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# A MODIFIED CAYLEY TRANSFORM FOR THE DISCRETIZED NAVIER-STOKES EQUATIONS

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*Summary.* This paper is concerned with the problem of computing a small number of eigenvalues of large sparse generalized eigenvalue problems. The matrices arise from mixed finite element discretizations of time dependent equations modelling viscous incompressible flow. The eigenvalues of importance are those with smallest real part and are used to determine the linearized stability of steady states, and could be used in a scheme to detect Hopf bifurcations. We introduce a modified Cayley transform of the generalized eigenvalue problem which overcomes a drawback of the usual Cayley transform applied to such problems. Standard iterative methods are then applied to the transformed eigenvalue problem. Numerical experiments are performed on large matrices arising from a discretization of the flow over a backward facing step.

*Keywords*: block matrices, eigenvalues, Cayley transform, Navier-Stokes.

*AMS classification*: 15A18, 65F15, 65F50, 76M10

## 1. INTRODUCTION

Let $A$ and $B$ be $N \times N$ real large matrices with the following block structure

$$A = \begin{bmatrix} K & C \\ C^T & 0 \end{bmatrix}, \quad B = \begin{bmatrix} M & 0 \\ 0 & 0 \end{bmatrix}, \tag{1.1}$$

with $K$ $n \times n$ sparse *nonsymmetric*, $C$ $n \times m$ sparse of rank $m$, $M$ $n \times n$ sparse symmetric and positive definite, $n > m$, and $N = n+m$. We consider the generalized eigenvalue problem

$$A\omega = \mu B\omega \tag{1.2}$$

and assume that the eigenvalues $\mu_i$ (i.e. the finite values $\mu_i \in \mathbf{C}$ such that $\det(A - \mu_i B) = 0$) are ordered by increasing real part, i.e. $i < j \implies \mathrm{Re}(\mu_i) \leqslant \mathrm{Re}(\mu_j)$. This paper is concerned with *the derivation and analysis of an iterative method for the calculation of the eigenvalues of* (1.2) *of smallest real part.* In our applications we are mainly concerned with the case where $\mu_1$ is complex, thus $\mu_2 = \bar{\mu}_1$, and so there are

(at least) two eigenvalues of smallest real part. Note that since (1.2) is a large sparse problem, standard software such as the QZ algorithm [8] will be at best inefficient or almost certainly not be feasible. Matrices of this type, with $n \approx 2m$, arise in mixed finite element methods for time dependent 2-D Navier-Stokes equations modelling viscous incompressible flow. Briefly, such discretizations produce nonlinear finite dimensional systems of the form

$$M\dot{x}_1 + H(x_1, \lambda)x_1 + Lx_1 + Cx_2 = b_1, \quad C^T x_1 = b_2 \tag{1.3}$$

where $x_1, b_1 \in \mathbf{R}^n$, $x_2, b_2 \in \mathbf{R}^m$ and $\lambda \in \mathbf{R}$ is a parameter, say Reynolds number or Rayleigh number. Here $M$ is a mass matrix. The study of the linearised stability of a steady state, $(x_1^0, x_2^0, \lambda^0)$ say, gives rise to the generalized eigenvalue problem (1.2) where $K = H(x_1^0, \lambda^0) + H_x(x_1^0, \lambda^0)x_1^0 + L$ and a steady state is *stable* if all eigenvalues of (1.2) lie in the *positive* half plane. Clearly if the eigenvalue(s) of smallest real part are known then the linearised stability of the steady state is known.

Our motivation is the design and analysis of algorithms for the detection of Hopf bifurcations which occur when complex conjugate pairs of eigenvalues of (1.2) cross the imaginary axis. An obvious idea is to calculate the eigenvalue(s) of (1.2) of smallest real part corresponding to the steady states as $\lambda$ varies and note the occurrence of a sign change in the real part of a complex conjugate pair. In applications the eigenvalues of interest are often called the "dangerous" eigenvalues and we shall use this nomenclature here. In this short paper we shall restrict attention to discussion of an algorithm to compute the dangerous eigenvalue of (1.2), and hence will determine the stability of the corresponding steady solution of (1.3), but shall not discuss its implementation in a routine to detect Hopf bifurcations. For more details of the problem and the techniques used here we refer the reader to [3], [6].

