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A Rigorous Implicit C^1 Chebyshev Integrator for Delay Equations

Jean-Philippe Lessard[1] · J. D. Mireles James[2]

Abstract

We present a new approach to validated numerical integration for systems of delay differential equations. We focus on the case of a single constant delay though the method generalizes to systems with multiple lags. The method provides mathematically rigorous existence results as well as error bounds for both the solution and the Fréchet derivative of the solution with respect to a given past history segment. We use Chebyshev series to discretize the problem, and solve approximately using a standard numerical scheme corrected via Newton's method. The existence/error analysis exploits a Newton–Kantorovich argument. We present examples of the rigorous time stepping procedure, and illustrate the use of the method in computer-assisted existence proofs for periodic solutions of the Mackey–Glass equation.

Keywords Delay equations · Validated numerics · Numerical integration · Chebyshev series

1 Introduction

Use of the digital computer as a tool for proving theorems in nonlinear analysis has its roots in the work of R.E. Moore on interval analysis [1,2], and has increased steadily since the groundbreaking work of Lanford, Eckman, Wittwer, and Koch on computer assisted analysis of renormalization group operators and the Feigenbaum conjectures in the early 1980s [3–5]. For a general overview of the literature we refer to the review articles [6,7] and to the book of Tucker [8].

✉ J. D. Mireles James
  jmirelesjames@fau.edu

  Jean-Philippe Lessard
  jp.lessard@mcgill.ca

[1] Department of Mathematics and Statistics, McGill University, 805 Sherbrooke Street West, Montreal, QC H3A 0B9, Canada

[2] Department of Mathematical Sciences, Florida Atlantic University, Science Building, Room 234, 777 Glades Road, Boca Raton, Florida 33431, USA

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Since the main objective of nonlinear dynamics is to understand the organization and interconnectedness of invariant sets, it is natural that validated numerical methods for computing mathematically rigorous enclosures of orbit segments play an indispensable role. The simplest case is a finite dimensional discrete time dynamical system, where computing an orbit segment requires iterating a function. This reduces to validated range bounding for nonlinear functions, and is one of the foundational problems of interval analysis [2,8]. The case of a finite dimensional continuous time system is more difficult, as an orbit segment is the solution of an initial value problem. Tremendous effort has gone into developing rigorous integrators for ordinary differential equations (ODEs) for precisely this purpose. The literature on this topic is substantial and, while a thorough review is beyond the scope of the present work, we will refer the interested reader to the works of [9–15] and the references therein.

Analogous problems for infinite dimensional discrete and continuous time dynamical systems are even more challenging, as in these cases the state space is itself a function space. There is a great deal of research interest in validated numerical methods for infinite dimensional discrete time dynamics, going back to work the mid 1980's on renormalization operators in the context of computer assisted proofs of the Feigenbaum conjectures and their generalizations [3–5,16–18] See also the works of [19–23] on computer-assisted existence proofs for fixed points, periodic orbits, attracting Morse sets, chaotic dynamics, and homoclinic connecting orbits for infinite dimensional discrete time dynamical systems. More recently there has been substantial progress in validated numerical methods for continuous time infinite dimensional systems. We refer the interested reader to the works of [24–30] on time stepping procedures for parabolic partial differential equations (PDEs), and to the recent computer aided proofs of the existence of chaotic dynamics in the Kuramoto–Sivashinsky PDE [31] and heteroclinic orbits in the Ohta–Kawasaki model [32]. The work of [33] develops a C^0 validated integration techniques for scalar delay differential equations (DDEs), where functions are represented by piecewise Taylor expansions. We direct the interested reader also to the recent resolution of both Jone's and Wright's conjectures in [34,35], which required development of a whole suit of validated numerical techniques for DDEs.

In contrast to the Taylor based C^0 approach of [33], our work develops a validated C^1 time stepping procedure based on Chebyshev series expansions for nonlinear systems of DDEs given by

$$y'(t) = f(y(t), y(t - \tau)), \tag{1}$$

where $f : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}^d$ is a smooth function and $\tau > 0$. We derive an implicit time stepping scheme based on the so called *method of steps* (see Sect. 1.1 for the formal definition). The method of steps leads to a fixed point problem for the evolution of the initial history segment, which is projected into an appropriate finite dimensional space and approximately solved numerically by iterating a Newton scheme. We then formulate an a-posteriori argument, which is based on a Newton–Kantorovich theorem, and which provides mathematically rigorous error bounds on the difference between the true and the approximate solution.

One novelty of our approach is the use of Chebyshev series to represent both the past history and the solution space. Chebyshev series provide accurate low density representations of smooth functions on an interval. Moreover the regularity of the solutions translates directly into decay rates for the Chebyshev coefficients, and this information is useful for choosing appropriate Banach spaces of infinite sequences in which to study the fixed point problem.

Another feature of our method is that it is C^1. That is, the method provides mathematically rigorous information about the derivative of the time step with respect to initial conditions. Such information is needed for local stability analysis in many areas of dynamical systems theory (though we do not consider these applications in this work).

Another fundamental difference between the method developed in the present work and the methods of previous works is that we treat the problem as implicitly defining an infinite dimensional discrete time dynamical system, rather than treating it as an infinite dimensional flow. This aspect of the approach is discussed in more detail in the next section. As an application of our method, we prove the existence of some periodic orbits in the Mackey–Glass Equation.

1.1 Problem Description: The Method of Steps

The *method of steps* is a classical technique for studying DDEs. The idea is to integrate both sides of Eq. (1) and observe that for $0 \le t \le \tau$ a solution $y(t)$ satisfies

$$y(t) = y(0) + \int_0^t f(y(s), y(s - \tau)) \, ds, \qquad t \ge 0. \tag{2}$$

This formulation makes it explicitly clear that the function y must be given on the interval $[-\tau, 0]$ so that the right hand side is defined for $t \in [0, \tau]$. The expression in Eq. (2) suggests we pass to an appropriate fixed point problem.

To this end suppose that a smooth initial history segment $y_0 \in C([-\tau, 0], \mathbb{R}^d)$ is specified. The function $y_1 \colon [0, \tau] \to \mathbb{R}^d$ is a *solution* of the DDE on the interval $[0, \tau]$ if f is continuous in both variables and y_1 is a fixed point of the operator

$$T(y_1, y_0)(t) = y_0(0) + \int_0^t f(y_1(s), y_0(s - \tau)) \, ds, \qquad t \in [0, \tau].$$

Define the mapping $\Phi_1 \colon C([-\tau, 0], \mathbb{R}^d) \to C([0, \tau], \mathbb{R}^d)$ by the rule that

$$\Phi_1(x) = y,$$

if and only if y is the unique fixed point of

$$y(t) = T(y, x)(t).$$

We refer to Φ_1 as the first *step map* for the DDE and write $\Phi_1(y_0) = y_1$ when y_1 solves Eq. (2) on $[0, \tau]$ with past history y_0 on $[-\tau, 0]$. If $y_1 \colon [0, \tau] \to \mathbb{R}^d$ solves the fixed point problem, then it is C^1 by the fundamental theorem of calculus. We remark that, while uniqueness of y_1 on $[0, \tau]$ follows from standard existence and uniqueness results for ODEs as soon as f is Lipschitz continuous in the first variable and y_0 is continuous, the constructive methods developed in the present work obtain existence and uniqueness without assuming that f is globally Lipschitz.

Iterating the procedure leads to subsequent step maps $\Phi_{n+1} \colon C([(n - 1)\tau, n\tau], \mathbb{R}^d) \to C([n\tau, (n + 1)\tau], \mathbb{R}^d)$ by the rule that

$$\Phi_{n+1}(x) = y,$$

if and only if y is the unique fixed point of

$$y(t) = x(n\tau) + \int_{n\tau}^t f(y(s), x(s - \tau)) \, ds, \qquad t \in [n\tau, (n + 1)\tau],$$

for $n \ge 0$. Clearly the step maps improve regularity by one derivative in each application, so that the maps have a discrete smoothing property akin to the infinitesimal smoothing property of parabolic PDEs. Indeed the Φ_{n+1} are compact mappings.

Moreover taking K compositions of the first K step maps is equivalent to solving the DDE over K units of the delay τ. More precisely, if $y_0 \colon [-\tau, 0] \to \mathbb{R}^d$ is a given history on $[-\tau, 0]$, then $y \colon [0, K\tau] \to \mathbb{R}^d$ solves Equation (1) with history y_0 if and only if

$$
y(t) = \begin{cases}
y_0(t), & t \in [-\tau, 0) \\
\Phi_1(y_0)(t), & t \in [0, \tau) \\
\Phi_2(y_1)(t), & t \in [\tau, 2\tau) \\
\vdots & \\
\Phi_K(y_{K-1})(t), & t \in [(K-1)\tau, K\tau].
\end{cases}
$$

The fact that integrating the DDE leads to a sequence of distinct step maps, each defined between different function spaces, prevents the scheme above from defining a discrete time dynamical systems. This inconvenience is easily overcome by shifting and rescaling time. More precisely, we shift and re-scale the time interval $[0, \tau]$ to $[-1, 1]$ (Chebyshev series are defined for functions on $[-1, 1]$) and define $T \colon C([-1, 1], \mathbb{R}^d) \times C([-1, 1], \mathbb{R}^d) \to C([-1, 1], \mathbb{R}^d)$ by

$$
T(y, x)(t) = x(1) + \frac{\tau}{2} \int_{-1}^{t} f(y(s), x(s))\, ds, \qquad t \in [-1, 1], \tag{3}
$$

and the mapping $\Phi \colon C([-1, 1], \mathbb{R}^d) \to C([-1, 1], \mathbb{R}^d)$ by the rule

$$
\Phi(x) = y \qquad \Longleftrightarrow \qquad y = T(y, x) \quad \text{(uniquely)}.
$$

We refer to Φ as the *step map* for the DDE. Given $y_0 \in C([-1, 1], \mathbb{R}^d)$ define

$$
y_n = \Phi(y_{n-1}),
$$

for $n = 1, \ldots K$. Shifting and rescaling back to the original domains recovers the solution of Eq. (1).

1.2 Chebyshev Discretization for the Method of Steps

We are interested in numerically iterating the step map, and discretize an appropriate subset of $C([-1, 1], \mathbb{R}^d)$ (to be specified later) using Chebyshev series expansions. Throughout this section we use freely a number of standard facts about Chebyshev series. Indeed we remark that Chebyshev series are an excellent tool for studying nonperiodic solutions of nonlinear differential equations as

- Chebyshev series have excellent (in some sense optimal) uniform approximation properties.
- The derivative is a diagonally dominant operator in Chebyshev coefficient space.
- Multiplication of scalar valued functions corresponds to discrete cosine convolution in Chebyshev coefficient space.

Excellent references for this material is [36,37].

