Functional-input Gaussian processes with applications to inverse scattering problems

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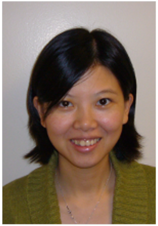
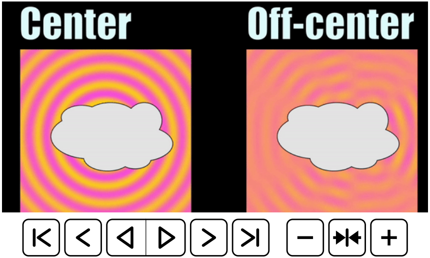


Ying Hung (Rutgers)

Outline

Inverse Scattering Problems

- **Inverse scattering problem** is the problem of determining characteristics of an object, based on data of how it scatters incoming radiation or particles.



Credit to YouTube: Inverse Scattering 101 (Feat. Fioralba Cakoni) by Inverse Problems Channel

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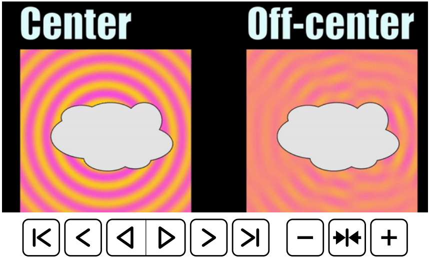

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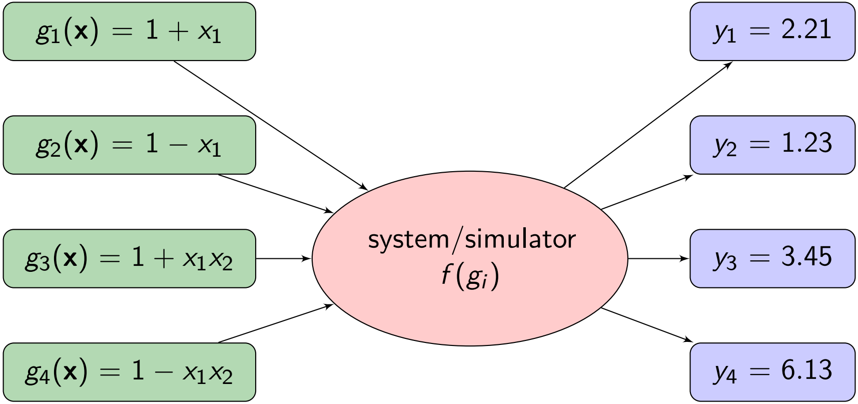
- Typically **the input is a function** that represents the material properties of an inhomogeneous isotropic scattering region of interest

Inverse Scattering Problems



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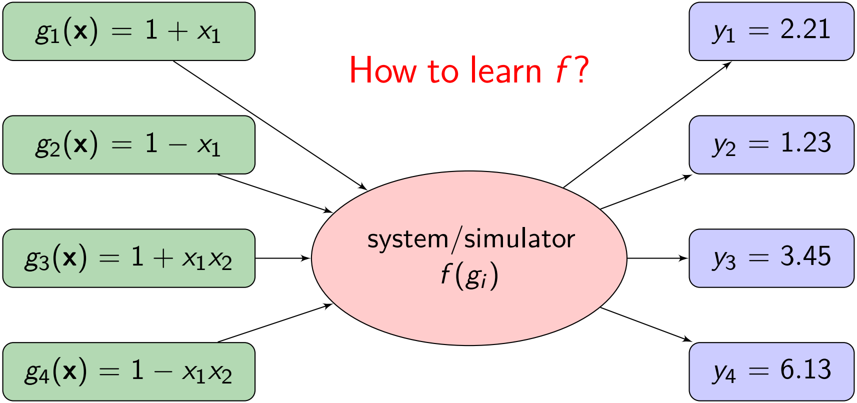

