

Computation of pseudospectral abscissa for large-scale nonlinear eigenvalue problems

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We present an algorithm to compute the pseudospectral abscissa for a nonlinear eigenvalue problem. The algorithm relies on global under-estimator and over-estimator functions for the eigenvalue and singular value functions involved. These global models follow from eigenvalue perturbation theory. The algorithm has three particular features. First, it converges to the globally rightmost point of the pseudospectrum, and it is immune to nonsmoothness. The global convergence assertion is under the assumption that a global lower bound is available for the second derivative of a singular value function depending on one parameter. It may not be easy to deduce such a lower bound analytically, but assigning large negative values works robustly in practice. Second, it is applicable to large-scale problems since the dominant cost per iteration stems from computing the smallest singular value and associated singular vectors, for which efficient iterative solvers can be used. Furthermore, a significant increase in computational efficiency can be obtained by subspace acceleration, that is, by restricting the domains of the linear maps associated with the matrices involved to small but suitable subspaces, and solving the resulting reduced problems. Occasional restarts of these subspaces further enhance the efficiency for large-scale problems. Finally, in contrast to existing iterative approaches based on constructing low-rank perturbations and rightmost eigenvalue computations, the algorithm relies on computing only singular values of complex matrices. Hence, the algorithm does not require solutions of nonlinear eigenvalue problems, thereby further increasing efficiency and reliability. This work is accompanied by a robust implementation of the algorithm that is publicly available.

Keywords: pseudospectra; nonlinear eigenvalue problem; eigenvalue perturbation theory; nonsmooth optimization; subspace methods, global optimization.

1. Introduction

We consider nonlinear eigenvalue problems of the form

$$F(\lambda)x = 0, \quad (1.1)$$

where $F : \Omega \rightarrow \mathbb{C}^{n \times n}$ is an analytic matrix-valued function on $\Omega \subseteq \mathbb{C}$. The scalar $\lambda \in \Omega$ satisfying the equation above for an $x \in \mathbb{C}^n \setminus \{0\}$ is called an eigenvalue, while x is called the corresponding eigenvector. Such eigenvalue problems when F is a matrix polynomial, especially the quadratic eigenvalue problem, arise from various engineering applications, for instance, from applications in structural design and fluid mechanics (Tisseur & Meerbergen, 2001). Nonpolynomial nonlinear eigenvalue problems are also of

great interest: finite element discretizations of boundary value problems, for instance, in photonics, lead to eigenvalue problems of the form (1.1), where $F(\lambda)$ is a rational function of λ (Mehrmann & Voss, 2004; Effenberg, 2013); delay systems in control theory necessitate nonlinear eigenvalue problems where $F(\lambda)$ involves exponentials of λ (Michiels & Niculescu, 2007). For recent progresses on the topic, we refer to the survey paper Mehrmann & Voss (2004) and theses Effenberg (2013) and Van Beeumen (2015).

Stability of the continuous dynamical system associated with the nonlinear eigenvalue problem is a fundamental issue. In terms of the nonlinear eigenvalue problem (1.1), this amounts to the inclusion of all of the eigenvalues on the left half of the complex plane. However, the system is often subject to uncertainties, and thus it is often desired that a system remains stable under small perturbations of parameters. This is reflected in the nonlinear eigenvalue problem (1.1) as the inclusion of the eigenvalues of the original problem as well as all perturbed problems in the left half of the complex plane. Moreover, a stable system can still exhibit transient behavior before reaching the equilibrium eventually. For instance, for the standard eigenvalue problem $Av = \lambda v$ and the associated dynamical system $x'(t) = Ax(t)$, this is explained by the Kreiss matrix theorem (Trefethen & Embree, 2005, Theorem 18.5). A corollary of this theorem is that a stable system $x'(t) = Ax(t)$ becoming unstable under small perturbations of A must exhibit transient growth.

For robustness against uncertainties and to assess the transient behavior of solutions of a stable system, a modern approach is the consideration of the ϵ -pseudospectrum of F . This is the set in the complex plane to which the eigenvalues of F can be shifted when perturbations at a distance ϵ or closer are taken into account. The ϵ -pseudospectral abscissa, the supremum of the real parts of the elements of the ϵ -pseudospectrum, constitutes a uniform bound on the asymptotic growth rate of the solutions for all perturbations at a distance ϵ or closer. Consequently, it assesses robust stability (Burke et al., 2003). The ϵ -pseudospectral abscissa is also closely related to the distance to instability (Verhees et al., 2014) and the H-infinity norm of transfer functions defined appropriately (see Zhou et al., 1996 for relations between H-infinity norms and robust stability criteria).

A standard approach to solve polynomial eigenvalue problems is to reformulate this type of eigenvalue problem as standard generalized linear eigenvalue problems, the so-called linearization, with the same eigenvalues as the original polynomial (Mackey et al., 2006; Amiraslani et al., 2009). The obtained linear eigenvalue problem can next be solved by a standard method of choice. For solving general nonlinear eigenvalue problems (1.1), first a polynomial or rational approximation is constructed (Van Beeumen, 2015) or the nonlinear eigenvalue problem is transformed into an equivalent infinite-dimensional operator eigenvalue problem, e.g., as for the delay eigenvalue problem (Jarlebring et al., 2010). Next, a linearization process follows to obtain a linear eigenvalue problem whose spectrum approximates the spectrum of the original nonlinear eigenvalue problem. For state-of-the-art general nonlinear eigenvalue solvers, we refer to Güttel et al. (2014) and Van Beeumen et al. (2015). Here, we will not consider the unstructured pseudospectra of a particular type of linearization. Instead, as in Tisseur & Higham (2001), Michiels & Guglielmi (2012) and Verhees et al. (2014), we will explicitly take the structure of the original nonlinear eigenvalue problem into account in the definition of its pseudospectra.

1.1 Formal definition

Formally, the analytic matrix-valued function F can always be expressed in the form

$$F(\lambda) = \sum_{j=0}^m f_j(\lambda)A_j, \quad (1.2)$$

where $A_j \in \mathbb{C}^{n \times n}$, the scalar function $f_j : \Omega \rightarrow \mathbb{C}$ is analytic on its entire domain Ω for $j = 0, \dots, m$, and $m \leq n^2 - 1$. The spectrum of F given by

$$\Lambda(F) := \left\{ \lambda \in \mathbb{C} : \det \left(\sum_{j=0}^m f_j(\lambda) A_j \right) = 0 \right\}, \quad (1.3)$$

more specifically the *spectral abscissa*

$$\alpha(F) := \sup \{ \Re \lambda : \lambda \in \Lambda(F) \}, \quad (1.4)$$

is responsible for the asymptotic behavior of the associated dynamical system, yet it does not say much about the transient behavior by itself.

To take the uncertainties and transient behavior into account, we are interested in the perturbed eigenvalue problem

$$\left(\sum_{j=0}^m f_j(\lambda) (A_j + \delta A_j) \right) x = 0. \quad (1.5)$$

We quantify the distance between the original matrix-valued function (1.2) and the perturbed one in (1.5) by introducing the norm

$$\|\Delta\|_{\text{glob}} := \left\| \begin{bmatrix} w_0 \|\delta A_0\|_2 \\ \vdots \\ w_m \|\delta A_m\|_2 \end{bmatrix} \right\|_\infty, \quad (1.6)$$

where $\Delta := (\delta A_0, \dots, \delta A_m) \in \mathbb{C}^{n \times n \times (m+1)}$ for given non-negative real scalars w_j (possibly ∞) for $j = 0, \dots, m$; equivalently we equip the vector space of analytic matrix-valued functions of the form (1.2) with variable coefficient matrices A_j but fixed scalar functions f_j with a norm.

We then define the ϵ -pseudospectrum of F by

$$\Lambda_\epsilon(F) := \bigcup_{\|\Delta\|_{\text{glob}} \leq \epsilon} \left\{ \lambda \in \mathbb{C} : \det \left(\sum_{j=0}^m f_j(\lambda) (A_j + \delta A_j) \right) = 0 \right\}, \quad (1.7)$$

and the ϵ -pseudospectral abscissa by

$$\alpha_\epsilon(F) := \sup \{ \Re \lambda : \lambda \in \Lambda_\epsilon(F) \} \quad (1.8)$$

as an indicator of the robust stability of the dynamical system associated with (1.1). The following characterization of $\Lambda_\epsilon(F)$ was derived in Michielis *et al.* (2006).

PROPOSITION 1.1 We have

$$\Lambda_\epsilon(F) = \left\{ \lambda \in \mathbb{C} : \sigma_{\min} \left(\sum_{j=0}^m f_j(\lambda) A_j \right) \leq \epsilon \|w(\lambda)\|_1 \right\}, \quad (1.9)$$

where $\sigma_{\min}(\cdot)$ denotes the smallest singular value of its matrix argument, and

$$w(\lambda) := \begin{bmatrix} f_0(\lambda) & \dots & f_n(\lambda) \\ w_0 & & w_m \end{bmatrix}^T. \quad (1.10)$$

Throughout the text, we assume that the portion of $\Lambda_\epsilon(F)$ to the right-hand side of each vertical line in the complex plane is bounded. Formally, letting

$$\mathbb{C}_{\geq \delta} := \{z \in \mathbb{C} : \Re z \geq \delta\}$$

for a given $\delta \in \mathbb{R}$, it is assumed that $\Lambda_\epsilon(F) \cap \mathbb{C}_{\geq \delta}$ is bounded for all $\delta \in \mathbb{R}$. This assumption ensures the well-posedness of $\alpha_\epsilon(F)$ defined by (1.8). For a thorough discussion on this condition, we refer to Michielis & Guglielmi (2012).

1.2 Literature

The ϵ -pseudospectrum for matrices, that is, when $F(\lambda) = \lambda I - A$, has been popularized by Trefethen in the last two decades (Trefethen & Embree, 2005). This set has found various applications in the literature in connection with robust stability and transient behavior, for instance, to analyse the cutoff phenomenon in Markov chains (Jónsson & Trefethen, 1998) and in stability analysis in hydrodynamics (Trefethen et al., 1993). Its computation benefits from its singular value characterization. The most standard approaches (Trefethen, 1999; Wright & Trefethen, 2002) are based on discretizing the complex plane and relying on powerful tools of numerical linear algebra such as the Lanczos method and Schur factorization. Some curve-tracing approaches have also been suggested (Brühl, 1996; Bekas & Gallopoulos, 2001).

Extensions to nonlinear eigenvalue problems have been considered throughout the last two decades. For polynomial eigenvalue problems, the connection with the backward error of an eigenvalue has been studied, singular value characterizations has been derived, and numerical approaches have been proposed for its computation in Tisseur & Higham (2001). This has been extended to rectangular matrix polynomials in homogeneous form in Higham & Tisseur (2002). The boundary and components of the ϵ -pseudospectrum have been studied, and a curve-tracing algorithm has been proposed in the matrix polynomial setting in Lancaster & Psarrakos (2005). More recent research has concentrated on the nonpolynomial setting. In particular, Green & Wagenknecht (2006) concerns the computation of the pseudospectra in the delay eigenvalue problem setting. In Michielis et al. (2006), the pseudospectra for a general analytic matrix-valued function have been formally introduced, and singular value characterizations have been derived. This has been extended to analytic matrix-valued functions subject to structured perturbations with multiplicative structure in Wagenknecht et al. (2008).

Particular attention has been paid to the computation of the pseudospectral abscissa. For the pseudospectral abscissa of a matrix, the first globally convergent algorithm was proposed in Burke et al. (2003). Since every iteration of this algorithm requires computing all eigenvalues of a matrix of twice the dimensions of the original matrix, it is restricted to problems of moderate size. In Guglielmi & Overton (2011), a locally convergent algorithm for large-scale matrices is proposed, where every iteration relies on computing the rightmost eigenvalue of the original matrix plus a rank-one perturbation (see also Kressner & Vandereycken, 2014 for an improvement of this algorithm based on subspace acceleration). The algorithm of Guglielmi & Overton (2011) has been extended to nonlinear eigenvalue problems in Michielis & Guglielmi (2012), and it has also been adopted to compute the distance to instability from a nonlinear dynamical system in Verhees et al. (2014). In a different direction, an implicit determinant

method is proposed to compute the distance to instability from a matrix (Freitag & Spence, 2011). This approach is based on solutions of certain linear systems only and can be coupled with a bisection method to compute the pseudospectral abscissa. In the next subsection, we situate the proposed algorithm with respect to these works.

1.3 Motivation and outline

We present a globally convergent algorithm for the computation of $\alpha_\epsilon(F)$, particularly suitable for large-scale problems, that is, when A_j are large matrices. Three main components of the algorithm are introduced in Mengi (2016), Mengi *et al.* (2014) and Kressner & Vandereycken (2014). In Mengi (2016), a locally convergent algorithm is presented for optimizing a linear function subject to a constraint on a smallest eigenvalue function. The algorithm is immune to the nonsmooth nature of the smallest eigenvalue function. In Section 2, we describe how this algorithm can be adopted to compute $\alpha_\epsilon(F)$ based on the characterization (1.9) of $\Lambda_\epsilon(F)$.

Unfortunately, this yields a locally rightmost point, which is possibly not rightmost globally. We overcome this by performing a vertical search by means of the algorithm introduced in Mengi *et al.* (2014) for the global optimization of a prescribed eigenvalue of a Hermitian and analytic matrix-valued function. We fix the real part α of the locally rightmost point and perform the minimization of

$$\frac{\sigma_{\min} \left(\sum_{j=0}^m f_j(\alpha + i\omega) A_j \right)}{\|w(\alpha + i\omega)\|_1}, \quad (1.11)$$

over all $\omega \in \mathbb{R}$ globally. This global minimization assumes the availability of a global lower bound on the second derivative of the function above with respect to α . In practice, choosing a large negative value for this bound works robustly. If the globally minimal value is less than ϵ , then we repeat the local search starting from $\alpha + i\omega_*$, where ω_* is a global minimizer of (1.11). We refer to Fig. 5 (in the numerical examples section towards the end of this text) for an illustration of the interplay between the local searches and vertical searches. In this illustration, local searches yield locally (but not globally) rightmost points twice. In each of these two cases, a vertical search provides a point strictly inside $\Lambda_\epsilon(F)$ whose real part is the same as the locally rightmost point. The vertical search idea is discussed in Section 3.

