

Validated numerics for equilibria of analytic vector fields: invariant manifolds and connecting orbits

J.D. Mireles James, *

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Abstract

The goal of these notes is to illustrate the use of validated numerics as a tool for studying the dynamics near and between equilibrium solutions of ordinary differential equations. We examine Taylor methods for computing local stable/unstable manifolds and also for expanding the flow in a neighborhood of a given initial condition. The Taylor methods discussed here have the advantage that the first N terms in the series are computed by recursion relations. Bounds on the tail of the series follow from a contraction mapping argument. As an application we apply these validated local computations to prove the existence of a heteroclinic connecting orbit in the Lorenz system.

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*Florida Atlantic University. Email: jmirelesjames@fau.edu.

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1 Introduction

Equilibria, periodic orbits, and connections between them occupy a central place in the qualitative theory of dynamical systems, as these special solutions are examples of low dimensional invariant sets which carry global information. Smale’s theorem for example tells us that a single non degenerate homoclinic for a periodic orbit forces the existence of infinitely many periodic orbits of arbitrarily long period, of chaotic motions, and mixing. Connecting orbits are fundamental in the study of nonlinear waves and for understanding pattern formation. Equilibria and connecting orbits make up the chain groups and boundary operators in Morse homology theory, allowing one to recover the homology of a compact N -dimensional manifold from zero and one dimensional data. Yet, for applications with strong nonlinearities, connecting orbits are difficult if not impossible to analyze by hand.

The lectures contained in the present volume describe mathematically rigorous tools in nonlinear analysis, which exploit in a fundamental way the power of the digital computer. The present lecture is a tutorial on local analysis for analytic vector fields. Suppose we are given a hyperbolic equilibrium point. We would like to understand the dynamics nearby—where are the local stable/unstable manifolds? Suppose on the other hand we are given a non-equilibrium point. Then we want to understand the flow nearby – what happens to nearby points for nearby times? With enough local information a global picture of the dynamics begins to emerge. By the end of this note we will construct some computer assisted arguments which prove the existence for transverse saddle-to-saddle connecting orbits.

The main tools used in the present note is Taylor series. We discuss a functional analytic framework for computer assisted proofs involving unknown analytic functions of several complex variables. The discussion is formulated in certain Banach spaces of infinite sequences (or infinite multi-sequences). Framing arguments in sequence space keeps us “close to the numerics,” and avoids some function space technicalities. The sequence space framework applies immediately to both the high order parameterization of an invariant manifold, and to the high order Taylor series solution of a initial value problem (we expand solutions of initial value problems in the spatial variables as well as in time). For both manifold and flow box computations an elementary contraction mapping argument bounds the truncation errors in the tail. For numerical applications we fix our attention on the familiar example of the Lorenz system.

Throughout the notes we make liberal use of the validated numerical algorithms discussed in [1], and the employ the interval arithmetic library IntLab [2] which runs under MatLab.

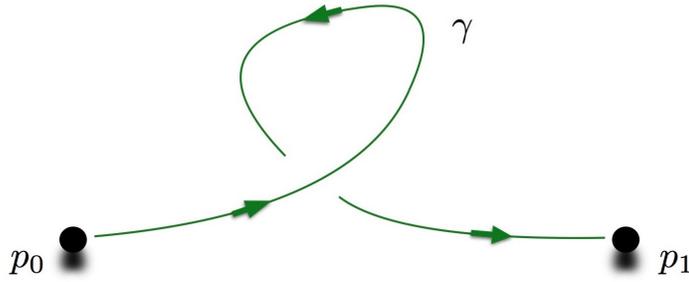


Figure 1: A heteroclinic connecting orbit from p_0 to p_1 .

1.1 Connecting orbits between equilibrium solutions of ordinary differential equations

Suppose that $f: \mathbb{R}^n \rightarrow \mathbb{R}^n$ is a real analytic vector field, and that $p_0, p_1 \in \mathbb{R}^n$ are equilibrium solutions of the differential equation

$$x' = f(x), \tag{1}$$

i.e. that p_0 and p_1 have that $f(p_0) = f(p_1) = 0$. A *heteroclinic connecting orbit* from p_0 to p_1 is a smooth curve $\gamma: (-\infty, \infty) \rightarrow \mathbb{R}^n$ which satisfies Equation (1) and which is subject to the constraints

$$\lim_{t \rightarrow -\infty} \gamma(t) = p_0, \quad \text{and} \quad \lim_{t \rightarrow \infty} \gamma(t) = p_1.$$

In other words γ is the solution of a boundary value problem on the unbounded domain \mathbb{R} with prescribed asymptotic behavior at plus and minus infinity. The situation is illustrated in Figure 1.

A standard method for treating the boundary conditions at infinity is the *method of projected boundaries* [3, 4, 5, 6, 7, 8]. The idea is to look for an orbit segment $\gamma: [0, T] \rightarrow \mathbb{R}^n$ satisfying Equation (1) on $(0, T)$ and having that

$$\gamma(0) \in W_{\text{loc}}^u(p_0), \quad \text{and} \quad \gamma(T) \in W_{\text{loc}}^s(p_1).$$

In other words, by projecting onto local unstable/stable manifolds of the equilibria, one guaranties that the conditions at infinity are met.

Let $\mathbb{E}^u, \mathbb{E}^s$ denote the unstable and stable eigenspaces of p_0 and p_1 respectively. We write $m_0 = \dim(\mathbb{E}^u)$ and $m_1 = \dim(\mathbb{E}^s)$ and for the moment place no restrictions on m_0, m_1 (appropriate constraints will emerge momentarily). Lets postpone for the moment any approximation scheme for the local stable/unstable manifolds (though linear approximation is a common choice) and assume that we know exactly some one to one maps $P: \mathbb{E}^u \rightarrow \mathbb{R}^n$ and $Q: \mathbb{E}^s \rightarrow \mathbb{R}^n$ having

$$P(0) = p_0, \quad \text{with} \quad \text{image}(P) \subset W_{\text{loc}}^u(p_0),$$

and

$$Q(0) = p_1, \quad \text{with} \quad \text{image}(Q) \subset W_{\text{loc}}^s(p_1).$$

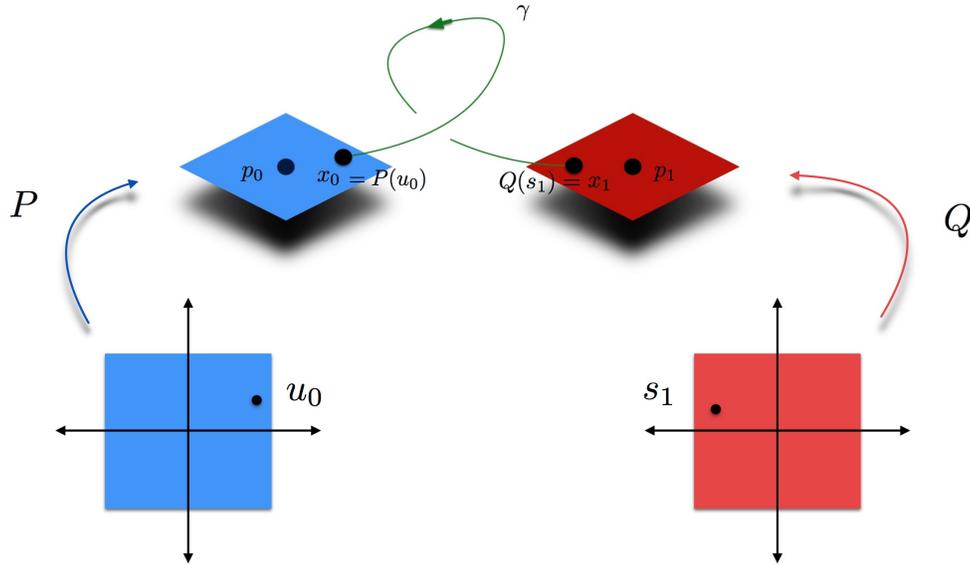


Figure 2: The meaning of the connecting orbit operator: Here P and Q are chart maps, or parameterizations of the local unstable and stable manifolds of p_0 and p_1 respectively. Using the charts, we are able to formulate a finite time boundary value problem for the connecting orbit. Namely we look for an orbit with initial conditions on the unstable manifold which arrives, after flowing for a time $L > 0$ on the stable manifold. The boundary conditions on the manifold are replaced with unknown coordinates u_0 and s_1 in the parameter spaces of the charts.

Then the problem of locating a heteroclinic orbit from p_0 to p_1 is reformulated as follows: find $u_0 \in \mathbb{E}^u$, $s_1 \in \mathbb{E}^s$, and a smooth curve $\gamma: [0, T] \rightarrow \mathbb{R}^n$ so that γ solves Equation (1) subject to the constraints

$$\gamma(0) = P(u_0), \quad \text{and} \quad \gamma(T) = Q(s_1).$$

The idea is illustrated in Figure 2.

Now, suppose that $\phi: \mathbb{R}^n \times \mathbb{R} \rightarrow \mathbb{R}^n$ is the flow generated by f , and define $F: \mathbb{E}^u \times \mathbb{E}^s \times \mathbb{R} \rightarrow \mathbb{R}^n$ by

$$F(u, s, T) = \phi(P(u), T) - Q(s). \quad (2)$$

If (u, s, T) is a zero of F , then

$$\gamma(t) = \phi(P(u), t),$$

is a solution of the projected boundary problem, hence a connecting orbit. We refer to F as the connecting orbit operator.

The goal driving these lectures is this: to deduce sufficient conditions for the existence of a zero of F in Equation (2). The sufficient conditions must be checkable via a finite number of operations. These will be carried out using the digital computer.

To achieve this goal it is necessary to understand P, Q , and ϕ precisely: and in typical applications none of these are known explicitly – they are all defined only implicitly by the vector field f . This is the technical hurdle which any computer analysis of a connecting

orbit must overcome. In these notes we develop Taylor series expansions for $P(u)$, $Q(s)$, and $\phi(x, t)$. Much effort goes into developing computer assisted methods for managing the truncation errors associated with these approximations. As we will see in Chapter 5, we also need to control derivatives of these functions if we want to obtain transversality.

Remark 1.1 (compatibility conditions). Note that if $\gamma: [0, T] \rightarrow \mathbb{R}^n$ is a heteroclinic orbit segment, then for any $h \in \mathbb{R}$ the function $\hat{\gamma}_h: [0, T] \rightarrow \mathbb{R}^n$ defined by

$$\hat{\gamma}_h(t) = \phi(\gamma(t), h),$$

is another heteroclinic orbit segment. Similarly, if $\tilde{T} > T$ then we can extend γ to the interval $[0, \tilde{T}]$ and will have yet another heteroclinic orbit segment.

These remarks imply that if (u_0, s_1, T) is a solution of F as defined in Equation (2), then by the implicit function theorem $DF(u_0, s_1, T)$ has at least a two dimensional kernel. If we want to isolate a solution of F we must somehow remove two variables. This well known issue is easily managed, and we describe in detail one solution in Section 5. For the moment just note that in order to have a balanced system of equations we need that

$$\dim(\mathbb{E}^u \times \mathbb{E}^s \times \mathbb{R}) - 2 = \dim(\mathbb{R}^n),$$

and a necessary condition for an isolated solution is that $m_0 + m_1 + 1 - 2 = n$ or

$$m_0 + m_1 = n + 1.$$

1.2 A brief survey of the surrounding literature

The aim of these notes is to present a moderately concise and self contained (if technical) explanation of a computer assisted proof for a heteroclinic connecting orbit. We choose an approach based entirely on manipulation of power series, giving all validations a similar flavor. Hopefully this notes could serve as a useful introduction to computer assisted proof using Taylor methods, and after examining these notes and the supporting codes the reader could implement the Taylor methods in any number of systems, or adapt the methods to closely related problems.

That being said, it is important to stress that this note represent the authors take on existing results and techniques. The only novelty is the presentation and the interested reader will want to consult the primary literature for a much more complete picture of what has been done in this area. The two main topics of these notes are validated solution of initial value problems (sometimes referred to as rigorous integration) and validated computer assisted analysis of stable/unstable manifolds. These topics are by now well established pillars of the field of computer assisted proof in dynamical systems theory, and some discussion of the literature is in order.

The reader interested in interval analysis/arithmetic will want to consult the work of Moore [9, 10, 11]. The 1966 book of Moore is more or less the beginning of the subject. An early example of the use of validated Taylor integrators as an ingredient in mathematically rigorous computer assisted proofs is found in the work of de la Llave and Fefferman [12], on the relativistic stability of matter. Modern and detailed discussion of rigorous Taylor integrators and their history, along with many supporting examples and implementation, is found in Chapter 6 of the book of Tucker [13]. Indeed, rigorous integrators played a critical role in Tucker's solution of Smale's 14-th problem [14, 15]. See also the work of Berz and Makino [16].

Foundational work on general rigorous integration schemes was done by Lohner, see for example [17, 18, 19]. Building on this work, Wilczak and Zgliczynski developed efficient

Taylor methods for simultaneous rigorous integration of vector fields and their variational equations [20, 21] that keep track the flow and its spatial derivatives. These algorithms form the core of the CAPD library for validated numerics (more information on the CAPD library is found at <http://capd.sourceforge.net/capdDynSys/people.php>). These methods are extended by Zgliczynski and Cyranka to infinite dimensional semi-flows such as parabolic PDEs [22, 23, 24, 25], and by Zgliczynski and Szczelina to semi-flows generated by delay differential equations [26]. Another approach to rigorous integration of parabolic PDEs is found in the work of Koch and Arioli [27]. Methods and software implementations mentioned in the previous two paragraphs are much more sophisticated than those discussed in the present introductory note.

Much of the community's interest in rigorous Taylor integrators is motivated by a desire to compute global dynamics. Rigorous integrators facilitate computer assisted proof of periodic orbits for ordinary differential equations [28, 29, 30, 31] and are used to prove the existence of connecting orbits [32, 33, 34] and topological horseshoes [35, 36, 37, 38, 28, 39, 40, 29]. Recently a computer assisted proof of chaos in the Kuramoto-Sivashinsky equation (a parabolic PDE) based on rigorous integration of the semi-flow has been announced by Wilczak and Zgliczynski [41].

To establish the existence of transverse connecting orbits, i.e. transverse intersections between stable/unstable manifolds, it is necessary to develop validated numerics for the local manifolds. Methods for studying local stable/unstable manifolds based on topological covering and cone conditions are developed by Zgliczynski and Capinski [42, 43]. These methods are used for example by Capinski, Roldan, and Wasieczko-Zajpolhk to prove the existence of center manifolds, transverse intersections of invariant manifolds in celestial mechanics problems, and to study strong stable/unstable manifolds [44, 45, 45]. We also mention that the Ph.D. dissertation of Alex Wittig contains a topological validation method for computer assisted analysis of stable/unstable manifolds which exploits high order polynomial enclosures of the invariant manifolds and cone conditions.

Another approach to computer assisted proof of transverse connecting orbits is based on the theory of exponential dichotomies and the notion of hyperbolic shadowing [46, 47]. Palmer, Coomes, and Koçak have developed validated numerical methods based on these ideas which apply to a wide variety of heteroclinic and homoclinic phenomena, including computer assisted proof of chaos [48]. We refer to [49, 50] and the references therein for more complete discussion.

Validated numerics for stable/unstable manifolds based on functional analytic tools are discussed at length below, and for the moment we only mention the work of Koch and Arioli [51, 52] on homoclinic connecting orbits traveling waves, and the Evans function; and also the work of the Breden, Lessard, Reinhardt, and the author on validated numerical methods for stable/unstable manifolds based on the parameterization method [53, 54]. Techniques based on the parameterization method lead also to validated numerics for stable/unstable manifolds of periodic orbits, as in the work of Castelli, Lessard and the author [55], and also to validated numerical methods for computing unstable manifolds and heteroclinic connecting orbits for parabolic PDEs [56]. Further discussion of the literature is found in these references.

Remark 1.2 (Taylor remainders and fixed point problems). A validated numerical integrator involves two essential components: first, a numerical stage which produces an approximate solution of the initial value problem; and second, a validation stage which provides mathematically rigorous bounds on all truncation and round off errors. Many of the references discussed above use Taylor series methods for the initial approximation stage. Validation strategies are sometimes based application of the Taylor remainder theorem, as

for example in the works of [19, 18, 17, 21, 20]. Other strategies treat the Taylor remainder using fixed point methods, as in [51, 52, 27].

More recently Lessard and Reinhardt introduced an approach to rigorous integration based on Chebyshev series approximation [57]. The Chebyshev series of a real analytic function $\gamma: [0, T] \rightarrow \mathbb{R}^n$ converges on an ellipse in the complex plane, whose foci are at 0 and T . Because of this, the Chebyshev series is much less sensitive to poles in the complex plane than the Taylor series, and very long time steps (often much greater than one time unit) are possible. Van den Berg and Sheombarsing have studied the problem of optimal meshing for longer validated time steps [58]. This work uses heuristic methods based on complex pole detection. Both of the works just mentioned exploit Newton's method in a Banach space of infinite sequences for rigorous error analysis.

Remark 1.3 (Fixed point analysis of recursion relations). Taylor series methods for local problems have the very convenient property that, via some power matching arguments, one works out exactly the recursion describing the power series coefficients of the unknown function. This observation is elaborated on at length below but, briefly this is due to the lower triangular structure of the Cauchy product of two analytic functions. Iterating the recursion numerically (using interval arithmetic) leads to rigorous enclosure of as many Taylor coefficients as one might desire. Judiciously rescaling the problem provides control over the decay rates of the Taylor coefficients and reduces the effects of the data dependence in the coefficient sequence.

In [52], Koch and Arioli develop computer assisted error bounds for analytic functions with coefficients defined via recursion. The idea is to view the recursion as a fixed point problem on a space of infinite sequences. Solving the recursion to a fixed finite order N provides a numerical approximation, which we view as an approximate fixed point. A contraction mapping argument on a suitable ball in a space of "tails" provides mathematically rigorous a-posteriori bounds for the truncation error.

Similar contraction mapping arguments, formulated in analytic function spaces, have been used by other authors to study local stable/unstable manifolds in [59, 60, 61, 62, 55], and analysis of local stable/unstable manifolds based on Newton's method in spaces of infinite sequence spaces is developed in [53, 54].

The exposition in the present lecture uses the fixed point/contraction mapping approach to recursion discussed in [52]. The main advantage of this method is that it does not require the inversion of any matrices (large or otherwise). This is a great virtue when working with analytic functions of several complex variables.

In an attempt to make transparent the computer assisted portion of the proofs, we formulate explicit a-posteriori validation theorems for each problem we consider. These theorems are framed in Banach algebras of infinite sequences, and the style of presentation is influenced by the radii-polynomial approach of Lessard, Day, Gameiro, van den Berg, and Mischaikow (see the notes of van den Berg and Lessard in the present volume). The hypotheses of our theorems involve certain finite sums which depend only on the numerical data (the approximate solution). Implementation of the computer assisted proofs is a matter of evaluating these finite sums using interval arithmetic to manage round off errors, and then checking that some quadratic polynomial has positive roots. As one sees by inspecting the codes, our a-posteriori theorems constitute digestible pseudo-code for the computer assisted proofs.

