Differential Equations for Roaming Pseudospectra: Paths to Extremal Points and Boundary Tracking

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Abstract. When studying the $\varepsilon$-pseudospectrum of a matrix, one is often interested in computing the extremal points having maximum real part or modulus. This is a crucial step, for example, when computing the distance to instability of a stable system. Using the property that the pseudospectrum is determined via perturbations by rank-1 matrices, we derive differential equations on the manifold of normalized rank-1 matrices whose solutions tend to the critical rank-1 perturbations associated with the extremal points of (locally) maximum real part and modulus. This approach also allows us to track the boundary contour of the pseudospectrum in a neighborhood of the extremal points. The technique we propose is related to an idea recently developed by Guglielmi and Overton, who derived discrete dynamical systems instead of the continuous ones we present. The method turns out to be fast in comparison with those previously proposed in the literature and appears to be promising in dealing with large sparse problems.

Key words. Pseudospectrum, pseudospectral abscissa, pseudospectral radius, rank-1 perturbations, low-rank dynamics.

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1. Introduction. The pseudospectrum is an important tool for the study of a linear operator; for non-normal operators it gives substantially more information than the spectrum (for a full discussion we refer the reader to the monograph by Trefethen and Embree [20]). The analysis of the pseudospectrum has been considered in a large number of applications (for an extensive list see, e.g., [19]), many of them relevant to problems of differential equations. In fact for an operator $A$ the knowledge of the pseudospectrum - and in particular of its extremal points - is important when studying the growth or decay of $\|A^n\|$ with growing $n$ as well as $\|e^{tA}\|$ for all positive times $t$.

The numerical approximation of the pseudospectrum has received increasing attention in the last few years, and several authors have considered this problem. For $\varepsilon > 0$, the $\varepsilon$-pseudospectrum of a matrix $A$ is the set of the complex numbers that are eigenvalues of a perturbed matrix, for some perturbation of norm smaller than $\varepsilon$ (in this paper we always consider the spectral norm). Denoting by $s_{\text{min}}$ the smallest singular value of a matrix and exploiting the property that $z \in \mathbb{C}$ belongs to the $\varepsilon$-pseudospectrum of a matrix $A$ if and only if $s_{\text{min}}(A - z I) \leq \varepsilon$ (where $I$ denotes the identity matrix), the most natural approach for computing the $\varepsilon$-pseudospectrum numerically is based on a repeated computation of the singular value decomposition of a collection of matrices associated with a chosen grid $\{z_k\}$ in the complex plane. The drawback of this approach is the computational cost which for large matrices makes this method unfeasible. Moreover, in many cases a complete computation of the pseudospectrum is not necessary and one is mainly interested in small subregions or even in single points of the pseudospectrum, typically, those with maximum real part or modulus.

Although several methods have been proposed for an efficient computation of the pseudospectrum, only a few of them have been focused on the computation of either

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restricted subregions or extremal points of the set. The computation of these points allows one, for example, to determine the robustness of a stable linear dynamical system subject to unstructured perturbations, which we shall quantify in Section 2.1, as well as the distance to instability of a stable system, which is an important indicator in systems theory and automatic control (see, e.g., [3, 7]).

In this paper we focus our attention on the computation of these extremal points and on the task of computing the boundary of the pseudospectrum in the neighbourhood of such points.

Let us first recall what methods have been proposed in the literature. A direct approach to compute these points is that of approximating the boundary of the pseudospectrum by a curve-tracing method computing the \( \varepsilon \)-level set of the function \( s_{\min}(A - z I) \). This is computationally demanding and does not provide any selection of a priori interesting regions. A more efficient approach is the one proposed by Burke, Lewis and Overton [2], which makes use of a so-called criss-cross algorithm to compute the points with maximal real part of the \( \varepsilon \)-pseudospectrum. This quadratically convergent iterative method, which alternates vertical and horizontal searches of boundary points of the pseudospectrum, is closely connected with an idea by Byers [3], which allows one to characterize points lying on the boundary of the pseudospectrum through an eigenvalue problem for a Hamiltonian matrix. These ideas have been further developed by Mengi and Overton [15] in order to adapt the criss-cross method to the computation of points with maximal modulus. Both algorithms have been implemented in EigTool [22]. They require the computation of several singular value decompositions; as a consequence they are suitable for dealing with matrices of moderate dimension (up to 1000, say). For problems of larger size they require too much computing time.

For this reason we are interested in finding methods that are able to work efficiently for large problems, possibly exploiting the sparsity of the matrix. Using the fact that for the computation of the pseudospectrum one can restrict the perturbations to be of rank one, recently Guglielmi and Overton [5] have proposed an iterative method which produces a sequence of rank-1 matrices \( \{E_k\} \) with \( \|E_k\| = 1 \) such that the real part (or modulus) of the leading eigenvalue \( \lambda_k \) of \( A + \varepsilon E_k \) converges - in most cases - to the pseudospectral abscissa (or radius). The sequence corresponds to the trajectory of a discrete dynamical system, whose analysis presents theoretical difficulties (in particular the local convergence to extremal points). The algorithm is fast since it basically requires at every step the computation of the leading left and right eigenvectors of the matrix \( A + \varepsilon E_k \), which can be computed efficiently by the power method or some variants (see, e.g., [12, 14]).

In this paper we extend the key idea in [5] of working with sequences of rank-1 matrices by considering a continuous dynamical system whose trajectories converge - at least locally - to the extremal points of the pseudospectrum. The behavior of the resulting method after discretization of the differential equation is very similar to that of the discrete method by Guglielmi and Overton, but the theoretical analysis turns out to be simpler. Both approaches explicitly provide rank-1 perturbations associated with the extremal points of the pseudospectrum. An additional property of the method we propose here is that it allows us to follow the contour of the pseudospectrum close to points with extremal abscissa or radius, providing in this way a zoom on the most interesting parts.

