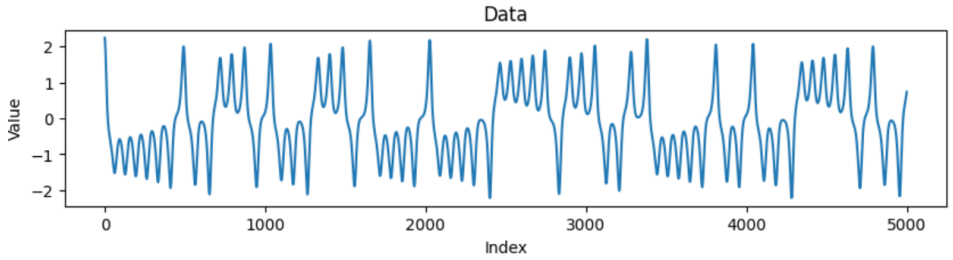
Selecting the best ML architecture for small-size 1-dim time series prediction among LSTM, GRU and Reservoir

Libraries such as TensorFlow and PyTorch fundamentally rely on backpropagation+gradient descent, and modifying that core algorithm is VERY DIFFICULT at the user level!!

$\Rightarrow$ I take a math-first approach to model design.

$\Rightarrow$ Propose a new Gradient descent.

Experimental setup for model comparison (1D Lorenz data)



Parameters fixed for fair accuracy comparison:

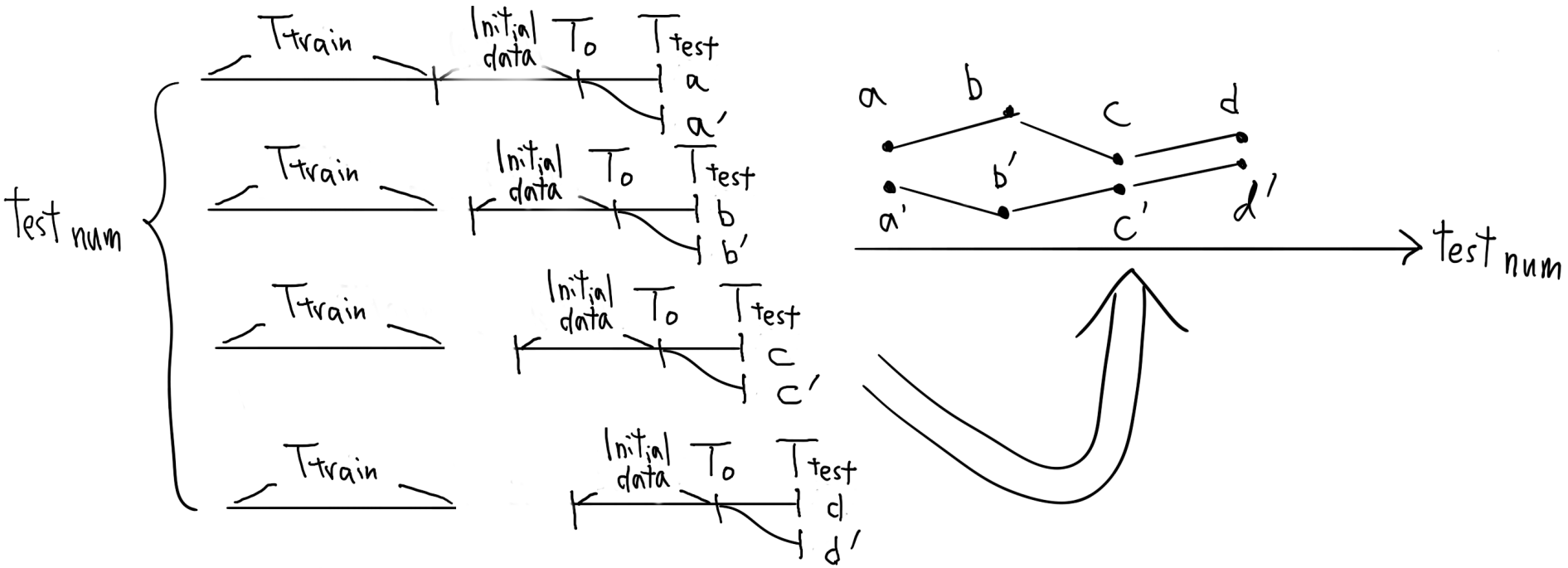
- Number of trainable parameters: 20,000
  (nodes: Reservoir ~ 150, LSTM ~ 70, GRU ~ 80)
- Training data size: 5,000
- Prediction horizon: 100 steps ahead
- L^2 regularization parameter: 0.0001

