

# Bayesian Methods for System Identification

Optimisation and Machine Learning in Process Systems Engineering

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Linear Regression

Ridge Regression

Extension to Gaussian processes

Stable Spline Kernel

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# System Identification

## Introduction

### Problem Statement

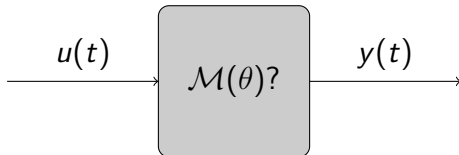
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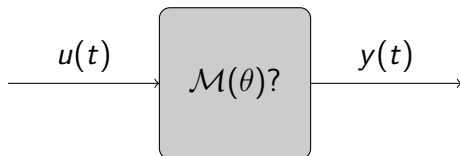


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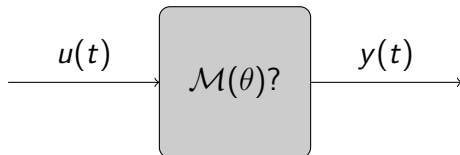
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$$y(t) = \overbrace{\theta_1 u(t)}^{\text{Linear model}} + \theta_2$$

$$y(t) = \underbrace{\theta_1 u(t)^n + \theta_2 u(t)^{n-1} + \dots + \theta_n}_{\text{n-th degree polynomial model}}$$

# System Identification

## Finite Impulse Response (FIR) Model



# System Identification

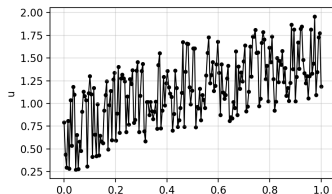
## Finite Impulse Response (FIR) Model

Given a time series of inputs  $u_0, u_1, u_2, \dots, u_k$  and outputs  $y_0, y_1, y_2, \dots, y_{k-1}$ , how to predict  $y_k$ ?

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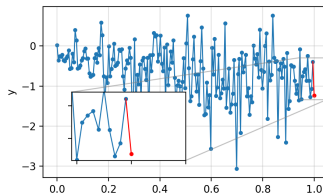
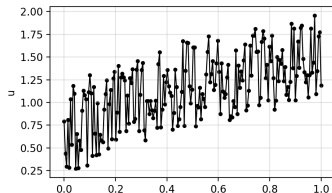
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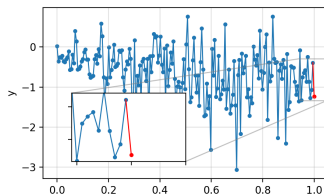
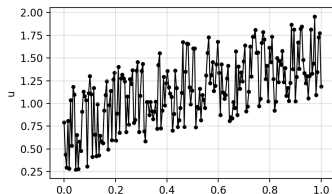
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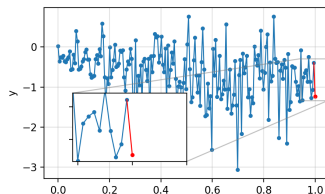
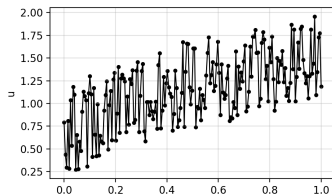


$$y_k = \theta_0 u_k + \theta_1 u_{k-1} + \dots + \theta_N u_{k-N} = \sum_{i=0}^N \theta_i \cdot u_{k-i}$$

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$$y_k = \theta_0 u_k + \theta_1 u_{k-1} + \dots + \theta_K u_{k-K} = \sum_{i=0}^K \theta_i \cdot u_{k-i}$$

Since the order  $K$  is finite, response is bounded and stable for a bounded input: bounded input, bounded output (BIBO).

