Padé approximation for Helmholtz frequency response problems

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Model Reduction for Parametrized Systems IV
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Parametric Helmholtz BVP

We consider the Helmholtz problem

\[-\Delta u - k^2 u = f \quad \text{in } D\]

coupled with either Dirichlet or Neumann homogeneous b.c. on \(\partial D\), where

- \(D\) is an open bounded regular domain in \(\mathbb{R}^d\), \(d = 1, 2, 3\)
- the wavenumber \(k^2\) is parametric and belongs to the interval of interest \(K := [k_{\min}^2, k_{\max}^2] \subset \mathbb{R}_{>0}\)
- \(f \in L^2(D)\)
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- \(f \in L^2(D)\)

We denote with \(V\) either \(H^1(D)\) or \(H^1_0(D)\) and assume the functions in \(V\) to be complex-valued.

**Weak formulation**: given \(f \in L^2(D)\) and \(k^2 \in K\), find \(u_{k^2} \in V\) such that

\[\int_D \nabla u_{k^2}(x) \cdot \nabla \overline{v(x)} dx - k^2 \int_D u_{k^2}(x) \overline{v(x)} dx = \int_D f(x) \overline{v(x)} dx \quad \forall v \in V\]
Helmholtz frequency response problem

We introduce the Helmholtz frequency response function (solution map)

\[ S : K \to V, \quad k^2 \mapsto S(k^2) = u_{k^2} \]

Goal: to know \( S(k^2) \) for any \( k^2 \in K \), where \( K \) contains high wavenumbers (mid- and high-frequency regime)
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Due to the oscillatory behavior of the solutions, the finite element approximation is accurate only on fine meshes or with high polynomial degrees. Hence, the direct numerical computation of \( u_{k^2} \) for a whole range of frequencies is out of reach.

**Method:** to reduce the computational cost by approximating \( S \) using a Padé-type technique

**OFFLINE:** compute evaluations of \( S \) (and of its derivatives) only at few frequencies

**ONLINE:** given a new frequency \( \bar{k}^2 \), estimate \( S(\bar{k}^2) \) by evaluating the constructed approximation of \( S \)
Outline

1. Regularity of the frequency response function

2. Rational (Padé) approximation of the solution map

3. Numerical results
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1. Regularity of the frequency response function
2. Rational (Padé) approximation of the solution map
3. Numerical results
We extend the solution map $S$ to the complex plane $\mathbb{C}$. $S$ associates each complex wavenumber $z \in \mathbb{C}$ with $u_z \in V$, where $u_z$ solves

$$\int_D \nabla u_z(x) \cdot \overline{\nabla v(x)} \, dx - z \int_D u_z(x) \overline{v(x)} \, dx = \int_D f(x) \overline{v(x)} \, dx \quad \forall v \in V$$

**Remark**: extending $S$ to the complex plane is equivalent to perturb the Helmholtz problem adding the damping term $i \text{Im}(z) u$. 

Denote with $\Lambda$ the set of eigenvalues of the Laplace bvp with the considered boundary conditions. Then $S$ is well-defined on $\mathbb{C} \setminus \Lambda$ (see [Bonizzoni–Nobile–Perugia2016]).
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A-priori bound for the Helmholtz solution

Given a positive real weight $w > 0$, we introduce the $H^1(D)$-weighted norm

$$
\| v \|_{1,w} := \sqrt{\| \nabla v \|_{L^2(D)}^2 + w^2 \| v \|_{L^2(D)}^2}
$$

**Remark:** $\| \cdot \|_{1,w}$ is equivalent to the standard $H^1(D)$-norm $\| \cdot \|_1$ (with $w = 1$).
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**Proposition** [Bonizzoni–Nobile–Perugia 2016]

Let \( z \in \mathbb{C}\setminus\Lambda \). Consider the Helmholtz problem with wavenumber \( z \)

\[
-\Delta u_z(x) - z u_z(x) = f(x), \quad x \in D
\]

with either Dirichlet or Neumann hom. b.c. on \( \partial D \). Let

\[
\lambda_{\min} := \min\{\lambda \in \Lambda\}. \quad \text{If } \min_{\lambda_j \in \Lambda} |\lambda_j - z| > \alpha > 0 \text{ then the unique solution } u_z \in V \text{ satisfies the a-priori bound}
\]

\[
\|u_z\|_{1,w} \leq \frac{\sqrt{|z-\lambda_{\min}| + |\text{Re}(z)| + w^2}}{\alpha} \|f\|_{L^2(D)}.
\]
Regularity of the frequency response function

