Probabilistic Numerics for Scientific Machine Learning

Jonathan Wenger

EBERHARD KARLS UNIVERSITÄT TÜBINGEN

imprs-is

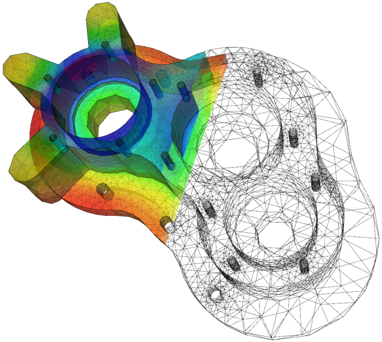
Mechanistic Models

Describing the laws of nature mathematically.

Scientific computing relies on mechanistic models.

Example: Physical processes modeled by linear PDEs

- thermal conduction (heat equation)
- electromagnetism (Maxwell's equations)
- wave mechanics (wave equation)



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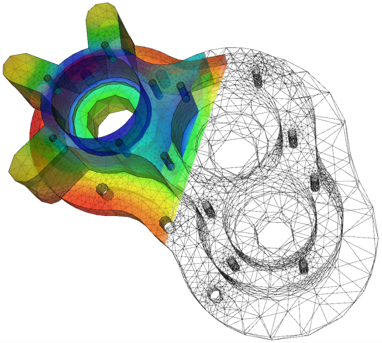

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Strengths

- Interpretable / causal relationships
- Experimentally validated

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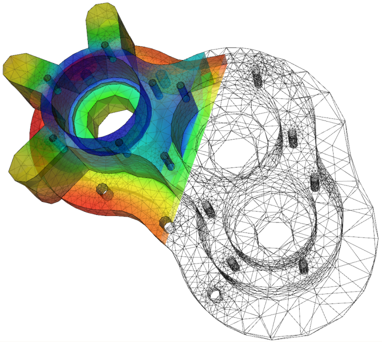
Weaknesses

- Unknown parameters
- Computationally expensive



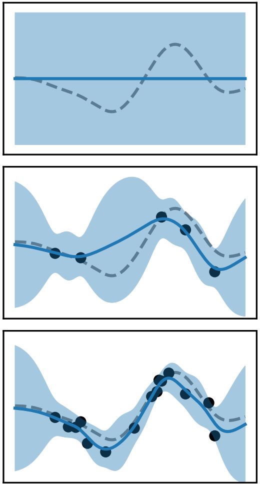
Machine Learning Models

Learning to predict from data.

Machine learning relies on statistical models.

Example: Supervised Learning

- parametric models (linear regression)
- hierarchical models (neural networks)
- probabilistic models (Gaussian processes)



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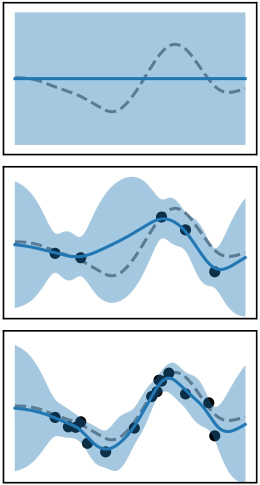
- Learn relationships from *unstructured* data
- Representation of uncertainty $\longrightarrow$ decision-making



Machine Learning Models

Learning to predict from data.

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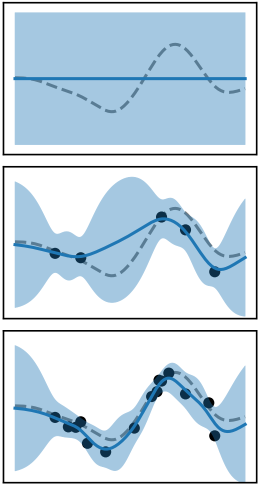
Strengths

- Learn relationships from *unstructured* data
- Representation of uncertainty $\longrightarrow$ decision-making

Weaknesses

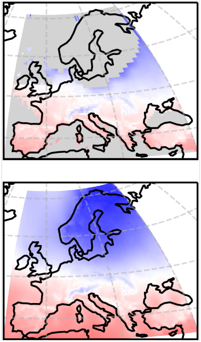
- Lack of guarantees
- Unclear or implicit assumptions



Combining Mechanistic and Statistical Models

...while retaining the benefits of both?

Modern science necessitates combining mechanistic and statistical models.



Axen et al. [2022]

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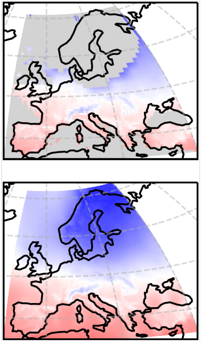
Why?

- Experiments produce volumes of unstructured, multi-modal data



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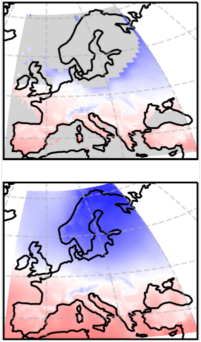

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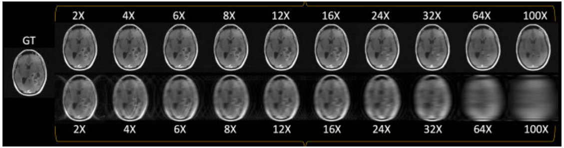

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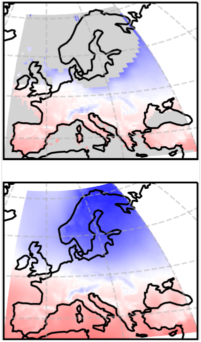

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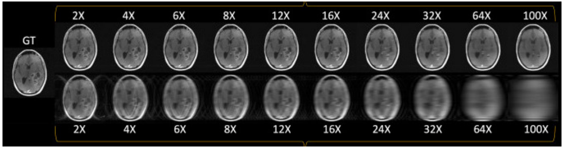