# System Identification

Impulse Signal (Dirac delta function)

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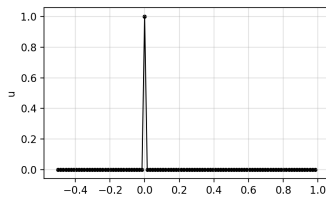
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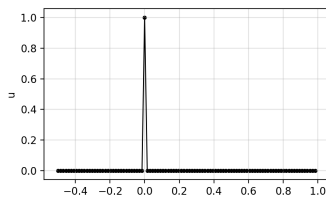
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Using our previous FIR model, consider the moving horizon of  $K$  time-steps it is clear that eventually the output  $y$  will eventually become 0 as  $t > K$ , hence finite.

# System Identification

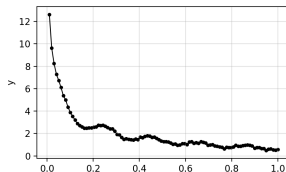
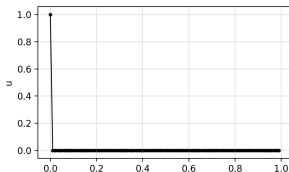
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What does the impulse response look like? For a stable system...

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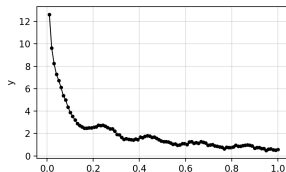
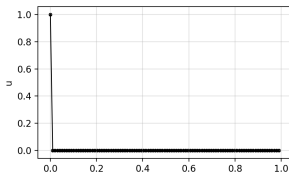
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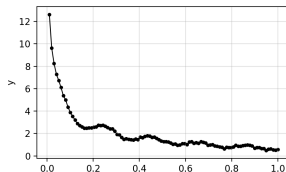
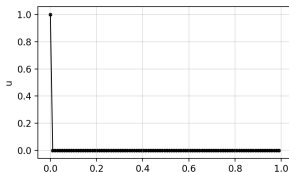


$$y_k = \theta_0 u_k + \theta_1 u_{k-1} + \dots + \theta_K u_{k-K}$$

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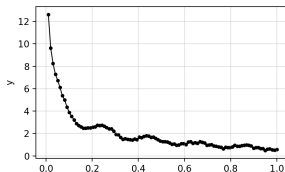
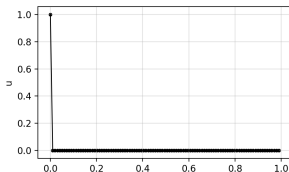
$$y_k = \theta_0 u_k + \theta_1 u_{k-1} + \dots + \theta_K u_{n-N}$$

$$y_K = \theta_0 \cdot 0 + \theta_1 \cdot 0 + \dots + \theta_{K-1} \cdot 0 + \theta_K \cdot 1$$

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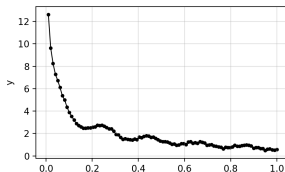
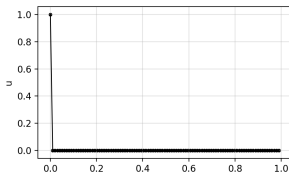
$$y_k = \theta_0 u_k + \theta_1 u_{k-1} + \dots + \theta_K u_{n-N}$$

$$y_{K-1} = \theta_0 \cdot 0 + \theta_1 \cdot 0 + \dots + \theta_{K-1} \cdot 1 + \theta_K \cdot 0$$

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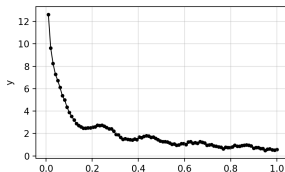
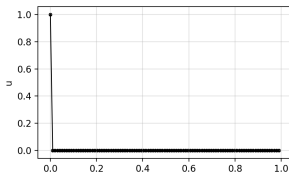
$$y_1 = \theta_0 \cdot 0 + \theta_1 \cdot 1 + \dots + \theta_{K-1} \cdot 0 + \theta_K \cdot 0$$



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What does the impulse response look like? For a stable system...



