Constraining Gaussian Processes to Systems of Linear Ordinary Differential Equations

Andreas Besginow, Markus Lange-Hegermann
OWL University of Applied Sciences and Arts

Why should you care?

- Many things run on differential equations
- Lotka-Volterra, fluid dynamics, ...
- For **systems of linear homogenuous ordinary differential equations with constant coeficients**
- Developed **symbolic** and **algorithmic** approach to constrain GPs to them
- Realizations of GPs **strictly** satisfy system of ODEs
- Approach also **extracts parameters** from system of ODEs **automatically**
- Learning parameters together with GPs
- We call them **LODE-GPs**

Prerequisites & assumptions

- Given a system of ODEs of the form

$$A \cdot \mathbf{f}(t) = 0 \qquad (1)$$

- Operator matrix $A \in \mathbb{R}[\partial_t]^{m \times n}$
- Smooth functions $f_i(t) \in C^\infty(\mathbb{R}, \mathbb{R})$ of $\mathbf{f}(t) = \big(f_1(t) \; \ldots \; f_n(t)\big)^T$

Theorem

For **every** system as in Equation 1 there exists a GP g, such that the **set of realizations of g is dense** in the set of solutions.

How we did it

$$\begin{aligned} & U \cdot A \cdot V \cdot V^{-1} \cdot \mathbf{f} = 0 \\ \Leftrightarrow \quad & D \cdot V^{-1} \cdot \mathbf{f} = 0 \\ \Leftrightarrow \quad & D \cdot \mathbf{p} = 0 \\ \Leftrightarrow \quad & \begin{cases} \bigwedge_{i=1}^{\min(n,m)} D_{i,i} \cdot \mathbf{p}_i = 0 \\ \wedge \bigwedge_{i=\min(n,m)+1}^{n} 0 \cdot \mathbf{p}_i = 0 \end{cases} \end{aligned}$$

- Decoupled **latent vector** $\mathbf{p} = V^{-1}\mathbf{f}$ of functions
- GP-prior for $h \sim \mathcal{GP}(\mathbf{0}, k)$ for $\mathbf{p}$ via **multi-output GP**
- **Pushforward** of h with V yields a GP g

The pushforward can be formulated as

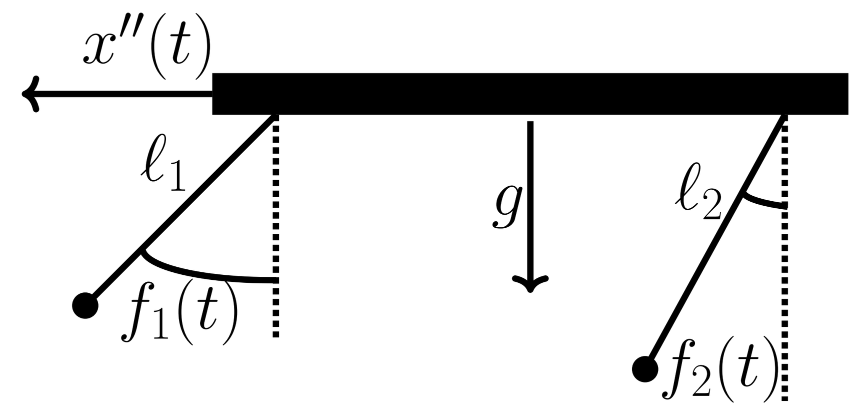
$$g \sim V_* h = \mathcal{GP}(\mathbf{0}, V \cdot k \cdot V')$$

with $V' = V^T$ applied on t_2.

- Zeroes of Ds diagonal entries are used to **construct** covariance function k of h (see table below)

d	$k(t_1, t_2)$
1	0
$(\partial_t - a)^j$	$\left(\Sigma_{i=0}^{j-1} t_1^i t_2^i\right) \cdot \exp(a \cdot (t_1 + t_2))$
$((\partial_t - a - ib)(\partial_t - a + ib))^j$	$\left(\Sigma_{i=0}^{j-1} t_1^i t_2^i\right) \cdot \exp(a \cdot (t_1 + t_2)) \cdot \cos(b \cdot (t_1 - t_2))$
0	k_{SE}

The linearized bipendulum



- With acceleration $u(t)$ proportional to $x''(t)$ we have system of ODEs:

$$f_1''(t) + g \cdot f_1(t) - u(t) = 0$$
$$f_2''(t) + \frac{g}{2} \cdot f_2(t) - \frac{u(t)}{2} = 0$$

- Which translates to operator matrix A:

$$\underbrace{\begin{bmatrix} \partial_t^2 + g & 0 & -1 \\ 0 & \partial_t^2 + \frac{g}{2} & -\frac{1}{2} \end{bmatrix}}_{A} \cdot \begin{bmatrix} f_1(t) \\ f_2(t) \\ u(t) \end{bmatrix}$$

- For rope lengths $\ell_1 \neq \ell_2$ the linearized Bipendulum (above) is controllable. For $\ell_1 = 1, \ell_2 = 2$:

