Parameterization of unstable manifolds for DDEs: formal series solutions and validated error bounds

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Abstract

This paper studies the local unstable manifold attached to an equilibrium solution of a system of delay differential equations (DDEs). Two main results are developed. The first is a general method for computing the formal Taylor series coefficients of a function parameterizing the unstable manifold. We derive linear systems of equations whose solutions are the Taylor coefficients, describe explicit formulas for assembling the linear equations for DDEs with polynomial nonlinearities. We also discuss a scheme for transforming non-polynomial DDEs into polynomial ones by appending auxiliary equations. The second main result is an a-posteriori theorem which – when combined with deliberate control of rounding errors – leads to mathematically rigorous computer assisted convergence results and error bounds for the truncated series. Our approach is based on the parameterization method for invariant manifolds and requires some mild non-resonance conditions between the unstable eigenvalues.

Key words. delay differential equations, invariant manifolds, parameterization method, formal power series, validated numerics, computer assisted proof

1 Introduction

Invariant manifolds are fundamental objects of study in dynamical systems theory. One standard approach to analyzing a nonlinear system is to locate some elementary compact invariant manifolds – for example equilibrium solutions, periodic orbits, and invariant tori – to study the linearized stability of these sets, and then to study their attached stable and unstable manifolds. Stable and unstable manifolds provide information about the way solutions approach the invariant object in forward and backward time, and intersections between stable/unstable manifolds trigger global bifurcations and illuminate transitions between different regions in phase space.

Numerical methods for computing stable/unstable manifolds is a topic of sustained interest thanks to their great theoretical and practical importance. In the present work we are especially interested in computational methods which lead to mathematically rigorous results. Such methods are used to prove theorems about systems with strong nonlinearities far from perturbative regimes where classical pen and paper methods may be unavailable. The utility of these techniques is not limited to finite dimensional settings, and computer assisted methods of proof for partial and delay differential

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equations (PDEs and DDEs) are active areas of research. A thorough discussion of the literature would take us far afield and we refer instead to the review articles of [1, 2, 3, 4, 5, 6], and to the books of [7, 8]. For the reader interested in computer assisted proofs for DDEs we recommend also the recent groundbreaking work of [9, 10, 11] on the resolution of both Wright's and Jones' conjectures about the global dynamics of Wright's equation.

The present work develops a general computational framework for studying unstable manifolds attached to equilibrium solutions of DDEs. There is much interest in computational techniques for studying invariant manifolds in equations with delays and we refer to work of [12, 13, 14, 15, 16, 17] for more discussion of the growing field. We focus on systems of DDEs having a single constant delay; however the content of this paper can be easily generalized for multiple constant delays. The nonlinearities of the systems are restricted to the one given by elementary functions (that is: polynomial, rational, trigonometric, inverse trigonometric, exponential, logarithmic, and more generally functions which can be expressed as the solutions of polynomial ordinary differential equations). Our main goals are to (A) develop formal series methods for approximating the unstable manifold to any desired order, and (B) to obtain mathematically rigorous convergence results and error bounds on all discretization and truncation errors so that our results can be validated and used as ingredients in more sophisticated computer assisted existence proofs involving connecting orbits and global bifurcations of DDEs (though such applications are not the topic of the present work).

Our approach is based on the parameterization method of [18, 19, 20], which provides a functional analytic framework for both theoretical and numerical studies of invariant manifolds in a wide variety of settings. The idea behind the parameterization method is to formulate an invariance equation describing chart maps for the manifold. The invariance equation is formulated in terms of a dynamical conjugacy to a simple well understood model system (in the present work we take the model to be linear), so that the parameterization method recovers the dynamics on the manifold in addition to its embedding. Moreover, the fact that the parameterization solves a functional equation is the basis of all our a-posteriori analysis hence is essential for formulating computer assisted proofs employing implicit function theory.

The interested reader will find in the book of [21] a clear exposition of the parameterization method, along with many worked examples and applications to problems in mathematical physics and engineering. The reference just mentioned provides also a thorough review of the now substantial literature, including discussion of its use in computer assisted proofs. For the purposes of the present work, which focuses on the dynamics of systems with constant delays, we refer also to the work of [17, 16] where parameterization methods for unstable manifolds attached to equilibrium and periodic solutions of scalar DDEs are developed. Indeed the present work is something of a sequel to [17], in that we generalize that work to systems of DDEs with non-polynomial nonlinearities, and more significantly, develop and implement the a-posteriori analysis necessary to obtain rigorous computer assisted error bounds.

The remainder of the paper is organized as follows. In the next section we give an overview of the main results of the paper. Section 2 develops formal power series expansions for the unstable manifold parameterizaitons. In particular, general formulas for the homological equations are derived. Section 3 developes a-posterior analysis for the formal series leading to a computer assisted strategy for bounding the series. Finally in Section 4 we apply the methods of the paper to a number of example problems. Julia implementations of the algorithms discussed in this paper are found at

`http://www.math.mcgill.ca/jplessard/ResearchProjects/unstableDDE/home.html`

1.1 Overview of main results

Throughout the paper, we discuss the case of DDEs with one constant delay. Nonetheless, the reader should bear in mind that all the results easily extend to DDEs with multiple constant delays. We

believe that this generalization is clear enough to allow us to formulate the paper in the more appealing form corresponding to the case of DDEs with one constant delay.

Let $F\colon \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}^d$ be smooth function and $\tau > 0$. Consider the system of DDEs with a single constant delay given by

$$\frac{d}{dt}x(t) = F(x(t), x(t-\tau)). \tag{1}$$

We recall a few well known facts about such equations, while remarking that the interested reader may refer to the classic texts [22, 23] for much more complete discussions. For example, we say that the function $x(t)$ is an *equilibrium solution* if and only if $x(t) = c$ for some $c \in \mathbb{R}^d$ and $x(t)$ solves Equation (1) for all $t \in \mathbb{R}$. This happens if and only if c is a solution of the equation

$$F(c, c) = 0,$$

so that finding equilibrium solutions reduces to finding roots of finite dimensional systems of non-linear equations. In the present work we assume that F is real analytic in both variables in some neighborhood of c.

The stability of an equilibrium is determined by the roots (real or complex) of the nonlinear *characteristic equation*

$$\det\left(D_1F(c,c) + D_2F(c,c)e^{-\lambda\tau} - \lambda\,\mathrm{Id}\right) = 0, \tag{2}$$

where D_iF denotes the derivative (a Jacobian matrix) of F with respect to its i^{th} variable ($i = 1, 2$). That is, such λ are the eigenvalues of the linearized DDE at c. In general there are infinitely many solutions of this equation, and we see the infinite dimensional character of the problem rear its head. One can show by examining Equation (2) that there are only ever finitely many eigenvalues to the right of any line in the complex plane of the form $\mathrm{Re}(z) = \alpha$ with $\alpha \in \mathbb{R}$. Here given $z \in \mathbb{C}$, we used the notation $\mathrm{Re}(z) \in \mathbb{R}$ to denote its real part. That is, the infinite part of the spectrum must have negative real part going to infinity. The number of unstable eigenvalues, when finite, is referred to as the *Morse index* of the equilibrium.

For a fixed $\lambda \in \mathbb{C}$ solving Equation (2), an associated eigenfunction is $\Xi(t) = e^{\lambda t}\xi$, where $\xi \in \mathbb{C}^d$ is in the kernel of the matrix

$$\Psi(\lambda) \stackrel{\text{def}}{=} D_1F(c,c) + D_2F(c,c)e^{-\lambda\tau} - \lambda\mathrm{Id}. \tag{3}$$

We refer to $\Psi(\lambda)$ as the *characteristic matrix* for the DDE at c. If λ has multiplicity one then the kernel of $\Psi(\lambda)$ is one dimensional and the function $\Xi(t)$ spans the eigenspace associated with λ. Note that ξ, and hence $\Xi(t)$, is only determined up to a scalar multiple.

An important fact is that a delay differential equation of the form Equation (1) generates a compact semi-flow on an appropriate Banach space, hence the linearization is a compact linear operator. This gives another, more functional analytic explanation for why the Morse index is well defined. Then for some $m \in \mathbb{N}$ there are m unstable eigenvalues which we denote by $\lambda_1, \ldots, \lambda_m \in \mathbb{C}$. These are the m unique complex numbers with

$$\mathrm{Re}(\lambda_j) > 0, \qquad 1 \le j \le m,$$

having that λ_j solves Equation (2). In that case, the Morse index is given by the number m.

We are interested in the power series of the m dimensional local unstable manifold attached to an equilibrium solution, and we build on the analysis found in the recent work of [17]. We refer the interested reader also to the masters dissertation of B. de Wolff [16]. Let $D^m \subset \mathbb{C}^m$ denote the complex unit poly-disk. We write $\sigma = (\sigma_1, \ldots, \sigma_m)$ to denote an element of $\mathbb{C}^m$. The following lemma summarizes the main result of [17]. We include an elementary proof in Appendix B for the sake of completeness. In fact [17] treated only scalar equations, hence the theorem and its proof are non-trivial generalizations.

Lemma 1.1 (Parameterization method for DDEs)**.** *Assume that $c \in \mathbb{R}^d$ is an equilibrium solution of Equation* (1) *with Morse index $m > 0$. Let $\lambda_1, \ldots, \lambda_m \in \mathbb{C}$ denote the m unstable eigenvalues, and assume that the λ_j, $1 \leq j \leq m$ are distinct. Suppose that $\xi_1, \ldots, \xi_m \in \mathbb{C}^d$ are associated eigenvectors – in the sense that each ξ_j is in the kernel of the matrix $\Psi(\lambda_j)$ defined in Equation* (3)*. Assume that $P\colon D^m \times (-\infty, 0] \to \mathbb{R}^d$ is a smooth solution of the invariance equation*

$$\lambda_1\sigma_1 \frac{\partial}{\partial \sigma_1} P(\sigma, t) + \ldots + \lambda_m \sigma_m \frac{\partial}{\partial \sigma_m} P(\sigma, t) = F(P(\sigma, t), P(\sigma, t-\tau)), \tag{4}$$

for all $t \leq 0$ and all $\sigma = (\sigma_1, \ldots, \sigma_m) \in D^m$. Assume also that P satisfies the first order constraints

$$P(0, t) = c, \tag{5}$$

and

$$\frac{\partial}{\partial \sigma_j} P(0, t) = e^{\lambda_j t}\xi_j, \tag{6}$$

for each $1 \leq j \leq m$. Finally, suppose that P has the shift invariance property

$$P(\sigma_1, \ldots, \sigma_m, t-\tau) = P(e^{-\lambda_1\tau}\sigma_1, \ldots, e^{-\lambda_m\tau}\sigma_m, t), \tag{7}$$

for all $t \leq 0$ and all $\sigma \in D^m$. Then P parameterizes a local unstable manifold at c.

Derivation of Equation (4) from first principles (for scalar DDEs) is treated in [17]. See also [16]. The idea behind the derivation is to combine the parameterization method of [18, 19, 20] with the classical theory of ordinary differential equations on function spaces as applied to DDEs in the classic work of [22, 23].

If F is analytic in both arguments then we expect the local unstable manifold to be analytic. In this case it is reasonable to look for analytic solutions of Equation (4). The following lemma from [17] provides the correct form of a power series solution.

Lemma 1.2 (Formal series solution of the invariance equation)**.** *If P is an analytic solution of Equation* (4) *then P has a power series expansion of the form*

$$P(\sigma_1, \ldots, \sigma_m, t) = \sum_{\alpha_1=0}^{\infty} \cdots \sum_{\alpha_m=0}^{\infty} \mathcal{A}_{\alpha_1,\ldots,\alpha_m} e^{(\lambda_1\alpha_1 + \ldots + \lambda_m\alpha_m)t} \sigma_1^{\alpha_1} \ldots \sigma_m^{\alpha_m}, \tag{8}$$

where $\lambda_1, \ldots, \lambda_m$ are the unstable eigenvalues and $\mathcal{A}_{\alpha_1,\ldots,\alpha_m} \in \mathbb{C}^d$ for all $0 \geq \alpha_j$, $1 \leq j \leq m$. The first order constraints of Equations (5) *and* (6) *of Lemma 1.1 require that*

$$\mathcal{A}_{\mathbf{0}} = c, \qquad \mathcal{A}_{e_1} = \xi_1, \qquad \ldots \qquad \mathcal{A}_{e_m} = \xi_m,$$

where $\mathbf{0} = (0, \ldots, 0) \in \mathbb{N}^m$ and $e_1, \ldots, e_m \in \mathbb{N}^m$ are the canonical basis vectors of $\mathbb{R}^m$.

One of the main results of the present work is that, so long as some mild non-resonance conditions hold between the unstable eigenvalues, the coefficients $\mathcal{A}_{\alpha_1,\ldots,\alpha_m} \in \mathbb{C}^d$ with $|\alpha| \geq 2$ are recursively and uniquely determined by systems of linear algebraic equations – where for each index $\alpha \in \mathbb{N}^m$ the linear equation determining the coefficient $\mathcal{A}_\alpha$ depends only on lower order coefficients. These equations are referred to as the *homological equations*, and we derive their general form for a large class of systems. First a definition.

Definition 1 (Non-resonant eigenvalues)**.** We say that the unstable eigenvalues $\lambda_1, \ldots, \lambda_m \in \mathbb{C}$ are *non-resonant* if

$$\alpha_1\lambda_1 + \ldots + \alpha_m\lambda_m \neq \lambda_j, \tag{9}$$

for all $|\alpha| = \alpha_1 + \cdots + \alpha_m \geq 2$ where $1 \leq j \leq m$.

Denote $\Lambda = (\lambda_1, \lambda_2, \ldots, \lambda_m)$ and

$$\langle \alpha, \Lambda \rangle \stackrel{\text{def}}{=} \sum_{j=1}^{m} \alpha_j \lambda_j = \alpha_1 \lambda_1 + \ldots + \alpha_m \lambda_m.$$

Using that notation, the power series (8) may be written as

$$P(\sigma, t) = \sum_{|\alpha| \geq 0} \mathcal{A}_\alpha e^{\langle \alpha, \Lambda \rangle t} \sigma^\alpha,$$

where, given $\alpha = (\alpha_1, \ldots, \alpha_m)$ and $\sigma = (\sigma_1, \ldots, \sigma_m)$ we used the standard multi-indices notations $|\alpha| = \alpha_1 + \cdots + \alpha_m$ and $\sigma^\alpha = \sigma_1^{\alpha_1} \ldots \sigma_m^{\alpha_m}$.

Since the Morse index m of c is finite and the $\alpha_1, \ldots, \alpha_m$ are positive integers, the non-resonance condition (9) is equivalent to asking that $\langle \alpha, \Lambda \rangle = \alpha_1 \lambda_1 + \ldots + \alpha_m \lambda_m$ is not in the spectrum of the linearized problem at c, for all $|\alpha| \geq 2$. Observe that, since there are only finitely many unstable eigenvalues and again, since $\alpha_1, \ldots, \alpha_m \geq 0$, there are only a finite number of opportunities for the eigenvalues to have a resonance. Hence Equation (9), despite first appearances, imposes only a finite number of conditions, for a fixed order $|\alpha|$.

We now state one of our main results, which says that if the unstable eigenvalues are non-resonant, then there exists a formal power series solution of the invariance Equation (4). We state the theorem for polynomial vector fields, though see Remark 1.6. (Note that the theorem does not provide that the radius of convergence is non-zero). Section 2.4 is devoted to the proof.

Theorem 1.3 (Homological equations for a DDE with one scalar delay)**.** *Suppose that $F \colon \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}^d$ is a polynomial mapping and that $F(c, c) = 0$ is an equilibrium solution. Assume that the unstable eigenvalues $\lambda_1, \ldots, \lambda_m$ are non-resonant in the sense of Definition 1. Then the power series solution $P(\sigma, t)$ of the invariance Equation (4) – where P has the form described in Lemma 1.2 – is formally well defined to all orders.*

Moreover, for each $\alpha \in \mathbb{N}^m$ with $|\alpha| \geq 2$ the coefficient $\mathcal{A}_\alpha \in \mathbb{C}^d$ of P is the unique solution of the homological equation

$$\Psi(\langle \alpha, \Lambda \rangle) \mathcal{A}_\alpha = -\hat{\mathcal{F}}_\alpha(\mathcal{A}, {}^\tau\mathcal{A}). \tag{10}$$

Here $\Psi(z)$ is the characteristic matrix defined in Equation (3), ${}^\tau\mathcal{A}$ is a "delayed" coefficient sequence as defined in Section 2.3, and $\hat{\mathcal{F}}_\alpha$ is, for each $\alpha \in \mathbb{N}^m$ with $|\alpha| \geq 2$ a polynomial function of lower order coefficients $\mathcal{A}_\beta$ with $|\beta| < |\alpha|$ given by Equation (17) in Section 2.2.

