A Jacobi-Davidson method for two real parameter nonlinear eigenvalue problems arising from delay differential equations

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SUMMARY

The critical delays of a delay-differential equation can be computed by solving a nonlinear two-parameter eigenvalue problem. The solution of this two-parameter problem can be translated to solving a quadratic eigenvalue problem of squared dimension. We present a structure preserving QR-type method for solving such quadratic eigenvalue problem that only computes real valued critical delays, i.e. complex critical delays, which have no physical meaning, are discarded. For large scale problems, we propose new correction equations for a Newton type or Jacobi-Davidson style method, that also forces real valued critical delays. We present three different equations: one real valued equation using a direct linear system solver, one complex valued equation using a direct linear system solver, and one Jacobi-Davidson style correction equation which is suitable for an iterative linear system solver. We show numerical examples for large scale problems arising from PDEs. Copyright © 2010 John Wiley & Sons, Ltd.

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1. Introduction

This paper considers the time-invariant linear delay-differential equation

$$M\dot{x}(t) + Ax(t) + Bx(t - \tau) = 0 \quad (1.1)$$

where, $M, A, B \in \mathbb{C}^{n \times n}$ are given system matrices and $\tau \geq 0$ is the delay. This system is (asymptotically) stable if, for every bounded initial condition, it holds that $x(t) \rightarrow 0$ as $t \rightarrow \infty$, and a necessary and sufficient condition is that the spectrum of the eigenvalue problem

$$\lambda Mu + Au + e^{-\tau\lambda}Bu = 0 \quad (1.2)$$

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is contained in the open left half-plane (cf. [8], e.g.). We assume that (1.1) does not have algebraic constraints, i.e. M is nonsingular.

Due to the continuous dependence of eigenvalues on the parameter τ , the stability behavior of (1.2) can only change as the delay τ varies if an eigenvalue of (1.2) crosses the imaginary axis. Hence, our goal is to find real parameters $\tau \geq 0$ called critical (or switching or crossing) delays such that $\lambda = i\omega$, $\omega \in \mathbb{R}$ is an eigenvalue of (1.2), i.e. such that the parameter dependent delay eigenvalue problem (DEVP)

$$T(\omega, \tau)u := i\omega Mu + Au + e^{-i\omega\tau}Bu = 0 \quad (1.3)$$

has a real nonzero eigenvalue ω . We exclude the case where $\omega = 0$ is a critical eigenvalue. In this case, $A + B$ is singular and any $\tau \in \mathbb{R}$ would be a critical delay.

Eq. (1.3) is a specific case of the more general problem appearing in the analysis of the stability of steady state solutions of a dynamical system: given a map $T : \mathbb{R} \times \mathbb{R} \rightarrow \mathbb{C}^{n \times n}$ the two real parameter eigenvalue problem is to find real values $\omega, \tau \in \mathbb{R}$ and a complex nonzero vector $u \in \mathbb{C}^n \setminus \{0\}$ such that

$$T(\omega, \tau)u = 0. \quad (1.4)$$

This problem is discussed in detail in [7] in the context of the determination of Hopf bifurcations of linear systems of differential equations. Other examples arise from the stability analysis of hydrodynamic systems [4] and chemical reactors [9], where the parameter τ is the Reynolds number or the temperature or another physical parameter. An obvious approach is continuation or homotopy, i.e. to follow an eigenvalue curve $\lambda(\tau)$ or a sequence of invariant subspaces solving a sequence of eigenvalue problems (1.2) for slightly changing τ . This is not only an inefficient process, but may also lead to wrong conclusions as was pointed out in [3].

Another approach to determine a critical delay consists of the transformation $\mu = e^{-i\omega\tau}$ in (1.3) and elimination of the eigenvalue ω using Kronecker products on the system matrices. This reduction from two to one parameter leads to the following quadratic eigenvalue problem in μ of order n^2 ,

$$\mu^2(B \otimes \bar{M})z + \mu(A \otimes \bar{M} + M \otimes \bar{A})z + (M \otimes \bar{B})z = 0 \quad (1.5)$$

called Kronecker eigenvalue problem (KEVP) [11][12]. Since we are only interested in real eigenvalues ω , we are looking for μ 's on the unit circle.

Kronecker products have been used in the literature for transforming a delay eigenvalue problem to a matrix pencil or a polynomial or a rational or a two parameter eigenvalue problem in order to determine critical delays [2, 5, 11, 12, 14, 18] for different classes of delay eigenvalue problems. Fassbender et al. [5] pointed out that the KEVP corresponding to (1.3) (even for a wider class of neutral time-delay systems) has a generalized palindromic structure which allows for structure preserving eigensolvers.

Unfortunately the complexity of this approach is $\mathcal{O}(n^6)$ such that it only applies to relatively small dimensions. To deal with medium sized to large scale problems, we combine the structure preserving eigensolver with an iterative projection method of Jacobi-Davidson type. Let $V \in \mathbb{C}^{n \times k}$, $k \ll n$ be an orthonormal basis of an ansatz space, and let (ω, τ, y) , $\omega, \tau \in \mathbb{R}$ be a solution of the projected k dimensional eigenvalue problem

$$V^H T(\omega, \tau) V y = 0 \quad (1.6)$$

which has the same structure as the original problem but can be solved by the structure preserving method of Section 2. If the resulting approximate solution (ω, τ, Vy) of (1.3) does

not satisfy our accuracy requirements then V is expanded following an analogous goal as in the Jacobi–Davidson method for nonlinear eigenvalue problems in [1, 21]: (an approximation to) the Newton direction of (1.3) has to be contained in the new search space $\text{Range}[V, v]$.

Since we require real ω and τ in the Newton step, the approach in [1, 21] does not apply directly. In Section 3 we construct a modified correction equation, and we discuss its iterative solution by a preconditioned Krylov solver. It is noteworthy that in the whole procedure only vectors of dimension n are involved.

The paper is organized as follows. In Section 2 we review the relationship between eigenpairs of the Kronecker eigenvalue problem (1.5) and eigentriples of the delay eigenvalue problem (1.3). In Subsection 2.2 we present a somewhat more efficient variant of the structure preserving method in [5] for the solution of (1.5). Section 3 develops a Jacobi–Davidson method for solving the large scale delay eigenvalue problems, and we discuss a practical algorithm for determining critical delays, including finding starting values for μ and ω . Section 4 illustrates the method for delay equations arising from discretized PDEs. They demonstrate that the method is very robust with respect to inexact solves of the correction equation, coarse preconditioners, and the starting vector. We formulate the main conclusions in Section 5.

2. A structure preserving method for the Kronecker eigenvalue problem

In this section, we derive a KEVP for the DEVP by eliminating ω . We then develop a structure preserving method for its solution.

2.1. The Kronecker eigenvalue problem

Recall the DEVP

$$(i\omega M + A + e^{-i\omega\tau} B)u = 0 \quad (2.1)$$

where $M, A, B \in \mathbb{C}^{n \times n}$. We are interested in solutions $(\omega, \tau, u) \in \mathbb{R} \times \mathbb{R} \times \mathbb{C}^n$.

