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# Efficient computation of analytic bases in Evans function analysis of large systems

Received: 16 July 2005 / Revised: 18 November 2005  
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**Abstract** In Evans function computations of the spectra of asymptotically constant-coefficient linearized operators of large systems, a problem that becomes important is the efficient computation of global analytically varying bases for invariant subspaces of the limiting coefficient matrices. In the case that the invariant subspace is spectrally separated from its complementary invariant subspace, we propose an efficient numerical implementation of a standard projection-based algorithm of Kato, for which the key step is the solution of an associated Sylvester problem. This may be recognized as the analytic cousin of a  $C^k$  algorithm developed by Dieci and collaborators based on orthogonal projection rather than eigenprojection as in our case. For a one-dimensional subspace, it reduces essentially to an algorithm of Bridges, Derks and Gottwald based on path-finding and continuation methods.

## 1 Introduction

A useful tool in the study of stability of traveling waves is the Evans function, an analytic function whose zeroes correspond to the eigenvalues of the linearized operator about the wave. More generally, let  $L$  be a differential operator with

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asymptotically constant coefficients along some preferred spatial direction  $x$ , and suppose that the eigenvalue equation  $(L - \lambda)w = 0$  may be expressed as a first-order ODE in an appropriate phase space:

$$W_x = A(\lambda, x)W, \quad \lim_{x \rightarrow \pm\infty} A(\lambda, x) = A_{\pm}(\lambda), \quad (1)$$

with  $A$  analytic in  $\lambda$  as a function from an open, simply connected subset  $\Omega$  of  $\mathbb{C}$  to  $C^1(\mathbb{R}, \mathbb{C}^{n \times n})$  and the dimension  $k$  of the stable subspace  $S_+$  of  $A_+$  and dimension  $n - k$  of the unstable subspace  $U_-$  of  $A_-$  summing to the dimension  $n$  of the entire phase space.

Then, one may construct analytic bases of solutions  $w_1^+, \dots, w_k^+$  and  $w_{k+1}^-, \dots, w_n^-$  respectively spanning the manifolds of solutions decaying as  $x \rightarrow +\infty$  and  $-\infty$  by essentially initializing them at infinity with values from the stable (resp. unstable) subspace of  $A_+$  (resp.  $A_-$ ) and solving toward  $x = 0$  using the ODE (1). The Evans function is then defined as

$$D(\lambda) := \det(W_1^+ \cdots W_k^+ W_{k+1}^- \cdots W_n^-), \quad (2)$$

for details, see, e.g., [2, 17, 21, 32, 34] and references therein.

Numerical approximation of the Evans function thus breaks into two problems: the computation of analytic bases for stable (resp. unstable) subspaces of  $A_+$  (resp.  $A_-$ ) and the solution of ODE (1) on a sufficiently large interval  $x \in [0, M]$  (resp.  $x \in [-M, 0]$ ). A difficulty in the latter problem is numerical stiffness for  $k, n - k \neq 1$ , due to the need to resolve modes of different exponential decay (resp. growth) rates. This was overcome in an elegant fashion in the 1998 doctoral thesis of Brin [8–10] by working in the exterior product space  $W_1^+ \wedge \cdots \wedge W_k^+ \in \mathbb{C}^{\binom{n}{k}}$  (resp.  $W_{k+1}^- \wedge \cdots \wedge W_n^- \in \mathbb{C}^{\binom{n}{n-k}}$ ), for which the desired subspace appears as a single, maximally stable (resp. unstable) mode.

This “exterior-product method” was rediscovered and further developed by Bridges et al. [3, 7], who pointed out also its mathematical equivalence to the much earlier “compound matrix method” introduced by Ng and Reid [27–30] for the numerical solution of stiff ODE, of which it may be regarded as a coordinate-independent implementation.

An earlier instance of the method may be found in a 1995 Evans function computation carried out by Pego in the Appendix of [1].

