SAMformer: Unlocking the Potential of Transformers in Time Series Forecasting

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école———
normale ———
supérieure ———
paris-saclay



Introduction

2 Failure of Transformers

3 SAMformer

- **4** Experiments
- **5** Take Home Message



Introduction

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- Our Experiments
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In many applications, data are gathered sequentially.









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

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

Challenges

- 1 Long-term temporal dependencies,
- **2** Highly correlated features.



D-dimensional time series of length $L \rightarrow$ predict next H values.

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

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

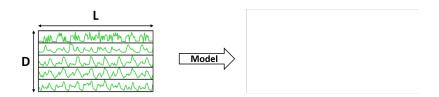




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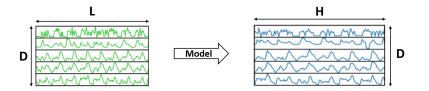




D-dimensional time series of length $L \rightarrow$ predict next *H* values.

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Standard methods:

- AR models (ARIMA)
- Seasonal naive

Deep learning methods

- RNN, CNN
- Transformer-based models



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Motivation

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

Main challenges

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



Main challenges

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



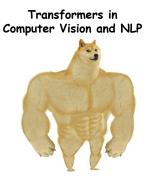
Main challenges

- 1 Quadratic complexity of self-attention
 - Sparse attention: LogTrans [5], Informer [13]
 - Modified attention: Pyraformer [6]
- Ocomplex 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.



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



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



Introduction

2 Failure of Transformers

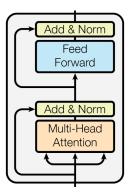
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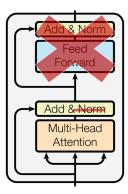
Starting Point: Linear Regression

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

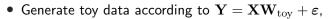


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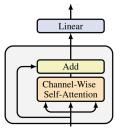






• Designing the simplest Transformer possible.

$$\begin{split} \mathbf{A}(\mathbf{X}) &= \texttt{softmax}\!\left(\frac{\mathbf{X}\mathbf{W}_{\mathbf{Q}}\mathbf{W}_{\mathbf{K}}^{\top}\mathbf{X}^{\top}}{\sqrt{d_{\mathrm{m}}}}\right) \\ f(\mathbf{X}) &= [\mathbf{X} + \mathbf{A}(\mathbf{X})\mathbf{X}\mathbf{W}_{V}\mathbf{W}_{O}]\mathbf{W} \end{split}$$



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$$f(\mathbf{X}) = [\mathbf{X} + \mathbf{A}(\mathbf{X})\mathbf{X}\mathbf{W}_{V}\mathbf{W}_{O}]\mathbf{W}$$

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., $f(\mathbf{X}) = \mathbf{X}\mathbf{W}_{toy}$.



Starting Point: Linear Regression

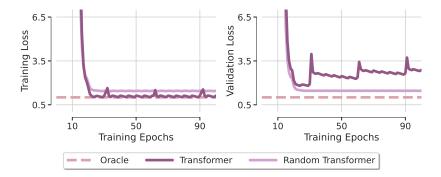
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In theory, our simplistic Transformer can be optimal. Is this the case in practice?

Poor Generalization

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



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

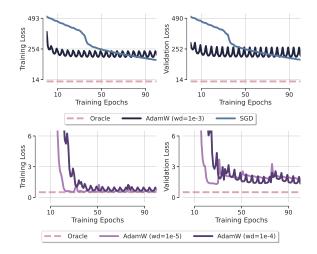
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Similar Behaviour with other Optimizers





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

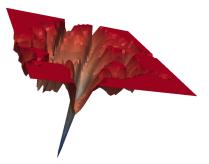
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Hypothesis from NLP and Computer Vision

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



Trainability Issues due to the Attention

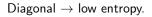


Hypothesis from NLP and Computer Vision

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

N

 \sim Uniform \rightarrow high entropy.

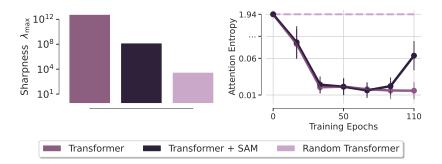


Trainability Issues due to the Attention



Hypothesis from NLP and Computer Vision

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

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1 σ Reparam [12]

Replace each weight matrix ${\bf W}$ by

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

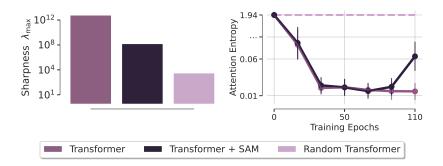
O Sharpness-Aware Minimization (SAM) [3]

Replace the training loss \mathcal{L}_{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}) + oldsymbol{arepsilon} \cdot rac{
abla \mathcal{L}_{ ext{train}}(oldsymbol{\omega})}{\|
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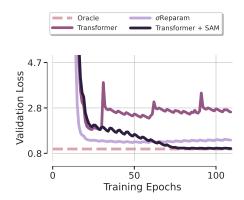
Contrary to NLP and Computer Vision, entropy collapse seems benign in time series forecasting while sharpness is harmful.