To help focus the discussion in the following sections we shall assume that the eigenvalues of the generalized eigenvalue problem (1.2) satisfy the following condition:

(P) Equation (1.2) has eigenvalues which satisfy $\mu_{1,2} = \nu_1 \pm i\omega_1$ $(\omega_1 > 0)$ and $\mu_3 \in \mathbf{R}$ with $\nu_1, \omega_1 \in \mathbf{R}$, and $\nu_1 < \mu_3$. (Thus the eigenvalues with smallest real part are complex, with $\mathrm{Re}(\mu_{1,2}) < \mu_3$.)

## 2. Some block matrix eigenvalue problems

In this section we discuss some theory for the eigenvalue problem (1.2) and its Cayley transform which we define below. Firstly we restate the problem:

Consider the $N \times N$ eigenvalue problem

$$Aw = \mu Bw \tag{2.1}$$

with

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

where $K$, $C$ and $M$ are as in the Introduction, and where in analogy with the application from the discretized Navier-Stokes equations we use $u \in \mathbf{R}^n$ and $p \in \mathbf{R}^m$ to correspond to velocity and pressure degrees of freedom respectively.

Since $C$ is full rank, the $QR$ factorisation of $C$ has the form

$$C = QR = [Q_1, Q_2] \begin{bmatrix} R_1, \\ 0 \end{bmatrix} \quad (= Q_1 R_1) \tag{2.2}$$

where $R$ is $n \times m$, $R_1$ is $m \times m$ nonsingular and upper triangular, $Q$ is $n \times n$ orthogonal, $Q_1$ is $n \times m$ and provides a basis for range $(C)$, and $Q_2$ is $n \times (n-m)$ and provides an basis for $C^{\perp}$.

The block structure of (2.1) and that fact that $C$ has full rank allows a particularly simple analysis of the eigenvalue problem which we now describe. The "second row" of (2.1) is $C^T u = 0$. Thus $u \in C^{\perp}$, and hence $\exists z \in \mathbf{R}^{n-m}$ such that $u = Q_2 z$. The "first row" of (2.1) gives $KQ_2 z + Cp = \mu M Q_2 z$ and multiplication on the left by $Q_2^T$ produces (since $Q_2^T C p = 0$) the $(n-m)$ dimensional eigenvalue problem

$$K_{22} z = \mu M_{22} z \tag{2.3}$$

where $K_{22} := Q_2^T K Q_2$, $M_{22} := Q_2^T M Q_2$. Since $M$ is positive definite it follows that $M_{22}$ is also positive definite, and hence (2.3) has precisely $n-m$ eigenvalues. It is not difficult to show that for any solution $(\mu, z)$ of (2.3) the corresponding $p$ in (2.1) is $p = -R_1^{-1} Q_1^T (K - \mu M) Q_2 z$. We thus have

**Theorem 1.** a) *The eigenvalue problem* (2.1) *has precisely* $n-m$ *eigenvalues* $\mu_i$, $i = 1, \ldots, n-m$, *which are those of the "reduced" eigenvalue problem* (2.3). *If* $z_i$ *is a corresponding eigenvector of* (2.3), *then corresponding eigenvectors of* (2.1) *are given by*

$$u_i = Q_2 z_i, \quad p_i = -R_1^{-1} Q_1^T (K - \mu_i M) u_i \quad i = 1, \ldots, n-m \tag{2.4}$$

b) *In addition* (2.1) *has an "infinite" eigenvalue of multiplicity* $2m$.

