Numerical Solution of Large Scale Structured Polynomial or Rational Eigenvalue Problems

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Abstract

This paper deals with the numerical solution of large scale polynomial or rational eigenvalue problems with Hamiltonian or symplectic symmetry in the spectrum. Applications where such problems arise are introduced briefly. It is shown how these problems may be formulated as linear generalized eigenvalue problems that have either symmetric/skew symmetric, skew Hamiltonian/Hamiltonian or symplectic pencils. The presented numerical methods are designed to preserve these structures.

Keywords: matrix polynomial, Hamiltonian matrix, skew-Hamiltonian matrix, skew-Hamiltonian/Hamiltonian pencil, symplectic pencil, matrix factorizations.

AMS(MOS) subject classification: 65F15, 15A18, 15A22

1 Introduction

In this paper we discuss numerical methods for the solution of large scale *non-linear eigenvalue problems*

$$P(\lambda)v = (\sum_{i=0}^{k} \lambda^{i-l} M_i)v = 0, \tag{1}$$

where l is some integer. Here, the coefficients M_i are real or complex matrices, and if $l = 0$ we have a polynomial eigenvalue problem, while if $l > 0$ then we have a rational eigenvalue problem. Eigenvalue problems of this form arise in

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a number of applications. We will present examples in Section 2. Typically one is interested in a small number of eigenvalues and associated eigenvectors. Polynomial eigenvalue problems (in particular quadratic problems) have recently received a lot of interest in the numerical analysis community, see for example the recent survey [30]. In this paper we are, in particular, interested in two special classes of such eigenvalue problems.

The first class consists of those polynomials, where the coefficient matrices are real or complex and form alternating sequences of real symmetric and real skew-symmetric matrices, or complex symmetric and skew-symmetric matrices, i.e., $M_i^T = (-1)^i M_i$ or $M_i^T = (-1)^{i+1} M_i$ for $i = 0, \ldots, k$. The matrices in this class have a nice symmetry in the spectrum.

Proposition 1 *[26] Consider the polynomial eigenvalue problem (1) with alternating (real or complex) coefficients, i.e., either $M_i^T = (-1)^i M_i$ or $M_i^T = (-1)^{i+1} M_i$ for $i = 0, \ldots, k$. Then $P(\lambda)v = 0$ if and only if $v^T P(-\lambda) = 0$.*

This means that v is a right eigenvector of P associated with eigenvalue λ if and only if v^T is a left eigenvector of P associated with eigenvalue $-\lambda$. This symmetry in the spectrum is called a *Hamiltonian eigensymmetry*, i.e., the spectrum consists of quadruplets $(\lambda, -\lambda, \bar{\lambda}, -\bar{\lambda})$ in the real case or pairs $(\lambda, -\lambda)$ in the complex case if the eigenvalues are not purely imaginary.

The second class of problems consists of rational eigenvalue problems with symmetrically placed coefficients of the form

$$P_1(\kappa)v = [M_0 + \sum_{j=1}^{k} (\frac{1}{\kappa^j} M_j + \kappa^j M_j^T)]v = 0 \tag{2}$$

where the coefficients are again real or complex matrices with $M_0 = M_0^T$.

The following simple result is the analogue of Proposition 1.

Proposition 2 *Consider an eigenvalue problem $P_1(\kappa)v = 0$ of the form (2). Then $P_1(\kappa)v = 0$ if and only if $v^T P_1(\frac{1}{\kappa}) = 0$.*

Proof. The result follows by setting $\lambda = \kappa^{-1}$ and transposing.

We have that v is a right eigenvector of P_1 associated with eigenvalue κ if and only if v^T is a left eigenvector of P_1 associated with eigenvalue $\frac{1}{\kappa}$. This symmetry in the spectrum is called a *symplectic eigensymmetry*, i.e., the spectrum consists of quadruplets $(\kappa, \kappa^{-1}, \bar{\kappa}, \bar{\kappa}^{-1})$ in the real case or pairs (κ, κ^{-1}) in the complex case if κ is not on the unit circle.

For the described classes of eigenvalue problems the following important questions are of interest and only partially solved as of today.

- How can we design efficient numerical methods to compute several eigenvalues and associated eigenvectors (possibly from the interior of the spectrum)?

- How can we make maximal use of the symmetry structure of the coefficients and the symmetry of the spectrum?

In the next section we briefly describe some applications that lead to eigenvalue problems of the described structures and discuss these structures. Unfortunately there are essentially no viable numerical methods available, that work directly on the data of polynomial or rational eigenvalue problems to compute the desired part of the spectrum. In Section 3 we therefore discuss the classical concept of *linearization*, i.e. of transforming the high degree polynomial or rational problem into a linear eigenvalue problem of higher dimension. Since our problems have a specific structure, it would be ideal if we had linearizations with analogous structure. We show how to obtain linear eigenvalue problems with the same structures and eigensymmetries. Then in Section 4 we present numerical algorithms that exploit these structures, and that guarantee that the symmetry in the spectum is also preserved even in finite precision arithmetic.

2 Applications

In order to demonstrate the importance of eigenvalue problems with Hamiltonian or symplectic spectra we will present in this section several applications, where such problems arise. We begin with two Hamiltonian examples.

