Continuation of invariant subspaces for parameterized quadratic eigenvalue problems

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Abstract

We consider quadratic eigenvalue problems with large and sparse matrices depending on a parameter. Problems of this type occur, for example, in the stability analysis of spatially discretized and parameterized nonlinear wave equations. The aim of the paper is to present and analyze a continuation method for invariant subspaces that belong to a group of eigenvalues the number of which is much smaller than the dimension of the system. The continuation method is of predictor-corrector type similar to the approach for the linear eigenvalue problem in [5], but we avoid linearizing the problem which will double the dimension and change the sparsity pattern. The matrix equations that occur in the predictor and the corrector step are solved by a bordered version of the Bartels-Stewart algorithm. Furthermore, we set up an update procedure that handles the transition from real to complex conjugate eigenvalues which occur when eigenvalues from inside the continued cluster collide with eigenvalues from outside. The method is demonstrated on several numerical examples: a homotopy between random matrices, a fluid conveying pipe problem, and a traveling wave of a damped wave equation.

1 Introduction

Quadratic eigenvalue problems are ubiquitous in applications to vibrating systems (see the surveys [26],[3],[2]) and usually derive from a second order system

$$Au'' + Bu' + Cu = f(t), \quad u(t), f(t) \in \mathbb{R}^m, A, B, C \in \mathbb{R}^{m,m}.$$

Typically the matrices in this equation are large and sparse and, in addition, depend on parameters. For the stability problem it is sufficient to compute the group of eigenvalues that is closest to the imaginary axis and to study how this group varies with the parameter (see e.g. [27] for such an application).

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This motivates to consider quadratic matrix polynomials that depend on a real parameter $s \in \mathbb{R}$

$$P(\lambda, s) = A(s)\lambda^2 + B(s)\lambda + C(s), \quad \lambda \in \mathbb{C}. \tag{1}$$

We assume the real matrices $A(s), B(s), C(s) \in \mathbb{R}^{m,m}$ to depend smoothly on s. Rather than computing single eigenvalues and eigenvectors we are interested in computing invariant pairs $(X, \Lambda) \in \mathbb{R}^{m,k} \times \mathbb{R}^{k,k}$, i.e. pairs (X, Λ) for which $\begin{pmatrix} X \\ X\Lambda \end{pmatrix}$ has rank k and which satisfy

$$P(\Lambda, s)X = A(s)X\Lambda^2 + B(s)X\Lambda + C(s)X = 0. \tag{2}$$

Note that Jordan pairs, as defined in [14],[26]), correspond to $k = 2m$ with Λ having a Jordan structure. Our interest is in $k \ll 2m$ where $\begin{pmatrix} X \\ X\Lambda \end{pmatrix}$ is a low-dimensional invariant subspace of a linearization. Once (X, Λ) has been computed one can solve the low-dimensional eigenvalue problem $\Lambda y = \lambda y$ (by any existing code) and obtain solutions $v = Xy$ to the quadratic eigenvalue problem

$$P(\lambda, s)v = (A(s)\lambda^2 + B(s)\lambda + C(s))v = 0.$$

The purpose of this paper is to investigate under which conditions smooth solution branches $(X, \Lambda) = (X(s), \Lambda(s))$ of (2) exist and how to compute them in an efficient way.

We will mainly generalize and adapt the techniques from [5] for the linear eigenvalue problem to the quadratic case. Note that related approaches have been developed for the linear invariant subpace problem in [10],[7], however, without discussing singular situations. Our approach will be to perform continuation directly on the quadratic subspace problem (2) rather than applying the known techniques to the linearized problem. The reason for doing this is two-fold. First, there are many ways of linearizing a quadratic (or polynomial) eigenvalue problem and the recent work in [26],[20], [21] shows that the conditioning of the linearized problem can strongly depend on the type of linearization. Second, we keep the original sparsity pattern of the matrices that dominates the structure of the linear systems to be solved. Linearization will generally destroy this pattern and increase the system size simultaneously.

In Section 2 we investigate the relations between the bifurcation problems induced by the quadratic and the linearized subspace problem. In particular, we show that, when using Newton's method for solving the subspace problem, there is a slight difference in the iterates due to second order terms. We also show that turning points for the subspace problem (2) relate to the occurrence of double eigenvalues and the transition from a pair of real eigenvalues to a complex conjugate pair and vice versa. This generalizes a result for single eigenvalues from [23] to invariant subspaces.

The details of the predictor corrector method for solving the system (2) are provided in Section 3. It turns out that in both steps linear matrix equations

with large and sparse bordered matrices have to be solved. We show how the Bartels Stewart algorithm [15] and its bordered version [5] can be generalized to reduce the numerical work to the solution of a sequence of bordered vector equations. Further, in Section 3 we show that the analysis of turning points from Section 2 leads to a switching algorithm for updating the invariant subspace when collisions with outside eigenvalues occur.

In Section 4 we demonstrate our method on several examples: a Galerkin approximation for a fluid conveying pipe problem [27], a traveling wave of a damped wave equation [12],[13], and a homotopy path between two random matrix polynomials,

2 Invariant pairs of quadratic eigenvalue problems and their linearizations

In this section we consider the parameter independent matrix polynomial

$$P(\lambda) = A\lambda^2 + B\lambda + C, \quad \lambda \in \mathbb{C}, \tag{3}$$

where $A, B, C \in \mathbb{K}^{m,m}$, $\mathbb{K} = \mathbb{R}, \mathbb{C}$. We assume that A is nonsingular, i.e the matrix pencil is regular.

2.1 Multiplicity of subspaces and regular solutions

As in [5] for the linear case we define the multiplicity of invariant subspaces for the quadratic case. Let $\sigma(A)$ denote the spectrum of a matrix A.

Definition 2.1. *A pair $(X, \Lambda) \in \mathbb{K}^{m,k} \times \mathbb{K}^{k,k}$ is called an invariant pair of rank k for the quadratic polynomial $P(\lambda)$ if the following two conditions hold*

(i) $\text{rank} \begin{pmatrix} X \\ X\Lambda \end{pmatrix} = k,$

(ii) $AX\Lambda^2 + BX\Lambda + CX = 0.$

The multiplicity of (X, Λ) is defined to be the number $\ell - k + 1$, where ℓ is the largest integer such that an invariant pair $(\tilde{X}, \tilde{\Lambda}) \in \mathbb{K}^{m,\ell} \times \mathbb{K}^{\ell,\ell}$ of rank ℓ satisfying $\sigma(\tilde{\Lambda}) = \sigma(\Lambda)$ exists. An invariant pair of multiplicity 1 is called simple.

The interpretation of this definition in terms of linearizations ([14]) is rather obvious. The columns of $\Phi = \begin{pmatrix} X \\ X\Lambda \end{pmatrix}$ span an invariant subpace of the linearization in first companion form

$$L(\lambda) = M\lambda - N = \begin{pmatrix} I & 0 \\ 0 & A \end{pmatrix} \lambda - \begin{pmatrix} 0 & I \\ -C & -B \end{pmatrix}, \tag{4}$$

i.e. $M\Phi\Lambda - N\Phi = 0$, $\operatorname{rank}(\Phi) = k$. The multiplicity of the pair (X, Λ) then coincides with the multiplicity of the invariant subspace $\operatorname{im}(\Phi)$ of $L(\lambda)$ as defined in [5] (see [25] for the notion of a simple invariant subspace). Note that any two linearizations $L_j(\lambda) = M_j\lambda - N_j, j = 1, 2$ of (3) are equivalent ([14, Ch.1.3]) and the matrices $M_j^{-1}N_j$ are similar, [14, Ch.S1]. Therefore, $L_1(\lambda)$ and $L_2(\lambda)$ have the same maximal dimension ℓ of an invariant subspace with corresponding spectrum equal to $\sigma(\Lambda)$.

In order to turn equation (ii) of Definition 2.1 into a well-posed square system for (X, Λ) we add k^2 normalization conditions. More specifically, we consider the operator

$$T(X, \Lambda) = \begin{pmatrix} AX\Lambda^2 + BX\Lambda + CX \\ \hat{X}^H(X - X_0) + \hat{Y}^H(X\Lambda - X_0\Lambda_0) \end{pmatrix} = 0, \tag{5}$$

where $\hat{X}, \hat{Y}, X_0 \in \mathbb{K}^{m,k}, \Lambda_0 \in \mathbb{K}^{k,k}$ are suitable initial approximations. Later on these matrices will be determined by the predictor in the continuation process. Simple invariant pairs can be characterized as regular solutions of (5) as follows.

