An efficient algorithm for Padé-type approximation of the frequency response for the Helmholtz problem

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Problem setting

Let $\Omega \subset \mathbb{R}^d$ ($d = 1, 2, 3$) be a bounded Lipschitz domain, with boundary partitioned into the (possibly empty) sets Γ_D and Γ_N . Given $k \in \mathbb{C}$ and $f \in L^2(\Omega)$, we consider the Helmholtz problem

$$\begin{cases} -\Delta u - k^2 u = f & \text{in } \Omega \\ u = 0 & \text{on } \Gamma_D \\ \partial_n u = 0 & \text{on } \Gamma_N \end{cases} \quad (\text{H})$$

whose solution is sought in the Hilbert space

$$V = H_{\Gamma_D}^1(\Omega) = \{v \in H^1(\Omega), v|_{\Gamma_D} = 0\}.$$

We can explicit the dependence on k of the solution of (H) by considering the Helmholtz solution map

$$\begin{aligned} \mathcal{S} : \quad \mathbb{C} &\rightarrow H_{\Gamma_D}^1(\Omega), \\ k^2 &\mapsto \mathcal{S}(k^2) \end{aligned}$$

which associates $z = k^2$ to the weak solution (if it exists) of (H), i.e.

$$\text{find } \mathcal{S}(z) \in V : (\mathcal{S}(z), v)_{H_0^1(\Omega)} - z(\mathcal{S}(z), v)_{L^2(\Omega)} = (f, v)_{L^2(\Omega)} \quad \forall v \in V. \quad (\text{HW})$$

The spectral properties of the Laplacian over bounded domains imply the existence of a discrete set $\Lambda = \{\lambda_\alpha\}_{\alpha=1}^\infty$ of real values of z for which (HW) is ill-posed, each associated to a finite-dimensional subspace $\{V_\alpha\}_{\alpha=1}^\infty \subset V$. In particular, the subspaces $\{V_\alpha\}_{\alpha=1}^\infty$ are pairwise orthogonal and have total direct sum V , and

$$\mathcal{S}(z) = \sum_{\alpha=1}^\infty \frac{s_\alpha}{\lambda_\alpha - z} \quad \text{with convergence in } V. \quad (*)$$

Due to the self-adjointness of problem (H), the elements of $\{s_\alpha\}_{\alpha=1}^\infty$ are pairwise orthogonal, each belonging to a different eigenspace V_α of the laplacian operator.

Conclusion: $\mathcal{S}$ is meromorphic over $\mathbb{C}$, having single poles (or removable singularities) at all $\lambda \in \Lambda$. As such, we wish to approximate it using a rational function, in a Padé-like fashion.

Remark: The construction of the meromorphic map (*) still holds for any problem to which the spectral theory for self-adjoint operators with compact resolvent applies.

Least-squares fast Padé approximants

Fix $z_0 \in \mathbb{C} \setminus \Lambda$, and let $M, N, E \in \mathbb{N}$, with $E \geq \max\{M, N\}$. We define a least-squares fast Padé approximant (LSFPA) of $\mathcal{S}$ of type $[M/N]$ centered at z_0 (which depends parametrically on E) as a rational function

$$\mathcal{S}_{[M/N]} = \mathcal{P}_{[M/N]}/\mathcal{Q}_{[M/N]} : \mathbb{C} \rightarrow V$$

such that:

- (i) $\mathcal{P}_{[M/N]} \in \mathbb{P}_M(\mathbb{C}; V) = \left\{ \sum_{j=0}^M p_j (\cdot - z_0)^j, \text{ with } \{p_j\}_{j=0}^M \subset V \right\};$
- (ii) $\mathcal{Q}_{[M/N]} \in \mathbb{P}_N^0(\mathbb{C}) = \left\{ \sum_{j=0}^N q_j (\cdot - z_0)^j, \text{ with } \{q_j\}_{j=0}^N \subset \mathbb{C}, \sum_{j=0}^N |q_j|^2 = 1 \right\};$
- (iii) $\|\mathcal{Q}_{[M/N]}(z) \mathcal{S}(z) - \mathcal{P}_{[M/N]}(z)\|_V = \mathcal{O}(|z - z_0|^{M+1});$
- (iv) $\mathcal{Q}_{[M/N]}$ achieves the minimum over $\mathbb{P}_N^0(\mathbb{C})$ of

