The waveguide eigenvalue problem and Tensor infinite Arnoldi

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Joint work with Elias Jarlebring and Olof Runborg

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Outline

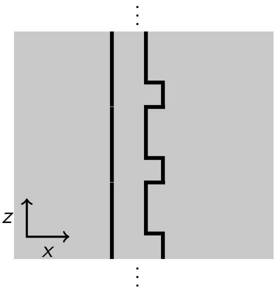
- WEP: Waveguide Eigenvalue Problem
- TIAR: Tensor infinite Arnoldi
- Specialization of TIAR to WEP and numerical simulations

WEP: the waveguide eigenvalue problem

Helmholtz equation (single-periodic coefficients):

$$\begin{aligned} \Delta u(x,z) + \kappa(x,z)^2 u(x,z) &= 0 \text{ when } (x,z) \in \mathbb{R} \times \mathbb{R} \\ u(x,\cdot) &\to 0 \text{ as } x \to \pm\infty \end{aligned}$$

- $\kappa(x,z)$ periodic z-direction.
- $\kappa(x,z)$ constant for $(x,z) \notin [x_-, x_+] \times \mathbb{R}$.



Some related computational works: [Tausch, Butler '02], [Engström, Hafner, Schmidt '09, Engström '10], [Schmidt, Hiptmair '13], [Spence, Poulton '05], [Cox, Stevens '99], ...

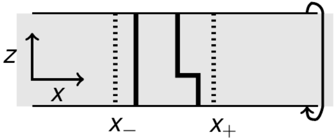
We look for normal modes (Bloch solutions)

$$\begin{aligned} u(x,z) &= e^{\lambda z} v(x,z) \\ v(x,z) &= v(x,z+1) \qquad \Rightarrow \end{aligned}$$

Periodic PDE-eigenvalue problem on a strip

Find $v \in \mathcal{C}^1(\mathbb{R} \times [0,1], \mathbb{R})$ and λ such that:

$$\begin{aligned} \Delta v + 2\lambda v_z + (\lambda^2 + \kappa(x,z)^2) v &= 0 \\ v(\cdot, z) &\to 0 \text{ as } x \to \pm\infty \\ v(x,z) &= v(x,z+1) \end{aligned}$$



Solutions of most interest: $\lambda \in \mathbb{C}_-$ close to imaginary axis.

Absorbing boundary conditions

DtN equivalence

Under generic conditions, equivalent in a weak sense

(i) A solution to PDE-eigenvalue problem on strip.

(ii) A solution to

$$\begin{aligned} \Delta v + 2\lambda v_z + (\lambda^2 + \kappa(x,z)^2) v &= 0, \quad (x,z) \in [x_-, x_+] \times [0,1] \\ v(x,z) &= v(x, z+1) \\ v_x(x_-, \cdot) &= \mathcal{T}_{-,\lambda}(v(x_-, \cdot)) \\ v_x(x_+, \cdot) &= \mathcal{T}_{+,\lambda}(v(x_+, \cdot)) \end{aligned}$$

For formalized weak-sense formulation in preprint

Dirichlet-to-Neumann maps in Fourier space:

$$\mathcal{T}_{\pm,\lambda}\left(\sum_{k=-\infty}^{\infty} a_{\pm,k} e^{i2\pi kz}\right) = \sum_{k=-\infty}^{\infty} s_{\pm,k}(\lambda) a_{\pm,k} e^{i2\pi kz}.$$

where $s_{\pm,k} = \rho_k \sqrt{((\lambda + 2i\pi k) + i\kappa_\pm)((\lambda + 2i\pi k) - i\kappa_\pm)}$

Discretization in the interior with FEM and truncation of DtN

A particular type of FEM discretization leads to

$$M(\lambda)v = \begin{pmatrix} Q(\lambda) & C_1(\lambda) \\ C_2^T & R^H P(\lambda) R \end{pmatrix} v = 0$$

- $Q(\lambda) = A_0 + A_1\lambda + A_2\lambda^2$ — A_i sparse
- $C_1(\lambda) = C_{1,0} + C_{1,1}\lambda + C_{1,2}\lambda^2$ — $C_{1,i}$ sparse
- R corresponds to FFT
- $P(\lambda) = \operatorname{diag}(s_{-,-p}(\lambda), \dots, s_{-,p}(\lambda), s_{+,-p}(\lambda), \dots, s_{+,p}(\lambda))$
- $s_{\pm,k}(\lambda) = \rho_k \sqrt{((\lambda + 2i\pi k) + i\kappa_\pm)((\lambda + 2i\pi k) - i\kappa_\pm)}$.
- $Q(\lambda) \in \mathbb{C}^{n \times n}$ and $P(\lambda) \in \mathbb{R}^{\sqrt{n} \times \sqrt{n}}$

n =discretization parameter

The nonlinear eigenvalue problem

Find $\lambda \in \mathbb{C}$, $v \neq 0$ such that

$$M(\lambda)v = 0$$

where M analytic in a disk $\Omega \subset \mathbb{C}$.

