

RATIONAL KRYLOV FOR REAL PENCILS WITH COMPLEX EIGENVALUES

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Abstract. A rational Krylov algorithm for eigenvalue computation is described. It is usable on a real matrix pencil with complex eigenvalues and builds up a real basis. The main purpose is to get real reduced models of a real linear dynamic system. Two variants are described, one where two real vectors are added to the Krylov space in each step and another where just one real vector is added in each step.

Results are reported from one small example that has been used earlier and where the solution is known, and one more realistic example, a linear descriptor system from a computational fluid dynamics application.

1. INTRODUCTION

We want to compute eigenvalues of a linear matrix pencil

$$(1) \quad (A - \lambda E)x = 0.$$

when the pencil is real but has complex eigenvalues.

Eigenvalues are of interest to understand the behavior of a linear time-invariant dynamical system

$$(2) \quad \begin{aligned} E\dot{x}(t) &= Ax(t) + bu(t), \\ y(t) &= cx(t), \end{aligned}$$

connecting input $u(t)$ and output $y(t)$ via the state $x(t)$. The poles of the transfer function are the eigenvalues of the pencil (1). Typically, for slowly damped systems, the eigenvalues are in the left half plane close to the imaginary axis.

Eigenvalue algorithms are by their nature complex, and special devices are needed to stay in real arithmetic and get solutions that give complex conjugate

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Work with Henrik Olsson, Zenon Mathews and Henrik Holst.

pairs of eigenvalues with real invariant subspaces. If the original matrices are small enough for transformation methods, there is the double shift QR or QZ algorithm. It computes a real Schur form and gives real bases for the invariant subspaces. Now we are interested in algorithms for larger problems, that can be treated with shift and invert Krylov space methods. The aim is to get real reduced order models for a real system (2).

We start this paper by describing the rational Krylov algorithm [10], implemented as shift invert Arnoldi with varying shifts [1, Ch. 8.5 p. 246]. A detailed description is given in the thesis by Olsson [5] and the paper [6]. In section 3, we treat the case with real matrices. First we describe a double shift variant, introduced in [8] and tested in the thesis by Holst [2]. Then we describe how to apply the original single vector variant, given by Parlett and Saad [7]. This variant promises to be the most interesting one for model reduction purposes, but we have yet to show how to change shifts.

We conclude in section 4, by reporting a few numerical tests. The reader is referred to the works by Olsson [5], Mathews [3] and Holst [2] for more details.

2. RATIONAL KRYLOV, GENERAL CASE

The rational Krylov algorithm is a shift invert Arnoldi decomposition

$$(3) \quad (A - \sigma E)^{-1} E V_j = V_{j+1} H_{j+1,j},$$

where the shift σ is changed in some of the steps j . The resulting matrix H is of Hessenberg form.

Consider step j ,

$$(A - \sigma_j E)^{-1} E v_j = V_{j+1} h_j,$$

where the $j + 1$ vector h_j consists of Gram Schmidt coefficients that assures that the next basis vector v_{j+1} is a unit vector orthogonal to the span of V_j , the previous vectors.

Multiply by $(A - \sigma_j E)$ and get

$$(A - \sigma_j E) V_{j+1} h_j = E v_j,$$

and separate A and E terms

$$A V_{j+1} h_j = E V_{j+1} (e_j + h_j \sigma_j).$$

Put earlier columns up front and get a rational Krylov recursion [10],

$$(4) \quad A V_{j+1} H_{j+1,j} = E V_{j+1} K_{j+1,j},$$

with two Hessenberg matrices, H consisting of the Gram Schmidt coefficients, and

$$(5) \quad K_{j+1,j} = I_{j+1,j} + H_{j+1,j} \text{diag}_{i=1}^j(\sigma_i)$$

We may now formulate the rational Krylov recursion (4) as an Arnoldi iteration with another starting vector w_1 , chosen from the Krylov space spanned by V_{j+1} . This is done by QR factorizing either H or K .

Let us choose to factorize H , which will give a *direct* iteration,

$$H_{j+1,j} = Q_{j+1}R_{j+1,j}$$

giving

$$(6) \quad \begin{aligned} AV_{j+1}Q_{j+1}R_{j+1,j} &= EV_{j+1}Q_{j+1}(Q'_{j+1}K_{j+1,j}) \\ AW_jR_{j,j} &= EW_{j+1}M_{j+1,j} \end{aligned}$$

with

$$W_{j+1} = V_{j+1}Q_{j+1} \text{ and } M_{j+1,j} = Q'_{j+1}K_{j+1,j}$$

In the unreduced case, when all the subdiagonal elements of H are nonzero, the orthogonal matrix is

$$Q_{j+1} = G_{1,2}G_{2,3} \cdots G_{j,j+1},$$

a product of j Givens rotations in the coordinate planes given by the subscripts.

