Spectral Division Methods for Block Generalized Schur Decompositions *

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Abstract. This paper describes from a new perspective the inverse-free spectral division methods for block generalized Schur decompositions and presents a more efficient, accurate and stable algorithm. Even in the case that only a right deflating subspace of a matrix pencil is of interest, as in many engineering application problems, the new algorithm can be used, with a low extra cost, to obtain posterior estimates on the backward accuracy of a computed orthonormal basis for the deflating subspace. The idea behind the new algorithm can be straightforwardly applied to non-inverse-free versions of spectral division algorithms.

1 Introduction

In this paper we discuss and present modifications on spectral division algorithms for computing block Schur decompositions [12, 26] of a matrix pencil (A, B), where A and B are square matrices of order n. In particular, we are interested in computing two unitary matrices $Q = (Q_1, Q_2)$ and $Z = (Z_1, Z_2)$ such that

$$Q^{\mathrm{H}} A Z = \begin{pmatrix} A_{11} & A_{12} \\ 0 & A_{22} \end{pmatrix} \quad \text{and} \quad Q^{\mathrm{H}} B Z = \begin{pmatrix} B_{11} & B_{12} \\ 0 & B_{22} \end{pmatrix}, \tag{1}$$

where $\lambda(A_{11}, B_{11})$, the eigenvalue set of (A_{11}, B_{11}), and $\lambda(A_{22}, B_{22})$ are disjoint. The idea of the so called spectral division methods, or deflating subspace methods, is to decompose the matrix pencil into two of smaller size by first separating two complementary deflating subspaces [2, 18, 4, 5]. When necessary, the same idea can be applied to one or two of the smaller matrix pencils, recursively. Such methods are attractive for that no re-grouping of

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eigenvalues is needed if the required eigenvalues are those of A_{11} or A_{22} and for that the algorithms can be easily implemented with level 3 BLAS, especially, in parallel computations.

There are two kinds of spectral division methods known in the literature: one is based on the Newton iteration for the matrix sign function; another is based on Malyshev's iteration for what we shall call the matrix disc function (cf. Section 3). The Newton iteration for computing the matrix sign function is first introduced by Roberts [22], and its version for matrix pencils, presented in [10], is defined as:

$$A_{k+1} = (A_k + BA_k^{-1}B)/2, \quad A_0 = A. \tag{2}$$

The pencil sequence (A_k, B) of (2) has the following property. If $A_k x = \lambda^{(k)} Bx$, where $x \neq 0$, then

$$A_{k+1}x = \frac{1}{2}\left(\lambda^{(k)} + \frac{1}{\lambda^{(k)}}\right) Bx.$$

There is a symmetrical result with the left eigenvectors. For $\lambda^{(0)} = \lambda \neq 0$, $\lambda^{(k)} \to \mathrm{sign}(\lambda)$ as $k \to \infty$, where $\mathrm{sign}(\lambda) = +1$ or -1, depending on $Re(\lambda) > 0$ or $Re(\lambda) < 0$. The sequence (2) is shown globally convergent if A is nonsingular and its asymptotic convergence rate is quadratic. Denote by (A_∞, B) the converged pencil. Then, $\mathcal{N}(A_\infty + B)$, the nullspace of $(A_\infty + B)$, and $\mathcal{N}(A_\infty - B)$ are the deflating subspaces of (A, B) corresponding to the eigenvalues, respectively, in the left and right complex planes. To extract a deflating subspace from, say, $A_\infty + B$ we need to separate the range and nullspace of $A_\infty + B$. Many effective numerical algorithms for such task have been further developed in recent years, such as rank-revealing QR factorizations (RR-QRF) [7,9,13,20,21], and rank-revealing URV [25]. Due to the inverse operation at each step, the Newton iteration is sensitive to perturbations and rounding errors in numerical computation when matrix A is poorly conditioned. There are inverse free iteration schemes for the matrix sign function, such as Newton-Schulz iteration [14], at the expense of loosing global convergence. For more details on numerical computation and high performance implementation of the Newton iteration, see, for example, [4,5,6,8,19].

Malyshev presented an alternative scheme, see Figure 1, for the spectral division [18]. Notice that there is no inverse involved in the iteration. We also note in passing that a singular pencil can be detected at the normalization step. The theoretical foundation of Malyshev's iteration is related to previous works of Godunov and Bulgakov, among others (see [11, 15, 16] and references therein). While the Newton iteration divides the spectrum along the imaginary axis, Malyshev's iteration divides the spectrum along the unit circle. In fact, these two approaches are dual with each other under Cayley transform if no eigenvalues lie on the imaginary axis or on the unit circle. Unlike the Newton iteration for matrix sign function, Malyshev's iteration does not apparently preserve both right and left deflating subspaces. However, Malyshev proves that $(A_k + B_k)$ are nonsingular and that

$$P_{\mathrm{rin}} = \lim_{k\to\infty} (A_k + B_k)^{-1} B_k, \quad \text{and} \quad P_{\mathrm{rout}} = \lim_{k\to\infty} (A_k + B_k)^{-1} A_k \tag{3}$$

are the spectral projectors into the respective right deflating subspaces of (A, B) corresponding to the eigenvalues inside and outside of the unit circle. The inverse operation is thus introduced at the step of computing the spectral projectors. Unfortunately, the stopping criterion used by Malyshev also involves matrix inverses.

1. Initial Normalization.
   Compute $(A, B) = L(A_0, B_0)$ so that $A_0 A_0^{\mathrm{H}} + B_0 B_0^{\mathrm{H}} = I_n$.
   Such normalization can be done, for example, by QR factorization.
2. For $k = 0, 1, \ldots$

$$\begin{pmatrix} Q_{11} & Q_{12} \\ Q_{21} & Q_{22} \end{pmatrix} \begin{pmatrix} B_k \\ -A_k \end{pmatrix} = \begin{pmatrix} R_k \\ 0 \end{pmatrix}, \quad \text{(QR factorization)}$$

$$A_{k+1} = Q_{21} A_k,$$
$$B_{k+1} = Q_{22} B_k.$$

Figure 1: Malyshev's iteration.

The drawbacks of Malyshev's algorithm are circumvented by Bai, Demmel and Gu [3]. Specifically, they propose an effective inverse-free stopping criterion using the Cholesky factors R_k of successive matrix pencils (cf. Figure 1):

$$\|R_k - R_{k-1}\|_1 \leq 10\, n\, \epsilon\, \|R_k\|_1, \tag{4}$$

where ϵ is the machine precision. Note that the Cholesky factors are readily available by the QR factorization in Malyshev's iteration. To avoid the inverse in computing spectral projectors, Bai, Demmel and Gu suggest applying the generalized QR factorization techniques to $(A_\infty + B_\infty)^{-1} B_\infty$. We shall describe the pioneering works of [3,18] in other aspects in later sections when related topics are discussed.