Selection of interesting works

[Ruhe '73], [Mehrmann, Voss '04], [Lancaster '02], [Tisseur, et al. '01], [Voss '05], [Unger '50], [Mackey, et al. '09], [Kressner '09], [Bai, et al. '05], [Meerbergen '09], [Breda, et al. '06], [Betcke, et al. '04, '10], [Asakura, et a. '10], [Beyn '12], [Szyld, Xue '13], [Hochstenbach, et al. '08], [Neumaier '85], [Gohberg, et al. '82], [Effenberger '13], [Van Beeumen, et al '15]
...

TIAR: tensor infinite Arnoldi

Properties / features of infinite Arnoldi method

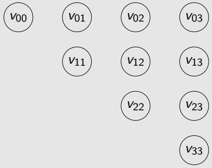
- Equivalent to Arnoldi's method on a companion matrix, for any truncation parameter N with $N > k$
- Equivalent to Arnoldi's method on an operator $\mathcal{B}$
- Reliability
- Convergence theory
- Requires adaption of computation of y_0. For Taylor version:

$$y_0 = M(\hat{\lambda})^{-1}(M'(\hat{\lambda})x_1 + \cdots + M^{(k)}(\hat{\lambda})x_k)$$

- Complexity of orthogonalization at step k: $O(k^2 n)$

Described in: [Jarlebring, et al. '11, '12, '15]

Observation: The basis matrix has a structure



Theorem (Implicit representation of the basis matrix [Jarlebring, M., Runborg '15])

There exists $Z = [z_1, \dots, z_k] \in \mathbb{C}^{n \times k}$ and tensor $[a_{i,j,\ell}]_{i,j,\ell=1}^{k}$, such that the blocks in the basis matrix generated by k steps of infinite Arnoldi method can factorized as

$$v_{i,j} = \sum_{\ell=1}^{k} a_{i,j,k} z_k.$$

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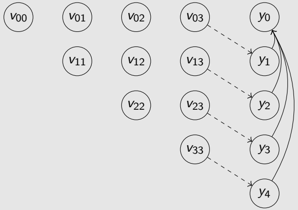

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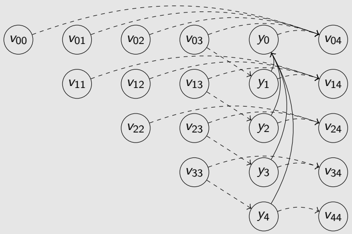

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Key ideas of TIAR

- Rephrase IAR using implicit representation of basis matrix as a $Z \in \mathbb{C}^{n \times k}$ and $[a_{i,j,\ell}]_{i,j,\ell=1}^{k}$.
- Maintain orthogonality of Z for numerical stability

TIAR vs IAR

- TIAR involves less memory $\mathcal{O}(nm^2)$ vs. $\mathcal{O}(nm)$,
- Complexity for m steps: $\mathcal{O}(nm^3)$ for both,
- TIAR involves less data and is much faster due to modern CPU-caching issues

Other literature with compact representations

- **TOAR**: [Zhang, Su, '13]
  Quadratic eigenvalue problem

$$M(\lambda) = A_0 + \lambda A_1 + \lambda^2 A_2$$

- **generalization of TOAR** [Kressner, Roman '14]
  Polynomial eigenvalue problem

$$M(\lambda) = A_0 + \lambda A_1 + \lambda^2 A_2 + \cdots + \lambda^d A_d$$

- **CORK**: [V. Beeumen, et al '15]
  Rational Krylov applied to (eventually growing) linearization of the NEP

TIAR is different in many ways: algorithm, derivation, application focus, extension to infinity, applicability to the WEP, . . .