The role of the non-resonance condition is precisely to guarantee the invertibility of the matrix $\Psi(\alpha_1 \lambda_1 + \ldots + \alpha_m \lambda_m)$, hence the main content of the Theorem is the explicit form of the homological Equation (10). We remark that, while the explicit formula for $\hat{\mathcal{F}}_\alpha$ requires developing some notation, it basically is an expression involving Cauchy products which is completely determined by the monomials of order two and higher in F.

Theorem 1.3 provides a solution of the invariance Equation (4) in the sense of formal power series. It does not provide a non-zero radius of convergence. A-posteriori criterion for the convergence of the series are given in the second main result of the present work, Theorem 3.3 of Section 3.3. To state and prove the bounds requires some technical developments, however the bounds depend in a completely explicit and fairly straightforward way on the coefficients of P computed to order N (using the homological equation of Theorem 1.3), and on the form of the polynomial map F – in particular on the monomial terms of order greater than or equal two in F and its derivative.

Remark 1.4 (Multiplicities and resonances)**.** It is important to remark that both the assumption that the eigenvalues are distinct, and the assumption that they are non-resonanant can be removed. The price is that one has to consider a more general invariance equation. Let m again denote the

number of eigenvalues counted with multiplicity. If the eigenvalues are non-distinct or resonant then we study the more general invariance equation

$$DP(\sigma,t)g(\sigma) = F(P(\sigma,t), P(\sigma,t-\tau)),$$

where $g\colon \mathbb{C}^m \to \mathbb{C}^m$ is a polynomial. In the case of distinct non-resonant eigenvalues we have

$$g(\sigma) = \begin{bmatrix} \lambda_1 & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & \lambda_m \end{bmatrix} \begin{pmatrix} \sigma_1, \\ \vdots \\ \sigma_m \end{pmatrix},$$

as discussed above. That is, g is a linear (in fact diagonal) vector field. When there are repeated and or resonant eigenvalues K must contain additional monomial terms, one monomial corresponding to each repeated or resonant eigenvalue. The order of the monomial is determined by the multiplicity/order of the resonance.

The form of the monomial "corrections" are determined as discussed in [18, 20]. The interested reader is referred also to the work of [24], where numerical implementations with computer assisted error bounds are developed and for explicit examples having multiplicities or resonances. The difference between the work just cited and the present work is that the former deals with ordinary rather than with delay differential equations. Multiplicities/resonances for DDEs can be dealt with precisely the same ideas as in [24], introducing only technical complications. In the present work we focus on distinct non-resonant eigenvalues to reduce the proliferation of technical details.

Remark 1.5 (Polynomial vector fields)**.** It is not necessary to assume that F in Theorem 1.3 is polynomial. Rather the theorem can be established under the weaker assumption that F is analytic in an open neighborhood of (c,c). Imitating the arguments of [18, 20] leads to the same homological equations given in Theorem 1.3, however in the general analytic case the explicit form of the right hand side is less straight forward than the one we will obtain in the present work. Indeed, development of the general case requires the multivariate Faâ di Bruno formula leading to expressions which are computationally cumbersome.

By focusing on polynomial problems we obtain explicit expressions for the right hand side in terms of Cauchy products whose implementation utilizes vector/matrix products, and can be speed up using the FFT. Moreover focusing on polynomial problems is less restrictive than it appears at first glance. See Remark 1.6 below.

Remark 1.6 (**Automatic differentiation**)**.** Many problems appearing in applications are transformed into equivalent polynomial problems by appending additional variables/equations. This is possible when the problem has nonlinear terms which are themselves solutions of polynomial differential equations, that is for most nonlinearities one encounters in practice. The procedure relies on the fact that the chain rule turns composition into multiplication.

The recent work of [25] develops a general framework describing these changes of coordinates and their properties in the general context of autonomous retarded functional differential equations (RFDE). Similar ideas have been used in computer assisted proofs for ordinary differential equations. The idea of using the differential equation solved by a nonlinear function to simplify formal series calculations has a long history and we refer the interested reader to the discussion of semi-numerical algorithms for polynomial manipulations in [26] (focusing on the one variable case) and to Chapter 2 of [21] for the multivariate case. See also [27] for a numerical software package for polynomial manipulations based on these ideas.

For the sake of completeness, we illustrate this discussion with the two following examples.

Example 1.7. Consider for example the scalar DDE given by

$$u'(t) = -u(t) + e^{-u(t-\tau)},$$

and define the new variable

$$v(t) \stackrel{\text{def}}{=} e^{-u(t)}.$$

Note that

$$v'(t) = -e^{-y(t)}y'(t) = -v(t)(-u(t) + e^{-u(t-\tau)}) = u(t)v(t) - v(t)v(t-\tau).$$

The original scalar equation with transcendental nonlinearity is then equivalent to

$$\begin{cases} u'(t) = -u(t) + v(t-\tau), \\ v'(t) = u(t)v(t) - v(t)v(t-\tau), \end{cases}$$

which can be re-written, letting $x(t) \stackrel{\text{def}}{=} (x_1(t), x_2(t)) = (u(t), v(t))$ and $y(t) \stackrel{\text{def}}{=} (y_1(t), y_2(t)) = (u(t-\tau), v(t-\tau))$, as a polynomial system

$$x'(t) = F(x(t), x(t-\tau)) = F(x(t), y(t)) \stackrel{\text{def}}{=} \begin{pmatrix} -x_1(t) + y_2(t) \\ -x_2(t)(-x_1(t) + y_2(t)) \end{pmatrix}.$$

Example 1.8. As a more practical example consider the Mackey-Glass equation

$$u'(t) = -\gamma u(t) + \beta \frac{u(t-\tau)}{1 + u(t-\tau)^\rho}, \tag{11}$$

for $\gamma, \beta, \tau > 0$ and $\rho \in \mathbb{R}$.

Assuming $\rho \in \mathbb{N}$, the new variable $v(t) \stackrel{\text{def}}{=} \dfrac{1}{1 + u(t)^\rho}$ turns Equation (11) into

$$\begin{cases} u'(t) = -\gamma u(t) + \beta u(t-\tau)v(t-\tau), \\ v'(t) = -\rho u(t)^{\rho-1} v(t)^2(-\gamma u(t) + \beta u(t-\tau)v(t-\tau)). \end{cases}$$

Letting $x(t) = (x_1(t), x_2(t)) \stackrel{\text{def}}{=} (u(t), v(t))$ and $y(t) = (y_1(t), y_2(t)) \stackrel{\text{def}}{=} (u(t-\tau), v(t-\tau))$, the above system gives a $(\rho+3)$-th order polynomial system

$$x'(t) = F(x(t), x(t-\tau)) = F(x(t), y(t)) \stackrel{\text{def}}{=} \begin{pmatrix} -\gamma x_1(t) + \beta y_1(t)y_2(t) \\ -\rho x_1(t)^{\rho-1} x_2(t)^2(-\gamma x_1(t) + \beta y_1(t)y_2(t)) \end{pmatrix}. \tag{12}$$

We observe that the above requires $\rho \in \mathbb{N}$ and corresponds a polynomial nonlinearity of degree $\rho + 3$. Thus, for large ρ, the computational cost increase drastically for large ρ.

Introducing $w(t) \stackrel{\text{def}}{=} u(t)^{\rho-1}$ and $z(t) \stackrel{\text{def}}{=} \dfrac{1}{u(t)}$ gives

$$\begin{cases} u'(t) = -\gamma u(t) + \beta u(t-\tau)v(t-\tau), \\ v'(t) = -\rho w(t)v(t)^2(-\gamma u(t) + \beta u(t-\tau)v(t-\tau)), \\ w'(t) = (\rho-1)w(t)z(t)(-\gamma u(t) + \beta u(t-\tau)v(t-\tau)), \\ z'(t) = -z(t)^2(-\gamma u(t) + \beta u(t-\tau)v(t-\tau)), \end{cases}$$

that is

$$x'(t) = F(x(t), x(t-\tau)) = F(x(t), y(t)) \stackrel{\text{def}}{=} \begin{pmatrix} -\gamma x_1(t) + \beta y_1(t)y_2(t) \\ -\rho x_3(t)x_2(t)^2(-\gamma x_1(t) + \beta y_1(t)y_2(t)) \\ (\rho-1)x_3(t)x_4(t)(-\gamma x_1(t) + \beta y_1(t)y_2(t)) \\ -x_4(t)^2(-\gamma x_1(t) + \beta y_1(t)y_2(t)) \end{pmatrix}. \tag{13}$$

Despite producing a higher dimensional system, this second polynomial embedding allows for $\rho \in \mathbb{R}$ and yields a polynomial nonlinearity of degree 5 (independent of ρ). This reformulation of the problem is used for example in the computer assisted existence proofs of periodic solutions to the Mackey-Glass equation to be found in [28]. Note that one can not consider (13) to compute the unstable manifold at 0 since the origin has been sent to infinity. Lastly, the equilibrium at 1 has no unstable manifold for $\rho \in [0, 5]$.

Therefore, for computing the unstable manifold at 0, one must use the first system (12), while for computing the unstable manifold at 1, one should consider using the second system (13).

2 Formal series solution of the invariance equation

The goal of this section is to prove Theorem 1.3. That is, we derive the homological equations defining the formal series solution to the invariance Equation 4. First we develop some notation.

2.1 Power series, Cauchy products, and Cauchy powers

It is convenient to introduce some notation which simplifies our work with multi-variable power series. So for $\alpha = (\alpha_1, \ldots, \alpha_m) \in \mathbb{N}^m$ an m-dimensional multi-index and $\sigma = (\sigma_1, \ldots, \sigma_m) \in \mathbb{C}^m$, define σ raised to the α power to be the number

$$\sigma^\alpha = \sigma_1^{\alpha_1} \ldots \sigma_m^{\alpha_m}.$$

Let $a = \{a_\alpha\}_{|\alpha|=0}^\infty$ be a collection of real (or complex) numbers indexed by an m-dimensional multi-index. We refer to a as an *m-dimensional infinite multi-sequence*. Given an m-dimensional infinite multi-sequence $a = \{a_\alpha\}_{|\alpha|=0}^\infty$ the formal power series p of m-complex variables with coefficients a is expressed as

$$p(\sigma) = \sum_{\alpha_1=0}^\infty \cdots \sum_{\alpha_m=0}^\infty a_{\alpha_1,\ldots,\alpha_m} \sigma_1^{\alpha_1} \ldots \sigma_m^{\alpha_m} = \sum_{|\alpha|=0}^\infty a_\alpha \sigma^\alpha,$$

which may converge only at $\sigma = 0$. Equality, addition, and scalar multiplication of formal power series are defined term by term in the usual way.

Let $p_1(\sigma), \ldots, p_d(\sigma)$ and $q_1(\sigma), \ldots, q_d(\sigma)$ be two collections of d many m-variable formal power series. It is convenient to think of two such collections as in our later work delayed and undelayed variables appear seperately. We write

$$p_j(\sigma) = \sum_{|\alpha|=0}^\infty a_\alpha^j \sigma^\alpha, \qquad \text{and} \qquad q_j(\sigma) = \sum_{|\alpha|=0}^\infty b_\alpha^j \sigma^\alpha,$$

for $1 \le j \le d$, where for each $1 \le j \le d$, the a^j, b^j are m-dimensional infinite multi-sequences.

Multiplicative operations on formal power series are defined by taking Cauchy products of coefficient sequences. More precisely, with $1 \le i, j \le d$ define for each $\alpha \in \mathbb{N}^m$ the sum

$$(a^i * b^j)_\alpha = \sum_{\substack{\beta+\omega=\alpha \\ \beta,\omega \in \mathbb{N}^m}} a_\beta^i b_\omega^j.$$

The m-dimensional infinite multi-sequence $\left\{(a^i * b^j)_\alpha\right\}_{|\alpha|=0}^\infty$ is called *the Cauchy product* of the sequences a^i and b^j, and the product $p_i \cdot q_j$ has formal power series representation

$$p_i(\sigma) q_j(\sigma) = \sum_{|\alpha|=0}^\infty \left(a^i * b^j\right)_\alpha \sigma^\alpha.$$

Next we establish notation helpful for expressing the power series expansion of a general monomial involving the $p_1, \ldots, p_d, q_1, \ldots, q_d$. Define

$$P(\sigma) = (p_1(\sigma), \ldots, p_d(\sigma)), \qquad \text{and} \qquad Q(\sigma) = (q_1(\sigma), \ldots, q_d(\sigma)),$$

so that for $\kappa = (\kappa_1, \ldots, \kappa_d)$, $\gamma = (\gamma_1, \ldots, \gamma_d) \in \mathbb{N}^d$ we have, via the multi-index notation, that

$$P(\sigma)^\kappa \cdot Q(\sigma)^\gamma = p_1(\sigma)^{\kappa_1} \ldots p_d(\sigma)^{\kappa_d} q_1(\sigma)^{\gamma_1} \ldots q_d(\sigma)^{\gamma_d}.$$

Let

$$\mathcal{A}_\alpha \stackrel{\text{def}}{=} (a_\alpha^1, \ldots, a_\alpha^d), \qquad \text{and} \qquad \mathcal{B}_\alpha \stackrel{\text{def}}{=} (b_\alpha^1, \ldots, b_\alpha^d),$$

denote the d-dimensional vectors of m-dimensional infinite multi-sequences.

The monomial $P^\kappa Q^\gamma$ can now be expressed in the convenient form

$$P(\sigma)^\kappa Q(\sigma)^\gamma = \sum_{|\alpha|=0}^{\infty} \left(\mathcal{A}^\kappa * \mathcal{B}^\gamma\right)_\alpha \sigma^\alpha$$

where for each $\alpha \in \mathbb{N}^m$

$$\left(\mathcal{A}^\kappa * \mathcal{B}^\gamma\right)_\alpha = \Big(\underbrace{a^1 * \ldots * a^1}_{\kappa_1 \text{ times}} * \ldots * \underbrace{a^d * \ldots * a^d}_{\kappa_d \text{ times}} * \underbrace{b^1 * \ldots * b^1}_{\gamma_1 \text{ times}} * \ldots * \underbrace{b^d * \ldots * b^d}_{\gamma_d \text{ times}} \Big)_\alpha .$$

2.2 Extracting top coefficients

In the formal series arguments to follow it is necessary to extract terms with index α from the α-th term of a Cauchy product. As motivation for the general notation to follow it is instructive to consider first the simplest case of the product of two power series.

Let $\mathbf{0} = (0, \ldots, 0) \in \mathbb{N}^m$ denote the zero multi-index. Then for $a = \{a_\alpha\}_{|\alpha|=0}^\infty$ and $b = \{b_\alpha\}_{|\alpha|=0}^\infty$ a pair of m-dimensional infinite multi-sequences we have that

$$\begin{aligned}(a * b)_\alpha &= \sum_{\beta+\omega=\alpha} a_\beta b_\omega \\ &= a_{\mathbf{0}} b_\alpha + b_{\mathbf{0}} a_\alpha + \widehat{(a * b)}_\alpha\end{aligned}$$

where, for $\alpha \in \mathbb{N}^m$, the *hat operation* is defined by

$$\widehat{(a * b)}_\alpha \stackrel{\text{def}}{=} \sum_{\substack{\beta+\omega=\alpha \\ \beta,\omega \in \mathbb{N}^d, \beta,\omega \neq \alpha}} a_\beta b_\omega, \tag{14}$$

Observe that

$$\widehat{(a * b)}_\alpha = (a * b)_\alpha - a_{\mathbf{0}} b_\alpha - b_{\mathbf{0}} a_\alpha = [(a * b)_\alpha]_{a_\alpha = b_\alpha = 0}.$$

The hat operation removes from the Cauchy product precisely the coefficients of order α. In fact the removed terms are related to the gradient of the monomial xy which induces the Cauchy product $a * b$ under consideration.

This idea generalizes as follows. For $\mathcal{A}, \mathcal{B}$ defined as in Section 2.1, for $\kappa = (\kappa_1, \ldots, \kappa_d)$, $\gamma = (\gamma_1, \ldots, \gamma_d) \in \mathbb{N}^d$ define the *hat operation* by

$$\widehat{(\mathcal{A}^\kappa * \mathcal{B}^\gamma)}_\alpha \stackrel{\text{def}}{=} \Big[\left(\mathcal{A}^\kappa * \mathcal{B}^\gamma\right)_\alpha \Big]_{\mathcal{A}_\alpha = \mathcal{B}_\alpha = 0}. \tag{15}$$

We then have the following identity.

