Implicitly restarted Arnoldi with purification for the shift-invert transformation

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April 1995

Abstract

The need to determine a few eigenvalues of a large sparse generalised eigenvalue problem $Ax = \lambda Bx$ with semi-positive definite B arises in many physical situations, for example, in a stability analysis of the discretised Navier-Stokes equation. A common technique is to apply Arnoldi's method to the shift-invert transformation, but this can suffer from numerical instabilities as is illustrated by a numerical example. In this paper, a new method that avoids instabilities is presented which is based on applying the implicitly restarted Arnoldi method with the B semi-inner product and a purification step. The paper contains a rounding error analysis and ends with brief comments on some extensions.

Keywords : sparse generalised eigenvalue problems, shift-invert, semi-inner product, implicitly restarted Arnoldi.

AMS Subject Classification : 65F15, 65F50

1 Introduction

The problem of finding a few eigenvalues of large sparse $N \times N$ generalised eigenvalue problems of the form

$$Ax = \lambda Bx \ , \tag{1}$$

with A nonsymmetric and B symmetric semi-positive definite, arises in many applications. For example, the block structured eigenvalue problem

$$\begin{bmatrix} K & C \\ C^T & 0 \end{bmatrix} \begin{bmatrix} u \\ p \end{bmatrix} = \lambda \begin{bmatrix} M & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} u \\ p \end{bmatrix} , \tag{2}$$

with $N = n + m$, $C \in \mathbb{R}^{n\times m}$ of full rank, $M \in \mathbb{R}^{n\times n}$ positive definite appears in the stability analysis of steady state solutions of Stokes (K symmetric) and Navier-Stokes (K nonsymmetric) equations for incompressible flow, where $u \in \mathbb{C}^n$ denotes the velocity component and $p \in \mathbb{C}^m$ the pressure, see for example Cliffe, Garratt, and Spence [1]. Here M is the mass matrix of the velocity elements and K is nonsymmetric because of the linearisation of the convection term in the Navier-Stokes equations. As is well known, see Malkus [7], Ericsson [3] and Cliffe, Garratt, and Spence [2], (2) can have infinite eigenvalues, corresponding to eigenvectors of the form $[0^T, p^T]^T$. These have no physical relevance and in applications one would only be concerned about the calculation of a small number of 'stability determining' finite eigenvalues.

A common approach for finding a few eigenvalues of (1) close to a given $\alpha \in \mathbb{C}$ is Arnoldi's method applied to the shift-invert transformation $S = (A - \alpha B)^{-1}B$. If (λ, x) is an eigenpair of (1), then (θ, x) with $\theta = 1/(\lambda - \alpha)$ is an eigenpair of S, and this relation allows the solution of (1) by finding eigenpairs of S. Throughout the paper, we take $\alpha = 0$ and use

$$S = A^{-1}B \;, \tag{3}$$

since there is no loss of generality at least in theory by making the shift $A \leftarrow A - \alpha B$. In fact, in many applications, a zero shift is very common, since the stability determining eigenvalues often lie close to the origin, though in other situations the accurate determination of an appropriate α is a major challenge, which we do not discuss here (see for example Grimes, Lewis and Simon [5]).

To illustrate the influence of a singular B on S, consider first the following simple example. Let $n = 2$, $m = 1$ (so $N = 3$), denote the columns of I_3 by $e_i, i = 1, 2, 3$, and let

$$K = \begin{bmatrix} 1 & 0 \\ 0 & \beta \end{bmatrix} \quad , \quad C = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \quad , \quad M = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} ,$$

with $\beta \neq 0$. Then

$$S = \begin{bmatrix} 0 & 0 & 0 \\ 0 & \beta^{-1} & 0 \\ 1 & 0 & 0 \end{bmatrix} ,$$

and clearly (β^{-1}, e_2) is an eigenpair of S, 0 is a double algebraic, simple geometric eigenvalue, e_3 is the corresponding eigenvector and e is the generalised eigenvector or principal eigenvector of grade 2. This behaviour is generic in $N \times N$ problems with the block structure of (2) as was shown by Malkus [7], who considered the Weierstrass-Kronecker canonical form of (2), and Ericsson [3], who considered the Jordan form for the shift-invert transformation of a variety of generalised eigenvalue problems. (Incidently, both authors restrict attention to problems with symmetric A but several of their results, at least to do with Jordan structure, extend to the case when A is nonsymmetric). To summarise the important results on S, where A and B have the block structure of (2), we have the following theorem, which can be readily deduced from Theorem 2.7 in Ericsson [3] :

Theorem 1 *S defined by (2) and (3) has $n - m$ nonzero eigenvalues, a zero eigenvalue of algebraic multiplicity $2m$ and geometric multiplicity m. The order of the Jordan blocks corresponding to the defective eigenvalue 0 is two. Clearly, $\mathcal{N} := \mathrm{Null}(S) = \mathrm{Null(B)}$ has* *dimension* m, *and* $\mathcal{G} := \mathrm{Null}(S^2) \setminus \mathrm{Null}(S)$ *(the generalised nullspace) also has dimension* m. *If* $\mathcal{R} := \mathrm{Range}(S^2)$ *then* $\mathbb{C}^N$ *can be decomposed as*

$$\mathbb{C}^N = \mathcal{R} + \mathcal{N} + \mathcal{G} \ .$$

Note finally that $S\mathcal{G} = \mathcal{N}$ *and* $S^2\mathcal{G} = S\mathcal{N} = \{0\}$.

If B in (1) were nonsingular then Arnoldi's method applied to $A^{-1}B$ would be expected to find the required eigenvalues fairly easily. However, in the case we consider here with B singular, Arnoldi's method can find approximations to the zero eigenvalue of S, with consequent confusion after back transformation using $\lambda = \theta^{-1}$. These approximations are known as 'spurious' eigenvalues and are sometimes hard to distinguish from approximations to wanted eigenvalues. Several techniques have been proposed to reduce the risk of computing spurious eigenvalues for the symmetric non-defective problem [8, 3] and the defective problem [3]. In this paper we shall concentrate on the nonsymmetric defective case, as exemplified by S derived from (2), because of its importance in applications. In exact arithmetic, when Arnoldi's method is applied with the initial vector $v_1 \in \mathcal{R}$, then only approximations to the nonzero eigenvalues of S can be computed. Such an initial vector can be chosen as $v_1 = S^2 v$ with $v \in \mathbb{C}^N$ since $S^2(\mathcal{N} + \mathcal{G}) = \{0\}$. Unfortunately, in practice, round-off errors perturb the exact Arnoldi vectors producing components in $\mathcal{N} + \mathcal{G}$ with a consequent corruption of the approximate eigenvalues and eigenvectors, (we show an example of this in Section 3) and this paper is concerned with the efficient control of these round-off errors. For the symmetric problem, both Ericsson [3] and Nour-Omid, Parlett, Ericsson and Jensen [8] use Lanczos method with B-orthogonalisation, i.e. use the B semi-inner product $x^H By$ instead of the classical $x^H y$. The important point is that $A^{-1}B$ is self adjoint with respect to the B semi-inner product and hence the Lanczos method can be used to produce the usual tridiagonal matrix. An important numerical feature is that this tridiagonal Lanczos matrix is *not* corrupted by the perturbations of the Lanczos vectors in $\mathcal{N}$, but *is* corrupted by perturbations of the Lanczos vectors in $\mathcal{G}$. Hence the Ritz values of S can be spurious. This cannot occur in the case considered by Nour-Omid, Parlett, Ericsson and Jensen [8] but is discussed by Ericsson [3, Theorem 3.8]. For completeness, we prove this statement later in Section 2. The Ritz vectors are more severely affected, being corrupted by round-off errors in both the $\mathcal{N}$ and $\mathcal{G}$ subspaces, but Ericsson shows that these errors may be eliminated by *two* applications of S, though in practice only one is in fact needed by use of a clever trick, called 'purification' in [8], but also discussed in [4] and [3]. In fact, we find it convenient to use the expression 'purification' in a more general way, so that it refers to the general operation of forming Sx from $x \in \mathbb{C}^N$. This arises in several places in the paper, though not always in relation to elimination of round-off errors.

