CHAPTER 6 : POLYNOMIAL EIGENVALUE PROBLEMS

Heinrich Voss

voss@tu-harburg.de

Hamburg University of Technology
Institute of Numerical Simulation

TUHH
Technische Universität Hamburg-Harburg

Polynomial eigenvalue problems

Consider the polynomial eigenproblem

$$P(\lambda)x = 0 \quad \text{and/or} \quad y^H P(\lambda) = 0$$

where

$$P(\lambda) = \sum_{j=0}^{\ell} \lambda^j C_j, \qquad C_j \in \mathbb{C}^{n\times n}.$$

Polynomial eigenvalue problems

Consider the polynomial eigenproblem

$$P(\lambda)x = 0 \quad \text{and/or} \quad y^H P(\lambda) = 0$$

where

$$P(\lambda) = \sum_{j=0}^{\ell} \lambda^j C_j, \qquad C_j \in \mathbb{C}^{n\times n}.$$

A thorough study of the mathematical properties of matrix polynomials can be found in the books of Gohberg, Lancaster & Rodman (1982) and Lancaster (2002, reprint of 1965).

Polynomial eigenvalue problems

Consider the polynomial eigenproblem

$$P(\lambda)x = 0 \quad \text{and/or} \quad y^H P(\lambda) = 0$$

where

$$P(\lambda) = \sum_{j=0}^{\ell} \lambda^j C_j, \qquad C_j \in \mathbb{C}^{n\times n}.$$

A thorough study of the mathematical properties of matrix polynomials can be found in the books of Gohberg, Lancaster & Rodman (1982) and Lancaster (2002, reprint of 1965).

If C_ℓ is nonsingular, then the polynomial eigenproblem is equivalent to a matrix pencil of dimension $n\ell$, and there are $n \cdot \ell$ eigenvalues.

Linearization

The polynomial eigenproblem $P(\lambda)x = 0$ is equivalent to the linear eigenproblem $Az = \lambda Bz$ where

$$A = \begin{pmatrix} -C_{\ell-1} & -C_{\ell-2} & \dots & -C_0 \\ I & & & \\ & \ddots & & \\ & & I & \end{pmatrix}, B = \begin{pmatrix} C_\ell & & & \\ & I & & \\ & & \ddots & \\ & & & I \end{pmatrix}, y = \begin{pmatrix} \lambda^{\ell-1}x \\ \lambda^{\ell-2}x \\ \vdots \\ x \end{pmatrix}.$$

Linearization

The polynomial eigenproblem $P(\lambda)x = 0$ is equivalent to the linear eigenproblem $Az = \lambda Bz$ where

$$A = \begin{pmatrix} -C_{\ell-1} & -C_{\ell-2} & \dots & -C_0 \\ I & & & \\ & \ddots & & \\ & & I & \end{pmatrix}, B = \begin{pmatrix} C_\ell & & & \\ & I & & \\ & & \ddots & \\ & & & I \end{pmatrix}, y = \begin{pmatrix} \lambda^{\ell-1}x \\ \lambda^{\ell-2}x \\ \vdots \\ x \end{pmatrix}.$$

Hence, any linear eigensolver of Arnoldi and Jacobi-Davidson type applies.

Linearization

The polynomial eigenproblem $P(\lambda)x = 0$ is equivalent to the linear eigenproblem $Az = \lambda Bz$ where

$$A = \begin{pmatrix} -C_{\ell-1} & -C_{\ell-2} & \dots & -C_0 \\ I & & & \\ & \ddots & & \\ & & I & \end{pmatrix}, B = \begin{pmatrix} C_\ell & & & \\ & I & & \\ & & \ddots & \\ & & & I \end{pmatrix}, y = \begin{pmatrix} \lambda^{\ell-1}x \\ \lambda^{\ell-2}x \\ \vdots \\ x \end{pmatrix}.$$

Hence, any linear eigensolver of Arnoldi and Jacobi-Davidson type applies.

BUT

- Dimension n grows to $\ell \cdot n$
- Useful structure (symmetry, Hamiltonian) which should be kept for efficiency and/or stability reasons is destroyed

Structure preservation

It is common wisdom in numerical analysis that any kind of extra structure (arising typically from the properties of the underlying physical problem) should be reflected as much as possible in the numerical method.

Structure preservation

It is common wisdom in numerical analysis that any kind of extra structure (arising typically from the properties of the underlying physical problem) should be reflected as much as possible in the numerical method.

In this way it is guaranteed that the approximate numerical solution properly reflects the physical properties of the system, and also structure preservation typically leads to a gain in efficiency and accuracy.

Structure preservation

It is common wisdom in numerical analysis that any kind of extra structure (arising typically from the properties of the underlying physical problem) should be reflected as much as possible in the numerical method.

In this way it is guaranteed that the approximate numerical solution properly reflects the physical properties of the system, and also structure preservation typically leads to a gain in efficiency and accuracy.

As an example consider problems with Hamiltonian eigensymmetry. It has been shown in Freiling, Mehrmann & Xu (2002) and Ran & Rodman (1988, 1989) that the problem may be well-conditioned under structured perturbations, but ill-posed under unstructured perturbations.

Structure preserving linearization

If the matrices C_j in

$$P(\lambda)x = \sum_{j=0}^{\ell} \lambda^j C_j x = 0, \quad C_j \in \mathbb{R}^{n\times n}$$

are alternating symmetric and skew-symmetric, i.e.

$$C_j^T = (-1)^j C_j \quad \text{or} \quad C_j^T = (-1)^{j+1} C_j, \quad j = 0, \ldots, \ell,$$

then it holds

$$P(\lambda)x = 0 \quad \Longleftrightarrow \quad x^T P(-\lambda) = 0.$$

Structure preserving linearization

If the matrices C_j in

$$P(\lambda)x = \sum_{j=0}^{\ell} \lambda^j C_j x = 0, \quad C_j \in \mathbb{R}^{n\times n}$$

are alternating symmetric and skew-symmetric, i.e.

$$C_j^T = (-1)^j C_j \quad \text{or} \quad C_j^T = (-1)^{j+1} C_j, \quad j = 0, \ldots, \ell,$$

then it holds

$$P(\lambda)x = 0 \quad \Longleftrightarrow \quad x^T P(-\lambda) = 0.$$

Hence, the spectrum of $P(\lambda)x = 0$ has Hamiltonian symmetry, i.e. the eigenvalues appear in quadruples $\{\lambda, -\lambda, \bar{\lambda}, -\bar{\lambda}\}$ (note that C_j are real matrices).