Lemma 2.1 (Composition Lemma). *Suppose that $F\colon \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}^d$ is a M-th order polynomial mapping*

$$F(x,y) = \sum_{|\rho|=0}^{M} \sum_{\kappa+\gamma=\rho} c_{\kappa,\gamma} x^\kappa y^\gamma, \qquad c_{\kappa,\gamma} = (c^1_{\kappa,\gamma}, \ldots, c^d_{\kappa,\gamma}) \in \mathbb{R}^d.$$

and that $P, Q\colon \mathbb{R}^m \to \mathbb{R}^d$ are formal power series with Taylor coefficients given by the infinite multi-sequences $\mathcal{A}, \mathcal{B}$. Then for each $\alpha \in \mathbb{N}^m$ with $|\alpha| \geq 2$ the formula for the α-th coefficient of the formal series of $F(P,Q)$ is

$$\mathcal{F}(\mathcal{A},\mathcal{B})_\alpha = D_1F(\mathcal{A}_0,\mathcal{B}_0)\mathcal{A}_\alpha + D_2F(\mathcal{A}_0,\mathcal{B}_0)\mathcal{B}_\alpha + \hat{\mathcal{F}}(\mathcal{A},\mathcal{B})_\alpha, \tag{16}$$

where

$$\hat{\mathcal{F}}(\mathcal{A},\mathcal{B})_\alpha = \sum_{|\rho|=2}^{M} \sum_{\kappa+\gamma=\rho} c_{\kappa,\gamma} \widehat{(\mathcal{A}^\kappa * \mathcal{B}^\gamma)}_\alpha. \tag{17}$$

Proof. By [29], for $\alpha \in \mathbb{N}^m$ with $|\alpha| \geq 2$,

$$\begin{aligned}
\mathcal{F}(\mathcal{A},\mathcal{B})_\alpha &= \frac{1}{\alpha!}\frac{\partial^{|\alpha|}}{\partial\sigma^\alpha}\Big|_{\sigma=0} F\left(P(\sigma), Q(\sigma)\right) \\
&= DF(P(0),Q(0))\frac{1}{\alpha!}\frac{\partial^{|\alpha|}}{\partial\sigma^\alpha}\Big|_{\sigma=0} \begin{pmatrix} P(\sigma) \\ Q(\sigma) \end{pmatrix} + R_\alpha(\mathcal{A},\mathcal{B}) \\
&= DF(\mathcal{A}_0,\mathcal{B}_0)\begin{pmatrix} \mathcal{A}_\alpha \\ \mathcal{B}_\alpha \end{pmatrix} + R_\alpha(\mathcal{A},\mathcal{B}).
\end{aligned}$$

Since R_α does not depend on $(\mathcal{A}_\alpha, \mathcal{B}_\alpha)$ it follows that $R_\alpha(\mathcal{A},\mathcal{B}) = [\mathcal{F}(\mathcal{A},\mathcal{B})_\alpha]_{\mathcal{A}_\alpha=\mathcal{B}_\alpha=0} = \hat{\mathcal{F}}(\mathcal{A},\mathcal{B})_\alpha$ which yields the desired identity. □

2.3 Delay operator on formal power series

Let $\alpha \in \mathbb{N}^m$ and suppose that $\Lambda = (\lambda_1, \ldots, \lambda_m) \in \mathbb{C}^m$ have

$$\mathrm{Re}(\lambda_j) > 0,$$

for $1 \leq j \leq m$. As before, we write

$$\langle \alpha, \Lambda \rangle = \alpha_1\lambda_1 + \ldots + \alpha_m\lambda_m.$$

Following Lemma 1.2, we are interested in formal power series whose coefficients are exponential functions of time with rates given by the λ_j, $1 \leq j \leq m$. For a single scalar delay equation, these can be written as

$$p(\sigma,t) = \sum_{|\alpha|=0}^{\infty} a_\alpha(t)\sigma^\alpha = \sum_{|\alpha|=0}^{\infty} a_\alpha e^{\langle\alpha,\Lambda\rangle t}\sigma^\alpha.$$

Such power series satisfy the shift invariance property of Lemma 1.1, as

$$p(\sigma, t-\tau) = p(e^{-\lambda_1\tau}\sigma_1, \ldots, e^{-\lambda_m\tau}\sigma_m, t).$$

Observe that for two such series $p(\sigma,t)$ and $q(\sigma,t)$ their product is a formal series of the same form. More precisely we have that

$$(p\cdot q)(\sigma,t) = \sum_{|\alpha|=0}^{\infty} e^{\langle\alpha,\Lambda\rangle t}(a*b)_\alpha\,\sigma^\alpha.$$

That is, the coefficients of the series product are once again given by Cauchy products. This remark generalizes directly to higher powers.

Now, for $\tau > 0$ define the operator $\tau(a)$ by the formula

$$\tau(a)_\alpha \stackrel{\text{def}}{=} e^{-\langle \alpha, \Lambda \rangle \tau} a_\alpha, \tag{18}$$

for all $\alpha \in \mathbb{N}^m$. We refer to this as the *delay operator* associated with the rates $\lambda_1, \ldots, \lambda_m$, and we have that

$$p(\sigma, t-\tau) = \sum_{|\alpha|=0}^{\infty} e^{-\langle \alpha, \Lambda \rangle \tau} a_\alpha e^{\langle \alpha, \Lambda \rangle t} \sigma^\alpha = \sum_{|\alpha|=0}^{\infty} \tau(a)_\alpha e^{\langle \alpha, \Lambda \rangle t} \sigma^\alpha.$$

More generally let $P = (p_1, \ldots, p_d)$ and $P^\tau = (p_1^\tau, \ldots, p_d^\tau)$ with

$$p_j(\sigma, t) = \sum_{|\alpha|=0}^{\infty} a_\alpha^j e^{\langle \alpha, \Lambda \rangle t} \sigma^\alpha,$$

for $1 \leq j \leq d$, so that

$$p_j(\sigma, t-\tau) = \sum_{|\alpha|=0}^{\infty} \tau(a^j)_\alpha e^{\langle \alpha, \Lambda \rangle t} \sigma^\alpha.$$

The goal of this section is to combine the notion of a delayed power series with the composition laws derived in the previous section. Let

$$\mathcal{A}_\alpha = (a_\alpha^1, \ldots, a_\alpha^d),$$

and

$$\mathcal{B}_\alpha = (\tau(a^1)_\alpha, \ldots, \tau(a^d)_\alpha).$$

Observe that

$$\mathcal{B}_\alpha = e^{-\langle \alpha, \Lambda \rangle \tau} \mathcal{A}_\alpha =: {}^\tau\mathcal{A}_\alpha. \tag{19}$$

By the Composition Lemma (2.1), we have that

$$F(P(\sigma, t), P(\sigma, t-\tau)) = \sum_{|\alpha|=0}^{\infty} \mathcal{F}(\mathcal{A}, {}^\tau\mathcal{A})_\alpha e^{\langle \alpha, \Lambda \rangle t} \sigma^\alpha,$$

has power series coefficients

$$\mathcal{F}(\mathcal{A}, {}^\tau\mathcal{A})_\alpha = \Big(D_1 F(c,c) + e^{-\langle \alpha, \Lambda \rangle \tau} D_2 F(c,c) \Big) \mathcal{A}_\alpha + \hat{\mathcal{F}}(\mathcal{A}, {}^\tau\mathcal{A})_\alpha, \tag{20}$$

for all $|\alpha| \geq 2$. Here $\hat{\mathcal{F}}$ is as defined by Equation (17) in the Composition Lemma (2.1) of Section 2.2.

2.4 Proof of Theorem 1.3

Consider again the polynomial function $F \colon \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}^d$ given by

$$F(x,y) = \sum_{|\rho|=0}^{M} \sum_{\kappa+\gamma=\rho} c_{\kappa,\gamma} x^\kappa y^\gamma, \qquad c_{\kappa,\gamma} = (c_{\kappa,\gamma}^1, \ldots, c_{\kappa,\gamma}^d) \in \mathbb{R}^d,$$

having $F(c,c) = 0$ and distinct unstable eigenvalues $\lambda_1, \ldots, \lambda_m \in \mathbb{C}$ with associated unstable eigenvectors ξ_j in the kernel of the matrix $\Psi(\lambda_j)$ for $1 \leq j \leq m$. Recall that the $d \times d$ matrix $\Psi(\lambda)$ is as defined in Equation (3), and also that Λ denotes the $m \times m$ diagonal matrix of unstable eigenvalues.

We seek a formal series solution of Equation (4) having the form

$$P(\sigma,t)=\sum_{|\alpha|=0}^{\infty}\mathcal{A}_\alpha e^{\langle\alpha,\Lambda\rangle t}\sigma^\alpha,$$

where $\mathcal{A}_\alpha$ is an n-dimensional vector of m-dimensional infinite multi-sequences. We begin by observing that

$$P(\sigma,t-\tau)=\sum_{|\alpha|=0}^{\infty}\mathcal{B}_\alpha e^{\langle\alpha,\Lambda\rangle t}\sigma^\alpha,$$

where $\mathcal{B}_\alpha={}^\tau\mathcal{A}$ using the notation defined in Equation (19). We require that $\mathcal{A}$ satisfies

$$\mathcal{A}_{\mathbf{0}}=c\quad\text{and}\quad\mathcal{A}_{e_j}=\xi_j,\quad\text{for } 1\le j\le m,$$

so that the first order constraints of Lemma 1.1 are satisfied.

Now, our goal is to find an infinite multi-sequence $\mathcal{A}$ corresponding to the coefficients of a formal series P solving the invariance Equation (4) in the sense of formal power series. Considering the left hand side of Equation (4), we must have that

$$\lambda_1\sigma_1\frac{\partial}{\partial\sigma_1}P(\sigma,t)+\ldots+\lambda_m\sigma_m\frac{\partial}{\partial\sigma_m}P(\sigma,t)=\sum_{|\alpha|=0}^{\infty}\langle\alpha,\Lambda\rangle\,\mathcal{A}_\alpha e^{\langle\alpha,\Lambda\rangle t}\sigma^\alpha,$$

while on the right we have

$$F(P(\sigma,t),P(\sigma,t-\tau))=\sum_{|\alpha|=0}^{\infty}\mathcal{F}(\mathcal{A},{}^\tau\mathcal{A})_\alpha e^{\langle\alpha,\Lambda\rangle t}\sigma^\alpha.$$

Matching like powers, employing Equation (20), and recalling that $\mathcal{A}_0=\mathcal{B}_0=c$ leads to

$$\langle\alpha,\Lambda\rangle\,\mathcal{A}_\alpha=\Big(D_1F(c,c)+e^{-\langle\alpha,\Lambda\rangle\tau}D_2F(c,c)\Big)\,\mathcal{A}_\alpha+\hat{\mathcal{F}}(\mathcal{A},{}^\tau\mathcal{A})_\alpha,$$

or

$$0=\Psi(\langle\alpha,\Lambda\rangle)\mathcal{A}_\alpha+\hat{\mathcal{F}}(\mathcal{A},{}^\tau\mathcal{A})_\alpha,\tag{21}$$

for $|\alpha|\ge 2$.

The proof of Theorem 1.3 now follows by rearranging Equation (21) into Equation (10). It follows that the homological equation has a unique solution for each $|\alpha|\ge 2$ by the non-resonance hypothesis.

Remark 2.2 (Uniqueness). The proof also shows that the coefficients of the formal series solution are unique for $|\alpha|\ge 2$. However the scalings of the ξ_j are arbitrary and we have uniqueness only up to the choice of scalings. This is a valuable freedom that allows us to choose a solution with advantageous coefficient decay in numerical work.

2.5 An example: homological equations by inspection

Consider a delayed van der Pol equation

$$\begin{cases}u'(t) &= v(t)\\ v'(t) &= -\mathrm{a}u(t)-\mathrm{b}u(t-\tau)+\mu(1-u^2(t-\tau))v(t),\end{cases}$$

with $\tau\ge 0$ and $\mathrm{a}+\mathrm{b}=1$. Observe that when $\tau\to 0$ the system converges to the classic van der Pol vector field. Let $(x_1(t),x_2(t),y_1(t),y_2(t))=(u(t),v(t),u(t-\tau),v(t-\tau))$, and define $F\colon\mathbb{R}^2\times\mathbb{R}^2\to\mathbb{R}^2$ by

$$F(x,y)=F(x_1,x_2,y_1,y_2)=\begin{pmatrix}x_2\\ -\mathrm{a}x_1-\mathrm{b}y_1+\mu(1-y_1^2)x_2\end{pmatrix}.\tag{22}$$

Note that

$$D_1F(x,y) = D_xF(x,y) = \begin{pmatrix} 0 & 1 \\ -\mathrm{a} & \mu(1-y_1^2) \end{pmatrix}$$

and

$$D_2F(x,y) = D_yF(x,y) = \begin{pmatrix} 0 & 0 \\ -\mathrm{b} - 2\mu y_1 x_2 & 0 \end{pmatrix},$$

and observe that $(\mathbf{0},\mathbf{0}) \in \mathbb{R}^4$ is the only equilibrium. Then the characteristic matrix at the origin is

$$\Psi(\lambda) = \begin{pmatrix} -\lambda & 1 \\ -\mathrm{a} - \mathrm{b}e^{-\lambda\tau} & \mu - \lambda \end{pmatrix}. \tag{23}$$

Suppose that the Morse index (i.e. the number of unstable eigenvalues) of the origin is m, and that the unstable eigenvalues are distinct and non-resonant. Let

$$P(\sigma,t) = \sum_{|\alpha|=0}^{\infty} \mathcal{A}_\alpha e^{\langle\alpha,\Lambda\rangle t}\sigma^\alpha = \sum_{|\alpha|=0}^{\infty} \begin{pmatrix} a_\alpha^1 \\ a_\alpha^2 \end{pmatrix} e^{\langle\alpha,\Lambda\rangle t}\sigma^\alpha,$$

denote the formal series for the parameterization. There is only one monomial term of order two or greater appearing in the second component of F, and it is $-\mu x_2 y_1^2$. Recalling the definition of the hat operation for a general monomial defined in Equation (15) we see that

$$\hat{\mathcal{F}}(\mathcal{A},\mathcal{B})_\alpha = -\begin{pmatrix} 0 \\ \mu\widehat{(a^2 * b^1 * b^1)}_\alpha \end{pmatrix}, \tag{24}$$

where

$$b_\alpha^1 = e^{-\tau(\alpha_1\lambda_1 + \ldots + \alpha_m\lambda_m)} a_\alpha^1.$$

Then the homological equations for this system are

$$\Psi(\langle\alpha,\Lambda\rangle)a_\alpha = \begin{pmatrix} -\langle\alpha,\Lambda\rangle & 1 \\ -\mathrm{a} - \mathrm{b}e^{-\tau\langle\alpha,\Lambda\rangle} & \mu - \langle\alpha,\Lambda\rangle \end{pmatrix} \begin{pmatrix} a_\alpha^1 \\ a_\alpha^2 \end{pmatrix} = \begin{pmatrix} 0 \\ \mu\widehat{(a^2 * b^1 * b^1)}_\alpha \end{pmatrix}, \tag{25}$$

for all $|\alpha| \geq 2$.

2.6 Numerical considerations

The discussion so far is summarized below in Algorithm 1 which, when provided with appropriate inputs, computes the Taylor coefficients of the unstable manifold parameterization to any desired order. The required inputs are the delay $\tau > 0$, an $N \in \mathbb{N}$ (the desired polynomial order of approximation, which should be two or more), an equilibrium solution $c \in \mathbb{R}^d$ whose Morse index (i.e. number of unstable eigenvalues) is $m > 0$, the unstable eigenvalues $\lambda_1, \ldots, \lambda_m \in \mathbb{C}$ stored in the $m \times m$ diagonal matrix Λ (the entries should be unique, and non-resonant in the sense of Definition 1), associated eigenvectors $\xi_1, \ldots, \xi_m \in \mathbb{C}^d$ (in the same order as the entries of Λ), and the polynomial vector field F. The algorithms returns the Taylor coefficients $\mathcal{A}_\alpha$ up to order $|\alpha| = N$.

It is assumed that all of the necessary conditions are checked outside of the program. It is also assumed that the program can compute and evaluate derivatives of F (in order to assemble the characteristic matrix Ψ), that it can extract monomials of F of order two and greater, evaluate Cauchy products associated with these monomials, and compute the delayed coefficient sequence $\mathcal{B} = {}^\tau\mathcal{A}$ (all this in order to compute $\hat{\mathcal{F}}_\alpha$ – which we recall depends only on coefficients of order less than $|\alpha|$), and that the procedure has access to a linear system solver.

