Efficient computation of characteristic roots of delay differential equations using LMS methods

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Abstract

We aim at the efficient computation of the rightmost, stability-determining characteristic roots of a system of delay differential equations. The approach we use is based on the discretization of the time integration operator by a linear multistep (LMS) method. The size of the resulting algebraic eigenvalue problem is inversely proportional to the steplength. We summarize theoretical results on the location and numerical preservation of roots. Furthermore, we select nonstandard LMS methods, which are better suited for our purpose. We present a new procedure that aims at computing efficiently and accurately all roots in any right half-plane. The performance of the new procedure is demonstrated for small- and large-scale systems of delay differential equations.

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1. Introduction

We consider a system of linear delay differential equations (DDEs) of the form

\[ y'(t) = A_0 y(t) + \sum_{j=1}^{m} A_j y(t - \tau_j) \quad \text{where} \quad y(t) \in \mathbb{R}^n, \]  

(1)

with \( A_0, A_j \in \mathbb{R}^{n \times n} \) and constant delays \( \tau_j \geq 0 \), for \( j = 1, \ldots, m \). The stability (of the zero steady state solution) of (1) is determined by the roots \( \lambda \) of the characteristic equation

\[ \det \left( \lambda I - A_0 - \sum_{j=1}^{m} A_j e^{-\lambda \tau_j} \right) = 0, \]  

(2a)

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which can equivalently be written in the form

\[ \lambda \in \sigma \left( A_0 + \sum_{j=1}^{m} A_j e^{-\lambda \tau_j} \right), \]  

(2b)

where \( \sigma(\cdot) \) denotes the spectrum of a matrix. System (1) is asymptotically stable if all characteristic roots \( \lambda \) of (2) lie in the open left half-plane, i.e., \( \Re(\lambda) < 0 \), see e.g., [10,4]. Note that (2) has an infinite number of roots \( \lambda \). However, the number of roots in any right half-plane, i.e., with \( \Re(\lambda) \geq r \in \mathbb{R} \), is finite. Hence, the stability of (1) is always determined by a finite number of roots. If the linearization of a nonlinear DDE system equals (1), then the local stability of the former is given by the stability of (1), cf. [4].

Most numerical methods to compute the rightmost characteristic roots of (2) discretize either the infinitesimal generator (cf. [2,14,3]) or the time integration operator (or solution operator) to (1) (cf. [7,1]).

We follow the approach presented in [7] and implemented in the software package DDE-BIFTOOL (cf. [6,5]) for the bifurcation and stability analysis of (nonlinear) DDE systems. In this procedure, the time integration operator is discretized by using a linear multistep (LMS) method with polynomial interpolation to evaluate the delayed terms. The size of the resulting algebraic eigenvalue problem is inversely proportional to the steplength used in the discretization. The steplength heuristic proposed in [7] is often too conservative, i.e., much more characteristic roots than desired are computed with a good accuracy.

In this paper we improve the above procedure in two ways. Firstly, the steplength heuristic is sharpened by using theoretical results on the spectrum of characteristic roots, cf. [13]. Secondly, we use nonstandard LMS methods which cannot be used to perform time integration, but which allow us to use a larger steplength in the computation of the rightmost roots. In particular, we use the maximal order LMS methods. The resulting procedure reduces the computational cost without sacrificing reliability.

The structure of this paper is as follows. In Section 2, we outline the computational procedure and the steplength heuristic of [7] and discuss the directions of improvement pursued here. Section 3 summarizes the main results of [13] on the location and numerical preservation of characteristic roots. Sections 4 and 5 form the core of this paper. In Section 4, we discuss why the discretization is improved by using the maximal order LMS methods. For the maximal order LMS methods, a new steplength heuristic is derived in Section 5. The significant reduction in computational cost is illustrated by examples in Section 6. In Section 7, we draw conclusions.

2. Motivation

Sections 2.1 and 2.2 outline the procedure to compute the rightmost, stability-determining characteristic roots and the steplength heuristic, respectively, proposed in [7] and implemented in DDE-BIFTOOL. We also introduce the directions of improvement on the LMS discretization scheme and the steplength heuristic pursued in this paper.

2.1. Computation of the rightmost characteristic roots

We approximate the rightmost characteristic roots \( \lambda \) of (2) by computing the dominant eigenvalues \( \tilde{\lambda} = e^{\tilde{\lambda} h} \) of the discretized time integration operator to (1) over one time step of length \( h \). Let \( y_i \) denote an approximation to \( y(ih) \).

First, the delayed terms in (1) are approximated by using Lagrange interpolating polynomials, as follows:

\[ y(ih - \tau_j) \approx \sum_{\ell = -s}^{s} \psi_\ell(\varepsilon_j) y_{i+\ell-L_j} \quad \text{where} \quad \psi_\ell(\varepsilon_j) := \sum_{\nu = -s}^{s} \frac{\varepsilon_j - \nu}{\ell - \nu}, \]

with \( L_j := \lfloor \tau_j / h \rfloor \) and \( \varepsilon_j := L_j - \tau_j / h \in [0, 1] \). Next, a \( k \)-step LMS method with steplength \( h \) is used to obtain the following discrete version of (1):

\[ \sum_{i=0}^{k} z_i y_i = h \sum_{i=0}^{k} \beta_i \left( A_0 y_i + \sum_{j=1}^{m} A_j \sum_{\ell = -s}^{s} \psi_\ell(\varepsilon_j) y_{i+\ell-L_j} \right), \]

(3)
where \( x_i \) and \( \beta_j \), for \( i = 0, \ldots, k \), are the LMS coefficients. Using (3), the time integration operator is discretized, resulting in a \( N \times N \) matrix, where

\[
N := n(k + \lceil \tau_{\text{max}} / h \rceil + s_-) \approx n \tau_{\text{max}} / h, \tag{4}
\]

with \( \tau_{\text{max}} := \max_j \tau_j \), the maximal delay. The eigenvalues \( \tilde{\mu} \) of this matrix can be computed by e.g., the QR method. This is a robust method, however, its cost grows like \( N^3 \approx n^3(\tau_{\text{max}} / h)^3 \).

To avoid the use of future mesh points \( y_{k+1}, \ldots \) in (3), we require that

\[
\begin{aligned}
    h &\leqslant h_{\text{max}} := \tau_{\text{min}} / s_+,
\end{aligned} \tag{5}
\]

where \( \tau_{\text{min}} := \min_j \tau_j \) is the minimal delay, since this implies that \( s_+ - L_j \leqslant 0 \), for \( j = 1, \ldots, m \). Moreover, condition (5) also ensures that \( L_j = s_+ \) only if \( \tau_j = L_j h \) (i.e., \( \epsilon_j = 0 \)). Additionally, we choose \( s_- \) and \( s_+ \) so that \( s_- \leqslant s_+ \leqslant s_- + 2 \). These conditions are necessary for the theoretical results of Section 3.

We now write the characteristic equation for (3) in a form similar to (2b). As in [7], we characterize the effect of the LMS method by the scalar function

\[
\text{LMS}(z) := \frac{\alpha(e^z)}{\beta(e^z)} \quad \text{with} \quad \alpha(e^z) := \sum_{i=0}^{k} \alpha_i e^{iz} \quad \text{and} \quad \beta(e^z) := \sum_{i=0}^{k} \beta_i e^{iz}. \tag{6}
\]

Note that \( \alpha(\cdot) \) and \( \beta(\cdot) \) in (6) are assumed to be \textit{irreducible}, i.e., without common zeros. If the LMS method of order \( p \geqslant 1 \) is irreducible, then

\[
\alpha(e^z) - z \beta(e^z) = \beta(1) C_{\text{err}} z^{p+1} + \mathcal{O}(z^{p+2}) \quad \text{if} \quad z \to 0 \tag{7a}
\]

—see e.g., [9]—or, equivalently,

\[
\text{LMS}(z) = z + C_{\text{err}} z^{p+1} + \mathcal{O}(z^{p+2}) \quad \text{if} \quad z \to 0. \tag{7b}
\]

Furthermore, we characterize the effect of the interpolation by the functions

\[
\text{Int}_j(z) := z - \frac{h}{\tau_j} \log \left( \sum_{\ell = -s_-}^{s_+} \psi_j(\varepsilon_j) e^{(\ell - \varepsilon_j)z} \right) \quad \text{for} \quad j = 1, \ldots, m. \tag{8}
\]

The characteristic equation for (3) is obtained by replacing \( y_i \) by \( \tilde{\mu} \). Let \( \tilde{\mu} = e^{\lambda} \) with \( -\pi < \Im \tilde{\mu} < \pi \) and \( z = \tilde{\lambda} h \). Using (6) and (8), the characteristic equation for the discretized system (3) can be written as

\[
\frac{1}{h} \text{LMS}(\tilde{\lambda} h) \in \sigma \left( A_0 + \sum_{j=1}^{m} A_j e^{-(\varepsilon_j / h) \text{Int}_j(\tilde{\lambda} h)} \right), \tag{9}
\]

which is the discrete counterpart of the characteristic equation (2b) of the DDE system (1).

