On the Equivalence of Certain Transformations of Block Matrices under Arnoldi's method

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Abstract

This paper is concerned with the relationship between the eigenvalues computed by a generalisation of the standard Arnoldi's method applied to certain preconditionings of the eigenvalue problem $Aw = \mu Bw$, where B is symmetric positive semidefinite. The matrices in the eigenvalue problem have a special block structure which arises after a mixed Finite Element Method discretization of the Navier-Stokes equations. Among the preconditionings considered are a Cayley Transform, a Modified Cayley Transform and a Shift-Invert Transform. The generalised Arnoldi method is similar to a generalisation of the Lanczos Algorithm presented by Nour-Omid et. al. (Maths Comp, 48, 1987 pp663-673). We prove that there is an exact relationship between the approximate eigenvalues computed when this generalised Arnoldi method is applied to the related transformations. The practical implications of these theoretical results are discussed briefly.

Keywords: Block matrices, spectral transformations, Arnoldi's method
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1 Introduction

In a previous paper in this journal, Cliffe, Garratt and Spence [2] discuss the numerical computation of the "leftmost" eigenvalues of the generalised eigenvalue problem

$$Aw = \mu Bw \tag{1}$$

where A and B are real $N \times N$ matrices, $w \in \mathbb{R}^N$, with the following block structure,

$$A = \begin{bmatrix} K & C \\ C^T & 0 \end{bmatrix}, \quad B = \begin{bmatrix} M & 0 \\ 0 & 0 \end{bmatrix}, \quad w = \begin{bmatrix} u \\ p \end{bmatrix}. \tag{2}$$

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Here $N = n+m,\ n > m,\ K$ is $n\times n$ non-symmetric, C is $n\times m$ of rank m, M is $n\times n$ symmetric positive definite, $u \in \mathbb{R}^n$ and $p \in \mathbb{R}^m$. As described in [2], matrices with this block structure arise after a mixed finite element discretization of incompressible fluid flow problems and of particular interest in [2] is the case when the leftmost eigenvalues are complex. In applications N is often large ($N > 2\times 10^5$ in [5]) and so iterative methods like Arnoldi's method [8] are used, since direct methods like the QZ algorithm [4] are out of the question.

The idea discussed in [2] is to apply Arnoldi's method to transformations, or preconditioners, of the original eigenvalue problem, with the transformations chosen so that the leftmost eigenvalues of (1) are mapped to dominant eigenvalues of the new eigenvalue problems. Specifically two transformations in [2] were "The Cayley Transform" ($\alpha_1, \alpha_2 \in \mathbb{R}$)

$$T_{\mathrm{C}} := \begin{bmatrix} K-\alpha_1 M & C \\ C^T & 0 \end{bmatrix}^{-1} \begin{bmatrix} K-\alpha_2 M & C \\ C^T & 0 \end{bmatrix} \tag{3}$$

and "The Modified Cayley Transform" ($\alpha_1, \alpha_3, \alpha_3 \in \mathbb{R}$)

$$T_{\mathrm{MC}} := \begin{bmatrix} K-\alpha_1 M & C \\ C^T & 0 \end{bmatrix}^{-1} \begin{bmatrix} K-\alpha_2 M & \alpha_3 C \\ \alpha_3 C^T & 0 \end{bmatrix} \tag{4}$$

Closely related, but not discussed in [2], is the "Shift-Invert Transformation" of (1), namely $(A-\alpha_1 B)^{-1}B$ $(\alpha_1 \in \mathbb{R})$, which in block form is

$$T_{\mathrm{SI}} := \begin{bmatrix} K-\alpha_1 M & C \\ C^T & 0 \end{bmatrix}^{-1} \begin{bmatrix} M & 0 \\ 0 & 0 \end{bmatrix}. \tag{5}$$

In each case it is assumed that α_1 is not an eigenvalue of (1), (2). Thus, if μ is a finite eigenvalue of (1) then T_{C} and T_{MC} have an eigenvalue $(\mu-\alpha_2)(\mu-\alpha_1)^{-1}$ (Theorem 13 of [2]) and T_{SI} has an eigenvalue $(\mu-\alpha_1)^{-1}$.

