A continuation framework for invariant subspaces and its application to traveling waves

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Abstract. We present a continuation method for low-dimensional invariant subspaces of a parameterized family of large and sparse matrices. Such matrices typically occur when linearizing about branches of steady states in reaction-diffusion equations. Our continuation method provides bases of the invariant subspaces depending smoothly on the parameter. From these we can compute the corresponding eigenvalues efficiently. The predictor and the corrector step are reduced to solving bordered matrix equations of Sylvester type. For these equations we develop a bordered version of the Bartels-Stewart algorithm. The numerical techniques are used to study the stability problem for traveling waves in two examples: the Ginzburg-Landau and the FitzHugh-Nagumo system. In these cases there always exists a simple or multiple eigenvalue zero while the remaining eigenvalues determine the stability. We demonstrate the difficulties of separating these critical eigenvalues from clusters of eigenvalues that are generated by the essential spectrum of the continuous problem.

1 Introduction

Spatial discretizations of reaction-diffusion systems lead to parameterized dynamical systems $\dot{u} = F(u, \lambda)$ of large dimension. A considerable amount of software has been developed for pathfollowing branches of steady states, periodic and homoclinic orbits and their bifurcations (see e.g. [6], [14]). However, transferring these techniques to large and sparse systems is still a partially developed subject. One topic in this area is the calculation of low-dimensional invariant subspaces of matrices that occur as Jacobians $A(s) = D_u F(u(s), \lambda(s))$ at branches $(u(s), \lambda(s))$ of steady states. While it is possible to use the (easier accessible) singular subspaces for the branches themselves [12], invariant subspaces seem to be indispensable for questions of stability and local approximation of invariant manifolds [1].

In this paper we set up the basics of a continuation method for low-dimensional invariant subspaces of parameter-dependent large matrices. Essentially, we combine well-known predictor-corrector methods with a generalization of the Bartels-Stewart algorithm ([9]) that allows us to reduce to linear systems with bordered matrices of the type

$$\begin{pmatrix} D_uF - \tau I & \phi \\ \hat{\phi}^T & 0 \end{pmatrix}, \ \tau \in C\,, \phi, \hat{\phi} \in R^{m,k}, k \ll m.$$

To these systems we apply the method of [10] which works with a black box solver for the large principle submatrix $D_uF - \tau I$ and which is robust even if this matrix is almost singular. As an application we consider the stability problem for traveling waves in reaction diffusion systems of spatial dimension one. The particular difficulties in this case arise from the essential spectrum (present in the infinite problem) that has to be separated from a few isolated eigenvalues which determine the stability.

This paper is largely based on the theses of the second [13] and the third author [19]. Full details will be provided in a forthcoming paper [2].

2 Continuation of invariant subspaces

We consider a family of matrices $A(s) \in R^{m,m}$ depending smoothly on a parameter $s \in R$. Our aim is to compute smooth matrices $\phi(s) \in R^{m,k}$ the columns of which form a basis of a k-dimensional subspace $R(\phi(s))$ invariant under $A(s)$, i.e.

$$A(s)\phi(s) = \phi(s)\Lambda(s) \tag{1}$$

for some $\Lambda(s) \in R^{k,k}$. With suitable choices of $\hat{\phi}, \phi_0 \in R^{m,k}$ we will normalize $\phi(s)$ according to

$$\hat{\phi}^T\phi(s) = \hat{\phi}^T\phi_0. \tag{2}$$

2.1 Existence and smooth dependence

Assume that for some $s_0 \in R$ we have a simple invariant subspace $R(\phi_0), \phi_0 \in R^{m,k}$ of $A(s_0)$ (see [18] for this notion) i.e. rank $\phi_0 = k$, $A(s_0)\phi_0 = \phi_0\Lambda_0$ for some $\Lambda_0 \in R^{k,k}$ and $R(\phi_0)$ is the unique maximal subspace $E \subset R^m$ satisfying $A(s_0)(E) \subset E, \sigma(A(s_0)_{|E}) \subset \sigma(\Lambda_0)$. Our continuation strategy is based on the following result (see [13]).