$$y_k = \theta_0 u_k + \theta_1 u_{k-1} + \dots + \theta_K u_{k-K}$$

$$y_0 = \theta_0 \cdot 1 + \theta_1 \cdot 0 + \dots + \theta_{K-1} \cdot 0 + \theta_K \cdot 0$$

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- ▶ The parameters  $\theta$  of our FIR model can be seen as the outputs of the system if subjected to an impulse signal  $\rightarrow$  predicting the impulse response.
- ▶ Useful as if you wanted to find out model parameters you just have to 'kick' the system and observe the response.
- ▶ What if we can't 'kick' the system?

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# Linear Regression

N observations, K inputs:

Given input matrix  $\mathbf{U} \in \mathbb{R}^{N \times K}$  and outputs  $\mathbf{y} \in \mathbb{R}^{N \times 1}$  along with a model  $\mathcal{M}$  in the form  $y = \mathbf{u}\theta^T$  where  $\theta \in \mathbb{R}^{K \times 1}$ :

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The diagram illustrates the dimensions of the matrices involved in the linear regression model. It consists of three parts: 1. A large square bracket representing the input matrix  $\mathbf{U}$ . To its left is a vertical double-headed arrow labeled  $N$ , indicating the number of rows (observations). Above the bracket is a horizontal double-headed arrow labeled  $K$ , indicating the number of columns (inputs). The letter  $\mathbf{U}$  is centered inside the bracket. 2. A smaller square bracket representing the output vector  $\mathbf{y}$ . To its left is a vertical double-headed arrow labeled  $N$ . Above the bracket is a horizontal double-headed arrow labeled  $1$ . The letter  $\mathbf{y}$  is centered inside the bracket. 3. A square bracket representing the parameter vector  $\theta$ . To its left is a vertical double-headed arrow labeled  $K$ . Above the bracket is a horizontal double-headed arrow labeled  $1$ . The letter  $\theta$  is centered inside the bracket.

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The diagram illustrates the dimensions of the matrices involved in linear regression. It consists of three parts: 1. A large square bracket representing matrix  $\mathbf{U}$ . To its left is a vertical double-headed arrow labeled  $N$ , indicating the number of rows (observations). Above the bracket is a horizontal double-headed arrow labeled  $K$ , indicating the number of columns (inputs). The letter  $\mathbf{U}$  is centered inside the bracket. 2. A second, smaller square bracket representing the output vector  $\mathbf{y}$ . To its left is a vertical double-headed arrow labeled  $N$ . Above the bracket is a horizontal double-headed arrow labeled  $1$ . The letter  $\mathbf{y}$  is centered inside the bracket. 3. A third, even smaller square bracket representing the parameter vector  $\theta$ . To its left is a vertical double-headed arrow labeled  $K$ . Above the bracket is a horizontal double-headed arrow labeled  $1$ . The letter  $\theta$  is centered inside the bracket.

Formulating the problem as least squares...

$$\hat{\theta} = \arg \min_{\theta} \|\mathbf{y} - \mathbf{U}\theta\|^2$$

# Linear Regression

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The diagram illustrates the dimensions of the matrices involved in linear regression. It shows three vertical column matrices. The first matrix is labeled  $\mathbf{U}$  and has a vertical double-headed arrow to its left labeled  $N$  and a horizontal arrow above it labeled  $K$ . The second matrix is labeled  $\mathbf{y}$  and has a vertical double-headed arrow to its left labeled  $N$  and a horizontal arrow above it labeled  $1$ . The third matrix is labeled  $\theta$  and has a vertical double-headed arrow to its left labeled  $K$  and a horizontal arrow above it labeled  $1$ .