Throughout this paper, we use the terminology 'B-orthogonal Arnoldi' to refer to Arnoldi's method applied with the B (semi)-inner product (see Algorithm 1) in comparison with the 'standard Arnoldi' method, where the usual inner product is employed.

The main numerical aim of our paper is to introduce and analyse a new improved way of carrying out the two purification steps needed when S is formed from nonsymmetric problems with the block structure in (2). The new approach is based on the use of the implicitly restarted Arnoldi method (IRA) [11] combined with the B semi-inner product. This leads to an improvement over the approach in [3] on two counts. First, the

Arnoldi upper Hessenberg matrix H_k is not seriously corrupted by round-off errors due to components in either $\mathcal{N}$ or $\mathcal{G}$, whereas in [3] significant round-off errors H_k could be present due to components in $\mathcal{G}$. Second, only *one* purification step is needed rather than two in [3], since the Arnoldi vectors could contain significant error components in $\mathcal{N}$ but *not* in $\mathcal{G}$. One other feature of our analysis is that from a theoretical viewpoint, we are able to show an equivalence result between the B-orthogonal Arnoldi method applied to S and an M-orthogonal Arnoldi method applied to a reduced eigenvalue problem (see Section 2), which helps our understanding of the absence of corruption in H_k in the nondefective case and the presence of corruptions of H_k due to components in $\mathcal{G}$ in the defective case.

Throughout the paper, we consider Arnoldi's method for nonsymmetric problems, though if K in (2) were symmetric we would be able to employ the Lanczos method, with corresponding simplifications to the theory.

The plan of the paper is as follows. In Section 2, we make some theoretical observations, and give a theoretical explanation of the B-orthogonal Arnoldi method with purification. In Section 3, we illustrate by an example that this method can produce spurious results for defective problems. We present and analyse our method based on the implicitly restarted Arnoldi method with B inner product, followed by purification. In Section 4, we analyse the error propagation in $\mathcal{N}$ and $\mathcal{G}$. Section 5 concludes with some comments and extensions.

2 The B-orthogonal Arnoldi method : theory

In this section we make three main theoretical observations. First, motivated by the approach in [3] we derive in Section 2.1 a reduced eigenvalue problem in $\mathbb{C}^n$ rather than the full problem in $\mathbb{C}^{n+m}$ for the case where B has the block structure in (2). Second, in Section 2.2 we prove an equivalence result about the B-orthogonal Arnoldi method applied to the full problem and the M-orthogonal Arnoldi algorithm applied to the reduced problem. Third, in Section 2.3, we discuss the reduced eigenvalue problem for the special case where A has the block structure in (2).

2.1 The reduced eigenvalue problem

Using (3), the generalised eigenproblem (1) is transformed to the standard eigenvalue problem

$$Sx = \theta x \ , \ x \in \mathbb{C}^{n+m} \tag{4}$$

that can now be solved by Arnoldi's method. Following Ericsson [3], we first present a decomposition of S, when B has the blockstructure in (2). In this case, S has the structure

$$S = A^{-1} \begin{bmatrix} M & 0 \\ 0 & 0 \end{bmatrix} = \begin{bmatrix} S_1 & 0 \\ S_2 & 0 \end{bmatrix} \ , \ S_1 \in \mathbb{R}^{n \times n}, S_2 \in \mathbb{R}^{m \times n} \ ,$$

and this leads to a useful reduction to a problem in $\mathbb{C}^n$. Of course S_1 and S_2 depend on blocks in A^{-1} which are unlikely to be known or be helpful in a practical application, so this decomposition of S is only of theoretical interest. Let $x = \begin{pmatrix} u \\ p \end{pmatrix}$, $u \in \mathbb{C}^n$, $p \in \mathbb{C}^m$, be an eigenvector of S, and so

$$\begin{bmatrix} S_1 & 0 \\ S_2 & 0 \end{bmatrix} \begin{pmatrix} u \\ p \end{pmatrix} = \theta \begin{pmatrix} u \\ p \end{pmatrix}$$

is equivalent to

$$S_1 u = \theta u \quad \text{and} \quad S_2 u = \theta p \ . \tag{5}$$

If $\theta \neq 0$ (which is the case if λ is finite), then

$$p = \theta^{-1} S_2 u \tag{6}$$

is a 'slave' to u and so the reduced problem

$$S_1 u = \theta u \tag{7}$$

determines precisely the nonzero eigenvalues and corresponding eigenvectors of S. Hence, in theory, it is sufficient to solve the reduced problem to solve (4). From (5), it follows that the zero eigenvalue of S has eigenvectors of the form $(0^T, p^T)^T$, but these obviously play no role in (7). Note that, the theory in [3] which leads to Theorem 1 is derived from analysis of this decomposition of S.

2.2 The B-orthogonal Arnoldi method and the equivalence theorem

In most practical cases we use the B-orthogonal Arnoldi method in a direct attempt to solve (4), rather than try to solve the reduced problem, so we first write down the method in detail.

Algorithm 1 *The B-orthogonal Arnoldi*
Given v_1 with $v_1^H B v_1 = 1$.
for $i = 1$ **to** k **do**
  Compute $w_{i+1} = A^{-1} B v_i$.
  Form $h_{ji} = v_j^H B w_{i+1}$, $j = 1, \ldots, i$.
  Form $w_{i+1} = w_{i+1} - \sum_{j=1}^{i} v_j h_{ji}$.
  Compute $h_{i+1,i} = \|w_{i+1}\|_B = \sqrt{w_{i+1}^H B w_{i+1}}$.
  Let $v_{i+1} = w_{i+1}/h_{i+1,i}$.
end for
Let $H_k = [h_{ji}]$.
Compute the eigenpairs (θ_j, z_j) $j = 1, \ldots, k$ of H_k.
Compute the approximate eigenpairs (λ_j, x_j) of $Ax = \lambda B x$ with $\lambda_j = 1/\theta_j$ and $x_j = V_k z_j$.

