# Modelling with Gaussian Processes

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## Jozef Stefan Institute



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## Department of systems and control

The domain of work

**CONTROL OF SYSTEMS AND PROCESSES** (cybernetics, informatics, automation)

#### Staff

→ 25 - 30 people (13-15 with PhD, 6-9 PhD students)

#### **Financing**

- ✤ 60% different ministries and state agencies
- ✤ 40% other sources (industry, international projects, etc.)

#### **Current areas of work**

- Modelling, control and optimization of (complex) systems
- Detection and localization of faults
- Smart factories
- Device and product development





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## An introduction to modelling

 Creating models of systems or signals with a specific purpose: design and construction, analysis, behavior prediction, etc.

# Modelling – why and how

Modelling

Various complex activities that make up the process of model development aiming to improve, e.g., the understanding of the functioning mechanisms of the modelled system, the prediction of its behaviour, the design and the evaluation of control systems, the estimation of the unmeasurable system states, the optimisation of the system behaviour, the development of simulators, as well as to enable the sensitivity analysis and the fault diagnosis.

- First-principles modelling (physics-based modelling, analytical modelling, etc.)
- System identification (experimental modelling , datadriven modelling, black-box modelling, statistical modelling, etc.)
- Hybrid modelling (integrated modelling, statistical postprocessing, explainable AI, etc.)

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(a)(a)

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## Linear regression

- Illustrative example,
- static input-output example

$$f(x) = x^3 + \epsilon$$

• 9 input data:

 $x_i, y_i \in \mathcal{N}_{(0, 0.01)}$ Prediction Error Method (PEM):

$$\phi(\mathbf{x}) = [f_1(\mathbf{x}), \dots, f_D(\mathbf{x})]^T$$
$$J = \sum_{i=1}^N (y_i - t_i)^2$$
$$y(\mathbf{x}, \mathbf{w}) = \sum_{j=0}^{M-1} w_j \phi_j(\mathbf{x}) = \mathbf{w}^T \phi(\mathbf{x})$$

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Random variables with a normal distribution at the output

• Random variables with a normal or Gaussian distribution at the output of a linear model,



• uncertainty of parameters,

$$cov\{\mathbf{w}\} = \sigma_n(\mathbf{\Phi}^{\mathrm{T}}\mathbf{\Phi})^{-1}$$

• prediction uncertainty.

 $cov\{y\} = \mathbf{\Phi}cov\{\mathbf{w}\}\mathbf{\Phi}^{\mathrm{T}}$ 

## Kernel methods for nonlinear systems

• Alternative to modelling with basis functions

$$y(\mathbf{x}, \mathbf{w}) = \sum_{j=0}^{M-1} w_j \phi_j(\mathbf{x}) = \mathbf{w}^{\mathrm{T}} \phi(\mathbf{x}) \quad y(\mathbf{x}, \mathbf{w}) = f\left(\sum_{j=1}^M w_j \phi_j(\mathbf{x})\right)$$

Linear and nonlinear models, e.g. MLP, fuzzy

• Substitute of large number of basis function with a kernel function  $k(\mathbf{x}, \mathbf{x}') = \boldsymbol{\phi}(\mathbf{x})^{\mathrm{T}} \boldsymbol{\phi}(\mathbf{x}')$ 

for linear system

 $k(\mathbf{x}, \mathbf{x}') = \mathbf{x}^{\mathrm{T}} \mathbf{x}'$ 

infinite number of basis functions

radial basis functions

 $k(\mathbf{x}, \mathbf{x}') = \exp\left(-\|\mathbf{x} - \mathbf{x}'\|^2 / 2\sigma^2\right)$  $k(\mathbf{x}, \mathbf{x}') = k(\|\mathbf{x} - \mathbf{x}'\|)$ 

- Kernel functions => kernel methods (e.g., SVM-support vector machines)
- memory-based methods, where model contains training data => nonparametric model
- Parameters of kernel functions are called hyperparameters => fewer optimisation parameters

## Gaussian process

- Gaussian process (GP) is a stochastic process: collection of random variables where each has a Gaussian distribution.
- Gaussian proces modelling is a nonparametric method that uses Bayesian learning for a model identification. Result is a Gaussian-process model (GP model).