Let $x, y : [-1, 1] \to \mathbb{R}^d$ have convergent expansions

$$
y(t) = a_0 + 2 \sum_{n \geq 1} a_n T_n(t) \quad \text{and} \quad x(t) = b_0 + 2 \sum_{n \geq 1} b_n T_n(t),
$$

where for $n \geq 0$ the coefficients $a_n, b_n \in \mathbb{R}^d$, and where the $T_n(t)$ are the *Chebyshev polynomials* defined recursively by $T_0(t) = 1$, $T_1(t) = t$ and $T_{n+1}(t) = 2t T_n(t) - T_{n-1}(t)$,

for $n \geq 1$. Denote the coefficient sequences by $a = (a_n)_{n\geq 0}$ and $b = (b_n)_{n\geq 0}$. Moreover, assume that the Chebyshev series expansion of $f(x, y)$ is convergent and given by

$$f(y(t), x(t)) = \phi_0 + 2 \sum_{n\geq 1} \phi_n T_n(t), \qquad \phi_n = \phi_n(a, b) \in \mathbb{R}^d. \tag{4}$$

As mentioned above, the product of two scalar Chebyshev series is given by discrete cosine convolution. Then if $f : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}^d$ is polynomial, the ϕ_n consist of discrete convolutions involving the components of a and b. Using that $\int T_0(s)\, ds = T_1(s) + const.$, $\int T_1(s)\, ds = \frac{T_0(s) + T_2(s)}{4} + const.$ and $\int T_n(s)\, ds = \frac{1}{2}\left(\frac{T_{n+1}(s)}{n+1} - \frac{T_{n-1}(s)}{n-1}\right) + const.$ for $n \geq 2$, yields

$$\int_{-1}^{t} f(y(s), x(s))\, ds$$
$$= \left(\phi_0 - \frac{\phi_1}{2} - 2\sum_{k\geq 2} \frac{(-1)^k}{k^2 - 1}\phi_k\right) T_0(t) + 2\sum_{n\geq 1} \frac{1}{2n}(\phi_{n-1} - \phi_{n+1})T_n(t).$$

Hence, the fixed point equation $y = T(y, x)$ becomes

$$y(t) = a_0 + 2\sum_{n\geq 1} a_n T_n(t)$$
$$= x(1) + \frac{\tau}{2}\int_{-1}^{t} f(y(s), x(s))$$
$$= b_0 + 2\sum_{n\geq 1} b_n + \frac{\tau}{2}\left(\left(\phi_0 - \frac{\phi_1}{2} - 2\sum_{k\geq 2} \frac{(-1)^k}{k^2 - 1}\phi_k\right) T_0(t)\right.$$
$$\left. + 2\sum_{n\geq 1} \frac{1}{2n}(\phi_{n-1} - \phi_{n+1})T_n(t)\right)$$

which is equivalent to solving $\tilde{\mathcal{F}}_0(a, b) + 2\sum_{n\geq 1} \tilde{\mathcal{F}}_n(a, b)T_n(t) = 0$ for all $t \in [-1, 1]$, with

$$\tilde{\mathcal{F}}_n(a, b) \overset{\text{def}}{=} \begin{cases} a_0 - \left(b_0 + 2\sum_{k\geq 1} b_k\right) - \frac{\tau}{2}\left(\phi_0 - \frac{\phi_1}{2} - 2\sum_{k\geq 2} \frac{(-1)^k}{k^2 - 1}\phi_k\right), & n = 0 \\ a_n - \frac{\tau}{4n}(\phi_{n-1} - \phi_{n+1}), & n \geq 1. \end{cases}$$

Observe that $\tilde{\mathcal{F}}_n(a, b) = 0$, for all $n \geq 1$ only if $a_n = \frac{\tau}{4n}(\phi_{n-1} - \phi_{n+1})$ for all $n \geq 1$, and we see that

$$a_0 - \left(b_0 + 2\sum_{k\geq 1} b_k\right) - \frac{\tau}{2}\left(\phi_0 - \frac{\phi_1}{2} - 2\sum_{k\geq 2} \frac{(-1)^k}{k^2 - 1}\phi_k\right)$$
$$= a_0 + 2\sum_{k\geq 1}(-1)^k a_k - \left(b_0 + 2\sum_{k\geq 1} b_k\right).$$

This leads to the equivalent zero finding problem $\mathcal{F}_n(a, b) = 0$ given component-wise by

$$\mathcal{F}_n(a, b) \stackrel{\text{def}}{=} \begin{cases} a_0 + 2\sum_{k\geq 1}(-1)^k a_k - \left(b_0 + 2\sum_{k\geq 1} b_k\right), & n = 0 \\ a_n - \dfrac{\tau}{4n}(\phi_{n-1} - \phi_{n+1}), & n \geq 1. \end{cases} \tag{5}$$

Define the operators

$$\mathcal{T} \stackrel{\text{def}}{=} \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & \cdots \\ 1 & 0 & -1 & 0 & \cdots & \\ 0 & 1 & 0 & -1 & 0 & \cdots \\ & \ddots & \ddots & \ddots & \ddots & \ddots \\ & \cdots & 0 & 1 & 0 & -1 \\ & & \cdots & \ddots & \ddots & \ddots \end{pmatrix} \quad \text{and} \quad \Lambda^{-1} \stackrel{\text{def}}{=} \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & \cdots \\ 0 & 1 & 0 & 0 & \cdots & \\ 0 & 0 & \frac{1}{2} & 0 & 0 & \cdots \\ & \ddots & \ddots & \ddots & \ddots & \ddots \\ & \cdots & 0 & 0 & \frac{1}{n} & 0 \\ & & \cdots & \ddots & \ddots & \ddots \end{pmatrix}. \tag{6}$$

The nonlinear map $\mathcal{F}$ defined in (5) is expressed as

$$\mathcal{F}_n(a, b) = \begin{cases} a_0 + 2\sum_{k\geq 1}(-1)^k a_k - \left(b_0 + 2\sum_{k\geq 1} b_k\right), & n = 0 \\ \left(a - \dfrac{\tau}{4}\Lambda^{-1}\mathcal{T}\phi(a, b)\right)_n, & n \geq 1. \end{cases} \tag{7}$$

We solve $\mathcal{F}(a, b) = (\mathcal{F}_n(a, b))_{n\geq 0} = 0$ on a space of infinite sequences, with b the fixed sequence of Chebyshev coefficients for the past history.

To recapitulate, if $a = (a_n)_{n\geq 0}$ is a zero of $\mathcal{F}(a, b)$ for fixed $b = (b_n)_{n\geq 0}$, and if $x(t)$ and $y(t)$ are the functions whose Chebyshev series have coefficient sequences a and b, then $y = T(y, x)$ and by rescaling the domains we have that y is a solution of the DDE (1) with previous history x. Regularity of the functions x, y leads to rapid decay of their Chebyshev series coefficients, and this fact is exploited to topologize the solution space of $\mathcal{F}$. We endow the coefficient space with a weighted "little-ell-one" norm. Such norms induce Banach space – in fact component-wise Banach algebra – structure, under discrete convolution. This results in a problem formulation amenable to Fréchet differential calculus, and Newton's method is an appropriate tool for studying the zero finding problem.

Thought of this way, the problem of time-stepping Eq. (1) is mathematically quite similar to the work of [38–41] on computer-assisted existence proofs for periodic orbits of DDEs. The works just cited reformulate a periodic solution of the DDE as a zero finding problem in a sequence space of rapidly decaying Fourier coefficients, and much of the technology developed in the references just cited is useful in the present work. The important difference being that we now employ discretization via Chebyshev series approximation, which are often described as *Fourier series in disguise*. In this sense the present work builds on earlier successful applications of Chebyshev series in validated numerical computations [42,43] and especially the work of [44–48] on computer-assisted proofs of solutions to initial and boundary value problems. We refer also to the computer-assisted existence proofs for spatial periodic orbits in a restricted four body problem in [49]. All of the works just cited exploit Chebyshev series approximation.

The remainder of the paper is organized as follows. Section 2 formalizes the problem description and presents the theoretical tools needed for the rest of the paper. Section 3

presents in details the a-posteriori analysis for Chebyshev discretization scheme for the method of steps, as well as how to get C^1 bounds. We apply the technique to Wright's equation. In Sect. 4 we present a method to obtain computer-assisted proofs of periodic orbits for DDEs, and we apply our approach to prove several periodic orbits in the Mackey–Glass equation.

Finally we remark that all of the programs discussed in this paper are implemented in MATLAB, some utilizing the IntLab library [50] for interval arithmetic and some the open-source package Chebfun. Our programs are freely available at
http://cosweb1.fau.edu/~jmirelesjames/methodOfSteps_CAP_DDE.html.

2 A-Posteriori Analysis and C^1 Bounds for the Method of Steps

In this section we develop the general setup used to study dynamical systems implicitly defined by certain fixed point problems throughout the remainder of the paper. The main tools are the implicit function theorem between Banach spaces, the contraction mapping theorem, and the Neumann series. The material in this section is agnostic toward problem specific details like the choice of function spaces and the projections used to study the problem numerically. Only in Sect. 3 do we return to the topic of Chebyshev series discretization for DDEs.

2.1 Functional Analytic Set up for Implicitly Defined Maps

Let X be a Banach space and $T: X \times X \to X$ be a smooth function. Given a norm $\| \cdot \|_X$ on X, denote by

$$B_r(c) \overset{\text{def}}{=} \{a \in X : \|a - c\|_X < r\} \subset X$$

the open ball of radius r centered at $c \in X$. We are interested in the dynamical system $\Phi: X \to X$ defined by the following rule: for $a, b \in X$ we say that

$$\Phi(b) = a,$$

if and only if a is the unique fixed point of the equation

$$T(a, b) = a,$$

for the given b. The domain of Φ is the set

$$D = \{b \in X : T(\cdot, b) \text{ has a unique fixed point } a \in X\},$$

which may or may not be empty. However, if $b_0 \in D$ then the implicit function theorem tells us when D contains an open neighborhood of b_0. To see this suppose that $(a_0, b_0) \in X \times X$ has that $T(a_0, b_0) = a_0$, and consider the function $\mathcal{F}: X \times X \to X$ defined by

$$\mathcal{F}(a, b) = a - T(a, b).$$

Note that $\mathcal{F}(a_0, b_0) = 0$. By the implicit function theorem we have the following: if the linear operator $D_1 \mathcal{F}(a_0, b_0): X \to X$ is an isomorphism then there is an $\epsilon > 0$ and a continuous function $a: B_\epsilon(b_0) \to X$ so that $a(b_0) = a_0$ and

$$\mathcal{F}(a(b), b) = 0 \qquad \text{for all } b \in B_\epsilon(b_0).$$

It follows that

$$T(a(b), b) = a(b),$$

for all $b \in B_\epsilon(b_0) \subset X$. That is, the function Φ is locally well defined near b_0 by the equation

$$T(\Phi(b), b) = \Phi(b), \tag{8}$$

and we have that

$$\Phi(b) = a(b).$$

This says precisely that $B_\epsilon(b_0) \subset D$. Note that, in terms of T we have that

$$D_1\mathcal{F}(a, b) = \mathrm{Id} - D_1T(a, b),$$

is the needed isomorphism, where Id denotes the identify operator on X.

The derivative of Φ is obtained by implicit differentiation. Differentiating Equation (8) with respect to b leads to

$$D\Phi(b) = D_1T(\Phi(b), b)D\Phi(b) + D_2T(\Phi(b), b),$$

so that

$$[\mathrm{Id} - D_1T(\Phi(b), b)] D\Phi(b) = D_2T(\Phi(b), b), \tag{9}$$

and since $\mathrm{Id} - D_1T(\Phi(b), b) = \mathrm{Id} - D_1T(a, b)$ is an isomorphism we obtain the useful formula

$$D\Phi(b) = [\mathrm{Id} - D_1T(a, b)]^{-1} D_2T(a, b) = - (D_1\mathcal{F}(a, b))^{-1} D_2\mathcal{F}(a, b). \tag{10}$$

We remark that the correspondence between iterates of Φ, fixed points of T, and zeros of $\mathcal{F}$ plays a central role in the discussion to follow. In the next section we discuss the a-posteriori theory for studying the solutions of $\mathcal{F} = 0$ – that is, we examine the question of when a "good enough" approximate solution implies the existence of a true solution "nearby".

2.2 A-Posteriori Existence and Error Bounds

The following result is a Newton–Kantorovich theorem with hypotheses suitable for computer assisted implementation. The theorem requires only an approximate solution, and approximate derivative and approximate inverse of the derivative. More precisely, given any vector $b \in X$ suppose that $\bar{a} \in X$ has $\mathcal{F}(\bar{a}, b) \approx 0$, and that operators $A^\dagger, A \in B(X)$ are linear operators approximating respectively $D_1\mathcal{F}(\bar{a}, b)$ and $D_1\mathcal{F}(\bar{a}, b)^{-1}$. In practice $\bar{a}$ will result by including an approximate numerical solution – an object sitting in the memory of our computer – into the function space X. Moreover, throughout the present work A and $A^\dagger$ will be finite dimensional matrices combined with identity mappings in the infinite dimensional "talis".

The theorem provides conditions sufficient for establishing the existence of an $r_0 > 0$ and a $\tilde{a} \in \overline{B_{r_0}(\bar{a})}$, so that $\tilde{a}$ is the unique solution of $\mathcal{F}(\tilde{a}, b) = 0$ in $\overline{B_{r_0}(\bar{a})}$. Here $\overline{B_{r_0}(\bar{a})}$ is the closure of the open ball $B_{r_0}(\bar{a})$. It is important to note that the invertibility of $D_1\mathcal{F}(\bar{a}, b)$ is not assumed; rather it emerges as a corollary (see Corollary 2.2 below).

