

Project Milestone: A Simple Parameter Inference with Transformers

Adam Kleman
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List of read articles:

- Vaswani et al. – Attention is All You Need <https://arxiv.org/abs/1706.03762>
- Jet: A Modern Transformer-Based Normalizing Flow <https://arxiv.org/html/2412.15129v1>
- Neural Spline Flows <https://arxiv.org/abs/1906.04032>
- Flow-based Conformal Prediction for Multi-dimensional Time Series <https://arxiv.org/abs/2502.05709>
- Normalizing Flows for Probabilistic Modeling and Inference <https://arxiv.org/abs/1912.02762>

Task overview:

The goal of this project is to predict the amplitude A_i and frequency ω_i of the periodic function $y_i(A_i, \omega_i, t) = A_i \cdot \sin(\omega_i \cdot t)$, where the input data consist of vectors $V_i(A_i, \omega_i)$ representing different time discretizations. The project focuses on searching for optimal hyperparameters, comparing a classical encoder-only transformer architecture using a regression head or a flow-based head for frequency prediction. Another goal is to examine the influence of dataset noise, dataset size, and time discretization on the stability and performance of the model.

Current progress:

At the beginning of the project, an initial encoder-only transformer model was implemented together with a synthetic dataset parameterized by amplitude, frequency, and time discretization. All data generation and experiments were performed with a fixed random seed to ensure full reproducibility. For a dataset of size $N=1000$, different frequency intervals – specifically $[0.0, 10.0]$, $[0.1, 10.0]$, and $[0.5, 10.0]$ – were compared to evaluate their effect on model behavior.

Suitable time discretization values were also tested, with $t_{disc} \in \{10, 20, 30, 40, 50, 100\}$. Training length was subsequently examined, and experiments showed that stable performance is achieved at approximately 160 epochs.

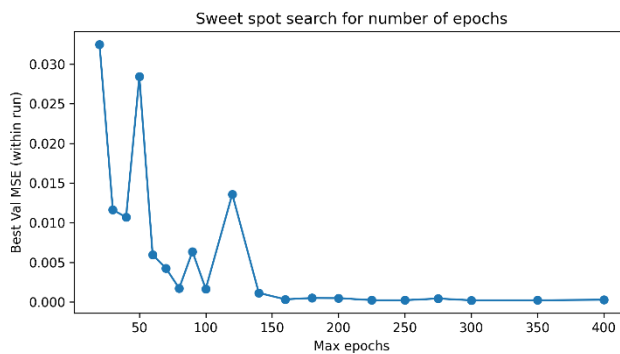


Fig. 1: Optimized number of sufficient epochs for training.

After selecting the interval $\omega \in [0.5, 10]$, time discretization $t_{disc}=100$, and 160 epochs, a slightly improvement in model performance was observed when the dataset was expanded. Therefore, datasets of size $N \in \{1000, 2500, 5000, 7500, 10000\}$ were tested together with $t_{disc} \in \{60, 70, 85, 100, 125, 150\}$.

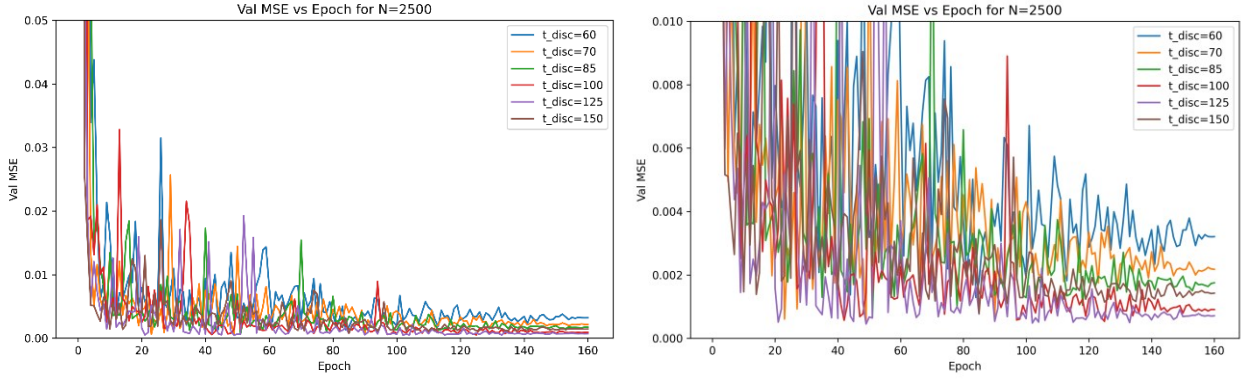


Fig. 2: Examples of different time discretizations and corresponding loss curves for $N=1000$ (left: slightly zoomed, right: fully zoomed).

In the next phase, systematic hyperparameter search was performed for $N=1000$ and $t_disc=100$. All combinations of parameter values $d_model \in \{32, 64, 128, 256\}$, $n_heads \in \{1, 2, 4, 8\}$, $num_layers \in \{1, 2, 3, 4\}$, and $dim_f \in \{64, 128, 256, 512\}$ were evaluated. I chose the fifth model from the table since it achieved similar performance to larger configurations but used significantly fewer parameters, making it a more efficient choice for further experiments.

Tab. 1: Top 5 model with performance at validation MSE.

d model	n heads	num layers	dim f	validation MSE
256	8	1	256	0.000172
256	8	1	64	0.000190
256	8	1	128	0.000204
256	8	1	512	0.000229
64	2	2	64	0.000239

Gaussian noise of the form $V_i = \sin(\omega_i t) + \mathcal{N}(\mu, \sigma)$ was then added to the dataset to analyze model behavior under more challenging conditions. The current stage of the project involves implementing a normalizing-flow output head for the transformer and improving both frequency prediction and uncertainty estimation.

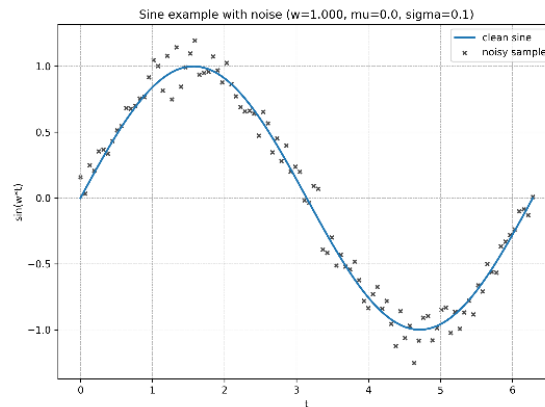


Fig. 3: Example of ideal wave without noise and created V_i with gaussian noise

Repository link: <https://gitlab.fit.cvut.cz/klemaada/mvi-sp> or <https://github.com/y4h1ko/mvi-sp>

Note: I also read lot of internet discussions, searched across lot GitHub repositories for multiple examples