### 2.2. Directions of improvements of previous work

This section outlines the steplength heuristic proposed in [7] and introduces the improvements (of the heuristic and the LMS coefficients) pursued in the following sections.

Denote the open and closed right half-plane by

\[
\mathbb{C}_R^+ := \{ \lambda \in \mathbb{C} : \Re(\lambda) > 0 \} \quad \text{and} \quad \mathbb{C}^+ := \{ \lambda \in \mathbb{C} : \Re(\lambda) \geqslant 0 \},
\]

respectively. Analogously, one can define the open and closed left half-plane, \( \mathbb{C}_L^0 \) and \( \mathbb{C}^- \), respectively. The closed right half-plane shifted horizontally by \( r \in \mathbb{R} \) is denoted as

\[
\mathbb{C}^+ + r := \{ \lambda \in \mathbb{C} : \Re(\lambda) \geqslant r \}.\n\]
We also use the notation $|D| := \{|c| : c \in D\}$, where $D \subseteq \mathbb{C}$. For ease of presentation, we denote the right-hand side of the characteristic equation (2b) by $\Sigma_\tau(\cdot)$, i.e.,

$$\Sigma_\tau(\lambda) := \sigma \left( A_0 + \sum_{j=1}^m A_j e^{-\lambda \tau_j} \right)$$

where $\lambda \in \mathbb{C}$. 

Furthermore, let $\Sigma_\tau(D) := \cup_{\lambda \in D} \Sigma_\tau(\lambda)$, where $D \subseteq \mathbb{C}$. By (2b) and (10), the roots $\lambda$ which lie in $\mathbb{C}^+ + r$ are included in $\Sigma_\tau(\mathbb{C}^+ + r)$.

The steplength heuristic proposed in [7] aims at approximating all roots $\lambda$ in $\mathbb{C}^+ + r$. This steplength heuristic was developed in two stages. In the first stage of the derivation, the case of $r = 0$ is considered. Here, this is illustrated with a system of four DDEs and one delay, $\tau = 1$, with

$$A_0 = \begin{bmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -10 & -4 \\ 0 & 0 & 4 & -10 \end{bmatrix} \quad \text{and} \quad A_1 = \begin{bmatrix} 3 & 3 & 3 & 3 \\ 0 & -1.5 & 0 & 0 \\ 0 & 0 & 3 & -5 \\ 0 & 5 & 5 & 5 \end{bmatrix}.$$ 

(11)

It holds that $\max \{ \Sigma_\tau(\mathbb{C}^+) \} \leq \sum_{j=0}^m \| A_j \|$, as is illustrated in Fig. 1 (left). This inequality can easily be shown, but it is typically a (large) overestimate. Denote by $\rho_{\text{LMS},\varepsilon}$ the radius of the disc in the complex plane centered at the origin in which $\text{LMS}(i[0, 2\pi])$ approximates the imaginary axis “up to a given tolerance” $\varepsilon > 0$, cf. Fig. 1 (right). One can prove that if

$$h = \frac{\rho_{\text{LMS},\varepsilon}}{\sum_{j=0}^m \| A_j \|},$$

(12)

then $\Sigma_\tau(\mathbb{C}^+) \cap (\mathbb{C}^+ + \varepsilon/h)$ belongs to $(1/h)\text{LMS}(\mathbb{C}_0^+)$ and $\Sigma_\tau(\mathbb{C}^+) \cap (\mathbb{C}^- - \varepsilon/h)$ belongs to $(1/h)\text{LMS}(\mathbb{C}_0^-)$. Next, [7] concludes that the delay-independent stability is preserved up to the tolerance $\varepsilon$. In that derivation, some technical conditions were used which guarantee, among others, that $\text{LMS}(i[0, 2\pi])$ is the boundary of $\text{LMS}(\mathbb{C}_0^-)$. We do not need these conditions in our approach, as will be explained in Section 4.

In the second stage, the steplength heuristic

$$h = 0.9 \frac{\rho_{\text{LMS},\varepsilon}}{\| A_0 \| + |r| + \sum_{j=1}^m \| A_j \| e^{-r \tau_j}}$$

(13)

was proposed to approximate roots $\lambda$ in the half-plane $\mathbb{C}^+ + r$. Here, 0.9 is a safety factor. Heuristic (13) is implemented in DDE-BIFTOOL.

Fig. 1. For the DDE system (11) with $n = 4$ and $m = 1 : \Sigma_\tau(\mathbb{C}^+)$ (colored in gray), $\Omega(0)$ (cf. Section 3.1, solid line) and the circle around the origin with radius $\sum_{j=0}^m \| A_j \|$ (dashed line). The right subplot also shows $(1/h)\text{LMS}(i[0, 2\pi])$ where $h$ is given by (12) (solid line) and parallel lines $\pm \varepsilon/h$ from the imaginary axis (dash-dotted lines) for the BDF method of fourth order (with a rather large $\varepsilon$ for visibility).
The second improvement is the use of LMS methods which are better suited for our purpose of computing the rightmost approximation of more characteristic roots than desired, see e.g., [7, Fig. 5.3]. This is partly caused by the (large) overestimate for \( \max |\Sigma_{\tau}(C^+ + r) \cap (C^+ + r) \) in the denominator of (13). Recall that the set \( \Sigma_{\tau}(C^+ + r) \cap (C^+ + r) \) is important because it contains all roots which lie in \( C^+ + r \).

The above motivates improving the procedure by locating more precisely \( \Sigma_{\tau}(C^+ + r) \) w.r.t. \( C^+ + r \), cf. Section 3. The second improvement is the use of LMS methods which are better suited for our purpose of computing the rightmost roots, cf. Section 4. In the choice of the LMS methods we also take the accuracy of the computed roots explicitly into account. Combining both ideas leads to a novel steplength heuristic, cf. Section 5. Clearly, a heuristic giving a large, but still reliable steplength \( h \) is advantageous, since the cost to compute the rightmost roots is proportional to \( 1/h^3 \), as mentioned in Section 2.1.

3. The location and numerical preservation of roots

In this and the next sections, we discuss our approach, which differs from the approach of [7]. This section summarizes the main results of [13] on the location and numerical preservation of characteristic roots. These properties will be used in Section 4.

3.1. The location of characteristic roots

We define the set-valued function \( \Omega(\cdot) \) which maps \( \vec{\chi} := (\chi_1, \ldots, \chi_m) \in \mathbb{R}^m \) onto

\[
\Omega(\vec{\chi}) := \bigcup_{\vec{\omega} \in [0,2\pi]^m} \sigma \left( A_0 + \sum_{j=1}^m A_j e^{-(\chi_j + i\omega_j)} \right).
\]  

Further, we use the notations \( \vec{\tau} := (\tau_1, \ldots, \tau_m) \) and \( \vec{\xi} := (\xi_1, \ldots, \xi_m) \), where \( \xi \in \mathbb{R} \). The closure of a set is denoted by “cl”.