Due to the fact that the computational cost is dominated by computing the smallest singular value and corresponding singular vectors, for which fast iterative methods are amenable, the proposed algorithm is applicable to large-scale problems. Moreover, a significant speed-up can be achieved by incorporating a subspace restriction, whose idea is originally proposed in Kressner & Vandereycken (2014) for the computation of the pseudospectral abscissa of a matrix. The remarkable low-rank property observed and exploited in that paper still holds in this more general nonlinear eigenvalue setting. In particular, there exists a one-dimensional subspace of \mathbb{C}^n such that the ϵ -pseudospectral abscissa of $F(\lambda)$ remains the same when the domain of the map $v \mapsto F(\lambda)v$ is restricted to this one-dimensional subspace. The details of this subspace idea for nonlinear eigenvalue problems are worked out in Section 4. The overall idea is to restrict the domain of $v \mapsto F(\lambda)v$ to very low-dimensional subspaces of \mathbb{C}^n and compute the ϵ -pseudospectral abscissa of the resulting smaller problems by means of the locally convergent algorithm in Mengi (2016). The vertical searches are performed on the original $F(\lambda)$. This is justified by the rare need for these vertical searches.

One genuine aspect of the algorithm is an occasional restart strategy for the subspaces as argued in Section 5. Since the essential task is to determine or capture a one-dimensional subspace, the algorithm erases the old subspaces occasionally. Thus after a vertical search, if a further application of the local

algorithm is deemed to be necessary, the algorithm starts with a one-dimensional subspace from scratch. Moreover, when the dimension of the subspace becomes large enough (still considerably smaller than n), the algorithm keeps only the last-added one-dimensional subspace, discarding the rest.

The overall framework is outlined in Algorithm 4. This algorithm features favorable properties over existing algorithms, for instance Michiels & Guglielmi (2012). Specifically, **(i)** it converges globally rather than locally (provided a sufficiently small global lower bound for the second derivative of the singular value function in (1.11) is chosen); **(ii)** it is immune to nonsmoothness, that is, even if $\alpha_\epsilon(F)$ is attained at a point say $z_* \in \mathbb{C}$ where $\sigma_{\min}(F(z_*))$ is not simple, it still converges; **(iii)** it handles large-scale problems well (the subspace method coupled with the restart strategy contributes to this largely, but the restarts would not be as effective without vertical searches that are performed globally); **(iv)** in contrast to the approach of Michiels & Guglielmi (2012), the algorithm does not rely on a nonlinear eigenvalue solver (provided it is initialized with the rightmost eigenvalue): instead of the rightmost eigenvalue of perturbed nonlinear eigenvalue problems, it is based on the repeated computation of the smallest singular value of complex matrices. Robust and efficient numerical algorithms are available, e.g., the implicitly restarted Arnoldi method of Lehoucq *et al.* (1998), for the smallest singular value.

2. Determination of locally rightmost points

Due to Proposition 1.9, the ϵ -pseudospectral abscissa of F can be cast as the following constrained eigenvalue optimization problem:

$$\begin{aligned} & \underset{z \in \mathbb{C}}{\text{maximize}} \quad \Re z \\ & \text{subject to} \quad \lambda(\Re z, \Im z) := \lambda_{\min}[F(\Re z, \Im z)^* F(\Re z, \Im z)] - \epsilon^2 \|w(\Re z, \Im z)\|_1^2 \leq 0, \end{aligned} \quad (2.1)$$

where we view the matrix-valued function in (1.2) as $F : \mathbb{R}^2 \rightarrow \mathbb{C}^{n \times n}$ and the weight function in (1.10) as $w : \mathbb{R}^2 \rightarrow \mathbb{R}$, by associating \mathbb{R}^2 with \mathbb{C} . Throughout the text, to ease the notation, $F(\cdot)$, $\lambda(\cdot)$, $w(\cdot)$ and $f_j(\cdot)$, $j = 0, \dots, m$ represent both the functions from \mathbb{C} and the functions from \mathbb{R}^2 . The functions with one parameter or supplied with a particular point in \mathbb{C} as the argument correspond to the ones with domain \mathbb{C} , and the functions with two parameters or supplied with a point in \mathbb{R}^2 as the argument have domain \mathbb{R}^2 . Furthermore, in (2.1) and in what follows, the notation $\lambda_{\min}[\cdot]$ and $\lambda_{\max}[\cdot]$ represents the smallest eigenvalue and the largest eigenvalue of the matrix argument, respectively.

An approach to maximize a linear objective subject to a smallest eigenvalue constraint was suggested in Mengi (2016). Below, we describe how this approach can be extended to deal with (2.1), in particular the additional nonsmoothness due to $\|w(\Re z, \Im z)\|_1^2$, that occurs whenever $f_j(\Re z, \Im z) = 0$ for some $j \in \{0, \dots, m\}$. The extension relies on the global over-estimators for $\lambda(\cdot)$ of the form specified in Theorem 2.1 below. These global over-estimators are defined in terms of global bounds γ_λ and γ_w satisfying

$$\lambda_{\max}\{\nabla^2 \lambda_{\min}[F(\Re z, \Im z)^* F(\Re z, \Im z)]\} \leq \gamma_\lambda \quad (2.2)$$

for all $z \in \mathbb{C}$ where $\sigma_{\min}[F(\Re z, \Im z)]$ is simple, and

$$\|\nabla^2 [\|w(\Re z, \Im z)\|_1^2]\|_2 \leq \gamma_w \quad (2.3)$$

for all $z \in \mathbb{C}$, respectively, where $f_j(\Re z, \Im z) \neq 0$ for each j , more specifically, in terms of $\gamma_h := \gamma_\lambda + \epsilon^2 \gamma_w$. Analytical deduction of such bounds is discussed in Section 2.1 below.

THEOREM 2.1 Suppose $z_k = (z_{k1}, z_{k2}) \in \mathbb{R}^2$ is a point such that $\sigma_{\min}[F(z_k)]$ is simple, and $f_j(z_k) \neq 0$ for each j . We have

$$\lambda(\Re z, \Im z) \leq q_k(\Re z, \Im z) := \lambda_k + \nabla \lambda_k^T((\Re z, \Im z) - z_k) + \frac{\gamma_h}{2} \|(\Re z, \Im z) - z_k\|_2^2 \quad \forall z \in \mathbb{C},$$

where $\lambda_k := \lambda(z_{k1}, z_{k2})$ and $\nabla \lambda_k := \nabla \lambda(z_{k1}, z_{k2})$.

The proof of Theorem 2.1 is in essence identical to the proof of Mengi (2016, Theorem 2.2), but $\lambda(\cdot)$ here takes the role of $\lambda_{\min}(\cdot)$ there. In this direction, we note the following:

- The function $\phi(\alpha) = \lambda((\Re z, \Im z) + \alpha p)$ for a given $p \in \mathbb{R}^2$ is the minimum of finitely many analytic functions, namely

$$\phi_{j,s_0,\dots,s_m}(\alpha) := \phi_j(\alpha) - \epsilon^2 \{s_0 f_0((\Re z, \Im z) + \alpha p) + \dots + s_m f_m((\Re z, \Im z) + \alpha p)\}^2$$

for $j = 1, \dots, n$, $s_0 = -1, 1, \dots, s_m = -1, 1$. Here, $\phi_1(\alpha), \dots, \phi_n(\alpha)$ represent the eigenvalues of $F((\Re z, \Im z) + \alpha p)^* F((\Re z, \Im z) + \alpha p)$ ordered so that each $\phi_j(\alpha)$ is analytic.

- The left-derivative $\phi'_-(\alpha)$ and the right-derivative $\phi'_+(\alpha)$ exist everywhere and satisfy $\phi'_-(\alpha) \geq \phi'_+(\alpha)$ at all α , since $\phi(\alpha)$ is the minimum of finitely many analytic functions.
- Furthermore, $\phi(\alpha)$ is analytic everywhere excluding finitely many points in a finite interval for the very same reason that it is the minimum of finitely many analytic functions.
- Finally, γ_h is such that

$$\begin{aligned} \lambda_{\max} [\nabla^2 \lambda(\Re z, \Im z)] &\leq \lambda_{\max} \{ \nabla^2 \lambda_{\min} [F(\Re z, \Im z)^* F(\Re z, \Im z)] \} + \lambda_{\max} \{ \nabla^2 [-\epsilon^2 \|w(\Re z, \Im z)\|_1^2] \} \\ &\leq \lambda_{\max} \{ \nabla^2 \lambda_{\min} [F(\Re z, \Im z)^* F(\Re z, \Im z)] \} + \epsilon^2 \|\nabla^2 [\|w(\Re z, \Im z)\|_1^2]\|_2 \\ &\leq \gamma_\lambda + \epsilon^2 \gamma_w = \gamma_h \end{aligned}$$

for all $z \in \mathbb{C}$ such that $\lambda(\Re z, \Im z)$ is twice differentiable.

Replacing the eigenvalue constraint in (2.1) with the over-estimator of Theorem 2.1 results in the following convex and smooth problem:

$$\begin{aligned} &\underset{(\alpha, \beta) \in \mathbb{R}^2}{\text{maximize}} \quad \alpha \\ &\text{subject to} \quad \lambda_k + \nabla \lambda_k^T((\alpha, \beta) - z_k) + \frac{\gamma_h}{2} \|(\alpha, \beta) - z_k\|_2^2 \leq 0. \end{aligned} \tag{2.4}$$

The algorithm generates a sequence $\{z_k\}$ in \mathbb{R}^2 such that z_{k+1} is the maximizer of (2.4) given z_k . Since the feasible set of (2.4) (a disk) is a subset of the feasible set of the original problem (2.1), each z_k remains feasible with respect to the original problem provided z_0 is feasible. By applying the first-order optimality conditions to (2.4), two consecutive iterates in the sequence $\{z_k\}$ are tied by the recurrence

$$z_{k+1} = z_k + \frac{1}{\gamma_h} \left[\frac{1}{\mu_+} \cdot (1, 0) - \nabla \lambda_k \right], \quad \text{where } \mu_+ = \frac{1}{\sqrt{\|\nabla \lambda_k\|_2^2 - 2\gamma_h \lambda_k}}, \tag{2.5}$$

$$\nabla \lambda_k = \begin{bmatrix} \text{Real} \left(v_k^* \frac{\partial F(z_k)^*}{\partial \Re z} F(z_k) v_k + v_k^* F(z_k)^* \frac{\partial F(z_k)}{\partial \Re z} v_k \right) - 2\epsilon^2 \|w(z_k)\|_1 \frac{\partial \|w(z_k)\|_1}{\partial \Re z} \\ \text{Real} \left(v_k^* \frac{\partial F(z_k)^*}{\partial \Im z} F(z_k) v_k + v_k^* F(z_k)^* \frac{\partial F(z_k)}{\partial \Im z} v_k \right) - 2\epsilon^2 \|w(z_k)\|_1 \frac{\partial \|w(z_k)\|_1}{\partial \Im z} \end{bmatrix},$$

$$\frac{\partial \|w(z_k)\|_1}{\partial \Re z} = \sum_{j=0}^m \frac{1}{w_j} \frac{\partial |f_j(z_k)|}{\partial \Re z}, \quad \frac{\partial \|w(z_k)\|_1}{\partial \Im z} = \sum_{j=0}^m \frac{1}{w_j} \frac{\partial |f_j(z_k)|}{\partial \Im z},$$

and $v_k \in \mathbb{C}^n$ is a unit right-singular vector corresponding to $\sigma_{\min}[F(z_k)]$. Here, we benefit from the analytical formulas for the derivatives of eigenvalue functions (Lancaster, 1964), in particular to calculate the derivatives of $\lambda_{\min}[F(\Re z, \Im z)^* F(\Re z, \Im z)]$. Recurrence (2.5) holds under the assumption that $\nabla q_k(z_{k+1}) \neq 0$. The condition $\nabla q_k(z_{k+1}) = 0$ is rather unlikely, and it occurs only if $\nabla \lambda_k = 0$ and $\lambda_k = 0$ (see Mengi, 2016, Theorem 2.3).

2.1 Upper bounds on second derivatives

In this section, we present bounds γ_λ and γ_w satisfying (2.2) and (2.3), respectively. An application of Mengi (2016, Theorem 6.1) yields

$$\lambda_{\max} \{ \nabla^2 \lambda_{\min} [F(\Re z, \Im z)^* F(\Re z, \Im z)] \} \leq \lambda_{\max} \{ \nabla^2 [F(\Re z, \Im z)^* F(\Re z, \Im z)] \} \quad (2.6)$$

for $z \in \mathbb{C}$ such that $\sigma_{\min}[F(z)]$ is simple, where

$$\nabla^2 [F(\Re z, \Im z)^* F(\Re z, \Im z)] := \begin{bmatrix} \frac{\partial^2 [F(\Re z, \Im z)^* F(\Re z, \Im z)]}{\partial \Re z^2} & \frac{\partial^2 [F(\Re z, \Im z)^* F(\Re z, \Im z)]}{\partial \Re z \cdot \partial \Im z} \\ \frac{\partial^2 [F(\Re z, \Im z)^* F(\Re z, \Im z)]}{\partial \Im z \cdot \partial \Re z} & \frac{\partial^2 [F(\Re z, \Im z)^* F(\Re z, \Im z)]}{\partial \Im z^2} \end{bmatrix}.$$

Above, $\partial^2 [F(\Re z, \Im z)^* F(\Re z, \Im z)] / \partial \Re z^2$ denotes the second derivative of the matrix-valued function $F(\Re z, \Im z)^* F(\Re z, \Im z)$ with respect to $\Re z$ and is an $n \times n$ matrix obtained from $F(\Re z, \Im z)^* F(\Re z, \Im z)$ by differentiating each of its entries with respect to $\Re z$ twice. The other second derivatives of $F(\Re z, \Im z)^* F(\Re z, \Im z)$ above are defined similarly.