- $S$ is continuous in $\mathbb{C} \setminus \Lambda$, i.e. $\lim_{h \to 0} \|S(z + h) - S(z)\|_{1,w} = 0$

- $S$ admits a complex derivative $\frac{dS}{dz}(z) := \lim_{h \to 0} \frac{S(z + h) - S(z)}{h}$ for $z \in \mathbb{C} \setminus \Lambda$, which is the unique solution of

$$
\int_D \nabla \frac{dS}{dz} \cdot \nabla v \; dx - z \int_D \frac{dS}{dz} \overline{v} \; dx = \int_D S(z) \overline{v} \; dx \quad \forall v \in V
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$\Longrightarrow$ Then $S$ is holomorphic in $\mathbb{C} \setminus \Lambda$
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\int_D \nabla \frac{dS}{dz} \cdot \nabla \bar{v} \ dx - z \int_D \frac{dS}{dz} \bar{v} \ dx = \int_D S(z) \bar{v} \ dx \quad \forall v \in V
\]

$\implies$ Then $S$ is holomorphic in $\mathbb{C} \setminus \Lambda$

Moreover, $S$ is meromorphic in $\mathbb{C}$ with poles of order 1.

Indeed, let $\mu_j$ be the (finite) multiplicity of each eigenvalue of the Laplacian $\lambda_j \in \Lambda$, and $\{\varphi_j\}_{j=1}^{\mu_j}$ the corresponding eigenfunctions. Then, the frequency response function can be expanded as

\[
S(z) = u_z = \sum_{j=1}^{\infty} \sum_{i=1}^{\mu_j} \frac{f_{j,i}}{\lambda_j - z} \varphi_{j,i}
\]
Outline

1. Regularity of the frequency response function

2. Rational (Padé) approximation of the solution map

3. Numerical results
For Hilbert space-valued functions a rational (Padé) approximation
\[ S_{[M/N]} : \mathbb{C} \to V \] is the ratio of two polynomials of degree \( M \) and \( N \) respectively

\[ S_{[M/N]}(z) = \frac{P_{[M/N]}(z)}{Q_{[M/N]}(z)} \]

with

- numerator: \( P_{[M/N]} \in \mathbb{P}_M(\mathbb{C}; V) \), i.e., \( P_{[M/N]}(z) = \sum_{i=0}^{M} p_i(z)z^i \), with coefficients \( p_i(z) \in V \)
- denominator: \( Q_{[M/N]} \in \mathbb{P}_N(\mathbb{C}) \), i.e., \( Q_{[M/N]}(z) = \sum_{i=0}^{N} q_i z^i \), with coefficients \( q_i \in \mathbb{C} \).
Least Square Padé approximant for $S$

[Guillame–Huard–Robin1997], [Huard–Robin1999]

**Notation**: we denote with $S_\alpha$ the $\alpha$-th order Taylor coeff. of $S$ in $z_0$, and with $(S(z))^E$ the Taylor pol. of degree $E$, i.e. $(S(z))^E = \sum_{\alpha=0}^{E} S_\alpha (z - z_0)^\alpha$
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**Functional** $j_{\rho,E}$: given $P(z) = \sum_{i=0}^{M} p_i(z)(z - z_0)^i \in \mathbb{P}_M(\mathbb{C}; V)$, $Q(z) = q_i(z - z_0)^i \in \mathbb{P}_N(\mathbb{C})$, $\rho \in \mathbb{R}^+$ and $E \in \mathbb{N}$, we define

$$j_{\rho,E}(P, Q) := \left( \sum_{\alpha=0}^{E} \| (Q(z)S(z) - P(z))_\alpha \|_{1,w}^2 \rho^{2\alpha} \right)^{1/2}$$
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**Functional $j_{\rho,E}:** given $P(z) = \sum_{i=0}^{M} p_i(z)(z - z_0)^i \in \mathbb{P}_M(C;V)$, $Q(z) = q_i(z - z_0)^i \in \mathbb{P}_N(C)$, $\rho \in \mathbb{R}^+$ and $E \in \mathbb{N}$, we define