Newton–Kantorovich theorems and their many variations are used frequently in computer-assisted proofs, We refer the interested reader to the references [5,38,51–57] for a number of different related approaches. Denote by $B(X)$ the set of bounded linear operators on the Banach space X and $\| \cdot \|_{B(X)}$ the corresponding bounded linear operator norm.

Theorem 2.1 *Let X be a Banach space and $\mathcal{F}\colon X \times X \to X$ be a Fréchet differentiable mapping with respect to both variables. Suppose that $\bar{a}, b \in X$, $A^\dagger \in B(X)$, and $A \in B(X)$ with A is injective. Assume that Y_0, Z_0, and Z_1 are positive constants and that $Z_2\colon (0, r_*) \to \mathbb{R}^+$ is a non-negative function satisfying*

$$\|A\mathcal{F}(\bar{a}, b)\|_X \leq Y_0, \tag{11}$$

$$\|\mathrm{Id} - AA^\dagger\|_{B(X)} \leq Z_0, \tag{12}$$

$$\|A[D_1\mathcal{F}(\bar{a}, b) - A^\dagger]\|_{B(X)} \leq Z_1, \tag{13}$$

$$\|A[D_1\mathcal{F}(a, b) - D_1\mathcal{F}(\bar{a}, b)]\|_{B(X)} \leq Z_2(r)r, \quad \forall a \in \overline{B_r(\bar{a})} \text{ and for } r \in (0, r_*). \tag{14}$$

Define

$$p(r) \stackrel{\text{def}}{=} Z_2(r)r - (1 - Z_0 - Z_1)r + Y_0.$$

If there is an $r_0 \in (0, r_*)$ such that $p(r_0) < 0$, then there exists a unique $\tilde{a} \in B_{r_0}(\bar{a})$ satisfying $\mathcal{F}(\tilde{a}, b) = 0$.

In practice, $b \in X$ is a fixed data point and $\bar{a} \in X$ is an approximate solution of $\mathcal{F}(\cdot, b) = 0$. The operator $A^\dagger$ is an approximation of the Fréchet derivative $D_1\mathcal{F}(\bar{a}, b)$, and the operator A is an approximate inverse of $A^\dagger$ making it an "even more" approximate inverse of $D_1\mathcal{F}(\bar{a}, b)$. The function $Z_2(r)$ is a local Lipschitz estimate of the first derivative of $\mathcal{F}$ at $\bar{a}$ which needs only to hold up to distance r_* from $\bar{a}$. In many applications $\mathcal{F}$ is twice continuously differentiable in its first variable and we simply take

$$Z_2(r) = \|A\|_{B(X)}Cr,$$

where C is any bound of the form

$$\sup_{a \in \overline{B_{r_*}(\bar{a})}} \|D_1^2\mathcal{F}(a, b)\|_{\text{bi-linear}(X)} \leq C.$$

Here r_* may be chosen somewhat arbitrarily –though "small" – and the norm is an appropriate norm on the space of bi-linear operators. The estimate of Eq. (14) is seen to hold for any $0 < r < r_*$ by applying the mean value inequality to $D_1\mathcal{F}$. Moreover in this case we have that $p(r)$ is a quadratic polynomial whose roots are easily determined from the quadratic equation.

Since several details from the proof of Theorem 2.1 are needed in the proof of the corollary below, we now sketch the argument. The idea is to look for a fixed point of the Newton-like operator

$$\mathcal{N}(a) \stackrel{\text{def}}{=} a - A\mathcal{F}(a, b),$$

where we have suppressed the dependance of $\mathcal{N}$ on b, as the parameter b is fixed throughout the following discussion. Observe that

$$D\mathcal{N}(a) = \mathrm{Id} - AD_1\mathcal{F}(a, b),$$

so that

$$\begin{aligned}
\|D\mathcal{N}(a)\|_{B(X)} &\leq \|\mathrm{Id} - AD_1\mathcal{F}(a, b)\|_{B(X)} \\
&\leq \|\mathrm{Id} - AA^\dagger\|_{B(X)} + \|A[A^\dagger - D_1\mathcal{F}(\bar{a}, b)]\|_{B(X)} \\
&\quad + \|A[D_1\mathcal{F}(a, b) - D_1\mathcal{F}(\bar{a}, b)]\|_{B(X)}
\end{aligned}$$

for all $a \in \overline{B_{r_0}(\bar{a})}$. Then, by the hypotheses of Theorem 2.1 we have the bound

$$\sup_{a \in \overline{B_{r_0}(\bar{a})}} \|D\mathcal{N}(a)\|_{B(X)} \le Z_2(r_0) + Z_1 + Z_0, \tag{15}$$

for any $0 < r_0 < r_*$. Now the condition $p(r_0) < 0$ encodes two valuable pieces of information, namely that $Z_2(r_0)r_0 + (Z_1 + Z_0)r_0 + Y_0 < r_0$, and, since $Y_0, r_0 > 0$, that $Z_2(r_0) + Z_1 + Z_0 < 1$. From the first it follows that

$$
\begin{aligned}
\|\mathcal{N}(a) - \bar{a}\|_{B(X)} &\le \|\mathcal{N}(a) - \mathcal{N}(\bar{a})\|_{B(X)} + \|\mathcal{N}(\bar{a}) - \bar{a}\|_{B(X)} \\
&\le \sup_{c \in B_{r_0}(\bar{a})} \|D\mathcal{N}(c)\|_{B(X)} \|a - \bar{a}\|_{B(X)} + \|A\mathcal{F}(\bar{a}, b)\|_{B(X)} \\
&\le (Z_2(r_0) + Z_1 + Z_0)\, r_0 + Y_0 < r_0,
\end{aligned}
$$

so that $\mathcal{N}$ maps the ball $\overline{B_{r_0}(\bar{a})}$ into $B_{r_0}(\bar{a})$. From the second it follows by (15) and the mean value theorem that $\mathcal{N}$ is a strict contraction on $\overline{B_{r_0}(\bar{a})}$, with Lipschitz constant $Z_2(r_0) + Z_1 + Z_0 < 1$. From the contraction mapping theorem follows the existence of a unique fixed point $\tilde{a} \in B_{r_0}(\bar{a})$ of $\mathcal{N}$, and from the injectivity of A it follows that $\tilde{a}$ is a unique zero of $\mathcal{F}(\cdot, b)$.

In the applications to follow we are interested not only in the existence of a zero $\tilde{a}$ of $\mathcal{F}(\cdot, b)$, but also in some information about the derivative. The following corollary provides some control over the norm of the inverse of $D_1\mathcal{F}(\tilde{a}, b)$, and when A is invertible provides some control over the difference between the true and approximate inverse at the true zero. Note that the corollary recycles several bounds already used in Theorem 2.1.

Corollary 2.2 (Bounds on the inverse derivative composed with A) *Suppose that X, $\mathcal{F}$, $\bar{a}$, b, A, $A^\dagger$, Z_0, Z_1, $Z_2(r)$ and $p(r)$ are as in Theorem 2.1, and that $r_0 > 0$ has $p(r_0) < 0$. Let $\tilde{a}$ be the unique solution of $\mathcal{F}(\cdot, b) = 0$ in $B_{r_0}(\bar{a})$ given by Theorem 2.1. Then*

1. *$AD_1\mathcal{F}(\tilde{a}, b)$ is boundedly invertible with*

$$\left\| \left[AD_1\mathcal{F}(\tilde{a}, b)\right]^{-1} \right\|_{B(X)} \le \frac{1}{1 - (Z_2(r_0) + Z_1 + Z_0)}. \tag{16}$$

2. *If A is invertible so is $D_1\mathcal{F}(\tilde{a}, b)$. In this case we have the bound*

$$\left\| D_1\mathcal{F}(\tilde{a}, b)^{-1} \right\|_{B(X)} \le \frac{\|A\|_{B(X)}}{1 - (Z_2(r_0) + Z_1 + Z_0)}. \tag{17}$$

3. *When A is invertible we also have the bound*

$$\left\| D_1\mathcal{F}(\tilde{a}, b)^{-1} - A \right\|_{B(X)} \le \frac{Z_0 + Z_1 + Z_2(r_0)}{1 - (Z_0 + Z_1 + Z_2(r_0))} \|A\|_{B(X)}. \tag{18}$$

Proof To prove (16) we write

$$D_1\mathcal{F}(\tilde{a}, b) = D_1\mathcal{F}(\tilde{a}, b) - D_1\mathcal{F}(\bar{a}, b) + D_1\mathcal{F}(\bar{a}, b) - A^\dagger + A^\dagger$$

so that

$$
\begin{aligned}
A\, D_1\mathcal{F}(\tilde{a}, b) &= A\left[D_1\mathcal{F}(\tilde{a}, b) - D_1\mathcal{F}(\bar{a}, b) + D_1\mathcal{F}(\bar{a}, b) - A^\dagger + A^\dagger\right] + \mathrm{Id} - \mathrm{Id} \\
&= \mathrm{Id} - \left(A\left[D_1\mathcal{F}(\bar{a}, b) - D_1\mathcal{F}(\tilde{a}, b)\right] + A\left[A^\dagger - D_1\mathcal{F}(\bar{a}, b)\right] + \left[\mathrm{Id} - AA^\dagger\right]\right)
\end{aligned}
$$

or

$$A\, D_1\mathcal{F}(\tilde{a}, b) = \mathrm{Id} - B, \tag{19}$$

where

$$B \overset{\text{def}}{=} \text{Id} - AD_1\mathcal{F}(\tilde{a}, b).$$

Combining the definition of B with the calculation above gives

$$B = A\left[D_1\mathcal{F}(\bar{a}, b) - D_1\mathcal{F}(\tilde{a}, b)\right] + A\left[A^\dagger - D_1\mathcal{F}(\tilde{a}, b)\right] + \left[\text{Id} - AA^\dagger\right].$$

The fact that $\tilde{a} \in B_{r_0}(\bar{a})$ and the estimate of Equation (15) (the contraction constant) leads to the bound

$$\begin{aligned}
\|B\|_{B(X)} &\leq \left\|A\left[D_1\mathcal{F}(\bar{a}, b) - D_1\mathcal{F}(\tilde{a}, b)\right]\right\|_{B(X)} + \left\|A\left[A^\dagger - D_1\mathcal{F}(\tilde{a}, b)\right]\right\|_{B(X)} \\
&\quad + \left\|\text{Id} - AA^\dagger\right\|_{B(X)} \\
&\leq Z_2(r_0) + Z_1 + Z_0 < 1.
\end{aligned}$$

This uses the hypothesis that $p(r_0) < 0$, just as in the proof of Theorem 2.1 sketched above. Now, by the Neumann theorem, we have that $\text{Id} - B$ is invertible with the desired bound.

The proof of (17) is as follows. Since A is invertible, we multiply both sides of Equation (19) by A^{-1} to obtain

$$D_1\mathcal{F}(\tilde{a}, b) = A^{-1}(\text{Id} - B). \tag{20}$$

Since both operators on the right hand side of Equation (20) are invertible we have that the product is invertible and that $D_1\mathcal{F}(\tilde{a}, b)^{-1} = (\text{Id} - B)^{-1}A$. Taking norms and employing the bound from Eq. (16) gives inequality (17). Finally, to establish (18) we recall that

$$\|B\|_{B(X)} = \|\text{Id} - AD_1\mathcal{F}(\tilde{a}, b)\|_{B(X)} < 1,$$

again exploiting $p(r_0) < 0$. Observing that

$$D_1\mathcal{F}(\tilde{a}, b)^{-1} - A = \left[\text{Id} - AD_1\mathcal{F}(\tilde{a}, b)\right]\left[D_1\mathcal{F}(\tilde{a}, b)\right]^{-1},$$

the bound (17) gives the inequality of Eq. (18). □

2.3 The Implicit Time Stepping Scheme

We now apply the results of Sect. 2.2 to the method of steps for DDEs. The main task is simply to write down explicit formulas for the function $\mathcal{F}$ and the fixed point operator T defined in Eq. (3) for the method of steps. These in turn implicitly define the step map Φ.

Let $X = C([-1, 1], \mathbb{R}^d)$ and define $\mathcal{F}: X \times X \to X$ by

$$\begin{aligned}
\mathcal{F}(y, x)(t) &= y(t) - x(1) - \frac{\tau}{2}\int_{-1}^{t} f(y(s), x(s))\,ds \\
&= y(t) - T(y, x)(t), \tag{21}
\end{aligned}$$

where T is the fixed point operator defined in Eq. (3). Observe that we change from (a, b) to (y, x) when we want to stress that the variables are functions. We save the (a, b) notation for later after we transform the problem to the space of infinite Chebyshev sequences.