For LSTM architecture, small-size data,

Backprop+GD VS Bayes+GD with Delay coordinate

Model performance comparison (rolling-window validation)

- Perform predictions 3000 times (test num), each shifted by one step, and compute the MAE (mean absolute error).
- Repeat the same process until the average MAE stabilizes (80 times).



Bayes+GD with Delay coordinate VS Backprop+GD

Delay Coordinates (see for e.g. Nakai-Saiki '21)

$U_t = (data(t), data(t-\tau), \cdots, data(t-(M-1)\tau))$

We train by using this U_t.

Backprop+GD (TensorFlow): Input $\tau = 1$, M is chosen prior to training

Output $\tau = 1$, $M = 1$

Bayes+GD with Delay coordi: τ and M are also learned during training

Sigmoid function h, $\odot$: element-wise product

LSTM

$$
\begin{aligned}
\text{Input gate} \quad & i_t = h(W_{datain} U_t + W_{gatein} x_{t-1} + bias), \\
\text{Forget gate} \quad & f_t = h(W_{dataforget} U_t + W_{forget} x_{t-1} + bias), \\
\text{Output gate} \quad & o_t = h(W_{dataout} U_t + W_{gateout} x_{t-1} + bias), \\
\text{Memory cell} \quad & c_t = i_t \odot \tanh(W_{datacell} U_t + W_{cell} c_{t-1} + bias) + f_t \odot c_{t-1}, \\
\text{Output} \quad & x_t = o_t \odot \tanh(c_t), \quad \widehat{U}_{t+1} = W_{out} x_t
\end{aligned}
$$

What is Bayes+GD with Delay coordinate?

Bayes+GD is the only way that we can adopt Delay coordinate!!

Random matrices

$W_{datain}, W_{dataforget}, W_{dataout}, W_{datacell}, W_{gatein}, W_{forget}, W_{gateout}, W_{cell}$

By ridge regression (convexity), we first determine the following W_{out}:

$$U_{t+1} \simeq W_{out} x_t \qquad \text{(the idea of the conventional Reservoir)}.$$

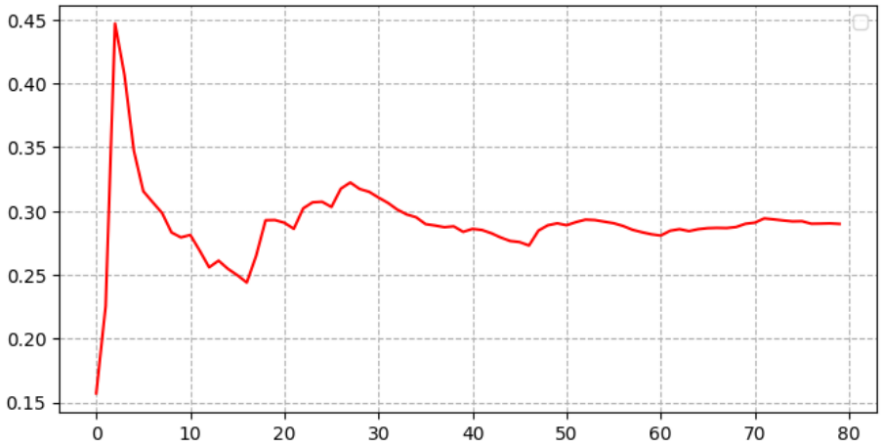
- By the convexity, W_{out} is explicitly obtained
- At this stage, not directly measuring $U_{t+1} - \widehat{U}_{t+1}$ so far

In the hyper-parameter space, we apply Bayesian Optimization (Optuna) to minimize the following objective function (RMSE):

