# Introduction to Uncertainty Quantification (UQ)

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**FLOW Winter School on Machine Learning and Data-Driven Methods**

## HANDS-ON, LSE

https://github.com/salrm8/UQcourse_HandsOn.git

## Frequentist's View - Example

- **Damped Harmonic Oscillator**

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

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

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

**Synthetic Data:**

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

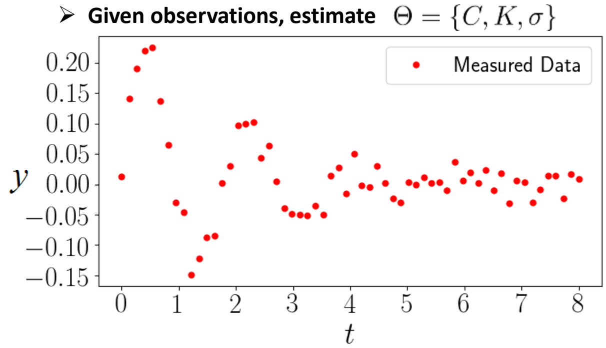
$$n = 60$$

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

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

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

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



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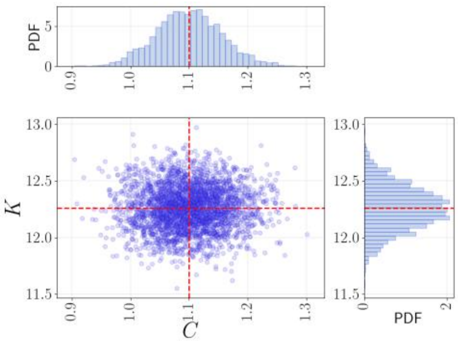


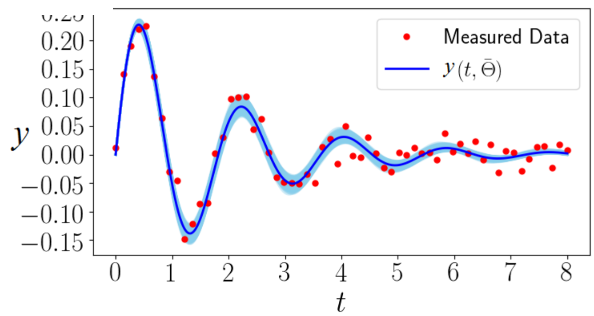

$$\Theta = \{C, K\}$$

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

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

$$\Theta_i = \bar{\Theta}_i \pm t_{n-p,1-\alpha/2} \sqrt{[\mathbb{V}_\Theta]_{ii}}$$

$$i = 1, 2$$




# 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.

$$\Theta_i = \bar{\Theta}_i \pm \underbrace{t_{n-p,1-\alpha/2}}_{1.96} \sqrt{[\mathbb{V}_\Theta]_{ii}}\,, \quad i = 1, 2$$

(for 95% confidence)