Apply the QZ algorithm to the leading $j \times j$ square pencil $(M_{j,j}, R_{j,j})$ of the recursion (6). A Ritz approximation $(\theta^{(j)}, y^{(j)})$ to an eigenpair of the pencil (1) is given by

$$M_{j,j}s_j = R_{j,j}s_j\theta^{(j)} \quad y^{(j)} = W_jR_{j,j}s_j.$$

Its residual is,

$$(7) \quad r^{(j)} = Ay^{(j)} - Ey^{(j)}\theta^{(j)} = Ew_{j+1}m_{j+1},s_j.$$

It is in the direction of the next basis vector Ew_{j+1} . Its length is given by the inner product between the $j + 1$ st and last row of M and the eigenvector s_j . We note that the transformed matrix $M_{j,j}$ is full. We may transform it into Hessenberg form, using the algorithm described in [9], but this may be ill conditioned if $R_{j,j}$ is close to singular.

3. RATIONAL KRYLOV FOR REAL MATRICES

We have developed a double shift variant, that gives a real Hessenberg pair when the original pencil (A, E) is real, but the shifts σ and the eigenvalues λ are complex.

In each step, add two vectors, given by the real and imaginary parts of

$$(8) \quad r = (A - \sigma E)^{-1} E v_j$$

orthogonalized to the previous basis vectors V_j , to give v_{j+1} and v_{j+2} . The matrix $\text{diag}(\sigma_i)$ in (5) will have 2×2 blocks, $\begin{pmatrix} \rho_i & \theta_i \\ -\theta_i & \rho_i \end{pmatrix}$ in those positions where the shift σ is complex, with real and imaginary parts

$$(9) \quad \sigma = \rho + i\theta.$$

This gives the double vector variant, described in [8] and [2].

We are now testing the original, single vector variant, given by Parlett and Saad [7]. In each step j , we take either the real *or* the imaginary part of r (8), adding one vector to the basis V_j and one column to H .

We get

$$(10) \quad B V_j = V_{j+1} H_{j+1,j}$$

where either

$$B = B_+ = \text{real}((A - \sigma E)^{-1} E)$$

or

$$B = B_- = \text{imag}((A - \sigma E)^{-1} E).$$

Note that

$$B_+ = \frac{1}{2} ((A - \sigma E)^{-1} + (A - \bar{\sigma} E)^{-1}) E$$

and similarly for B_- . It will get the same real invariant subspaces as the pencil (1) but other complex conjugate eigenvalues μ_+ and μ_- .

If we partition the shift into real and imaginary parts $\sigma = \rho + i\theta$ (9), we get

$$(11) \quad \begin{aligned} \mu_+ = \lambda(B_+) &= \frac{1}{2} \left(\frac{1}{\lambda - \sigma} + \frac{1}{\lambda - \bar{\sigma}} \right) \\ &= \frac{1}{2} \left(\frac{\lambda - \sigma + \lambda - \bar{\sigma}}{(\lambda - \sigma)(\lambda - \bar{\sigma})} \right) \\ &= \frac{\lambda - \rho}{(\lambda^2 - 2\rho\lambda + |\sigma|^2)} \end{aligned}$$

$$(12) \quad \mu_- = \lambda(B_-) = \frac{\theta}{(\lambda^2 - 2\rho\lambda + |\sigma|^2)}$$

If we compute any of these from the Hessenberg matrix H in (10), we can get approximations to the pencil eigenvalues λ by solving a quadratic equation.

In the first case, we get from (11) that $\lambda = \rho + \xi$ where ξ is a solution of

$$(13) \quad \xi^2 - \frac{1}{\mu_+} \xi + \theta^2 = 0,$$

and in the second, (12) implies that

$$(14) \quad \xi^2 - \frac{\theta}{\mu_-} + \theta^2 = 0$$

The sign has to be chosen properly, for each of the j eigenvalues μ we get two λ suggested. As of now, we do this by checking the Rayleigh quotients of the original pencil (1).

4. NUMERICAL EXAMPLES

Hopf bifurcation

This small problem was reported by Parlett and Saad [7]. It describes reaction and transport interaction of two chemical solutions in a tubular reactor. A simple finite difference approximation over the unit interval with 100 interior points gives a matrix of order $n = 200$ with a 2 by 2 block structure. It depends on a bifurcation parameter L . For interesting values of L , most eigenvalues are real and negative. We seek the pair of eigenvalues that is close to imaginary axis.