$\sigma {\rm Reparam}$ 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).

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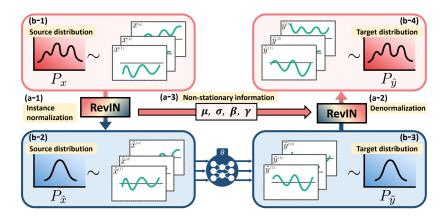


RevIN [4] \rightarrow Reduce distribution shift between input and target.

- 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 $ilde{\mathbf{Y}} = f(ilde{\mathbf{X}})$,
- Denormalize each feature $\tilde{\mathbf{Y}}_i \leftarrow \hat{\mathbf{Y}}_i = \frac{\tilde{\mathbf{Y}}_i \beta}{\gamma} \leftarrow \sigma \hat{\mathbf{Y}}_i + \mu.$



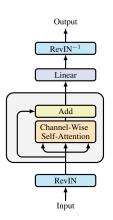
RevIN [4] \rightarrow Reduce distribution shift between input and target.



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],
- Channel-wise attention $\mathbf{A}(\mathbf{X}) \in \mathbb{R}^{D \times D}$,
- Smooth loss landscape with SAM [3].

$$egin{aligned} \mathbf{A}(\mathbf{X}) &= \mathtt{softmax}igg(rac{\mathbf{X}\mathbf{W}_{\mathbf{Q}}\mathbf{W}_{\mathbf{K}}^{ op}\mathbf{X}^{ op}}{\sqrt{d_{\mathrm{m}}}}igg) \ f(\mathbf{X}) &= [\mathbf{X} + \mathbf{A}(\mathbf{X})\mathbf{X}\mathbf{W}_{V}\mathbf{W}_{O}]\mathbf{W} \end{aligned}$$



SAMformer is a shallow transformer trained with SAM. \rightarrow One head, one encoder, 15 lines of code!



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

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

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

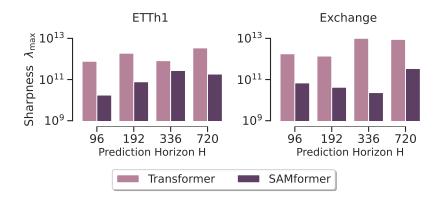
Dataset	ETTh1/ETTh2	ETTm1/ETTm2	Electricity	Exchange	Traffic	Weather
<pre># features # time steps</pre>	$7 \\ 17420$	7 69680	$321 \\ 26304$	8 7588	862 17544	21 52696
Granularity	1 hour	15 minutes	1 hour			10 minutes



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 i	mprovement	$\mathbf{6.58\%}$	8.79%	$\mathbf{13.2\%}$	22.5 %	35.9 %

SAMformer outperforms all baselines while having significantly fewer parameters.

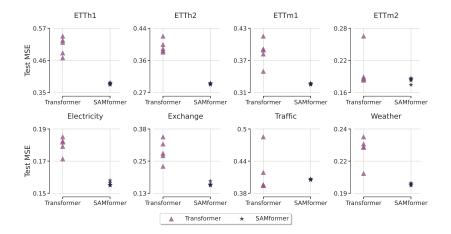




SAM provides a smoother loss landscape

Better Generalization

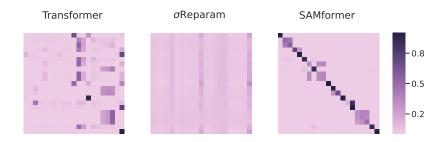




... leading to better generalization and robustness.

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

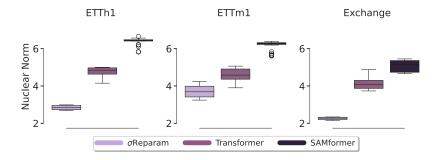


Theorem (Ilbert, O., Feofanov et al.)