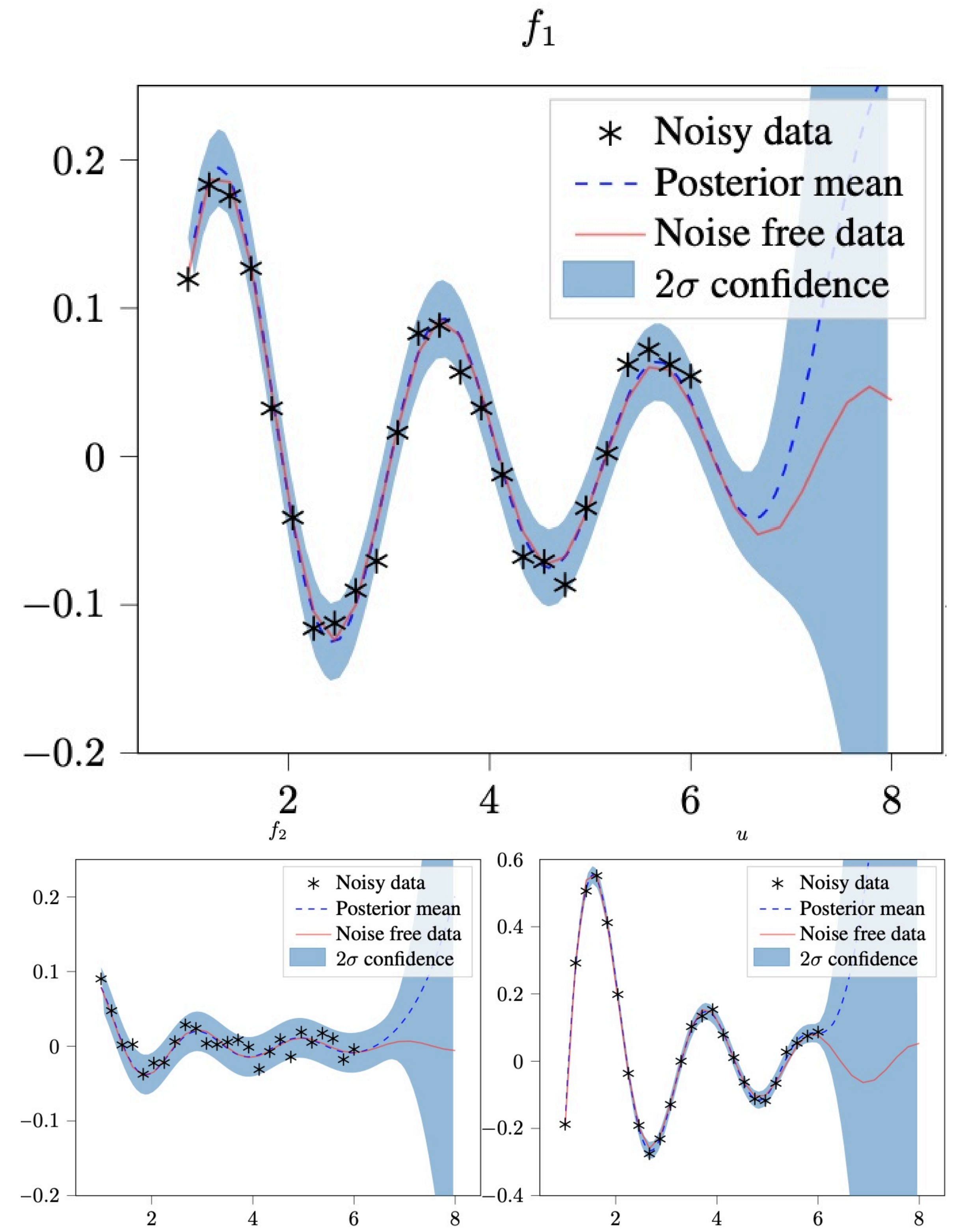
$$\underbrace{\begin{bmatrix} 1 & 0 \\ -\frac{1}{2} & 1 \end{bmatrix}}_{U} \underbrace{\begin{bmatrix} \partial_t^2 + g & 0 & -1 \\ 0 & \partial_t^2 + \frac{g}{2} & -\frac{1}{2} \end{bmatrix}}_{A} \underbrace{\begin{bmatrix} 0 & -\frac{4}{g} & \frac{2\partial_t^2 + g}{2} \\ 0 & -\frac{2}{g} & \frac{\partial_t^2 + g}{2} \\ -1 & -\frac{4\partial_t^2 + 4g}{g} & (\partial_t^2 + \frac{g}{2})(\partial_t^2 + g) \end{bmatrix}}_{V}$$

$$= \underbrace{\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix}}_{D}$$

- From D we construct prior cov. fkt. k with diagonal entries $(0, 0, k_{\mathrm{SE}})$
- Where $k_{\mathrm{SE}} = \exp(-\frac{1}{2}(t_1 - t_2)^2)$

- The LODE-GP kernel is defined by

$$V \cdot k \cdot V' = \begin{bmatrix} \frac{2\partial_{t_1}^2 + g}{2} \\ \frac{\partial_{t_1}^2 + g}{2} \\ (\partial_{t_1}^2 + \frac{g}{2})(\partial_{t_1}^2 + g) \end{bmatrix} \cdot \begin{bmatrix} k_{\mathsf{SE}} \end{bmatrix} \cdot \begin{bmatrix} \frac{2\partial_{t_2}^2 + g}{2} & \frac{\partial_{t_2}^2 + g}{2} & (\partial_{t_2}^2 + \frac{g}{2})(\partial_{t_2}^2 + g) \end{bmatrix}$$



Acknowledgement

This research was supported by the research training group "Dataninja" (Trustworthy AI for Seamless Problem Solving: Next Generation Intelligence Joins Robust Data Analysis) funded by the German federal state of North Rhine-Westphalia.

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PtJ Projektträger Jülich Forschungszentrum Jülich
Ministerium für Kultur und Wissenschaft des Landes Nordrhein-Westfalen
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