Structure preserving linearization

If the matrices C_j in

$$P(\lambda)x = \sum_{j=0}^{\ell} \lambda^j C_j x = 0, \quad C_j \in \mathbb{R}^{n\times n}$$

are alternating symmetric and skew-symmetric, i.e.

$$C_j^T = (-1)^j C_j \quad \text{or} \quad C_j^T = (-1)^{j+1} C_j, \quad j = 0, \ldots, \ell,$$

then it holds

$$P(\lambda)x = 0 \quad \Longleftrightarrow \quad x^T P(-\lambda) = 0.$$

Hence, the spectrum of $P(\lambda)x = 0$ has Hamiltonian symmetry, i.e. the eigenvalues appear in quadruples $\{\lambda, -\lambda, \bar{\lambda}, -\bar{\lambda}\}$ (note that C_j are real matrices).

It should be noted that for eigenvalues with real part zero (for instance for gyroscopic quadratic eigenproblems), where $\lambda = -\overline{\lambda}$, the quadruples are only pairs.

Structure preserving linearization ct.

There are linearizations that preserve the Hamiltonian symmetry

Structure preserving linearization ct.

There are linearizations that preserve the Hamiltonian symmetry

THEOREM (Mehrmann & Watkins) 2001,2002

$P(\lambda)x = 0$ has the same eigenvalues as the pencil $A - \lambda B$ where

$$A = \left(\begin{array}{c|cccc} -C_0 & O & O & O & \dots & O \\ \hline O & -C_2 & -C_3 & -C_4 & \dots & -C_\ell \\ O & C_3 & C_4 & & & O \\ O & -C_4 & & & & O \\ \vdots & \vdots & & & & \vdots \\ O & \pm C_\ell & O & O & \dots & O \end{array}\right),$$

$$B = \left(\begin{array}{cccc|c} C_1 & C_2 & C_3 & \dots & C_{\ell-1} & C_\ell \\ \hline -C_2 & -C_3 & -C_4 & \dots & -C_\ell & O \\ C_3 & C_4 & & & O & O \\ -C_4 & & & & O & O \\ \vdots & & & & \vdots & \vdots \\ \pm C_\ell & O & O & \dots & O & O \end{array}\right).$$

Structure preserving linearization ct.

The pencil $A - \lambda B$ obviously is skew-symmetric/symmetric.

Structure preserving linearization ct.

The pencil $A - \lambda B$ obviously is skew-symmetric/symmetric.

If the dimension of the linearized problem is even then multiplying by

$$J := \begin{pmatrix} O & I \\ -I & O \end{pmatrix}$$

one gets a skew-Hamiltonian/Hamiltonian pencil

$$\lambda H_1 - H_2$$

with $(JH_1)^T = -JH_1$ and $(JH_2)^T = JH_2$.

Structure preserving linearization ct.

The pencil $A - \lambda B$ obviously is skew-symmetric/symmetric.

If the dimension of the linearized problem is even then multiplying by

$$J := \begin{pmatrix} O & I \\ -I & O \end{pmatrix}$$

one gets a skew-Hamiltonian/Hamiltonian pencil

$$\lambda H_1 - H_2$$

with $(JH_1)^T = -JH_1$ and $(JH_2)^T = JH_2$.

If H_1 can be represented in product form $H_1 = Z_1 Z_2$ such that $Z_2^T J = \pm J Z_1$ then this pencil is equivalent to the standard eigenvalue problem

$$Z_1^{-1} H_2 Z_2^{-1} - \lambda I =: W - \lambda I$$

in which the matrix W can be easily shown to be Hamiltonian.

Structure preserving linearization ct.

Applying Arnoldi's method to the skew-Hamiltonian matrix $-W$ then (in exact arithmetic) the Krylov space $\mathcal{K}_k(q^1, W)$ is isotropic, i.e.

$$x^T Jy = 0 \quad \text{for all } x, y \in \mathcal{K}_k(q^1, W).$$

Structure preserving linearization ct.

Applying Arnoldi's method to the skew-Hamiltonian matrix $-W$ then (in exact arithmetic) the Krylov space $\mathcal{K}_k(q^1, W)$ is isotropic, i.e.

$$x^T Jy = 0 \quad \text{for all } x, y \in \mathcal{K}_k(q^1, W).$$

Therefore, to keep the Hamiltonian structure in the Arnoldi process one should not only orthogonalize against $q^1, \ldots, q^k$, but also against $Jq^1, \ldots, Jq^k$.

Structure preserving linearization ct.

Applying Arnoldi's method to the skew-Hamiltonian matrix $-W$ then (in exact arithmetic) the Krylov space $\mathcal{K}_k(q^1, W)$ is isotropic, i.e.

$$x^T Jy = 0 \quad \text{for all } x, y \in \mathcal{K}_k(q^1, W).$$

Therefore, to keep the Hamiltonian structure in the Arnoldi process one should not only orthogonalize against $q^1, \ldots, q^k$, but also against $Jq^1, \ldots, Jq^k$.

Moreover, for the same reason shifts have to be used in pairs $\{\sigma, -\sigma\}$ (if eigenvalues are real or purely imaginary) or in quadruples $\{\sigma, -\sigma, \bar{\sigma}, -\bar{\sigma}\}$.

Structure preserving linearization ct.

Applying Arnoldi's method to the skew-Hamiltonian matrix $-W$ then (in exact arithmetic) the Krylov space $\mathcal{K}_k(q^1, W)$ is isotropic, i.e.

$$x^T Jy = 0 \quad \text{for all } x, y \in \mathcal{K}_k(q^1, W).$$

Therefore, to keep the Hamiltonian structure in the Arnoldi process one should not only orthogonalize against $q^1, \ldots, q^k$, but also against $Jq^1, \ldots, Jq^k$.

Moreover, for the same reason shifts have to be used in pairs $\{\sigma, -\sigma\}$ (if eigenvalues are real or purely imaginary) or in quadruples $\{\sigma, -\sigma, \bar{\sigma}, -\bar{\sigma}\}$.

This results in SHIRA, a structure-preserving skew-Hamiltonian, isotropic, implicitly restarted shift-and-invert Arnoldi algorithm proposed by Mehrmann & Watkins (2001).

Gyroscopic eigenproblem

Consider the gyroscopic eigenproblem

$$Q(\lambda)x := \lambda^2 Mx + \lambda Gx + Kx,$$

where $K = K^T$, $M = M^T$ and $G = -G^T$.

Gyroscopic eigenproblem

Consider the gyroscopic eigenproblem

$$Q(\lambda)x := \lambda^2 Mx + \lambda Gx + Kx,$$

where $K = K^T$, $M = M^T$ and $G = -G^T$.