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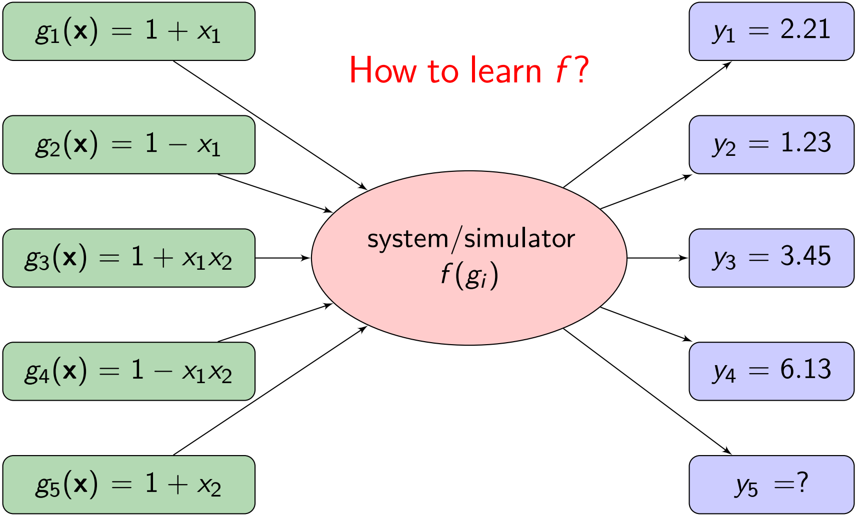

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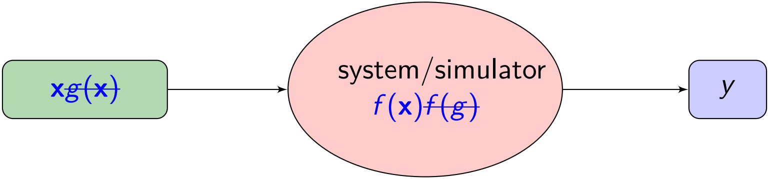

- $\mathbf{x}$ is the input in a Euclidean space.

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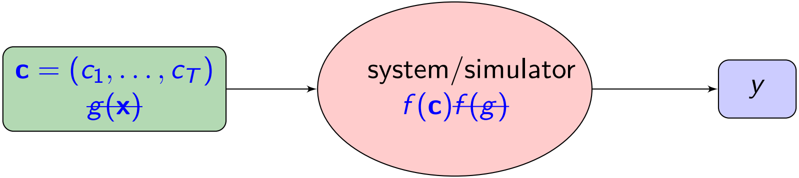

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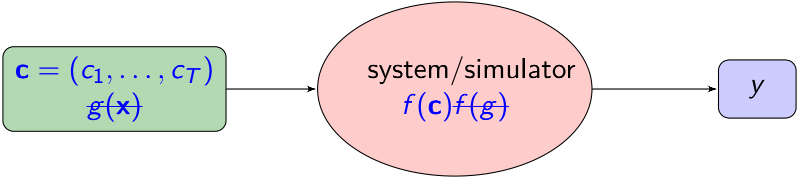

- How to choose T? How to take the approximation error into account?
- What if the dimension of $\mathbf{x}$ is greater than 3? Curse of dimensionality!

Our contributions

- We propose a new model (called FIGP) that directly uses the functional input without the need of basis expansion!
- Like conventional Gaussian processes (GPs), FIGP provides predictions as well as uncertainty quantification (confidence intervals).
- Theoretical properties are provided, including the convergence rates of the mean squared prediction errors (MSPE) and the connections to experimental design.

Functional-input Gaussian Process (FIGP)

- Suppose that V is a functional space consisting of functions defined on a compact and convex region $\Omega \subseteq \mathbb{R}^d$.

- $g \in V$ are continuous on Ω, i.e., $V \subset C(\Omega)$.

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- A functional-input GP, $f : V \to \mathbb{R}$, is denoted by

$$f(g) \sim \mathcal{FIGP}(\mu, K(g, g')),$$

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- How to define $K(g, g')$? Will go back to this soon.