In [10, 18, 22], the solution of the algebraic Riccati equation [17] is concerned and in such case only the right deflating subspace is of interest. The idea of the deflating subspace methods is generalized in [3,5] to computing the block Schur decomposition of matrix pencils as shown in (1). The approach is to have an additional Newton iteration (2) or Malyshev's iteration starting with $(A^{\mathrm{H}}, B^{\mathrm{H}})$ and then compute the left spectral projectors. As we indicated earlier, with one sequence of the Newton iteration, we can get both the right and left deflating subspaces with respect to the same division in the spectrum. Thus, the gap in arithmetic cost between the Newton iteration approach and the Malyshev iteration approach is not only in each iteration but also in the total number of iterations. In more details, each Newton iteration of (2) takes about $O(6n^3)$ floating-point arithmetic operations (flops); each Malyshev iteration as shown in Figure 1 uses about $O(13.3n^3)$ flops. Moreover, the two-sided

Malyshev iteration approach takes twice as many iterations as the one-sequence Newton iteration. An approach to compute the left spectral projectors without the left iteration is mentioned in [3] but it introduces the inverse of the converged Cholesky factor, which is possibly ill-conditioned.

In this paper we present a stable inverse-free block generalized Schur decomposition method based on one-sided subspace iteration and an accurate subspace extraction scheme. This method costs no more than the less stable one in [3] and reduces the arithmetic cost by half compared to its counterparts with two-sided iterations. Even in the case that only a right deflating subspace is of interest, our algorithm can be used, with relatively low extra cost, to obtain posterior estimates on the backward accuracy of a computed orthonormal basis for the desired subspace. The idea can be applied straightforwardly to the methods based on the Newton iteration for the matrix sign function. Our paper is organized as follows. In Section 3, we review the theory on block generalized Schur decompositions; our computational objects are block Schur decompositions, and our computational approach is more directly related to the theory underpinning the decompositions. In Section 3, we describe from a new perspective the algebraic preliminaries on Malyshev's iteration and characterize a family of Malyshev-like iterations, which we will call CS-AB iterations. It is hoped that our description of the essentials for the inverse free algorithms is more understandable. In Section 4, we introduce a primary version of our deflation method with one-sided iteration. In particular, we introduce a truly inverse-free scheme for obtaining both right and left deflating subspaces, without resorting to $(A_\infty + B_\infty)^{-1} B_\infty$ or its approximation. In Section 5, we give a proof convergence of (A_k, B_k) without assuming either A_k or B_k be nonsingular. In Section 6, we provide a modified version of our algorithm, taking into account the numerical difficulties in subspace extractions. In Section 7 we describe the initial inverse-free spectral transformations that allow spectral division methods to divide the spectrum in various ways. In Section 8, we present some of our numerical experiments, which have consistently shown that the numerical behaviors of our one-sided approach are about the same as the two-sided iteration approach in some cases, and superior to its two-sided counterparts in other cases. Our concluding remarks are in Section 9.

The following notation and conventions will be used throughout the paper unless stated otherwise. We will use $\|\cdot\|$ to denote the matrix 2-norm. We will use MATLAB's colon notation for (sub)matrices and permuted matrices. By $\mathcal{R}(A)$ we denote the range of A; and $\mathcal{N}(A)$, the nullspace of A. We denote by Π a permutation matrix (or a unitary matrix) in a rank-revealing decomposition.

2 Block Schur decompositions

Our stable scheme to obtain both right and left deflating subspaces with one-sided iteration is based on the very idea of a direct construction proof for the generalized Schur decomposition of matrix pencils, see, for example, [26].

Theorem 1 (Generalized Schur Decomposition - *Moler and Stewart, 1973) If A and B are in $\mathbb{C}^{n\times n}$, then there exist unitary matrices Q and Z such that $Q^{\mathrm{H}}AZ = S$ and $Q^{\mathrm{H}}BZ = T$ are upper triangular.*

Proof: The theorem obviously holds when $n = 1$. Assume it holds for all matrices of order $n-1$ or less. If $Ax = \lambda Bx$ or $\gamma Ax = Bx$ for some scalars γ and λ and vector $x \neq 0$, then there exist a pair of unitary matrices Z and Q such that

$$Q^{\mathrm{H}}AZ = \begin{array}{cc} \begin{pmatrix} \alpha_{11} & a^{\mathrm{H}} \\ 0 & A_{n-1} \end{pmatrix} & \begin{array}{c} 1 \\ n-1 \end{array} \end{array}, \quad Q^{\mathrm{H}}BZ = \begin{array}{cc} \begin{pmatrix} \beta_{11} & b^{\mathrm{H}} \\ 0 & B_{n-1} \end{pmatrix} & \begin{array}{c} 1 \\ n-1 \end{array} \end{array}, \tag{5}$$

where Z is chosen so that $Ze_1 = x/\|x\|$, and Q is chosen so that

$$Q^{\mathrm{H}}(Ax, Bx) = \begin{array}{cc} \begin{pmatrix} \alpha_{11} & \beta_{11} \\ 0 & 0 \end{pmatrix} & \begin{array}{c} 1 \\ n-1 \end{array} \end{array}. \tag{6}$$

In details, if $Ax = Bx = 0$, then Q can be any orthogonal matrix, particularly the identity matrix; if both Ax and Bx are nonzero, then Q can be a Householder reflection so that $Qe_1 = Bx/\|Bx\| = Ax/\|Ax\|$; otherwise, Qe_1 is proportional to the nonzero vector among Ax and Bx. By induction, there are unitary matrices Q_{n-1} and Z_{n-1} such that $\left(Q_{n-1}^{\mathrm{H}}A_{n-1}Z_{n-1}, Q_{n-1}^{\mathrm{H}}B_{n-1}Z_{n-1}\right) = (T_{n-1}, S_{n-1})$. If $Q_n = Q\mathrm{diag}(1, Q_{n-1})$ and $Z_n = Z\mathrm{diag}(1, Z_{n-1})$ then $\left(Q_n^{\mathrm{H}}AZ_n, Q_n^{\mathrm{H}}BZ_n\right)$ has the requisite form. ∎

The following should be noticed:

a) The proof presented here for the general Schur form recovers the Schur form when B is the identity matrix, I. Since $Bx = x \neq 0$, we can always let $Q = Z$ in the induction step and have, by induction, $Q_n = Z_n$.