Applying the structure preserving linearization yields the symmetric/skew-symmetric pencil

$$\begin{pmatrix} -K & O \\ O & -M \end{pmatrix} - \lambda \begin{pmatrix} G & M \\ -M & O \end{pmatrix},$$

and multiplying by $-J$ we obtain the skew-Hamiltonian/Hamiltonian pencil

$$\begin{pmatrix} O & M \\ -K & O \end{pmatrix} - \lambda \begin{pmatrix} M & O \\ G & M \end{pmatrix}$$

...

Gyroscopic eigenproblem ct.

which with

$$\begin{pmatrix} M & O \\ G & M \end{pmatrix} = \begin{pmatrix} M & O \\ 0.5G & I \end{pmatrix} \begin{pmatrix} I & O \\ 0.5G & M \end{pmatrix} = Z_1 Z_2$$

can be reduced to the skew-Hamiltonian eigenproblem

$$Wy := \begin{pmatrix} M & O \\ 0.5G & I \end{pmatrix}^{-1} \begin{pmatrix} O & M \\ -K & O \end{pmatrix} \begin{pmatrix} I & O \\ 0.5G & M \end{pmatrix}^{-1} y = \lambda y.$$

Gyroscopic eigenproblem ct.

which with

$$\begin{pmatrix} M & O \\ G & M \end{pmatrix} = \begin{pmatrix} M & O \\ 0.5G & I \end{pmatrix} \begin{pmatrix} I & O \\ 0.5G & M \end{pmatrix} = Z_1 Z_2$$

can be reduced to the skew-Hamiltonian eigenproblem

$$Wy := \begin{pmatrix} M & O \\ 0.5G & I \end{pmatrix}^{-1} \begin{pmatrix} O & M \\ -K & O \end{pmatrix} \begin{pmatrix} I & O \\ 0.5G & M \end{pmatrix}^{-1} y = \lambda y.$$

Introducing shifts σ and $-\sigma$ one has to apply the isotropic Arnoldi process to

$$\begin{aligned} R &= (W-\sigma I)^{-1}(W+\sigma I)^{-1} = Z_2(H_2-\sigma H_1)^{-1} Z_1 Z_2 (H_2+\sigma H_1)^{-1} Z_1 \\ &= \begin{pmatrix} I & O \\ 0.5G & M \end{pmatrix} \begin{pmatrix} I & O \\ \sigma I & I \end{pmatrix} \begin{pmatrix} O & M^{-1} \\ -Q(\sigma)^{-1} & O \end{pmatrix} \times \\ &\quad \times \begin{pmatrix} M & O \\ G & M \end{pmatrix} \begin{pmatrix} O & M^{-1} \\ -Q(-\sigma)^{-1} & O \end{pmatrix} \begin{pmatrix} I & O \\ -\sigma I & I \end{pmatrix} \begin{pmatrix} M & O \\ 0.5G & I \end{pmatrix} \end{aligned}$$

Second order Krylov subspace

Consider the quadratic eigenvalue problem

$$(\lambda^2 C_2 + \lambda C_1 + C_0)x = 0$$

and its linearization

$$Ay = \begin{pmatrix} -C_1 & -C_0 \\ I & 0 \end{pmatrix} y = \lambda \begin{pmatrix} C_2 & 0 \\ 0 & I \end{pmatrix} y.$$

Second order Krylov subspace

Consider the quadratic eigenvalue problem

$$(\lambda^2 C_2 + \lambda C_1 + C_0)x = 0$$

and its linearization

$$Ay = \begin{pmatrix} -C_1 & -C_0 \\ I & 0 \end{pmatrix} y = \lambda \begin{pmatrix} C_2 & 0 \\ 0 & I \end{pmatrix} y.$$

To apply a Krylov subspace-based method we need the Krylov space $\mathcal{K}_k(y^0, H)$, where

$$H = B^{-1}A = \begin{pmatrix} -C_2^{-1}C_1 & -C_2^{-1}C_0 \\ I & 0 \end{pmatrix} =: \begin{pmatrix} E & F \\ I & 0 \end{pmatrix}.$$

Second order Krylov subspace

Consider the quadratic eigenvalue problem

$$(\lambda^2 C_2 + \lambda C_1 + C_0)x = 0$$

and its linearization

$$Ay = \begin{pmatrix} -C_1 & -C_0 \\ I & 0 \end{pmatrix} y = \lambda \begin{pmatrix} C_2 & 0 \\ 0 & I \end{pmatrix} y.$$

To apply a Krylov subspace-based method we need the Krylov space $\mathcal{K}_k(y^0, H)$, where

$$H = B^{-1}A = \begin{pmatrix} -C_2^{-1}C_1 & -C_2^{-1}C_0 \\ I & 0 \end{pmatrix} =: \begin{pmatrix} E & F \\ I & 0 \end{pmatrix}.$$

We study the Krylov space for the particular initial vector

$$y^0 := \begin{pmatrix} u \\ 0 \end{pmatrix}$$

for some vector $u \neq 0$.

Second order Krylov subspace ct.

$$
\begin{aligned}
y^1 &:= Hy^1 = \begin{pmatrix} E & F \\ I & 0 \end{pmatrix} \begin{pmatrix} u \\ 0 \end{pmatrix} = \begin{pmatrix} Eu \\ u \end{pmatrix} =: \begin{pmatrix} u^1 \\ u^0 \end{pmatrix} \\
y^2 &:= Hy^1 = \begin{pmatrix} E & F \\ I & 0 \end{pmatrix} \begin{pmatrix} u^1 \\ u^0 \end{pmatrix} = \begin{pmatrix} Eu^1 + Fu^0 \\ u^1 \end{pmatrix} =: \begin{pmatrix} u^2 \\ u^1 \end{pmatrix} \\
y^3 &:= Hy^2 = \begin{pmatrix} E & F \\ I & 0 \end{pmatrix} \begin{pmatrix} u^2 \\ u^1 \end{pmatrix} = \begin{pmatrix} Eu^2 + Fu^1 \\ u^2 \end{pmatrix} =: \begin{pmatrix} u^3 \\ u^2 \end{pmatrix} \\
&\dots \\
y^{j+1} &= Hy^j = \begin{pmatrix} E & F \\ I & 0 \end{pmatrix} \begin{pmatrix} u^j \\ u^{j-1} \end{pmatrix} = \begin{pmatrix} Eu^j + Fu^{j-1} \\ u^j \end{pmatrix} =: \begin{pmatrix} u^{j+1} \\ u^j \end{pmatrix}
\end{aligned}
$$

Second order Krylov subspace ct.