Prediction and Uncertainty Quantification

- Suppose that $g_1, g_2, \ldots, g_n$ are the inputs and the outputs $\{f(g_i)\}_{i=1}^n$ are observed.

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- The outputs $\{f(g_i)\}_{i=1}^n$ follow a multivariate normal distribution,

$$(f(g_1), \ldots, f(g_n))' \sim \mathcal{N}_n(\boldsymbol{\mu}_n, \mathbf{K}_n),$$

where mean $\boldsymbol{\mu}_n = \mu \mathbf{1}_n$ and covariance $\mathbf{K}_n$ with $(\mathbf{K}_n)_{j,k} = K(g_j, g_k)$.

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- The hyperparameters in the kernel function K and mean parameter μ can be estimated by likelihood-based approaches or Bayesian approaches

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Prediction and Uncertainty Quantification

- Suppose $g \in V$ is an untried new input.
- The corresponding output $f(g)$ follows a normal distribution with the mean and variance,

$$f(g) \sim \mathcal{N}(\mu(g), \sigma^2(g)),$$

where

$$\mu(g) = \mu + \mathbf{k}_n(g)^T \mathbf{K}_n^{-1}(\mathbf{y}_n - \boldsymbol{\mu}_n),$$

$$\sigma^2(g) = K(g,g) - \mathbf{k}_n(g)^T \mathbf{K}_n^{-1}\mathbf{k}_n(g),$$

where $\mathbf{y}_n^T = (f(g_1), \ldots, f(g_n))$ and $\mathbf{k}_n(g) = (K(g,g_1), ..., K(g,g_n))^T$.

A New Class of Kernel Functions

- How to define a kernel function $K(g, g')$ on $V \times V$?

A New Class of Kernel Functions

- How to define a kernel function $K(g, g')$ on $V \times V$?
- We propose a new class of kernel functions:
  - linear kernels and nonlinear kernels.
- The asymptotic convergence properties of the resulting MSPEs will be provided.

Linear Kernel

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- By Mercer's theorem, we have

$$\Psi(\mathbf{x},\mathbf{x}')=\sum_{j=1}^{\infty}\lambda_j\phi_j(\mathbf{x})\phi_j(\mathbf{x}'),$$

where $\mathbf{x},\mathbf{x}'\in\Omega$, and $\lambda_1\geq\lambda_2\geq\ldots>0$ and $\{\phi_k\}_{k\in\mathbb{N}}$ are the eigenvalues and the orthonormal basis in $L_2(\Omega)$, respectively.

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- We construct a GP via the Karhunen–Loève expansion:

$$f(g\cancel{\mathbf{x}})=\sum_{j=1}^{\infty}\sqrt{\lambda_j}\langle\phi_j,g\cancel{\mathbf{x}}\rangle_{L_2(\Omega)}Z_j,$$

where Z_j's are independent standard normal random variables.

Linear Kernel

Definition: linear kernel function for FIGP

For $g_1, g_2 \in V$,

$$K(g_1, g_2) = \int_\Omega \int_\Omega g_1(\mathbf{x}) g_2(\mathbf{x}') \Psi(\mathbf{x}, \mathbf{x}') \mathrm{d}\mathbf{x} \mathrm{d}\mathbf{x}',$$

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Proposition 2: linearity

The FIGP, $f(g)$, constructed based on the linear kernel is linear, i.e., for any $a, b \in \mathbb{R}$ and $g_1, g_2 \in V$, it follows that

$$f(ag_1 + bg_2) = af(g_1) + bf(g_2).$$

Theoretical Properties of Linear Kernels

Assumption: Matérn kernel Ψ

$$\Psi(\mathbf{x},\mathbf{x}')=\psi(\|\Theta(\mathbf{x}-\mathbf{x}')\|_2)$$

with

$$\psi(r)=\frac{\sigma^2}{\Gamma(\nu)2^{\nu-1}}(2\sqrt{\nu}r)^{\nu}B_{\nu}(2\sqrt{\nu}r),$$