## Gaussian-process models

• Kernel model + Bayesian statistics = GP model

$$\mathbf{y} = f\left(\mathbf{X}\right) + \boldsymbol{\varepsilon}$$



- Output random variables, GP mapping function, kernel model
- <u>Input</u> is a regression vector of samples,
- <u>Output</u> is a random variable with normal distribution
- <u>Mapping function</u> is a Gaussian process
- Kernels in GP models are covariance functions
- Motives for GP use:
  - Optimisation of complex model structure can be avoided
  - Dealing with limited amount of data
  - Reducing the potential for overfitting

## Gaussian-process model



## Gaussian-process model

- Probabilistic (Bayes) model. Nonparametric model no predetermined structure (basis functions) depending on system likelihood prior distribution posterior distribution
- Determined by:
  - Input/output data  $X_i, y_i$  (data points, not signals)  $\mathcal{D} = \{X, y\}$ (training data – identification data):  $\mathbf{K} = \begin{bmatrix} K_{11} & \dots & K_{1N} \\ \vdots & \ddots & \vdots \\ K_{N1} & \dots & K_{NN} \end{bmatrix}$
  - Covariance matrix:

$$K_{ij} = \operatorname{cov}\left(y_i, y_j\right)$$

 $\operatorname{cov} (f(\mathbf{x}_i), f(\mathbf{x}_i)) = C(\mathbf{x}_i, \mathbf{x}_i)$ 

 $\overbrace{p(w|y;\theta,\mathcal{M})}^{f} = \frac{\int p(y|w,f;\mathcal{M}) p(w,f;\theta,\mathcal{M}) df}{p(y;\theta,\mathcal{M})}$ 

marginal likelihood





 $\mathcal{GP}\left(f\left(\cdot\right)|\mathbf{y}\right) = \frac{p\left(\mathbf{y}|\mathbf{f}\right)\mathcal{GP}\left(f\left(\cdot\right)\right)}{p\left(\mathbf{y}\right)}$ 



 $\mathcal{GP}\left(f\left(\cdot\right)|\mathbf{y}\right) = \frac{p\left(\mathbf{y}|\mathbf{f}\right)\mathcal{GP}\left(f\left(\cdot\right)\right)}{p\left(\mathbf{y}\right)}$ 



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$$\mathcal{GP}(f(\cdot)|\mathbf{y}) = \frac{p(\mathbf{y}|\mathbf{f}) \mathcal{GP}(f(\cdot))}{p(\mathbf{y})}$$



$$\mathcal{GP}\left(f\left(\cdot\right)|\mathbf{y}\right) = \frac{p\left(\mathbf{y}|\mathbf{f}\right)\mathcal{GP}\left(f\left(\cdot\right)\right)}{p\left(\mathbf{y}\right)}$$



$$\mathcal{GP}(f(\cdot)|\mathbf{y}) = \frac{p(\mathbf{y}|\mathbf{f}) \mathcal{GP}(f(\cdot))}{p(\mathbf{y})}$$

## Training of hyperparameters

$$p\left(\boldsymbol{\theta}, \sigma_{n}^{2} | \mathbf{y}\right) = \frac{p\left(\mathbf{y} | \boldsymbol{\theta}, \sigma_{n}^{2}\right) p\left(\boldsymbol{\theta}, \sigma_{n}^{2}\right)}{p\left(\mathbf{y}\right)}$$

- Optimisation:
  - Cost function: marginal likelihood

$$\hat{\theta}, \hat{\sigma}_n^2 = \operatorname*{arg\,max}_{\theta, \sigma_n^2} \left[ \log p\left(\mathbf{y}; \theta, \sigma_n^2\right) \right],$$

where

$$\log p\left(\mathbf{y}; \boldsymbol{\theta}, \sigma_n^2\right) = \underbrace{-\frac{1}{2} \mathbf{y}^T \left(\mathbf{K}_{f,f} + \mathbf{I}\sigma_n^2\right)^{-1} \mathbf{y}}_{\text{data fit term}} - \underbrace{\frac{1}{2} \log \left|\mathbf{K}_{f,f} + \mathbf{I}\sigma_n^2\right|}_{\text{regularization term}} - \underbrace{\frac{n}{2} \log 2\pi}_{\text{constant}}.$$