b) The proof can be extended to the real Schur decomposition for a real matrix pencil (A, B). If $Ax = \lambda\, B\, x$, where λ is complex and $x = \mathrm{Re}(x) + i\,\mathrm{Im}(x) \neq 0$, then we can find orthogonal matrices Z and Q in the induction step to satisfy instead:

$$\begin{aligned} (\mathrm{Re}(x), \mathrm{Im}(x)) &= Z \begin{array}{cc} \begin{pmatrix} R \\ 0 \end{pmatrix} & \begin{array}{c} 2 \\ n-2 \end{array} \end{array}, \\ Q^{\mathrm{T}}(AZ(:,1\!:\!2),\ BZ(:,1\!:\!2)) &= \begin{pmatrix} S_{11} & T_{11} \\ 0 & 0 \end{pmatrix}, \end{aligned}$$

where one of the 2×2 matrices, S_{11} and T_{11}, can be made upper triangular, and both Z and Q can be constructed as a product of two Householder reflections.

c) In general, (A, B) can be transformed into a block Schur form $(Q^{\mathrm{H}}AZ,\ Q^{\mathrm{H}}BZ) = (S, T)$ with S and T block upper triangular. If X is a basis matrix for a deflating subspace of

(A, B), i.e., $\dim(\mathcal{R}([AX, BX])) = \dim(\mathcal{R}(X))$, then there exist unitary matrices Z and Q such that

$$X = Z \begin{pmatrix} R_r \\ 0 \end{pmatrix} = Z_r R_r,$$

$$Q^{\mathrm{H}}(AZ_r,\, BZ_r) = \begin{pmatrix} A_{11} & B_{11} \\ 0 & 0 \end{pmatrix}.$$

d) Once a right deflating subspace corresponding to a subset of eigenvalues is obtained, the Q-Z transformations will decouple the matrix pencil into two of smaller size and, in addition, the left deflating subspace corresponding to the remaining eigenvalues is readily available.

e) The two matrices A and B in a matrix pencil are treated equally or symmetrically. There are cases where it is necessary to write the eigenvalue problem in the cross-product form $\beta Ax = \alpha Bx$ as suggested by Stewart [24]; in other cases we use for convenience the traditional, asymmetrical definition $Ax = \lambda Bx$.

3 Malyshev-like iterations

We introduce in this section basic algebraic properties of the Malyshev iteration and Malyshev-like iterations. A Malyshev-like iteration generates two matrix pencil sequences $\{(A_k, B_k)\}$ and $\{(C_k, S_k)\}$ from $(A_0, B_0) = (A, B)$ by the following two rules:

THE CS-AB EQUIVALENCE RULE

$$C_k A_k = S_k B_k, \quad k \geq 0, \tag{7}$$

THE SQUARING RECURRENCE

$$\begin{aligned} A_{k+1} &= S_k A_k, \\ B_{k+1} &= C_k B_k. \end{aligned} \tag{8}$$

For convenience, we call such iterations CS-AB iterations hereafter. The Malyshev iteration, see figure 1, uses the QR factorization of $(A_k^{\mathrm{T}}, B_k^{\mathrm{T}})^{\mathrm{T}}$ to generate C_k and S_k, which are Q_{22} and Q_{21}, respectively, at each iteration step k. The two rules can be combined into a single matrix equation:

$$\begin{pmatrix} S_k & C_k \end{pmatrix} \begin{pmatrix} B_k & A_k & 0 \\ -A_k & 0 & B_k \end{pmatrix} = \begin{pmatrix} 0 & A_{k+1} & B_{k+1} \end{pmatrix}.$$

There are many interesting relationships between the two matrix pencil sequences, between the pencils in each sequence, and between the two matrices in a pencil. First, if B_k in (7) are nonsingular, then (S_k, C_k) are equivalent to (A_k, B_k), for that

$$S_k = C_k A_k B_k^{-1}, \quad C_k = C_k B_k B_k^{-1},$$

i.e., for each k, (S_k, C_k) has the same eigenvalues as (A_k, B_k). We may therefore expect a squaring of the eigenvalues of (A_k, B_k) in (A_{k+1}, B_{k+1}). Indeed, if $A_k x = \lambda B_k x$ for some scalar λ and $x \neq 0$, then we have, by the CS-AB equivalence rule (7) and the squaring recurrence (8),

$$\begin{aligned} A_{k+1}x &= S_k A_k x = \lambda S_k B_k x = \lambda\, C_k A_k x \\ &= \lambda^2 C_k B_k x = \lambda^2 B_{k+1} x. \end{aligned} \tag{9}$$

In symmetric form, if $\beta A_0 x = \alpha B_0 x$, then $\beta^{2^k} A_k x = \alpha^{2^k} B_k x$, by induction. As $k \to \infty$,

$$\frac{\beta^{2^k}}{\beta^{2^k} + \alpha^{2^k}} \to 1 \quad \text{if} \quad |\beta| > |\alpha|, \qquad \frac{\beta^{2^k}}{\beta^{2^k} + \alpha^{2^k}} \to 0 \quad \text{if} \quad |\beta| < |\alpha|.$$

In corresponding matrix forms, it can be shown easily that if (A, B) has no eigenvalues on the unit circle $|\alpha| = |\beta|$, then $(A_\infty + B_\infty)$ is nonsingular and $(A_\infty + B_\infty)^{-1} B_\infty$ is the matrix *disc* function of (A, B). The disc function $\mathrm{disc}(\lambda)$ maps λ inside the unit circle to 1 and outside of the circle to 0. It is easy to check that $(A_\infty + B_\infty)^{-1} A_\infty$ is the matrix function corresponding to the scalar function $1-\mathrm{disc}(\lambda)$.

For the case that B_0 is nonsingular, the relationship between A_k and B_k can be simply expressed as in the following:

Lemma 2 *If B_0 is nonsingular, then $A_k = B_k (B_0^{-1} A_0)^{2^k}$, $k \geq 1$.*

Proof: For the case $k = 1$, we have by the CS-AB relation $S_0 = C_0 A_0 B_0^{-1}$ and hence $A_1 = S_0 A_0 = C_0 A_0 B_0^{-1} A_0 = B_1 (B_0^{-1} A_0)^2$. Assume the lemma holds for $k-1 \geq 1$, i.e., $A_{k-1} = B_{k-1} (B_0^{-1} A_0)^{2^{k-1}}$. Then,

$$\begin{aligned} A_k &= S_{k-1} A_{k-1} && \\ &= S_{k-1} B_{k-1} (B_0^{-1} A_0)^{2^{k-1}} && \text{(by induction hypothesis)} \\ &= C_{k-1} A_{k-1} (B_0^{-1} A_0)^{2^{k-1}} && \text{(by CS-AB equivalence rule)} \\ &= C_{k-1} B_{k-1} (B_0^{-1} A_0)^{2^k} && \text{(by induction hypothesis)} \\ &= B_k (B_0^{-1} A_0)^{2^k}. && \end{aligned} \tag{10}$$

The lemma is therefore proved for all $k \geq 1$. ■
In such case, B_k can be interpreted as a weight factor for $(B_0^{-1} A_0)^{2^k}$.