Theorem 2.2. *Let $A, B, C \in \mathbb{K}^{m,m}$, $\hat{X}, \hat{Y}, X_0 \in \mathbb{K}^{m,k}$, $\Lambda_0 \in \mathbb{K}^{k,k}$ be given such that $\hat{X}^H X_0 + \hat{Y}^H X_0\Lambda_0$ is nonsingular. Then (X_0, Λ_0) is a simple invariant pair of rank k for $P(\lambda)$ if and only if it is a regular solution of the equation (5).*

Remark 2.3. *Regularity means that the total derivative $DT(X_0, \Lambda_0)$ is nonsingular. Newton's method for solving (5) will then converge locally and quadratically.*

Proof. Adapted to the current setting, Theorem 2 in [5] states the following. Given $\hat{\Phi}, \Phi_0 \in \mathbb{K}^{2m,k}, \Lambda_0 \in \mathbb{K}^{k,k}$ such that $\hat{\Phi}^H\Phi_0$ is nonsingular, the pair (Φ_0, Λ_0) is a regular solution of the matrix equation

$$F(\Phi, \Lambda) = \begin{pmatrix} M\Phi\Lambda - N\Phi \\ \hat{\Phi}^H(\Phi - \Phi_0) \end{pmatrix} = 0 \tag{6}$$

if and only if (Φ_0, Λ_0) is a simple invariant pair of rank k for the linear pencil $L(\lambda) = M\lambda - N$. We apply this result to the linearization (4) with the settings

$$\hat{\Phi} = \begin{pmatrix} \hat{X} \\ \hat{Y} \end{pmatrix}, \quad \Phi_0 = \begin{pmatrix} X_0 \\ X_0\Lambda_0 \end{pmatrix}. \tag{7}$$

First note that $\hat{\Phi}^H\Phi_0$ is nonsingular by assumption and hence Φ_0 has rank k. Further, by the remarks preceding the theorem we infer that (X_0, Λ_0) is a simple invariant pair of rank k for $P(\lambda)$ iff (Φ_0, Λ_0) is a simple invariant pair of rank k for $L(\lambda)$. Therefore, it suffices to show that the regularity of solutions (X_0, Λ_0) to (5) and of (Φ_0, Λ_0) to (6) are equivalent. Using

$$P(\Lambda)X = AX\Lambda^2 + BX\Lambda + CX \tag{8}$$

the derivatives read

$$DT(X_0, \Lambda_0)(H, \Delta) = \begin{pmatrix} P(\Lambda_0)H + AX_0(\Lambda_0\Delta + \Delta\Lambda_0) + BX_0\Delta \\ \hat{X}^H H + \hat{Y}^H(H\Lambda_0 + X_0\Delta) \end{pmatrix} \tag{9}$$

$$DF(\Phi_0,\Lambda_0)(\Psi,\Delta)=\begin{pmatrix}M(\Phi_0\Delta+\Psi\Lambda_0)-N\Psi\\ \hat{\Phi}^H\Psi\end{pmatrix}. \tag{10}$$

Partitioning $\Psi=\begin{pmatrix}\Psi_1\\ \Psi_2\end{pmatrix}$, an easy calculation shows that

$$DF(\Phi_0,\Lambda_0)(\Psi,\Delta)=\begin{pmatrix}X_0\Delta+\Psi_1\Lambda_0-\Psi_2\\ G\end{pmatrix}$$

where $G=DT(X_0,\Lambda_0)(\Psi_1,\Delta)$ if

$$X_0\Delta+\Psi_1\Lambda_0=\Psi_2. \tag{11}$$

Hence, if $0\neq(H,\Delta)\in\ker(DT(X_0,\Lambda_0))$ then

$$0\neq\left(\begin{pmatrix}H\\ X_0\Delta+H\Lambda_0\end{pmatrix},\quad\Delta\right)\in\ker DF(\Phi_0,\Lambda_0).$$

Conversely, if $0\neq(\Psi,\Delta)\in\ker DF(\Phi_0,\Lambda_0)$ then $0\neq(\Psi_1,\Delta)\in\ker DT(X_0,\Lambda_0)$ where $\Psi=\begin{pmatrix}\Psi_1\\ \Psi_2\end{pmatrix}$. Note that $\Psi_1=0,\Delta=0$ implies $\Psi_2=0$ by (11). □

2.2 Nonequivalence of Newton's method

In the previous section we saw that regularity of the derivatives (9) and (10) transforms into each other. Thus local convergence of Newton's method for (6) and (5) is guaranteed under the same conditions. We now show that the Newton corrections of one step also transform into each other, whereas the Newton steps themselves don't.

Proposition 2.4. *Let the relations (7) for the normalizing matrices hold and consider one Newton step for (5)*

$$DT(X,\Lambda)(H,\Delta_T)=-T(X,\Lambda),\quad(\tilde{X},\tilde{\Lambda}_T)=(X,\Lambda)+(H,\Delta_T) \tag{12}$$

and one Newton step for (6)

$$DF(\Phi,\Lambda)(\Psi,\Delta_F)=-F(\Phi,\Lambda),\quad(\tilde{\Phi},\tilde{\Lambda}_F)=(\Phi,\Lambda)+(\Psi,\Delta_F). \tag{13}$$

If the initial data are related by $\Phi=\begin{pmatrix}X\\ X\Lambda\end{pmatrix}$ *then* $DT(X,\Lambda)$ *is nonsingular if and only if* $DF(\Phi,\Lambda)$ *is nonsingular, and in this case the following holds*

$$\begin{aligned}&\Delta_F=\Delta_T,\quad\Psi=\begin{pmatrix}H\\ H\Lambda+X\Delta_T\end{pmatrix},\\ &\tilde{\Delta}_F=\tilde{\Delta}_T,\quad\tilde{\Phi}=\begin{pmatrix}\tilde{X}\\ \tilde{X}\tilde{\Lambda}_T\end{pmatrix}-\begin{pmatrix}0\\ H\Delta_T\end{pmatrix}.\end{aligned} \tag{14}$$

Remark 2.5. *Equation (14) shows that the Λ-correction is identical for both systems whereas the invariant pair update differs by the second order term $H\Delta_T$. Therefore, the Newton iterates of (5) and (6) will generally not transform into each other through linearization.*

Proof. The equivalence of invertibility for $DF(\Phi,\Lambda)$ and $DT(X,\Lambda)$ was shown in the proof of Theorem 2.2. It remains to show (14). Using (7),(9) we find that the equations in (12) read

$$AH\Lambda^2+AX(\Lambda\Delta_T+\Delta_T\Lambda)+B(H\Lambda+X\Delta_T)+CH = -AX\Lambda^2-BX\Lambda-CX, \quad (15)$$

$$\hat{X}^H H + \hat{Y}(H\Lambda + X\Delta_T) = -\hat{X}(X - X_0) - \hat{Y}^H(X\Lambda - X_0\Lambda_0), \quad (16)$$

whereas (13) leads to

$$\begin{aligned} \Phi_1\Delta_F + \Psi_1\Lambda - \Psi_2 &= -\Phi_1\Lambda + \Phi_2, \\ A(\Phi_2\Delta_F + \Psi_2\Lambda) + C\Psi_1 + B\Psi_2 &= -(A\Phi_2\Lambda + C\Phi_1 + B\Phi_2), \\ \hat{X}^H\Psi_1 + \hat{Y}^H\Psi_2 &= -(\hat{X}^H(\Phi_1 - X_0) + \hat{Y}^H(\Phi_2 - X_0\Lambda_0)). \end{aligned} \quad (17)$$

Setting $\Phi_1 = X, \Phi_2 = X\Lambda, \Psi_1 = H, \Psi_2 = H\Lambda + X\Delta_T, \Delta_F = \Delta_T$ in (17) we see that the first equation is trivially satisfied while the second and the third agree exactly with (15),(16). Finally, we note that

$$\tilde{\Phi}_2 = \Phi_2 + \Psi_2 = X\Lambda + H\Lambda + X\Delta_T = (X + H)(\Lambda + \Delta_T) - H\Delta_T.$$

□

2.3 Equivalence of turning points

In this section we consider the simplest type of singular (i.e. nonregular) solution of (5) that occurs in real systems $\mathbb{K} = \mathbb{R}$. In one-parameter systems we find such singular solutions at turning points where the branch of solutions has a tangent that is vertical with respect to the parameter (see e.g. [1],[18],[4]). Two of the conditions for a quadratic turning point (X_0, Λ_0) are

$$\ker(DT(X_0,\Lambda_0)) = \operatorname{span}\{(H_0,\Delta_0)\} \quad \text{with } 0 \neq (H_0,\Delta_0) \in \mathbb{R}^{m,k} \times \mathbb{R}^{k,k}, \quad (18)$$

$$D^2T(X_0,\Lambda_0)(H_0,\Delta_0)^2 \notin \operatorname{im}(DT(X_0,\Lambda_0)). \quad (19)$$

The third condition describes transversality with respect to the parameter, see Proposition 3.1. A characterization of (18),(19) in terms of multiplicities was shown in [5] for the linear subspace problem. The following result generalizes this to the quadratic eigenvalue problem.

Theorem 2.6. *Let the assumptions of Theorem 2.2 hold. Then the following conditions are equivalent.*

(i) The pair $(X_0,\Lambda_0) \in \mathbb{R}^{m,k} \times \mathbb{R}^{k,k}$ is a singular solution of (5) that satisfies conditions (18),(19).