For the standard ϵ -pseudospectral abscissa of a matrix A , that is, when $F(z) = A - zI$, we have $\nabla^2 [F(\Re z, \Im z)^* F(\Re z, \Im z)] = 2I$. Consequently, inequality (2.6) leads to the upper bound $\lambda_{\max} \{ \nabla^2 \lambda_{\min} [F(\Re z, \Im z)^* F(\Re z, \Im z)] \} \leq 2$ for all $z \in \mathbb{C}$ such that $\sigma_{\min}[F(z)]$ is simple. In the general nonlinear setting (1.2), routine calculations yield

$$\nabla^2 [F(\Re z, \Im z)^* F(\Re z, \Im z)] = \sum_{k=0}^m \sum_{j=0}^m \left[\overline{F_{k,j}(\Re z, \Im z)} + F_{j,k}(\Re z, \Im z) \right] \otimes A_k^* A_j,$$

where

$$\begin{aligned} F_{j,k}(\Re z, \Im z) &:= \nabla^2 \overline{f_k(\Re z, \Im z)} \cdot f_j(\Re z, \Im z) + \nabla \overline{f_k(\Re z, \Im z)} \cdot \nabla f_j(\Re z, \Im z)^T \\ &= \overline{f_k''(z)} f_j(z) \begin{bmatrix} 1 & -i \\ -i & -1 \end{bmatrix} + \overline{f_k'(z)} f_j'(z) \begin{bmatrix} 1 & i \\ -i & 1 \end{bmatrix}, \end{aligned} \quad (2.7)$$

and \otimes denotes the Kronecker product. Above, $f'_k(z), f''_k(z)$ represent first, second complex derivatives of $f_k(z)$, thus functions from $\Omega \subseteq \mathbb{C}$ to \mathbb{C} . From here, by employing (2.6) and exploiting

$$\overline{F_{k,j}(\Re z, \Im z)} + F_{j,k}(\Re z, \Im z) = \left[\overline{F_{j,k}(\Re z, \Im z)} + F_{k,j}(\Re z, \Im z) \right]^*,$$

we deduce the following bound.

THEOREM 2.2 Suppose that $z \in \mathbb{C}$ is such that $\sigma_{\min}[F(z)]$ is simple. The following holds:

$$\lambda_{\max} \left\{ \nabla^2 \lambda_{\min} [F(\Re z, \Im z)^* F(\Re z, \Im z)] \right\} \leq 2 \cdot \sum_{k=0}^m \sum_{j=0}^m \|F_{k,j}(\Re z, \Im z)\|_2 \cdot \|A_k^* A_j\|_2.$$

EXAMPLE 2.3 (Polynomial Eigenvalue Problem) Consider $F(z) = \sum_{j=0}^m z^j A_j$ for given matrices $A_j \in \mathbb{C}^{n \times n}$ for $j = 0, \dots, m$. Noting that $f_j(z) = z^j$, Theorem 2.2 combined with expression (2.7) for $F_{j,k}(\Re z, \Im z)$ implies

$$\begin{aligned} \lambda_{\max} \left\{ \nabla^2 \lambda_{\min} [F(\Re z, \Im z)^* F(\Re z, \Im z)] \right\} &\leq \\ &4 \cdot \left[\sum_{k=0}^m \sum_{j=2}^m j \cdot (j-1) \cdot |z|^{j+k-2} \|A_k^* A_j\|_2 + \sum_{k=1}^m \sum_{j=1}^m k \cdot j \cdot |z|^{j+k-2} \|A_k^* A_j\|_2 \right]. \end{aligned}$$

Assuming that the ϵ -pseudospectrum of F is bounded and contained inside a ball of radius δ in the complex plane and letting $a := \max_{j=0, \dots, m} \|A_j\|_2$, we can set

$$\gamma_\lambda := 4a^2 \cdot \left[\left(\frac{\delta^{m+1} - 1}{\delta - 1} \right) \left(\frac{\delta^{m+1} - 1}{\delta - 1} \right)'' + \left(\left\{ \frac{\delta^{m+1} - 1}{\delta - 1} \right\}' \right)^2 \right],$$

where the derivatives are with respect to δ . Similarly, bounds can also be derived for delay and rational eigenvalue problems based on Theorem 2.2.

The following bound is the consequence of rudimentary calculations.

THEOREM 2.4 Suppose $z \in \mathbb{C}$ is such that $f_j(z) \neq 0$ for $j = 0, \dots, m$. The following holds:

$$\|\nabla^2 [\|w(\Re z, \Im z)\|_1^2]\|_2 \leq 2 \cdot \left[\sum_{j=0}^m \frac{1}{w_j} |f'_j(z)| \right]^2 + 2 \cdot \left[\sum_{j=0}^m \frac{1}{w_j} |f_j(z)| \right] \cdot \left[\sum_{j=0}^m \frac{1}{w_j} \left\{ 3 \cdot \frac{|f'_j(z)|^2}{|f_j(z)|} + |f''_j(z)| \right\} \right].$$

For instance, for the matrix polynomial $F(z) = \sum_{j=0}^m z^j A_j$ with $f_j(z) = z^j$, Theorem 2.4 gives rise to the bound

$$\|\nabla^2 [\|w(\Re z, \Im z)\|_1^2]\|_2 \leq 2 \cdot \left[\sum_{j=1}^m \frac{j \cdot |z|^{j-1}}{w_j} \right]^2 + 2 \cdot \left[\sum_{j=0}^m \frac{|z|^j}{w_j} \right] \cdot \left[\sum_{j=1}^m \frac{3j^2 \cdot |z|^{j-2}}{w_j} + \sum_{j=2}^m \frac{j \cdot (j-1) \cdot |z|^{j-2}}{w_j} \right].$$

If the ϵ -pseudospectral abscissa of F is contained inside the ball of radius δ and $\underline{w} := \min_{j=0,\dots,m} w_j$, we can choose

$$\gamma_w := \frac{2}{\underline{w}^2} \cdot \left[\left(\left\{ \frac{\delta^{m+1} - 1}{\delta - 1} \right\}' \right)^2 + \left(\frac{\delta^{m+1} - 1}{\delta - 1} \right) \left(\frac{3}{\delta} + 4 \left\{ \frac{\delta^{m+1} - 1}{\delta - 1} \right\}'' + 3 \left\{ \frac{\delta^{m+1} - 1}{\delta - 1} \right\}' \right) \right].$$

2.2 Convergence

Let us denote the components of $z_k \in \mathbb{R}^2$ with z_{k1} and z_{k2} . We call $\mathcal{C}(z_k) := z_{k1} + iz_{k2}$ the *complexification* of z_k . The sequence $\{z_{k1}\}$ is monotone increasing. This is because z_{k+1} is chosen among all $(\Re z, \Im z)$ satisfying $q_k(\Re z, \Im z) \leq 0$ such that $\Im z$ is as large as possible and, in particular, z_k satisfies $q_k(z_k) = 0$. Additionally, since it is assumed that $\Lambda_\epsilon(F) \cap \mathbb{C}_{\geq \delta}$ is bounded for all $\delta \in \mathbb{R}$, the sequence $\{z_{k1}\}$ is bounded above. This would imply the convergence of $\{z_{k1}\}$ as stated next.

THEOREM 2.5 Suppose that $\Lambda_\epsilon(F) \cap \mathbb{C}_{\geq \delta}$ is bounded for all $\delta \in \mathbb{R}$, $\sigma_{\min}[F(z_k)]$ is simple for each k , and $f_j(z_k) \neq 0$ for each j, k . Then the sequence $\{z_{k1}\}$ is convergent.

The boundedness of $\Lambda_\epsilon(F) \cap \mathbb{C}_{\geq \delta}$ for all $\delta \in \mathbb{R}$, rather than the boundedness of $\Lambda_\epsilon(F)$, is also sufficient for the convergence of the sequence $\{z_k\}$ to a desired point, provided $\|\nabla \lambda_k\|_2$ remains bounded away from zero.

THEOREM 2.6 (Convergence) Suppose that $\Lambda_\epsilon(F) \cap \mathbb{C}_{\geq \delta}$ is bounded for all $\delta \in \mathbb{R}$, $\sigma_{\min}[F(z_k)]$ is simple for each k , and $f_j(z_k) \neq 0$ for each j, k .

- (i) If $\nabla \lambda_k \neq 0$ for each k sufficiently large, then $\lambda_k \rightarrow 0$ as $k \rightarrow \infty$.
- (ii) If there exists a real scalar $L > 0$ such that $\|\nabla \lambda_k\|_2 > L$ for each k sufficiently large, then

$$\frac{(1, 0) \cdot \nabla \lambda_k}{\|\nabla \lambda_k\|_2} \rightarrow 1 \quad \text{as } k \rightarrow \infty.$$

The proofs of parts (i) and (ii) are similar to the proofs of Mengi (2016, Lemma 3.5, Theorem 3.6). Part (i) means that $\mathcal{C}(z_k)$ approaches the boundary of $\Lambda_\epsilon(F)$ as $k \rightarrow \infty$. Moreover, part (ii) amounts to $\nabla \lambda(z_k)$ pointing in the direction of $(1, 0)$ as $k \rightarrow \infty$. Thus, eventually $\mathcal{C}(z_k)$ becomes aligned with the points on the boundary of $\Lambda_\epsilon(F)$ with the vertical tangent line. The assertions of Theorem 2.6 amount to the satisfaction of the first-order optimality conditions by the sequence $\{z_k\}$ in the smooth and nonsmooth sense, that is, regardless of the multiplicity of $\sigma_{\min}[F(z_*)]$ whenever the limit $z_* = \lim_{k \rightarrow \infty} z_k$ exists. Formally, the first-order optimality conditions for (2.1) are given by

$$\exists \mu > 0 \quad \text{s.t.} \quad (1, 0) \in \mu \cdot \partial \lambda(\Re z, \Im z) \quad \text{and} \quad \lambda(\Re z, \Im z) = 0,$$

where the generalized gradient $\partial \lambda(\Re z, \Im z)$ is defined by (Clarke, 1990, page 11)

$$\partial \lambda(\Re z, \Im z) := \text{Co} \left\{ \lim_{k \rightarrow \infty} \nabla \lambda(\tilde{z}_k) \mid \tilde{z}_k \rightarrow (\Re z, \Im z), \tilde{z}_k \notin \Omega \right\}, \quad (2.8)$$

the set Ω is a subset of \mathbb{R}^2 (of measure zero) on which λ is not differentiable and $\text{Co}(H)$ denotes the convex hull of the set H . The property $\lambda(z_*) = 0$ is immediate from part (i) of Theorem 2.6. Additionally, part (ii) of Theorem 2.6 implies

$$(1, 0) = \lim_{k \rightarrow \infty} \frac{\nabla \lambda(z_k)}{\|\nabla \lambda(z_k)\|_2} \in \mu_* \cdot \partial \lambda(z_*),$$

where $\mu_* := 1 / \lim_{k \rightarrow \infty} \|\nabla \lambda(z_k)\|_2$, amounting to the satisfaction of the first-order optimality conditions.

The assumptions of Theorem 2.6 that $f_j(z_k) \neq 0$ and $\sigma_{\min}[F(z_k)]$ is simple are satisfied generically. The set of points z where $f_j(z)$ vanish, or $\sigma_{\min}[F(z)]$ is not simple is a subset of Ω of measure zero. The algorithm never encounters such points in practice. It can generate points close to such points of nonsmoothness, but this has no effect on the convergence of the algorithm. On the other hand, the nonsmoothness at an optimal point has a different nature. Smooth algorithms may not converge to such points. But the algorithm here converges to optimal points regardless of whether they are smooth.

We conclude this section with a description of the algorithm below. This description is given in the more general rectangular setting, when $F : \Omega \rightarrow \mathbb{C}^{n \times p}$ is analytic on Ω . The ϵ -pseudospectrum can be defined for a rectangular analytic matrix-valued function in a similar fashion by (1.9). The algorithm extends without any modification to this rectangular setting. Throughout this text, in the descriptions of the algorithms, we state the termination criteria in exact terms to keep the descriptions neat. Obviously, numerical implementations would require the satisfaction of these conditions up to specified tolerances.

Algorithm 1 Local search

Require: A matrix-valued function $F : \Omega \rightarrow \mathbb{C}^{n \times p}$ analytic on Ω and a positive scalar $\epsilon \in \mathbb{R}$.

1. $z_0 \leftarrow (\Re z_R, \Im z_R)$, where z_R is any point in $\Lambda_\epsilon(F)$ and $k \leftarrow 0$.
 2. Calculate $\sigma_0 := \sigma_{\min}[F(z_0)]$ and an associated unit right-singular vector v_0 .
 3. Calculate $\lambda_0, \nabla \lambda_0$ using σ_0, v_0, z_0 .
 4. **while** ($\lambda_k \neq 0$) or ($\nabla \lambda_k \neq c \cdot (1, 0)$ $\forall c \in \mathbb{R}^+$) **do**
 5. Apply the recurrence (2.5) to find z_{k+1} given $z_k, \lambda_k, \nabla \lambda_k$.
 6. Calculate $\sigma_{k+1} := \sigma_{\min}[F(z_{k+1})]$ and an associated unit right-singular vector v_{k+1} .
 7. Calculate $\lambda_{k+1}, \nabla \lambda_{k+1}$ using $\sigma_{k+1}, v_{k+1}, z_{k+1}$.
 8. Increment k .
 9. **end while**
 10. **Output:** z_k .
-

3. Vertical search

It is essential that $\mathcal{C}(z_0) \in \Lambda_\epsilon(F)$ for the locally convergent algorithm of the previous section. In this section, we further impose $\mathcal{C}(z_0)$ to be the rightmost eigenvalue of $F(\lambda)$. This turns out to be essential for global convergence. The sequence $\{z_k\}$ defined by the update rule (2.5), when it converges, yields a point $z_* = (\alpha_*, \beta_*)$ such that

- (1) $\mathcal{C}(z_*)$ is on the boundary of $\Lambda_\epsilon(F)$ with vertical tangent line, or
- (2) $0 \in \partial \lambda(z_*)$.

Recall that $\partial\lambda(z_*)$ denotes the generalized gradient of λ at z_* defined by (2.8). Case (2) can occur after finitely many iterations if it happens that $\lambda_k = 0$ and $\nabla\lambda_k = 0$ for some k . In this case, $z_\ell = z_k$ for each $\ell > k$ due to the fact that z_{k+1} is the local maximizer of (2.4). In the more probable infinite convergence case, unless $0 \in \partial\lambda(z_*)$, the point $\mathcal{C}(z_*)$ must be on the boundary of $\Lambda_\epsilon(F)$ with a vertical tangent line by Theorem 2.6.