We remark also that if interval enclosures of the input data are provided, and if derivatives, Cauchy products, and solution routines for linear systems are all provided with interval versions, then

Algorithm 1 Compute unstable manifold parameterization

Inputs: real $\tau > 0$, integer $N \geq 2$, real $c \in \mathbb{R}^d$, complex $\xi_1, \ldots, \xi_m \in \mathbb{C}^d$,
$m \times m$ diagonal, unique, non-resonant complex Λ,
real polynomial $F \colon \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}^d$

$\mathcal{A}_{\mathbf{0}} = c$
$\mathcal{A}_{e_1} = \xi_1, \ldots, \mathcal{A}_{e_m} = \xi_m$
for $|\alpha| = 2$ to $|\alpha| = N$ **do**
  $\Psi(\langle \alpha, \Lambda \rangle) \stackrel{\text{def}}{=} D_1 F(c,c) + e^{-\tau \langle \alpha, \Lambda \rangle} D_2 F(c,c) - \langle \alpha, \Lambda \rangle \, \mathrm{Id}$
  $d = \hat{\mathcal{F}}(\mathcal{A}, {}^{\tau}\mathcal{A})_\alpha$
  $\mathcal{A}_\alpha = \mathrm{linearSystemSolve}(\Psi(\langle \alpha, \Lambda \rangle), d)$
end for
Return: $\mathcal{A} = \{\mathcal{A}_\alpha\}_{|\alpha|=0}^{N}$

the returned coefficients will be interval enclosures of the Taylor coefficients. Finding an interval enclosure of the equilibrium solution c requires a finite dimensional validated nonlinear system solver. This is a classic problem in interval analysis going back at least to the work of [30, 31]. We refer also to the more modern discussion in [7, 32]. The problem of obtaining validated bounds on the unstable eigenvalues is similar, perhaps easier, as they are solutions of the nonlinear complex scalar equation $\det(\Psi(\lambda)) = 0$. Similarly, the problem of computing validated bounds on solutions of linear systems and on eigenvectors associated with distinct eigenvalues is also quite standard and is discussed in any of the references just cited. Checking the non-resonance is then just a matter of multiplication by the relevant multi-indices.

Somewhat more subtle is to validate that the Morse index of the equilibrium c is exactly m. That is, if we prove the existence of m unstable eigenvalue(s) by solving the equation $\det(\Psi(\lambda)) = 0$, how do we know they are these and no others? The problem is addressed in a recent work [33] by the second and third authors. Rather than recapulating the details here, we direct the interested reader to the reference just cited. The point we hope to make is that there exist validated numerical methods which allow us to obtain mathematically rigorous interval enclosures on all the input data for Algorithm 2.6, and that once this is done obtaining validated enclosures on the Taylor coefficients is just a matter of obtaining validated interval enclosures on the solutions of some linear systems of equations.

The last point is that the scalings of the eigenvectors are not unique, and must be chosen as inputs to the algorithm. This problem is already present in the parameterization method for stable/unstable manifolds attached to equilibrium (or periodic) solutions of finite dimensional vector fields, and has been treated in a number of places. See for example the work of [34]. The main observation is this: suppose that $s_1, \ldots, s_m \neq 0$ are a collection of scale factors, and that we define

$$\eta_j = s_j \xi_j, \qquad 1 \leq j \leq m.$$

Now, using Algorithm 1, make the function calls

$$\{\mathcal{A}\}_{|\alpha|=0}^{N} = \text{Compute unstable manifold parameterization}(\tau, N, c, \xi_1, \ldots, \xi_m, \Lambda, F),$$

and

$$\{\mathcal{C}\}_{|\alpha|=0}^{N} = \text{Compute unstable manifold parameterization}(\tau, N, c, \eta_1, \ldots, \eta_m, \Lambda, F).$$

Then

$$\mathcal{C}_\alpha = s^\alpha \mathcal{A}_\alpha = s_1^{\alpha_1} \ldots s_m^{\alpha_m} \mathcal{A}_{\alpha_1, \ldots, \alpha_m}. \tag{26}$$

The proof is almost identical to the argument given in [34].

The rescaling law of Equation (26) is utilized in numerical calculations as follows. First make an arbitrary choice of the scalings, say taking $\xi_1, \ldots, \xi_m$ all scaled to have unit length. Then compute

$$\left\{\tilde{\mathcal{A}}\right\}_{|\alpha|=0}^{N_0} = \text{Compute unstable manifold parameterization}(\tau, N_0, c, \xi_1, \ldots, \xi_m, \Lambda, F),$$

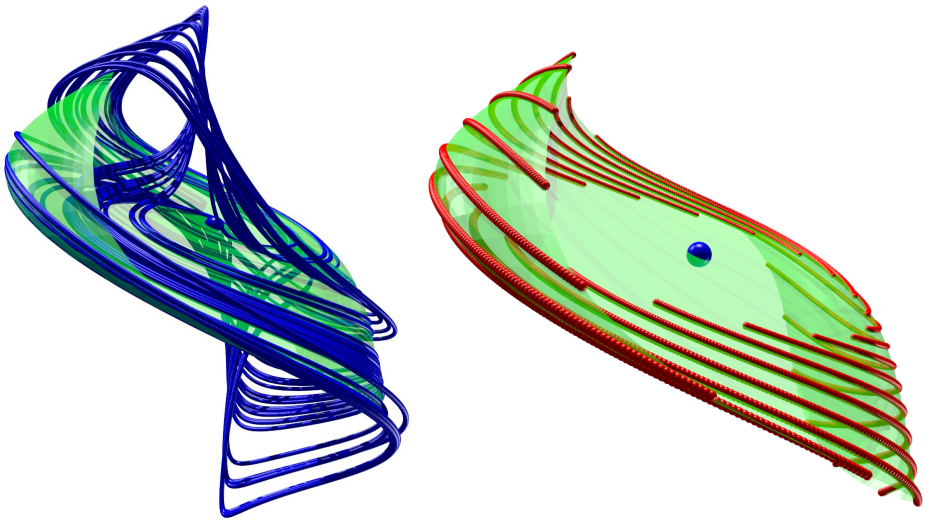


Figure 1: **2D unstable manifold of origin for a delayed van der Pol:** the green surface in both frames illustrates the local unstable manifold of the origin, parameterized to order $N = 60$ when $\tau = 2$. We use three coordinates $u(t)$, $v(t)$, and $u(t-\tau)$ to generate a three dimensional representation of the infinite dimensional dynamics. Observe that the parameterization follows a fold in the embedding, that is the manifold is not the graph of any function over the unstable eigenspace. The blue curve in the left frame result from simulating a typical initial initial condition until the transients have died out, and illustrates how the unstable manifold sits inside the attractor. The red curves on the right illustrate the fact that points on the manifold are actually functions. Each one of the 20 red curves is obtained by evaluating P at a (σ_1, σ_2) with $\sigma_1^2+\sigma_2^2 = 1$. This results in a function $P(\sigma, t) = P(\sigma_1, \sigma_2, t)$ which we evaluate and plot for $t \in [-\tau, 0]$.

with $N_0 \ll N$, where N is the desired order of the final approximation. Now compute the exponential best fit for the decay rate of $\tilde{\mathcal{A}}$. Using the empirically computed decay rate and the rescaling law of Equation (26) calculate $s_1, \ldots, s_m$ so that $\mathcal{A}$ has the desired decay. Then compute

$$\{\mathcal{A}\}_{|\alpha|=0}^{N} = \text{Compute unstable manifold parameterization}(\tau, N, c, s_1\xi_1, \ldots, s_m\xi_m, \Lambda, F).$$

A useful condition is to choose $s_1, \ldots, s_m$ as large as possible so that $\|\mathcal{A}_\alpha\|_{\mathbb{C}^d}$ is on the order of *machine epsilon*. This works well because the magnitude of the highest order coefficients is roughly the magnitude of the truncation error on the unit poly-disk. Of course if we take our domain to be the unit disk (or any other fixed domain) then the scaling of the eigenvectors determines the size of the parameterization in phase space, so that we do not want to take the scalings any smaller than necessary to obtain the desired error bounds.

2.7 An example calculation

Returning to the example of the van der Pol system defined in Section 2.5, observe that $c = (0, 0) \in \mathbb{R}^2$ is the only solution of $F(c, c) = 0$, and hence the zero solution is the only equilibrium. Observe also that the characteristic equation for the system is

$$\det(\Psi(z)) = \det\left(\begin{bmatrix} -z & 1 \\ -\mathrm{a} - \mathrm{b}e^{-\tau z} & \mu - z \end{bmatrix}\right) = z^2 + \mathrm{b}e^{-\tau z} - \mu z + \mathrm{a} = 0.$$

Consider the parameters $\tau = 2$, $\mu = 1$, a $= 0.9$, and b $= 0.1$. A numerical search of the complex plane finds that

$$\bar{\lambda}_{1,2} = 0.521837944044436 \pm 0.805637509255934i,$$

is a complex conjugate pair of unstable eigenvalues, and finds no other unstable eigenvalues. So, we look for a two dimensional unstable manifold attached to the origin.

The eigenfunctions are

$$\Xi_{1,2}(t) = \xi_{1,2} e^{\lambda_{1,2} t},$$

where

$$\bar{\xi}_{1,2} = \begin{pmatrix} 0.721431128547296 \\ 0.376470136890778 \pm 0.581211977502541i \end{pmatrix},$$

are found by solving the equation $\Psi(\bar{\lambda}_{1,2})\bar{\xi} = 0$. We are now in a position to run Algorithm 1, where $|\alpha| = m = 2$, $d = 2$, and $c = (0, 0)$, with τ, and $\bar{\xi}_{1,2}$ as above. After some numerical experimentation we find that taking $N = 60$ and rescaling the eigenvectors to have a length of 3.5 leads to decay such that the coefficients of order 60 have maximum magnitude on the order of 10^{-14}. This results in a polynomial approximation of the unstable manifold to order sixty. The resulting approximation is valid on the unit disk, and its image in function space is illustrated in Figure 1.

3 A-posteriori analysis for the nonlinear recurrence

The computer assisted error bounds derived and implemented in this section exploit in a crucial way that we are working with nonlinear recursions. The ideas used here were introduced in [35] to study initial value problems and stable/unstable manifolds of ordinary differential equations. See also the lecture notes [32].

The following theorem (slightly modified version from [36]), whose elementary proof we provide for the sake of completeness in Appendix C, provides a-posteriori criteria for the existence of a fixed point of a Fréchet differentiable map T.

Given a Banach space $(X, \|\cdot\|_X)$, denote by $B_r(x) = \{y \in X : \|x - y\| \leq r\}$ the closed ball of radius $r > 0$ centred at a given $x \in X$.

Theorem 3.1 (A-posteriori quadratic fixed point theorem)**.** *Let X be a Banach space and $T \colon X \to X$ a Fréchet differentiable mapping. Let $x_0 \in X$, and suppose that $r_*, Y, Z_1, Z_2 > 0$ such that*

$$\begin{aligned} \|T(x_0) - x_0\|_X &\leq Y, \\ \|DT(x_0)\|_{B(X)} &\leq Z_1, \\ \sup_{h \in B_{r^*}(x_0)} \|D^2 T(h)\|_{B(X,B(X))} &\leq Z_2. \end{aligned}$$

Define

$$p(r) = \frac{Z_2}{2} r^2 + (Z_1 - 1) r + Y.$$

If $r_0 \in [0, r_*]$ has that

$$p(r_0) \leq 0 \qquad \text{and} \qquad Z_1 + Z_2 r_0 < 1,$$

then there is a unique $\tilde{x} \in B_{r_0}(x_0)$ so that

$$T(\tilde{x}) = \tilde{x}.$$

3.1 Banach algebras of infinite multi-sequences

In this section we lay the ground work to apply Theorem 3.1 by endowing the spaces of infinite multi-sequences defined in Sections 2.1, 2.2 and 2.3 with Banach space structure. For $a = \{a_\alpha\}_{|\alpha|=0}^{\infty}$ an m-dimensional infinite multi-sequence define the norm

$$\|a\|_1 = \sum_{|\alpha|=0}^{\infty} |a_\alpha|.$$

The normed linear space

$$\ell^1_m = \left\{ a = \{a_\alpha\}_{|\alpha|=0}^{\infty} \,|\, a_\alpha \in \mathbb{C} \text{ for all } \alpha \in \mathbb{N}^m, \text{ and } \|a\|_1 < \infty \right\},$$

is a Banach space. Given $a, b \in \ell^1_m$ define for each $\alpha \in \mathbb{N}^m$ the number

$$(a * b)_\alpha = \sum_{\substack{\beta+\omega=\alpha \\ \beta,\omega\in\mathbb{N}^d}} a_\beta b_\omega.$$

This operation defines a new infinite multi-sequence and is referred to as the *Cauchy product* on ℓ^1_m. Indeed, defining $c = a * b$ by

$$c_\alpha = (a * b)_\alpha, \qquad\qquad \alpha \in \mathbb{N}^m,$$

one verifies that $a * b = b * a$ and that

$$\|a * b\|_1 \leq \|a\|_1 \|b\|_1,$$

for all $a, b \in \ell^1_m$. Then $*\colon \ell^1_m \times \ell^1_m \to \ell^1_m$ is a binary operation and moreover $(\ell^1_m, *)$ is a commutative Banach algebra. Naturally, powers in the Banach algebra are defined by iterated Cauchy products. Recall that the $*$ operation is Fréchet differentiable on any Banach algebra, and by commutativity, a polynomial mapping on ℓ^1_m is differentiable with the usual derivative formula for polynomials.

One of the fundamental steps in deriving the homological equations was – for a given multi-index $\alpha \in \mathbb{N}^m$ – extracting from a Cauchy product all coefficients of order α. This led to the so called "hat-product" which we now study as an operation on ℓ^1_m.

The hat operation encodes the process of top coefficient extraction, so for example, recalling Equation (14), we have that

$$\|\widehat{a * b}\|_1 \leq \|a * b\|_1. \tag{27}$$

This generalizes. Define the Banach space

$$\mathcal{X} \stackrel{\text{def}}{=} \left(\ell^1_m\right)^d$$

by endowing the d fold product of ℓ^1_m with the norm

$$\|\mathcal{A}\|_{\mathcal{X}} \stackrel{\text{def}}{=} \left\| \begin{pmatrix} \|a^1\|_1 \\ \vdots \\ \|a^m\|_1 \end{pmatrix} \right\|_{\mathbb{C}^d}. \tag{28}$$

For $\kappa = (\kappa_1, \ldots, \kappa_d), \gamma = (\gamma_1, \ldots, \gamma_d) \in \mathbb{N}^d$ and $\mathcal{A}, \mathcal{B} \in \mathcal{X}$, the estimate (27) implies

$$\|\widehat{\mathcal{A}^\kappa * \mathcal{B}^\gamma}\|_1 \leq \|\mathcal{A}^\kappa * \mathcal{B}^\gamma\|_1 \leq \|a^1\|_1^{\gamma_1} \cdots \|a^d\|_1^{\gamma_d} \cdot \|b^1\|_1^{\kappa_1} \cdots \|b^d\|_1^{\kappa_d}. \tag{29}$$

This observation is useful for bounding derivatives when combined with the fact that the hat product commutes with the Fréchet derivative. These results will be exploited in Section 3.3 to obtain explicit forms for the bounds of Theorem 3.1.

Lastly, for $\tau > 0$ and $\lambda_1, \ldots, \lambda_m \in \mathbb{C}$ complex numbers with positive real parts, the *delay operator* defined in Equation (18) is a mapping $\tau \colon \ell^1_m \to \ell^1_m$. In fact, $\tau \in B(\ell^1_m)$ with

$$\|\tau\|_{B(\ell^1_m)} = 1.$$

(Inequality is clear, and equality is seen by acting on a multi-sequence whose only non-zero term is at order $|\alpha| = 1$).