Formulating the problem as least squares...

$$\hat{\theta} = \arg \min_{\theta} \|\mathbf{y} - \mathbf{U}\theta\|^2$$

Analytical solution of:

$$\hat{\theta} = (\mathbf{U}^T \mathbf{U})^{-1} \mathbf{U}^T \mathbf{y}$$

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$$\begin{array}{ccc} \xrightarrow{K} & \xrightarrow{1} & \xrightarrow{1} \\ \begin{array}{c} N \\ \downarrow \end{array} \left[ \begin{array}{c} \mathbf{U} \end{array} \right] & \begin{array}{c} N \\ \downarrow \end{array} \left[ \begin{array}{c} \mathbf{y} \end{array} \right] & \begin{array}{c} K \\ \downarrow \end{array} \left[ \begin{array}{c} \theta \end{array} \right] \end{array}$$

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What about bias vs variance?  $\rightarrow$  Needs to be considered in linear regression.

# Linear Regression

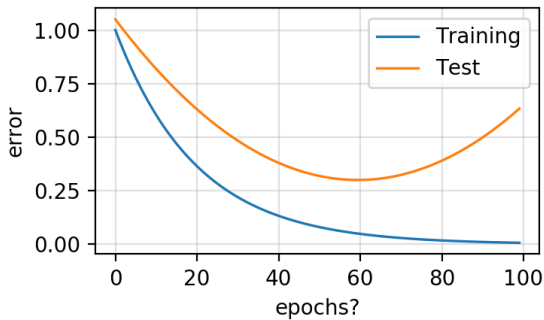
Trading off bias / variance.

For neural networks...

# Linear Regression

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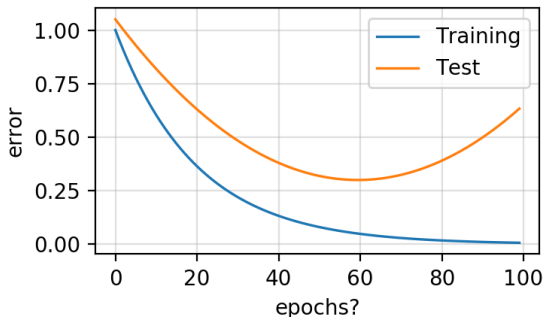
For neural networks...



# Linear Regression

Trading off bias / variance.

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What is the equivalent of epochs for a model with analytical parameters?

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# Ridge Regression

Regularisation technique

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Regularisation technique

$$\hat{\theta} = \arg \min_{\theta} ||\mathbf{y} - \mathbf{U}\theta||^2$$

# Ridge Regression

Regularisation technique

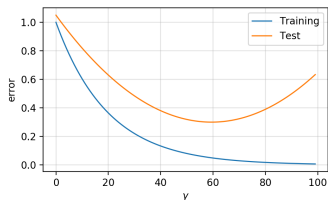
$$\hat{\theta} = \arg \min_{\theta} ||\mathbf{y} - \mathbf{U}\theta||^2 + \underbrace{\gamma ||\theta||^2}_{\text{Ridge term}}$$

# Ridge Regression

Regularisation technique

$$\hat{\theta} = \arg \min_{\theta} ||\mathbf{y} - \mathbf{U}\theta||^2 + \underbrace{\gamma ||\theta||^2}_{\text{Ridge term}}$$

By varying  $\gamma$ , bias and variance can be traded off.



For any  $\gamma$ , analytical solution of  $\hat{\theta} = (\mathbf{U}^T \mathbf{U} + \gamma \mathbf{I})^{-1} \mathbf{U}^T \mathbf{y}$

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What if instead of the identity matrix we used some other matrix?