The paper is organized as follows. In Section 2 we recall the definition of the pseudospectrum of a matrix and introduce the quantities we are interested in, the
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pseudospectral abscissa and the pseudospectral radius. In Section 3 we describe the
algorithm developed by Guglielmi and Overton [5], whose discrete nature is opposed
to the continuous character of the method we propose. In Section 4 we present the
ordinary differential equations that lead to the pseudospectral abscissa. This is a dif-
ferential equation for rank-1 matrices $E(t) = u(t)v(t)^*$ of unit norm, or equivalently
a coupled pair of differential equations for unit vectors $u(t)$ and $v(t)$, constructed
such that the real part of the eigenvalue $\lambda(t)$ of largest real part of $A + \varepsilon E(t)$ grows
with $t$. When the dynamics runs into a stationary point such that the corresponding
stationary eigenvalue of $A + \varepsilon E$ lies on the boundary of the pseudospectrum, then it
is at a local maximum of the real part. In Section 5 we explain how to escape from
internal stationary points. In Section 6 we present an exponential Euler method for
the numerical integration of the differential equations. In Section 7 we show modified
differential equations which lead in a straight line to the boundary of the pseudospec-
trum. In Section 8 we show that starting from the boundary of the pseudospectrum,
the dynamics follows the boundary contour. Subsequently in Section 9, we show how
finally we conclude with a section illustrating the behavior of the method on some
examples.

2. Pseudospectral abscissa and radius. In this section we describe the basic
framework of the paper.

2.1. Pseudospectrum of a matrix. Let $A \in \mathbb{C}^{n \times n}$ be a square matrix, where
the interest is in non-normal matrices. The spectrum $\sigma(A)$ is the set of eigenvalues
of $A$. The $\varepsilon$-pseudospectrum $\sigma_\varepsilon(A)$ admits the following characterizations [20] (here $\| \cdot \| = \| \cdot \|_2$ is the spectral norm and $s_{\text{min}}$ refers to the smallest singular value):

$$
\lambda \in \sigma_\varepsilon(A) \iff \| (A - \lambda I)^{-1} \| \geq \varepsilon^{-1}
$$
$$
\iff s_{\text{min}}(A - \lambda I) \leq \varepsilon
$$
$$
\iff \lambda \in \sigma(A + \varepsilon E) \text{ for some } E \in \mathbb{C}^{n \times n} \text{ of norm } \leq 1
$$
$$
\iff \lambda \in \sigma(A + \varepsilon E) \text{ for some rank-1 matrix } E \in \mathbb{C}^{n \times n} \text{ of norm } \leq 1.
$$

The last characterization has first been noted and used in [17]. It will be of major
importance for the approach of this paper. It is obtained readily from the second
characterization by noting that if $\eta \leq \varepsilon$ is a singular value of $A - \lambda I$ and $u$ and $v$
are corresponding left and right singular vectors, then the matrix $A - \lambda I - \eta uv^*$ has a
singular value 0, that is, $\lambda$ is an eigenvalue of $A - \eta uv^*$.

We further note that the boundary $\partial \sigma_\varepsilon(A)$ of the $\varepsilon$-pseudospectrum is charac-
terized by the condition $s_{\text{min}}(A - \lambda I) = \varepsilon$. This is clearly a subset of the union of
the level sets $\Gamma_k(\varepsilon) = \{ \mu \in \mathbb{C} : s_k(A - \mu I) = \varepsilon \}$ for $k = 1, \ldots, n$, where $s_k$
refers to the $k$th singular value. The $\varepsilon$-level sets for the non-minimal singular values are either
empty or unions of curves in the interior of the $\varepsilon$-pseudospectrum.

2.2. Pseudospectral abscissa and radius. The $\varepsilon$-pseudospectral abscissa of
$A$ is the real part of the rightmost point in the $\varepsilon$-pseudospectrum:

$$
\alpha_\varepsilon(A) = \max_{\lambda \in \sigma_\varepsilon(A)} \Re \lambda.
$$

The $\varepsilon$-pseudospectral radius is

$$
\rho_\varepsilon(A) = \max_{\lambda \in \sigma_\varepsilon(A)} |\lambda|.
$$
The pseudospectral abscissa and radius are of interest in bounding the matrix exponential $e^{tA}$ or matrix powers $A^n$ of the matrix $A$ or of perturbations of $A$. For example, there is the following obvious, but important robust stability result from the third characterization of the $\varepsilon$-pseudospectrum: If $\alpha_\varepsilon(A) < 0$, then
\[ e^{t(A+\varepsilon E)} \to 0 \quad \text{as} \quad t \to +\infty \quad \text{for every } E \text{ of norm } \leq 1. \]

If $\rho_\varepsilon(A) < 1$, then
\[ (A + \varepsilon E)^n \to 0 \quad \text{as} \quad n \to +\infty \quad \text{for every } E \text{ of norm } \leq 1. \]

Using the Kreiss matrix theorem \cite{10, 20} and the first characterization of the pseudospectrum, one obtains bounds of $e^{tA}$ for all $t \geq 0$ in terms of the pseudospectral abscissa, and of $A^n$ for all positive integers $n$ in terms of the pseudospectral radius. Furthermore, with Laplace transforms and the Plancherel formula one obtains the spectrum, one obtains bounds of $e^{tA}$ for all $t \geq 0$ in terms of the pseudospectral abscissa, and of $A^n$ for all positive integers $n$ in terms of the pseudospectral radius.

3. Guglielmi and Overton’s iterative algorithm. Very recently, Guglielmi and Overton \cite{5} proposed an iterative algorithm for computing the pseudospectral abscissa and radius. The standard algorithm for computing the pseudospectral abscissa is the criss-cross algorithm of Burke, Lewis and Overton \cite{2}. It is a robust iterative algorithm that is globally convergent, but it is computationally expensive, requiring many eigenvalue and singular value decompositions of $2n \times 2n$ and $n \times n$ matrices, respectively. There is also a variant of this algorithm for the computation of the pseudospectral radius \cite{15}.

Initialize: Let $x_0$ and $y_0$ be left and right eigenvectors, respectively, for the rightmost eigenvalue of $A$, both normalized to unit norm and with $x_0^*y_0 > 0$.

Iterate: for $k = 1, 2, \ldots$, let $x_k, y_k$ be left and right eigenvectors, respectively, for the rightmost eigenvalue $\lambda_k$ of $A + \varepsilon x_{k-1}^*y_{k-1}$, of unit norm with $x_k^*y_k > 0$.

The expectation for this strikingly simple algorithm is that $\lambda_k$ converges to a $\lambda_*$ with $\text{Re } \lambda_* = \alpha_\varepsilon(A)$. The algorithm works very well and fast in practice, requiring at each iteration only the rightmost eigenvalue of $A + \varepsilon x_{k-1}^*y_{k-1}$, which can be computed at small computational cost for large sparse matrices $A$; see, e.g., \cite{12, 13, 14}. It turns out, however, that the algorithm is difficult to analyze.