The characteristic roots \( \lambda \) can be located in the complex plane by using the property that the region \( \text{cl} \bigcup_{\xi \geq r} \Omega(\vec{\xi}) \) contains all roots \( \lambda \) with real part larger than \( r \). This implies by the identity \( \text{cl} \bigcup_{\xi \geq r} \Omega(\vec{\xi}) = \text{cl} \Sigma_{\tau}(C^+ + r) \), cf. [13]. Furthermore, the boundary of the region \( \text{cl} \bigcup_{\xi \geq r} \Omega(\vec{\xi}) \), that contains all roots \( \lambda \) of (2) lying in \( C^+ + r \), belongs to the set \( \Omega(r\vec{\tau}) \).

Here, we illustrate these results with a system of four DDEs and one delay, \( \tau = 1 \), with \( A_0 \) and \( A_1 \) defined in (11). The region \( \text{cl} \bigcup_{\xi \geq r} \Omega(\vec{\xi}) \), is colored in gray in Fig. 2, for \( r = 0 \) (left) and \( r = -1 \) (right). This figure illustrates that this region contains all roots \( \lambda \) with real part larger than \( r \). Fig. 2 also shows that the region \( \text{cl} \bigcup_{\xi \geq r} \Omega(\vec{\xi}) \) is bounded by the set \( \Omega(r\vec{\tau}) \). However, note that part of \( \Omega(r\vec{\tau}) \) can lie in the interior of \( \bigcup_{\xi \geq r} \Omega(\vec{\xi}) \). Furthermore, \( \Omega(r\vec{\tau}) \) is in general a two-dimensional subset of the complex plane. However, in the case of commensurate delays or a single delay, \( \Omega(r\vec{\tau}) \) is a union of curves.
If the set \([0, 2\pi t^m]\) in the right-hand side of (14) is replaced by \([0, \pi] \times [0, 2\pi t^{m-1}]\), then only “half of” the points in \(\Omega(\bar{\gamma})\) are obtained. However, since the matrices \(A_j\) are real, the whole of \(\Omega(\bar{\gamma})\) is regained by adding the complex conjugates of the points.

3.2. The numerical preservation of roots in \(\mathbb{C}^+ + r\)

This section introduces the theoretical results on what we call the (numerical) preservation of roots in \(\mathbb{C}^+ + r\) (with \(r \leq 0\)). Let us first explain this notion. Clearly, it is desirable that the discretization errors \(|\tilde{\lambda} - \lambda|\) are small. Additionally, one may want to compute (approximations to) all roots \(\lambda\) in \(\mathbb{C}^+ + r\), if any. E.g., if \(r = 0\), the absence of roots in \(\mathbb{C}^+\) proves the stability of (1). Here, we give a condition for the approximation of roots \(\hat{\lambda}\) of (2) in \(\mathbb{C}^+ + r\) by roots \(\tilde{\lambda}\) of (9) which belong to the same half-plane \(\mathbb{C}^+ + r\).

Before stating the main result, let us consider the right-hand sides of the “fixed-point condition” (2b) and its discrete counterpart (9) with \(h \in [0, h_{\text{max}}]\) (where \(h_{\text{max}}\) is defined in (5)). By (7b), LMS(\(\cdot\)) approximates the identity mapping. Analogously, \(\text{Int}_j(\cdot)\) approximates the identity mapping, for \(j = 1, \ldots, m\). In order to quantify the latter approximations when mapping half-planes, we introduce a function \(\rho(r)\) (for \(r \leq 0\)) so that \(\mathbb{C}^+ + \rho(r)\) is the largest half-plane whose images \((1/h)\text{Int}_j(\mathbb{C}^+ + \rho(r)h)\) belong to \(\mathbb{C}^+ + r\), or, equivalently,

\[
\rho(r) := \min \left\{ q \in \mathbb{R} : r \leq \text{Re} \left( \frac{1}{h} \text{Int}_j(gh + i\omega) \right), \quad \text{for } j = 1, \ldots, m \text{ & } \omega \in \mathbb{R} \right\}.
\]

Clearly, \(\rho(r) \approx r\), since the effect of polynomial interpolation is small. Moreover, \(r \leq \rho(r) \leq 0\), which can easily be proven along the lines of [7, Lemma 4.2]. The main result on the (delay-dependent) preservation of roots is:

**Theorem 1.** Let \(r \leq 0, \bar{\gamma} > \bar{0}, h \in [0, h_{\text{max}}]\) and \(s_- \leq s_+ \leq s_- + 2\).

\(^{(i)}\) If \(\Omega(\bar{\gamma}) \cap (\mathbb{C}^+ + r) = \emptyset\), then
- Eq. (2) has no roots \(\lambda\) in \(\mathbb{C}^+ + r\) and
- Eq. (9) has no roots \(\tilde{\lambda}\) which satisfy both
  - \((1/h)\text{Int}_j(\tilde{\lambda}h) \subset \mathbb{C}^+ + r\), for \(j = 1, \ldots, m\),
  - \((1/h)\text{LMS}(\tilde{\lambda}h) \subset \mathbb{C}^+ + r\).

\(^{(ii)}\) Let \(\bar{A} \subset \mathbb{C}^+ + \rho(r) \subset (\mathbb{C}^+ + r)\) be multiple connected. If \(c\) connected components of \(\Omega(\bar{\gamma})\) lie in the interior of \((1/h)\text{LMS}(h\bar{A}) \cap (\mathbb{C}^+ + r)\), then
- Eq. (2) has at least \(c\) roots \(\lambda\) (counting multiplicities) in the interior of \((1/h)\text{LMS}(h\bar{A}) \cap (\mathbb{C}^+ + r)\),
- those roots are approximated by \(c\) roots \(\tilde{\lambda}\) of (9) (counting multiplicities) which lie in the interior of \(\tilde{\lambda} \subset (\mathbb{C}^+ + r)\).

Its proof is analogous to the proof of [13, Theorem 3].

Let us now focus on the case of \(r = 0\). We define the stability preserving region of an LMS method as

\[
\mathcal{R}_{\text{pr}}^+: = \{ z \in \mathbb{C}^+ : \text{LMS}(z) \in \mathbb{C}^+ \}.
\]

(15)

Roughly speaking, \(\mathcal{R}_{\text{pr}}^+\) is the set of “unstable points which are mapped onto unstable points” by LMS(\(\cdot\)). This term is inspired by part (i) of the following corollary (proven in [13]), which specifies when the scaled stability preserving region \((1/h)\mathcal{R}_{\text{pr}}^+\) is free of approximate roots \(\tilde{\lambda}\).

**Corollary 2.** Let \(\bar{\gamma} > \bar{0}\) and \(s_- \leq s_+ \leq s_- + 2\).

\(^{(i)}\) If \(\Omega(\bar{\gamma}) \cap \mathbb{C}^+ = \emptyset\), then (2) has no roots in \(\mathbb{C}^+\) and (9) has no roots in \((1/h)\mathcal{R}_{\text{pr}}^+\). for all \(\overline{\gamma} > \bar{0}\) and \(h \in [0, h_{\text{max}}]\).

\(^1\) At the expense of greater complexity, a more detailed result is obtained in [13].

\(^2\) The stability preserving region differs from the stability region, defined roughly as the subset of the complex plane where no \(z \in \mathbb{C}^+\) are mapped upon by LMS(\(\cdot\)).
Let \( \tilde{A} \subseteq (1/h)\mathcal{S}^+_\text{pr} \) (\( \subseteq \mathbb{C}^+ \)) be multiple connected and \( h \in [0, h_{\text{max}}] \). If \( c \) connected components of \( \Omega(\tilde{0}) \) lie in the interior of \( (1/h)\text{LMS}(\tilde{A}) \) (\( \subseteq \mathbb{C}^+_r \)), then (2) has at least \( c \) roots \( \tilde{\lambda} \) (counting multiplicities) in the interior of \( (1/h)\text{LMS}(\tilde{A}) \) and its approximations \( \tilde{\lambda} \) (i.e., the roots of (9)) lie in the interior of \( \tilde{A} \) for all \( \tilde{r} > 0 \).