Theorem 1. *Under the above assumptions choose $\hat{\phi} \in R^{m,k}$ such that $\hat{\phi}^T\phi_0$ is nonsingular. Then the implicit function theorem applies to the operator equation*

$$T(\phi, \Lambda, s) = \begin{pmatrix} A(s)\phi - \phi\Lambda \\ \hat{\phi}^T\phi - \hat{\phi}^T\phi_0 \end{pmatrix} = 0 \tag{3}$$

at $\phi = \phi_0, \Lambda = \Lambda_0, s = s_0$. In particular, the partial derivative

$$D_{\phi,\Lambda}T(\phi_0, \Lambda_0, s_o)(H, \Delta) = \begin{pmatrix} A(s_0)H - H\Lambda_0 - \phi_0\Delta \\ \hat{\phi}^T H \end{pmatrix}, \ H \in R^{m,k}, \Delta \in R^{k,k}$$

is nonsingular and for s close to s_0 there is a unique branch of solutions $\phi(s), \Lambda(s)$ of (1), (2). Moreover, $R(\phi(s))$ is a simple invariant subspace of $A(s)$.

2.2 The predictor and the corrector step

Assuming the conditions of Theorem 1 we can 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 a linear system of dimension $(m+k)k$

$$\begin{pmatrix} A(s_0)H_0 - H_0\Lambda_0 - \phi_0\Delta_0 \\ \hat{\phi}^T H_0 \end{pmatrix} = \begin{pmatrix} -A'(s_0)\phi_0 \\ 0 \end{pmatrix} \tag{4}$$

This system is a Sylvester type matrix equation for H_0 (cf. [9]) bordered by k^2 extra equations and unknowns. Since $\sigma(\Lambda_0) \subset \sigma(A(s_0))$ the Sylvester equation is singular and it is essential to use the bordering for a stable solution algorithm (see 2.3). Given a step size δ the predictor is given by $(\phi_1, \Lambda_1, s_1) = (\phi_0, \Lambda_0, s_0) + \delta(H_0, \Delta_0, 1)$.

In the corrector step we solve the system (3) with $(s, \hat{\phi}, \phi_0)$ replaced by (s_1, ϕ_0, ϕ_1). Starting at the predictor (ϕ_1, Λ_1), Newton's method generates the sequence $(\phi_\nu, \Lambda_\nu), \nu \geq 1$ defined by

$$\begin{pmatrix} A(s_1)\phi_{\nu+1} - \phi_{\nu+1}\Lambda_\nu - \phi_\nu\Lambda_{\nu+1} \\ \phi_0^T\phi_{\nu+1} \end{pmatrix} = \begin{pmatrix} -\phi_\nu\Lambda_\nu \\ \phi_0^T\phi_1 \end{pmatrix} \tag{5}$$

This system is of the same type as (4) and it is solved by the algorithm in 2.3. We notice that this approach differs from the conventional realization of Newton's method ([5], [4]) where $\Lambda_{\nu+1}$ is eliminated from the first equation of (5) with the help of the second equation.

2.3 A bordered Bartels-Stewart algorithm

The linear systems to be solved in (4) and (5) are of the form

$$\begin{pmatrix} AH - H\Lambda - \phi\Delta \\ \hat{\phi}^T H \end{pmatrix} = \begin{pmatrix} B \\ C \end{pmatrix} \tag{6}$$

where $H, B, \hat{\phi} \in R^{m,k},\ C, \Lambda, \Delta \in R^{k,k}$ and $\sigma(\Lambda) \subset \sigma(A)$. We compute the complex Schur decomposition of the matrix Λ (see [9]).

$$Q^H \Lambda Q = \tilde{\Lambda}, \quad Q^H Q = I, \quad \tilde{\Lambda} \text{ upper triangular.} \tag{7}$$

This involves solving an eigenvalue problem of low dimension $k \ll m$. The system (6) may then be transformed by replacing the matrices H, Δ, B, C, Λ by $\tilde{H} = HQ, \tilde{\Delta} = \Delta Q, \tilde{B} = BQ, \tilde{C} = CQ, \tilde{\Lambda}$. 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 ([9], 7.6.3) by a sequence of bordered linear systems

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

Notice that the upper left block $A - \tilde{\Lambda}_{j,j} I$ is a large sparse and (almost) singular matrix, but that the bordered matrix is generally well conditioned. Linear systems of this type occur quite frequently in bifurcation problems and numerous approaches have been developed for their stable and efficient solution. We propose to use the mixed block elimination method of Govaerts, Pryce [10]. It requires for $A - \tilde{\Lambda}_{j,j} I$ and its transpose a black box solver which is normwise backward stable. It is obvious how to compute the matrices H and Δ from $\tilde{H}$ and $\tilde{\Delta}$. Moreover, we can avoid complex arithmetic by transforming to quasi upper triangular form in (7) (see [13] for the details).

