Introduction to Uncertainty Quantification (UQ)

Saleh Rezaeiravesh

salehr@kth.se

FLOW Winter School on Machine Learning and Data-Driven Methods

HANDS-ON, LSE

Frequentist's View - Example

- **Damped Harmonic Oscillator**

$$\begin{cases} \ddot{y} + C\dot{y} + Ky = 0, \\ y(0) = y_0,\ \dot{y}(0) = v_0 \end{cases}$$

$$y(t) = e^{-\frac{c}{2}t}\left(c_1 \cos \omega t + c_2 \sin \omega t\right)$$

$$\omega = \sqrt{K - C^2/4},\ c_1 = y_0,\ c_2 = (v_0 + cy_0/2)/\omega$$

Synthetic Data:

$$\begin{cases} Y_{\text{obs}_i} = f(t_i, C_0, K_0) + \varepsilon_i, \quad i = 1, 2 \cdots, n \\ \varepsilon_i \sim \mathcal{N}(0, \sigma_0^2) \end{cases}$$

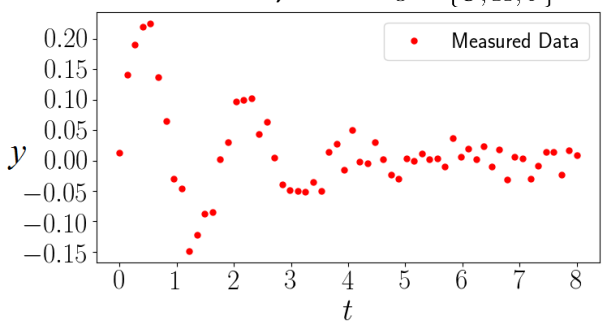
$$n = 60$$

$$t \in [0, 8]$$

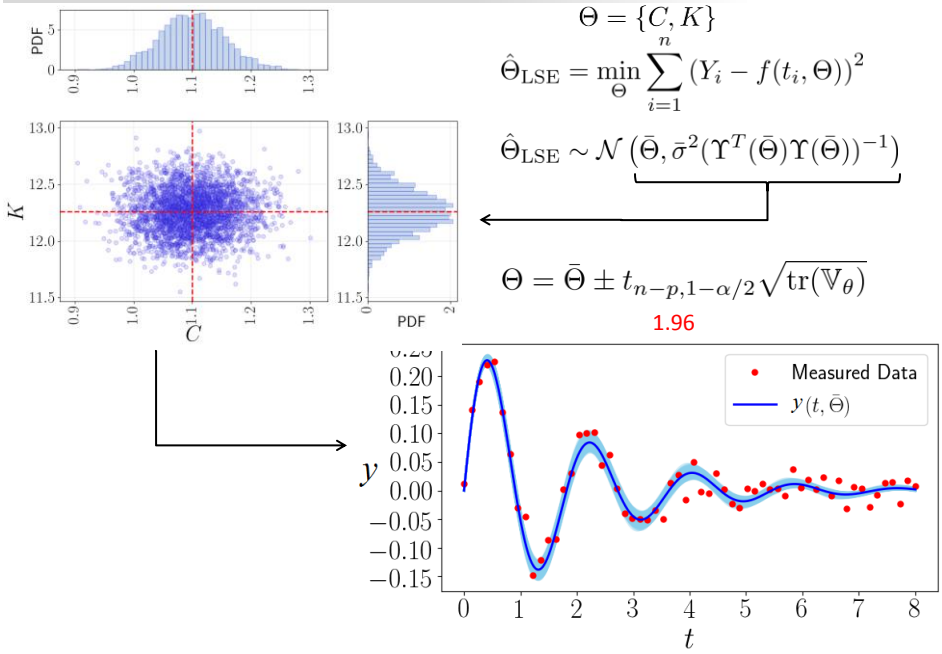
$$x_0 = 0\,, v_0 = 1$$

$$\begin{cases} C_0 = 1 \\ K_0 = 12 \\ \sigma_0 = 0.02 \end{cases}$$

- **Given observations, estimate** $\Theta = \{C, K, \sigma\}$



Frequentist's View - Example



$$\Theta = \{C, K\}$$

$$\hat{\Theta}_{\text{LSE}} = \min_{\Theta} \sum_{i=1}^{n} (Y_i - f(t_i, \Theta))^2$$

$$\hat{\Theta}_{\text{LSE}} \sim \mathcal{N}\left(\bar{\Theta}, \bar{\sigma}^2 (\Upsilon^T(\bar{\Theta})\Upsilon(\bar{\Theta}))^{-1}\right)$$

$$\Theta = \bar{\Theta} \pm t_{n-p,1-\alpha/2}\sqrt{\text{tr}(\mathbb{V}_\theta)}$$

1.96

Warm-up Task

- We have mean ($\bar{\Theta}$) and covariance matrices ($\mathbb{V}_\Theta$) of the parameters $\Theta = \{C, K\}$ estimated by LSE.

Task: Construct 95% confidence interval for these parameters.

$$\Theta = \bar{\Theta} \pm t_{n-p,1-\alpha/2}\sqrt{\text{tr}(\mathbb{V}_\theta)}$$

1.96