Example 1 The study of corner singularities in anisotropic elastic materials [1, 2, 16, 19, 25, 27] leads to real quadratic eigenvalue problems of the form

$$\begin{aligned} &\lambda^2 M(p)v + \lambda G(p)v + K(p)v = 0, \\ &M = M^T, \quad G = -G^T, \quad K = K^T \end{aligned} \tag{3}$$

The coefficient matrices are large and sparse, having been produced by a finite element discretization. M is a positive definite mass matrix, and $-K$ is a stiffness matrix. Typically the coefficients depend on a set of material or geometry parameters p which are varied.

Example 2 [26] The optimality conditions for the optimal control problem to minimize the cost functional

$$\int_{t_0}^{t_1} \sum_{i=0}^{k} (q^{(i)})^T Q_i q^{(i)} + u^T R u \, dt$$

with $Q_i = Q_i^T$, $i = 0, \ldots, k$, positive semidefinite and $R = R^T$ positive definite, subject to the control system

$$\sum_{i=0}^{k} M_i q^{(i)} = Bu(t), \tag{4}$$

with control input $u(t)$ and initial conditions

$$q^{(i)}(t_0) = q_{i,0}, \; i = 0, 1, \ldots, k-1, \tag{5}$$

lead to the polynomial two-point boundary value problem

$$\begin{aligned}\sum_{j=1}^{k-1}\left[\begin{array}{cc}(-1)^{j-1}Q_j & M_{2j}^T\\ M_{2j} & 0\end{array}\right]\left[\begin{array}{c}q^{(2j)}\\ \mu^{(2j)}\end{array}\right]+&\\ \sum_{j=1}^{k-1}\left[\begin{array}{cc}0 & -M_{2j+1}^T\\ M_{2j+1} & 0\end{array}\right]\left[\begin{array}{c}q^{(2j+1)}\\ \mu^{(2j+1)}\end{array}\right]+&\\ \left[\begin{array}{cc}-Q_0 & M_0^T\\ M_0 & -BR^{-1}B^T\end{array}\right]\left[\begin{array}{c}q\\ \mu\end{array}\right]=0,&\end{aligned} \tag{6}$$

with initial conditions (5) and $\mu^{(i)}(t_1)=0$ for $i=0,\ldots k-1$. Here we have (for simpler notation) introduced the virtual coefficients $M_{k+1}=M_{k+2}=\ldots=M_{2k}=0$. We observe that all coefficients of derivatives higher than k are singular. If the weighting matrices Q_i are chosen to be zero for all $i\geq k/2$, then we have that all coefficients of derivatives higher than k vanish and (after possibly multiplying the second block row by -1) we obtain an alternating sequence of real symmetric and skew-symmetric coefficient matrices. The solution of this polynomial boundary value problem can then be obtained via the solution of the corresponding polynomial eigenvalue problem.

As a special case we may study the optimal control of linear mechanical systems, e.g. in robotics, which are governed by a second order differential equation of the form

$$M\ddot{q}+D\dot{q}+Kq=Bu,$$

where x and u are vectors of state and control variables, respectively. The task of computing the optimal control u that minimizes the cost functional

$$\int_{t_0}^{t_1} q^TQ_0q+\dot{q}^TQ_1\dot{q}+u^TRu\,dt$$

leads to the system

$$\left[\begin{array}{cc}Q_1 & M^T\\ M & 0\end{array}\right]\left[\begin{array}{c}\ddot{q}\\ \ddot{\mu}\end{array}\right]+\left[\begin{array}{cc}0 & -D^T\\ D & 0\end{array}\right]\left[\begin{array}{c}\dot{q}\\ \dot{\mu}\end{array}\right]+\left[\begin{array}{cc}-Q_0 & K^T\\ K & -BR^{-1}B^T\end{array}\right]\left[\begin{array}{c}q\\ \mu\end{array}\right]=0,$$

which is a special case of (6). The substitution

$$\left[\begin{array}{c}q\\ \mu\end{array}\right]=e^{\lambda t}\left[\begin{array}{c}v\\ w\end{array}\right]$$

then yields the quadratic eigenvalue problem

$$\left(\lambda^2\left[\begin{array}{cc}Q_1 & M^T\\ M & 0\end{array}\right]+\lambda\left[\begin{array}{cc}0 & -D^T\\ D & 0\end{array}\right]+\left[\begin{array}{cc}-Q_0 & K^T\\ K & -BR^{-1}B^T\end{array}\right]\right)\left[\begin{array}{c}v\\ w\end{array}\right]=0. \tag{7}$$

Other applications with similar structures arise for example in the analysis of gyroscopic systems [13, 17] or the control of semidiscretized (in space) parabolic partial differential equations [14, 13].

Our third example discusses an application that leads to an eigenvalue problem with symplectic eigensymmetry.

