Distribution of model parameters and causality

IA pour la Science

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Distribution of model parameters and causality

The research focuses on the causal inference for the model selection in machine learning. To select a model we need to estimate the distribution of model parameters.
PyTorch provides a well-developed automated differentiation framework to estimate the parameters of the model. The nearest goal is to propose a method to build Causal Structural Model through the distribution of model parameters and use it for model selection purposes.
Below:

1. Causal machine and Control Problem
2. Clarification of the CI for time series
3. Applications of the Causal Discovery

Causal Inference and Control Problem

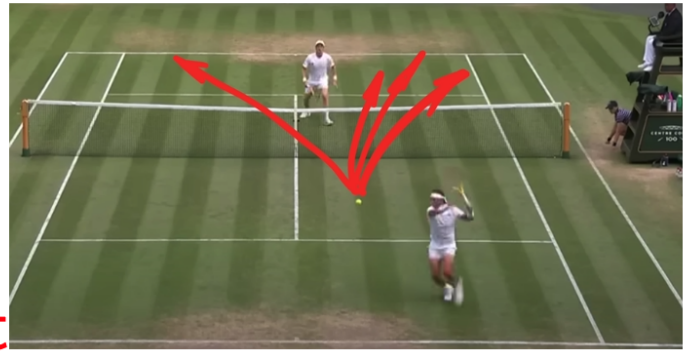
Control

Stimulus

$$
\begin{tikzcd}
 & & z \arrow[d, "\text{Exogenous}"] \\
u = C(\varepsilon) \arrow[rr, "\text{Control}"] & & y = f(x, y, u, z) \arrow[d, "\text{Measurement}"] \\
\hat{f}, \varepsilon \arrow[u, "\text{Decision}"] & & \hat{x}, \hat{y}, \hat{z} \arrow[ll, "\text{Modelling}"']
\end{tikzcd}
$$

Action

Game with opponent



Game with nature

Proportional integral derivative PID controller

$$u(t) = C_{\mathrm{p}}\varepsilon(t) + C_{\mathrm{i}} \int_0^t \varepsilon(\tau)\, d\tau + C_{\mathrm{d}} \frac{d\varepsilon(t)}{dt}$$

Time-delay embedding in Singula Spectrum Analysis

1. Construct the Hankel matrix with time series,

$$\boldsymbol{X} = \begin{bmatrix} \boldsymbol{x}_1 \\ \boldsymbol{x}_2 \\ \boldsymbol{x}_3 \\ \vdots \\ \boldsymbol{x}_t \end{bmatrix} = \begin{bmatrix} x_1 & x_2 & x_3 & \cdots & x_n \\ x_2 & x_3 & x_4 & \cdots & x_{n+1} \\ x_3 & x_4 & x_5 & \cdots & x_{n+2} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ x_t & x_{t+1} & x_{t+2} & \cdots & x_{t+n} \end{bmatrix}.$$

2. Decompose the matrix and take the k first components,

$$\boldsymbol{X} = \boldsymbol{X}_1 + \cdots + \boldsymbol{X}_n = \boldsymbol{U}\Lambda\boldsymbol{V}^{\mathsf{T}} = \sum_{k=1}^{n} \lambda_k \boldsymbol{u}_k \boldsymbol{v}_k^{\mathsf{T}}.$$

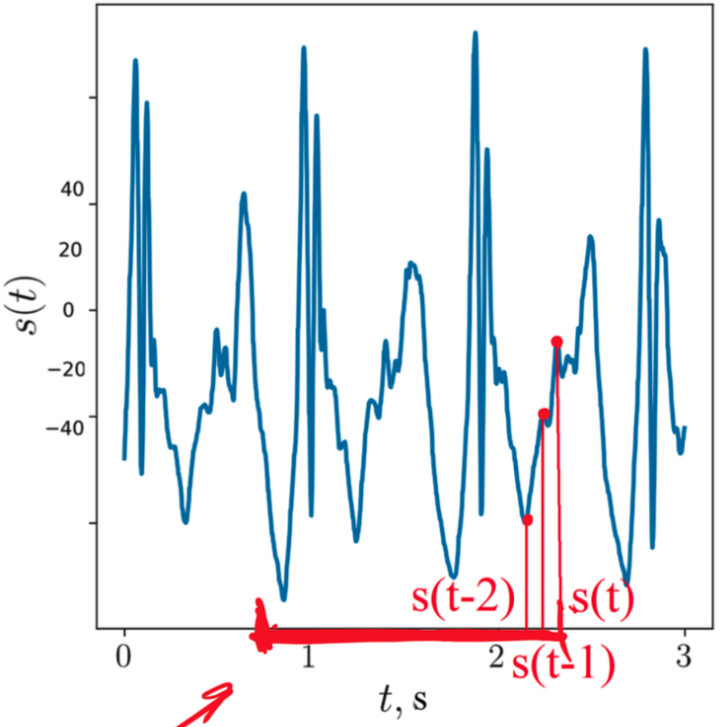
3. Reconstruct the time series by anti-diagonal average