2 Background: infinite multi-sequences

Fix $m \in \mathbb{N}$ and consider a function $a: \mathbb{N}^m \rightarrow \mathbb{C}$. We refer to a as an *infinite multi-sequence* of complex numbers, and write

$$a = \{a_\alpha\}_{\alpha \in \mathbb{N}^m}.$$

With $m = 1$ we recover the standard notion of an infinite sequence. It is natural then to think of a multi-sequence as an infinite m -dimensional array of complex numbers, i.e. an array whose coordinates are addressed by m -dimensional vectors of natural numbers. The m -dimensional vectors $\alpha = (\alpha_1, \dots, \alpha_m) \in \mathbb{N}^m$ are called *multi-indices*. The order of a multi-index α is the non-negative integer $|\alpha| := \alpha_1 + \dots + \alpha_m$.

In the next chapters we are interested in proving, with computer assistance, some theorems about analytic functions of several complex variables. Our arguments are formulated in Banach spaces and Banach algebras of infinite multi-sequences, because these spaces provide a natural framework for efficiently manipulating analytic functions of several complex variables on the digital computer. As motivation for the more thorough discussion of multi-sequences to come, we first sketch – somewhat informally – the reduction of a nonlinear problem in functional analysis to an equivalent fixed point problem on a space of infinite multi-sequences. For the sake of simplicity we focus for a moment on the case $m = 1$.

Consider an operator equation of the form

$$\Psi(f(z)) = 0, \tag{3}$$

where $f(z)$ is an unknown analytic function. We think of Ψ as a mapping taking values in some space of analytic functions, and do not rule out the possibility that Ψ contains unbounded operators which are only densely defined. We look for a series solution of the form

$$f(z) = \sum_{n=0}^{\infty} a_n z^n.$$

Suppose that the power series coefficients of $\Psi \circ f$ are smooth functions of the unknown Taylor coefficients $\{a_n\}_{n=0}^{\infty}$. More precisely we assume that there are smooth, complex valued functions $\Psi_n(\{a_n\}_{n=0}^{\infty})$ having that

$$\Psi(f(z)) = \sum_{n=0}^{\infty} \Psi_n(\{a_n\}_{n=0}^{\infty}) z^n.$$

Since an analytic function is the zero function if and only if all its Taylor coefficients are zero, the terms of the sequence $\{a_n\}_{n=0}^{\infty}$ are the Taylor coefficients of an analytic solution of Equation (3) if and only if

$$\Psi_n(\{a_n\}_{n=0}^{\infty}) = 0, \tag{4}$$

for all $n \in \mathbb{N}$. This standard “power matching scheme” reduces Equation (3) to a coupled system of countably many scalar equations in countably many scalar unknowns. Instead of an unknown function we now seek an unknown collection of complex numbers.

To further reduce the problem we observe that –very loosely speaking– the implicit function theorem allows us to solve Equation (4) for a_n in terms of the remaining variables. So for each $n \in \mathbb{N}$ we find a function T_n so that $\{a_n\}_{n=0}^{\infty}$ satisfies

$$a_n = T_n(a_0, \dots, a_{n-1}, a_{n+1}, \dots), \tag{5}$$

if and only if $\{a_n\}_{n=0}^{\infty}$ satisfies Equation (4).

Indeed for the applications considered in these lectures, and for many other applications whose nonlinearities involve multiplication of analytic functions or composition with elementary functions, the functions T_n in Equation (5) are easily derived from the Ψ_n of Equation (4) without any appeal to the implicit function theorem. Moreover the resulting nonlinear functionals T_n often have the form

$$a_n = T_n(a_0, \dots, a_{n-1}), \quad (6)$$

for all $n \in \mathbb{N}$, where each T_n depends only on terms of order less than n .

Let $a = \{a_n\}_{n=0}^\infty$ denote the unknown coefficient sequence and define the map $T(a) = \{T_n(a)\}_{n=0}^\infty$. We now see that proving the existence of an analytic solution of Equation (3) is reduced to proving the existence of an infinite sequence $\{a_n\}_{n=0}^\infty$ solving the fixed point problem

$$T(a) = a.$$

A computer assisted solution of this problem has two major steps.

- **Step 1: Finite dimensional approximation:** We view Equation (6) as *recursion relations* for the unknown Taylor coefficients. Assuming that we have enough initial data to seed this recursion (a matter which must be addressed on a problem by problem basis) we compute a_n inductively from the known lower order terms a_0, \dots, a_{n-1} . This recursion is repeated to any desired finite order N .
- **Step 2: Infinite dimensional validation:** Let $\bar{a}^N = (\bar{a}_0, \dots, \bar{a}_N) \in \mathbb{C}^{N+1}$ denote the approximate solution obtained in Step 1. Since \bar{a}^N is an *exact fixed point of T to order N* , we only have to prove the existence of a tail sequence $h = (0, \dots, 0, h_{N+1}, h_{N+2}, \dots)$ so that $\hat{a} = \bar{a}^N + h$ is an exact fixed point of the full operator T . In the present work this task is aided by the contraction mapping theorem. The idea is that, because Taylor coefficients of analytic functions satisfy classical growth estimates, we can choose a norm in which the tail mapping $\{T_n(\bar{a}^N + h)\}_{n=N+1}^\infty$ is a contraction in an appropriate ball about the known finite dimensional fixed point \bar{a}^N .

2.1 Banach algebras of infinite multi-sequences

Let \mathcal{S}_m denote the set of all m -dimensional infinite multi-sequences of complex numbers. Note that \mathcal{S}_m is a vector space, and with $\nu > 0$ define the quantity

$$\|a\|_{\nu, m}^1 := \sum_{\alpha_1=0}^\infty \dots \sum_{\alpha_m=0}^\infty |a_{\alpha_1, \dots, \alpha_m}| \nu^{\alpha_1 + \dots + \alpha_m} = \sum_{|\alpha|=0}^\infty |a_\alpha| \nu^{|\alpha|},$$

The set

$$\ell_{\nu, m}^1 := \{a = \{a_\alpha\} \in \mathcal{S}_m : \|a\|_{\nu, m}^1 < \infty\},$$

is a Banach space. Let $B(\ell_{\nu, m}^1)$ denote the collection of all bounded linear operators from $\ell_{\nu, m}^1$ into itself, and note that $B(\ell_{\nu, m}^1)$ is a Banach space.

The sequence spaces $\ell_{\nu, m}^1$ are related to Banach spaces of analytic functions. More precisely, let $z = (z_1, \dots, z_m) \in \mathbb{C}^m$ and $r > 0$. Define the poly-disk of radius r centered at z by

$$D_r^m(z) := \left\{ w = (w_1, \dots, w_m) \in \mathbb{C}^m : \max_{1 \leq j \leq m} |w_j - z_j| < r \right\},$$

where $|\cdot|$ denotes the usual complex absolute value. Endow \mathbb{C}^m with the norm

$$\|z\| := \max_{1 \leq j \leq m} |z_j|,$$

and note that poly-disks are the balls induced by this norm. The poly-disk $D_r^m(0)$, i.e. “the ball of radius r at the origin of \mathbb{C}^m ” is especially important in the discussion to follow and we often drop the (0) notation and write simply D_r^m .

Let $C^\omega(D_r^m)$ denote the set of all analytic functions on D_r^m taking values in \mathbb{C} . Then for any $a = \{a_\alpha\}_{\alpha \in \mathbb{N}^m} \in \ell_{\nu,m}^1$, the function f defined by

$$f(z) = \sum_{|\alpha|=0}^{\infty} a_\alpha z^\alpha,$$

has $f \in C^\omega(D_\nu^m)$. A partial converse is given by the following observation: if $f \in C^\omega(D_r^m)$, then the Taylor coefficients of f are in $\ell_{\nu,m}^1$ for all $\nu < r$.

Recall also that the product of two analytic functions is again analytic, i.e. $C^\omega(D_\nu^m)$ is a Banach algebra under pointwise multiplication of functions. The sequence space $\ell_{\nu,m}^1$ inherits this Banach algebra structure, as we now discuss. Define the binary product $*$: $\ell_{\nu,m}^1 \times \ell_{\nu,m}^1 \rightarrow \mathcal{S}_m$ by

$$(a * b)_\alpha = \sum_{\beta_1=0}^{\alpha_1} \cdots \sum_{\beta_m=0}^{\alpha_m} a_{\alpha_1-\beta_1, \dots, \alpha_m-\beta_m} b_{\beta_1, \dots, \beta_m},$$

with $a, b \in \ell_{\nu,m}^1$. Note that the product is commutative. We refer to $*$ as the *Cauchy product*, and for $a, b \in \ell_{\nu,m}^1$ have

•

$$\|a * b\|_{\nu,m}^1 \leq \|a\|_{\nu,m}^1 \|b\|_{\nu,m}^1,$$

i.e. the pair $(\ell_{\nu,m}^1, *)$ is a Banach algebra.

• If $f, g \in C^\omega(D_r^m)$ have Taylor series expansions

$$f(z) = \sum_{|\alpha|=0}^{\infty} a_\alpha z^\alpha, \quad \text{and} \quad g(z) = \sum_{|\alpha|=0}^{\infty} b_\alpha z^\alpha,$$

then $f \cdot g \in C^\omega(D_r^m)$ and has power series representation

$$(f \cdot g)(z) = \sum_{|\alpha|=0}^{\infty} (a * b)_\alpha z^\alpha,$$

i.e. pointwise multiplication in the function domain corresponds to Cauchy products in sequence space.

In the applications to come we are interested in the operation of differentiation. This does not define a bounded linear operator on $C^\omega(D_r^m)$, hence cannot induce a bounded linear map on $\ell_{\nu,m}^1$. But, as usual in complex analysis, we recover bounds on the derivative after giving up some portion of the domain. More precisely we have the following Lemma, whose proof is an exercise.

Lemma 2.1 (Cauchy Bounds in Several Complex Variables). *Let $\nu > 0$, and $a = \{a_\alpha\}_{\alpha \in \mathbb{N}^m} \in \ell_{\nu,m}^1$. Define $f: D_\nu^m \rightarrow \mathbb{C}$*

$$f(z) := \sum_{|\alpha|=0}^{\infty} a_\alpha z^\alpha.$$

Let $0 < \sigma \leq 1$ and

$$\tilde{\nu} = e^{-\sigma} \nu.$$

Then

$$\sup_{z \in D_{\tilde{\nu}}^m} \left| \frac{\partial}{\partial z_j} f(z) \right| \leq \frac{1}{\nu \sigma} \|a\|_{\nu, m}^1,$$

for each $1 \leq j \leq m$.

Recall that polynomial operations on a Banach algebra are Fréchet differentiable. For example fix $c \in \ell_{\nu, m}^1$ and define the maps $F, G: \ell_{\nu, m}^1 \rightarrow \ell_{\nu, m}^1$ by

$$G(a) := c * a, \quad \text{and} \quad F(a) := a * a.$$

Then F and G are Fréchet differentiable, and the derivatives $DG(a), DF(a) \in B(\ell_{\nu, m}^1)$ have action given by

$$DG(a)h = c * h, \quad \text{and} \quad DF(a)h = 2(a * h),$$

for $h \in \ell_{\nu, m}^1$. This is as much calculus on Banach spaces as is needed in the present note.

2.2 Projection and truncation spaces

Define the linear subspaces

$$X_{\nu, m}^N = \{a = \{a_\alpha\} \in \ell_{\nu, m}^1 \mid a_\alpha = 0 \text{ when } |\alpha| \geq N + 1\},$$

and

$$X_{\nu, m}^\infty = \{a = \{a_\alpha\} \in \ell_{\nu, m}^1 \mid a_\alpha = 0 \text{ when } 0 \leq |\alpha| \leq N\},$$

and the canonical projection operators $\pi_N: \ell_{\nu, m}^1 \rightarrow X_{\nu, m}^N$ and $\pi_\infty: \ell_{\nu, m}^1 \rightarrow X_{\nu, m}^\infty$ by

$$\pi_N(a)_\alpha = \begin{cases} a_\alpha & \text{if } 0 \leq |\alpha| \leq N \\ 0 & \text{if } |\alpha| \geq N + 1 \end{cases},$$

and

$$\pi_\infty(a)_\alpha = \begin{cases} 0 & \text{if } 0 \leq |\alpha| \leq N \\ a_\alpha & \text{if } |\alpha| \geq N + 1 \end{cases}.$$

Note that

- $X_{\nu, m}^N$, and $X_{\nu, m}^\infty$ are closed linear subspaces of $\ell_{\nu, m}^1$, hence Banach spaces in their own right (endowed with the $\ell_{\nu, m}^1$ norm).
- $\ell_{\nu, m}^1 = X_{\nu, m}^N \oplus X_{\nu, m}^\infty$, i.e. each $a \in \ell_{\nu, m}^1$ has unique decomposition

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

Moreover, the projections are bounded linear operators.

- $X_{\nu, m}^\infty$ inherits the Banach algebra structure of $\ell_{\nu, m}^1$, i.e. if $u, v \in X_{\nu, m}^\infty$, then $u * v \in X_{\nu, m}^\infty$, and we have

$$\|u * v\|_{X_{\nu, m}^\infty} = \|u * v\|_{\ell_{\nu, m}^1} \leq \|u\|_{\ell_{\nu, m}^1} \|v\|_{\ell_{\nu, m}^1} = \|u\|_{X_{\nu, m}^\infty} \|v\|_{X_{\nu, m}^\infty},$$

as the norm on $X_{\nu,m}^\infty$ is the norm inherited from $\ell_{\nu,m}^1$. On the other hand, note that $X_{\nu,m}^N$ does not inherit directly the Banach algebra structure. This is because a typical pair $a, b \in X_{\nu,m}^N$ has product $a * b \in \ell_{\nu,m}^1$ with nonzero projection into $X_{\nu,m}^\infty$. These remarks make sense when we view the elements of $\ell_{\nu,m}^1$ as Taylor coefficients. Recall that the product of two polynomials of degree N is a polynomial of degree $2N$, yet if two analytic functions are zero to order N then their product is zero to order N as well. (In fact their product is zero to order $2N$, but this does not play an important role).

- Taking the previous remark a step further, note that if $a^N \in X_{\nu,m}^N$ and $u \in X_{\nu,m}^\infty$ then $a^N * u \in X_{\nu,m}^\infty$, as a consequence of the fact that when we multiply an analytic function by an analytic function which is zero to order N the resulting product is zero to order N .

While $X_{\nu,m}^N$ does not inherit a Banach algebra structure from the Cauchy product, there is a truncated Cauchy product on $X_{\nu,m}^N$ defined as follows. For $a^N, b^N \in X_{\nu,m}^N$ define $(\cdot * \cdot)^N : X_{\nu,m}^N \oplus X_{\nu,m}^N \rightarrow X_{\nu,m}^N$ by

$$(a^N * b^N)^N := \pi_N(a^N * b^N),$$

so that product $(a^N * b^N)^N$ has components

$$(a^N * b^N)_\alpha^N = \begin{cases} \sum_{\beta_1=0}^{\alpha_1} \cdots \sum_{\beta_m=0}^{\alpha_m} a_{\alpha-\beta} b_\beta & \text{if } 0 \leq |\alpha| \leq N \\ 0 & \text{if } |\alpha| \geq N + 1 \end{cases}.$$

The pair $(X_{\nu,m}^N, (\cdot * \cdot)^N)$ is a Banach algebra.

The neglected terms define yet another product $(\cdot * \cdot)^\infty : X_{\nu,m}^N \oplus X_{\nu,m}^N \rightarrow X_{\nu,m}^\infty$ by

$$(a^N * b^N)^\infty := \pi_\infty(a^N * a^N),$$

so that $(a^N * b^N)^\infty$ has components

$$(a^N * b^N)_\alpha^\infty = \begin{cases} 0 & \text{if } 0 \leq |\alpha| \leq N \\ \sum_{\beta_1=0}^{\alpha_1} \cdots \sum_{\beta_m=0}^{\alpha_m} a_{\alpha-\beta} b_\beta & \text{if } N + 1 \leq |\alpha| \leq 2N \\ 0 & \text{if } |\alpha| \geq 2N + 1 \end{cases}.$$

Remark 2.2 (Derivatives of truncation errors). The projection operators commute with Fréchet derivatives. This follows from the observation that the projection operators are bounded. So for example

$$D_u \pi_\infty((a^N + u) * (b^N + v))h = b^N * h + v * h,$$

and

$$D_u \pi_\infty((a^N + u) * (a^N + u))h = 2a^N * h + 2u * h,$$

for $h \in X_{\nu,m}^\infty$. Other derivatives are similar.

2.3 Error analysis for two specialized product operations

This section contains some more technical generalizations of the material above, which is used in the computer assisted analysis of invariant manifolds and Taylor integrators to follow. The two product operations defined below allow us to, in various settings, solve the recursion relations for some Taylor series problems without the use of the implicit function theorem.

2.3.1 The “hat” product for invariant manifolds

When analyzing invariant manifolds we encounter operator equations containing terms of the form

$$cz_j \frac{\partial}{\partial z_j} f(z_1, \dots, z_m) = g(z_1, \dots, z_m) f(z_1, \dots, z_m), \quad (7)$$

with $c \in \mathbb{C}$, g a known and f an unknown function. Further motivation for this equation is discussed in Section 3.1, and for now we just note that the first order partial differential operator on the left hand side is the push forward of the vector field $z'_j = cz_j$ under f . Considering $1 \leq j \leq m$ the operators on the left hand side of Equation (7) form a basis for more general push forwards.

On the level of power series Equation (7) is

$$\sum_{|\alpha|=0}^{\infty} c\alpha_j a_\alpha z^\alpha = \sum_{|\alpha|=0}^{\infty} (a * b)_\alpha z^\alpha,$$

which, after matching like powers, is

$$c\alpha_j a_\alpha = (a * b)_\alpha = \sum_{\beta_1=0}^{\alpha_1} \dots \sum_{\beta_m=0}^{\alpha_m} a_{\alpha_1-\beta_1, \dots, \alpha_m-\beta_m} b_{\beta_1, \dots, \beta_m}. \quad (8)$$

To solve for the coefficient a_α we remove from the sum on the right any terms whose multi-index is α . Note that a_α appears in the sum if and only if $\beta = 0$, and that b_α appears if and only if $\beta = \alpha$. So, define

$$\hat{\delta}_\beta^\alpha := \begin{cases} 0 & \text{if } \beta = 0 \\ 0 & \text{if } \beta = \alpha \\ 1 & \text{otherwise} \end{cases}, \quad (9)$$

and observe that

$$(a * b)_\alpha = a_\alpha b_0 + b_\alpha a_0 + \sum_{\beta_1=0}^{\alpha_1} \dots \sum_{\beta_m=0}^{\alpha_m} \hat{\delta}_\beta^\alpha a_{\alpha_1-\beta_1, \dots, \alpha_m-\beta_m} b_{\beta_1, \dots, \beta_m}.$$

(This $\hat{\delta}$ is related to the usual *Kronecker delta* δ_β^α by $\hat{\delta}_\beta^\alpha = 1 - \delta_\beta^\alpha$).

This operation – namely extracting terms containing the multi-index α from the Cauchy product – is important enough that we define a new binary product based on the discussion above. The following discussion is somewhat tedious, but makes quite transparent the analysis of invariant manifolds in the sequel. The reader may want to skip the remainder of this section on first reading and refer back only as needed.