Introducing the parameter $\mu = e^{-i\omega\tau}$ translates the problem to the two-parameter problem

$$i\omega Mu + Au + \mu Bu = 0. \quad (2.2)$$

Note that μ lies on the unit circle, thus $\bar{\mu} = \mu^{-1}$. Hence the complex conjugate equation of (2.2) reads

$$-i\omega \bar{M}\bar{u} + \bar{A}\bar{u} + \mu^{-1}\bar{B}\bar{u} = 0. \quad (2.3)$$

Using (2.2) and (2.3) we arrive at

$$\begin{aligned} 0 &= -(i\omega Mu) \otimes \bar{M}\bar{u} - Mu \otimes (-i\omega \bar{M}\bar{u}) \\ &= (Au + \mu Bu) \otimes \bar{M}\bar{u} + Mu \otimes (\bar{A}\bar{u} + \mu^{-1}\bar{B}\bar{u}) \\ &= ((A + \mu B) \otimes \bar{M} + M \otimes (\bar{A} + \mu^{-1}\bar{B}))(u \otimes \bar{u}). \end{aligned} \quad (2.4)$$

The last equation is a rational eigenvalue problem. Expanding and multiplication by μ yields the quadratic eigenvalue problem

$$\mu^2(B \otimes \bar{M})z + \mu(A \otimes \bar{M} + M \otimes \bar{A})z + (M \otimes \bar{B})z = 0. \quad (2.5)$$

We have thus shown that if (ω, τ, u) is a solution of (2.1) and $\mu = e^{-i\omega\tau}$ with real ω and τ , then $(\mu, u \otimes \bar{u})$ is an eigenpair of (2.5). This is a standard result, see e.g. [12] or [5]. The converse statement is also true:

Theorem 1. *Let $M, A, B \in \mathbb{C}^{n \times n}$ with M nonsingular. Then any eigenvector $z \in \mathbb{C}^{n^2}$ of (2.5) corresponding to a simple eigenvalue $\mu \in \mathbb{C}$ can be written as $z = \alpha u_1 \otimes u_2$ for some vectors $u_1, u_2 \in \mathbb{C}^n$ and some $\alpha \in \mathbb{C}$.*

Moreover, if $|\mu| = 1$ then $u_1 = \bar{u}_2 = u$ and there is an $\omega \in \mathbb{R}$ such that (2.2) holds.

Proof. The proof follows a similar reasoning as the proofs of Theorem 2.2 in [15] and Theorem 1 in [16]. $\square$

Note that when M is singular and x is a nullvector of M , then (1.3) is a singular two-parameter eigenvalue problem [17], as, in this case, any μ is an eigenvalue of (2.4) with eigenvector $x \otimes \bar{x}$. Such situation occurs when the delay differential equation has an algebraic constraint, a situation that we do not consider in this paper.

We have thus transformed the problem of finding solutions of (2.2) to the problem of finding eigenvalues of modulus one of (2.5). We defer its solution to Section 2.2. Once an eigenpair (μ, z) of (2.5) is known, u can be recovered from $z = \alpha u \otimes \bar{u}$. One possibility is to compute the dominant singular vector of the $n \times n$ matrix Z with $z = \text{vec}(Z)$. Alternatively, one could choose u as a column of Z scaled such that u has norm one. Subsequently ω can be obtained by projecting (2.2), i.e.

$$\omega = \frac{-\text{Im}((Mu)^H(Au + \mu Bu))}{\|Mu\|_2^2}. \quad (2.6)$$

Finally, τ may be computed from μ and ω as $\tau = -\text{Im}(\ln(\mu))/\omega$.

2.2. A structure preserving eigenvalue solver

We need to compute all eigenpairs (μ, z) of (2.5) with $|\mu| = 1$. For small n , it is feasible to compute all eigenvalues of (2.5) and then discard those not on the unit circle. An obstacle occurs however: with rounding errors it is difficult to decide whether a computed eigenvalue is on or only close to the unit circle. We will exploit the structure in (2.5) to circumvent this difficulty. The following is essentially the method from [5], but specialized to quadratic problems with symmetric permutation P . This simplifies the method considerably, because the factorization (2.9) can be written down explicitly without computations.

Recall that the Kronecker product does, in general, not commute, i.e. $A \otimes B \neq B \otimes A$. However there is a symmetric permutation matrix P such that $A \otimes B = P(B \otimes A)P$. The permutation vector p , corresponding to P , is obtained by `p=reshape(reshape(1:n^2,n,n)',1,n^2)` in MATLAB. Note that using this permutation, (2.5) is of the form

$$(\mu^2 A_2 + \mu A_1 + A_0)z = 0, \quad \text{where } A_2 = P \bar{A}_0 P, \quad A_1 = P \bar{A}_1 P, \quad \text{where } P = P^{-1} = P^T \in \mathbb{R}^{n^2 \times n^2}. \quad (2.7)$$

Such problems are called PCP-palindromic eigenvalue problems. Their solution is discussed in [5].

The method can be divided into three steps. First, the quadratic eigenvalue problem is reformulated as

$$\left(\mu \begin{bmatrix} 0 & P \\ P & 0 \end{bmatrix} \begin{bmatrix} \bar{A}_1 - \bar{A}_2 & \bar{A}_0 \\ \bar{A}_0 & \bar{A}_0 \end{bmatrix} \begin{bmatrix} 0 & P \\ P & 0 \end{bmatrix} + \begin{bmatrix} A_1 - A_2 & A_0 \\ A_0 & A_0 \end{bmatrix} \right) \begin{bmatrix} \mu z \\ z \end{bmatrix} = 0, \quad (2.8)$$

which is a linear PCP-palindromic problem, because with P also $\begin{bmatrix} P & \\ & P \end{bmatrix}$ is a real symmetric permutation.

Second, using the factorization

$$\begin{bmatrix} 0 & P \\ P & 0 \end{bmatrix} = UU^T, \quad \text{where} \quad U = \frac{1}{\sqrt{2}} \begin{bmatrix} I & iP \\ P & -iI \end{bmatrix} \quad (2.9)$$

we define

$$C := U^H \begin{bmatrix} A_1 - A_2 & A_0 \\ A_0 & A_0 \end{bmatrix} \bar{U}. \quad (2.10)$$

Since U is unitary, i.e. $U^H U = I = U^T \bar{U}$, the pencil in (2.8) is equivalent to

$$\begin{aligned} & U^H \left(\mu \begin{bmatrix} 0 & P \\ P & 0 \end{bmatrix} \begin{bmatrix} \bar{A}_1 - \bar{A}_2 & \bar{A}_0 \\ \bar{A}_0 & \bar{A}_0 \end{bmatrix} \begin{bmatrix} 0 & P \\ P & 0 \end{bmatrix} + \begin{bmatrix} A_1 - A_2 & A_0 \\ A_0 & A_0 \end{bmatrix} \right) \bar{U} \\ &= \mu U^T \begin{bmatrix} \bar{A}_1 - \bar{A}_2 & \bar{A}_0 \\ \bar{A}_0 & \bar{A}_0 \end{bmatrix} U + U^H \begin{bmatrix} A_1 - A_2 & A_0 \\ A_0 & A_0 \end{bmatrix} \bar{U} \\ &= \mu \bar{C} + C. \end{aligned}$$

Third, consider an eigenpair (θ, x) of the real generalized eigenvalue problem

$$\operatorname{Re}(C)x = \theta \operatorname{Im}(C)x \quad (2.11)$$

or, equivalently,

$$Cx + \frac{i + \theta}{i - \theta} \bar{C}x = 0. \quad (2.12)$$

Note that $\mu := (i + \theta)/(i - \theta)$ is on the unit circle if and only if θ is real or $\theta = \infty$ (the latter resulting in $\mu = -1$).