3.2 Truncation spaces and operators

Define the bounded linear operators $\pi_N, \pi_\infty \colon \ell^1_m \to \ell^1_m$ by

$$\pi_N(a)_\alpha = \begin{cases} a_\alpha & \text{if } |\alpha| \leq N \\ 0 & \text{otherwise,} \end{cases}$$

and

$$\pi_\infty = \mathrm{Id}_{\ell^1_m} - \pi_N,$$

so that

$$\pi_\infty(a)_\alpha = \begin{cases} 0 & \text{if } |\alpha| \leq N \\ a_\alpha & \text{otherwise.} \end{cases}$$

Define the closed linear subspaces $X^N, X^\infty \subset \ell^1_m$ by

$$X^N = \pi_N(\ell^1_m),$$

and

$$X^\infty = \pi_\infty(\ell^1_m).$$

Observe that

$$X^N \oplus X^\infty = \ell^1_m,$$

as every $a \in \ell^1_m$ has a unique decomposition

$$a = \pi_N(a) + \pi_\infty(a).$$

Recall that $\mathcal{X} = \left(\ell^1_m\right)^d$ denotes d products of ℓ^1_m, and that we write $\mathcal{A} = (a^1, \ldots, a^d)$ to denote an element of $\mathcal{X}$. Recall the norm (28) on the Banach space $\mathcal{X}$. Define the bounded linear operators $\Pi_N, \Pi_\infty \colon \mathcal{X} \to \mathcal{X}$ by

$$\Pi_N(\mathcal{A}) = (\pi_N(a^1), \ldots, \pi_N(a^d)),$$

and

$$\Pi_\infty(\mathcal{A}) = \left(\mathrm{Id}_{\mathcal{X}} - \Pi_N\right)(\mathcal{A}) = (\pi_\infty(a^1), \ldots, \pi_\infty(a^d)).$$

The spaces

$$\mathcal{X}^N = \Pi_N(\mathcal{X})$$

and

$$\mathcal{X}^\infty = \Pi_\infty(\mathcal{X})$$

are closed linear subspaces of $\mathcal{X}$ with the obvious norm, such that

$$\mathcal{X}^N \oplus \mathcal{X}^\infty = \mathcal{X}.$$

3.3 Bounds for parameterized unstable manifolds for DDEs

Suppose we are in the context of Theorem 1.3. Since the $\lambda_1, \ldots, \lambda_m$ are non-resonant we have that the homological equations give the explicit recursion

$$\mathcal{A}_\alpha = -\Psi(\langle \alpha, \Lambda \rangle)^{-1} \hat{\mathcal{F}}(\mathcal{A}, {}^\tau\mathcal{A})_\alpha.$$

where $\Psi(\langle \alpha, \Lambda \rangle) = \Psi(\alpha_1\lambda_1 + \ldots + \alpha_m\lambda_m)$ is the characteristic matrix evaluated at $\langle \alpha, \Lambda \rangle \in \mathbb{C}$. Consider the map T defined on $\mathcal{X}$ by

$$T(\mathcal{A})_\alpha = \begin{cases} c & \alpha = \mathbf{0} \\ \xi_j & \alpha = e_j, 1 \le j \le m \\ -\Psi(\langle \alpha, \Lambda \rangle)^{-1} \hat{\mathcal{F}}(\mathcal{A}, {}^\tau\mathcal{A})_\alpha & |\alpha| \ge 2. \end{cases}$$

The operator $T \colon \mathcal{X} \to \mathcal{X}$ is well defined. To see this let $\mathcal{A} \in \mathcal{X}$. According to the definition of the norm on $\mathcal{X}$ given by (28), observe that

$$\|T(\mathcal{A})\|_{\mathcal{X}} \le \sum_{|\alpha|=0}^{\infty} \|T(\mathcal{A})_\alpha\|_{\mathbb{C}^d}.$$

Hence,

$$\|T(\mathcal{A})\|_{\mathcal{X}} \le \|c\|_{\mathbb{C}^d} + \|\xi_1\|_{\mathbb{C}^d} + \ldots + \|\xi_m\|_{\mathbb{C}^d} + \sum_{|\alpha|=2}^{\infty} \|T(\mathcal{A})_\alpha\|_{\mathbb{C}^d}$$

where, letting $\mathcal{B} = {}^\tau\mathcal{A}$,

$$\begin{aligned} \sum_{|\alpha|=2}^{\infty} \|T(\mathcal{A})_\alpha\|_{\mathbb{C}^d} &\le \sum_{|\alpha|=2}^{\infty} \|\Psi(\langle \alpha, \Lambda \rangle)^{-1}\|_{B(\mathbb{C}^d)} \|\hat{\mathcal{F}}(\mathcal{A}, \mathcal{B})_\alpha\|_{\mathbb{C}^d} \\ &\le \sum_{|\alpha|=2}^{\infty} \frac{C}{|\langle \alpha, \Lambda \rangle|} \left\| \sum_{|\rho|=2}^{M} \sum_{\kappa+\gamma=\rho} c_{\kappa,\gamma} (\widehat{\mathcal{A}^\kappa * \mathcal{B}^\gamma})_\alpha \right\|_{\mathbb{C}^d} \\ &\le \sum_{|\rho|=2}^{M} \sum_{\kappa+\gamma=\rho} \sum_{|\alpha|=2}^{\infty} \frac{C\|c_{\kappa,\gamma}\|_{\mathbb{C}^d}}{|\langle \alpha, \Lambda \rangle|} |(\widehat{\mathcal{A}^\kappa * \mathcal{B}^\gamma})_\alpha| \\ &\le \sum_{|\rho|=2}^{M} \sum_{\kappa+\gamma=\rho} C\|c_{\kappa,\gamma}\|_{\mathbb{C}^d} \sum_{|\alpha|=2}^{\infty} \frac{1}{|\langle \alpha, \Lambda \rangle|} |(\widehat{\mathcal{A}^\kappa * \mathcal{B}^\gamma})_\alpha| \\ &< \infty, \end{aligned}$$

as by (29)

$$\sum_{|\alpha|=2}^{\infty} \left\| (\widehat{\mathcal{A}^\kappa * \mathcal{B}^\gamma})_\alpha \right\|_{\mathbb{C}^d} \le \|a_1\|_1^{\kappa_1} \ldots \|a^d\|_1^{\kappa_d} \|b^1\|_1^{\gamma_1} \ldots \|b^d\|_1^{\gamma_d} < \infty,$$

and

$$\lim_{|\alpha| \to \infty} \frac{1}{|\langle \alpha, \Lambda \rangle|} = 0.$$

Choose $N \in \mathbb{N}$ and consider $\Pi_N(\mathcal{A}) \in \mathcal{X}^N$, i.e.

$$\Pi_N(\mathcal{A})_\alpha = \begin{cases} c & \alpha = \mathbf{0} \\ \xi_j & \alpha = e_j, 1 \le j \le m \\ -\Psi(\langle \alpha, \Lambda \rangle)^{-1} \hat{\mathcal{F}}(\mathcal{A}, {}^\tau\mathcal{A})_\alpha & 2 \le |\alpha| \le N \\ 0 & |\alpha| \ge N+1 \end{cases}$$

Define the operators $T^N\colon \mathcal{X} \to \mathcal{X}^N$ and $T^\infty\colon \mathcal{X} \to \mathcal{X}^\infty$ by

$$T^N(\mathcal{A}) = \Pi_N(T(\mathcal{A}))$$

and

$$T^\infty(\mathcal{A}) = \Pi_\infty(T(\mathcal{A}))$$

so that

$$T(\mathcal{A}) = T^N(\mathcal{A}) + T^\infty(\mathcal{A}).$$

Finally, define the operator $\mathcal{T}\colon \mathcal{X}^\infty \to \mathcal{X}^\infty$ by

$$\mathcal{T}(\mathcal{H}) = T^\infty(\Pi_N(\mathcal{A}) + \mathcal{H}), \qquad \mathcal{H} \in \mathcal{X}^\infty.$$

It is now clear that we have the following.

Proposition 3.2. *Let $\Pi_N(\mathcal{A}) \in \mathcal{X}^N$ be a fixed point of T^N, and suppose that $\tilde{\mathcal{H}} \in \mathcal{X}^\infty$ has*

$$\mathcal{T}(\tilde{\mathcal{H}}) = \tilde{\mathcal{H}}.$$

Then $\Pi_N(\mathcal{A}) + \tilde{\mathcal{H}} \in \mathcal{X}$ is a fixed point of T.

Define the operator $\mathfrak{L}\colon \mathcal{X}^\infty \to \mathcal{X}^\infty$ by

$$\mathfrak{L}(\mathcal{H})_\alpha = -\Psi(\langle \alpha, \Lambda \rangle)^{-1}\mathcal{H}_\alpha,$$

and note that $\mathfrak{L}$ is a bounded linear operator with

$$\|\mathfrak{L}\|_{B(\mathcal{X}^\infty)} = C_N(\lambda_1, \ldots, \lambda_m),$$

where

$$C_N = \sup_{|\alpha| \geq N+1} \left\| \Psi(\langle \alpha, \Lambda \rangle)^{-1} \right\|_{B(\mathbb{C}^d)}.$$

The non-resonance assumption insures that each $\Psi(\langle \alpha, \Lambda \rangle)^{-1}$ is invertible and the bounds in Appendix A insure that

$$\lim_{|\alpha| \to \infty} \left\| \Psi(\langle \alpha, \Lambda \rangle)^{-1} \right\|_{B(\mathbb{C}^d)} = 0.$$

Then $C_N < \infty$.

In the notation afforded by $\mathfrak{L}$ we see that $\mathcal{T}$ is expressed as

$$\mathcal{T}(\mathcal{H}) = \mathfrak{L}\Pi_\infty \hat{\mathcal{F}}(\Pi_N(\mathcal{A}) + \mathcal{H}, \Pi_N({}^\tau\mathcal{A}) + {}^\tau\mathcal{H}),$$

a formula which is easy to differentiate as the derivative commutes with the bounded linear operators $\mathfrak{L}$ and Π_∞.

Lemma 3.3 (A-posteriori bounds)**.** *Suppose that $F\colon \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}^d$ is a polynomial mapping*

$$F(x,y) = \sum_{|\rho|=2}^{M} \sum_{\kappa+\gamma=\rho} c_{\kappa,\gamma} x^\kappa y^\gamma = \begin{pmatrix} \sum_{|\rho|=0}^{M_1} \sum_{\kappa+\gamma=\rho} c^1_{\kappa,\gamma} x^\kappa y^\gamma \\ \vdots \\ \sum_{|\rho|=0}^{M_d} \sum_{\kappa+\gamma=\rho} c^d_{\kappa,\gamma} x^\kappa y^\gamma \end{pmatrix}, \qquad c_{\kappa,\gamma} = (c^1_{\kappa,\gamma}, \ldots, c^d_{\kappa,\gamma}) \in \mathbb{R}^d,$$

where $M = \max(M_1, \ldots, M_d)$. Let $M_{i,j}$ be the order of the polynomial $\partial_j F_i$ for $i = 1, \ldots, d$ and $j = 1, \ldots, 2d$.

Assume the context of Theorem 1.3. Fix $r_* > 0$. The bounds $Y, Z_1, Z_2 > 0$ of Theorem 3.1 for the operator $\mathcal{T}$ read

$$Y = C_N \left\| \begin{pmatrix} \sum_{|\alpha|=N+1}^{M_1 N} \left| \sum_{|\rho|=2}^{M_1} \sum_{\kappa+\gamma=\rho} c^1_{\kappa,\gamma} \left(\Pi_N(\mathcal{A})^\kappa * \Pi_N({}^\tau\mathcal{A})^\gamma \right)_\alpha \right| \\ \vdots \\ \sum_{|\alpha|=N+1}^{M_d N} \left| \sum_{|\rho|=2}^{M_d} \sum_{\kappa+\gamma=\rho} c^d_{\kappa,\gamma} \left(\Pi_N(\mathcal{A})^\kappa * \Pi_N({}^\tau\mathcal{A})^\gamma \right)_\alpha \right| \end{pmatrix} \right\|_{\mathbb{C}^d}, \tag{30}$$

$$Z_1 = C_N \left\| \begin{pmatrix} \sum_{i=1}^{d} \left(\sum_{|\alpha|=0}^{M_{1,i} N} \left| \sum_{|\rho|=3}^{M_{1,i}+1} \sum_{\kappa+\gamma=\rho} c^1_{\kappa,\gamma\kappa_i} \left(\Pi_N(\mathcal{A})^{\kappa-e_i} * \Pi_N({}^\tau\mathcal{A})^\gamma \right)_\alpha \right| + \sum_{|\alpha|=0}^{M_{1,i+d} N} \left| \sum_{|\rho|=3}^{M_{1,i+d}+1} \sum_{\kappa+\gamma=\rho} c^1_{\kappa,\gamma\gamma_i} \left(\Pi_N(\mathcal{A})^\kappa * \Pi_N({}^\tau\mathcal{A})^{\gamma-e_i} \right)_\alpha \right| \right) \\ \vdots \\ \sum_{i=1}^{d} \left(\sum_{|\alpha|=0}^{M_{d,i} N} \left| \sum_{|\rho|=3}^{M_{d,i}+1} \sum_{\kappa+\gamma=\rho} c^d_{\kappa,\gamma\kappa_i} \left(\Pi_N(\mathcal{A})^{\kappa-e_i} * \Pi_N({}^\tau\mathcal{A})^\gamma \right)_\alpha \right| + \sum_{|\alpha|=0}^{M_{d,i+d} N} \left| \sum_{|\rho|=3}^{M_{d,i+d}+1} \sum_{\kappa+\gamma=\rho} c^d_{\kappa,\gamma\gamma_i} \left(\Pi_N(\mathcal{A})^\kappa * \Pi_N({}^\tau\mathcal{A})^{\gamma-e_i} \right)_\alpha \right| \right) \end{pmatrix} \right\|_{\mathbb{C}^d}, \tag{31}$$

$$Z_2 = C_N \left\| \begin{pmatrix} \sum_{i,j=1}^{d} \partial_{x_i}\partial_{y_j}|F_1|(\mathbf{z}) + \partial_{x_i}\partial_{x_j}|F_1|(\mathbf{z}) + \partial_{y_i}\partial_{y_j}|F_1|(\mathbf{z}) \\ \vdots \\ \sum_{i,j=1}^{d} \partial_{x_i}\partial_{y_j}|F_d|(\mathbf{z}) + \partial_{x_i}\partial_{x_j}|F_d|(\mathbf{z}) + \partial_{y_i}\partial_{y_j}|F_d|(\mathbf{z}) \end{pmatrix} \right\|_{\mathbb{C}^d}, \tag{32}$$

where $\mathbf{z} = (\|\pi_N(a^1)\|_{\ell^1} + r_*, \ldots, \|\pi_N(a^d)\|_{\ell^1} + r_*, \|\pi_N(\tau(a^1))\|_{\ell^1} + r_*, \ldots, \|\pi_N(\tau(a^d))\|_{\ell^1} + r_*)$ *and*

$$|F|(x,y) = \sum_{|\rho|=0}^{M} \sum_{\kappa+\gamma=\rho} |c_{\kappa,\gamma}| x^\kappa y^\gamma.$$

Before the proof of the theorem some remarks about the form of the bounds are in order.

Remark 3.4 (The Y bound)**.** By definition the Y bound given by given by Equation (30) corresponds to the norm of the tail of absolutely converging series; Y is naturally small. Still, the sum involved in the Y bound will usually contain a tremendous number of terms and in practice the most efficient method for computing the monomials $(\Pi_N(\mathcal{A})^\kappa * \Pi_N({}^\tau\mathcal{A})^\gamma)$ is to use the FFT rather than using explicit order-by-order formulas.

Remark 3.5 (The Z_1 bound)**.** The Z_1 bound of Equation (31) is the most delicate one. Indeed, its size depends on both our choice of N and requiring that N is large enough we could guarantee C_N is small enough to make $Z_1 < 1$, no matter how large the remaining terms are. The point is that in applications we do not want to be forced to take N very large, and it may in fact be better to control the norm terms in the Z_1 bound by taking the scalings of the eigenvectors small. That Z_1 is balanced by N and the eigenvector scalings is a fact we exploit in our computer assisted proofs to obtain results that are optimized for the particular problem at hand.

Remark 3.6 (The Z_2 bound)**.** The Z_2 bound determines the curvature of the *radii polynomial* p appearing in Theorem 3.1. As Y bounds is in a vicinity of 0, it follows that Z_2 bears little impact. A fortiori, the choice of r_* is fairly arbitrary and hence not critical.