Let $\hat{*}: \ell_{\nu, m}^1 \oplus \ell_{\nu, m}^1 \rightarrow \ell_{\nu, m}^1$ have components defined by

$$(a \hat{*} b)_\alpha := \sum_{\beta_1=0}^{\alpha_1} \dots \sum_{\beta_m=0}^{\alpha_m} \hat{\delta}_\beta^\alpha a_{\alpha-\beta} b_\beta.$$

Then

$$(a * b)_\alpha = a_0 b_\alpha + a_\alpha b_0 + (a \hat{*} b)_\alpha,$$

where $(a \hat{*} b)_\alpha$ depends only on terms of order strictly less than $|\alpha|$. Returning to Equation (8), we see that the power series coefficients of the solution of Equation (7) satisfy the recursion

$$a_\alpha = \frac{1}{c\alpha_j - b_0} (a_0 b_\alpha + (a \hat{*} b)_\alpha),$$

as long as the *non-resonance condition* $\alpha_j c \neq b_0$ for all $|\alpha| \geq 1$ is satisfied.

Define the binary operations (or products) $(\hat{\cdot})^N: X_{\nu,m}^N \oplus X_{\nu,m}^N \rightarrow X_{\nu,m}^N$ and $(\hat{\cdot})^\infty: X_{\nu,m}^N \oplus X_{\nu,m}^N \rightarrow X_{\nu,m}^\infty$ by

$$(a^N \hat{*} b^N)^N = \pi_N(a^N \hat{*} b^N) = \begin{cases} \sum_{\beta_1=0}^{\alpha_1} \cdots \sum_{\beta_m=0}^{\alpha_m} \hat{\delta}_\beta^\alpha a_{\alpha-\beta} b_\beta & \text{if } 0 \leq |\alpha| \leq N \\ 0 & \text{if } |\alpha| \geq N+1 \end{cases}$$

and

$$(a^N \hat{*} b^N)^\infty = \pi_\infty(a^N \hat{*} a^N) = \begin{cases} 0 & \text{if } 0 \leq |\alpha| \leq N \\ \sum_{\beta_1=0}^{\alpha_1} \cdots \sum_{\beta_m=0}^{\alpha_m} \hat{\delta}_\beta^\alpha a_{\alpha-\beta} b_\beta & \text{if } N+1 \leq |\alpha| \leq 2N, \\ 0 & \text{if } |\alpha| \geq 2N+1 \end{cases}$$

so that

$$a \hat{*} b = \pi_N(a \hat{*} b) + \pi_\infty(a \hat{*} b)$$

where

$$\pi_N(a \hat{*} b) = (\pi_N(a) \hat{*} \pi_N(b))^N,$$

and

$$\pi_\infty(a \hat{*} b) = (\pi_N(a) \hat{*} \pi_N(b))^\infty + \pi_N(a) \hat{*} \pi_\infty(b) + \pi_N(b) \hat{*} \pi_\infty(a) + \pi_\infty(a) \hat{*} \pi_\infty(b). \quad (10)$$

The following estimate is used in the truncation analysis of invariant manifolds.

Lemma 2.3. *Let $a^N, b^N \in X_{\nu,m}^N$ and $u, v \in X_{\nu,m}^\infty$. Then*

$$\|a^N \hat{*} u\|_{\nu,m}^1 \leq \left(\sum_{|\alpha|=1}^N |a_\alpha^N| \nu^{|\alpha|} \right) \|u\|_{\nu,m}^1,$$

so that

$$\begin{aligned} \|\pi_\infty((a^N + u) \hat{*} (b^N + v))\|_{X_{\nu,m}^\infty} &\leq \sum_{|\alpha|=N+1}^{2N} \left| \sum_{\beta_1=0}^{\alpha_1} \cdots \sum_{\beta_m=0}^{\alpha_m} \hat{\delta}_\beta^\alpha a_{\alpha-\beta}^N b_\beta^N \right| \nu^{|\alpha|} \\ &\quad + \left(\sum_{|\alpha|=1}^N |a_\alpha^N| \nu^{|\alpha|} \right) \|v\|_{\nu,m}^1 \\ &\quad + \left(\sum_{|\alpha|=1}^N |b_\alpha^N| \nu^{|\alpha|} \right) \|u\|_{\nu,m}^1 \\ &\quad + \|u\|_{\nu,m}^1 \|v\|_{\nu,m}^1. \end{aligned}$$

Proof. Consider the bound on $\|a^N \hat{*} u\|_{\nu,m}^1$ and define the sequence

$$\hat{a}_\alpha^N = \begin{cases} 0 & \text{if } \alpha = 0 \\ a_\alpha^N & \text{if } 1 \leq |\alpha| \leq N. \\ 0 & \text{if } |\alpha| \geq N+1 \end{cases}$$

Note that

$$\|a^N \hat{*} u\|_{\nu, m}^1 = \|\hat{a} * u\|_{\nu, m}^1 \leq \|\hat{a}\|_{\nu, m}^1 \|u\|_{\nu, m}^1 = \left(\sum_{|\alpha|=1}^N |a_\alpha^N| \nu^{|\alpha|} \right) \|u\|_{\nu, m}^1,$$

as desired. To complete the proof we apply the estimate above in conjunction with the Banach algebra estimate to the decomposition given in Equation (10). \square

2.3.2 A shift operator for initial value problems

In our study of Taylor integrators we encounter equations of the form

$$\frac{\partial}{\partial z_j} f(z_1, \dots, z_m) = f(z_1, \dots, z_m) g(z_1, \dots, z_m), \quad (11)$$

subject to the constraint

$$f(0, \dots, 0) = w_0 \in \mathbb{C},$$

where, for the moment we consider g a known function. The motivation for this equation is that the right hand side provides a basis for the push forward of constant vector fields, which in turn are the foundation of the flow box theorem for initial value problems.

On the level of power series Equation (11) becomes

$$\sum_{|\alpha|=0}^{\infty} (\alpha_j + 1) a_{\alpha_1, \dots, \alpha_j+1, \dots, \alpha_m} z^\alpha = \sum_{|\alpha|=0}^{\infty} (a * b)_\alpha z^\alpha,$$

which, after matching like powers becomes

$$a_0 = w_0,$$

and

$$(\alpha_j + 1) a_{\alpha_1, \dots, \alpha_j+1, \dots, \alpha_m} = (a * b)_\alpha, \quad \text{for } |\alpha| \geq 0.$$

We prefer to write the equation indexed to order α , so that

$$a_\alpha = \frac{1}{\alpha_j} (a * b)_{\alpha_1, \dots, \alpha_j-1, \dots, \alpha_m},$$

for $|\alpha_j| > 1$. Note that the expression on the right does not involve any terms of order $|\alpha|$.

The operation of lowering an index and then reindexing, which occurs any time we consider first order partial differential operators, is important enough to warrant special consideration and is formalized as follows. Again, the reader may want to skip ahead and refer back to the remainder of the section only as needed.

For $1 \leq j \leq m$ define the shift operator $S_j: \ell_{\nu, m}^1 \rightarrow \ell_{\nu, m}^1$ by

$$S_j(a)_\alpha = \begin{cases} 0 & \text{if } \alpha_j = 0 \\ a_{\alpha_1, \dots, \alpha_j-1, \dots, \alpha_m} & \text{if } \alpha_j \geq 1 \end{cases}.$$

The following lemma codifies some useful bounds.

Lemma 2.4. *Suppose that $a^N \in X_{\nu, m}^N$ and $u \in X_{\nu, m}^\infty$. Then*

$$\|\pi_\infty (S_j(a^N + u))\|_{\nu, m}^1 \leq \nu^{N+1} \left(\sum_{|\alpha|=N} |a_{\alpha_1, \dots, \alpha_j, \dots, \alpha_m}^N| \right) + \nu \|u\|_{\nu, m}^1.$$

Proof. Since S_j and π_∞ are both linear operators, we have that

$$\|\pi_\infty S_j(a^N + u)\|_{\nu, m}^1 = \|\pi_\infty S_j(a^N) + \pi_\infty S_j(u)\|_{\nu, m}^1 \leq \|\pi_\infty S_j(a^N)\|_{\nu, m}^1 + \|\pi_\infty S_j(u)\|_{\nu, m}^1.$$

Then we will bound the pieces singly. For the first term we have that

$$\begin{aligned} \|\pi_\infty S_j(a^N)\|_{\nu, m}^1 &= \sum_{|\alpha|=0}^{\infty} |[\pi_\infty S_j(a^N)]_\alpha| \nu^{|\alpha|} \\ &= \sum_{|\alpha|=N+1}^{\infty} |S_j(a^N)_\alpha| \nu^{|\alpha|} \\ &= \sum_{|\alpha|=N+1}^{\infty} \left| a_{\alpha_1, \dots, \alpha_j-1, \dots, \alpha_m}^N \right| \nu^{|\alpha|} \\ &= \sum_{|\alpha|=N+1}^{\infty} \left| a_{\alpha_1, \dots, \alpha_j-1, \dots, \alpha_m}^N \right| \nu^{N+1} \\ &= \nu^{N+1} \left(\sum_{|\alpha|=N}^{\infty} \left| a_{\alpha_1, \dots, \alpha_j, \dots, \alpha_m}^N \right| \right) \end{aligned}$$

as $a_\alpha^N = 0$ for all $\alpha \in \mathbb{N}^m$ with $|\alpha| \geq N+1$.

For the second term we have that

$$\begin{aligned} \|\pi_\infty S_j(u)\|_{\nu, m}^1 &= \sum_{|\alpha|=0}^{\infty} |[\pi_\infty S_j(u)]_\alpha| \nu^{|\alpha|} \\ &= \sum_{|\alpha|=N+1}^{\infty} |S_j(u)_\alpha| \nu^{|\alpha|} \\ &= \sum_{|\alpha|=N+1}^{\infty} \left| u_{\alpha_1, \dots, \alpha_j-1, \dots, \alpha_m} \right| \nu^{\alpha_1 + \dots + \alpha_j + \dots + \alpha_m} \\ &= \nu \sum_{|\alpha|=N+1}^{\infty} \left| u_{\alpha_1, \dots, \alpha_j-1, \dots, \alpha_m} \right| \nu^{\alpha_1 + \dots + \alpha_j - 1 + \dots + \alpha_m} \\ &= \nu \sum_{|\alpha|=N}^{\infty} \left| u_{\alpha_1, \dots, \alpha_j, \dots, \alpha_m} \right| \nu^{\alpha_1 + \dots + \alpha_j + \dots + \alpha_m} \\ &\leq \nu \sum_{|\alpha|=0}^{\infty} \left| u_{\alpha_1, \dots, \alpha_j, \dots, \alpha_m} \right| \nu^{\alpha_1 + \dots + \alpha_j + \dots + \alpha_m} \\ &= \nu \|u\|_{\nu, m}^1, \end{aligned}$$

where the inequality exploits the fact that $u_\alpha = 0$ when $|\alpha| \leq N$. Combining the estimates of the first and second terms gives the result. \square

Now for $1 \leq j \leq m$ consider the nonlinear operation $S_j(a * b)$. We have the following estimate.

Lemma 2.5. *Let $a^N, b^N \in X_{\nu, m}^N$ and $u, v \in X_{\nu, m}^\infty$. Then*

$$\begin{aligned} \|\pi_\infty(S_j((a^N + u) * (b^N + v)))\|_{\nu, m}^1 &\leq \nu^{N+1} \left(\sum_{|\alpha|=N} |(a^N * b^N)_\alpha| \right) \\ &\quad + \nu \sum_{|\alpha|=N+1}^{2N} |(a^N * b^N)_\alpha| \nu^{|\alpha|} \\ &\quad + \nu \|a^N\|_{\nu, m}^1 \|v\|_{\nu, m}^1 \\ &\quad + \nu \|b^N\|_{\nu, m}^1 \|u\|_{\nu, m}^1 \\ &\quad + \nu \|u\|_{\nu, m}^1 \|v\|_{\nu, m}^1 \end{aligned}$$

Proof. First note that

$$\begin{aligned} \pi_\infty(S_j((a^N + u) * (b^N + v))) &= \pi_\infty(S_j(a^N * b^N + a^N * v + b^N * u + u * v)) \\ &= \pi_\infty S_j(a^N * b^N) + \pi_\infty S_j(a^N * v) + \pi_\infty S_j(b^N * u) + \pi_\infty S_j(u * v). \end{aligned}$$

So we consider each of the four terms singly.

For the first term, recall that

$$(a^N * b^N) = (a^N * b^N)^N + (a^N * b^N)^\infty,$$

with $(a^N * b^N)^N \in X_{\nu, m}^1$ and $(a^N * b^N)^\infty \in X_{\nu, m}^\infty$. Then, by Lemma 2.4, we have that

$$\begin{aligned} \|\pi_\infty S_j(a^N * b^N)\|_{\nu, m}^1 &= \|\pi_\infty S_j((a^N * b^N)^N + (a^N * b^N)^\infty)\|_{\nu, m}^1 \\ &\leq \nu^{N+1} \left(\sum_{|\alpha|=N} |(a^N * b^N)_\alpha^N| \right) + \nu \|(a^N * b^N)^\infty\|_{\nu, m}^1 \\ &= \nu^{N+1} \left(\sum_{|\alpha|=N} |(a^N * b^N)_\alpha| \right) + \nu \left(\sum_{|\alpha|=N+1}^{2N} |(a^N * b^N)_\alpha| \nu^{|\alpha|} \right). \end{aligned}$$

For the remaining terms we note that $a^N * v, b^N * u$, and $u * v$ are all in $X_{\nu, m}^\infty$ and hence have zero projections into $X_{\nu, m}^N$. Combining this observation with Lemma 2.4 and the Banach algebra estimate completes the proof. \square

2.4 Two a-posteriori existence theorems

We now state two theorems sufficient for any computer assisted analysis in the remainder of the note. Both theorems are ‘‘a-posteriori’’ in the sense that given a good enough approximate fixed point/zero of some operator they provide conditions sufficient to conclude the existence of a true solution nearby. Indeed, the theorems provide explicit bounds on what is meant by ‘‘nearby’’. We state the proof of the first for the sake of completeness, while the proof of the second is found in the literature. In both cases we refer the interested reader to the works of [63, 64, 65, 66, 67, 68, 69] for more thorough discussion and historical context.

Proposition 2.6. *Let X be a Banach space, $\bar{x} \in X$, and suppose that $T: X \rightarrow X$ is a Fréchet differentiable mapping. Suppose that Y_0, Z_1 are positive constants and that $Z_2: (0, \infty) \rightarrow [0, \infty)$ is a positive function, having*

$$\|T(\bar{x}) - \bar{x}\| \leq Y_0,$$

and that

$$\sup_{x \in \overline{B_r(0)}} \|DT(\bar{x} + x)\| \leq Z_1 + Z_2(r)r,$$

for all $r > 0$.

If there is an $r > 0$ so that

$$Z_2(r)r^2 - (1 - Z_1)r + Y_0 \leq 0, \quad (12)$$

then there is unique $\hat{x} \in \overline{B_r(\bar{x})}$ with $T(\hat{x}) = \hat{x}$.

Proof. Note that $\overline{B_r(\bar{x})}$ is a complete metric space. Now for $x \in \overline{B_r(\bar{x})}$ consider

$$\begin{aligned} \|T(x) - \bar{x}\| &\leq \|T(x) - T(\bar{x})\| + \|T(\bar{x}) - \bar{x}\| \\ &\leq \sup_{z \in \overline{B_r(\bar{x})}} \|DT(z)\| \|x - \bar{x}\| + Y_0 \\ &\leq (Z_1 + Z_2(r)r) \|x - \bar{x}\| + Y_0 \\ &\leq Z_2(r)r^2 + Z_1r + Y_0 \\ &\leq r, \end{aligned}$$

by the hypothesis given in Equation (12). Then T maps $\overline{B_r(\bar{x})}$ into itself.

Now choose $x, y \in \overline{B_r(\bar{x})}$, and consider

$$\begin{aligned} \|T(x) - T(y)\| &\leq \sup_{z \in \overline{B_r(\bar{x})}} \|DT(z)\| \|x - y\| \\ &\leq (Z_1 + Z_2(r)r) \|x - y\|. \end{aligned}$$

From Equation (12) we have that

$$Z_2(r)r^2 + Z_1r + Y_0 \leq r,$$

or

$$Z_2(r)r + Z_1 + \frac{Y_0}{r} \leq 1.$$

Now since $Z_2(r), Z_1, Y_0$ and r are strictly positive, it follows that

$$Z_2(r)r + Z_1 < 1,$$

so that T is a strict contraction on $\overline{B_r(\bar{x})}$. The existence of a unique fixed point now follows from the Banach fixed point theorem. \square

The following theorem provides for a-posteriori analysis of finite dimensional systems of nonlinear equations.

Proposition 2.7. *Let $U \subset \mathbb{R}^n$ be an open set, $F: U \rightarrow \mathbb{R}^n$ be twice continuously differentiable on U , $\bar{x} \in U$, A be an $n \times n$ matrix, and $r_* > 0$ be such that $\overline{B_{r_*}(\bar{x})} \subset U$. Suppose that Y_0, Z_0, Z_2 are positive constants with*

$$\begin{aligned} \|AF(\bar{x})\| &\leq Y_0, \\ \|Id - ADF(\bar{x})\| &\leq Z_0, \\ \|A\| \sup_{x \in \overline{B_{r_*}(\bar{x})}} \|D^2F(x)\| &\leq Z_2. \end{aligned}$$

Define the polynomial

$$p(r) := Z_2 r^2 - (1 - Z_0)r + Y_0.$$

If $0 < r \leq r_*$ has that

$$p(r) \leq 0,$$

then A is invertible and there exists a unique $x_* \in \overline{B_r(\bar{x})}$ so that

$$F(x_*) = 0.$$

Moreover $DF(x_*)$ is invertible and

$$\|DF(x_*)^{-1}\| \leq \frac{\|A\|}{1 - Z_2 r - Z_0}.$$

A proof is found, for example in [70]. The interested reader can easily supply a proof by applying Theorem 2.6 to the “Newton-like” operator

$$T(x) = x - AF(x),$$

on a ball about \bar{x} .

2.5 A classic example: the Lorenz system

For all the numerical examples in the remainder of the notes we fix our attention on the familiar Lorenz system. This is the ordinary differential equation associated with the vector field $f: \mathbb{R}^3 \rightarrow \mathbb{R}^3$ given by

$$f(x, y, z) = \begin{pmatrix} \sigma(y - x) \\ x(\rho - z) - y \\ xy - \beta z \end{pmatrix}.$$

For $\rho > 1$ there are three equilibrium points

$$p^0 = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}, \quad \text{and} \quad p^{1,2} = \begin{pmatrix} \pm\sqrt{\beta(\rho - 1)} \\ \pm\sqrt{\beta(\rho - 1)} \\ \rho - 1 \end{pmatrix}.$$

It is an exercise to work out the eigenvalues and eigenvectors by hand.

Remark 2.8 (Validated numerics for existence and localization of an equilibrium solution). Even though the equilibrium solutions for the Lorenz system can be worked out by hand, for more difficult nonlinearities –especially in higher dimensions – this could be impossible. A typical strategy for studying equilibrium solutions is to compute a numerical zero using Newton’s method, and then validate the existence of a true zero a-posteriori nearby using Theorem 2.7 or one of its variants. This issue is discussed in detail in the review paper of Rump [1] and in the book of Tucker [13], and the interval arithmetic package IntLab [2] has a number of built-in nonlinear solvers.