(ii) The pair $(X_0, \Lambda_0) \in \mathbb{R}^{m,k} \times \mathbb{R}^{k,k}$ *is an invariant pair of rank* k *for the quadratic polynomial* $P(\lambda)$ *that has multiplicity two. There exists a real eigenvalue* $\lambda_0 \in \sigma(\Lambda_0)$ *of multiplicity two such that*

$$P(\lambda_0)v_0 = 0, \quad P(\lambda_0)v_1 = P'(\lambda_0)v_0, \tag{20}$$

for some $v_0 \in \mathrm{im}(X_0)\backslash\{0\}$ *and* $\begin{pmatrix} v_1 \\ \lambda_0 v_1 - v_0 \end{pmatrix} \notin \mathrm{im} \begin{pmatrix} X_0 \\ X_0\Lambda_0 \end{pmatrix}$.

Remark 2.7. *We give an interpretation of condition (ii). Equation (20) states that there is an eigenvector* v_0 *with eigenvalue* $\lambda_0 \in \sigma(\Lambda_0)$ *and a generalized eigenvector* v_1 *that is not represented by the invariant pair* (X_0, Λ_0) *in the following sense. Note that* $\begin{pmatrix} X_0 \\ X_0\Lambda_0 \end{pmatrix}$ *has rank* k *by our assumptions and that* $\begin{pmatrix} v_0 \\ \lambda_0 v_0 \end{pmatrix} \in \mathrm{im} \begin{pmatrix} X_0 \\ X_0\Lambda_0 \end{pmatrix}$ *by the proof below. Hence there exists a unique* $c_0 \in \mathbb{R}^k$ *such that*

$$v_0 = X_0 c_0, \quad X_0(\Lambda_0 - \lambda_0 I)c_0 = 0.$$

But, according to condition (ii), there is no $c_1 \in \mathbb{R}^k$ *such that*

$$v_1 = X_0 c_1, \quad X_0((\Lambda_0 - \lambda_0 I)c_1 + c_0) = 0.$$

Proof. Similar to Theorem 2.2 we use the characterization of singular solutions of the linearized system (6) from [5, Theorem 3]. For matrices $\hat{\Phi}, \Phi_0 \in \mathbb{R}^{2m,k}$, $\hat{\Phi}^T\Phi_0$ nonsingular, the following are equivalent

(i′) $(\Phi_0, \Lambda_0) \in \mathbb{R}^{2m,k} \times \mathbb{R}^{k,k}$ is a singular solution of (6) satisfying

$$\ker(DF(\Phi_0, \Lambda_0)) = \mathrm{span}\{(\Psi_0, \Delta_0)\} \quad \text{with } 0 \neq (\Psi_0, \Delta_0) \in \mathbb{R}^{2m,k} \times \mathbb{R}^{k,k}, \tag{21}$$

$$D^2F(\Phi_0, \Lambda_0)(\Psi_0, \Delta_0)^2 \notin \mathrm{im}(DF(\Phi_0, \Lambda_0)). \tag{22}$$

(ii′) (Φ_0, Λ_0) is an invariant pair of $L(\lambda) = \lambda M - N$ of rank k and with multiplicity 2. There exist $\lambda_0 \in \sigma(\Lambda_0) \cap \mathbb{R}$ and $\varphi_0 \in \mathrm{im}(\Phi_0)$, $\varphi_1 \notin \mathrm{im}(\Phi_0)$ such that

$$\lambda_0 M\varphi_0 - N\varphi_0 = 0, \quad \lambda_0 M\varphi_1 - N\varphi_1 = M\varphi_0. \tag{23}$$

With the settings (4),(7) it is sufficient to prove the equivalences $(i) \iff (i')$ and $(ii) \iff (ii')$.

Proof of (i) $\iff$ (i′)

Using the arguments from the end of the proof of Theorem 2.2 we find that (18) implies (21) with

$$\Psi_0 = \begin{pmatrix} H_0 \\ X_0\Delta_0 + H_0\Lambda_0 \end{pmatrix}. \tag{24}$$

Conversely, if (21) holds for (Ψ_0, Δ_0) and we set $\Psi_0 = \begin{pmatrix} H_0 \\ \Psi_2 \end{pmatrix}$ then we obtain $\Psi_2 = X_0\Delta_0 + H_0\Lambda_0$ from (11) and condition (18) follows. Next we evaluate the second derivative of F. Using (10), (7), (24) we find that the condition

$$DF(\Phi_0, \Lambda_0)(\Psi, \tilde{\Delta}) = D^2F(\Phi_0, \Lambda_0)(\Psi_0, \Delta_0)^2$$

holds for some $\Psi = \begin{pmatrix} \Psi_1 \\ \Psi_2 \end{pmatrix} \in \mathbb{R}^{2m,k}$, $\tilde{\Delta} \in \mathbb{R}^{k,k}$ if and only if the following equations are satisfied

$$\begin{aligned} X_0\tilde{\Delta} + \Psi_1\Lambda_0 - \Psi_2 &= 2H_0\Delta_0 && (25)\\ A(X_0\Lambda_0\tilde{\Delta} + \Psi_2\Lambda_0) + B\Psi_2 + C\Psi_1 &= 2A(X_0\Delta_0 + H_0\Lambda_0)\Delta_0 && (26)\\ \hat{X}^T\Psi_1 + \hat{Y}^T\Psi_2 &= 0. && (27) \end{aligned}$$

Similarly, the condition

$$DT(X_0, \Lambda_0)(H, \Delta) = D^2T(X_0, \Lambda_0)(H_0, \Delta_0)^2$$

is equivalent to the set of equations

$$\begin{aligned} P(\Lambda_0)H + AX_0(\Lambda_0\Delta + \Delta\Lambda_0) + BX_0\Delta = 2AH_0(\Lambda_0\Delta_0 + \Delta_0\Lambda_0) \\ + BH_0\Delta_0 + AX_0\Delta_0^2 \end{aligned} \quad (28)$$

$$\hat{X}^TH + \hat{Y}(H\Lambda_0 + X_0\Delta) = 2\hat{Y}^TH_0\Delta_0. \quad (29)$$

If one solves (25) for Ψ_2 and inserts this into (26), (27) then one obtains equations (28),(29). Therefore, if $(\Psi, \tilde{\Delta})$ is a solution of (25)-(27), then $(H, \Delta) = (\Psi_1, \tilde{\Delta}))$ solves (28),(29). Conversely, any solution (H, Δ) of (28),(29) leads to a solution

$$\Psi = \begin{pmatrix} H \\ X_0\Delta + H\Lambda_0 - 2H_0\Delta_0 \end{pmatrix}, \quad \tilde{\Delta} = \Delta$$

of the system (25)-(27). This proves that (19) and (22) are equivalent.

Proof of (ii) $\Longleftrightarrow$ (ii′) By the discussion following Definition 2.1 we know that the multiplicities of the invariant pairs (X_0, Λ_0) for $P(\lambda)$ and of (Φ_0, Λ_0) for $L(\lambda)$ are the same (see (7) for the definition of Φ_0).

First, let (ii) be satisfied. We define

$$\varphi_0 = \begin{pmatrix} v_0 \\ \lambda_0 v_0 \end{pmatrix}, \quad \varphi_1 = \begin{pmatrix} v_1 \\ \lambda_0 v_1 - v_0 \end{pmatrix} \quad (30)$$

and with (20) readily verify that

$$\lambda_0 M\varphi_0 - N\varphi_0 = 0 \quad \lambda_0 M\varphi_1 - N\varphi_1 = M\varphi_0. \quad (31)$$

By assumption we have $\varphi_1 \notin \mathrm{im}(\Phi_0)$, therefore it remains to show $\varphi_0 \in \mathrm{im}(\Phi_0)$. Since (Φ_0, Λ_0) has multiplicity 2 there exist an invariant subspace $Y \supset \mathrm{im}(\Phi_0)$,

$\dim(Y) = k+1$ of $M^{-1}N$ which belongs to the spectral set $\sigma(\Lambda_0)$ and which is maximal with this property. From (31) and $\lambda_0 \in \sigma(\Lambda_0)$ we conclude $\varphi_1 \in Y$. Since $\varphi_1 \notin \mathrm{im}(\Phi_0)$ we have $Y = \mathrm{im}(\Phi_0) \oplus \mathrm{span}\{\varphi_1\}$. Therefore, there are unique $c \in \mathbb{R}^k$ and $\rho \in \mathbb{R}$ such that $\varphi_0 = \Phi_0 c + \rho\varphi_1$. If $\rho = 0$ then $\varphi_0 \in \mathrm{im}(\Phi_0)$ as claimed. If $\rho \neq 0$ then

$$\begin{aligned} 0 &= M^{-1}N\varphi_0 - \lambda_0\varphi_0 \\ &= (M^{-1}N\Phi_0 - \lambda_0\Phi_0)c + \rho(M^{-1}N\varphi_1 - \lambda_0\varphi_1) \\ &= \Phi_0(\Lambda_0 - \lambda_0 I)c - \rho\varphi_0 \end{aligned}$$

implies $\varphi_0 \in \mathrm{im}(\Phi_0)$.

The implication $(ii') \Longrightarrow (ii)$ is shown easily. Let us write $\varphi_0 = \begin{pmatrix} v_0 \\ w_0 \end{pmatrix}$ and $\varphi_1 = \begin{pmatrix} v_1 \\ w_1 \end{pmatrix}$. Then (23) implies (20) as well as the relations

$$w_0 = \lambda_0 v_0, \quad w_1 = \lambda_0 v_1 - v_0.$$

Therefore, the last conditions in (ii) follow from $\varphi_0 \in \mathrm{im}(\Phi_0)$ and $\varphi_1 \notin \mathrm{im}(\Phi_0)$. □

For later purposes in Section 3.3.2 we note that one can actually use the pair (H_0, Δ_0) in the kernel (see (18)) for computing an invariant pair (X_1, Λ_1) of rank $k+1$ that extends the pair (X_0, Λ_0).

