Continuation of low-dimensional invariant subspaces in dynamical systems of large dimension

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Abstract

We present a continuation method for low-dimensional invariant subspaces of a parameterized family of large and sparse real matrices. Such matrices typically occur when linearizing about branches of steady states in dynamical systems that are obtained by spatial discretization of time-dependent PDE's. The main interest is in subspaces that belong to spectral sets close the imaginary axis. Our continuation procedure provides bases of the invariant subspaces that depend smoothly on the parameter as long as the continued spectral subset does not collide with another eigenvalue. Generalizing results from [32] we show that this collision generically occurs when a real eigenvalue from the continued spectral set meets another eigenvalue from outside to form a complex conjugate pair. Such a situation relates to a turning point of the subspace problem and and we develop a method to inflate the subspace at such points.

We show that the predictor and the corrector step during continuation lead to bordered matrix equations of Sylvester type. For these equations we develop a bordered version of the Bartels-Stewart algorithm which allows to reduce the linear algebra to solving a sequence of bordered linear systems.

The numerical techniques are illustrated by studies of the stability problem for traveling waves in parabolic systems, in particular for the Ginzburg-Landau and the FitzHugh-Nagumo equation.

1 Introduction

This paper is a special outcome of the DANSE project on 'Connecting orbits in dynamical systems of large dimension'. It focusses on a certain part of the project which deals with the realization of numerical techniques for dynamical systems (bifurcation, invariant manifolds, stability and spectral analysis) in higher dimensions, in particular with the efficient approximation of parameter dependent invariant subspaces. The specific results on connecting orbits will

be documented elsewhere. We first summarize the main results of the paper and then relate our work to known approaches in the literature, in particular to other projects of the DANSE program.

1.1 Outline of the paper

Low-dimensional invariant subspaces of parametrized large matrices $A(s)$ play an important role in the numerical analysis of dynamical systems. They typically occur as Jacobians $A(s) = D_u F(u(s), \lambda(s))$ at branches $(u(s), \lambda(s))$ of steady states for a dynamical system

$$\dot{u} = F(u, \lambda).$$

If this system arises from a spatial discretization of a partial differential equation then the matrices will be large and sparse. Invariant subspaces that belong to parts of the spectrum which is close to zero or to the imaginary axis provide the information about stability, bifurcation and, more generally, about locally invariant manifolds, see e.g. [5], [17], [27], [3], [6]. In current bifurcation and continuation packages such as [11], [28] the associated eigenvalues are used for detecting and locating singular points on branches as well as for branch switching. However, these eigenvalues are usually obtained from a full resolution of the spectrum. For transferring the bifurcation techniques to large and sparse systems it will be important to incorporate the continuation of low-dimensional invariant subspaces into such software.

In this paper we develop the details of a predictor-corrector method for low-dimensional invariant subspaces of parameter-dependent large matrices. By a bordered version of the well-known Bartels-Stewart algorithm (cf. [14]) we are able to reduce the linear algebra work to solving several linear systems with bordered matrices of the type

$$\begin{pmatrix} A(s) - \tau I & \Phi \\ \hat{\Phi}^T & 0 \end{pmatrix}, \ \tau \in \mathbb{C}, A(s) \in \mathbb{R}^{m,m}, \ \Phi, \hat{\Phi} \in \mathbb{R}^{m,k}, k \ll m. \qquad (1)$$

Here τ is in or close to the spectrum of $A(s)$ and k is the dimension of the invariant subspaces. Linear systems of this type occur quite frequently in bifurcation problems and several approaches have been developed for their stable and efficient solution, see [7], [15], [25], [36]. We use the method of mixed block elimination [15], [19] which requires only a black box solver for the (almost singular) principle submatrix $A(s) - \tau I$ and its transpose. This solver should be normwise backward stable in the sense of [22].

Our continuation method is independent of any multiplicities of eigenvalues that occur within the invariant subspace. However, we are forced to update the dimension when a real eigenvalue of the continued spectral subset meets an eigenvalue from outside to form a complex conjugate pair (the opposite movement presents no difficulties since real and imaginary parts of complex conjugate eigenvectors are always included in the subspace which then passes smoothly through the formation of a pair of real eigenvalues). In this case we inflate the

subspace by generalizing the method from [30], [32] where the continuation of single eigenvalues is considered. In this situation the given parameter s (which is usually some arclength from the original nonlinear problem) is no longer suitable for parametrization and another arclength parameter for the subspace problem is introduced. The double real eigenvalue then appears as a turning point of the subspace problem and from this the relevant update vectors can be computed easily. Again, the linear systems can be reduced to solving with matrices of type (1) where now the size of the bordering increases by 1.

Several additional features of the current implementation of the algorithm will be discussed in section 5, such as starting procedures, reorthogonalization of the matrices in the normalizing conditions, computation of invariant subspaces for the adjoint matrices and weighted inner products for the pseudo arclength condition. A particular issue is the coupling of subspace continuation and nonlinear branch continuation, called simultaneous branch following. For systems where the matrices are not available analytically this seems to be the only approach which is conceptionally clear and at the same time avoids nested iterations and conflicts of different step size controls.

Our approach is tested on the spectra of several large matrices that occur for linearizations about traveling waves in parabolic systems. More details on the specific properties of these examples will be given below.

1.2 Related references and projects

As mentioned above, the papers [30], [32], [20] treat the transition between real eigenvalues and complex conjugate pairs (and more general singularities of higher codimension) from the bifurcation point of view. There the focus is on the homotopy method for analyzing the spectrum of a single matrix and no precautions are taken to handle large and sparse systems.

A related approach has been developed in [37] where an extra attempt is made to ensure that the continued eigenvalue is the rightmost one which is currently not intended in our approach. To achieve such a goal it seems necessary to use repeatedly along the branch some potentially slow iterations such as inverse subspace iteration or even integration of the time-dependent system (compare the work of Lubich and others [31], [23]). In general this question is related to the so called Hopf detection problem, i.e. to detect parameter values where complex conjugate pairs (that do not belong to the current subspace) cross the imaginary axis. We refer to [13] for various approaches and an overview of this problem.

Another continuation strategy for invariant subspaces is proposed in the recent work [9] where it is used to update the boundary conditions for connecting orbits. In order to obtain a neighboring block Schur decomposition the authors take a deflation approach (apply Newton's method to the associated Riccati equation and solve a Sylvester equation in each step) in contrast to the inflation approach of the current paper (apply Newton's method to a bordered invariant subspace equation and use a bordered Bartels Stewart algorithm in each step). There is no proposal in [9] on how to handle large, sparse systems.

The current paper is an extension of an earlier version [3]. The method grew out of the thesis of the second author [26] (supported by DANSE) and was further developed and applied in the diploma thesis of the third author [42]. In [26], [2] the techniques of this paper are transferred to the problem of computing higher order Taylor terms of locally invariant manifolds. It turns out that the higher derivatives satisfy so-called multilinear Sylvester equations. Using Bartels-Stewart techniques as above these equations can be arranged in such a way that only a series of equations with bordered matrices as in (1) has to be solved. The number τ in (1) is now a sum of eigenvalues from the subspace and the well-posedness of the matrix in (1) is guaranteed by nonresonance conditions (or the stronger gap conditions) for the decomposition of the spectrum.

Our bordering approach for subspaces is strongly related to the so-called generalized Liapunov-Schmidt method pursued in Böhmer's project, see [5], [6]. There the nonlinear system itself is bordered by extra unknowns and extra equations and this is used to analyze bifurcation points numerically and to investigate approximation methods. We also mention the work in [39], [40] where Lanczos and Arnoldi procedures in Krylov spaces are discussed in the context of continuation. It is, however, not clear how these iterative methods perform for bordered systems of the type (1). Moreover, when applied directly (i.e. without a rational pretransformation) to the subspace problem, Arnoldi methods tend to produce invariant subspaces that belong to extremal eigenvalues. Therefore it may be difficult to treat some of the examples below. There the critical part of the spectrum is almost enclosed by the remaining parts and it seems inevitable to use some type of Newton's method to obtain the invariant subspace.

In our applications we consider the stability problem for traveling waves in reaction diffusion systems in 1D space. The particular difficulties in this case arise from the essential spectrum that appears for the second order linear operator on the real line. For discretizations (truncation to a finite interval with asymptotic boundary conditions plus discretization on a mesh) this creates clusters of eigenvalues that have to be separated from a few isolated eigenvalues. In [4] we investigate the influence of asymptotic boundary conditions on the point spectra of the linearized equations. More specific information on how the essential spectrum breaks up is obtained in the work of Sandstede and Scheel [38].