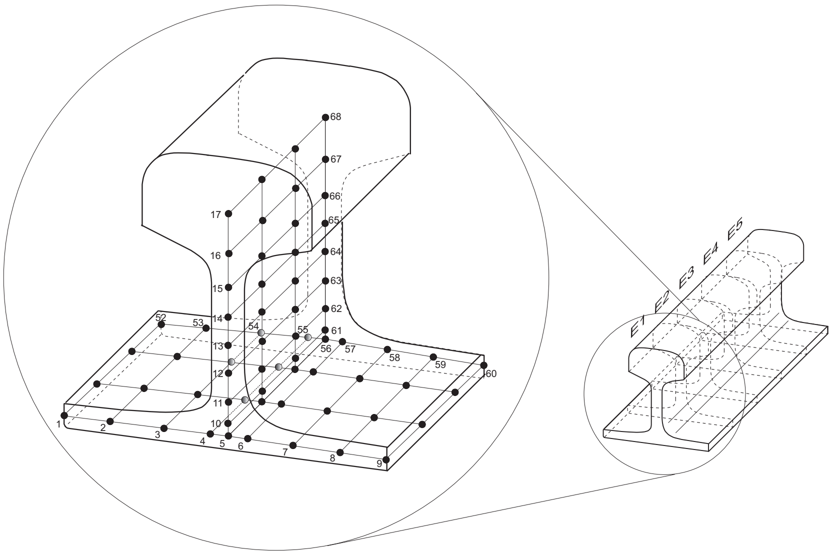

Figure 1: Finite element model of rail

Example 3 In [15] the vibration of rails under the excitation arising from fast trains is studied. Partitioning the rail into a finite number of pieces between two crossties, see Figure 3, and using classical finite element discretization leads under the assumption of an infinite rail to an infinite second order system of differential equations of the form

$$M\ddot{x} + D\dot{x} + Kx = F, \tag{8}$$

with infinite block tridiagonal coefficient matrices M, D, K, where

$$M = \begin{bmatrix} \ddots & \ddots & 0 & \dots & 0 \\ \ddots & M_{j-1,0} & M_{j,1} & 0 & \dots \\ 0 & M_{j,1}^T & M_{j,0} & M_{j+1,1} & 0 \\ \vdots & \ddots & M_{j+1,1}^T & M_{j+1,0} & M_{j+2,1} \\ 0 & \dots & 0 & \ddots & \ddots \end{bmatrix}, \; x = \begin{bmatrix} \vdots \\ x_{j-1} \\ x_j \\ x_{j+1} \\ \vdots \end{bmatrix}, \; F = \begin{bmatrix} \vdots \\ F_{j-1} \\ F_j \\ F_{j+1} \\ \vdots \end{bmatrix}.$$

The matrices D, K have the same structure with blocks $D_{j,0}, D_{j,1}$ and $K_{j,0}, K_{j,1}$, respectively. Here $M_{j,0}$ is symmetric positive definite and $D_{j,0}, K_{j,0}$ are positive semidefinite. There are several ways to approach the solution of this problem, which presents a mixture between a differential equation (time derivatives of x) and a difference equation (space differences in j).

Since one is interested in studying the behaviour of the system under excitation, the ansatz $F_j = \hat{F}_j e^{i\omega t}$, $x_j = \hat{x}_j e^{i\omega t}$, where ω is the excitation frequency, leads to a second order difference equation with variable coefficients. The discretized system for the $\hat{x}_j$ is given by

$$A_{j,j+1}^T \hat{x}_{j-1} + A_{j,j}\hat{x}_j + A_{j,j+1}\hat{x}_{j+1} = \hat{F}_j \tag{9}$$

with the coefficent matrices

$$A_{j,j+1} = -\omega^2 M_{j,1} + i\omega D_{j,1} + K_{j,1}, \ A_{j,j} = -\omega^2 M_{j,0} + i\omega D_{j,0} + K_{j,0}.$$

Observing that the system matrices vary periodically due to the identical form of the track between two crossties we may combine the (say $l = 5$) parts belonging to the rail in this space interval (see Figure 3) into one vector

$$y_j = \begin{bmatrix} \hat{x}_j \\ \hat{x}_{j+1} \\ \vdots \\ \hat{x}_{j+l} \end{bmatrix}$$

and thus obtain a constant coefficient second order difference equation

$$A_1^T y_{j-1} + A_0 y_j + A_1 y_{j+1} = G_j \tag{10}$$

with the coefficent matrices

$$\begin{aligned} A_0 &= \begin{bmatrix} A_{j,j} & A_{j,j+1} & & & \\ A_{j+1,j+2}^T & A_{j+1,j+1} & A_{j+1,j+2} & & \\ & \ddots & \ddots & \ddots & \\ & & A_{j+l-1,j+l}^T & A_{j+l-1,j+l-1} & A_{j+l-1,j+l} \\ & & & A_{j+l,j+l+1}^T & A_{j+l,j+l} \end{bmatrix}, \\ A_1 &= \begin{bmatrix} 0 & 0 & \dots & \dots & 0 \\ 0 & \ddots & \ddots & & \\ & \ddots & \ddots & \ddots & \\ 0 & 0 & \dots & \dots & 0 \\ A_{j+l,j+l+1} & 0 & \dots & \dots & 0 \end{bmatrix}. \end{aligned}$$

For this system we make the ansatz $y_{j+1} = \kappa y_j$, which leads to the rational eigenvalue problem

$$(\frac{1}{\kappa} A_1^T + A_0 + \kappa A_1) y = 0.$$

Note that, since in general A_1 is singular, this is necessarily a *second order discrete time descriptor system.*

We have seen in this section that several applications lead to polynomial or rational eigenvalue problems with particular symmetry structures. In the interest of efficiency and stability, any good numerical method for solving problems of this type should preserve and exploit these structures.