Besides the Malyshev iteration there are other procedures to generate two matrix sequences that satisfy (7) and (8). For example, if A and B are commutative in multiplication, i.e., $AB = BA$, then $S_k \stackrel{\text{def}}{=} A_k$ and $C_k \stackrel{\text{def}}{=} B_k$ satisfy (7), $k \geq 0$. We thus have $A_{k+1} = A_k^2 = A_0^{2^{k+1}}$ and $B_{k+1} = B_k^2 = B_0^{2^{k+1}}$. This is in fact the Cayley power method [14] for the matrix sign function with $B_0 = A - B$ and $A_0 = A + B$. It can also be described as a block LU version of the CS-AB iteration compared to Malyshev's QR version in that

$$\begin{pmatrix} I & 0 \\ A & B \end{pmatrix} \begin{pmatrix} B \\ -A \end{pmatrix} = \begin{pmatrix} B \\ 0 \end{pmatrix}.$$

The explicit squaring in A_k and B_k, however, entails explicit scaling strategies to avoid overflow, underflow or both, if possible.

4 A deflation algorithm with one-sided iteration

We see from (9) that the matrix pencil sequence $\{(A_k, B_k)\}$ preserves the right deflating subspaces of (A, B) and couple them into three subspaces corresponding to the eigenvalues inside the unit circle, outside the circle and on the circle, by squaring the eigenvalues successively. By Weierstrass's canonical form [26], or, the spectral resolution theorem by Stewart and J-G Sun [26], we may let X_{in} be a basis matrix for the deflating subspace corresponding to the eigenvalues inside the unit circle $\Lambda \subseteq \{|\lambda| < 1\}$, i.e., $A\,X_{in} = BX_{in}\Lambda$. Then we have for $k = 0$:

$$\begin{aligned} A_{k+1}X_{in} &= S_k\,A_k\,X_{in} = S_k\,B_k\,X_{in}\,\Lambda^{2^k} = C_k\,A_k\,X_{in}\,\Lambda^{2^k} \\ &= C_k\,B_k\,X_{in}\,\Lambda^{2^{k+1}} = B_{k+1}\,X_{in}\,\Lambda^{2^{k+1}}. \end{aligned} \tag{11}$$

By induction, it is true for all $k \geq 0$. Symmetrically, for the deflating subspace corresponding to the eigenvalues outside the unit circle, we have $BX_{ex} = AX_{ex}\Gamma$, where the eigenvalues of Γ are reciprocal to the exterior eigenvalues of (A, B) and hence are smaller than 1 in magnitude, and we have

$$\begin{aligned} B_{k+1}X_{ex} &= Y_{ex}^{\mathrm{H}}C_k\,B_k\,X_{ex} = C_k\,A_k\,X_{ex}\,\Lambda = S_k\,B_k\,X_{ex}\,\Gamma^{2^k} \\ &= S_k\,A_k\,X_{ex}\,\Gamma^{2^{k+1}} = A_{k+1}\,X_{ex}\,\Gamma^{2^{k+1}}, \quad k \geq 0. \end{aligned} \tag{12}$$

The eigenvalues on the unit circle remain on the circle but do not converge as $k \to \infty$, except at 1.

Assume that (A, B) has eigenvalues outside and inside the unit circle but has no eigenvalues on the unit circle and that (A_k, B_k) converges to a matrix pencil, denoted by (A_∞, B_∞). Then, $\mathcal{R}(X_{in}) \subseteq \mathcal{N}(A_\infty)$ and $\mathcal{R}(X_{ex}) \subseteq \mathcal{N}(B_\infty)$. If $(A_\infty^{\mathrm{T}}, B_\infty^{\mathrm{T}})^{\mathrm{T}}$ is of full column rank, then $\mathcal{R}(X_{in}) = \mathcal{N}(A_\infty)$ and $\mathcal{R}(X_{ex}) = \mathcal{N}(B_\infty)$. In such case, X_{in} or X_{ex} can be obtained by separating the right range and nullspace of A_∞ or B_∞, respectively. Similarly, one can get the left deflating subspaces with respect to the same spectrum division by another CS-AB iteration starting with $(A^{\mathrm{H}}, B^{\mathrm{H}})$. If both right and left deflating subspaces are required, the arithmetic cost would be doubled.

In Figure 2 we present our primary algorithm that applies the CS-AB iteration on one side only. The idea is as shown in the the proof for block Schur decompositions (see Section 2); we employ the CS-AB iteration on one side, extract the desired subspace, $\mathcal{R}(Z_1)$, by orthonormal rank-revealing techniques, and obtain a deflating subspace on the other side by a QR factorization of (AZ_1, BZ_1). The matrix pencil can thus be decoupled into two of smaller size. If (S_{11}, T_{11}) is desired to posses the exterior eigenvalues, A_∞ in step 2 should be replaced by B_∞, and B_0 in step 3 should be replaced by A_0. It is then easy to see that we can get, via one-sided CS-AB iterations, both the right and left deflating subspaces

1. **CS-AB iteration** with given (A_0, B_0) and stopping criterion (4).
2. **Extract the right deflating subspace** corresponding to the interior eigenvalues:
$$A_\infty Z = \hat{S} = \begin{pmatrix} 0 & \hat{S}_{12} \\ 0 & \hat{S}_{22} \end{pmatrix}, \quad \text{(RR-QRF/URV)}$$
where $Z = (Z_1, Z_2)$ is unitary with $\mathcal{R}(Z_1) = \mathcal{N}(A_\infty) = \mathcal{R}(X_{in})$.
3. **Extract the left deflating subspace** corresponding to the exterior eigenvalues
$$Q^{\mathrm{H}} B_0 Z_1 = \begin{pmatrix} T_{11} \\ 0 \end{pmatrix}. \quad \text{(QR factorization)}$$
4. **Decouple the matrix pencil**
$$Q^{\mathrm{H}} A_0 Z = \begin{pmatrix} S_{11} & S_{12} \\ 0 & S_{22} \end{pmatrix}, \; Q^{\mathrm{H}} B_0 Z = \begin{pmatrix} T_{11} & T_{12} \\ 0 & T_{22} \end{pmatrix},$$
where (S_{11}, T_{11}) has the interior eigenvalues of (A, B) and (S_{22}, T_{22}) has the exterior eigenvalues.

