# Parallelized reservoir computing scheme and results

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.

# My research topic (prediction for parallelized data)

- Forecasting of stock price data and weather data, focusing on small-size datasets (less than 10,000 samples).

## Architecture selection

Reservoir computing performs best for the small-size datasets.

- See my GitHub repository, **"compare-LSTM-GRU-Reservoir"** .

Data structure for my research: at $u.shape[0]$ fixed observation points generate $u.shape[0]$-elements time series data.

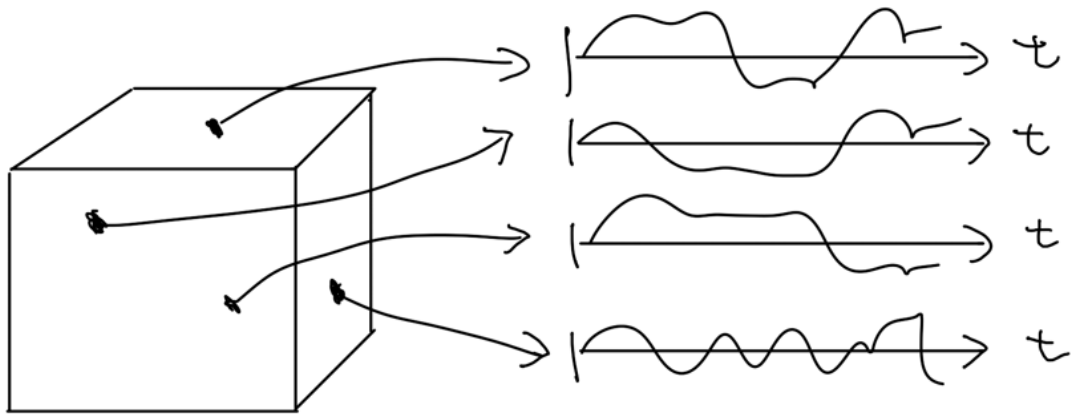



Figure: This case $u.shape[0] = 4$

## Case 1: the set of time series data contains rich spatial information

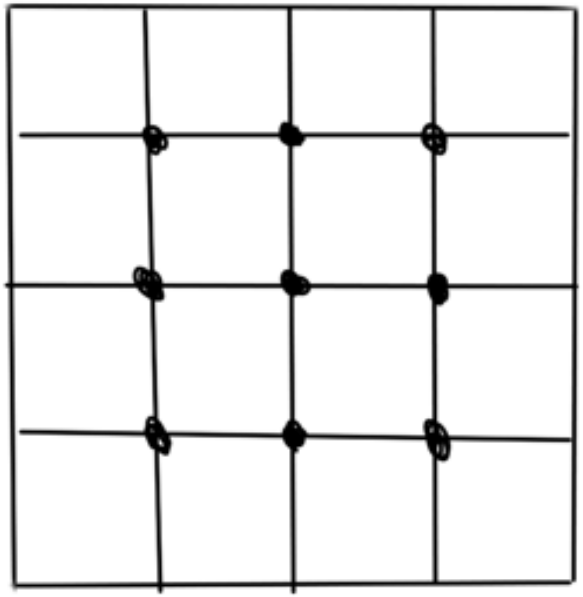
- Apply FFT (fast Fourier transform)
  Example: in periodic box turbulence obtained from DNS
- Focus on time evolution of the amplitudes. See Nakai-Saiki (2018).
- Spatial filters (e.g. low-pass, band-pass) are appropriate.

## Case 2: the set of time series data contains little spatial information

- Filters in the spatial direction may not be appropriate.
- Time filtering can still be applied
  but need assumption: underlying systems generating each time series are considered to be nearly identical.

## case 3: Intermediate case

- Graph Neural Networks might be one of them?