A model problem for traveling waves is provided by the complex Ginzburg-Landau equations the analysis of which is part of Mielke's project, see [33], [34], [35]. In fact, our project benefitted a lot from A. Mielke's suggestion to investigate the stability of the classical Hocking-Stewartson pulse [24] in certain parameter regions. Due to extra symmetries of the Ginzburg-Landau equation a double zero eigenvalue appears which even becomes triple at a certain parameter value, compare [34]. Since the corresponding eigenfunctions are all captured by the continued subspace this behavior could be resolved easily. Our numerical computations suggest that the Hocking-Stewartson pulse is always unstable, see section 3 for details.

In section 5 we apply our method to the classical equations of FitzHugh Nagumo for nerve conduction [12] . There we encounter an isolated eigenvalue

in the continued invariant subspace that moves towards a cluster of eigenvalues. At such a point our continuation procedure currently terminates and an update procedure for such situations has still to be developed.

2 Smooth branches of invariant subspaces

In this section we consider a family of matrices $A(s) \in \mathbb{R}^{m,m}$ that depends smoothly on a parameter $s \in \mathbb{R}$ and we ask for a smooth family of invariant subspaces of dimension $k \ll m$. Formally we try to find smooth matrices $\Phi(s) \in \mathbb{R}^{m,k}$, each of rank k, such that $\mathcal{R}(\Phi(s))$ is an invariant subspace of $A(s)$, i.e.

$$A(s)\Phi(s) = \Phi(s)\Lambda(s) \tag{2}$$

for some $\Lambda(s) \in \mathbb{R}^{k,k}$. The matrices $\Phi(s)$ will be normalized by

$$\hat{\Phi}^T\Phi(s) = \hat{\Phi}^T\Phi_0 \tag{3}$$

where $\hat{\Phi}, \Phi_0 \in \mathbb{R}^{m,k}$ are suitable rank k matrices.

First we extend the notion of a simple invariant subspace from [41] as follows.

Definition 2.1. For $\mathbb{K} = \mathbb{R}$ or $\mathbb{C}$ let $X \subset \mathbb{K}^m$ be an invariant subspace of $A \in \mathbb{K}^{m,m}$ and let $E \subset \mathbb{K}^m$ be the unique maximal invariant subspace of A satisfying

$$X \subset E,\ \sigma(A|_E) = \sigma(A|_X). \tag{4}$$

Then the subspace X is called *simple* if $X = E$ and it is called *multiple* in case $X \subsetneq E$ with *multiplicity*

$$\dim E - \dim X + 1. \tag{5}$$

It is clear from this definition that the multiplicity of a subspace is obtained from the Jordan normal form of A by collecting and completing all blocks that have a diagonal entry in the spectrum of $A|_X$. In the real case $A \in \mathbb{R}^{m,m}$ this spectrum is always symmetric with respect to the real axis.

The following theorem extends the well known fact that simple eigenvalues and their eigenvectors are regular solutions of a suitably normalized system of equations.

Theorem 2.2. *Let $A \in \mathbb{R}^{m,m}$, $\hat{\Phi}, \Phi_0 \in \mathbb{R}^{m,k}$, $\Lambda_0 \in \mathbb{R}^{k,k}$ be given such that $\hat{\Phi}^T\Phi_0$ is nonsingular.*

Then $\mathcal{R}(\Phi_0)$ is a simple invariant subspace of A with $A\Phi_0 = \Phi_0\Lambda_0$ if and only if the pair $(\Phi_0, \Lambda_0) \in \mathbb{R}^{m,k} \times \mathbb{R}^{k,k}$ is a regular solution of the equation

$$T(\Phi, \Lambda) = \begin{pmatrix} A\Phi - \Phi\Lambda \\ \hat{\Phi}^T\Phi - \hat{\Phi}^T\Phi_0 \end{pmatrix} = 0. \tag{6}$$

Proof. Regularity means that the total derivative

$$DT(\Phi_0, \Lambda_0)(H, \Delta) = \begin{pmatrix} AH - H\Lambda_0 - \Phi_0\Delta \\ \hat{\Phi}^T H \end{pmatrix} \tag{7}$$

is a nonsingular linear map in $\mathbb{R}^{m,k} \times \mathbb{R}^{k,k}$. Note that $\operatorname{rank}(\Phi_0) = k$ follows from the nonsingularity of $\hat{\Phi}^T\Phi_0$.

First, assume that $\mathcal{R}(\Phi_0)$ is a simple invariant subspace and consider $(H, \Delta) \in \mathcal{N}(DT(\Phi_0, \Lambda_0))$. Then this implies

$$A(\Phi_0, H) = (\Phi_0, H) \begin{pmatrix} \Lambda_0 & \Delta \\ 0 & \Lambda_0 \end{pmatrix} \tag{8}$$

and hence $\mathcal{R}(\Phi_0, H)$ is an invariant subspace of A with spectrum $\sigma(\Lambda_0)$. By our assumption $\mathcal{R}(\Phi_0, H) = \mathcal{R}(\Phi_0)$ and hence $H = \Phi_0 B$ for some $B \in \mathbb{R}^{k,k}$. Furthermore

$$0 = \hat{\Phi}^T H = \hat{\Phi}^T \Phi_0 B$$

implies $B = 0$ and $H = 0$, $\Delta = 0$. Thus $DT(\Phi_0, \Lambda_0)$ is nonsingular.

Conversely, if (Φ_0, Λ_0) solves (6) and $\mathcal{R}(\Phi_0)$ has multiplicity ≥ 2 then there exists an eigenvalue $\mu \in \sigma(\Lambda_0)$ and a vector $\varphi \in \mathbb{C}^m$, $\varphi \notin \Phi_0(\mathbb{C}^k)$ such that

$$(A - \mu I)\varphi = \Phi_0 c \tag{9}$$

for some $c \in \mathbb{C}^k$. Choose $Q \in \mathbb{C}^{k,k}$ such that $Q^{-1}\Lambda_0 Q$ is upper triangular with (k, k)-entry μ. Then with arbitrary $\gamma \in \mathbb{C}^k$ we define

$$H = (0, \ldots, 0, \Phi_0\gamma + \varphi)Q^{-1}$$

and obtain from (9)

$$\begin{aligned} AH - H\Lambda_0 &= [(0, \ldots, 0, A\varphi + \Phi_0\Lambda_0\gamma) - (0, \ldots, 0, \varphi + \Phi_0\gamma)Q^{-1}\Lambda_0 Q]Q^{-1} \\ &= \Phi_0(0, \ldots, 0, c + (\Lambda_0 - \mu I)\gamma)Q^{-1} = \Phi_0\Delta \end{aligned}$$

Determining γ from $\hat{\Phi}^T\Phi_0\gamma = -\hat{\Phi}^T\varphi$ we find that $(H, \Delta) \in \mathbb{C}^{m,k} \times \mathbb{C}^{k,k}$ is a nontrivial element in the (complex) nullspace of $DT(\Phi_0, \Lambda_0)$. Since $DT(\Phi_0, \Lambda_0)$ is a real operator, this proves the assertion. □

We return to the parameter dependent setting and note that $(\Phi(s), \Lambda(s))$ from (2),(3) are solutions of

$$T(\Phi, \Lambda, s) = \begin{pmatrix} A(s)\Phi - \Phi\Lambda \\ \hat{\Phi}^T\Phi - \hat{\Phi}^T\Phi_0 \end{pmatrix} = 0. \tag{10}$$

If $\mathcal{R}(\Phi_0)$ is a simple invariant subspace of $A(s_0)$ then, according to Theorem 2.2, we can apply the implicit function theorem to (10) at (Φ_0, Λ_0, s_0) and obtain a branch of solutions $(\Phi(s), \Lambda(s))$ for small $|s - s_0|$. This branch can be continued as long as the subspaces stay simple (see the next section for the details of the continuation method).

As is well known from bifurcation theory the parametrization by the given parameter breaks down at a *turning point* of (10) and this is the only possibility in generic one-parameter systems. A turning point (Φ_0, Λ_0, s_0) of (10) satisfies

$$\dim \mathcal{N}(D_{\Phi,\Lambda} T^0) = 1, \text{ e.g. } \mathcal{N}(D_{\Phi,\Lambda} T^0) = \operatorname{span}\{(H_0, \Delta_0)\} \tag{11}$$

$$D_s T^0 \notin \mathcal{R}(D_{\Phi,\Lambda} T^0), \tag{12}$$

where the upper index "0" indicates evaluation at (Φ_0, Λ_0, s_0). Then there is a smooth branch

$$(\Phi(t), \Lambda(t), s(t)), \ |t| < t_0, \ s(0) = s_0, \ s'(0) = 0 \tag{13}$$

passing through (Φ_0, Λ_0, s_0). Generically, the turning point will be quadratic, i.e. $s''(0) \neq 0$ which is known to be equivalent to the second order condition

$$D^2_{\Phi,\Lambda} T^0 (H_0, \Delta_0)^2 \notin \mathcal{R}(D_{\Phi,\Lambda} T^0). \tag{14}$$

In the context of single eigenvalues and eigenvectors this situation (and more general ones) have been analyzed in [20], [30], [32]

The following theorem characterizes conditions (11), (14) and is a generalization of [32] to invariant subspaces. For this result we can omit the parameters.