Proof. Part a) was proved above. Part b) follows by considering $\frac{1}{\mu} Aw = Bw$, or may be deduced by considering the Weierstrass-Kronecker Canonical Form [10]. □

A technique for transforming the eigenvalues of a matrix to help numerical methods is the *(Generalized) Cayley transform* [5], [11], [2], [6], [3]: for $\alpha_1, \alpha_2 \in \mathbf{R}$ with

$$\text{(2.5)} \qquad \text{a)} \quad \alpha_1 < \alpha_2 \qquad \text{b)} \quad \alpha_1 \neq \{\mu_i\}_1^{n-m}$$

define the Cayley transform of (2.3) by

$$\text{(2.6)} \qquad C := C(K_{22}, M_{22}) = (K_{22} - \alpha_1 M_{22})^{-1}(K_{22} - \alpha_2 M_{22})$$

which has eigenvalues $\theta_i$, satisfying

$$\text{(2.7)} \qquad \theta_i = (\mu_i - \alpha_2)/(\mu_i - \alpha_1) \quad i = 1, \ldots, n-m.$$

(Note that under (2.5a), $\theta_i \neq 1$.)

It is straightforward to show that under (2.5b) the matrix $\begin{bmatrix} K - \alpha_1 M & C \\ C^T & 0 \end{bmatrix}$ is nonsingular and hence we may introduce the Cayley transform of (2.1), namely,

$$\text{(2.8)} \quad C(A, B) := (A - \alpha_1 B)^{-1}(A - \alpha_2 B) = \begin{bmatrix} K - \alpha_1 M & C \\ C^T & 0 \end{bmatrix}^{-1} \begin{bmatrix} K - \alpha_2 M & C \\ C^T & 0 \end{bmatrix}$$

which has $(n+m)$ eigenvalues $\theta_i$, satisfying

$$\text{(2.9)} \qquad \begin{aligned} \theta_i &= \frac{\mu_i - \alpha_2}{\mu_i - \alpha_1} \quad i = 1, \ldots, n-m \\ \theta_i &= 1 \quad i = n-m+1, \ldots, n+m. \end{aligned}$$

It is easy to verify that the eigenvector(s) of $C(A, B)$ corresponding to $\theta_i$ are precisely the eigenvectors of (2.1) corresponding to $\mu_i$.

The key property of the Cayley transform (2.7) is that eigenvalues $\mu_i$ to the right (left) of the line $\mathrm{Re}(\mu) = \frac{1}{2}(\alpha_1 + \alpha_2)$ in the $\mu$ plane are mapped into (outside) the unit circle in the $\theta$ plane. Specifically

**Lemma 2.** $\mathrm{Re}(\mu_i) > (<) \, 0 \; \frac{\alpha_1 + \alpha_2}{2} \iff |\theta_i| < (>) \, 1.$

Thus an approach to finding the dangerous eigenvalues of (2.1) is now clear: Choose $\alpha_1$ and $\alpha_2$ such that $\mathrm{Re}(\mu_{1,2}) < \frac{\alpha_1 + \alpha_2}{2}$ and that $\mathrm{Re}(\mu_i) \geqslant \frac{\alpha_1 + \alpha_2}{2}$ for $i = 3, \ldots, n-m$. Hence the eigenvalues of (2.8) given by (2.9) satisfy

$$|\theta_{1,2}| > 1, \quad |\theta_i| \leqslant 1 \quad i = 3, \ldots, n+m.$$

Now the idea is to apply Arnoldi's method [1] or subspace iteration [12] to $C(A, B)$ to find the dominant eigenvalues $\theta_{1,2}$ and hence recover $\mu_{1,2}$ from $\mu = (\alpha_1\theta - \alpha_2)/(\theta - 1)$. In fact the $2m$ eigenvalues at 1 can cause difficulties in large systems when $|\theta_{1,2}| \approx 1$, but a minor modification can eliminate this feature with no extra computational cost, and this is the topic of the next section.