2.4 Some details on the implementation

The previous sections just describe the core linear algebra used in our continuation method. The whole framework has several additional numerical features which will be briefly mentioned here (see [13], [2] for the details).

- An initial guess for an invariant subspace of prescribed dimension k is obtained by well known methods such as Cayley transforms combined with orthogonal subspace iteration. ([9], [8])
- A standard step-size selection strategy is used. If the matrices $A(s)$ arise from linearizing about a steady state branch of a dynamical system $\dot{u} = F(u, \lambda)$ then both continuation methods must be well suited to each other.
- The corresponding k-dimensional invariant subspace $R(\Psi(s))$ of $A^T(s)$ can be computed from one additional linear system.
- The normalizing matrices $\hat{\phi}$ are constantly re-orthogonalized along the branch in order to avoid ill-conditioning.
- Along the branch one tries to keep the dimension of the invariant subspace minimal but above k. Typically, changes in dimension occur when two real eigenvalues collide and become complex or vice versa. The bases of the left and right invariant subspaces are used to detect changes in dimension and provide initial guesses for the updated subspaces. Currently no device is implemented to guarantee that the continued part of the spectrum contains the rightmost eigenvalues in the complex plane. For some interesting algorithms in this direction we refer to [17], [8].

3 Stability of traveling waves

Consider a parabolic system

$$u_t = A u_{xx} + f(u, u_x), \qquad x \in R, \quad t \geq 0, \tag{8}$$

where $u(x,t) \in R^n, A \in R^{n,n}$. Traveling wave solutions of this system are special types of bounded solutions $u(x,t) = \bar{v}(x - ct)$ where

$$\lim_{\xi \to \pm\infty} \bar{v}(\xi) = u_\pm, \quad \lim_{\xi \to \pm\infty} \bar{v}'(\xi) = 0$$

A necessary condition for the asymptotic states $u_\pm$ is $f(u_\pm, 0) = 0$. In case $u_- = u_+$ we have a pulse and a front solution otherwise. In a moving coordinate frame $v(\xi,t) = u(\xi + ct, t)$ equation (8) transforms into

$$v_t = Av_{\xi\xi} + cv_\xi + f(v, v_\xi), \quad \xi \in R, \quad t \geq 0, \tag{9}$$

with stationary solution $v(\xi,t) := \bar{v}(\xi)$. The stability is determined by the spectrum of the linearization of (9) at $\bar{v}$ given by

$$\begin{aligned} u_t &= Au_{xx} + B(\cdot)u_x + C(\cdot)u =: Pu \\ \text{where} \quad B(x) &= cI + D_2 f(\bar{v}(x), \bar{v}'(x)), \quad C(x) = D_1 f(\bar{v}(x), \bar{v}'(x)). \end{aligned}$$

Since (8) is autonomous, the operator P has the eigenvalue zero. If the remaining spectrum is in the half plane $Re \leq -\gamma < 0$ then the wave turns out to be stable with asymptotic phase. We assume that the traveling wave has been computed on a finite interval $[x_-, x_+]$ to sufficient accuracy by standard methods for homoclinic or heteroclinic orbits in the steady state equation of (9) ([6]). Then we consider the eigenvalue problem $Pu = \lambda u$ on $[x_-, x_+]$ with either periodic or Dirichlet boundary conditions. An analysis of the perturbation of the spectra under this process is carried out in [3]. The finite problem is further discretized with constant stepsize $h = (x_+ - x_-)/M$ using centered second-order differences. One obtains a large block tridiagonal matrix (with some bordering due to the boundary conditions) for which we compute small invariant subspaces by the methods of section 2.