$$
\begin{aligned}
y^1 &:= Hy^1 = \begin{pmatrix} E & F \\ I & 0 \end{pmatrix} \begin{pmatrix} u \\ 0 \end{pmatrix} = \begin{pmatrix} Eu \\ u \end{pmatrix} =: \begin{pmatrix} u^1 \\ u^0 \end{pmatrix} \\
y^2 &:= Hy^1 = \begin{pmatrix} E & F \\ I & 0 \end{pmatrix} \begin{pmatrix} u^1 \\ u^0 \end{pmatrix} = \begin{pmatrix} Eu^1 + Fu^0 \\ u^1 \end{pmatrix} =: \begin{pmatrix} u^2 \\ u^1 \end{pmatrix} \\
y^3 &:= Hy^2 = \begin{pmatrix} E & F \\ I & 0 \end{pmatrix} \begin{pmatrix} u^2 \\ u^1 \end{pmatrix} = \begin{pmatrix} Eu^2 + Fu^1 \\ u^2 \end{pmatrix} =: \begin{pmatrix} u^3 \\ u^2 \end{pmatrix} \\
&\dots \\
y^{j+1} &= Hy^j = \begin{pmatrix} E & F \\ I & 0 \end{pmatrix} \begin{pmatrix} u^j \\ u^{j-1} \end{pmatrix} = \begin{pmatrix} Eu^j + Fu^{j-1} \\ u^j \end{pmatrix} =: \begin{pmatrix} u^{j+1} \\ u^j \end{pmatrix}
\end{aligned}
$$

Hence, the whole information on the Krylov space $\mathcal{K}_k(y^0, H)$ is contained in the sequence $\{u^j\}$ which has the dimension n of the original problem.

Second order Krylov subspace ct.

$$
\begin{aligned}
y^1 &:= Hy^1 = \begin{pmatrix} E & F \\ I & 0 \end{pmatrix} \begin{pmatrix} u \\ 0 \end{pmatrix} = \begin{pmatrix} Eu \\ u \end{pmatrix} =: \begin{pmatrix} u^1 \\ u^0 \end{pmatrix} \\
y^2 &:= Hy^1 = \begin{pmatrix} E & F \\ I & 0 \end{pmatrix} \begin{pmatrix} u^1 \\ u^0 \end{pmatrix} = \begin{pmatrix} Eu^1 + Fu^0 \\ u^1 \end{pmatrix} =: \begin{pmatrix} u^2 \\ u^1 \end{pmatrix} \\
y^3 &:= Hy^2 = \begin{pmatrix} E & F \\ I & 0 \end{pmatrix} \begin{pmatrix} u^2 \\ u^1 \end{pmatrix} = \begin{pmatrix} Eu^2 + Fu^1 \\ u^2 \end{pmatrix} =: \begin{pmatrix} u^3 \\ u^2 \end{pmatrix} \\
&\dots \\
y^{j+1} &= Hy^j = \begin{pmatrix} E & F \\ I & 0 \end{pmatrix} \begin{pmatrix} u^j \\ u^{j-1} \end{pmatrix} = \begin{pmatrix} Eu^j + Fu^{j-1} \\ u^j \end{pmatrix} =: \begin{pmatrix} u^{j+1} \\ u^j \end{pmatrix}
\end{aligned}
$$

Hence, the whole information on the Krylov space $\mathcal{K}_k(y^0, H)$ is contained in the sequence $\{u^j\}$ which has the dimension n of the original problem.

Bai & Su (2005) proposed SOAR, a second order Arnoldi method for the solution of quadratic eigenvalue problems which is based on this sequence.

Definition For $E, F \in \mathbb{R}^{n\times n}$, and $u \in \mathbb{R}^n$, $u \neq 0$ the sequence

$$\begin{aligned} u^0 &:= u \\ u^1 &:= Eu^0 \\ u^j &:= Eu^{j-1} + Fu^{j-1},\ j \geq 2 \end{aligned}$$

is called a second order Krylov sequence based on E, F, and u. The space

$$\mathcal{G}_k(u^0, E, F) = \text{span}\{u^0, u^1, \ldots, u^{k-1}\}$$

is called a kth second order Krylov subspace.

Definition For $E, F \in \mathbb{R}^{n\times n}$, and $u \in \mathbb{R}^n$, $u \neq 0$ the sequence

$$\begin{aligned} u^0 &:= u \\ u^1 &:= Eu^0 \\ u^j &:= Eu^{j-1} + Fu^{j-1},\ j \geq 2 \end{aligned}$$

is called a second order Krylov sequence based on E, F, and u. The space

$$\mathcal{G}_k(u^0, E, F) = \text{span}\{u^0, u^1, \ldots, u^{k-1}\}$$

is called a kth second order Krylov subspace.

Note the subspace $\mathcal{G}_k(u^0, E, F)$ generalizes the standard Krylov subspace $\mathcal{K}_k(u^0, E)$ since $\mathcal{K}_k(u^0, E) = \mathcal{G}_k(u^0, E, O)$.

SOAR

$q^1 = u/\|u\|$
$p^0 = 0$
for $k = 1, 2, \ldots$ **do**
  $r = Eq^j + Fp^j$
  $s = q^j$
  for i=1,2,. . . ,j **do**
    $t_{ij} = (q^i)^T r$
    $r = r - q^i t_{ij}$
    $s = s - p^i t_{ij}$
  end for
  $t_{j+1,j} = \|r\|$
  if $t_{j+1,j} = 0$ **stop end if**
  $q^{j+1} = r/t_{j+1,j}$
  $p^{j+1} = s/t_{j+1,j}$
end for

Comments on SOAR

The matrices E and F are referenced only via the matrix-vector multiplication in line 4 of the SOAR algorithm. Therefore, it is ideal for sparse matrices E and F.

Comments on SOAR

The matrices E and F are referenced only via the matrix-vector multiplication in line 4 of the SOAR algorithm. Therefore, it is ideal for sparse matrices E and F.

The **for**-loop in lines 6-10 is an orthonormalization procedure with respect to the q^i vectors. The vector sequence p^j is an auxiliary sequence. There exists a modified version of the algorithm in Bai & Su (2005) which avoids the vectors p^j thus reducing the memory requirements by almost one half.

Comments on SOAR

The matrices E and F are referenced only via the matrix-vector multiplication in line 4 of the SOAR algorithm. Therefore, it is ideal for sparse matrices E and F.

The **for**-loop in lines 6-10 is an orthonormalization procedure with respect to the q^i vectors. The vector sequence p^j is an auxiliary sequence. There exists a modified version of the algorithm in Bai & Su (2005) which avoids the vectors p^j thus reducing the memory requirements by almost one half.

The SOAR algorithm stops prematurely when the norm of r computed in line 12 vanishes at certain step j. In this case, we encounter either deflation or breakdown.

SOAR ct.