Theorem 2.8. *Let the assumptions of Theorem 2.2 hold and let condition (i) of Theorem 2.6 be satisfied. Then the matrix H_0 is of rank 1 and has the form*

$$H_0 = v_1\psi^T, \quad \textit{where} \quad 0 \neq \psi \in \mathbb{R}^k, \psi^T\Lambda_0 = \lambda_0\psi^T. \tag{32}$$

The extended matrices

$$X_1 = \begin{pmatrix} X_0 & v_1 \end{pmatrix} \in \mathbb{R}^{m,k+1}, \quad \Lambda_1 = \begin{pmatrix} \Lambda_0 & \frac{1}{\psi^T\psi}\Delta_0\psi \\ 0 & \lambda_0 \end{pmatrix} \in \mathbb{R}^{k+1,k+1} \tag{33}$$

form an invariant pair for $P(\lambda)$ of rank $k+1$.

Proof. We use the the property (21) for the linearized system (6). It is shown in [5, Theorem 3] that the matrix Ψ_0 in (21) is of rank 1 and has the form

$$\Psi_0 = \varphi_1\psi^T, \quad 0 \neq \psi \in \mathbb{R}^k, \tag{34}$$

where φ_1 is the generalized eigenvector from (23). Using (34),(23) in (21) yields

$$\begin{aligned} 0 &= M\Psi_0\Lambda_0 - N\Psi_0 + M\Phi_0\Delta_0 \\ &= M\varphi_1\psi^T\Lambda_0 - N\varphi_1\psi^T + M\Phi_0\Delta_0 \\ &= M\left[\varphi_1\psi^T(\Lambda_0 - \lambda_0 I) + \varphi_0\psi^T + \Phi_0\Delta_0\right]. \end{aligned}$$

From the nonsingularity of M and $\varphi_0 \in \mathrm{im}(\Phi_0)$, $\varphi_1 \notin \mathrm{im}(\Phi_0)$ we conclude $\psi^T(\Lambda_0 - \lambda_0 I) = 0$. Multiplying by ψ from the right yields $\varphi_0 \psi^T \psi = -\Phi_0 \Delta_0 \psi$. We combine this with (23) to obtain

$$\begin{aligned}\begin{pmatrix} N\Phi_0 & N\varphi_1 \end{pmatrix} &= \begin{pmatrix} M\Phi_0\Lambda_0 & \lambda_0 M\varphi_1 - M\varphi_0 \end{pmatrix} \\ &= M \begin{pmatrix} \Phi_0 & \varphi_1 \end{pmatrix} \begin{pmatrix} \Lambda_0 & \frac{1}{\psi^T\psi}\Delta_0\psi \\ 0 & \lambda_0 \end{pmatrix}. \end{aligned} \tag{35}$$

Therefore, $\Phi_1 = \begin{pmatrix} \Phi_0 & \varphi_1 \end{pmatrix}$ and Λ_1 form an invariant pair of rank $k+1$ for the linearization $L(\lambda) = M\lambda - N$. By (7),(30) the matrix X_1 from (33) is the upper block of Φ_1 and hence, together with Λ_1, forms an invariant pair of rank $k+1$ for $P(\lambda)$. □

3 Continuation of invariant pairs

3.1 Existence and smooth dependence of branches

In this section we consider the quadratic matrix polynomial $P(\lambda, s)$ from (1) that depends smoothly on a parameter $s \in \mathbb{R}$ and we ask for a smooth family of invariant pairs $(X(s), \Lambda(s))$ of rank $k \leq 2m$, i.e.

$$P(\Lambda(s), s)X(s) = A(s)X(s)\Lambda(s)^2 + B(s)X(s)\Lambda(s) + C(s)X(s) = 0.$$

The matrices $X(s) \in \mathbb{R}^{m,k}$ will be normalized by

$$\hat{X}^T(X(s) - X_0) + \hat{Y}^T(X(s)\Lambda(s) - Y_0) = 0,$$

where $\hat{X}, \hat{Y}, X_0 \in \mathbb{R}^{m,k}, \hat{\Lambda}, \Lambda_0 \in \mathbb{R}^{k,k}, Y_0 = X_0\Lambda_0$ are suitable rank k matrices. These will be fixed during a single predictor and corrector step, but they will vary during global continuation along the branch.

Suppose that, initially, we have a simple invariant pair (X_0, Λ_0) of rank k for $P(\lambda, s_0)$ and we set $\hat{X} = X_0, \hat{Y} = Y_0 = X_0\Lambda_0$. By Theorem 2.2 we can apply the implicit function theorem near (X_0, Λ_0, s_0) to the equation

$$T(X, \Lambda, s) = \begin{pmatrix} A(s)X\Lambda^2 + B(s)X\Lambda + C(s)X \\ \hat{X}^T(X - X_0) + \hat{Y}^T(X\Lambda - Y_0) \end{pmatrix} = 0. \tag{36}$$

This yields a locally unique and smooth branch $(X(s), \Lambda(s))$, $|s - s_0| \leq \varepsilon$ of simple invariant pairs of rank k for the polynomial $P(\lambda, s)$ such that $X(s_0) = X_0, \Lambda(s_0) = \Lambda_0$.

In the following we first consider the continuation of these simple pairs. Then we treat the case of turning points on the branch where the continued subspace will be inflated.

3.2 Continuation of simple branches

We discuss the details of implementing a standard predictor corrector method (see e.g. [1],[18],[4]) for continuing a branch of simple invariant pairs $(X(s), \Lambda(s))$ as above.

3.2.1 Predictor

Assume that (X_0, Λ_0) is a regular solution of (36) at $s = s_0$. Then we compute the tangent

$$(H_0, \Delta_0) = (X'(s_0), \Lambda'(s_0))$$

to the branch $(X(s), \Lambda(s))$ at $s = s_0$ from

$$D_{(X,\Lambda)}T(X_0, \Lambda_0, s_0)(H_0, \Delta_0) = -D_sT(X_0, \Lambda_0, s_0).$$

Using (9) and the operator $P(\Lambda_0, s_0)$ from (2) we obtain the following linear system of dimension $(m + k)k$ for (H_0, Δ_0)

$$\begin{pmatrix} P(\Lambda_0, s_0)H_0 + A(s_0)X_0(\Delta_0\Lambda_0 + \Lambda_0\Delta_0) + B(s_0)X_0\Delta_0 \\ \hat{X}^T H_0 + \hat{Y}^T(X_0\Delta_0 + H_0\Lambda_0) \end{pmatrix} = \begin{pmatrix} -(A'(s_0)X_0\Lambda_0^2 + B'(s_0)X_0\Lambda_0 + C'(s_0)X_0) \\ 0 \end{pmatrix}. \tag{37}$$

This matrix system for H_0, Δ_0 contains a singular part $H_0 \to P(\Lambda_0, s_0)H_0$ bordered by k^2 extra unknowns and equations. When linearizing $P(\Lambda_0, s_0)$ one obtains a matrix equation of Sylvester type (see [15]) that is again singular. It is essential to use the bordering for a stable solution. An algorithm for solving (37) that exploits this structure will be provided in Section 3.2.3 below.

Given a stepsize $\delta > 0$ and the solution (H_0, Δ_0) of (37) we compute the predictor from

$$(X_1, \Lambda_1, s_1) = (X_0, \Lambda_0, s_0) + \delta(H_0, \Delta_0, 1). \tag{38}$$

3.2.2 Corrector

In the corrector step we solve the system (36) with $(s, \hat{X}, X_0, \hat{Y}, Y_0)$ replaced by $(s_1, X_0, X_1, X_0\Lambda_0, X_1\Lambda_1)$, i.e. we use the predicted values and adapt the normalization condition. We note that Theorem 2.2 does no longer apply directly to this adapted equation. But for small δ we have changed the system (36) only slightly and thus still expect to have a unique solution. Starting at (X_1, Λ_1), Newton's method generates the sequence (X_ν, Λ_ν), $\nu \geq 1$ defined by $(X_{\nu+1}, \Lambda_{\nu+1}) = (X_\nu, \Lambda_\nu) + (H_\nu, \Delta_\nu)$ where

$$\begin{aligned} P(\Lambda_\nu, s_1)H_\nu + A(s_1)X_\nu(\Lambda_\nu\Delta_\nu + \Delta_\nu\Lambda_\nu) + B(s_1)X_\nu\Delta_\nu &= -P(\Lambda_\nu, s_1), \\ \hat{X}^T H_\nu + \hat{Y}^T(X_\nu\Delta_\nu + H_\nu\Lambda_\nu) &= 0. \end{aligned} \tag{39}$$

Note that the right hand side of the normalization equation stays always zero during iteration. The system (39) is of the same type as (37) and is solved by the algorithm below.