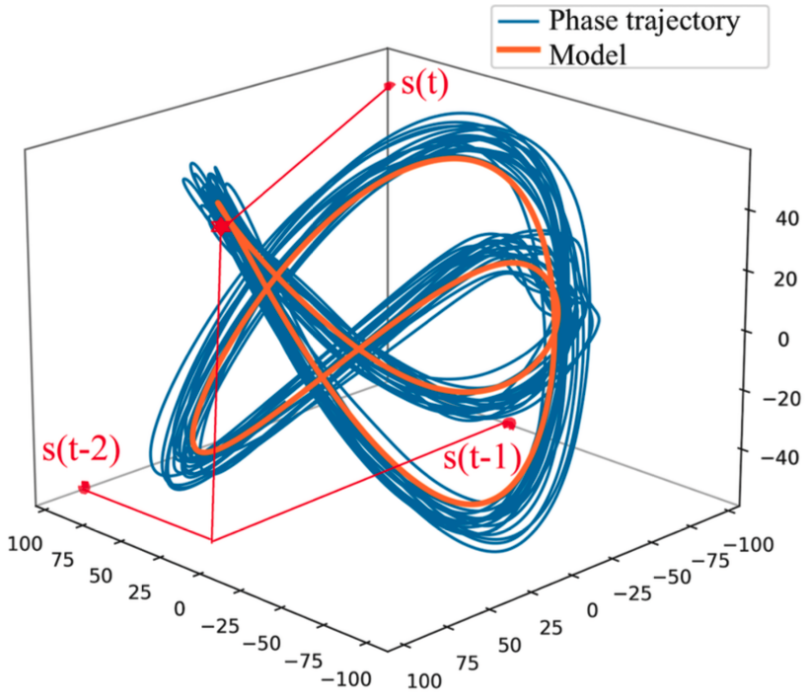
$$\hat{x}_t = \text{mean}\boldsymbol{X}(i,j), \quad i + j = t - 1.$$

State space models describe the change of state $\boldsymbol{x}$ in time $\frac{d\boldsymbol{x}}{dt} = \boldsymbol{f}(\boldsymbol{z})$

Define the state space by vectors $\{\boldsymbol{x}_1, \ldots, \boldsymbol{x}_t\}$, the phase trajectory $\boldsymbol{X}$.