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# Extension to Gaussian processes

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What if instead of the identity matrix we used some other matrix?

$$\arg \min_{\theta} ||\mathbf{y} - \mathbf{U}\theta||^2 + \gamma \theta^T \mathbf{K}^{-1} \theta$$

This has an analytical solution of:

$$\hat{\theta} = (\mathbf{K}\mathbf{U}^T\mathbf{U} + \gamma \mathbf{I}_K)^{-1} \mathbf{K}\mathbf{U}^T \mathbf{y}$$

# Extension to Gaussian processes

$$\hat{\theta} = \underbrace{(K\mathbf{U}^T\mathbf{U} + \gamma I_K)^{-1}K\mathbf{U}^T\mathbf{y}}_{\text{regularised least squares estimate}}$$

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$$\hat{\theta} = \underbrace{(K\mathbf{U}^T\mathbf{U} + \gamma I_K)^{-1}K\mathbf{U}^T\mathbf{y}}_{\text{regularised least squares estimate}}$$

For jointly Gaussian variables ( $\theta \sim \mathcal{N}(0, K)$ ,  $\mathbf{e}_y \sim \mathcal{N}(0, \sigma)$ )

$$\begin{bmatrix} \theta \\ \mathbf{y} \end{bmatrix} \sim \mathcal{N} \left( \begin{bmatrix} 0 \\ 0 \end{bmatrix}, \begin{bmatrix} K & K\mathbf{U}^T \\ \mathbf{U}K & \mathbf{U}K\mathbf{U}^T + \sigma^2 I_N \end{bmatrix} \right)$$

# Extension to Gaussian processes

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The posterior distribution of  $\theta$  given  $\mathbf{y}$  is given as:

$$\theta|\mathbf{y} \sim \mathcal{N}(\hat{\theta}, K^*)$$

# Extension to Gaussian processes

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The posterior distribution of  $\theta$  given  $\mathbf{y}$  is given as:

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$$\hat{\theta} = \underbrace{(K\mathbf{U}^T\mathbf{U} + \sigma^2 I_N)^{-1}K\mathbf{U}^T\mathbf{y}}_{\text{Posterior distribution of } \theta}$$

# Extension to Gaussian processes

$$\underbrace{(K\mathbf{U}^T\mathbf{U} + \gamma I_K)^{-1}K\mathbf{U}^T\mathbf{y}}_{\text{kernel-regularised least squares estimate}} \quad \underbrace{(K\mathbf{U}^T\mathbf{U} + \sigma^2 I_N)^{-1}K\mathbf{U}^T\mathbf{y}}_{\text{Posterior distribution of } \theta}$$

# Extension to Gaussian processes

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They're equivalent! What does this mean?



# Extension to Gaussian processes

$$\underbrace{(K\mathbf{U}^T\mathbf{U} + \gamma I_K)^{-1}K\mathbf{U}^T\mathbf{y}}_{\text{kernel-regularised least squares estimate}} \quad \underbrace{(K\mathbf{U}^T\mathbf{U} + \sigma^2 I_N)^{-1}K\mathbf{U}^T\mathbf{y}}_{\text{Posterior distribution of } \theta}$$

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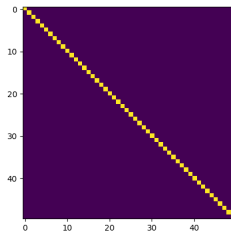
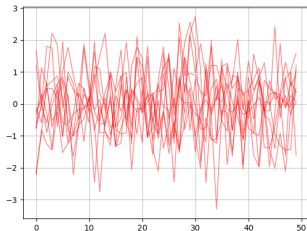
- ▶ Ridge regression and Gaussian processes are equivalent when the covariance matrix  $= I$ . e.g. when prior samples look like this...

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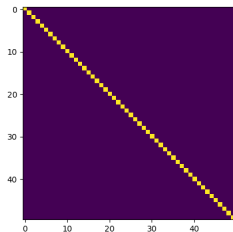
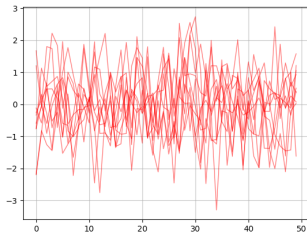
- Ridge regression and Gaussian processes are equivalent when the covariance matrix =  $I$ . e.g. when prior samples look like this...



