



#### Gaussian Process Regression for Complex-valued Frequency Response Functions

with J. Bect<sup>3</sup>, U. Römer<sup>1</sup> and S. Schöps<sup>2</sup>; ECCOMAS YIC 2021

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#### Overview

- Introduction
- Approximation of Frequency Response Functions
- Numerical results
- Conclusion

## Frequency Response Functions (FRFs)

- Response to harmonic (sinusoidal) excitation with a certain frequency f
  - FRF: Measure of magnitude and phase of the output, relative to the input



- Frequency sweep requires many simulation runs
- Goal: Approximation of FRFs based on a few training points
- Approach: Describe FRF with a complex Gaussian Process

- Gaussian Process
   f(x) ∼ GP(m(x), k(x, x'))
  - Mean function m(x)
  - Covariance function k(x, x')
- Gaussian Process Regression (GPR): infer unobserved values by conditioning on training data
- Posterior mean: minimum norm interpolant in the RKHS associated to k
- Approximation of complex functions
  - 1. Use separate Gaussian Process approximations for real and imaginary part
  - 2. Use complex Gaussian Process  $f(x) \sim CGP(m(x), k(x, x'), c(x, x'))$ 
    - Covariance function  $k(x, x') = \mathbb{E}[(f(x) m(x))\overline{(f(x) m(x'))}]$
    - Pseudo-covariance function  $c(x, x') = \mathbb{E}[(f(x) m(x))(f(x) m(x'))]$



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## **Parametric Problem**

· We address linear parametric problems in the form

$$(\mathbf{K} + s\mathbf{D} + s^2\mathbf{M})\mathbf{u} = \mathbf{g}$$

- Stiffness, damping and mass matrix **K**, **D**,  $\mathbf{M}$ ,  $\in \mathbb{R}^{n_h \times n_h}$
- Complex frequency variable  $s = i\omega$ , where  $\omega \in \Omega \subset \mathbb{R}^+$
- Quantity of Interest (QoI)

 $F:\mathbb{C} \to \mathbb{C}$ ,  $s \mapsto \mathcal{J}(\mathbf{u}(s))$ 

• Assumption:  $F \in H^2(\Gamma_{\alpha})$ , where

$$\Gamma_{lpha}:=\{s\in\mathbb{C}\,|\,\mathcal{R}[s]>-lpha\}$$
 ,  $lpha>0$ 

• Hardy space  $H^2(\Gamma_{\alpha})$  is an RKHS with the Szegö kernel

$$k(s_k, s_l) = \frac{1}{2\pi(2\alpha + s_k + \overline{s_l})}$$





## **Choice of Pseudo-Covariance**

- FRF  $F(i\omega)$  is the Laplace transform of a real-valued signal  $\tilde{f}(t)$ , hence  $F \in H^2_{sub}(\Gamma_{\alpha}) := \{ u \in H^2(\Gamma_{\alpha}) \mid \mathcal{L}^{-1}[u](t) \text{ real-valued} \}$
- Information can be incorporated by choosing the pseudo-covariance<sup>1</sup>

$$c(s_k, s_l) = \mathbb{E}[f(s_k)f(s_l)] = \mathbb{E}[f(s_k)\overline{f(\overline{s_l})}] = k(s, \overline{s_l})$$
(1)

of a mean-free complex GP, i.e.,  $f(s) \sim \mathsf{CGP}(\mathbf{0}, \mathit{k}, \mathit{c})$ 

• Numerical example: third order rational function  $g \in H^2_{\mathrm{sub}}(\Gamma_{\alpha})$ ,  $\omega \in [0, 1]$ 



<sup>1</sup>J. Lataire and T. Chen. "Transfer function and transient estimation by Gaussian process regression in the frequency domain." Automatica (2016)

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# Approach: GPR + Rational Basis (Sz.-Rat.)