Model of the phase trajectory in the state space





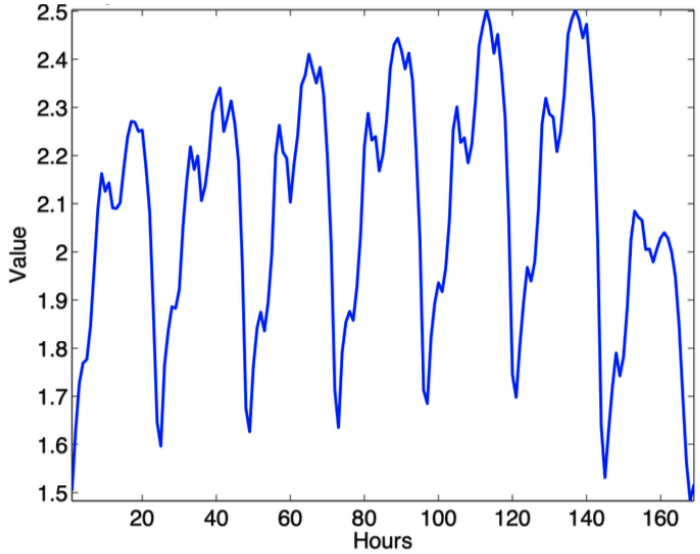
t - 1000

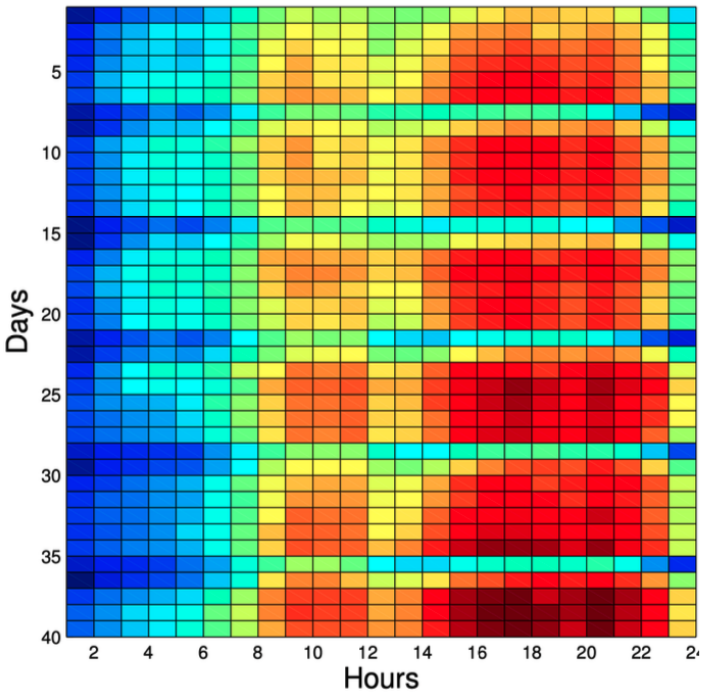
dim(s) $\approx$ 1000 $\longrightarrow$ dim(x) $= 4$

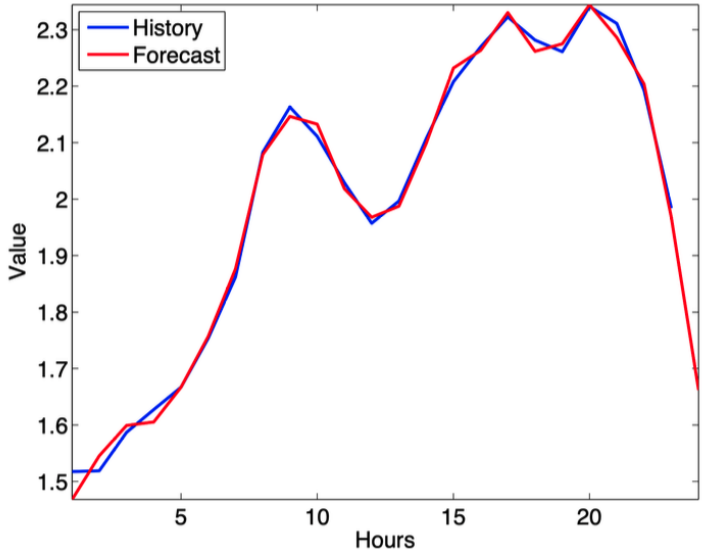
Reduce dimensionality with the principal component analysis, autoencoder $\boldsymbol{z} = \boldsymbol{W}^{\mathsf{T}}\boldsymbol{x}$ where $\boldsymbol{W}$ is an orthogonal (rotation) matrix. The first principal components are given by Singular Values Decomposition

$$\sqrt{\lambda_k}\boldsymbol{V_k} = \boldsymbol{X}^{\mathsf{T}}\boldsymbol{U}_k \quad \text{the SVD is} \quad \boldsymbol{X} = \boldsymbol{U}\Lambda\boldsymbol{V}^{\mathsf{T}}$$

