The waveguide eigenvalue problem and the Tensor Infinite Arnoldi method

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The waveguide eigenvalue problem

The following PDE–eigenvalue problem arises in the study of waves traveling in a periodic medium [3]

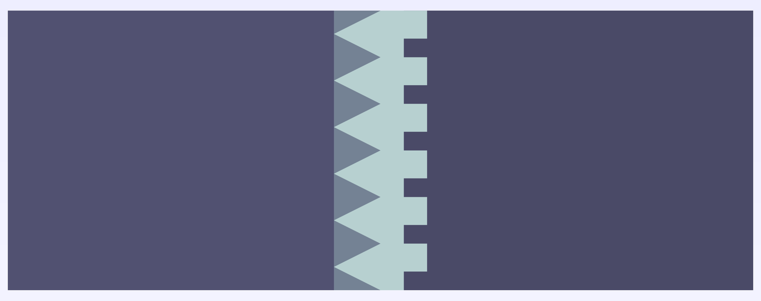
$$\begin{aligned}\Delta u(x,z) \;+\; 2\gamma u_z(x,z) + (\gamma^2 + \kappa(x,z)^2)u(x,z) &= 0, \quad (x,z) \in \mathbb{R}^2,\\ u(x,z) &= u(x,z+1) \;\text{ for all } (x,z) \in \mathbb{R}^2,\\ u(x,\cdot) &\to 0 \text{ when } x \to -\infty,\\ u(x,\cdot) &\to 0 \text{ when } x \to +\infty.\end{aligned}$$

The eigenvalues of interest are in the region

$$\Omega = \{\lambda \in \mathbb{C} \mid Re\lambda < 0, -2\pi < Im\lambda < 0\}$$

The function $\kappa(x,z)$ (wavenumber) is:

- piecewise constant,
- $\kappa(x,z) = \kappa_- \text{ when } x \le x_-$
- $\kappa(x,z) = \kappa_+ \text{ when } x \ge x_+$
- $\kappa(x,z) = \kappa(x,z+1)$



Wavenumber of a sample waveguide.

In the infinite domain $D_{\text{out}} = ([-\infty, x_-] \cup [x_+, +\infty]) \times \mathbb{R}$ the wavenumber is constant, therefore the problem has an analytic solution. Using the Dirichlet to Neumann (DtN) map we reformulate the problem in $D_{\text{in}} = [x_-, x_+] \times \mathbb{R}$ imposing artificial boundary conditions in order to match the solution in $D_{\text{in}} \cap D_{\text{out}}$.

$$\begin{aligned}\Delta u(x,z) + 2\gamma u_z(x,z) + (\gamma^2 + \kappa(x,z)^2)u(x,z) &= 0, \quad (x,z) \in D_{\text{in}},\\ u(x,z) &= u(x,z+1) \;\text{ for all } (x,z) \in \mathbb{R}^2,\\ \mathcal{T}_{-,\gamma}[u(x_-,\cdot)] &= -u_x(x_-,\cdot),\\ \mathcal{T}_{+,\gamma}[u(x_+,\cdot)] &= u_x(x_+,\cdot).\end{aligned}$$

A particular type of FEM discretization leads to the following nonlinear eigenvalue problem, which consists of finding pairs $(\gamma, v) \in \mathbb{C} \times (\mathbb{C}^n \setminus \{0\})$ such that

$$M(\lambda)v = \begin{pmatrix} Q(\gamma) & C_1(\gamma) \\ C_2^T & R\Lambda(\gamma)R^{-1} \end{pmatrix} v = 0.$$

Properties of the problem:

- the size of the problem is n (large number) and $\Lambda(\gamma) \in \mathbb{C}^{\sqrt{n} \times \sqrt{n}}$,
- the matrices $Q(\gamma)$ and $C_1(\gamma)$ are sparse and polynomials of second degree in γ,
- the matrix $\Lambda(\gamma)$ is diagonal and involves square roots of polynomials in γ,
- the functions involved in $\Lambda(\gamma)$ have singularities in the imaginary axis, therefore close to the region where the eigenvalues of interest lie,
- there is a closed formula for the derivatives of $M(\lambda)$,
- the matrix-vector product corresponding to R and R^{-1} can be computed with the Fast Fourier Transform (FFT).

Through a Cayley transformation the eigenvalues of interest are mapped in the unitary disk and the singularities in the unitary circle. The structure of the eigenvalue problem is preserved.