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**Normalization of $Q$:** $\mathbb{P}^*_N(C) = \left\{ Q(z) = \sum_{i=0}^{N} q_iz^i \in \mathbb{P}_N(C) : \sum_{i=0}^{N} |q_i|^2 = 1 \right\}$
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**Least squares Padé approximant:** Let $E \geq M + N$.

$$S_{[M/N]}(z) = \frac{P(z)}{Q(z)}, \quad (P, Q) = \arg \min_{P \in \mathbb{P}_M(\mathbb{C}; V), \ Q \in \mathbb{P}_N^*(\mathbb{C})} j_{\rho,E}(P, Q)$$

The Padé minimization problem admits at least one solution (minimization of a continuous functional on a compact set).
Construction of the least squares Padé approximant

**Starting point:** Compute $S(z_0)$ and the first $E$ derivatives $S_\alpha$, $\alpha = 1, 2, \ldots, E$ by

$$
\int_D \nabla S_\alpha(z) \cdot \overline{\nabla v} \, dx - z \int_D S_\alpha(z) \overline{v} \, dx = \alpha \int_D S_{\alpha-1}(z) \overline{v} \, dx \quad \forall \, v \in V
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**Reduced functional:**

$$
 j_{\rho,E}(P, Q)^2 = \sum_{\alpha=0}^E \| (QS - P)_\alpha \|_{1,w,\rho}^2
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$$j_{\rho,E}(P, Q)^2 = \sum_{\alpha=0}^E \| (QS - P)_\alpha \|_{1,w}^2 \rho^{2\alpha}$$

$$= \sum_{\alpha=0}^M \| (QS - P)_\alpha \|_{1,w}^2 \rho^{2\alpha} + \sum_{\alpha=M+1}^E \| (QS - P)_\alpha \|_{1,w}^2 \rho^{2\alpha}$$
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$$

Take $P$ such that $P_{\alpha} = (QS)_{\alpha}$ for $0 \leq \alpha \leq M$, and define the reduced functional

$$
\tilde{j}_{\rho,E}(Q)^2 = \sum_{\alpha=M+1}^{E} \|(QS)_{\alpha}\|_{1,w}^2 \rho^{2\alpha} \quad \text{(quadratic form in } \{q_i\})
$$
Construction of the least squares Padé approximant

Starting point: Compute $S(z_0)$ and the first $E$ derivatives $S_\alpha$, $\alpha = 1, 2, \ldots, E$ by

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\int_D \nabla S_\alpha(z) \cdot \nabla v \, dx - z \int_D S_\alpha(z) v \, dx = \alpha \int_D S_{\alpha-1}(z) v \, dx \quad \forall \ v \in V
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Reduced functional:

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$$

Eigenvalue problem: $Q$ corresponds to the “smallest” eigenvector of $\bar{j}_{\rho,E}(Q)$

$$
\min_{Q \in \mathbb{P}_N(\mathbb{C})} \bar{j}_{\rho,E}(Q), \quad \text{s.t. } \sum_{i=0}^N |q_i|^2 = 1
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**Reduced functional:**

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\tilde{j}_{\rho,E}(P, Q)^2 = \sum_{\alpha=0}^{E} \| (QS - P)_\alpha \|_{1,w}^2 \rho^{2\alpha} = \sum_{\alpha=0}^{M} \| (QS - P)_\alpha \|_{1,w}^2 \rho^{2\alpha} + \sum_{\alpha=M+1}^{E} \| (QS - P)_\alpha \|_{1,w}^2 \rho^{2\alpha}
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$$

**Eigenvalue problem:** $Q$ corresponds to the “smallest” eigenvector of $\tilde{j}_{\rho,E}(Q)$

$$
\min_{Q \in P_N(\mathbb{C})} \tilde{j}_{\rho,E}(Q), \quad \text{s.t.} \quad \sum_{i=0}^{N} |q_i|^2 = 1
$$

A fast version of the algorithm is under investigation: see the poster presented by D. Pradovera!
Convergence result

**Theorem** [Bonizzoni–Nobile–Perugia 2016]

Let $N \in \mathbb{N}$ be fixed, and $R > 0$ s.t. $B(z_0, R)$ contains exactly $N$ poles $\lambda_l, \ldots, \lambda_{l+N}$ of $S$. Denote $G = \{\lambda_l, \ldots, \lambda_{l+N}\}$. Then

$$\lim_{M \to \infty} \| S(z) - S_{[M/N]}(z) \|_{1,w} = 0$$

uniformly on all compact subsets of $B(z_0, R) \setminus G$.