3 Linearization

The classical approach to solving a k-th degree polynomial eigenvalue problem of dimension m is to *linearize* it, [12], i.e. to transform it to an equivalent first-degree equation $Ax - \lambda Bx = 0$ of dimension km. There are many different such linearizations with very different numerical properties, see [26, 29]. Since the problems that we have presented in Section 2 have a specific symmetry structure we will demonstrate now how we can preserve this structure in the linearization. For problems with alternating coefficients the following result has been shown in [26].

Theorem 3 *Consider the polynomial eigenvalue problem $P(\lambda)v = 0$ given by (1) with either $M_i^T = (-1)^i M_i$ or $M_i^T = (-1)^{i+1} M_i$ and with M_k nonsingular. Then the pencil $A - \lambda B \in \mathbb{C}^{mk,mk}$, where*

$$A = \left[\begin{array}{c|ccccc} -M_0 & 0 & 0 & 0 & \cdots & 0 \\ \hline 0 & -M_2 & -M_3 & -M_4 & \cdots & -M_k \\ 0 & M_3 & M_4 & & & 0 \\ 0 & -M_4 & & & & 0 \\ \vdots & \vdots & & & & \vdots \\ 0 & \pm M_k & 0 & 0 & \cdots & 0 \end{array}\right] \tag{11}$$

and

$$B = \left[\begin{array}{ccccc|c} M_1 & M_2 & M_3 & \cdots & M_{k-1} & M_k \\ \hline -M_2 & -M_3 & -M_4 & \cdots & -M_k & 0 \\ M_3 & M_4 & & & 0 & 0 \\ -M_4 & & & & 0 & 0 \\ \vdots & & & & \vdots & \vdots \\ \pm M_k & 0 & 0 & \cdots & 0 & 0 \end{array}\right], \tag{12}$$

has the same eigenvalues as P. Here $\pm M_k$ is shorthand for $(-1)^{k-1}M_k$. If $M_i^T = (-1)^i M_i$, then A is symmetric and B is skew symmetric. If $M_i^T = (-1)^{i+1} M_i$, then B is symmetric and A is skew symmetric. If $P(\lambda)v = 0$, then $\left[\begin{array}{cccc} v^T & \lambda v^T & \cdots & \lambda^{k-1} v^T \end{array}\right]^T$ is an eigenvector of $A - \lambda B$.

It is obvious that the pencil $A - \lambda B$ specified by (11) and (12) is a linear eigenvalue problem, with alternating coefficients and thus by Proposition 1 we again have the Hamiltonian symmetry of the spectrum. If the dimension of $A - \lambda B$ is even then multiplying by J, we obtain a *skew Hamiltonian/Hamiltonian* pencil

$$\lambda H_1 - H_2 \tag{13}$$

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

Example 4 *If we apply Theorem 3 to the quadratic eigenvalue problem (3), we obtain the symmetric/skew-symmetric pencil*

$$\left[\begin{array}{cc} -K & 0 \\ 0 & -M \end{array}\right] - \lambda \left[\begin{array}{cc} G & M \\ -M & 0 \end{array}\right].$$

If we then multiply by $-J$, we obtain the skew Hamiltonian/Hamiltonian pencil

$$\begin{bmatrix} 0 & M \\ -K & 0 \end{bmatrix} - \lambda \begin{bmatrix} M & 0 \\ G & M \end{bmatrix}.$$

This is essentially the linearization that was used in [25].

To get a similar linearization in the symplectic case (2) is more difficult. First of all we have to discuss what is the analgoue to skew Hamiltonian/Hamiltonian pencils as in (13). Note that the discrete time analogue to Hamiltonian matrices are the *symplectic matrices* S, which satisfy $S^TJS = J$. See [22, 23, 24] for an analysis of the analogy. When it comes to pencils there are two well studied generalizations of Hamiltonian matrices, the *Hamiltonian pencils* $\lambda H_1 - H_2$ such that $H_1^TJH_2 = H_2^TJH_1$ and the skew Hamiltonian/Hamiltonian pencils (13).

The analogue to the Hamiltonian pencils are the *symplectic pencils* $\lambda S_1 - S_2$ such that $S_1^TJS_1 = S_2^TJS_1$ which are obtained from a Cayley transformation of Hamiltonian pencils [23, 24].

To see what is the analogue to skew Hamiltonian/Hamiltonian pencils, we perform a Cayley transformation $\lambda = \frac{\kappa-1}{\kappa+1}$ with a skew Hamiltonian/Hamiltonian pencil $\lambda H_1 - H_2$. Reordering the pencil we obtain a pencil $\kappa(H_1 - H_2) - (H_1 + H_2) =: \kappa W_1 - W_2$ with the property that

$$W_2 = JW_1^TJ^T, \tag{14}$$

i.e. we have a pencil of the form

$$\kappa S - JS^TJ^T.$$

We call such pencils *proper symplectic pencils.*

For problems of the form (2) it is much more difficult to a obtain appropriate linearizations. For the second order case of Example 3, i.e.,

$$(\kappa^{-1}A_1^T + A_0 + \kappa A_1)y = 0. \tag{15}$$

we may set $\kappa z = A_1^Ty$ and obtain the linear problem

$$(\kappa S_1 + S_2)\begin{bmatrix} y \\ z \end{bmatrix} := (\kappa \begin{bmatrix} A_1 & 0 \\ 0 & I \end{bmatrix} + \begin{bmatrix} A_0 & I \\ -A_1^T & 0 \end{bmatrix})\begin{bmatrix} y \\ z \end{bmatrix} = 0. \tag{16}$$

We immediately obtain that this linearization preserves the symplecticity of the spectrum.