Linear model for time series forecasting







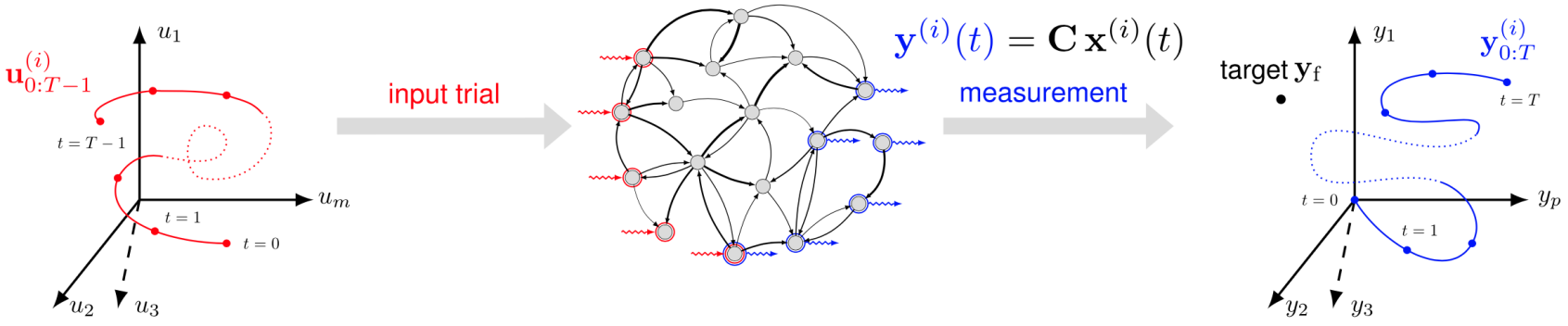
The design matrix is

$$\begin{array}{c|c} \underset{1\times 1}{y_{t+1}} & \underset{1\times n}{\boldsymbol{x}_t} \\ \hline \underset{t\times 1}{\boldsymbol{y}} & \underset{t\times n}{\boldsymbol{X}} \end{array},$$

the forecasting model $\hat{\boldsymbol{y}} = \boldsymbol{w}^\top \boldsymbol{X}$,
the forecast $\hat{y}_{t+1} = \boldsymbol{w}^\top \boldsymbol{x}_t$.

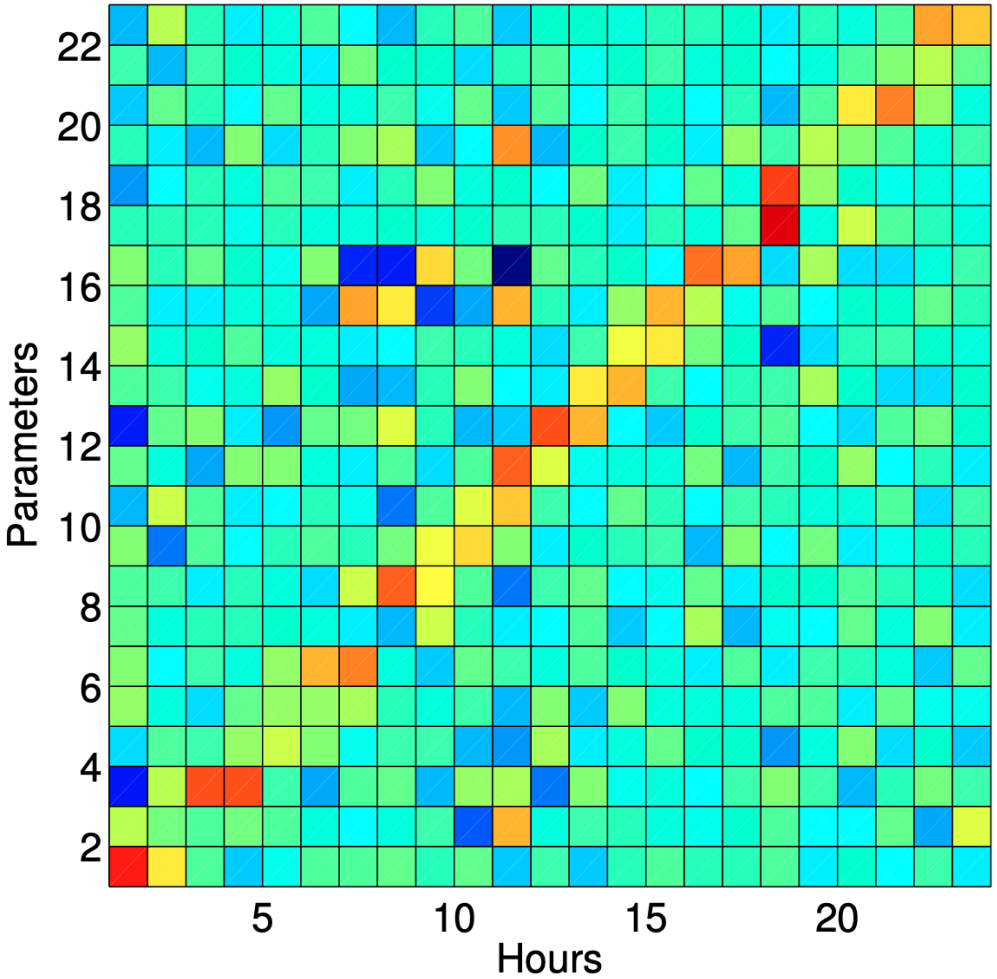
Conrol problem for time series forecasting

$$\mathbf{x}^{(i)}(t+1) = \mathbf{A}\,\mathbf{x}^{(i)}(t) + \mathbf{B}\,\mathbf{u}^{(i)}(t)$$



Covariance matrix of forecasting model parameters

Estimate parameters $\mathrm{w}(\tau) = (\mathrm{X}^{\mathsf{T}}\mathrm{X})^{-1}\mathrm{X}^{\mathsf{T}}\mathrm{y}$, then calculate the sample $s(\tau) = \mathrm{w}^{\mathsf{T}}(\tau)\mathrm{X}_{m+1}$ for each τ of the next $m+1$-th period.