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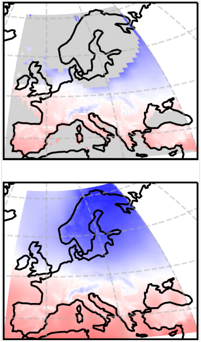

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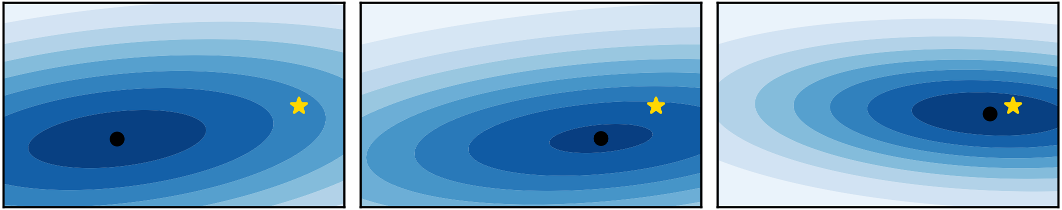
Sources of error / uncertainty: Limited computation and limited data.

Core Insights

- The solution to any numerical problem is fundamentally uncertain.



★ Solution $\boldsymbol{x}_*$ ● Estimate $\boldsymbol{x}_i = \mathbb{E}(\boldsymbol{x}_*)$ ▬ Belief $p(\boldsymbol{x}_*)$

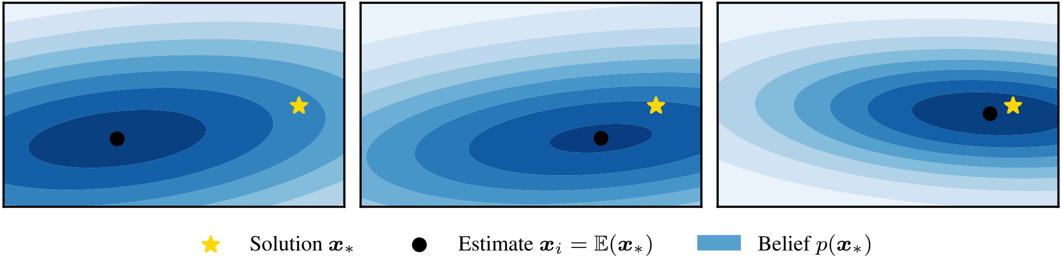
Probabilistic Numerics

Interpreting problems from numerical analysis as statistical inference.

Hennig et al. [2015], Cockayne et al. [2019]

Core Insights

- The solution to any numerical problem is fundamentally uncertain.
- Numerical algorithms are learning agents, which actively collect data and make predictions.



Linear Partial Differential Equations

Mechanistic models for thermal conduction, electromagnetism, wave mechanics, …

We look for a function $\boldsymbol{u} : \mathbb{D} \to \mathbb{R}^{d'}$ which solves the equation

$$\mathcal{D}_{\boldsymbol{\theta}}[\boldsymbol{u}] = f$$

on an open and bounded domain $\mathbb{D} \subset \mathbb{R}^d$, where $\mathcal{D}_{\boldsymbol{\theta}}$ is a linear differential operator and $f : \mathbb{D} \to \mathbb{R}$.

Typically, we require $\boldsymbol{u} \in \mathbb{U}$ and $f \in \mathbb{V}$ for Banach spaces $\mathbb{U}, \mathbb{V}$.

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Problems

- Usually no analytic solution $\Rightarrow$ numerical solvers necessary $\Rightarrow$ discretization error
- Parameters of the PDE (diffop parameters, right-hand side, etc.) are usually not known exactly

Physics-Informed Gaussian Process Regression

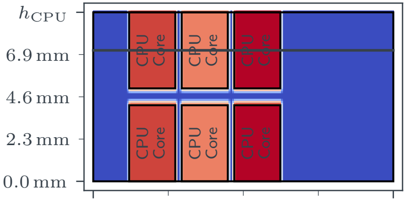
Case Study: The Heat Distribution in a CPU

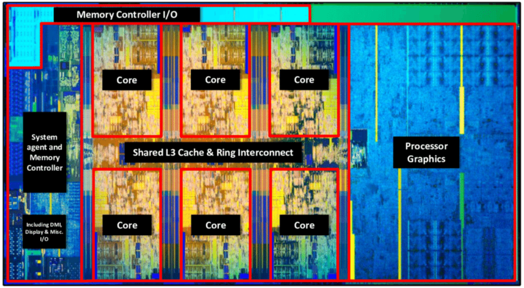
A Computer Scientist's Linear PDE

The Heat Distribution in a CPU

Spatial Domain: $\mathbb{D}_{\mathrm{CPU}} = [0, l_{\mathrm{CPU}}] \times [0, w_{\mathrm{CPU}}] \times [0, d_{\mathrm{CPU}}] \subset \mathbb{R}^3$

Spatial Domain: $\mathbb{D}_{\text{CPU,2D}} = [0, l_{\text{CPU}}] \times [0, w_{\text{CPU}}] \subset \mathbb{R}^2$





from Hebbar [2018]

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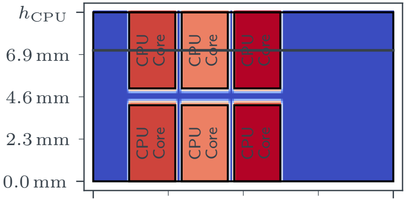
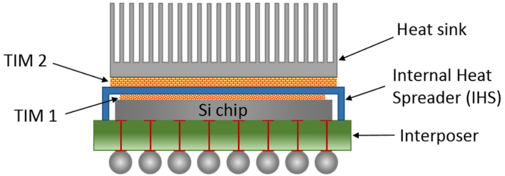
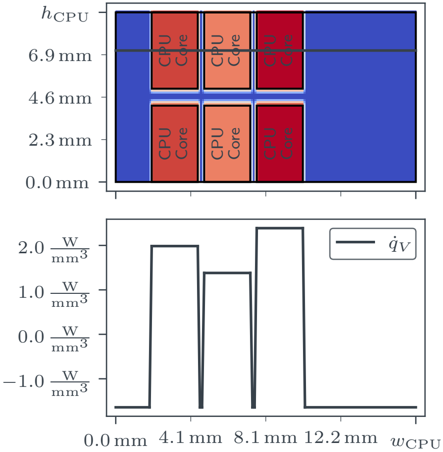
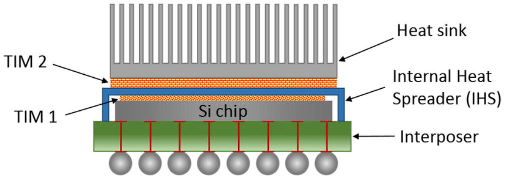




from Nylander [2018]