We applied the single vector algorithm of Parlett and Saad [7] with basis size $j = 30$ and constant shift $\sigma = 0.5 + 2.1i$. In Figure 1, we plot the eigenvalue approximations together with the exact eigenvalues for comparison. Notice that those closest to the shift σ are the first to converge. In Figure 2, we plot the eigenvalues μ of the shifted and inverted pencil

$$B = (A - \sigma E)^{-1}E$$

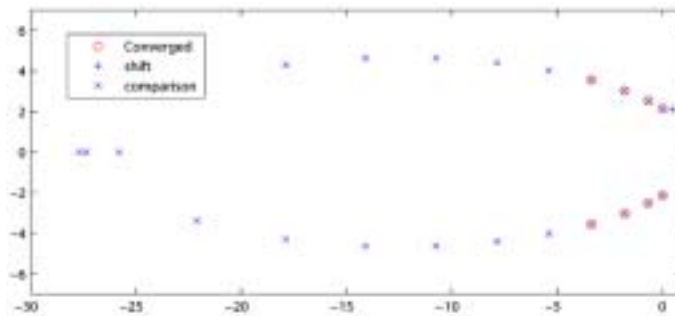


Fig. 1. Hopf bifurcation, eigenvalues.

and μ_+ and μ_- , those of its real and imaginary parts B_+ and B_- , (11) and (12). Note that the eigenvalues of B are not in complex conjugate pairs, while those of B_+ and B_- are. All three matrices have some well separated eigenvalues μ ,

expected to converge fast, and many eigenvalues close to zero that correspond to eigenvalues λ far from the shift σ .

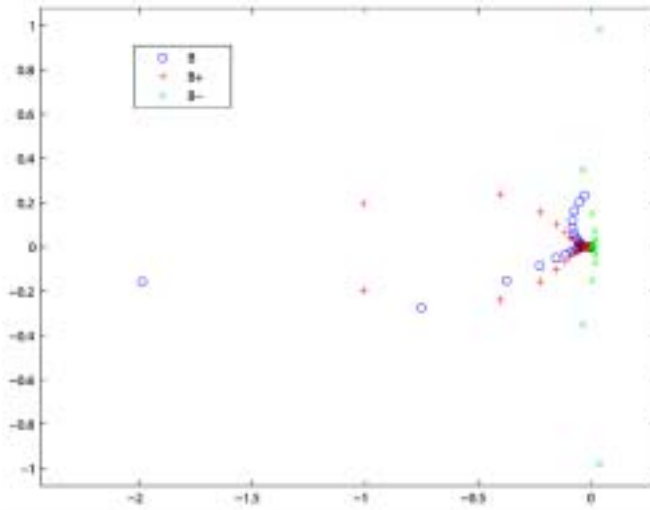


Fig. 2. Hopf bifurcation, transformed eigenvalues.

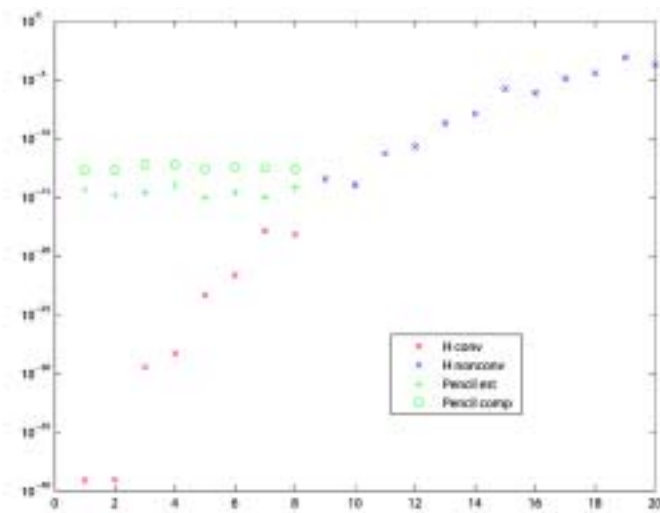


Fig. 3. Hopf bifurcation, residuals.

We plot the leading 20 residuals in Figure 3. The estimates of the transformed H residuals in (10) with $B = B_+$, plotted as crosses, are used to signal convergence. We check by computing and plotting the pencil residuals (7) and see that we indeed

have 8 converged eigenvalues.