## Prediction with GP model

 Prediction of the output based on similarity test input – training inputs

$$\mathcal{GP}(f(\cdot)|\mathbf{y}) = \frac{p(\mathbf{y}|\mathbf{f}) \mathcal{GP}(f(\cdot))}{p(\mathbf{y})}$$

• Output: normal distribution



μ-2σ

μ

 $\mu + 2\sigma$ 

$$\mathbb{E}[\mathbf{f}_*|\mathbf{y}] = \mathbf{K}_{*,f} \left( \mathbf{K}_{f,f} + \mathbf{I}\sigma_n^2 \right)^{-1} \mathbf{y},$$
$$\mathbb{V}[\mathbf{f}_*|\mathbf{y}] = \mathbf{K}_{*,*} - \mathbf{K}_{*,f} \left( \mathbf{K}_{f,f} + \mathbf{I}\sigma_n^2 \right)^{-1} \mathbf{K}_{f,*}$$



Probabilistic Graphical Model - PGM

(b) PGM of a GP regression model.

## Static illustrative example

- Static example:  $f(x) = x^3 + \epsilon$   $f(x) = x^3 + \epsilon$
- $x_i, y_i$   $\mathcal{N}(0, 0.01)$
- 9 measured data:
- Gray belt
- Sparse data →
   increased variance
   (higher uncertainty).



The absolute error of prediction and the band of double standard deviation of the prediction



Properties of GP models ( compared to a model based on basis functions ) :

- a smaller number of optimization and design parameters,
- prediction uncertainty depends on the amount of identification data,
- overfitting is minimised,
- works satisfactorily even with a small number of identification data,
- smoothing data with noise,
- enables the use of prior knowledge, \*
- easy to use ( engineering practice ),
- the computational load increases with the amount of identification data,
- a relatively young methodology, still in development
- nonparametric model.

\* Also possible with some other models

# Example of smoothing - the power curve of wind turbine



• Static system

## Power curve (2)

1/10 data for training

complete data



Power curve (3)



NRMSE = 0.051

## Static vs. dynamic

## • Dynamic system

A system in which time-dependent qualitative or quantitative changes are taking place. The output of such a system depends not only on the current input value but also on the previous input values.

A dynamic system is a system or process in which motion occurs, or includes active forces, as opposed to static conditions with no motion.

## • Dynamic models (system identification):

conventional approach (ANN, decision trees, fuzzy models, etc.) delayed inputs and outputs as regressors.

# Modelling – why and how

### Modelling

Various complex activities that make up the process of model development aiming to improve, e.g., the understanding of the functioning mechanisms of the modelled system, the prediction of its behaviour, the design and the evaluation of control systems, the estimation of the unmeasurable system states, the optimisation of the system behaviour, the development of simulators, as well as to enable the sensitivity analysis and the fault diagnosis.

- First-principles modelling (physics-based modelling, analytical modelling, etc.)
- System identification (experimental modelling, data-driven modelling, black-box modelling, statistical modelling, etc.)
- Hybrid modelling (integrated modelling, statistical postprocessing, explainable AI, etc.)
- What is **system identification**?

Methods to build mathematical models of **dynamic systems** from measured data.

• Purpose: prediction, forecasting, simulation, control design, systems analysis, etc.

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# Identification - why and how

- Application: unknown detailed physical background of the systems.
- Application: constraints of the engineering practice.



- ✓ Identification of **nonlinear** dynamic systems.
- $\checkmark$  Connection with statistics and machine learning.
  - Various methods → artificial neural networks (UNM), decision trees, fuzzy models, etc.
  - Difficult to use (structure selection, large number of optimization parameters and structure complexity, large amount of data required for optimization, bias-variance, inadequate fit, overfitting).
  - Planning in practice: the problem of confidence in the model.

- Dynamic models:
- A common approach (UNM, fuzzy models, etc.) is that the regressor vector contains delayed samples of the input and output signal.