Remark 2.9 (Validated numerics for linear stability analysis of an equilibrium solution). Similar comments apply to the eigendata. In fact, for vector fields of up to a few hundred or even a thousand dimensions we can obtain approximate eigenvalues and eigenvectors using

standard numerical solvers. Note that once we have an approximate eigenvalue/eigenvector pair, we study the system of (nonlinear) equations

$$Df(p)\xi - \lambda\xi = 0, \quad \|\xi\|^2 - 1 = 0,$$

once again using Theorem 2.7 or a variant. (The constraint above works for real eigenvalue/eigenvector pair. See [71, 1] for more general discussion). Again, we refer to the review paper of Rump [1] for more thorough review of the literature and remark that Int-Lab [2] is equipped with built in eigenvalue/eigenvector validation algorithms.

3 The local problem: equilibria, stability, and local invariant manifolds

As per the philosophy of Section 2, we formulate an operator equation whose solution is a chart map for the desired local invariant manifold. Two such classical approaches are the graph transform method and the Lyapunov-Perron method (see Chapter 5 of [72] for more complete discussion of this literature). Yet another is that of Irwin [73], and still another is the parameterization method [74, 75, 76], which we utilize here.

The idea of the parameterization method is to formulate a conjugacy between the invariant manifold of interest and some simpler dynamical model. The user of the method is free to choose the model system, though a poor choice may well lead to no solution. This freedom makes the method very flexible, and it applies to problems as diverse as invariant circles and their stable/unstable manifolds [77, 78, 79], breakdown/collisions of invariant bundles associated with quasi periodic dynamics [80, 81], stable/unstable manifolds of periodic orbits of differential equations and diffeomorphisms [76, 82, 83, 84, 85], study slow stable manifolds [74, 76] and their invariant vector bundles [86], and invariant tori for differential equations [87, 81]. The parameterization methods has also been used to develop KAM strategies not requiring action angle variables [88, 89, 90, 91], as well as to study invariant objects for PDEs [92, 93, 56] and DDEs [94, 95, 96]. Moreover the short list above is far from complete. A thorough description of the method, as well as many more examples and much more complete discussion of the literature, is found in a recent book devoted to the subject [97].

Since it is based on the study of conjugacy equations, the parameterization method naturally lends itself to a-posteriori validation and computer assisted proof. In addition to reading the present notes, the interested reader may also want to refer to [60, 98, 99, 53, 70, 54] for more discussion of validated numerics for stable/unstable manifolds based which use the parameterization method. See also [100] for a modern approach to validated numerics for invariant tori based on the parameterization method. Again, we refer also to [97] for more discussion.

3.1 Representation of the local invariant manifold by a conjugating chart: the parameterization method for vector fields on \mathbb{R}^n

In this section we review enough parameterization method basics to facilitate the validated computer assisted analysis of stable/unstable manifolds needed in the sequel. Focusing for the moment on the stable manifold, suppose that $p \in \mathbb{R}^n$ is an equilibrium point for an analytic vector field $f: \mathbb{R}^n \rightarrow \mathbb{R}^n$, and that $Df(p)$ has $m \leq n$ stable eigenvalues, which we denote by $\lambda_1, \dots, \lambda_m \in \mathbb{R}$. We assume for the present discussion that the eigenvalues

are real and distinct. Then $Df(p)$ is diagonalizable, and we choose $\xi_1, \dots, \xi_m \in \mathbb{R}^n$ an associated set of real eigenvectors.

In this context the parameterization method looks for solutions of the invariance equation

$$\lambda_1 s_1 \frac{\partial}{\partial s_1} P(s_1, \dots, s_m) + \dots + \lambda_m s_m \frac{\partial}{\partial s_m} P(s_1, \dots, s_m) = f(P(s_1, \dots, s_m)). \quad (13)$$

Our interest in Equation (13) is due to the fact that a function $P: (-1, 1)^m \rightarrow \mathbb{R}^n$ solving Equation (13) and subject to the first order constraints

$$P(0, \dots, 0) = p, \quad \text{and} \quad \frac{\partial}{\partial s_j} P(0, \dots, 0) = \xi_j, \quad 1 \leq j \leq m, \quad (14)$$

is a chart for a local stable manifold patch at p .

This claim is made precise in Proposition 3.1 below. First let Λ denote the $m \times m$ matrix with $\lambda_1, \dots, \lambda_m$ on the diagonal entries and zeros elsewhere. Rewriting Equation (13) as

$$DP(s)\Lambda s = f(P(s)),$$

makes the geometric meaning clear. Namely, the equation requires that the vector field f , restricted to the image of P , is tangent to (in fact equal to) the push forward of the linear vector field

$$\sigma' = \Lambda \sigma,$$

by the map P . Since the two vector fields are equal, they generate the same orbits, hence Equation (13) provides an infinitesimal conjugacy between the linear and nonlinear systems. The well understood dynamics of the linear system model the more complex dynamics of the nonlinear system restricted to the image of P .

Proposition 3.1. *Let ϕ denote the flow generated by f , and suppose that P is a solution of Equation (13) satisfying also the linear constraints of Equation (14). Then P is a one-to-one mapping and the image of P is a local stable manifold at p . Moreover, P has*

$$\phi(P(s_1, \dots, s_m), t) = P(e^{\lambda_1 t} s_1, \dots, e^{\lambda_m t} s_m), \quad (15)$$

for all $s = (s_1, \dots, s_m) \in (-1, 1)^m$ and $t \geq 0$.

An elementary proof is found in [86]. So, in addition to recovering the embedding of the local stable manifold, P provides also the dynamics on the manifold via this simple conjugacy. The geometric meaning of Equation (15) is illustrated in Figure 3. Note also that the parameterization is not required to be the graph of a function over the stable/unstable eigenspace, hence the method can follow folds in the embedding of the manifold.

We know that if p is hyperbolic then the stable/unstable manifolds exist and are as smooth as f , in this case analytic. Then it is reasonable to ask if an analytic solution of Equation (13) always exists? The answer is no, and the obstruction is expressed in terms of certain algebraic conditions between the stable eigenvalues.

Definition 3.2. The eigenvalues $\lambda_1, \dots, \lambda_m$ are said to have a *resonance* of order $\alpha \in \mathbb{N}^m$ if

$$\alpha_1 \lambda_1 + \dots + \alpha_m \lambda_m - \lambda_j = 0,$$

for some $1 \leq j \leq m$ with $|\alpha| \geq 2$. If there are no resonances at any order $|\alpha| \geq 2$ then the eigenvalues are non-resonant.

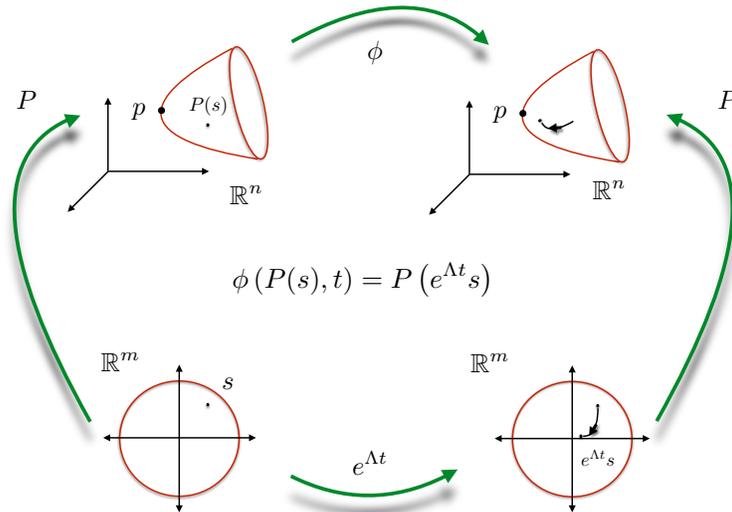


Figure 3: The figure illustrates the dynamical meaning of Equation (15). The unknown function P maps orbits of the linear $e^{\Lambda t}$ to orbits of the flow ϕ generated by f . Since orbits in the stable eigenspace converge to zero, and since $P(0) = p$, we have that the image of P is a local stable manifold.

We have the following theorem, whose proof is found in [56]. Much more general results are found in [74].

Theorem 3.3. *Suppose that the stable eigenvalues are non-resonant. Then there is a power series $P(s) = \sum_{|\alpha|=0}^{\infty} p_{\alpha} s^{\alpha}$ satisfying the constraints of Equation (14) which solves Equation (13) in the sense of formal series. The solution is unique up to the choice of the scalings of the eigenvectors, and for each choice of eigenvectors there is an $R > 0$ so that P has radius of convergence R .*

The reason for this non-resonance condition will become more clear in the next two sections when we consider formal series solutions. For the moment, note that (despite first appearances) the non-resonance condition imposes only a finite number of algebraic constraints between the eigenvalues. To see this simply note that there is an N so that if $|\alpha| \geq N$ then $\alpha_1 \lambda_1 + \dots + \alpha_m \lambda_m$ is larger than λ_j for each $1 \leq j \leq m$, and a resonance is only possible for $2 \leq |\alpha| \leq N$. So, the hypotheses of Theorem 3.3 are satisfied generically, i.e. given a “typical” fixed point p we expect the eigenvalues to be non-resonant at all orders. Or to put it another way: we usually expect an analytic solution of Equation (13). Moreover, given a particular collection of stable eigenvalues $\lambda_1, \dots, \lambda_m$, there is a finite procedure for determining if the non-resonance hypothesis holds. We also remark that the appearance of additional conditions in the parameterization method is not surprising, as the method provides more information than just the embedding.

The discussion above motivates our approach to solving Equation (13). Since we expect an analytic solution it is reasonable to make a power series *ansatz*, and try to work out the form of the unknown Taylor coefficients as discussed in the introduction of Section 2. This procedure is illustrated in detail in the next several sections.

Remark 3.4. The diagonalizable assumption is made for the sake of convenience. It can be removed, but this introduces some minor complications. See for example [53]. The reference just cited also describes how to modify the parameterization method so that it succeeds when there is a resonance (the idea is that one must conjugate to a polynomial rather than a linear model system. The order of the polynomial is the order of the resonance). It is also possible to treat complex conjugate eigenvalues using the method described above, as is described in detail in [62]. Nearly identical comments apply to the unstable manifold, as is seen by considering the vector field $-f$. Finally, while we work exclusively with analytic vector fields in these notes, the finite differentiability case is treated in [74, 75].

3.2 Formal series solutions: parameterized stable/unstable manifolds for the Lorenz system

Choose one of the three fixed points of the Lorenz system and denote it by $\hat{p} \in \mathbb{R}^3$. Let λ denote an eigenvalue of $Df(\hat{p})$, and let ξ denote an associated choice of eigenvector. If λ is a stable eigenvalue, assume it is the only stable eigenvalue, so that the remaining two eigenvalues are unstable (or vice versa if λ is unstable).

In this case $m = 1$, and the invariance equation (13) reduces to

$$\lambda s \frac{d}{ds} P(s) = f[P(s)].$$

We look for a power series solution

$$P(s) = \sum_{n=0}^{\infty} \begin{pmatrix} a_n \\ b_n \\ c_n \end{pmatrix} s^n.$$

Imposing the first order constraints, we have

$$\begin{pmatrix} a_0 \\ b_0 \\ c_0 \end{pmatrix} = \hat{p}, \quad \text{and} \quad \begin{pmatrix} a_1 \\ b_1 \\ c_1 \end{pmatrix} = \xi.$$

Validated numerics for the first order data was discussed in Section 2.5.

Now

$$\lambda s \frac{d}{ds} P(s) = \sum_{n=0}^{\infty} n\lambda \begin{pmatrix} a_n \\ b_n \\ c_n \end{pmatrix} s^n,$$

and

$$f(P(s)) = \sum_{n=0}^{\infty} \begin{pmatrix} \sigma(b_n - a_n) \\ \rho a_n - b_n - \sum_{k=0}^n a_{n-k} c_k \\ -\beta c_n + \sum_{k=0}^n a_{n-k} b_k \end{pmatrix} s^n.$$

Then matching like powers gives

$$n\lambda \begin{pmatrix} a_n \\ b_n \\ c_n \end{pmatrix} = \begin{pmatrix} \sigma(b_n - a_n) \\ \rho a_n - b_n - \sum_{k=0}^n a_{n-k} c_k \\ -\beta c_n + \sum_{k=0}^n a_{n-k} b_k \end{pmatrix},$$

for all $n \geq 2$. We isolate terms of order n on the left, and have

$$\begin{pmatrix} \sigma(b_n - a_n) - n\lambda a_n \\ \rho a_n - b_n - a_0 c_n - c_0 a_n - n\lambda b_n \\ -\beta c_n + a_0 b_n + b_0 a_n - n\lambda c_n \end{pmatrix} = \begin{pmatrix} 0 \\ \sum_{k=1}^{n-1} a_{n-k} c_k \\ -\sum_{k=1}^{n-1} a_{n-k} b_k \end{pmatrix}.$$

When expressed in matrix form the above system of equations is

$$[Df(\hat{p}) - n\lambda\text{Id}] p_n = R_n, \quad (16)$$

where $p_n = (a_n, b_n, c_n)^T$ and

$$R_n := \begin{pmatrix} 0 \\ \sum_{k=1}^{n-1} a_{n-k} c_k \\ -\sum_{k=1}^{n-1} a_{n-k} b_k \end{pmatrix}.$$

The linear equations (16) are referred to as the *homological equations*, and determine the power series coefficients of P for all orders $n \geq 2$.

The left hand side of Equation (16) is invertible as long as $n\lambda$ is not an eigenvalue of $Df(p_0)$. But we assumed that λ is the only stable eigenvalue. Since $n\lambda < \lambda < 0$ for all $n \geq 2$, i.e. $n\lambda$ is never an eigenvalue, the matrix is always invertible, and the Taylor coefficients of P are uniquely defined to all orders.

Solving Equation (16) recursively leads to Taylor coefficients for P to any finite order. Let

$$P^N(s) = \sum_{n=0}^N p_n s^n,$$

denote the N -th order approximation obtained by solving Equation (16) for $2 \leq n \leq N$ be our approximation of the stable/unstable manifold.

Returning to the remaining eigenvalues we proceed in a similar fashion to compute the two dimensional invariant manifold. So we take λ_1 and λ_2 with the same stability (both stable or both unstable) and assume that the remaining eigenvalue has opposite stability (unstable or stable). Since $m = 2$ the invariance equation (13) reduces to

$$\lambda_1 s_1 \frac{\partial}{\partial s_1} P(s_1, s_2) + \lambda_2 s_2 \frac{\partial}{\partial s_2} P(s_1, s_2) = f[P(s_1, s_2)],$$

and we look for

$$P(s_1, s_2) = \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} \begin{pmatrix} a_{mn} \\ b_{mn} \\ c_{mn} \end{pmatrix} s_1^m s_2^n.$$

Power matching as above leads to the homological equations

$$[Df(\hat{p}) - (m\lambda_1 + n\lambda_2)\text{Id}] p_{mn} = R_{mn}, \quad (17)$$

where

$$p_{mn} = \begin{pmatrix} a_{mn} \\ b_{mn} \\ c_{mn} \end{pmatrix},$$

and

$$R_{mn} = \begin{pmatrix} 0 \\ \sum_{k=0}^m \sum_{l=0}^n \hat{\delta}_{kl}^{mn} a_{(m-k)(n-l)} c_{kl} \\ -\sum_{k=0}^m \sum_{l=0}^n \hat{\delta}_{kl}^{mn} a_{(m-k)(n-l)} b_{kl} \end{pmatrix}.$$

Here $\hat{\delta}_{kl}^{mn}$ is as defined in Section 2.2 (see 2.3.1 Equation (9)), that is this coefficient appears to remove terms containing the multi-index α from the summation.

Now, if

$$m\lambda_1 + n\lambda_2 \neq \lambda_{1,2} \quad (18)$$

for all $m, n \in \mathbb{N}$ with $m + n \geq 2$, then the matrix in the left hand side of Equation (17) is invertible, and hence the formal series solution P is defined to all orders. Supposing that this is the case, solving the homological equations for all $2 \leq |\alpha| \leq N$ leads to our numerical approximation

$$P^N(s_1, s_2) = \sum_{n=0}^N \sum_{m=0}^n p_{n-m,m} s_1^{n-m} s_2^m.$$

Remark 3.5 (Resonance conditions). The conditions supposed in Equation (18) are the *non-resonance* conditions which always appear in the parameterization method. As one can easily verify, these conditions give rise to only a finite number of constraints between the eigenvalues and hence are typically (generically) satisfied on an open set of parameters. Nevertheless, resonances sometimes occur (for example they *will* occur if one continues along a one parameter family of equilibrium solutions), and can be treated for example using the approach discussed in [53].

Again, a much more general treatment of this material is found in [74, 75, 76]. For example one can choose to look for P only a C^k conjugation to the flow, in which case the eigenvalues need only satisfy non-resonance conditions to order $m + n < k$. Moreover the techniques employed above can be extended to many infinite dimensional contexts, and can be used to study other invariant manifolds including invariant tori and their invariant manifolds.

3.3 Numerical considerations

In implementing the numerical computations outlined in Section 3.2 two important issues must be addressed.

- **Scaling:** the initial choice of scalings for the eigenvectors is free. How best to choose them?
- **Numerical domain:** the method provides a polynomial approximation, and this polynomial is defined on all of \mathbb{R}^m . Yet we don't expect that a Taylor series is a good approximation globally. On the other hand, we want to use the largest domain on which the polynomial is an accurate approximation. How best to restrict the domain of P^N so that we obtain meaningful results?

First, we consider the effect of rescaling the eigenvectors on the Taylor coefficients. We have the following.

Lemma 3.6. *Let $p \in \mathbb{R}^n$ be an equilibrium solution for a real analytic vector field $f: \mathbb{R}^n \rightarrow \mathbb{R}^n$. Suppose that $Df(p)$ is diagonalizable with m -stable eigenvalues $\lambda_1, \dots, \lambda_m \in \mathbb{C}$. Assume that $\lambda_1, \dots, \lambda_m$ are non-resonant, so that a formal series solution of Equation (13) exists for every fixed choice of eigenvectors (and is unique up to this choice).*

Let $\xi_1, \dots, \xi_m \in \mathbb{C}^n$ be a collection of eigenvectors with

$$\|\xi_j\| = 1, \quad 1 \leq j \leq m,$$

and suppose that $P(s) = \sum_{|\alpha|=0}^{\infty} p_{\alpha} s^{\alpha}$ is the unique formal series solution of Equation (13) with

$$p_{e_j} = \frac{\partial}{\partial s_j} P(0) = \xi_j.$$

For any collection of non-zero constants $\tau_1, \dots, \tau_m \in \mathbb{R}$, define $\tilde{\xi}_1, \dots, \tilde{\xi}_m \in \mathbb{C}^n$ by

$$\tilde{\xi}_j = \tau_j \xi_j, \quad 1 \leq j \leq m.$$

Then $\tilde{P}(s) = \sum_{|\alpha|=0}^{\infty} \tilde{p}_\alpha s^\alpha$ is the unique formal series solution of Equation (13) with

$$\tilde{p}_{e_j} = \frac{\partial}{\partial s_j} \tilde{P}(0) = \tau_j \xi_j, \quad 1 \leq j \leq m,$$

if and only if

$$\tilde{p}_\alpha = \tau_1^{\alpha_1} \dots \tau_m^{\alpha_m} p_\alpha, \quad (19)$$

for all $\alpha \in \mathbb{N}^m$.

