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A data-driven surrogate model
for uncertainty quantification of
dynamical systems

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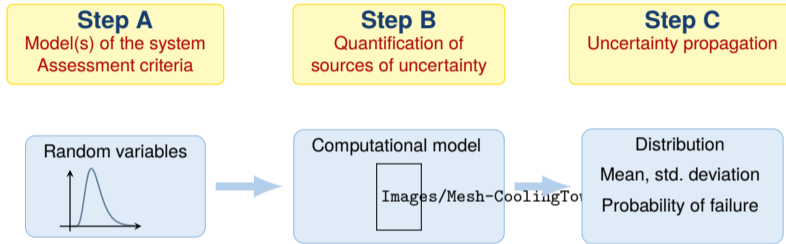
Outline

1. Problem statement
2. Surrogate models for dynamical systems
3. Case study

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Global framework for uncertainty quantification



Sudret, B. Uncertainty propagation and sensitivity analysis in mechanical models. Habilitation à diriger des recherches, 2007.

- ▶ Requires many evaluations of the **costly computational model**
- ▶ Solution: replace the computational model with a **cheap-to-evaluate surrogate**

Problem setup

Static system

- ▶ The surrogate is build from **experimental design** inputs

$$\mathcal{X} = \{\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(N_{ED})}\}$$

and corresponding model outputs

$$\mathcal{Y} = \{\mathbf{y}^{(1)}, \dots, \mathbf{y}^{(N_{ED})}\}$$

- ▶ Typically, the surrogate maps a set of **scalar inputs** to one or more **scalar quantities of interest** (outputs)

$$\tilde{\mathcal{M}} : \mathcal{D}_{\mathbf{x}} \subset \mathbb{R}^M \rightarrow \mathbb{R}$$

Dynamical system

- ▶ System has **time-dependent** exogenous **inputs and output**

$$\mathbf{x} : \mathcal{T} \rightarrow \mathbb{R}^M \text{ and } \mathbf{y} : \mathcal{T} \rightarrow \mathbb{R}$$

that evolve along a time axis

$$\mathcal{T} = \{0, \delta t, 2\delta t, \dots, N\delta t\}$$

- ▶ The surrogate predicts the output at time t based on the input up to and including time t

$$\mathbf{y}(t) = \mathcal{M}(\mathbf{x}(\mathcal{T} \leq t)) \approx \tilde{\mathcal{M}}(\mathbf{x}(\mathcal{T} \leq t))$$

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Surrogate models for dynamical systems

Dynamical systems can often be modelled using **AutoRegressive with eXogenous inputs** (ARX) models

- ▶ Autoregressive: model uses its own past predictions
- ▶ Exogenous input: excitation that governs the system response

Images/narx.png

We denote such models as:

$$y(t) = \mathcal{M}(\varphi(t), \mathbf{c})$$

- ▶ $\varphi(t) \in \mathbb{R}^{M_\varphi}$: **gathers** the exogenous **inputs** and system **output** at different time steps
- ▶ \mathbf{c} : finite set of model parameters, e.g. regression coefficients or weights

Calibrating an ARX model

Building an ARX model can be cast into ordinary **regression problem** $\mathbf{y} = \tilde{\mathcal{M}}(\Phi, \mathbf{c})$ with regression matrix Φ and output vector \mathbf{y} :

$$\Phi = \begin{pmatrix} \varphi(t_0) \\ \varphi(t_0 + \delta t) \\ \vdots \\ \varphi((N-1)\delta t) \end{pmatrix}, \quad \mathbf{y} = \begin{pmatrix} \mathbf{y}(t_0) \\ \mathbf{y}(t_0 + \delta t) \\ \vdots \\ \mathbf{y}((N-1)\delta t) \end{pmatrix},$$

where each row $\varphi(\bullet)$ reads

$$\begin{aligned} \varphi(t) = & \{ \mathbf{y}(t - \ell_1^y), \mathbf{y}(t - \ell_2^y), \dots, \mathbf{y}(t - \ell_{n_y}^y), \\ & x_1(t - \ell_1^{x_1}), x_1(t - \ell_2^{x_1}), \dots, x_1(t - \ell_{n_{x_1}}^{x_1}), \\ & x_2(t - \ell_1^{x_2}), x_2(t - \ell_2^{x_2}), \dots, x_2(t - \ell_{n_{x_2}}^{x_2}), \\ & \dots, \\ & x_M(t - \ell_1^{x_M}), x_M(t - \ell_2^{x_M}), \dots, x_M(t - \ell_{n_{x_M}}^{x_M}) \} \end{aligned}$$