Theorem 2.3. *Let the assumptions of Theorem 2.2 hold and let* (Φ_0, Λ_0) *be a solution of (6). Then the turning point conditions*

$$\mathcal{N}(DT^0) = \operatorname{span}\{(H_0, \Delta_0)\} \text{ for some } (H_0, \Delta_0) \neq 0 \tag{15}$$

$$D^2 T^0 (H_0, \Delta_0)^2 \notin \mathcal{R}(DT^0) \tag{16}$$

hold if and only if $\mathcal{R}(\Phi_0)$ *is an invariant subspace of multiplicity 2 and the vector needed to make* $\mathcal{R}(\Phi_0)$ *maximal invariant is a generalized eigenvector that belongs to a real eigenvalue* $\mu \in \sigma(\Lambda_0)$ *of algebraic multiplicity 2. This generalized eigenvector spans the columns of* H_0 *which is a rank 1 matrix.*

Proof. First from (7) one calculates that

$$D^2 T^0 (H, \Delta)^2 = (-2H\Delta, 0), \ H \in \mathbb{R}^{m,k}, \Delta \in \mathbb{R}^{k,k}. \tag{17}$$

Therefore equations (15), (16) state that (H_0, Δ_0) is the only solution (up to constant multiples) of the system

$$AH - H\Lambda_0 - \Phi_0 \Delta = 0, \qquad \hat{\Phi}^T H = 0 \tag{18}$$

and there is no solution (H, Δ) of the system

$$AH - H\Lambda_0 - \Phi_0 \Delta = H_0 \Delta_0, \quad \hat{\Phi}^T H = 0. \tag{19}$$

Let us first assume that (15), (16) hold. From (18) and (8) we have that $\mathcal{R}(\Phi_0, H_0)$ is an invariant subspace of A with spectrum $\sigma(\Lambda_0)$. Since $\hat{\Phi}^T \Phi_0$

is nonsingular and $\hat{\Phi}^T H_0 = 0$ we obtain that $\mathcal{R}(\Phi_0)$ is a proper subspace of $\mathcal{R}(\Phi_0, H_0)$ and hence $\mathcal{R}(\Phi_0)$ has multiplicity $p+1 \geq 2$. Therefore we find a matrix $\Phi_1 \in \mathbb{R}^{m,p},\ p \geq 1$ such that $\operatorname{rank}(\Phi_0, \Phi_1) = k + p$ and

$$A(\Phi_0, \Phi_1) = (\Phi_0, \Phi_1) \begin{pmatrix} \Lambda_0 & \Lambda_{01} \\ 0 & \Lambda_1 \end{pmatrix},\ \sigma(\Lambda_1) \subset \sigma(\Lambda_0). \tag{20}$$

By a similarity transformation with $\left(\begin{smallmatrix} Q_{00} & Q_{01} \\ 0 & Q_{11} \end{smallmatrix}\right) \in \mathbb{C}^{m+p,m+p}$ we can assume that the matrix $\left(\begin{smallmatrix} \Lambda_0 & \Lambda_{01} \\ 0 & \Lambda_1 \end{smallmatrix}\right)$ is in Jordan normal form. Then the matrices $\Lambda_\nu,\ \Phi_\nu$ $(\nu = 0, 1)$ and $H_0,\ \Delta_0,\ \Lambda_{01}$ become complex but the solvability conditions for (18), (19) still hold in $\mathbb{C}^{m,k} \times \mathbb{C}^{k,k}$. Moreover, by deleting columns in Φ_1 we can assume $p \leq 2$. The assertion is proved if $p = 1$ and Φ_1 extends a Jordan chain of an eigenvalue μ of algebraic multiplicity exactly 2. Therefore the following cases have to be excluded

case 1

$p = 2$ and the vectors in $\Phi_1 = (\varphi_0, \varphi_1)$ belong to different Jordan chains in (20) (they may be eigenvectors themselves), i.e.

$$\begin{pmatrix} \Lambda_0 & \Lambda_{01} \\ 0 & \Lambda_1 \end{pmatrix} = \begin{pmatrix} \ddots & & & & \\ & J_0 & & 0 & 0 \\ & & & 1 & 0 \\ & & J_1 & 0 & 0 \\ & & & 0 & 1 \\ & & & \mu_0 & 0 \\ & & & 0 & \mu_1 \end{pmatrix},\quad J_\nu = \begin{pmatrix} \mu_\nu & 1 & & \\ & \ddots & \ddots & \\ & & \ddots & 1 \\ & & & \mu_\nu \end{pmatrix},\ \nu = 0, 1.$$

Defining $\gamma_\nu \in \mathbb{R}^k$ by $\hat{\Phi}^T \Phi_0 \gamma_\nu = -\hat{\Phi}^T \varphi_\nu,\ \nu = 0, 1$ one then verifies that

$$\begin{aligned} &H = (0, \ldots, 0, \Phi_0\gamma_0 + \varphi_0, 0, \ldots, 0), \\ &\Delta = (0, \ldots, 0, (\Lambda_0 - \mu_0 I)\gamma_0 + e^{k_0}, 0, \ldots, 0) \\ \text{and} \qquad & \\ &H = (0, \ldots, 0, \Phi_0\gamma_1 + \varphi_1), \\ &\Delta = (0, \ldots, 0, (\Lambda_0 - \mu_1 I)\gamma_1 + e^{k_1}) \end{aligned} \tag{21}$$

are linearly independent solutions of (18). The vector $e^{k_\nu},\ \nu = 0, 1$ is taken to be zero if φ_ν is an eigenvector and a proper Cartesian basis vector otherwise.

case 2

$p = 1,\ \Phi_1 = \varphi_1,\ \Lambda_1 = (\mu_1),\ \varphi_1$ extends a Jordan block $J_1 = (\mu_1)$ in Λ_0 and μ_1 appears in another block of Λ_0 with eigenvector φ_2. This leads to the same contradiction as above because in addition to (21) we have a linearly independent solution of type

$$H = (0, \ldots, 0, \Phi_0\gamma_2 + \varphi_2, 0, \ldots, 0),\ \Delta = (0, \ldots, 0, (\Lambda_0 - \mu_1 I)\gamma_2, 0, \ldots, 0).$$

case 3

$1 \le p \le 2$ and the columns of Φ_1 belong to a Jordan chain of length ≥ 3 for some eigenvalue μ_0. This leads to two subcases:

case 3a $p = 1$, $\Lambda_1 = (\mu_0)$, $\Lambda_0 = \begin{pmatrix} \ddots & \\ & \begin{smallmatrix} \mu_0 & 1 \\ & \mu_0 \end{smallmatrix} \end{pmatrix}$, $\Phi_1 = (\varphi_1)$.

case 3b $p = 2$, $\Lambda_1 = \left(\begin{smallmatrix} \mu_0 & 1 \\ 0 & \mu_0 \end{smallmatrix}\right)$, $\Lambda_0 = \begin{pmatrix} \ddots & \\ & \begin{smallmatrix} 0 & \\ & \mu_0 \end{smallmatrix} \end{pmatrix}$, $\Phi_1 = (\varphi_1, \varphi_2)$.

Note that the case $p = 2$ with μ_0 being multiple in Λ_0 can be reduced to case 3a by deleting φ_2. For both subcases the unique solvability of (18) leads to

$$H_0 = (0, \dots, 0, \Phi_0\gamma_0 + \varphi_1), \ \Delta_0 = (0, \dots, 0, (\Lambda_0 - \mu_0 I)\gamma_0 + e^k)$$

where $\hat{\Phi}^T\Phi_0\gamma_0 = -\hat{\Phi}^T\varphi_1$. Since the last entry of $(\Lambda_0 - \mu_0 I)\gamma_0$ vanishes we obtain $H_0\Delta_0 = H_0$ in (19). One then verifies that (19) has a solution, namely

in case 3a

$$\begin{aligned} H &= (0, \dots, 0, \Phi_0\gamma_1 - \varphi_1, \Phi_0\gamma_2 + \varphi_1), \\ \Delta &= (0, \dots, 0, (\Lambda_0 - \mu_0 I)\gamma_1 - e^k, (\Lambda_0 - \mu_0 I)\gamma_2 + e^k - \gamma_1 - \gamma_0) \end{aligned}$$

in case 3b

$$\begin{aligned} H &= (0, \dots, 0, \Phi_0\gamma_2 + \varphi_2), \\ \Delta &= (0, \dots, 0, (\Lambda_0 - \mu_0 I)\gamma_2 - \gamma_0) \end{aligned}$$

Here the vectors γ_1, γ_2 are chosen to satisfy the normalization condition.