The computation of an analytic basis is likewise straightforward in the exterior-product framework, since it reduces to the calculation of a single eigenvector. Two quite satisfactory approaches to this problem (described further below) were given in [10] and [7], each of order  $\binom{n}{k}^3$  equal to the cost of a matrix inversion or the multiplication of two matrices in dimension  $\binom{n}{k} \times \binom{n}{k}$ : negligible compared to the cost of integrating the exterior-product version of (1). The “direct” method of [10] has the advantage of simplicity, featuring a simple structure involving only calls to standard linear-algebra subroutines, while the method of [7] (only slightly more difficult to code) has the advantage of greater efficiency in the sense that the coefficient  $C$  in the complexity estimate  $C \binom{n}{k}^3$  is smaller.

Together, these two steps give an extremely fast and well-conditioned shooting algorithm for the computation of the Evans function, for moderate values of  $n$ . However, for equations of large dimension  $n$ , such as those that arise in complicated

physical systems or through transverse discretization of a multi-dimensional problem on a cylindrical domain [24], the exterior-product method quickly becomes impractical, since the typical value  $k \sim n/2$  leads to a working dimension  $\binom{n}{n/2}$  growing as  $n^{n/2}$ . For example, for the typical values  $n \sim 10^2$  found in [24], this is clearly out of computational range.

In this situation, Sandstede [31] has suggested in place of the high-dimensional shooting methods described above, to recast (1) as a boundary-value problem with appropriate projective boundary conditions, which may be solved in the original space  $\mathbb{C}^n$  for individual modes by robust and highly accurate collocation/continuation techniques, thus reducing the cost to polynomial order  $C(n)kn^2$ , where  $C(\cdot)$  counts the number of mesh points required as the number of operations rises. However, it remains to provide a correspondingly efficient initialization routine prescribing analytic basis/projection for the stable (resp. unstable) subspace of  $A_+$  (resp.  $A_-$ ).

The direct method of [10] admits a straightforward generalization to this case. Namely, given matrix  $A$ , one may efficiently ( $\sim 32n^3$  operations; see [18,33]) compute by “ordered” Schur decomposition,<sup>1</sup> i.e., Schur decomposition  $A = QUQ^{-1}$ ,  $Q$  orthogonal and  $U$  upper triangular, for which also the diagonal entries of  $U$  are ordered in increasing real part, orthonormal bases of its stable (resp. unstable) subspaces, and thereby the stable (resp. unstable) eigenprojection  $P$  (resp.  $I - P$ ). Once these projections are known, the desired analytic basis may be obtained by solution of a linear analytic ODE

$$S_\lambda = B(P(\lambda))S, \quad (3)$$

introduced by Kato [(6) below] for a block-diagonalizing unitary transformation  $S$ . However, in the computationally intensive large- $n$  regime, it is desirable also to generalize the more efficient method of [7].

In this note, we describe such an algorithm based on a reformulation of the standard ODE construction of Kato by which existence of an analytic basis is usually proved. More precisely, we derive a Riccati-type ODE in  $\lambda$ :

$$S_\lambda = F(S, \lambda), \quad (4)$$

((16)–(17) below) equivalent to (3) for which the computation of  $F$  costs fewer than  $3.5n^3$  operations, for the coordinate transformation  $S$  reducing the desired  $k$ -dimensional basis (resp. projection) to the standard Euclidean one. Moreover, the computations involved are standard matrix operations permitting use of readily available fast subroutines.

The algorithm so derived is closely related to an algorithm derived from quite different considerations by Dieci and collaborators [11, 13–16] for efficient computation of *local, smoothly varying* bases of invariant subspaces. More precisely, both algorithms may be regarded as instances of the same method for numerically integrating Kato’s ODE (3), with different choices of projection  $P$ : analytic eigenprojection in our case, nonanalytic but uniformly well-conditioned orthogonal projection in the case of [11, 13–16]. Their development, having its origins in the work of Beyn [4], proceeds from local principles of “least variation” in the associated Schur factorization, rather than analytic dependence.