- ▶ System response $\mathbf{y} \in \mathbb{R}^N$
- ▶ Exogenous input $\mathbf{x} \in \mathbb{R}^{N \times M}$
- ▶ Autoregressive lags
 $\ell_i^y \in \{\delta t, 2\delta t, \dots, (N-1)\delta t\}$
- ▶ Exogenous input lags
 $\ell_i^{x_j} \in \{\mathbf{0}, \delta t, \dots, (N-1)\delta t\}$

Challenges with ARX models

Only one timestep at a time:

$$\hat{y}(t) = \hat{\mathcal{M}}(\mathbf{x}(\mathcal{T} \leq t), \hat{y}(\mathcal{T} < t))$$

- ▶ **past predictions** $\hat{y}(\mathcal{T} < t)$
- ▶ **exogenous input** $\mathbf{x}(\mathcal{T} \leq t)$

Main difficulties

1. **Curse of dimensionality**
2. Control systems making the response **non-smooth**
3. Dampers, nonlinear springs and coupling introducing **nonlinearities**

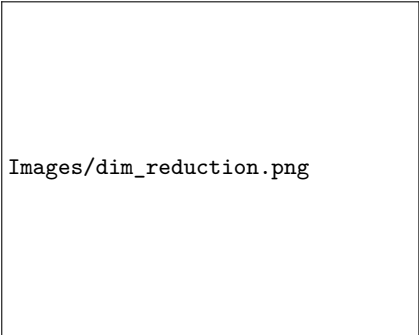
Dealing with high-dimensional exogenous inputs

Reduce dimensionality of the system excitation x along **non-temporal coordinates**:

$$\tilde{x} = \mathcal{G}(x)$$

where $x \in \mathbb{R}^{N \times M}$ and $\tilde{x} \in \mathbb{R}^{N \times m}$ such that $m \ll M$

- ▶ **Original time scale** \mathcal{T} is preserved
- ▶ Wide array of methods available, e.g.:
 - n-dimensional discrete cosine transform
 - principal component analysis
 - (deep) autoencoders



Images/dim_reduction.png

Dealing with complex dynamical systems

- ▶ Building a surrogate solely on the **original exogenous input** $\mathbf{x} \in \mathbb{R}^{N \times M}$ input can be suboptimal:

$$\tilde{\mathcal{M}} : \mathbf{x}(\mathcal{T} \leq t) \rightarrow \mathbf{y}(t)$$

- ▶ A **more informative set of features** $\zeta \in \mathbb{R}^{N \times M_\zeta}$ can simplify the mapping to \mathbf{y} :

$$\tilde{\mathcal{M}} : \zeta(\mathcal{T} \leq t) \rightarrow \mathbf{y}(t) \text{ where } \zeta = \mathcal{F}(\mathbf{x})$$

- ▶ The feature set ζ :
 - does not necessarily have a reduced dimensionality (i.e. $M_\zeta > M$)
 - can and should incorporate prior knowledge about the system

How can we construct and select these features?

Construction of auxiliary quantities

Auxiliary quantities z_i are constructed incrementally by applying any transform \mathcal{F}_i :

$$z_1(t) = \mathcal{F}_1(\mathbf{x}(\mathcal{T} \leq t), z_1(\mathcal{T} < t))$$

$$z_2(t) = \mathcal{F}_2(z_1(\mathcal{T} \leq t), \mathbf{x}(\mathcal{T} \leq t), z_2(\mathcal{T} < t))$$

⋮

$$z_i(t) = \mathcal{F}_i(z_1(\mathcal{T} \leq t), \dots, z_{i-1}(\mathcal{T} \leq t), \mathbf{x}(\mathcal{T} \leq t), z_i(\mathcal{T} < t))$$

$$\tilde{\mathcal{M}} : \zeta(\mathcal{T} \leq t) \rightarrow y(t) \text{ where } \zeta = \{\mathbf{x}, z_1, \dots, z_i\}$$

- ▶ Transform \mathcal{F}_i can be an ARX model
- ▶ An auxiliary quantity can depend on other auxiliary quantities
- ▶ Possible auxiliary quantities are e.g.:
 - control system outputs
 - moving averages, integrals/derivates