Spatial Domain: $\mathbb{D}_{\text{CPU,1D}} = [0, l_{\text{CPU}}] \subset \mathbb{R}$





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Heat Equation

$$c_p \rho \frac{\partial u}{\partial t} - \kappa \Delta u = \dot{q}_V,$$

where

- $u \colon [0, T] \times \mathbb{D} \to \mathbb{R}$ temperature
- c_p, ρ, κ material parameters
- $\dot{q}_V \colon [0, T] \times \mathbb{D} \to \mathbb{R}$ heat source

A Computer Scientist's Linear PDE II

The Heat Distribution in a CPU

Lienhard and Lienhard [2020]

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Stationary Heat Equation

$$-\kappa \Delta u = \dot{q}_V$$

where

- $u \colon \mathbb{D} \to \mathbb{R}$ temperature
- κ thermal conductivity
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Lienhard and Lienhard [2020]

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How can we phrase this as a learning problem?

(Linear) PDEs are Indirect Observations of Their Solution

Conservation Laws and Information Operators

Classic Notion of an Observation

$$u(\boldsymbol{x}_i) = f(\boldsymbol{x}_i) \iff \delta_{\boldsymbol{x}_i}[u] - f(\boldsymbol{x}_i) = 0$$

- Observations are point evaluations.
- Interpret as applying evaluation functional.

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- Observations are point evaluations.
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Generalized "Observation"

$$-\kappa \Delta u = \dot{q}_V \iff \mathcal{D}[u] - f = 0$$

- Heat equation is a conservation law.
- A conservation law is an observation of the behavior of the system u!

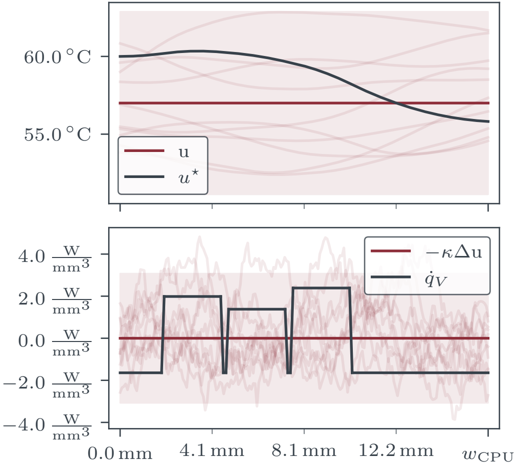
Idea: Relax notion of an observation to an *information operator* $\mathcal{I}[\mathbf{u}] := \mathcal{D}[\mathbf{u}] - f = 0$.

Prior

$$u \sim \mathcal{GP}(m, k)$$

Observations / Information Operators

$$\mathcal{I}_{\text{PDE}}[u] := -\kappa \Delta u(X_{\text{PDE}}) - \dot{q}_V(X_{\text{PDE}}) = \mathbf{0}$$



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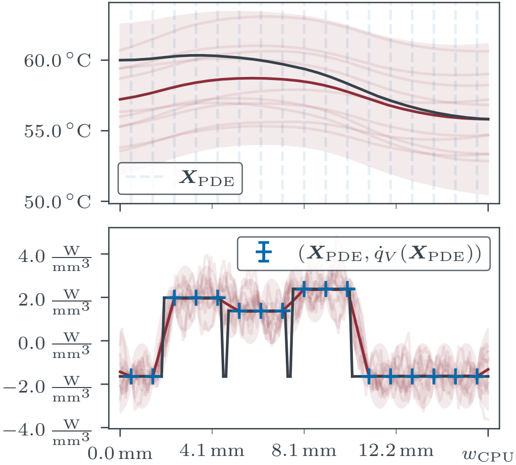
Posterior

$$\left(\mathrm{u} \mid \mathcal{I}_{\mathrm{PDE}}[\mathrm{u}] = \mathbf{0}\right) \Big| \mathcal{I}_{\mathrm{DBC}}[\mathrm{u}] = \mathbf{0} \sim \mathcal{GP}$$



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$$\mathcal{I}_{\mathsf{DBC}}[\mathsf{u}] := \mathsf{u}(X_{\mathsf{BC}}) - u^\star(X_{\mathsf{BC}}) = \mathbf{0}$$

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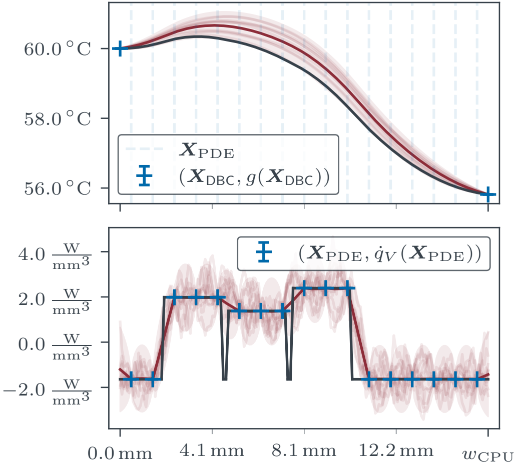
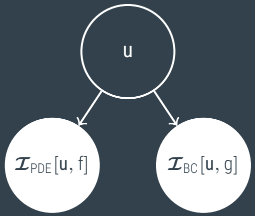


We have seen that GP inference can produce

- an approximate solution of the BVP, and
- an estimate of the approximation error.