A second style of transformation was introduced in Section 3 of [2], namely

$$T_1 := \begin{bmatrix} M & C \\ C^T & 0 \end{bmatrix}^{-1} \begin{bmatrix} K & 0 \\ 0 & 0 \end{bmatrix} \tag{6}$$

From Theorem 12 of [2], it is known that the finite eigenvalues of (1) are eigenvalues of T_1, and, additionally, T_1 has a zero eigenvalue of multiplicity $2m$. A shift transformation

$$T_2 := \begin{bmatrix} M & C \\ C^T & 0 \end{bmatrix}^{-1} \begin{bmatrix} K-\gamma M & 0 \\ 0 & 0 \end{bmatrix}, \quad \gamma \in \mathbb{R}, \tag{7}$$

was introduced in Section 3.2 of [2], and a generalisation of T_2 (see [1]) is

$$T_3 := \begin{bmatrix} M & C \\ C^T & 0 \end{bmatrix}^{-1} \begin{bmatrix} K-\gamma M & \delta_1 C \\ \delta_1 C^T & 0 \end{bmatrix}, \quad \gamma, \delta_1 \in \mathbb{R}. \tag{8}$$

If μ is a finite eigenvalue of (1) then T_2 and T_3 have an eigenvalue $\mu - \gamma$ (Theorem 3.1 of [1]). The δ_1 in (8) is used to shift the zero eigenvalue of T_1. In [2], the hybrid Chebyshev-Arnoldi algorithm [8] was applied to T_2 to find the leftmost eigenvalues of (1).

Eigenvalue problems of the form (1) and (2) are intimately related to problems with constraints. If K is symmetric then (1), (2) is equivalent to the problem [3]:

Find the extrema of $u^T K u$, subject to $u^T M u = 1$ and $C^T u = 0$.

(In (1), (2), $p \in \mathbb{R}^m$ provides the Lagrange multipliers corresponding to the m constraints $C^T u = 0$.) This connection indicates that a natural setting for the eigenvalue problem (1), (2) is the subspace

$$\mathcal{C}^\perp := \left\{ w = \begin{bmatrix} u \\ p \end{bmatrix} \in \mathbb{C}^N \ : \ C^T u = 0 \right\}. \tag{9}$$

Continuing with the assumption that K is symmetric for the moment, we note that even though the shift-invert matrix $T_{\mathrm{SI}} = (A - \alpha_1 B)^{-1} B$ is not symmetric, it is self adjoint with respect to the semi-inner product induced by B, namely

$$< x, y >_B := < Bx, y >, \quad x, y \in \mathbb{C}^N, \tag{10}$$

where $< x, y >$ denotes the usual inner product $y^H x$. This fact is used in [6], along with the requirement to work in Range(T_{SI}), to develop a Generalised Lanczos algorithm based on using $< \cdot, \cdot >_B$ rather than $< \cdot, \cdot >$. For problems with the block structure (2) we note that $w = \begin{bmatrix} u \\ p \end{bmatrix} \in$ Range(T_{SI}) if and only if $C^T u = 0$. Also $< w, w >_B = 1$ if and only if $u^H M u = 1$, and so the use of the semi-inner product in the Lanczos method is natural in view of the normalisation in the optimization problem quoted above.

The main point of this paper is to make the observation that if a Generalised Arnoldi method, based on restriction to $\mathcal{C}^\perp$ and the use of a B-semi-inner product as in [6], is used as an iterative eigenvalue solver, then the three transformations (3), (4) and (5) of the nonsymmetric eigenvalue problem (1) are equivalent in a sense to be made precise in Sections 2 and 3. This result is stated formally in Theorem 1. Similar reasoning shows the equivalence of (6), (7) and (8) which is stated in Theorem 2.

2 The Cayley and Shift-Invert Transformations

Consider Arnoldi's method with l steps and starting vector v_1 ([8],p172) applied to the matrix eigenvalue problem A. Let $\lambda_i^{(l)}, \quad i = 1, \ldots, l$, denote the approximate eigenvalues of A obtained from Arnoldi. Consider also Arnoldi's method with l steps and starting vector v_1 applied to the linear transformation $\alpha I + \beta A$. The following Lemma is easily proved by induction and is a consequence of the linear invariance property of the Krylov subspace ([7],p238).

LEMMA 1 *"Equivalence of A and $\alpha I + \beta A$". Let $\theta_i^{(l)}$, $i = 1, \dots, l$, denote the approximate eigenvalues of A obtained using Arnoldi's method ([8],p172) with starting vector v_1. Then the approximate eigenvalues of $\alpha I + \beta A$ $(\alpha, \beta \in \mathbb{R})$ obtained using Arnoldi's method with starting vector v_1 are $\alpha + \beta\theta_i^{(l)}$, $i = 1, \dots, l$.*

The implication of this result is that if Arnoldi's method is used to find eigenvalues of A then there is no gain in attempting to improve the rate of convergence by applying Arnoldi's method to a linear transformation of A. This is in contrast to the situation when simultaneous iteration is used, where such linear shifts are often used to accelerate convergence ([9],p572).

An immediate Corollary is the equivalence of T_{C} and T_{SI}.