An illustration is given in Fig. 3 for the randomly chosen $6 \times 6$ matrix
\[ A = \begin{pmatrix}
0.1019 & -0.8350 & 0.2966 & -0.0756 & -2.2079 & 1.2682 \\
1.1813 & -1.4224 & -0.8664 & 0.8003 & -1.3413 & 1.3547 \\
-1.2457 & -0.1737 & -1.1910 & -0.3194 & -0.2909 & 0.8230 \\
-0.7830 & -0.5115 & -0.0109 & 0.8860 & 0.4878 & 0.3246 \\
-0.5740 & 0.0268 & 1.1950 & -0.1729 & 0.9966 & -0.8003 \\
-0.3815 & -0.4476 & -0.9740 & 1.4030 & 1.0361 & 0.7399
\end{pmatrix}. \quad (3.1) \]
The closed curves drawn with different colours in Fig. 3 (and also in the subsequent ones) represent the level sets of the function \( f(z) = s_{\min}(A - zI) = \varepsilon \) for different values \( \varepsilon = 10^\kappa \), where the exponents \( \kappa \) which correspond to different colours are shown in the colour bar on the right. The black points are the eigenvalues of the considered unperturbed matrix.

Guglielmi and Overton’s algorithm is an iterative algorithm on the manifold of normalized rank-1 matrices \( M = \{ E \in \mathbb{C}^{n \times n} : \text{rank}(E) = 1, \|E\| = 1 \} \), producing a sequence of rank-1 perturbations to \( A \),

\[ E_0 \rightarrow E_1 \rightarrow E_2 \rightarrow E_3 \rightarrow \ldots \]

The present paper originated from the following question: *Can we find a continuous path \( E(t) \) on \( M \) such that the real part of an eigenvalue of \( A + \varepsilon E(t) \) tends to the pseudospectral abscissa \( \alpha_\varepsilon(A) \) as \( t \rightarrow \infty \)?* There are a number of cases in numerical analysis where considering a continuous counterpart to an iterative algorithm yields new insight or improved algorithms. The reader might recall, for example, the Newton path motivating the damped Newton method for finding zeros of a function, the gradient flow for minimization problems, or the QR isospectral flow interpolating the iterates of the QR algorithm; see, e.g., [1, 4, 6] and the early paper [18].

### 4. A differential equation leading to the pseudospectral abscissa.

In this section we present the continuous dynamical system on the manifold of normalized rank-1 matrices that produces paths to points with locally maximal real part in the pseudospectrum, and we study its properties. A main feature of the dynamics is the monotonicity of the real part of the rightmost eigenvalue of \( A + \varepsilon E(t) \) along the flow.

#### 4.1. A tangent space projection.

We work on the manifold of normalized rank-1 matrices,

\[ M = \{ uv^* : u, v \in \mathbb{C}^n, \|u\| = \|v\| = 1 \} \]

\[ = \{ E \in \mathbb{C}^{n \times n} : \text{rank}(E) = 1, \|E\| = 1 \}. \quad (4.1) \]

We note that the representation of \( E \in M \) as \( E = uv^* \) is not unique: replacing \( u \rightarrow e^{i\varphi}u, \ v \rightarrow e^{i\varphi}v \) does not change \( E \). Moreover, we can equivalently write the manifold as \( M = \{ uv^* : u, v \in \mathbb{C}^n, \|u\|^2 \|v\|^2 = 1 \} \). With this observation, the tangent space at \( E = uv^* \) is characterized as

\[ T_E M = \{ \delta u v^* + u \delta v^* : \delta u, \delta v \in \mathbb{C}^n, \ \text{Re}(u^* \delta u + v^* \delta v) = 0 \}. \]
An essential ingredient in our construction of a differential equation on $\mathcal{M}$ leading to the pseudospectral abscissa is the following oblique projection onto $T_E\mathcal{M}$.

**Lemma 4.1.** Let $E = uv^* \in \mathcal{M}$. For $Z \in \mathbb{C}^{n \times n}$, set

$$P_E(Z) = i \operatorname{Im}(u^*Zv)uv^* + (I - uu^*)Zv^* + uu^*Z(I - vv^*).$$

Then, $P_E$ is a projection of $\mathbb{C}^{n \times n}$ onto the tangent space $T_E\mathcal{M}$.

**Proof.** Rewriting

$$P_E(Z) = \left( \frac{i}{2} \operatorname{Im}(u^*Zv)u + (I - uu^*)Zv \right)v^* + u\left( \frac{i}{2} \operatorname{Im}(v^*Z^*u)v + (I - vv^*)Z^*u \right),$$

we see that $P_E(Z) \in T_E\mathcal{M}$, since $\operatorname{Re}(u^*\delta u + v^*\delta v) = 0$.

On the other hand, if $Z = \delta u v^* + u \delta v^* \in T_E\mathcal{M}$ for some $\delta u, \delta v \in \mathbb{C}^n$ with $\operatorname{Re}(u^*\delta u + v^*\delta v) = 0$, then $u^*Zv = u^*\delta u + \delta v^*v$ and hence $\operatorname{Re}(u^*Zv) = 0$, so that $i \operatorname{Im}(u^*Zv) = u^*Zv$. It then follows that

$$P_E(Z) = uu^*Zv^* + (I - uu^*)Zv^* + uu^*Z(I - vv^*)$$

$$= uu^*\delta u v^* + u \delta v^*v^* + (I - uu^*)\delta uv^* + u \delta v^*(I - vv^*)$$

$$= \delta u v^* + u \delta v^* = Z,$$

and hence $P_E$ is a projection onto $T_E\mathcal{M}$. □

**4.2. A differential equation on $\mathcal{M}$.** We consider the differential equation for $E(t) = u(t)v^*(t)$, $t \geq 0$,

$$\dot{E} = P_E(xy^*),$$

(4.3)

where $x$ and $y$ are left and right eigenvectors, respectively, to the rightmost eigenvalue $\lambda$ of $A + \varepsilon E$, both of unit norm and with $x^*y > 0$. This equation on $\mathcal{M}$ can be translated into differential equations for $u, v$ in $E = uv^*$ (compare with (4.2)):

$$\dot{u} = \frac{i}{2} \operatorname{Im}(u^*x y^*v)u + (I - uu^*)xy^*v$$

$$\dot{v} = \frac{i}{2} \operatorname{Im}(v^*y x^*u)v + (I - vv^*)yx^*u.$$

(4.4)
In Fig. 4.2 we plot, for the matrix $A$ of (3.1) and several values of $\varepsilon$, the rightmost eigenvalue $\lambda(t)$ of the matrix $A + \varepsilon E(t)$, where $E(t) = u(t)v(t)^*$ follows the differential equation (4.3) or equivalently (4.4). We observe that $\lambda(t)$ tends to a point on the boundary of the $\varepsilon$-pseudospectrum that has maximal abscissa. We now explain this behavior.