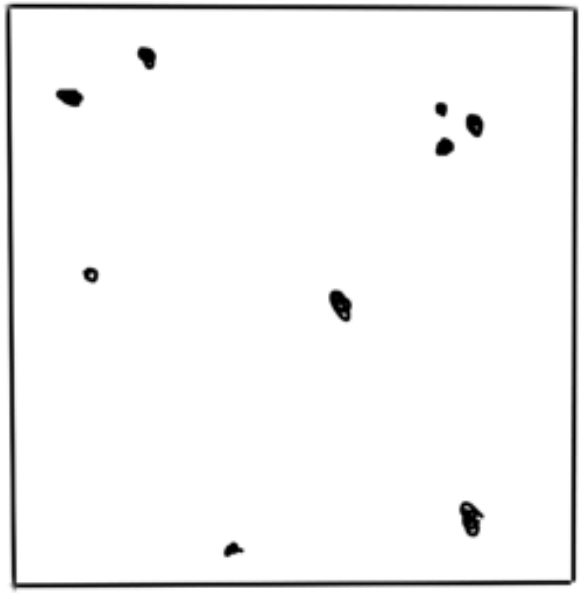


Figure: Left: suitable for FFT, RIGHT: try to apply GNN in the future

Focus on the case 2

- Wind-speed data seems having little spatial information
- Stock data clearly do not have such spatial information

# Overview of the Learning Scheme (Case 2)

Parallelized data can be written as:

$$\{u_{j,t}\}_{j\in[0,1,\cdots,u.shape[0]-1],t\in[0,1,\cdots,u.shape[1]-1]}$$

- the number of discrete data points: $u.shape[1]$
- the number of time series data: $u.shape[0]$

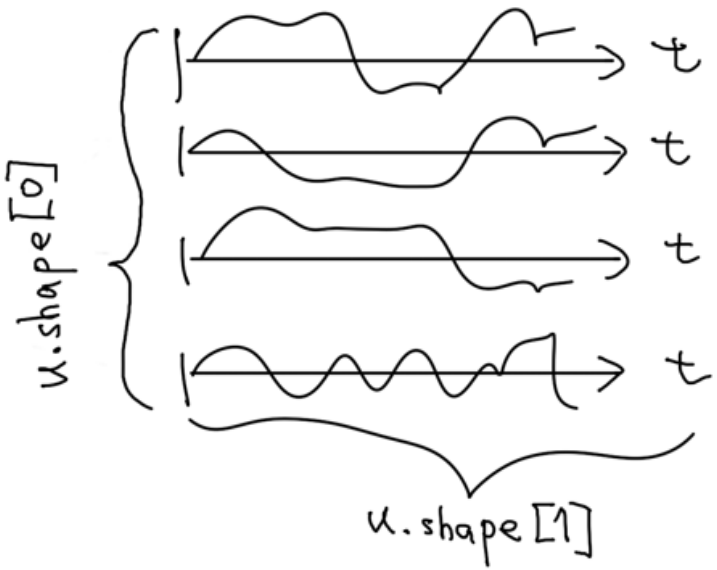



Figure: Image of data shape

# Delay coordinate (see Nakai-Saiki 2021)

Rewrite the data in a form of *dim*-dimensional vector as the following:

$$U_{j,t} = \begin{pmatrix} u_{j,t} \\ u_{j,t-lag} \\ \vdots \\ u_{j,t-(dim-1)lag} \end{pmatrix}.$$