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

$$\|\mathbf{X}\mathbf{W}_{Q}\mathbf{W}_{K}^{\top}\mathbf{X}^{\top}\|_{*} \leq \underbrace{\|\mathbf{W}_{Q}\mathbf{W}_{K}^{\top}\|_{2}}_{\mathbf{W}_{K}} \|\mathbf{X}\|_{\mathrm{F}}^{2}.$$

goes to 0 with σ Reparam



Strong Competitor to MOIRAI



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

Dataset	Full-shot	Zero-shot		
	SAMformer	MOIRAI _{Small}	$MOIRAI_{Base}$	MOIRAILarge
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	<u>0.188</u>
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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Findings

- Transformer failure \rightarrow 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].



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.

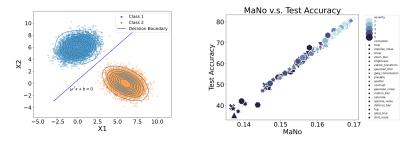
- * Paper: https://arxiv.org/pdf/2402.10198
- * Code: https://github.com/romilbert/samformer



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



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



https://arxiv.org/pdf/2405.18979

Thanks for your attention !

References I



- Chen, S.-A., Li, C.-L., Arik, S. O., Yoder, N. C., and Pfister, T. (2023). TSMixer: An all-MLP architecture for time series forecasting. *Transactions on Machine Learning Research*.
- [2] Chen, X., Hsieh, C.-J., and Gong, B. (2022). When vision transformers outperform resnets without pre-training or strong data augmentations. In *International Conference on Learning Representations*.
- [3] Foret, P., Kleiner, A., Mobahi, H., and Neyshabur, B. (2021). Sharpness-aware minimization for efficiently improving generalization. In *International Conference on Learning Representations*.
- [4] Kim, T., Kim, J., Tae, Y., Park, C., Choi, J.-H., and Choo, J. (2021). Reversible instance normalization for accurate time-series forecasting against distribution shift. In *International Conference on Learning Representations*.

References II



- [5] Li, S., Jin, X., Xuan, Y., Zhou, X., Chen, W., Wang, Y.-X., and Yan, X. (2019). Enhancing the locality and breaking the memory bottleneck of transformer on time series forecasting. In Wallach, H., Larochelle, H., Beygelzimer, A., d'Alché-Buc, F., Fox, E., and Garnett, R., editors, *Advances in Neural Information Processing Systems*, volume 32. Curran Associates, Inc.
- [6] Liu, S., Yu, H., Liao, C., Li, J., Lin, W., Liu, A. X., and Dustdar, S. (2022). Pyraformer: Low-complexity pyramidal attention for long-range time series modeling and forecasting. In *International Conference on Learning Representations*.
- [7] Liu, Y., Hu, T., Zhang, H., Wu, H., Wang, S., Ma, L., and Long, M. (2024). itransformer: Inverted transformers are effective for time series forecasting. In *The Twelfth International Conference on Learning Representations*.

References III



- [8] Nie, Y., Nguyen, N. H., Sinthong, P., and Kalagnanam, J. (2023). A time series is worth 64 words: Long-term forecasting with transformers. In *The Eleventh International Conference on Learning Representations*.
- [9] Woo, G., Liu, C., Kumar, A., Xiong, C., Savarese, S., and Sahoo, D. (2024). Unified training of universal time series forecasting transformers.
- [10] Wu, H., Xu, J., Wang, J., and Long, M. (2021). Autoformer: Decomposition transformers with Auto-Correlation for long-term series forecasting. In Advances in Neural Information Processing Systems.
- [11] Zeng, A., Chen, M., Zhang, L., and Xu, Q. (2023). Are transformers effective for time series forecasting? In *Proceedings* of the AAAI Conference on Artificial Intelligence.



- [12] Zhai, S., Likhomanenko, T., Littwin, E., Busbridge, D., Ramapuram, J., Zhang, Y., Gu, J., and Susskind, J. M. (2023). Stabilizing transformer training by preventing attention entropy collapse. In Krause, A., Brunskill, E., Cho, K., Engelhardt, B., Sabato, S., and Scarlett, J., editors, *Proceedings of the 40th International Conference on Machine Learning*, volume 202 of *Proceedings of Machine Learning Research*, pages 40770–40803. PMLR.
- [13] Zhou, H., Zhang, S., Peng, J., Zhang, S., Li, J., Xiong, H., and Zhang, W. (2021). Informer: Beyond efficient transformer for long sequence time-series forecasting. In *The Thirty-Fifth AAAI Conference on Artificial Intelligence, AAAI 2021, Virtual Conference*, volume 35, pages 11106–11115. AAAI Press.



[14] Zhou, T., Ma, Z., Wen, Q., Wang, X., Sun, L., and Jin, R. (2022). FEDformer: Frequency enhanced decomposed transformer for long-term series forecasting. In *Proc. 39th International Conference on Machine Learning (ICML 2022).*