The color shows the value of a parameter for each hour.

Probabilistic model selection

Bayesian inference delivers the error function $S(\mathbf{w})$

Posterior Likelihood Prior

$$p(\mathbf{w}|\mathfrak{D}, \mathbf{A}, \mathbf{B}, \mathbf{f}) = \frac{p(\mathfrak{D}|\mathbf{w}, \mathbf{B}, \mathbf{f})p(\mathbf{w}|\mathbf{A}, \mathbf{f})}{p(\mathfrak{D}|\mathbf{A}, \mathbf{B}, \mathbf{f})}.$$

Evidence
(to select a model)

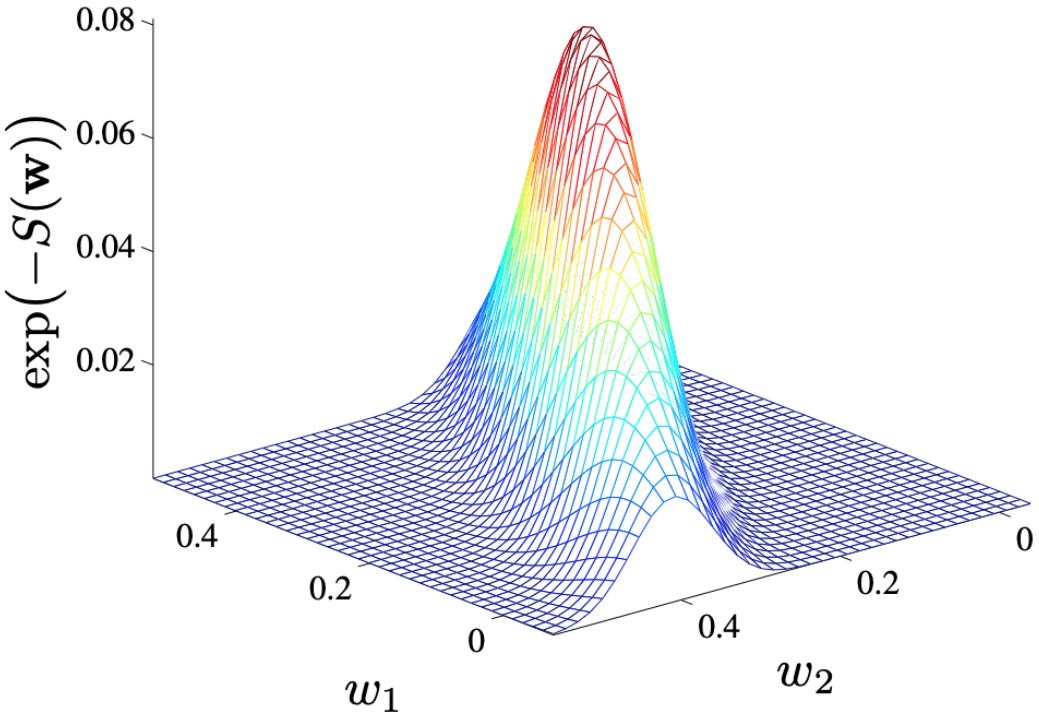
Write the error function given hyperparameters $\mathbf{A}, \mathbf{B}$