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<sup>1</sup> Supported, for example, in MATLAB and LAPACK.

It is somewhat remarkable that these quite different criteria lead to a common method.

In the special case  $k = 1$ , our algorithm reduces essentially to one developed in [7] based on continuation methods. However, the latter does not appear to directly generalize in the form given to case  $k > 1$ , nor was there made a connection to Kato's ODE (6) (a crucial point in verifying analyticity; see Remark 4.1).

Though the relation of (3) to Kato's ODE seems to be well-known among experts on smooth continuation, at least in principle (L. Dieci, private communication), there does not seem to be any explicit discussion in the literature of this fact, or of the problem of global analytic continuation. Nor, likewise, does there appear in the Evans function literature reference to the large body of work by Dieci and others on efficient continuation algorithms [11, 13–16]. Thus, it seems useful to make clearly and explicitly these connections, as we do here without claim to originality.

## 2 The algorithm of Kato

We first recall the theorem of Kato on which our algorithm is based.

**Proposition 2.1** ([22, § II.4.2]) *Let  $P(\lambda)$  be an analytically varying projection on a simply connected domain  $\Omega \subset \mathbb{C}$ . Then, the linear analytic ODE*

$$r'_j = [P', P]r_j; \quad r_j(\lambda_0) = r_j^0 \tag{5}$$

*defines a global analytically varying basis  $\{r_j(\lambda)\}$  of the associated invariant subspace  $\text{Range } P(\lambda)$ , where “'” denotes  $d/d\lambda$  and  $[A, B] := AB - BA$  the commutator of  $A$  and  $B$ .*

*More generally,*

$$S' = [P', P]S; \quad S(\lambda_0) = I. \tag{6}$$

*defines a global analytic coordinate change such that*

$$S^{-1}PS \equiv \text{constant} = P_0. \tag{7}$$

*Proof* Relation (7) follows from  $(S^{-1}PS)' = 0$ , as may be established by direct calculation using the key relations  $PP'P = 0$  and  $(I - P)(I - P)'(I - P) = 0$ , which in turn follow by differentiation of the projective equation  $P^2 - P = 0$ . Observing that  $S^{-1}$  satisfies the “transpose” ODE

$$(S^{-1})' = -S^{-1}S'S^{-1} = -S^{-1}[P', P]SS^{-1} = -S^{-1}[P', P], \tag{8}$$

we have that both  $S$  and its inverse satisfy linear analytic ODEs, hence have global bounded analytic solutions in  $\Omega$  by standard analytic ODE theory [12]. Finally,  $\text{Range } P = S \text{Range } P_0$  is spanned by the columns of  $SR_0$ , where the columns of  $R_0$  are chosen to span  $\text{Range } P_0$ , verifying (5).  $\square$

*Remark 2.2* From (8) we see that  $S$  (hence  $R$ ) is unitary if  $P$  is self-adjoint (i.e., an orthogonal projection), since in that case  $[P', P]^* = -[P', P]$ , so that  $S^*$  and  $S^{-1}$  satisfy the same ODE with same initial conditions  $I$ . Likewise, the relation  $P = SP_0S^{-1} = SP_0S^*$  shows that, for  $P_0$  self-adjoint,  $S$  is unitary only if  $P$  is self-adjoint for all  $\lambda$ .

**Definition 2.3** For a given matrix  $A$ , a subspace  $E$  is  $A$ -invariant if  $AE \subset E$ ; a projection  $P$  is  $A$ -invariant if  $PA = AP$ .

Every spectrally separated  $A$ -invariant subspace is the range of a unique  $A$ -invariant projection  $P$ ; likewise, both range and kernel of an  $A$ -invariant projection are  $A$ -invariant.