In particular, let $K_{\alpha} := \bigcup_{\lambda \in \Lambda \cap K} (\lambda - \alpha, \lambda + \alpha) \subset K$, where $K = [k_{min}^2, k_{max}^2]$ is the interval of interest, and $\alpha > 0$. Then $\exists M^* \text{ s.t. } \forall M \geq M^*$,

$$\| S(z) - S_{[M/N]}(z) \|_{1,w} \leq C \frac{1}{\alpha} \left( \frac{\rho}{R} \right)^{M+1}, \quad \forall z \in K \setminus K_{\alpha}$$

where $\rho_K < \rho < R$, with $\rho_K = \min_{z \in K} |z_0 - z|$, and $C$ depends on $\rho_K$, $\rho$, $R$, $N$, $g_{K,\alpha} := \min_{z \in K \setminus K_{\alpha}} |g(z)|$, $z_0$, $\lambda_{min} = \min \lambda \in \Lambda$ and $\| f \|_{L^2(D)}$. 
Example to clarify the ideas...

1. $K = [k_{min}^2, k_{max}^2]$ interval of interest, which contains 4 poles
2. Fix $z_0$ with $\text{Im}(z_0) \neq 0$ and $\rho > 0$ s.t. $K \subset B(z_0, \rho)$
3. Take $N = 4$ and $R > \rho$ s.t. $B(z_0, R)$ contains exactly 4 poles
4. Construct the Padé approximant $S_{[M/N]}$. The convergence rate is $(\frac{\rho}{R})^{M+1}$
5. If $N = 5$, we can choose $R$ larger s.t. $B(z_0, R)$ contains exactly 5 poles. The convergence is faster!

**Geometrical interpretation:**
- $\rho$: it is the radius of the smallest disk $B(z_0, \rho)$ which contains the interval of interest.
- $R$: it is the radius of the biggest disk $B(z_0, R)$ which contains $N$ poles of $S$ (i.e. $N$ eigenvalues of the Laplacian).
Random wave number - Convergence result

- Consider $k^2 \in K := [k_{\text{min}}^2, k_{\text{max}}^2]$ random with given distribution $\mu$
- Qol: $X(k^2) = \mathcal{L}(S(k^2))$, with $\mathcal{L} : V \to \mathbb{R}$ a linear and bounded functional
- Approximate Qol: $X_P(k^2) = \mathcal{L}(S_{[M/N]}(k^2))$
- Characteristic function $\phi_X(t) = \mathbb{E}[e^{i X t}]$; cdf $F_X(t) = \mathbb{P}\{X \leq t\}$

From the uniform convergence of the Padé approximant $S_{[M/N]}$ on compact subsets of $K \setminus G$, we infer the convergence of $\phi_{X_P}$ and $F_{X_P}$:

- for any $t \in \mathbb{R}_+$
  \[
  |\phi_X(t) - \phi_{X_P}(t)| \leq 2 |K_\alpha| + tL C \frac{1}{\alpha} \left( \frac{\rho}{R} \right)^{M+1} |K \setminus K_\alpha|
  \]

- for any $0 < p < +\infty$ and $\delta \in \mathbb{R}$
  \[
  |F_X(\delta) - F_{X_P}(\delta)| \leq 2 |K_\alpha| + 3 \left( \frac{D_X(\delta L C)}{\alpha} \left( \frac{\rho}{R} \right)^{M+1} \right)^{\frac{p}{p+1}} |K \setminus K_\alpha|^{\frac{1}{p+1}}
  \]

where $0 < D_X(\delta) \leq \sup_x f_X(x)$, with $f_X$ the pdf of $X$. 

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1. Regularity of the frequency response function

2. Rational (Padé) approximation of the solution map

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Test 1: Setting

Let $D = [0, \pi] \times [0, \pi]$, and consider the Helmholtz problem with homogeneous Dirichlet boundary conditions on $\partial D$. Let $\nu^2 \in \mathbb{R}^+ \setminus \Lambda$, and $d = (d_1, d_2) \in \mathbb{R}^2$. The loading term $f(x) = f(x_1, x_2)$ is such that the unique solution of the considered Helmholtz problem with wavenumber $\nu^2$ is the product between the plane wave traveling along the direction $d$, $v(x) = e^{-i\nu d \cdot x}$, and the bubble $w(x) = \frac{16}{\pi^2} x_1 x_2 (x_1 - \pi)(x_2 - \pi)$.

\[\nu = \sqrt{12}, \quad d = (\cos(\pi/6), \sin(\pi/6))\]
Test 1

Consider $K = [7, 11]$, which contains two eigenvalues of the Laplace operator: $\lambda = 8$ (multiplicity one) and $\lambda = 10$ (multiplicity two), i.e. $K$ contains two simple poles of $S$.