4.3. Growing real part of the rightmost eigenvalue. As the following result shows, the real part of $\lambda(t)$ increases monotonically.

**Theorem 4.2.** Let $E(t)$ satisfy the differential equation (4.3). If $\lambda(t)$ is a simple eigenvalue of $A + \varepsilon E(t)$, then

\[ \Re \dot{\lambda}(t) \geq 0. \]

**Proof.** The standard perturbation theory of eigenvalues (see, e.g., [9, 21]) shows that

\[ \dot{\lambda} = \frac{x^* d}{d\varepsilon} (A + \varepsilon E) y}{x^* y} = \varepsilon \frac{x^* E y}{x^* y} = \varepsilon \frac{x^* P_E(xy^*) y}{x^* y}. \]  

(4.5)

We calculate, for $E = uv^*$ and with $\alpha = u^*x$, $\beta = v^*y$,

\[ x^* P_E(xy^*) y = \pi \beta \cdot i \Im (\alpha \overline{\beta}) + |\alpha|^2 \cdot \|y - \beta v\|^2 + |\beta|^2 \cdot \|x - \alpha u\|^2 \]

(4.6)

and hence

\[ \Re \left( x^* P_E(xy^*) y \right) = (\Im (\pi \beta))^2 + |\alpha|^2 \cdot \|y - \beta v\|^2 + |\beta|^2 \cdot \|x - \alpha u\|^2 \geq 0. \]

(4.7)

Since $\varepsilon > 0$ and $x^* y > 0$, this yields $\Re \dot{\lambda} \geq 0$. □

4.4. Stationary points. The boundary of the $\varepsilon$-pseudospectrum is characterized as the set of complex $\lambda$ for which $s_{\min}(A - \lambda I) = \varepsilon$. At the pseudospectral abscissa the tangent to this boundary is vertical. Boundary points with vertical tangent are among the stationary points of the motion of the eigenvalue $\lambda(t)$ driven by the differential equation (4.3), but there may be further stationary points.

We characterize the stationary points as follows. We assume again that $\lambda$ is a simple eigenvalue of $A + \varepsilon uv^*$ with left and right eigenvectors $x$ and $y$, of unit norm with $x^* y > 0$.

**Theorem 4.3.** $\Re \dot{\lambda} = 0$ holds if and only if one of the following two situations is met:

1. For some $k$, the $k$th singular value of $A - \lambda I$ equals $\varepsilon$ with singular vectors $u$ and $v$, and the level contour $\Gamma_k(\varepsilon) = \{ \mu \in \mathbb{C} : s_k(A - \mu I) = \varepsilon \}$ has a vertical tangent at $\mu = \lambda$.
2. The left and right eigenvectors $x$ and $y$ of $A + \varepsilon uv^*$ to the eigenvalue $\lambda$ are orthogonal to $u$ and $v$, respectively. In this case they are also eigenvectors of $A$ to the same eigenvalue $\lambda$.

Moreover, if $\Re \dot{\lambda} = 0$, then $E = uv^*$ is a stationary point of the differential equation (4.3).

**Proof.** From (4.5) and (4.7) we see that $\Re \dot{\lambda} = 0$ only in two cases:

1. $x = \alpha u$, $y = \beta v$, $\beta = \pm \alpha$
2. $\alpha = \beta = 0$. 

\((\text{Note that we cannot have } \alpha = 0 \text{ and } x = \alpha u, \text{ since } x \neq 0. \text{ If } x = \alpha u \text{ and } y = \beta v, \text{ then } |\alpha| = |\beta| = 1, \text{ and therefore } \text{Im}(\alpha \beta) = 0 \text{ implies } \beta = \pm \alpha.\)\)

In the second case we see that \(x, y\) are actually left and right eigenvectors of \(A\) with eigenvalue \(\lambda\). The first case is more interesting. Here we have \(|\alpha| = |\beta| = 1\) and

\[
(\mathbf{A} + \varepsilon \mathbf{u} \mathbf{v}^\ast) \mathbf{v} = \lambda \mathbf{v} \tag{4.8}
\]
\[
\mathbf{u}^\ast (\mathbf{A} + \varepsilon \mathbf{u} \mathbf{v}^\ast) = \lambda \mathbf{u}^\ast \tag{4.9}
\]
or equivalently

\[
\begin{pmatrix} -\varepsilon \\ -\mathbf{v} \end{pmatrix} = \lambda \begin{pmatrix} -\mathbf{u} \\ -\mathbf{v} \end{pmatrix}.
\tag{4.10}
\]

which states that \(A - \lambda I\) has the singular value \(\varepsilon\), with left and right singular vectors \(-\mathbf{u} \) and \(\mathbf{v} \), respectively.

For any parametrization \(\mu(\theta)\) of the level contour \(\Gamma_k(\varepsilon)\) with \(\mu(0) = \lambda\), we have \(s_k(A - \mu(\theta) I) = \varepsilon\). If this is a simple singular value, then we obtain (with \(\prime = d/d\theta\))

\[
0 = \left. \frac{d}{d\theta} s_k(A - \mu(\theta) I) \right|_{\theta = 0} = \frac{(-\mathbf{u}^\ast \mathbf{v}^\ast) \begin{pmatrix} 0 & -\mu'(0) I \\ -\mu'(0) I & 0 \end{pmatrix} \begin{pmatrix} -\mathbf{u}^\ast \\ -\mathbf{v}^\ast \end{pmatrix}}{\mathbf{u}^\ast \mathbf{u} + \mathbf{v}^\ast \mathbf{v}}
\]

\[
= \text{Re} (\mu'(0) \mathbf{u}^\ast \mathbf{v}) = \text{Re} (\mu'(0) \alpha \beta) x^* y.
\]

With \(\alpha = \pm \beta\), this requires \(\text{Re} (\mu'(0)) = 0\), i.e., \(\Gamma_k(\varepsilon)\) has a vertical tangent at \(\lambda\).