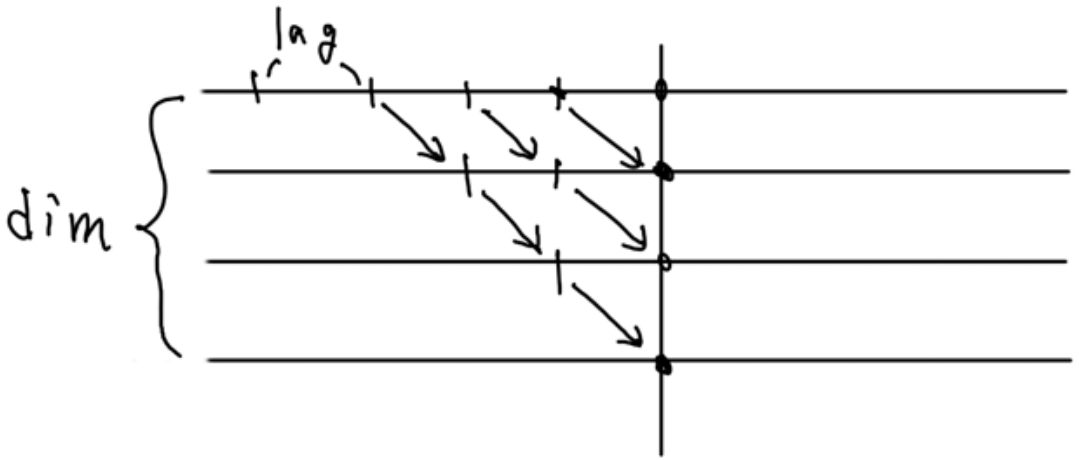



Figure: Image of $U_{j,t}$

# Overview of our ML architecture

- $M$: the number of learnable parameters
- $\{w_i\}_{i=1}^{M}$: learnable parameters (reservoir's $W_{in}$, $W$, $W_{out}$)

For a function $F_j : \mathbb{R}^M \times \mathbb{R}^{dim} \to \mathbb{R}^{dim}$, the prediction value $\widehat{U}_{j,t+1}$ is

$$\widehat{U}_{j,t+1} = F_j\left(\{w_i\}_{i=0}^{M-1}, \{U_{j,t}\}_{j=0}^{u.shape[0]-1}\right).$$

We then select the $\{w_i\}_i$ that minimizes the following energy:

$$\sum_{j=0}^{u.shape[0]-1} \sum_{t=0}^{T_{train}-1} |\widehat{U}_{j,t+1} - U_{j,t+1}|^2$$

(we omit regularization term here). Assume that underlying systems are almost identical, then $F_j$ can be unified into a single $F$ independent of $j$:

$$\widehat{U}_{j,t+1} = F\left(\{w_i\}_{i=0}^{M-1}, U_{j,t}\right).$$

This significantly simplifies the learning model.

# Reservoir Computing (overview)

## Trainable parameters

- Input weight matrix: $W^{in} \in \mathbb{R}^{N_x \times dim}$
- Recurrent weight matrix: $W \in \mathbb{R}^{N_x \times N_x}$
- Output weight matrix: $W^{out} \in \mathbb{R}^{dim \times N_x}$

Substitute data $U_{j,t} \in \mathbb{R}^{dim}$ and feature vector $x_{j,t} \in \mathbb{R}^{N_x}$
Output predicted value $\widehat{U}_{j,t+1} \in \mathbb{R}^{dim}$ and feature vector $x_{j,t+1} \in \mathbb{R}^{N_x}$

$$(U_{j,t}, x_{j,t}) \mapsto (\widehat{U}_{j,t+1}, x_{j,t+1}),$$

$$\begin{cases} x_{j,t+1} &= (1-\alpha)x_{j,t} + \alpha \tanh(W^{in}U_{j,t} + Wx_{j,t}), \\ \widehat{U}_{j,t+1} &= W^{out}x_{j,t+1}. \end{cases}$$