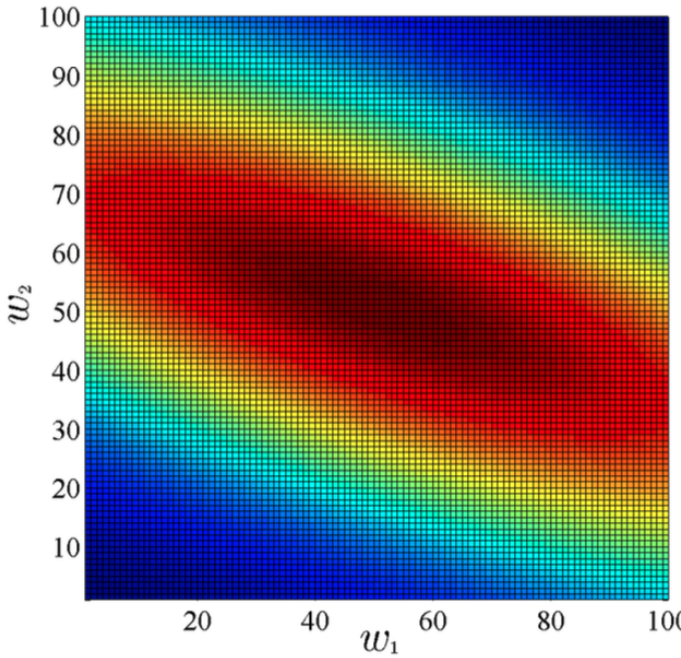
$$S(\mathbf{w}) = \underbrace{\frac{1}{2}(\mathbf{y} - \mathbf{f})^\mathsf{T}\mathbf{B}(\mathbf{y} - \mathbf{f})}_{\text{approximation error}} + \underbrace{\frac{1}{2}(\mathbf{w} - \hat{\mathbf{w}})^\mathsf{T}\mathbf{A}(\mathbf{w} - \hat{\mathbf{w}})}_{\text{regularisation error}},$$

$$S = E_D + E_\mathbf{w} = \boldsymbol{\lambda}^\mathsf{T}\mathbf{s}, \qquad \text{metaparameters } \lambda = \frac{1}{2}.$$

Empirical distribution of model parameters

The value of error function $S(\mathbf{w}|\mathfrak{D}, f)$ depends on parameters.