3.2.3 The bordered Bartels Stewart algorithm

Both linear systems (37), (39) are of the form

$$\begin{pmatrix} P(\Lambda)H + AX(\Delta\Lambda + \Lambda\Delta) + BX\Delta \\ \hat{X}^T H + \hat{Y}^T(X\Delta + H\Lambda) \end{pmatrix} = \begin{pmatrix} R \\ S \end{pmatrix} \tag{40}$$

where $H, R, \hat{X}, \hat{Y} \in \mathbb{R}^{m,k}$, $S, \Lambda, \Delta \in \mathbb{R}^{k,k}$ and $\sigma(\Lambda) \subset \sigma(P(\cdot))$ with P as in (8). Using the underlying idea of the Bartels Stewart algorithm for Sylvester equations [15] we reduce equation (40) to a sequence of linear systems with borderings of matrices $P(\lambda), \lambda \in \sigma(\Lambda_0)$. As in [5] we call this the *bordered Bartels-Stewart algorithm.*

First compute the complex Schur decomposition of the matrix Λ (see [15])

$$Q^H \Lambda Q = \tilde{\Lambda}, \quad Q^H Q = I, \quad \tilde{\Lambda} \text{ upper triangular.} \tag{41}$$

This involves solving an eigenvalue problem of very small dimension $k \ll 2m$. Using $\Lambda^2 Q = Q\tilde{\Lambda}^2$ we transform (40) into

$$\begin{pmatrix} P(\tilde{\Lambda})\tilde{H} + AX\tilde{\Delta}\tilde{\Lambda} + (AX\Lambda + BX)\tilde{\Delta} \\ \hat{X}^T\tilde{H} + \hat{Y}^T(\tilde{H}\tilde{\Lambda} + X\tilde{\Delta}) \end{pmatrix} = \begin{pmatrix} \tilde{R} \\ \tilde{S} \end{pmatrix}$$

where

$$\tilde{R} = RQ, \ \tilde{S} = SQ, \ \tilde{H} = HQ, \ \tilde{\Delta} = \Delta Q. \tag{42}$$

Since $\tilde{\Lambda}$ is upper triangular we can compute the columns $\tilde{H}_j, \tilde{\Delta}_j$ of $\tilde{H}, \tilde{\Delta}$ recursively as in the Bartels-Stewart algorithm (see [15], Ch. 7.6.3) from a sequence of k bordered (complex) linear systems

$$\begin{pmatrix} P(\tilde{\Lambda}_{jj}) & AX(\Lambda + \tilde{\Lambda}_{jj}I) + BX \\ \hat{X}^T + \tilde{\Lambda}_{jj}\hat{Y}^T & \hat{Y}^T X \end{pmatrix} \begin{pmatrix} \tilde{H}_j \\ \tilde{\Delta}_j \end{pmatrix} = \\ \begin{pmatrix} \tilde{R}_j - \sum_{\nu=1}^{j-1} \left[\tilde{\Lambda}_{\nu j}(AX\tilde{\Delta}_\nu + B\tilde{H}_\nu) + (\tilde{\Lambda}^2)_{\nu j} A\tilde{H}_\nu \right] \\ \tilde{S}_j - \sum_{\nu=1}^{j-1} \tilde{\Lambda}_{\nu j}\hat{Y}^T\tilde{H}_\nu \end{pmatrix}, \quad j = 1, \ldots, k. \tag{43}$$

Using (42) the solution H, Δ is obtained from $\tilde{H}, \tilde{\Delta}$. Note that, although the system is complex, the final solution H, Δ will be real. The important feature of the system above is that the upper left block $P(\tilde{\Lambda}_{jj})$ is typically a large sparse, almost singular matrix. Systems of this type occur quite frequently in bifurcation problems and several approaches for their efficient and stable solution have been developed that use several calls of a black box solver for $P(\tilde{\Lambda}_{jj})$ or its transpose, [6],[16],[17], [22], [24]. During the continuation of k-dimensional simple invariant pairs we can expect that its rank drops at most by k which can be compensated for by the bordering.

3.3 Turning points and subspace updates

3.3.1 Pseudo-arclength continuation

Rather than parameterizing solution branches of (36) by the given parameter s we apply a path following algorithm to compute smooth solution branches of

the form

$$(X(t), \Lambda(t), s(t)) \in \mathbb{R}^{m,k} \times \mathbb{R}^{k,k} \times \mathbb{R}, \quad t \in \mathbb{R}. \tag{44}$$

Using Theorem 2.6 we show that at a turning point (i.e. $\frac{ds}{dt}(t) = 0, \frac{d^2s}{dt^2}(t) \neq 0$) a real eigenvalue from the continued cluster $\sigma(\Lambda(t))$ collides with an eigenvalue from outside to form a complex conjugate pair, see the discussion in Section 3.3.2. In order to deal with such bifurcations of real eigenvalues, but also for reasons of computational efficiency, we use a pseudo arclength method for (36) which adds an extra equation of the form

$$\langle \dot{X}, X - X_0 \rangle + \langle \dot{\Lambda}, \Lambda - \Lambda_0 \rangle + \dot{s}(s - s_0) = \delta. \tag{45}$$

Here δ is some step-size, the matrices $\dot{X} \in \mathbb{R}^{m,l}$, $\dot{\Lambda} \in \mathbb{R}^{k,k}$ and $\dot{s} \in \mathbb{R}$ are approximate tangent vectors from the previous point on the branch, and we use a (suitably scaled) inner product for rectangular matrices

$$\langle A, B \rangle = \frac{1}{\ell k} \operatorname{trace}(A^T B) \quad \text{for } A, B \in \mathbb{R}^{\ell,k}.$$

For completeness we write down the analogs of (37)-(39) in this setting. The tangent (H_0, Δ_0, τ_0) to the branch at (X_0, Λ_0, s_0) is computed from

$$\begin{pmatrix} D_{(X,\Lambda)}T^0 & D_s T^0 \\ \langle \dot{X}| & \langle \dot{\Lambda}| \quad \dot{s} \end{pmatrix} \begin{pmatrix} (H_0, \Delta_0) \\ \tau_0 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \tag{46}$$

where T is given in (36) and the upper index 0 indicates evaluation at (X_0, Λ_0, s_0). The predicted point is

$$(X_1, \Lambda_1, s_1) = (X_0, \Lambda_0, s_0) + \delta(H_0, \Delta_0, \tau_0).$$

The corrector solves the system

$$\begin{pmatrix} T(X, \Lambda, s) \\ \langle \dot{X}, X - X_1 \rangle + \langle \dot{\Lambda}, \Lambda - \Lambda_1 \rangle + \dot{s}(s - s_1) \end{pmatrix} = 0.$$

Starting at (X_1, Λ_1, s_1) the Newton steps are

$$(X_{\nu+1}, \Lambda_{\nu+1}, s_{\nu+1}) = (X_\nu, \Lambda_\nu, s_\nu) + (H_\nu, \Delta_\nu, \sigma_\nu), \quad \nu \geq 1 \tag{47}$$

where

$$\begin{pmatrix} D_{(X,\Lambda)}T^\nu & D_s T^\nu \\ \langle \dot{X}| & \langle \dot{\Lambda}| \quad \dot{s} \end{pmatrix} \begin{pmatrix} (H_\nu, \Delta_\nu) \\ \sigma_\nu \end{pmatrix} = - \begin{pmatrix} T^\nu \\ 0 \end{pmatrix}. \tag{48}$$

Equations (46) and (48) lead to linear systems for $H \in \mathbb{R}^{m,k}$, $\Delta \in \mathbb{R}^{k,k}$ and $\mu \in \mathbb{R}$ of the following type (compare (40))

$$\begin{aligned} P(\Lambda)H + AX(\Delta\Lambda + \Lambda\Delta) + BX\Delta + \Gamma\mu &= R \in \mathbb{R}^{m,k} \\ \hat{X}^T H + \hat{Y}^T(X\Delta + H\Lambda) &= S \in \mathbb{R}^{k,k} \\ \langle \dot{X}, H \rangle + \langle \dot{\Lambda}, \Delta \rangle + \dot{s}\mu &= d \in \mathbb{R} \end{aligned} \tag{49}$$

where $\Gamma \in \mathbb{R}^{m,k}$. For example, in the predictor step we have

$$\Gamma = D_s P(\Lambda_0, s_0) X_0 = A'(s_0) X_0 \Lambda_0^2 + B'(s_0) X_0 \Lambda_0 + C'(s_0) X_0.$$

The bordered Bartels-Stewart from Section 3.2.3 can be modified for this case as follows. First, put Λ into upper triangular form as in (41) and transform the data as in (42) where in addition $\tilde{X} = \dot{X}Q, \tilde{\Lambda} = \dot{\Lambda}Q$. For simplicity we drop the "˜" and work with (49) where Λ is upper triangular. We compute the columns H_j, Δ_j of H, Δ and the value μ via the ansatz

$$(H_j, \Delta_j, \mu) = (H_j^0, \Delta_j^0, \mu_j^0) + \sum_{i=1}^{j} \alpha_i (H_j^i, \Delta_j^i, \mu_j^i), \ j = 1, \ldots, k. \tag{50}$$