The point $\mathcal{C}(z_*)$ may or may not be a rightmost point globally in $\Lambda_\epsilon(F)$. To check whether $\mathcal{C}(z_*)$ is indeed a rightmost point globally in $\Lambda_\epsilon(F)$, we globally minimize

$$\sigma(\alpha_*, \omega) := \frac{\sigma_{\min}[F(\alpha_*, \omega)]}{\|w(\alpha_*, \omega)\|_1}, \quad (3.1)$$

over all $\omega \in \mathbb{R}$, which we call a vertical search. This global minimization is achieved by means of the algorithm in Mengi *et al.* (2014) for the optimization of a prescribed eigenvalue of a Hermitian and analytic matrix-valued function. If the globally smallest value of $\sigma(\alpha_*, \omega)$ is ϵ , then $\mathcal{C}(z_*)$ is indeed a rightmost point of $\Lambda_\epsilon(F)$ globally. We draw this conclusion based on the assumption that z_0 is the rightmost eigenvalue of F and by the fact that each connected component of $\Lambda_\epsilon(F)$ must contain an eigenvalue. If the globally minimal value of $\sigma(\alpha_*, \omega)$ is strictly less than ϵ , then we repeat the locally convergent algorithm of the previous section starting from (α_*, ω_*) , where ω_* is the computed global minimizer of $\sigma(\alpha_*, \omega)$. The point $\mathcal{C}(\alpha_*, \omega_*)$ lies strictly inside $\Lambda_\epsilon(F)$.

Figure 5 illustrates this vertical search idea combined with the local search of the previous section on a nonlinear delay eigenvalue problem. (Note that the approach in this figure also benefits from the subspace idea, described in detail in the next section.) In this example, the local search converges to a locally rightmost point (α_*, ω_*) initially. A vertical search determines that there are points with real part equal to α_* that lie strictly inside the ϵ -pseudospectrum. Such a point is given by (α_*, ω_{**}) where ω_{**} is the global minimizer of $\sigma(\alpha_*, \omega)$ over ω . Thus, the local search is resumed from (α_*, ω_{**}) . The local search again leads to a locally rightmost point, which is followed by another vertical search. A third application of the local search ends up at a point that is globally rightmost. This globally rightmost assertion is drawn by a final vertical search. It is determined in this final vertical search that the smallest value of the singular value function $\sigma(\cdot)$ along the dashed vertical line is ϵ .

The algorithm in Mengi *et al.* (2014) to minimize $\sigma(\alpha_*, \omega)$ constructs piecewise quadratic functions of the form

$$Q_k(\omega) := \max_{\ell=0,\dots,k} q_\ell(\omega) \quad \text{where} \quad q_\ell(\omega) := \sigma(\alpha_*, \omega_\ell) + \frac{\partial\sigma(\alpha_*, \omega_\ell)}{\partial\omega}(\omega - \omega_\ell) - \frac{\gamma}{2}(\omega - \omega_\ell)^2$$

and γ is required to satisfy $\partial^2\sigma(\alpha_*, \omega)/\partial\omega^2 \geq \gamma$ for all ω such that $\sigma(\alpha_*, \omega)$ is differentiable. This function is constructed so as to satisfy $\sigma(\alpha_*, \omega) \geq Q_k(\omega)$ for all ω and $\sigma(\alpha_*, \omega_\ell) = Q_k(\omega_\ell)$, as well as $\partial\sigma(\alpha_*, \omega_\ell)/\partial\omega = Q'_k(\omega_\ell)$ for $\ell = 0, \dots, k$. The overall algorithm generates the sequence $\{\omega_k\}$ for a given ω_0 such that $\omega_{k+1} := \arg \min_\omega Q_k(\omega)$. Every convergent subsequence of this sequence is shown to converge to a global minimizer of $\sigma(\alpha_*, \omega)$ in Mengi *et al.* (2014). Thus the algorithm makes use of the derivative

$$\frac{\partial\sigma(\alpha_*, \omega)}{\partial\omega} = \frac{1}{\|w(\alpha_*, \omega)\|_1} \cdot \Re \left(u^* \frac{\partial F(\alpha_*, \omega)}{\partial\omega} v \right) - \frac{1}{\|w(\alpha_*, \omega)\|_1^2} \cdot \frac{\partial \|w(\alpha_*, \omega)\|_1}{\partial\omega} \cdot \sigma_{\min}[F(\alpha_*, \omega)]$$

where u, v represent a consistent pair of unit left- and unit right-singular vectors associated with $\sigma_{\min}[F(\alpha_*, \omega)]$, whenever $\sigma_{\min}[F(\alpha_*, \omega)]$ is simple and $f_j(\alpha_*, \omega) \neq 0$ for each $j \in \{0, \dots, m\}$. Unlike

the previous section, which offered analytical means to choose γ_λ and γ_w , analytical determination of the lower bound γ on the second derivatives of $\sigma(\alpha_*, \omega)$ does not seem easy. The additional difficulty is due to a lower bound sought, rather than an upper bound, on the second derivatives of a smallest eigenvalue function. In practice, assigning a large negative real value to γ works robustly. A numerical example is given at the end of Section 6.3 to illustrate the effect of the choice of γ on the number of iterations of this algorithm for vertical searches.

In special cases, it may be possible to adapt the level set approach proposed to minimize $\sigma_{\min}(A - i\omega I)$ over $\omega \in \mathbb{R}$ in Byers (1988) and its quadratically convergent variants Boyd & Balakrishnan (1990) and Bruinsma & Steinbuch (1990) for the minimization of $\sigma(\alpha_*, \omega)$ as in (3.1). But the applicability of these approaches depends on the particular form of $F(z)$, in particular the scalar functions $f_j(z)$. For the standard eigenvalue problem (i.e., when $F(z) = A - zI$) and the polynomial eigenvalue problem, such approaches would require the solution of the eigenvalue problems of the same kind but twice the size of the original problem. For the delay eigenvalue problem, this would give rise to a nonlinear eigenvalue problem of twice the original dimension involving positive and negative powers of $\exp(\lambda)$; see Michiels & Gumussoy (2010) where the level set approach is fully worked out for the problem of the \mathcal{H}_∞ norm computation.

A description of the vertical search combined with the local search is given in Algorithm 2 below. This yields a globally convergent algorithm to compute $\alpha_\epsilon(F)$. Vertical searches also apply regardless of whether F is a square or a rectangular matrix-valued function.

Algorithm 2 Computation of ϵ -pseudospectral abscissa for matrix-valued functions

Require: A matrix-valued function $F : \Omega \rightarrow \mathbb{C}^{n \times p}$ analytic on Ω and a positive scalar $\epsilon \in \mathbb{R}$.

1. $z_0 \leftarrow (\Re z_R, \Im z_R)$, where z_R is a rightmost eigenvalue of F .
 2. *Convergence* \leftarrow False.
 3. **while** \neg *Convergence* **do**
 4. **Local search:** Apply Algorithm 1 starting from z_0 to find $z_* = (\alpha_*, \beta_*)$ such that $\mathcal{C}(z_*) \in \partial \Lambda_\epsilon(F)$ with a vertical tangent line (or $0 \in \partial \lambda(z_*)$).
 5. **Vertical search:** $\omega_* \leftarrow \arg \min_{\omega \in \mathbb{R}} \sigma(\alpha_*, \omega)$ and $\sigma_* \leftarrow \sigma(\alpha_*, \omega_*)$.
 6. **if** $\sigma_* = \epsilon$ **then**
 7. *Convergence* \leftarrow True.
 8. **else**
 9. $z_0 \leftarrow (\alpha_*, \omega_*)$.
 10. **end if**
 11. **end while**
 12. **Output:** z_* .
-

4. Subspace methods

To cope with large-scale problems, we consider the map $v \mapsto F(\lambda)v$ when its domain is restricted to a subspace \mathcal{S} of \mathbb{C}^n . Let S be an isometry (i.e., S is a matrix with more rows than columns satisfying $S^*S = I$) whose columns form an orthonormal basis for \mathcal{S} . The matrix representation of the linear map acting on \mathcal{S} with respect to this basis becomes

$$F_S(\lambda) := F(\lambda)S = \sum_{j=0}^m f_j(\lambda)A_j S.$$

Such a subspace idea is introduced in Kressner & Vandereycken (2014) for the computation of the ϵ -pseudospectral abscissa of a matrix, that is, when $F(\lambda) = \lambda I - A$. Here we extend it to the general setting when $F(\lambda)$ is an analytic matrix-valued function of the form (1.2). In this section, we use the following definitions of the ϵ -pseudospectrum and the ϵ -pseudospectral abscissa of F_S :

$$\Lambda_\epsilon(F_S) := \left\{ \lambda \in \mathbb{C} : \sigma_{\min} \left(\sum_{j=0}^m f_j(\lambda) A_j S \right) \leq \epsilon \|w(\lambda)\|_1 \right\} \quad \text{and}$$

$$\alpha_\epsilon(F_S) := \sup \left\{ \Re \lambda : \lambda \in \Lambda_\epsilon(F_S) \right\}.$$

This terminology and notation is slightly illusive. Indeed, the set $\Lambda_\epsilon(F_S)$ and the quantity $\alpha_\epsilon(F_S)$ are intrinsic to the underlying linear map acting on S and independent of the choice of the orthonormal basis (given by the columns of S) for S . We pursue them in order to remain consistent with the previous sections.

Theorem 4.3 below shows the existence of small subspaces S such that $\alpha_\epsilon(F) = \alpha_\epsilon(F_S)$, where the columns of the matrix S form an orthonormal basis for S . The notation $\mathcal{V}(z)$ is used in this result for the set consisting of right-singular vectors corresponding to $\sigma_{\min}[F(z)]$ for a given $z \in \mathbb{C}$. Additionally, $\text{Col}(S)$ represents the column space of the matrix S . Lemma 4.1 below concerning the monotonicity of $\Lambda_\epsilon(F_S)$ with respect to $\text{Col}(S)$ is a generalization of Kressner & Vandereycken (2014, Lemma 3.1), which specifically addresses the matrix case. Theorem 4.3 generalizes Kressner & Vandereycken (2014, Lemma 3.2), similarly, from the matrix setting to the nonlinear eigenvalue setting.

LEMMA 4.1 (Monotonicity) Two isometries S_1, S_2 such that $\text{Col}(S_1) \subseteq \text{Col}(S_2)$ satisfy

$$(1) \quad \Lambda_\epsilon(F_{S_1}) \subseteq \Lambda_\epsilon(F_{S_2}) \quad \text{and} \quad (2) \quad \alpha_\epsilon(F_{S_1}) \leq \alpha_\epsilon(F_{S_2}).$$

Proof. Let $S_j := \text{Col}(S_j)$ for $j = 1, 2$. Suppose $z \in \Lambda_\epsilon(F_{S_1})$, that is,

$$\sigma_{\min} \left(\sum_{j=0}^m f_j(z) A_j S_1 \right) \leq \epsilon \|w(z)\|_1 \tag{4.1}$$

holds. Notice that

$$\begin{aligned} \sigma_{\min} \left(\sum_{j=0}^m f_j(z) A_j S_1 \right) &= \min_{v \in S_1, \|v\|_2=1} \left\| \sum_{j=0}^m f_j(z) A_j v \right\|_2 \\ &\geq \min_{v \in S_2, \|v\|_2=1} \left\| \sum_{j=0}^m f_j(z) A_j v \right\|_2 = \sigma_{\min} \left(\sum_{j=0}^m f_j(z) A_j S_2 \right), \end{aligned}$$

where the inequality is due to $S_1 \subseteq S_2$. Combining this with inequality (4.1), we deduce that $z \in \Lambda_\epsilon(F_{S_2})$ proving (1). Furthermore, (2) is an immediate consequence of (1). \square

LEMMA 4.2 For $z \in \Lambda_\epsilon(F)$ and a unit right-singular vector v associated with $\sigma_{\min}[F(z)]$, we have $z \in \Lambda_\epsilon(F_v)$.

Proof. This is immediate from

$$\epsilon \|w(z)\|_1 \geq \sigma_{\min} \left(\sum_{j=0}^m f_j(z) A_j \right) = \left\| \sum_{j=0}^m f_j(z) A_j v \right\|_2 = \sigma_{\min} \left(\sum_{j=0}^m f_j(z) A_j v \right). \quad \square$$

THEOREM 4.3 (Low dimensionality) Suppose that S is an isometry. Then $\alpha_\epsilon(F) = \alpha_\epsilon(F_S)$ if and only if $\mathcal{V}(z_*) \cap \text{Col}(S) \neq \emptyset$ for some globally rightmost point z_* of $\Lambda_\epsilon(F)$.

Proof. First observe that $\alpha_\epsilon(F) = \alpha_\epsilon(F_{v_*})$ for any unit right-singular vector v_* associated with $\sigma_{\min}[F(z_*)]$. This is due to $\alpha_\epsilon(F) \geq \alpha_\epsilon(F_{v_*})$ by Lemma 4.1, as well as Lemma 4.2, which implies $z_* \in \Lambda_\epsilon(F_{v_*})$, so $\alpha_\epsilon(F) = \Re z_* \leq \alpha_\epsilon(F_{v_*})$.

Suppose $\mathcal{V}(z_*) \cap \text{Col}(S) \neq \emptyset$ for some globally rightmost point z_* of $\Lambda_\epsilon(F)$. Consider any $v_* \in \mathcal{V}(z_*) \cap \text{Col}(S)$, which we assume to be a unit vector without loss of generality. We have $\text{span}\{v_*\} \subseteq \text{Col}(S)$, so by Lemma 4.1, we obtain

$$\alpha_\epsilon(F_{v_*}) \leq \alpha_\epsilon(F_S) \leq \alpha_\epsilon(F).$$

Thus the equality $\alpha_\epsilon(F_{v_*}) = \alpha_\epsilon(F)$ leads us to $\alpha_\epsilon(F_S) = \alpha_\epsilon(F)$.