The B-orthogonal Arnoldi algorithm is merely the standard Arnoldi algorithm with the usual inner product $x^H y$ replaced by the semi-inner product $x^H B y$. To be precise, the method computes a B-orthonormal basis $v_1, \ldots, v_{k+1}$ of the Krylov space

$$\mathcal{K}_{k+1}(v_1, S) = \text{span}\{v_1, S v_1, S^2 v_1, \ldots, S^k v_1\} \ ,$$

with the matrix $H_k = V_k^H BSV_k$ being upper Hessenberg, and $V_k^H BV_k = I$ with $V_k = [v_1, \ldots, v_k]$. It looks a little strange that a singular matrix is used to compute the inner product, but as we shall see later in this section, it is a natural thing to do for generalised problems of the form (2). The approximate eigenpairs of (θ, x) are computed from the eigenpairs of H_k in the usual way, see Algorithm 1. Similarly, one can use the M-orthogonal Arnoldi method to solve the reduced problem. As we now prove, there is a precise connection between the B-orthogonal Arnoldi method applied to S and the M-orthogonal Arnoldi method applied to S_1, which we now state.

Theorem 2 Equivalence Theorem
If k steps of M-orthogonal Arnoldi applied to S_1 starting with $y_1 \in \mathbb{C}^n$ produces an eigenpair (θ, u), then k steps of B-orthogonal Arnoldi applied to S starting with v_1, given by

$$v_1 = \begin{pmatrix} y_1 \\ q_1 \end{pmatrix} \tag{8}$$

with $q_1 \in \mathbb{C}^m$ arbitrary, produces an eigenpair (θ, x) with $x^T = (u^T, p^T)$.

Proof. In the B-orthogonal Arnoldi method, we have that

$$w_{l+1} = Sv_l - \sum_{j=1}^{l} h_{jl} v_j \ , \tag{9}$$

with $h_{jl} = v_j^H BSv_l$, $j = 1, \ldots, l$, $h_{l+1,l} = \|w_{l+1}\|_B$ and $v_{l+1} = w_{l=1}/h_{l+1,l}$, for $l = 1, \ldots, k$. In the M-orthogonal Arnoldi method, the relations are

$$s_{l+1} = S_1 y_l - \sum_{j=1}^{l} g_{jl} y_j \ , \tag{10}$$

with $g_{jl} = y_j^H MS_1 y_l$, $j = 1, \ldots, l$, $g_{l+1,l} = \|s_{l+1}\|_M$ and $y_{l+1} = s_{l+1}/g_{l+1,l}$, for $l = 1, \ldots, k$. First, we show that

$$h_{jl} = g_{jl} \quad \text{and} \quad v_j = \begin{bmatrix} y_j \\ q_j \end{bmatrix} \ , \ j = 1, \ldots, l+1 \tag{11}$$

for $l = 1, \ldots, k$ by induction on l. We first prove (11) under the assumption that it is valid for $l - 1$. From (11) for $l - 1$ and (9), it follows that

$$\begin{aligned} h_{jl} &= v_j^H BSv_l = [y_j^H \ p_j^H] \begin{bmatrix} M & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} S_1 & 0 \\ S_2 & 0 \end{bmatrix} \begin{bmatrix} y_l \\ q_l \end{bmatrix} \\ &= y_j^H MS_1 y_l = g_{jl} \ , \ j = 1, \ldots, l \ . \end{aligned} \tag{12}$$

Hence, using the block-structure of S and (10),

$$w_{l+1} = \begin{bmatrix} S_1 y_l - \sum_{j=1}^{l} g_{jl} y_l \\ S_2 y_l - \sum_{j=1}^{l} g_{jl} q_l \end{bmatrix} = \begin{pmatrix} s_{l+1} \\ q_{l+1}^* \end{pmatrix} \ , \tag{13}$$

and $h_{l+1,l} = \|w_{l+1}\|_B = \|s_{l+1}\|_M = g_{l+1,l}$. Thus $v_{l+1}^T = (y_{l+1}^T, q_{l+1}^T)$ with $q_{l+1} = q_{l+1}^*/g_{l+1,l}$. Using (8), (12) and (13), it is easy to see that (11) holds for $l = 1$, which completes the prove by induction. So, both Arnoldi processes compute the same upper Hessenberg matrix and thus the computed eigenpairs (θ, z) of this matrix are equal. In M-orthogonal Arnoldi on S_1, the computed eigenvector of S_1 is $u = [y_1, \ldots, y_k]z$, and in the B-orthogonal Arnoldi method on S,

$$x = \begin{bmatrix} y_1, \ldots, y_k \\ q_1, \ldots, q_k \end{bmatrix} z = \begin{bmatrix} u \\ p \end{bmatrix} ,$$

and the result is proved. □

The equivalence theorem shows that solving (4) with B-orthogonal Arnoldi and (7) with M-orthogonal Arnoldi for the initial vector chosen as in (8) compute the same eigenvalues. The u-component of x corresponds to the computed eigenvector of S_1. However, the p-component does not play a role in the B-orthogonal Arnoldi method and cannot be guaranteed to be correct. The correct p is obtained by the slave relation (6), so that if (θ, u) is an exact eigenpair of S_1, then, following (6), $(\theta, \begin{pmatrix} u \\ \theta^{-1} S_2 u \end{pmatrix})$ is an exact eigenpair of S. If $x = \begin{pmatrix} u \\ p \end{pmatrix}$ is computed by B-orthogonal Arnoldi, (6) should be computed explicitly. The practical way to do this is to apply S to x, since

$$Sx = \begin{bmatrix} S_1 & 0 \\ S_2 & 0 \end{bmatrix} \begin{pmatrix} u \\ p \end{pmatrix} = \begin{pmatrix} S_1 u \\ S_2 u \end{pmatrix} = \theta \begin{pmatrix} u \\ \theta^{-1} S_2 u \end{pmatrix}$$

is an eigenvector belonging to θ. In the B-orthogonal Arnoldi method, Sx can be computed without extra vector operations with S. The Arnoldi vectors namely satisfy the relation

$$SV_k = V_k H_k + h_{k+1,k} v_{k+1} e_k^H , \tag{14}$$

with e_k the k-th unit vector of length k. Hence

$$Sx = SV_k z = V_k H_k z + h_{k+1,k} v_{k+1} e_k^H z$$

and since z is an eigenvector of H_k,

$$SV_k z = \theta_j V_k z + h_{k+1,k} v_{k+1} e_k^H z . \tag{15}$$

This expression was used by Ericsson and Ruhe [4] as a means of improving accuracy in eigenvectors, but Nour-Omid, Parlett, Ericsson and Jensen [8] considered especially the case B singular and called the correction of $V_k z$ 'purification', because it has the potential for removing significant round-off error components in the $\mathcal{N}$ space. Since this is a rather important result for our method, we describe why this is so in Section 4.