Now, let $\Phi: C([-1, 1], \mathbb{R}^d) \to C([-1, 1], \mathbb{R}^d)$ denote the step map as defined in Section 1.1. For fixed $x \in C([-1, 1], \mathbb{R}^d)$ we have that $y(t)$ corresponds (after shifting and rescaling of the domain) to a solution of the DDE with history $x(t)$ if and only if $\Phi(x) = y$, if and only if y is a fixed point of $T(\cdot, x)$, if and only if y is a solution of the equation $\mathcal{F}(\cdot, x) = 0$.

In the following we write D, D_1, D_2 to denote Fréchet derivatives and partial Fréchet derivatives with respect to infinite dimensional variables, and ∂_1, ∂_2 to denote the usual partial derivatives with respect to finite dimensional (vector valued) variables. Then

$$D_1 \mathcal{F}(y, x) = \text{Id} - D_1 T(y, x), \tag{22}$$

where for $h \in X$ this operator has action

$$[D_1 \mathcal{F}(y, x)h](t) = h(t) - \frac{\tau}{2} \int_{-1}^{t} \partial_1 f(y(x), x(s))h(s)\, ds. \tag{23}$$

It is worth recording also that the partial Fréchet derivative with respect to the second variable – the past history – is

$$[D_2 T(y, x)h](t) = -[D_2 \mathcal{F}(y, x)h](t) = h(1) + \frac{\tau}{2} \int_{-1}^{t} \partial_2 f(y(x), x(s))h(s)\, ds. \tag{24}$$

In Sect. 3 we use Eq. (23) to define the approximate derivative $A^\dagger$ and approximate inverse A hypothesized in Theorem 2.1. The formula in Eq. (24) is needed to compute the validated C^1 bounds for the step map.

Suppose that $x \in C([-1, 1], \mathbb{R}^d)$ is given and that $y \in C([-1, 1], \mathbb{R}^d)$ is a fixed point of $T(\cdot, x)$. Recall from Sect. 2.1 that the step map is well defined near x if $\text{Id} - D_1 T(y, x)$ is an isomorphism. We now see that this is equivalent to the nondegeneracy of $D_1 \mathcal{F}(y, x)$ in the sense of Corollary 2.2. So, if we prove the existence of a zero of $\mathcal{F}(y, x)$ using Theorem 2.1 then the step map is locally well defined near x. Moreover the step map Φ is differentiable at x with $D\Phi(x)$ given by Eq. (10), which can now be rewritten as

$$D\Phi(x) = -D_1 \mathcal{F}(y, x)^{-1} D_2 \mathcal{F}(y, x) = (\text{Id} - D_1 T(y, x))^{-1} D_2 T(y, x). \tag{25}$$

We stress that if y is found through a successful application of Theorem 2.1 and if A is invertible, then Corollary 2.2 provides invertibility and norm bounds on $D_1 \mathcal{F}(y, x)$.

2.4 Validated Bounds on the Derivative

Suppose $y, x \in C([-1, 1], \mathbb{R}^d)$ have that $\mathcal{F}(y, x) = 0$, so that $\Phi(x) = y$. Then, by the discussion above $D\Phi(x)$ exists and is given by Eq. (25). Suppose that y results from a successful application of Theorem 2.1, and that we would like to obtain information about the derivative. We need to introduce a new operator $A_2^\dagger$, which approximates $D_2 \mathcal{F}(\bar{y}, x)$. Indeed in practice $A_2^\dagger$ is a finite matrix with zero tail.

Recall that $A^\dagger$ is an approximation of $D_1 \mathcal{F}(\bar{y}, x)$ and that A is an approximate inverse of $A^\dagger$. Then, recalling the formula for the derivative of the implicitly defined mapping Φ given in Eq. (10), we have in fact that that

$$D\Phi(x) \approx -A A_2^\dagger.$$

This is a convenient approximation as A and $A_2^\dagger$ are known quantities. The next theorem provides a quantitative bound on the approximation.

Theorem 2.3 (C^1 bounds for an implicit time step) *Suppose that $X = C([-1, 1], \mathbb{R}^d)$, that $\mathcal{F}$ is as defined in Eq. (21), and that $\bar{y}, x \in X$, $A \in B(X)$, Z_0, Z_1, $Z_2(r)$ and $p(r)$ satisfy the hypotheses of Theorem 2.1. Assume that A is invertible and that $A_2^\dagger \in B(X)$. Assume further*

that $r_0 > 0$ has $p(r_0) < 0$. Let $\tilde{y}$ be the unique solution of $\mathcal{F}(\cdot, x) = 0$ in $B_{r_0}(\bar{y})$ given by Theorem 2.1. Let

$$M \stackrel{\text{def}}{=} -AA_2^\dagger \in B(X). \tag{26}$$

If $\delta_0, \delta_1, \delta_2 \geq 0$ are constants with

$$\|D_2\mathcal{F}(\tilde{y}, x)\|_{B(X)} \leq \delta_0 \tag{27}$$

$$\left\| A[D_2\mathcal{F}(\bar{y}, x) - A_2^\dagger] \right\|_{B(X)} \leq \delta_1 \tag{28}$$

$$\|A[D_2\mathcal{F}(\tilde{y}, x) - D_2\mathcal{F}(\bar{y}, x)]\|_{B(X)} \leq \delta_2 \tag{29}$$

then

$$\|D\Phi(x) - M\|_{B(X)} \leq \left(\frac{Z_0 + Z_1 + Z_2(r_0)}{1 - (Z_0 + Z_1 + Z_2(r_0))} \right) \|A\|_{B(X)}\delta_0 + \delta_1 + \delta_2. \tag{30}$$

Proof The idea of the proof is that M approximately solves Eq. (9). That is

$$\|D_1\mathcal{F}(\tilde{y}, x)M + D_2\mathcal{F}(\tilde{y}, x)\|_{B(X)} \ll 1.$$

Then M approximates the derivative and we seek an a-posteriori bound on the approximation. Recalling (26) and that $D\Phi(x) = -D_1\mathcal{F}(\tilde{y}, x)^{-1}D_2\mathcal{F}(\tilde{y}, x)$ we have that

$$D\Phi(x) - M = -[D_1\mathcal{F}(\tilde{y}, x)^{-1} - A]D_2\mathcal{F}(\tilde{y}, x) - A[D_2\mathcal{F}(\tilde{y}, x) - D_2\mathcal{F}(\bar{y}, x)]$$
$$- A[D_2\mathcal{F}(\bar{y}, x) - A_2^\dagger].$$

Applying triangle's inequality gives the desired result:

$$\|D\Phi(x) - M\|_{B(X)}$$
$$\leq \|[D_1\mathcal{F}(\tilde{y}, x)^{-1} - A]D_2\mathcal{F}(\tilde{y}, x)\|_{B(X)} + \|A[D_2\mathcal{F}(\tilde{y}, x) - D_2\mathcal{F}(\bar{y}, x)]\|_{B(X)}$$
$$+ \|A[D_2\mathcal{F}(\bar{y}, x) - A_2^\dagger]\|_{B(X)}$$
$$\leq \|[D_1\mathcal{F}(\tilde{y}, x)^{-1} - A]\|_{B(X)}\|D_2\mathcal{F}(\tilde{y}, x)\|_{B(X)} + \delta_2 + \delta_1$$
$$\leq \frac{Z_0 + Z_1 + Z_2(r_0)}{1 - (Z_0 + Z_1 + Z_2(r_0))}\|A\|_{B(X)}\delta_0 + \delta_2 + \delta_1.$$

$\square$

3 Computer-Assisted Proofs for the Method of Steps

In this section, we introduce the necessary steps to apply the Newton–Kantorovich approach of Theorem 2.1 to prove existence of zeros of the nonlinear map $\mathcal{F}$ given by (5). First, we introduce in Sect. 3.1 the Banach space X in which we look for solutions of $\mathcal{F} = 0$. Then in Sect. 3.2, we introduce the finite dimensional projection used to compute numerical approximations. Third, we introduce in Sect. 3.3 the bounded linear operators $A, A^\dagger : X \to X$ required to apply Theorem 2.1.

3.1 Banach Spaces of Infinite Sequences with Rapid Decay

Recall from Sect. 1.2 that we employ Chebyshev series to pass from analysis in function spaces to sequence spaces, and that in doing so differentiation is represented by a (diagonally

dominant) infinite matrix, multiplication is given by discrete cosine convolution, and the C^0 norm is bounded by an appropriate weighted little ell-one norm. Again we refer to [36,37] for more general discussion.

Then, given a sequence of weights $\omega = (\omega_n)_{n \geq 0}$ given by

$$\omega_n \overset{\text{def}}{=} \begin{cases} 1, & n = 0 \\ 2\nu^n, & n > 1 \end{cases} \tag{31}$$

for a given real number $\nu \geq 1$, define

$$\ell_\omega^1 \overset{\text{def}}{=} \left\{ \alpha = (\alpha_n)_{n \geq 0} : \alpha_n \in \mathbb{R} \quad \text{and} \quad \|\alpha\|_\omega \overset{\text{def}}{=} \sum_{n \geq 0} |\alpha_n| \omega_n < \infty \right\}. \tag{32}$$

For $a, b \in \ell_\omega^1$, denote by $a * b$ the discrete convolution given component-wise by

$$(a * b)_n = \sum_{\substack{n_1 + n_2 = n \\ n_1, n_2 \in \mathbb{Z}}} a_{|n_1|} b_{|n_2|}.$$

It is a classical result that for the weights given in (31), $(\ell_\omega^1, *)$ is a Banach algebra, that is $\|a * b\|_\omega \leq \|a\|_\omega \|b\|_\omega$ for all $a, b \in \ell_\omega^1$. Indeed this is an example of a Beurling algebra, whose elementary properties are explored in [58].

Given $b \in \ell_\omega^1$ we look for a solution of $\mathcal{F}(a, b) = 0$ in the space

$$X \overset{\text{def}}{=} (\ell_\omega^1)^d = \{ a = (a_1, a_2, \ldots, a_d) : a_j \in \ell_\omega^1, \quad \text{for } j = 1, \ldots, d \}$$

with norm

$$\|a\|_X \overset{\text{def}}{=} \max_{j=1,\ldots,d} \{ \|a_j\|_\omega \}. \tag{33}$$

Remark 3.1 When $f : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}^d$ is polynomial, the terms ϕ_n as in (4) are discrete convolutions (in a and b) and if $b \in X$, that if $b_j \in \ell_\omega^1$ for each $j = 1, \ldots, d$, since ℓ_ω^1 defined in (32) is a Banach algebra under discrete convolution, then the map $\mathcal{F}$ satisfies $\mathcal{F} : X \times X \to X$.

Given an initial condition $b \in X$, the idea of the computer-assisted proof of existence of a zero of $\mathcal{F}(\cdot, b)$ is to demonstrate that a certain Newton-like operator is a contraction on a closed ball centered at a numerical approximation $\bar{a}$. Computing a numerical approximation requires considering a finite dimensional projection of the nonlinear map (5).

Remark 3.2 (Choice of weights and regularity) Adjusting the weights $\{\omega_n\}$ in the space (32) provides control over the regularity of the fixed point argument. Throughout this paper, we choose the weights given in (31) for a given real number $\nu \geq 1$. Suppose that we obtain a fixed point $\tilde{a} \in \ell_\omega^1$ with $\nu = 1$. The resulting $y_1 : [-1, 1] \to \mathbb{R}^n$ with Chebyshev coefficients given by $\tilde{a}$ is then in $C^0([-1, 1], \mathbb{R}^n)$ and moreover is differentiable almost everywhere (absolutely continuous). On the other hand, taking $\nu > 1$ results in y_1 real analytic on $[-1, 1]$. Of course a given b may be in some spaces and not others, and in practice this will limit our choices. On the other hand, we are often guided by theoretical results, for example when f is real analytic we know that any periodic solution of the DDE is real analytic [59], suggesting the use of exponential. That said, other weights could be used to represent C^k functions, namely

$$\omega_n \overset{\text{def}}{=} \begin{cases} 1, & n = 0 \\ 2(n + 1)^k, & n > 1 \end{cases},$$

which still makes ℓ_ω^1 a Banach algebra (e.g. see [60]).