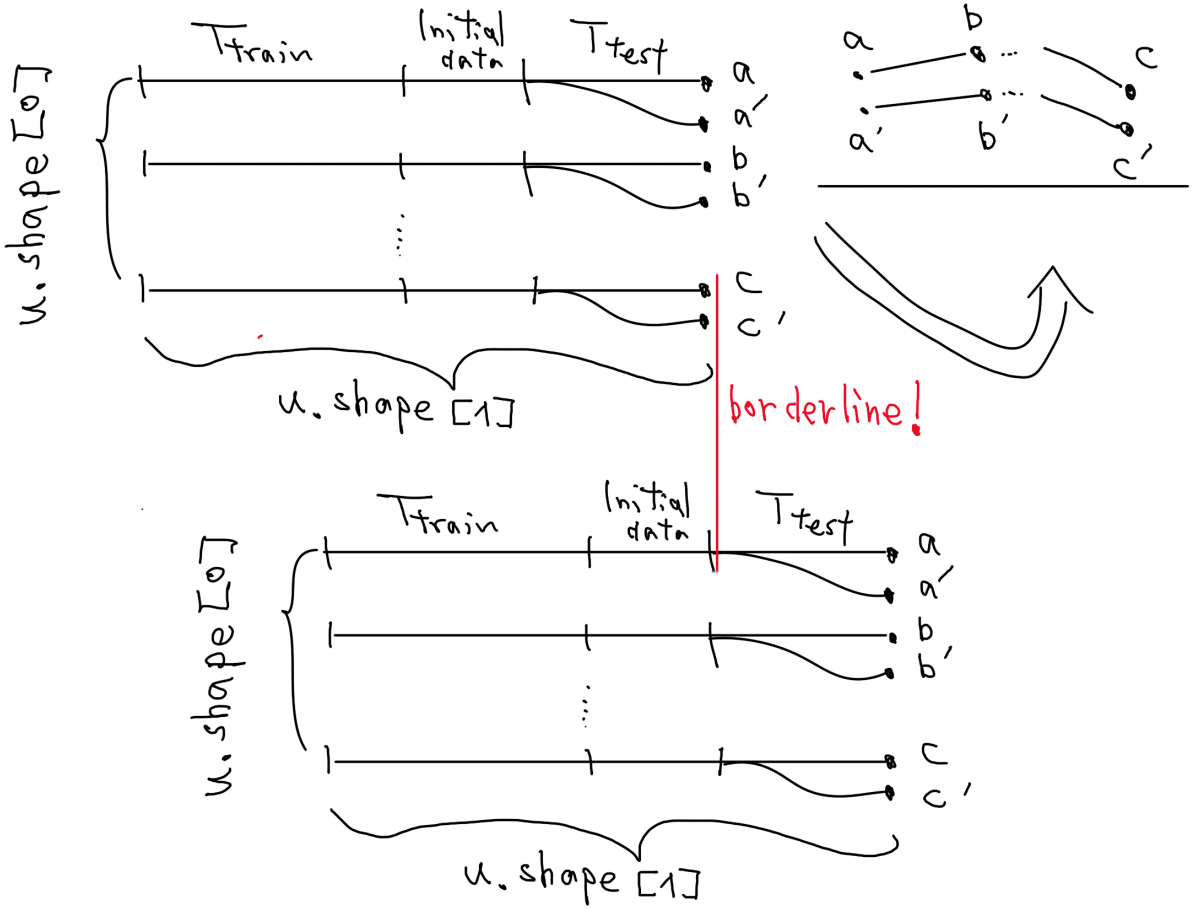
$\alpha \in (0, 1]$ is called the leaking rate, which is similar to the well-known concept of residual connections.

# Conceptual diagram of the learning scheme

The scheme has two stages:

- Model selection
- Generalization performance evaluation

Each of them are including a training phase



# Training phase

We select $W^{out}$ that minimizes the following $E$:

## Evaluation function

$$E = \frac{1}{2} \sum_{j=0}^{u.shape[0]-1} \sum_{t=0}^{T_{train}-1} |U_{j,t} - W^{out} x_t|^2 + \frac{\beta}{2} \sum_{i=0}^{dim-1} \sum_{j=0}^{N_x-1} |W_{ij}^{out}|^2.$$

- $\beta > 0$ is a regularization parameter
- $T_{train}$ is the number of training data points
- due to convexity, $W^{out}$ can be solved analytically

