Reservoir computing

1.a) Input data $\underline{u}(t) \in \mathbb{R}^M$

$t \in [-T, 0]$

These data will be used to train the 'machine' for the purpose of making predictions for $t > 0$.

b) Reservoir computer

State vector $\underline{r}(t) \in \mathbb{R}^d$, with $d >> M$. As shown below, the reservoir will be constructed as a dynamical system on a weighted random network.

c) Output data $\underline{v}(t) \in \mathbb{R}^N$

The desired output data

d) $\hat{R}_{in} : \mathbb{R}^M \to \mathbb{R}^d$ maps the input data to the reservois stack, hence

$$\underline{r}(t) = \hat{R}_{in}\left[\underline{u}(t)\right]$$

$\hat{R}_{out} : \mathbb{R}^d \to \mathbb{R}^N$ maps the reservois stack to the output, i.e.,

$$\underline{v}(t) = \hat{R}_{out}\left[\underline{r}(t)\right]$$

2. Reservoir dynamics

The reservoir is often chosen as a random weighted directed network which is constructed in the following way (# nodes = d)

(i) Generate a directed ER (random) network with mean $\langle k_{in} \rangle = \langle k_{out} \rangle = \langle k \rangle$

(ii) Choose edge weights from a $\mathcal{U}[-1, 1]$ (uniform) distribution.

(iii) Determine adjacency matrix $\tilde{A}$: d x d

(iv) Rescale A with a constant c ($A = cA$) so that the norm of the largest eigenvalue is equal to 1 (the spectral radius).

Let $\hat{R}_{in}[\underline{u}(t)] = W_{in}\,\underline{u}(t)$

where $W_{in} : d \times M$, where each row has exactly one element $\in U[-\sigma, \sigma]$. The discrete dynamics on the network is then given by

$$\underline{r}(t+\Delta t) \overset{\text{component wise}}{=} \tanh\left(A\,\underline{r}(t) + W_{in}\,\underline{u}(t)\right)$$

Note that we introduced already several hyperparameters:

- d: # nodes
- σ: coupling constant in W_{in}
- $\langle k \rangle$: mean degree
- c or
- ρ: spectral radius of A

3. Training of the network

- Over the period $[-T, 0]$, the reservoir evolves according to

$$\underline{r}(t) = \tanh\left(A\,\underline{r}(t) + W_{in}\,\underline{u}(t) \right)$$

so we have $\frac{T}{\Delta t} = n$ vectors

$$\left(\underline{r}_1, \dots, \underline{r}_n \right).$$

- Sometimes the following is used

$$r_j^* = \begin{cases} r_j, & j \text{ odd} \\ r_j^2, & j \text{ even} \end{cases}$$

but we will omit this here

- Define W_{out} as an $M \times d$ matrix of weights, and define $(j = 1, \ldots, n)$:

$$\underline{V}_j = \hat{R}_{out}(\underline{r}_j) = W_{out}\,\underline{r}_j$$

- Let the input vectors $\underline{u}(t)$ over the discrete times be indicated by $(\underline{u}_1, \ldots, \underline{u}_n)$, then the W^*_{out} is determined from

$$W^*_{out} = \min_W \left\{ \frac{1}{2} \sum_{j=1}^{n} \| \underline{u}_j - \underline{V}_j \|^2 + \right.$$

$$\left. + \beta/2 \, \| W_{out} \|^2 \right\}$$

where $\|W_{out}\|^2$ is the matrix norm (sum over all squares).

4. Solution of the optimization problem.

Example: $M = 2$, $d = 3$, $n = 1$

$$W_{out} = \begin{pmatrix} w_{11} & w_{12} & w_{13} \\ w_{21} & w_{22} & w_{23} \end{pmatrix}$$

$$\underline{r}(t) = \begin{pmatrix} r_1 \\ r_2 \\ r_3 \end{pmatrix}(t) \; ; \; \begin{cases} \underline{u}(t) = \begin{pmatrix} u_1 \\ u_2 \end{pmatrix}(t) \\ \underline{v}(t) = \begin{pmatrix} v_1 \\ v_2 \end{pmatrix}(t) \end{cases}$$

Hence:

$$\begin{pmatrix} v_1 \\ v_2 \end{pmatrix} = \begin{pmatrix} w_{11} r_1 + w_{12} r_2 + w_{13} r_3 \\ w_{21} r_1 + w_{22} r_2 + w_{23} r_3 \end{pmatrix}$$

which can be written as

$$\begin{pmatrix} v_1 \\ v_2 \end{pmatrix} = \begin{pmatrix} r_1 & r_2 & r_3 & 0 & 0 & 0 \\ 0 & 0 & 0 & r_1 & r_2 & r_3 \end{pmatrix} \times \begin{pmatrix} \underline{w} \\ \text{III} \\ w_{11} \\ w_{12} \\ w_{13} \\ w_{21} \\ w_{22} \\ w_{23} \end{pmatrix}$$

Cost function is in this case:

$$E(\underline{w}) = \frac{1}{2}\left(\underline{u} - \underline{v}\right)^2 + \beta/2 \|w\|^2$$

$$= \frac{1}{2}\left(\underline{u} - X\underline{w}\right)^2 + \beta/2 \|w\|^2$$

Minimum, need again ∇E

$$\nabla E = -X^T\left(\underline{u} - X\underline{w}\right) + \beta I \underline{w}$$

6x1 ← 6x2 · 2x1 2x6 6x1

$\underline{w}_* = \min_{\underline{w}} J(\underline{w})$ determined from $\nabla J = 0 \longrightarrow$

$$-X^T(\underline{y} - X\underline{w}) + \beta I \underline{w} = 0$$

$$\longrightarrow \quad \underline{w} = (\beta I + X^T X)^{-1} X^T \underline{y}$$

This is just a linear regression problem. If $n > 1$, then

$$X = \begin{pmatrix} \overleftrightarrow{d} & & \\ \underline{r}_1^T & 0 & 0 \\ 0 & \underline{r}_1^T & 0 \\ 0 & 0 & \underline{r}_1^T \\ \vdots & & \\ \underline{r}_n^T & 0 & 0 \\ 0 & \underline{r}_n^T & 0 \\ 0 & 0 & \underline{r}_n^T \end{pmatrix} \updownarrow H$$

$\underline{r}_j : d \times 1$

When $\beta = 0$:

$$\underline{w} = \underbrace{\left(X^T X\right)^{-1}}_{\text{Moore-Penrose inverse}} X^T \underline{y}$$

5. Prediction

Once the weights are determined, forecasts can be made for $t > 0$ using:

$$\begin{cases} \underline{r}(t+\Delta t) = \tanh\left(A\,\underline{r}(t) + W_{in}\,\underline{v}(t)\right) \\ \underline{v}(t) = W_{out}\,\underline{r}(t) \end{cases}$$

- Initial conditions:
  - $\underline{u}(0)$ is the last input of the training set.
  - we want to choose $\underline{r}(0)$ such that $\underline{v}(0) = \underline{r}(0)$
    hence $\underline{u}(0) = W_{out}\,\underline{r}(0)$

Multiplying by W_{in}, we find

$$W_{in}\,\underline{u}(0) = \underbrace{W_{in}W_{out}}_{\psi}\,\underline{r}(0)$$

$$\longrightarrow \quad \underline{r}(0) = \left(W_{in}W_{out}\right)^{-1} W_{in}\,\underline{u}(0)$$

$d \times 1$ $\quad$ $d \times M$ $\quad$ $M \times d$ $\quad$ $d \times M$ $\quad$ $M \times 1$

Exercise : Lorenz system

- notebook
- test effect hyper-parameters.