Input-output identification pairs  $\mathbf{x}_i / y_i$ :

 $\boldsymbol{x}_{i} \dots$  Regressor vector

[u(k-1),..,u(kL), y(k-1),..,y(kL)]

y<sub>i</sub>... Output value of the model

y(k)

# Why modeling dynamic systems with GP-models?

- Dynamic systems in engineering.
- Relatively large dimensions of the entrance space.
- Specific distribution of input data.
- Dynamic systems:
  - prediction, simulation,
  - simulation evaluation,
  - noise handling,
  - convergence.

## Model prediction and simulation



- ARX model

- OE model

## Dynamic model simulation

- A simulation
  - <u>"naive" ... m(k),</u>
  - by propagating m(k),v(k):
    - analytical approximation:
      - The Taylor method,
      - Model matching,
    - numerical approximation:
      - Monte Carlo method.



## Example of identification – bioreactor

Identification process, properties of the identified GP-model  $\rightarrow$ 

Bioreactor - discrete dynamic nonlinear system of the 2nd order:

$$\begin{aligned} x_1(k+1) &= x_1(k) + 0.5 \frac{x_1(k)x_2(k)}{x_1(k) + x_2(k)} - 0.5u(k)x_1(k) \\ x_2(k+1) &= x_2(k) - 0.5 \frac{x_1(k)x_2(k)}{x_1(k) + x_2(k)} - 0.5u(k)x_2(k) + 0.05u(k) \\ y(k) &= x_1(k) + \epsilon(k) \end{aligned}$$

 $x_1$ ... concentration of microorganisms,  $x_2$ ... substrate concentration, u... output flow,  $0 \le u(k) \le 0.7$ ,  $\epsilon$ . white Gaussian noise,  $\sigma = 0.5\%$  (ymaxymin).



# Bioreactor (2)

- 1. Definition of the purpose of the model: response to an input signal.
- 2. Experiment design:
  - input and output signal ightarrow
  - ~ 600 points for identification.

- 3. Conducting an experiment, data processing.
- 4. Selection of a model structure:
  - Gaussian covariance function (iterative) (stationarity, smoothness),
  - selection of regressors. [y(k-1)...y(kL) u(k-1)...u(kL)], y(k)



## Bioreactor (3)

- validation  $\rightarrow$  n=2,
- ARD  $\rightarrow$  reduction of the number of regressors, [u (k-1) u (k-2) y (k-2)]

### [u(k-1)u(k-2)y(k-2)]

Table 2.3 Values of the validation performance measures and the hyperparameters of different bioreactor GP models with the best measure values in bold.

Model	Model Ident. data		Valid. data		Hyperparameters									noise <sup>‡</sup>	
order	<i>ℓ</i> <sub>1</sub>	SMSE <sub>2</sub>	MSLL <sub>2</sub>	SMSE	MSLL	$ly_4 = \frac{1}{\sqrt{wy_4}}$	$ly_3 = \frac{1}{\sqrt{wy_3}}$	$ly_2 = \frac{1}{\sqrt{wy_4}}$	$ly_1 = \frac{1}{\sqrt{wy_1}}$	$lu_4 = \frac{1}{\sqrt{wu_4}}$	$lu_3 = \frac{1}{\sqrt{wu_3}}$	$l_{u_2} = \frac{1}{\sqrt{w_{u_2}}}$	$l_{u_1} = \frac{1}{\sqrt{w_{u_1}}}$	°f	$\sigma_n$
- 4	1628	3.1.10-3	-3.31	$5.1 \cdot 10^{-3}$	-3.22	9.2	6.3	4.8	977	406	7.2	7.0	8.9	2.5 5	$5.0 \cdot 10^{-4}$
3	1621	$2.3 \cdot 10^{-3}$	-3.38	$3.8 \cdot 10^{-3}$	-3.32	×	20.0	3.90	49.3	×	17.4	17.3	15.6	4.2 5	$5.1 \cdot 10^{-4}$
2	1612	$1.2 \cdot 10^{-3}$	-3.55	$1.9 \cdot 10^{-3}$	-3.50	×	×	5.8	29.8	×	×	13.3	14.7	5.3 5	$5.3 \cdot 10^{-4}$
2 🔷	1603	$7.8 \cdot 10^{-4}$	-3.57	$1.2 \cdot 10^{-3}$	-3.49	×	×	5.2	×	×	×	13.1	14.4	5.6 5	$5.4 \cdot 10^{-4}$
2	785	$3.5 \cdot 10^{-3}$	-2.36	$3.1 \cdot 10^{-4}$	-2.37	×	×	4.07	×	×	×	10.7	8.7	3.3 2	$2.1 \cdot 10^{-3}$