Eigenvectors of (2.8) and (2.11) are related by

$$\begin{bmatrix} \mu z \\ z \end{bmatrix} = \bar{U}x = \frac{1}{\sqrt{2}} \begin{bmatrix} I & -iP \\ P & iI \end{bmatrix} x. \quad (2.13)$$

Hence, (a multiple of) an eigenvector of the original quadratic problem (2.7) respectively (2.5) is given by the lower (as well as the upper) half of $\bar{U}x$:

$$z = \frac{1}{\sqrt{2}} \begin{bmatrix} I & -iP \end{bmatrix} x \text{ or } z = \frac{1}{\sqrt{2}} \begin{bmatrix} P & iI \end{bmatrix}. \quad (2.14)$$

From the equations above we then derive the following algorithm for solving small scale DEVPs.

Algorithm 1.

Input: $M, A, B \in \mathbb{C}^{n \times n}$

Output: solutions $(\omega_j, \tau_j, u_j)_{j=1, \dots}$ of $(i\omega M + A + e^{-i\omega\tau} B)u = 0$

- 1: $A_0 = M \otimes \bar{B}$, $A_1 = A \otimes M + M \otimes \bar{A}$
- 2: Construct the permutation P
- 3: $C = \frac{1}{2} \begin{bmatrix} I & iP \\ P & -iI \end{bmatrix}^H \begin{bmatrix} A_1 - P\bar{A}_0P & A_0 \\ A_0 & A_0 \end{bmatrix} \overline{\begin{bmatrix} I & iP \\ P & -iI \end{bmatrix}}$
- 4: Compute all eigenpairs (θ_j, x_j) of $\operatorname{Re}(C)x = \theta \operatorname{Im}(C)x$ where θ_j is real
- 5: **for** $j=1, \dots$ **do**
- 6: $\mu_j = \frac{i + \theta_j}{i - \theta_j}$

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7:   $z_j = [I - iP]x_j$ 
8:  Compute  $u_j$  as dominant singular vector of  $\text{mat}(z_j)$ 
9:   $\omega_j = \frac{-\text{Im}((Mu_j)^H(Au_j + \mu_j Bu_j))}{\|Mu_j\|_2^2}$ 
10:  $\tau_j = \frac{-\text{Im}(\ln(\mu_j))}{\omega_j}$ 
11: end for

```

The dominant computational step in Algorithm 1 is step 4 with a complexity of $\mathcal{O}(n^6)$. Since the real eigenvalues of a real pencil can be determined in a stable way by the real QZ algorithm, the eigenvalues of (1.5) on the unit circle, and therefore the critical delays can be identified in a reliable way.

3. A Jacobi-Davidson method for the two real parameter eigenvalue problem

Due to its high numerical complexity the structure preserving algorithm in Section 2.2 is only applicable to problems of relatively small dimension. For medium sized to large scale problems we combine it with a subspace method of Jacobi–Davidson type.

The Jacobi–Davidson method is an iterative projection method which was introduced by Sleijpen and van der Vorst [22] for linear eigenvalue problems and generalized to one parameter nonlinear ones [1, 21]. Here the search space is expanded in a way that the Newton iterate at the current approximate eigenpair is contained in the expanded subspace, and it was shown to be very robust with respect to inexact Newton iterates [22, 24] which makes it particularly qualified for large-scale problems. In this section we develop a Jacobi–Davidson type method for the nonlinear two-parameter eigenvalue problem (1.3) with the particularity that the parameters are required to be real.

Algorithm 2 contains a template of the Jacobi–Davidson method.

Algorithm 2.

Input: $T : \mathbb{R} \times \mathbb{R} \mapsto \mathbb{C}^{n \times n}$, its partial derivatives, and tolerance $\eta > 0$

Input: orthonormal basis $V \in \mathbb{C}^{n \times k_0}$, $V^H V = I$ of initial search space

Output: solutions $(\omega_j, \tau_j, u_j)_{j=1, \dots} \in \mathbb{R} \times \mathbb{R} \times \mathbb{C}^n$ of $T(\omega, \tau)u = 0$

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1: for  $k = k_0, k_0 + 1, \dots$  do
2:   compute all eigentriples  $(\hat{\omega}_i, \hat{\tau}_i, \hat{z}_i)$  with real  $\hat{\omega}_i$  and  $\hat{\tau}_i$  of the projected eigenvalue problem

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$$V^H T(\omega, \tau) V z = 0 \quad (3.1)$$

using Algorithm 1

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3:   compute the associated Ritz vectors  $\hat{u}_i = V \hat{z}_i$ 
4:   check for convergence:  $\|T(\hat{\omega}_i, \hat{\tau}_i) \hat{u}_i\|_2 \leq \eta$ 
5:   (append  $\hat{u}_i$  to  $V$  if  $(\hat{\omega}_i, \hat{\tau}_i, \hat{u}_i)$  has converged and  $\hat{u}_i \notin \text{Range}(V)$ )
6:   STOP if enough eigentriples have converged
7:   determine an approximate eigentriple  $(\hat{\omega}, \hat{\tau}, \hat{u}) \in \mathbb{R} \times \mathbb{R} \times \text{Range}(V)$ 
8:   reduce search space if necessary
9:   determine a correction  $c$  to  $\hat{u}$ 
10:  expand search space  $V = \text{orth}([V, c])$ 
11: end for

```

Some comments on the respective steps are in order.

Input: Algorithm 2 requires an orthonormal basis V of an initial search space. Here we can introduce pre-knowledge, for instance known symmetry properties of solutions or the solution of a nearby problem which may have been solved before. Usually, however, such initial information is not at hand, and we start with a normalized random vector $V \in \mathbb{C}^{n \times 1}$.

- 2: The method to solve the projected problem depends on the individual two parameter eigenvalue problem at hand. In case of the delay eigenvalue problem (1.3) we solve

$$i\omega \widehat{M}z + \widehat{A}z + e^{-i\tau\omega} \widehat{B}z = 0 \quad (3.2)$$

with $\widehat{M} = V^H M V$, $\widehat{A} = V^H A V$, and $\widehat{B} = V^H B V$, by the structure preserving Algorithm 1.