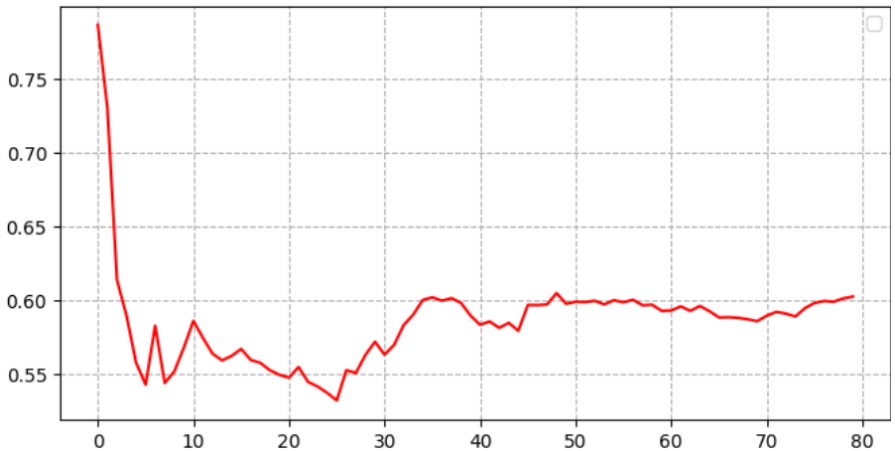
$$\left(\frac{1}{T} \sum_{t=0}^{T-1} |U_{t+1} - W_{out} x_t|^2 \right)^{1/2}.$$

Note: Random matrices must be continuously depending on seed value!

Result: Bayes+GD with Delay coordi VS Backprop+GD



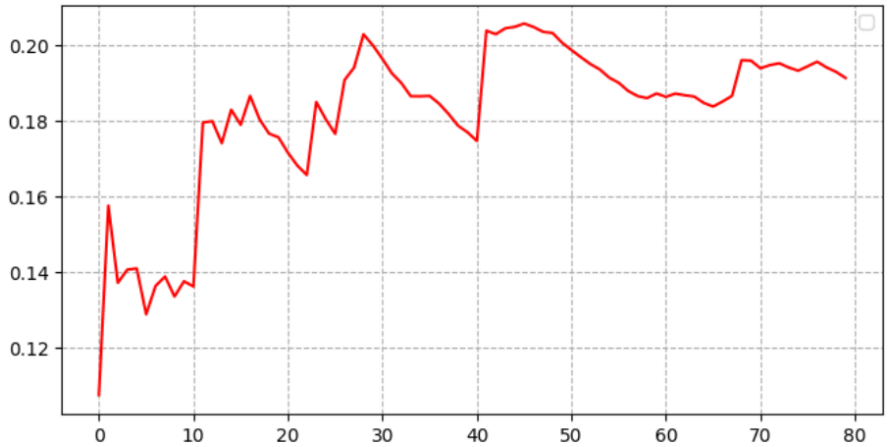
LSTM-BayesOpt-DelayCoordi: MAE 0.29



LSTM-TensorFlow: MAE 0.60

In this competition, all components other than the delay coordinates are the same. Therefore, this big difference in MAE arises from the presence or absence of the delay coordinates!

Replication test: GRU



GRU-Bayes+GD-DelayCoordi: MAE 0.19

Just only changing the LSTM to GRU architecture (simpler architecture than LSTM), we simply get better result!

Do we really need the complicated LSTM architecture?

Further simplified LSTM (only memory cell)

$$\begin{aligned} \text{input gate:} \quad & i_t = tanh(W_{datain} U_t) \\ \text{forget gate:} \quad & f_t = h(W_{dataforget} U_t + bias) \\ \text{memory cell:} \quad & c_t = i_t + f_t \odot c_{t-1} \\ \text{Ridge regression:} \quad & U_{t+1} \simeq W_{out} c_t \end{aligned}$$

$$\text{induction arg:} \quad c_t = \sum_{s=0}^{t} \left(i_s \prod_{r=s+1}^{t} (\odot f_r) \right), \quad \prod_{r=t+1}^{t} f_r := 1.$$