4 The complex Ginzburg-Landau equation

The complex Ginzburg-Landau equation is a well known modulation equation, used in physics, and chemistry [15] which depends on two parameters $\alpha, \beta \in R$. We consider a two-parametric version ([16])

$$u_t = (1 + i\alpha)(u_{xx} - (1 + i\beta)^2 u + (1 + i\beta)(2 + i\beta)|u|^2 u). \tag{10}$$

We investigate the stability of the stationary solution $\bar{v}(x) = \cosh(x)^{-(1+i\beta)}$ of (10) (see [11]) where $u_\pm = \lim_{x \to \pm\infty} \bar{v}(x) = 0$. The linearization $L_{\alpha,\beta}$ of (10) at $\bar{v}$ is given in real and imaginary parts by the following two-dimensional system

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

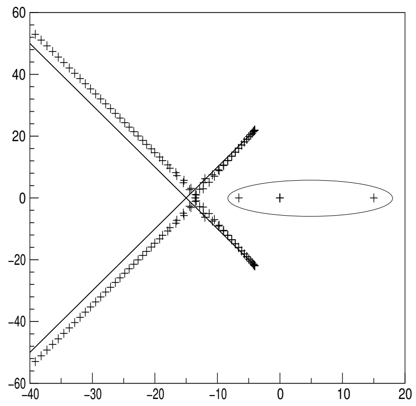
where

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

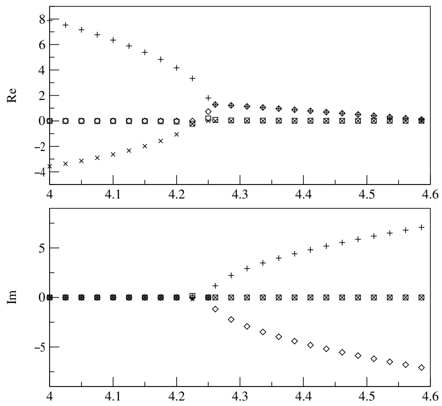
The operator $L_{\alpha,\beta}$ has a zero eigenvalue with geometric multiplicity at least two and corresponding eigenfunctions $\bar{v}'$ and $i\bar{v}$. The full spectrum for the values $x_\pm = \pm 20, h = 0.04, \alpha = -2, \beta = 3$ and the essential spectrum are shown in Fig. 1(a). The essential spectrum consists of two half-lines which cross the imaginary axis on the critical curve (cf. [3]).

$$\beta(\beta + 2\alpha) - 1 = 0. \tag{11}$$

We continue a four-dimensional subspace that belongs to the zero eigenvalues and the two real eigenvalues encircled in Fig. 1(a). With increasing β the stable eigenvalue passes zero (as shown by Mielke this happens precisely on the curve (11) where a generalized eigenvector corresponding to $i\bar{v}$ 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 motion appears in 1(b) (see [3] for details). This sensitive behaviour could only be revealed since the 4D-subspace stays separated and the remaining 4×4 eigenvalue problem can be solved very accurately.



(a) part of the essential and numerical spectrum



(b) real and imaginary part vs. β

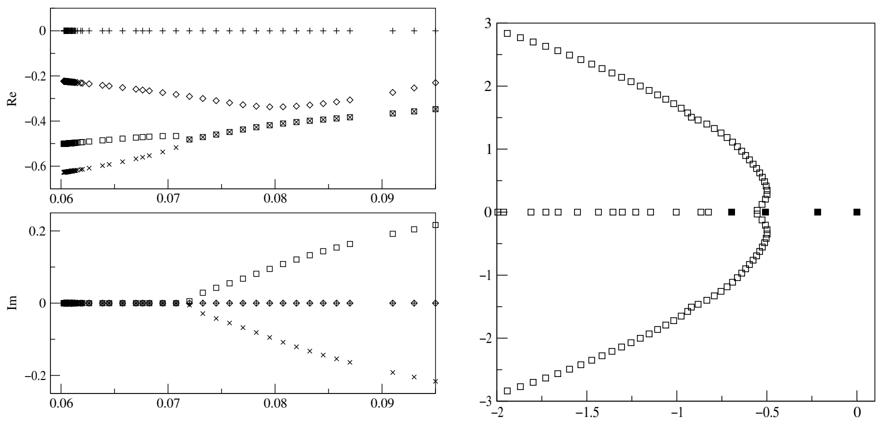
Fig. 1. Ginzburg-Landau equation, $\alpha = -2$

5 The FitzHugh-Nagumo system

The FitzHugh-Nagumo equation is a model equation for the propagation of nerve impulses [7]. We consider a two-dimensional system with a small additional diffusive term