Note that the B inner product is not affected by the portions of v_j in the nullspace of B, since for $x = (u^T, p^T)^T$ and $y = (v^T, q^T)^T$, $x^H B y = u^H M v$. Since B and S have the same nullspace, H_k is independent of components of V_k in the $\mathcal{N}$ space.

There is another way to explain the B-orthogonal Arnoldi method. Since B is semi positive-definite there exists a Cholesky like factorisation $B = P^T P$ with $P \in \mathbb{R}^{N \times N}$ singular. Nour-Omid, Parlett, Ericsson and Jensen [8] point out to an equivalence result between B-orthogonal Arnoldi applied to $A^{-1}B$ and standard Arnoldi applied to

$PA^{-1}P^T$. It appears that with appropriate initial vectors, the eigenvalues computed by both methods are equal and that one needs a purification step to find the eigenvectors of $A^{-1}B$ in the B-orthogonal Arnoldi method.

Finally, note that if S_1 is nonsingular, the B-orthogonal Arnoldi method applied to S would not be expected to compute approximations to the zero eigenvalue of S since the method is equivalent to M-orthogonal Arnoldi applied to S_1. This is essentially the case described in [8].

2.3 Application of B-orthogonal Arnoldi to the Navier-Stokes problem (2)

Now consider the problem with block structure (2) which provides the main motivation for this paper. From $S = A^{-1}B$ we have that

$$\begin{bmatrix} K & C \\ C^T & 0 \end{bmatrix} \begin{bmatrix} S_1 & 0 \\ S_2 & 0 \end{bmatrix} = \begin{bmatrix} M & 0 \\ 0 & 0 \end{bmatrix} ,$$

which yields $C^T S_1 = 0$. Also, since $C \in \mathbb{R}^{n\times m}$ is of full rank, $S_1 \in \mathbb{R}^{n\times n}$ has at least m independent left null vectors and so, $\mathrm{rank(S_1)} \leq \mathrm{n-m}$. Since A is nonsingular, $\mathrm{rank(S)} = \mathrm{rank(B)} = \mathrm{n}$. Since $S_2 \in \mathbb{R}^{m\times n}$, $\mathrm{rank(S_2)} \leq \mathrm{m}$, and, since $\mathrm{rank(S)} \leq \mathrm{rank(S_1)} + \mathrm{rank(S_2)}$,

$$\mathrm{rank(S_1)} \geq \mathrm{rank(S)} - \mathrm{rank(S_2)} \geq \mathrm{n-m}$$

so, $\mathrm{rank(S_1)} = \mathrm{n-m}$. Clearly, the nullspace of S_1, $\mathcal{N}_1$ say, has dimension m, and the range, $\mathcal{R}_1$ say, has dimension $n-m$. Note that for $u \in \mathcal{R}_1$, it can easily be shown that $C^T u = 0$ and this agrees with the second equation in (2).

We can now be more precise about the link between S_1 and S as follows. For u and x defined as $S_1 u = \theta u$ and $Sx = \theta x$,

$$u \in \mathcal{R}_1 \quad \Leftrightarrow \quad x = \begin{pmatrix} u \\ \theta^{-1} S_2 u \end{pmatrix} \in \mathcal{R} \tag{16}$$

and

$$u \in \mathcal{N}_1 \quad \Leftrightarrow \quad \begin{pmatrix} u \\ 0 \end{pmatrix} \in \mathcal{G} \ . \tag{17}$$

Equivalence (16) follows from (5) and (6), and (17) follows from the fact that

$$S \begin{pmatrix} u \\ 0 \end{pmatrix} = \begin{pmatrix} S_1 u \\ S_2 u \end{pmatrix} = \begin{pmatrix} 0 \\ S_2 u \end{pmatrix} \in \mathcal{N}$$

and thus

$$S^2 \begin{pmatrix} u \\ 0 \end{pmatrix} = \begin{pmatrix} S_1^2 u \\ S_2 S_1 u \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} .$$

Since S_1 has an eigenvalue zero, M-orthogonal Arnoldi (and B-orthogonal Arnoldi) may compute the zero eigenvalue in practice. Nevertheless, if $y_1 \in \mathcal{R}_1$,

$$\mathcal{K}_k(S_1, y_1) \subset \mathcal{R}_1$$

and so in exact arithmetic, the zero eigenvalue cannot be computed. $y_1 \in \mathcal{R}_1$ can be achieved by $y_1 \leftarrow S_1 y_1$. To apply B-orthogonal Arnoldi to S, one should start with v_1, given by (8). This is achieved by $v_1 \leftarrow S v_1$, since

$$Sv_1 = S \begin{pmatrix} y_1 \\ q_1 \end{pmatrix} = \begin{pmatrix} S_1 y_1 \\ S_2 y_1 \end{pmatrix} .$$

Note that then in exact arithmetic $\mathcal{K}_k(S, Sv_1) \subset \mathcal{R} + \mathcal{N}$. Of course, in practice, round-off errors cannot be avoided and in the following two sections we derive and analyse a new approach to mitigate the effect of round-off for this problem.

3 The B-orthogonal Arnoldi method : practice

In this section, we present and describe a new approach which significantly reduces the effects of errors in $\mathcal{G}$ and $\mathcal{N}$. The approach is based on a combination of the implicitly restarted Arnoldi method of Sorensen [11] with B-inner product and purification. However, before going into details we present a simple numerical example to show how round-off error can grow in the Arnoldi vectors and how spurious eigenvalues can be obtained even although care is taken with the starting vector. Results for both the B-orthogonal Arnoldi method with purification and standard Arnoldi are given.

3.1 Example

Consider the matrices A and B computed using the following Matlab code.

```
rand('seed',1); n=200; m=100;
C = [rand(m,m) ; zeros(n-m,m)];
K = rand(n);
A = [K C ; C' zeros(m,m)];
B = [eye(n,n) zeros(n,m) ; zeros(m,n+m)];
```

The rightmost eigenvalues of $Ax = \lambda Bx$ are 49.9129, 2.7017, $2.2521 \pm 1.4533i$ and 2.0517. To compute them we use $S = (A - 60B)^{-1}B$. We used $k = 20$ steps of the standard Arnoldi method (i.e. using the usual inner product $x^H y$ and no purification step) with initial vector

$$v_1 = S^2 [1 \cdots 1]^T \in \mathcal{R} .$$

(Note that in exact arithmetic the Arnoldi vectors would lie in $\mathcal{R}$ so that spurious eigenvalues should not be computed.) It is easy to check that for this example, S has the block form

$$S = \begin{bmatrix} 0 & 0 & 0 \\ 0 & S_{22} & 0 \\ S_{31} & S_{32} & 0 \end{bmatrix}$$

where $S_{22} \in \mathbb{R}^{n-m \times n-m}$ and $S_{31} \in \mathbb{R}^{m \times n}$ are nonsingular. Then

$$\mathcal{G} := \{ \begin{pmatrix} u \\ 0 \\ 0 \end{pmatrix} : u \in \mathbb{C}^m \} \ , \ \mathcal{N} := \{ \begin{pmatrix} 0 \\ 0 \\ p \end{pmatrix} : p \in \mathbb{C}^m \} \text{ and } \mathcal{R} := \{ \begin{pmatrix} 0 \\ u \\ S_{32} S_{22}^{-1} u \end{pmatrix} : \mathrm{u} \in \mathbb{C}^{\mathrm{n-m}} \} .$$