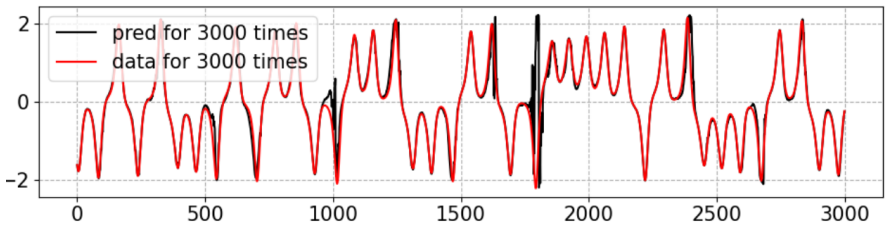
Now assume that the following probability:

$$\gamma := P(f_r \cdot e_j \neq 0) \quad (0 < \gamma < 1)$$

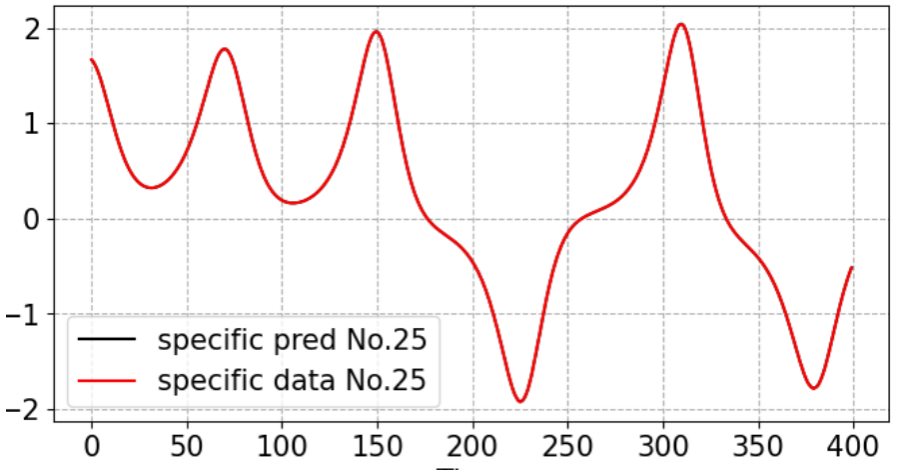
is independent of j and r, where e_j is the j'th unit vector. Also assume f_r and $f_{r'}$ $(r \neq r')$ are probabilistically independent. Then we have ESP:

$$P\left(\prod_{r=s+1}^{t} f_r \cdot e_j \neq 0 \right) = \prod_{r=s+1}^{t} P(f_r \cdot e_j \neq 0) = \gamma^{t-s} \to 0 \quad (s \ll t \to \infty).$$

Result: Further simplified LSTM (only memory cell)