Tensor Infinite Arnoldi Method

Our approach is based on the infinite Arnoldi method [2] which is an iterative algorithm with the following characteristics:

- it is equivalent to the Arnoldi method (for an infinite dimensional eigenproblem),
- k steps result in an Arnoldi relation
$$B_k V_k = V_{k+1} H_{k+1,k}$$
with $V_k \in \mathbb{C}^{nk \times k}$,
- it requires, for each step, the computation of
$$y_0 = M(0)^{-1} \sum_{\ell=1}^{k} M^{(\ell)}(0) v_\ell \qquad (1)$$
- in each step is performed the Gram-Schmidt orthogonalization between vectors of length kn (operations involving a huge amount of data).
- it has complexity (k steps): $O(k^3 n)$ due to the Gram–Schmidt orthogonalization.

Theorem. *[1] It exists a tensor $a \in \mathbb{C}^{k \times k \times k}$ and a matrix $Z_k \in \mathbb{C}^{n \times k}$ such that*

$$V_k = \sum_{\ell=1}^{k} \begin{pmatrix} a_{1,1,\ell} & \cdots & a_{1,k,\ell} \\ \vdots & & \vdots \\ a_{k,1,\ell} & \cdots & a_{k,k,\ell} \end{pmatrix} \otimes z_\ell$$

moreover all the steps of the Infinite Arnoldi method can be done using this factorization of the matrix V_k.

The new algorithm that use this representation of V_k is called Tensor Infinite Arnoldi [1] and has the following properties:

- it requires less memory,
- the Gram-Schmidt orthogonalization is performed involving vectors of length n,
- it is much faster than [2] in practice,
- it has complexity $O(k^3 n)$ due to the computation of y_0, see equation (1).

Remark 1. *In contrast to Infinite Arnoldi method, tensor infinite Arnoldi method involves less data. This implies that on modern computer architectures, where CPU caching makes operations on smaller data-sets more efficiently, the new algorithm is in practice considerably faster.*

Adaption to the waveguide eigenvalue problem

Notice that if $k > 3$ the derivatives of $M(\lambda)$ have the following structure

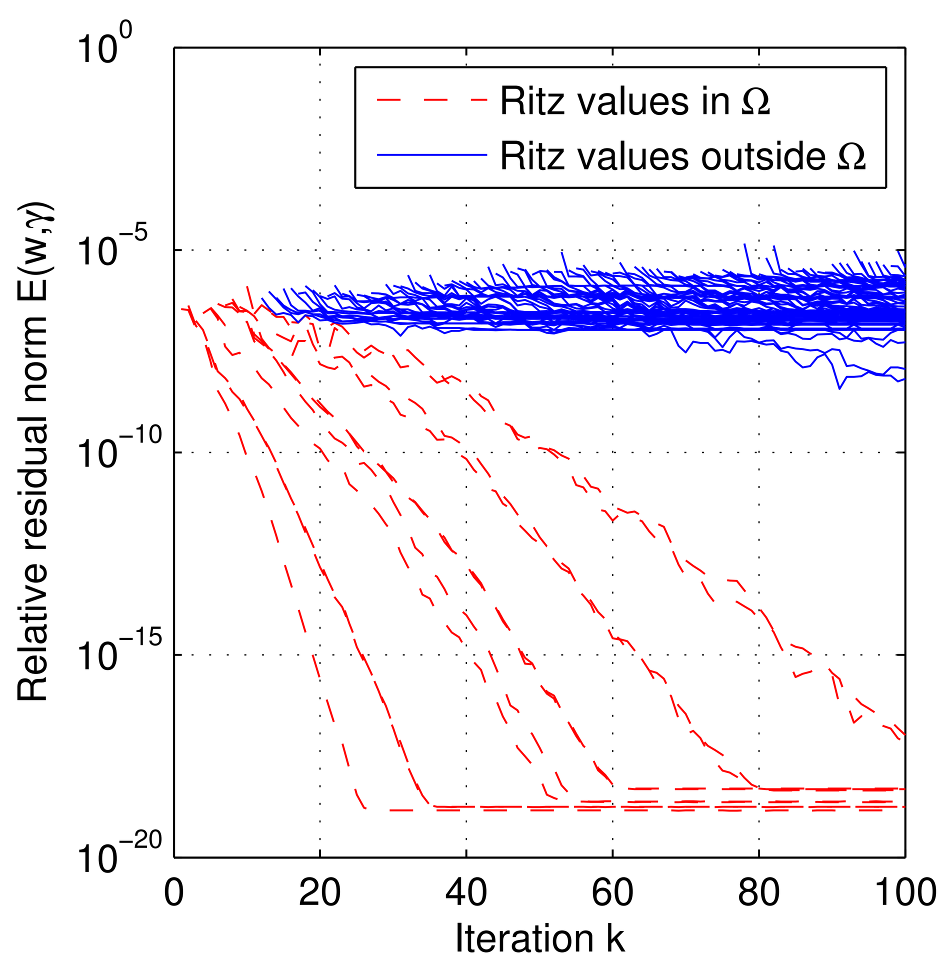
$$M^{(k)}(\lambda) = \begin{pmatrix} 0 & 0 \\ 0 & R\Lambda(\gamma)^{(k)}R^{-1} \end{pmatrix}$$