Proof. Define the $m \times m$ diagonal matrix

$$\Gamma = \begin{pmatrix} \tau_1 & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & \tau_m \end{pmatrix},$$

and the reparameterization

$$P_\Gamma(s) = P(\Gamma s).$$

Observe that

$$\frac{\partial}{\partial s_j} P_\Gamma(s) = \frac{\partial}{\partial s_j} (P(\Gamma s)) = \frac{\partial}{\partial s_j} P(\Gamma s) \tau_j, \quad (20)$$

for each $1 \leq j \leq m$. Then

$$DP_\Gamma(s) \Lambda s = DP(\Gamma s) \Gamma \Lambda s = DP(\Gamma s) \Lambda \Gamma s = f(P(\Gamma s)) = f(P_\Gamma(s)),$$

as Γ and Λ commute and recalling that P is a solution of Equation (13). This shows that P_Γ is a solution of Equation (13). Moreover, by evaluating at zero in Equation (20), we have that

$$\frac{\partial}{\partial s_j} P_\Gamma(0) = \tau_j \frac{\partial}{\partial s_j} P(0) = \tau_j \xi_j.$$

Since \tilde{P} is the unique formal series solution of Equation (13) associated with these eigenvectors, we see that $\tilde{P} = P_\Gamma$ in the sense of formal series. Since these are equal as power series we have

$$\begin{aligned} \sum_{|\alpha|=0}^{\infty} \tilde{p}_\alpha s^\alpha &= \tilde{P}(s) \\ &= P_\Gamma(s) \\ &= P(\Gamma s) \\ &= \sum_{|\alpha|=0}^{\infty} p_\alpha (\Gamma s)^\alpha \\ &= \sum_{|\alpha|=0}^{\infty} \tau_1^{\alpha_1} \dots \tau_m^{\alpha_m} p_\alpha s^\alpha, \end{aligned}$$

and matching like powers gives the result. The reverse implication is left as an exercise. \square

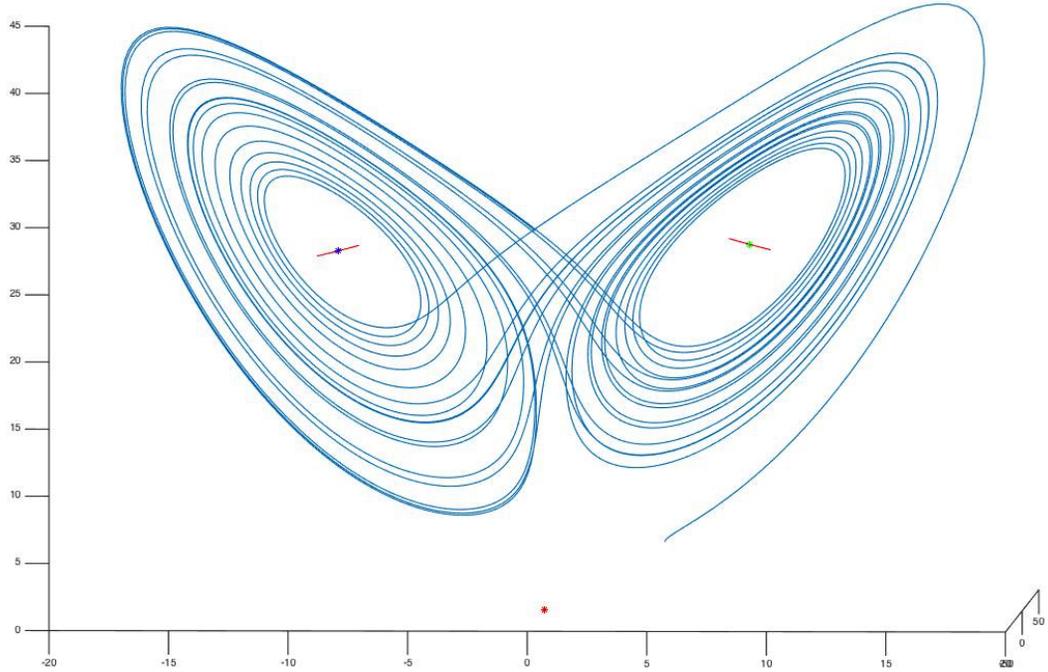


Figure 4: Parameterized local stable manifolds of the non-trivial equilibria, computed to polynomial order $N = 50$. For these parameterizations we choose an eigenvector scaled to length one, and evaluate the polynomial approximations on the unit interval $[-1, 1]$. The results illustrate that these seemingly standard choices can lead to unsatisfactory results.

So, not only are solutions of Equation (13) unique up to the choice of eigenvectors, but given the Taylor series coefficients of one solution we obtain the Taylor coefficients of another solution associated with different eigenvector scalings simply applying the transformation of Equation (19) term by term. This fact helps us choose appropriate eigenvector scalings in numerical applications.

Example: one dimensional stable manifolds in the Lorenz system: Consider the Lorenz system with classic parameter values $\sigma = 10$, $\beta = 8/3$, $\rho = 28$, and the non-trivial equilibrium solution at

$$p \approx \begin{pmatrix} 8.485281374238570 \\ 8.485281374238570 \\ 27 \end{pmatrix}.$$

Then $Df(p)$ has a single stable eigenvalue

$$\lambda^s \approx -13.854577914596042.$$

We are free to choose any eigenvector we wish, and a natural choice might be to take

$$\xi^s \approx \begin{pmatrix} 0.855665024602210 \\ -0.329822750612395 \\ -0.398816146677856 \end{pmatrix},$$

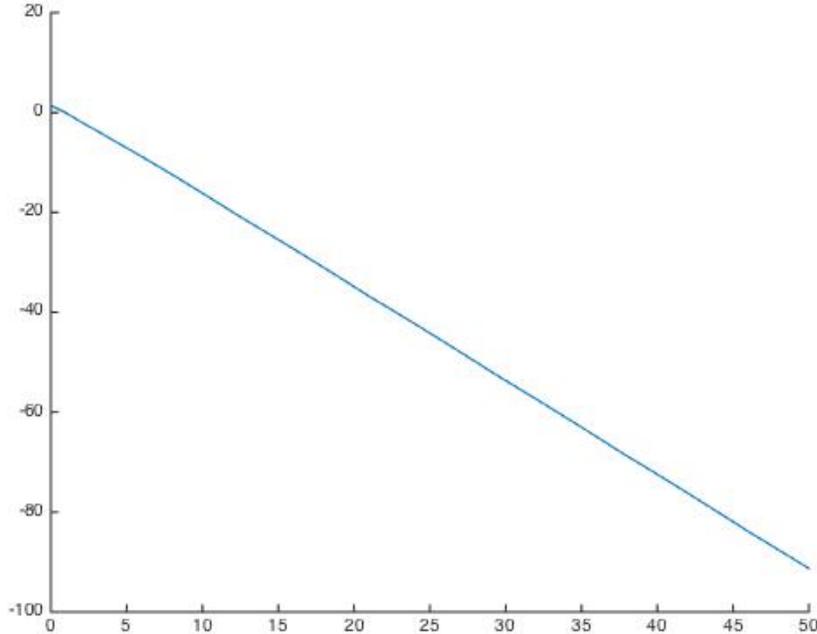


Figure 5: Plot of $\log_{10} \|p_n\|$ versus n for the parameterization illustrated in Figure 4. The linear appearance of the curve illustrates the exponential decay of the power series coefficients. Note that the $N = 50$ coefficient has magnitude on the order of 10^{-90} . The exponential decay rate not only suggests that we need to rescale the eigenvectors, it also suggests the correct choice for the rescaled length.

with $\|\xi^s\| = 1$. Letting $p_0 = p$ and $p_1 = \xi^s$, we then solve recursively the homological equations (17) for $2 \leq n \leq N = 50$ to obtain the polynomial

$$P^{50}(s) = \sum_{n=0}^{50} p_n s^n.$$

The next question is “what should we take as the domain of P^{50} ?” Again, a natural choice is to take the unit interval $[-1, 1]$. The resulting parametric arcs are plotted in Figure 4. (The manifold at the second nontrivial equilibrium is obtained by the symmetry $(x, y) \rightarrow (-x, -y)$).

The results are rather unsatisfactory, in the sense that we used $N = 50$ terms and obtain only a rather small portion of the manifold. To obtain better results we should either rescale the eigenvectors, or evaluate the polynomial on a larger domain. Since these two approaches are equivalent we will hold the domain $[-1, 1]$ fixed, and look for a better scaling of the eigenvectors. The reason we choose this approach is simply that evaluating power series for $s \in [-1, 1]$ is more numerically stable than on larger domains.

We start with the question: how fast were the Taylor coefficients $\{p_n\}_{n=0}^{50}$ decaying in the previous computation? The question is answered in Figure 5, where the decay rates

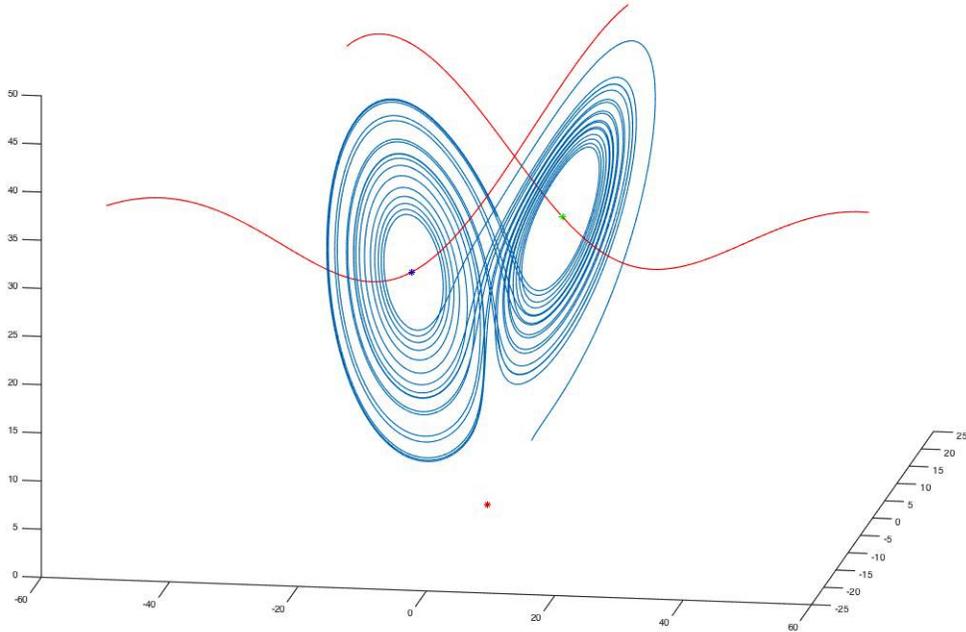


Figure 6: Parameterized local stable manifolds of the non-trivial equilibria, computed to polynomial order $N = 50$. For these parameterizations we rescaled the eigenvector to have length 58, but still evaluate the polynomial approximations on the unit interval $[-1, 1]$. The rescaled parameterization yields a much larger embedding of the local stable manifold.

are plotted on a base ten logarithmic scale. The figure makes it clear that the coefficients are decaying far too rapidly to be numerically useful, as their magnitudes appear to dip below machine epsilon (approximately 2.2204×10^{-16}) after about the tenth coefficient. This illustrates the problem with arbitrarily fixing the scaling of the eigenvectors: an eigenvector with length one may lead to undesirably fast exponential decay (or growth!)

To get a better result we rescale the eigenvector so that the new Taylor coefficients $\{\tilde{p}_n\}_{n=0}^{50}$ have $\|\tilde{p}_{50}\| \approx 10^{-2}$. Here we are aided by the formula of Equation (19) and choose a rescaling factor τ so that

$$\|\tau^{50}\xi^s\| = \tau^{50}10^{-90} = 10^{-2},$$

or $\tau = 10^{88/50} \approx 57.544$.

So, take $\hat{\xi}^s = 58\xi^s$ and recompute the Taylor coefficients by recursively solving the homological equations again. The reason that we recompute is that, once we fix a good scaling, it is more numerically stable to find \tilde{p}_n , $2 \leq n \leq 50$ from scratch using the recursion than it is to employ the transformation given by Equation (19) directly to the known coefficients $\{p_n\}_{n=0}^{50}$. The recomputed Taylor coefficients decay exponentially fast but at a much more practical rate, i.e. we do not let the high order coefficients get too small. The results are much more satisfactory as illustrated in Figure 6.

This discussion leads to the following heuristic: *rescaling the eigenvectors controls the size of the embedding of $[-1, 1]$ in the phase space.* Taking larger or smaller scalings we parameterize larger or smaller patches of the local stable/unstable manifolds. In general there is no reason not to fix a domain of unit size.

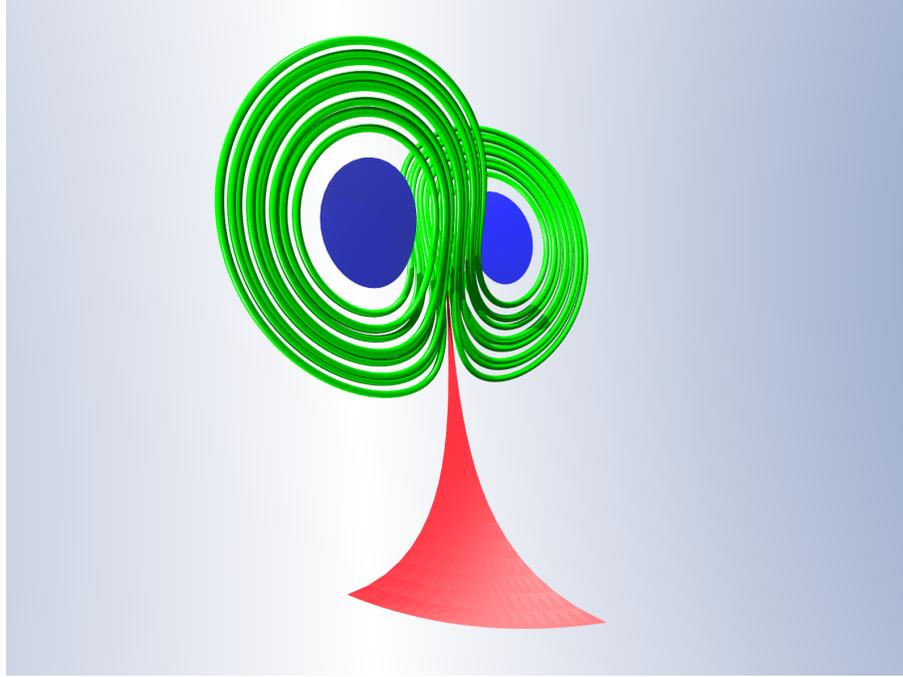


Figure 7: Parameterized two dimensional local unstable manifolds of the non-trivial equilibria (blue), and local stable manifold of the origin (red), computed to polynomial order $N = 150$ and $N = 50$ respectively. At the nontrivial equilibrium the unstable unit eigenvectors are rescaled by $\tau = 3.6$ and at the origin the stable unit eigenvectors are rescaled by $\tau_1 = 20$ in the slow direction and $\tau_2 = 2$ in the fast direction.

Example: Similar considerations apply when we compute two dimensional parameterizations of local stable/unstable manifolds. Consider first the two dimensional unstable manifold at the nontrivial equilibrium. The eigenvalues are complex conjugates with

$$\lambda_1^u \approx 0.093955623964686 - i10.194505220927850, \quad \text{and} \quad \lambda_2^u = \overline{\lambda_1^u}.$$

Note that the real part of the unstable eigenvalues is small, i.e. orbits move slowly away from the equilibrium even though they oscillate rather rapidly. We choose complex conjugate eigenvectors $\xi_{1,2}^u$ of length one and, since we want to absorb as much of the slow escape into the parameterization as possible, compute the manifold to order $N = 150$.

The Taylor coefficients of order $N = 150$ have magnitude on the order to 10^{-100} , i.e. they are numerically useless. We would prefer that the final coefficients had magnitude on the order of machine epsilon, and returning to Equation (19) we choose to rescale to

$$\hat{\xi}_1^u = \tau \xi_1^u,$$

where $\tau = 3.6$ so that $\tau^N 10^{-100} \approx 10^{-16}$. Upon recomputing the coefficients we obtain the desired decay rate (i.e. rate with coefficients of order $N = 150$ at machine precision).

At the origin the situation is a little different. There we have stable eigenvalues

$$\lambda_1^s \approx -2.667, \quad \text{and} \quad \lambda_2^s \approx -22.828.$$

Now, our interest is in connections from p_0 to p_1 (non-trivial to the origin) and we expect such connecting orbits to approach the origin along the slow stable manifold (sub-manifold of the stable manifold where the dynamics is analytically conjugate to the linear dynamics given by the smaller of the two stable eigenvalues. See [86] for more discussion). So we are more interested in the portion of the manifold tangent to the slow eigenspace. Since $\lambda_2^s \approx 10\lambda_1^s$ we scale the slow eigenvector to ten times longer than the fast eigenvalue.

So, we choose $\|\xi_1^s\| = 1$ and $\|\xi_2^s\| = 0.1$, compute the Taylor coefficients to order $N = 50$, and find that the largest coefficients $p_\alpha \in \mathbb{R}^3$ with $|\alpha| = 50$ have magnitude approximately 10^{-80} (this time we suppress the log base 10 plot). Being conservative, we would prefer that the largest coefficients of order $|\alpha| = 50$ have magnitudes close to machine epsilon. This is achieved by taking

$$\hat{\xi}_1^s = \tau \xi_1^s, \quad \text{and} \quad \hat{\xi}_2^s = \tau \xi_2^s,$$

with $\tau = 20$.

3.4 Fixed point formulation for the truncation error

For the applications considered below we are interested in the two dimensional stable/unstable manifolds of the Lorenz system, hence we discuss only the validation of these manifolds.

Recall that $Df(\hat{p})$ is diagonalizable, and that the eigenvalues $\lambda_1, \lambda_2, \lambda_3 \in \mathbb{C}$, and the associated eigenvectors $\xi_1, \xi_2, \xi_3 \in \mathbb{C}^3$ are known (at least up to interval enclosures). Suppose also, using the notation of the previous section, that λ_1, λ_2 have the same stability (either both stable or both unstable). We write

$$Q = [\xi_1, \xi_2, \xi_3],$$

for the matrix whose columns are the eigenvectors. By the assumption of diagonalizability Q is invertible, and we let Q^{-1} denote its inverse. Let

$$\Lambda = \begin{pmatrix} \lambda_1 & 0 & 0 \\ 0 & \lambda_2 & 0 \\ 0 & 0 & \lambda_3 \end{pmatrix},$$

denote the diagonal matrix of eigenvalues.