- 4: The stopping criterion is based on the residual $r = T(\hat{\omega}, \hat{\tau})\hat{u}$ as a measure of the backward error of the eigentriple. An eigentriple is considered accurate when $\|r\| \leq \eta$ for a prescribed tolerance η .
- 5: This step applies to DEVPs with real matrices M, A, B only. If (ω, τ, u) is an eigentriple then the same holds true for $(-\omega, \tau, \bar{u})$. Hence, for every converged eigentriple we append $\bar{u}$ to $\text{span}(V)$ to obtain $(-\omega, \tau, \bar{u})$ immediately. Otherwise several JD iterations have to be performed until $\bar{u}$ appears in the search space.
- 7: The projected problem (3.1) often has more than one real eigenpair $(\hat{\omega}, \hat{\tau})$. We choose the eigentriple which has not yet converged with the minimal residual. If (3.2) does not produce any unconverged eigentriples with $\hat{\omega} \in \mathbb{R}$ and $\hat{\tau} \in \mathbb{R}$, we use an alternative selection as described in Subsection 3.4.
- 8: As the dimension of the search space grows, the cost of solving the projected problem (3.1) can become prohibitively large. In the case of the DEVP the cost for the QZ algorithm in the structure preserving eigensolver of the projected eigenvalue problem swells like $\mathcal{O}(k^6)$. Hence, the search space has to be reduced whenever k exceeds a prescribed limit. We continue the algorithm with an orthonormal basis of the space spanned by the already converged eigenvectors and additionally all or a selection of vectors corresponding to the not yet converged eigentriples of the current projected problem (3.1) with the smallest residual norm.
- 9: The orthogonal correction for an eigenvector approximation by Newton's method is given by a linear system, and we only have to make sure that the corrections of ω and τ are real. However, for truly large problems this linear system can not be solved by a direct solver. For this case we have to provide a correction equation which can be solved efficiently by an iterative solver. This will be discussed in Subsections 3.1, 3.2 and 3.3.
- 10: Any orthogonalization procedure can be employed. We use classical Gram Schmidt with reorthogonalization.

In the following subsections we shall discuss the expansion of the search space.

3.1. Correction equation for medium sized problems

Let $(\hat{\omega}, \hat{\tau}, \hat{u})$ be an approximate eigentriple of the DEVP (1.3). We are looking for a correction $(\hat{\omega} + \delta, \hat{\tau} + \varepsilon, \hat{u} + c)$ where δ, ε are real and c is complex and is orthogonal to $\hat{u}$. This orthogonality constraint makes the direction of c unique.

Applying a single step of Newtons method to the root finding problem for

$$f : \mathbb{C}^n \times \mathbb{R} \times \mathbb{R} \rightarrow \mathbb{C}^{n+1}, (c, \delta, \varepsilon) \mapsto \begin{bmatrix} T(\hat{\omega} + \delta, \hat{\tau} + \varepsilon)(\hat{u} + c) \\ \hat{u}^H c \end{bmatrix} \quad (3.3)$$

with zero initial guess leads to

$$\begin{bmatrix} T(\hat{\omega}, \hat{\tau}) & T_\omega(\hat{\omega}, \hat{\tau})\hat{u} & T_\tau(\hat{\omega}, \hat{\tau})\hat{u} \\ \hat{u}^H & 0 & 0 \end{bmatrix} \begin{bmatrix} c \\ \delta \\ \varepsilon \end{bmatrix} = \begin{bmatrix} -T(\hat{\omega}, \hat{\tau})\hat{u} \\ 0 \end{bmatrix}. \quad (3.4)$$

This is a linear system of $(n + 1)$ complex equations in n complex and 2 real unknowns. We therefore call this the mixed correction equation.

To determine a solution of (3.4) with real components δ and ε , and to take advantage of existing software for solving linear systems we separate real and imaginary parts in (3.4) leading to the equivalent real linear system of dimension $2n + 2$

$$\begin{bmatrix} \text{Re}(\hat{T}) & -\text{Im}(\hat{T}) & \text{Re}(\hat{T}_\omega \hat{u}) & \text{Re}(\hat{T}_\tau \hat{u}) \\ \text{Im}(\hat{T}) & \text{Re}(\hat{T}) & \text{Im}(\hat{T}_\omega \hat{u}) & \text{Im}(\hat{T}_\tau \hat{u}) \\ \text{Re}(\hat{u}^H) & -\text{Im}(\hat{u}^H) & 0 & 0 \\ \text{Im}(\hat{u}^H) & \text{Re}(\hat{u}^H) & 0 & 0 \end{bmatrix} \begin{bmatrix} \text{Re}(c) \\ \text{Im}(c) \\ \delta \\ \varepsilon \end{bmatrix} = \begin{bmatrix} \text{Re}(-\hat{T}\hat{u}) \\ \text{Im}(-\hat{T}\hat{u}) \\ 0 \\ 0 \end{bmatrix}, \quad (3.5)$$

which we call the real correction equation. Here we used the notation $\hat{T} := T(\hat{\omega}, \hat{\tau})$, $\hat{T}_\omega := T_\omega(\hat{\omega}, \hat{\tau})$, and $\hat{T}_\tau := T_\tau(\hat{\omega}, \hat{\tau})$.

A different approach that guarantees the realness of δ and ε is to complement system (3.4) by its complex conjugate counterpart, which we call the complex correction equation. The name ‘complex’ comes from the fact that we join the correction equations for both u and $\bar{u}$.

$$\begin{bmatrix} \hat{T} & 0 & \hat{T}_\omega \hat{u} & \hat{T}_\tau \hat{u} \\ 0 & \hat{\bar{T}} & \hat{\bar{T}}_\omega \hat{u} & \hat{\bar{T}}_\tau \hat{u} \\ \hat{u}^H & 0 & 0 & 0 \\ 0 & \hat{\bar{u}}^H & 0 & 0 \end{bmatrix} \begin{bmatrix} d_1 \\ d_2 \\ d_3 \\ d_4 \end{bmatrix} = \begin{bmatrix} -\hat{T}\hat{u} \\ -\hat{\bar{T}}\hat{u} \\ 0 \\ 0 \end{bmatrix}. \quad (3.6)$$

In [19], it was argued that complex linear systems that respect the sparse structure are preferred to real valued linear system such as (3.5) that lose this structure. Indeed, (3.6) can be solved by a single factorization of $\hat{T}$, provided $\hat{T}$ is nonsingular.

To show that the components d_3 and d_4 of a solution of (3.6) are real and d_1 and d_2 are complex conjugate of each other we first show the following results.

Lemma 1. *If the complex valued linear system*

$$\begin{bmatrix} \alpha_1 & \alpha_2 \\ \bar{\alpha}_1 & \bar{\alpha}_2 \end{bmatrix} \begin{bmatrix} \xi_1 \\ \xi_2 \end{bmatrix} = \begin{bmatrix} \beta \\ \bar{\beta} \end{bmatrix} \quad (3.7)$$

has a unique solution, then ξ_1 and ξ_2 are real.

Proof. By linear combination of the rows of the complex system, we find the real system

$$\begin{bmatrix} \text{Re}(\alpha_1) & \text{Re}(\alpha_2) \\ \text{Im}(\alpha_1) & \text{Im}(\alpha_2) \end{bmatrix} \begin{bmatrix} \xi_1 \\ \xi_2 \end{bmatrix} = \begin{bmatrix} \text{Re}(\beta) \\ \text{Im}(\beta) \end{bmatrix}$$

which proves the lemma. $\square$

Theorem 2. *Let the linear system (3.6) be nonsingular. Then its solution is $(c^T, \bar{c}^T, \delta, \epsilon)^T$ where c , δ and ϵ satisfy (3.4) and δ and ϵ are real.*

Proof. We first prove that d_3 and d_4 are real and $d_2 = \bar{d}_1$. Since the linear system is nonsingular, Gaussian elimination (if needed with pivoting) on the first and third block rows and similarly the second and fourth block rows produces

$$\begin{bmatrix} I & 0 & h_\omega & h_\tau \\ 0 & I & \bar{h}_\omega & \bar{h}_\tau \\ 0 & 0 & \alpha_\omega & \alpha_\tau \\ 0 & 0 & \bar{\alpha}_\omega & \bar{\alpha}_\tau \end{bmatrix} \begin{bmatrix} d_1 \\ d_2 \\ d_3 \\ d_4 \end{bmatrix} = \begin{bmatrix} g \\ \bar{g} \\ \gamma \\ \bar{\gamma} \end{bmatrix}. \quad (3.8)$$

Then d_3 and d_4 are solved from the subsystem consisting of the third and fourth rows of (3.8). Following Lemma 1, d_3 and d_4 are real. Since d_3 and d_4 are real, it is easy to see from (3.8) that $d_2 = \bar{d}_1$.