Finally, in both cases 1. and 2. we calculate \(P_E(xy^*) = 0\), so that \(E\) is a stationary point of (4.3). \(\square\)

### 4.5. Special cases

We consider the behavior of solutions to the differential equations (4.4) in two particular cases, the case where \(A\) is normal and the case where \(A\) is non-negative. We have the following results for arbitrary \(\varepsilon > 0\).

**Theorem 4.4.**

(a) If \(A\) is normal and \(u(0) = v(0)\) is the (left and right) eigenvector of \(A\) to the eigenvalue \(\lambda_0\) of largest real part, then the solution of (4.3) satisfies \(u(t) = u(0)\) and \(v(t) = v(0)\) for all \(t\).

(b) If \(A\) has non-negative entries and \(u(0)\) and \(v(0)\) are the non-negative left and right leading eigenvectors of \(A\), then the entries of the solution \(u(t)\) and \(v(t)\) of (4.4) are real and non-negative for all \(t\).

**Proof.** (a) We note that \(A + \varepsilon u(0) u(0)^\ast\) is normal with eigenvector \(u(0)\). It is then checked directly that \(u(t) = v(t) = u(0)\) solves (4.4) with initial values \(u(0) = v(0)\).

(b) We first show the result when “non-negative” is everywhere replaced by “positive” in the statement. By the Perron-Frobenius theorem, we then have \(u(0) > 0\) and \(v(0) > 0\) with componentwise inequalities. Let \(t^* = \sup \{t : u(t) > 0, v(t) > 0\}\). We will show that \(t^* = +\infty\). For \(t < t^*\), all entries of the matrix \(A + \varepsilon u(t) v(t)^\ast\) are positive, and by the Perron-Frobenius theorem its leading left and right eigenvectors are real and satisfy \(x(t) > 0\) and \(y(t) > 0\). With \(\alpha = u^\ast x > 0, \beta = v^\ast y > 0\) and \(\omega = \alpha \beta\), the differential equations (4.4) read

\[
\dot{u} = \beta x - \omega u
\]
\[
\dot{v} = \alpha y - \omega v.
\]
Setting $\Omega(t) = \int_0^t \omega(s) \, ds$, we therefore obtain

$$u(t) = e^{-\Omega(t)} u(0) + \int_0^t e^{-(\Omega(t)-\Omega(s))} \beta(s) \, x(s) \, ds$$

and the analogous formula for $v(t)$. For all $t < t^*$ we thus have $u(t) \geq e^{-\Omega(t)} u(0)$ with $u(0) > 0$ and similarly for $v(t)$. In view of the definition of $t^*$, this contradicts a finite $t^*$. Hence, $t^* = +\infty$. Finally, the “non-negative” version of the result follows from the “positive” version by a continuity argument. \[ \square \]

We note the following for the rightmost eigenvalue $\lambda(t)$ of $A + \varepsilon u(t) v(t)^*$: in case (a) $\lambda(t) = \lambda_0 + \varepsilon$ for all $t$ (with $\lambda_0$ the rightmost eigenvalue of $A$) and hence $\text{Re} \, \lambda(t)$ equals the $\varepsilon$-pseudospectral abscissa for all $t$, and in case (b) the rightmost eigenvalue $\lambda(t)$ of the non-negative matrix $A + \varepsilon u(t) v(t)^*$ is real and non-negative for all $t$.

5. Escaping from interior stationary points. A point in the $\varepsilon$-pseudospectrum with maximal real part corresponds to a stationary point of the differential equation (4.3), as is every point with vertical tangent. According to Theorem 4.3, however, stationary points are not necessarily on the boundary of the $\varepsilon$-pseudospectrum, since at such points only some singular value of $A - \lambda I$, not necessarily the smallest one, equals $\varepsilon$. Our numerical experiments indicate, however, that the stationary points in the interior of the $\varepsilon$-pseudospectrum are unstable. A heuristic explanation is that by a perturbation we may increase the real part of $\lambda$, and then it must increase further along the trajectory of the differential equation. It appears delicate, however, to make this argument rigorous. As an alternative to relying on the instability of interior stationary points we now propose a simple strategy to avoid getting trapped at such points.

Theorem 4.3 does not guarantee that $\lambda(t)$ tends to a point on $\partial \sigma_{\varepsilon}(A)$ with a local maximum of the real part, but it might instead tend to a stationary point $\lambda_0$ with $\eta := s_{\min}(A - \lambda_0 I) < s_k(A - \lambda_0 I) = \varepsilon$ for some $k$. Let $u_0, v_0$ be the singular vectors corresponding to the minimal singular value $\eta$. Then, $\lambda_0$ is an eigenvalue of $A + \eta E_0$ with $E_0 = u_0 v_0^*$. The idea is now to consider the rightmost eigenvalue $\lambda(t)$ of $A + \zeta(t) E_0$, where $\zeta(0) = \eta$ and

$$\dot{\zeta} = \frac{x^* y}{x^* E_0 y}$$

with $x$ and $y$ the left and right eigenvectors to the eigenvalue $\lambda$ of $A + \zeta E_0$, of unit norm with $x^* y > 0$. Note that by condition 1 of Theorem 4.3, $x(0)$ and $y(0)$ are multiples of $u_0$ and $v_0$, respectively, so that at $t = 0$ the denominator has absolute value 1. We then have, provided that $\lambda(t)$ remains a simple eigenvalue,

$$\dot{\lambda} = \frac{x^* \frac{d}{ds} (A + \zeta(t) E_0) y}{x^* y} = \dot{\zeta} \frac{x^* E_0 y}{x^* y} = 1,$$

continued until a time $t_1$ at which $|\zeta(t_1)| = \varepsilon$ (which exists apart from exceptional situations where a singularity is hit in (5.1)). We then restart the differential equation (4.3) from $A + \zeta(t_1) E_0$, with $\text{Re} \, \lambda(t_1) > \text{Re} \, \lambda_0$.

6. Discretizing the differential equation. In computing the spectral abscissa using a numerical solution of the differential equation (4.3), it is not important to follow accurately a trajectory of the differential equation, but to increase the real part of the rightmost eigenvalue of $A + \varepsilon E$ in every time step. A possible approach,
which we present here, is to apply a projected exponential Euler method \[8\] together with a stepsize selection strategy based on a line search.