**Corollary 2.4** Let  $A(\lambda) \in \mathbb{C}^{n \times n}$  be an analytically varying matrix on a simply connected domain  $\Omega$  and  $E(\lambda)$  a spectrally separated  $A$ -invariant subspace. Then, there exists a global analytic basis of  $E(\lambda)$  defined by (5), where  $P$  is the unique  $A$ -invariant projection associated with  $E$ .

*Proof* Under the assumption of spectral separation, the  $A$ -invariant projection  $P(\lambda)$  associated with  $E$  is analytic, by standard matrix perturbation theory [22]. Applying Proposition 2.1, we obtain the result.  $\square$

*Remark 2.5* Corollary 2.4 includes Proposition 2.1 as a special case, with  $A = P$  and  $E = \text{Range } P$ . Thus, there is no loss of generality in working with this matrix-based formulation, as we shall do throughout the sequel.

The following standard result (proof deferred to the following section) gives a useful geometric characterization of the basis obtained through (5).

**Proposition 2.6** Let  $R(\lambda) = (r_1 \cdots r_k) \in \mathbb{C}^{n \times k}$ , be the matrix of basis vectors of  $E(\lambda)$  defined by ODE (5) and  $L \in \mathbb{C}^{k \times n}$  be the matrix whose rows form the dual basis of  $\tilde{E}(\lambda) := \text{Range } P^*$ ,  $LR \equiv I_k \in \mathbb{C}^{k \times k}$ . Then,

$$LR' \equiv L'R \equiv 0. \quad (9)$$

*Remark 2.7* Property (9) is a standard normalization favorable for spectral perturbation calculations; see, e.g., [19, 20, 25, 26]. Thus, the Kato basis is in some sense optimal. This property, together with  $A$ -invariance, uniquely determines the Kato ODE.

### 3 Projection-independent version

Let  $P(\lambda)$  denote an analytically varying projection that maps  $\Omega \subset \mathbb{C}$  into  $\mathbb{C}^{n \times n}$  with  $P(\lambda_0) = P_0$ , then we may, without loss of generality, set

$$P_0 = \begin{pmatrix} I_k & 0 \\ 0 & 0 \end{pmatrix}, \quad (10)$$

where  $k := \dim \text{Range } P$ . Then, we have:

**Lemma 3.1** For  $S$  satisfying (6),  $P_0$  as in (10), the matrix  $Y := S^{-1}S'$  vanishes on diagonal blocks, i.e.,

$$Y = \begin{pmatrix} 0_k & * \\ * & 0_{n-k} \end{pmatrix}. \quad (11)$$

*Proof* Multiplying (6) on the left by  $S^{-1}$  and rearranging using (7), we obtain

$$Y = [S^{-1}P'S, P_0]. \tag{12}$$

Observing that a commutator with the block-diagonal matrix  $P_0$  (or any block-diagonal matrix whose diagonal blocks are multiples of the identity) vanishes on diagonal blocks, we are done.  $\square$

*Proof of Proposition 2.6* By coordinate-independence of (6), we may without loss of generality take (10), whence  $R = \begin{pmatrix} S_{11} \\ S_{21} \end{pmatrix}$ ,  $L = ((S^{-1})_{11} \ (S^{-1})_{12})$ , and (9) follows from (11).  $\square$

*Remark 3.2* For applications, it is more convenient to substitute for the normalization (10), involving an additional change of coordinates, the more general algorithm

$$S' = [P', P]S; \quad S(\lambda_0) = S_0, \tag{13}$$

with normalization  $S_0^{-1}P_0S_0 = \begin{pmatrix} I_k & 0 \\ 0 & 0 \end{pmatrix}$ , or, equivalently,

$$S_0^{-1}A_0S_0 = \begin{pmatrix} \alpha_0 & 0 \\ 0 & \beta_0 \end{pmatrix}. \tag{14}$$

It is easily seen that the conclusion of Proposition 2.1 then holds with (7) replaced by

$$S^{-1}PS \equiv \text{constant} = \begin{pmatrix} I_k & 0 \\ 0 & 0 \end{pmatrix},$$

with the desired analytic basis given by the first  $k$  columns of  $S$ .

