#### Latent Forces Models: related work

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#### Contenido

#### Introduction

Gaussian processes for Multiple outputs

Parameter estimation in differential equations

Gaussian processes for systems identification

# Different Views of the LFM (I)

 Gaussian processes over latent forces plus linear differential equations lead to multiple output Gaussian process.

This multi-output Gaussian process uses a covariance function that encodes the interactions between the different mechanistic models.

 $\Box$  Marginal likelihood to estimate the hyperparameters  $\theta$  of the covariance function equals estimating the parameters of differential equations.

## Different Views of the LFM (II)

The related work can be seen from different perspectives.

- We focus on three
  - Gaussian processes for multiple outputs.
  - Parameter estimation in differential equations.
  - Gaussian processes for systems identification.

#### Contenido

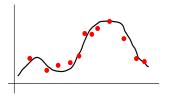
Introduction

Gaussian processes for Multiple outputs

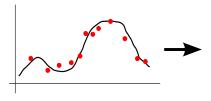
Parameter estimation in differential equations

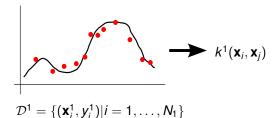
Gaussian processes for systems identification

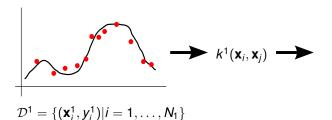
Gaussian process priors for multiple outputs have been thoroughly studied in the spatial analysis and geostatistics literature (Higdon, 2002; Boyle and Frean, 2005; Journel and Huijbregts, 1978; Cressie, 1993; Goovaerts, 1997; Wackernagel, 2003).

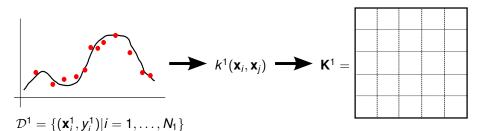


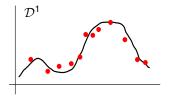
$$\mathcal{D}^1 = \{(\bm{x}_i^1, y_i^1) | i = 1, \dots, N_1\}$$

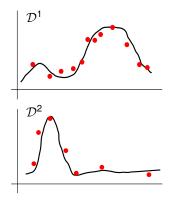


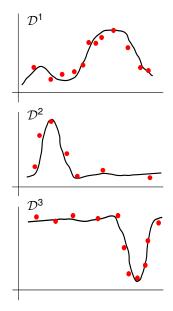


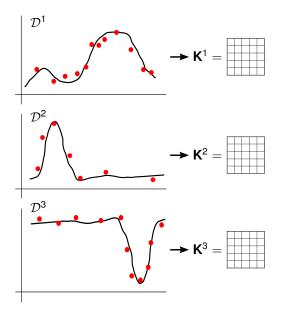


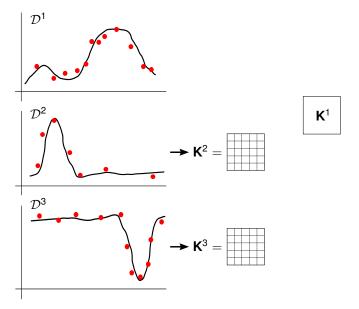


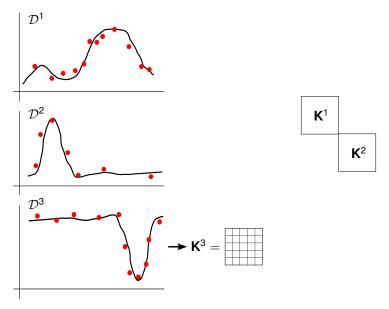


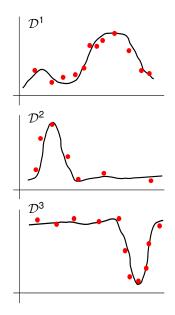


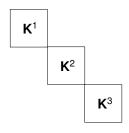


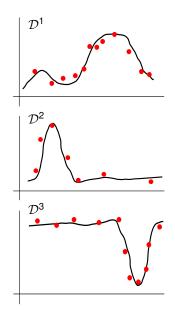


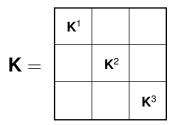


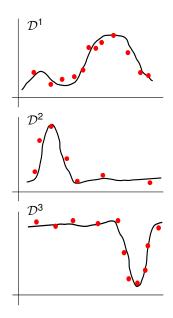












#### Joint covariance

K =	<b>K</b> <sup>1</sup>	?	?
	?	<b>K</b> <sup>2</sup>	?
	?	?	<b>K</b> <sup>3</sup>

K be a valid covariance matrix

Assume we have D outputs,  $\{f_d(\mathbf{x})\}_{d=1}^D$ . The covariance between  $f_d(\mathbf{x})$  and  $f_{d'}(\mathbf{x}')$  follows (Higdon, 2002; Boyle and Frean, 2005; Álvarez et al., 2012)

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#### Discrete convolutions

Murray-Smith and Pearlmutter (2005) introduced the idea of transforming a Gaussian process prior using a discretized version of the integral operator of the equation before.