Defining the bordered matrix

$$M_j = \begin{pmatrix} P(\Lambda_{jj}, s_0) & AX(\Lambda + \Lambda_{jj} I) + BX & \Gamma_j \\ \hat{X}^T + \Lambda_{jj} \hat{Y}^T & \hat{Y}^T X & 0 \\ \frac{1}{mk} \dot{X}_j^T & \frac{1}{k^2} \dot{\Lambda}_j^T & \frac{\dot{s}}{k} \end{pmatrix} \tag{51}$$

we determine the unknowns in (50) for $j = 1, \ldots, k$ from

$$M_j \begin{pmatrix} H_j^0 \\ \Delta_j^0 \\ \mu_j^0 \end{pmatrix} = \begin{pmatrix} R_j - \sum_{i=1}^{j-1} \Lambda_{ij} (AX\Delta_i^0 + BH_i^0) + (\tilde{\Lambda}^2)_{ij} AH_i^0 \\ \tilde{S}_j - \sum_{i=1}^{j-1} \Lambda_{ij} \hat{Y}^T H_i^0 \\ 0 \end{pmatrix},$$

$$M_j \begin{pmatrix} H_j^i \\ \Delta_j^i \\ \mu_j^i \end{pmatrix} = \begin{pmatrix} -\sum_{\nu=1}^{j-1} \Lambda_{\nu j} (AX\Delta_\nu^i + BH_\nu^i) + (\Lambda^2)_{\nu j} AH_\nu^i \\ -\sum_{\nu=1}^{j-1} \Lambda_{\nu j} \hat{Y}^T H_\nu^i \\ 0 \end{pmatrix} \quad \text{for } i = 1, \ldots, j-1,$$

$$M_j \begin{pmatrix} H_j^j \\ \Delta_j^j \\ \mu_j^j \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}.$$

The last entry $\frac{\dot{s}}{k}$ guarantees that M_j is nonsingular even in the predictor step where we normalize with $(\dot{X}, \dot{\Lambda}, \dot{s}) = (0, 0, 1)$. Finally, the α_i are calculated from the k-dimensional system

$$\begin{pmatrix} \mu_2^1 - \mu_1^1 & \mu_2^2 & & \\ \vdots & \vdots & \ddots & \\ \mu_k^1 - \mu_1^1 & \mu_k^2 & \cdots & \mu_k^k \\ 1 & \cdots & & 1 \end{pmatrix} \begin{pmatrix} \alpha_1 \\ \vdots \\ \alpha_k \end{pmatrix} = \begin{pmatrix} \mu_1^2 - \mu_2^3 \\ \vdots \\ \mu_1^2 - \mu_k^{k+1} \\ d \end{pmatrix} \tag{52}$$

Setting $\mu = \mu_1^0 + \alpha_1 \mu_1^1$ one verifies that the desired solution is given by (50).

Contrary to (43) the linear systems above involve a bordering of the singular matrix $P(\Lambda_{jj}, s_0)$ of width $k+1$. They can be expected to be well-conditioned even at the turning points which correspond to double real eigenvalues. We note, however, that the overall method is rather expensive since one has to solve $\frac{1}{2}(k+1)(k+2)$ bordered systems.

3.3.2 Update of invariant pairs at turning points

The parameter dependent version of the linearized problem (6) is

$$F(\Phi, \Lambda, s) = \begin{pmatrix} M(s)\Phi\Lambda - N(s)\Phi \\ \hat{\Phi}^H(\Phi - \Phi_0) \end{pmatrix} = 0, \tag{53}$$

where

$$L(\lambda, s) = M(s)\lambda - N(s) = \begin{pmatrix} I & 0 \\ 0 & A(s) \end{pmatrix} \lambda - \begin{pmatrix} 0 & I \\ -C(s) & -B(s) \end{pmatrix}. \tag{54}$$

As an easy consequence of Section 2.3 we note the following.

Proposition 3.1. *Let $\hat{X}, \hat{Y}, X_0 \in \mathbb{R}^{m,k}, \Lambda_0 \in \mathbb{R}^{k,k}$ be given such that $\hat{X}^T X_0 + \hat{Y}^T X_0 \Lambda_0$ is nonsingular and define $\hat{\Phi}, \Phi_0$ by (7). Then the triple (X_0, Λ_0, s_0) is a quadratic turning point of the system (36) if and only if the triple (Φ_0, Λ_0, s_0) is a quadratic turning point of the linearized system (53).*

Proof. By definition a quadratic turning point (Φ_0, Λ_0, s_0) of (53) satisfies conditions (21), (22) at $s = s_0$ and the transversality condition

$$D_s F(\Phi_0, \Lambda_0, s_0) \notin \mathrm{im} D_{(\Phi,\Lambda)} F(\Phi_0, \Lambda_0, s_0). \tag{55}$$

By the proof of Theorem 2.6 it is sufficient to prove that (55) is equivalent to

$$D_s T(X_0, \Lambda_0, s_0) \notin \mathrm{im} D_{(X,\Lambda)} T(X_0, \Lambda_0, s_0). \tag{56}$$

Note that equation (55) leads to a system of type (25)-(27) with right-hand sides 0,$D_s P(\Lambda_0, s_0)X_0$,0 and (56) is of the form (28),(29) with right-hand sides $D_s P(\Lambda_0, s_0)X_0$,0. From this the assertion follows. □

Suppose now that we have detected and computed a quadratic turning point on a branch (44), see [4], [8], [9], [11], [18] for appropriate methods and implementations. Then a continuation method will reverse the s- direction and follow a branch of invariant pairs that differs from the previous invariant pairs by just one real eigenvalue. As follows from [19],[23] the turning point for the real system can be interpreted as a complex bifurcation point for the complexified equation. At this point two real eigenvalues meet to form a double eigenvalue which, when keeping the parameter direction, form a complex conjugate pair of eigenvalues associated to a two-dimensional real invariant subspace. In our situation one of the real eigenvalues is in the continued group before the turning point and the other one is picked up upon turning back. Otherwise the spectral sets are identical.

Rather than turning back we want our method to continue in the s-direction. Therefore we update the invariant pair of rank k to one of rank $k+1$ by including the generalized eigenvector. The corresponding invariant pair then continues in the same direction and includes the real and imaginary parts of the eigenvectors and the corresponding complex conjugate eigenvalues. Theorem 2.8 shows how to achieve this.

Let $(X_0, \Lambda_0, s_0) = (X(0), \Lambda(0), s(0))$ denote the computed turning point on the branch (44) and let $(H_0, \Delta_0, \tau_0) \neq 0$ with $\tau_0 = 0$ denote the tangent to the branch computed from (46). Differentiating $T(X(t), \Lambda(t), s(t)) = 0$ at $t = 0$ shows that (H_0, Δ_0) spans the kernel of $D_{(X,\Lambda)}T(X_0, \Lambda_0, s_0)$. In view of (32) we compute the singular value decomposition

$$H_0 = \sigma_1 v_1 \psi_1^T, \quad \sigma_1 > 0, v_1 \in \mathbb{R}^m, \psi_1 \in \mathbb{R}^k, v_1^T v_1 = \psi_1^T \psi_1 = 1. \tag{57}$$

A comparison with (32) shows $\psi = \sigma_1 \psi_1$ and hence (33) leads to the update formula

$$X_1 = \begin{pmatrix} X_0 & v_1 \end{pmatrix}, \quad \Lambda_1 = \begin{pmatrix} \Lambda_0 & \frac{1}{\sigma_1}\Delta_0\psi_1 \\ 0 & \lambda_0 \end{pmatrix}. \tag{58}$$

If λ_0 is not yet available one can compute it from (32) via

$$\lambda_0 = \frac{\psi^T \Lambda_0 \psi}{\psi^T \psi} = \psi_1^T \Lambda_0 \psi_1. \tag{59}$$

4 Algorithmic details and numerical examples

4.1 A summary of the algorithm

We summarize the essential steps in the continuation of invariant pairs $(X(s), \Lambda(s))$ for the quadratic eigenvalue problem (2).

Step1: Initial data
Choose $k_0 \leq k \leq k_1$ where $k_0 < k_1 \in \mathbb{N}$ denote the minimal and the maximal rank of invariant pairs to be continued,
Choose $X_1 \in \mathbb{R}^{m,k}$, $\Lambda_1 \in \mathbb{R}^{k,k}$ and $s_1 \in J$, where $J \subset \mathbb{R}$ is the prescribed interval for the parameter s,
$n_{step} = 0$ step counter, $\delta = \delta_0 > 0$ step-size,

$$\dot{X} = 0, \quad \dot{\Lambda} = 0, \quad \dot{s} = \dot{s}_0 = \begin{cases} +1 & \text{increase } s \text{ on the branch} \\ -1 & \text{decrease } s \text{ on the branch} \end{cases}$$

Step2: Corrector
Generate the Newton sequence $(X_\nu, \Lambda_\nu, s_\nu)$, $\nu \geq 1$ from (47),(48). Use the bordered Bartels Stewart algorithm (49)- (52) for the linear systems.
No convergence: Stop if $n_{step} = 0$, otherwise decrease step-size δ and return to the predictor in step 4 or the update in step 6.
Convergence: Let (X_0, Λ_0, s_0) denote the last Newton iterate. Stop if $s_0 \notin J$, otherwise set $n_{step} = n_{step} + 1$ and increase δ appropriately.