Figure 2: Deflation with One-sided CS-AB Iteration (primary version).

corresponding to, say, the interior eigenvalues. We will give modifications of the primary algorithm in Section 6, taking into account the numerical difficulties in subspace extractions.

5 Convergence analysis

Recall that the there are two necessary conditions for our algorithm (see Figure 2) to work. First, (A_k, B_k) must converge, to a limit matrix pencil (A_∞, B_∞), and secondly, $(A_\infty^{\mathrm{T}}, B_\infty^{\mathrm{T}})^{\mathrm{T}}$ must be of full column rank. Within the framework of CS-AB iterations, Malyshev iteration is overflow free and guarantees global convergence with the assumptions that (A_0, B_0) is regular with respect to the unit circle [18], i.e., $\det(A - \lambda B) \neq 0$ with $|\lambda| = 1$, and that (A_0, B_0) has eigenvalues on both sides of the unit circle. The regularity with respect to the unit circle implies the regularity; the iteration would be meaningless if all the eigenvalues lie on the same side of the unit circle. There should be no additional requirement that one of A_0 and B_0 be nonsingular; we have seen that if the sequence (A_k, B_k) converges, it converges to a pair of singular matrices, i.e., both A_∞ and B_∞ are singular. Notice that equations (9), (11) and (12) are based only on the CS-AB equivalence rule (7) and the squaring recurrence (8).

Since S_k and C_k are subblocks of a unitary matrix with Malyshev's iteration, $\|A_{k+1}\| \leq \|A_k\|$ and $\|B_{k+1}\| \leq \|B_k\|$, and consequently, $|A_k|$ and $|B_k|$ are bounded from above. It is then easy to see that $(\|A_k\|, \|B_k\|)$ converges as $k \to \infty$, and all convergent subsequences of (A_k, B_k) must converge to the same limit, by the continuity of the 2-norm. According to Malyshev [18] and Bai-Demmel-Gu [3], the smallest singular value of $(A_\infty^{\mathrm{T}}, B_\infty^{\mathrm{T}})^{\mathrm{T}}$ is bounded away from 0. More precisely, it is shown in [3] that

$$\sigma_{\min}\left(\begin{pmatrix} A_\infty \\ B_\infty \end{pmatrix}\right) \geq \min_\theta \sigma(A_0 - e^{i\theta} B_0) = d_{(A_0,B_0)}, \tag{13}$$

where $d_{(A,B)}$ is defined as the distance of (A, B) to matrix pencils singular with respect to the unit circle:

$$d_{(A,B)} \stackrel{\text{def}}{=} \inf\{\, \|E\| + \|F\| : \det((A+E) - e^{i\theta}(B+F)) = 0 \text{ for some } \theta\}. \tag{14}$$

The matrix $(A_\infty^{\mathrm{T}}, B_\infty^{\mathrm{T}})^{\mathrm{T}}$ is therefore of full column rank and we have $\mathcal{N}(A_\infty) = \mathcal{R}(X_{in})$ and $\mathcal{N}(B_\infty) = \mathcal{R}(X_{ex})$. Moreover, we know from (11) and (12) that the farther the eigenvalues of (A_0, B_0) are away from the unit circle, the faster (A_k, B_k) converges.

The asymptotic convergence rate of $(A_k^{\mathrm{T}}, B_k^{\mathrm{T}})^{\mathrm{T}}$ can be described via the convergence rate of the Cholesky factor, which we also denote by R_k. For convenience we write the QR factorization at each step as $\begin{pmatrix} A_k \\ B_k \end{pmatrix} = Q \begin{pmatrix} R_k \\ 0 \end{pmatrix}$ and partition Q conformally into 2×2 blocks. Since $\mathcal{N}(B_k) \cap \mathcal{N}(A_k) \to \mathcal{R}(X_{in}) \cap \mathcal{R}(X_{ex}) = 0$, as $k \to \infty$, we know by the CS decomposition theory [12,26] that $Q_{11}^{\mathrm{H}} Q_{21} \to 0$ as $k \to \infty$. Let

$$F_k = Q_{11}^{\mathrm{H}} Q_{21}, \quad R_{k+1} = (I + E_k) R_k, \tag{15}$$

where E_k is upper triangular. By $A_{k+1} = Q_{22}^{\mathrm{H}} Q_{11} R_k$ and $B_{k+1} = Q_{12}^{\mathrm{H}} Q_{21} R_k$, we have

$$\begin{aligned}(I + E_k)^{\mathrm{H}}(I + E_k) &= R_k^{-\mathrm{H}}(A_{k+1}^{\mathrm{H}} A_{k+1} + B_{k+1}^{\mathrm{H}} B_{k+1}) R_k^{-1} \\ &= I - (F_k F_k^{\mathrm{H}} + F_k^{\mathrm{H}} F_k),\end{aligned}$$

and hence $\|E_k\| = O(\|F_k\|^2)$. We show the quadratic convergence of $\|E_k\|$ to zero by establishing the relationship between F_{k+1} and F_k. Let

$$\begin{pmatrix} A_{k+1} \\ B_{k+1} \end{pmatrix} = \begin{pmatrix} \tilde{Q}_{11} \\ \tilde{Q}_{21} \end{pmatrix} R_{k+1}, \qquad (\text{ QR factorization }).$$

Then,

$$\tilde{Q}_{11}(I + E_k) = Q_{22}^{\mathrm{H}} Q_{11}, \quad \tilde{Q}_{21}(I + E_k) = Q_{12}^{\mathrm{H}} Q_{21}.$$

By the CS decomposition theory,

$$Q_{11} = U_1 \Sigma_1 V_1^{\mathrm{H}}, \quad Q_{21} = U_2 \Sigma_2 V_1^{\mathrm{H}},$$

for some unitary matrices U_1, U_2 and V_1, where Σ_1 and Σ_2 are diagonal. It is easy to check that

$$Q_{12} = -U_1\Sigma_2 V_2, \quad Q_{22} = U_2\Sigma_1 V_2,$$

with some unitary matrix V_2. Then,

$$\begin{aligned} F_{k+1} &= \tilde{Q}_{11}^{\mathrm{H}}\tilde{Q}_{21} \\ &= (I+E_k)^{-\mathrm{H}}Q_{11}^{\mathrm{H}}Q_{22}Q_{12}^{\mathrm{H}}Q_{21}(I+E_k)^{-1} \\ &= (I+E_k)^{-\mathrm{H}}Q_{11}^{\mathrm{H}}U_2\Sigma_1\Sigma_2U_1Q_{21}(I+E_k)^{-1} \\ &= -(I+E_k)^{-\mathrm{H}}(Q_{11}^{\mathrm{H}}Q_{21})^2(I+E_k)^{-1} \\ &= -(I+E_k)^{-\mathrm{H}}F_k^2(I+E_k)^{-1}. \end{aligned}$$

Recalling that $\|E_k\| = O(\|F_k\|^2)$, we now have $\|F_{k+1}\| = O(\|F_k\|^2)$. Our proof of this result is an improvement on the one given in [3] in that none of A_k and B_k is assumed nonsingular.