# Extension to Gaussian processes

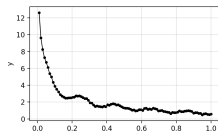
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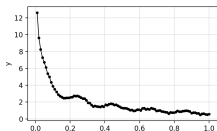
- ▶ Now we can look at this system identification problem from a Bayesian point of view; can we fully embrace the framework and incorporate prior knowledge into our prediction of  $\hat{\theta}$ ?

# Extension to Gaussian processes

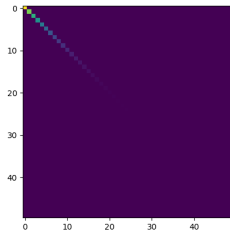
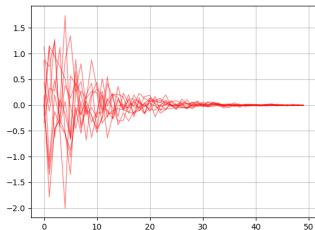


Instead of doing Ridge regression (i.e. using the identity prior) or some other covariance function (i.e. squared exponential) what about if we let it decay exponentially?

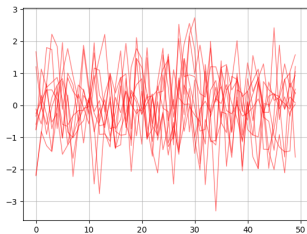
# Extension to Gaussian processes



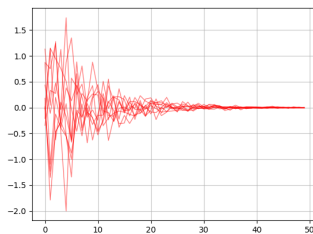
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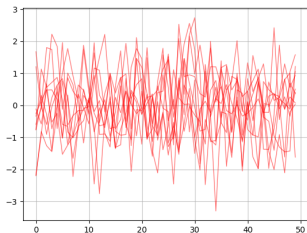


$$K_{ij} = \delta_{ij}$$

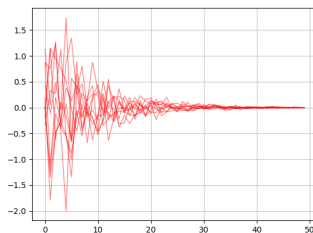


$$K_{ij} = \alpha^i \delta_{ij}$$

# Extension to Gaussian processes



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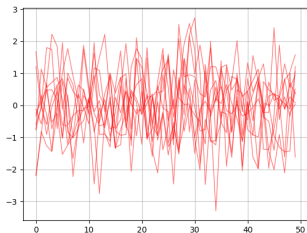


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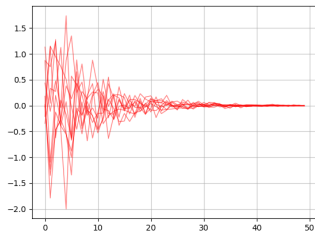
Remaining issue:

Each neighbouring value of  $\theta$ , i.e.  $\theta_1, \theta_2 \dots$  is uncorrelated (off diagonal terms in the covariance matrix are all 0)  $\rightarrow$  non-smooth.

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This is a false assumption!



# Table of Contents

System Identification

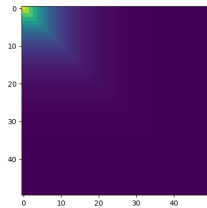
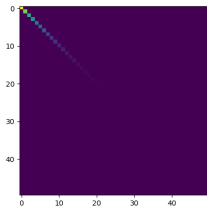
Linear Regression