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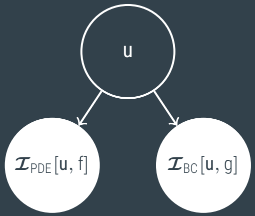
Unfortunately,

- the boundary values are unknown in deployment, and
- the values of the heat source distribution are uncertain.



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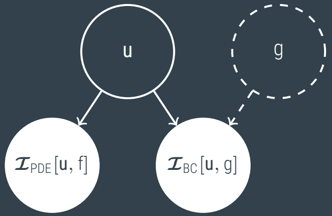

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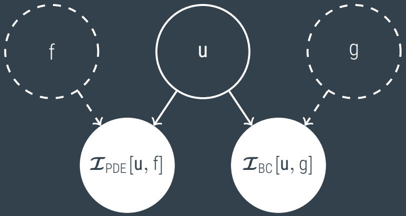

Epistemic Parameter Uncertainty and Measured Data

Uncertain Right-Hand Side

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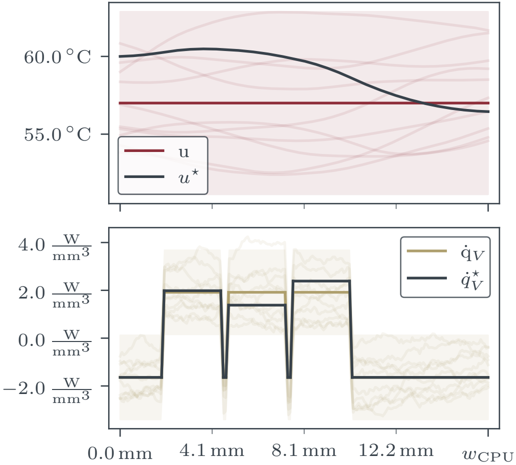
$$u \sim \mathcal{GP}(m_u, k_u)$$
$$\dot{q}_V \sim \mathcal{GP}(m_{\dot{q}_V}, k_{\dot{q}_V})$$

Information Operators



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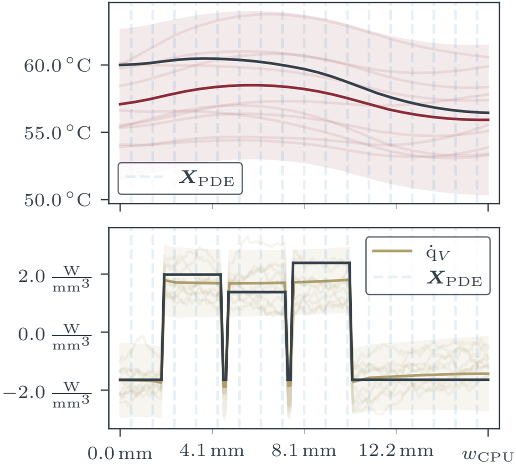
Information Operators

$$\mathcal{I}_{\mathrm{PDE}}[\mathrm{u}, \dot{q}_V] = -\kappa \Delta \mathrm{u}(X_{\mathrm{PDE}}) - \dot{q}_V(X_{\mathrm{PDE}}) = \mathbf{0}$$



Epistemic Parameter Uncertainty and Measured Data

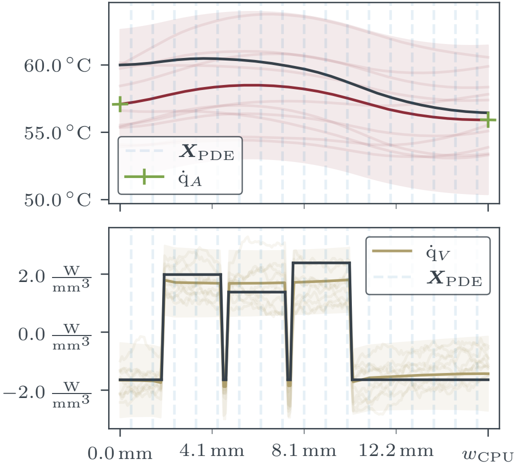
Uncertain Neumann Boundary Conditions

Prior

$$\mathrm{u} \sim \mathcal{GP}\left(m_{\mathrm{u}}, k_{\mathrm{u}}\right)$$
$$\dot{\mathrm{q}}_V \sim \mathcal{GP}\left(m_{\dot{\mathrm{q}}_V}, k_{\dot{\mathrm{q}}_V}\right)$$
$$\dot{\mathrm{q}}_A \sim \mathcal{GP}\left(m_{\dot{\mathrm{q}}_A}, k_{\dot{\mathrm{q}}_A}\right)$$

Information Operators

$$\mathcal{I}_{\mathrm{PDE}}[\mathrm{u}, \dot{\mathrm{q}}_V] = -\kappa \Delta \mathrm{u}\left(X_{\mathrm{PDE}}\right) - \dot{\mathrm{q}}_V\left(X_{\mathrm{PDE}}\right) = \mathbf{0}$$
$$\mathcal{I}_{\mathrm{NBC}}[\mathrm{u}, \dot{\mathrm{q}}_A] = -\kappa \partial_{\nu(X_{\mathrm{BC}})} \mathrm{u}\left(X_{\mathrm{BC}}\right) - \dot{\mathrm{q}}_A\left(X_{\mathrm{BC}}\right) = \mathbf{0}$$



Epistemic Parameter Uncertainty and Measured Data

Noisy Sensor Data

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$$u \sim \mathcal{GP}(m_u, k_u)$$
$$\dot{q}_V \sim \mathcal{GP}(m_{\dot{q}_V}, k_{\dot{q}_V})$$
$$\dot{q}_A \sim \mathcal{GP}(m_{\dot{q}_A}, k_{\dot{q}_A})$$
$$\epsilon_{\mathrm{DTS}} \sim \mathcal{N}(\mathbf{0}, \Sigma_{\mathrm{DTS}})$$