### 3.1 The algorithm

Let  $S, P$  be as in (13), (14), with  $P$  an  $A$ -invariant projection (i.e.,  $AP = PA$ ) with spectrally separated range  $E$ , associated with some analytically varying matrix  $A(\lambda)$ ,

so that

$$S^{-1}AS = \begin{pmatrix} \alpha(\lambda) & 0 \\ 0 & \beta(\lambda) \end{pmatrix}. \tag{15}$$

Then, we have:

**Proposition 3.3** *The matrix  $S$  defined in (13) is uniquely determined by*

$$S' = SY, \quad Y = \begin{pmatrix} 0 & Y_{12} \\ Y_{21} & 0 \end{pmatrix}, \tag{16}$$

where  $Y$  satisfies the Sylvester problem

$$Y \begin{pmatrix} \alpha & 0 \\ 0 & \beta \end{pmatrix} - \begin{pmatrix} \alpha & 0 \\ 0 & \beta \end{pmatrix} Y = \begin{pmatrix} 0 & (S^{-1}A'S)_{12} \\ (S^{-1}A'S)_{21} & 0 \end{pmatrix}. \tag{17}$$

*Remark 3.4* As discussed in the introduction, ODE (16), (17) is quite similar to the one developed by Dieci and collaborators for the purpose of generating local, smoothly varying bases. In place of our similarity transform  $S$  diagonalizing  $A$ , they seek a unitary matrix  $Q$  effecting the decomposition  $Q^* A Q = \begin{pmatrix} R_{11} & R_{12} \\ 0 & R_{22} \end{pmatrix}$ , leading to the 1-1 block of (16) for  $Y := Q^{-1} Q' = Q^* Q'$ , with  $Q$  substituted for  $S$  and  $R_{11}$  and  $R_{22}$  substituted for  $\alpha, \beta$ ; see (1)–(3) of [16]. Blocks  $Y_{11}$  and  $Y_{22}$  are again set to zero, while  $Y_{21} = -Y_{12}^*$  is forced by the fact that  $Q^* Q'$  is skew-symmetric.

The resulting (orthonormal) basis  $\Omega := Q(I, 0)^T$  thus satisfies

$$\Omega^* \Omega' = Y_{11} = 0,$$

which, by Remark 2.7, is the property uniquely characterizing the Kato ODE for projection  $\tilde{P}$  defined as orthogonal projection. Thus, we may conclude that the algorithm of Dieci et al. is exactly the Kato algorithm generated by orthogonal projection.

*Proof of Proposition 3.3* Differentiating the relation (15), we obtain

$$-S^{-1} S' S^{-1} A S + S^{-1} A S' = -S^{-1} A' S + \begin{pmatrix} \alpha' & 0 \\ 0 & \beta' \end{pmatrix}, \quad (18)$$

or, appealing to (15),

$$Y \begin{pmatrix} \alpha & 0 \\ 0 & \beta \end{pmatrix} - \begin{pmatrix} \alpha & 0 \\ 0 & \beta \end{pmatrix} Y = S^{-1} A' S - \begin{pmatrix} \alpha' & 0 \\ 0 & \beta' \end{pmatrix}, \quad (19)$$

for  $Y := S^{-1} S'$ . Noting that the left-hand side of (19) vanishes on diagonal blocks, as a commutator of a block-diagonal matrix and a matrix ( $Y$ ) with vanishing corresponding diagonal blocks, we obtain the result.  $\square$