Table 1: Arnoldi's method applied to the example in Section 3.1

	Arnoldi		B-Arnoldi	
j	$\Vert P_{\mathcal{N}} \cdot \Vert_2$	$\Vert P_{\mathcal{G}} \cdot \Vert_2$	$\Vert P_{\mathcal{N}} \cdot \Vert_2$	$\Vert P_{\mathcal{G}} \cdot \Vert_2$
1	6.59e-13	4.86e-16	3.40e-11	2.50e-14
2	4.74e-10	1.45e-12	5.70e-10	5.88e-12
3	2.88e-08	4.22e-11	1.57e-08	1.26e-10
4	1.46e-06	1.38e-09	3.86e-07	2.52e-09
5	3.30e-05	2.30e-08	1.05e-05	5.79e-08
6	9.61e-04	5.33e-07	2.76e-04	1.32e-06
7	3.04e-02	1.40e-05	6.69e-03	2.81e-05
8	7.96e-02	3.19e-05	1.79e-01	6.72e-04
9	5.28e-03	2.70e-05	4.31e+00	1.46e-02
10	2.62e-02	4.84e-04	7.70e+01	2.38e-01
11	8.91e-03	6.97e-04	1.20e+02	3.27e-01
12	1.46e-02	6.36e-04	1.88e+02	3.03e-02
$\vdots$				
15	1.30e-02	6.52e-04	1.34e+04	3.15e-01
$\vdots$				
20	1.30e-02	6.52e-04	1.40e+04	3.29e-01
	$\lambda_1 = 60.0823 + 0.1292i$		$\lambda_1 = 60.0072 + 0.0228i$	
x_1	3.e-3	9.e-5	3.e-3	6.e-16

Hence, for any vector y, the size of $\mathcal{N}$ and $\mathcal{G}$ components can be measured by calculating $\|P_{\mathcal{N}}y\|_2$ and $\|P_{\mathcal{G}}y\|_2$ where

$$\begin{aligned} P_{\mathcal{N}} &= [0 \quad -S_{32}S_{22}^{-1} \quad I_m] \in \mathbb{R}^{m \times n+m} \\ P_{\mathcal{G}} &= [S_{31} \quad 0 \quad 0] \in \mathbb{R}^{m \times n+m} , \end{aligned}$$

though obviously replacing S_{31} by I_m would also be sufficient in $P_{\mathcal{G}}$. In practice we first normalise so that $\|P_{\mathcal{N}}\|_2 = \|P_{\mathcal{G}}\|_2 = 1$. One would expect that the eigenvalue 49.9 would be found in a few Arnoldi steps, since it is clearly much closer to α than any other eigenvalues. In fact, this is not the case, as the results in the first and second columns of Table 1 demonstrate. At the bottom of the table we give the computed rightmost eigenvalue of $Ax = \lambda Bx$, denoted λ_1, after 20 steps of standard Arnoldi. We see that λ_1 is rather far from 49.9. Also plotted are measures of the $\mathcal{N}$ and $\mathcal{G}$ components of x_1, the corresponding unpurified eigenvector, and these are also rather large.

The same problem was solved with the B-orthogonal Arnoldi method with purification. We see that λ_1 is a very poor approximation to 49.9. However, though $\|P_{\mathcal{N}}x_1\|$ is large, $\|P_{\mathcal{G}}x_1\|$ is small, since purification wipes out the $\mathcal{N}$ component in the unpurified form and maps the $\mathcal{G}$ component to $\mathcal{N}$. The practical effect of the purification step given by (15) in the presence of large error components in the Arnoldi vectors is striking (cf. Table 1 in [8]). We also show in Table 1 the measures $\|P_{\mathcal{N}}v_j\|_2$ and $\|P_{\mathcal{G}}v_j\|_2$ for the Arnoldi vectors. Recall that at the end of Section 2.3 it was shown that B-orthogonal Arnoldi in exact arithmetic should not compute spurious eigenvalues if $v_1, \ldots, v_{k+1} \in \mathcal{R} + \mathcal{N}$ and to achieve this, one should use B-orthogonal Arnoldi with starting vector Sv_1. (In fact, to obtain the numerical results we used the starting vector $S^2v_1 \in \mathcal{R}$, as recommended by Ericsson [3].)

Clearly, in this example, during the computation of $v_1, \ldots, v_{k+1}$, the Arnoldi vectors contain large components in $\mathcal{G}$ which then produce 'spurious' eigenvalues. We know this since all the finite eigenvalues of $Ax = \lambda Bx$ are known, and none lies to the right of α. Thus we can infer that S has no eigenvalues with positive real part. It has zero eigenvalues corresponding to vectors with components in $\mathcal{N}$ and $\mathcal{G}$. Round-off error introduces these components into the Arnoldi vectors and H_{20} has eigenvalues of positive real part which approximate zero. λ_1 arises from such an eigenvalue, and is thus spurious. In fact, in this example, we found no eigenvalue of H_{20} that is a reasonable approximation to 49.9.

3.2 A new approach

In order to present the details of our method, we need first to understand the steps of the implicitly restarted Arnoldi method by Sorensen [11], and to do this we present the following theorem, which is a compilation of results from [11], but is stated and proved here for completeness.

Theorem 3 *Let* $v_1, \ldots, v_{k+2}$, $\bar{H}_{k+1} = \begin{bmatrix} H_{k+1} \\ 0 \cdots 0 \; h_{k+2,k+1} \end{bmatrix}$ *be computed by* B*-orthogonal Arnoldi on* S*. Consider the* QR *factorisation* $\bar{H}_{k+1} = \bar{Q}_{k+1}R_{k+1}$ *with* $\bar{Q}_{k+1} \in \mathbb{C}^{k+2 \times k+1}$ *orthogonal and* $R_{k+1} \in \mathbb{C}^{k+1 \times k+1}$ *upper triangular. Let* $\bar{Q}_k$ *be the* $k+1 \times k$ *upper left part of* $\bar{Q}_{k+1}$ *and define*

$$W_{k+1} = V_{k+2}\bar{Q}_{k+1} \qquad \text{and} \qquad \mathrm{\bar{G}_k} = \mathrm{R_{k+1}\bar{Q}_k} \in \mathbb{C}^{\mathrm{k+1 \times k}} .$$

Then W_{k+1} and $\bar{G}_k$ have the following properties :

1. $W_{k+1}^H B W_{k+1} = I$.
2. $\mathrm{span}(\mathrm{w}_1, \ldots, \mathrm{w}_{\mathrm{k+1}}) = \mathrm{span}(\mathrm{Sv}_1, \ldots, \mathrm{Sv}_{\mathrm{k+1}})$.
3. *$\bar{G}_k$ is upper Hessenberg and for $W_{k+1} = [W_k \; w_{k+1}]$,*

$$SW_k = W_{k+1}\bar{G}_k$$

with $w_1 = Sv_1/\|Sv_1\|_B$.