Exploiting this structure, the computation of y_0 can be done more efficiently and the complexity becomes $O(nk^2 + \sqrt{n}k^3)$.

Remark 2. *If the size of the problem n is large, performing $k \ll n$ steps of tensor infinite Arnoldi method exploiting the structure of the waveguide eigenvalue problem has the same complexity as the Arnoldi method on a classic eigenvalue problem of the same size.*

Numerical experiments

Here are presented the results of the algorithms tested on the sample problem.

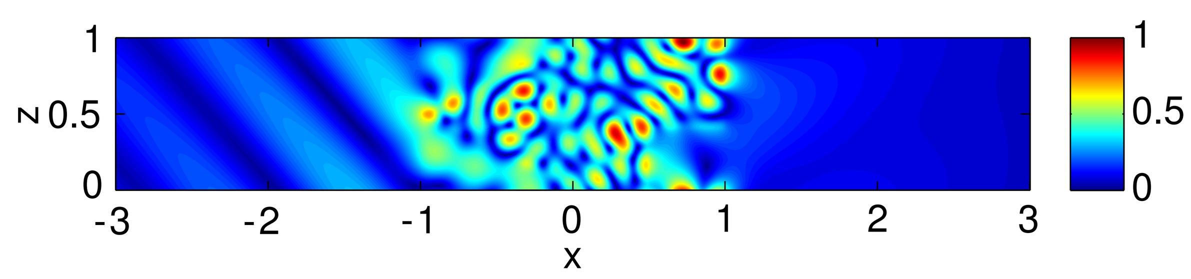


In the pictures there are:

- convergence history of Tensor infinite Arnoldi for a problem of size $n = 411{,}522$ (left),
- one of the eigenfunctions in the region of interest Ω (below).

Conclusions:

- the algorithm solves efficiently the problem,
- large problems can be solved:
  - size more than one million on a laptop (16GB of RAM),
  - size more than ten millions on a server (60GB of RAM).



	CPU time		storage of V_m	
n	IAR	WTIAR	IAR	WTIAR
462	8.35 secs	2.58 secs	35.24 MB	7.98 MB
1,722	28.90 secs	2.83 secs	131.38 MB	8.94 MB
6,642	1 min and 59 secs	4.81 secs	506.74 MB	12.70 MB
26,082	8 mins and 13.37 secs	13.9 secs	1.94 GB	27.52 MB
103,362	out of memory	45.50 secs	out of memory	86.48 MB
411,522	out of memory	3 mins and 30.29 secs	out of memory	321.60 MB
1,642,242	out of memory	15 mins and 20.61 secs	out of memory	1.23 GB

CPU time and estimated memory required to perform $m = 100$ iterations of Infinite Arnoldi (IAR) and Waveguide Tensor Infinite Arnoldi (WTIAR).

References

[1] E. Jarlebring, G. Mele, and O. Runborg. The waveguide eigenvalue problem and the tensor infinite Arnoldi method. *arXiv preprint arXiv:1503.02096*, 2015.

[2] E. Jarlebring, W. Michiels, and K. Meerbergen. A linear eigenvalue algorithm for the nonlinear eigenvalue problem. Technical report, 2010.

[3] J. Tausch and J. Butler. Floquet multipliers of periodic waveguides via Dirichlet-to-Neumann maps. 159(1):90–102, 2000.