Gaussian Process Regression for Complex-valued Frequency Response Functions

with J. Bect\textsuperscript{3}, U. Römer\textsuperscript{1} and S. Schöps\textsuperscript{2}; ECCOMAS YIC 2021

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Overview

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

- Gaussian Process
  \[ f(x) \sim \text{GP}(m(x), k(x, x')) \]
  - 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 \( f(x) \sim \text{CGP}(m(x), k(x, x'), c(x, x')) \)
     - Covariance function \( k(x, x') = \mathbb{E}[(f(x) - m(x))(f(x') - m(x'))] \)
     - 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

\[(K + sD + s^2M)u = g\]

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

- Quantity of Interest (QoI)

\[F : \mathbb{C} \to \mathbb{C}, s \mapsto J(u(s))\]

- Assumption: \(F \in H^2(\Gamma_\alpha)\), where

\[\Gamma_\alpha := \{s \in \mathbb{C} | \Re[s] > -\alpha\}, \alpha > 0\]

- Hardy space \(H^2(\Gamma_\alpha)\) is an RKHS with the Szegö kernel

\[k(s_k, s_l) = \frac{1}{2\pi(2\alpha + s_k + s_l)}\]
Choice of Pseudo-Covariance

- FRF $F(i\omega)$ is the Laplace transform of a real-valued signal $\tilde{f}(t)$, hence
  
  $$F \in H^2_{\text{sub}}(\Gamma_\alpha) := \{ u \in H^2(\Gamma_\alpha) \mid \mathcal{L}^{-1}[u](t) \text{ real-valued} \}$$

- Information can be incorporated by choosing the pseudo-covariance\(^1\)
  
  $$c(s_k, s_l) = \mathbb{E}[f(s_k)f(s_l)] = \mathbb{E}[f(s_k)\overline{f(s_l)}] = k(s, \overline{s_l})$$

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

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

\(^1\)J. Lataire and T. Chen. "Transfer function and transient estimation by Gaussian process regression in the frequency domain." Automatica (2016)
Approach: GPR + Rational Basis (Sz.-Rat.)

- Problem: slow convergence of Szegö-GPR prediction $f_N(i\omega; \alpha)$ if $F$ has a few dominant poles limiting $\Gamma_\alpha$

- Idea: combine GPR with rational basis functions\(^2\)

$$f_N^{(K)}(i\omega; p, \alpha) = f_N(i\omega; \alpha) + \sum_{i=1}^{K} \frac{1}{i\omega - p_i} r_i + \frac{1}{i\omega - \overline{p_i}} \overline{r_i},$$

- Approach: heuristic algorithm starting with $K_{\text{max}}$ 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 $\{f^{(K)}\}_{K=0}^{K_{\text{max}}}$

- $\Rightarrow$ Model selection using a novel criterion based on leave-on-out cross-validation with an additional instability penalty

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Electric Circuit

- Parallel connection of \( n \) underdamped series RLC circuits

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

- Setting 1: \( n_1 = 1000 \) random series RLC elements

\[
C_i \sim \mathcal{U}(1, 20) \ \mu \text{F}, \quad L_i \sim \mathcal{U}(0.1, 2) \ \text{mH}, \quad R_i = L_i(1 + \mathcal{U}(-0.2, 0.2)) \frac{\Omega}{\text{mH}}
\]

- Setting 2: two additional circuit elements with very low damping

![Diagram of an electric circuit with series RLC components and a pole-zero diagram]
Electric Circuit

- Parallel connection of $n$ underdamped series RLC circuits

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

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- Setting 2: two additional circuit elements with very low damping
Electric Circuit - Setting 1

\[
\begin{align*}
\text{Re}[Y(i\omega)] & \quad \omega = 1 \cdot 10^4 \quad 1 \quad 1.5 \quad 2 \quad 2.5 \\
\text{Im}[Y(i\omega)] & \quad \omega = 1 \cdot 10^4 \quad 1 \quad 1.5 \quad 2 \quad 2.5 \\
|Y(i\omega)| & \quad \omega = 1 \cdot 10^4 \quad 1 \quad 1.5 \quad 2 \quad 2.5 
\end{align*}
\]

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**Electric Circuit - Setting 1**

![Graphs](attachment:image.png)

**Introduction**

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**Setting 1**

- **Re**[$\mathcal{Y}(i\omega)$]
- **Im**[$\mathcal{Y}(i\omega)$]
- $|\mathcal{Y}(i\omega)|$

**RMSE**

- Number of training points $N$

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Electric Circuit - Setting 1

![Graphs showing Electric Circuit - Setting 1](image)

Setting 1 (100 runs)

Median RMSE vs. Number of training points $N$

- **AAA**
- **VF**
- **Sz.-Rat.**
- **Szegö**
- **Gauss**

---

Electric Circuit - Setting 2

![Graphs showing the real part, imaginary part, and magnitude of the frequency response function for Setting 2.]

**Setting 2 (1 run)**

![Graph showing the RMSE for different algorithms with varying number of training points.]

$$\omega \cdot 10^4$$

**Introduction**

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Electric Circuit - Setting 2

\[ \text{Setting 2 (100 runs)} \]

\[ \text{Median RMSE} \]

<table>
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<tr>
<th>Number of training points ( N )</th>
<th>AAA(^1)</th>
<th>VF(^2)</th>
<th>Sz.-Rat.</th>
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\(^1\)Y. Nakatsukasa et al. "The AAA algorithm for rational approximation" (2018)

\(^2\)B. Gustavsen et al. "Rational approximation of frequency domain responses by vector fitting" (1999)
Benchmark Problem: Acoustic Scattering

- PACMAN shape: vibrating surface (frequency $f = \frac{\omega}{2\pi}$)
- Acoustic pressure $p_i$ at black dot
- Approximation using 28 training points (blue crosses)
- Method:

\begin{align*}
\mathcal{R}[p_i] & \quad 2,000 & 2,500 & 3,000 & 3,500 & 4,000 \\
\mathcal{I}[p_i] & \quad 2,000 & 2,500 & 3,000 & 3,500 & 4,000
\end{align*}

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$\mathcal{R}[p_i]$ $\mathcal{I}[p_i]$

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- Method: AAA (rational approximation)

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- PACMAN shape: vibrating surface (frequency $f = \frac{\omega}{2\pi}$)
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- Approximation using 28 training points (blue crosses)
- Method: Vector Fitting (rational approximation)

$\mathcal{R}[p_i]$ and $\mathcal{I}[p_i]$ graphs with training points and approximations.

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Benchmark Problem: Acoustic Scattering

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- Method: GPR (Szegö kernel) + rational basis

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Conclusion

- 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

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Thank you for your attention!

Please ask questions now or contact

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