It is also quite clear that the solution of (3.6) satisfies (3.4): the first and third rows on the one hand and the complex conjugate of the second and fourth rows of (3.6) on the other hand correspond to (3.4). $\square$

Both systems of equations, (3.5) and (3.6) are called correction equations of the Jacobi–Davidson method. Expanding the search space by the solution c of one of them we can expect quadratic convergence [22]. However, solving them directly becomes too expensive for truly large problems, and so they are only appropriate for medium sized problem.

3.2. Correction equation for large-scale problems

In this subsection we eliminate d_3 and d_4 from system (3.6) to obtain a form of the correction equations which is suitable for solving it by a preconditioned Krylov solver. A similar technique was used in [10] to derive a second-order correction equation for two-parameter linear eigenvalue problems.

With

$$\mathbb{T} = \begin{bmatrix} \hat{T} & 0 \\ 0 & \hat{\bar{T}} \end{bmatrix}, \quad K = \begin{bmatrix} \hat{T}_\omega \hat{u} & \hat{T}_\tau \hat{u} \\ \hat{\bar{T}}_\omega \hat{u} & \hat{\bar{T}}_\tau \hat{u} \end{bmatrix}, \quad U = \begin{bmatrix} \hat{u} & 0 \\ 0 & \hat{\bar{u}} \end{bmatrix}$$

and $r = \hat{T}\hat{u}$ equation (3.6) reads

$$\begin{bmatrix} \mathbb{T} & K \\ U^H & 0 \end{bmatrix} \begin{bmatrix} c \\ \bar{c} \\ \delta \\ \epsilon \end{bmatrix} = \begin{bmatrix} -r \\ -\bar{r} \\ 0 \\ 0 \end{bmatrix}. \quad (3.9)$$

Assume that $U^H K$ has rank two (i.e. full rank). Then we deduce from (3.9) that

$$U^H \mathbb{T} \begin{bmatrix} c \\ \bar{c} \end{bmatrix} + U^H K \begin{bmatrix} \delta \\ \epsilon \end{bmatrix} = -U^H \begin{bmatrix} r \\ \bar{r} \end{bmatrix}.$$

Solving this equation for δ and ϵ and plugging them back into (3.9) we obtain

$$(\mathbb{T} - K(U^H K)^{-1}U^H \mathbb{T}) \begin{bmatrix} c \\ \bar{c} \end{bmatrix} = -(I - K(U^H K)^{-1}U^H) \begin{bmatrix} r \\ \bar{r} \end{bmatrix}. \quad (3.10)$$

Imposing that $\hat{u}^H c = 0$ we finally arrive at

$$(I - K(U^H K)^{-1} U^H) \mathbb{T}(I - UU^H) \begin{bmatrix} c \\ \bar{c} \end{bmatrix} = -(I - K(U^H K)^{-1} U^H) \begin{bmatrix} r \\ \bar{r} \end{bmatrix}. \quad (3.11)$$

which looks like the common correction equation of the Jacobi–Davidson method for nonlinear eigenvalue problems: the equation $\mathbb{T}[c^T, \bar{c}^T]^T = -[r^T, \bar{r}^T]^T$ is complemented by the oblique projector $I - K(U^H K)^{-1} U^H$ which provokes that the Newton direction is contained in $\text{span}\{\hat{u}, c\}$. We call (3.11) the JD correction equation.

The same procedure could be used to obtain a correction equation from (3.5) which does not depend on δ and ε . However, it will be demonstrated in the next subsection that preconditioned Krylov solvers can be applied easily to (3.11). In particular, given a preconditioner P of $\hat{T}$ one can easily implement the preconditioner $\text{diag}\{P, \bar{P}\}$ for system (3.11) which does not make sense for the real system corresponding to (3.11) obtained from (3.5).

3.3. Preconditioning the correction equation

When an iterative solver is used for (3.11), a preconditioner is highly recommended. Let P be a preconditioner for $\hat{T} = T(\hat{\omega}, \hat{\tau})$. Define

$$\mathbb{P} = \begin{bmatrix} P & 0 \\ 0 & \bar{P} \end{bmatrix}.$$

Then the projected matrix

$$(I - K(U^H K)^{-1} U^H) \mathbb{P}(I - UU^H) \quad (3.12)$$

is an approximation to $(I - K(U^H K)^{-1} U^H) \mathbb{T}(I - UU^H)$ which we use as preconditioner for (3.11). The inverse of (3.12) in the range of $(I - UU^H)$ is

$$(I - UU^H) \mathbb{P}^{-1} (I - K(U^H \mathbb{P}^{-1} K)^{-1} U^H \mathbb{P}^{-1}).$$

In every step of a left preconditioned Krylov solver for (3.11) we have to determine

$$\begin{bmatrix} t \\ \bar{t} \end{bmatrix} = [(I - UU^H) \mathbb{P}^{-1} (I - K(U^H \mathbb{P}^{-1} K)^{-1} U^H \mathbb{P}^{-1})] (I - K(U^H K)^{-1} U^H) \mathbb{T}(I - UU^H) \begin{bmatrix} v \\ \bar{v} \end{bmatrix}$$

for some given v with $\hat{u}^H v = 0$.

Simplifications produce the following equations.

$$\begin{aligned} \begin{bmatrix} t \\ \bar{t} \end{bmatrix} &= (I - UU^H) \mathbb{P}^{-1} (I - K(U^H \mathbb{P}^{-1} K)^{-1} U^H \mathbb{P}^{-1}) \mathbb{T}(I - UU^H) \begin{bmatrix} v \\ \bar{v} \end{bmatrix} \\ \begin{bmatrix} t \\ \bar{t} \end{bmatrix} &= (I - UU^H) (I - \mathbb{P}^{-1} K(U^H \mathbb{P}^{-1} K)^{-1} U^H) \mathbb{P}^{-1} \mathbb{T}(I - UU^H) \begin{bmatrix} v \\ \bar{v} \end{bmatrix} \\ \begin{bmatrix} t \\ \bar{t} \end{bmatrix} &= (I - \mathbb{P}^{-1} K(U^H \mathbb{P}^{-1} K)^{-1} U^H) \mathbb{P}^{-1} \mathbb{T}(I - UU^H) \begin{bmatrix} v \\ \bar{v} \end{bmatrix} \end{aligned} \quad (3.13)$$

The vector t can be computed very efficiently taking advantage of the fact $\hat{u}^H t = 0$. (Of course, $\bar{t}$ is not computed explicitly.) Using the structure of U , $\mathbb{T}$ and $\mathbb{P}$, (3.13) becomes

$$\begin{bmatrix} t \\ \bar{t} \end{bmatrix} = (I - \mathbb{P}^{-1} K(U^H \mathbb{P}^{-1} K)^{-1} U^H) \begin{bmatrix} P^{-1} \hat{T}(I - \hat{u} \hat{u}^H) v \\ \bar{P}^{-1} \bar{\hat{T}}(I - \hat{u} \hat{u}^H) \bar{v} \end{bmatrix}$$

or since $(I - \hat{u}\hat{u}^H)v = v$

$$t = P^{-1}Tv + P^{-1}[\hat{T}_\omega\hat{u}, \hat{T}_\tau\hat{u}]a \quad (3.14)$$

$$\bar{t} = \bar{P}^{-1}\bar{T}v + \bar{P}^{-1}[\bar{\hat{T}}_\omega\bar{u}, \bar{\hat{T}}_\tau\bar{u}]a \quad (3.15)$$

where a is chosen so that $\hat{U}^H t = 0$.