- ν: smoothness parameter
- Θ: lengthscale parameter
- σ^2: scalar parameter
- B_ν: the modified Bessel function of the second kind

Theoretical Properties of Linear Kernels

Corollary 1: MSPE convergence

Suppose g_j, $j = 1, \ldots, n$ are the first n eigenfunctions of Ψ, i.e, $g_j = \phi_j$. For $g \in \mathcal{N}_\Psi(\Omega)$, there exists a constant $C_1 > 0$ such that

$$\mathbb{E}\left(f(g) - \mu(g)\right)^2 \leq C_1 \|g\|^2_{\mathcal{N}_\Psi(\Omega)} n^{-\frac{4\nu}{d}}.$$

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Corollary 2: MSPE convergence

Define $\mathbf{X}_n \equiv \{\mathbf{x}_1, \ldots, \mathbf{x}_n\}$. Suppose $\mathbf{X}_n$ is quasi-uniform and $g_j(\mathbf{x}) = \Psi(\mathbf{x}, \mathbf{x}_j)$, where $\mathbf{x}, \mathbf{x}_j \in \Omega$ for $j = 1, \ldots, n$. For $g \in \mathcal{N}_\Psi(\Omega)$, there exists a constant $C_2 > 0$ such that

$$\mathbb{E}\left(f(g) - \mu(g)\right)^2 \leq C_2 \|g\|^2_{\mathcal{N}_\Psi(\Omega)} n^{-\frac{2\nu}{d}}.$$

Extension to Nonlinear Kernel

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$$f(g) = \sum_{j=1}^{\infty} \sqrt{\lambda_j} \langle \phi_j, \mathcal{M} \circ g \rangle_{L_2(\Omega)} Z_j,$$

which results in a nonlinear kernel function

$$K(g_1, g_2) = \int_\Omega \int_\Omega \mathcal{M} \circ g_1(\mathbf{x}) \mathcal{M} \circ g_2(\mathbf{x}') \Psi(\mathbf{x}, \mathbf{x}') \mathrm{d}\mathbf{x} \mathrm{d}\mathbf{x}'$$

- How to specify $\mathcal{M}$? There are many possible ways!

Nonlinear Kernel

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- Let $\psi(r) : \mathbb{R}^+ \to \mathbb{R}$ be a radial basis function whose corresponding kernel in $\mathbb{R}^d$ is strictly positive definite for any $d \geq 1$.

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- For example, if ψ is the radial basis function whose corresponding kernel is a Gaussian kernel, then

$$K(g_1, g_2) = \exp(-\gamma^2 \|g_1 - g_2\|^2_{L_2(\Omega)}).$$

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Corollary 3: MSPE convergence

Suppose that Φ is a Matérn kernel function with smoothness ν_1, and ψ is the radial basis function whose corresponding kernel is Matérn with smoothness ν. For any $n > N_0$ with a constant N_0, there exist n input functions such that for any $g \in \mathcal{N}_\Phi(\Omega)$ with $\|g\|_{\mathcal{N}_\Phi(\Omega)} \leq 1$, the MSPE can be bounded by

$$\mathbb{E}\left(f(g) - \mu(g)\right)^2 \leq C_3(\log n)^{-\frac{(\nu_1+d/2)\tau}{d}} \log\log n.$$

Selection of kernels

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- Leave-one-out cross-validation (LOOCV) error:

$$\frac{1}{n}\sum_{i=1}^{n}(y_i-\tilde{y}_i)^2=\frac{1}{n}\|\mathbf{\Lambda}_n^{-1}\mathbf{K}_n^{-1}(\mathbf{y}_n-\mu\mathbf{1}_n)\|_2^2,$$

  where $\mathbf{\Lambda}_n$ is a diagonal matrix with the element $(\mathbf{\Lambda}_n)_{j,j}=(\mathbf{K}_n^{-1})_{j,j}$.

- Choose the one that has a smaller LOOCV error.