Step3: Tangent vector
Solve (46) for $H_0 \in \mathbb{R}^{m,k}$,$\Delta_0 \in \mathbb{R}^{k,k}$, $\tau_0 \in \mathbb{R}$ using the bordered Bartels Stewart algorithm (49)-(52).
If $\dot{s}\tau_0 < 0$ a turning point is detected, proceed with Step 5.
Let $\dot{X} = H_0$, $\dot{\Lambda} = \Delta_0$, $\dot{s} = \tau_0$.

Step4: Predictor

$$(X_1, \Lambda_1, s_1) = (X_0, \Lambda_0, s_0) + \delta(H_0, \Delta_0, \tau_0).$$

Goto Step 2.

Step5: Turning point
Compute the turning point (X_*, Λ_*, s_*) of (36) that is close to (X_0, Λ_0, s_0) and the tangent $(H_0, \Delta_0, \tau_0 = 0)$ at the turning point from (46).

Step6: Update of dimension
Compute the singular value decomposition (57) of H_0,
update $X_1 \in \mathbb{R}^{m,k+1}$, $\Lambda_1 \in \mathbb{R}^{k+1,k+1}$ according to (58),(59).
Set $k = k + 1$ and $\dot{X} = 0$, $\dot{\Lambda} = 0$, $\dot{s} = \dot{s}_0$.
Validate the estimate X_1, Λ_1 by performing some corrector steps (see (47),(48)) and, upon convergence, let (X_1, Λ_1) be the final iterate.
If $k > k_1$, then depending on the spectrum of Λ_*, reduce k to some $k \in [k_0, k_1]$ and adapt X_1, Λ_1 correspondingly.
Set $s_1 = s_* + \delta_0 \dot{s}_0$.
Proceed with Step 2.

In step 5 we use cubic Hermite interpolation to get a good initial estimate of the turning point (cf. [8, Ch.5.2]) and then compute an approximate turning point on the branch. In the update step 6 the dimension of the subspace increases by one at every turning point. Therefore, it is reasonable to take precautions for reducing the dimension (we decided to keep the dimension within prescribed bounds $k_0 < k_1$). For example, if stability is the principal issue, one may eliminate the eigenvalues of smallest real part. This can be achieved by solving the eigenvalue problem for the small matrix Λ_* (see the step (41) during the linear solves) and then reducing to an invariant pair with columns complementary to the eliminated eigenvectors. This strategy will guarantee that we follow the rightmost group of eigenvalues within the continued cluster. But, of course, due to the local nature of the method, this does not guarantee that the algorithm follows the rightmost group of eigenvalues within the whole spectrum.

4.2 Fluid conveying pipes

The analysis of vibration of fluid conveying pipes [27] leads to the following PDE

$$u_{xxxx} + s^2 u_{xx} + \gamma(x-1)u_{xx} + 2\sqrt{\beta}\, s\, u_{xt} + \gamma u_x + u_{tt} = 0, \quad x \in [0,1], t \geq 0, \tag{60}$$

where $\beta = m_f/m_p$ denotes the quotient of the mass of fluid m_f and the mass of pipe m_p and γ denotes the gravity constant. The continuation parameter s is the fluid velocity.

From spatial discretization with a Galerkin ansatz one obtains a parameterized ODE

$$I\ddot{v} + B(s)\dot{v} + C(s)v = 0, \quad B(s), C(s) \in \mathbb{R}^{m,m},$$

where

$$B(s) = 2\sqrt{\beta}\, s\, \tilde{B}, \quad C(s) = \tilde{A} + (s^2 - \gamma)G + \gamma(D + \tilde{B}),$$

and the matrices $\tilde{A}$, $\tilde{B}$, G and D stem from the Galerkin discretization. The standard stability analysis leads to the quadratic eigenvalue problem

$$X(s)\Lambda^2(s) + B(s)X(s)\Lambda(s) + C(s)X(s) = 0.$$

For more details on the derivation of this quadratic eigenvalue problem see [27].

At parameter values $\beta = 0.4$, $\gamma = 10$, $m = 100$ we continue a 6 dimensional invariant pair from $s = 0$ to $s = 14$. At $s = 0$ we start with the eigenvalues of smallest imaginary part on the $y-$axis. Figure 2 shows the dependence of the real part and the imaginary part w.r.t. the parameter s as obtained by our method. No collisions with outside eigenvalues occur, but there are two real to complex transitions inside the group. These do not affect our step-size control and only become visible a-posteriori when plotting the eigenvalues of the reduced matrix $\Lambda(s)$. For comparison we show in Figure 1 the full spectrum at the endpoints $s = 0$ and $s = 14$. In the blow-up we indicate the continued group of eigenvalues by boxes.

The pipe becomes unstable at $s \approx 9.2$ through one complex conjuagte pair indicating a Hopf bifurcation. This is in agreement with the results in [27], where a simple continuation method for an extended system (obtained by using Kronecker products) was used to follow two eigenvalues.

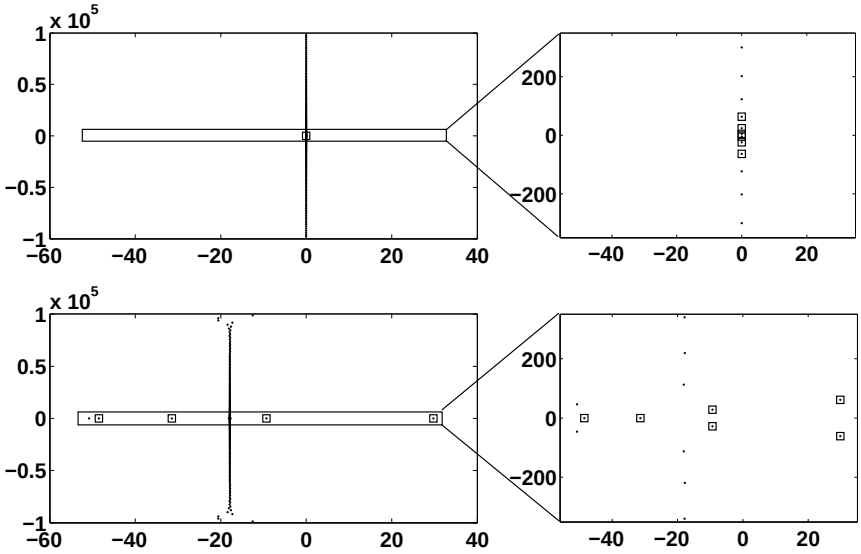

Figure 1: Fluid conveying pipes, full spectrum at $s = 0$ (top) and $s = 14$ (bottom).

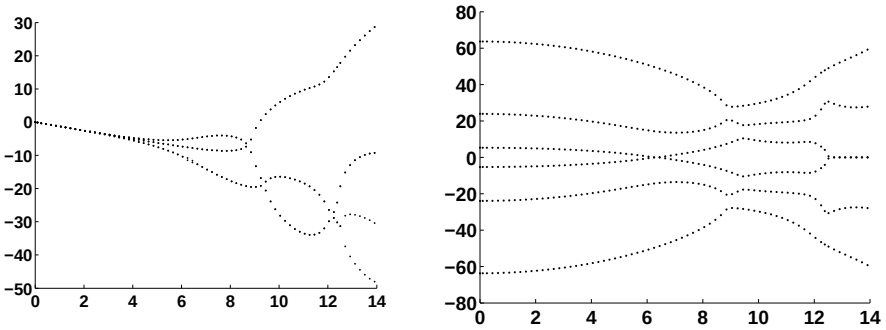

Figure 2: Fluid conveying pipes, continuation of 6 dimensional invariant pair, real part (left) and imaginary part (right).

4.3 Damped hyperbolic wave equation

The damped hyperbolic wave equation with parameter s reads

$$su_{tt} + u_t = u_{\xi\xi} + f(u), \tag{61}$$

Following [12],[13] we transform (61) via $u(\xi, t) = v(\sqrt{1 + sc^2}\xi - ct, t)$ into

$$sv_{tt} + v_t - 2scv_{xt} = v_{xx} + cv_x + f(v). \tag{62}$$

Stationary solutions $\bar{v}(x)$ of this equation, i.e. $\bar{v}'' + c\bar{v}' + f(\bar{v}) = 0$, then lead to traveling waves $u(\xi, t) = \bar{v}(\sqrt{1 + sc^2}\xi - ct)$ of the given system (61). For example, for the Nagumo nonlinearity $f(u) = u(1 - u)(u - \mu)$ we obtain

$$\bar{v}(x) = (1 + \exp(-\frac{x}{\sqrt{2}}))^{-1}, \quad c = -\sqrt{2}(\frac{1}{2} - \mu). \tag{63}$$

In order to examine stability of the traveling wave we linearize about $\bar{v}$. The ansatz $v(x, t) = e^{\lambda t}w(x)$ leads to the eigenvalue problem

$$(s\lambda^2 + \lambda)w - 2s\lambda cw' = w'' + cw' + f'(\bar{v})w, \quad x \in \mathbb{R}. \tag{64}$$

We truncate to a finite interval $J = [-20, 20]$, use zero Dirichlet boundary conditions, and discretize (64) with finite differences and $m = 200$ gridpoints. With the notation $u_n \approx w(x_n), n = 0, \ldots, m$ we obtain the quadratic eigenvalue problem

$$\lambda^2 A(s)u + \lambda B(s)u - Cu = 0,$$

where $A(s) = sI$, $B(s) = I - 2scD_0$, $C = -(D_-D_+ + cD_0 + \mathrm{diag}(f'(\bar{v})))$ and $D_\pm$, D_0 are matrices generated by forward/backward and central differencing.