Proof. (See also Sorensen [11]) The proof of statement 1 is easy and is omitted. $\bar{H}_{k+1}$ and V_{k+2} are computed from

$$\begin{aligned} SV_{k+1} &= V_{k+1}H_{k+1} + v_{k+2}h_{k+2,k+1}e_{k+1}^H \\ &= V_{k+2}\bar{H}_{k+1} \ , \end{aligned} \tag{18}$$

and replacing $\bar{H}_{k+1}$ by its QR factorisation, we obtain

$$SV_{k+1} = W_{k+1}R_{k+1} \ . \tag{19}$$

Since $\mathrm{rank}(\mathrm{R}_{\mathrm{k+1}}) = \mathrm{rank}(\bar{\mathrm{H}}_{\mathrm{k+1}}) = \mathrm{k} + 1$,

$$W_{k+1} = SV_{k+1}R_{k+1}^{-1} \tag{20}$$

which proves statement 2.

Let W_k be the first k columns of W_{k+1}, then $W_k = V_{k+1}\bar{Q}_k$. Multiply (19) on the right by $\bar{Q}_k$, then

$$SW_k = W_{k+1}\bar{G}_k$$

with $\bar{G}_k = R_{k+1}\bar{Q}_k$. It is well known (see Sorensen [11]) that if $\bar{H}_{k+1}$ is upper Hessenberg, $\bar{Q}_k$ and $\bar{Q}_{k+1}$ are upper Hessenberg too, and therefore $\bar{G}_k$ is upper Hessenberg. Since w_1 is the first column of (20),

$$w_1 = Sv_1r_{11}^{-1}$$

and since $\|w_1\|_B = 1$, $r_{11} = \|Sv_1\|_B$. □

In other words, the theorem says that W_{k+1} and $\bar{G}_k$ can be viewed as having been computed by the B-orthogonal Arnoldi method with starting vector $Sv_1/\|Sv_1\|_B$, which is exactly what we wish to do, but is accomplished implicitly by the QR-factorisation of $\bar{H}_{k+1}$.

In Algorithm 2 we write down the different steps that are needed to perform one implicit restart step. Our approach consists of three stages :

(1) the computation of V_{k+2},

(2) an implicit application of S to V_{k+1} (achieved by the QR step for $\bar{H}_{k+1}$), which has the effect of removing the $\mathcal{N}$ portion of V_{k+1} and mapping the $\mathcal{G}$ portion into $\mathcal{N}$,

(3) the purification of $W_k z$ that achieves the removal of the remaining $\mathcal{N}$ component (which is a second implicit application of S).

Table 2: Schematic representation of the flow of the error components in $\mathcal{N}$ and $\mathcal{G}$ by implicit application of S using first implicitly restarted B-orthogonal Arnoldi and then purification (Here the notation $V_{k+2}(\mathcal{N},\mathcal{G})$ means that V_{k+2} contains components in $\mathcal{N}$ and $\mathcal{G}$).

stage 1 (B-orthog. Arn.)	V_{k+2} ($\mathcal{N}$,$\mathcal{G}$)	$\bar{H}_{k+1}$ ($\mathcal{G}$)
implicit S :	$\Downarrow$ $\downarrow$ $\downarrow$	$\Downarrow$
stage 2 (implicit restart)	$W_{k+1}(\{0\},\mathcal{N})$	$\bar{G}_k$ ( )
implicit S :	$\Downarrow$ $\downarrow$	
stage 3 (purification)	x_j ($\{0\}$)	

Table 2 gives a schematic representation of the impact of these implicit applications of S on the $\mathcal{N}$ and $\mathcal{G}$ components of V_{k+2}, W_{k+1} and $W_k z$, and on the Arnoldi upper Hessenberg matrices $\bar{H}_{k+1}$ and $\bar{G}_k$. We assume that V_{k+2} has components in $\mathcal{N}$ and $\mathcal{G}$ which we represent by $V_{k+2}(\mathcal{N},\mathcal{G})$ and we trace the propagation of these components through the 3 stages of Algorithm 2. We see that $\bar{G}_k$ and the purified x_j do not depend on $\mathcal{N}$ and $\mathcal{G}$ components.

Algorithm 2 *Implicitly restarted B-orthogonal Arnoldi with purification*

Compute in $k+1$ steps of B-orthogonal Arnoldi the matrices V_{k+2} and $\bar{H}_{k+1}$.
Compute the QR factorisation $\bar{H}_{k+1} = Q_{k+1}R_{k+1}$.
Perform one restart : $W_{k+1} = V_{k+2}Q_{k+1}$, $\bar{G}_k = R_{k+1}Q_k$.
Let G_k be the $k \times k$ upper part of $\bar{G}_k$.
Compute the eigenpairs (θ_j, z_j), $j = 1, \ldots, k$ of G_k.
Compute the eigenpairs (λ_j, x_j) of $Ax = \lambda Bx$ as $\lambda_j = \theta_j^{-1}$
  and $x_j = \theta_j W_k z_j + g_{k+1,k} w_{k+1} e_k^H z_j$.

3.3 Example revisited

Recall Section 3.1. After 20 steps of the B-orthogonal Arnoldi method, we have $\|P_{\mathcal{N}}V_{21}\|_2 \simeq 4.\,10^4$ and $\|P_{\mathcal{G}}V_{21}\|_2 \simeq 1.\,10^0$. After one implicit restart, $\|P_{\mathcal{N}}W_{20}\|_2 \simeq 2.\,10^4$ and is essentially unchanged, but $\|P_{\mathcal{G}}W_{20}\|_2 \simeq 2.\,10^{-9}$. By the implicit operation with S, the $\mathcal{N}$ component of V_{k+2} is wiped out and the $\mathcal{G}$ component is mapped to the $\mathcal{N}$ component of W_{k+1}. Since $\|P_{\mathcal{G}}W_{20}\|_2$ is small, G_{19} is not seriously corrupted by components in $\mathcal{N}$ and $\mathcal{G}$. The eigenvalue of G_{19} closest to $\alpha = 60$ is $\lambda_1 = 49.9129$, which is indeed the sought eigenvalue with an accuracy of at least 6 digits. The purified eigenvector x_1 has $\|P_{\mathcal{N}}x_1\|_2 \simeq 3.\,10^{-11}$ and $\|P_{\mathcal{G}}x_1\|_2 \simeq 3.\,10^{-14}$. Even though, W_{k+1} does have small $\mathcal{G}$ components, G_k is not affected by components in $\mathcal{N}$ and $\mathcal{G}$, and the purified x_1 has small $\mathcal{N}$ and $\mathcal{G}$ portions in spite of large $\mathcal{N}$ and $\mathcal{G}$ components in V_{k+1}.