The linear operator in  $Y$  determined by the left-hand side of (17) is invertible and numerically well-conditioned if and only if  $\alpha$  and  $\beta$  have disjoint spectrum. Thus, when  $E$  is spectrally separated from its complementary  $A$ -invariant subspace, (16), (17) together give the desired projection-independent algorithm for the computation of  $S$  and the basis  $r_j(\lambda) = S(\lambda)e_j$ . If needed, the projection  $P(\lambda)$  may be recovered through (7) and (10) as

$$P = RL = S \begin{pmatrix} I_k & 0 \\ 0 & 0 \end{pmatrix} S^{-1}. \quad (20)$$

Since the Sylvester problem is known to be of complexity  $O(n^3)$  (see, e.g., [18]), as is the matrix multiplication involved in the calculation of the right-hand side, Proposition 3.3 yields an  $O(n^3)$  algorithm as claimed.

More precisely, if  $A$  is  $n \times n$ ,  $B$  is  $m \times m$ , and both  $X$  and  $C$  are  $n \times m$ , then problem  $AX + XB = C$  may be solved with  $4mn(m+n)$  operations [18], yielding cost  $4n(n-k)k$ . Likewise, it is easily calculated that the multiplications in the calculation of  $SY$  and the right-hand side of (17) together cost  $2n^3 + 2n(n-k)k$ , for a total cost of

$$2n^3 + 6nk(n-k) \leq 3.5n^3, \quad (21)$$

with equality in the worst (and typical) case  $k = n/2$ .

### 3.2 Proposed implementation

A typical application (cf. [7–10]) is to compute the winding number of the Evans function about a large closed contour  $\Gamma$  in the non-stable complex half plane  $\Re\lambda \geq 0$ , thus determining the number of unstable eigenvalues enclosed in  $\Gamma$ . The requisite initialization at spatial infinity may be efficiently accomplished by (i) computing a starting value  $S_0 = (E_0 \ F_0)$  for the transformation  $S$  at a base point  $\lambda_0$  by ordered Schur decomposition as discussed in the introduction, where the columns of  $E_0$  and  $F_0$  are bases for the  $A_0$ -invariant subspace  $E(0)$  and its  $A$ -invariant complement  $F(0)$ , then (ii) advancing these values analytically by the ODE algorithm described in section 3.2 above.

Specifically, in step (ii) we solve an ODE

$$S' = F(S, \lambda) = SY(S, \lambda),$$

where  $Y$  is determined by the property that it must vanish on diagonal blocks together with the off-diagonal blocks of Sylvester problem (17). To determine the off-diagonal blocks of (17), we must invert  $S$ , then compute the diagonal blocks  $\alpha, \beta$  of  $S^{-1}AS$  and the off-diagonal blocks of  $S^{-1}A'S$ . These steps, solution of the resulting pair of Sylvester problems corresponding to the off-diagonal blocks, and the multiplication  $SY$  (taking account that  $Y$  vanishes on off-diagonal blocks) together cost  $\sim 3.5n^3$  operations, as described in the previous subsection, This is the cost of each functional evaluation of  $F$ .

The ODE may then be integrated by a standard Runge–Kutta or Euler method, for a total cost of  $\mathcal{O}(n^3N)$  operations, where  $N$  denotes the number of mesh points involved in the prescribed contour. (Note: since the ODE has analytic coefficients, it may be solved by an extremely high-order accuracy scheme for further savings.)

*Remark 3.5* One might also think of evolving  $S^{-1}$  by the associated ODE  $(S^{-1})' = -YS^{-1}$ . However, this would be more expensive ( $3.5n^3$  vs.  $n^3/3$  operations) and, due to accumulated roundoff error, less accurate than the direct matrix inversion prescribed above.

*Remark 3.6* Alternatively, (17) might be viewed as an  $N \times N$  system of linear equations in the  $N := k^2 + (n-k)^2$  nonzero entries of  $Y$ , which is invertible when  $E, F$  are spectrally separated. However, the cost of solution by this method would be order  $N^3 = n^6 \gg n^3$ .