Proof. Taking $\mathbf{0} \in \mathcal{X}^\infty$ as our approximate fixed point for $\mathcal{T}$ we have

$$\begin{aligned}\|\mathcal{T}(\mathbf{0})\|_{\mathcal{X}^\infty} &= \left\| \mathfrak{L}\Pi_\infty \hat{\mathcal{F}}(\Pi_N(\mathcal{A}), \Pi_N({}^\tau\mathcal{A})) \right\|_{\mathcal{X}^\infty} \\ &\leq \|\mathcal{L}\|_{B(\mathcal{X}^\infty)} \left\| \Pi^\infty \hat{\mathcal{F}}(\Pi_N(\mathcal{A}), \Pi_N({}^\tau\mathcal{A})) \right\|_{\mathcal{X}^\infty} \\ &= C_N \left\| \Pi^\infty \hat{\mathcal{F}}(\Pi_N(\mathcal{A}), \Pi_N({}^\tau\mathcal{A})) \right\|_{\mathcal{X}^\infty} \\ &= Y.\end{aligned}$$

Observe that the Fréchet derivative of $\hat{\mathcal{F}}$ at some $(\mathcal{U}_1, \mathcal{U}_2) \in \mathcal{X} \times \mathcal{X}$ acting on $\mathcal{V}_1, \mathcal{V}_2 \in \mathcal{X}$ is

$$\begin{aligned}&D\hat{\mathcal{F}}(\mathcal{U}_1, \mathcal{U}_2)(\mathcal{V}_1, \mathcal{V}_2) \\ &= \begin{pmatrix} \sum_{i=1}^d \left(\sum_{|\rho|=3}^{M_{1,i}+1} \sum_{\kappa+\gamma=\rho} c^1_{\kappa,\gamma} \kappa_i \widehat{\mathcal{U}_1^{\kappa-e_i} * \mathcal{U}_2^\gamma} * \mathcal{V}_1^{e_i} + \sum_{|\rho|=3}^{M_{1,i+d}+1} \sum_{\kappa+\gamma=\rho} c^1_{\kappa,\gamma} \gamma_i \mathcal{U}_1^\kappa \widehat{* \mathcal{U}_2^{\gamma-e_i}} * \mathcal{V}_2^{e_i} \right) \\ \vdots \\ \sum_{i=1}^d \left(\sum_{|\rho|=3}^{M_{d,i}+1} \sum_{\kappa+\gamma=\rho} c^d_{\kappa,\gamma} \kappa_i \widehat{\mathcal{U}_1^{\kappa-e_i} * \mathcal{U}_2^\gamma} * \mathcal{V}_1^{e_i} + \sum_{|\rho|=3}^{M_{d,i+d}+1} \sum_{\kappa+\gamma=\rho} c^d_{\kappa,\gamma} \gamma_i \mathcal{U}_1^\kappa \widehat{* \mathcal{U}_2^{\gamma-e_i}} * \mathcal{V}_2^{e_i} \right) \end{pmatrix}.\end{aligned}$$

From the estimate (29), we have, for $j = 1, \ldots, d$ and $i = 1, \ldots, d$,

$$\sup_{\|\mathcal{V}_1\|_{\mathcal{X}}=1} \left\| \left(\sum_{|\rho|=3}^{M_{j,i}+1} \sum_{\kappa+\gamma=\rho} c^j_{\kappa,\gamma} \widehat{\mathcal{U}_1^{\kappa-e_i} * \mathcal{U}_2^\gamma} \right) * \mathcal{V}_1^{e_i} \right\|_1 \leq \left\| \sum_{|\rho|=3}^{M_{j,i}+1} \sum_{\kappa+\gamma=\rho} c^j_{\kappa,\gamma} \mathcal{U}_1^{\kappa-e_i} * \mathcal{U}_2^\gamma \right\|_1$$

and similarly

$$\sup_{\|\mathcal{V}_2\|_{\mathcal{X}}=1} \left\| \left(\sum_{|\rho|=3}^{M_{j,i+d}+1} \sum_{\kappa+\gamma=\rho} c^j_{\kappa,\gamma} \mathcal{U}_1^\kappa \widehat{* \mathcal{U}_2^{\gamma-e_i}} \right) * \mathcal{V}_2^{e_i} \right\|_1 \leq \left\| \sum_{|\rho|=3}^{M_{j,i+d}+1} \sum_{\kappa+\gamma=\rho} c^j_{\kappa,\gamma} \mathcal{U}_1^\kappa * \mathcal{U}_2^{\gamma-e_i} \right\|_1.$$

Thus,

$$\begin{aligned}&\|D\mathcal{T}(\mathbf{0})\|_{B(\mathcal{X}^\infty)} \\ &\leq \|\mathcal{L}\|_{B(\mathcal{X}^\infty)} \left\|\Pi^\infty\right\|_{B(\mathcal{X}^\infty)} \left\|D\hat{\mathcal{F}}(\Pi_N(\mathcal{A}), \Pi_N({}^\tau\mathcal{A}))\right\|_{B(\mathcal{X})} \\ &\leq C_N \left\| \begin{pmatrix} \sum_{i=1}^d \left(\sum_{|\alpha|=0}^{M_{1,i}{}^N} \left| \sum_{|\rho|=3}^{M_{1,i}+1} \sum_{\kappa+\gamma=\rho} c^1_{\kappa,\gamma} \kappa_i \left(\Pi_N(\mathcal{A})^{\kappa-e_i} * \Pi_N({}^\tau\mathcal{A})^\gamma \right)_\alpha \right| + \sum_{|\alpha|=0}^{M_{1,i+d}{}^N} \left| \sum_{|\rho|=3}^{M_{1,i+d}+1} \sum_{\kappa+\gamma=\rho} c^1_{\kappa,\gamma} \gamma_i \left(\Pi_N(\mathcal{A})^\kappa * \Pi_N({}^\tau\mathcal{A})^{\gamma-e_i} \right)_\alpha \right| \right) \\ \vdots \\ \sum_{i=1}^d \left(\sum_{|\alpha|=0}^{M_{d,i}{}^N} \left| \sum_{|\rho|=3}^{M_{d,i}+1} \sum_{\kappa+\gamma=\rho} c^d_{\kappa,\gamma} \kappa_i \left(\Pi_N(\mathcal{A})^{\kappa-e_i} * \Pi_N({}^\tau\mathcal{A})^\gamma \right)_\alpha \right| + \sum_{|\alpha|=0}^{M_{d,i+d}{}^N} \left| \sum_{|\rho|=3}^{M_{d,i+d}+1} \sum_{\kappa+\gamma=\rho} c^d_{\kappa,\gamma} \gamma_i \left(\Pi_N(\mathcal{A})^\kappa * \Pi_N({}^\tau\mathcal{A})^{\gamma-e_i} \right)_\alpha \right| \right) \end{pmatrix} \right\|_{\mathbb{C}^d} \\ &= Z_1.\end{aligned}$$

We now consider the second derivative of $\mathcal{T}$ in the neighbourhood $B_{r_*}(\mathbf{0}) \subset \mathcal{X}^\infty$. From the

estimate (29),

$$
\begin{aligned}
&\sup_{\mathcal{H}\in B_{r_*}(\mathbf{0})} \left\|D^2\mathcal{T}(\mathcal{H})\right\|_{B(\mathcal{X}^\infty)} \\
&\leq \sup_{\mathcal{H}\in B_{r_*}(\mathbf{0})} \|\mathcal{L}\|_{B(\mathcal{X}^\infty)} \|\Pi^\infty\|_{B(\mathcal{X}^\infty)} \left\|D^2\hat{\mathcal{F}}(\Pi_N(\mathcal{A})+\mathcal{H}, \Pi_N({}^\tau\mathcal{A})+{}^\tau\mathcal{H})\right\|_{B(\mathcal{X},B(\mathcal{X}))} \\
&\leq C_N \begin{pmatrix} \sum_{i,j=1}^{d} \partial_{x_i}\partial_{y_j}|F_1|(\mathbf{z}) + \partial_{x_i}\partial_{x_j}|F_1|(\mathbf{z}) + \partial_{y_i}\partial_{y_j}|F_1|(\mathbf{z}) \\ \vdots \\ \sum_{i,j=1}^{d} \partial_{x_i}\partial_{y_j}|F_d|(\mathbf{z}) + \partial_{x_i}\partial_{x_j}|F_d|(\mathbf{z}) + \partial_{y_i}\partial_{y_j}|F_d|(\mathbf{z}) \end{pmatrix} \\
&= Z_2
\end{aligned}
$$

where $\mathbf{z} \stackrel{\text{def}}{=} \big(\|\pi_N(a^1)\|_1 + r_*, \ldots, \|\pi_N(a^d)\|_1 + r_*, \|\pi_N(\tau(a^1))\|_1 + r_*, \ldots, \|\pi_N(\tau(a^d))\|_1 + r_*\big)$. □

3.4 Numerical considerations

The result described in Lemma 3.3 leads to a straight forward implementation for computer assisted analysis of the unstable manifold parameterization. Suppose that the coefficients of the parameterization have been computed numerically (and rigorously enclosed via interval arithmetic) for all $2 \leq |\alpha| \leq N$ by solving the homological equations.

- **Step 1:** Compute Y using the formula given in Equation (30). Observe that this is a finite calculation involving only known data. If Y is too large (more than a few hundred multiples of machine precision) then consider shortening the eigenvalue scalings and/or increasing the order of the computation.
- **Step 2:** Compute the quantity Z_1 using the formula given in Equation (31). This can be done first without interval arithmetic to provide a good indication of the expected size of Z_1. If Z_1 is not less than one then the calculation of $\Pi_N(\mathcal{A})$ must be repeated using either higher order and/or shorter eigenvalue scalings.
- **Step 3:** Choose some $r_* > 0$ a-priori and compute Z_2 using the formula given in Equation (32). As a rule of thumbs, we choose it a few order below 1 and increase it only if the roots of p are larger than r_*.
- **Step 4:** If there exists $r_0 > 0$ satisfying Theorem 3.1, i.e. $p(r_0) = \dfrac{Z_2}{2}r_0^2 + Z_1 r_0 - r_0 + Y < 0$, $Z_1 + Z_2 r_0 < 1$ and $r_0 \in [0, r_*]$, then r_0 is a rigorous a-posteriori error bound for the tail of the Taylor series of the parametrization. Otherwise, one can recompute with higher order and/or smaller eigenvector scalings and/or larger r_*.

Further adjustments can be made to refine the bounds effectively and even reduce the computation time. For instance, notable improvements can be done with the following changes:

1. in the Z_1 bound (31), one could have chosen to keep the "hat-product" instead of the Cauchy product which, we recall, removes the terms involving the top coefficients;
2. one could also consider only the multiindices $\alpha \in \mathbb{N}^m$ such that the Z_1 bound is less than 1. More precisely, the set of multiindices such that the latter condition holds depends on C_N, that is the eigenvalues Λ. This is particularly relevant if the eigenvalues are of different orders.

4 Applications

Codes associated with the computations discussed in this section are found at [37]. It is important to keep in mind that r_0 is a bound on the tail of the Taylor series representation of the parametrization. In particular, it does not immediately provide a C^0 error between the polynomial approximation and the true parameterization of the unstable manifold. Indeed, we have to include the wrapping error involved in the exact computation of the Taylor coefficients.

More specifically, let P be the true solution of the invariance equation (4) which from Lemma 1.2 is given by Equation (8). Denote by $\overline{P}$ its polynomial approximation and by $\overline{\mathcal{A}} = (\overline{a^1}, \dots, \overline{a^d})$ its Taylor coefficients. Then,

$$\begin{aligned}\sup_{\sigma\in B_1(0)}\sup_{t\le 0}\left\|P(\sigma,t)-\overline{P}(\sigma,t)\right\|_{\mathbb{C}^d} &\le \|\mathcal{A}-\overline{\mathcal{A}}\|_{\mathcal{X}}\\ &\le \|\Pi_N(\mathcal{A}-\overline{\mathcal{A}})\|_{\mathcal{X}} + \|\Pi_\infty(\mathcal{A}-\overline{\mathcal{A}})\|_{\mathcal{X}}\\ &= \|\Pi_N(\mathcal{A}) - \Pi_N(\overline{\mathcal{A}})\|_{\mathcal{X}} + \|\Pi_\infty(\mathcal{A})\|_{\mathcal{X}}\\ &= \max_{1\le k\le d}\sum_{|\alpha|=0}^{N}\|a_\alpha^k - \overline{a^k}_\alpha\|_1 + r_0.\end{aligned}$$

Consequently, while the bounds Lemma 3.3 may give a r_0 below *machine epsilon*, the C^0 error bound will be at best of its order.

4.1 A delayed van der Pol equation

Consider again the delayed van der Pol system defined in Section 2.5. We would like to develop validated error bounds for numerical parameterizations like the ones computed in Section 2.7. Once again we take $\mu = 1$, $\tau = 2$, a = 0.9 and b = 0.1. The equilibrium is known exactly (it is at the origin). Using the methods developed in [33] we obtain computer assisted proof that the Morse index at the origin is two, and that the two unstable eigenvalues are a complex conjugate pair $\lambda_{1,2}$.

Moreover, from the characteristic matrix given by (23), it follows that for an eigenvalue λ, the associated eigenvector is determined by

$$\xi = s\begin{pmatrix}1\\ \lambda\end{pmatrix}, \qquad s\in\mathbb{R}.$$

A rigorous Newton's method (see [38] for more details) allows us to show that

$$\begin{aligned}\bar{\lambda}_1 &= 0.5218379440444361 + 0.8056375092559337i,\\ |\bar{\lambda}_1 - \lambda_1| &\le 5.2636242474841115\times 10^{-16}.\end{aligned}$$

The remaining eigenvalue $\bar{\lambda}_2$ is the complex conjugates of the above and enjoy the same same error bound; the associated eigenvectors are given by .

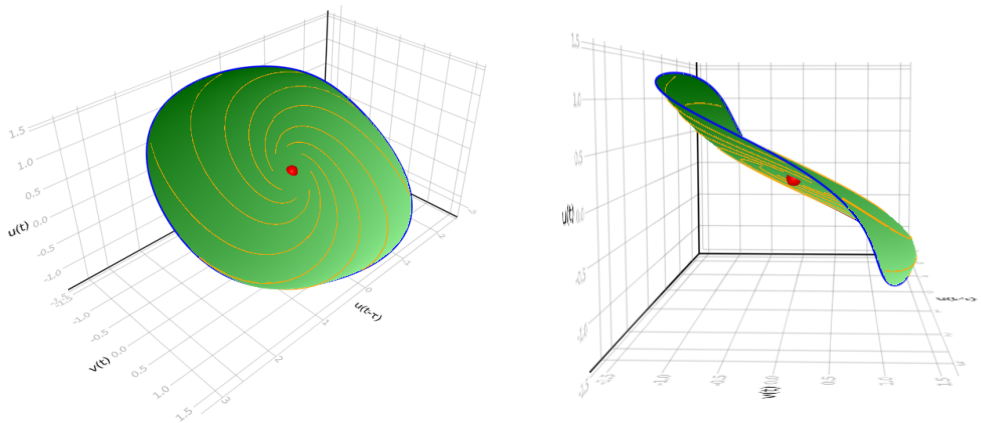
With this data we have all the inputs necessary to run the interval arithmetic version of Algorithm 2.6 to any desired order.

We choose the order $N = 99$ to obtain our polynomial approximation of the unstable manifold with a total of 5050 coefficients $(\pi_N(p)_{mn}, \pi_N(q)_{mn}) \in \mathbb{C}^2$ $(m, n = 0, \dots, N,\ m+n \le N)$ to compute. We note that the largest coefficient of order 99 has norm less than 1.9×10^{-38}.

One can visualize the manifold in Figure 2.

Combining the explicit form of $\hat{\mathcal{F}}_\alpha$ for the van der Pol system as given in Equation (24) with the formula for the Y bound given in Equation (30) leads to the expression

$$Y = C_N\sum_{n=N+1}^{3N}\sum_{m=0}^{n}\left|\mu(\pi_N(q)\,\widehat{*}\,\pi_N(\tau(p))^2)_{m,n-m}\right|,$$



(a) (b)

Figure 2: In green, the unstable manifold of the origin for the delayed van der Pol equation. In orange, the trajectories on the unstable manifold obtained via the conjugacy relation satisfied by the parameterization. In blue the boundary of the manifold.

which we evaluate using interval arithmetic to obtain that

$$Y \in [1.17146 \times 10^{-36}, 1.17147 \ \times 10^{-36}].$$

Observe that this is roughly a hundred times larger than the bound on the magnitude of the coefficients of order $N = 99$. That is, the coefficient size is in this case is an excellent indicator of the defect.

We obtain $C_N \in [0.0198871, 0.0198872]$, so that

$$Z_1 \in [0.886818, 0.886819],$$

and for $r_* = 10^{-3}$ we have

$$Z_2 \in [0.769352, 0.769353].$$

This yields

$$r_0 = 1.0350358132422712 \times 10^{-35}.$$

Then r_0 is a bound on the tail of the parameterization of the unstable manifold in the van der Pol system. We check that the C^0 error bound has

$$\sup_{\sigma \in B_1(0)} \sup_{t \leq 0} \left\| P(\sigma, t) - \overline{P}(\sigma, t) \right\|_{\mathbb{C}^2} \leq 1.2922996006636825 \times 10^{-13},$$

a bound which takes into account the round off errors in the Taylor coefficient computations as well as the bound on the tail.

4.2 An epidemiological model

Consider the following *SEIR* epidemiological system studied in [39]

$$\begin{cases} S'(t) = \mu N(t) - \nu \dfrac{S(t)I(t)}{N(t)} - \mu S(t), \\ E'(t) = \nu \dfrac{S(t)I(t)}{N(t)} - \nu \dfrac{S(t-\tau)I(t-\tau)}{N(t)} e^{-\mu\tau} - \mu E(t), \\ I'(t) = \nu \dfrac{S(t-\tau)I(t-\tau)}{N(t)} e^{-\mu\tau} - \gamma I(t) - \mu I(t), \\ R'(t) = \gamma I(t) - \mu R(t), \end{cases}$$

where $\gamma, \mu, \nu, \tau > 0$ are parameters, and where $S(t)$ represents the number of individuals susceptible to the disease, $I(t)$ represents the number of infected individuals who are infectious and are able to spread the disease by contact with susceptible individuals, $E(t)$ represents the number of exposed (in the latent period) individuals and $R(t)$ represents the number of individuals who have been infected and then removed from the possibility of being infected again or of spreading at time t. In this case, the delay $\tau \geq 0$ represents the time describing the latent period of the disease and the term $\nu \frac{S(t-\tau)I(t-\tau)}{N(t)}$ represents the individuals surviving in the latent period τ and becoming infective at time t.