For the converse statement assume that φ_1 is the generalized eigenvector belonging to the double eigenvalue μ and let

$$\Lambda_0 = \begin{pmatrix} \Lambda_{00} & 0 \\ 0 & \mu \end{pmatrix}, \quad (A - \mu I)\varphi_1 = \varphi_0 \tag{22}$$

Then a solution of (18) is given by

$$H_0 = (0, \dots, 0, \Phi_0\gamma_1 + \varphi_1), \quad \Delta_0 = (0, \dots, 0, (\Lambda_0 - \mu I)\gamma_1 + e^k) \tag{23}$$

where γ_1 is defined by $\hat{\Phi}^T\Phi_0\gamma_1 = -\hat{\Phi}^T\varphi_1$. Let (H_1, Δ_1) be another solution of (18), then

$$A(\Phi_0, H_0, H_1) = (\Phi_0, H_0, H_1) \begin{pmatrix} \Lambda_0 & \Delta_0 & \Delta_1 \\ 0 & \Lambda_0 & 0 \\ 0 & 0 & \Lambda_0 \end{pmatrix}.$$

Hence $\mathcal{R}(\Phi_0, H_0, H_1)$ is an invariant subspace of A with spectrum $\sigma(\Lambda_0)$. Since $\mathcal{R}(\Phi_0)$ has multiplicity 2 and $\dim \mathcal{R}(\Phi_0, H_0) = \dim \mathcal{R}(\Phi_0, \varphi_1) = k+1$ we obtain

$\mathcal{R}(H_1) \subset \mathcal{R}(\Phi_0, \varphi_1)$. Therefore we can write any $\varphi \in \mathcal{R}(H_1)$ as $\varphi = \Phi_0\gamma + \alpha\varphi_1$ and from $\hat{\Phi}^T H_1 = 0$ we get $\hat{\Phi}^T\Phi_0\gamma = -\alpha\hat{\Phi}^T\varphi_1$ and hence $\varphi = \alpha(\Phi_0\gamma_1 + \varphi_1)$ for some $\alpha \in \mathbb{R}$. Therefore we can write for some vector $\alpha^T = (\alpha_1, \ldots, \alpha_{k-1})$, $\alpha_k \in \mathbb{R}$

$$H_1 = H_0 D, \quad D = \begin{pmatrix} 0 & 0 \\ \alpha^T & \alpha_k \end{pmatrix}$$

Using (18) for (H_1, Δ_1) and (H_0, Δ_0) we obtain

$$0 = AH_0D - H_0D\Lambda_0 - \Phi_0\Delta_1 = H_0(\Lambda_0 D - D\Lambda_0) + \Phi_0(\Delta_0 D - \Delta_1)$$

Now

$$(\Lambda_0 D - D\Lambda_0) = \begin{pmatrix} 0 & 0 \\ \alpha^T(\mu I - \Lambda_{00}) & 0 \end{pmatrix} \quad \text{and} \quad \varphi_1 \notin \mathcal{R}(\Phi_0)$$

imply $\alpha^T(\mu I - \Lambda_{00}) = 0$, $\Delta_0 D - \Delta_1 = 0$. Since $\mu \notin \sigma(\Lambda_{00})$ we finally have $\alpha = 0$ and $H_1 = \alpha_k H_0$, $\Delta_1 = \alpha_k\Delta_0$. Thus the nullspace is one-dimensional.

Now assume that (H_2, Δ_2) is a solution of (19). Then

$$A(\Phi_0, H_0, H_2) = (\Phi_0, H_0, H_2)\begin{pmatrix} \Lambda_0 & \Delta_0 & \Delta_2 \\ 0 & \Lambda_0 & \Delta_0 \\ 0 & 0 & \Lambda_0 \end{pmatrix},$$

and with the same argument as before $\mathcal{R}(H_2) \subset \mathcal{R}(H_0) = \operatorname{span}\{\Phi_0\gamma_1 + \varphi_1\}$. In particular $H_2 e^k = \alpha(\Phi_0\gamma_1 + \varphi_1)$ for some $\alpha \in \mathbb{R}$. Now apply the matrix $AH_2 - H_2\Lambda_0 - \Phi_0\Delta_2 = H_0$ to the vector e^k and find with (22)

$$\begin{aligned} H_0 e^k &= \Phi_0\gamma_1 + \varphi_1 = \alpha(A - \mu I)(\Phi_0\gamma_1 + \varphi_1) - \Phi_0(\Delta_2)_k \\ &= \alpha(\Phi_0\Lambda_{00}\gamma_1 + \varphi_0) - \Phi_0(\Delta_2)_k \end{aligned}$$

This contradicts $\varphi_1 \notin \mathcal{R}(\Phi_0)$. □

Similar to the homotopy method for eigenvalues in [32] we suggest in this paper to apply a path-following algorithm to the invariant subspace system (10). If we encounter a turning point on the branch, Theorem 2.3 shows that the original parameter s will reverse its direction and a real eigenvalue from the continued spectral set collides with a real eigenvalue from outside. In fact, a pair of complex conjugate eigenvalues is created at this point if the parameter s moves beyond the turning point, see [20]. However, following the branch with the new parameter t the whole subspace passes smoothly through the multiplicity. Note that the rank of H_0 and Δ_0 is one at the turning point. In section 4 we will use this information to update the dimension of the subspace.

3 Continuation methods for invariant subspaces

First we consider the case of continuing simple invariant subspaces, i.e. we compute a branch $(\Phi(s), \Lambda(s))$ for the equation (10).

3.1 The predictor and the corrector step

Assume that (Φ_0, Λ_0) is a regular solution of (10) at $s = s_0$. Then we compute the tangent

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

to the branch $(\Phi(s), \Lambda(s))$ at $s = s_0$ from the following linear system of dimension $(m + k)k$ (cf. (7))

$$\begin{pmatrix} A(s_0)H_0 - H_0\Lambda_0 - \Phi_0\Delta_0 \\ \hat{\Phi}^T H_0 \end{pmatrix} = \begin{pmatrix} -A'(s_0)\Phi_0 \\ 0 \end{pmatrix}. \tag{24}$$

This system contains a matrix equation for H_0 which is of Sylvester type (see [14]) and which is bordered by k^2 extra unknowns and equations. Since $\sigma(\Lambda_0) \subset \sigma(A(s_0))$ the Sylvester part $A(s_0)H_0 - H_0\Lambda_0$ is singular and it is essential to use the bordering for a stable solution (see the next subsection).

Given a stepsize δ and the solution (H_0, Δ_0) from (24) we compute the predictor from

$$(\Phi_1, \Lambda_1, s_1) = (\Phi_0, \Lambda_0, s_0) + \delta(H_0, \Delta_0, 1) \tag{25}$$

In the corrector step we solve the system (10) with $(s, \hat{\Phi}, \Phi_0)$ replaced by (s_1, Φ_0, Φ_1), i.e. we adapt the normalization condition. Starting at (Φ_1, Λ_1), Newton's method generates the sequence (Φ_ν, Λ_ν), $\nu \geq 1$ defined by

$$\begin{pmatrix} A(s_1)\Phi_{\nu+1} - \Phi_{\nu+1}\Lambda_\nu - \Phi_\nu\Lambda_{\nu+1} \\ \Phi_0^T\Phi_{\nu+1} \end{pmatrix} = \begin{pmatrix} -\Phi_\nu\Lambda_\nu \\ \Phi_0^T\Phi_1 \end{pmatrix}. \tag{26}$$

This system is of the same type as (24) and we use again the algorithm below. Note that the form (26) differs from the conventional realization of Newton's method (see [8], [10]) where $\Lambda_{\nu+1}$ is eliminated from the first equation in (26) with the help of the second. Our approach keeps the bordering structure.