Proposition 4 *The pencil $\kappa S_1 + S_2$ from (16) is a* symplectic pencil, *i.e. $S_1JS_1^T = S_2JS_2^T$. The pencil $\kappa S_1 + S_2$ is regular, i.e., its determinant does not vanish identically, if and only if the rational pencil $\kappa^{-1}A_1^T + A_0 + \kappa A_1$ is regular.*

Proof. The proof of symplecticity follows by direct calculation. For the regularity observe that if the dimension of A_0 is n, then

$$\det(\kappa S_1 + S_2) = \kappa^n \det(\kappa^{-1}A_1^T + A_0 + \kappa A_1).$$

□

Note that it is not needed that the matrix A_1 is invertible to obtain a symplectic pencil, i.e. this linearization applies to Example 3. If, however, S_1 is invertible then clearly $S_1^{-1}S_2$ is a symplectic matrix. If A_1 is singular with rank defect $n-r$ then the pencil (16) has $n-r$ eigenvalues at 0 and $n-r$ eigenvalues at ∞ and hence the pairing is preserved. For more details on symplectic pencils see [11, 23].

To obtain a proper symplectic linearization we make use of the fact that a block partitioning of (14) gives a pencil of the form

$$\kappa \begin{bmatrix} A_{1,1} & A_{1,2} \\ A_{2,1} & A_{2,2} \end{bmatrix} - \begin{bmatrix} A_{1,1}^T & -A_{1,2}^T \\ -A_{2,1}^T & A_{1,1}^T \end{bmatrix}. \tag{17}$$

We can easily obtain such a linearization for (15) as

$$\kappa \begin{bmatrix} A_1 & A_1 \\ -A_1 & A_1^T - A_0 \end{bmatrix} - \begin{bmatrix} A_1 - A_0 & -A_1^T \\ A_1^T & A_1^T \end{bmatrix}. \tag{18}$$

This is easily seen by a multiplication of (17) by $\begin{bmatrix} \kappa x \\ x \end{bmatrix}$ and setting this to be zero, yields the pencils

$$\begin{aligned} (\kappa^2 A_{1,1} + \kappa(A_{1,2} - A_{2,2}^T) + A_{1,2}^T)x &= 0 \\ (\kappa^2(-A_{2,1}) + \kappa(-A_{2,2} - A_{2,1}^T) + A_{1,1}^T)x &= 0 \end{aligned}$$

which yields two copies of (15) if we choose the blocks as in (18).

It is much more difficult to obtain a linearization which is a symplectic pencil or a proper symplectic pencil for higher order rational problems of the form (2).

4 Numerical methods to preserve the structures

Motivated by the fact that a numerical method to solve the eigenvalue problem should preserve existing structures as much as possible, we have shown in the previous section how to transform polynomial or rational eigenvalue problems to linear generalized eigenvalue problems with the same structure.

To these problems we may then apply structure preserving methods. The development of such methods for problems with Hamiltonian or symplectic eigensymmetry has been an important research topic for many years, see [11, 23] and even though much progress has been made for problems with Hamiltonian eigensymmetry, see [4, 8, 9] for small scale methods and [1, 5, 7, 6, 25, 26, 32] for large scale problems, completely satisfactory methods, i.e. methods which are backward stable and completely structure preserving, are not yet available. This holds for both the Hamiltonian and symplectic cases.

Recently several structure-preserving Krylov subspace methods have been developed [1, 5, 6, 25, 26, 32]. Each of these requires that the Hamiltonian or symplectic pencil be reduced further to a Hamiltonian or symplectic matrix.

This can be done efficiently in many cases. For example, consider the skew-symmetric/symmetric pencil in Example 4. Since

$$\begin{bmatrix} G & M \\ -M & 0 \end{bmatrix} = \begin{bmatrix} I & 0 \\ 0 & M \end{bmatrix} \begin{bmatrix} I & -\frac{1}{2}G \\ 0 & I \end{bmatrix} \begin{bmatrix} 0 & I \\ -I & 0 \end{bmatrix} \begin{bmatrix} I & 0 \\ \frac{1}{2}G & I \end{bmatrix} \begin{bmatrix} I & 0 \\ 0 & M \end{bmatrix},$$

that pencil is equivalent to the Hamiltonian matrix

$$H = J \begin{bmatrix} I & \frac{1}{2}G \\ 0 & I \end{bmatrix} \begin{bmatrix} K & 0 \\ 0 & M^{-1} \end{bmatrix} \begin{bmatrix} I & 0 \\ -\frac{1}{2}G & I \end{bmatrix},$$

as is shown in [25]. There is no need to assemble the matrix H, nor is there any need to compute M^{-1} explicitly. We just need to compute and use the Cholesky decomposition of M. Notice also that

$$H^{-1} = \begin{bmatrix} I & 0 \\ \frac{1}{2}G & 0 \end{bmatrix} \begin{bmatrix} K^{-1} & 0 \\ 0 & M \end{bmatrix} \begin{bmatrix} I & -\frac{1}{2}G \\ 0 & I \end{bmatrix} J^T,$$

so H^{-1}, which is also Hamiltonian, is no less accessible than H itself. This is important; if one wants the eigenvalues of H that are closest to the origin, one had better work with H^{-1}.