6 Accurate extraction of deflating subspaces

There are two factors affecting the accuracy of the computed deflating subspaces: first, how well the CS-AB iteration preserve the deflating subspaces of the initial matrix pencil (A_0, B_0), and secondly how accurately the subspaces are extracted from the converged matrix pencil (A_∞, B_∞). For perturbation analysis and error analysis of subspace preserving, see [18] and [3]. We shall be concerned in this section with subspace extraction approaches.

In presence of rounding errors, the nullspace of A_∞ computed by Step 2 of the primary algorithm in Figure 2 may be drifted away from the numerical deflating subspace of (A_∞, B_∞) if the Cholesky factor of (A_∞, B_∞) is poorly conditioned. To overcome this problem, we use the following two steps to replace Step 2 of the primary algorithm:

<u>2. Extract the right deflating subspace</u>

2.1) $\begin{pmatrix} A & B \end{pmatrix} = R\begin{pmatrix} P_A & P_B \end{pmatrix}$, (RQ factorization)

2.2) $\Pi P_A Z = \begin{pmatrix} \tilde{E}_{11} & \tilde{S}_{12} \\ \tilde{E}_{21} & \tilde{S}_{22} \end{pmatrix}$ (RR-RQF)

where $\tilde{E}$ is small with respect to the threshold for numerical rank of P_A. By the CS decomposition theory, $(P_A, P_B) = (W\Sigma_a U^{\mathrm{H}}, W\Sigma_b V^{\mathrm{H}})$ for some unitary matrices W, U and V, where Σ_a and Σ_b are diagonal matrices satisfying $\Sigma_a^2 + \Sigma_b^2 = I$. We also have $\Sigma_a\Sigma_b = 0$ from $\mathcal{N}(A) \cap \mathcal{N}(B) = 0$. Thus, we have not only $\mathcal{N}(A) = \mathcal{N}(P_A)$ and $\mathcal{N}(B) = \mathcal{N}(P_B)$, but also $\mathcal{R}(P_A) = \mathcal{R}^\perp(P_B)$. We see that Step 2.1 serves the purpose of aligning and preconditioning A_∞ and B_∞ for subspace extraction.

In step 3 of the primary algorithm, Figure 2, if B_0Z_1 is not well conditioned, a computed left nullspace of B_0Z_1 may not be a good left null space of A_0Z_1. Based on the proof for block Schur decomposition, we compute an orthonormal rank-revealing decomposition of (A_0Z_1, B_0Z_1) instead:

3. Extract the left deflating subspace

$$Q^{\mathrm{H}}(A_0Z_1, B_0Z_1)\Pi = \begin{pmatrix} S_{11} & T_{11} \\ E_{21} & F_{21} \end{pmatrix}$$

7 Transformations of Spectral Divisions

The CS-AB iteration algorithms divide the spectrum of (A, B) along the unit circle. With the appropriate transformation on (A, B), the CS-AB iteration algorithms can divide the spectrum in various ways. Though such concept is applied in [18], the technique presented by Bai, Demmel and Gu [3] for the class of Möbius transformations on matrix pencils is extremely simple. The general theory behind their technique can be found in an early work by Stewart and J-G Sun [26]:

Theorem 3 *Let M be a nonsingular matrix. Given the matrix pencil (A, B), set $(C, D) = (A, B)(M \otimes I_2)$. Given the pair $(\alpha, \beta) \neq (0, 0)$ so that $\det(\beta A - \alpha B) \neq 0$, define (γ, δ) by*

$$\begin{pmatrix} \delta \\ -\gamma \end{pmatrix} = M^{-1} \begin{pmatrix} \beta \\ -\alpha \end{pmatrix}.$$

Then $\det(\beta A - \alpha B) \neq 0$ if and only if $\det(\delta C - \gamma D) \neq 0$.

With the initial matrix pencil transformed by $W \otimes I_2$, the CS-AB iteration algorithms divide the spectrum of (A, B) along the curve $|\delta| = |\gamma|$ without inverse introduced. For the special case of

$$W = \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}, \quad (A_0, B_0) = (A, B) \begin{pmatrix} I & I \\ I & -I \end{pmatrix},$$

the Cayley transform is performed in the initial pencil and the CS-AB iteration divides the spectrum of (A, B) along the imaginary axis. Figures 3 and 4 depict the progressive changes of the eigenvalues with Malyshev's iteration starting, respectively, from (A, B) and $(A+B, A-B)$, where A and B are the matrices in Example 2 of Section 8. In Figure 3, the eigenvalues converge to their sign function values ± 1; in Figure 4, we show only the eigenvalues inside the unit circle, which converge to 0. The reciprocal of the eigenvalues outside of the circle is symmetric to those inside with respect to the imaginary axis, cf. Section 3. Each figure consists of 4 snapshots, showing the distribution of the initial eigenvalues (top left) and the eigenvalues at the end of iteration 1 (top right), iteration 2 (bottom left) and iteration 5 (bottom right).

Among other Möbius transformations there are those scaling the unit circle, shifting the circle center, and shifting and/or rotating the imaginary axis. It should be noted that the concept and approach of such inverse-free transformations on the initial matrix pencil can be applied to other algorithms for generalized eigenvalue problems.