OnlyMemoryCellLSTM: MAE 0.11, prediction 400 steps ahead



OnlyMemoryCellLSTM: MAE 0.11, prediction 400 steps ahead

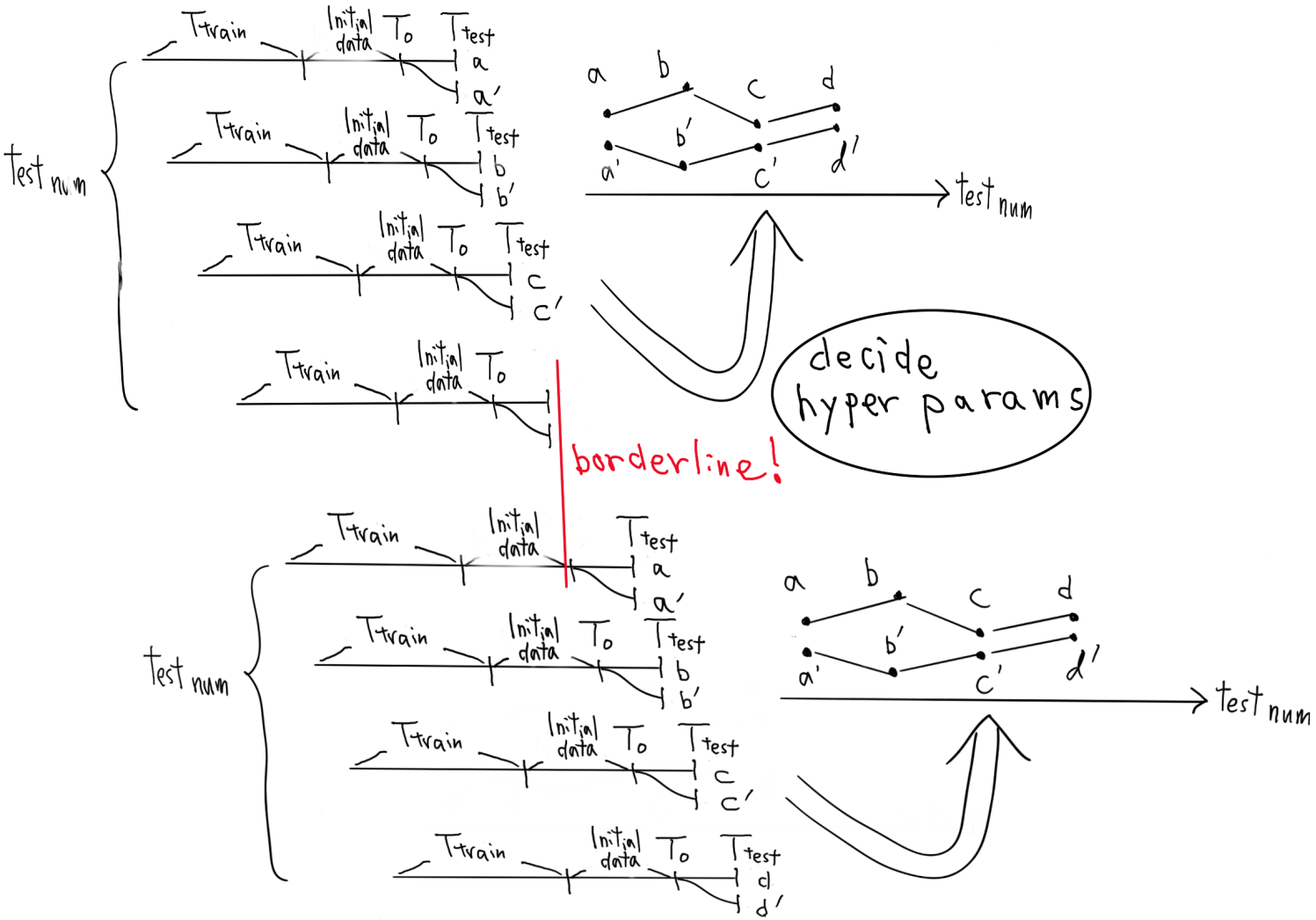
At least, for the small-size data prediction, we do not need the complicated conventional LSTM!

Model selection phase VS Conventional Grad descent

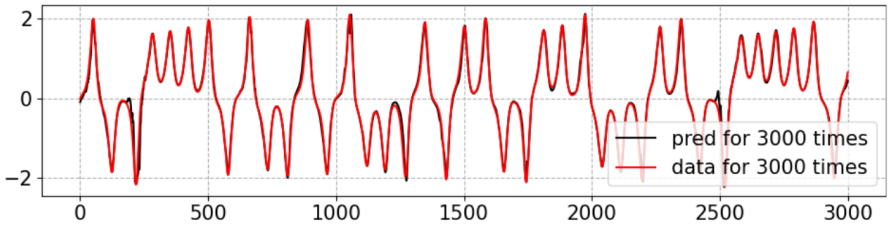
When Bayesian optimization is used, conventional gradient descent is no longer required. Accordingly, we propose adding a model-selection phase to the procedure.

Online Reservoir with model selection phase (diagram)

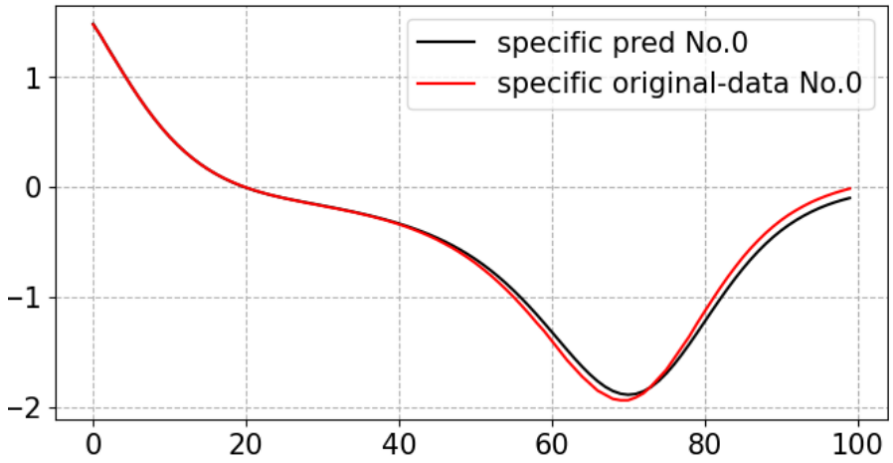
The first loop: Ridge regression, The second loop: Bayesian optimization using model selection data.