To prove the converse, suppose $\alpha_\epsilon(F) = \alpha_\epsilon(F_S)$. Denote a globally rightmost point of $\Lambda_\epsilon(F_S)$ with z_S . Due to Lemma 4.1, we have $z_S \in \Lambda_\epsilon(F)$ and $\Re z_S = \alpha_\epsilon(F_S) = \alpha_\epsilon(F)$, so z_S is also a rightmost point of $\Lambda_\epsilon(F)$ globally. Furthermore, letting v_S be a unit right-singular vector associated with $\sigma_{\min}[F_S(z_S)]$, observe

$$\left\| \sum_{j=0}^m f_j(z_S) A_j S v_S \right\|_2 = \sigma_{\min}[F_S(z_S)] = \sigma_{\min}[F(z_S)].$$

Thus $S v_S$ is a unit right-singular vector associated with $\sigma_{\min}[F(z_S)]$, that is, $\mathcal{V}(z_S) \cap \text{Col}(S) \neq \emptyset$, completing the proof. \square

Theorem 4.3 gives the initiative to work on an $n \times p$ matrix-valued function F_S for $p \ll n$ and for a properly chosen subspace $\mathcal{S} = \text{Col}(S)$ (rather than working on the full $n \times n$ matrix-valued function F). A natural choice for \mathcal{S} appears to be the span of right-singular vectors of $\sigma_{\min}[F(z)]$ for various $z \in \mathbb{C}$ close to globally rightmost points of $\Lambda_\epsilon(F)$. The following observations lead us to this choice: **(i)** the right-singular vectors of $\sigma_{\min}[F(z)]$ are continuous w.r.t. z : if $z \approx z_*$, then $\mathcal{V}(z) \approx \mathcal{V}(z_*)$; **(ii)** $\alpha_\epsilon(F_S)$ is continuous w.r.t. $\text{Col}(S)$: if $\text{Col}(S) \approx \text{Col}(S_*)$ for any isometry S_* such that $\text{Col}(S_*) \cap \mathcal{V}(z_*) \neq \emptyset$, then $\alpha_\epsilon(F_S) \approx \alpha_\epsilon(F_{S_*}) = \alpha_\epsilon(F)$. Initially, we could consider the rightmost eigenvalue z_R of F as a good approximation for the globally rightmost point of $\Lambda_\epsilon(F)$ (this is especially true for $\epsilon \approx 0$). Setting $z_0 := z_R$, we could then generate a sequence $\{z_k\}$ in \mathbb{C} such that

Framework 1 (Subspace selection based on smallest singular value)

- (1) S_k is an isometry s.t. its columns form an orthonormal basis for $\mathcal{S}_k := \text{span}\{v_0, \dots, v_k\}$, where v_j is a right-singular vector corresponding to $\sigma_{\min}[F(z_j)]$,
 - (2) z_{k+1} is a rightmost point of $\Lambda_\epsilon(F_{S_k})$,
-

for $k \in \mathbb{N}$.

REMARK 4.4 There is a natural alternative to this way of choosing subspaces. Theorem 4.3 could be interpreted in terms of eigenvectors corresponding to rightmost eigenvalues of perturbed matrix-valued functions $F + \Delta$. In Michielis & Guglielmi (2012, Proposition 3.1), it is shown that each $z \in \mathbb{C}$ on the boundary of $\Lambda_\epsilon(F)$ is an eigenvalue of

$$(F + \Delta_z)(\lambda) := \sum_{j=0}^m f_j(\lambda)(A_j + \delta A_{z,j}) \quad \text{where } \delta A_{z,j} := -\frac{\epsilon \cdot \overline{f_j(z)}}{w_j \cdot |f_j(z)|} uv^*,$$

and u, v are consistent unit left-, unit right-singular vectors corresponding to $\sigma_{\min}[F(z)]$. Indeed, u, v are left, right eigenvectors associated with the eigenvalue z of $F + \Delta_z$. Furthermore, if z_* is a globally rightmost point of $\Lambda_\epsilon(F)$, then it is a rightmost eigenvalue of $F + \Delta_{z_*}$. Thus, $\mathcal{V}(z_*)$ in Theorem 4.3 could be interpreted as the set of all eigenvectors associated with a rightmost eigenvalue of $F + \Delta_{z_*}$. These observations suggest forming the subspace \mathcal{S} from eigenvectors associated with a rightmost eigenvalue of $F + \Delta_z$ for various z close to globally rightmost points of $\Lambda_\epsilon(F)$. Setting $z_0 := z_R$ the rightmost eigenvalue of F , an alternative sequence $\{z_k\}$ in \mathbb{C} is defined by

Alternative framework for subspace selection

- (1) S_k is an isometry s.t. its columns form an orthonormal basis for $\mathcal{S}_k := \text{span}\{v_0, \dots, v_k\}$, where v_j is an eigenvector associated with a rightmost eigenvalue of $F + \Delta_{z_j}$,
 - (2) z_{k+1} is a rightmost point of $\Lambda_\epsilon(F_{S_k})$,
-

for $k \in \mathbb{N}$. Note that the alternative framework above requires the solution of a nonlinear eigenvalue problem in every iteration, whereas Framework 1 involves only standard singular value problems. Furthermore, numerical estimation of the rightmost eigenvalue of a nonlinear eigenvalue problem is, in general, harder than that of the smallest singular value of a matrix. Thus, we abandon this alternative framework, rather we adopt Framework 1 based on standard smallest singular value computations.

Below, we illustrate how the subspace idea can be put in use for large-scale F by coupling Framework 1 above with Algorithm 1 of Section 2. This results in Algorithm 3, which returns a locally rightmost point of $\Lambda_\epsilon(F)$. Approaches other than Algorithm 1 of Section 2 can be employed at the local search stage on line 5 to determine a point on the boundary of $\Lambda_\epsilon(F_{S_k})$ with vertical tangent line. For instance, it is possible to adopt the approach of Michielis & Guglielmi (2012), which would require the rightmost eigenvalues of rank-one perturbations of the original matrix-valued function. As mentioned above, the numerical computation of a rightmost nonlinear eigenvalue is usually harder than the computation of a smallest singular value, on which Algorithm 1 is based. Consequently, we rely on Algorithm 1 for this local search. In the description of this algorithm, we adopt the notation $\sigma(\Re z, \Im z) := \sigma_{\min}[F(\Re z, \Im z)] / \|w(\Re z, \Im z)\|_1$. We disregard the possibility that the local search (on line 5) converges to a point where the generalized gradient of λ (associated with F_{S_k}) contains zero, which is extremely unlikely. Such an unlikely case can be dealt with, for instance, by occasional vertical searches at additional cost. Furthermore, when $\sigma(z_{k+1}) = \epsilon$ holds, the condition $c \cdot (1, 0) \in \partial\sigma(z_{k+1}) \exists c \in \mathbb{R}^+$ on line 6 (recall that $\partial\sigma(z_{k+1})$ represents the generalized gradient of σ at z_{k+1}) amounts to having a vertical tangent line on the boundary of $\Lambda_\epsilon(F)$ at z_{k+1} in the nonsmooth sense. In the smooth case, when $\sigma(z_{k+1})$ is simple, this condition reduces to $\nabla\sigma(z_{k+1}) = c \cdot (1, 0) \exists c \in \mathbb{R}^+$.

Algorithm 3 Large-scale local search

Require: A matrix-valued function $F : \Omega \rightarrow \mathbb{C}^{n \times n}$ analytic on Ω and a positive scalar $\epsilon \in \mathbb{R}$.

1. $z_0 \leftarrow$ a rightmost eigenvalue of F and $k \leftarrow 0$.
 2. $\mathcal{S}_0 \leftarrow \text{span}\{v_0\}$, where v_0 is a right-singular vector associated with $\sigma_{\min}[F(z_0)]$.
 3. $\text{Convergence} \leftarrow \text{False}$.
 4. **while** $\neg \text{Convergence}$ **do**
 5. **Local search:** Apply Algorithm 1 to find $z_{k+1} = (\alpha_*, \beta_*)$ such that $\mathcal{C}(z_{k+1}) \in \partial \Lambda_\epsilon(F_{S_k})$ with a vertical tangent line.
 6. **if** $(\sigma(z_{k+1}) = \epsilon) \text{ and } (c \cdot (1, 0) \in \partial \sigma(z_{k+1}) \exists c \in \mathbb{R}^+)$ **then**
 7. $\text{Convergence} \leftarrow \text{True}$.
 8. **else**
 9. $\mathcal{S}_{k+1} \leftarrow \text{span}(\mathcal{S}_k \cup \{v_{k+1}\})$, where v_{k+1} is a right-singular vector associated with $\sigma_{\min}[F(z_{k+1})]$.
 10. Increment k .
 11. **end if**
 12. **end while**
 13. **Output:** z_{k+1} .
-

5. Restarts

In the subspace $\mathcal{S}_k = \text{span}\{v_0, \dots, v_k\}$ of Framework 1, the vectors added lately are more relevant to the set of optimal right-singular vectors $\mathcal{V}(z_*)$ of Theorem 4.3. This is because the sequence $\{\Re z_k\}$ is monotone increasing and later points in $\{z_k\}$ usually represent the optimal z_* better. This brings up a subspace-restart idea: when the subspace \mathcal{S}_k becomes of high dimension, erase the earlier vectors and keep the last-added few vectors among v_0, \dots, v_k , possibly only v_k . Thus redefine $\mathcal{S}_j := \text{span}\{v_{k-j}, \dots, v_k\}$ and restart. Such restart strategies have already been employed in the context of large-scale eigenvalue computation based on Krylov subspace methods (Lehoucq & Sorensen, 1996) and incorporated into modern software, for instance ARPACK (Lehoucq *et al.*, 1998).

The vertical searches described in Section 3 can also benefit from this restart strategy. A vertical search, when it determines that a point is not globally rightmost, also provides a new point z_0 to start with. Then the subspace could be reset to $\text{span}\{v_0\}$ where v_0 is a right-singular vector associated with $\sigma_{\min}[F(z_0)]$.

5.1 Quality of subspace approximations

To further motivate the restart strategy and to discard poor approximations in the subspace, below we relate the quality of a subspace \mathcal{S}_k (specifically its proximity to v_*) with the quality of $\alpha_\epsilon(F_{S_k})$ (specifically its proximity to $\alpha_\epsilon(F)$). Here and throughout this subsection, S_k is a matrix whose columns form an orthonormal basis for \mathcal{S}_k , and z_* is as defined in Theorem 4.3. Furthermore, let u_*, v_* be consistent unit left-, right-singular vectors associated with $\sigma_{\min}[F(z_*)]$, that is,

$$F(z_*)v_* = \sigma_{\min}[F(z_*)]u_* \quad \text{and} \quad u_*^*F(z_*) = \sigma_{\min}[F(z_*)]v_*^*.$$

We measure the quality of \mathcal{S}_k in terms of $\delta = v_* - v_{k*}$ where $v_{k*} := \arg \min_{v \in \mathcal{S}_k, \|v\|_2=1} \|v_* - v\|_2$, and focus on the error $\alpha_\epsilon(F) - \alpha_\epsilon(F_{S_k})$ as $\delta \rightarrow 0$. This issue of relating the quality of the restricted pseudospectral

abscissa to the quality of the subspace has been addressed in the more simple matrix setting by Kressner & Vandereycken (2014, Theorem 3.3).

Our approach has two stages. In the first stage, we establish

$$\|F(z_*)v_{k*}\|_2/\|w(z_*)\|_1 = \epsilon + \mathcal{O}(\|\delta\|_2^2). \quad (5.1)$$

In the second stage, starting from this equality, we deduce the existence of a $z_{k*} \in \mathbb{C}$ satisfying

$$\|F(z_{k*})v_{k*}\|_2/\|w(z_{k*})\|_1 = \epsilon \quad (5.2)$$

and $\Re z_* - \Re z_{k*} = \mathcal{O}(\|\delta\|_2^2)$. The last equality implies that $z_{k*} \in \Lambda_\epsilon(F_{S_k})$, meaning $\Re z_{k*} \leq \alpha_\epsilon(F_{S_k})$. The desired relation between the ϵ -pseudospectral abscissa of F and F_{S_k} follows from $\alpha_\epsilon(F) - \alpha_\epsilon(F_{S_k}) \leq \Re z_* - \Re z_{k*}$.

To prove equality (5.1), let us define the vector-valued function

$$v : \mathbb{R} \rightarrow \mathbb{R}^n, \quad v(t) := \left[v_* + \frac{v_{k*} - v_*}{\|v_{k*} - v_*\|_2} t \right] / \left\| v_* + \frac{v_{k*} - v_*}{\|v_{k*} - v_*\|_2} t \right\|_2,$$

and the scalar function

$$\mu : \mathbb{R} \rightarrow \mathbb{R}, \quad \mu(t) := \|F(z_*)v(t)\|_2,$$

which is real analytic near 0. We benefit from a Taylor expansion of $\mu(t)$ about 0 to obtain (5.1). Specifically, since $v(\|\delta\|_2) = v(\|v_{k*} - v_*\|_2) = v_{k*}$, we have

$$\begin{aligned} \frac{\|F(z_*)v_{k*}\|_2}{\|w(z_*)\|_1} &= \frac{\|F(z_*)v(\|\delta\|_2)\|_2}{\|w(z_*)\|_1} = \frac{\mu(\|\delta\|_2)}{\|w(z_*)\|_1} \\ &= \frac{\mu(0) + \mu'(0)\|\delta\|_2 + \mathcal{O}(\|\delta\|_2^2)}{\|w(z_*)\|_1}. \end{aligned}$$

The desired equality (5.1) follows from the observations $\mu(0) = \sigma_{\min}[F(z_*)] = \epsilon\|w(z_*)\|_1$ (since $v(0) = v_*$), and

$$\mu'(0) = \Re(u_*^* F(z_*) v'(0)) = \Re(\sigma_{\min}[F(z_*)] v_*^* v'(0)) = \epsilon\|w(z_*)\|_1 \Re(v_*^* v'(0)) = 0,$$

where $\Re(v_*^* v'(0)) = 0$ due to $\|v(t)\|_2^2 = 1$ for all t .