3.2 Finite Dimensional Projection

To compute $\bar{a}$, we consider a finite dimensional projection of the map $\mathcal{F} : X \times X \to X$. Given a *projection dimension* number $N \in \mathbb{N}$, and given a vector $\alpha = (\alpha_n)_{n\geq0} \in \ell_\omega^1$, consider the projection $\pi^N : \ell_\omega^1 \to \mathbb{R}^{N+1} : \alpha \mapsto \pi^N\alpha \stackrel{\text{def}}{=} (\alpha_n)_{n=0}^N \in \mathbb{R}^{N+1}$. We extend this to product spaces, defining $\pi_d^N : X \to \mathbb{R}^{d(N+1)}$ by $\pi_d^N(a_1, \ldots, a_d) \stackrel{\text{def}}{=} (\pi^N a_1, \ldots, \pi^N a_d) \in \mathbb{R}^{d(N+1)}$. Often, given $a \in X$, we denote

$$a^{(N)} \stackrel{\text{def}}{=} \pi_d^N a \in \mathbb{R}^{d(N+1)}.$$

Moreover, we define the natural inclusion $\iota^N : \mathbb{R}^{N+1} \hookrightarrow \ell_\omega^1$ as follows. For $\alpha = (\alpha_n)_{n=0}^N \in \mathbb{R}^{N+1}$ let $\iota^N\alpha \in \ell_\omega^1$ be defined component-wise by

$$\left(\iota^N\alpha\right)_n = \begin{cases} \alpha_n, & n = 0, \ldots, N \\ 0, & n \geq N+1. \end{cases}$$

Similarly, let $\iota_d^N : \mathbb{R}^{d(N+1)} \hookrightarrow X$ be the natural inclusion defined as follows: given $a = (a_1, \ldots, a_d) \in (\mathbb{R}^{N+1})^d \cong \mathbb{R}^{d(N+1)}$,

$$\iota_d^N a \stackrel{\text{def}}{=} \left(\iota^N a_1, \ldots, \iota^N a_d\right) \in X.$$

Consider the *finite dimensional projection* $\mathcal{F}^{(N)} : \mathbb{R}^{d(N+1)} \times \mathbb{R}^{d(N+1)} \to \mathbb{R}^{d(N+1)}$ of the map $\mathcal{F}$, for $a \in \mathbb{R}^{d(N+1)}$, as

$$\mathcal{F}^{(N)}(a, b) = \pi_d^N \mathcal{F}(\iota_d^N a, \iota_d^N b). \tag{34}$$

Given an initial condition vector $b \in X$, denote by $\bar{b} \stackrel{\text{def}}{=} \pi_d^N b \in \mathbb{R}^{d(N+1)}$. Assume that, using Newton's method, a numerical approximation $\bar{a} \in \mathbb{R}^{d(N+1)}$ of (34) has been obtained, that is $\mathcal{F}^{(N)}(\bar{a}, \bar{b}) \approx 0$. We slightly abuse the notation and denote $\bar{a} \in \mathbb{R}^{d(N+1)}$ and $\iota_d^N \bar{a} \in X$ both using $\bar{a}$. We use a similar identification for $\bar{b}$.

3.3 Definition of the Operators $A^\dagger$ and A

Consider the finite dimensional projection $\mathcal{F}^{(N)} : \mathbb{R}^{d(N+1)} \times \mathbb{R}^{d(N+1)} \to \mathbb{R}^{d(N+1)}$ and assume that we computed (e.g. using Newton's method) $\bar{a} \in \mathbb{R}^{d(N+1)}$ such that $\mathcal{F}^{(N)}(\bar{a}, \bar{b}) \approx 0$. Denote by $D_1\mathcal{F}^{(N)}(\bar{a}, \bar{b}) \in M_{d(N+1)}(\mathbb{R})$ the Jacobian matrix of $\mathcal{F}^{(N)}$ at $\bar{a}$. Given $a \in X$, define

$$A^\dagger a = \iota_d^N \pi_d^N A^\dagger a + (\text{Id} - \iota_d^N \pi_d^N)A^\dagger a, \tag{35}$$

where $\pi_d^N A^\dagger a = D_1\mathcal{F}^{(N)}(\bar{a}, \bar{b})a^{(N)}$ and $(\text{Id} - \iota_d^N \pi_d^N)A^\dagger a = (\text{Id} - \iota_d^N \pi_d^N)a$. Since $A^\dagger \to D_1 F(\bar{a}, \bar{b})$ as $N \to \infty$ we expect that for N large enough, $A^\dagger$ is a good approximation of the Fréchet derivative $D_1\mathcal{F}(\bar{a}, \bar{b})$. Its action on the finite dimensional projection is the Jacobian matrix (the derivative) of $\mathcal{F}^{(N)}$ at $\bar{a}$ while its action on the tail is the identity.

Consider now a matrix $A^{(N)} \in M_{d(N+1)}(\mathbb{R})$ computed so that $A^{(N)} \approx D_1\mathcal{F}^{(N)}(\bar{a}, \bar{b})^{-1}$. In other words, this means that $\|\text{Id} - A^{(N)} D_1\mathcal{F}^{(N)}(\bar{a}, \bar{b})\| \ll 1$, where here Id refers to as the $d(N+1) \times d(N+1)$ identity matrix. This step is performed using numerical linear algebra

software (MATLAB in our case). We decompose the matrix $A^{(N)}$ block-wise as

$$A^{(N)} = \{A_{i,j}^{(N)}\}_{i,j=1}^{d},$$

so that it acts on $a^{(N)} = (a_1^{(N)}, \ldots, a_d^{(N)}) \in \mathbb{R}^{d(N+1)}$. The operator A is defined block-wise as

$$A = \{A_{i,j}\}_{i,j=1}^{d}, \tag{36}$$

where the action of each block of A is finite (that is they act on $a^{(N)} = \pi_d^N a$ only) except for the d diagonal blocks $A_{j,j}$ ($j = 1, \ldots, n$) which have infinite (identity) tails. More explicitly, for each $j = 1, \ldots, d$,

$$(A_{i,j}a_j)_n = \begin{cases} (A_{i,j}^{(N)}\pi^N a_j)_n & n = 0, \ldots, N+1, \\ \delta_{i,j}(a_j)_n & n \geq N+1. \end{cases} \tag{37}$$

Having defined the operators A and $A^\dagger$, the last step in applying the a-posteriori method of Theorem 2.1 is the construction of the bounds Y_0, Z_0, Z_1 and Z_2 satisfying (11)–(14), respectively. The construction of these bounds reduces to calculations which are by now standard in the field of rigorous numerics. See for example the works of [61–63]. Then, rather than developing the bounds in full generality, we focus instead on the specific case of Wright's equation

$$u'(t) = f(u(t), u(t-\tau)) \overset{\text{def}}{=} -\alpha u(t-\tau)(1+u(t)), \quad \alpha \in \mathbb{R}. \tag{38}$$

Fixing a scalar DDE with quadratic nonlinearity minimizes the proliferation of technical details, while still illustrating all the main steps of the procedure. The reader interested in the construction of Y_0, Z_0, Z_1 and Z_2 bounds for general polynomial problems is referred to [41,49].

3.4 Explicit Bounds for the Rigorous C^1 Integration of Wright's Equation

Equation (38) is referred to as Wright's Equation, and is a classic example of a simple DDE with long period stable oscillatory dynamics. For Wright's equation, the Banach space is simply $X = \ell_\omega^1$ as this is a scalar equation. Recall that we use the weights ω_n given by (31).

3.4.1 The Bound Y_0

Assume that the initial condition with Chebyshev coefficients $b = (b_n)_{n \geq 0}$ is given with an error bound of the form

$$\|b - \bar{b}\|_X = \max_{j=1,\ldots,d} \{\|b_j - \bar{b}_j\|_\omega\} \leq \varepsilon_0,$$

where $\bar{b}$ is the center of the ball of initial conditions, which we take to have the same number of non zero components as $\bar{a}$. In the context of a calculation involving multiple time steps the truncation error ε_0 on the initial history comes from the rigorous error bound in the previous

time step. Denote $b^\varepsilon \overset{\text{def}}{=} b - \bar{b} \in X$ with $\|b^\varepsilon\|_X \leq \varepsilon_0$. Then, at $a = \bar{a}$

$$
\mathcal{F}_n(\bar{a}, b) = \mathcal{F}_n(\bar{a}, \bar{b} + b^\varepsilon)
$$

$$
= \begin{cases}
\bar{a}_0 + 2 \displaystyle\sum_{k=1}^{N} (-1)^k \bar{a}_k - \left(\bar{b}_0 + 2 \sum_{k=1}^{N} \bar{b}_k \right) - \left(b_0^\varepsilon + 2 \sum_{k \geq 1} b_k^\varepsilon \right), & n = 0 \\[2ex]
\bar{a}_n - \dfrac{\tau}{4n} (\phi_{n-1}(\bar{a}, \bar{b} + b^\varepsilon) - \phi_{n+1}(\bar{a}, \bar{b} + b^\varepsilon)), & n \geq 1.
\end{cases}
$$

For each $n \geq 0$, write

$$
\phi_n(\bar{a}, \bar{b} + b^\varepsilon) = \phi_n(\bar{a}, \bar{b}) + \psi_n(\bar{a}, \bar{b}, b^\varepsilon),
$$

where the terms $\psi_n(\bar{a}, \bar{b}, b^\varepsilon)$ may either be computed exactly using an expansion (in case the equations are polynomials) or can be estimated (using for instance the mean value inequality in Banach spaces). Note that $\mathcal{F}(\bar{a}, b)$ can be split as a sum of two terms, that is $\mathcal{F}(\bar{a}, b) = \mathcal{F}(\bar{a}, \bar{b}) + \mathcal{G}(\bar{a}, \bar{b}, b^\varepsilon)$, where

$$
\mathcal{G}_n(\bar{a}, \bar{b}, b^\varepsilon) \overset{\text{def}}{=}
\begin{cases}
- \left(b_0^\varepsilon + 2 \displaystyle\sum_{k \geq 1} b_k^\varepsilon \right), & n = 0 \\[2ex]
- \dfrac{\tau}{4n} (\psi_{n-1}(\bar{a}, \bar{b}, b^\varepsilon) - \psi_{n+1}(\bar{a}, \bar{b}, b^\varepsilon)), & n \geq 1.
\end{cases}
$$

For Wright's equation, $\phi(a, b) = -\alpha b - \alpha a * b$ and therefore

$$
\begin{aligned}
\psi(\bar{a}, \bar{b}, b^\varepsilon) &= \phi(\bar{a}, \bar{b} + b^\varepsilon) - \phi(\bar{a}, \bar{b}) \\
&= -\alpha(\bar{b} + b^\varepsilon) - \alpha \bar{a} * (\bar{b} + b^\varepsilon) + \alpha \bar{b} + \alpha \bar{a} * \bar{b} \\
&= -\alpha(b^\varepsilon + \bar{a} * b^\varepsilon) \\
&= -\alpha(\hat{1} + \bar{a}) * b^\varepsilon,
\end{aligned}
$$

where $\hat{1} \overset{\text{def}}{=} (1, 0, 0, 0, \dots,) \in \ell_\omega^1$.

Compute $Y_0^{(1)}$ with interval arithmetic such that

$$
\|A\mathcal{F}(\bar{a}, \bar{b})\|_\omega \leq Y_0^{(1)}.
$$

The computation of $Y_0^{(1)}$ involves the rigorous evaluation of $\mathcal{F}(\bar{a}, \bar{b})$. If $f : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}^d$ in (1) is polynomial, then the resulting map $\mathcal{F}(\bar{a}, \bar{b})$ involves discrete convolutions with only finitely many nonzero terms. This rigorous evaluation can be done using the *Fast Fourier Transform* (FFT) algorithm combined with Banach algebra estimates (see [60]). If f is non-polynomial having nonlinearities that are solutions of polynomial ODEs, it is possible to introduce a higher dimensional polynomial embedding which will recover the dynamics of the original DDE (e.g. see [64,65]).

