The waveguide eigenvalue problem and Tensor infinite Arnoldi

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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):
\[
\Delta u(x, z) + \kappa(x, z)^2 u(x, z) = 0 \quad \text{when} \quad (x, z) \in \mathbb{R} \times \mathbb{R}
\]
\[
u(x, \cdot) \to 0 \quad \text{as} \quad x \to \pm \infty
\]

- \( \kappa(x, z) \) 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)

\[ u(x, z) = e^{\lambda z} v(x, z) \]
\[ v(x, z) = v(x, z + 1) \implies \]

Periodic PDE-eigenvalue problem on a strip

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

\[ \Delta v + 2\lambda v_z + (\lambda^2 + \kappa(x, z)^2)v = 0 \]
\[ v(\cdot, z) \to 0 \text{ as } x \to \pm\infty \]
\[ v(x, z) = v(x, z + 1) \]

Solutions of most interest: \( \lambda \in \mathbb{C}_- \) close to imaginary axis.
### Absorbing boundary conditions

<table>
<thead>
<tr>
<th>DtN equivalence</th>
</tr>
</thead>
<tbody>
<tr>
<td>Under generic conditions, equivalent in a weak sense</td>
</tr>
<tr>
<td>(i) A solution to PDE-eigenvalue problem on strip.</td>
</tr>
<tr>
<td>(ii) A solution to</td>
</tr>
</tbody>
</table>

\[
\Delta v + 2\lambda v_z + (\lambda^2 + \kappa(x, z)^2)v = 0, \quad (x, z) \in [x_-, x_+] \times [0, 1]
\]

\[
v(x, z) = v(x, z + 1)
\]

\[
v_x(x_-, \cdot) = T_{-},\lambda(v(x_-, \cdot))
\]

\[
v_x(x_+, \cdot) = T_{+},\lambda(v(x_+, \cdot))
\]

For formalized weak-sense formulation in preprint

### Dirichlet-to-Neumann maps in Fourier space:

\[
T_{\pm},\lambda \left( \sum_{k=-\infty}^{\infty} a_{\pm, k} e^{i2\pi k z} \right) = \sum_{k=-\infty}^{\infty} s_{\pm, k}(\lambda) a_{\pm, k} e^{i2\pi k z}.
\]

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

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

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

\[ n = \text{discretization parameter} \]
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 al. '10], [Beyn '12],
[Szyld, Xue '13], [Hochstenbach, et al. '08], [Neumaier '85],
[Gohberg, et al. '82], [Effenberger '13], [Van Beeumen, et al '15]...

The waveguide eigenvalue problem and Tensor infinite Arnoldi

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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 $k$: $O(k^2 n)$

Observation: The basis matrix has a structure

\[
\begin{array}{cccc}
  v_{00} & v_{01} & v_{02} & v_{03} \\
  v_{11} & v_{12} & v_{13} \\
  v_{22} & v_{23} \\
  v_{33} \\
\end{array}
\]

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

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

\[
v_{i,j} = \sum_{\ell=1}^{k} a_{i,j,k} z_{k}.
\]
Observation: The basis matrix has a structure

\[
\begin{array}{cccc}
  v_{00} & v_{01} & v_{02} & v_{03} \\
  v_{11} & v_{12} & v_{13} & y_0 \\
  v_{22} & v_{23} & y_1 & y_2 \\
  v_{33} & y_3 & y_4 \\
\end{array}
\]

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

There exists \( Z = [z_1, \ldots, z_k] \in \mathbb{C}^{n \times k} \) 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

\[
v_{i,j} = \sum_{\ell=1}^{k} a_{i,j,k} z_{k}.
\]
Observation: The basis matrix has a structure

\[ v_{00} \quad v_{01} \quad v_{02} \quad v_{03} \quad v_{04} \]
\[ v_{11} \quad v_{12} \quad v_{13} \quad v_{14} \]
\[ v_{22} \quad v_{23} \quad v_{24} \]
\[ v_{33} \quad v_{34} \]
\[ y_0 \quad y_1 \quad y_2 \quad y_3 \quad y_4 \quad v_{44} \]

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

There exists \( Z = [z_1, \ldots, z_k] \in \mathbb{C}^{n \times k} \) 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

\[ v_{i,j} = \sum_{\ell=1}^k a_{i,j,k} z_{k}. \]
### 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 $O(nm^2)$ vs. $O(nm)$.
- Complexity for $m$ steps: $O(nm^3)$ 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 \( C_1(\lambda) = C_{1,0} + C_{1,1} \lambda + C_{1,2} \lambda^2 \)

\[ P(\lambda) = \text{diag}(s_{-,-p}(\lambda), \ldots, s_{-},p(\lambda), s_{+},-p(\lambda), \ldots, s_{+},p(\lambda)) \]

where

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

**Bad news:** \( O(\sqrt{n}) \) 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 $O(\sqrt{n})$ non-zero elements (reduces dominant $O(n)$-term to $O(\sqrt{n})$)
- 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: \( n \approx 10^7 \).
Using different computer: $n = 9,009,002$, several hours CPU-time.

<table>
<thead>
<tr>
<th>$n$</th>
<th>$n_x$</th>
<th>$n_z$</th>
<th>IAR</th>
<th>WTIAR</th>
<th>IAR</th>
<th>TIAR</th>
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<td>out of memory</td>
<td>1.23 GB</td>
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CONCLUSIONS

New contributions

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

Online material:

- Preprint:
- Software:
  http://www.math.kth.se/~gmele/waveguide