Result: Online Reservoir with model selection phase



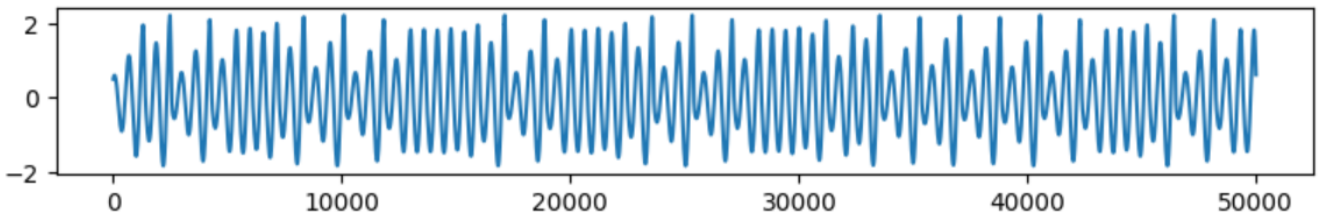
Reservoir: MAE 0.067,
1500+150 training samples



Reservoir: MAE 0.067,
1500+150 training samples

At least, for the small-size data prediction, adding model-selection phase seems much better!

Replication Test: Rössler Equation



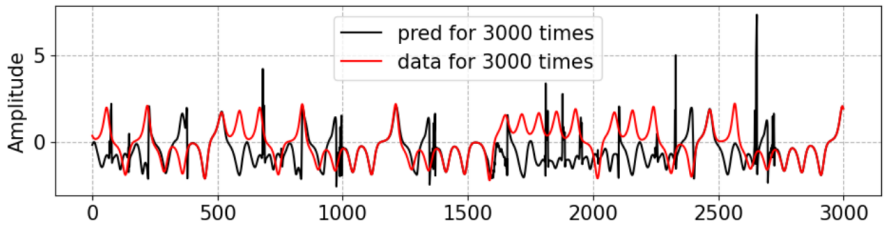
- Number of trainable parameters: 20,000
  (Reservoir ∼150 nodes, LSTM ∼70, GRU ∼80)
- Training data size: 5,000 (Reservoir uses 1,500+150)
- Pred: 100 steps ahead (OnlyMemoryCellLSTM: 400 steps ahead)
- L^2 regularization parameter: 0.0001

Learning Results (MAE)

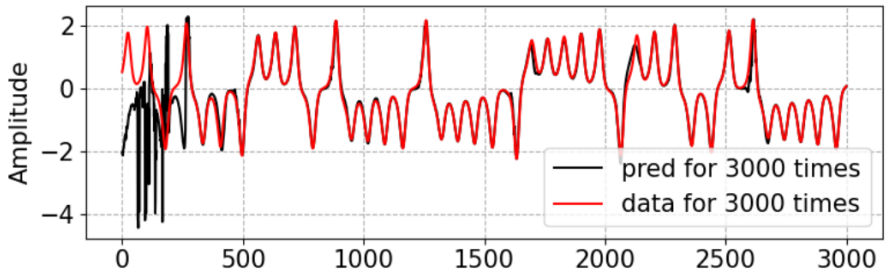
- OnlyMemoryCellLSTM: 0.005
  (prediction 400 steps ahead)
- Res-ModelSelect: 0.030
  (1,500+150 training samples)
- DelayCoodi-LSTM: 0.055
- DelayCoordi-GRU: 0.061
- TensorFlow-LSTM: 0.52

Choose OnlyMemoryCell-LSTM or Reservoir

To assess robustness, we examine progressively smaller datasets to evaluate how the accuracy behaves.



OnlyMemoryCellLSTM: MAE 0.854, 650 train data



Res: MAE 0.188, 500+150 train data

- With only 650 data points, a significant difference emerged between the Only-Memory-Cell-LSTM and reservoir computing. Future research should adopt reservoir computing as the optimal approach.