Information Operators

$$\mathcal{I}_{\mathrm{PDE}}[u, \dot{q}_V] = -\kappa \Delta u(X_{\mathrm{PDE}}) - \dot{q}_V(X_{\mathrm{PDE}}) = \mathbf{0}$$
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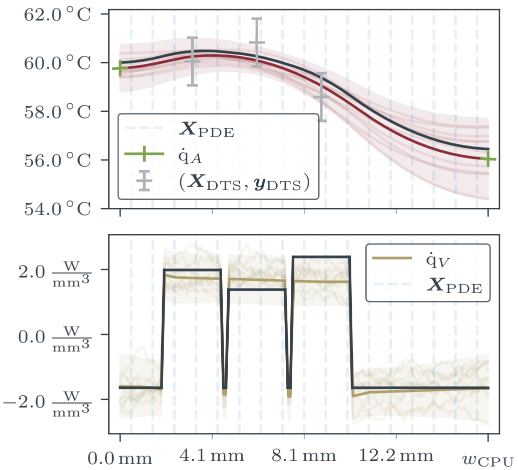
$$\mathcal{I}_{\mathrm{DTS}}[u, \epsilon_{\mathrm{DTS}}] = u(X_{\mathrm{DTS}}) + \epsilon_{\mathrm{DTS}} = y_{\mathrm{DTS}}$$



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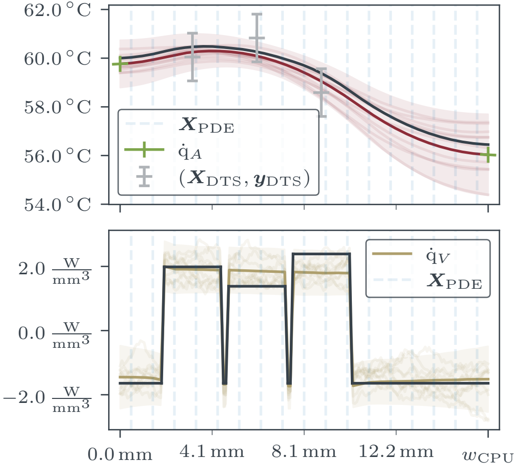
$$\mathcal{I}_{\mathrm{DTS}}[\mathrm{u}, \boldsymbol{\epsilon}_{\mathrm{DTS}}] = \mathrm{u}(X_{\mathrm{DTS}}) + \boldsymbol{\epsilon}_{\mathrm{DTS}} = y_{\mathrm{DTS}}$$
$$\mathcal{I}_{\mathrm{STAT}}[\dot{\mathrm{q}}_V, \dot{\mathrm{q}}_A] = d_{\mathrm{CPU}} \int_{\mathbb{D}} \dot{\mathrm{q}}_V \, dx - \int_{\partial \mathbb{D}} \dot{\mathrm{q}}_A \, dS = 0$$



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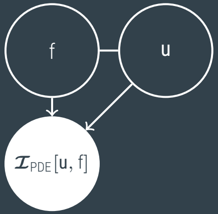

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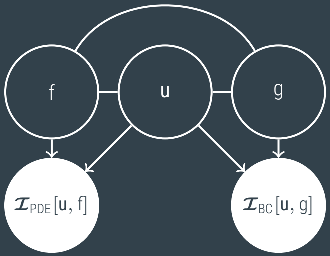
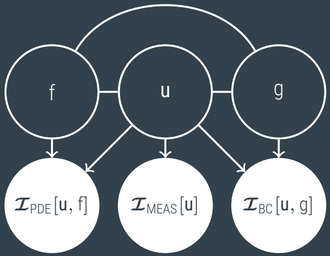
- mechanistic knowledge in the form of linear PDEs with uncertain right-hand sides,
- uncertain boundary conditions, and



The GP approach integrates enables seamless integration of

- prior knowledge about the solution,
- mechanistic knowledge in the form of linear PDEs with uncertain right-hand sides,
- uncertain boundary conditions, and
- noisy empirical measurements,



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- prior knowledge about the solution,
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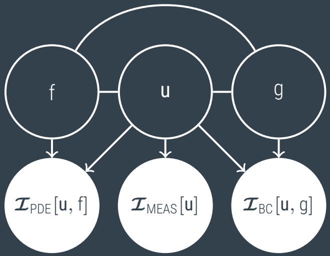

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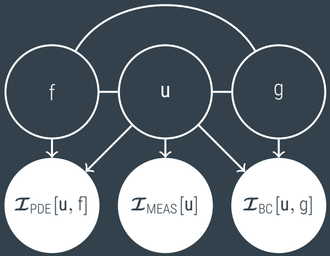

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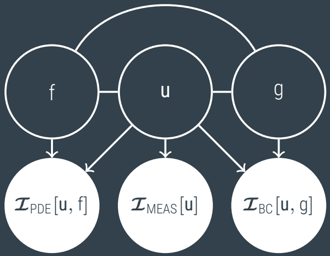

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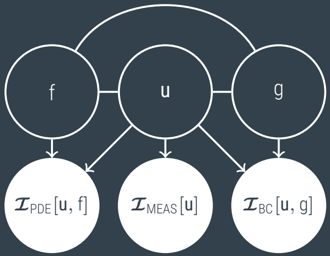
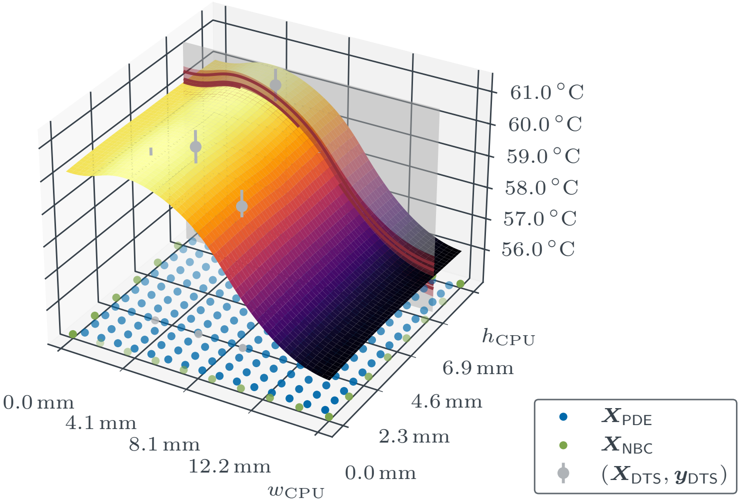
- a Bayesian solution to the inverse problem of estimating the right-hand side and boundary function from data.