COROLLARY 1 *Assume that α_1 is not an eigenvalue of (1),(2), and that the same α_1 is used in (3), and (5). Then T_{C} and T_{SI} are equivalent in the sense of Lemma 1*

Proof $T_{\mathrm{C}} = I + (\alpha_1 - \alpha_2)T_{\mathrm{SI}}$. $\square$

The practical implication of Corollary 1 is that if Arnoldi's method is the chosen numerical method, then T_{SI} is to be preferred over T_{C} since there is no need to introduce the second parameter α_2. Indeed, if $\theta_i^{(l)}$ denotes the eigenvalues obtained by Arnoldi's method applied to T_{SI}, then the corresponding approximate eigenvalues of (1), denoted by $\mu_i^{(l)}$, are given by

$$\mu_i^{(l)} = \alpha_1 + 1/\theta_i^{(l)}. \tag{11}$$

It is easy to verify that precisely the same expression is obtained after applying Arnoldi's method to the transformation T_{C} and then back transforming to find eigenvalues of (1).

3 The Generalised Arnoldi algorithm and the equivalence results

We now introduce a generalised Arnoldi algorithm in the spirit of the generalised Lanczos method of [6]. There are two modifications from Algorithm 6.1 in [8]. First, we replace the usual inner product $< \cdot, \cdot >$ by the semi-inner product $< \cdot, \cdot >_B$ defined by (10) with B given in (2). Correspondingly $\| w \|_2$ is replaced by $\| w \|_B := \sqrt{< w, w >_B} = < Bw, w >^{\frac{1}{2}}$, and hence in the notation of (2), $\| w \|_B = u^H M u$. Second, we restrict attention to $\mathcal{C}^\perp$, the subspace of $\mathbb{C}^N$ defined by (9). For completeness the algorithm is as follows (cf [8],p172)

ALGORITHM 1 *Generalised Arnoldi with l steps.*

For $A : \mathcal{C}^\perp \to \mathcal{C}^\perp$ with $\mathcal{C}^\perp$ defined by (9) and $< \cdot, \cdot >_B$ defined by (10).

A Start: *Choose a vector $v_1 \in \mathcal{C}^\perp$ with $< v_1, v_1 >_B = 1$*

B Eigenvalue computation:
1. Iterate. For $j = 1, 2, \dots, l$ compute:

$$\begin{aligned} h_{i,j} &= < Av_j, v_i >_B, \quad i = 1, 2, \dots, j \\ w_j &= Av_j - \sum_{i=1}^{j} h_{i,j} v_i \\ h_{j+1,j} &= \sqrt{< w_j, w_j >_B} \\ v_{j+1} &= w_j / h_{j+1,j} \end{aligned}$$

2. Compute the eigenvalues, $\theta_i^{(l)}$, $i = 1, \dots, l$, of the upper Hessenberg matrix $H_l = (h_{i,j})$, $i, j = 1, \dots, l$.

The following straightforward Lemma provides the key to the equivalence results below.

LEMMA 2 *Let A and D be $N \times N$ matrices satisfying*
a) $A, D : \mathcal{C}^\perp \to \mathcal{C}^\perp$,
b) $< Dx, y >_B = 0 \quad \forall x, y \in \mathcal{C}^\perp$.
Let H_l denote the $l \times l$ upper Hessenberg matrix derived by Algorithm 1 applied to A with starting vector $v_1 \in \mathcal{C}^\perp$. Then Algorithm 1 applied to $A + \beta D \quad (\beta \in \mathbb{R})$ with the same starting vector produces the same upper Hesenberg matrix H_l. Hence the algorithm applied to A and $A + \beta D$ produces the same approximate eigenvalues.

Proof The proof consists of working through the steps of Algorithm 1. The calculation of all the $h_{i,j}$, the elements of the upper Hessenberg matrix for $A + \beta D$ involves an operation with $< \cdot, \cdot >_B$ and hence from *b)* above, the contribution from the βD term is zero. Note however that the bases for the corresponding Krylov subspaces are not identical for $l > 1$. $\Box$

It is easily verified that the transformations given by (3)-(8) all satisfy condition a), and that two examples of matrices satisfying the conditions on D in Lemma 3 are:

$$a) \; D_1 := \begin{bmatrix} K - \alpha_1 M & C \\ C^T & 0 \end{bmatrix}^{-1} \begin{bmatrix} 0 & C \\ C^T & 0 \end{bmatrix}, \quad b) \; D_2 := \begin{bmatrix} M & C \\ C^T & 0 \end{bmatrix}^{-1} \begin{bmatrix} 0 & C \\ C^T & 0 \end{bmatrix}. \tag{12}$$

Lemma 2 provides the following corollary.

COROLLARY 2 *Assume that α_1 is not an eigenvalue of (1), (2), and that the same α_1 is used in (3), (4). Then Algorithm 1 applied to T_{C} and T_{MC} produces the same eigenvalues.*

Proof $T_{\mathrm{MC}} = T_{\mathrm{C}} + (\alpha_3 - 1)D_1$ with D_1 given by (12a). $\square$

Corollary 1 and Corollary 2 combine to provide the main result of this paper on the equivalence of the three spectral transformations (3),(4) and (5).