Let $Q_k := [q^1, \ldots, q^k] \in \mathbb{R}^{n\times k}$ and $P_k := [p^1, \ldots, p^k] \in \mathbb{R}^{n\times k}$, and let $T \in \mathbb{R}^{k\times k}$ be the upper Hessenberg matrices with nonzero entries t_{ij} as defined in the SOAR algorithm. Then the following relations hold true

$$\begin{aligned} EQ_k + FP_k &= Q_k T_k + t_{k+1,k} q^{k+1} (e^k)^T \\ Q_k &= P_k T_k + t_{k+1,k} p^{k+1} (e^k)^T. \end{aligned}$$

SOAR ct.

Let $Q_k := [q^1, \ldots, q^k] \in \mathbb{R}^{n\times k}$ and $P_k := [p^1, \ldots, p^k] \in \mathbb{R}^{n\times k}$, and let $T \in \mathbb{R}^{k\times k}$ be the upper Hessenberg matrices with nonzero entries t_{ij} as defined in the SOAR algorithm. Then the following relations hold true

$$\begin{aligned} EQ_k + FP_k &= Q_k T_k + t_{k+1,k} q^{k+1} (e^k)^T \\ Q_k &= P_k T_k + t_{k+1,k} p^{k+1} (e^k)^T. \end{aligned}$$

Let

$$\tilde{T}_k = \begin{pmatrix} T_k \\ t_{k+1,k}(e^k)^T \end{pmatrix}.$$

Then these equations can be written in compact form as

$$H \begin{pmatrix} Q_k \\ P_k \end{pmatrix} = \begin{pmatrix} E & F \\ I & O \end{pmatrix} \begin{pmatrix} Q_k \\ P_k \end{pmatrix} = \begin{pmatrix} Q_{k+1} \\ P_{k+1} \end{pmatrix} \tilde{T}_k.$$

SOAR ct.

Let $Q_k := [q^1, \ldots, q^k] \in \mathbb{R}^{n\times k}$ and $P_k := [p^1, \ldots, p^k] \in \mathbb{R}^{n\times k}$, and let $T \in \mathbb{R}^{k\times k}$ be the upper Hessenberg matrices with nonzero entries t_{ij} as defined in the SOAR algorithm. Then the following relations hold true

$$\begin{aligned} EQ_k + FP_k &= Q_k T_k + t_{k+1,k} q^{k+1} (e^k)^T \\ Q_k &= P_k T_k + t_{k+1,k} p^{k+1} (e^k)^T. \end{aligned}$$

Let

$$\tilde{T}_k = \begin{pmatrix} T_k \\ t_{k+1,k}(e^k)^T \end{pmatrix}.$$

Then these equations can be written in compact form as

$$H \begin{pmatrix} Q_k \\ P_k \end{pmatrix} = \begin{pmatrix} E & F \\ I & O \end{pmatrix} \begin{pmatrix} Q_k \\ P_k \end{pmatrix} = \begin{pmatrix} Q_{k+1} \\ P_{k+1} \end{pmatrix} \tilde{T}_k.$$

This relation assembles the similarity between the SOAR method and the Arnoldi procedure. We shall use this connection to prove that the SOAR algorithm determines an orthonormal basis of the second order Krylov subspace $\mathcal{G}_k(u, E, F)$.

SOAR ct.

If $V_k = [v^1, \ldots, v^k] \in \mathbb{R}^{2n\times k}$ denotes the orthonormal basis of $\mathcal{K}_k(v^1, H)$ obtained by the Arnoldi method and U_k the corresponding Hessenberg matrix, then it holds

$$HV_k = V_k U_k + \ell_{k+1,k} v^{k+1} (e^k)^T$$

and in compact form

$$HV_k = V_{k+1}\tilde{U}_k, \quad \text{where } \tilde{U}_k = \begin{pmatrix} U_k \\ u_{k+1,k}(e^k)^T \end{pmatrix}$$

SOAR ct.

If $V_k = [v^1, \ldots, v^k] \in \mathbb{R}^{2n\times k}$ denotes the orthonormal basis of $\mathcal{K}_k(v^1, H)$ obtained by the Arnoldi method and U_k the corresponding Hessenberg matrix, then it holds

$$HV_k = V_k U_k + \ell_{k+1,k} v^{k+1} (e^k)^T$$

and in compact form

$$HV_k = V_{k+1}\tilde{U}_k, \quad \text{where } \tilde{U}_k = \begin{pmatrix} U_k \\ u_{k+1,k}(e^k)^T \end{pmatrix}$$

The following lemma reveals the connection between this Arnoldi recurrence and the one obtained from SOAR.

Lemma

Let $A \in \mathbb{R}^{n\times n}$. Let $V_{k+1} = [V_k v^{k+1}] \in \mathbb{R}^{k\times k+1}$ such that

$$AV_k = V_{k+1}\tilde{H}_k$$

for an upper Hessenberg matrix $\tilde{H}_k$. Then there is an upper triangular matrix R_k such that

$$V_k R_k = [v^1 Av^1 \dots A^{k-1}v^1]. \qquad (1)$$

Furthermore, if the first $k-1$ subdiagonal elements of $\tilde{H}_k$ are nonzero, then R_k is nonsingular, and

$$\operatorname{span} V_k = \mathcal{K}_k(v^1, A). \qquad (2)$$

Lemma

Let $A \in \mathbb{R}^{n\times n}$. Let $V_{k+1} = [V_k v^{k+1}] \in \mathbb{R}^{k\times k+1}$ such that

$$AV_k = V_{k+1}\tilde{H}_k$$

for an upper Hessenberg matrix $\tilde{H}_k$. Then there is an upper triangular matrix R_k such that

$$V_k R_k = [v^1 Av^1 \dots A^{k-1}v^1]. \qquad (1)$$

Furthermore, if the first $k-1$ subdiagonal elements of $\tilde{H}_k$ are nonzero, then R_k is nonsingular, and

$$\operatorname{span} V_k = \mathcal{K}_k(v^1, A). \qquad (2)$$

Proof We prove (1) by induction. For $k = 1$ equation (1) obvious holds with $R = (1)$.

Lemma

Let $A \in \mathbb{R}^{n\times n}$. Let $V_{k+1} = [V_k v^{k+1}] \in \mathbb{R}^{k\times k+1}$ such that

$$AV_k = V_{k+1}\tilde{H}_k$$

for an upper Hessenberg matrix $\tilde{H}_k$. Then there is an upper triangular matrix R_k such that

$$V_k R_k = [v^1 Av^1 \dots A^{k-1}v^1]. \qquad (1)$$

Furthermore, if the first $k-1$ subdiagonal elements of $\tilde{H}_k$ are nonzero, then R_k is nonsingular, and

$$\operatorname{span} V_k = \mathcal{K}_k(v^1, A). \qquad (2)$$

Proof We prove (1) by induction. For $k = 1$ equation (1) obvious holds with $R = (1)$.