Recall the linear Equations (17), i.e. the homological equations which define the Taylor coefficients for a parameterization of a local stable/unstable manifold of an equilibrium for Lorenz. Using the notation above the left hand side of the homological equations becomes

$$\begin{aligned} Df(p_0) - (m\lambda_1 + n\lambda_2)\text{Id} &= Q\Lambda Q^{-1} - (m\lambda_1 + n\lambda_2)QQ^{-1} \\ &= Q[\Lambda - (m\lambda_1 + n\lambda_2)\text{Id}]Q^{-1}. \end{aligned}$$

Assuming that λ_1, λ_2 are non-resonant, we have that

$$[Df(p_0) - (m\lambda_1 + n\lambda_2)\text{Id}]^{-1} = Q[\Lambda - (m\lambda_1 + n\lambda_2)\text{Id}]^{-1}Q^{-1},$$

where

$$[\Lambda - (m\lambda_1 + n\lambda_2)\text{Id}]^{-1} = \begin{pmatrix} (\lambda_1 - m\lambda_1 - n\lambda_2)^{-1} & 0 & 0 \\ 0 & (\lambda_2 - m\lambda_1 - n\lambda_2)^{-1} & 0 \\ 0 & 0 & (\lambda_3 - m\lambda_1 - n\lambda_2)^{-1} \end{pmatrix}.$$

With $(m, n) \in \mathbb{N}^2$, define the matrices

$$A_{mn} = Q[\Lambda - (m\lambda_1 + n\lambda_2)\text{Id}]^{-1}Q^{-1},$$

and constants

$$K_{mn} := \max \left(\frac{1}{|\lambda_1 - m\lambda_1 - n\lambda_2|}, \frac{1}{|\lambda_2 - m\lambda_1 - n\lambda_2|}, \frac{1}{|\lambda_3 - m\lambda_1 - n\lambda_2|} \right). \quad (21)$$

Note that $K_{mn} \rightarrow 0$ as $(m+n) \rightarrow \infty$, and that

$$\|A_{mn}\| = \|(Df(p_0) - (m\lambda_1 + n\lambda_2)\text{Id})^{-1}\| \leq \|Q\| \|Q^{-1}\| K_{mn}.$$

Now, using the hat product notation of Section 2.3.1, the homological equations become

$$\begin{pmatrix} a_{mn} \\ b_{mn} \\ c_{mn} \end{pmatrix} = A_{mn} \begin{pmatrix} 0 \\ (a \hat{*} c)_{mn} \\ -(a \hat{*} b)_{mn} \end{pmatrix},$$

where the right hand side does not depend on coefficients of order $m+n$ (but rather depends only on “lower order terms”) suggesting that unknown Taylor coefficient sequences $\{a_{mn}\}, \{b_{mn}\}, \{c_{mn}\}$ together solve a fixed point problem.

Endow $(\ell_{1,2}^1)^3 = \ell_{1,2}^1 \oplus \ell_{1,2}^1 \oplus \ell_{1,2}^1$, with the product space norm

$$\|(a, b, c)\|_{(\ell_{1,2}^1)^3} := \max(\|a\|_{1,2}^1, \|b\|_{1,2}^1, \|c\|_{1,2}^1),$$

and consider the operator $\Psi: (\ell_{1,2}^1)^3 \rightarrow (\ell_{1,2}^1)^3$ given by

$$\Psi(a, b, c)_{mn} = \begin{pmatrix} \Psi(a, b, c)_{mn}^1 \\ \Psi(a, b, c)_{mn}^2 \\ \Psi(a, b, c)_{mn}^3 \end{pmatrix} = A_{mn} \begin{pmatrix} 0 \\ (a \hat{*} c)_{mn} \\ -(a \hat{*} b)_{mn} \end{pmatrix}. \quad (22)$$

Note that a fixed point of Ψ solves the homological equations to all orders, i.e. if $(a, b, c) \in (\ell_{1,2}^1)^3$ is a fixed point of Ψ , then $p_{mn} = (a_{mn}, b_{mn}, c_{mn})$ are the Taylor coefficients of the desired parameterization.

To prove that Ψ has a fixed point, consider the terms of order $m+n \leq N$ and the tail terms separately. Define the subspaces $X_{1,2}^N, X_{1,2}^\infty \subset \ell_{1,2}^1$ and projections $\pi_N: \ell_{1,2}^1 \rightarrow X_{1,2}^N$ and $\pi_\infty: \ell_{1,2}^1 \rightarrow X_{1,2}^\infty$ as in Section 2.2. Let $\Psi^N := \pi_N \circ \Psi$ and $\Psi^\infty := \pi_\infty \circ \Psi$, so that Ψ has the decomposition

$$\Psi(a, b, c) = \Psi^N(a^N, b^N, c^N) + \Psi^\infty(u, v, w, a^N, b^N, c^N).$$

Note that $\Psi^N: (X_{1,2}^N)^3 \rightarrow (X_{1,2}^N)^3$ and $\Psi^\infty: (X_{1,2}^\infty)^3 \oplus (X_{1,2}^N)^3 \rightarrow (X_{1,2}^\infty)^3$. Here the nonzero components of Ψ^N are just the homological equations for $0 \leq m+n \leq N$. So, suppose that $\bar{a}^N, \bar{b}^N, \bar{c}^N \in X_{1,2}^N$ are obtained by solving these homological equation exactly (at least in the sense of interval arithmetic). Define the map $T: (X_{1,2}^\infty)^3 \rightarrow (X_{1,2}^\infty)^3$ by

$$T(u, v, w) := \Psi^\infty(u, v, w, \bar{a}^N, \bar{b}^N, \bar{c}^N),$$

where the “barred” data is considered fixed. Since solving the recursion relations to N -th order gives the fixed point of Ψ^N , we need now only prove the existence of a fixed point of the map T in order to obtain a fixed point of the full map Ψ .

The operator T is written explicitly as

$$T(u, v, w)_{mn} = \begin{pmatrix} T(u, v, w)_{mn}^1 \\ T(u, v, w)_{mn}^2 \\ T(u, v, w)_{mn}^3 \end{pmatrix} = A_{mn} \begin{pmatrix} 0 \\ (\bar{a}^N + u) \hat{*} (\bar{c}^N + w)_{mn} \\ -(\bar{a}^N + u) \hat{*} (\bar{b}^N + v)_{mn} \end{pmatrix}, \quad (23)$$

for $m + n \geq N + 1$.

To write the operators on a higher level, let A_{mn}^{ij} denote the i -th row and j -th column of the matrix A_{mn} , and define the bounded linear operators $A^{ij} : X_{1,2}^\infty \rightarrow X_{1,2}^\infty$ by

$$(A^{ij}u)_{mn} = \begin{cases} 0 & \text{if } 0 \leq m + n \leq N \\ A_{mn}^{ij}u_{mn} & \text{if } m + n \geq N + 1 \end{cases}.$$

It is worth remarking that the explicit form of these operators will play no role in the analysis to follow. What is essential is that each of these operators satisfies the bound

$$\|A^{ij}\| \leq \sup_{m+n \geq N+1} K_{mn}.$$

Also recall that in Section 2.2 we derived the decompositions

$$\pi_\infty(\bar{a}^N + u) \hat{*} (\bar{c}^N + w) = (\bar{a}^N \hat{*} \bar{c}^N)^\infty + (u \hat{*} \bar{c}^N) + (w \hat{*} \bar{a}^N) + (u \hat{*} w)$$

and

$$\pi_\infty(\bar{a}^N + u) \hat{*} (\bar{b}^N + v) = (\bar{a}^N \hat{*} \bar{b}^N)^\infty + (u \hat{*} \bar{b}^N) + (v \hat{*} \bar{a}^N) + (u \hat{*} v).$$

Then for $j = 1, 2, 3$ we have

$$T(u, v, w)^j = A^{j2}((\bar{a}^N \hat{*} \bar{c}^N)^\infty + (u \hat{*} \bar{c}^N) + (w \hat{*} \bar{a}^N) + (u \hat{*} w)) \quad (24)$$

$$- A^{j3}((\bar{a}^N \hat{*} \bar{b}^N)^\infty + (u \hat{*} \bar{b}^N) + (v \hat{*} \bar{a}^N) + (u \hat{*} v)). \quad (25)$$

Note that T is Fréchet differentiable and that (suppressing for a moment the (u, v, w) arguments) $DT : (X_{1,2}^\infty)^3 \rightarrow (X_{1,2}^\infty)^3$ is given by

$$DT = \begin{pmatrix} D_1 T^1 & D_2 T^1 & D_3 T^1 \\ D_1 T^2 & D_2 T^2 & D_3 T^2 \\ D_1 T^3 & D_2 T^3 & D_3 T^3 \end{pmatrix},$$

where, for $h \in X_{1,2}^\infty$ these partial derivatives have the action

$$D_1 T^j(u, v, w)h = A^{j2}(\bar{c}^N \hat{*} h + h \hat{*} w) - A^{j3}(\bar{b}^N \hat{*} h + h \hat{*} v)$$

$$D_2 T^j(u, v, w)h = -A^{j3}(\bar{a}^N \hat{*} h + u \hat{*} h),$$

and

$$D_3 T^j(u, v, w)h = A^{j2}(\bar{a}^N \hat{*} h + u \hat{*} h),$$

for $j = 1, 2, 3$.

3.5 A validated computation via the contraction mapping theorem

Given the data $\bar{a}^N, \bar{b}^N, \bar{c}^N \in X_{1,2}^N$, we hope to show that T is a contraction in some (hopefully small) neighborhood of the origin in $(X_{1,2}^\infty)^3$. Recalling Proposition 2.6 and the ‘‘hat star’’ bounds of Lemma 2.3, we have the following.

Lemma 3.7. *Let $\{K_{mn}\}_{(m,n) \in \mathbb{N}^2}$ be as defined in Equation (21), and*

$$K^N := \|Q\| \|Q^{-1}\| \sup_{m+n \geq N+1} K_{mn}.$$

Define

$$Y_0 := K^N \left(\sum_{m+n=N+1}^{2N} |(\bar{a}^N \hat{*} \bar{b}^N)_{mn}| + |(\bar{a}^N \hat{*} \bar{c}^N)_{mn}| \right),$$

$$Z_1 := K^N \left(\sum_{1 \leq m+n \leq N} 2|\bar{a}_{mn}^N| + \sum_{1 \leq m+n \leq N} (|\bar{b}_{mn}^N| + |\bar{c}_{mn}^N|) \right),$$

and

$$Z_2 := 4K^N.$$

Then

$$\|T(0, 0, 0)\|_{(X_{1,2}^\infty)^3} \leq Y_0.$$

Moreover, for $r > 0$ let $B_r(0)$ denote the ball of radius r about the origin in $(X_{1,2}^\infty)^3$. Then

$$\sup_{(u,v,w) \in \overline{B_r(0)}} \|DT(u, v, w)\|_{B((X_{1,2}^\infty)^3)} \leq Z_1 + Z_2 r.$$

Proof. Consider

$$\begin{aligned} \|T(0, 0, 0) - 0\|_{(X_{1,2}^\infty)^3} &\leq \max_{1 \leq j \leq 3} \|T(0, 0, 0)^j\|_{X_{1,2}^\infty} \\ &\leq \|A^{j2}\|_{B(X_{1,2}^\infty)} \|(\bar{a}^N \hat{*} \bar{c}^N)^\infty\|_{1,2}^1 + \|A^{j3}\|_{B(X_{1,2}^\infty)} \|(\bar{a}^N \hat{*} \bar{b})^\infty\|_{1,2}^1 \\ &\leq K^N \left(\sum_{m+n=N+1}^{2N} |(\bar{a}^N \hat{*} \bar{b}^N)_{mn}| + |(\bar{a}^N \hat{*} \bar{c}^N)_{mn}| \right) \\ &= Y_0, \end{aligned}$$

where the estimate of Lemma 2.3 provides the bound on the hat products.

Now consider $(u, v, w) \in \overline{B_r(0)} \subset (X_{1,2}^\infty)^3$. In light of the estimates in Lemma 2.3 one has that

$$\begin{aligned} \|DT(u, v, w)\|_{B((X_{1,2}^\infty)^3)} &\leq \max_{1 \leq j \leq 3} \sum_{k=1}^3 \|D_k T^j(u, v, w)\|_{B(X_{1,2}^\infty)} \\ &\leq \max_{1 \leq j \leq 3} \sum_{k=1}^3 \sup_{\|h\|_{X_{1,2}^\infty} = 1} \|D_k T^j(u, v, w)h\|_{X_{1,2}^\infty} \\ &\leq K^N \left(2 \sum_{1 \leq m+n \leq N} |\bar{a}_{mn}^N| + \sum_{1 \leq m+n \leq N} (|\bar{b}_{mn}^N| + |\bar{c}_{mn}^N|) + 2\|u\|_{X_{1,2}^\infty} + \|v\|_{X_{1,2}^\infty} + \|w\|_{X_{1,2}^\infty} \right) \\ &\leq K^N \left(\sum_{1 \leq m+n \leq N} 2|\bar{a}_{mn}^N| + \sum_{1 \leq m+n \leq N} (|\bar{b}_{mn}^N| + |\bar{c}_{mn}^N|) + 4r \right) \\ &\leq Z_1 + Z_2 r. \end{aligned}$$

□

Example: Consider the two dimensional manifold at the origin. Using interval arithmetic we check that

$$\lambda^u \in [11.82772345116345, 11.82772345116347],$$

$$\lambda_1^s \in [-2.666666666666667, -2.666666666666666],$$

and

$$\lambda_2^s \in [-22.82772345116347, -22.82772345116345].$$

and that the eigenvectors satisfy the inclusions

$$\xi^u \in \begin{pmatrix} [-0.41650417819291, -0.41650417819290] \\ [-0.90913380178490, -0.90913380178489] \\ [-0.000000000000001, 0.000000000000001] \end{pmatrix},$$

$$\xi_1^s = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix},$$

and

$$\xi_2^s \in \begin{pmatrix} [-0.61481678521648, -0.61481678521647] \\ [0.78866996938902, 0.78866996938903] \\ 0 \end{pmatrix}.$$

Then we recursively solve the homological equations and obtain interval enclosures of the coefficients to order $N = 50$. The fact that we can solve the homological equations with validated error bounds up to order $N = 50$ shows that there are no resonances with below order fifty.

Note that if $(m, n) \in \mathbb{N}^2$ with $|(m, n)| = m + n \geq 51$, then since $N = 50 > |\lambda_2^s| > |\lambda_1^s|^2$ we have that

$$\frac{1}{|m\lambda_1^s + n\lambda_2^s - \lambda_1^s|} \leq \frac{1}{|(m+n)\lambda_1^s - \lambda_1^s|} = \frac{1}{|m+n-1||\lambda_1^s|} \leq \frac{1}{50|\lambda_1^s|} \leq 0.0075,$$

$$\frac{1}{|m\lambda_1^s + n\lambda_2^s - \lambda_2^s|} \leq \frac{1}{|(m+n)\lambda_1^s - \lambda_2^s|} = \frac{1}{(m+n)|\lambda_1^s| - |\lambda_2^s|} \leq \frac{1}{50|\lambda_1^s| - |\lambda_2^s|} \leq 0.0089,$$

and

$$\frac{1}{|m\lambda_1^s + n\lambda_2^s - \lambda^u|} \leq \frac{1}{|(m+n)|\lambda_1^s| + |\lambda^u|} \leq \frac{1}{50|\lambda_1^s| + |\lambda^u|} \leq 0.0068.$$

Then choose

$$K^N = 0.009.$$

We scale the slow eigenvector to have length 15 and the fast eigenvector to have length 1.5 (as the difference in the magnitudes of the eigenvalues is about ten). We obtain a validated contraction mapping error bound of 7.5×10^{-20} , which is below machine precision, but we need order $N = 50$ with this choice of scalings in order to get

$$Z_1 = 0.71 < 1.$$

We could take lower order and smaller scalings to validate a smaller portion of the manifold.

At “the eye” we have unstable eigenvalue enclosures

$$\lambda_1^u \in D(0.0939556239647 - 10.19450522092785i, 6 \times 10^{-15}),$$

and similar for the complex conjugate eigenvectors. We choose eigenvectors scaled to unit length. More importantly we check that for the complex conjugate eigenvalue, if $\lambda_1^u = a + ib$ and $\lambda_2^u = \overline{\lambda_1^u}$ then

$$\begin{aligned} \frac{1}{|m\lambda_1^u + n\lambda_2^u - \lambda_{1,2}^u|} &= \frac{1}{|m(a + ib) + n(a - ib) - (a \pm ib)|} \\ &\leq \frac{1}{|(m + n - 1)a \pm ib|} \\ &\leq \frac{1}{|Na \pm ib|} \\ &\leq \frac{1}{N|\text{real}(\lambda_1^u)|} \\ &\leq 0.054, \end{aligned}$$

where we take $N = 200$ the order of approximation. The contraction mapping proof succeeds and we have that the tail of the parameterization has norm less than 10^{-90} . This is fantastically small, but we need to take $N = 200$ in order to get

$$Z_1 = 0.846 < 1.$$

If we choose smaller scalings the proof is much easier, but the local manifold is smaller. Having a larger local unstable manifold is helpful for the connecting orbit proof later.

4 The flow box problem: propagating and differentiating sets of initial conditions

In the previous section we studied the dynamics near a equilibrium solution. To connect one equilibrium to another it is necessary to study the flow generated by the vector field. In this section we develop Taylor series expansions with validated error bounds for the flow map in a neighborhood of a given initial condition.

4.1 Formal series solutions: a Taylor integrator for the Lorenz system

Given a non-equilibrium point $(x_0, y_0, z_0) \in \mathbb{R}^3$, we look for a locally defined flow map of the form

$$\phi(t, x_0 + x, y_0 + y, z_0 + z) = \sum_{n=0}^{\infty} \sum_{k=0}^{\infty} \sum_{l=0}^{\infty} \sum_{m=0}^{\infty} \begin{pmatrix} a_{klmn} \\ b_{klmn} \\ c_{klmn} \end{pmatrix} x^k y^l z^m t^n, \quad (26)$$

having that

$$\frac{\partial}{\partial t} \phi(t, x_0 + x, y_0 + y, z_0 + z) = \tau f(\phi(t, x_0 + x, y_0 + y, z_0 + z)), \quad (27)$$

for all $(x, y, z, t) \in (-1, 1)^4 \subset \mathbb{R}^4$. Here we take f to be the Lorenz vector field. The parameter $\tau > 0$ simply rescales time so that we can take $t \in (-1, 1)$ and parameterize the time interval $(-\tau, \tau)$ for the differential equation. We take

$$\begin{pmatrix} a_{0,0,0,0} \\ b_{0,0,0,0} \\ c_{0,0,0,0} \end{pmatrix} = \begin{pmatrix} x_0 \\ y_0 \\ z_0 \end{pmatrix},$$

and with $c > 0$ take

$$\begin{pmatrix} a_{1,0,0,0} \\ b_{1,0,0,0} \\ c_{1,0,0,0} \end{pmatrix} = \begin{pmatrix} c \\ 0 \\ 0 \end{pmatrix}, \quad \begin{pmatrix} a_{0,1,0,0} \\ b_{0,1,0,0} \\ c_{0,1,0,0} \end{pmatrix} = \begin{pmatrix} 0 \\ c \\ 0 \end{pmatrix}, \quad \begin{pmatrix} a_{0,0,1,0} \\ b_{0,0,1,0} \\ c_{0,0,1,0} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ c \end{pmatrix}, \quad (28)$$

and

$$\begin{pmatrix} a_{klm0} \\ b_{klm0} \\ c_{klm0} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix},$$

for all $(k, l, m) \in \mathbb{N}^3$ having $k + l + m \geq 2$. These conditions enforce that

$$\phi((-1, 1), (-1, 1), (-1, 1), 0) = (x_0 - c, x_0 + c) \times (y_0 - c, y_0 + c) \times (z_0 - c, z_0 + c),$$

i.e. our power series at time $t = 0$ maps into a cube of radius c .

We now plug the power series of Equation (26) into Equation (27) and matching like powers leads to

$$\begin{pmatrix} a_{klmn} \\ b_{klmn} \\ c_{klmn} \end{pmatrix} = \frac{\tau}{n} \begin{pmatrix} \sigma(b_{klmn-1} - a_{klmn-1}) \\ \rho a_{klmn-1} - b_{klmn-1} - (a * c)_{klmn-1} \\ -\beta c_{klmn-1} + (a * b)_{klmn-1} \end{pmatrix} \quad (29)$$

for $n \geq 1$.