To establish (5.2) for some $z_{k*} \in \mathbb{C}$ such that $\Re z_* - \Re z_{k*} = \mathcal{O}(\|\delta\|_2^2)$, let us suppose that $\sigma_{\min}[F(z_*)]$ is simple, and $f_j(z_*) \neq 0$ for $j = 0, \dots, m$. In this case, all of the functions

$$\begin{aligned} \sigma(\Re z, \Im z) &:= \frac{\sigma_{\min}[F(\Re z, \Im z)]}{\|w(\Re z, \Im z)\|_1}, \quad \hat{\sigma}(\Re z, \Im z) := \frac{\|F(\Re z, \Im z)v_*\|_2}{\|w(\Re z, \Im z)\|_1} \\ \text{and} \quad \tilde{\sigma}(\Re z, \Im z) &:= \frac{\|F(\Re z, \Im z)v_{k*}\|_2}{\|w(\Re z, \Im z)\|_1} \end{aligned}$$

are continuously differentiable at $(\Re z, \Im z) = (\Re z_*, \Im z_*)$. Target equality (5.2) can be written as $\tilde{\sigma}(\Re z_{k*}, \Im z_{k*}) = \epsilon$, whereas (5.1) can be expressed as

$$\tilde{\sigma}(\Re z_*, \Im z_*) = \epsilon + \mathcal{O}(\|\delta\|_2^2). \quad (5.3)$$

Assuming that the gradient of $\sigma(\Re z, \Im z)$ does not vanish at $(\Re z_*, \Im z_*)$, the first-order optimality conditions imply

$$\nabla \sigma(\Re z_*, \Im z_*) = \nabla \hat{\sigma}(\Re z_*, \Im z_*) = c \cdot (1, 0) \quad (5.4)$$

for some positive $c \in \mathbb{R}$. But then, by continuity and the second equality in (5.4), we have

$$\eta := p^T \nabla \tilde{\sigma}(\Re z_*, \Im z_*) < 0, \quad \text{where } p = -(1, 0). \quad (5.5)$$

Employing (5.3) and due to (5.5), there exists $\alpha > 0$ such that

$$\tilde{\sigma}(\Re z_* - \alpha, \Im z_*) = \frac{\|F(\Re z_* - \alpha, \Im z_*)v_{k*}\|_2}{\|w(\Re z_* - \alpha, \Im z_*)\|_1} = \epsilon.$$

Defining z_{k*} by $\Re z_{k*} := \Re z_* - \alpha$ and $\Im z_{k*} := \Im z_*$, we deduce (5.2). To quantify $\alpha = \Re z_* - \Re z_{k*}$, we expand $\tilde{\sigma}(\Re z, \Im z)$ about $(\Re z_*, \Im z_*)$ only varying $\Re z$ (note that $\tilde{\sigma}(\Re z, \Im z_*)$ is real analytic with respect to $\Re z$ near $\Re z_*$). This leads to

$$\tilde{\sigma}(\Re z_* - \alpha, \Im z_*) = \tilde{\sigma}(\Re z_*, \Im z_*) + \eta\alpha + \mathcal{O}(\alpha^2) \implies \alpha = \mathcal{O}(\|\delta\|_2^2).$$

Finally, since $v_{k*} \in \mathcal{S}_k$, we have

$$\frac{\sigma_{\min}[F_{S_k}(z_{k*})]}{\|w(z_{k*})\|_1} \leq \frac{\|F(z_{k*})v_{k*}\|_2}{\|w(z_{k*})\|_1} = \epsilon,$$

meaning $z_{k*} \in \Lambda_\epsilon(F_{S_k})$. From $\alpha_\epsilon(F) = \Re z_*$ and $\alpha_\epsilon(F_{S_k}) \geq \Re z_{k*}$, we obtain $\alpha_\epsilon(F) - \alpha_\epsilon(F_{S_k}) \leq \Re z_* - \Re z_{k*} = \alpha$. Hence,

$$\alpha_\epsilon(F) - \alpha_\epsilon(F_{S_k}) = \mathcal{O}(\|\delta\|_2^2).$$

5.2 Overall algorithm

We apply the subspace method, specifically Framework 1 in Section 4. Initially, z_0 is chosen as the rightmost eigenvalue of F , and \mathcal{S}_0 is the associated one-dimensional subspace. The subspace method requires the determination of a rightmost point of $\Lambda_\epsilon(F_{S_k})$ for several k , each of which we achieve by the local algorithm in Section 2. In practice, this results in convergence to a point $z_* = (z_{*1}, z_{*2}) \in \mathbb{R}^2$ such that $\mathcal{C}(z_*)$ is (up to a tolerance) on the boundary of $\Lambda_\epsilon(F)$ with a vertical tangent line for a rather small subspace \mathcal{S}_k . We do not allow \mathcal{S}_k to expand arbitrarily and restart with a one-dimensional subspace once its dimension reaches a prescribed value. We perform the vertical search discussed in Section 3 along the line $\{z \in \mathbb{C} \mid \Re z = z_{*1}\}$. The vertical search is performed on the full matrix-valued function F in order to ensure global convergence. Termination occurs if this vertical search yields ϵ as the smallest value of the singular value function involved (up to a specified tolerance in practice). Otherwise, we restart the subspace method from a global minimizer on the vertical line and with the associated one-dimensional subspace. A detailed description is given in Algorithm 4 below.

The computational work is usually dominated by the vertical search on line 7, which is needed only a few times in practice. Each vertical search requires the computation of the smallest singular value of

the full matrix-valued function $F(z)$ at several z , and this constitutes the main computational burden. On the other hand, the local search on line 5 is performed quite a few times, but that computational cost is quite low, since it involves small matrix-valued functions.

Algorithm 4 Computation of ϵ -pseudospectral abscissa for large-scale matrix-valued functions

Require: A matrix-valued function $F : \Omega \rightarrow \mathbb{C}^{n \times n}$ analytic on Ω , a positive scalar $\epsilon \in \mathbb{R}$ and the maximal subspace dimension allowed $k_{\max} \in \mathbb{Z}^+$.

1. $z_0 \leftarrow$ a rightmost eigenvalue of F and $k \leftarrow 0$.
2. $\mathcal{S}_0 \leftarrow \text{span}\{v_0\}$, where v_0 is a right-singular vector associated with $\sigma_{\min}[F(z_0)]$.
3. *Convergence* \leftarrow False.
4. **while** \neg *Convergence* **do**
5. **Local search:** Apply Algorithm 1 to find $z_{k+1} = (\alpha_*, \beta_*)$ such that $\mathcal{C}(z_{k+1}) \in \partial \Lambda_\epsilon(F_{\mathcal{S}_k})$ with a vertical tangent line.
6. **if** $(\sigma(z_{k+1}) = \epsilon) \text{ and } (c \cdot (1, 0) \in \partial \sigma(z_{k+1}) \exists c \in \mathbb{R}^+)$ **then**
7. **Vertical search:** $\omega_* \leftarrow \arg \min_{\omega \in \mathbb{R}} \sigma(\alpha_*, \omega)$ and $\sigma_* \leftarrow \sigma(\alpha_*, \omega_*)$.
8. **if** $\sigma_* = \epsilon$ **then**
9. *Convergence* \leftarrow True.
10. **else**
11. $z_0 \leftarrow \mathcal{C}(\alpha_*, \omega_*)$ and $k \leftarrow 0$.
12. $\mathcal{S}_0 \leftarrow \text{span}\{v_0\}$, where v_0 is a right-singular vector associated with $\sigma_{\min}[F(z_0)]$.
13. **end if**
14. **else**
15. **if** $k = k_{\max}$ **then**
16. $z_0 \leftarrow z_{k+1}$ and $k \leftarrow 0$.
17. $\mathcal{S}_0 \leftarrow \text{span}\{v_0\}$, where v_0 is a right-singular vector associated with $\sigma_{\min}[F(z_0)]$.
18. **else**
19. $\mathcal{S}_{k+1} \leftarrow \text{span}(\mathcal{S}_k \cup \{v_{k+1}\})$, where v_{k+1} is a right-singular vector associated with $\sigma_{\min}[F(z_{k+1})]$.
20. Increment k .
21. **end if**
22. **end if**
23. **end while**
24. **Output:** z_{k+1} .

6. Numerical examples

A practical implementation of Algorithm 4 requires several parameters, most notably the upper and lower bounds for the second derivatives of the eigenvalue functions involved for local and vertical searches, as well as the maximal subspace dimension. In the examples in this section and for local searches, we set the upper bound γ equal to 2 for the standard eigenvalue problem, and 40000 for other nonlinear eigenvalue problems. The former is an analytical upper bound, while the latter is a heuristic that works well in practice. For the latter case, alternatively, the bounds implied by Theorems 2.2 and 2.4 could be used. We set the lower bound γ for vertical searches equal to -4 , which again is a heuristic that works well in our experience. The maximal subspace dimension is by default chosen as $n/4$ for an $n \times n$

matrix-valued function. This excludes the delay example in Section 6.3 for which the maximal subspace dimension is chosen as 10.

We always start the algorithm with the rightmost eigenvalue computed by MATLAB for the standard and polynomial eigenvalue problems. This is computed by means of the QR algorithm (i.e., eig command in MATLAB) for matrices of size up to 300 and by Arnoldi's method (i.e., eigs command in MATLAB) for matrices of size beyond 300. We linearize the matrix polynomials and compute the eigenvalues of linearizations by means of the QR algorithm for small-scale problems (i.e., polyeig command in MATLAB). For large-scale problems the current state-of-the art-CORK algorithm (Van Beeumen *et al.*, 2015) should be used. This algorithm fully exploits the Kronecker structure of the linearization pencils. For other nonlinear eigenvalue problems, we expect the user to specify the rightmost eigenvalue as an input parameter. This eigenvalue can, e.g., be computed via the software NLEIGS (Güttel *et al.*, 2014) for generic nonlinear eigenvalue problems or by the algorithm of Wu & Michielis (2012) for the delay eigenvalue problem. All of the numerical experiments below are performed with MATLAB R2011a on a Mac Pro with a quad-core Intel Xeon processor and 16 GB memory.

6.1 Standard eigenvalue problem

Algorithm 4 is especially suitable for the computation of the pseudospectral abscissa for large-scale matrices, that is, when $F(z) = A - zI$ for a given large matrix A and weights are given by $[1 \infty]$. The *criss-cross algorithm* (Burke *et al.*, 2003) is the most reliable choice for the computation of the pseudospectral abscissa of a matrix at the moment, but its use is limited mainly to small- up to medium-scale matrices. We compare Algorithm 4 with the criss-cross algorithm in this subsection.

In our numerical experiments, Algorithm 4 in practice is terminated after a vertical search, whenever it is determined that the globally smallest value of $\sigma_{\min}[A - (\alpha_* + \omega i)I]$ over ω (for an α_* converged by the local search algorithm) does not differ from ϵ by more than a tolerance, $10^{-6}\|A\|_2$ for the examples below. The criss-cross algorithm also performs vertical searches, but they are based on extracting all imaginary eigenvalues of $2n \times 2n$ Hamiltonian matrices from which the intersection points of a vertical line with the ϵ -pseudospectrum boundary are inferred. It terminates either if a vertical search fails to find any intersection point or if two consecutive estimates for the ϵ -pseudospectral abscissa are not increasing due to rounding errors.

We start with a random 50×50 matrix formed by typing `randn(50) + 0.7*i*randn(50)` in MATLAB. Algorithm 4 applies the subspace iteration initially. Each subspace iteration amounts to a local search on a small problem. When the subspace becomes eight-dimensional, it stops expanding as the local searches on seven- and eight-dimensional subspaces return nearly identical rightmost points. Instead, it performs a vertical search and terminates. In Fig. 1, the progress of the subspace iteration on this example is shown for two-, four- and six-dimensional subspaces. The results of Algorithm 4 and the criss-cross algorithm match up to 12 decimal digits.

The next three sets of examples illustrate the superiority of Algorithm 4 over the criss-cross algorithm for medium- to large-scale matrices. All these examples can be generated using EigTool (Wright, 2014). Each one of the three test sets consists of four matrices of size 200, 400, 800 and 1200 chosen from a particular family. The matrices in the first set are Landau matrices arising from an integral equation in laser theory (Landau, 1977). The matrices in the second set are Hatano–Nelson matrices, which are tridiagonal and arise from quantum mechanics (Hatano & Nelson, 1996). The matrices in the third set are Davies matrices originating from a spectral method discretization of an anharmonic oscillator, that is, a second-order differential operator subject to boundary conditions in one dimension (Davies, 1999). A comparison of running times of the algorithms is given in Table 1. In all cases, Algorithm 4 becomes

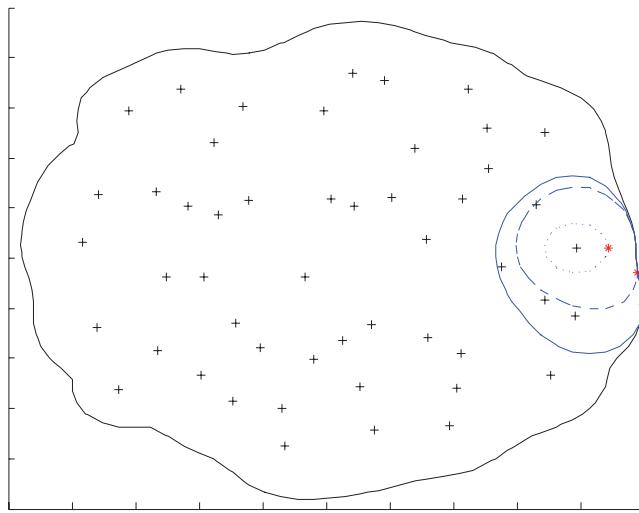


FIG. 1. Subspace iteration on a 50×50 random matrix is displayed. The outermost curve represents the boundary of the ϵ -pseudospectrum of this matrix for $\epsilon = 1$, while each + represents an eigenvalue. The ϵ -pseudospectrum for the restricted problem F_{S_k} is shown with dotted, dashed and solid inner curves for $k = 2, 4, 6$, respectively. The asterisks mark the rightmost points for these restricted problems.

TABLE 1 *Running times for the algorithms in seconds with respect to the sizes of the matrices and the computed pseudospectral abscissa; the running times of the criss-cross algorithm are omitted for Hatano and Davies matrices of size 1200, since its computations take excessive time*

Landau, $\epsilon = 10^{-0.5}$	200	400	800	1200
Algorithm 4	7	20	78	176
Criss-cross algorithm	7	43	223	662
α_ϵ	1.3153	1.3161	1.3161	1.3161
Hatano, $\epsilon = 1$	200	400	800	1200
Algorithm 4	14	29	89	207
Criss-cross algorithm	7	46	2030	
α_ϵ	4.0765	4.0903	4.0678	4.1474
Davies, $\epsilon = 10^5$	200	400	800	1200
Algorithm 4	8	9	19	40
Criss-cross algorithm	3	41	223	
α_ϵ	$4.0355 \cdot 10^5$	$4.8867 \cdot 10^6$	$7.6266 \cdot 10^7$	$3.8504 \cdot 10^8$

superior in terms of the running times, as soon as n (the size of the matrix) is slightly larger than 200. The gap grows quickly as n increases. Furthermore, the roughly quadratic dependence of the running time for Algorithm 4 on the sizes of the matrices is apparent. This is due to the fact that the required smallest eigenvalues and singular values and the corresponding eigenvectors and singular vectors are computed by means of ARPACK (Lehoucq *et al.*, 1998), which is based on Arnoldi's method. The results computed by the two algorithms differ by amounts on the order of the double machine precision in a relative sense. More precisely, denoting the results returned by Algorithm 4 and the criss-cross algorithm by f_1 and f_2 , respectively, and the 2-norm of the input matrix by $\|A\|_2$, the quantity $|f_1 - f_2|/\|A\|_2$ does not exceed 10^{-14} .