THEOREM 1 *Assume that α_1 is not an eigenvalue of (1),(2) and that the same α_1 is used in (3),(4) and (5). Let $\theta_i^{(l)}$, $i = 1, \ldots, l$, denote the eigenvalues of T_{SI} obtained from Algorithm 1 (the Generalised Arnoldi Algorithm), then Algorithm 1 applied to T_{C} and T_{MC} produces the eigenvalues $1 + (\alpha_1 - \alpha_2)\theta_i^{(l)}$, $i = 1, \ldots, l$.*

An alternative statement of Theorem 1 is that using Algorithm 1, T_{SI}, T_{C} and T_{MC} are equivalent in the sense of Lemma 1. The practical implication is that if Algorithm 1 is to be used in a scheme to find the leftmost eigenvalues of (1),(2) then there is no gain in using T_{C} or T_{MC} over T_{SI}. Indeed T_{SI} is to preferred since (i) there is only one parameter to be found, namely α_1, and (ii) it is probably the quickest in terms of operation counts because of the simple form of the right hand side matrix in (5).

The corresponding result for the transformations (6),(7) and (8) follows in a similar manner by noting that

$$T_1 = T_2 + \gamma I - \gamma D_2$$

and

$$T_1 = T_3 + \gamma I - (\delta_1 + \gamma) D_2$$

with D_2 given by (12b). For completeness we state

THEOREM 2 *Let $\theta_i^{(l)}$, $i = 1, \ldots, l$ denote the eigenvalues of T_1 obtained from Algorithm 1. Then Algorithm 1 applied to T_2 and T_3 produces the eigenvalues $\theta_i^{(l)} - \gamma$, $i = 1, \ldots, l$.*

Note that Algorithm 1 stops when $h_{j+1,j} = 0$. This can occur for two reasons. First, if $w_j = 0$, then $\mathrm{span}\{v_1, \ldots, v_j\}$ is an invariant subspace and the eigenvalues of H_l are eigenvalues of A. Once these eigenvalues are found the algorithm can be restarted with a new starting vector orthogonal to the invariant subspace. Second, if $w_j \neq 0$, but $< w_j, w_j >_B = 0$, then $u_j^H M u_j = 0$ and w_j has the form $\begin{bmatrix} 0 \\ p_j \end{bmatrix}$, which cannot correspond to an eigenvector of a finite eigenvalue of (1),(2) (or any corresponding transformed eigenvalue of (3) - (8)). Thus the algorithm stops before any unwanted vectors are introduced.

We also mention that (10) is not the only semi-inner product for which the above theory holds. Let L be any $n \times n$ symmetric positive definite matrix and define the $N \times N$ matrix $\hat{B}$ by $\hat{B} := \begin{bmatrix} L & 0 \\ 0 & 0 \end{bmatrix}$. Now define a new semi-inner product

$$< x, y >_{\hat{B}} := < \hat{B}x, y > = u^H L v \tag{13}$$

where $x = \begin{bmatrix} u \\ p \end{bmatrix}$, $y = \begin{bmatrix} v \\ q \end{bmatrix}$. If $< \cdot, \cdot >_B$ is replaced by $< \cdot, \cdot >_{\hat{B}}$ in Algorithm 1 then it is straightforward to show that property *b*) in Lemma 2 holds for D_1 and D_2 defined by (12) and the above theory goes through. For completeness we state:

THEOREM 3 *If the semi-inner product (13) is used instead of (10) in Algorithm 1 then the conclusions of Theorem 1 and Theorem 2 remain true.*

The choice $L = I_n$ leads to $< x, y >_{\hat{B}} := u^T v$ and it is clear that Algorithm 1 reduces to an Arnoldi method which ignores the pressure components (i.e. the last m components) when computing all inner products.

Finally we note that similar results apply to the following generalisation of (1):

$$\begin{bmatrix} K & C_1 \\ C_2^T & 0 \end{bmatrix} \begin{bmatrix} u \\ p \end{bmatrix} = \mu \begin{bmatrix} M & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} u \\ p \end{bmatrix} \tag{14}$$

where C_1 and C_2 are $n \times m$ matrices of rank m with $C_2^T C_1$ invertible (see (2.7) of [1]). T_{SI}, T_{C} and T_{MC} are defined in an obvious way. The definition of $\mathcal{C}^\perp$ is modified to

$$\mathcal{C}^\perp := \left\{ w = \begin{bmatrix} u \\ p \end{bmatrix} \in \mathbb{C}^N \ : \ C_2^T u = 0 \right\}, \tag{15}$$

but otherwise Theorems 1,2 and 3 remain unchanged.

Numerical results on several examples confirm the equivalence theory described above and are not repeated here.

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