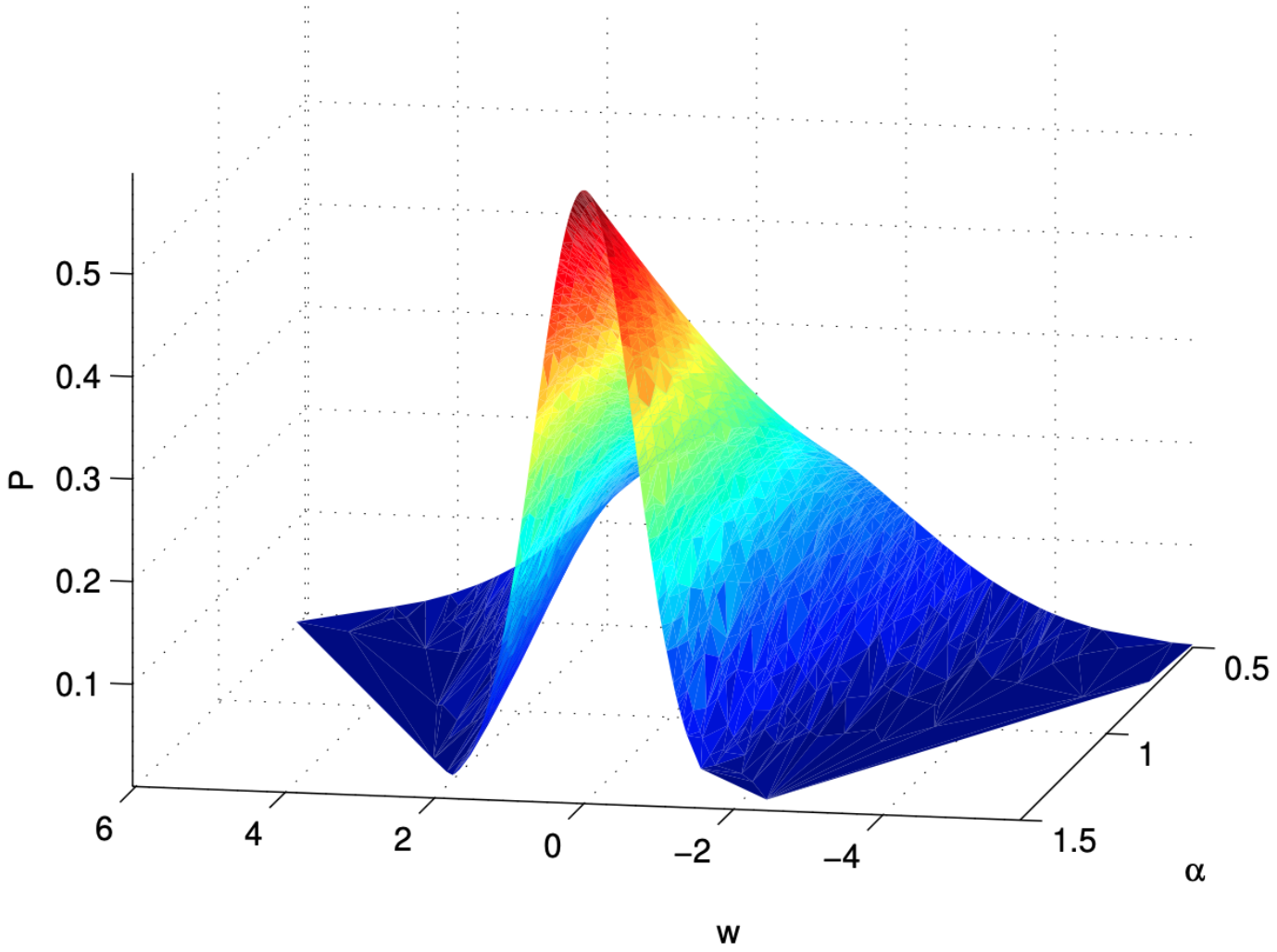




x-axis and y-axis: parameters $\mathbf{w}$, z-axis: $\exp(-S(\mathbf{w}))$

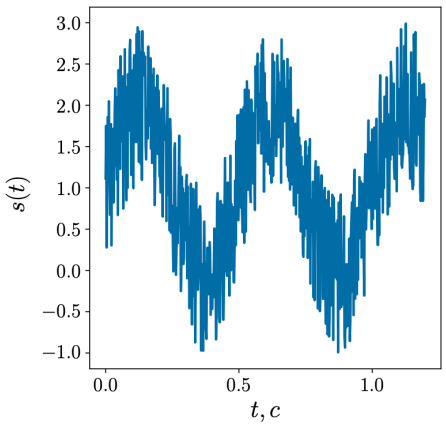
Evidence of the model

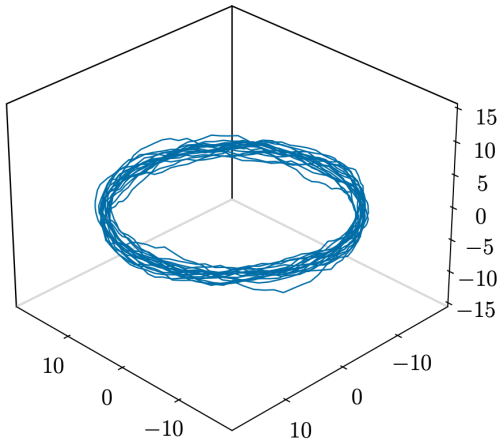
depends on both, error E_D (likelihood) and regularisation $E_{\mathbf{w}}$ (prior).



Parameters $\mathbf{w}$, variance α^{-2}, and $p(\mathbf{w}|\mathfrak{D}, \alpha)$ is the evidence.