Notes:

The index 1 denotes the first set of data for identification

The index 2 denotes the second set of data for identification

 $\ddagger$  the identified standard deviation of noise  $\sigma_n$ 

• reduced number of regressors by masking the regressor y(k-1)

• identified on the output signal with the increased standard deviation of noise,  $\sigma_{\nu} = 0.002$ 

Kocijan (2016) Modeling and control of dynamic systems with Gaussian process models, Springer.

# Bioreactor (4)

$2^{nd}$ order model	Ident. data				
Covariance function	$\ell_1$	$SMSE_2$	$MSLL_2$		
Squared exponential $+$ ARD	1603	$7.8 \cdot 10^{-4}$	-3.57		
Matérn + ARD $d = \frac{3}{2}$	1591	$7.2 \cdot 10^{-4}$	-3.54		
Rational quadratic $+$ ARD	1603	$4.1 \cdot 10^{-3}$	-3.31		
Linear + ARD	1281	$1.7 \cdot 10^{-2}$	-1.46		
Matérn $d = \frac{3}{2}$	1587	$1.2 \cdot 10^{-3}$	-2.03		
Matérn $d = \frac{5}{2}$	1597	$1.7 \cdot 10^{-3}$	-1.58		
Neural network	1596	$5.2 \cdot 10^{-3}$	-1.00		
Squared exponential	1600	$1.6 \cdot 10^{-3}$	-1.35		

Kocijan (2016) Modeling and control of dynamic systems with Gaussian process models, Springer.

### 5. Hyperparameter training

## Bioreactor (5)

### 6. Model validation:

- plausibility ("looks", "behaves" logically),
- falseness (validation of input-output behaviour),
- purposiveness (satisfying the purpose of modelling).

## Bioreactor (6)

### Model evaluation:

variance

- Falseness:
  - qualitative (visual assessment of response)
  - quantitative price lists:
    - mean squared error (MSE),
    - Mean Relative Square Error (MRSE),
    - The logarithm of the prediction error density (LD),
    - The negative logarithm of the optimization data likelihood (LL),
    - <u>SMSE</u>, <u>MSLL</u>, NRMSE etc.

$$SE = \frac{1}{N} \sum_{i=1}^{N} e_i^2, \qquad LD = \frac{1}{2} log(2\pi) + \frac{1}{2N} \sum_{i=1}^{N} \left( log(\sigma_i^2) + \frac{e_i^2}{\sigma_i^2} \right),$$
  

$$MRSE = \sqrt{\frac{\sum_{i=1}^{N} e_i^2}{\sum_{i=1}^{N} y_i^2}}, \qquad LL = \frac{1}{2} \log |\mathbf{K}| + \frac{1}{2} \mathbf{y}^T \mathbf{K}^{-1} \mathbf{y} + \frac{N}{2} \log(2\pi)$$
  

$$SMSE = \frac{1}{N} \frac{\sum_{i=1}^{N} (y_i - E(\hat{y}_i))^2}{\sigma_y^2} \qquad MSLL = \frac{1}{2N} \sum_{i=1}^{N} \left[ ln(\sigma_i^2) + \frac{(y_i - E(\hat{y}_i))^2}{\sigma_i^2} \right] - \frac{1}{2N} \sum_{i=1}^{N} \left[ ln(\sigma_y^2) + \frac{(y_i - E(\mathbf{y}))^2}{\sigma_y^2} \right]$$

## Bioreactor (7)

### Simulation in the domain of identification data, but not with an identification signal.



## Bioreactor (8)

Simulation outside the domain of identification data:

u(k) > 0.7.