Often we prefer to shift before we invert. If we know that the eigenvalues of interest lie near τ, we might prefer to work with $(H - \tau I)^{-1}$. However, the shift destroys the Hamiltonian structure, so we need ways to effect shifts while preserving the structure. One simple remedy is to work with the matrix

$$(H - \tau I)^{-1}(H + \tau I)^{-1},$$

which is not Hamiltonian but skew Hamiltonian. If τ is neither real nor purely imaginary, we prefer to work with the skew-Hamiltonian

$$(H - \tau I)^{-1}(H - \overline{\tau} I)^{-1}(H + \tau I)^{-1}(H + \overline{\tau} I)^{-1},$$

in order to stay within the real number system.

If we wish to use a shift *and* keep the Hamiltonian structure, we can work with the Hamiltonian matrix

$$H^{-1}(H - \tau I)^{-1}(H + \tau I)^{-1}$$

or

$$H(H - \tau I)^{-1}(H + \tau I)^{-1},$$

for example.

Another possibility is to work with the Cayley transform

$$(H - \tau I)^{-1}(H + \tau I), \tag{19}$$

which is symplectic. Of course, the Cayley transform can also be used to transform a symplectic problem to one that is Hamiltonian. Structure-preserving Krylov subspace methods exist for each of these structures.

In practice a Krylov subspace method is never run to completion, but if it were, it would effect a similarity transformation that transforms the operator to a condensed form such as upper Hessenberg or tridiagonal. The transforming matrix is the matrix whose columns are the vectors that were generated by the process. Since in actuality a Krylov subspace method is not run to completion, it only effects a partial similarity transform.

Whether A is Hamiltonian, skew Hamiltonian, or symplectic, the structure is preserved under a symplectic similarity transformation. That is, if S is symplectic, then $S^{-1}AS$ is Hamiltonian as A is, and so on. If we write $S = [\, S_1 \; S_2 \,]$, where S_1 and S_2 are both $2n \times n$, then the symplectic property $S^T JS = J$ implies that $S_1^T JS_1 = 0$, $S_2^T JS_2 = 0$, and $S_1^T JS_2 = I$. Recall that a subspace of $\mathbb{R}^n$ is called *isotropic* if $x^T Jy = 0$ for all x and y in the subspace. The condition $S_i^T JS_i = 0$ implies that the space spanned by the columns of S_i is isotropic, and so are all of its subspaces.

A Krylov subspace method will preserve Hamiltonian, skew-Hamiltonian, or symplectic structure if it generates a symplectic similarity transformation when run to completion. To achieve this it must generate vectors that span isotropic subspaces.

The skew-Hamiltonian form is easiest to preserve, since Krylov subspaces generated by skew-Hamiltonian operators are automatically isotropic [25]. Consequently the standard Arnoldi and unsymmetric Lanczos processes preserve the structure automatically in theory. In practice the isotropy is steadily eroded by roundoff errors, so it must be enforced by an additional orthogonalization step. In the context of the Arnoldi process, this means that the vector q_{j+1} generated on step j must be made orthogonal to $Jq_1, \ldots, Jq_j$ as well as $q_1, \ldots, q_j$.

All of our algorithms employ short Arnoldi or Lanczos runs with repeated implicit restarts in the spirit of Sorensen's implicitly restarted Arnoldi (IRA) process [21, 28]. The skew-Hamiltonian implicitly-restarted Arnoldi (SHIRA) algorithm [25] is a variant of IRA that includes the extra orthogonalization to enforce isotropy. SHIRA has been used in [1] for the efficent computation of corner singularities in three-dimensional anisotropic elastic structures.

A skew-Hamiltonian implicitly-restarted Lanczos (SHIRL) process can be built on the same principle. So far we have not pursued this possibility.

For the Hamiltonian case an essentially new algorithm was needed. Benner and Faßbender [5] developed a Hamiltonian Lanczos process with implicit restarts. This process has to preserve structure in both phases. In the Lanczos phase it must build isotropic subspaces, and in the restart phase it must preserve the isotropy. The latter is done by using the SR algorithm to effect the restarts, instead of the QR algorithm, which is used in IRA and SHIRA. In the algorithm of [5] there are several parameters that can be chosen freely, resulting in different variants of the algorithm. One particularly simple parameter choice leads to a simplified algorithm that uses the HR algorithm, which is much simpler than the SR algorithm, to do the restarts. This Hamiltonian implicitly restarted Lanczos (HIRL) process is outlined in [32]. HIRL has been applied successfully to the corner singularity problems of Example 1. It is roughly as fast and accurate as SHIRA. Since it produces both left and right eigenvec-