Multiplying by $\hat{u}^H$ and $\bar{u}$, respectively we obtain a linear system like (3.7), and it follows from Lemma 1 that a must be real.

The preconditioned right-hand side for the iterative solver is

$$\begin{aligned} \begin{bmatrix} b \\ \bar{b} \end{bmatrix} &= -[(I - UU^H)\mathbb{P}^{-1}(I - K(U^H\mathbb{P}^{-1}K)^{-1}U^H\mathbb{P}^{-1})](I - K(U^H K)^{-1}U^H) \begin{bmatrix} r \\ \bar{r} \end{bmatrix} \\ &= -(I - UU^H)\mathbb{P}^{-1}(I - K(U^H\mathbb{P}^{-1}K)^{-1}U^H\mathbb{P}^{-1}) \begin{bmatrix} r \\ \bar{r} \end{bmatrix} \\ &= -(I - \mathbb{P}^{-1}K(U^H\mathbb{P}^{-1}K)^{-1}U^H)\mathbb{P}^{-1} \begin{bmatrix} r \\ \bar{r} \end{bmatrix} \end{aligned}$$

which can again be written as

$$b = P^{-1}r - P^{-1}[\hat{T}_\omega\hat{u}, \hat{T}_\tau\hat{u}]a_r \quad (3.16)$$

with $a_r \in \mathbb{C}^2$. With the same reasoning as before, using $\hat{u}^H b = 0$ and Lemma 1, it can be seen that a_r must be real. (Of course, $\bar{b}$ is not computed explicitly.)

Equations (3.14) and (3.16) demonstrate how the preconditioned Krylov solver for (3.11) can be implemented efficiently. The matrix $D := P^{-1}[\hat{T}_\omega\hat{u}, \hat{T}_\tau\hat{u}]$ is independent of v and r and can be pre-calculated. Then the vector t is obtained from

$$t = P^{-1}\hat{T}v + Da \quad \text{where } a \text{ solves} \quad \begin{bmatrix} \text{Re}(\hat{u}^H D) \\ \text{Im}(\hat{u}^H D) \end{bmatrix} a = - \begin{bmatrix} \text{Re}(\hat{u}^H P^{-1}\hat{T}v) \\ \text{Im}(\hat{u}^H P^{-1}\hat{T}v) \end{bmatrix},$$

and b is obtained similarly. Hence, each iteration requires only one matrix-vector product $\hat{T}v$ and one solve with the preconditioner, and the only additional cost taking into account the projectors in the preconditioning are two matrix-vector products and three solves with the preconditioner P to determine D and to initialize the Krylov solver. This favorable property that the inclusion of the projectors into the preconditioner comes nearly for free was already pointed out by Sleijpen and van der Vorst in [22].

3.4. Alternative selection

The expansion of the search space with a solution of the correction equation (3.4) requires an approximate eigentriple $(\hat{\omega}, \hat{\tau}, \hat{u})$ with $\hat{u}$ from the search space. As a natural choice we take an unconverged Ritz triple of (3.1). However, in particular in very early stages of the algorithm such a Ritz triple often does not exist, and this may also happen in JD iterations right after a Ritz triple has converged and the current projected problem yields no unconverged approximate eigentriples. Then an alternative selection strategy has to be employed.

It turned out to be successful and robust to choose $\hat{u} = V\hat{z}$ where $\hat{z}$ solves the minimization problem

$$\|(i\hat{\omega}M + A + e^{-i\hat{\tau}\hat{\omega}}B)V\hat{z}\| = \min \quad \text{s.t. } \|\hat{z}\| = 1,$$

where V is the basis of the current search space and $\hat{\omega}$ and $\hat{\tau}$ are randomly chosen real parameters. Notice that the number of columns of V is usually very small and the right singular vector $\hat{z}$ of $(i\hat{\omega}M + A + e^{-i\hat{\tau}\hat{\omega}}B)V$ corresponding to its smallest singular value can be found efficiently. With this triple $(\hat{\omega}, \hat{\tau}, \hat{u})$ we solve the Newton correction equation (3.4), and expand the search space by its solution c .

The strategy is implemented by replacing step 7 of Algorithm 2 by

- 1: **if** an unconverged Ritz triple exists **then**
- 2: select the unconverged Ritz triple with smallest residual norm
- 3: **else**
- 4: select random parameters $\hat{\omega} \neq 0$ and $\hat{\tau} \neq 0$
- 5: compute $\hat{u} = V\hat{z}$, with $\|\hat{z}\|_2 = 1$ so that $\|(i\hat{\omega}M + A + e^{-i\hat{\tau}\hat{\omega}}B)V\hat{z}\|_2$ is minimal
- 6: **end if**

4. Numerical examples

4.1. Example 1

The first example is taken from [13]: Consider the partial delay differential equation

$$-\frac{\partial}{\partial t}x(\xi, t) + \frac{\partial^2}{\partial \xi^2}x(\xi, t) + a(\xi)x(\xi, t) + b(\xi)x(\pi - \xi, t - \tau) = 0 \quad \text{for } \xi \in (0, \pi), \quad t > 0 \quad (4.1)$$

with boundary conditions $\frac{\partial}{\partial \xi}x(0, t) = 0 = \frac{\partial}{\partial \xi}x(\pi, t)$. Discretization in space with central differences (i.e. $x(t) = [x_1(t), \dots, x_n(t)]^T$ with $x_i(t) = x((i-1)h, t)$ and $h = \pi/(n-1)$) yields

$$I\dot{x}(t) + \left(\frac{1}{h^2} \begin{bmatrix} 1 & -1 & & & \\ -1 & 2 & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 2 & -1 \\ & & & -1 & 1 \end{bmatrix} - \begin{bmatrix} a(0) & & & & \\ & a(h) & & & \\ & & \ddots & & \\ & & & a(\pi-h) & \\ & & & & a(\pi) \end{bmatrix} \right) x(t) - \begin{bmatrix} & & & & b(0) \\ & & & b(h) & \\ & & \ddots & & \\ & b(\pi-h) & & & \\ b(\pi) & & & & \end{bmatrix} x(t-\tau) = 0.$$

We used $n = 500$, $a(\xi) = -2\sin(\xi)$, and $b(\xi) = 2\sin(\xi) + 1$. (In [13] $b(\xi) = 2\sin(\xi)$ is used, but then the problem has a double solution.)