We first describe an exponential Euler method for (4.4), starting from \(u_n, v_n\). We denote by \(x_n, y_n\) the left and right eigenvectors to the rightmost eigenvalue \(\lambda_n\) of \(A + \varepsilon u_n v_n^*\), and we set \(\alpha_n = u_n^* x_n\), \(\beta_n = v_n^* y_n\), and \(\gamma_n = \frac{1}{2} \text{Im}(\alpha_n \beta_n^*)\). With the function \(\varphi(z) = (e^z - 1)/z\) (and \(\varphi(0) = 1\)), a step with stepsize \(h\) then reads

\[
\begin{align*}
\tilde{u}(h) &= e^{i\gamma_n h} u_n + h \varphi(i\gamma_n h) \overline{\beta_n}(x_n - \alpha_n u_n) \\
\tilde{v}(h) &= e^{-i\gamma_n h} v_n + h \varphi(-i\gamma_n h) \overline{\alpha_n}(y_n - \beta_n v_n),
\end{align*}
\]

(6.1)

and we normalize

\[
\tilde{u}(h) = \frac{\tilde{u}(h)}{\|\tilde{u}(h)\|}, \quad \tilde{v}(h) = \frac{\tilde{v}(h)}{\|\tilde{v}(h)\|}.
\]

The motivation for choosing this method is that near a stationary point, the motion is nearly vertical and close to the boundary of the pseudospectrum, where \(x = \alpha u\) and \(y = \beta v\). The dominating term driving the motion is then the first term on the right-hand side of (4.4), which is integrated out exactly in this scheme. Moreover, this scheme preserves stationary points.

The stepsize \(h\) can, for example, be selected by the following algorithm.

1. initialize the stepsize by the previous stepsize, \(h = h_{n-1}\)
2. compute the rightmost eigenvalue \(\tilde{\lambda}(h)\) of \(A + \varepsilon \tilde{u}(h) \tilde{v}(h)^*\)
3. if \(\text{Re} \tilde{\lambda}(h) \leq \text{Re} \lambda_n\), then halve the stepsize, \(h := h/2\), and repeat from 2.
4. else if \(h = h_{n-1}\), then compute \(\tilde{\lambda}(2h)\) and if \(\text{Re} \tilde{\lambda}(2h) \leq \text{Re} \tilde{\lambda}(2h)\), then double the stepsize, \(h := 2h\)
5. set \(h_n = h\), \(\lambda_n = \tilde{\lambda}(h)\), and determine the starting values for the next step as \(u_{n+1} = \tilde{u}(h), \; v_{n+1} = \tilde{v}(h)\).

This algorithm requires in each step two computations of rightmost eigenvalues and associated eigenvectors of rank-1 perturbations to the matrix \(A\), which can be computed at relatively small computational cost for large sparse matrices \(A\), combining the Cayley transformation approach of \([13, 14]\) with the Sherman-Morrison formula or using an implicitly restarted Arnoldi method as implemented in ARPACK \([12]\) and used in the MATLAB function \(eigs\).

In implementing this algorithm we encountered the difficulty that very close to the stationary points the method often exhibits small oscillations in the imaginary part of the leading eigenvalue, which is not controlled by the above algorithm. This undesired feature can be avoided by restricting the stepsize such that the recursion becomes stable. We require

\[
|e^{i\gamma_n h} - \varphi(i\gamma_n h) \alpha_n \overline{\beta}_n| \leq 1 + \delta
\]

with a moderately small parameter \(\delta\), e.g., \(\delta = 0.1\).

7. Going horizontally to the boundary of the pseudospectrum. We consider the projection into a subspace of \(T_E M\),

\[
\tilde{P}_E(Z) = (I - uu^*) Z vv^* + uu^* Z (I - vv^*),
\]

(7.1)

and instead of (4.3) the differential equation

\[
\dot{E} = \tilde{P}_E(xy^*),
\]

(7.2)
where again $x, y$ with $x^*y > 0$ are left and right eigenvectors, respectively, to the rightmost eigenvalue $\lambda$ of $A + \epsilon E$. This leads to horizontal motion of $\lambda$ to the right.

**Theorem 7.1.** Let $E(t)$ satisfy the differential equation (7.2). If $\lambda(t)$ is a simple eigenvalue of $A + \epsilon E(t)$, then $\dot{\lambda}(t)$ is real and non-negative.

**Proof.** We have (cf. (4.6))

$$\dot{\lambda} = \epsilon \frac{x^*y}{x^*y} \left( |\alpha|^2 \cdot \|y - \beta v\|^2 + |\beta|^2 \cdot \|x - \alpha u\|^2 \right) \in \mathbb{R}, \geq 0,$$  \hspace{1cm} (7.3)

which gives the result. □

Observe that if we apply (7.2) to the rotated matrix $e^{i\theta} A$, we obtain a motion along any given ray $\lambda(t) \in \{ \lambda(0) + e^{-i\theta} r, r > 0 \}$.

By the argument of the proof of Theorem 4.3, this motion becomes stationary when a singular value of $A - \lambda I$ equals $\epsilon$, which holds in particular, but not necessarily at the boundary $\partial \sigma_\epsilon(A)$. To avoid getting stuck at an interior level contour $\Gamma_k(\epsilon)$, we can proceed as in the previous section.

We note the following consequence of (7.3) for boundary points of the $\epsilon$-pseudospectrum. It shows that generically for $\lambda \in \partial \sigma_\epsilon(A)$, there is a unique rank-1 matrix $E$ of unit norm such that $\lambda$ is an eigenvalue of $A + \epsilon E$.

**Lemma 7.2.** Let $\lambda \in \partial \sigma_\epsilon(A)$, and let $u, v \in \mathbb{C}^n$ of unit norm be such that $\lambda$ is a simple eigenvalue of $A + \epsilon uv^*$. Then $-u$ and $v$ are left and right eigenvectors of $A + \epsilon uv^*$, and are left and right singular vectors of $A - \lambda I$. Therefore, $uv^*$ is uniquely determined if $\epsilon$ is a simple singular value of $A - \lambda I$.