Ridge Regression

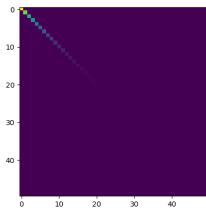
Extension to Gaussian processes

Stable Spline Kernel

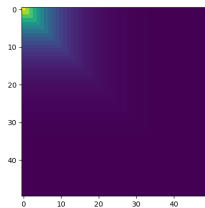
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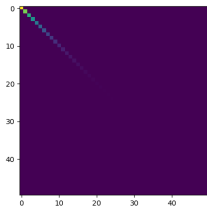


$$K_{ij} = \alpha^i \delta_{ij}$$

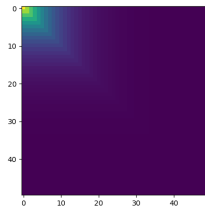


$$K_{ij} = \alpha^{\max(i,j)}$$

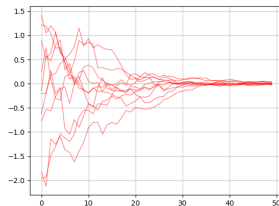
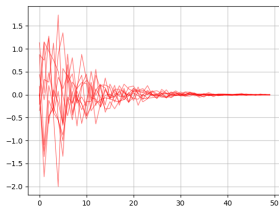
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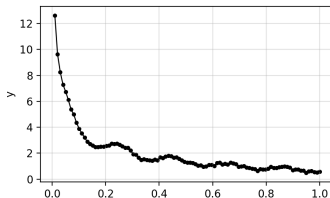
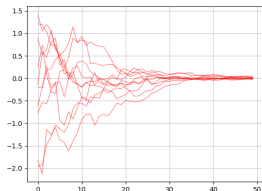
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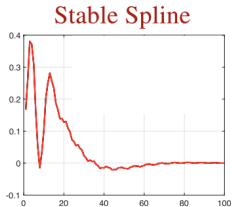
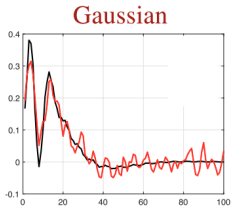
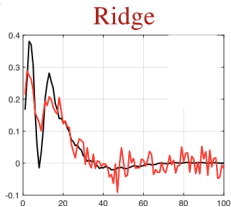
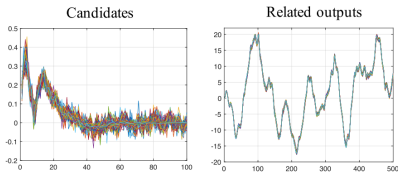
Can also extend the estimation of the parameter vector to continuous time. Continuous system identification  $\rightarrow$  function approximation using an informative prior.





# Results

100 different impulse responses generated, with a single 'true' response. Note how the predicted outputs with each impulse response varies by very little.



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- ▶ Regularised linear regression and Gaussian processes inherently linked
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- ▶ Continuous system identification enabled using GPs as a function approximator.

# Thanks!

# References

- ▶ Pillonetto, G., Dinuzzo, F., Chen, T., De Nicolao, G., & Ljung, L. (2014). Kernel methods in system identification, machine learning and function estimation: A survey. Automatica, 50(3), 657–682. <https://doi.org/10.1016/j.automatica.2014.01.001>
- ▶ Pillonetto, G. (n.d.). REGULARIZED KERNEL-BASED APPROACHES TO SYSTEM IDENTIFICATION. Retrieved from [https://www.google.com/url?sa=t&rct=j&q=&esrc=s&source=web&cd=&cad=rja&uact=8&ved=2ahUKEwjWse28\\_Y3sAhUKSxUIHXVNCW0QFjABegQIARAB&url=https%3A%2F%2Fwww.kth.se%2Fsocial%2Ffiles%2F5b716a5b56be5bd565e07e4f%2Fgianluigi\\_pillonetto\\_sysid2018.pdf&usg=AOvVaw2uRQRyV2Tb9jo3l04T06zj](https://www.google.com/url?sa=t&rct=j&q=&esrc=s&source=web&cd=&cad=rja&uact=8&ved=2ahUKEwjWse28_Y3sAhUKSxUIHXVNCW0QFjABegQIARAB&url=https%3A%2F%2Fwww.kth.se%2Fsocial%2Ffiles%2F5b716a5b56be5bd565e07e4f%2Fgianluigi_pillonetto_sysid2018.pdf&usg=AOvVaw2uRQRyV2Tb9jo3l04T06zj)