Images/auxiliary_quantities.png

Automatic selection of auxiliary quantities

Function `SelectFeatures(\tilde{x}, z, y)`

```
 $\zeta \leftarrow \{\}, \tilde{y} \leftarrow y$   
while  $\tilde{x} \neq \{\}$  or  $z \neq \{\}$  do  
   $\rho \leftarrow \text{Correlate}(\{\tilde{x}, z\}, \tilde{y})$   
  if  $\max(|\rho|) < \theta$  then  
    break  
   $\zeta_i \leftarrow \arg \max(|\rho|)$   
  if  $\zeta_i \in \tilde{x}$  then  
     $\zeta \leftarrow \{\zeta, \zeta_i\}$   
     $\tilde{x} \leftarrow \tilde{x} \setminus \zeta_i$   
  else if  $\zeta_i \in z$  then  
     $\zeta' \leftarrow \text{SelectFeatures}(\{\tilde{x}, \zeta\}, z \setminus \zeta_i, \zeta_i)$   
     $\tilde{x} \leftarrow \{\tilde{x}, z \cap \zeta'\}$   
     $z \leftarrow z \setminus z \cap \zeta'$   
     $\zeta \leftarrow \{\zeta, \zeta_i\}$   
     $z \leftarrow z \setminus \zeta_i$   
   $\tilde{y} \leftarrow y - \tilde{\mathcal{M}}(\zeta)$   
return  $\zeta$ 
```

- ▶ \tilde{x} : features only depending on exogenous input
- ▶ z : auxiliary quantities
- ▶ y : system response
- ▶ ζ : selected features
- ▶ ρ : measure of association, e.g Kendall's tau
- ▶ θ : minimum correlation to stop algorithm
- ▶ $\tilde{\mathcal{M}}$: ARX model

$$\rho(\mathbf{x}_i, \mathbf{y}) = \frac{2}{n(n-1)} \sum_{k < \ell} \text{sgn}(x_{i,k} - x_{i,\ell}) \text{sgn}(y_k - y_\ell)$$

Function `Correlate(x, y)`

```
 $\rho \leftarrow \{\}$   
for  $x_i \leftarrow x_1, \dots, x_M$  do  
   $\rho \leftarrow \{\rho, \text{KendallTau}(x_i, y)\}$   
return  $\rho$ 
```

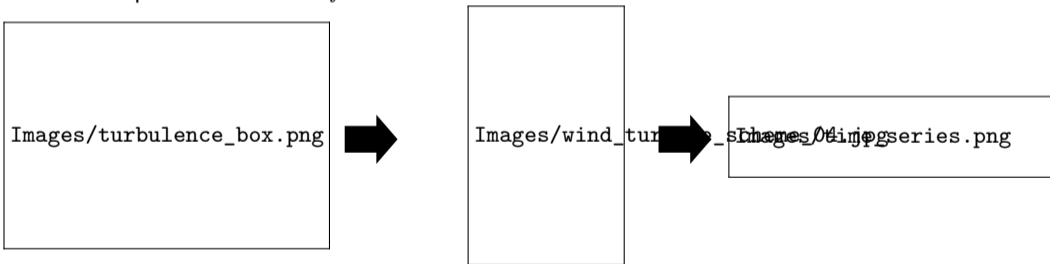
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Case study - aero-servo-elastic simulation of a wind turbine

- ▶ Input **turbulence box** $v : \mathcal{T} \rightarrow \mathbb{R}^{\nu_w \times \nu_y \times \nu_z}$
 - Discrete time axis $\mathcal{T} = \{0, \delta t, 2\delta t, \dots, N\delta t\}$
 - Wind speed components ν_w
 - Discrete spatial grid $\nu_y \times \nu_z$
- ▶ Response **time series** $f : \mathcal{T} \rightarrow \mathbb{R}$

Find a surrogate $\tilde{\mathcal{M}}$ for the
aero-servo-elastic wind turbine
simulator \mathcal{M} :
 $f(t) = \mathcal{M}(v(\mathcal{T} \leq t)) \approx \tilde{\mathcal{M}}(v(\mathcal{T} \leq t))$



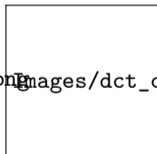
Dimensionality reduction

- ▶ Only dominant **longitudinal wind speed component** v_x is kept
- ▶ Decompose each slice $v_x(t)$ into its spectral coefficients $\xi_{i,j}(t)$ using the **2-dimensional discrete cosine transform**
- ▶ Dimensionality is reduced by choosing $n_i < \nu_y$ and $n_j < \nu_z$