## 3. The modified Cayley transform

In this section we consider a small modification of the Cayley transform defined by (2.8). Specifically, for $\alpha_1, \alpha_2 \in \mathbf{R}$ satisfying (2.5) we define the *modified Cayley transform* by

$$M(A,B) := \begin{bmatrix} K-\alpha_1 M & C \\ C^T & 0 \end{bmatrix}^{-1} \begin{bmatrix} K-\alpha_2 M & 0 \\ 0 & 0 \end{bmatrix} \tag{3.1}$$

where we note that the difference between $M(A,B)$ and $C(A,B)$ is that the $C$ and $C^T$ blocks have been dropped from the rightmost matrix in (2.8). The next theorem tells us about the eigenvalues and eigenvectors of $M(A,B)$ and shows the reason for the introduction of $M(A,B)$. Let us denote the eigenvalues of $M(A,B)$ by $\beta_i$, $i = 1, \ldots, n+m$.

**Theorem 3.** *Assume* (2.5), *and in addition*

$$\alpha_2 \neq \{\mu_i\}_1^{n-m} \tag{3.2}$$

a) *For* $i = 1, \ldots, n-m$, $\beta_i = (\mu_i - \alpha_2)/(\mu_i - \alpha_1)$ *with corresponding eigenvector* $[\nu_i, q_i]$ *given by*

$$\nu_i = Q_2 z_i \ (= u_i), \quad q_i = \Big(\frac{\beta_i}{1-\beta_i}\Big) p_i$$

*where* $u_i$, $p_i$ *and* $z_i$ *are as in Theorem 1.*

b) $\beta_i = 0$, $i = n-m+1, \ldots, n+m$.

Proof. The eigenvalues of $M(A,B)$ satisfy

$$\begin{bmatrix} K-\alpha_2 M & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} \nu \\ q \end{bmatrix} = \beta \begin{bmatrix} K-\alpha_1 M & C \\ C^T & 0 \end{bmatrix} \begin{bmatrix} \nu \\ q \end{bmatrix} \tag{3.3}$$

First we determine the non-zero eigenvalues of (3.3). For $\beta \neq 0$, the "second row" of (3.3) implies $C^T \nu = 0$. Hence $\nu = Q_2 z$ for some $z \in \mathbf{R}^{n-m}$ and similar analysis to that in Section 2 now follows: The "first row" of (3.3) provides $(K-\alpha_2 M)Q_2 z = \beta(K-\alpha_1 M)Q_2 z + \beta C q$. Premultiplication by $Q_2^T$ shows that $(K_{22} - \alpha_2 M_{22})z = \beta(K_{22} - \alpha_1 M_{22})z$, which is precisely the Cayley transform $C(K_{22}, M_{22})$ given by (2.6), and has $(n-m)$ eigenvalues $(\mu_i - \alpha_2)/(\mu_i - \alpha_1)$, $i = 1, \ldots, n-m$. Note that (2.5a) and (3.3) ensure that $\beta_i \notin \{0, 1\}$, $i = 1 \ldots, n-m$. The eigenvector corresponding to $\beta_i$ has the form $[\nu_i, q_i] = [u_i, \beta_i p_i/(1-\beta_i)]$ with $[u_i, p_i]$ as in (2.4). $\beta = 0$ provides the remaining $2m$ eigenvalues. [If in addition $K - \alpha_2 M$ is nonsingular, then $\beta = 0$ has precisely $m$ null vectors of the form $[\nu, q]^T = [0, q]^T$, $q \in \mathbf{R}^m$.] □

The advantage of $M(A, B)$ over $C(A, B)$ is now clear. First, the modified Cayley transform leaves the important eigenvalues unchanged, i.e. the eigenvalues $\beta_i$, $i = 1, \ldots, n - m$ are precisely the $\theta_i$ given by (2.8). Second, the $2m$ infinite eigenvalues of (2.1), which play no role in the stability analysis of (1.3) are mapped by $M(A, B)$ to zero, clearly the best place for them. In contrast $C(A, B)$ maps the $2m$ infinite eigenvalues to 1, which may slow up convergence of an iterative algorithm applied to $C(A, B)$. Note that in the applications of interest here, $n \approx 2m$ and so $N \approx 3m$. Thus the $\theta_i = 1$ and $\beta_i = 0$ eigenvalues of (2.9) and (3.1) respectively correspond to about $\frac{2}{3}$ of the eigenvalues of (2.1). In Section 4 we have a case where $N \approx 2 \times 10^5$ and hence $2m \approx 1.4 \times 10^5$.

