Learned Infinite Elements

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Abstract

We propose a new type of transparent boundary conditions which shares the algebraic structure with standard transparent boundary conditions, while the matrix entries are not derived analytically from the exterior PDE, but optimized or "learned" from a given Dirichlet-to-Neumann (DtN) operator. We study scalar time-harmonic second-order wave equations, which are separable in the exterior domain such that DtN can be written as a functional calculus of (typically) the Laplace-Beltrami operator on the coupling boundary. The optimization problem reduces to a rational approximation problem for the symbol of DtN. Convergence rates are determined by the singularities of the holomorphic extension of the symbol, and they are typically exponential. Learned Infinite Elements outperform classical methods such as Perfectly Matched Layers for the Helmholtz equation and also work seamlessly for strongly inhomogeneous layered media such as the atmosphere of the Sun.

Keywords: transparent boundary conditions, rational approximation, stratified media, exponential convergence

1 Introduction

We consider a linear second-order elliptic PDE

 $\mathcal{L}u = f$ in Ω + radiation condition, (1)

on some unbounded domain $\Omega \subset \mathbb{R}^d$ which is the disjoint union of a bounded interior domain Ω_{int} with supp $f \subset \Omega_{int}$, an unbounded exterior domain Ω_{ext} where \mathcal{L} is separable and a smooth coupling boundary $\Gamma = \partial \Omega_{int} \cap \partial \Omega_{ext}$. For computing accurate approximations of the solution u in Ω_{int} with as little as possible computational effort for the treatment of Ω_{ext} a number of different methods have been proposed and analyzed including Perfectly Matched Layers, different type of infinite elements, local transparent boundary conditions, and others.



Figure 1: Learned Infinite Elements can be seen as classical finite elements on some artificial domain, the voilet are indicates one such element. System matrices are learned within the algebraic structure of finite element discretizations to approximate a given DtN operator.

2 Reduction to a rational approximation problem

By separability we mean that there exists a diffeomorphism $\Psi : [a, \infty) \times \Gamma \to \overline{\Omega}_{ext}$ such that $\Psi(\{a\} \times \Gamma) = \Gamma, |\partial_r \Psi(a, \hat{x})|_2 = 1, \hat{x} \in \Gamma$ and

$$(\mathcal{L}u) \circ \Psi = [\mathcal{A} \otimes \mathrm{Id}_{\Gamma} + \mathcal{B} \otimes (-\Delta_{\Gamma})] (u \circ \Psi) \quad (2)$$

Here \mathcal{A} is a second-order differential operator in r, \mathcal{B} is a multiplication operator on $L^2([a, \infty))$, Δ_{Γ} is the Laplace-Beltrami operator on Γ , and Id_{Γ} the identity operator on $L^2(\Gamma)$. Then the exterior PDE separates into a sequence of ordinary differential equations $(\mathcal{A} + \lambda_{\ell}\mathcal{B})\varphi_{\ell}$ indexed by the eigenvalues λ_{ℓ} of $-\Delta_{\Gamma}$. If $\{v_{\ell} : \ell \in \mathbb{N}\}$ is a corresponding orthonormal L^2 basis of eigenvectors of Δ_{Γ} , the Dirichlet-to-Neumann map DtN on Γ can be written as a functional calculus

DtN
$$u_0 = \operatorname{dtn}(-\Delta_{\Gamma})u_0 = \sum_{\ell=1}^{\infty} \operatorname{dtn}(\lambda_{\ell}) \langle u_0, v_{\ell} \rangle v_{\ell}$$

with a function $dtn(\lambda_{\ell}) = \varphi'_{\ell}(a)/\varphi_{\ell}(a)$ that we will refer to as symbol of DtN.



(a) Homogen:: dtn^{hom} (b) Waveguide: dtn^{guide} Figure 2: Symbols dtn of DtN operators for (a): homogeneous Helmholtz equation in the exterior of a ball , (b) homogeneous wave-guide with Dirichlet boundary conditions. First row: geometries, second row: real and imaginary part of the dtn functions, third row: structure of the singularities of analytic extensions of the dtn functions, which are poles in (a) and a branch cut in (b).

It turns out that for tensor product discretizations of Perfectly Matched Layers, infinite elements and other methods, the discrete analog $\underline{\text{DtN}}$ of DtN has a similar form,

$$\underline{\mathrm{DtN}} = \mathrm{dtn}_N(-\underline{\Delta}_{\Gamma})$$

with a discrete approximation $\underline{\Delta}_{\Gamma}$ of $\underline{\Delta}_{\Gamma}$. Here dtn_N is a rational function which is given explicitly in terms of the matrix representations $\underline{A}, \underline{B} \in \mathbb{C}^{(N+1)\times(N+1)}$ of the operators \mathcal{A} and \mathcal{B} in (2) (or transformations of these operators), more precisely dtn_N = r/q with polynomial r, qof degrees deg(r) = N + 1 and deg(q) = N (see Fig. 1).

In Learned Infinite Elements the matrices \underline{A} and \underline{B} are not derived analytically, but "learned" from the symbol dtn of DtN by solving a rational approximation problem in a preprocessing step. If dtn_N has only simple poles (and such rational functions are dense in the set of rational functions of the given degrees), then the right lower $N \times N$ blocks of \underline{A} and \underline{B} can be chosen diagonal such that Learned Infinite Elements lead to sparser system matrices than most other methods.



Figure 3: Error plot for Learned Infinite Elements, Hardy space infinite elements, adaptive PML and tensor product PML in terms of the number of degrees of freedom (left) and the number of non-zero matrix elements (right) for a point source.

3 holomorphic extensions of the symbol and convergence rates

The error of the DtN approximation can be bounded in terms of a weighted error of the rational dtn approximation. It is known that the approximation rate of the latter is usually exponential in N if dtn has a holomorphic extension, and it is determined by the position of singularities of this holomorphic extension. E.g. for the Helmholtz equation, $\mathcal{L} = \Delta + k^2$ in the exterior of a disk with radius a, the symbol $dtn^{hom}(\lambda) =$ $kH^{(1)}_{a\sqrt{\lambda}}(ka)/H^{(1)}_{a\sqrt{\lambda}}(ka)$ has simple poles tending to infinity along an implicitly defined curve (see Fig. 2a and [2]). We get exponential convergence, which is considerably faster than for competing methods (see Fig. 3). For a homogeneous waveguide, rational approximations to $dtn^{guide}(\lambda) = -i\sqrt{k^2 - \lambda}$ are also known to converge of order $\mathcal{O}(\exp(-\sqrt{N}))$ as $N \to \infty$.

For stratified media exhibiting internal reflections where dtn is usually not explicitly known, in particular the solar atmosphere, we observed poles close to the real axis, but only very few. This is in line with the observed very rapid convergence of Learned Infinite Elements in our numerical experiments.

References

- T. Hohage, C. Lehrenfeld and J. Preuß, Learned Infinite Elements, SIAM Journal of Scientific Computing 43 (2021), pp. A3552–A3579.
- [2] W. Magnus and L. Kotin, The zeros of the Hankel function as a function of its order, *Numer. Math.* 2 (1960), p. 228-244-