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

For the parameters $a = 0.7, b = 0.8$ there is a branch containing stable and unstable waves (for details see [2]). We consider a specific part of the stable branch and follow again a four dimensional subspace with decreasing parameter Φ. Fig. 2(a) shows real and imaginary parts of the eigenvalues on this branch. While the two largest real eigenvalues remain separated from the essential spectrum the other two move towards it. The situation at $\Phi_{crit} = 0.062$ is shown in Fig. 2(b). At this point our algorithm breaks down (due to stagnation of the continuation steps) because these two eigenvalues can no longer be separated from the cluster that approximates the essential spectrum. Of course, concerning the stability problem there is no need to further include these eigenvalues in the continuation.



(a) real and imaginary parts vs. Φ

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

Fig. 2. FitzHugh-Nagumo, stable wave, $x_- = 0, x_+ = 65, h = 0.1$

References

1. W.-J. Beyn and W. Kleß. Numerical Taylor expansions of invariant manifolds in large dynamical systems. *Numerische Mathematik*, 80:1–38, 1998.
2. W.-J. Beyn, W. Kleß, and V. Thümmler. Continuation methods for low-dimensional invariant subspaces with applications to dynamical systems of large dimension. in preparation, 1999.
3. W.-J. Beyn and J. Lorenz. Stability of traveling waves: Dichotomies and eigenvalue conditions on finite intervals. *Numer. Funct. Anal. and Optimiz.*, 20:201–244, 1999.
4. F. Chatelin. *Eigenvalues of matrices.* John Wiley & Sons, 1993.
5. J. W. Demmel. Three methods for refining estimates of invariant subspaces. *Computing*, 38:43–57, 1987.
6. E. Doedel, T. Champneys, T. Fairgrieve, Y. Kuznetsov, B. Sandstede, and X.-J. Wang. *AUTO97 Continuation and bifurcation software for ordinary differential equations (with HomCont).* Concordia Univ. Montreal, 1997. available via ftp.cs.concordia.ca/pub/doedel/auto.
7. R. FitzHugh. Impulses and physiological states in theoretical models of nerve membrane. *Biophysical Journal*, 1:445–466, 1961.
8. T. J. Garratt, G. Moore, and A. Spence. A generalised Cayley transform for the numerical detection of Hopf bifurcations in large systems. In *Contributions in numerical mathematics*, pages 177–195. World Sci. Publ., 1993.
9. G. H. Golub and C. F. van Loan. *Matrix Computations.* The John Hopkins University Press, 2 edition, 1989.
10. W. Govaerts and J. D. Pryce. Mixed block elimination for linear systems with wider borders. *IMA J. Numer. Anal.*, 13:161–180, 1993.
11. L. M. Hocking and K. Stewartson. On the nonlinear response of a marginally unstable plane parallel flow to a two-dimensional disturbance. *Proc. Roy. Soc. London Ser. A*, 326:289–313, 1972.
12. H. Jarausch. Analyzing stationary and periodic solutions of systems of parabolic partial differential equations by using singular subspaces as reduced basis. *Math. Comput. Modelling*, 20:69–87, 1994.
13. W. Kleß. *Numerische Approximation lokal invarianter Mannigfaltigkeiten in großen dynamischen Systemen.* PhD thesis, University of Bielefeld, 1997.
14. Y. Kuznetsov and V. Levitin. *CONTENT: A multiplatform environment for analyzing dynamical systems.* GWI Amsterdam, 1997. available via ftp.cwi.nl/pub/CONTENT.
15. C. D. Levermore and M. Oliver. The complex Ginzburg-Landau equation as a model problem. In *Dynamical systems and probabilistic methods in partial differential equations*, pages 141–190. Amer. Math. Soc., 1996.
16. A. Mielke. The complex Ginzburg-Landau equation on large and unbounded domains: sharper bounds and attractors. *Nonlinearity*, 10:199–222, 1997.
17. R. Neubert. Predictor-corrector techniques for detecting Hopf bifurcation points. *Internat. J. Bifur. Chaos Appl. Sci. Engrg.*, 3(5):1311–1318, 1993.
18. G. W. Stewart and J. Sun. *Matrix perturbation theory.* Academic press, 1990.
19. V. Thümmler. Numerische Stabilitätskriterien für wandernde Wellen. Master's thesis, University of Bielefeld, 1998.