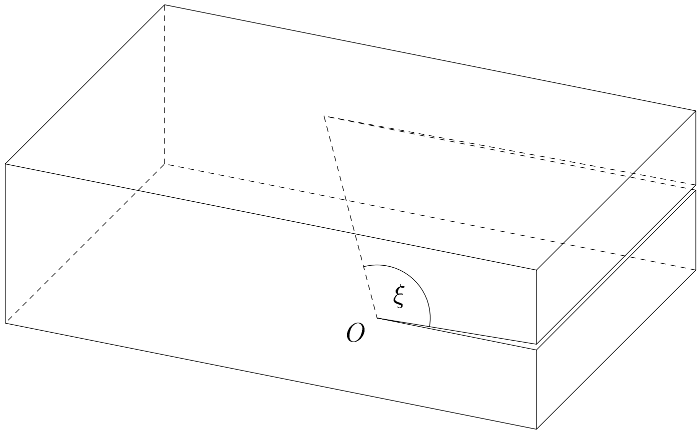

Figure 2: Illustration of the crack example

tors, along with the eigenvalues, it is also able to compute residuals, as well as condition numbers for the eigenvalues.

There have been analogous developments for the symplectic case. Benner and Faßbender [6] developed a symplectic implicitly restarted Lanczos process that uses the symplectic SR algorithm for the restarts. Just as in the Hamiltonian case, it is possible to choose the parameters so that the algorithm takes a simple form that allows for restarts by the simpler HR algorithm. The resulting symplectic implicitly restarted Lanczos (SIRL) algorithm is outlined in [32]. SIRL has been tested on the singularity problems of Example 1, transformed to symplectic form by a Cayley transform (19). The algorithm was as accurate as HIRL and SHIRA but less efficient. The effectiveness of SIRL on symplectic problems of the types outlined in Example 3 has not yet been tested.

5 Numerical Example

For a numerical test of some of the methods mentioned we investigate the following problem which originates from [3, 19]. Consider a specimen in form of a brick with a crack as illustrated in Figure 2. The (homogeneous) material has Poisson ratio $\nu = 0.32$, the Young modulus does not influence the result and can be set arbitrarily. The stress concentration near the point O where the crack intersects the surface of the brick can be investigated within the linear elasticity framework, as long as the material is brittle, see e.g. [18, 19, 20]. The stress field is derived from the displacement field which can be represented by a regular part and several singular terms of the form $kr^\alpha u(\varphi, \theta)$ where (r, φ, θ) are spherical coordinates centered in the point of interest, k is called stress intensity factor, and α is the characteristic (singular) exponent with the associated mode u. These terms are singular when $\operatorname{Re}\alpha < 1$ and $\operatorname{Re}\alpha \neq 0$.

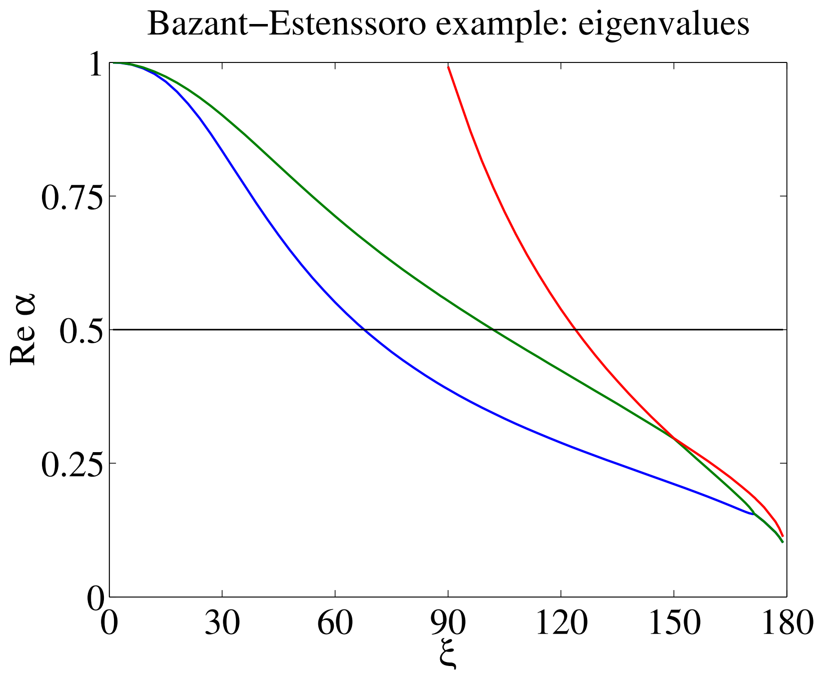

Figure 3: Real part of the interesting eigenvalues against the angle ξ between the crack and the surface of the brick