All this is only possible because we give up on trying to identify a single unique solution in favor of a probability measure over infinitely many solution candidates.

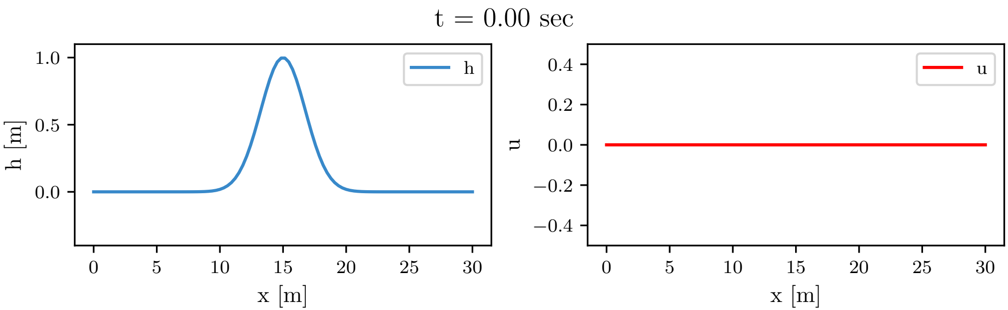
2D Version of the CPU Simulation



Example: Systems of Time-Dependent PDEs

The (Linearized) Shallow Water / Saint-Venant Equations

Credit: Tim Weiland



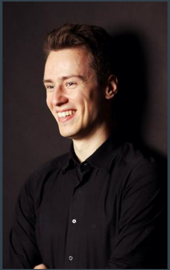
Physics-Informed Gaussian Process Regression Generalizes Linear PDE Solvers

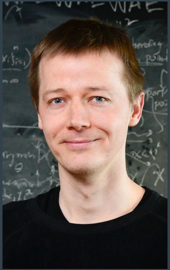
Marvin Pförtner, Ingo Steinwart, Philipp Hennig, Jonathan Wenger

- PDEs can be solved via GP inference $\Rightarrow$ structured uncertainty
- GPs provide a rigorous framework for probabilistic inference of unknown functions from heterogeneous information sources provided by affine information operators
- A vast class of classical PDE solvers (methods of weighted residuals) can be recovered in the mean of a GP posterior
- Proof of GP inference theorem with bounded linear operator observations in separable Banach path spaces

Paper / 2212.12474

Code / marvinpfoertner / linpde-gp





Generalized Gaussian Process Inference

A well-known conjecture...

Prior $\mathrm{u} \sim \mathcal{GP}(m, k)$ with paths in $\mathbb{U} \subset \mathbb{R}^{\mathbb{D}}$

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Observations $\mathbf{y} = \mathcal{L}[\mathrm{u}] + \boldsymbol{\epsilon}$, where

- $\mathcal{L} : \mathbb{U} \to \mathbb{R}^n$ linear (e.g. $\mathcal{L}_i = \mathcal{D}[\cdot](\boldsymbol{x}_i)$)
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Predictive $\boldsymbol{\mathcal{L}}[\mathrm{u}] + \boldsymbol{\epsilon} \sim \mathcal{N}\left(\boldsymbol{\mathcal{L}}[m], \boldsymbol{\mathcal{L}} k \boldsymbol{\mathcal{L}}' + \boldsymbol{\Sigma}\right)$, where

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Posterior $\mathrm{u} \mid \boldsymbol{\mathcal{L}}[\mathrm{u}] + \boldsymbol{\epsilon} = \boldsymbol{y} \sim \mathcal{GP}\left(m^{\mathrm{u}|\boldsymbol{y}}, k^{\mathrm{u}|\boldsymbol{y}}\right)$, where

$$m^{\mathrm{u}|\boldsymbol{y}}(\boldsymbol{x}) := m(\boldsymbol{x}) + \boldsymbol{\mathcal{L}}[k(\cdot, \boldsymbol{x})]^\top \left(\boldsymbol{\mathcal{L}} k \boldsymbol{\mathcal{L}}' + \boldsymbol{\Sigma}\right)^\dagger (\boldsymbol{y} - \boldsymbol{\mathcal{L}}[m])$$

$$k^{\mathrm{u}|\boldsymbol{y}}(\boldsymbol{x}_1, \boldsymbol{x}_2) := k(\boldsymbol{x}_1, \boldsymbol{x}_2) - \boldsymbol{\mathcal{L}}[k(\cdot, \boldsymbol{x}_1)]^\top \left(\boldsymbol{\mathcal{L}} k \boldsymbol{\mathcal{L}}' + \boldsymbol{\Sigma}\right)^\dagger \boldsymbol{\mathcal{L}}[k(\cdot, \boldsymbol{x}_2)]$$

Connections to Classical Methods

MWR Information Operators

MWR Information Operators

From Dirac to Galerkin

[Pförtner et al., 2022, Section 3.3]

$$\mathcal{I}^{\mathrm{PDE}}[\mathrm{u}, \mathrm{f}] = \mathcal{D}[\mathrm{u}](X_{\mathrm{PDE}}) - \mathrm{f}(X_{\mathrm{PDE}})$$

- $\mathbb{U}, \mathbb{V}$ (separable) Banach spaces
- paths $(\mathrm{u}) \subset \mathbb{U}$ and paths $(\mathrm{f}) \subset \mathbb{V}$ (or continuously embedded)
- $\mathcal{D} \colon \mathbb{U} \to \mathbb{V}$ linear and bounded