Specialization of TIAR to WEP and numerical simulations

Recall WEP:

$$M(\lambda) = \begin{pmatrix} Q(\lambda) & C_1(\lambda) \\ C_2^T & R^H P(\lambda) R \end{pmatrix}$$

and $Q(\lambda) = A_0 + A_1\lambda + A_2\lambda^2$
and $C_1(\lambda) = C_{1,0} + C_{1,1}\lambda + C_{1,2}\lambda^2$

$$P(\lambda) = \text{diag}(s_{-,-p}(\lambda), \dots, s_{-,p}(\lambda), s_{+,-p}(\lambda), \dots, s_{+,p}(\lambda))$$

where

$$s_{\pm,k}(\lambda) = \rho_k \sqrt{((\lambda + 2i\pi k) + i\kappa_\pm)((\lambda + 2i\pi k) - i\kappa_\pm)}.$$

Bad news: $\mathcal{O}(\sqrt{n})$ branch-point singularities
Good news: All singularities are on $i\mathbb{R}$

Solution

Cayley transformation brings all singularities to unit circle.
Apply algorithm to Cayley transformed problem.

In order to implement IAR or TIAR: We need an efficient way to compute

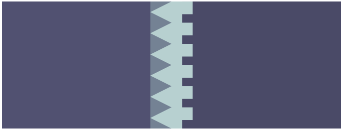
$$y_0 = M(0)^{-1}(M'(0)x_1 + \cdots + M^{(k)}(0)x_k)$$

Compute by exploiting structure

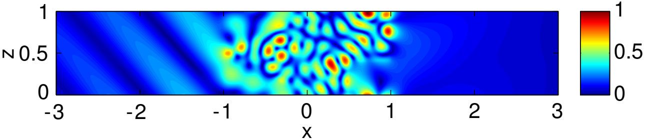
- Derivatives of $\sqrt{a\lambda^2 + b\lambda + c}$ after Cayley transformation computable with Gegenbauer polynomials (inspired by [Tausch, Butler 02'])
- Use FFT-for dense (2,2)-block
- Higher order derivatives have $\mathcal{O}(\sqrt{n})$ non-zero elements (reduces dominant $\mathcal{O}(n)$-term to $\mathcal{O}(\sqrt{n})$)
- Use Schur complement and LU-factorization of $(1,1)$-block

Numerical experiments

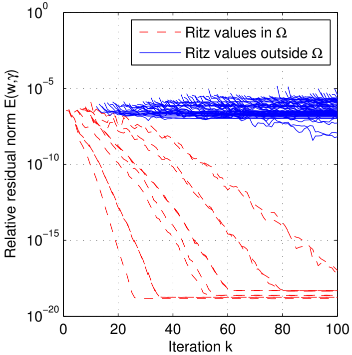
Simulations for a (more difficult) variant of the waveguide in [Tausch, Butler '02]

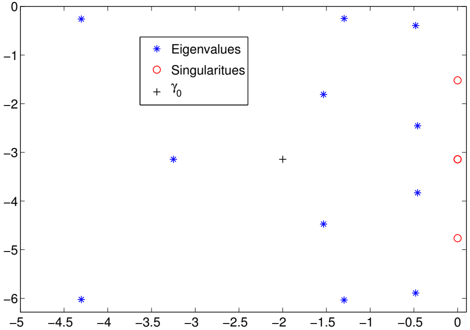


One of the eigenfunctions of interest



Largest problem with our approach: $n \approx 10^7$.





			CPU time		storage of Q_m	
n	n_x	n_z	IAR	WTIAR	IAR	TIAR
462	20	21	8.35 secs	2.58 secs	35.24 MB	7.98 MB
1,722	40	41	28.90 secs	2.83 secs	131.38 MB	8.94 MB
6,642	80	81	1 min and 59 secs	4.81 secs	506.74 MB	12.70 MB
26,082	160	161	8 mins and 13.37 secs	13.9 secs	1.94 GB	27.52 MB
103,362	320	321	out of memory	45.50 secs	out of memory	86.48 MB
411,522	640	641	out of memory	3 mins and 30.29 secs	out of memory	321.60 MB
1,642,242	1280	1281	out of memory	15 mins and 20.61 secs	out of memory	1.23 GB

Using different computer: $n = 9,009,002$, several hours CPU-time.

CONCLUSIONS

New contributions

- A structured discretization of a waveguide eigenvalue problem (WEP)
- A new algorithm: TIAR
- Specialization of TIAR to WEP

Online material:

- Preprint: `http://arxiv.org/abs/1503.02096`
- Software: `http://www.math.kth.se/~gmele/waveguide`