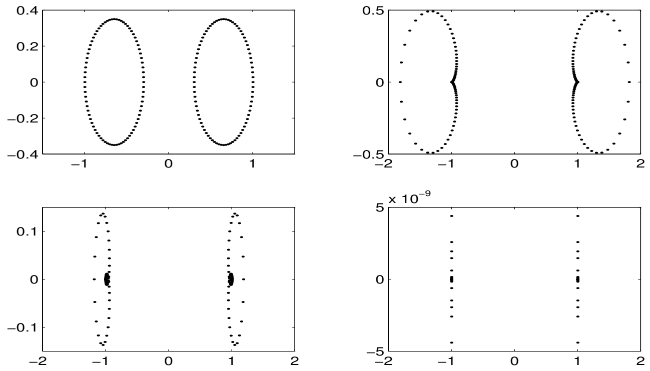

Figure 3: Iterations for the sign function

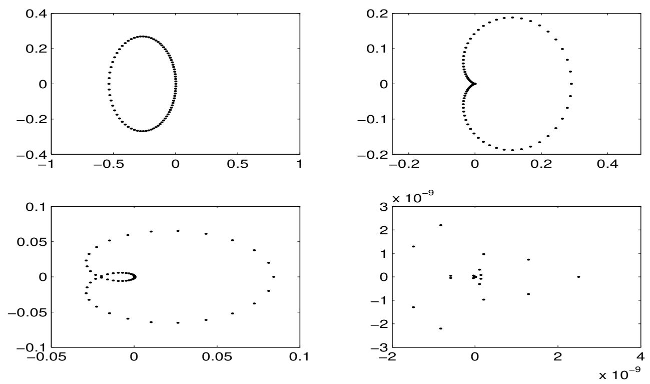

Figure 4: Iterations for the disc function

8 Numerical experiments

In this section we present some of our numerical experiments with three spectral division algorithms named individually by MM-INV, MM-GQR and M-ABQR. Algorithm MM-INV uses two-sided Malyshev's iterations and involves inverse operations in subspace extraction; algorithm MM-GQR uses two-sided Malyshev's iteration and the generalized QR factorization scheme in subspace extraction as suggested in [3]; algorithm M-ABQR uses only one-sided Malyshev's iteration and our subspace extraction scheme, which treats A_∞ and B_∞ equally without referring to $(A_\infty + B_\infty)^{-1}$, cf. Section 4 and Section 6.

The stopping criterion (4), by Bai, Demmel and Gu, is employed for all three algorithms. To measure and compare the backward accuracy of the algorithms, we evaluate the *relative decoupling residual*:

$$\|(E_{21}, F_{21})\|_F / \|(A, B)\|_F. \tag{16}$$

All the experiments were performed in MATLAB 4.2 on a SUN SPARC-20 workstation using IEEE arithmetic and $\epsilon \approx 2.2 \times 10^{-16}$.

We conducted two sets of experiments. The matrix pencils (A, B) in the first set are 100×100 random matrices with entries independent and normally distributed within $[-1, 1]$. We test the algorithms for both the case of division along the imaginary axis and the case along the unit circle, cf. Section 7. Because of using the same stopping criterion, all the three algorithms require about the same number of iterations to compute the right deflating subspace. With two-sided iterations, the number of the right side iterations and the number of the left iterations are very close. The decoupling residuals with MM-GQR and M-ABQR are about the same for both division cases, whereas the decoupling residuals by MM-INV are more sensitive to the condition number of $(A_\infty + B_\infty)$ with respect to inverse.

The second set of experiments consists of matrix pencils specially designed with known eigenvalue structures. We present our results on three examples used in [1, 3]. Since the examples are designed for computing the matrix sign function of A or (A, I), we carry out the experiments for the generalized matrix sign function on both the pencil (A, I) and the equivalent pencil (R, Q^{H}) where $A = QR$ is a QR factorization. There are no noticeable differences between the two options.

Following the notation in [3] we use $\Delta(A)$ to denote the gap between the eigenvalues and the imaginary axis:

$$\Delta(A) = \min_{\lambda_j \in \lambda(A)} |Re(\lambda_j)|$$

The bigger the gap $\Delta(A)$ is, the faster (A_k, B_k) converges, cf. Section 5. To estimate the sensitivity of subspaces to perturbations in matrix pencils, we compute a lower bound of the quantity *dif* introduced by Stewart [23]:

$$\mathrm{dif}[(A_{11}, B_{11}), (A_{22}, B_{22})] \stackrel{\mathrm{def}}{=} \inf_{\max\{\|P\|_{\mathrm{F}}, \|Q\|_{\mathrm{F}}\}} \max\{\|QA_{11} + A_{22}P\|_{\mathrm{F}}, \|QB_{11} + B_{22}P\|_{\mathrm{F}}\}.$$

The lower bound we compute is the smallest singular value of the matrix operator T that maps (Q, P) to $(QA_{11} + A_{22}P, QB_{11} + B_{22}P)$, cf. [23].

Example 1. The matrix A is constructed as follows:

$$A = Q^{\mathrm{T}} \begin{pmatrix} F & S \\ G & -F^{\mathrm{T}} \end{pmatrix} Q$$

where

$$F = \begin{pmatrix} -\eta & 1 & 0 & 0 \\ -1 & -\eta & 0 & 0 \\ 0 & 0 & \eta & 1 \\ 0 & 0 & -1 & \eta \end{pmatrix}, \quad S = G = \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \end{pmatrix} \begin{pmatrix} 1 & 1 & 1 & 1 \end{pmatrix},$$

and Q is an orthogonal matrix obtained from the QR factorization of a random matrix. Notice that A is a real Hamiltonian matrix and hence has eigenvalues symmetric to, but not on, the imaginary axis and symmetric to the real axis. This type of matrices arise in a linear-quadratic optimal control problem [1,17]. For this particular example, there are four eigenvalues in a neighborhood of $\pm\eta^2 \pm i$. Table 1 lists the computed results with a few different values of η. As $\eta \to 0$ the eigenvalues at about $\pm\eta^2 \pm i$ approach two points $\pm i$ on the imaginary axis and the division along this axis becomes more difficult. Table 1 shows that all three algorithms behave about the same with the matrix in Example 1.

Example 2. The matrix is of Hamiltonian-like structure:

$$A = Q^{\mathrm{T}} \begin{pmatrix} A_{11} & A_{12} \\ 0 & A_{22} \end{pmatrix} Q$$

where

$$A_{11} = \begin{pmatrix} 1-\alpha & & & \alpha \\ \alpha & 1-\alpha & & \\ & \ddots & \ddots & \\ & & \alpha & 1-\alpha \end{pmatrix}, \quad A_{22} = -A_{11}^{\mathrm{T}} \,,$$

A_{12} is a $k \times k$ random matrix (not necessarily symmetric), and Q is an orthogonal matrix obtained from the QR factorization of a random matrix. The matrix A_{11} is a circulant matrix having the eigenvalues evenly distributed on a circle with center at $1-\alpha$ and radius α. The eigenvalues of A are therefore on two circles symmetric to the imaginary axis, the left and right circles are in the left and right half planes, respectively, for $\alpha \in (0, 0.5)$, cf. Figure 3. Table 2 lists two groups of experimental tests. In the first group, we let $\alpha \to 0.5$ so that the two circles get closer to each other toward the imaginary axis. Both $\Delta(A)$ and dif decrease at the same time. In the second group, we fix α at 0.45 and shift A so that $\Delta(A)$ gets smaller and dif remains the same. Algorithm MM-ABQR is better in both cases.