**Proof.** Without loss of generality we may assume that $\sigma_\epsilon(A)$ lies locally to the left of a curve passing through $\lambda$ with a non-horizontal tangent. (Otherwise we rotate $A \to e^{i\theta} A$.) Then, the solution of the differential equation (7.2) starting from $E(0) = uv^*$ must have $\dot{\lambda} = 0$, which by (7.3) implies $x = \alpha u$ and $y = \beta v$, so that $-u$ and $v$ are left and right eigenvectors of $A + \epsilon uv^*$. By the equivalence of formulas (4.9) and (4.10), this also implies that these vectors are singular vectors of $A - \lambda I$. □

![Fig. 7.1](image_url)  \hspace{1cm} 8. Tracking the boundary of the $\epsilon$-pseudospectrum. The following result shows that the differential equation (4.3) allows for tracking smooth segments of the boundary of the pseudospectrum.

**Theorem 8.1.** Let $E(t) \in \mathcal{M}$ satisfy the differential equation (4.3) and let $\lambda(t)$ be a continuous path of simple eigenvalues of $A + \epsilon E(t)$ for $0 \leq t \leq T$. If $\lambda(0) \in \partial \sigma_\epsilon(A)$, then $\lambda(t) \in \partial \sigma_\epsilon(A)$ for all $t$ as long as $\epsilon$ is a simple singular value of $A - \lambda(t)I$. □
1.4 1.6 1.8 2 2.2 2.4 2.6 2.8
1.2 1.4 1.6 1.8 2
2.2 2.4 2.6

Fig. 9.1. Path of the eigenvalue $\lambda(t)$ with largest modulus of $A + \varepsilon E(t)$ with $A$ of (3.1) and $\varepsilon = 1$, where $E(t)$ satisfies the differential equation (4.3) with $x$ replaced by $\lambda x$. The initial vectors $u(0)$ and $v(0)$ are randomly chosen and scaled to have norm 1. In black the circle centered at the origin with radius $\rho_1(A)$. Right: zoom.

Proof. Let $E = uv^\ast$. By Lemma 7.2, the normalized left and right eigenvectors $x, y$ with $x^\ast y > 0$ of $A + \varepsilon E$ to the eigenvalue $\lambda$ are complex multiples of $u$ and $v$: $x = \alpha u$, $y = \beta v$ with $|\alpha| = |\beta| = 1$. It follows from (4.6) that then $\dot{\lambda}$ is a real multiple of $\overline{\alpha}\beta$, or equivalently, $\Re(\overline{\alpha}\beta) = 0$. By the final argument in the proof of Theorem 4.3, it follows that $\dot{\lambda}$ is tangent to $\partial\sigma_\varepsilon(A)$. Since this holds for every $t$, $\lambda(t)$ stays on the boundary as long as $\varepsilon$ remains a simple singular value of $A - \lambda(t)I$. \[\square\]

From a computational point of view, in contrast to Section 6, we here follow the differential equation with standard error control, based on a local error estimate in the leading eigenvalue. In order to draw sections of the boundary of the pseudospectrum not only close to local maxima of the real part, we can apply (7.2) to a rotated matrix $e^{i\theta}A$ to hit the boundary along the ray with angle $-\theta$ and continue from the boundary point with the differential equation (4.3). In this way we can roam around the whole pseudospectrum.

9. A differential equation leading to the pseudospectral radius. At $E = uv^\ast \in \mathcal{M}$, let $x, y$ be left and right eigenvectors with $x^\ast y > 0$ to the eigenvalue $\lambda$ of largest absolute value of $A + \varepsilon uv^\ast$. We modify the differential equation (4.3) to

\[\dot{E} = P_E(\lambda xy^\ast),\]

that is, we replace $x$ by $\lambda x$ in (4.3) and correspondingly in the differential equations (4.4) for $u$ and $v$. We then obtain the following analog of Theorem 4.2 for the modulus instead of the real part.

Theorem 9.1. Let $E(t)$ satisfy the differential equation (4.3). If $\lambda(t)$ is a simple eigenvalue of $A + \varepsilon E(t)$, then $|\lambda(t)|$ increases monotonically with $t$.

Proof. We have

\[\frac{d}{dt}|\lambda|^2 = 2 \Re(\lambda \dot{\lambda}) = 2 \Re\left(\overline{\lambda} \frac{x^\ast \dot{E} y}{x^\ast y}\right)\]

\[= 2\varepsilon \frac{x^\ast y}{x^\ast y} \Re((\lambda x)^* P_E(\lambda xy^\ast)y) \geq 0,\]

using (4.7) with $\lambda x$ in place of $x$ and with $\alpha = u^\ast \lambda x$. \[\square\]

As the following analog of Theorem 4.3 shows, the motion is stationary at boundary points where the tangent to $\partial\sigma_\varepsilon(A)$ is orthogonal to $\lambda$. 

Theorem 9.2. \( \frac{d}{dt} |\lambda|^2 = 0 \) holds if and only if one of the following situations is met:

1. For some \( k \), the \( k \)-th singular value of \( A - \lambda I \) equals \( \varepsilon \) with singular vectors \( u \) and \( v \), and the level contour \( \Gamma_k(\varepsilon) = \{ \mu \in \mathbb{C} : s_k(A - \mu I) = \varepsilon \} \) has a tangent at \( \mu = \lambda \) that is orthogonal to \( \lambda \).

2. The left and right eigenvectors \( x \) and \( y \) of \( A + \varepsilon uv^* \) to the eigenvalue \( \lambda \) are orthogonal to \( u \) and \( v \), respectively. In this case they are also eigenvectors of \( A \) to the same eigenvalue \( \lambda \).

3. \( \lambda = 0 \).

Moreover, if \( \frac{d}{dt} |\lambda(t)|^2 = 0 \), then \( E = uv^* \) is a stationary point of the differential equation (9.1).

Proof. The proof uses the same argument as that of Theorem 4.3, starting now from \( \lambda x = \alpha u \) and \( y = \beta v \) in case 1. and ending up with \( \text{Re} (\mu'(0)X) = 0 \), i.e., \( \mu''(0) \perp \lambda \).

For the practical computation of the pseudospectral radius we discretize the differential equation (9.1) by the exponential Euler algorithm of Section 6, replacing again \( x_n \) by \( \lambda x_n \) on every occurrence.

10. Numerical experiments with dense and sparse matrices. In this section we consider two matrices from the Eigtool demo, the dense Landau matrix and the sparse elliptic-PDE matrix.

