ilbert, O., Feofanov et al.)

Given fixed attention weights $\mathbf{W}_Q, \mathbf{W}_K, \mathbf{W}_V, \mathbf{W}_O$, there exists an infinity of optimal \mathbf{W} reaching the oracle, i.e., $f(\mathbf{X}) = \mathbf{X}\mathbf{W}_{tov}$.



- ullet Generate toy data according to $\mathbf{Y} = \mathbf{X}\mathbf{W}_{\mathrm{tov}} + oldsymbol{arepsilon}$,
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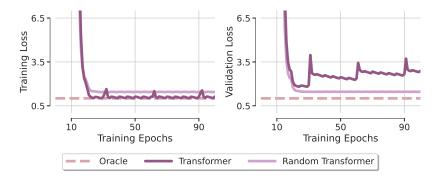


In theory, our simplistic Transformer can be optimal. Is this the case in practice?

Poor Generalization



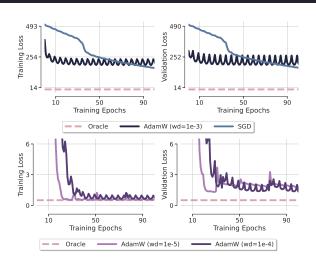
- Oracle: optimal solution,
- ullet Transformer with $\mathbf{W}_Q, \mathbf{W}_K, \mathbf{W}_V, \mathbf{W}_O, \mathbf{W}$ trainable,
- ullet Random Transformer: only ${f W}$ is trainable.



Despite its simplicity, Transformer overfits a lot. Fixing the attention weight improves generalization.

Similar Behaviour with other Optimizers





Poor generalization of Transformer with SGD, Adam, and AdamW.

Trainability Issues due to the Attention



Hypothesis from NLP and Computer Vision

- Transformers have sharp loss landscape [2]
 - Convergence to sharp minima \rightarrow poor generalization,
 - Computed as λ_{max} , the largest singular value of the Hessian.



Trainability Issues due to the Attention

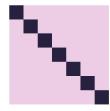


Hypothesis from NLP and Computer Vision

- Transformers have sharp loss landscape [2],
- Attention suffers from entropy collapse [12].
 - ${\sf Entropy} = {\sf average} \ {\sf entropy} \ {\sf of} \ {\sf the} \ {\sf rows},$
 - It causes training instability,
 - [12]
 ightarrow entropy collapse and sharpness appear in tandem.



 \sim Uniform \rightarrow high entropy.



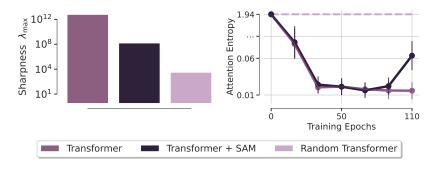
Diagonal \rightarrow low entropy.

Trainability Issues due to the Attention



Hypothesis from NLP and Computer Vision

- Transformers have **sharp loss landscape** [2],
- Attention suffers from **entropy collapse** [12].



Training the attention induces an entropy collapse and a sharp loss landscape.

Existing Solutions



\bullet Reparam [12]

Replace each weight matrix ${f W}$ by

$$\widehat{\mathbf{W}} = rac{\gamma}{\|\mathbf{W}\|_2} \mathbf{W}, \ ext{with} \ \gamma \in \mathbb{R} \ ext{learnable} \ ,$$

Sharpness-Aware Minimization (SAM) [3]

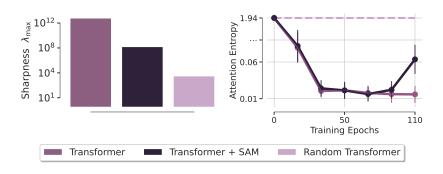
Replace the training loss $\mathcal{L}_{\mathrm{train}}$ by

$$\mathcal{L}_{ ext{train}}^{ ext{SAM}}(oldsymbol{\omega}) = \max_{\|oldsymbol{arepsilon}\| <
ho} \mathcal{L}_{ ext{train}}(oldsymbol{\omega} + oldsymbol{arepsilon}) pprox \mathcal{L}_{ ext{train}}(oldsymbol{\omega}) pprox \mathcal{L}_{ ext{train}}(oldsymbol{\omega}) \|_2 igg).$$

σ Reparam doesn't solve the problem, but SAM does.