Numerical Studies

- $\Omega \in [0,1]^2$
- test function 1: $f_1(g) = \int_\Omega \int_\Omega g(\mathbf{x}) \mathrm{d}x_1 \mathrm{d}x_2$ (linear)
- test function 2: $f_2(g) = \int_\Omega \int_\Omega g(\mathbf{x})^3 \mathrm{d}x_1 \mathrm{d}x_2$ (nonlinear)
- test function 3: $f_3(g) = \int_\Omega \int_\Omega \sin(g(\mathbf{x})^2) \mathrm{d}x_1 \mathrm{d}x_2$(nonlinear)

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$g(\mathbf{x})$	$x_1 + x_2$	x_1^2	x_2^2	$1 + x_1$	$1 + x_2$	$1 + x_1 x_2$	$\sin(x_1)$	$\cos(x_1 + x_2)$
$f_1(g)$	1	0.33	0.33	1.5	1.5	1.25	0.46	0.50
$f_2(g)$	1.5	0.14	0.14	3.75	3.75	2.15	0.18	0.26
$f_3(g)$	0.62	0.19	0.19	0.49	0.49	0.84	0.26	0.33

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$f_3(g)$	0.62	0.19	0.19	0.49	0.49	0.84	0.26	0.33

$g(\mathbf{x})$	$\sin(0.3x_1 + 0.7x_2)$	$0.2 + x_1^2 + x_2^3$	$\exp\{-0.6x_1x_2\}$
$f_1(g)$	?	?	?
$f_2(g)$	?	?	?
$f_3(g)$	?	?	?

Numerical Studies

	Kernel	$f_1(g) = \int_\Omega \int_\Omega g$	$f_2(g) = \int_\Omega \int_\Omega g^3$	$f_3(g) = \int_\Omega \int_\Omega \sin(g^2)$
LOOCV	linear	$\mathbf{8.0 \times 10^{-7}}$	0.380	0.095
	nonlinear	2.1×10^{-6}	**0.227**	**0.017**

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$g(\mathbf{x})$		$\sin(0.3x_1 + 0.7x_2)$	$0.2 + x_1^2 + x_2^3$	$\exp\{-0.6x_1x_2\}$
$f_1(g)$	ture	0.468	0.783	0.868
	FIGP	0.468 [0.4674, 0.4684]	0.783 [0.7745, 0.7921]	0.868 [0.8673, 0.8686]
$f_2(g)$	ture	0.152	0.919	0.683
	FIGP	0.137 [-0.1868, 0.4609]	0.831 [0.2083, 1.4540]	0.774 [0.0346, 1.513]
$f_3(g)$	ture	0.248	0.483	0.682
	FIGP	0.240 [0.0404, 0.4395]	0.455 [0.1801, 0.7305]	0.482 [0.1412, 0.8231]

Numerical Studies

- test input 1: $g_9(\mathbf{x}) = \sin(\alpha_1 x_1 + \alpha_2 x_2)$ with $\alpha_1, \alpha_2 \sim U(0,1)$
- test input 2: $g_{10}(\mathbf{x}) = \beta + x_1^2 + x_2^3$ with $\beta \sim U(0,1)$
- test input 3: $g_{11}(\mathbf{x}) = \exp\{-\kappa x_1 x_2\}$ with $\kappa \sim U(0,1)$
- Simulate 100 times:

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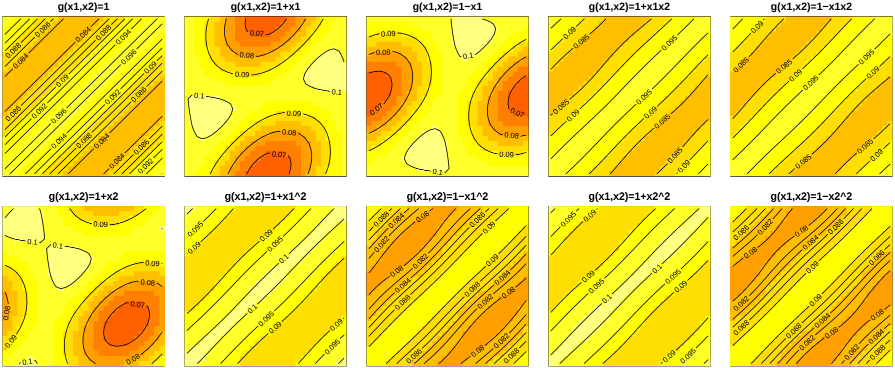
Measurements	Method	$f_1(g) = \int_\Omega \int_\Omega g$	$f_2(g) = \int_\Omega \int_\Omega g^2$	$f_3(g) = \int_\Omega \int_\Omega \sin(g)$
MSE	FIGP	$\mathbf{8.3 \times 10^{-8}}$	**1.176**	**1.640**
	FPCA	0.0017	8.870	2.356
	Taylor	6.144	108.928	6.954
Coverage (%)	FIGP	**100**	**100**	**100**
	FPCA	75.33	79.00	49.67
	Taylor	**100**	**100**	66.67
Score	FIGP	**14.740**	**2.571**	**3.458**
	FPCA	4.587	-1.991	-12.208
	Taylor	2.0597	-1.0283	0.4039

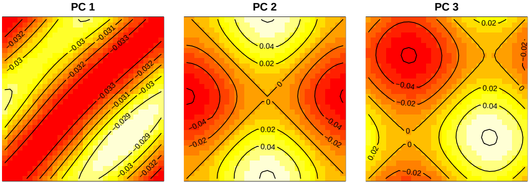
Application: Inverse Scattering Problems



Training data

Application: Inverse Scattering Problems

- The outputs are images!
- The folllowing 3 principle components can explain more than 99.9% variations of the data.



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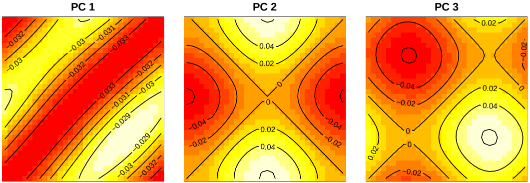

- The output becomes a 3-dimensional vector: $f_1(g), f_2(g)$ and $f_3(g)$
- Fit an FIGP separately on these three outputs

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- test input: $g(\mathbf{x}) = 1 - \sin(x_2)$

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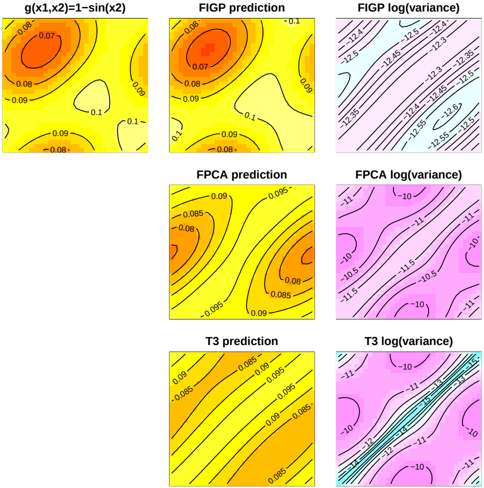


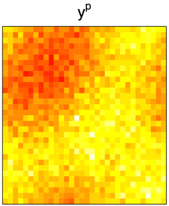
Conclusion

- We propose a new model (FIGP) for problems with functional inputs.
- Numerical studies show that the FIGP provides accurate predictions and uncertainty quantification.
- Theoretical properties of the convergence rate of the mean squared prediction error for FIGP are developed.
- Inverse scattering problems?