4 Rounding error analysis

It is clear that in exact arithmetic, the implicit restart and the purification operations implicitly perform multiplication by S. In this section we provide a detailed analysis of the effect of round-off error in several of the important operations when S satisfies Theorem 1. To be precise we shall discuss the following results :

(a) the $\mathcal{N}$ and $\mathcal{G}$ component in v_j may increase as j increases ;

(b) the purification operation (15) produces an approximate eigenvector with no $\mathcal{G}$ component but which may have a component in $\mathcal{N}$ arising from a $\mathcal{G}$ component in the unpurified vector.

(c) one implicit restart in B-orthogonal Arnoldi produces a $\bar{G}_k$ that is not corrupted by $\mathcal{N}$ or $\mathcal{G}$ components, and a W_{k+1} which has no $\mathcal{G}$ component.

The combination of the results in (b) and (c) produce the rounding error analysis for our proposed method (Algorithm 2), which we state as follows.

> *Rounding Error Conclusion for Algorithm 2 :*
> One implicit restart in B-orthogonal Arnoldi with purification using (15) produces a $\bar{G}_k$ uncorrupted by $\mathcal{G}$ or $\mathcal{N}$ components with the consequence that no spurious eigenvalues are found. In addition, the eigenvectors purified among (15) have no significant components in $\mathcal{N}$ and $\mathcal{G}$.

(Note that, as in all analyses of round-off error, statements like *removes the $\mathcal{N}$ components in the computed eigenvector* should really be interpreted as *removes the significant parts of round-off error in the $\mathcal{N}$ components in the computed eigenvector.*)

The numerical results in our examples agree with these statements, and we now proceed to justify them. We introduce the projectors $\mathcal{P}_\mathcal{R}$, $\mathcal{P}_\mathcal{N}$, and $\mathcal{P}_\mathcal{G}$ that map a vector into $\mathcal{R}$, $\mathcal{N}$, and $\mathcal{G}$ respectively, and so an arbitrary vector x can be decomposed uniquely as $x = \mathcal{P}_\mathcal{R}x + \mathcal{P}_\mathcal{N}x + \mathcal{P}_\mathcal{G}x$. Note that

$$\mathcal{P}_\mathcal{N}S = S\mathcal{P}_\mathcal{G} \qquad \text{and} \qquad \mathcal{P}_\mathcal{G}\mathrm{S} = 0 \ . \tag{21}$$

Recall from the end of Section 2.2 that with a proper implementation of the B inner product, x^HBy is unaffected by any $\mathcal{N}$ component in x and y.

Throughout this section, round-off errors are denoted by Greek characters.

Statement (a) is proved as follows (cf. analysis in [8]). The (computed) Arnoldi vector v_{j+1} satisfies the following relation, resulting from the Gram-Schmidt orthogonalisation of Sv_j :

$$h_{j+1,j}v_{j+1} = Sv_j - \sum_{i=1}^{j} h_{ij}v_i + \psi_j \tag{22}$$

and

$$h_{ij} = v_i^H BSv_j + \delta_{ij} \ , \ j = 1, \ldots, i+1 \ ,$$

where $\psi_j \in \mathbb{C}^N$ and $\delta_{ij} \in \mathbb{C}$ are typically small rounding errors arising from the matrix-vector multiply with S, the calculation of h_{ij} and the Gram-Schmidt orthogonalisation. To increase the stability of the orthogonalisation process, one often uses modified Gram-Schmidt with re-orthogonalisation [6] or even orthogonal transformations [12]. In block form, the equations are written as

$$V_{k+1}\bar{H}_k = SV_k + \Psi_{k+1} \ , \tag{23}$$

$$\bar{H}_k = V_{k+1}^H BSV_k + \Delta_k \ , \tag{24}$$

with $\|\Psi_{k+1}\|$ and $\|\Delta_k\|$ small compared to $\|SV_{k+1}\|$ and $\|\bar{H}_k\|$. The portion of v_{j+1} in $\mathcal{N}$ and $\mathcal{G}$ is found by applying the projectors $\mathcal{P}_\mathcal{N}$ and $\mathcal{P}_\mathcal{G}$ to (22) and using (21) :

$$\begin{aligned} h_{j+1,j}\mathcal{P}_\mathcal{N} v_{j+1} &= S\mathcal{P}_\mathcal{G} v_j - \sum_{i=1}^{j} h_{ij}\mathcal{P}_\mathcal{N} v_i + \mathcal{P}_\mathcal{N}\psi_j \ , \\ h_{j+1,j}\mathcal{P}_\mathcal{G} v_{j+1} &= \sum_{i=1}^{j} h_{ij}\mathcal{P}_\mathcal{G} v_i + \mathcal{P}_\mathcal{G}\psi_j \ . \end{aligned}$$

There is no reason to assume that $\|\mathcal{P}_\mathcal{N} v_{j+1}\|$ and $\|\mathcal{P}_\mathcal{G} v_{j+1}\|$ do not grow.

Statement (b) is proved as follows. The purified x_j computed by (15), satisfies

$$\begin{aligned} x_j &= \theta_j V_k z_j + h_{k+1,k} v_{k+1} e_k^H z_j + \pi_i' \\ &= V_k H_k z_j + h_{k+1,k} v_{k+1} e_k^H z_j + \pi_i \end{aligned} \tag{25}$$

with V_k, H_k and $h_{k+1,k}$ satisfying (23), and where π_i' and π_i are the round-off errors arising from the computation of (15), which is in general small. At first sight, it is not obvious why this form provides the necessary cancellation of spurious $\mathcal{G}$ components, but this is in fact easily shown : from (23), it follows that

$$SV_k z_j = V_k H_k z_j + h_{k+1,k} v_{k+1} e_k^H z_j - \Psi_k z_j \ , \tag{26}$$

and combining (25) and (26), we obtain $x_j = SV_k z_j + \xi_j$ with $\xi_j = \pi_j + \Psi_k z_i$ small. Hence, using (21),

$$\begin{aligned} \mathcal{P}_\mathcal{N} x_j &= \mathcal{P}_\mathcal{N} SV_k z_j + \mathcal{P}_\mathcal{N}\xi_j = S\mathcal{P}_\mathcal{G} V_k z_j + \mathcal{P}_\mathcal{N}\xi_j \\ \mathcal{P}_\mathcal{G} x_j &= \mathcal{P}_\mathcal{G} SV_k z_j + \mathcal{P}_\mathcal{G}\xi_j = \mathcal{P}_\mathcal{G}\xi_j \ . \end{aligned}$$

Observe that the $\mathcal{N}$ component in x_j arises from the $\mathcal{G}$ component in $V_k z_j$ and that the $\mathcal{N}$ component in $V_k z_j$ is wiped out.