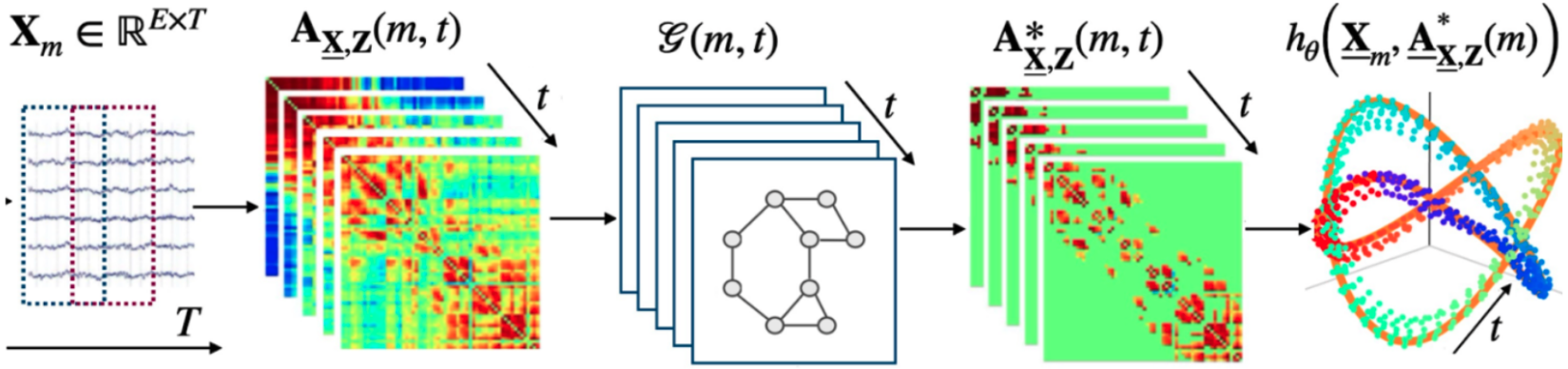
Do-operations and tests





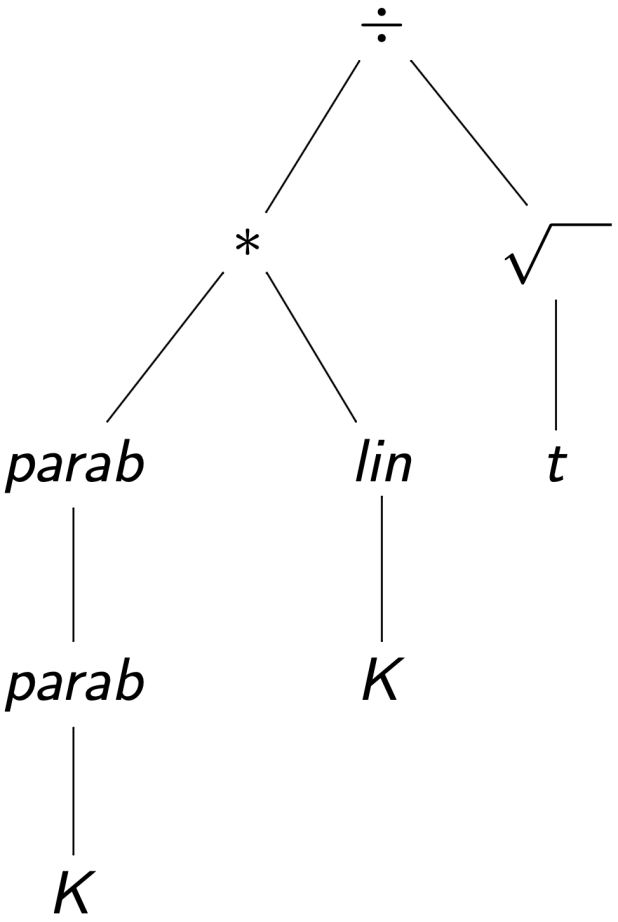
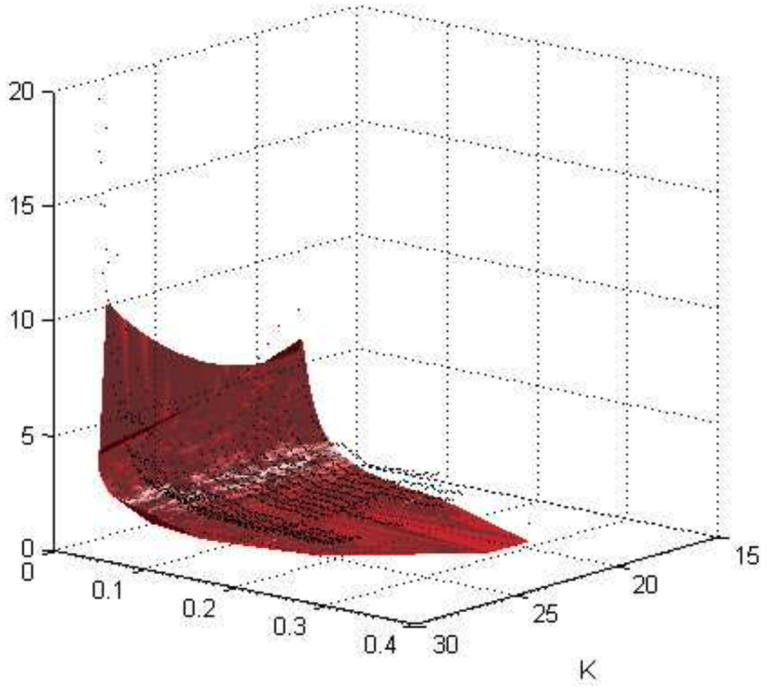
High variance and high co-variance in time series

Dynamic graph reflects dependencies between the time series.



To reconstruct the dependencies

1. Reconstruct phase trajectories through time-delay embedding.
2. Define distance between points of the phase trajectories.
3. Make low-rank decomposition, prune the dependency graph.
4. Reconstruct time series.

Causal discovery for syblolic regression modeling

$$\sigma = \frac{(w_1 K + w_2)(w_1 K^2 + w_2 K + w_3)}{\sqrt{t}}$$