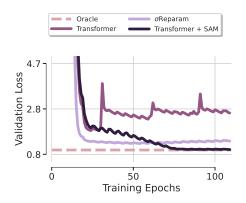
Contrary to NLP and Computer Vision, entropy collapse seems benign in time series forecasting while sharpness is harmful.



σ Reparam doesn't solve the problem, but SAM does.



Contrary to NLP and Computer Vision, entropy collapse seems benign in time series forecasting while sharpness is harmful.



 σ Reparam helps but is not sufficient while using SAM leads to the optimal solution (oracle).

Good Practices: RevIN



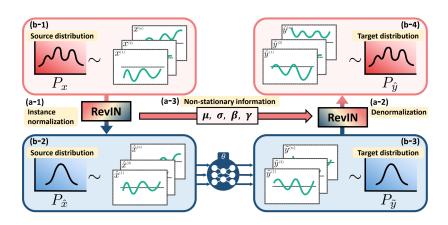
RevIN [4] \rightarrow Reduce distribution shift between input and target.

- Multivariate time series $\mathbf{X} \in \mathbb{R}^{D \times L}$, learnable γ, β .
- Normalize each feature $\mathbf{X}_i \leftarrow \tilde{\mathbf{X}}_i = \frac{\mathbf{X}_i \mu}{\sigma} \leftarrow \gamma \tilde{\mathbf{X}}_i + \beta$,
- Apply model on multivariate time series $\tilde{\mathbf{Y}} = f(\tilde{\mathbf{X}})$,
- Denormalize each feature $\tilde{\mathbf{Y}}_i \leftarrow \hat{\mathbf{Y}}_i = \frac{\tilde{\mathbf{Y}}_i \beta}{\gamma} \leftarrow \sigma \hat{\mathbf{Y}}_i + \mu$.

Good Practices: RevIN



RevIN [4] \rightarrow Reduce distribution shift between input and target.

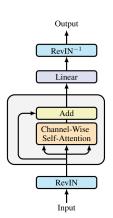


SAMformer: SAM & Channel-Wise Attention



- Input $\mathbf{X} \in \mathbb{R}^{D \times L}$, output $f(\mathbf{X}) \in \mathbb{R}^{D \times H}$,
- Reduce distribution shift with RevIN [4],
- ullet Channel-wise attention $\mathbf{A}(\mathbf{X}) \in \mathbb{R}^{D imes D}$,
- Smooth loss landscape with SAM [3].

$$\begin{aligned} \mathbf{A}(\mathbf{X}) &= \mathtt{softmax}\bigg(\frac{\mathbf{X}\mathbf{W}_{\mathbf{Q}}\mathbf{W}_{\mathbf{K}}^{\top}\mathbf{X}^{\top}}{\sqrt{d_{\mathrm{m}}}}\bigg) \\ f(\mathbf{X}) &= [\mathbf{X} + \mathbf{A}(\mathbf{X})\mathbf{X}\mathbf{W}_{V}\mathbf{W}_{O}]\mathbf{W} \end{aligned}$$



SAMformer is a shallow transformer trained with SAM.

→ One head, one encoder, 15 lines of code!

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Baselines & Datasets



All-MLP model (2023): TSMixer [1].

Transformers (2021-2022): FEDformer [14], Autoformer [10].

Recent Transformers (2023-2024): iTransformer [7], PatchTST [8].

Dataset	ETTh1/ETTh2	ETTm1/ETTm2	Electricity	Exchange	Traffic	Weather
# features	7	7	321	8	862	21
# time steps	17420	69680	26304	7588	17544	52696
Granularity	1 hour	15 minutes	1 hour	1 day	1 hour	10 minutes

SOTA Performance

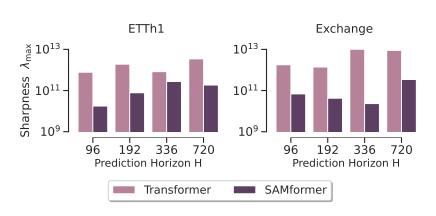


Dataset	SAMformer -	iTransformer 2024	PatchTST 2023	TSMixer 2023	FEDformer 2022	Autoformer 2021
ETTh1	0.410	0.454	0.469	0.437	0.440	0.496
ETTh2	0.344	0.383	0.387	0.357	0.437	0.450
ETTm1	0.373	0.407	0.387	0.385	0.448	0.588
ETTm2	0.269	0.288	0.281	0.289	0.305	0.327
Traffic	0.425	0.428	0.481	0.620	0.610	0.628
Weather	0.260	0.258	0.259	0.267	0.309	0.338
Overall	improvement	$\boldsymbol{6.58\%}$	8.79%	13.2 %	22.5 %	35.9 %

SAMformer outperforms all baselines while having significantly fewer parameters.