Denote by A_0 the first column of the operator A and $A_{1,\infty}$ the operator A "take away" the first column A_0. More explicitly, denoting the operator A entry-wise by $A = (A_{m,n})_{m,n \geq 0}$, the operator $A_{1,\infty}$ is defined entry-wise by $A_{1,\infty} = (A_{m,n})_{m \geq 0, n \geq 1}$. Then,

$$
A\mathcal{G}(\bar{a}, \bar{b}, b^\varepsilon) = -A_0 \left(b_0^\varepsilon + 2 \sum_{k \geq 1} b_k^\varepsilon \right) + \frac{\tau \alpha}{4} A_{1,\infty} \left(\left(\Lambda^{-1} \mathcal{T}(\hat{1} + \bar{a}) * b^\varepsilon \right)_n \right)_{n=1}^{\infty},
$$

and therefore, using the Banach algebra and that $\left|b_0^\varepsilon + 2\sum_{k\geq 1} b_k^\varepsilon\right| \leq \|b^\varepsilon\|_\omega \leq \varepsilon_0$,

$$\|A\mathcal{G}(\bar{a},\bar{b},b^\varepsilon)\|_\omega \leq Y_0^{(2)} \stackrel{\text{def}}{=} \left(\|A_0\|_\omega + \frac{\tau|\alpha|}{4}\|A_{1,\infty}\left(\left(\Lambda^{-1}\mathcal{T}(\hat{1}+\bar{a})\right)_n\right)_{n=1}^\infty\|_\omega\right)\varepsilon_0.$$

The computation of $Y_0^{(2)}$ involves first computing the vector $\Lambda^{-1}\mathcal{T}(\hat{1}+\bar{a})$, which has only finitely many nonzero terms. Indeed, recalling the linear operators $\mathcal{T}$ and Λ^{-1} in (6),

$$v_n \stackrel{\text{def}}{=} \left(\Lambda^{-1}\mathcal{T}(\hat{1}+\bar{a})\right)_n = \begin{cases} 0, & n = 0 \\ 1 + \bar{a}_0 - \bar{a}_2, & n = 1 \\ \frac{1}{n}(\bar{a}_{n-1} - \bar{a}_{n+1}), & n \in \{2, \ldots, N-1\} \\ \frac{1}{n}\bar{a}_{n-1}, & n \in \{N, N+1\} \\ 0, & n \geq N+2. \end{cases}$$

Then, recalling from (37) that the operator consists of a finite dimensional block matrix in $M_{N+1}(\mathbb{R})$ and a diagonal (identity) tail,

$$\|A_{1,\infty}\left(\left(\Lambda^{-1}\mathcal{T}(\hat{1}+\bar{a})\right)_n\right)_{n=1}^\infty\|_\omega = \sum_{m=0}^N \left|\sum_{n=1}^N A_{m,n}^{(N)} v_n\right|\omega_m + \frac{1}{N+1}|\bar{a}_N|\omega_{N+1},$$

which is used to compute $Y_0^{(2)}$. Finally, set

$$Y_0 \stackrel{\text{def}}{=} Y_0^{(1)} + Y_0^{(2)}. \tag{39}$$

3.4.2 The Bound Z_0

The following result is useful when computing bounded linear operator norms on ℓ_ω^1. For an elementary proof see [62].

Lemma 3.3 *Consider a linear operator $Q: \ell_\omega^1 \to \ell_\omega^1$ of the form*

$$Q = \begin{bmatrix} Q^{(N)} & & & 0 \\ & q_{N+1} & & \\ & & q_{N+2} & \\ 0 & & & \ddots \end{bmatrix}$$

where $Q^{(N)} = \left(Q_{m,n}^{(N)}\right)_{0\leq m,n\leq N}$ and $q_n \in \mathbb{R}$. Assume that $|q|_\infty = \sup_{n>N}|q_n| < \infty$. Then

$$\|Q\|_{B(\ell_\omega^1)} = \max\left(\max_{0\leq n\leq N}\frac{1}{\omega_n}\sum_{m=0}^N |Q_{m,n}^{(N)}|\omega_m, \; |q|_\infty\right). \tag{40}$$

Let $B \stackrel{\text{def}}{=} \text{Id} - AA^\dagger$. By construction of the tails of A and $A^\dagger$, $B_{m,n} = 0$ for $m > N$ or $n > N$. Letting

$$Z_0 \stackrel{\text{def}}{=} \max_{0\leq n\leq N}\frac{1}{\omega_n}\sum_{0\leq m\leq N}|B_{m,n}|\omega_m, \tag{41}$$

Lemma 3.3 gives $\|\text{Id} - AA^\dagger\|_{B(\ell_\omega^1)} \leq Z_0$.

3.4.3 The Bound Z_1

Let $h \in \ell^1_\omega$ with $\|h\|_\omega \leq 1$ and let

$$z \stackrel{\text{def}}{=} (D_1 \mathcal{F}(\bar{a}, b) - A^\dagger) h.$$

Set

$$h^{(I)} \stackrel{\text{def}}{=} (\text{Id} - \iota^N \pi^N) h = (0, \ldots, 0, h_{N+1}, h_{N+2}, \ldots) \in \ell^1_\omega.$$

Recalling that $\pi_1^N A^\dagger a = D_1 \mathcal{F}^{(N)}(\bar{a}, \bar{b}) a^{(N)}$, then

$$z_n = \begin{cases} 2 \sum\limits_{k \geq N+1} (-1)^k h_k, & n = 0 \\ \dfrac{\tau \alpha}{4n} \left(\mathcal{T}(h^{(I)} * \bar{b} + h * b^\varepsilon) \right)_n, & n = 1, \ldots, N \\ \dfrac{\tau \alpha}{4n} \left(\mathcal{T}(h * \bar{b} + h * b^\varepsilon) \right)_n, & n > N. \end{cases}$$

Denote

$$z_n^{(1)} \stackrel{\text{def}}{=} \begin{cases} 2 \sum_{k \geq N+1} (-1)^k h_k, & n = 0 \\ \frac{\tau \alpha}{4n} \left(\mathcal{T}(h^{(I)} * \bar{b}) \right)_n, & n = 1, \ldots, N \\ \frac{\tau \alpha}{4n} \left(\mathcal{T}(h * \bar{b}) \right)_n, & n > N. \end{cases} \quad \text{and} \quad z_n^{(2)} \stackrel{\text{def}}{=} \begin{cases} 0, & n = 0 \\ \frac{\tau \alpha}{4n} \left(\mathcal{T}(h * b^\varepsilon) \right)_n, & n = 1, \ldots, N \\ \frac{\tau \alpha}{4n} \left(\mathcal{T}(h * b^\varepsilon) \right)_n, & n > N \end{cases}$$

so that $z = z^{(1)} + z^{(2)}$. More explicitly, $z^{(2)} = \frac{\tau \alpha}{4} \Lambda^{-1} \mathcal{T}(h * b^\varepsilon)$, and hence

$$\begin{aligned} \|A z^{(2)}\|_\omega &\leq \frac{\tau \alpha}{4} \|A \Lambda^{-1} \mathcal{T}(h * b^\varepsilon)\|_\omega \\ &\leq \frac{\tau \alpha}{4} \|A \Lambda^{-1} \mathcal{T}\|_{B(\ell^1_\omega)} \varepsilon_0 \\ &\leq Z_1^{(2)} \stackrel{\text{def}}{=} \frac{\tau \alpha}{4} \|A \Lambda^{-1}\|_{B(\ell^1_\omega)} (\hat{\omega} + \check{\omega}) \varepsilon_0, \end{aligned} \tag{42}$$

where we used the rather straightforward result

$$\|\mathcal{T}\|_{B(\ell^1_\omega)} \leq \hat{\omega} + \check{\omega}, \tag{43}$$

where

$$\hat{\omega} \stackrel{\text{def}}{=} \sup_{k \geq 0} \frac{\omega_{k+1}}{\omega_k} \quad \text{and} \quad \check{\omega} \stackrel{\text{def}}{=} \sup_{k \geq 2} \frac{\omega_{k-1}}{\omega_k}.$$

Recalling that the weights are given by $\omega_k = 1$, for $k = 0$ and $\omega_k = 2\nu^k$ for $k \geq 1$,

$$\hat{\omega} = \max \left(\frac{2\nu}{1}, \sup_{k \geq 1} \frac{2\nu^{k+1}}{2\nu^k} \right) = 2\nu \quad \text{and} \quad \check{\omega} = \sup_{k \geq 2} \frac{2\nu^{k-1}}{2\nu^k} = \frac{1}{\nu}.$$

The more involved estimate is to bound $\|A z^{(1)}\|_\omega$. First note that $|z_0^{(1)}| \leq \frac{1}{\nu^{N+1}}$.

The following technical lemma, which is a slight modification of Corollary 3 in [62]), will be useful when bounding $\|A z^{(1)}\|_\omega$.

Lemma 3.4 *Fix a truncation Chebyshev mode to be N. Let $M \in \mathbb{N}$ and let $\bar{\alpha} = (\bar{\alpha}_0, \ldots, \bar{\alpha}_M, 0, 0, \ldots) \in \ell^1_\omega$. Then, for all $h \in \ell^1_\omega$ such that $\|h\|_\omega \leq 1$, and for $k = 0, \ldots, N$,*

$$\left| (\bar{\alpha} * h^{(I)})_k \right| \leq \Psi_k(\bar{\alpha}) \stackrel{\text{def}}{=} \max_{\ell = N+1, \ldots, k+M} \frac{|\bar{\alpha}_{k+\ell} + \bar{\alpha}_{|k-\ell|}|}{\omega_\ell}. \tag{44}$$

Defining $\hat{z}^{(1)} \in \mathbb{R}_+^{N+1}$ component-wise by

$$
\hat{z}_n^{(1)} = \begin{cases} \dfrac{1}{\nu^{N+1}}, & n = 0 \\ \dfrac{\tau \alpha}{4n} \left(|\mathcal{T}^{(N)}| \Psi(\bar{b}) \right)_n, & n = 1, \ldots, N \end{cases}
$$

we have

$$
\begin{aligned}
\|Az^{(1)}\|_\omega &= \sum_{n \geq 0} |[Az^{(1)}]_n| \omega_n \\
&\leq \sum_{n=0}^{N} |[Az^{(1)}]_n| \omega_n + \sum_{n > N} |[Az^{(1)}]_n| \omega_n \\
&\leq \sum_{n=0}^{N} [|A^{(N)}| \hat{z}^{(1)}]_n \omega_n + \frac{\tau \alpha}{4(N+1)} \sum_{n > N} |[\mathcal{T}(h * \bar{b})]_n| \omega_n \\
&\leq \sum_{n=0}^{N} [|A^{(N)}| \hat{z}^{(1)}]_n \omega_n + \frac{\tau \alpha}{4(N+1)} \sum_{n \geq 0} |[\mathcal{T}(h * \bar{b})]_n| \omega_n \\
&\leq Z_1^{(1)} \overset{\text{def}}{=} \sum_{n=0}^{N} [|A^{(N)}| \hat{z}^{(1)}]_n \omega_n + \frac{\tau \alpha}{4(N+1)} (\hat{\omega} + \check{\omega}) \|\bar{b}\|_\omega, \quad (45)
\end{aligned}
$$

where we used (43) to establish the last inequality. Combining (45) and (42), we see that

$$
Z_1 \overset{\text{def}}{=} Z_1^{(1)} + Z_1^{(2)} \tag{46}
$$

satisfies (13).

3.4.4 The Bound Z_2

Since for Wright's equation, $\phi(a, b) = -\alpha b - \alpha a * b$ is linear in a, then $D_1 \mathcal{F}(c, b) - D_1 \mathcal{F}(\bar{a}, b) = 0$. Hence, we set $Z_2 = 0$.

In the next subsections, we compute the bounds δ_0, δ_1 and δ_2, satisfying (27)–(29), respectively. Recall that via Theorem 2.3 these bounds are used to compute C^1-bounds for the step map F.