Bayesian Approach for Functional Inverse

- Assume $g(\mathbf{x})$ follows a GP prior:

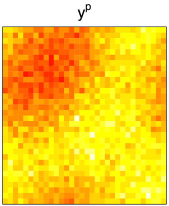
$$g(\mathbf{x})|\boldsymbol{\eta}, \sigma_g^2 \sim \mathcal{GP}(0, \tau_g^2 \Phi_{\boldsymbol{\eta}}(\mathbf{x}, \mathbf{x}'))$$

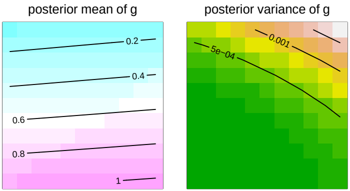


Bayesian Approach for Functional Inverse

- Assume $g(\mathbf{x})$ follows a GP prior:

$$g(\mathbf{x})|\boldsymbol{\eta}, \sigma_g^2 \sim \mathcal{GP}(0, \tau_g^2 \Phi_{\boldsymbol{\eta}}(\mathbf{x}, \mathbf{x}'))$$





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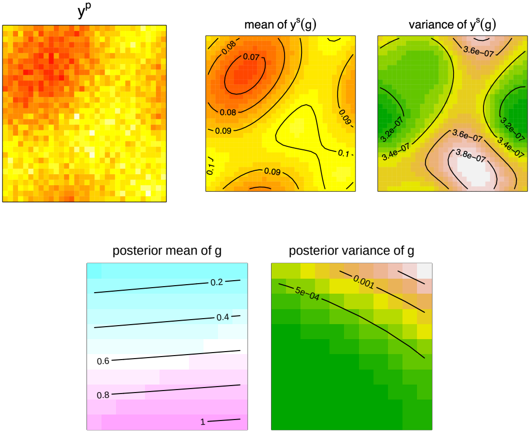

Arxiv

- **Sung, C.-L.**, Wang, W., Cakoni, F., Harris, I., & Hung, Y. (2024). Functional-input Gaussian processes with applications to inverse scattering problems. *Statistica Sinica*, 34(4), to appear.
- **Sung, C.-L.**, Song, Y., & Hung, Y. (2024+). Advancing inverse scattering with surrogate modeling and Bayesian inference for functional inputs. arXiv preprint arXiv:2305.01188.

Cornell University

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[Submitted on 5 Jan 2022 (v1), last revised 16 Mar 2022 (this version, v2)]

Functional-Input Gaussian Processes with Applications to Inverse Scattering Problems

Chih-Li Sung, Wenjia Wang, Fioralba Cakoni, Isaac Harris, Ying Hung

Surrogate modeling based on Gaussian processes (GPs) has received increasing attention in the analysis of complex problems in science and engineering. Despite extensive studies on GP modeling, the developments for functional inputs are scarce. Motivated by an inverse scattering problem in which functional inputs representing the support and material properties of the scatterer are involved in the partial differential equations, a new class of kernel functions for functional inputs is introduced for GPs. Based on the proposed GP models, the asymptotic convergence properties of the resulting mean squared prediction errors are derived and the finite sample performance is demonstrated by numerical examples. In the application to inverse scattering, a surrogate model is constructed with functional inputs, which is crucial to recover the reflective index of an inhomogeneous isotropic scattering region of interest for a given far-field pattern.

Subjects: **Methodology (stat.ME)**; Applications (stat.AP)

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Functional-Input Gaussian Processes with Applications to Inverse Scattering Problems (Reproducibility)

Chih-Li Sung March 15, 2022

This instruction aims to reproduce the results in the paper "*Functional-Input Gaussian Processes with Applications to Inverse Scattering Problems*" by Sung et al. (https://arxiv.org/abs/2201.01682). Hereafter, functional-Input Gaussian Process is abbreviated by *FIGP*.

The following results are reproduced in this file

- The sample path plots in Section 4.1 (Figures 2 and 3)
- The prediction results in Section 4.2 (Tables 1, 2, and 3)
- The plots and prediction results in Section 5 (Figures 4, 5, and 6)

Step 0.1: load functions and packages

```
library(randtoolbox)
library(R.matlab)
library(cubature)
library(plgp)
```

Thank You!

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