 Applications mentioned include fusing the information from multiple sensors or for solving inverse problems in reconstruction of images (Shi et al., 2005).

### Contenido

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## Differential equations and statistics

- Differential equations are the cornerstone of a diverse range of engineering fields and applied sciences.
- Combination with probabilistic models and use within machine learning and statistics has been less explored.
- Functional data analysis (Ramsay and Silverman, 2005).

## Classical point of view in frequentist statistics

Given a differential equation with unknown coefficients  $\{\mathbf{A}_m\}_{m=0}^M$ , how do we use data to fit those parameters?

- Classical approaches to fitting parameters  $\theta \ (= \{\mathbf{A}_m\}_{m=0}^M)$  of differential equations observed data include (Ramsay et al., 2007; Brewer et al., 2008)
  - Numerical approximations of initial value problems.
  - collocation methods

## Numerical approximations

- Iterative process given an initial set of parameters  $\theta_0$  and initial conditions  $\mathbf{y}_0$ ,
- A numerical method is used to solve the differential equation.
- ☐ The parameters of the differential equation are then optimized by minimizing an error criterion between the approximated solution and the observed data.

# Collocation methods (I)

- □ The solution of the differential equation is approximated using a set of basis functions,  $\{\phi_i(t)\}_{i=1}^J$ , this is  $y(t) = \sum_{i=1}^J \beta_i \phi_i(t)$ .
- □ The basis functions must be sufficiently smooth so that to compute  $\mathcal{D}^m y(t) = \sum \beta_i \mathcal{D}^m \phi_i(t)$ .
- Collocation methods also use an iterative procedure for fitting the additional parameters involved in the differential equation.
- Minimization of an error criteria is used to estimate the parameters of the differential equation.

## Collocation methods (II)

 Principal differential analysis (PDA) (Ramsay, 1996) is one example of a collocation method in which the basis functions are *splines*.

Parameters are obtained by minimizing the squared residuals of the higher order derivative  $\mathcal{D}^M y(t)$ , and the weighted sum of derivatives  $\{\mathcal{D}^m y(t)\}_{m=0}^{M-1}$ .

# Collocation methods (III)

- Collocation method augmented with Gaussian process priors (Graepel, 2003).
- The solution of the differential equation  $\mathcal{D}_0^M y(t)$  is assumed to follow a Gaussian process prior with covariance  $k_{\mathcal{D}_{0,t}^M,\mathcal{D}_{0,t'}^M}(t,t')$
- An approximated solution  $\widetilde{y}(t)$  can then be computed through the expansion  $\widetilde{y}(t) = \sum_{n=1}^{N} \alpha_n k_{\mathcal{D}_{0,t'}^M, \mathcal{D}_{0,t'}^M}(t, t_n)$ .
- $\alpha_n$  is an element of the vector  $(\mathbf{K}_{\mathcal{D}_{0,t'}^M,\mathcal{D}_{0,t'}^M} + \sigma_y^2 \mathbf{I}_N)^{-1} \hat{\mathbf{y}}$ , and  $\hat{\mathbf{y}}$  is a vector of noisy observations of  $\mathcal{D}_0^M y(t)$ .

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### Systems Identification

- In control engineering, systems identification refers to a set of techniques used for representing a dynamical system by a mathematical model (mostly a linear model).
- □ A detailed description of the dynamical system is usually unknown, and parameters of the surrogate model are estimated from measured data.

# GPs for systems identification

- Gaussian processes have been used as models for systems identification (Solak et al., 2003; Kocijan et al., 2005; Calderhead et al., 2009; Thompson, 2009).
- A non-linear dynamical system is linearized around an equilibrium point by means of a Taylor series expansion (Thompson, 2009),  $y(t) = \sum_{j=0}^{\infty} \frac{y^{(j)}(a)}{j!} (t-a)^j$ , with a the equilibrium point.
- Covariates correspond to the terms  $(t a)^j$  and the derivatives  $y^{(j)}(a)$  to regression coefficients.
- The derivatives are assumed to follow a Gaussian process prior with a covariance function that is obtained as  $k^{(j,j')}(t,t')$ .

### State space models

- Representation of the possible nonlinear relationships between the latent space and between the latent space and the observation space (Ko et al., 2007; Deisenroth et al., 2009; Turner et al., 2010).
- Latent process is a GP (Hartikainen and Särkkä, 2011; Hartikainen et al., 2012), improving computational complexity.

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