3.2 The bordered Bartels-Stewart algorithm

The linear systems (24), (25) are of the form

$$\begin{pmatrix} AH - H\Lambda - \Phi\Delta \\ \hat{\Phi}^T H \end{pmatrix} = \begin{pmatrix} B \\ C \end{pmatrix} \tag{27}$$

where $H, B, \hat{\Phi} \in \mathbb{R}^{m,k}$, $C, \Lambda, \Delta \in \mathbb{R}^{k,k}$ and $\sigma(\Lambda) \subset \sigma(A)$. We reduce the equations to systems of type (1) by the following algorithm which we call the *bordered Bartels-Stewart algorithm*. First compute the complex Schur decomposition of the matrix Λ (see [14]).

$$Q^H\Lambda Q = \tilde{\Lambda}, \quad Q^H Q = I, \quad \tilde{\Lambda} \text{ upper triangular.} \tag{28}$$

Note that this involves solving an eigenvalue problem of very small dimension $k \ll m$. Then we transform (27) into

$$\begin{pmatrix} A\tilde{H} - \tilde{H}\tilde{\Lambda} - \Phi\tilde{\Delta} \\ \hat{\Phi}^T\tilde{H} \end{pmatrix} = \begin{pmatrix} \tilde{B} \\ \tilde{C} \end{pmatrix} \tag{29}$$

where

$$\tilde{B} = BQ,\ \tilde{C} = CQ,\ \tilde{H} = HQ,\ \tilde{\Delta} = \Delta Q \tag{30}$$

Since $\tilde{\Lambda}$ is upper triangular we can compute the columns $\tilde{H}_j, \tilde{\Delta}_j$ of $\tilde{H}, \tilde{\Delta}$ similar to the Bartels-Stewart algorithm (see [14], Ch. 7.6.3) from a sequence of k bordered linear systems

$$\begin{pmatrix} A - \tilde{\Lambda}_{jj} I & -\Phi \\ \hat{\Phi}^T & 0 \end{pmatrix} \begin{pmatrix} \tilde{H}_j \\ \tilde{\Delta}_j \end{pmatrix} = \begin{pmatrix} \tilde{B}_j + \sum_{\nu=1}^{j-1} \tilde{\Lambda}_{\nu j} \tilde{H}_\nu \\ \tilde{C}_j \end{pmatrix},\ j = 1, \ldots, k. \tag{31}$$

Finally the solution H, Δ is obtained from $\tilde{H}, \tilde{\Delta}$ in (30). We notice that the upper left block $A - \tilde{\Lambda}_{jj} I$ is typically a large sparse, almost singular matrix. During the continuation of k-dimensional simple invariant subspaces we can expect that its rank drops at most by k which can be compensated for by the bordering (see [18], [16] for some estimates of condition numbers for this case).

Bordered systems of the above type occur quite frequently in bifurcation problems and various approaches have been developed for their stable and efficient solution (see [7], [19], [36]). We propose to use the mixed block elimination of Govaerts and Pryce [19] which requires only a black box solver for the principle submatrix and its transpose. If this solver is normwise backward stable in the sense of [22] and if the inverse of the principal submatrix times machine accuracy has a moderate bound then the block elimination can be shown to be forward stable [19].

3.3 The complex Ginzburg-Landau equation

As a first example we investigate the stability of a pulse solution due to Hocking and Stewartson [24] in the complex Ginzburg Landau equation. The latter is a well known modulation equation used in physics and chemistry [29] and we use the following form with two parameters $\alpha, \beta \in \mathbb{R}$. ([33], [34])

$$u_t = (1 + i\alpha)(u_{xx} - (1 + i\beta)^2 u + (1 + i\beta)(2 + i\beta)|u|^2 u). \tag{32}$$

The stationary solution is $\bar{u}(x) = \cosh(x)^{-(1+i\beta)} = \bar{v} + i\bar{w}$ (see [24]) where $\lim_{x \to \pm\infty} \bar{u}(x) = 0$. The linearization $L_{\alpha,\beta}$ of (32) at $\bar{u}$ is given in real and imaginary parts by the following two-dimensional system

$$L_{\alpha,\beta} \begin{pmatrix} v \\ w \end{pmatrix} = \begin{pmatrix} 1 & -\alpha \\ \alpha & 1 \end{pmatrix} \left[\begin{pmatrix} v_{xx} \\ w_{xx} \end{pmatrix} + (M_2\, M_3 - M_1) \begin{pmatrix} v \\ w \end{pmatrix} \right]$$

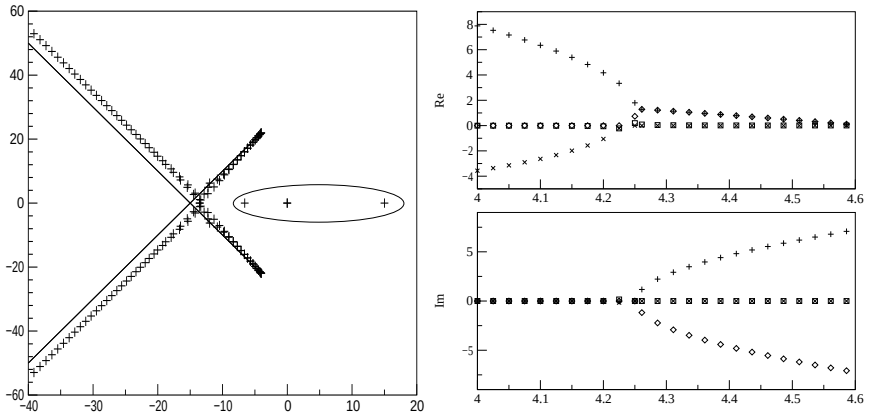
where

$$M_1 = \begin{pmatrix} 1 - \beta^2 & -2\beta \\ 2\beta & 1 - \beta^2 \end{pmatrix},\ M_2 = \begin{pmatrix} 2 - \beta^2 & -3\beta \\ 3\beta & 2 - \beta^2 \end{pmatrix},$$
$$M_3 = \begin{pmatrix} 3\bar{v}^2 + \bar{w}^2 & 2\bar{v}\bar{w} \\ 2\bar{v}\bar{w} & \bar{v}^2 + 3\bar{w}^2 \end{pmatrix}.$$

The operator $L_{\alpha,\beta}$ has a zero eigenvalue with geometric multiplicity at least two and corresponding eigenfunctions $\bar{u}'$ and $i\bar{u}$. The essential spectrum consists of two half-lines which cross the imaginary axis on the critical curve (cf. [4]).

$$\beta(\beta + 2\alpha) - 1 = 0. \tag{33}$$

We consider $L_{\alpha,\beta}$ in the finite interval $[x_-, x_+]$ subject to Dirichlet boundary conditions and we discretize by a centered finite difference scheme with step-size h. The changes in the spectrum caused by truncation to a finite interval have been analyzed in [4].



(a) part of the essential and numerical spectrum

(b) real and imaginary part vs. β

Figure 1: Ginzburg-Landau equation, $\alpha = -2$

Figure 1(a) shows the two half lines of the essential spectrum and the full numerical spectrum for the case $x_\pm = \pm 10$, $h = 0.04$ and $\alpha = -2, \beta = 3$.

We continue a four-dimensional subspace that belongs to the two (almost) zero eigenvalues and the two real eigenvalues encircled in Fig. 1(a). With increasing β the stable eigenvalue passes zero (as shown by Mielke [34] this happens precisely on the curve (33) where a generalized eigenvector corresponding to $i\bar{u}$ appears), then forms a complex pair with the unstable eigenvalue which finally moves to the left half plane. For the numerical eigenvalues ($x_\pm = \pm 10, h = 0.004$) a perturbation of this appears in Figure 1(b) (see [4] for details).

A schematic drawing of the motion of the 4 eigenvalues in the infinite case and in the discretized case is shown in Fig. 2, 3. This sensitive behavior can only be revealed since the 4D-subspace stays separated from the rest of the spectrum and the remaining 4×4 eigenvalue problem can be solved very accurately. The double or even triple zero eigenvalue does not affect the continuation of the subspace which could be done with uniform step-size in the parameter β.