An alternative for the local searches (Algorithm 1) in this matrix setting is the approach suggested in Guglielmi & Overton (2011), which computes repeatedly the rightmost eigenvalues of rank-one perturbations of the matrix whose ϵ -pseudospectral abscissa is sought. We have performed comparisons of Algorithm 1 and this approach on four families of matrices (without subspace restrictions and vertical searches). Two of these families are composed of dense matrices, namely the Landau and Hatano matrices of Table 1. The other two families are the Poisson matrices and Wathen matrices, which are sparse and available through the MATLAB gallery. The Poisson matrices arise from the application of the five-point finite difference formula to the two-dimensional Poisson equation, whereas the Wathen matrices arise from a two-dimensional finite element discretization. In our experiments, we have observed that the particular implementation¹ of the algorithm in Guglielmi & Overton (2011) that we rely on has terminated with failure occasionally on the sparse Poisson and Wathen matrices, which we attribute to the Arnoldi solver (i.e., `eigs` in MATLAB) to retrieve the rightmost eigenvalue. On successful attempts, the running times of the two approaches together with their number of iterations are listed in Table 2. In these runs, both algorithms are terminated when the modulus of the difference between two consecutive estimates for a rightmost eigenvalue does not differ by more than 10^{-8} . The particular implementation of Guglielmi & Overton (2011) that we depend on uses the QR algorithm (i.e., calls `eig`) for dense matrices. This is partly the reason for the excessive amount of time this algorithm takes on the Landau and Hatano matrices. But beyond the running time considerations, this algorithm also requires quite a few additional iterations compared to Algorithm 1 on these dense matrices. For the 200×200 Landau and Hatano matrices, the first few iterations of Algorithm 1 and the algorithm in Guglielmi & Overton (2011) are given in Table 3. Faster convergence of Algorithm 1 is apparent from this table. It requires only 5 and 4 iterations so that two consecutive iterations do not differ by more than 10^{-8} for the Landau and Hatano matrices, respectively. (Note that the row of $k = 0$ lists the initial estimates in the table.) On the other hand, the algorithm in Guglielmi & Overton (2011) performs 46 and 24 iterations to satisfy the same criterion. On the sparse Poisson and Wathen matrices, the two algorithms exhibit similar convergence behavior, and both require only a few iterations. For matrices on the order of ten thousands in Table 1, the algorithm in Guglielmi & Overton (2011) runs faster than Algorithm 1. We attribute this to the fact that the estimation of a smallest singular value based on the Arnoldi iteration requires computation of a sparse Cholesky or an LU factorization followed by sparse forward and back substitutions, which may not be needed to compute a rightmost eigenvalue. But this comes at the expense of reliability. The particular implementation of Guglielmi & Overton (2011) that we use terminates with failure in most of the attempts on the Poisson and Wathen matrices.

¹ PSAPSR version 1.2 that is available at <http://www.cs.nyu.edu/overton/software/psapsr/index.html>.

TABLE 2 Comparison of the running times and number of iterations of Algorithm 1 and the algorithm in Guglielmi & Overton (2011) on four families of matrices: Landau and Hatano matrices are dense, whereas Poisson and Wathen matrices are sparse. In each table in the second and third rows, the numbers separated by a comma correspond to the running time in seconds and the number of iterations, respectively. These entries are omitted for the algorithm in Guglielmi & Overton (2011) and for the 800×800 , 1200×1200 Landau matrices, as well as for the 1200×1200 Hatano matrices, since the computations take an excessive amount of time

Landau , $\epsilon = 10^{-0.5}$	200	400	800	1200
Algorithm 1	0.8, 5	2.3, 5	10.7, 5	21.2, 5
Algorithm in Guglielmi & Overton (2011)	25.5, 46	509, 176		
Hatano , $\epsilon = 1$	200	400	800	1200
Algorithm 1	0.5, 4	0.7, 4	2, 4	4.4, 4
Algorithm in Guglielmi & Overton (2011)	11, 24	57.3, 29	225.6, 22	
Poisson , $\epsilon = 10^2$	225	900	2500	10000
Algorithm 1	0.07, 2	0.4, 2	1, 2	5.4, 2
Algorithm in Guglielmi & Overton (2011)	0.16, 2	1, 2	1.8, 2	8.5, 2
Wathen , $\epsilon = 10^2$	341	560	1281	2821
Algorithm 1	0.1, 2	0.3, 2	0.4, 2	0.9, 2
Algorithm in Guglielmi & Overton (2011)	0.1, 2	0.5, 2	0.6, 2	1.3, 2

TABLE 3 A comparison of the iterations of Algorithm 1 and the algorithm in Guglielmi & Overton (2011) on two matrices: (left) first five iterations of these algorithms on the 200×200 Landau matrix for $\epsilon = 10^{-0.5}$. For this example $\alpha_\epsilon(A) = 1.3153$ rounded to four decimal digits; (right) first four and five iterations of Algorithm 1 and the algorithm in Guglielmi & Overton (2011) on the 200×200 Hatano matrix for $\epsilon = 1$. Algorithm 1 converges after 5 iterations. In this case, $\alpha_\epsilon(A) = 4.0765$ rounded to four decimal digits

k	Algorithm in Guglielmi & Overton (2011)		Algorithm in Guglielmi & Overton (2011)	
	Algorithm 1	(2011)	k	Algorithm 1 (2011)
0	0.998463500946449	0.998463500946449	0	2.975503186571108
1	1.314691266963286	1.314183947855148	1	3.975503186571105
2	1.315321099396864	1.314549337187003	2	4.076353694550083
3	1.315321120654854	1.314742547970619	3	4.076461835403093
4	1.315321120661175	1.314870338002996	4	4.076461835511952
5	1.315321120661177	1.314963416776238	5	4.074749026199803

6.2 Polynomial eigenvalue problem

In this subsection, we experiment with several polynomial eigenvalue problems available in the collection [Betcke et al. \(2010\)](#). In all of these experiments, Algorithm 4 is terminated in practice whenever a vertical search determines that the globally smallest value of $\sigma_{\min}[F(\alpha_*, \omega)] / \|w(\alpha_*, \omega)\|_1$ over ω does not differ from ϵ by more than $10^{-6} \|A_m\|_2$, where A_m denotes the leading coefficient matrix of the matrix polynomial $F(\lambda) := \sum_{j=0}^m \lambda^j A_j$ whose ϵ -pseudospectral abscissa is sought. Furthermore, in all experiments in this subsection, all weights are set equal to 1, unless otherwise stated. All of the plots of the pseudospectra are generated by computing the singular value function $\sigma_{\min}[P(z)] / \|w(z)\|_1$ on a grid.

6.2.1 Wing example. The first one arises from the analysis of oscillations of a wing of an airplane, leading to a 3×3 quadratic eigenvalue problem $Q(\lambda) = A_0 + \lambda A_1 + \lambda^2 A_2$ where

$$A_0 = \begin{bmatrix} 121 & 18.9 & 15.9 \\ 0 & 2.7 & 0.145 \\ 11.9 & 3.64 & 15.5 \end{bmatrix}, \quad A_1 = \begin{bmatrix} 7.66 & 2.45 & 2.1 \\ 0.23 & 1.04 & 0.223 \\ 0.60 & 0.756 & 0.658 \end{bmatrix}, \quad A_2 = \begin{bmatrix} 17.6 & 1.28 & 2.89 \\ 1.28 & 0.824 & 0.413 \\ 2.89 & 0.413 & 0.725 \end{bmatrix}.$$

The progress of Algorithm 4 on this example with $\epsilon = 10^{-0.8}$ is illustrated in Fig. 2. The algorithm starts with a rightmost eigenvalue $z_r = 0.0947 + 2.2529i$. However, this eigenvalue is considerably less sensitive as compared to the eigenvalues $-0.8848 \pm 8.4415i$. The first few iterations yield estimates in the component of $\Lambda_\epsilon(Q)$ containing z_r . When the rightmost point in this component is obtained, a vertical search is performed, and the algorithm jumps into the component of the eigenvalue $-0.8848 - 8.4415i$. A few more subspace iterations result in convergence to a rightmost point globally. The computed value $\alpha_\epsilon(Q) = 9.25817665382$ matches the result reported in [Michielis & Guglielmi \(2012\)](#).

6.2.2 Butterfly example. We next experiment on the butterfly example in [Betcke et al. \(2010\)](#). This involves a 64×64 quartic polynomial $P(\lambda) = B_0 + \lambda B_1 + \lambda^2 B_2 + \lambda^3 B_3 + \lambda^4 B_4$ for which the computation of $\alpha_\epsilon(P)$ appears notoriously difficult. A particular application of Algorithm 4 for the computation of $\alpha_\epsilon(P)$ for $\epsilon = 0.08$ is illustrated in Fig. 3. The algorithm converges to (nonglobal) local solutions twice. It escapes from these local solutions by means of vertical searches. Consequently, it generates iterates with imaginary parts about -2 . But slow convergence occurs, and our numerical implementation applies another vertical search. This is an artifact of the numerical implementation; this vertical search is not essential for convergence to a globally rightmost point, as the pseudospectra is symmetric with respect to the real axis. But it speeds up the convergence. This leads to iterates with imaginary parts about 2 and eventually termination with $\alpha_\epsilon(P) = 1.3858189142$.

It has been proven in [Kressner & Vandereycken \(2014\)](#) that the subspace approach for the computation of a pseudospectral abscissa of a matrix converges superlinearly with respect to the subspace dimension. Even faster quadratic convergence has been reported in practice in the same paper. In the more general nonlinear eigenvalue setting, we still observe quadratic convergence. For instance, for the butterfly example above, the first five iterations of the subspace approach before the first vertical search are given on the left in Table 4, where quadratic convergence is apparent.

To illustrate the effect of the weights, the algorithm is applied to the butterfly example for $\epsilon = 0.2$ with weights $[1 \ 1 \ 1 \ 1 \ 1]$, $[1 \ 1 \ 1 \ 1 \ \infty]$, $[1 \ 1 \ 1 \ \infty \ \infty]$ and $[1 \ 1 \ \infty \ \infty \ \infty]$. The iterates generated on the associated ϵ -pseudospectrum for each of these four cases are provided in Fig. 4. The computed $\alpha_\epsilon(P)$ are 3.6758307326, 1.4144528011, 1.2006081257 and 1.1221784200, respectively. The decrease in the ϵ -pseudospectral abscissa is dramatic when perturbations of the leading coefficient are not allowed. The

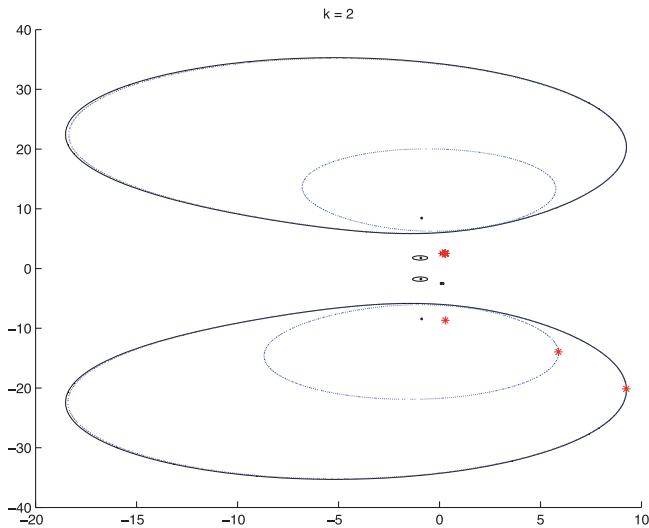


FIG. 2. The progress of the algorithm on the wing example Q for $\epsilon = 10^{-0.8}$ is shown. The eigenvalues are marked with dots, and the iterates of the algorithm are marked with asterisks. The outermost solid curve corresponds to the boundary of $\Lambda_\epsilon(Q)$ for $\epsilon = 10^{-0.8}$, whereas the inner dotted curves represent the boundary of this ϵ -pseudospectrum when the domain of the map $v \mapsto Qv$ is restricted to one- and two-dimensional subspaces.

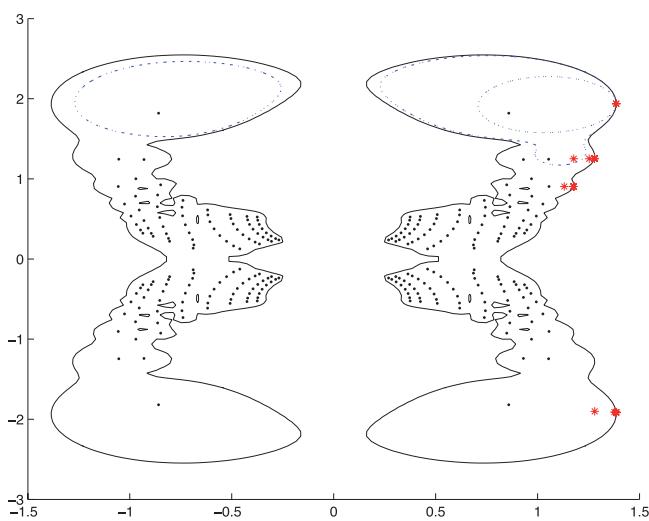


FIG. 3. The algorithm is depicted on the butterfly example with $\epsilon = 0.08$. Once again, the eigenvalues and the iterates of the algorithm are marked with dots and asterisks, respectively. The outermost solid curve corresponds to the boundary of the ϵ -pseudospectrum. The dotted curve and dashed dotted curve represent the ϵ -pseudospectrum when the domain is restricted to a one-dimensional subspace and a three-dimensional subspace just a few iterations before termination.

TABLE 4 The real parts of the rightmost points are listed with respect to the subspace dimension k for the following examples: (left) the butterfly example illustrated in Fig. 3 before the first vertical search with all weights equal to 1 and $\epsilon = 0.08$; (right) the delay example of Fig. 5 after the first vertical search with weights $[\infty \ 1 \ 1]$ and $\epsilon = 0.45$

k	$\alpha_\epsilon(P_{S_k})$	k	$\alpha_\epsilon(D_{S_k})$
1	1.13113137749520	1	14.77293966129789
2	1.17557525555857	2	15.54331045219255
3	1.17810581840297	3	15.58945602178569
4	1.17824505975687	4	15.58946152761596
5	1.17824509591110	5	15.58946153015292
6	1.17824509591110	6	15.58946153015296

algorithm does not require any vertical searches on the top-left figure, and it performs vertical searches on the other three figures to avoid locally rightmost points.