3.3. Previous results for the case of \( r = 0 \)

3.3. Previous results for the case of \( r = 0 \)

The following corollary can be proven using Theorem 1 (for \( r = 0 \)) and the property \( \text{cl}\bigcup_{\tilde{r} > \tilde{0}}\Omega(\tilde{r}) = \text{cl}\bigcup_{\tilde{r} > 0}\Omega(\tilde{r}) \), cf. [13]. These (delay-independent) results were proven in another way in [7] and used there to derive a (conservative) steplength heuristic (see also the brief summary in Section 2.2).

**Corollary 3.** (Parts (i) and (ii) of Theorems 3.4 and 4.3 in [7].) Assume that \( \text{LMS}(\mathbb{C}^+) \cap \text{LMS}(\mathbb{C}^-) = \emptyset \) and \( s_- \leq s_+ \leq s_- + 2 \).

(i) If \( \Omega(\tilde{r}) \subseteq \mathbb{C}^- \) for all \( \tilde{r} \geq \tilde{0} \), then \( (1) \) is stable for all \( \tilde{r} > \tilde{0} \).

If \( \Omega(\tilde{r}) \subseteq (1/h)\text{LMS}(\mathbb{C}^-) \) for all \( \tilde{r} \geq \tilde{0} \), then \( (3) \) is stable for all \( \tilde{r} > \tilde{0} \).

(ii) If \( \Omega(\tilde{r}) \subseteq \mathbb{C}^+ \) for all \( \tilde{r} \geq \tilde{0} \), then \( (1) \) is unstable for all \( \tilde{r} > \tilde{0} \).

If \( \Omega(\tilde{r}) \subseteq (1/h)\text{LMS}(\mathbb{C}^+) \) for all \( \tilde{r} \geq \tilde{0} \), then \( (3) \) is unstable for all \( \tilde{r} > \tilde{0} \).

4. Choosing which LMS methods to use

This section lays the basis for the new procedure to compute the rightmost roots, which is proposed in the next section. Section 4.1 considers which properties of LMS methods are desirable for our purpose to preserve the characteristic roots in the half-plane \( \mathbb{C}^+ + r \). Additionally, and contrary to [7], we also explicitly require a minimal accuracy of the computed roots in \( \mathbb{C}^+ + r \). Our requirements differ from those imposed for accurate time integration. In Section 4.2, we choose the LMS methods which best satisfy these requirements. In Section 4.3, the order of magnitude of the relative error on a computed root is derived.

4.1. Requirements on the LMS methods

At the end of this section, the requirements on the LMS method used are formulated. Besides the results on the preservation of roots of Section 3, we now also use the estimate

\[
\frac{\mid \lambda - \tilde{\lambda} \mid}{\mid \tilde{\lambda} \mid} = C \left( \frac{\mid \text{LMS}(\tilde{\lambda} h) - \tilde{\lambda} h \mid}{\tilde{\lambda} h} \right)
\]

for the order of magnitude of the relative error on a computed root \( \tilde{\lambda} \). At the end of this section, we will derive (16) for the LMS methods which will be used. The presence of the LMS(\cdot)-mapping in the estimate (16) can intuitively be explained by a comparison of the characteristic equation (2b) for the DDE system and its discrete counterpart (9).

The error estimate (16) highlights the importance of the region in the complex plane where LMS(\cdot) approximates the identity mapping well. Let \( \delta > 0 \) be a given relative tolerance. Motivated by (16), we define the trust-region \( \mathcal{S}_\delta \) by

\[
\mathcal{S}_\delta := \text{LMS}(\mathcal{S}_\delta), \quad \mathcal{S}_\delta := \{ z \in C^-_0 \cup \mathcal{S}^+_\text{pr} : |\Im(z)| < \pi, |\text{LMS}(z) - z| \leq h|z| \}.
\]

The restriction to \( C^-_0 \cup \mathcal{S}^+_\text{pr} \) in (17) is explained as follows. In this section, we make use of Theorem 1 for \( r \leq 0 \) and with

\[
\tilde{A} = \frac{1}{h} \mathcal{S}_\delta \cap (\mathbb{C}^+ + \rho(r)).
\]

In the case of \( r = 0 \), (17) and the property \( \rho(0) = 0 \) (cf. Section 3.2) imply that \( \tilde{A} \subseteq (1/h)\mathcal{S}^+_\text{pr} \). Hence, Corollary 2 can also be used. From this point on, we denote \( \mathcal{S}_\delta \) by \( \text{LMS}^{-1}(\mathcal{S}_\delta) \). This slight abuse of notation simplifies the presentation.

Theorem 1 and Corollary 2 only guarantee the numerical preservation of a root in the half-plane \( \mathbb{C}^+ + r \) under a strict condition. Roughly speaking, the root \( \lambda \) must belong to a connected component of \( \Omega(\tilde{r}) \) which lies completely
As a consequence, LMS and the condition that LMS is irreducible. By (7b), one expects to obtain a large trust-region $\mathcal{T}_\delta$ if the LMS method has a high order $p$ and a small error constant $C_{err}$. The latter requirements call for a maximal order LMS method, i.e., the unique $k$-step LMS method (with $k \geq 1$) of order $p = 2k$, cf. [8]. Table 1 shows the coefficients of the maximal order LMS methods of fourth, sixth and eighth order, i.e., with $k = 2, 3$ and 4, respectively. $(k = 1$ corresponds to the trapezoidal rule, which has second order.) Table 1 also lists the remarkably small error constants. In addition to these favorable properties, the maximal order LMS methods also satisfy condition (18), which we need. The latter is shown as follows. In the case of the maximal order LMS methods, $\alpha(e^z) - z\beta(e^z)$ in the left-hand side of (7a) is an odd function, i.e., its Taylor expansion contains only odd terms, or, equivalently,

$$\alpha_i = -\alpha_{k-i} \quad \text{and} \quad \beta_i = \beta_{k-i} \quad \text{for} \quad i = 0, \ldots, \lfloor k/2 \rfloor.$$  

As a consequence, LMS(-) is symmetrical w.r.t. the imaginary axis, which immediately implies (18). Furthermore, it is easily checked that the maximal order methods listed in Table 1 are irreducible and that LMS(-) has no poles on $i \pi$, $i\pi$. The latter conditions are also imposed in the previous section.

It is important to note that, apart from the trapezoidal rule, the maximal order LMS methods are not used for time integration. The reason for this is that their stability regions are empty. However, as explained in the previous section, the stability region is not important for our purpose of accurately computing the rightmost characteristic roots. The following paragraphs discuss some properties of the maximal order LMS methods which are desirable in the light of our purpose.
Fig. 3. $\mathcal{P}_{pr}$ (bounded by the thick dash-dotted line), $\mathcal{T}_\delta$ for $\delta = 0.1$ (colored in gray and bounded by the solid line), $\text{LMS}^{-1}(\mathcal{T}_\delta)$ (bounded by the dashed line) and (a part of) the image of lines parallel to the imaginary axis (with integer $\Re(\cdot)$) under $\text{LMS}(\cdot)$ (dotted lines) for the maximal order methods of fourth, sixth and eighth order.

Fig. 4. The same regions as in Fig. 3, but for the BDF methods of fourth and sixth order.

**Fig. 3** shows the location of $\mathcal{P}_{pr}$, $\mathcal{T}_\delta$ and $\text{LMS}^{-1}(\mathcal{T}_\delta)$, with $\delta = 0.1$, for the maximal order methods listed in Table 1. For the sixth order method, $\mathcal{P}_{pr}$ is large but does not equal $\mathbb{C}^+$. **Fig. 3** also shows (a part of) the image of lines parallel to the imaginary axis by the $\text{LMS}(\cdot)$-mapping. These curves illustrate the good approximation of the identity mapping by $\text{LMS}(\cdot)$ in a large region around the origin. Obviously this goes together with the small error constants listed in Table 1.