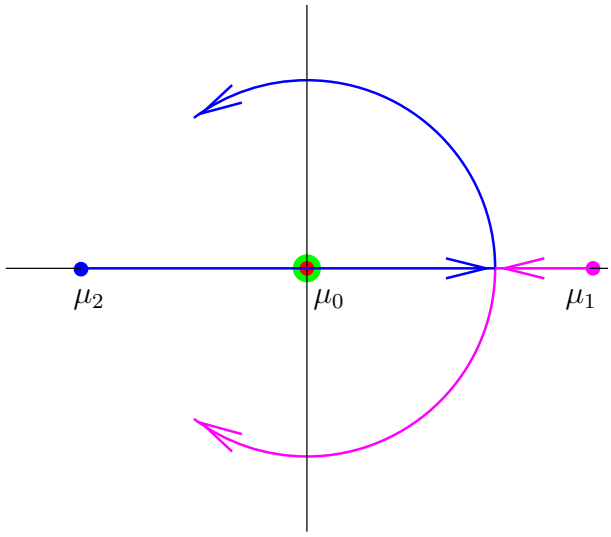
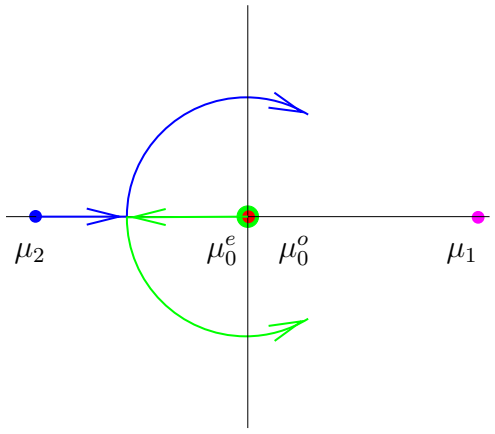
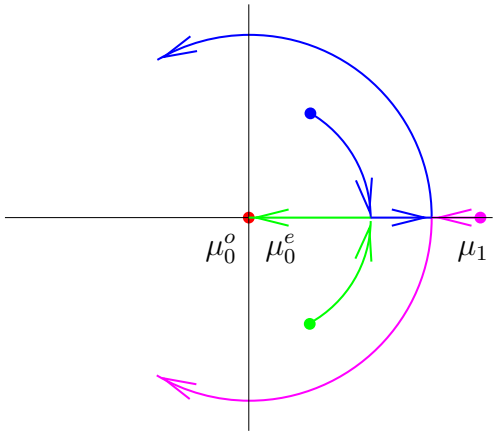


Figure 2: Behavior of complex eigenvalues when β increases from 4 to 5



(a) $4 \leq \beta \lesssim \beta_{crit}$



(b) $\beta_{crit} \lesssim \beta \leq 5$

Figure 3: Behavior of numerical eigenvalues for $4 \leq \beta \leq 5$

3.4 Passing through nonsimple subspaces

As explained at the end of section 2 we can apply a general continuation method to the system (10) in order to pass through double real eigenvalues. But it may also be advantageous along branches of simple invariant subspaces due to the better adaptation of step-sizes. For example in a pseudo arclength method the extra equation is of the form

$$\langle \dot\Phi, \Phi - \Phi_0\rangle + \langle \dot\Lambda, \Lambda - \Lambda_0\rangle + \dot\lambda(\lambda - \lambda_0) = \delta \tag{34}$$

where we have used the inner product $\langle A, B\rangle = \mathrm{trace}(A^T B)$ for rectangular matrices and where $\dot\Phi, \dot\Lambda, \dot\lambda$ are approximate tangent vectors at the previous point on the branch.

Similar to (24)-(26), both the predictor and the corrector step for (10), (34) lead to linear systems for $H \in \mathbb{R}^{m,k}$, $\Delta \in \mathbb{R}^{k,k}$ and $\mu \in \mathbb{R}$ as follows (compare (27))

$$\begin{aligned} AH - H\Lambda - \Phi\Delta + \Gamma\mu &= B \in \mathbb{R}^{m,k} \\ \hat\Phi^T H &= C \in \mathbb{R}^{k,k} \\ \langle \dot\Phi, H\rangle + \langle \dot\Lambda, \Delta\rangle + \dot\lambda\mu &= d \in \mathbb{R} \end{aligned} \tag{35}$$

where $\Gamma \in \mathbb{R}^{m,k}$. For example, $\Gamma = A'(s_0)\Phi_0$ holds in the predictor step. We can solve this system with the standard block elimination method [25]. This requires to solve two linear (H, Δ) systems with right hand sides $\binom{B}{C}$ and $\binom{\Gamma}{0}$ by the bordered Bartels-Stewart algorithm above and then form a suitable linear combination which satisfies the last equation in (35). However, very close to or at the turning point this is not reliable and the bordering by Γ is needed for stability, see Theorem 2.3 and (18), (19).

For this case the algorithm from 3.2 can be modified as follows. First, Λ is put into upper triangular form as in (28) and the data are transformed as in (30) where in addition $\tilde{\dot\Phi} = \dot\Phi Q$, $\tilde{\dot\Lambda} = \dot\Lambda Q$. For simplicity we drop the "˜" and work with (35). For the columns H_j, Δ_j of H, Δ and for μ we use the ansatz

$$(H_j, \Delta_j, \mu) = (H_j^0, \Delta_j^0, \mu_j^0) + \sum_{i=1}^{j} \alpha_i (H_j^i, \Delta_j^i, \mu_j^i),\ j = 1, \ldots, k \tag{36}$$

in the first two equations of (35). With the matrix

$$M_j = \begin{pmatrix} A^0 - \Lambda_{jj} I_m & -\Phi & -\Gamma_j \\ \hat\Phi^T & 0 & 0 \\ \dot\Phi_j^T & \dot\Lambda_j^T & 0 \end{pmatrix} \tag{37}$$

we determine the unknowns in (36) for $j = 1, \ldots, k$ from

$$M_j \begin{pmatrix} H_j^0 \\ \Delta_j^0 \\ \mu_j^0 \end{pmatrix} = \begin{pmatrix} B_j + \sum_{i=1}^{j-1} \Lambda_{ij} H_i^0 \\ C_j \\ 0 \end{pmatrix}, \quad M_j \begin{pmatrix} H_j^j \\ \Delta_j^j \\ \mu_j^j \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

$$M_j \begin{pmatrix} H_j^i \\ \Delta_j^i \\ \mu_j^i \end{pmatrix} = \begin{pmatrix} \sum_{\nu=i}^{j-1} \Lambda_{\nu j} H_\nu^i \\ 0 \\ 0 \end{pmatrix} \quad \text{for } i = 1, \ldots, j-1$$

Finally the α_i and μ are calculated from the $(k+1)$-dimensional system

$$\begin{pmatrix} \mu_1^1 & & & -1 \\ \vdots & \ddots & & \vdots \\ \mu_k^1 & \ldots & \mu_k^k & -1 \\ 1 & \ldots & 1 & \dot{\lambda} \end{pmatrix} \begin{pmatrix} \alpha_1 \\ \vdots \\ \alpha_k \\ \mu \end{pmatrix} = \begin{pmatrix} -\mu_1^0 \\ \vdots \\ -\mu_k^0 \\ d \end{pmatrix} \tag{38}$$

One readily verifies that this yields the desired solution via (36). Moreover, the matrix M_j now has a bordering of width $k+1$ and can be expected to be well conditioned even at the double real eigenvalue. However, the overall method is rather expensive since one has to solve $\frac{1}{2}(k+1)(k+2)$ bordered systems.

4 Updating the dimension

If the matrices $A(s)$ arise from linearizing about a steady state branch then one does not want the subspace continuation to reverse the direction of the parameter s (which is usually arclength for the nonlinear problem). Rather, if a real eigenvalue from the continued spectral set meets another one from outside then one should increase the dimension of the subspace by 1 and follow the complex conjugate pair in the original s-direction. This is precisely the situation that has been analyzed for single eigenvalues in [32]. We now deal with this problem in the context of general subspaces.

4.1 Inflating the subspace

Suppose (Φ_0, Λ_0, s_0) is a quadratic turning point, i.e. (11), (12) and (14) hold. According to Theorem 2.3 there is a smooth branch $(\Phi(t), \Lambda(t), s(t))$ passing through (Φ_0, Λ_0, s_0) at some $t = t^*$. Therefore $\Phi_0 = \Phi(t^*), \Lambda_0 = \Lambda(t^*), s_0 = s(t^*)$ and

$$A(s(t))\Phi(t) - \Phi(t)\Lambda(t) = 0 \tag{39}$$

$$(\dot{\Phi}(t^*), \dot{\Lambda}(t^*)) = c(H_0, \Delta_0) \quad \text{for some } c \in \mathbb{R} \tag{40}$$

Since H_0 has rank 1 we obtain that after the turning point there is one new eigenvalue created by the one which becomes double, but all the other eigenvalues of $\Lambda(t)$ are identical with those that have been passed before the turning point.