Assume that it holds for some $k-1$. then for k

Proof ct.

$$
\begin{aligned}
[v^1 Av^1 \dots A^{k-1}v^1] &= [v^1, A[v^1 Av^1 \dots A^{k-2}v^1]] \\
&= [v^1, AV_{k-1}R_{k-1}] \\
&= [V_k e^1, V_k \tilde{H}_{k-1}R_{k-1}] \\
&= V_k[e^1, \tilde{H}_{k-1}R_{k-1}] =: V_k R_k.
\end{aligned}
$$

Proof ct.

$$\begin{aligned}
[v^1 Av^1 \dots A^{k-1}v^1] &= [v^1, A[v^1 Av^1 \dots A^{k-2}v^1]] \\
&= [v^1, AV_{k-1}R_{k-1}] \\
&= [V_k e^1, V_k \tilde{H}_{k-1}R_{k-1}] \\
&= V_k[e^1, \tilde{H}_{k-1}R_{k-1}] =: V_k R_k.
\end{aligned}$$

The fact of the upper triangularity of R_k follows immediately by its definition.

Proof ct.

$$\begin{aligned}
[v^1 Av^1 \dots A^{k-1}v^1] &= [v^1, A[v^1 Av^1 \dots A^{k-2}v^1]] \\
&= [v^1, AV_{k-1}R_{k-1}] \\
&= [V_k e^1, V_k \tilde{H}_{k-1}R_{k-1}] \\
&= V_k[e^1, \tilde{H}_{k-1}R_{k-1}] =: V_k R_k.
\end{aligned}$$

The fact of the upper triangularity of R_k follows immediately by its definition.

The diagonal elements of R_k are 1 and the products of the first $k-1$ subdiagonal elements of $\tilde{H}_k$. Thus, if these subdiagonal elements are nonzero, then R_k is nonsingular.

Proof ct.

$$\begin{aligned}
[v^1 Av^1 \dots A^{k-1}v^1] &= [v^1, A[v^1 Av^1 \dots A^{k-2}v^1]] \\
&= [v^1, AV_{k-1}R_{k-1}] \\
&= [V_k e^1, V_k \tilde{H}_{k-1}R_{k-1}] \\
&= V_k[e^1, \tilde{H}_{k-1}R_{k-1}] =: V_k R_k.
\end{aligned}$$

The fact of the upper triangularity of R_k follows immediately by its definition.

The diagonal elements of R_k are 1 and the products of the first $k-1$ subdiagonal elements of $\tilde{H}_k$. Thus, if these subdiagonal elements are nonzero, then R_k is nonsingular.

Finally, (2) is established by (1) and the nonsingularity of R_k. $\square$

Theorem

If $t_{j+1,j} \neq 0$ for $j \geq 1$ in the SOAR algorithm, then the vector sequence $\{q^1, \ldots, qj\}$ forms an orthonormal basis of the second-order Krylov subspace $\mathcal{G}_j(u, E, F)$.

Theorem

If $t_{j+1,j} \neq 0$ for $j \geq 1$ in the SOAR algorithm, then the vector sequence $\{q^1, \ldots, qj\}$ forms an orthonormal basis of the second-order Krylov subspace $\mathcal{G}_j(u, E, F)$.

Proof

$$
\begin{aligned}
\mathcal{G}_j(u,E,F) &= \operatorname{span}\{u^0, u^1, \ldots, u^{j-1}\} \\
&= \operatorname{span}\left\{ [I\ O] \begin{pmatrix} u^0 & u^1 & \ldots & u^{j-1} \\ 0 & u^0 & \ldots & u^{j-2} \end{pmatrix} \right\} \\
&= \operatorname{span}\left\{ [I\ O][v^1\, Hv^1 \ldots H^{j-1}v^1] \right\} \\
&= \operatorname{span}\left\{ [I\ O] \begin{pmatrix} Q_j \\ P_j \end{pmatrix} R_j \right\} \\
&= \operatorname{span}\left\{ [I\ O] \begin{pmatrix} Q_j \\ P_j \end{pmatrix} \right\} \\
&= \operatorname{span}\{Q_j\}. \qquad \square
\end{aligned}
$$

SOAR projection

The theorem suggests the following Rayleigh–Ritz method for quadratic eigenproblems:

SOAR projection

The theorem suggests the following Rayleigh–Ritz method for quadratic eigenproblems:

1: Run the SOAR procedure with $E = -C_2^{-1}C_1$ and $F = -C_2^{-1}C_0$ and a starting vector u to generate the matrix $Q_k \in \mathbb{R}^{n\times k}$ whose columns are orthonormal and span $\mathcal{G}_k(u, E, F)$

2: Compute the projected matrices

$$C_j^{(k)} := Q_k^T C_j Q_k,\ j = 0, 1, 2$$

3: Solve the reduced eigenvalue problem

$$\lambda^2 C_j^{(k)} z + \lambda C_1^{(k)} z + C_0^{(k)} z = 0$$

and obtain the Ritz pair (θ, x), $x = Q_m z$.

4: Test for convergence

Example: Accelerator cavity

We consider the simulation of an accelerator cavity with external coupling. Discretizing the Maxwell equations in the cavity with waveguide boundary conditions yields the nonlinear eigenvalue problem:

$$Kx + i\sum_{j=1}^{d}\sqrt{k^2 - k_{cj}^2}W_j x = k^2 Mx, \qquad (1)$$

where d is the number of waveguides which are leading into this cavity, and k_{cj} are coefficients of the corresponding waveguides.

Example: Accelerator cavity

We consider the simulation of an accelerator cavity with external coupling. Discretizing the Maxwell equations in the cavity with waveguide boundary conditions yields the nonlinear eigenvalue problem:

$$Kx + i\sum_{j=1}^{d}\sqrt{k^2 - k_{cj}^2}W_j x = k^2 Mx, \qquad (1)$$

where d is the number of waveguides which are leading into this cavity, and k_{cj} are coefficients of the corresponding waveguides.

The eigenvalues are the resonant frequencies and the eigenvectors describe the corresponding electromagnetic field. Eigenvalues with smallest magnitude are of interest.

Example: Accelerator cavity

We consider the simulation of an accelerator cavity with external coupling. Discretizing the Maxwell equations in the cavity with waveguide boundary conditions yields the nonlinear eigenvalue problem:

$$Kx + i\sum_{j=1}^{d}\sqrt{k^2 - k_{cj}^2}W_j x = k^2 Mx, \qquad (1)$$

where d is the number of waveguides which are leading into this cavity, and k_{cj} are coefficients of the corresponding waveguides.

The eigenvalues are the resonant frequencies and the eigenvectors describe the corresponding electromagnetic field. Eigenvalues with smallest magnitude are of interest.