First example. The matrix \( A \) is given by the Landau matrix, which is a dense matrix of dimension 250, here multiplied by \( e^{i\pi/2} \) so that the pseudospectrum is rotated by \( \pi/2 \). The Landau matrix arises from an integral equation in laser theory (see [11]).

![Fig. 10.1. Path of the eigenvalues with largest modulus (north) and largest real part (east) obtained by applying the exponential Euler method with \( A \) the rotated Landau matrix and \( \varepsilon = 0.1 \). The circumscribing circle centered in the origin has radius \( \rho_1(A) \). Middle: zoom close to the rightmost point. Right: zoom close to the point with maximum modulus.](image)
A with largest real part (for computing the pseudospectral abscissa) or with largest modulus (for computing the pseudospectral radius).

When computing the pseudospectral radius we note that the eigenvalue of largest modulus of $A + \varepsilon u_0 v_0^* $ is already very close to $\rho_\varepsilon(A) $ (the relative error is around $10^{-4}$). This explains the behavior of the algorithm illustrated in Fig. 10, where the disk centered in zero with radius $\rho_\varepsilon(A) $ is drawn in black.

The algorithms based on the exponential Euler method of Section 6 compute the pseudospectral abscissa and radius with an accuracy of 6 digits in 14 and 19 steps, respectively. They have been coded in Matlab and executed on a laptop of average performance; the computation time is about 30 seconds in each case. In order to compute the leading eigenvalue and eigenvectors we have made use of the Matlab function \textit{eigs}, which makes use of the ARPACK libraries (see [12]).

In Tables 10.1 and 10.2 we report the results of the new algorithms compared to the Eigtool routines. We have made use of the stopping criterion $|\lambda_n - \lambda_{n-1}| \leq \min\left(10^{-10}, 10^{-8}\varepsilon\right)$. The values of the pseudospectral abscissa and radius, the time (in seconds) for the computation and the obtained accuracy are reported for several values of $\varepsilon \in [10^{-5}, 10^{-1}]$.

<table>
<thead>
<tr>
<th>$\varepsilon$</th>
<th>$\alpha_\varepsilon(A)$</th>
<th>time (Eigtool)</th>
<th>time (New)</th>
<th>accuracy</th>
</tr>
</thead>
<tbody>
<tr>
<td>$10^{-5}$</td>
<td>0.71551936009653</td>
<td>37s</td>
<td>2.4s</td>
<td>$1.10 \cdot 10^{-10}$</td>
</tr>
<tr>
<td>$10^{-4}$</td>
<td>0.7158743258394</td>
<td>50.6s</td>
<td>6.3s</td>
<td>$2.65 \cdot 10^{-11}$</td>
</tr>
<tr>
<td>$10^{-3}$</td>
<td>0.71936257485625</td>
<td>43.3s</td>
<td>10.7s</td>
<td>$7.34 \cdot 10^{-10}$</td>
</tr>
<tr>
<td>$10^{-2}$</td>
<td>0.74963767306566</td>
<td>56.4s</td>
<td>7.4s</td>
<td>$1.25 \cdot 10^{-11}$</td>
</tr>
<tr>
<td>$10^{-1}$</td>
<td>0.92654015790866</td>
<td>78.3s</td>
<td>14.4s</td>
<td>$9.13 \cdot 10^{-10}$</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>$\varepsilon$</th>
<th>$\rho_\varepsilon(A)$</th>
<th>time (Eigtool)</th>
<th>time (New)</th>
<th>accuracy</th>
</tr>
</thead>
<tbody>
<tr>
<td>$10^{-5}$</td>
<td>0.99967346120266</td>
<td>209s</td>
<td>1.1s</td>
<td>$1.41 \cdot 10^{-12}$</td>
</tr>
<tr>
<td>$10^{-4}$</td>
<td>0.99976363162005</td>
<td>45.1s</td>
<td>1.1s</td>
<td>$3.92 \cdot 10^{-13}$</td>
</tr>
<tr>
<td>$10^{-3}$</td>
<td>1.0006532404045</td>
<td>94.2s</td>
<td>1.3s</td>
<td>$9.56 \cdot 10^{-10}$</td>
</tr>
<tr>
<td>$10^{-2}$</td>
<td>1.0098114991932</td>
<td>114s</td>
<td>18.5s</td>
<td>$2.37 \cdot 10^{-12}$</td>
</tr>
<tr>
<td>$10^{-1}$</td>
<td>1.09977564493406</td>
<td>111.5s</td>
<td>29.8s</td>
<td>$1.38 \cdot 10^{-12}$</td>
</tr>
</tbody>
</table>

Second example. We consider the sparse matrix $A$ of dimension 2961 from the Eigtool demo that is denoted as Elliptic-PDE matrix. As the name indicates, it arises from the discretization of an elliptic boundary value problem; see [23] for a detailed description. We choose $\varepsilon = 10^{-1.5}$. It is possible to exploit the sparsity of $A$ in the computation of the leading eigenvectors of the matrices arising in the integration of (4.3). This can be done efficiently in Matlab through the function \textit{eigs} which uses an implicitly restarted Arnoldi method as implemented in ARPACK [12].
The algorithm of Section 6 computes the pseudospectral abscissa to an accuracy of 6 digits in 10 steps, which are performed in 35 seconds (to be compared to about 8 seconds for the first computation of the leading eigenvectors of $A$, which means a ratio of less than 5). Similarly to what is observed in [5], we have that the cpu time for the overall computation does not exceed significantly the cpu time for the computation of the leading eigenvectors of the original matrix, since in the later steps one can start from excellent starting values, which makes the restarted Arnoldi method converge with very few Krylov steps.

Fig. 10 shows the pseudospectrum (for several values of $\varepsilon$) and the rightmost eigenvalues associated to the matrices $A + \varepsilon u_n v_n^*$ obtained by the exponential Euler method. We note that the sequence follows closely the boundary of the pseudospectrum.

Since the matrix $A$ is large a comparison with the criss-cross algorithm used by Eigtool is not possible. It would be interesting to compare the algorithms presented in this paper with those given in [5]. For the sparse example we are considering we get 8 correct digits in about 50 seconds using the method described in Section 6 and in about 30 seconds using the algorithm by Guglielmi and Overton. In the near future we plan to do a systematic comparison, after a careful optimization of the numerical integrator and in particular of the stepsize control strategy.

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