Under the assumption that the population is constant $N(t) = N = E(t) + I(t) + R(t)$ and noticing that $E(t)$ only appears in $E'(t)$, it is sufficient to look at $S'(t)$ and $I'(t)$:

$$\begin{cases} S'(t) = \mu - \nu S(t)I(t) - \mu S(t), \\ I'(t) = \nu S(t-\tau)I(t-\tau)e^{-\mu\tau} - \gamma I(t) - \mu I(t), \end{cases}$$

where we did the normalization $(S, I) \mapsto (S/N, I/N)$.

The fixed points (S^*, I^*) are given by

$$\begin{cases} 0 = \mu - \nu S^* I^* - \mu S^*, \\ 0 = \nu S^* I^* e^{-\mu\tau} - \gamma I^* - \mu I^*. \end{cases}$$

The second equation implies $I^* = 0$ or $S^* = 1/R_0^\tau$ with $R_0^\tau = \frac{\nu}{\mu+\gamma} e^{-\mu\tau}$; R_0^τ is referred to as the *basic reproduction number*. Plugging this into the first equation, we have the two steady-states

$$(S_1, I_1) = (1, 0) \qquad \text{and} \qquad (S_2, I_2) = \left(\frac{1}{R_0^\tau}, \frac{\mu}{\nu}(R_0^\tau - 1) \right).$$

We find that the characteristic matrix is given by

$$\Psi(\lambda) = \begin{pmatrix} -\nu I^* - \mu - \lambda & -\nu S^* \\ \nu I^* e^{-\mu\tau} e^{-\lambda\tau} & -\mu - \gamma + \nu S^* e^{-\mu\tau} e^{-\lambda\tau} - \lambda \end{pmatrix}.$$

We focus on the disease free equilibrium $(S_1, I_1) = (1, 0)$, such that an eigenvalue λ is a solution of

$$\det \left| \begin{pmatrix} -\mu - \lambda & -\nu \\ 0 & -\mu - \gamma + \nu e^{-\mu\tau} e^{-\lambda\tau} - \lambda \end{pmatrix} \right| = (\lambda + \mu)(\lambda + \gamma + \mu - \nu e^{-\mu\tau} e^{-\lambda\tau})$$

and the associated eigenvector is determined by

$$\xi = s \begin{pmatrix} \nu \\ -(\lambda + \mu) \end{pmatrix}, \qquad s \in \mathbb{R}.$$

Let $\lambda = x + iy$. The imaginary part of $\lambda + \mu + \gamma - \nu e^{-\mu\tau} e^{-\lambda\tau}$ reads $y + \alpha \sin y\tau$, where $\alpha = \nu e^{-\mu\tau} e^{-x\tau}$. Provided $x > 0$ and $\nu\tau \in (0, 1)$, we have $\dfrac{d}{dy}(y + \alpha \sin y\tau) > 0$ for all $y \in \mathbb{R}$. Thus, $y = 0$ is the unique zero of g and we have a unique unstable eigenvalue λ.

One can visualize the manifold in Figure 3.

Set $\gamma = 0.1$, $\mu = 0.1$, $\nu = 0.5$ and $\tau = 1$. By using a rigorous Newton's method (see [38] for more details), we obtain

$$\bar{\lambda} = 0.1784703538844722, \qquad |\bar{\lambda} - \lambda| \leq 7.255548872917566 \times 10^{-16}.$$

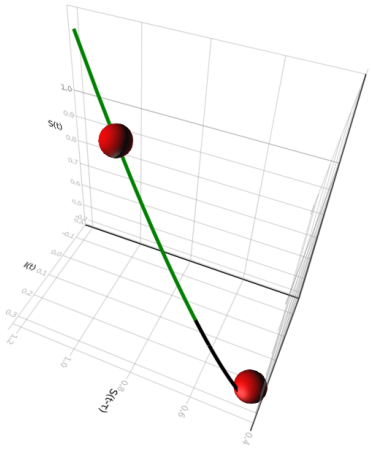


Figure 3: In green, the proven unstable manifold of the equilibrium $(S_2, I_2) = \left(\frac{1}{R_0^\tau}, \frac{\mu}{\nu}(R_0^\tau - 1)\right)$ for the SEIR model with $\gamma = 0.1$, $\mu = 0.1$, $\nu = 0.5$ and $\tau = 1$. In black, a non rigorous numerical integration suggesting a possible heteroclinic connection between the disease free equilibria $(S_1, I_1) = (1, 0)$ and (S_2, I_2).

The bounds for $N = 200$ and $r_* = 10^{-3}$ are

$$\begin{aligned} Y &\in [3.39957 \times 10^{-12}, 3.39958 \times 10^{-12}], \\ C_N &\in [0.0283506, 0.0283507], \\ Z_1 &\in [0.957894, 0.957895], \\ Z_2 &\in [0.0283506, 0.0283507]. \end{aligned}$$

Thus, we find

$$r_0 = 8.073867668235697 \times 10^{-11}.$$

However, in our computation, we find that

$$\max_{1 \le k \le d} \sum_{|\alpha|=0}^{N} \|a_\alpha^k - \overline{a^k}_\alpha\|_1 \le 7.855938122247608 \times 10^{-13}.$$

Consequently, we can hope to reach as low as the order 10^{-13}. To illustrate how much control on r_0 our method gives, suppose one would be willing to compute 1000 Taylor coefficients (as our problem is a one dimensional manifold and a quadratic differential equation, this bears little computational cost), then for $r_* = 10^{-3}$ we obtain

$$\begin{aligned} Y &\in [3.24923 \times 10^{-94}, 3.24924 \times 10^{-94}], \\ C_N &\in [0.00561643, 0.00561644], \\ Z_1 &\in [0.189764, 0.189765], \\ Z_2 &\in [0.00561643, 0.00561644], \end{aligned}$$

and the corresponding root of the radii polynomial is $r_0 = [4.010231975551042 \times 10^{-94}]$. Thus, the C^0 error bound is

$$\sup_{\sigma \in B_1(0)} \sup_{t \le 0} \left\| P(\sigma, t) - \overline{P}(\sigma, t) \right\|_{\mathbb{C}^2} \le 7.85593812224761 \times 10^{-13}.$$

4.3 The Mackey-Glass model for white blood cell

Recall the Mackey-Glass Equation (11), which was originally introduced in [40] to model the concentration of white blood cells in a subject. Its equilibria are

$$u_0 = 0, \qquad u_1 = \left(\frac{\beta}{\gamma} - 1\right)^{1/n}$$

and the characteristic equation reads

$$0 = \det(\Psi(\lambda)) = -\gamma + \beta\frac{1-(\rho-1)(u^*)^\rho}{(1+(u^*)^\rho)^2}e^{-\lambda\tau} - \lambda = \begin{cases} -\gamma + \beta e^{-\lambda\tau} - \lambda, & u^* = u_0, \\ -\gamma + \frac{\gamma^2}{\beta}\left(\rho - \frac{\beta}{\gamma}(\rho-1)\right)e^{-\lambda\tau} - \lambda, & u^* = u_1. \end{cases} \tag{33}$$

For computational purposes, we focus on the polynomial form of the Mackey-Glass equation given by Equation (12). According to [25], (11) and (12) admits the same equilibria and the same corresponding eigenvalues; also, the associated eigenvectors for the system (12) are determined by

$$\xi = s\begin{pmatrix} 1 \\ -\rho(u^*)^{\rho-1} \end{pmatrix}, \qquad s \in \mathbb{R}.$$

It is clear from Equation (33) that for u_0 we have one unstable eigenvalue λ. Let $\tau = 2$, $\beta = 2$ and $\gamma = 1$. We compute the eigenvalue via a rigorous Newton's method (see [38] for more details)

$$\bar{\lambda} = 0.2393001697495648, \qquad |\bar{\lambda} - \lambda| \leq 2.735639747364635 \times 10^{-16}.$$

For $\rho \geq 6$, a hopf bifurcation has occurred and u_1 has now two unstable directions. For such ρ, the workload increases drastically and the two dimensional unstable manifold of u_1 can be proven after a very long runtime and scaling $s < 10^{-1}$.

Table 1 shows the bounds for the one dimensional unstable manifold associated to u_0 for different values of the parameter ρ; note that for a given scaling s, increasing ρ helps for the decay of Y as more convolutions are involved. From Figure 4, we observe numerically heteroclinic connections between the equilibria u_0 and u_1 for $\rho = 2, 3, 4, 5$. At $\rho = 6$, Figure 5 shows that the unstable manifold of u_0 seems to go towards a periodic orbit about u_1.

ρ	s	Y	Z_1	Z_2	r_0	C^0 error bound
2	0.7	$[0, 7.07451 \times 10^{-17}]$	$[0.974922, 0.97493]$	$[4.76185, 4.76187]$	$2.8217933626969985 \times 10^{-15}$	$8.936693615517724 \times 10^{-15}$
3	0.7	$[0, 6.41125 \times 10^{-54}]$	$[0.128703, 0.128704]$	$[1.83918, 1.83919]$	$7.358282103472888 \times 10^{-54}$	$1.262878690511116 \times 10^{-15}$
4	0.7	$[0, 3.82093 \times 10^{-70}]$	$[0.0648989, 0.064899]$	$[1.69807, 1.69808]$	$4.086110681933862 \times 10^{-70}$	$5.065392549852279 \times 10^{-16}$
5	0.7	$[0, 1.36263 \times 10^{-78}]$	$[0.0414152, 0.0414153]$	$[1.68682, 1.68683]$	$1.421499690866838 \times 10^{-78}$	$3.339387096700201 \times 10^{-16}$
6	0.9	$[0, 2.16623 \times 10^{-17}]$	$[0.556393, 0.556394]$	$[19.1673, 19.1674]$	$4.883199523552479 \times 10^{-17}$	$5.380240154610301 \times 10^{-16}$
10	0.9	$[0, 6.8496 \times 10^{-25}]$	$[0.298606, 0.298607]$	$[21.7748, 21.7749]$	$9.765696825614624 \times 10^{-25}$	$4.313375009670121 \times 10^{-16}$

Table 1: Bounds associated to the one dimensional unstable manifold of u_0 for different values of $\rho \in \mathbb{N}$. In every cases $N = 600$ and $r_* = 10^{-3}$, for which $C_N \in [0.00700184, 0.00700185]$.

A Resolvent bound for DDEs

Throughout this section we assume that $\lambda_1, \ldots, \lambda_m \in \mathbb{C}$ are non-resonant in the sense of Definition 1.

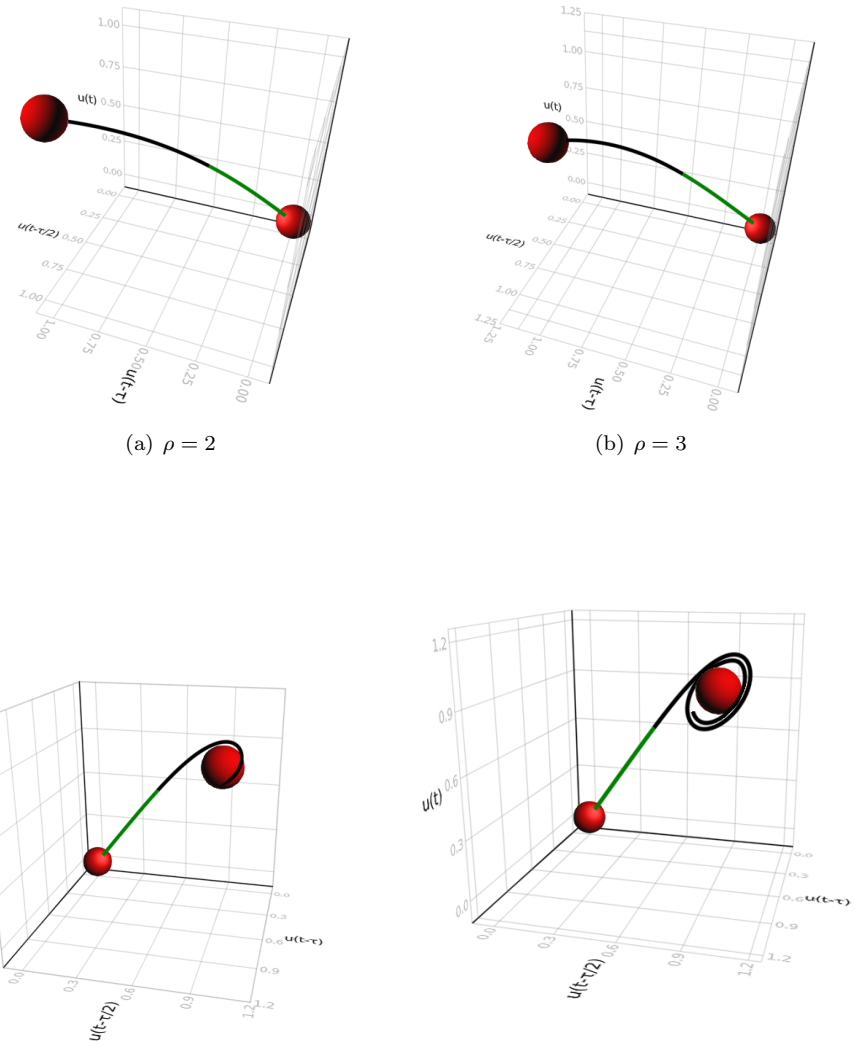
Recall that given $z \in \mathbb{C}$, denote by $\mathrm{Re}(z) \in \mathbb{R}$ its real part.

Proposition A.1 (Resolvent bound)**.** *Suppose that $\tau > 0$, that K_1, K_2 are complex $n \times n$ matrices, and that z is a complex number with*

$$|z| > \|K_1\|, \tag{34}$$

and

$$\mathrm{Re}(z) > \frac{1}{\tau}\ln\left(\frac{\|K_2\|}{|z| - \|K_1\|}\right). \tag{35}$$



(a) $\rho = 2$ (b) $\rho = 3$

(c) $\rho = 4$ (d) $\rho = 5$

Figure 4: In green, the proven unstable manifold of the equilibrium $u_0 = 0$ for the Mackey-Glass equation with $\tau = 2$, $\beta = 2$ and $\gamma = 1$. In black, a non rigorous numerical integration suggesting a possible heteroclinic connection between the equilibria u_0 and $u_1 = 1$.

Then the matrix

$$\Psi(z) = K_1 + e^{-\tau z} K_2 - zId,$$

is invertible with

$$\left\|\Psi(z)^{-1}\right\| \leq \frac{1}{|z| - \left(\|K_1\| + e^{-\tau \mathrm{Re}(z)} \|K_2\|\right)}. \tag{36}$$

Proof. Suppose that $z \in \mathbb{C}$ satisfies the conditions given in Equations (34) and (35). Consider the family of matrices

$$\Psi_0(z) = K_1 - z\mathrm{Id} = -z\left(\mathrm{Id} - \frac{1}{z}K_1\right).$$

Since

$$\frac{\|K_1\|}{|z|} < 1,$$

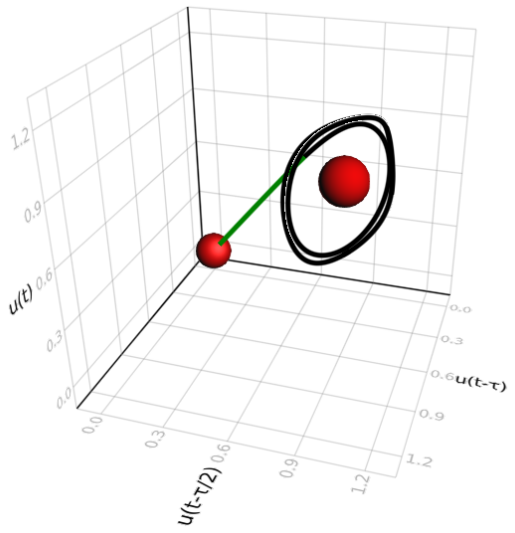


Figure 5: In green, the proven unstable manifold of the equilibrium $u_0 = 0$ for the Mackey-Glass equation with $\tau = 2$, $\beta = 2$ and $\gamma = 1$. In black, a non rigorous numerical integration suggesting a possible heteroclinic connection between the equilibrium u_0 and a periodic orbit about $u_1 = 1$.