Assuming $k_{cj} = 0$, $j = 1, \ldots, d$ and setting $\lambda = \sqrt{k^2}$ simplifies problem (1) to the quadratic eigenvalue problem

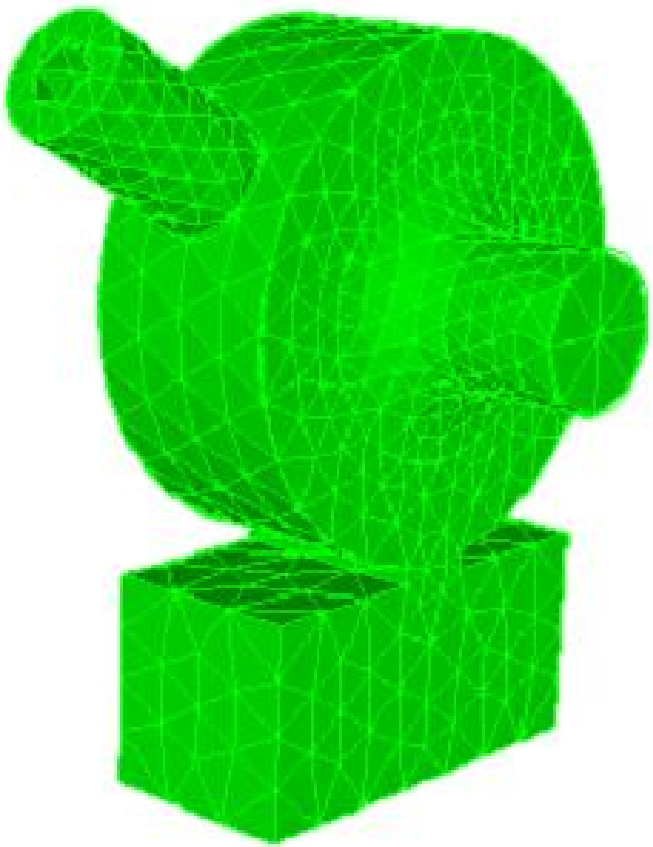
$$Q(\lambda)x := \Big(\lambda^2 M - i\lambda\sum_{j=1}^{d} W_j - K\Big)x = 0.$$

Accelerator cavity ct.

In particular we consider a finite element model with $N = 9956$ degrees of freedom of a cavity connecting two waveguides, which is named gun-cavity and is shown below.

Accelerator cavity ct.

In particular we consider a finite element model with $N = 9956$ degrees of freedom of a cavity connecting two waveguides, which is named gun-cavity and is shown below.



Accelerator cavity ct.

The quadratic eigenproblem (2) obtains the form

$$\Big(\lambda^2 M - i\lambda(W_1 + W_2) - K\Big)x = 0. \qquad (3)$$

Accelerator cavity ct.

The quadratic eigenproblem (2) obtains the form

$$\left(\lambda^2 M - i\lambda(W_1 + W_2) - K\right)x = 0. \qquad (3)$$

The system matrices have got the following properties:

$N = 9956$	$\|\cdot\|_1$	real	sym.	pos. def.	nnz
M	17.04	yes	yes	yes	148318
$W_1 + W_2$	0.95	yes	yes	no	350
K	14.75	yes	yes	no	148308

Accelerator cavity ct.

The quadratic eigenproblem (2) obtains the form

$$\left(\lambda^2 M - i\lambda(W_1 + W_2) - K\right)x = 0. \qquad (3)$$

The system matrices have got the following properties:

$N = 9956$	$\|\cdot\|_1$	real	sym.	pos. def.	nnz
M	17.04	yes	yes	yes	148318
$W_1 + W_2$	0.95	yes	yes	no	350
K	14.75	yes	yes	no	148308

Since all matrices are real, we have

$$Q(\lambda)x = 0 \quad \Longleftrightarrow \quad x^H Q(-\overline{\lambda}) = 0.$$

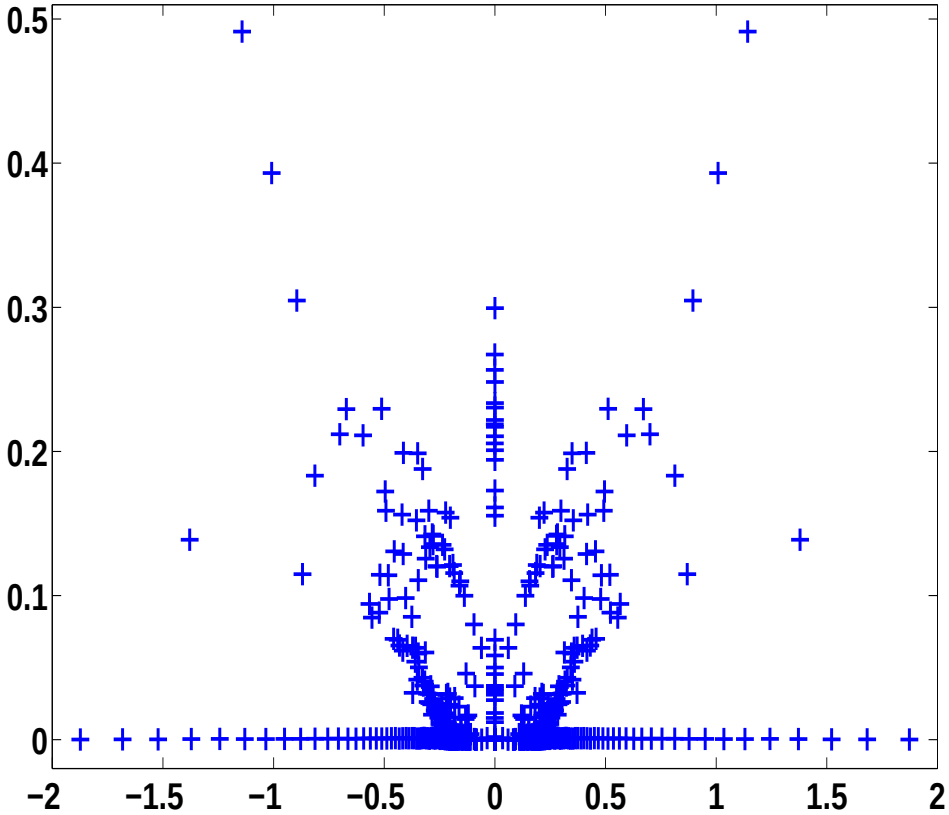
Hence, the spectrum of (3) is symmetric about the imaginary axis.

Accelerator cavity ct.

The following figure shows 600 eigenvalues with smallest magnitude which have been calculated via a projection method of high order and which serve as reference values when evaluating the approximations.

Accelerator cavity ct.

The following figure shows 600 eigenvalues with smallest magnitude which have been calculated via a projection method of high order and which serve as reference values when evaluating the approximations.