Supersonic engine inlet

The second system we study here comes from *Active Control of a Supersonic Engine Inlet* by Willcox, Lassaux, and Gratton [4]. It is a descriptor system (2) of size $n = 11730$ coming from a linearization of two-dimensional Euler equations describing unsteady flow through a supersonic diffuser. The descriptor matrix E is singular. There are two inputs and one output, which means that $b \in \mathbb{R}^{n \times 2}$ and $c \in \mathbb{R}^{1 \times n}$. This is an interesting test problem to us, since it is reasonably large and has quite a lot of eigenvalues along the imaginary axis.

Some of the eigenvalues in the second quadrant, as reported in [6] are seen in Figure 4. The shifts are chosen adaptively along the imaginary axis, so that for each shift about the same number of eigenvalues converge. Note that we get nearly all eigenvalues with real part above -10 and imaginary between 0 and 140 . Let us show just one snapshot of the eigenvalue approximations. In Figure 5, we plot approximations at a basis size $j = 100$ of the double vector algorithm when the shift has stepped up to $\sigma = 20i$. Observe that the approximations are expanding in a circle like region around the shift, finding all eigenvalues inside.

We also plot one case of transformed eigenvalues μ_+ after $j = 20$ steps in Figure 6. Here we do not see an accumulation at zero like in Figure 2, because now we have a long time to go before those eigenvalues converge. We see a circle like configuration as implied by the convergence behaviour shown in Figure 5.

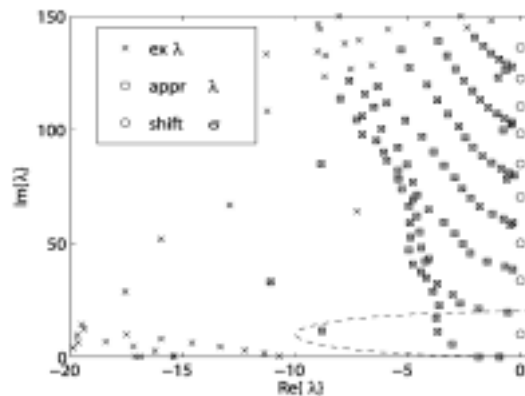


Fig. 4. Supersonic engine inlet: Some eigenvalue approximations computed with rational Krylov, compared with the exact spectrum found with eigs. Also included is a (half-)circle with radius 10 centered at $\sigma = 10i$ for indicating the axis scales and the shape of a typical convergence region of a shift invert method.

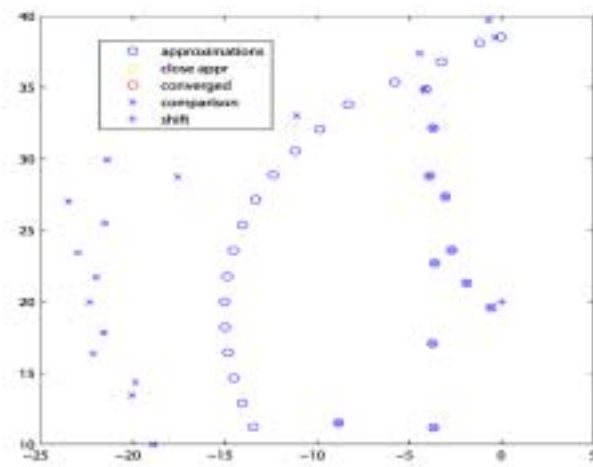


Fig. 5. Supersonic engine inlet: Progress at step $j = 100$ when shift $\sigma = 20i$. Comparison computed with eigs.

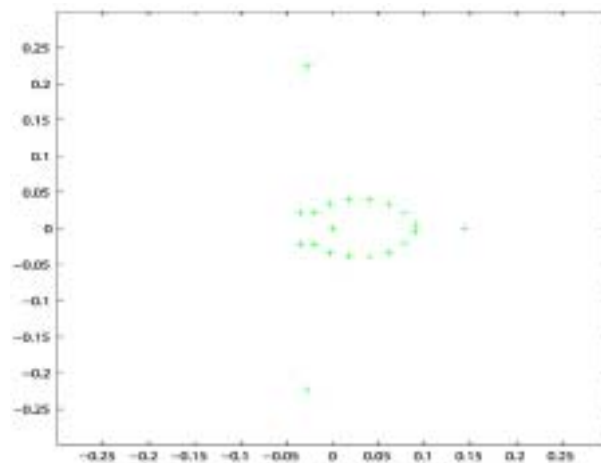


Fig. 6. Supersonic engine inlet: Transformed Ritz approximations μ_+ at step $j = 20$.

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