Comparing Figs. 3 and 4, it is clear that the trust-regions $\mathcal{T}_\delta$ of the maximal order methods are significantly larger than the $\mathcal{T}_\delta$ of the BDF methods. By construction of the maximal order methods, $\mathcal{P}_{pr}$ and $\mathcal{T}_\delta$ contain part of the imaginary axis. It is important to note that this desired property does not hold for the BDF methods—nor for the Adams–Bashford or Adams–Moulton methods.
Remark that the maximal order LMS methods for \( k \geq 2 \) are not zero-stable (or D-stable). By definition, an LMS method is zero-stable if and only if all zeros of the polynomial \( z(\bar{\mu}) \) lie in the closed unit disc and the zeros on the unit circle are simple, see e.g., [8]. Because we impose no requirements on the stability region of the LMS method used, the LMS method does not have to be zero-stable either. Note that the so-called Dahlquist barrier states that the order of zero-stable \( k \)-step LMS methods is limited to \( k + 2 \) if \( k \) is even and \( k + 1 \) if \( k \) is odd, cf. [8]. Remark that the fourth order method in Table 1, the so-called Milne–Simpson method, is the zero-stable LMS method of order \( p \geq 2 \) for which the line segment LMS([\( i \pi \), \( i \pi \)]) \( \subseteq i \mathbb{R} \) is maximal, namely \( i[-\sqrt{3}, \sqrt{3}] \), cf. [9].

4.3. The accuracy of computed roots

In this section, we derive the estimate (16) for the error on a computed root \( \hat{\lambda} \).

We assume that \( \lambda \) is a simple characteristic root. By (2), \( \lambda \) is an eigenvalue of the matrix \( \sum_{j=0}^{m} A_j e^{-\lambda \tau_j} \). We replace \( \lambda \) by its approximation \( \tilde{\lambda} \approx \lambda \) and consider the matrix \( \sum_{j=0}^{m} A_j e^{-\lambda \tau_j} \). Consequently, one of its eigenvalues, say \( \lambda_e \), tends to \( \lambda \) if \( \hat{\lambda} \) tends to \( \lambda \). Let \( v \) and \( w \) be the right and left eigenvectors which belong to \( \lambda_e \), and which are normalized so that \( w^H v = 1 \). Then, a small calculation gives the Taylor expansion about \( \lambda \) for \( \lambda_e \) as a function of \( \tilde{\lambda} \):

\[
\tilde{\lambda} = \lambda + \left(-\sum_{j=1}^{m} w^H A_j v \tau_j e^{-\lambda \tau_j}\right) (\lambda - \tilde{\lambda}) + O((\lambda - \tilde{\lambda})^2) \approx \lambda + \left(-\sum_{j=1}^{m} w^H A_j v \tau_j e^{-\lambda \tau_j}\right) (\lambda - \tilde{\lambda}) \quad (20a)
\]

Analogously, (9) implies that

\[
\frac{1}{h} \text{LMS}(\tilde{\lambda} h) = \lambda_e + \sum_{j=1}^{m} (-w^H A_j v \tau_j e^{-\lambda \tau_j}) \left(\frac{1}{h} \text{Int}_j(\tilde{\lambda} h) - \lambda\right) + O\left(\left(\frac{1}{h} \text{Int}_j(\tilde{\lambda} h) - \lambda\right)^2\right). \quad (20b)
\]

It follows from (20) that

\[
\frac{\lambda - \tilde{\lambda}}{2\tilde{\lambda}} \approx \kappa_0(\tilde{\lambda}) \left(\frac{\text{LMS}(\tilde{\lambda} h) - \tilde{\lambda} h}{\tilde{\lambda} h}\right) + \sum_{j=1}^{m} \kappa_j(\tilde{\lambda}) \left(\frac{\text{Int}_j(\tilde{\lambda} h) - \tilde{\lambda} h}{\tilde{\lambda} h}\right), \quad (21a)
\]

where

\[
\kappa_0(\tilde{\lambda}) := \frac{1}{1 + \sum_{j=1}^{m} w^H A_j v \tau_j e^{-\lambda \tau_j}} \quad \text{and} \quad \kappa_j(\tilde{\lambda}) := \frac{w^H A_j v \tau_j e^{-\lambda \tau_j}}{1 + \sum_{j=1}^{m} w^H A_j v \tau_j e^{-\lambda \tau_j}}. \quad (21b)
\]

Hence, \( \sum_{j=0}^{m} \kappa_j(\tilde{\lambda}) = 1 \). Remark that all values in (21) are complex nonreal unless \( \lambda \) (and its approximation \( \tilde{\lambda} \)) are real. One could use (21) as an a posteriori error estimator. Here, we simplify (21) based on the following two arguments.

Firstly, \( |\kappa_j(\tilde{\lambda})| \approx |\kappa_j(\lambda)| \), for \( j = 0, \ldots, m \), are typically \( O(1) \)—or smaller. Ample numerical evidence for this claim can be found in Table 2 which lists \( |\kappa_j(\lambda)| \) for the rightmost roots \( \lambda \) of the DDE systems of Sections 6.1–6.3.

Secondly, for the maximal order methods, the worst-case “interpolation error”—defined as the maximum of \( |\text{Int}_j(z) - z|/|z| \) over \( j = 1, \ldots, m \)—is of the same order of magnitude as the “LMS error”, defined as

\[
A_{\text{LMS}} := |\text{LMS}(z) - z|/|z|. \quad (22)
\]

Let us develop this argument. Denote by \( \text{rad}_{\text{LMS}} \) the radius of the largest circle centered around the origin, inscribed in \( \mathcal{F}_\delta \). Thus, by (17), \( \text{rad}_{\text{LMS}} \) equals the minimal value of \( |\text{LMS}(z)| \) when \( A_{\text{LMS}} \) is kept constant (assuming that the
Table 2
The moduli of the coefficients $k_j(\lambda)$ in error estimate (16) for the rightmost $\lambda$ of the DDE systems of Sections 6.1–6.3

| (Section 6.1) $\lambda$ | $|k_0(\lambda)|$ | $|k_1(\lambda)|$ |
|------------------------|---------------|---------------|
| 0.61764                | 0.38202       | 0.61798       |
| 0.27277 ± i0.88038     | 1.0850        | 1.2389        |
| −0.45272 ± i6.8812     | 0.091661      | 0.91183       |
| −0.45303 ± i1.1797     | 0.091794      | 0.91173       |
| −0.47992 ± i4.8199     | 0.19787       | 0.95923       |

| (Section 6.2) $\lambda$ | $|k_0(\lambda)|$ | $|k_1(\lambda)|$ | $|k_2(\lambda)|$ | $|k_3(\lambda)|$ |
|------------------------|---------------|---------------|---------------|---------------|
| 0.30887                | 2.9086        | 0.41828       | 0.41828       | 2.7452        |
| −0.097128              | 2.3623        | 0.36845       | 0.36845       | 4.0992        |
| −0.45585 ± i1.6885     | 0.27709       | 0.046433      | 0.046433      | 0.82352       |
| −0.88327 ± i5.3251     | 0.16345       | 0.029835      | 0.029835      | 0.92233       |
| −1.296 ± i5.0575       | 0.10106       | 0.020034      | 0.020034      | 1.0591        |
| −1.3445 ± i9.2985      | 0.086974      | 0.017409      | 0.017409      | 0.98031       |
| −1.6238 ± i9.3967      | 0.059818      | 0.012661      | 0.012661      | 1.0250        |
| −1.7048 ± i3.450       | 0.051967      | 0.011179      | 0.011179      | 1.0055        |

| (Section 6.3) $\lambda$ | $|k_0(\lambda)|$ | $|k_1(\lambda)|$ |
|------------------------|---------------|---------------|
| 0                      | 0.076061      | 0.92394       |
| ±i47.709               | 0.22880       | 0.78554       |
| −0.091454 ± i5.8356    | 0.067976      | 0.93766       |
| −0.22501 ± i4.2457     | 0.11148       | 0.92312       |
| −0.28499 ± i11.796     | 0.051810      | 0.96001       |
| −0.47107 ± i17.878     | 0.035826      | 0.97545       |
| −0.55646 ± i36.422     | 0.034593      | 0.98159       |
| −0.59908 ± i24.035     | 0.021680      | 0.98389       |
| −0.64281 ± i30.230     | 0.012921      | 0.98717       |
| −1.1905                | 1.0007        | 0.00068       |

Fig. 5. For orders 4, 6 and 8 (from bottom to top): radLMS versus $A_{\text{LMS}}$ (thick lines) for the maximal order LMS methods (cf. Fig. 3) and radInt versus $A_{\text{Int}}$ (thin lines).

restriction to $S^+_{pr}$ in (17) nor $|\Im m(z)| < \pi$ are “active constraints”, as is the case below). Fig. 5 shows radLMS versus $A_{\text{LMS}}$ for $p = 4, 6, 8$.