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Example (Ritz-Galerkin Method)

- $\mathbb{U} = H^1(\mathbb{D})$, $\mathbb{V} = H^1_0(\mathbb{D})$
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- $\ell^{(i)}$ induced by test functions $\psi^{(i)} \in \mathbb{V} \hookrightarrow \mathbb{V}''$

  $\Rightarrow \ell^{(i)}[\mathcal{D}^{W}[u]] = \mathcal{D}^{W}[u](\psi^{(i)})$

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- choose $\mathcal{P}_{\hat{\mathbb{U}}}$ e.g. as L_2 projection onto $\hat{\mathbb{U}}$

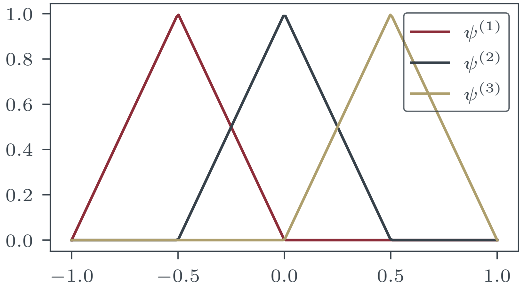
$$\mathcal{P}_{\hat{\mathbb{U}}}[\mathsf{u}] = \sum_{i=1}^{n} \phi^{(i)} \sum_{j=1}^{n} (P^{-1})_{ij} \langle \phi^{(j)}, \mathsf{u} \rangle_{L_2},$$

where $P_{ij} = \langle \phi^{(i)}, \phi^{(j)} \rangle_{L_2}$

Example: The Finite Element Method for the 1D Poisson Equation

A Ritz-Galerkin Method with Locally Supported Trial Functions

Test Functions: Linear Lagrange Elements



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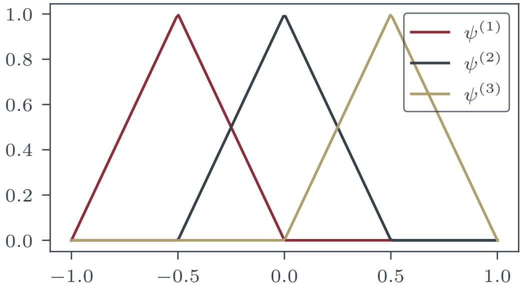
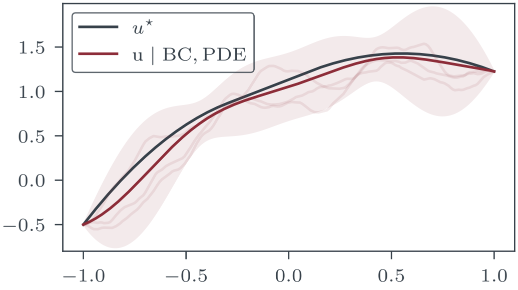
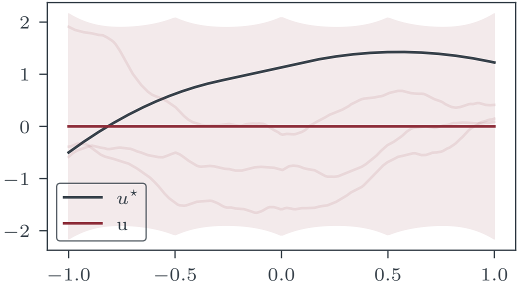


GP Posterior



Matérn-$\frac{3}{2}$ Prior Covariance $\Rightarrow$ paths $(\mathrm{u}) \subset H^1(\mathbb{D})$

MWR Recovery Prior



$$
\begin{aligned}
k^{\mathrm{MWR}} &:= \mathcal{P}_{\hat{\mathbb{U}}} k \mathcal{P}'_{\hat{\mathbb{U}}} + \mathcal{P}_{\ker(\mathcal{P}_{\hat{\mathbb{U}}})} k \mathcal{P}'_{\ker(\mathcal{P}_{\hat{\mathbb{U}}})} \\
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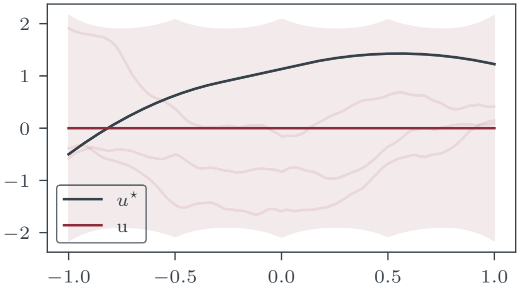

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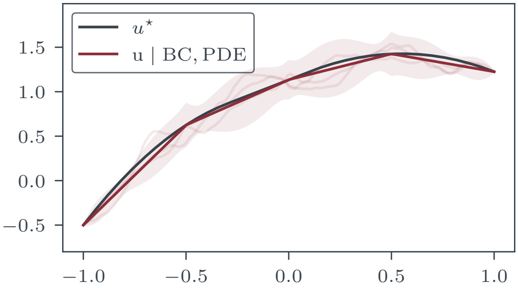
Posterior



Connections to Classical Methods

Weighted Residual Methods Through the Lens of GP Inference

[Pförtner et al., 2022, Section 3.3]

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$\Rightarrow$ GP-based approaches as uncertainty-aware drop-in replacements for classical methods

Theoretical Backbone

Gaussian Process Regression with Linear Operator Observations

Definition (Gaussian Process)

A Gaussian process is a family of random variables $\{\omega \mapsto \mathrm{f}(x, \omega)\}_{x \in \mathbb{X}}$ on a common Borel probability space $(\Omega, \mathcal{B}(\Omega), \mathrm{P})$ such that every finite combination $f(x_1, \cdot), \dots, f(x_n, \cdot)$ of the random variables follows a multivariate normal distribution.