*Remark 3.7* Defining  $R \in \mathbb{C}^{n \times k}$  and  $L \in \mathbb{C}^{k \times n}$  as in Proposition 3.1, we may obtain from the first block of (16) an evolution equation

$$\begin{aligned} \bar{\beta}R' - R'\alpha &= (I - RL)A'R, \\ L'\bar{\beta} - \alpha L' &= LA'(I - RL) \end{aligned} \tag{22}$$

in  $R, L$  alone, where  $\alpha = LAR, \bar{\beta} := (I - RL)A(I - RL)$ , and  $LR' = L'R = 0_k$ . This is likewise a Sylvester problem, and so well-conditioned when  $E$  is spectrally separated. However, this reduction seems to be mainly of theoretical interest, since the solution of (22) appears to require either inversion of an enlarged  $(kn) \times (kn)$  system analogous to that described in Remark 3.6 or else coordinatization of  $F$  and  $\tilde{F}$  by the calculation of bases orthogonal to  $\tilde{E}$  and  $E$ .



### 3.3 Stability

Finally, we comment briefly on stability of the proposed algorithm. An inherent limitation of the method, both numerically and analytically, is that the spectra of  $\alpha$  and  $\beta$ , i.e., the spectra of  $A$  associated with the invariant subspace  $E$  to be computed and its invariant complement  $F$ , must remain separated in the domain of computation. This condition is essentially always satisfied in the Evans function context, where  $E$  and  $F$  are the stable and unstable subspaces of  $A$  and  $\Re\lambda \geq 0$  is the computational domain; indeed, it is a consequence of the standard, “consistent splitting” assumption (see, e.g., [2, 17, 32]), roughly equivalent to linearized stability of the limiting endstates of the traveling wave under study as a constant solutions of the underlying evolution equation, that  $A(\lambda)$  possess no pure imaginary eigenvalues on  $\Re\lambda \geq 0$ .

Numerical well-conditioning requires, further, that, possibly after preconditioning by an appropriate coordinate transformation, (i) the spectra of  $\alpha$  and  $\beta$  remain uniformly separated relative to the norm of  $A$ , and (ii) the spaces  $E$  and  $F$  remain uniformly transverse. These conditions are satisfied quite generally in applications for high frequencies  $|\lambda| \gg 1$ . For example, a general second-order parabolic evolution equation in one dimension,  $u_t + f(u, u_x) = (B(u)u_x)_x$ ,  $B$  symmetric, linearized about a constant solution  $u \equiv u_o$ , yields an eigenvalue equation  $Bu'' + Cu' + Du = \lambda u$ , which, written as a first-order equation after the parabolic rescaling  $x \rightarrow |\lambda|^{1/2}x$ ,  $u' \rightarrow |\lambda|^{-1/2}u'$ , appears as an ODE  $U' = AU$ ,  $U = (u^T, u'^T)^T$ , for which the coefficient matrix

$$A = \begin{pmatrix} 0 & I \\ B^{-1}\lambda/|\lambda| & 0 \end{pmatrix} + O(|\lambda|^{-1/2})$$

satisfies (i), (ii) for  $|\lambda| \gg 1$ , assuming uniform ellipticity  $B \geq \theta > 0$ .

For low frequencies and large  $n$ , it is often the case that, when consistent splitting can be verified, it can be verified by an *energy estimate* yielding at the same time (i) and (ii). However, clearly (i), (ii) amount to additional structural conditions on the equations, which in general may be violated as  $n \rightarrow \infty$ .

For the specific examples considered in [24], arising through transverse discretization of a multi-dimensional second-order parabolic evolution equation problem on a cylindrical domain, higher modes correspond to higher transverse frequencies, and we can conclude, similarly as in the large  $|\lambda|$  case that (i), (ii) are satisfied assuming only uniform ellipticity of the second-order term. Thus, at least in our main motivating example, the problem is indeed numerically feasible by the method we propose.