Statement (c) follows by similar reasoning. Let the QR-factorisation of $\bar{H}_{k+1}$ (in finite arithmetic) be

$$\bar{H}_{k+1} = \bar{Q}_{k+1} R_{k+1} + \Omega_{k+1} \ , \tag{27}$$

with $\bar{Q}_{k+1} \in \mathbb{C}^{k+2 \times k+1}$, $R_{k+1} \in \mathbb{C}^{k+1 \times k+1}$ and

$$W_{k+1} = V_{k+2}\bar{Q}_{k+1} + \Pi_{k+1} \ , \tag{28}$$

where $\Omega_{k+1} \in \mathbb{C}^{k+2 \times k+1}$ and $\Pi_{k+1} \in \mathbb{C}^{N \times k+1}$ are of the order of machine precision. The extension of (23) is

$$SV_{k+1} = V_{k+2}\bar{H}_{k+1} - \Psi_{k+2}$$

and by applying (27) and (28) in that order,

$$\begin{aligned} SV_{k+1} &= V_{k+2}\bar{Q}_{k+1} R_{k+1} + V_{k+2}\Omega_{k+1} - \Psi_{k+2} \\ &= W_{k+1} R_{k+1} - \Pi_{k+1} R_{k+1} + V_{k+2}\Omega_{k+2} - \Psi_{k+2} \ , \end{aligned} \tag{29}$$

so

$$W_{k+1} = SV_{k+1} R_{k+1}^{-1} + \Xi_k$$

with $\Xi_k = \Pi_{k+1} - (V_{k+2}\Omega_{k+1} - \Psi_{k+2})R_{k+1}^{-1}$, which only consists of small terms. Thus, using (21),

$$\begin{array}{rclcrclcl} \mathcal{P}_{\mathcal{N}}W_{k+1} & = & \mathcal{P}_{\mathcal{N}}SV_{k+1}R_{k+1}^{-1} & + & \mathcal{P}_{\mathcal{N}}\Xi_k & = & S\mathcal{P}_{\mathcal{G}}V_{k+1}R_{k+1}^{-1} & + & \mathcal{P}_{\mathcal{N}}\Xi_k \\ \mathcal{P}_{\mathcal{G}}W_{k+1} & = & \mathcal{P}_{\mathcal{G}}SV_{k+1}R_{k+1}^{-1} & + & \mathcal{P}_{\mathcal{G}}\Xi_k & = & & & \mathcal{P}_{\mathcal{G}}\Xi_k \ . \end{array}$$

The analysis for $\bar{G}_k$ is given next. In the implicit restart step, $\bar{G}_k$ is computed (in finite precision arithmetic) as

$$\bar{G}_k = R_{k+1}\bar{Q}_k + \Sigma_k \ ,$$

with $\bar{Q}_k \in \mathbb{C}^{k+1\times k}$. By applying (27) and (24) in this order,

$$\begin{aligned} \bar{G}_k &= \bar{Q}_{k+1}^H \bar{H}_{k+1} Q_k - \bar{Q}_{k+1}^H \Omega_{k+1} + \Sigma_k \\ &= \bar{Q}_{k+1}^H V_{k+2}^H BSV_{k+1}\bar{Q}_k + \bar{Q}_{k+1}^H \Delta_{k+1}\bar{Q}_k - \bar{Q}_{k+1}^H \Omega_{k+1} + \Sigma_k \end{aligned}$$

The first term is dominant since the other terms are small rounding errors. From (29),

$$V_{k+2}\bar{Q}_{k+1} = SV_{k+1}R_{k+1}^{-1} - (V_{k+2}\Omega_{k+1} + \Psi_{k+2})R_{k+1}^{-1} \ ,$$

and so $V_{k+2}\bar{Q}_{k+1}$ has no significant component in $\mathcal{G}$ but still contains significant components in $\mathcal{N}$. This also shows that $SV_{k+1}\bar{Q}_k$ has no significant component in $\mathcal{N}$ or $\mathcal{G}$. The action of the B-inner product in the calculation of $(V_{k+2}\bar{Q}_{k+1})^H B(SV_{k+1}\bar{Q}_k)$ eliminates any contribution from the $\mathcal{N}$ component of $V_{k+2}\bar{Q}_{k+1}$. Hence $\bar{G}_k$ is free from significant errors in $\mathcal{N}$ and $\mathcal{G}$.

The final, and for this paper the most important, result concerns the round-off error in the implicitly restarted B-orthogonal Arnoldi method with purification (Algorithm 2), and is given by the 'Round-off Error Conclusion' at the beginning of this section. The proof consists of combining the arguments in (b) and (c) and is omitted.

5 Conclusions

We end this paper with a summary of the main points and some brief comments on related work.

The main conclusion to draw is that the Algorithm 2 which does two implicit multiplications by S, is less susceptible to round-off errors than the algorithm in Ericsson [3] for the shift-invert operator S derived from problems with block-structure (2). In fact, Algorithm 2 requires two fewer matrix-vector multiplications than the one in [3] (since Algorithm 2 needs no premultiplication of the initial vector v_1 by S^2) with the only (minor) addition of the QR-step for $\bar{H}_{k+1}$ and the formation of W_{k+1}.

On an aesthetic level, the purification approach of [8] using (15) rather than direct multiplication by S was very elegant. We think that the use of implicitly restarted Arnoldi to carry out implicitly a second multiplication by S is similarly pleasing.

Note that one could avoid the need for the purification step at stage 3 of Algorithm 2 by performing two steps of IRA. In fact, for *any* S which is singular with generalised null vectors of grade 2 we see that 2 steps of IRA with standard inner product will remove elements from $\mathcal{N}$ and $\mathcal{G}$. This can clearly be extended to cases where grade r generalised null vectors arise when r IRA steps would be required. If S arises from a generalised problem with B of the form (2) then one fewer IRA step is needed with the addition of a purification step.

It appears that the IRA method may help to stabilise calculations of eigenvalues (which is a known property of this method). The analysis here, where S is singular and defective helps to illustrate why this might be the case since there is an implicit subspace iteration step (see statement 2 in Theorem 3), which is another nice feature of this method. In fact, Philippe and Sadkane [9] use a few steps of subspace iteration in an explicit way to purify the Arnoldi vectors in an application coming from Maxwell's equations.

The theoretical analysis of iterative methods for the reduced problem $S_1 u = \theta u$ helps in an understanding of the performance of iterative methods for $Sx = \theta x$. The fact that implicitly restarted B-orthogonal Arnoldi applied to S works could, following the analysis in Section 2.2, also be explained by analysing the implicitly restarted M-orthogonal Arnoldi method applied to S_1, since one implicit matrix vector multiplication by S_1 maps the initial vector into $\mathcal{R}_1$.

Finally note that the B-inner product has been used in subspace iteration by Scott [10]. Ericsson [3] and Nour-Omid, Parlett, Ericsson and Jensen [8] mention that it is also a useful tool when B is non singular, but very ill conditioned.

6 Acknowledgements

The authors are grateful to the British Council and the Belgian National Fund for Scientific Research (NFWO) for supporting the collaboration between the Katholieke Universiteit Leuven and the University of Bath.

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