Figure 4 show the continuation of invariant pairs for $s = [0, 1.5]$. Initially, at $s = 0$, the spectrum is real and we choose the four dimensional group of rightmost real eigenvalues (including the zero eigenvalue which is always present). A total of 3 real-to-complex updates as in step 6 occur at parameter values

indicated by vertical lines. At $s = 1.5$ we have an invariant pair of rank 7 that corresponds to the zero eigenvalue and to 3 complex conjugate pairs. Note that we never decrease the dimension in step 6, which corresponds to taking $k_0 = 4, k_1 \geq 7$ in step 1. For comparison we show again the full spectrum for the endpoints in Figure 3. The waves are always stable (with asymptotic phase), for growing values of s real eigenvalues continue to form complex conjugate pairs and the hyperbolic character of the equation becomes more and more dominant.

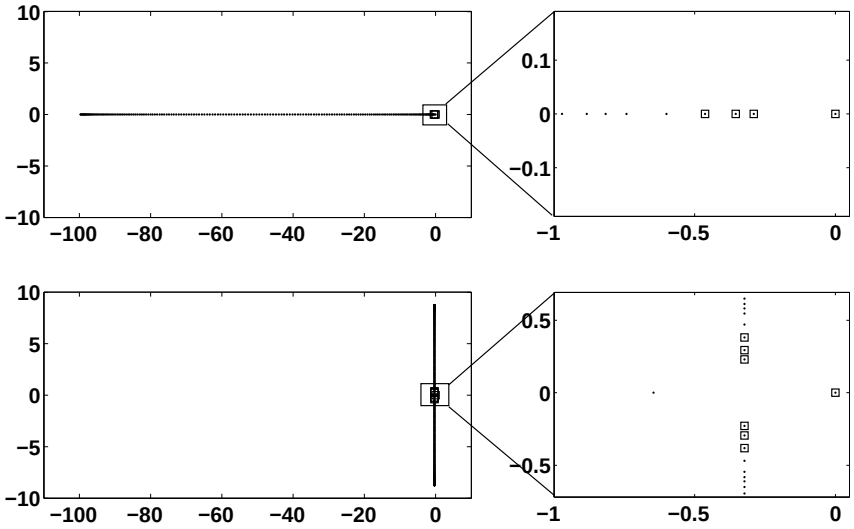

Figure 3: Damped hyperbolic wave equation, full spectrum at $s = 0$ (top) and $s = 1.5$ (bottom).

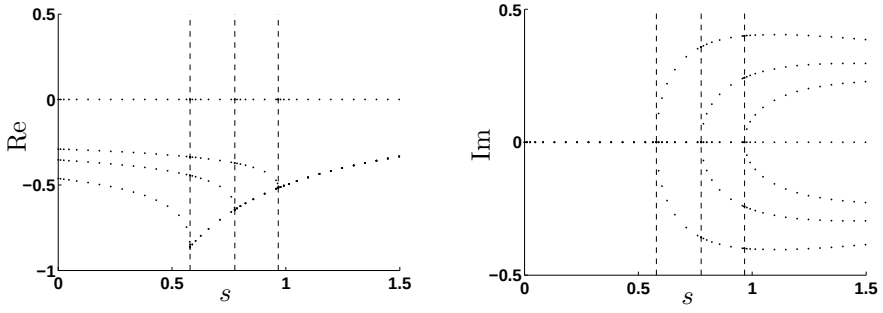

Figure 4: Damped hyperbolic wave equation, continuation of 4 dimensional invariant pair, real part (left) and imaginary part (right).

4.4 Homotopy of random matrices

For the last example we use a homotopy of matrices $A(s) = sA_1 + (1-s)A_0$, where $A_0, A_1 \in \mathbb{R}^{m,m}$ are chosen at random and $B(s),\ C(s)$ are built analogously. For dimension $m = 60$ we continue a four dimensional invariant subspace from $s = 0$ (see the boxes in Figure 5) until $s = 1$. Figure 6 shows that the dimension of the subspaces alternates between 4 and 5 which corresponds to taking $k_0 = 4,\ k_1 = 5$ in the algorithm. The subspace is enlarged two times due to collision with other real eigenvalues (dashed vertical lines) and it also deflated two times (solid vertical lines). Whenever the eigenvalue with smallest real part was real, the dimension was reduced to 4 causing a deflation. During continuation the eigenvalues in the group are not always well separated from the rest of the spectrum. Nevertheless the continuation method works without problems.

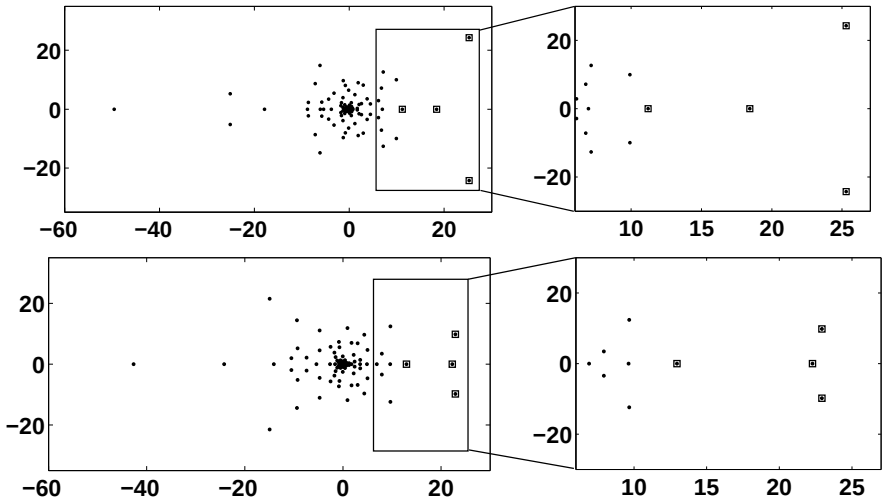

Figure 5: Homotopy of random matrices (dimension = 60), full spectrum at $s = 0$ (top) and $s = 1$ (bottom).

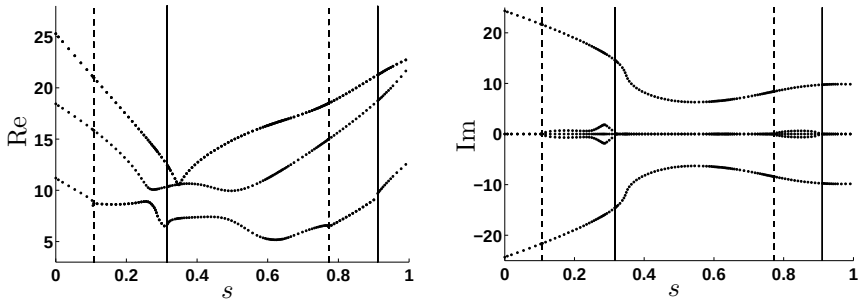

Figure 6: Homotopy of random matrices (dimension = 60), continuation of 4 dimensional invariant pair, real part (left) and imaginary part (right).

5 Conclusions

We have developed the details of an algorithm for computing branches of invariant pairs for parameter-dependent quadratic eigenvalue problems. Invariant pairs are matrix solutions to the quadratic eigenvalue problem (see (2)) that are in one-to-one correspondence with invariant subspaces of linearizations. In our approach we extend the quadratic equation for an invariant pair by suitable normalization conditions and then solve by a Newton-like process. The emphasis is on low dimensional invariant pairs of large and sparse quadratic matrix polynomials as they typically arise in finite element or finite difference discretizations of PDE's that are of second order in time. We avoid linearizing the system which will double its size and may destroy sparsity patterns.

Several numerical issues have been resolved successfully. The linear matrix equations that arise during the predictor corrector method can be solved by a *bordered Bartels Stewart algorithm*. The algorithm involves the Schur decomposition of a small matrix and the solution of a small number of linear vector equations with a bordering of the matrix polynomial. It is shown that turning points on the branch correspond exactly to a double real eigenvalue where two real eigenvalues collide to form a complex conjugate pair. At such points the dimension of the invariant pair is increased by one and the theory is used to compute initial approximations of the updated pair. The method proposed is strictly local in the sense that invariant pairs can only be updated when such collisions occur with eigenvalues that are already inside the group.

Quite a few challenging problems remain. While it is rather obvious how to generalize the techniques of this paper to higher order matrix polynomials it is not at all clear how to treat genuinely nonlinear eigenvalue problems. In particular, it is not obvious how to define invariant pairs in general and whether it makes sense to compute branches that belong to groups of eigenvalues. More importantly, for the application to stability problems one needs algorithms that can detect globally all eigenvalues that pass certain critical lines, such as the imaginary axis, and thus should be included in the continued invariant pair.

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