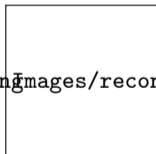
$$v_x^{\kappa,\ell}(t) = \sum_{i=0}^{n_i-1} \sum_{j=0}^{n_j-1} \xi_{i,j}(t) \cos \left[\frac{\pi}{n_i} \left(\kappa + \frac{1}{2} \right) i \right] \cos \left[\frac{\pi}{n_j} \left(\ell + \frac{1}{2} \right) j \right]$$



Original frame
 $v_x(t = t^*)$



Spectral coefficients
 $\log |\xi(t = t^*)|$



Reconstructed frame
 $\tilde{v}_x(t = t^*)$



Time-dependent spectral coefficients

Feature selection

- ▶ Quantity of interest: **Power output P**
- ▶ Pool of **features**
 - Spectral coefficients $\xi_{0,0}, \dots, \xi_{6,6}$
 - Blade pitch ϕ
 - Rotor speed ω
- ▶ Stopping criterion: $\rho < \theta = 0.05$
- ▶ Using **Polynomial NARX model**:

$$y(t) = \sum_{\alpha \in \mathcal{A}} c_{\alpha} \mathcal{P}_{\alpha}(\varphi(t))$$

where

$$\mathcal{P}_{\alpha}(\varphi(t)) = \prod_{i=1}^{M_{\varphi}} \varphi_i(t)^{\alpha_i}$$

Power output P

Images/feature_selection_GenPwr.png

Rotor speed ω

Images/feature_selection_RotSpeed.png

Blade pitch ϕ

Images/feature_selection_BldPitch1.png

Results - Blade pitch

Auxiliary quantity

$$\hat{\phi}(t) = \tilde{\mathcal{M}}(\xi(\mathcal{T} \leq t), \hat{\phi}(\mathcal{T} < t))$$

- ▶ Root-mean-squared (RMSE) error on the **out-of-sample validation dataset**
- ▶ Simulation with **lowest** and **highest** RMSE
- ▶ Surrogate shows high accuracy
- ▶ Surrogate is slightly less responsive than the turbine controller

Images/BldPitch1_RMSE.png

Images/BldPitch1_trace_low_rmse.png

Images/BldPitch1_trace_high_rmse.png

Results - Rotor speed

Auxiliary quantity

$$\hat{\omega}(t) = \tilde{\mathcal{M}}(\xi(\mathcal{T} \leq t), \hat{\phi}(\mathcal{T} \leq t), \hat{\omega}(\mathcal{T} < t))$$

- ▶ Surrogate shows high accuracy
- ▶ Prediction is missing very high-frequency components
- ▶ **Prediction remains stable** also when relying on the blade pitch prediction

Images/RotSpeed_RMSE.png

Images/RotSpeed_trace_low_rmse.png

Images/RotSpeed_trace_high_rmse.png

Results - Generator power

Quantity of interest

$$\hat{P}(t) = \tilde{\mathcal{M}}(\xi(\mathcal{T} \leq t), \hat{\phi}(\mathcal{T} \leq t), \hat{\omega}(\mathcal{T} \leq t), \hat{P}(\mathcal{T} < t))$$

- ▶ Surrogate tends to slightly overestimate power output (< 2 % in average)
- ▶ Sharp dips are not captured well by the surrogate
- ▶ Accurate surrogate **over the full 10 minutes**, even when relying on blade pitch and rotor speed prediction

Images/GenPwr_scatter_and_err.png

Images/GenPwr_trace_low_err.png

Images/GenPwr_trace_high_err.png

Conclusion and outlook

Conclusion

- ▶ **Multistep surrogate modelling approach** can be favourable as it simplifies the input-output mapping at each step
- ▶ The final surrogate **prediction is stable** over extended time periods, even when relying on auxiliary quantities
- ▶ Construction order of auxiliary quantities can be determined in a **data-driven recursive fashion**

Outlook

- ▶ Investigate the effect of different **stopping criteria** and **measures of association**
- ▶ Application to other problems, such as buildings under wind loads and ground motion

Images/Chair2022-1.jpg

Chair of Risk, Safety & Uncertainty Quantification
www.rsuq.ethz.ch

Images/funded_by_EU.pdf

The Uncertainty Quantification Software

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The Uncertainty Quantification Community

www.uqworld.org

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