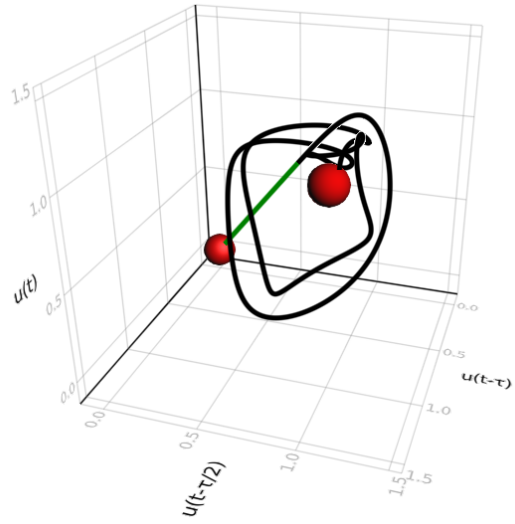


Figure 6: In green, the proven unstable manifold of the equilibrium $u_0 = 0$ for the Mackey-Glass equation with $\tau = 2$, $\beta = 2$ and $\gamma = 1$. In black, a non rigorous numerical integration showing a longer term behaviour in the attractor.

we have that $\left(\mathrm{Id} - \frac{1}{z}K_1\right)$ is invertible with

$$\left\| \left(\mathrm{Id} - \frac{1}{z}K_1\right)^{-1} \right\| \leq \frac{1}{1 - \|K_1\|/|z|}.$$

It follows that $\Psi_0(z)$ is invertible, that

$$\Psi_0(z)^{-1} = -\frac{1}{z}\left(\mathrm{Id} - \frac{1}{z}K_1\right)^{-1},$$

and that we have the bound

$$\left\|\Psi_0(z)^{-1}\right\| \leq \frac{1}{|z| - \|K_1\|}.$$

We now consider the family

$$\Psi(z) = K_1 + e^{-\tau z}K_2 - z\mathrm{Id}.$$

We have that

$$\begin{aligned}\Psi(z) &= K_1 - z\mathrm{Id} + e^{-\tau z}K_2 \\ &= \Psi_0(z) + e^{-\tau z}K_2 \\ &= \Psi_0(z)\left[\mathrm{Id} + e^{-\tau z}\Psi_0(z)^{-1}K_2\right]\end{aligned}$$

Since

$$\begin{aligned}\left\|e^{-\tau z}\Psi_0(z)^{-1}K_2\right\| &\leq e^{-\tau \mathrm{Re}(z)}\|K_2\|\frac{1}{|z| - \|K_1\|} \\ &< 1,\end{aligned}$$

we have that $\mathrm{Id} + e^{-\tau z}\Psi_0(z)^{-1}K_2$ is invertible with

$$\left\|\left(\mathrm{Id} + e^{-\tau z}\Psi_0(z)^{-1}K_2\right)^{-1}\right\| \leq \frac{1}{1 - \frac{e^{-\tau \mathrm{Re}(z)}\|K_2\|}{|z| - \|K_1\|}}.$$

It follows that $\Psi(z)$ is invertible, that

$$\Psi(z)^{-1} = \left[\mathrm{Id} + e^{-\tau z}\Psi_0(z)^{-1}K_2\right]^{-1}\Psi_0(z)^{-1}$$

and that

$$\left\|\Psi(z)^{-1}\right\| \leq \frac{1}{1 - \frac{e^{-\tau \mathrm{Re}(z)}\|K_2\|}{|z| - \|K_1\|}}\frac{1}{|z| - \|K_1\|} = \frac{1}{|z| - \left(\|K_1\| + e^{-\tau \mathrm{Re}(z)}\|K_2\|\right)}.$$

□

Corollary A.2. *Define*

$$\mu_* = \min_{1 \leq j \leq m} |\lambda_j|,$$

and

$$\mu^* = \min_{1 \leq j \leq m} \mathrm{Re}(\lambda_j).$$

Let

$$N = \max\left(\left\lceil \frac{\|K_1\| + 1}{\mu_*} \right\rceil, \left\lceil \frac{1}{\tau\mu^*}\log(\|K_2\|) \right\rceil + 1\right).$$

Then for any $\alpha \in \mathbb{N}^m$ with $|\alpha| \geq N$ we have that

$$\Psi(\langle \alpha, \Lambda \rangle) = K_1 + e^{-\langle \alpha, \Lambda \rangle \tau}K_1 - \langle \alpha, \Lambda \rangle \, Id,$$

is invertible with

$$\left\|\Psi(\langle \alpha, \Lambda \rangle)^{-1}\right\| \leq \frac{C}{|\langle \alpha, \Lambda \rangle|}.$$

where $C > 0$ can be taken as

$$C = \frac{1}{1 - \frac{\|K_1\| + e^{-\tau\mu^* N}\|K_2\|}{N\mu_*}}.$$

Proof. Note that $\mu_*, \mu^* > 0$ as the λ_j are unstable. Note also that the hypotheses on N give

$$N\mu_* \geq \|K_1\| + 1 > \|K_1\|,$$

and

$$N\mu^* \geq \frac{1}{\tau}\log(\|K_2\|) + 1 > \frac{1}{\tau}\log(\|K_2\|),$$

so that

$$e^{-\tau\mu^* N}\|K_2\| < 1.$$

Now assume that $\alpha \in \mathbb{N}^m$ has $|\alpha| \geq N$. Then

$$|\alpha_1\lambda_1 + \ldots + \alpha_m\lambda_m| \geq N\mu_* > \|K_1\|,$$

and

$$\mathrm{Re}\,(\alpha_1\lambda_1 + \ldots + \alpha_m\lambda_m) \geq N\mu^* > \frac{1}{\tau}\log(\|K_2\|).$$

Then

$$e^{-\tau(\alpha_1\lambda_1+\ldots+\alpha_m\lambda_m)}\|K_2\| \leq e^{-\tau\mu^* N}\|K_2\| < 1$$

So, we have that

$$z = \alpha_1\lambda_1 + \ldots + \alpha_m\lambda_m,$$

satisfies the hypotheses of Proposition A.1, and $\Psi(\alpha_1\lambda_1 + \ldots + \alpha_m\lambda_m)$ is invertible.

Noting that

$$N\mu_* \geq \|K_1\| + 1 > \|K_1\| + e^{-\tau\mu^* N}\|K_2\|,$$

we have that

$$\frac{\|K_1\| + e^{-\tau\mathrm{Re}(\alpha_1\lambda_1+\ldots+\alpha_m\lambda_m)}\|K_2\|}{|\alpha_1\lambda_1 + \ldots + \alpha_m\lambda_m|} \leq \frac{\|K_1\| + e^{-\tau\mu^* N}\|K_2\|}{N\mu_*} < 1,$$

and from Proposition A.1 we have the estimate

$$\begin{aligned}
\left\|\Psi(\langle\alpha,\Lambda\rangle)^{-1}\right\| &\leq \frac{1}{|\alpha_1\lambda_1 + \ldots + \alpha_m\lambda_m| - \left(\|K_1\| + e^{-\tau\mathrm{Re}(\alpha_1\lambda_1+\ldots+\alpha_m\lambda_m)}\|K_2\|\right)} \\
&= \frac{1}{|\alpha_1\lambda_1 + \ldots + \alpha_m\lambda_m|\left(1 - \frac{\|K_1\|+e^{-\tau\mathrm{Re}(\alpha_1\lambda_1+\ldots+\alpha_m\lambda_m)}\|K_2\|}{|\alpha_1\lambda_1+\ldots+\alpha_m\lambda_m|}\right)} \\
&\leq \frac{1}{|\alpha_1\lambda_1 + \ldots + \alpha_m\lambda_m|\left(1 - \frac{\|K_1\|+e^{-\tau\mu^* N}\|K_2\|}{N\mu_*}\right)},
\end{aligned}$$

as desired. □

A.1 Example: delayed van der Pol

In a specific problem we sometimes derive resolvent bounds by hand rather than using the general estimates of Corollary A.2. For example consider the delayed van der Pol equation defined in Section 2.5 and take parameters a = 0.9, b = 0.1, $\mu = 1$, and $\tau = 2$. Then

$$K_1 = \begin{pmatrix} 0 & 1 \\ -0.9 & 1 \end{pmatrix}, \qquad \text{and} \qquad K_2 = \begin{pmatrix} 0 & 0 \\ -0.1 & 0 \end{pmatrix},$$

and we see that

$$\|K_1\| \leq 1.9, \qquad \text{and} \qquad \|K_2\| \leq 0.1,$$

as the matrix norm is the infinity norm. Note that if $|z| > 2$ then $|z| - \|K_1\| > 0.1$, so that $\|K_2\|/(|z| - \|K_1\|) < 1$. In this case the logarithm is negative. So, for all z in the right half plane we have that $\mathrm{Re}(z) > \log(\|K_2\|/(|z| - \|K_1\|))/\tau$. Taking z in the right half plane with $|z| > 2$ guarantees that all the hypotheses of Proposition A.1 hold, and for such $|z|$ we have that $\Psi(z)$ is invertible and that the bound given in Equation (36) holds.

Let $c \pm id = \lambda_{1,2}$. Recalling the result from Section 4.1 that

$$\lambda_{1,2} \approx 0.52183794404443 \pm 0.80563750925593i,$$

with an error of less than 10^{-15}, we are safe in saying that $\mathrm{Re}(\lambda_{1,2}) = c > 0.5$. Then

$$|\alpha_1\lambda_1 + \alpha_2\lambda_2| = \sqrt{|\alpha|^2c^2 + (\alpha_1 - \alpha_2)^2d^2} \geq |\alpha|c > \frac{|\alpha|}{2},$$

as $a = \mathrm{Re}(\lambda_{1,2}) > 0.5$. Then taking $|\alpha| > 4$ is sufficient to guarantee that the resolvent bound holds. That is, as long as we parameterize the manifold to order $N \geq 5$ or higher we have that

$$\begin{aligned}
\|\Psi(\alpha_1\lambda_1 + \alpha_2\lambda_2)^{-1}\| &\leq \frac{1}{|\alpha_1\lambda_1 + \alpha_2\lambda_2| - \left(1.9 + 0.1e^{-|\alpha|}\right)} \\
&\leq \frac{1}{0.5N - (1.9 + 0.1e^{-N})}
\end{aligned}$$

For example when $N = 25$ we have that

$$\sup_{|\alpha|\geq 26}\left\|\Psi(\alpha_1\lambda_1 + \alpha_2\lambda_2)^{-1}\right\| \leq 0.09434.$$

Taking $C_N = 0.1$ we have the bound

$$\sup_{|\alpha|> 25}\left\|\Psi(\alpha_1\lambda_1 + \alpha_2\lambda_2)^{-1}\right\| \leq C_N = 0.1.$$

This estimate is simple to work out by hand and illustrates what is happening in the bounds. Nevertheless it is quite conservative, and better bounds are obtained in our general codes by using interval arithmetic to enclose the expressions.

B Proof of Lemma 1.1

Suppose that $P\colon D^m \times (-\infty, 0] \to \mathbb{R}^n$ satisfies the hypotheses of Lemma 1.1. Choose any $\hat{\sigma} \in D^m$ and define the function $\hat{x}\colon (-\infty, 0] \to \mathbb{R}^n$ by

$$\hat{x}(t) = P(\hat{\sigma}_1, \ldots, \hat{\sigma}_m, t).$$

Observe that

$$\hat{x}(t) = P(\hat{\sigma}_1 e^{\lambda_1 t}, \ldots, \hat{\sigma}_m e^{\lambda_m t}, 0),$$

by the shift invariance. Note that $\hat{x}(t)$ is well defined for all $t \leq 0$. We claim that $\hat{x}(t)$ is a solution of the DDE on the time interval $(-\infty, 0]$. To see this, differentiate with respect to time and obtain

$$\begin{aligned}
\frac{d}{dt}\hat{x}(t) &= \frac{d}{dt} P(\hat{\sigma}_1 e^{\lambda_1 t}, \ldots, \hat{\sigma}_m e^{\lambda_m t}, 0) \\
&= \hat{\sigma}_1 \lambda_1 e^{\lambda_1 t} \frac{\partial}{\partial \sigma_1} P(\hat{\sigma}_1 e^{\lambda_1 t}, \ldots, \hat{\sigma}_m e^{\lambda_m t}, 0) + \ldots + \hat{\sigma}_m \lambda_m e^{\lambda_m t} \frac{\partial}{\partial \sigma_m} P(\hat{\sigma}_1 e^{\lambda_1 t}, \ldots, \hat{\sigma}_m e^{\lambda_m t}, 0) \\
&= F(P(\hat{\sigma}_1 e^{\lambda_1 t}, \ldots, \hat{\sigma}_m e^{\lambda_m t}, 0), P(\hat{\sigma}_1 e^{\lambda_1 t}, \ldots, \hat{\sigma}_m e^{\lambda_m t}, -\tau)) \\
&= F(P(\hat{\sigma}_1 e^{\lambda_1 t}, \ldots, \hat{\sigma}_m e^{\lambda_m t}, 0), P(\hat{\sigma}_1 e^{\lambda_1 t} e^{-\lambda_1 \tau}, \ldots, \hat{\sigma}_m e^{\lambda_m t} e^{-\lambda_m \tau}, 0)) \\
&= F(P(\hat{\sigma}_1 e^{\lambda_1 t}, \ldots, \hat{\sigma}_m e^{\lambda_m t}, 0), P(\hat{\sigma}_1 e^{\lambda_1 (t-\tau)}, \ldots, \hat{\sigma}_m e^{\lambda_m (t-\tau)}, 0)) \\
&= F(\hat{x}(t), \hat{x}(t-\tau)).
\end{aligned}$$

To see that $\hat{x}(t)$ is on the unstable manifold of c we exploit the fact that the backwards flow of a known solution of the DDE is obtained by shifting backwards in time along the solution curve. Then, by taking the limit

$$\begin{aligned}
\lim_{t \to -\infty} \hat{x}(t) &= \lim_{t \to -\infty} P(\hat{\sigma}, t) \\
&= \lim_{t \to -\infty} P(\hat{\sigma}_1 e^{\lambda_1 t}, \ldots, \hat{\sigma}_m e^{\lambda_m t}, 0) \\
&= P(0, \ldots, 0, 0) \\
&= c,
\end{aligned}$$

we have that that a point in the image of P is a solution of the DDE with backward history accumulating at the equilibrium solution. Since the image of P is an m-dimensional smooth disk tangent to the unstable eigenspace at c, we have that P parameterizes a local unstable manifold at c as desired.

C Proof of Theorem 3.1

Suppose there exists $r_* > 0$ such that $p(r_0) = \frac{Z_2}{2} r_0^2 + (Z_1 - 1) r_0 + Y \leq 0$ for some $r_0 \in [0, r_*]$.

For $h \in B_{r_0}(x_0) \subset B_{r_*}(x_0)$,

$$\begin{aligned}
\|T(h) - x_0\|_X &\leq \|T(x_0) - x_0\|_X + \|T(h) - T(x_0)\|_X \\
&\leq Y + \int_0^1 \|DT(x_0 + t(h - x_0))(h - x_0)\|_X \, dt \\
&\leq Y + r_0 \int_0^1 \|DT(x_0 + t(h - x_0))\|_{B(X)} \, dt \\
&= Y + r_0 \int_0^1 \|DT(x_0 + t(h - x_0)) + DT(x_0) - DT(x_0)\|_{B(X)} \, dt \\
&\leq Y + \|DT(x_0)\|_{B(X)} r_0 + r_0 \int_0^1 \|DT(x_0 + t(h - x_0)) - DT(x_0)\|_{B(X)} \, dt \\
&\leq Y + Z_1 r_0 + r_0 \int_0^1 \left(\sup_{z \in [x_0, x_0 + t(h - x_0)]} \|D^2 T(z)\|_{B(X, B(X))} \right) t \|h - x_0\|_X \, dt \\
&\leq Y + Z_1 r_0 + r_0 \int_0^1 \left(\sup_{z \in B_{r_*}(x_0)} \|D^2 T(z)\|_{B(X, B(X))} \right) t \|h - x_0\|_X \, dt \\
&\leq Y + Z_1 r_0 + Z_2 r_0^2 \int_0^1 t \, dt \\
&\leq Y + Z_1 r_0 + \frac{Z_2}{2} r_0^2 \\
&\leq r_0
\end{aligned}$$

that is T maps the ball into itself.

Finally, since $Z_1 + Z_2 r_0 < 1$, for $h_1, h_2 \in B_{r_0}(x_0)$ we have

$$\begin{aligned}
\|T(h_1) - T(h_2)\|_X &\leq \|h_1 - h_2\|_X \int_0^1 \|DT(h_1 + t(h_2 - h_1))\|_{B(X)}\, dt \\
&\leq \|h_1 - h_2\|_X \left(\int_0^1 \|DT(x_0)\|_{B(X)}\, dt + \int_0^1 \|DT(z_1 + t(h_2 - h_1)) - DT(x_0)\|_{B(X)}\, dt \right) \\
&\leq \|h_1 - h_2\|_X \, (Z_1 + Z_2 r_0) \\
&< \|h_1 - h_2\|_X
\end{aligned}$$

which proves that T is a contraction.

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