Differentiating (39) at $t = t^*$ and using $s'(t^*) = 0$ leads to

$$A_0\dot{\Phi}(t^*) = \dot{\Phi}(t^*)\Lambda_0 + \Phi_0\dot{\Lambda}(t^*) \tag{41}$$

Since $\dot{\Phi}(t^*)$ has rank one a singular value decomposition yields

$$\dot{\Phi}(t^*) = \mu u v^T \quad \text{for some } \mu > 0,\ \|u\| = \|v\| = 1.$$

Here u is the generalized eigenvector. Insert this into (41) and multiply by v to obtain

$$\mu A_0 u = \mu u v^T \Lambda_0 v + \Phi_0 \dot{\Lambda}(t^*) v.$$

Therefore the following two steps are sufficient to update the subspace

1. SVD:
$$\dot{\Phi}(t^*) = \mu u v^T,\ \mu > 0$$

2. Update:
$$\Phi_{up} = \begin{pmatrix} \Phi(t^*) & u \end{pmatrix}, \quad \Lambda_{up} = \begin{pmatrix} \Lambda(t^*) & \frac{1}{\mu}\dot{\Lambda}(t^*)v \\ 0 & v^T\Lambda(t^*)v \end{pmatrix}$$

4.2 A traveling wave example

As an example for the turning of the eigenvalues we use a variant of the Nagumo equation with an additional parameter ρ.

$$u_t = u_{xx} + f(u,\rho), \quad u(x) : \mathbb{R} \to \mathbb{R},\ t > 0, \tag{42}$$
$$f(u,\rho) = \rho\ u(1-u)(u-\mu),\ \mu \in (0,\frac{1}{2})$$

We continue traveling wave fronts of (42) i.e. solutions $\bar{u}(x,t) = \bar{v}(x-ct)$ which satisfy

$$\lim_{\xi\to\infty} \bar{v}(\xi) = 1, \quad \lim_{\xi\to-\infty} \bar{v}(\xi) = 0$$

At $\rho = 1$ the following explicit solution is known, see [21], p. 130.

$$\bar{v}_1(x) = \frac{1}{1+\exp(-\frac{x}{\sqrt{2}})}, \quad c = -\sqrt{2}\ (\tfrac{1}{2} - \mu) \tag{43}$$

The function $\bar{v}$ and the parameter c satisfy the second order equation

$$F(v) = v_{xx} + cv_x + f(v,\rho) = 0, \quad -\infty < x < \infty \tag{44}$$

and the stability of the wave is governed by the spectrum of the linearized operator (see [21],[43])

$$Pu = u_{xx} + cu_x + D_v f(\bar{v},\rho)u \tag{45}$$

We restrict to a finite interval $J = [x_-, x_+]$ and use Dirichlet boundary conditions (see [1] for the general approach).

Then the resulting boundary value problem is discretized with finite differences and the spectrum of the matrix obtained by linearizing about the solution (i.e. the discrete analog of (45)) is analyzed, for our example $J = [-10, 10]$, $h = 0.1$, $\mu = \frac{1}{4}$. We start the continuation at $\rho = 1$ with the known solution (43) and decrease ρ. We use periodic boundary conditions which tend to give good approximations of the essential spectrum but at the same time tend to produce complex eigenvalues (cf. [4]).

Figure 4 shows the result of following the three dimensional invariant subspace which belongs to the three eigenvalues with largest real part. The real and imaginary part are shown as functions of the arclength t of the subspace continuation. The eigenvalue close to zero (which always exists and is exactly zero for the continuous problem) stays real while the other two eigenvalues form a complex pair at $t = 0.4,\ \rho = 0.6$. (for the latter value see also figure 5(b))

Suppose we had started the continuation with the largest two real eigenvalues. Then the pictures in 5(a), 5(b) result where we pass a turning point at $t = 0.37,\ \rho = 0.63$.

Both eigenvalues and the parameter ρ are plotted versus arclength t and also the eigenvalue which turns is shown versus the parameter ρ. While the

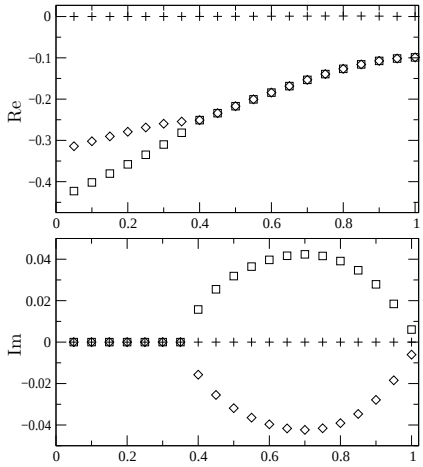
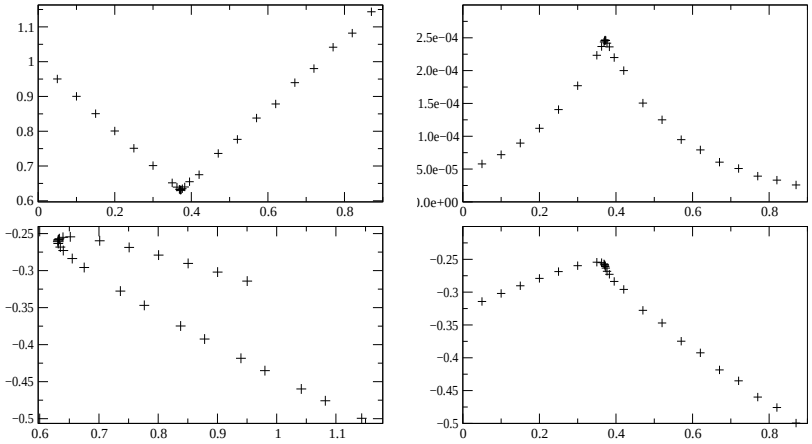


Figure 4: eigenvalues for $k = 3$ vs. arclength t

zero eigenvalue returns to itself the nonzero eigenvalue passes on to the third eigenvalue.

Finally, we show in Fig.6 the result of the update procedure when starting with the same two dimensional subspace as above. Near the turning point the continuation first slows down until the turn in the parameter ρ is detected. After inflating the subspace the step-size increases again and a comparison with Figures 4, 5 shows a good correspondence.



(a) parameter ρ vs. arclength t and the second eigenvalue vs. ρ

(b) two real eigenvalues vs. arclength t for two-dimensional subspace continuation

Figure 5: Nagumo equation, $\mu = \frac{1}{4}, J = [-10, 10]$

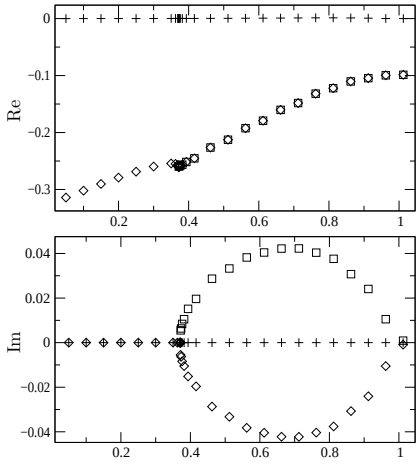


Figure 6: real and imaginary parts of the eigenvalues vs. arclength t

5 Application and examples

In this section we discuss some extensions and further issues which turn out to be important for the actual implementation.

5.1 Algorithmic details

Getting the subspace continuation started is a crucial problem. If no complete spectrum is available initially we use a combination of Caley-transforms (see [13]) and orthogonal subspace iteration ([14]). In this way we obtain an invariant subspace that belongs to a spectral set in a prescribed vertical strip of the complex plane.

During continuation we keep the dimension of the invariant subspace minimal but above some critical number k. After each complex-real transition it is tested whether the eigenvalues with smallest real part (either a real eigenvalue or a complex conjugate pair) can be omitted without getting below dimension k. However, no device is currently implemented to guarantee that the continued spectral set contains the rightmost eigenvalues. This is a global problem and for some algorithms in this direction we refer to [13] and [37]. In order to avoid ill-conditioning of the matrices $\Phi(s)$ these matrices are constantly reorthogonalized after the successful corrector step. For example the predictor in (24) is computed with an orthogonal Φ_0 so that in the succeeding corrector step (26) the matrix $\Phi_0^T\Phi_1$ is close to the identity.

5.2 The left invariant subspaces

If a solution (Φ_0, Λ_0) of (6) has been computed then the corresponding pair (Ψ_0, M_0) for the adjoint can be computed by solving just one extra linear system as the following proposition shows.

Proposition 5.1. *Under the assumptions of Theorem 2.2 let (Φ_0, Λ_0) be a regular solution of (6). Then the linear system*

$$\begin{aligned} A^T\Psi - \Psi\Lambda_0^T - \Phi_0 M &= 0 \\ \Phi_0^T\Psi &= I \end{aligned} \tag{46}$$

has a unique solution $\Psi_0 \in \mathbb{R}^{m,k}$, $M_0 \in \mathbb{R}^{k,k}$. This solution satisfies $M_0 = 0$ and $\mathcal{R}(\Psi_0)$ is a simple invariant subspace of A^T with respect to the spectral set $\sigma(\Lambda_0)$.