Gaussian Process Regression with Linear Operator Observations I

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EBERHARD KARLS UNIVERSITÄT TÜBINGEN

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- for a generic GP, we can only reason about finitely many evaluations
- some of the observation operators we care about (partial derivatives and integrals) implicitly operate on an infinite set of evaluations
- to apply existing results, we need $\omega \mapsto (\mathrm{f}(\boldsymbol{X}, \omega), \boldsymbol{\mathcal{L}}[\mathrm{f}(\cdot, \omega)])$ to be a Gaussian random variable, but it is unclear if this is even measurable

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Definition (Gaussian Process)

A Gaussian process is a family of random variables $\{\omega \mapsto \mathrm{f}(\boldsymbol{x}, \omega)\}_{\boldsymbol{x} \in \mathbb{X}}$ on a common Borel probability space $(\Omega, \mathcal{B}(\Omega), \mathrm{P})$ such that every finite combination $f(\boldsymbol{x}_1, \cdot), \dots, f(\boldsymbol{x}_n, \cdot)$ of the random variables follows a multivariate normal distribution.

- for a generic GP, we can only reason about finitely many evaluations
- some of the observation operators we care about (partial derivatives and integrals) implicitly operate on an infinite set of evaluations
- to apply existing results, we need $\omega \mapsto (\mathrm{f}(\boldsymbol{X}, \omega), \boldsymbol{\mathcal{L}}[\mathrm{f}(\cdot, \omega)])$ to be a Gaussian random variable, but it is unclear if this is even measurable
- theoretical results should be easily applicable to GPs specified via their mean and covariance functions (as opposed to projections of Gaussian measures in functions spaces)

Gaussian Process Regression with Linear Operator Observations II

EBERHARD KARLS UNIVERSITÄT TÜBINGEN

Theorem (Pförtner et al. 2022, Theorem 1)

Let $\mathrm{f} \sim \mathcal{GP}(m, k)$ *be a Gaussian process prior with index set* $\mathbb{X}$ *on the probability space* $(\Omega, \mathcal{F}, \mathrm{P})$*, whose paths lie in a real separable reproducing kernel Banach space (RKBS)* $\mathbb{B} \subset \mathbb{R}^{\mathbb{X}}$ *such that* $\omega \mapsto \mathrm{f}(\cdot, \omega)$ *is a* $\mathbb{B}$*-valued Gaussian random variable. Let* $\mathcal{L} \colon \mathbb{B} \to \mathbb{R}^n$ *be a bounded linear operator. Then*

$$\mathcal{L}[\mathrm{f}] \sim \mathcal{N}\left(\mathcal{L}[m], \mathcal{L}k\mathcal{L}'\right).$$

Let $\boldsymbol{\epsilon} \sim \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$ *be an* $\mathbb{R}^n$*-valued Gaussian random vector with* $\boldsymbol{\epsilon} \perp\!\!\!\perp \mathrm{f}$*. Then, for any* $\boldsymbol{y} \in \mathbb{R}^n$*,*

$$\mathrm{f} \mid \mathcal{L}[\mathrm{f}] + \boldsymbol{\epsilon} = \boldsymbol{y} \sim \mathcal{GP}\left(m^{\mathrm{f}|\boldsymbol{y}}, k^{\mathrm{f}|\boldsymbol{y}}\right),$$

with conditional mean and covariance function given by

$$m^{\mathrm{f}|\boldsymbol{y}}(\boldsymbol{x}) = m(\boldsymbol{x}) + \mathcal{L}[k(\boldsymbol{x}, \cdot)]^\top \left(\mathcal{L}k\mathcal{L}' + \boldsymbol{\Sigma}\right)^\dagger (\boldsymbol{y} - (\mathcal{L}[m] + \boldsymbol{\mu})), \quad \text{and}$$

$$k^{\mathrm{f}|\boldsymbol{y}}(\boldsymbol{x}_1, \boldsymbol{x}_2) = k(\boldsymbol{x}_1, \boldsymbol{x}_2) - \mathcal{L}[k(\boldsymbol{x}_1, \cdot)]^\top \left(\mathcal{L}k\mathcal{L}' + \boldsymbol{\Sigma}\right)^\dagger \mathcal{L}[k(\cdot, \boldsymbol{x}_2)].$$

- We show that the assumptions of the theorem are fulfilled for Gaussian processes with
  - paths in any separable reproducing kernel Hilbert space $\mathbb{H}$
    $\Rightarrow \mathbb{B} = \mathbb{H}$
    $\Rightarrow$ Sobolev spaces [see Steinwart, 2019, Kanagawa et al., 2018]

Gaussian Process Regression with Linear Operator Observations III

On Prior Selection

[Pförtner et al., 2022, Sections B.2 and B.4]

- We show that the assumptions of the theorem are fulfilled for Gaussian processes with
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  - continuous paths on a compact domain $\Rightarrow \mathbb{B} = C(\mathbb{D})$

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  - continuous paths on a compact domain $\Rightarrow \mathbb{B} = C(\mathbb{D})$
  - continuously differentiable paths with bounded and uniformly continuous partial derivatives
    $\Rightarrow \mathbb{B} = C^k(\overline{\mathbb{D}})$ or $\mathbb{B} = C^{\boldsymbol{\alpha}}(\overline{\mathbb{D}})$
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- in these spaces, the most important observation operators (point evaluated partial derivatives and integrals) are bounded
- path properties can be verified from properties of the covariance function [see e.g. Adler and Taylor, 2007]

- a GP whose covariance function is a tensor product of 1D Matérn-$(p_i + \frac{1}{2})$ kernels has paths in $\mathbb{B} = C^{(p_1, \dots, p_d)}(\overline{\mathbb{D}})$ [Wang et al., 2021]

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- a GP with Gaussian covariance function has smooth paths (i.e. $\mathbb{B} = C^k(\overline{\mathbb{D}})$ for any $k \geq 0$)
- a GP with Matérn-($p + \frac{1}{2}$) covariance function has paths in an RKHS which is norm-equivalent to the Sobolev space $H^p(\mathbb{D})$ (under mild assumptions on the domain $\mathbb{D}$, see Kanagawa et al. 2018)

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