3.4.5 The Bound δ_0

Recall that δ_0 is a bound for $\|D_2 \mathcal{F}(\tilde{a}, b)\|_{B(\ell_\omega^1)}$. Let $h \in B_1(0) \subset X$ and denote by $z \overset{\text{def}}{=} D_2 \mathcal{F}(\tilde{a}, b)h$ which is given component-wise by

$$
z_n = \begin{cases} -\left(h_0 + 2 \sum_{k \geq 0} h_k \right), & n = 0 \\ \dfrac{\tau \alpha}{4n} (\mathcal{T}(h + \tilde{a} * h))_n, & n \geq 1, \end{cases}
$$

and which satisfies (recalling the definition of the weights ω_n in (32))

$$
\begin{aligned}
\|z\|_\omega = |z_0| + 2\sum_{n\geq 0}|z_n|\nu^n &\leq \left(|h_0| + 2\sum_{k\geq 0}|h_k|\right) + 2\sum_{n\geq 1}\left|\frac{\tau\alpha}{4n}\left(\mathcal{T}(h+\tilde{a}*h)\right)_n\right|\nu^n \\
&\leq 1 + \frac{\tau\alpha}{4}\|\mathcal{T}\|_{B(\ell^1_\omega)}\|h+\tilde{a}*h\|_\omega \\
&\leq 1 + \frac{\tau\alpha}{4}(\hat{\omega}+\check{\omega})(1+\|\tilde{a}\|_\omega) \\
&\leq 1 + \frac{\tau\alpha}{4}(\hat{\omega}+\check{\omega})(1+\|\bar{a}\|_\omega + r_0).
\end{aligned}
$$

Hence, we set

$$
\delta_0 \overset{\text{def}}{=} 1 + \frac{\tau\alpha}{4}(\hat{\omega}+\check{\omega})(1+\|\bar{a}\|_\omega + r_0). \tag{47}
$$

3.4.6 The Bound δ_1

Recall that δ_1 satisfies $\left\|A[D_2\mathcal{F}(\bar{a},b) - A_2^\dagger]\right\|_{B(\ell^1_\omega)} \leq \delta_1$. Denote by $D_2\mathcal{F}^{(N)}(\bar{a},\bar{b}) \in M_{N+1}(\mathbb{R})$. Given $h \in \ell^1_\omega$, define

$$
A_2^\dagger h = \iota_1^N \pi_1^N A_2^\dagger h + (\text{Id} - \iota_1^N \pi_1^N)0, \tag{48}
$$

where $\pi_1^N A_2^\dagger h = D_2\mathcal{F}^{(N)}(\bar{a},\bar{b})h^{(N)}$. Again we note that as $N \to \infty$, $A_2^\dagger$ approaches the Fréchet derivative $D_2\mathcal{F}(\bar{a},\bar{b})$, and hence we expect the approximation to be good when N is large enough. The action of $A^\dagger$ on the finite dimensional projection is the Jacobian matrix (the derivative w.r.t b) of $\mathcal{F}^{(N)}$ while its action on the tail is zero. Let $h \in \ell^1_\omega$ with $\|h\|_\omega \leq 1$ and let

$$
z \overset{\text{def}}{=} (D_2\mathcal{F}(\bar{a},b) - A_2^\dagger)h.
$$

Recalling that $\pi_1^N A_2^\dagger h = D_2\mathcal{F}^{(N)}(\bar{a},\bar{b})h^{(N)}$, we have

$$
z_n = \begin{cases} -2\sum_{k\geq N+1} h_k, & n = 0 \\ \frac{\tau\alpha}{4n}\left(\mathcal{T}(\bar{a}*h^{(I)})\right)_n, & n = 1,\ldots,N \\ \frac{\tau\alpha}{4n}(\mathcal{T}(h+\bar{a}*h))_n, & n > N. \end{cases}
$$

Defining $\hat{z} \in \mathbb{R}_+^{N+1}$ component-wise by

$$
\hat{z}_n = \begin{cases} \dfrac{1}{\nu^{N+1}}, & n = 0 \\ \dfrac{\tau\alpha}{4n}\left(|\mathcal{T}^{(N)}|\Psi(\bar{a})\right)_n, & n = 1,\ldots,N \end{cases}
$$

we see that

$$
\begin{aligned}
\|Az\|_\omega &\leq \sum_{n=0}^{N} |[Az]_n|\omega_n + \sum_{n>N} |[Az]_n|\omega_n \\
&\leq \sum_{n=0}^{N} [|A^{(N)}|\hat{z}]_n\omega_n + \frac{\tau\alpha}{4(N+1)} \sum_{n>N} |[\mathcal{T}(h + \bar{a} * h)]_n|\omega_n \\
&\leq \sum_{n=0}^{N} [|A^{(N)}|\hat{z}]_n\omega_n + \frac{\tau\alpha}{4(N+1)} \sum_{n\geq 0} |[\mathcal{T}(h + \bar{a} * h)]_n|\omega_n \\
&\leq \delta_1 \stackrel{\text{def}}{=} \sum_{n=0}^{N} [|A^{(N)}|\hat{z}]_n\omega_n + \frac{\tau\alpha}{4(N+1)} \|\mathcal{T}\|_{B(\ell^1_\omega)}(1 + \|\bar{a}\|_\omega).
\end{aligned}
\tag{49}
$$

3.4.7 The Bound δ_2

Since for Wright's equation, $\phi(a, b) = -\alpha b - \alpha a * b$ is linear in b, then $D_2\mathcal{F}(\tilde{a}, b) - D_2\mathcal{F}(\bar{a}, b) = 0$. Hence, we set $\delta_2 = 0$.

Having defined all the bounds hypothesized in Theorems 2.1 and 2.3 we now present some applications.

3.5 Rigorous C^1 Integration for Wright's Equation

The bounds Y_0, Z_0 and Z_1 given by (39), (41) and (46) are implemented in the MATLAB program `script_iterate_wright_cheb.m` which uses the interval arithmetic library INTLAB [50] and Chebfun [66]. We fixed the parameter value to $\alpha \approx 2.350319657675625$, since at that value, there is a periodic orbit of period roughly equal to 5. We fixed an initial condition $b \in \mathbb{R}^{27}$ close to 0 with fast decay (the Chebyshev coefficients of b can be found in the file `b0.mat` available on the codes' website mentioned in Section 1), fixed $\nu = 1.1$ and the number of Chebyshev coefficients per step to be $N = 40$. The code verified successfully the hypothesis of Theorem 2.1 for 17 consecutive steps. At each step, the program verifies the existence of $r_0 > 0$ such that $p(r_0) < 0$. The orbit is visualized in Figure 1 and the values of r_0 are found in Table 1.

The bounds δ_0 and δ_1 given respectively by (47) and (49) are also implemented in the program and Theorem 2.3 and applied to prove, still with $N = 40$ and $\nu = 1.1$, that in the first step we have $\|D\Phi(x) - M\|_{B(\ell^1_\omega)} \leq 0.229$, with M an explicitly known matrix stored during the program execution. We changed $N = 200$, and obtained a proof that $\|D\Phi(x) - M\|_{B(\ell^1_\omega)} \leq 0.0172$. Fixing $\nu = 1.01$ and $N = 1000$, we proved that

$$
\|D\Phi(x) - M\|_{B(\ell^1_\omega)} \leq 0.00369.
$$

It is clear that the accuracy of the C^1 bounds improve as N is increased, and that there is hope of obtaining qualitative information about stability using these bounds. Yet, in many problems such bounds are not needed as we illustrate in the next section.
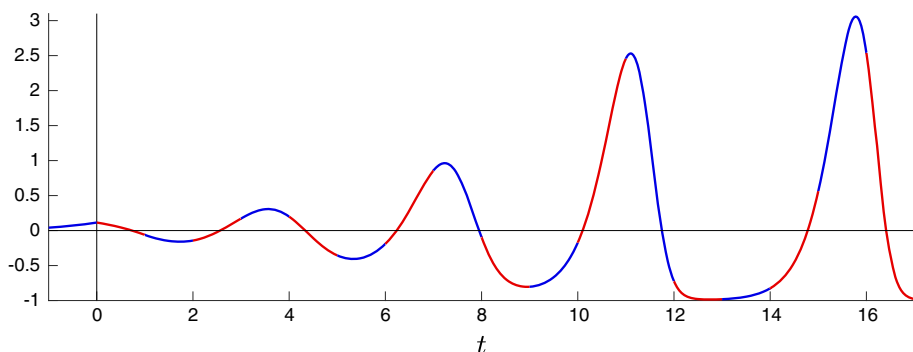
Fig. 1 A rigorously computed 17-step orbit in Wright's equation at the parameter value $\alpha \approx 2.350319657675625$. The final step appears to be close to an attracting periodic solution of Wright's. This illustrates an integration starting near an unstable equilibrium and terminating near the global attractor

4 Proofs of Existence of *m*-Steps Periodic Solutions in DDEs

Using the rigorous method of steps of this paper, we can obtain computer-assisted proofs of existence of some specific type, namely *m*-steps periodic solutions, which we now define.

Definition 4.1 Given an integer $m \in \mathbb{N}$, a differentiable function $\psi : \mathbb{R} \to \mathbb{R}^d$ is said to be an *m-steps periodic solution* of the delay equation $y'(t) = f(y(t), y(t - \tau))$ if ψ solves the equation, $\psi(t + T) = \psi(t)$ for all $t \in \mathbb{R}$ and $T = m\tau$.

An m-steps periodic solution of the delay equation $y'(t) = f(y(t), y(t-\tau))$ is represented with a sequence of m sequences $a^{(1)}, a^{(2)}, \ldots, a^{(m)} \in (\ell^1_\omega)^d$ satisfying

$$\begin{pmatrix} \mathcal{F}(\tau, a^{(2)}, a^{(1)}) \\ \mathcal{F}(\tau, a^{(3)}, a^{(2)}) \\ \vdots \\ \mathcal{F}(\tau, a^{(m)}, a^{(m-1)}) \\ \mathcal{F}(\tau, a^{(1)}, a^{(m)}) \end{pmatrix} = 0 \in (\ell^1_\omega)^{md}, \tag{50}$$

where $\mathcal{F}$ is given by (5). More explicitly, given $i \in \{1, \ldots, m - 1\}$,

$$\mathcal{F}_n(\tau, a^{(i+1)}, a^{(i)}) \overset{\text{def}}{=} \begin{cases} a_0^{(i+1)} + 2\sum_{k \geq 1}(-1)^k a_k^{(i+1)} - \left(a_0^{(i)} + 2\sum_{k \geq 1} a_k^{(i)}\right), & n = 0 \\ a_n^{(i+1)} - \dfrac{\tau}{4n}(\phi_{n-1}(a^{(i+1)}, a^{(i)}) - \phi_{n+1}(a^{(i+1)}, a^{(i)})), & n \geq 1 \end{cases} \tag{51}$$

Remark 4.2 Given an integer $m \in \mathbb{N}$, solving for an m-steps periodic solution of the delay equation $y'(t) = f(y(t), y(t - \tau))$ requires having that $\frac{T}{\tau} = m \in \mathbb{N}$. Rather than solving for the period T (or equivalently the frequency), we solve for the delay τ for which we can find a solution to (57).

By construction, a solution of (50) yields the existence of an m-steps periodic solution of $y'(t) = f(y(t), y(t - \tau))$. Let us consider applications of this approach to prove existence of periodic solutions in the Mackey–Glass equation.