6.2.3 *Two-dimensional acoustic wave example.* This concerns a quadratic matrix polynomial $W(\lambda) = K_0 + \lambda K_1 + \lambda^2 K_2$ arising from a finite element discretization of a two-dimensional harmonic wave equation over the unit square $[0, 1] \times [0, 1]$. The size of the matrix polynomial W depends on the coarseness of the finite element grid. Running times of Algorithm 4 to compute $\alpha_\epsilon(W)$ for $\epsilon = 0.01$ with respect to the size of W are listed in Table 5.

The majority of the running time is consumed by the vertical searches for the examples in Table 5. Algorithm 3 without the vertical searches is applicable to large-scale matrix polynomials. This is illustrated in Table 6 on the matrix polynomials of size 1100×1100 , 2100×2100 and 4200×4200 arising from the acoustic wave equation. Here, only the subspace approach combined with the local searches is applied, in a way such that it terminates when the two consecutive estimates for the ϵ -pseudospectral abscissa differ by less than 10^{-12} . Thus, the computed values for $\alpha_\epsilon(W)$ can possibly correspond to the real parts of points in $\Lambda_\epsilon(W)$ that are locally rightmost. The rightmost eigenvalues are computed *a priori*, so the time consumed for their computation is not included in the overall running time. The running times in Table 6 are remarkable; given this rightmost eigenvalue, the subspace approach requires less than a minute to compute a locally rightmost point in $\Lambda_\epsilon(W)$. The majority of the running time for the subspace approach is taken by the smallest singular value computations on the full matrix polynomial. Recall that the right-singular vectors associated with these singular values are needed to form the subspaces.

6.3 Delay eigenvalue problem

We test Algorithm 4 on the following delay eigenvalue problem with weights $[\infty \ 1 \ 1]$:

$$D(\lambda) = \lambda I - D_0 - D_1 e^{-\lambda} - D_2 e^{-3\lambda}. \quad (6.1)$$

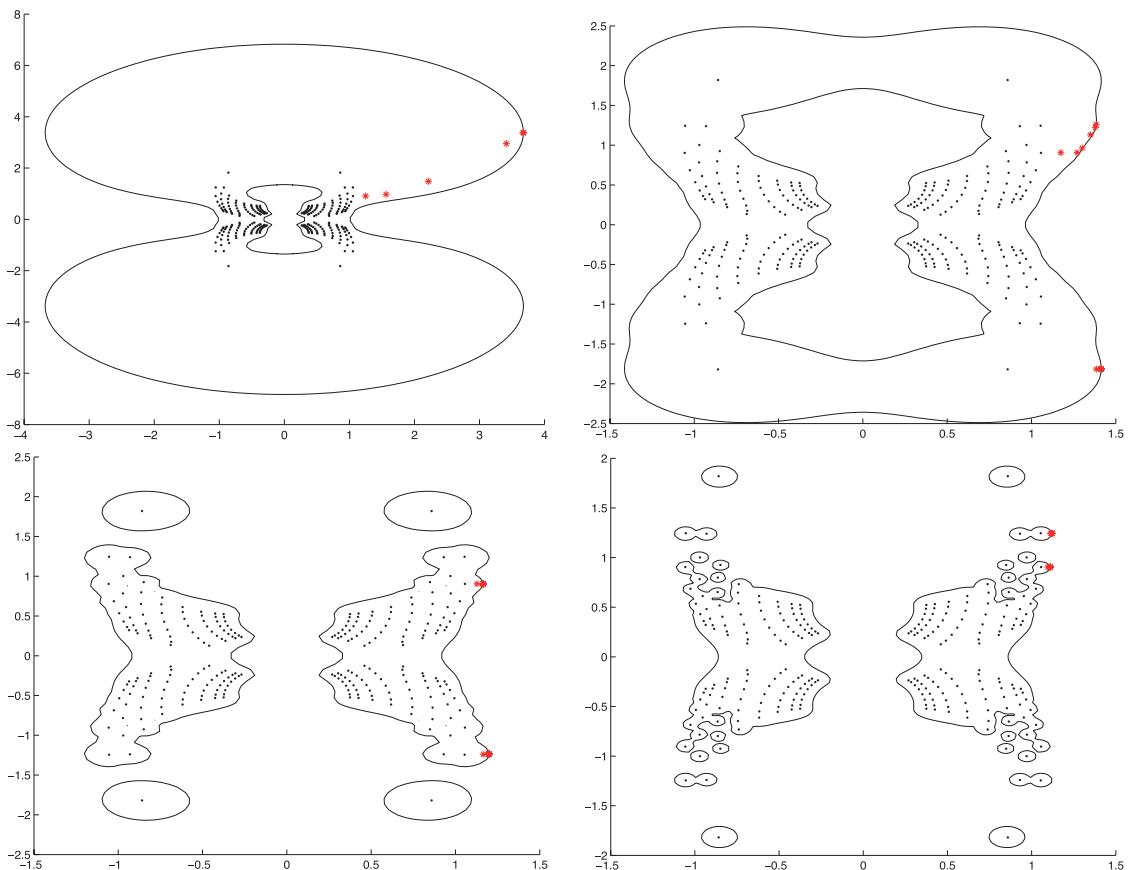


FIG. 4. The algorithm on the butterfly example with $\epsilon = 0.2$ is depicted for various choices of weights. The eigenvalues and the iterates are marked with dots and asterisks, respectively. The solid curve is the boundary of the ϵ -pseudospectrum. Weights are as follows: (**top left**) [1 1 1 1]; (**top right**) [1 1 1 ∞]; (**bottom left**) [1 1 1 $\infty \infty$]; (**bottom right**) [1 1 $\infty \infty \infty$].

TABLE 5 *Running time for Algorithm 4 in seconds on the two-dimensional acoustic wave equation with respect to the size of the quadratic matrix polynomial involved, and the computed pseudospectral abscissa*

Two-dimensional acoustic wave, $\epsilon = 0.01$	110	210	420
Running time	11	138	584
α_ϵ	4.99778	6.95044	$1.00718 \cdot 10^1$

The coefficient matrices D_0, D_1, D_2 are obtained by typing `randn(100) + 1.2*randn(100)*i, randn(100)` and `gallery('poisson', 10)` in MATLAB.² Thus D_0 and D_1 are complex and real

² The precise data is available on the web at <http://home.ku.edu.tr/~emengi/software/delay.mat>.

TABLE 6 *Running time for Algorithm 3 (without the vertical searches) in seconds on the two-dimensional acoustic wave equation with respect to the size of the quadratic matrix polynomial involved, the real part of the rightmost eigenvalue α , and computed pseudospectral abscissa α_ϵ*

Two-dimensional acoustic wave, $\epsilon = 0.0001$	1100	2100	4200
Running time	3	7	57
α	$3.50140 \cdot 10^2$	$6.68451 \cdot 10^2$	$1.33690 \cdot 10^3$
α_ϵ	$3.50631 \cdot 10^2$	$6.70238 \cdot 10^2$	$1.34408 \cdot 10^3$

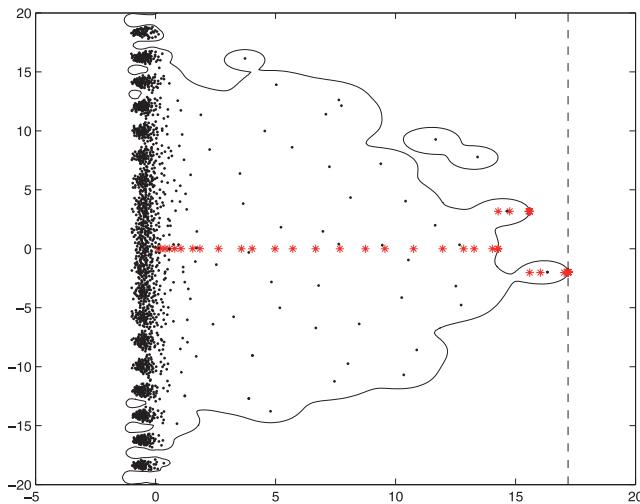


FIG. 5. The progress of the algorithm on delay example (6.1) for $\epsilon = 0.45$ is shown, when initiating at the origin. The iterates are marked with asterisks, the eigenvalues are indicated by dots, whereas the solid curve corresponds to the boundary of the ϵ -pseudospectrum. The dashed vertical line represents the points with real part equal to the computed ϵ -pseudospectral abscissa.

random matrices, respectively, whereas D_2 comes from the five-point finite difference discretization of the two-dimensional Poisson equation. For $\epsilon = 0.45$ the pseudospectrum $\Lambda_\epsilon(D)$ is shown in Fig. 5, for which the boundary is generated by calculating $\sigma_{\min}(D(z))/\|w(z)\|_1$ on a grid. The rightmost eigenvalue is given by $\lambda = 16.3300 - 1.9812i$. Initiating Algorithm 4 with this value, only one local search is needed to locate the globally rightmost point, leading to $\alpha_\epsilon(D) = 17.1899477706$.

A nice, didactic illustration of the interplay between the two components of Algorithm 4 (searching for a locally rightmost point and switching by vertical searches) is obtained by initializing the algorithm with the origin instead. Then the algorithm ends up at locally rightmost points twice; see Fig. 5. Each time this happens, a vertical search provides a better estimate strictly inside the ϵ -pseudospectrum and well away from the boundary. All together 53 subspace iterations are needed to retrieve the pseudospectral abscissa. The subspace dimension is never allowed to exceed 10; whenever the subspace dimension becomes 10, it is reset to a one-dimensional subspace based on the latest iterate. The algorithm concludes with convergence after an eventual vertical search, when it is found that the globally smallest value of

TABLE 7 *The number of iterations during the first and last vertical searches, as well as the total running time in seconds, with respect to γ for the delay example of Section 6.3*

γ	-4	-8	-16	-32	-100	-200
First vertical search	58	87	113	171	285	404
Last vertical search	46	72	103	144	244	342
Total running time (in seconds)	47.2	48.6	51.0	54.5	65.4	80.4

TABLE 8 *The number of iterations of a local search when the subspace dimension is nine, as well as the total running time in seconds, with respect to γ_h for the delay example*

γ_h	4×10^5	4×10^6	4×10^7	4×10^8
Number of iterations	330	1031	3200	8893
Total running time (in seconds)	47.2	55.8	113.7	154.9

$\sigma_{\min}[D(\alpha_*, \omega)] / \|w(\alpha_*, \omega)\|_1$ for fixed $\alpha_* = 17.1899477706$ over all ω does not differ from ϵ by more than $10^{-6}\|D_2\|_2$. The iterates of the subspace approach on this example after the first vertical search are listed on the right-hand side of Table 4, where we again observe a quadratic rate of convergence with respect to the subspace dimension. Note that by starting from an arbitrary point λ_0 satisfying $\sigma_{\min}[D(\lambda_0)] < \epsilon\|w(\lambda_0)\|_1$ does not by itself guarantee to find a globally rightmost point of the pseudospectrum, since, for instance, the possibility of the existence of an isolated component of the pseudospectrum to the right of the dashed line in Fig. 5 is not excluded. Such a situation is avoided by initiating the algorithm with the rightmost eigenvalue.

In this example, the global lower bound γ for the second derivatives of the singular value function minimized during the vertical searches is set equal to -4. As this lower bound is chosen smaller, the number of iterations required by the vertical searches to satisfy the prescribed error tolerance $10^{-6}\|D_2\|_2$ increases. But the increase in the number of iterations is typically sublinear with respect to γ . This is illustrated in Table 7 for the first and the last vertical searches for the particular delay example. The total running times in seconds with respect to γ are also listed in this table. The total running times increase even more slowly than the number of iterations during the vertical searches. This is due to the computations required by the other ingredients of the algorithm. For all the values of γ in the table, the retrieved values of the ϵ -pseudospectral abscissa are all the same up to at least prescribed accuracy.

The dependence of the number of iterations of a local search on the upper bound γ_h is also sublinear in our experience. This is demonstrated in Table 8, specifically for the delay example and for the local search performed with nine-dimensional subspace restrictions right before the first vertical search. The growth of the total running time with respect to γ_h also listed in the same table is again slower than the growth of the number of iterations. Employing Theorem 2.2, one can draw the conclusion that $\gamma_h = 4 \times 10^7$ leads to an analytical upper bound. However, the computed ϵ -pseudospectral abscissa for the values of γ_h used in the table are all the same up to at least prescribed accuracy. For a nonlinear eigenvalue problem, the bounds $\gamma = -4$ in vertical searches and $\gamma_h = 40000$ in local searches yield accurate results in our experiments on a wide range of examples.

7. Software

Algorithm 4 is implemented in MATLAB. This MATLAB software is available on the web publicly.³ For a nonpolynomial nonlinear eigenvalue problem, the user is expected to write down a routine calculating the functions $f_j(z)$ as in (1.2) and their first derivatives at a given $z \in \mathbb{C}$. The user must provide the name of this routine and a rightmost eigenvalue to the software as input parameters.

8. Conclusion

An algorithm is proposed for the computation of the ϵ -pseudospectral abscissa of an analytic matrix-valued function $F(\lambda)$ depending on one complex parameter. The algorithm is capable of handling large-scale problems. This is made possible by an adaptation of the subspace iteration (Kressner & Vandeheycken, 2014) for the nonlinear eigenvalue problem setting. Each subspace iteration involves the computation of the ϵ -pseudospectral abscissa when the domain of the map $v \mapsto F(\lambda)v$ is restricted to a small subspace. This computation is realized locally, but in a robust way against nonsmoothness, by adapting the support-based algorithm of Mengi (2016) for optimization subject to eigenvalue constraints. Repeated applications of the subspace iteration result in a point on the boundary of the ϵ -pseudospectrum with a vertical tangent line. Vertical searches are performed to check whether these converged points are globally rightmost in the ϵ -pseudospectrum. These vertical searches are realized by means of the support-based algorithm of Mengi *et al.* (2014), which determines the globally smallest value of a prescribed eigenvalue of a Hermitian and analytic matrix-valued function. They depend on the availability of a global lower bound γ for the second derivative of a certain singular value function. Assigning a large, negative value to γ works robustly in practice. A restarting strategy for the subspaces further enhances the efficiency of the algorithm.

The algorithm is both globally convergent and well suited for large-scale problems. The accompanying software that is publicly available aims for large-scale standard, polynomial and more general nonlinear eigenvalue problems.

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³ http://home.ku.edu.tr/~emengi/software/nonlinear_pseudoabscissa.

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