An analysis similar to the proof of Theorem 3 provides the generalization:

**Corollary 4.** *The matrix*

$$\begin{bmatrix} K - \alpha_1 M & C \\ C^T & 0 \end{bmatrix}^{-1} \begin{bmatrix} K - \alpha_2 M & \alpha_3 C \\ \alpha_3 C^T & 0 \end{bmatrix}$$

*has eigenvalues* $\beta_i = (\mu_i - \alpha_2)/(\mu_i - \alpha_1)$, $i = 1, \ldots, n-m$, *and* $\beta_i = \alpha_3$, $i = n-m+1, \ldots, n+m$.

Though it is natural to make the choice $\alpha_3 = 0$, the choice $\alpha_3 = \frac{1}{2}$ proves to be more appropriate in certain instances (see [3]). In many situations it is important to check the sensitivity of the eigenvalues of a matrix. This is measured by the condition number of the eigenvalue defined for the standard eigenvalue problem $Aw = \mu w$ by $s_i = y_i^H w_i$ where $Aw_i = \mu_i w_i$, $y_i^H A = \mu_i y_i^H$ with $y_i^H y_i = 1$, $w_i^H w_i = 1$ [13]. It is straightforward to show that the corresponding condition number of an eigenvalue of (2.1) is

$$s_i = y_i^H M w_i \tag{3.4}$$

where $y_i^H M y_i = 1$, $w_i^H M w_i = 1$.

The strategy used to find the dangerous eigenvalues of (2.1) is essentially to apply an algorithm for finding the dominant eigenvalues of a matrix to $M(A, B)$ defined by (3.1) (see [3] for details). This is the technique used to provide the numerical results in Section 4, where the subspace iteration method [12] was the iterative eigenvalue solver used. Initial estimates for $\alpha_1$ and $\alpha_2$ were obtained by first finding the eigenvalues of (2.1) nearest the origin by inverse iteration. Note also that the (matrix)×(vector) operation $M(A, B)x = y$ can be implemented as $y = x + z$, where

$$\begin{bmatrix} K - \alpha_1 M & C \\ C^T & 0 \end{bmatrix} z = \begin{bmatrix} (\alpha_1 - \alpha_2) M & -C \\ -C^T & 0 \end{bmatrix} x$$

which is preferred when multiplications with the nonsymmetric matrix $K$ are expensive.

Finally we note that to check the accuracy of a computed eigensolution, say $(\tilde{\mu}, [\tilde{u}, \tilde{p}])$, we form the relative residual $\|(A - \tilde{\mu}B)[\tilde{u}, \tilde{p}]\|_2 / \|\tilde{u}\|_2$ which is easily shown to equal the standard residual for the "reduced" problem $\|(K_{22} - \tilde{\mu}M_{22})z\|_2 / \|z\|_2$ where $z = Q_2^T \tilde{u}$.

## 4. Numerical results

The strategy outlined at the end of the previous section (and given in more detail in [3]) was used to compute the dangerous eigenvalue in a classical problem in fluid mechanics, namely, the stability of the flow over a backward facing step [4], [7], and we refer to the reader to these papers for the details of the equations and their discretization. The equations were discretized using 4 different meshes, giving rise to 4 eigenvalue problems. The dangerous eigenvalue in this case is real and approximations to $\tilde{\mu}_1$ are computed with residuals less than $10^{-5}$. Subspace iteration with 10 vectors was applied to $M(A, B)$ to find its dominant eigenvalues. The numerical results for Reynolds number 800 are given in Table 1.

| $N$ | 8 426 | 22 842 | 89 682 | 200 522 |
|---|---|---|---|---|
| $\tilde{\mu}_1$ | 16.584 | 14.946 | 15.068 | 15.065 |

Table 1: The calculation of the dominant eigenvalue at Re = 800 for the backward facing step problem [7], [4].

Numerical results for other problems in fluid mechanics, for example, flow past a circular cylinder where the dangerous eigenvalues are complex [9] will be reported elsewhere.

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