- Given $N = 2$ we construct the Padé approximant $S_{[M/N]}$ centered in $z_0 = 10 + 0.5i$.
- We partition uniformly $K$ in 100. At each point $z$ of the mesh, the solution $S_h(z) = u_h(z, \cdot)$ is computed via the $P^3$ continuous FE method.

Comparison between the norm of the FE solution $\|u_h(z, \cdot)\|_{1,w}$ (dashed line), and the norm of the Padé approximant $\|u_{P,h}(z, \cdot)\|_{1,w}$ (solid line).
Test 1: Random wavenumber

Here $k^2 \sim \mathcal{U}([7.5; 8.5])$; QoI $X(k^2) = \| u_k^2 \|_{1,w}$
Test 2: Transmission/Reflection problem

Consider the square domain $D = (-1, 1)^2$ with two different refractive indices. The interface is located in $y = 0$. Problem: find $u \in H^1(D)$ s.t.

$$
\begin{align*}
-\Delta u - k^2 \varepsilon_r u &= 0 \quad \text{in } \Omega \\
u|_{\partial D} &= g_\theta \\
\end{align*}
$$

where $\varepsilon_r = \begin{cases} 
4, & \text{if } y < 0 \\
1, & \text{if } y > 0
\end{cases}$
Test 2: Transmission/Reflection problem

Consider the square domain $D = (-1, 1)^2$ with two different refractive indices. The interface is located in $y = 0$. Problem: find $u \in H^1(D)$ s.t.

$$\begin{cases} -\Delta u - k^2 \varepsilon_r u = 0 \quad \text{in } \Omega \\ u|_{\partial D} = g_\theta \end{cases}$$

where $\varepsilon_r = \begin{cases} 4, & \text{if } y < 0 \\ 1, & \text{if } y > 0 \end{cases}$

Incident plane wave $u^i = e^{i z d \cdot x}$, with $d = (\cos(\theta), \sin(\theta))$.

Depending on the value of the parameter $\theta$, the solution $u$ behaves differently. There exists a critical value $\theta_c$ s.t.

- if $\theta > \theta_c$, the wave is refracted
- if $\theta < \theta_c$, we have internal reflection
We let $k$ vary in the interval of interest $K$

- The frequency response map is meromorphic in $\mathbb{C}$, with (real) poles of order one (see [Bonizzoni–Nobile–Perugia–Pradovera2018])
- The Padé approximant $S_{[M/N]}$ is able to catch the singularities of $S$
- The approximation error decays as the predicted rate $\frac{\rho}{R}^{(M+1)}$
Test 3: Scattering problem

Consider the scattering of acoustic waves at a scatterer occupying the domain $\mathcal{B}(0, 0.5) \subset \mathbb{R}^2$. Let $g$ be the impedance trace of the incident plane wave $u^i = e^{izd \cdot x}$, i.e., $g = \frac{\partial u^i}{\partial n} - izu^i$. Problem: find $u \in H^1_{\Gamma_D}(D)$ ($\Gamma_D = \partial \mathcal{B}(0, 0.5)$) s.t.

$$\begin{cases} -\Delta u - z^2 u = 0 & \text{in } D \\ u = 0 & \text{on } \Gamma_D \\ \frac{\partial u}{\partial n} - izu = g & \text{on } \Gamma_N \end{cases}$$

(1)

- Problem (1) admits a unique solution for any $z$ with $\text{Im}(z) \geq 0$
- The frequency response map $S : z \rightarrow u_z$ is meromorphic in $\mathbb{C}$, with poles in the half-plane $\{\text{Im}(z) < 0\}$ (see [Bonizzoni–Nobile–Perugia–Pradovera2018])
Conclusions

- We have designed a Least-Square Padé-type approximation for Hilbert space-valued meromorphic maps
- We have proved that the Padé approximation error converges exponentially in the degree of the denominator
- Numerical examples which show the effectiveness of our approach are provided
Thank you for your attention!
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