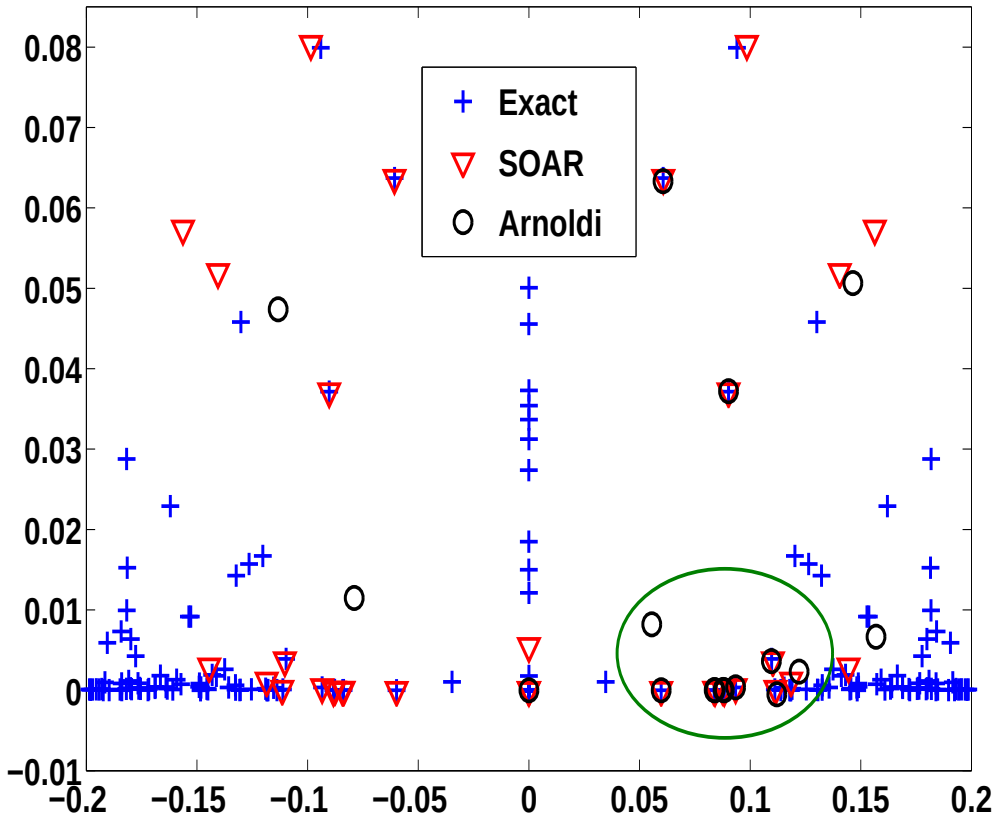


Accelerator cavity ct.

The following picture exhibits the approximate eigenvalues obtained by the SOAR-algorithm (triangles) and by the Arnoldi-procedure applied to the linearized problem (circles). In both cases the dimension of the reduced model is $n = 20$.

Accelerator cavity ct.

The following picture exhibits the approximate eigenvalues obtained by the SOAR-algorithm (triangles) and by the Arnoldi-procedure applied to the linearized problem (circles). In both cases the dimension of the reduced model is $n = 20$.



Accelerator cavity ct.

In the following we compare the accuracy of the approximations to eigenvalues with smallest magnitude obtained with the SOAR- and the Arnoldi-procedure. The two smallest eigenvalues with positive real part are

$$\begin{aligned}\lambda_1 &= 0.05979318129849 + 0.00000060564291 * i,\\ \lambda_2 &= 0.08377031861983 + 0.00001865296741 * i.\end{aligned}$$

Accelerator cavity ct.

In the following we compare the accuracy of the approximations to eigenvalues with smallest magnitude obtained with the SOAR- and the Arnoldi-procedure. The two smallest eigenvalues with positive real part are

$$\begin{aligned}\lambda_1 &= 0.05979318129849 + 0.00000060564291 * i,\\ \lambda_2 &= 0.08377031861983 + 0.00001865296741 * i.\end{aligned}$$

The Arnoldi-procedure ($n = 10$) yields the approximations

$$\begin{aligned}\lambda_1^{Ar} &= \underline{0.05979322}105350 + \underline{0.00000070}031027 * i,\\ \lambda_2^{Ar} &= \underline{0.08356811}958546 + \underline{0.00004068}274681 * i\end{aligned}$$

Accelerator cavity ct.

In the following we compare the accuracy of the approximations to eigenvalues with smallest magnitude obtained with the SOAR- and the Arnoldi-procedure. The two smallest eigenvalues with positive real part are

$$\begin{aligned}\lambda_1 &= 0.05979318129849 + 0.00000060564291 * i,\\ \lambda_2 &= 0.08377031861983 + 0.00001865296741 * i.\end{aligned}$$

The Arnoldi-procedure ($n = 10$) yields the approximations

$$\begin{aligned}\lambda_1^{Ar} &= \underline{0.05979322}105350 + \underline{0.00000070}031027 * i,\\ \lambda_2^{Ar} &= \underline{0.08356811}958546 + \underline{0.00004068}274681 * i\end{aligned}$$

and the SOAR-algorithm ($n = 10$)

$$\begin{aligned}\lambda_1^{S} &= \underline{0.05979318}141426 + \underline{0.00000060}548039 * i,\\ \lambda_2^{S} &= \underline{0.08379}343875125 + \underline{0.00002}471127141 * i\end{aligned}$$

where we have underlined the leading correct digits.

Accelerator cavity ct.

After $n = 20$ iterations 16 leading digits of λ_1^S and λ_1 match.

Accelerator cavity ct.

After $n = 20$ iterations 16 leading digits of λ_1^S and λ_1 match.

The eigenvalue approximations with the SOAR-algorithm are more exact than the ones with the Arnoldi-procedure.

Accelerator cavity ct.

After $n = 20$ iterations 16 leading digits of λ_1^S and λ_1 match.

The eigenvalue approximations with the SOAR-algorithm are more exact than the ones with the Arnoldi-procedure.

The elapsed time for generating the orthonormal basis was $t_{Ar} = 25.1s$ with the Arnoldi-method and only $t_S = 7.7s$ with the SOAR-method.

Accelerator cavity ct.

After $n = 20$ iterations 16 leading digits of λ_1^S and λ_1 match.

The eigenvalue approximations with the SOAR-algorithm are more exact than the ones with the Arnoldi-procedure.

The elapsed time for generating the orthonormal basis was $t_{Ar} = 25.1s$ with the Arnoldi-method and only $t_S = 7.7s$ with the SOAR-method.

The eigenvalue approximations from the SOAR-algorithm preserve the symmetry about the imaginary axis which is not the case for for the Arnoldi-procedure.