$$j_E(Q) = \left\| (QS)^{(E)}(z_0) \right\|_V = \left\| \sum_{j=0}^N \binom{E}{j} Q^{(j)}(z_0) \mathcal{S}^{(E-j)}(z_0) \right\|_V. \quad (\text{F})$$

Theoretical results [1]

Pole convergence. Let N be fixed, and consider λ among the N elements of Λ which are closest to z_0 . Then there exists a root λ^* of $\mathcal{Q}_{[M/N]}$ and C independent of E such that

$$|\lambda - \lambda^*| \leq C \left(\frac{\rho}{R} \right)^{2E} \quad \text{for } E \text{ large enough,}$$

with ρ and R being the distance from z_0 to the N -th and $(N+1)$ -th closest elements of Λ .

Remark: Numerical experiments suggest that ρ may be replaced by $|\lambda - z_0|$.

LSFPA exponential convergence. Let $z_0 \in \mathbb{C} \setminus \Lambda$ and $R > 0$ be fixed, so that $\mathcal{B}(z_0, R)$ contains exactly $\overline{N}$ poles of $\mathcal{S}$, and no pole lies on $\partial\mathcal{B}(z_0, R)$. Consider a sequence

$$(M_k, N_k)_{k=1}^\infty \subset \{(M, N) \in \mathbb{N}^2, M+1 \geq N\},$$

such that $M_{k+1} \geq M_k$ and $N_{k+1} \geq N_k$ for all k . Moreover, assume that

$$\infty > \lim_{k \rightarrow \infty} N_k \geq \overline{N} \quad \text{and} \quad \lim_{k \rightarrow \infty} M_k = \infty.$$

Let $\mathcal{S}_{[M_k/N_k]}$ be a LSFPA of $\mathcal{S}$, computed with $E \in \{M_k, M_k + 1\}$ for all values of k . Then, for any $\delta > 0$, there exists C_δ independent of k (which depends on $\lim_{k \rightarrow \infty} N_k$) such that

$$\|\mathcal{S}(z) - \mathcal{S}_{[M_k/N_k]}(z)\|_V \leq C_\delta \left(\frac{|z - z_0|}{R} \right)^{M_k+1} \quad \text{for } k \text{ large enough,}$$

for all $z \in \mathcal{B}(z_0, R) \setminus \mathcal{E}_\delta$, with $|\mathcal{E}_\delta| < \delta$.

LSFPA convergence in measure. Take the hypotheses above except for the boundedness assumption on the sequence $(N_k)_{k=1}^\infty$. There exists a set of zero measure $\mathcal{E}_0$ such that

$$\lim_{k \rightarrow \infty} \|\mathcal{S}(z) - \mathcal{S}_{[M_k/N_k]}(z)\|_V = 0$$

for all $z \in \mathcal{B}(z_0, R) \setminus \mathcal{E}_0$.

Conclusion: LSFPAAs converge to the target map with exponential rate along rows of the Padé table, and with no specific rate on more general paths along the Padé table.

Remark: More refined estimates on the general convergence rate of LSFPAAs can be obtained if information about Λ is available.

M \ N	0	1	2	...
0				
1				
2				
3				
...				

Figure 1: Padé table. In blue the region of convergence.

Implementation-oriented remarks

The numerical computation of LSFPAAs relies on three steps:

- Evaluation of derivatives.** The derivatives of the Helmholtz map are computed up to degree E , according to the recursive definition (which follows from (HW))

$$\text{find } \mathcal{S}^{(j)}(z_0) \in V :$$

$$(\mathcal{S}^{(j)}(z_0), v)_{H_0^1(\Omega)} - z_0 (\mathcal{S}^{(j)}(z_0), v)_{L^2(\Omega)} = j (\mathcal{S}^{(j-1)}(z_0), v)_{L^2(\Omega)} \quad \forall v \in V,$$

for $j = 1, \dots, E$, with the base case being $\mathcal{S}^{(0)}(z_0) = \mathcal{S}(z_0)$.