## 4 The algorithm of Bridges, Derks and Gottwald

In the one-dimensional case  $k = 1$ , (17) reduces to a pair of standard matrix equations of dimension  $(n - 1) \times (n - 1)$ :

$$\begin{aligned} Y_{12}(\beta - \alpha I_{n-k}) &= (S^{-1}A'S)_{12}, \\ (\beta - \alpha I_{n-k})Y_{21} &= -(S^{-1}A'S)_{21}. \end{aligned} \tag{23}$$

We may compare this to the  $(2n + 1) \times (2n + 1)$  system

$$\begin{aligned} \begin{pmatrix} A - \alpha & -R \\ -L & 0 \end{pmatrix} \begin{pmatrix} R' \\ \alpha' \end{pmatrix} &= \begin{pmatrix} -A'R \\ 0 \end{pmatrix}, \\ (L' \ \alpha') \begin{pmatrix} A - \alpha & -R \\ -L & 0 \end{pmatrix} &= (-LA' \ 0), \end{aligned} \tag{24}$$

proposed by Bridges et al. in [7] as an alternative to Kato's ODE, motivated by similar methods used in continuation [23]. The cost of either algorithm is mainly that of a single matrix inversion, of dimension  $(n - 1)$  and  $(n + 1)$ , respectively. From the relation  $LR' = 0$ , we see that (24) is equivalent to Kato's ODE and thus to (23). The link between the two algorithms is the standard relation  $\alpha' = LA'R$ .

*Remark 4.1* Global solubility of (16), (17) or the related one-dimensional algorithms (23), (24) follows from the corresponding property of Kato's ODE (6). However, it is not immediately apparent from the original formulation, since the associated ODE are (at least apparently) nonlinear and so not necessarily uniformly Lipschitz in the respective arguments  $S$  and  $(R, L, \alpha)$ .

In the scalar case (23), (24), we may alternatively observe directly that

$$\begin{pmatrix} A - \alpha & -R \\ -L & 0 \end{pmatrix}^{-1} = \begin{pmatrix} (A - \alpha + P)^{-1}(I - P) & -R \\ -L & 0 \end{pmatrix},$$

where  $P(\lambda)$  denotes the eigenprojection of  $A(\lambda)$  associated with eigenvalue  $\alpha(\lambda)$ , hence (24) reduces to  $\alpha' = LA'R$  and equations

$$\begin{aligned} R' &= -(A - \alpha + P)^{-1}(I - P)A'R, \\ L' &= -LA'(I - P)(A - \alpha + P)^{-1} \end{aligned} \tag{25}$$

(a special case of (22)) that, considering  $\alpha$  as a known globally analytic function of  $\lambda$ , are linear in  $(R, L)$ , hence globally soluble. This repairs a minor omission in [7], proof of Lemma 5.1, p. 202, which cites the theorem that an ODE (4) with  $F$  globally Lipschitz in  $S$  on compact sets of  $\lambda$  and analytic in  $\lambda$  is globally analytically soluble on a simply connected domain  $\Omega$ , but without verifying or explicitly stating the condition that  $F$  be *globally* Lipschitz. (For  $F$  locally Lipschitz, an easy counterexample is the complex Riccati equation  $S' = S^2$ .)

## 5 Further comments

Matrices  $A$  coming from PDE are often sparse as well, so it is desirable also to design algorithms exploiting this property. This has been studied, for example, in [5,6].

**Acknowledgements** Research of J.H. was partially supported under Ohio State University NSF VIGRE grant DMS-0135308. Research of B.S. was partially supported under NSF grant DMS-0203854 and by a Royal Society–Wolfson Research Merit Award. Research of K.Z. was partially supported under NSF grants number DMS-0070765 and DMS-0300487. Thanks to Luca Dieci for helpful conversations regarding the numerical literature on continuation of invariant subspaces.

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