# Model selection phase

- We forecast $T_{test}$ steps ahead
- The initial value for model selection is $U_{j,T_{train}}$
- $x_{j,T_{train}}$ is already obtained during the training phase

Based on these, the next step is estimated as follows:

$$\begin{cases} x_{j,T_{train}+1} &= (1-\alpha)x_{j,T_{train}} + \alpha \tanh(W^{in}U_{j,T_{train}} + Wx_{j,T_{train}}), \\ \widehat{U}_{j,T_{train}+1} &= W^{out}x_{j,T_{train}+1}. \end{cases}$$

The resulting $\widehat{U}_{j,t}, x_{j,t}$ are then sequentially fed into the following recurrence relation to generate the predicted data:

$$\begin{cases} x_{j,t+1} &= (1-\alpha)x_{j,t} + \alpha \tanh(W^{in}\widehat{U}_{j,t} + Wx_{j,t}), \\ \widehat{U}_{j,t+1} &= W^{out}x_{j,t+1} \end{cases}$$

for $t = T_{train}+1, \cdots, T_{train}+T_{test}$.

# Bayesian optimization phase

Apply **Bayesian opt (Optuna)** using the prediction data $\widehat{U}_{j,T_{train}+T_{test}}$.
More specifically, minimize the following MAE-based evaluation function:

## Evaluation function

$$\frac{1}{u.shape[0]} \sum_{j=0}^{u.shape[0]-1} |\widehat{U}_{j,T_{train}+T_{test}} - U_{j,T_{train}+T_{test}}|$$

in the selection of the following parameters:

$$\text{dim, lag, } \alpha, \ W, \ W^{in}.$$

# Generalization Performance: re-training Phase

After selecting dim, lag, $\alpha$, $W$, and $W^{in}$ in the previous phase, we implement a new test to evaluate generalization performance. We re-select $W^{out}$ that minimizes the following $E$:

## Evaluation function

$$E = \frac{1}{2} \sum_{j=0}^{u.shape[0]-1} \sum_{t=T_{test}}^{T_{train}+T_{test}-1} |U_{j,t} - W^{out} x_{j,t}|^2 + \frac{\beta}{2} \sum_{i=0}^{dim-1} \sum_{j=0}^{N_x-1} |W_{ij}^{out}|^2.$$

- We evaluate the generalization performance from $T_{train} + T_{test}$
- The initial value is $U_{j,T_{train}+T_{test}}$
- $x_{j,T_{train}+T_{test}}$ is already obtained during the re-training phase

# Generalization Performance: evaluation phase

We generate the next step as follows.

$$\begin{cases} x_{j,T_{train}+T_{test}+1} &= (1-\alpha)x_{j,T_{train}+T_{test}} \\ & \quad +\alpha\tanh(W^{in}U_{j,T_{train}+T_{test}} + Wx_{j,T_{train}+T_{test}}), \\ \widehat{U}_{j,T_{train}+T_{test}+1} &= W^{out}x_{j,T_{train}+T_{test}+1}. \end{cases}$$

The $(\widehat{U}_{j,t}, x_{j,t})$ obtained in this manner are then sequentially fed into the following recurrence relation to generate the prediction data:

$$\begin{cases} x_{j,t+1} &= (1-\alpha)x_{j,t} + \alpha\tanh(W^{in}\widehat{U}_{j,t} + Wx_{j,t}), \\ \widehat{U}_{j,t+1} &= W^{out}x_{j,t+1} \end{cases}$$

for $t = T_{train} + T_{test} + 1, \cdots, T_{train} + 2T_{test}$. Then, finally, the generalization performance is evaluated using the following MAE:

## Evaluation function

$$\frac{1}{u.shape[0]} \sum_{j=0}^{u.shape[0]-1} |\widehat{U}_{j,T_{train}+2T_{test}} - U_{j,T_{train}+2T_{test}}|$$

Thank you!