Define $\mathcal{I}_N \subset \mathbb{N}^4$ to be the set of all four dimensional multi-indices of order less than N , i.e.

$$\mathcal{I}_N := \{(k, l, m, n) \in \mathbb{N}^4 : 0 \leq k + l + m + n \leq N\}.$$

These recursion relations are solved to any desired finite order N , resulting in Taylor a coefficient $(a_{klmn}, b_{klmn}, c_{klmn}) \in \mathbb{R}^3$ for each multi-index $(k, l, m, n) \in \mathcal{I}_N$. We approximate the flow near (x_0, y_0, z_0) using the polynomial

$$\phi^N(x_0 + x, y_0 + y, z_0 + z, t) = \sum_{(k,l,m,n) \in \mathcal{I}_N} \begin{pmatrix} a_{klmn} \\ b_{klmn} \\ c_{klmn} \end{pmatrix} x^k y^l z^m t^n,$$

taking $(x, y, z, t) \in (-1, 1)^4$.

4.2 Numerical considerations

Given an initial condition $(x_0, y_0, z_0) \in \mathbb{R}^3$ fix a desired polynomial approximation order $N \in \mathbb{N}$. We choose a rescaling of time $\tau > 0$ and a reparametrization of space $c > 0$ so that $\phi^N(x_0 + x, y_0 + y, z_0 + z, t)$ is a good approximation of the flow for $(x, y, z, t) \in (-1, 1)^4$. These rescaling give us control over the decay rates of the Taylor coefficients. As with the manifold computations, our strategy is to compute the coefficients once – guess the appropriate decay rate – and compute a second time with the optimal choice of rescaling.

Example: Consider the initial condition $(-15, -15, 40) \in \mathbb{R}^3$ for the Lorenz system. The point is “near the attractor” and its behavior is fairly typical. We choose a polynomial approximation of order $N = 30$ and recursively compute the Taylor coefficients with $\tau = c = 1$. The resulting Taylor coefficient grow exponentially fast, and the last coefficient has magnitude on the order of 10^{25} .

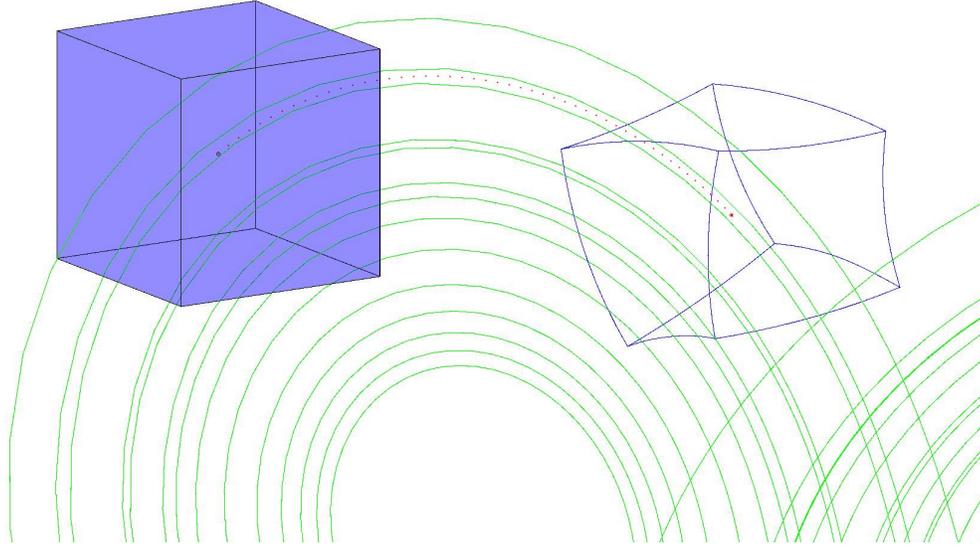


Figure 8: Taylor integration of a “phase box” near the attractor. The time step is $\tau = 0.1$ forward in time and the box of initial conditions has a radius $c = 4$. The advected box is illustrated as a blue wire frame and shows that the nonlinearities have time to twist and stretch the phase box.

As is well known, rescaling time by a factor of τ has the effect of rescaling the power series coefficients by powers of τ . If we want the last coefficient on the order of 10^{-5} we take $\tau = 0.1$, so that $\tau^{30}10^{25} = 10^{-5}$ gives the correct rescaling of time. A little experimentation shows that the coefficient growth is much less sensitive to the spatial parameterization, and we can take $c = 4$ without significantly effecting the decay rates of the Taylor coefficients. We resolve the recursion with these weights and obtain a new series whose order $N = 30$ Taylor coefficients have magnitudes on the order of 10^{-5} as desired. Figure 8 illustrates the results. We see that the box, when advected for a time $\tau = 0.1$ is already distorted in a nonlinear way.

Remark 4.1 (*h*-sets, and covering relations, and well aligned windows). An important technique for developing validated integrators is the choice of special, adapted coordinates for the Taylor expansion. This idea goes back to [19, 18, 17] and is used extensively in the CAPD library [20, 21]. The idea, loosely speaking, is to modify the first order conditions given in Equation (28) so that they better represent the geometry of the flow. For example we could pre-compute the solution of the initial value problem along with the solution of the first order variational equations using a standard and inexpensive numerical integration scheme (perhaps Runge-Kutta). Computing an eigenbasis for the solution of the variational equation provides a frame which is best adapted to the flow to first order.

In the references discussed above, this technique is used to minimize “wrapping effect”. In the language of analytic decay rates employed in the present notes, choosing an adapted frame leads to even better decay rates for the Taylor coefficients of the flow map in the spatial directions. But, in the applications to come such considerations will not play an important role. This is because, in some sense, we brute force the computations by taking high order expansions in space. That being said, control over higher order spatial derivatives

will play an important role in the Newton-like argument for the connecting orbit, especially in the transversality argument.

4.3 Fixed point formulation for the truncation error

Define the operator $\Psi: (\ell_{\nu,4}^1)^3 \rightarrow (\ell_{\nu,4}^1)^3$ by

$$\Psi(a, b, c) = \begin{pmatrix} \Psi_1(a, b, c) \\ \Psi_2(a, b, c) \\ \Psi_3(a, b, c) \end{pmatrix} \quad (30)$$

where the operators $\Psi_1, \Psi_2, \Psi_3: (\ell_{\nu,4}^1)^3 \rightarrow (\ell_{\nu,4}^1)$ are defined by

$$\Psi_1(a, b, c)_{klmn} := \begin{cases} x_0 & \text{if } k = l = m = n = 0 \\ 1 & \text{if } k = 1 \text{ and } l = m = n = 0 \\ 0 & \text{if } l = 1, \text{ and } k = m = n = 0 \\ 0 & \text{if } m = 1, \text{ and } k = l = n = 0 \\ 0 & \text{if } n = 0, \text{ and } k + l + m \geq 2 \\ \frac{\tau\sigma}{n}(b_{klm,n-1} - a_{klm,n-1}) & \text{if } n \geq 1 \end{cases}$$

$$\Psi_2(a, b, c)_{klmn} := \begin{cases} y_0 & \text{if } k = l = m = n = 0 \\ 0 & \text{if } k = 1 \text{ and } l = m = n = 0 \\ 1 & \text{if } l = 1, \text{ and } k = m = n = 0 \\ 0 & \text{if } m = 1, \text{ and } k = l = n = 0 \\ 0 & \text{if } n = 0, \text{ and } k + l + m \geq 2 \\ \frac{\tau}{n}(\rho a_{klm,n-1} - b_{klm,n-1} - (a * c)_{klm,n-1}) & \text{if } n \geq 1 \end{cases}$$

and

$$\Psi_3(a, b, c)_{klmn} := \begin{cases} z_0 & \text{if } k = l = m = n = 0 \\ 0 & \text{if } k = 1 \text{ and } l = m = n = 0 \\ 0 & \text{if } l = 1, \text{ and } k = m = n = 0 \\ 1 & \text{if } m = 1, \text{ and } k = l = n = 0 \\ 0 & \text{if } n = 0, \text{ and } k + l + m \geq 2 \\ \frac{\tau}{n}(-\beta c_{klm,n-1} + (a * b)_{klm,n-1}) & \text{if } n \geq 1 \end{cases}.$$

Consider the decomposition

$$\Psi(a, b, c) = \pi_N(\Psi(a, b, c)) + \pi_\infty(\Psi(a, b, c)),$$

and suppose that $\bar{a}^N, \bar{b}^N, \bar{c}^N \in X_{\nu,4}^N$ provide an exact fixed point of $\pi_N(\Psi)$. Note that this fixed point is given exactly by solving the recursion relations to order N . For fixed $\tau > 0$ define the operator $T: (X_{\nu,4}^\infty)^3 \rightarrow (X_{\nu,4}^\infty)^3$ by

$$T(u, v, w) := \pi_\infty(\Psi(\bar{a}^N, \bar{b}^N, \bar{c}^N, u, v, w)). \quad (31)$$

Let $L: X_{\nu,4}^\infty \rightarrow X_{\nu,4}^\infty$ be the linear operator defined by

$$L(a)_{klmn} = \begin{cases} 0 & \text{if } 0 \leq k + l + m + n \leq N \\ 0 & \text{if } k + l + m + n \geq N + 1, \text{ and } n = 0 \\ \frac{\tau}{n} a_{klmn} & \text{if } k + l + m + n \geq N + 1, \text{ and } n \geq 1 \end{cases}.$$

Then the components of T are given explicitly by

$$T_1(u, v, w) = \sigma L(\pi_\infty(S_4(\bar{b}^N + v)) - \pi_\infty(S_4(\bar{a}^N + u))),$$

$$T_2(u, v, w) = L(\rho\pi_\infty S_4(\bar{a}^N + u) - \pi_\infty S_4(\bar{b}^N + v) - \pi_\infty S_4((\bar{a}^N + u) * (\bar{c}^N + w))),$$

and

$$T_3(u, v, w) = L(-\beta\pi_\infty S_4(\bar{c}^N + w) + \pi_\infty S_4((\bar{a}^N + u) * (\bar{b}^N + v))).$$

Note then that DT is the “three-by-three matrix” of linear operators

$$DT(u, v, w) = \begin{pmatrix} D_1 T_1(u, v, w) & D_2 T_1(u, v, w) & D_3 T_1(u, v, w) \\ D_1 T_2(u, v, w) & D_2 T_2(u, v, w) & D_3 T_2(u, v, w) \\ D_1 T_3(u, v, w) & D_2 T_3(u, v, w) & D_3 T_3(u, v, w) \end{pmatrix},$$

where, for $h \in X_{\nu,4}^\infty$ the operators have the action given by

$$D_1 T_1(u, v, w)h = -\sigma L\pi_\infty S_4(h),$$

$$D_2 T_1(u, v, w)h = \sigma L\pi_\infty S_4(h),$$

$$D_3 T_1(u, v, w)h = 0,$$

$$D_1 T_2(u, v, w)h = \rho L\pi_\infty S_4(h) - L\pi_\infty S_4(\bar{c}^N * h) - L\pi_\infty S_4(h * w),$$

$$D_2 T_2(u, v, w)h = -L\pi_\infty S_4(h),$$

$$D_3 T_2(u, v, w)h = -L\pi_\infty S_4(\bar{a}^N * h) - L\pi_\infty S_4(h * u),$$

$$D_1 T_3(u, v, w)h = L\pi_\infty S_4(\bar{b}^N * h) + L\pi_\infty S_4(h * v),$$

$$D_2 T_3(u, v, w)h = L\pi_\infty S_4(\bar{a}^N * h) + L\pi_\infty S_4(u * h),$$

$$D_3 T_3(u, v, w)h = -\beta L\pi_\infty S_4(h).$$

4.4 Validated Taylor integration of a phase box via the contraction mapping theorem

Applying the estimates of Lemmas 2.4 and 2.5 to the expressions for $T(u, v, w)$ and $DT(u, v, w)$ yields the following proposition.

Proposition 4.2. *Suppose that $\bar{a}^N, \bar{b}^N, \bar{c}^N \in X_{\nu,m}^N$ are fixed, and that $T: (X_{\nu,4}^\infty)^3 \rightarrow (X_{\nu,4}^\infty)^3$ is as defined in Equation (31). Define the positive constants Y_{01}, Y_{02}, Y_{03} by*

$$\begin{aligned} Y_{01} &= |\sigma| |\tau| \nu^{N+1} \sum_{k+l+m+n=N} \frac{1}{n+1} (|\bar{b}_{klmn}^N| + |\bar{a}_{klmn}^N|) \\ Y_{02} &= |\rho| |\tau| \nu^{N+1} \sum_{k+l+m+n=N} \frac{1}{n+1} |\bar{a}_{klmn}^N| \\ &\quad + |\tau| \nu^{N+1} \sum_{k+l+m+n=N} \frac{1}{n+1} |\bar{b}_{klmn}^N| \\ &\quad + |\tau| \nu^{N+1} \sum_{k+l+m+n=N} \frac{1}{n+1} |(\bar{a}^N * \bar{c}^N)_{klmn}| \\ &\quad + |\tau| \nu \sum_{k+l+m+n=N+1}^{2N} \frac{1}{n+1} |(\bar{a}^N * \bar{c}^N)_{klmn}| \nu^{k+l+m+n}, \end{aligned}$$

$$\begin{aligned}
Y_{03} &= |\beta| |\tau| \nu^{N+1} \sum_{k+l+m+n=N} \frac{1}{n+1} |\bar{c}_{klmn}^N| \\
&+ |\tau| \nu^{N+1} \sum_{k+l+m+n=N} \frac{1}{n+1} |(\bar{a}^N * \bar{b}^N)_{klmn}| \\
&+ |\tau| \nu \sum_{k+l+m+n=N+1}^{2N} \frac{1}{n+1} |(\bar{a}^N * \bar{b}^N)_{klmn}| \nu^{k+l+m+n}
\end{aligned}$$

and let

$$Y_0 := \max(Y_{01}, Y_{02}, Y_{03}).$$

Similarly, define the positive constants $Z_{11}, Z_{12}, Z_{13}, Z_{21}, Z_{22}, Z_{23}, Z_{31}, Z_{32},$ and Z_{33} by

$$Z_{11} = Z_{12} = |\sigma| |\tau| \nu, \quad Z_{13} = 0,$$

$$Z_{21} = |\tau| (|\rho| + 1 + \|\bar{c}^N\|_{\nu, m}^1) \nu, \quad Z_{22} = |\tau| \nu, \quad \text{and} \quad Z_{23} = |\tau| \|\bar{a}^N\|_{\nu, m}^1 \nu,$$

$$Z_{31} = |\tau| \|\bar{b}^N\|_{\nu, m}^1 \nu, \quad Z_{32} = |\tau| \|\bar{a}^N\|_{\nu, m}^1 \nu, \quad \text{and} \quad Z_{33} = |\beta| |\tau| \nu$$

and let

$$Z_1 = \max_{1 \leq i \leq 3} \sum_{j=1}^3 Z_{ij},$$

and

$$Z_2 = 2|\tau|.$$

Then

$$\|T(0, 0, 0)\|_{(X_{\nu, m}^\infty)^3} \leq Y_0,$$

and

$$\|DT(u, v, w)\|_{B((X_{\nu, m}^\infty)^3)} \leq Z_1 + Z_2 r,$$

for all $u, v, w \in X_{\nu, m}^\infty$ with $\|u\|_{\nu, m}^1, \|v\|_{\nu, m}^1, \|w\|_{\nu, m}^1 \leq r$.

Proof. Define the linear operator $A: \ell_{\nu, m}^1 \rightarrow \ell_{\nu, m}^1$ by

$$A(a)_{kmln} = \frac{\tau}{n+1} a_{klmn}, \quad a \in \ell_{\nu, m}^1.$$

One easily checks that

$$L\pi_\infty S_j(a) = \pi_\infty S_j A(a),$$

for all $a \in \ell_{\nu, m}^1$. Then

$$\begin{aligned}
\|T_1(0, 0, 0)\|_{X_{\nu, m}^\infty} &= \|\sigma L(\pi_\infty S_4(\bar{b}^N) - \pi_\infty S_4(\bar{a}^N))\|_{\nu, m}^1 \\
&= \|\sigma(\pi_\infty S_4 A(\bar{b}^N) - \pi_\infty S_4 A(\bar{a}^N))\|_{\nu, m}^1 \\
&\leq |\sigma| |\tau| \nu^{N+1} \sum_{k+l+m+n=N} \frac{1}{n+1} (|\bar{b}_{klmn}^N| + |\bar{a}_{klmn}^N|) \\
&= Y_{01},
\end{aligned}$$

and similarly that

$$\begin{aligned}
\|T_2(0, 0, 0)\|_{X_{\nu, m}^\infty} &= \|L(\rho\pi_\infty S_4(\bar{a}^N) - \pi_\infty S_4(\bar{b}^N) - \pi_\infty S_4(\bar{a}^N * \bar{c}^N))\|_{\nu, m}^1 \\
&= \|(\rho\pi_\infty S_4 A(\bar{a}^N) - \pi_\infty S_4 A(\bar{b}^N) - \pi_\infty S_4 A(\bar{a}^N * \bar{c}^N))\|_{\nu, m}^1 \\
&\leq |\rho||\tau|\nu^{N+1} \sum_{k+l+m+n=N} \frac{1}{n+1} |\bar{a}_{klmn}^N| \\
&\quad + |\tau|\nu^{N+1} \sum_{k+l+m+n=N} \frac{1}{n+1} |\bar{b}_{klmn}^N| \\
&\quad + |\tau|\nu^{N+1} \sum_{k+l+m+n=N} \frac{1}{n+1} |(\bar{a}^N * \bar{c}^N)_{klmn}| \\
&\quad + |\tau|\nu \sum_{|\alpha|=N+1}^{2N} \frac{1}{n+1} |(\bar{a}^N * \bar{c}^N)_\alpha| \nu^{|\alpha|} \\
&= Y_{02},
\end{aligned}$$

and that

$$\begin{aligned}
\|T_3(0, 0, 0)\|_{X_{\nu, m}^\infty} &= \|L(-\beta\pi_\infty S_4(\bar{c}^N) + \pi_\infty S_4(\bar{a}^N * \bar{b}^N))\|_{\nu, m}^1 \\
&= \|(-\beta\pi_\infty S_4 A(\bar{c}^N) + \pi_\infty S_4 A(\bar{a}^N * \bar{b}^N))\|_{\nu, m}^1 \\
&\leq |\beta||\tau|\nu^{N+1} \sum_{k+l+m+n=N} \frac{1}{n+1} |\bar{c}_{klmn}^N| \\
&\quad + |\tau|\nu^{N+1} \sum_{k+l+m+n=N} \frac{1}{n+1} |(\bar{a}^N * \bar{b}^N)_{klmn}| \\
&\quad + |\tau|\nu \sum_{k+l+m+n=N+1}^{2N} \frac{1}{n+1} |(\bar{a}^N * \bar{b}^N)_{klmn}| \nu^{k+l+m+n} \\
&= Y_{03}.
\end{aligned}$$

It follows that

$$\begin{aligned}
\|T(0, 0, 0)\|_{(X_{\nu, m}^\infty)^3} &= \max\left(\|T_1(0, 0, 0)\|_{X_{\nu, m}^\infty}, \|T_2(0, 0, 0)\|_{X_{\nu, m}^\infty}, \|T_3(0, 0, 0)\|_{X_{\nu, m}^\infty}\right) \\
&\leq \max(Y_{01}, Y_{02}, Y_{03}) \\
&= Y_0.
\end{aligned}$$