Example 3. The matrix is constructed as

$$A = Q^{\mathrm{T}} \begin{pmatrix} A_{11} & A_{12} \\ 0 & A_{22} \end{pmatrix} Q$$

where Q is an orthogonal matrix obtained from the QR factorization of a random matrix, A_{12} is a 5×5 random matrix, A_{11} is a random upper triangular matrix with positive diagonal entries scaled by a parameter d, and A_{22} is a random upper triangular matrix with its diagonal elements replaced by those of A_{11} with negative sign. As d gets smaller, dif decreases by orders but $\Delta(A)$ remains of the same order. Table 3 shows again the superior behavior of the one-sided algorithm to that of the two-sided algorithms.

Our experimental results confirm that the dominant factor for the number of iterations is $\Delta(A)$ and that the decoupling residual depends on how well converged the last matrix

$\varDelta(A) \approx \eta^2/2$	dif	iter	MM-INV	MM-GQR	M-ABQR
5.00 e-1	4.26 e-1	8	2.04 e-16	2.31 e-16	1.81 e-16
5.00 e-3	5.04 e-3	15	4.66 e-15	4.75 e-15	6.52 e-15
5.00 e-5	5.00 e-5	22	3.84 e-13	3.84 e-13	2.55 e-13
5.00 e-7	5.00 e-7	28	3.91 e-11	3.91 e-11	1.53 e-11

Table 1: Experimental Results with Example 1.

$\varDelta(A)$	dif	iter	MM-INV	MM-GQR	M-ABQR
10^{-1}	1.41 e-1	10	6.49 e-16	5.10 e-16	2.77 e-16
10^{-3}	1.41 e-3	17	6.77 e-14	3.58 e-14	5.32e-16
10^{-5}	1.41 e-5	23	5.71 e-11	4.56 e-12	3.28 e-15
10^{-7}	1.41 e-7	29	6.95 e-08	1.42 e-10	3.64 e-14
10^{-3}	1.41 e-1	16	2.59 e-15	1.03 e-15	2.90 e-16
10^{-5}	1.41 e-1	23	2.25 e-14	1.32 e-14	3.27 e-16
10^{-7}	1.41 e-1	30	1.62 e-13	1.42 e-13	3.00 e-16

Table 2: Experimental results with Example 2 ($k = 20$).

d	$\varDelta(A)$	dif	iter	MM-INV	MM-GQR	M-ABQR
1.0	2.43 e-1	2.56 e-2	9	1.63 e-15	7.42 e-16	4.58 e-16
0.5	1.21 e-1	2.19 e-3	10	1.61 e-14	2.67 e-15	5.08 e-16
0.3	7.20 e-2	2.33 e-4	11	1.34 e-13	3.67 e-14	7.05 e-16
0.2	4.86 e-2	2.46 e-5	11	1.41 e-11	1.31 e-12	4.50 e-15
0.1	2.43 e-2	1.23 e-7	12	6.57 e-10	6.57 e-10	4.83 e-14

Table 3: Experimental Results with Example 3.

pencil (A_∞, B_∞) (a premature stop of Malyshev's iteration would render a poor decoupling residual), and how accurately the deflating subspaces can be extracted from (A_∞, B_∞). In other words, the decoupling residual is affected by $\varDelta(A)$, dif, and the methods used. In the first set of experimental tests on random matrix pencils, the problems are well-conditioned in terms of $\varDelta(A)$ and dif, and all three algorithms behave well numerically. In the case that both $\varDelta(A)$ and dif are small, which we consider difficult, all three algorithms behave about the same in Example 1 but the one-sided algorithm performs better in Example 2. When $\varDelta(A)$ or dif is not too small and the other is small, the algorithm with one-sided iteration gives significantly better decoupling residuals, which seem affected only by the milder one of the two conditions $\varDelta(A)$ and dif. We shall mention that we observed from our experiments that $\|E_{21}\|_{\mathrm{F}}$ and $\|F_{21}\|_{\mathrm{F}}$ by the two-sided algorithms are not well balanced.

9 Concluding remarks

We have presented a framework of spectral division algorithms for block generalized Schur decompositions (1) with one-sided subspace iteration and an accurate subspace extraction scheme. In the case of employing inverse free subspace iteration, such as Malyshev's iteration, there is no inverse re-introduced in the subspace extraction step. The theory on decoupling a matrix pencil into two of smaller size with one known or computed deflating subspace is long established, see, for example, Stewart and J-G. Sun [26]. The same technique is used by Van Dooren [27] for computing reducing subspaces of singular pencils. Our contributions to the inverse free methods are mainly in the following aspects: 1) we use the subspace-preserving theory and subspace extraction techniques on the matrix pencil sequence (A_k, B_k) instead of computing or resorting to approximate spectral projectors $(A_k + B_k)^{-1}A_k$ or $(A_k + B_k)^{-1}B_k$, which involve inverse operations on possibly poorly-conditioned matrices; 2) we have removed the possible inconsistency with two-sided iteration methods [3] due to two independent iterations on (A_0, B_0) and $(A_0^{\mathrm{H}}, B_0^{\mathrm{H}})$; 3) we have eliminated the assumption that either A_k or B_k is nonsingular in the convergence proof of (A_k, B_k); 4) we provide an effective subspace extraction scheme that treats A_k and B_k symmetrically and allows us to save the left-sided subspace iterations. In our experimental tests our algorithm has shown consistently superior numerical behavior than its two-sided counterparts, except in some difficult cases, such as Example 1, where our algorithm behaves about the same as its counterparts. Thus, even in the case that only a right (or left) deflating subspace is of interest, our algorithm can be used, with relatively low extra cost, to obtain posterior estimates on computed quantities. Moreover, the ideas behind our approach are simple and can be straightforwardly applied to other spectral division methods, such as methods based on Newton iteration for the matrix sign function.

Inverse free spectral methods need further development to be more accurate, efficient and hence practical. Our algorithm has taken a step further in this direction.

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