Table 1 At each step, the values of $r_0 > 0$ such that $p(r_0) < 0$

step	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17
r_0	1.3e-15	9.3e-15	7.5e-14	5.9e-13	3e-12	1.7e-11	2.2e-10	2e-09	5.3e-09	5.4e-08	1.5e-06	1.5e-05	2.3e-05	3.4e-04	7.8e-03	0.23	3.84

4.1 Applications to the Mackey–Glass Equation

Consider the scalar delay differential equation

$$u'(t) = g(u(t), u(t-\tau)) = -\gamma u(t) + \beta \frac{u(t-\tau)}{1+u(t-\tau)^\rho}, \qquad \gamma, \beta, \rho > 0. \tag{52}$$

Typically ρ is chosen large and possibly non-integer [67,68]. Denote $y_1(t) \overset{\text{def}}{=} u(t)$. Letting

$$y_2(t) \overset{\text{def}}{=} \frac{y_1(t)}{1+y_1(t)^\rho} = h(y_1(t)),$$

then $y_1'(t) = -\gamma y_1(t) + \beta y_2(t-\tau)$. Letting $y_3(t) \overset{\text{def}}{=} y_1(t)^{\rho-2}$ and $y_4(t) \overset{\text{def}}{=} y_1(t)^{-1}$ allows us considering the following system of polynomial DDEs

$$y_1'(t) = -\gamma y_1(t) + \beta y_2(t-\tau), \tag{53a}$$

$$y_2'(t) = y_2(t)\,(y_4(t) - \rho y_2(t)y_3(t))\,(-\gamma y_1(t) + \beta y_2(t-\tau)), \tag{53b}$$

$$y_3'(t) = (\rho-2)y_4(t)y_3(t)\,(-\gamma y_1(t) + \beta y_2(t-\tau)), \tag{53c}$$

$$y_4'(t) = -y_4(t)^2\,(-\gamma y_1(t) + \beta y_2(t-\tau)). \tag{53d}$$

Denote $y(t) = (y_1(t), y_2(t), y_3(t), y_4(t))$, $x(t) = (x_1(t), x_2(t), x_3(t), x_4(t)) = y(t-\tau) = (y_1(t-\tau), y_2(t-\tau), y_3(t-\tau), y_4(t-\tau))$ and

$$f(y(t), x(t)) \overset{\text{def}}{=} \begin{pmatrix} -\gamma y_1(t) + \beta x_2(t) \\ y_2(t)\,(y_4(t) - \rho y_2(t)y_3(t))\,(-\gamma y_1(t) + \beta x_2(t)) \\ (\rho-2)y_4(t)y_3(t)\,(-\gamma y_1(t) + \beta x_2(t)) \\ -y_4(t)^2\,(-\gamma y_1(t) + \beta x_2(t)) \end{pmatrix}.$$

To compute periodic orbits of the Mackey–Glass equation via the system of polynomial delay equations (53a)–(53d), one must introduce the unfolding parameters (as the ones considered in [41]) together with the extra scalar equations included to impose the correct initial conditions on the auxiliary differential equations describing the nonlinearities. More explicitly, one solves

$$y_1'(t) = -\gamma y_1(t) + \beta y_2(t-\tau), \qquad\qquad\qquad y_1(0) = 1, \tag{54a}$$

$$y_2'(t) = -\gamma y_1(t)y_2(t)y_4(t) + \beta y_2(t)y_4(t)y_2(t-\tau) + \rho\gamma y_1(t)y_2(t)^2 y_3(t)$$
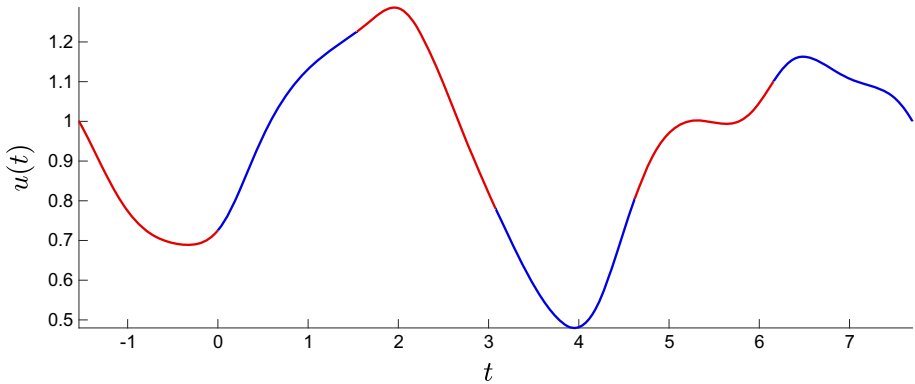$$\qquad - \rho\beta y_2(t)^2 y_3(t)y_2(t-\tau) + \eta_1, \qquad\qquad y_2(0) = 1/2, \tag{54b}$$

$$y_3'(t) = -\gamma(\rho-2)y_1(t)y_3(t)y_4(t) + \beta(\rho-2)y_3(t)y_4(t)y_2(t-\tau) + \eta_2, \quad y_3(0) = 1, \tag{54c}$$

$$y_4'(t) = \gamma y_1(t)y_4(t)^2 - \beta y_4(t)^2 y_2(t-\tau) + \eta_3, \qquad\qquad y_4(0) = 1. \tag{54d}$$

Hence, in this case

$$\phi_n(a, b, \eta) \overset{\text{def}}{=} \begin{pmatrix} (-\gamma a_1 + \beta b_2)_n \\ (-\gamma a_1 a_2 a_4 + \beta a_2 a_4 b_2 + \rho\gamma a_1 a_2^2 a_3 - \rho\beta a_2^2 a_3 b_2 + \hat\eta_1)_n \\ (-\gamma(\rho-2)a_1 a_3 a_4 + \beta(\rho-2)a_3 a_4 b_2 + \hat\eta_2)_n \\ (\gamma a_1 a_4^2 - \beta a_4^2 b_2 + \hat\eta_3)_n \end{pmatrix}, \tag{55}$$

where $\hat\eta_j \overset{\text{def}}{=} (\eta_j, 0, 0, 0, \dots) \in \ell_\omega^1$ for $j = 1, 2, 3$.

Fig. 2 A rigorously validated 6-step periodic orbit of the Mackey–Glass equation at the parameter values $\alpha = 2$, $\beta = 1$ and $\rho = 10$. For the proof, we used $N = 55$ Chebyshev coefficients per component and fixed $\nu = 1.05$. The radius enclosure of the orbit is given by $r = 2.5 \times 10^{-8}$ and the delay τ is given by the rigorous enclosure $\tau \in 1.539575123 \pm [-r, r]$. The code which performs the proof is `script_proof_PO_Fig3_MG_period_6.m`
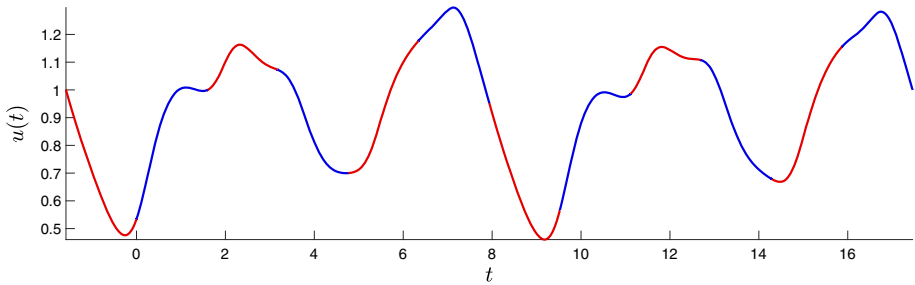
Fig. 3 A rigorously validated 12-step periodic orbit in the Mackey–Glass equation at the parameter values $\alpha = 2$, $\beta = 1$ and $\rho = 10$. For the proof, we used $N = 60$ Chebyshev coefficients per component and fixed $\nu = 1.033$. The radius enclosure of the orbit is given by $r = 4.3 \times 10^{-8}$ and the delay τ is given by the rigorous enclosure $\tau \in 1.587078323 \pm [-r, r]$. The code which performs the proof is `script_proof_PO_Fig4_MG_period_12.m`

The unknowns describing the m-steps periodic solutions in the Mackey–Glass equations are given by the time delay $\tau \in \mathbb{R}$, the unfolding parameters $\eta = (\eta_1, \eta_2, \eta_3) \in \mathbb{R}^3$ and the Chebyshev coefficients of each step $a^{(i)} \in X = (\ell^1_\omega)^d$ for $i = 1, \ldots, m$. Denote
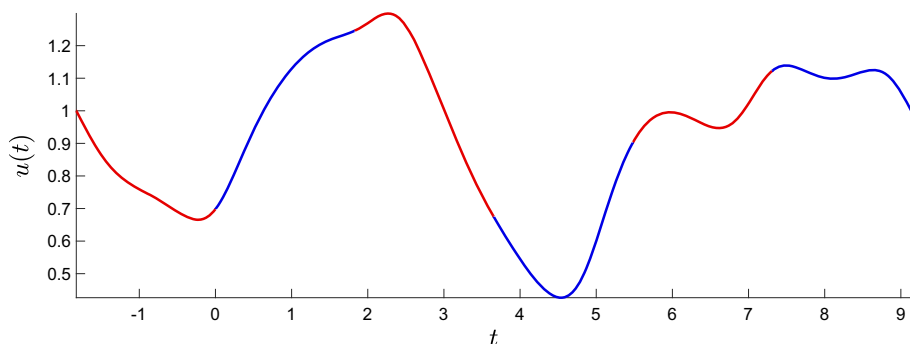
$$x \overset{\text{def}}{=} (\tau, \eta, a^{(1)}, \ldots, a^{(m)}) \in \mathcal{X} \overset{\text{def}}{=} \mathbb{R}^4 \times X \times \cdots \times X = \mathbb{R} \times \mathbb{R}^3 \times X^m.$$

We endow the Banach space $\mathcal{X}$ with the product norm

$$\|x\|_{\mathcal{X}} \overset{\text{def}}{=} \max\{|\tau|, |\eta_1|, |\eta_2|, |\eta_3|, \|a^{(1)}\|_X, \ldots, \|a^{(m)}\|_X\}.$$

Using Chebyshev series expansion of the solution $y(t)$ on the first time step interval $[0, \tau]$, the four extra scalar equations $y_1(0) = 1$, $y_2(0) = 1/2$, $y_3(0) = 1$ and $y_4(0) = 1$ become

$$P_j \overset{\text{def}}{=} (a^{(1)}_j)_0 + 2\sum_{k \geq 1} (-1)^k (a^{(1)}_j)_k - \alpha_j = 0, \quad j = 1, 2, 3, 4$$

Fig. 4 A rigorously validated 6-step periodic orbit in the Mackey–Glass equation at the parameter values $\alpha = 2$, $\beta = 1$ and $\rho = 9.65$. For the proof, we used $N = 54$ Chebyshev coefficients per component and fixed $\nu = 1.05$. The radius enclosure of the orbit is given by $r = 3.5 \times 10^{-8}$ and the delay τ is given by the rigorous enclosure $\tau \in 1.827334865 \pm [-r, r]$. The code which performs the proof is `script_proof_PO_Fig5_MG_period_6.m`

where $\alpha_1 = \alpha_3 = \alpha_4 = 1$ and $\alpha_2 = 1/2$. Denote $P(a^{(1)}) \stackrel{\text{def}}{=} \left(P_1(a^{(1)}), P_2(a^{(1)}), P_3(a^{(1)}), P_4(a^{(1)}) \right) \in \mathbb{R}^4$. This leads to the zero finding problem $\mathcal{F}^{(\text{po})} : \mathcal{X} \to \mathcal{X}$ given by

$$
\mathcal{F}^{(\text{po})}(x) \stackrel{\text{def}}{=}
\begin{pmatrix}
P(a^{(1)}) \\
\mathcal{F}(\tau, \eta, a^{(2)}, a^{(1)}) \\
\vdots \\
\mathcal{F}(\tau, \eta, a^{(m)}, a^{(m-1)}) \\
\mathcal{F}(\tau, \eta, a^{(1)}, a^{(m)})
\end{pmatrix}, \tag{56}
$$

where

$$
\mathcal{F}_n(\tau, \eta, a, b) \stackrel{\text{def}}{=}
\begin{cases}
a_0 + 2 \sum_{k \geq 1} (-1)^k a_k - \left(b_0 + 2 \sum_{k \geq 1} b_k \right), & n = 0 \\
a_n - \dfrac{\tau}{4n} (\phi_{n-1}(a, b, \eta) - \phi_{n+1}(a, b, \eta)), & n \geq 1
\end{cases} \tag{57}
$$

with $\phi_n(a, b, \eta)$ given in (55). By construction, a solution $x \in \mathcal{X}$ to $\mathcal{F}^{(\text{po})}(x) = 0$ yields an m-steps periodic solution of (52). To prove the existence of solutions to $\mathcal{F}^{(\text{po})} = 0$, we may apply Theorem 2.1, or any Newton–Kantorovich type theorem. In this way we proved the existence of two 6-step and one 12-step periodic solutions of the Mackey–Glass equation. These validated solutions are illustrated in Figs. 2, 3 and 4 . Details about the parameters are given in the captions.

Note that we have not computed the C^1 bounds associated to the periodic orbits in Mackey–Glass, as this would involve more than just computing $D\Phi$ at each step of the orbit. More explicitly, this involves computing a bound on the derivative of a composition operator. While we believe this can be done, this is the subject of future investigation. Finally note that the polynomial embedding approach does not create any obstruction in obtaining information about the Floquet multipliers associated to the periodic orbit (e.g. see [64]).

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