We first used Algorithm 2, where the complex correction equation (3.6) was solved using the considerations from §3.1. A linear system with $\hat{T}$ was solved with a direct sparse solver, using MATLAB's backslash. We accepted an eigentriple as converged if its residual norm was less than 10^{-10} . Table I shows the Ritz values ω and τ for the different iterations with their residual norms. In the last column we indicated by 'Ritz sel.' that the associated Ritz pair was selected for solving the correction equation, by 'alt. sel.' that no eigenvalues of the Kronecker eigenvalue problem were found on the unit circle and the search space was expanded by the

method described in Subsection 3.4, and we marked a row by ‘conv.’ if a Ritz triple (ω, τ, u) had converged. In this case we complemented the search space by the complex conjugate $\bar{u}$ of the Ritz vector u such that $(-\omega, \tau, \bar{u})$ was found immediately.

Starting with a random vector $x = \text{randn}(500, 1) + i \cdot \text{randn}(500, 1)$ it is not surprising that the projected problem has no real eigenpair (ω, τ) . It took two alternative selection steps to obtain a projected problem with a real eigenpair. Three expansions of the search space with Newton steps produced a residual $1.69 \cdot 10^{-12}$ such that the first eigentriple has converged. After complementing the search space by $\bar{u}$ the next eigentriple was found, but there was no further real eigenpair (ω, τ) corresponding to a non-converged eigentriple. After two alternative selection steps two more real eigenpairs of the projected problem were found. Two further Newton expansions made one eigenpair converge, and complementing the search space again by $\bar{u}$ yielded the missing eigentriple. The development of the residuals indicates quadratic convergence.

We then used Algorithm 2, where the correction equation (3.11) was solved with GMRES [20]. It turned out that the method is extremely robust with respect to inexact solves of the correction equation. As preconditioner we used an incomplete Cholesky factorization of the real matrix A with drop tolerance 10^{-2} , but incomplete LU factorizations of $T(\omega, \tau)$ for various choices of real ω and τ worked similarly well. The GMRES method was terminated after at most 5 steps or if the initial residual was reduced by at least 10^{-1} .

Columns two, three and four of Table II show the Ritz values for the different iterations with their residual norms. Column 5 contains the number of iteration steps of GMRES which were required to reduce the residual of the correction equation by 10^{-1} , and Column 6 contains remarks similar to Table I.

4.2. Example 2

Consider the equation

$$u_t - \nabla((1 + x^2 + y^2)\nabla u) - \alpha(1 + xy)u(t - \tau) = 0 \quad (4.2)$$

with spatial variables x and y on $\Omega = (0, 1) \times (0, 1)$ with Dirichlet boundary condition $u = 0$ on $\partial\Omega$. We used COMSOL[†] for a discretization with finite elements using piecewise quadratic ansatz functions on a triangular grid which led to an eigenvalue problem of the form (1.2) of dimension $n = 104257$.

We solved the problem for $\alpha = 23$ which is close to a delay-independent stable system (actually for $\alpha = 22.6$ the system is stable for all non-negative delay values τ), and therefore the domain of attraction of Newton’s method should be quite small. We preconditioned with `P=luinc(A,1e-3)`, and we terminated the GMRES method for solving the correction equation after at most 10 iteration steps or if the residual was reduced at least by 10^{-1} and we started Algorithm 2 by a complex random vector.

For the alternative selection we considered two alternatives. Choosing $\omega = \text{randn}$ and $\tau = \text{randn}$ the average number of initial alternative selection steps for ten different initial vectors was 6.6 (where at least 4 and at most 9 alternative steps were required to find a projected problem with a real eigenpair) and convergence was obtained after 14.4 steps on

[†]<http://www.comsol.com>

Iteration	$\hat{\omega}$	$\hat{\tau}$	residual norm	remark
1	0.298280	5.266183	$6.49 \cdot 10^{-1}$	alt. sel.
2	1.226607	1.280603	$4.04 \cdot 10^{-4}$	alt. sel.
3	1.682195	1.315610	$5.56 \cdot 10^{-5}$	Ritz sel.
	-1.682195	1.315610	$5.29 \cdot 10^{-5}$	
4	1.785471	1.226493	$4.76 \cdot 10^{-5}$	Ritz sel.
	-1.785471	1.226493	$4.81 \cdot 10^{-7}$	
5	1.785556	1.226393	$3.27 \cdot 10^{-5}$	compl. by $\bar{u}$
	-1.785556	1.226393	$1.69 \cdot 10^{-12}$	conv.
6	1.785556	1.226393	$3.18 \cdot 10^{-12}$	alt. sel.
	-1.785556	1.226393	$1.69 \cdot 10^{-12}$	
	0.189676	8.281467	$2.11 \cdot 10^{-5}$	
7	1.785556	1.226393	$1.65 \cdot 10^{-12}$	alt. sel.
	-1.785556	1.226393	$2.04 \cdot 10^{-12}$	
	0.301713	5.206255	$2.12 \cdot 10^{-5}$	
8	1.785556	1.226393	$2.10 \cdot 10^{-12}$	Ritz sel.
	-1.785556	1.226393	$1.31 \cdot 10^{-12}$	
	0.041958	0.542808	$1.52 \cdot 10^{-5}$	
	-0.041958	0.542808	$1.47 \cdot 10^{-5}$	
9	1.785556	1.226393	$1.63 \cdot 10^{-12}$	Ritz sel.
	-1.785556	1.226393	$3.22 \cdot 10^{-13}$	
	0.119168	0.542465	$1.05 \cdot 10^{-6}$	
	-0.119168	0.542465	$2.33 \cdot 10^{-7}$	
10	1.785556	1.226393	$1.62 \cdot 10^{-12}$	compl. by $\bar{u}$
	-1.785556	1.226393	$1.94 \cdot 10^{-13}$	
	0.119263	0.542468	$5.73 \cdot 10^{-8}$	
	-0.119263	0.542468	$1.16 \cdot 10^{-13}$	
11	1.785556	1.226393	$5.57 \cdot 10^{-13}$	
	-1.785556	1.226393	$1.13 \cdot 10^{-12}$	
	0.119263	0.542468	$8.94 \cdot 10^{-14}$	
	-0.119263	0.542468	$1.35 \cdot 10^{-13}$	

Table I. Results for Example 1 using a direct linear system solver

average (at least 12 and at most 17). Determining only ω randomly and choosing $\tau = \text{const}/\omega$ with the same set of initial vectors only 4.6 (at least 4 and at most 5) initial alternative selections were required and convergence was obtained after 12.6 iterations on average (at least 12 and at most 13). Here we used $\text{const} = \pi/2$ which turned out to be most efficient. Actually the method behaved very similar in a wide interval around $\pi/2$ and only close to 0 and π the convergence deteriorated.