Fig. 5 also shows a similar curve for the worst-case interpolation error, constructed as follows. If $s_+ + s_- + 1$ in (8) equals $p$, then simple roots are approximated with order $h^p$, cf. [7]. Therefore we choose $s_+ = s_- + 1 = p/2 = k$. Substitution of $\tau_j/h \geq s_+ + 1 - e_j$ (cf. Section 2.1) gives the following conservative upper bound for $|\text{Int}_j(z) - z|/|z|$ (for $j = 1, \ldots, m$):

$$A_{\text{Int}} := \max_{0 < \epsilon < 1} \frac{1}{|z|(k + 1 - \epsilon)} \left| \log \left( \sum_{\ell=-k+1}^{k} \psi_{\ell}(\epsilon)e^{(\ell-\epsilon)z} \right) \right|.$$ (23)
Table 3
The parameters of ellipses (24) inscribed in $T_\delta$ for $\delta = 0.1$ and $\text{rad}_{\text{LMS}}$, i.e., the radius of the largest inscribed circle centered around the origin

<table>
<thead>
<tr>
<th>order</th>
<th>4</th>
<th>6</th>
<th>8</th>
</tr>
</thead>
<tbody>
<tr>
<td>$a_{\text{ell}}$</td>
<td>2.193</td>
<td>1.345</td>
<td>2.958</td>
</tr>
<tr>
<td>$b_{\text{ell}}$</td>
<td>1.679</td>
<td>2.442</td>
<td>2.010</td>
</tr>
<tr>
<td>$\text{rad}_{\text{LMS}}$</td>
<td>1.679</td>
<td>2.1000</td>
<td>2.205</td>
</tr>
</tbody>
</table>

Analogous to (22), formula (23) is evaluated for a range of $z$-values in the complex plane. Next, $\text{rad}_{\text{Int}}$ is determined as the minimal value of $|\text{LMS}(z)|$ for constant $A_{\text{Int}}$. The curves of $\text{rad}_{\text{Int}}$ versus $A_{\text{Int}}$ (cf. Fig. 5) are nonsmooth due to properties of the LMS($\cdot$)-mapping, the explanation of which lies outside the scope of this paper.

Fig. 5 illustrates that the magnitude of the worst-case interpolation error, i.e., $A_{\text{Int}}$, is smaller than the LMS error $A_{\text{LMS}}$ (except for a small part of the fourth order curves). Remark that in the one-delay case, $h$ can be chosen so that $A_{\text{Int}}$ is integer, which avoids interpolation altogether.

In conclusion, we may use the estimate (16), although, in practice, the error on the computed roots is often much smaller, cf. Section 6.

5. The novel steplength heuristic

In this section, we derive a novel steplength heuristic for the maximal order LMS methods. Next, we prove that the new heuristic yields a larger steplength than heuristic (13) for any DDE system.

5.1. Derivation of the novel steplength heuristic

As argued in Section 4.1, we determine $h$ such that the part of $\Omega(r\tilde{\tau})$ (defined in (14)) which lies in $\mathbb{C}^+ + r$ also belongs to $(1/h)T_\delta$ (cf. Fig. 3). Recall that $r \leq 0$ and that $\delta > 0$ is a given relative tolerance. We aim at a simple formula for the steplength $h$ that can easily be implemented in software. For this reason, we avoid working directly with the trust-region $T_\delta$, but instead use ellipses of the form

$$(\Re(z)/a_{\text{ell}})^2 + (\Im(z)/b_{\text{ell}})^2 = 1,$$

which are inscribed in $T_\delta$. Table 3 shows possible values for $a_{\text{ell}}$ and $b_{\text{ell}}$ for $\delta = 0.1$.\(^3\) This table also lists $\text{rad}_{\text{LMS}}$, the radius of the largest circle centered around the origin and inscribed in $T_\delta$, which can be read from Fig. 5. Note that for the sixth order method, we use by default the first ellipse listed in Table 3, because it gave the smallest steplengths in almost all our tests. This could be expected from the typical wedge-like form of the rightmost part of the spectrum.

Our heuristic choice of the steplength is formulated as follows. First, for a given value of $r$, a (finite) number of points $q_K \in \Omega(r\tilde{\tau})$, for $K = 1, 2, \ldots$, is computed. By Section 3.1, these points can be obtained as the eigenvalues of the matrix

$$A_0 + \sum_{j=1}^{m} (A_j e^{-r\tau_j}) e^{-i\omega_j},$$

for a number of $m$-vectors $\tilde{\omega} := (\omega_1, \ldots, \omega_m)$ chosen from $[0, \pi] \times [0, 2\pi]^{n-1}$. Clearly, the size of the matrix eigenvalue problem (25), $n$, is much smaller than $N$ in (4), i.e., the size of the approximate algebraic eigenvalue problem. Additionally, $\Omega(r\tilde{\tau})$ does not have to be determined very accurately. However, these points should be well spread out over $\Omega(r\tilde{\tau})$. Next, the points with real parts larger than $r - \Delta r$ for some $\Delta r > 0$ are selected. We use the safety margin $\Delta r$ because only a limited number of points is computed. Typical values are $r = -1, -2$ and $\Delta r = 0.1$. Finally, the largest value of $h$ is determined such that the selected points scaled by $h/0.9$ fit into an ellipse of the

\(^3\) Note that $\delta = 0.1$ equals the default value $\varepsilon = 0.1$ used in the old heuristic (13).
form (24), where 0.9 is a safety factor. Hence, \( h \) is given by

\[
0.9 \sqrt{\max \Re(q_K) \geq r - \Delta r \left( (\Re(q_K)/a_{\ell})^2 + (\Im(q_K)/b_{\ell})^2 \right)}.
\]

(26)

5.2. Discussion

Let us now consider two heuristics that are “intermediate” between the old heuristic (13) (using traditional LMS methods) and the new heuristic (26) (using the maximal order LMS methods):

- Adaptation 1 uses the maximal order LMS methods with a steplength given by

\[
h = \frac{\text{rad}_{\text{LMS}}}{\|A_0\| + |r| + \sum_{j=1}^m \|A_j\| e^{-r \tau_j}},
\]

where \( \text{rad}_{\text{LMS}} \) is taken from Table 3.