Proof. Since $\mathcal{R}(\Phi_0)$ is a simple invariant subspace we have a block diagonalization of A

$$A(\Phi_0, \Phi_1) = (\Phi_0, \Phi_1)\begin{pmatrix} \Lambda_0 & 0 \\ 0 & \Lambda_1 \end{pmatrix}, \quad \sigma(\Lambda_1) \cap \sigma(\Lambda_0) = \emptyset$$

where $\Phi_1 \in \mathbb{R}^{m,m-k}$, $\Lambda_1 \in \mathbb{R}^{k,k}$ and (Φ_0, Φ_1) is nonsingular. Defining

$$(\Phi_0, \Phi_1)^{-1} = (\Psi_0, \Psi_1)^T, \quad \Psi_0 \in \mathbb{R}^{m,k}, \ \Psi_1 \in \mathbb{R}^{m,m-k}$$

we obtain that $\mathcal{R}(\Psi_0)$ is a simple invariant subspace of A^T with spectrum $\sigma(\Lambda_0^T) = \sigma(\Lambda_0)$. Since $\Phi_0^T\Psi_0 = I$ we see that $\Psi = \Psi_0,\ M = 0$ solves (46). Now, for uniqueness, suppose that (Ψ, M) solves the homogenous equation (46). Then multiply the first equation in (46) by Φ_0^T and use the second to obtain

$$0 = (A\Phi_0)^T\Psi - \Phi_0^T\Psi\Lambda_0^T - \Phi_0^T\Phi_0 M = \Lambda_0^T\Phi_0^T\Psi - \Phi_0^T\Phi_0 M = -\Phi_0^T\Phi_0 M.$$

Since $\Phi_0^T\Phi_0$ is nonsingular we find $M = 0$. Therefore, $A^T\Psi - \Psi\Lambda_0^T = 0$ and from the simplicity of $\mathcal{R}(\Psi_0)$ we obtain $\Psi = \Psi_0 B$ for some $B \in \mathbb{R}^{k,k}$. Finally, this implies

$$0 = \Phi_0^T\Psi = \Phi_0^T\Psi_0 B = B$$

as well as $\Psi = 0$. □

We notice that the data Φ_0, Λ_0 of the linear system (46) are assumed to be known at this stage of the computation and that the linear system (46) can be solved by the bordered Bartels-Stewart algorithm with A replaced by A^T. Though we have not used the adjoint in our continuation method the "left invariant subspaces" provide useful information for evaluating test functions or computing singularities (see [16], [28]).

5.3 Simultaneous branch following

In the previous sections we always assumed that the matrices $A(s)$ are available analytically. If, however $A(s) = D_u F(u(s), \lambda(s))$ for a branch $(u(s), \lambda(s))$ of some nonlinear system $F(u, \lambda) = 0$, then any evaluation of $A(s)$ requires a new solution of the nonlinear system. This is particularly annoying when - as in section 3 - the value of s is constantly changed during the Newton iteration for the subspace problem. In order to avoid such nested iterations and to coordinate different step-size controls for the two problems we have implemented a single continuation algorithm for a very large system. It is of the form

$$S(\Phi, \Lambda, u, \lambda) = \begin{pmatrix} F(u, \lambda) \\ T(\Phi, \Lambda, u, \lambda) \end{pmatrix} = 0 \tag{47}$$

where $F : \mathbb{R}^n \times \mathbb{R} \to \mathbb{R}^n$ and

$$T(\Phi, \Lambda, u, \lambda) = \begin{pmatrix} A(u, \lambda)\Phi - \Phi\Lambda \\ \hat{\Phi}^T(\Phi - \Phi_0) \end{pmatrix}, \quad \Phi \in \mathbb{R}^{m,k},\ \Lambda \in \mathbb{R}^{k,k}.$$

Here $A(u, \lambda) \in \mathbb{R}^{m,m}$ are matrices that depend smoothly on $(u, \lambda) \in \mathbb{R}^{n+1}$. Usually we have $n = m$ and $A(u, \lambda) = D_u F(u, \lambda)$, but other cases occur where e.g. $F(u, \lambda)$ contains boundary conditions which have to be eliminated for the spectral problem (compare the examples in this paper). We have implemented a continuation method for the large system (47) which needs only one step-size control and uses a weighted norm for $(\Phi, \Lambda, u, \lambda)$

$$\|(\Phi, \Lambda, u, \lambda)\|^2 = \frac{1}{mk}\|\Phi\|_F^2 + \frac{1}{k^2}\|\Lambda\|_F^2 + \frac{\|u\|_2^2}{n} + \lambda^2 \tag{48}$$

where $\|\Phi\|_F^2 = \mathrm{tr}(\Phi^T\Phi)$ is the Frobenius norm.

The linear systems arising during the predictor and the corrector step for (47) have a special structure (the first n equations do not depend on Φ, Λ) and they can be reduced to solving

- two linear systems with a bordering of $D_u F$
- three linear systems with a bordering of $D_{\Phi,\Lambda} T$.

The reduction is rather obvious and we do not display the details here.

During continuation turning points with respect to λ can occur for two different reasons, first because the branch of the nonlinear system $F(u, \lambda) = 0$ turns and second because a double real eigenvalue for the subspace problem occurs. The second case is indicated by

$$\dot{u}_1^T \dot{u}_0 \leq 0 \tag{49}$$

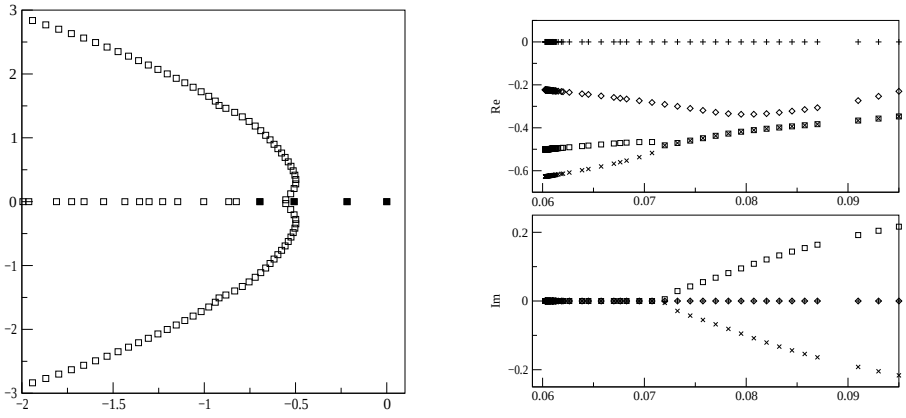
where $\dot{u}_0, \dot{u}_1$ are successive tangents to the u-part of the (u, λ)-branch. Then the update procedure for the subspace is invoked. In fact, if we pass a turning point of the (u, λ)-branch we expect $\dot{u}_1^T \dot{u}_0 > 0$ while (49) indicates that the tangent of this branch is reversed due to a turning point with respect to the parameter s as in section 4.

5.4 The FitzHugh-Nagumo system, a final example

The FitzHugh-Nagumo equation is a model equation for the propagation of nerve impulses [12]. We consider a two-dimensional system with a small additional diffusive term

$$v_t = v_{xx} + F(v,w), \quad w_t = \epsilon w_{xx} + G(v,w)$$
$$F(v,w) = v - \frac{1}{3}v^3 - w, \quad G(v,w) = \Phi(v + a - bw), \quad a,b,\Phi \in \mathbb{R}.$$

For the parameters $a = 0.7, b = 0.8$ there is a branch containing stable and unstable waves. We consider a specific part of the stable branch and follow again a four dimensional subspace with decreasing parameter Φ. For the actual calculation we restrict to $[x_-, x_+] = [0, 65]$, use Dirichlet boundary conditions and discretize with step-size $h = 1$ (more details can be found in [4]). Fig. 7(b) shows real and imaginary parts of the eigenvalues on the stable branch. The complex conjugate pair undergoes a transition to two real eigenvalues which is harmless for our method. However while the two largest real eigenvalues remain separated from the essential spectrum the other two move towards it. The situation for the full spectrum at the critical value $\Phi_{crit} = 0.062$ is shown in Fig. 7(a). At this point our algorithm breaks down due to stagnation of the continuation steps. The two eigenvalues can no longer be separated from the cluster that approximates the essential spectrum. Of course, concerning the stability problem for the original wave there is no need to further include these eigenvalues in the continuation. This shows that there can be reasons for deflating the subspace other than the minimality requirement discussed in 5.1.



(a) part of the numerical spectrum at Φ_{crit}

(b) real and imaginary parts vs. Φ

Figure 7: FitzHugh-Nagumo, stable wave, $x_- = 0, x_+ = 65, h = 1$

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