Figure 1 shows a typical convergence history. Four alternative selection steps (marked by triangles) are required until a pair of eigentriples is detected for the projected problem. Thereafter the method needs seven Jacobi–Davidson steps until the residual for one of the solutions (ω, τ, u) does not exceed 10^{-10} (the residuals are marked by bullets whereas the

Iteration	$\hat{\omega}$	$\hat{\tau}$	residual norm	# it.step.	remark
1	0.715967	2.193951	$6.49 \cdot 10^{-1}$		alt. sel.
2	0.244171	12.313196	$3.04 \cdot 10^{-4}$		
	-0.244171	12.313196	$3.04 \cdot 10^{-4}$	3	Ritz sel.
3	1.603328	1.458382	$2.45 \cdot 10^{-4}$		
	-1.603328	1.458382	$2.07 \cdot 10^{-4}$	2	Ritz sel.
4	1.791874	1.222252	$7.75 \cdot 10^{-5}$		
	-1.791874	1.222252	$5.68 \cdot 10^{-6}$	2	Ritz sel.
5	1.785402	1.226548	$6.89 \cdot 10^{-5}$		
	-1.785402	1.226548	$1.53 \cdot 10^{-7}$	3	Ritz sel.
6	1.785556	1.226393	$3.36 \cdot 10^{-5}$		
	-1.785556	1.226393	$4.26 \cdot 10^{-9}$	3	Ritz sel.
7	1.785556	1.226393	$2.89 \cdot 10^{-5}$		
	-1.785556	1.226393	$1.40 \cdot 10^{-10}$	2	Ritz sel.
8	1.785556	1.226393	$2.35 \cdot 10^{-5}$		compl. by $\bar{u}$
	-1.785556	1.226393	$1.51 \cdot 10^{-11}$	2	conv.
9	1.785556	1.226393	$6.92 \cdot 10^{-12}$		
	-1.785556	1.226393	$1.51 \cdot 10^{-11}$		
	1.598648	0.982578	$1.32 \cdot 10^{-5}$		alt. sel.
10	1.785556	1.226393	$1.19 \cdot 10^{-11}$		
	-1.785556	1.226393	$1.56 \cdot 10^{-11}$		
	0.022410	0.542613	$1.79 \cdot 10^{-5}$		
	-0.022410	0.542613	$1.79 \cdot 10^{-5}$	2	Ritz sel.
11	1.785556	1.226393	$1.50 \cdot 10^{-11}$		
	-1.785556	1.226393	$8.37 \cdot 10^{-13}$		
	0.119220	0.542466	$8.89 \cdot 10^{-7}$		
	-0.119220	0.542466	$5.11 \cdot 10^{-7}$	2	Ritz sel.
12	1.785556	1.226393	$8.64 \cdot 10^{-13}$		
	-1.785556	1.226393	$1.50 \cdot 10^{-11}$		
	0.119263	0.542468	$7.87 \cdot 10^{-8}$		
	-0.119263	0.542468	$4.52 \cdot 10^{-9}$	2	Ritz sel.
13	1.785556	1.226393	$3.38 \cdot 10^{-13}$		
	-1.785556	1.226393	$1.51 \cdot 10^{-11}$		
	0.119263	0.542468	$7.19 \cdot 10^{-8}$		
	-0.119263	0.542468	$1.85 \cdot 10^{-10}$	1	Ritz sel.
14	1.785556	1.226393	$5.52 \cdot 10^{-13}$		
	-1.785556	1.226393	$1.52 \cdot 10^{-11}$		
	0.119263	0.542468	$2.19 \cdot 10^{-8}$		compl. by $\bar{u}$
	-0.119263	0.542468	$1.62 \cdot 10^{-12}$		conv.
15	1.785556	1.226393	$5.07 \cdot 10^{-12}$		
	-1.785556	1.226393	$1.00 \cdot 10^{-11}$		
	0.119263	0.542468	$1.57 \cdot 10^{-12}$		
	-0.119263	0.542468	$1.62 \cdot 10^{-12}$		

Table II. Results for Example 1 using GMRES for solving the correction equation

residuals of the second solution of the projected problems are marked by plus signs). Appending $\bar{u}$ to the search space the residual of the second solution is also reduced to less than 10^{-10} . The computations were performed on a Pentium (R) D computer with 3.2 GHz and 3.5 GB RAM under MATLAB R2008b. 40.5 seconds were needed for computing both Ritz triples and additionally 13.4 seconds to determine the preconditioner.

Figure 1. Convergence history for Example 2 with parameter $\alpha = 23$

For $\alpha = 89$ the system has four pairs of eigentriples. We solved it using the same preconditioner and the same parameters for the GMRES solver of the correction equation. We restarted the method if the dimension of the search space exceeded $k = 12$ (recall the complexity $\mathcal{O}(k^6)$ of the structure preserving solver of the projected problems), and we retained the Ritz vectors found so far in the search space after restart [23, 6]. 157.6 seconds were needed to compute all 8 eigentriples. The convergence history is shown in Figure 2. Four restarts were necessary after steps 12, 20, 24 and 28 but this loss of information does not seem to slow down the convergence.

Two alternative selection steps are needed to find the first eigentriple (marked with black triangles) of the projected problem. After 9 Jacobi–Davidson steps the first eigentriple (ω, τ, u) has converged (black bullets). The residual of the approximation to $(-\omega, \tau, \bar{u})$ at that time is nearly untouched (marked by a black square), but appending $\bar{u}$ to the search space convergence is obtained in the next step. A second, third and fourth pair of eigentriples appears in the projected problems in steps 6, 7, and 20, respectively. The convergence of these Ritz triples is displayed in the same way as for the first one in blue, red and green, where we marked the residuals with bullets if the Jacobi–Davidson method is aiming at them and with plus signs otherwise.

Figure 2. Convergence history for Example 2 with parameter $\alpha = 89$

4.3. Example 3

Consider

$$u_t - \nabla((1 + x^2 + y^2 + z^2)\nabla u) + [1, 0, -1]\nabla u + u - \alpha(1 + x^2)u(t - \tau) = 0 \quad (4.3)$$

with spatial variables x, y and z on $\Omega = (0, 1) \times (0, 1) \times (0, 1)$ with Dirichlet boundary condition $u = 0$ on $\partial\Omega$. A discretization with piecewise quadratic ansatz functions on a tetrahedral grid using COMSOL yielded an eigenvalue problem (1.2) of dimension $n = 80623$. For $\alpha = 100$ the problem has four pairs of eigentriples.

Again we used `P=luinc(A,1e-3)` as preconditioner (which due to the higher population of the matrix A required a CPU time of 94.4 seconds) and the same restart strategy and the same parameters for the GMRES solver as in Example 2. The method determined all 8 eigentriples needing 188.4 seconds. The convergence history is shown in Figure 3. It is organized in the same way as in Example 2.

5. Conclusions

We presented a new Jacobi-Davidson type method for the solution of the two-real-parameter eigenvalue problem governing critical delays of a linear system of delay differential equations. The paper contributed in two important ways. Firstly, a structure preserving method was presented for solving the small scale problem, arising from the projection of the large scale problem on the search space. This method only computes real eigen pairs (ω, τ) . Secondly, a

Figure 3. Convergence history for Example 3 with parameter $\alpha = 100$

correction equation was presented that forces (ω, τ) to be real, as desired. We observed that one cannot always rely on the availability of Ritz triples to continue the JD iteration. We proposed an alternative selection strategy that in all cases managed to bridge the steps until Ritz triples could be used. For all test problems, the method converges well, and (if the correction equations are solved accurately enough) shows quadratic convergence behaviour which is typical to this type of methods. We also showed that the method is robust with respect to inexact solves of the correction equation, coarse preconditioners and the choice of starting vector.

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