The estimates for the derivative are very similar. Note that the derivative can be decomposed as

$$DT(u, v, w) = \mathcal{L} + \mathcal{M}(u, v, w),$$

where for $H = (h_1, h_2, h_3) \in (X_{\nu, m}^1)^3$ the actions of \mathcal{L} and \mathcal{M} are given by

$$\mathcal{L}(h_1, h_2, h_3) = \begin{pmatrix} -\sigma L\pi_\infty S_4(h_1) + \sigma L\pi_\infty S_4(h_2) \\ \rho L\pi_\infty S_4(h_1) - L\pi_\infty S_4(\bar{c}^N * h_1) - L\pi_\infty S_4(h_2) - L\pi_\infty S_4(\bar{a}^N * h_3) \\ L\pi_\infty S_4(\bar{b}^N * h_1) + L\pi_\infty S_4(\bar{a}^N * h_2) - \beta L\pi_\infty S_4(h_3) \end{pmatrix}$$

and

$$\mathcal{M}(u, v, w)(h_1, h_2, h_3) = \begin{pmatrix} 0 \\ -L\pi_\infty S_4(h_1 * w) - L\pi_\infty S_4(h_3 * u) \\ L\pi_\infty S_4(h_1 * v) + L\pi_\infty S_4(h_2 * u) \end{pmatrix}$$

Then

$$\begin{aligned}
& \|\mathcal{L}\|_{B((X_{\nu,m}^1)^3)} = \sup_{\|H\|=1} \|\mathcal{L}H\|_{(X_{\nu,m}^1)^3} \\
& \leq \sup_{\|H\|=1} \left\| \begin{pmatrix} -\sigma L\pi_\infty S_4(h_1) + \sigma L\pi_\infty S_4(h_2) \\ \rho L\pi_\infty S_4(h_1) - L\pi_\infty S_4(\bar{c}^N * h_1) - L\pi_\infty S_4(h_2) - L\pi_\infty S_4(\bar{a}^N * h_3) \\ L\pi_\infty S_4(\bar{b}^N * h_1) + L\pi_\infty S_4(\bar{a}^N * h_2) - \beta L\pi_\infty S_4(h_3) \end{pmatrix} \right\|_{(X_{\nu,m}^1)^3} \\
& \leq \max_{1 \leq i \leq 3} \sum_{j=1}^3 Z_{ij} \\
& = Z_1,
\end{aligned}$$

and, if $\|u\|_{\nu,m}^1, \|v\|_{\nu,m}^1, \|w\|_{\nu,m}^1 \leq r$, then

$$\begin{aligned}
\|\mathcal{M}(u, v, w)\|_{B((X_{\nu,m}^1)^3)} &= \sup_{\|H\|=1} \|\mathcal{M}(u, v, w)H\|_{(X_{\nu,m}^1)^3} \\
&\leq \sup_{\|H\|=1} \left\| \begin{pmatrix} 0 \\ -L\pi_\infty S_4(h_1 * w) - L\pi_\infty S_4(h_3 * u) \\ L\pi_\infty S_4(h_1 * v) + L\pi_\infty S_4(h_2 * u) \end{pmatrix} \right\|_{(X_{\nu,m}^1)^3} \\
&\leq 2|\tau|r \\
&= Z_2 r
\end{aligned}$$

□

Example: Consider the initial conditions $x_0 = -15$, $y_0 = -15$, and $z_0 = 40$ near the attractor but otherwise arbitrary. We compute to order $N = 7$ and take a time step of size $\tau = 0.002$. Recall that the step size is controlled by rescaling the vector field by τ . We take $c = 1/4$, i.e. we reparameterize to a spatial cube of size a half. With these choices the largest coefficient of order $N = 7$ is approximately 10^{-8} .

We check that we have the bounds $Y_0 = 1.4 \times 10^{-9}$, $Z_1 = 0.44$, and $Z_2 = 0.01$. Then we obtain a validated contraction on a ball of radius $r = 2.4 \times 10^{-9}$, i.e. the order to the last coefficient computed numerically. Then, for example, the C^0 error between the exact solution and our approximation is less than or equal to r for all $x, y, z, t \leq 1$ (these are the rescaled variables).

5 The global problem: connecting one local picture to another

5.1 The method of projected boundaries (slight return)

We now set up the operator used to establish the existence of a heteroclinic connection. Lets focus on only the set up actually used in the next section, and avoid the temptation to generalize.

Let

$$D := \{z \in \mathbb{C} \mid |z| < 1\},$$

denote the unit disk at the origin in the complex plane and $D^2 = D \times D$ denote the unit poly-disk. Let

$$B^2 := \left\{ (x, y) \in \mathbb{R}^2 \mid \sqrt{x^2 + y^2} < 1 \right\},$$

be the unit disk at the origin in the Euclidean plane.

Definition 5.1 (Focus to fast-slow saddle assumptions). Let $f: \mathbb{R}^3 \rightarrow \mathbb{R}^3$ be a real analytic vector field and assume that

- (i) $p_0 \in \mathbb{R}^3$ is an equilibrium solution with a complex conjugate pair of unstable eigenvalues $\lambda_1^u, \lambda_2^u \in \mathbb{C}$. Let $\xi_1^u, \xi_2^u \in \mathbb{C}^3$ denote a complex conjugate pair of eigenvectors.
- (ii) $p_1 \in \mathbb{R}^3$ is an equilibrium solution with two distinct, real, stable eigenvectors λ_1^s, λ_2^s having

$$\text{real}(\lambda_2^s) < \text{real}(\lambda_1^s) < 0.$$

Let $\xi_1^s, \xi_2^s \in \mathbb{R}^3$ be associated eigenvectors.

- (iii) $P: D^2 \rightarrow \mathbb{C}^3$ is a solution of Equation (13) subject to the first order constraints

$$P(0, 0) = p_0, \quad \text{and} \quad \partial_1 P(0, 0) = \xi_1^u, \quad \partial_2 P(0, 0) = \xi_2^u.$$

Assume moreover that the (complex conjugate) Taylor coefficients $p \in (\ell_{1,2}^1)^3$ have $\|p\|_{(\ell_{1,2}^1)^3} \leq C_1$. Define the map $\hat{P}: B^2 \rightarrow \mathbb{R}^3$ by

$$\hat{P}(u, v) = P(u + iv, u - iv).$$

- (iv) $Q: [-1, 1]^2 \rightarrow \mathbb{R}^3$ is a solution of Equation (13) subject to the first order constraints

$$Q(0, 0) = p_1, \quad \text{and} \quad \partial_1 Q(0, 0) = \xi_1^s, \quad \partial_2 Q(0, 0) = \xi_2^s.$$

Assume moreover that the (real) Taylor coefficients $q \in (\ell_{1,2}^1)^3$ have $\|q\|_{(\ell_{1,2}^1)^3} \leq C_2$.

Proposition 5.2 (Connecting orbit operator). *Assume the existence of data as in Definition 5.1. For $0 < r_u, r_s < 1$ define the $F: \mathbb{R} \times (0, \infty) \times [-1, 1] \rightarrow \mathbb{R}^3$, by*

$$F(\theta, h, T) = \phi(\hat{P}(r_u \cos(\theta), r_u \sin(\theta)), T) - Q(h, r_s). \quad (32)$$

If there is a $(\hat{\theta}, \hat{h}, \hat{T}) \in \mathbb{R}^3$ so that

$$F(\hat{\theta}, \hat{h}, \hat{T}) = 0,$$

then $\gamma: \mathbb{R} \rightarrow \mathbb{R}^3$ defined by

$$\gamma(t) = \phi\left(\hat{P}(r_u \cos(\hat{\theta}), r_u \sin(\hat{\theta})), t\right),$$

is a heteroclinic connecting orbit from p_0 to p_1 . We refer to F as the connecting orbit operator.

Proof. Note that for each $t \in \mathbb{R}$, $\gamma(t)$ is a solution to the differential equation due to the fact that ϕ is the flow map.

Consider $t \geq 0$ and let $z_0 := r_u \cos(\hat{\theta}) + ir_u \sin(\hat{\theta})$. By Proposition 3.1, P conjugates the nonlinear to the linear flow so that

$$\begin{aligned}\gamma(-t) &= \phi\left(\hat{P}(r_u \cos(\hat{\theta}), r_u \sin(\hat{\theta})), -t\right) \\ &= \phi\left(P(z_0, \bar{z}_0), -t\right) \\ &= P\left(z_0 e^{-\lambda_u^1 t}, \bar{z}_0 e^{-\bar{\lambda}_u^1 t}\right).\end{aligned}$$

Then

$$\begin{aligned}\lim_{t \rightarrow -\infty} \gamma(t) &= \lim_{t \rightarrow \infty} P\left(z_0 e^{-\lambda_u^1 t}, \bar{z}_0 e^{-\bar{\lambda}_u^1 t}\right) \\ &= P(0, 0) \\ &= p_0,\end{aligned}$$

as P is continuous (in fact analytic).

Similarly, suppose that $t > \hat{T}$. Then we can write $t = \hat{T} + s$ with $s > 0$, and by combining the conjugacy of Proposition 3.1 with the definition of the connecting orbit operator and the fact that $(\hat{\theta}, \hat{h}, \hat{T})$ is a zero, have that

$$\begin{aligned}\gamma(t) &= \phi\left(\hat{P}(r_u \cos(\hat{\theta}), r_u \sin(\hat{\theta})), \hat{T} + s\right) \\ &= \phi\left(\phi\left(\hat{P}(r_u \cos(\hat{\theta}), r_u \sin(\hat{\theta})), \hat{T}\right), s\right) \\ &= \phi(Q(\hat{h}, r_s), s) \\ &= Q(e^{\lambda_s^1 s} \hat{h}, e^{\lambda_s^2 s} r_s).\end{aligned}$$

Then

$$\begin{aligned}\lim_{t \rightarrow \infty} \gamma(t) &= \lim_{s \rightarrow \infty} Q(e^{\lambda_s^1 s} \hat{h}, e^{\lambda_s^2 s} r_s) \\ &= Q(0, 0) \\ &= p_1,\end{aligned}$$

again by the continuity of Q . □

Remark 5.3. This argument actually only requires that ϕ is defined in a neighborhood of the orbit segment $\gamma([0, \hat{T}])$.

In applications it is desirable to subdivide the time interval \hat{T} , and consider the following “multiple-shooting” scheme.

Proposition 5.4 (Multiple-shooting connecting orbit operator). *Assume the existence of data as in Definition 5.1. For $0 < r_u, r_s < 1$ define the map $F^K: \mathbb{R} \times \mathbb{R}^{3(K+1)} \times (0, \infty) \times (-1, 1) \rightarrow \mathbb{R}^{3(K+2)}$ by*

$$F^K(\theta, x_0, x_1, x_2, \dots, x_{K-1}, x_K, h, \tau) := \begin{pmatrix} \hat{P}(r_u \cos(\theta), r_u \sin(\theta)) - x_0 \\ \phi(x_0, \tau) - x_1 \\ \phi(x_1, \tau) - x_2 \\ \vdots \\ \phi(x_{K-1}, \tau) - x_K \\ \phi(x_K, \tau) - Q(h, r_s) \end{pmatrix}. \quad (33)$$

If $\hat{x} = (\hat{\theta}, \hat{x}_0, \dots, \hat{x}_K, \hat{h}, \hat{\tau}) \in \mathbb{R}^{3(K+2)}$ has that

$$F^K(\hat{x}) = 0,$$

then $(\hat{\theta}, \hat{h}, (K+1)\hat{\tau})$ is a zero of the connecting orbit operator defined in Proposition 5.2.

We refer to F^K as the multiple shooting connecting orbit operator.

The proof is an elementary application of the properties of a flow. In particular if \hat{x} is a zero of F^K then

$$\phi(\hat{x}_0, \hat{\tau}) = \hat{x}_1,$$

and

$$\phi(\hat{x}_1, \hat{\tau}) = \hat{x}_2,$$

which imply

$$\phi(\hat{x}_0, 2\hat{\tau}) = \hat{x}_2.$$

Repeated application of this idea gives that

$$\phi(\hat{x}_0, (K+1)\tau) = Q(\hat{h}, r_s).$$

Noting that

$$\hat{x}_0 = \hat{P}(r_u \cos(\hat{\theta}), r_u \sin(\hat{\theta})),$$

yields the result desired zero of the connecting orbit operator F of Proposition 5.2.

Remark 5.5 (Derivatives and transversality). Observe that F^K is differentiable and that the $3(K+2) \times 3(K+2)$ Jacobian matrix of F^K is given by

$$DF^K(\theta, x_0, x_1, x_2, \dots, x_{K-1}, x_K, h, \tau) = \begin{pmatrix} d_P(\theta) & -\text{Id}_3 & 0 & 0 & 0 & \dots & 0 & 0 & 0 & 0 \\ 0 & D_1\phi(x_0, \tau) & -\text{Id}_3 & 0 & 0 & \dots & 0 & 0 & 0 & f(\phi(x_0, \tau)) \\ 0 & 0 & D_1\phi(x_1, \tau) & -\text{Id}_3 & 0 & \dots & 0 & 0 & 0 & f(\phi(x_1, \tau)) \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & 0 & \dots & D_1\phi(x_{K-1}, \tau) & -\text{Id}_3 & 0 & f(\phi(x_{K-1}, \tau)) \\ 0 & 0 & 0 & 0 & 0 & \dots & 0 & D_1\phi(x_K, \tau) & d_Q(h) & f(\phi(x_K, \tau)) \end{pmatrix}$$

Here

$$d_P(\theta) := r_u \partial_1 P(z, \bar{z})w + r_u \partial_2 P(z, \bar{z})\bar{w},$$

where $z = \cos(\theta) + i \sin(\theta)$ and $w = -\sin(\theta) + i \cos(\theta)$, and

$$d_Q(h) := \partial_1 Q(h, r_s).$$

The explicit form of the derivative is critical for numerical calculations, but it is also useful in theoretical arguments. For example, an argument similar to that given in Section 6 of [62] shows that the connecting orbit $\gamma(t)$ of Proposition 5.2 is transverse if and only if the matrix $DF^K(\hat{x})$ is invertible. As we will see below, the invertibility of $DF^K(\hat{x})$ is obtained as a consequence of our computer assisted a-posteriori analysis of the multiple shooting connecting orbit operator.

Remark 5.6 (Approximate connecting orbit). It is in general quite difficult to locate approximate connecting orbits, and indeed this is often the most challenging part of a computer assisted proof. For some problems it is possible to find an approximate orbit as the limit of a family of periodic orbits. Other times perturbative methods are used.

For the example at hand we perform some numerical experiments. The idea is to sample points on the boundary of the unstable manifold, and to integrate these until they pass near

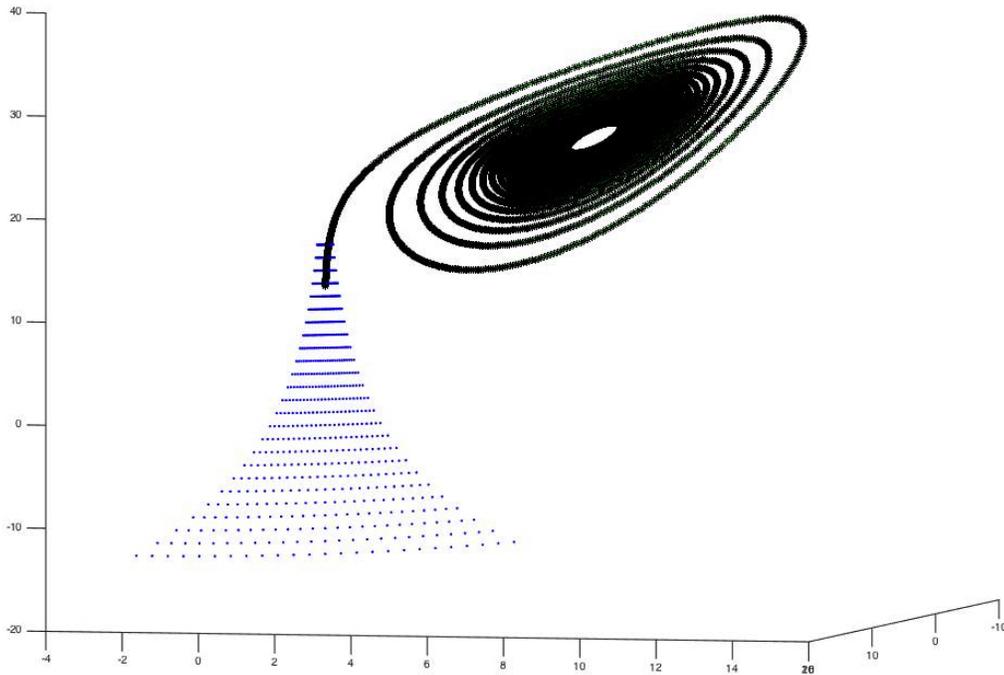


Figure 9: A transverse heteroclinic connecting orbit from p_0 to p_1 . The existence of the orbit is validated using Theorem 2.7, in conjunction with the validated local stable/unstable manifolds and the validated Taylor integrator of Sections 3.5 and 4.4.

the stable manifold. The orbits are examined by eye until we find a reasonable candidate. Bisection is used to refine the guess. Since the boundary of the unstable manifold is one dimensional this scheme is relatively efficient, and a few minutes of experimentation provided a viable initial guess for the multiple shooting connecting orbit operator. This initial guess is refined via Newton's method until we have defect on the order of machine precision.

Remark 5.7 (Generalized connecting orbit operators). While we have written the connecting orbit operators in a very specific form, namely the one used to study connections from eye to origin in the Lorenz system. However, the functional analytic setup introduced here generalizes to vector fields in any dimension and to hyperbolic equilibria with any stability type. The details are found for example in [62], and are generalized for connections between periodic orbits in [101].

5.2 Computer assisted proof of a transverse connecting orbit via a finite dimensional Newton like argument

Once we have an approximate connecting orbit via numerical experimentation as described above, it is a simple matter of applying Proposition 2.7 to get the computer assisted proof of existence *as long as we have the requisite bounds* $\phi(x, t)$, $P(u)$ and $Q(s)$. But the methods of Sections 3.5 and 4.4 provide these bounds.

For example, using the validated parameterizations discussed in Sections 3.5 and 4.4 i.e.

orders $N = 150$ for the unstable and $N = 50$ for the stable manifold, and expanding ϕ to order $N = 8$ at each of the points $\bar{x}_0, \dots, \bar{x}_K$, with $K = 8,875$, and taking $\bar{\tau} = 0.002$, we check the conditions of Proposition 2.7 for the multiple shooting connecting orbit operator and obtain a true heteroclinic connection within a ball of radius $r = 10^{-4}$ about $\bar{x} \in \mathbb{R}^{3(K+1)}$. Since the proof succeeds we have that $DF^K(\hat{x})$ is invertible, and hence the connection is transverse.

Remark 5.8 (Second derivatives). Theorem 2.7 (which is necessary to obtain invertibility of the derivative and hence transversality) requires bounds on second derivatives near the approximate solution \bar{x} . But the connecting orbit operator involves derivatives of $\phi(x, \tau)$ with respect to x , as well as derivatives of \hat{P} and Q . This explains the role of $r_u, r_s < 1$ in the definition of the connecting orbit operators: we need to make sure that we have some domain to “trade in” for bounds on derivatives. The necessary trade is negotiated via the Cauchy bounds of Lemma 2.1.

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