## Bioreactor (9)

More noise:

$$\sigma = 2\% (y_{max} - y_{min}).$$

Increased variance:

- increased noise,
- insufficient data.



## Bioreactor (10)

Unmodeled input z = 0.05 for t > = 30s.

Confidence in the forecast does not change in the field of identification data.



# Selected examples of GP modeling applications

- Gas-liquid separation process engineering.
- Gear life-span prognosis mechanical production.
- Dispersion of nuclear pollution environmental science.
- Online modelling with GP models various fields.
- Modelling and forecasting of ozone values environmental science.
- Predictive control of the gas-liquid separation process engineering.
- Online adaptive control automatic.
- Adaptive predictive control of bioreactor biotechnology.

### Modelling of the gas-liquid separator



KOCIJAN, Juš, LIKAR, Bojan. Gas - liquid separator modelling and simulation with Gaussian process models . Simulation modelling practice and theory , 2008, vol. 16, well. 18, p. 910-922.



### Gear life-span prognostics





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Fig. 4. The modelling of feature evolution for the gear with the model containing the sum of Matérn and polynomial covariance function (a) and neural network covariance function (b) for 144 training data points



Kocijan , Juš , Tanko , Vesna . Prognosis of gear health using Gaussian process model. In: *IEEE EUROCON 2011* , International Conference on Computer as a Tool. 2011, Lisbon, Portugal, 2011, 4 p.





Mean predicted time

Confidence interval

Modeling weather variables to analyze the spread of nuclear contamination



KRIVEC, Tadej, KOCIJAN, Juš, PERNE, Matija, GRAŠIČ, Boštjan, BOŽNAR, Marija, MLAKAR, Primož. Data-driven method for the improving forecasts of local weather dynamics. Engineering applications of artificial intelligence, Elsevier, 2021, vol. 105, 104423-1-104423-14.



Online modelling - a scheme of the concept of online learning of an evolving GP-model





Petelin , Dejan , Kocijan , Juš . Streaming-data selection for Gaussian-process modeling . In: Borgelt , Christian. *Towards advanced data analysis by combining soft computing and statistics* . Heidelberg: Springer, 2013, p. 177-190.



### Modelling and forecasting of ozone values - a study of a mobile pollution measurement station





Kocijan, Juš, Gradisar, Dejan, Božnar, Marija, Grašič, Boštjan, Mlakar, Primož. On-line algorithm for ground-level ozone prediction with a mobile station. *Atmospheric environment*, 2016, vol. 131, p. 326-333

### Predictive control of the gas preparation unit



Kocijan (2016) Modelling and control of dynamic systems with Gaussian process models , Springer.



Control demonstration using evolving GP-model



Control demonstration using evolving GP-model





Identification data (black dots) and data with the most information (red circles) displayed on the surface of the selected nonlinear system



STEPANČIČ, Martin, GRANCHAROVA, Alexandra, KOCIJAN, Juš . Adaptive MPC based on probabilistic blackbox input-output model. *Comptes rendus de l' Academie bulgare des Sciences*, ISSN 1310-1331, 2015, vol. 68, well. 6, p. 767-774.

## Summary

- GP modelling is a flexible, probabilistic, approach to experimental modelling
- Applicable for uncertain, missing and corrupted data
- A promising method for engineering practice, especially for control design.

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Toolbox <u>https://github.com/Dynamic-</u> <u>Systems-and-GP/GPdyn.git</u> or <u>http://extras.springer.com</u>

AIC

Models

🖄 Springer



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#### RESEARCH DIRECTIONS

The objectives of the proposed research topic for PhD project are to develop methods for dynamic system modelling based on machine learning methods like kernel methods or to improve the existing data-driven modelling procedures to be better suited for the targeted application. The models obtained are meant for different applications, each representing a potential PhD project, which are as follows.

- Modelling of spatiotemporal systems using Gaussian processes and image or video forecasting, e.g., for modelling pollution dispersion
- Designing of adaptive and robust control systems that handle signal and safety constraints in complex dynamic systems.