Remark: The span of the derivatives of $\mathcal{S}$ is a Krylov subspace of V generated by the resolvent at z_0 $(-\Delta - z_0)^{-1} : H^{-1}(\Omega) \rightarrow H_{\Gamma_D}^1(\Omega)$. Hence, the sequence of problems above can be solved efficiently by computing and storing a single operator factorization.

- Optimizing.** The minimization of (F) can be recast as a constrained quadratic programming problem, effectively coinciding with the computation of the minimal eigenpair of a $(N+1) \times (N+1)$ Hermitian matrix. The components of the eigenvector provide the coefficients of the LSFPA denominator.

- Assembling.** Once the denominator has been computed, the (unique) numerator satisfying (iii) can be found by matching the first Taylor coefficients (at z_0) of $\mathcal{P}_{[M/N]}$ with those of $\mathcal{Q}_{[M/N]}\mathcal{S}$.

Numerical example: damaged elastic membrane

We consider a membrane $\Omega = [0, 2] \times [0, 1] \setminus T$, with T being a thin triangular “crack” in the upper side of the rectangle, see figure below. We consider a time-periodic Gaussian load

$$f^*(\mathbf{x}, t) = \text{Re} \left(\exp \left\{ ikt - \frac{|\mathbf{x} - \mathbf{x}_0|^2}{2\sigma^2} \right\} \right)$$

centered at $\mathbf{x}_0 = (\frac{1}{2}, \frac{1}{2})^\top$ and with standard deviation $\sigma = \frac{1}{10}$. We assume that the membrane is held in place over all its border, except on the stress-free crack.

We seek the solution $u = \mathcal{S}(z)$ of the Helmholtz equation (H) with $f(\mathbf{x}) = f^*(\mathbf{x}, 0)$, which represents the asymptotic amplitude of a monochrome (with wavenumber k) solution of the wave equation (with normalized wave speed) whose forcing term is f^* [4].

In order to approximate the solution map $\mathcal{S}$ for several values of $k^2 = z \in [78, 122]$, we apply LSFPAAs with center at $z_0 = 100 + \frac{1}{2}i$ and several values of M, N and E . In particular, we do not approximate the solution of (H) – or more properly (HW) – directly, but we consider a discretization of the problem with $\mathbb{P}^3$ Finite Elements on a triangular mesh.

Figure 2: Amplitude f of the load term (left) and solution of (H) for $k^2 = z = 100$ (right).

Figure 3: V -norm of $\mathcal{S}$ and of $\mathcal{S}_{[M/N]}$ (left) and of the approximation error (right) for sub-diagonal approximants of type $[N-1/N]$ for $N \in \{3, 6, 9\}$, with $z \in [78, 122]$. In all cases, E is equal to N .

Figure 4: Convergence of the approximation error in the V -norm at $z = 105$ for several choices of N . In all cases, E is set equal to M .

Figure 5: Convergence of the roots of LSFPAAs denominators for $N = 3$ to the N poles of $\mathcal{S}$ which are closest to z_0 .

Conclusion: On rows of the Padé table, i.e. for fixed N , the theoretical convergence rates for both the approximation error and the distance between exact and estimated poles have been verified. Moreover, the convergence along the sub-diagonal sequence $([N-1/N])_{N=1}^\infty$ has been confirmed numerically.

Remark: The V -norm used in the experiments above is a suitably weighted version

$$\|\cdot\|_V = \left(\|\cdot\|_{H_0^1(\Omega)}^2 + \text{Re}(z_0)^2 \|\cdot\|_{L^2(\Omega)}^2 \right)^{1/2}$$

of the usual $H^1(\Omega)$ norm to account for the harmonic nature of the solution.

References

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