Smoother Loss Landscape

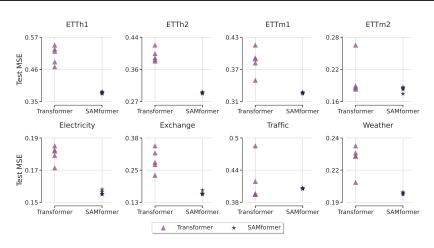




SAM provides a smoother loss landscape ...

Better Generalization

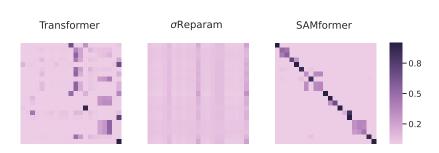




... leading to better generalization and robustness.

Better Signal Propagation





Channel-wise attention improves the propagation of the signal with self-feature correlations as in ViTs.

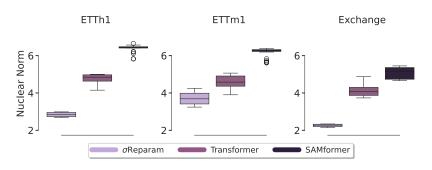
Intuition behind the Failure of σ Reparam



Theorem (Ilbert, O., Feofanov et al.)

Applying σ Reparam [12] leads to attention rank collapse.

$$\|\mathbf{X}\mathbf{W}_{Q}\mathbf{W}_{K}^{\top}\mathbf{X}^{\top}\|_{*} \quad \leq \underbrace{\|\mathbf{W}_{Q}\mathbf{W}_{K}^{\top}\|_{2}}_{\text{goes to 0 with } \sigma \textit{Reparam}} \|\mathbf{X}\|_{\mathrm{F}}^{2}.$$



Strong Competitor to MOIRAI



- MOIRAI [9]: foundation model trained on 27B samples,
- ullet Nb. params: small (14M), base (91M) and large (314M).

Dataset _	Full-shot	Zero-shot		
	SAMformer	${\tt MOIRAI_{Small}}$	${\tt MOIRAI_{Base}}$	${\tt MOIRAI_{Large}}$
ETTh1	0.410	0.400	0.434	0.510
ETTh2	0.344	0.341	0.345	0.354
ETTm1	0.373	0.448	0.381	0.390
ETTm2	0.269	0.300	0.272	0.276
Electricity	0.181	0.233	0.188	0.188
Weather	0.260	0.242	0.238	0.259
Overall MSE	improvement	6.9%	1.1%	7.6%

SAMformer outperforms MOIRAI while having significantly fewer parameters!

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Easier, Better, Faster, Stronger



Findings

- ullet Transformer failure o trainability issues of the attention,
- In time series forecasting, entropy collapse is benign,
- But sharpness prevents good generalization.

Proposal

- SAMformer: RevIN + channel-wise attention + SAM,
- SOTA and lightest model,
- Strong competitor to MOIRAI [9].

To Know More



This work has been accepted as an **Oral at ICML 2024, Vienna**. You may find the links to the paper and the code below. To know more about my research, check my website: ambroiseodt.github.io and feel free to contact me.

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* Paper: https://arxiv.org/pdf/2402.10198
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* Code: https://github.com/romilbert/samformer

Acknowledgements

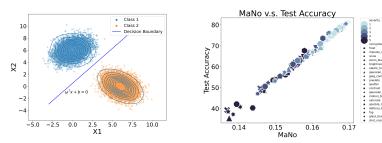


This project was led by Romain Ilbert and myself with our co-authors Vasilii Feofanov, Aladin Virmaux, Giuseppe Paolo, Themis Palpanas, and levgen Redko.

Self-Promotion



MANO: Exploiting Matrix Norm for Unsupervised Accuracy Estimation Under Distribution Shifts



https://arxiv.org/pdf/2405.18979

Thanks for your attention!

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