Mathematically, the pair (α, u) is eigenpair of a quadratic operator pencil [16, 19]. Approximation by the finite element method leads to a finite-dimensional problem, an eigenvalue problem for a quadratic matrix pencil, see [2] for discretization error estimates. After substitution $\lambda = \alpha + 0.5$ this problem has the more convenient form (3), see Example 1 in Section 2. Figure 5 displays the real part of the (approximated) eigenvalues from the strip $0 < \operatorname{Re}\alpha < 1$ for the whole possible range of the angle ξ between the crack and the surface. A crack in progress has curved shape and the angle between the crack and the surface adjusts such that the corresponding eigenvalue α has real part 0.5, in our case $\xi \in \{67°, 101°, 124°\}$ where the angles are rounded to integer values. Which angle actually appears depends on the load applied. For the computation of the 2 or 3 eigenvalues of interest we computed 9 eigenvalues. Note that $\alpha = 0$ $(\lambda = 0.5)$ and $\alpha = 1$ $(\lambda = 1.5)$ are both triple eigenvalues corresponding to rigid body motion and without theoretical interest. We compare HIRL (with shift $\tau = 0.0$) and SHIRA with shift values $\tau = 1.0$ (useful shift in the middle of the strip of interest $0.5 < \operatorname{Re}\lambda < 1.5$) and $\tau = 0.0$. As a benchmark we include also a simple method that does not exploit the structure of the problem and that computes in general also eigenvalues in the left half of the complex plane if not an appropriate shift is applied; therefore we compute 18 eigenvalues in

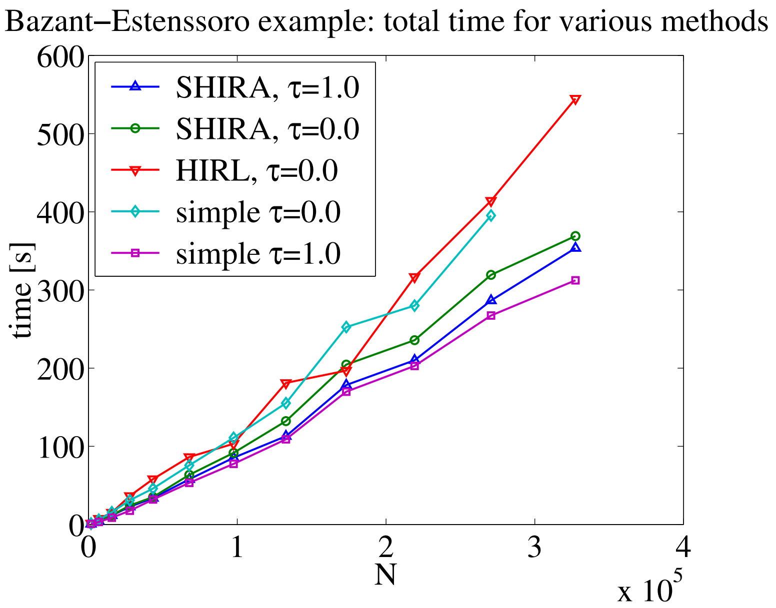

Figure 4: Computing time for the crack with $\xi = 120°$ and various discretization parameters

the case $\tau = 0.0$. For this test we chose $\xi = 120°$ where the three eigenvalues of interest are well separated. The total computing times with various discretization parameters are displayed in Figure 4 where N is the size of the matrices K, G, and M. Note that the times include the assembly of the matrices which is independent of the solution methods used.

To evaluate the algorithms we give some implementational details. The implementation of the SHIRA algorithm is based on the ARPACK package [21]. Only a slight modification is made to enforce isotropy, as discussed in Section 4. To apply the operator, we have to solve systems with the sparse matrices. In the case of SHIRA this matrix is in general ($\tau \neq 0$) non-symmetric and we use the LU-decomposition from version 2.0 of the package SuperLU [10]. In the case of HIRL we can use a Cholesky decomposition. After some comparisons we decided to use the TAUCS package for this [31]. The simple method mentioned above is the application of ARPACK to the matrix $(H - \tau I)^{-1}$ which has no structure. Again, we used version 2.0 of the package SuperLU for the factorization necessary. In all cases we used a stopping tolerance of 10^{-12} for the Krylov iteration. The tests were carried out on an Intel Pentium 4 CPU with 1.60 GHz, 1 GB main memory and 256 kB cache.

We conclude that SHIRA is a competitive algorithm to compute eigenvalues of quadratic skew-Hamiltonian/Hamiltonian pencils. HIRL in the current implementation is much slower which can be traced back to a much larger number of iterations in comparison with SHIRA that cannot be explained satisfactorily at this time. We are still analyzing all kinds of tolerances used in both the SHIRA and the HIRL packages. The simple method applied with the optimal shift is superior; the number of solves is nearly equal to that of SHIRA with the same shift, but some overhead, e.g. due to the additional reorthogonalization, does not occur. In extreme cases, however, we expect more stability with structure preserving methods like SHIRA.

Note that the comparison of HIRL with the other methods is not quite fair, since HIRL computes eigenvectors and both SHIRA and the simple method do not. If eigenvectors are desired these methods (in the current implementation) apply one step of inverse iteration which needs another LU factorization for each eigenvector.

A second strength of HIRL is that it computes both right and left eigenvectors, and this allows the computation of a condition number for each eigenvalue. Since we have eigenvectors to go with the eigenvalues, we can also compute residuals. If the residual is tiny and the condition number is good, the eigenvalue is guaranteed accurate.

6 Conclusion

We have discussed the numerical solution of large scale polynomial or rational eigenvalue problems with a Hamiltonian or symplectic symmetry in the spectrum. Several applications are presented that lead to such structures. We discuss recent developments in numerical methods and presented numerical examples.

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