- Adaptation 2 still uses the traditional LMS methods, but with a steplength given by

\[
h = \frac{\rho_{\text{LMS},\epsilon}}{\max \{\Omega(r \tilde{\tau}) \cap (C^+ + r - \Delta r)\}}.
\]

(28)

Adaptation 1 (cf. (27)) is obtained by replacing \( \rho_{\text{LMS},\epsilon} \) in (13) by \( \text{rad}_{\text{LMS}} \). Hence, it guarantees that \( \Omega(r \tilde{\tau}) \) belongs to \( (1/h)\mathcal{F}_\delta \). The resulting \( h \) benefits from the improvement by the maximal order LMS methods, but still uses an overestimate in the denominator which severely restricts the steplength. Adaptation 2 (cf. (28)) uses a more realistic bound for \( |\Omega(r \tilde{\tau}) \cap (C^+ + r)\). Let us compare \( \rho_{\text{LMS},\epsilon} \) and \( \text{rad}_{\text{LMS}} \) with the maximum of \( a_{\ell} \) and \( b_{\ell} \) in Table 3 for LMS methods of orders 4 and 6. Specifically, we assume that (28) and the old heuristic (13) are used with a BDF method. One then has to compare \( \rho_{\text{LMS},\epsilon} \approx 0.57 \) and \( \text{rad}_{\text{LMS}} \approx 0.70 \), respectively, for the BDF methods (and \( \epsilon = 0.1 \)) to the values in Table 3 (where \( \delta = 0.1 \)) for the maximal order LMS methods of fourth and sixth order. The latter values are significantly larger. Hence, both adaptations improve the old steplength heuristic and the new heuristic combines the merits of both. In conclusion, the novel heuristic (26) yields a larger steplength than the old heuristic (13) for any DDE system. In Section 6.1, this is illustrated by examples.

Remark that the steplength \( h \) given by heuristic (26) has to be bounded above by \( h_{\text{max}} \), cf. (5).

5.3. An a posteriori safeguard

Section 4.1 provides no (heuristic) guarantee about the correctness of computed roots \( \tilde{\tau} \) which do not belong to \( (0.9/h)\text{LMS}^{-1}(\mathcal{F}_\delta) \). If such a root also belongs to \( C^+ + r \) (which is rare), then it is safe to assume that it is artificial, i.e., only caused by the discretization scheme. Therefore, our algorithm removes all computed roots in \( C^+ + r \) which lie outside \( (0.9/h)\text{LMS}^{-1}(\mathcal{F}_\delta) \).

6. Examples

This section presents examples to illustrate the efficiency of the new procedure to compute the rightmost characteristic roots. We consider two small-scale DDE systems and one large-scale DDE system. For the first example, we also assess the merits of the two “intermediate” adaptations introduced in Section 5.

6.1. A small-scale system of DDEs with one delay

This section considers the system of four DDEs and one delay, \( \tau = 1 \), with

\[
A_0 = \begin{bmatrix}
-1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 \\
0 & 0 & -10 & -4 \\
0 & 0 & 4 & -10
\end{bmatrix}
\quad \text{and} \quad
A_1 = \begin{bmatrix}
3 & 3 & 3 & 3 \\
0 & -1.5 & 0 & 0 \\
0 & 0 & 3 & -5 \\
0 & 5 & 5 & 5
\end{bmatrix},
\]
Table 4
Quantities used in the computation of the steplength for different \( r \)

<table>
<thead>
<tr>
<th>( r )</th>
<th>( h )</th>
<th>( N )</th>
<th>( h )</th>
<th>( N )</th>
<th>( h )</th>
<th>( N )</th>
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<td>10^{-2}</td>
<td>168</td>
<td>8.95</td>
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<td>4.79</td>
<td>10^{-3}</td>
<td>476</td>
<td>4.79</td>
</tr>
</tbody>
</table>

Left column: using the old heuristic (13) for the BDF methods. Mid columns: using the adaptations (27) resp. (28). Right column: using the new heuristic (26) for the maximal order LMS methods.

Table 5
Values of the steplength \( h \) and size \( N \) of the eigenvalue problem for \( r = 0, -0.5, -1, -3 \)

<table>
<thead>
<tr>
<th>( r )</th>
<th>Old heuristic</th>
<th>Adaptation 1</th>
<th>Adaptation 2</th>
<th>New heuristic</th>
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</thead>
<tbody>
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<td>( N )</td>
<td>( h )</td>
<td>( N )</td>
<td>( h )</td>
</tr>
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<td>2.97</td>
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<tr>
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<td>4</td>
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<td>240</td>
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<tr>
<td>-1</td>
<td>4</td>
<td>1.29</td>
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<td>332</td>
</tr>
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<td>-3</td>
<td>4</td>
<td>2.33</td>
<td>10^{-3}</td>
<td>1740</td>
</tr>
</tbody>
</table>

Table 6
Ratios of the steplengths \( h_{new} / h_{old} \) and ratios of the sizes of the eigenvalue problem, \( N_{old} / N_{new} \), where \( h_{new} \) comes from heuristic (26) for maximal order LMS methods and \( h_{old} \) from heuristic (13) for the BDF methods

<table>
<thead>
<tr>
<th>Order</th>
<th>( h_{new} / h_{old} )</th>
<th>( N_{old} / N_{new} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>4</td>
<td>20.5</td>
<td>9.2</td>
</tr>
<tr>
<td>6</td>
<td>11.2</td>
<td>5.3</td>
</tr>
</tbody>
</table>

For \( r = 0 \), \( h_{new} > h_{max} \) and \( h_{new} \) is set to \( h_{max} \).

that was introduced in Section 2.2. We used, for comparison, the maximal order LMS methods of fourth, sixth and eighth order and the BDF methods of fourth and sixth order to compute roots \( \lambda \in \mathbb{C}^+ + r \) for \( r = 0, -0.5, -1, -3 \). The rightmost characteristic roots and the set \( \Omega(r \bar{r}) \) for \( r = 0 \) and \( -1 \) are shown in Fig. 2 and the quantities used in the steplength heuristics are given in Table 4.

Table 5 lists the steplength \( h \) and the size \( N \) of the corresponding eigenvalue problem for the novel heuristic (26) (with \( \Delta r = 0.1 \) and using the maximal order LMS methods of fourth, sixth and eighth order) and for the old heuristic (13) (using the BDF methods of fourth and sixth order). Obviously, \( h \) decreases with \( r \). If \( h > h_{max} = \tau_{min}/s_+ \), the steplength is set equal to \( h_{max} \). This is indicated by a “(s)” encryption. In this case, \( N = n(3k - 1) \) for the maximal order LMS method of order \( p = 2k \). In order to assess the merits of the two adaptations (the location of \( \Omega(r \bar{r}) \cap (\mathbb{C}^+ + r) \) and the maximal order LMS methods), Table 5 also lists the two heuristics presented in Section 5 (adaptations 1 and 2) that are “intermediate” between the old heuristic (13) and the new heuristic (26). We see that both adaptations improve the old steplength heuristic and that the new heuristic combines the merits of both adaptations.
We fix parameters of the same order. The novel heuristic (26) gives 
and 
and 
and 

Fig. 6. For the small-scale DDE system of Section 6.1: approximate roots \( \tilde{\lambda}(+) \), their corrections using Newton iterations (\( \diamond \)) and \((0.9/h)\) LMS \(-1(\mathcal{F}_\delta)\) (bounded by the dashed line) for the maximal order LMS methods of fourth order (top) and eighth order (bottom). Left column: \( r = -1 \). Right column: \( r = -3 \).

Table 6 gives the ratio of the steplengths and the ratio of the sizes of the eigenvalue problems for the new heuristic (26) and the old heuristic (13). Notice that the ratio \( \frac{N_{\text{old}}}{N_{\text{new}}} \) listed in Table 6 decreases with \( r \). However, the new heuristic remains superior.

Fig. 6 shows the approximate roots \( \tilde{\lambda} \) with their corrections for the maximal order LMS methods of fourth and eighth order for \( r = -1, -3 \). Computed roots \( \tilde{\lambda} \) in \( \mathbb{C}^+ \) \( + \) \( r \) which lie outside \((0.9/h)\) LMS \(-1(\mathcal{F}_\delta)\) (drawn in Fig. 6) were removed, for the reason explained in Section 5. Recall that the highest accuracy is achieved for roots \( \tilde{\lambda} \) close to the origin.