- Problem: slow convergence of Szegö-GPR prediction f<sub>N</sub>(iω; α) if F has a few dominant poles limiting Γ<sub>α</sub>
- Idea: combine GPR with rational basis functions<sup>2</sup>

$$f_{N}^{(K)}(i\omega;\mathbf{p},\alpha) = f_{N}(i\omega;\alpha) + \sum_{i=1}^{K} \frac{1}{i\omega - p_{i}}r_{i} + \frac{1}{i\omega - \overline{p_{i}}}\overline{r_{i}},$$

- Approach: heuristic algorithm starting with  $K_{max}$  initial pole pairs  $p_i$ ,  $\overline{p_i}$ 
  - 1. Tune kernel hyper-parameter  $\alpha$  and K pole pairs simultaneously (MLE)
  - 2. Store model  $f_N^{(K)}$
  - 3. Remove pole pair with smallest contribution to the likelihood and repeat
- Output: set of approximations  $\{f^{(K)}\}_{K=0}^{K_{max}}$
- ⇒ Model selection using a novel criterion based on leave-on-out cross-validation with an additional instability penalty

<sup>&</sup>lt;sup>2</sup>B. Gustavsen and A. Semlyen, "Rational approximation of frequency domain responses by vector fitting", IEEE Trans. Power Delivery (1999)

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## **Electric Circuit**

Parallel connection of n underdamped series RLC circuits

$$\Upsilon(i\omega) = \sum_{i=1}^{n} \frac{i\omega}{(i\omega)^2 L_i + i\omega R_i + C_i^{-1}}, \quad \omega \in [10 \text{ kHz}, 25 \text{ kHz}]$$

Setting 1: n<sub>1</sub> = 1000 random series RLC elements

$$C_i \sim \mathcal{U}(1, 20) \, \mu$$
F,  $L_i \sim \mathcal{U}(0.1, 2) \, m$ H,  $R_i = L_i (1 + \mathcal{U}(-0.2, 0.2)) rac{\Omega}{mH}$ 

Setting 2: two additional circuit elements with very low damping



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<sup>1</sup>Y. Nakatsukasa et al. "The AAA algorithm for rational approximation" (2018)

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Method:

- PACMAN shape: vibrating surface (frequency  $f = \frac{\omega}{2\pi}$ )
- Acoustic pressure p<sub>i</sub> at black dot
- Approximation using 28 training points (blue crosses)



<sup>3</sup>H. Ziegelwanger, P. Reiter. "The PAC-MAN model: Benchmark case for linear acoustics in computational physics." J. Comput. Phys. (2017)

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- Method: AAA (rational approximation)



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- PACMAN shape: vibrating surface (frequency  $f = \frac{\omega}{2\pi}$ )
- Acoustic pressure *p<sub>i</sub>* at black dot
- Approximation using 28 training points (blue crosses)
- Method: GPR (Szegö kernel) + rational basis



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- PACMAN shape: vibrating surface (frequency  $f = \frac{\omega}{2\pi}$ )
- Acoustic pressure *p<sub>i</sub>* at black dot
- Approximation using N training points



<sup>3</sup>H. Ziegelwanger, P. Reiter. "The PAC-MAN model: Benchmark case for linear acoustics in computational physics." J. Comput. Phys. (2017)

# **Conclusion**<sup>5</sup>

- Complex GPR using a suitable (pseudo-)kernel for FRFs
- Additional rational basis functions to capture dominant poles
- Model selection based on LOO and instability penalty
- Improvements w.r.t. AAA/VF for a number of benchmark problems

#### Outlook:

• Generalization to multivariate case  $\Rightarrow$  UQ for parametric PDEs<sup>4</sup>

<sup>&</sup>lt;sup>4</sup>M. Griebel and C. Rieger. "Reproducing kernel Hilbert spaces for parametric partial differential equations." SIAM-ASA J. Uncertain. (2017)

<sup>&</sup>lt;sup>5</sup>N. Georg, J. Bect, U. Römer, S. Schöps. *Rational kernel-based interpolation for complex-valued frequency response functions.* Will appear on ARXIV soon.

# Thank you for your attention!

#### Please ask questions now or contact

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