6.2. A small-scale system of DDEs with multiple delays

In [11], two coupled identical neurons with time-delayed connections are modelled by the system of \( n = 2 \) DDEs

\[
\begin{align*}
y'_1(t) &= -\lambda y_1(t) + \beta_0 \tanh(y_1(t - \tau_3)) + \beta_{1,2} \tanh(y_2(t - \tau_2)), \\
y'_2(t) &= -\lambda y_2(t) + \beta_0 \tanh(y_2(t - \tau_3)) + \beta_{2,1} \tanh(y_1(t - \tau_1)).
\end{align*}
\]

We fix parameters \( \lambda = 0.5, \beta_0 = -1, \beta_{1,2} = 1, \beta_{2,1} = 2.34, \tau_1 = 0.2, \tau_2 = 0.2 \) and \( \tau_3 = 1.5 \) and linearize the system about the zero steady state solution, cf. [6]. For this example, one can easily show that \( \bigcup_{z \geq 1} \Omega(z^2\tau) \) is the annulus given by 
\[
e^{-1.5r} - \sqrt{2.34}e^{-0.2r} \leq |z + 1/2| \leq e^{-1.5r} + \sqrt{2.34}e^{-0.2r}.
\]

The spectrum shown in Fig. 7 is computed using heuristic (26) with the maximal order LMS method of sixth order and \( r = -3, \Delta r = 0.1, \delta = 0.1 \) (left) and \( \delta = 0.01 \) (blow-up, right).

Let us first compare the novel heuristic with \( \delta = 0.1 \) and order 6 to the old heuristic with the BDF method of the same order. The novel heuristic (26) gives \( h = 1.31 \times 10^{-2} \) and \( N = 240 \). The old heuristic (13) gives \( h = 6.30 \times 10^{-3} \) and \( N = 494 \). Note that in this case, the denominator of the old heuristic is not a large overestimate; indeed, \( \|A_0\| + |r| + \sum_{j=1}^n \|A_j\|e^{-r\tau_j} \approx 99.603 \) is comparable to max \( |\Omega(r\tau) \cap (\mathbb{C}^+ + r)| \approx 92.819 \).
The steplength is larger using this ellipse since \( x = h \) is commensurate with the ellipse in Fig. 7. For the small-scale DDE system of Section 6.2 with \( 2^{24} \), \( K = 6.3 \) and \( \delta = 0.1 \) (left) and \( \delta = 0.01 \) (blow-up, right).

Using the novel heuristic with the second ellipse listed in Table 3 under “order 6” gives \( h = 1.95 \times 10^{-2} \) and \( N = 164 \). The steplength is larger using this ellipse since \( \Omega(r \bar{r}) \) with \( r = -3 \) is covered by a disc with radius \( \approx 92.804 \) and center \( -\frac{1}{2} \). Hence, for this example, one should prefer this alternative ellipse.

For the roots closest to the origin, the relative errors of the two procedures are comparable, namely \( \mathcal{O}(10^{-13}) \). Further away from the origin, the accuracy of the new procedure becomes slightly worse. E.g., for the complex conjugate pair of roots \( \lambda \approx -2.9811 \pm 184.797 \), the relative errors are \( 1.50 \times 10^{-4} \) for the new procedure and \( 2.50 \times 10^{-5} \) for the old procedure. This example illustrates that the right-hand side of (16) often overestimates the relative error.

Let us now consider the novel heuristic with \( \delta = 0.01 \). In this case, \( h = 1.55 \times 10^{-2} \) and \( N = 206 \), which is still a factor of \( \approx 2.3 \) smaller than the eigenvalue problem solved by the old procedure. For the above-mentioned complex conjugate pair of roots, the relative error is now \( 5.21 \times 10^{-5} \), cf. Fig. 7 (blow-up, right).

6.3. A large-scale system of DDEs

This section considers a hybrid DDE–PDE system modelling a semiconductor laser subject to conventional optical feedback and lateral carrier diffusion, cf. [12]. The system in the complex scalar variable \( A(t) \) and real \( Z(x, t) \), where \( x \in [-0.5, 0.5] \), reads as

\[
\frac{dA(t)}{dt} = (1 - i\phi) A(t) \zeta(t) + \eta A(t - \tau)e^{-i\phi} - ibA(t), \tag{29a}
\]

\[
T \frac{\partial Z(x, t)}{\partial t} = d \frac{\partial^2 Z(x, t)}{\partial x^2} - Z(x, t) + P(x) - F(x)(1 + 2Z(x, t))|A(t)|^2. \tag{29b}
\]

The functions \( \zeta(t) \), \( P(x) \) and \( F(x) \) are specified in [12]. Zero Neumann boundary conditions for \( Z(x, t) \) are imposed at \( x = \pm 0.5 \). We fix parameters \( \alpha = 3 \), \( \phi = 0 \), \( T = 1000 \), \( d = 1.68 \times 10^{-2} \) and delay \( \tau = 1000 \). For the numerical computations, the time variable is rescaled as \( t \leftarrow 1000t \). The symmetry about \( x = 0 \) is exploited by considering only the interval \([0, 0.5]\). We split (29a) into real and imaginary part and discretize (29b) in space using a second order central difference formula with constant stepsize \( \Delta x = 0.5/128 \). Hence, the resulting DDE system has size 131. For \( \eta \approx 2.5717 \times 10^{-3} \), a steady state Hopf bifurcation arises with \( |A| \approx 1.8209 \) and \( b \approx 1.1119 \times 10^{-3} \). The system is linearized about this steady state solution. The approximate roots \( \tilde{\lambda} \) and their corrections are shown in Fig. 8. Similar comments on the accuracy can be made as before. Note that, due to the rotational symmetry in the complex variable \( A \), there is always an additional characteristic root at zero.

The spectrum shown in Fig. 8 was computed using the maximal order LMS method of sixth order and with \( r = -1 \), \( \Delta r = 0.1 \) and \( \delta = 0.1 \) (left) and \( \delta = 0.01 \) (right). For this example, contrary to the previous ones, we use a steplength \( h \) commensurate with \( \tau \). That is, the value of \( h \) obtained from heuristic (26) is lowered until \( \tau/h \) is integer, so that interpolation is avoided. After this adaption, the novel heuristic (26) gives \( h = \tau/24 \) \((N = 3537)\) for \( \delta = 0.1 \) and \( h = \tau/36 \) \((N = 5109)\) for \( \delta = 0.01 \). The resulting eigenvalue problems are large, but still feasible. The old heuristic (13), using the BDF method of sixth order, gives \( h = \tau/7195 \), which would lead to an intractable eigenvalue problem of size \( N = 943 \times 331 \) (for \( \varepsilon = 0.1 \) in (13)).
The steplength resulting from heuristic (13) is so small because $\|A_0\| + |r| + \|A_1\|e^{-\tau} \approx 4.531.8$ severely overestimates $\max \{\Omega(r) \cap (\mathbb{C}^+ + r)\} \approx 52.5$. The former value is large because $\Omega(r)$ extends far to the left in $\mathbb{C}^-$. However, only the part of $\Omega(r)$ in $\mathbb{C}^+ + r$ is important. For space discretizations of reaction–diffusion systems, the tail of $\Omega(r)$ typically grows to the left when the discretization in space becomes finer, because the leftmost eigenvalues of $A_0$ tend to minus infinity. Remark that, by using $\Omega(r)$, we ensure that the purely imaginary complex conjugate roots with large imaginary part (shown in Fig. 8) are detected. This is important since roots on the imaginary axis indicate a so-called Hopf bifurcation point, see e.g., [10,4].

7. Conclusions

In this paper, we have described a procedure which computes efficiently and accurately the rightmost (stability-determining) characteristic roots of the system of DDEs (1). This is a modification to the procedure presented in [7] (and is incorporated in the new version of DDE-BIFTOOL). Our new procedure is more efficient while maintaining the reliability of the numerical results. To achieve this goal, we have used theoretical results on the location and numerical preservation of roots. Furthermore, we have argued that computing characteristic roots accurately imposes other requirements on the LMS method used in the discretization than for accurate time integration. Consequently, we have used the maximal order LMS methods, which satisfy these requirements, instead of using LMS methods traditionally used for time integration. Using a novel steplength heuristic for the maximal order LMS methods reduces the size of the algebraic eigenvalue problem. Hence, for all systems of DDEs the computational cost is lower compared with the procedure in [7], especially for (the space discretization of) delay PDEs of reaction–diffusion type.

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References


