

AMS Short Course on Rigorous Numerics in Dynamics: The Parameterization Method for Stable/Unstable Manifolds of Vector Fields

J.D. Mireles James, *

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Abstract

This lecture builds on the validated numerical methods for periodic orbits presented in the lecture of J. B. van den Berg. We discuss a functional analytic perspective on validated stability analysis for equilibria and periodic orbits as well as validated computation of their local stable/unstable manifolds. Building on this analysis we study heteroclinic and homoclinic connecting orbits between equilibria and periodic orbits of differential equations. We formulate the connecting orbits as solutions of certain projected boundary value problems which are amenable to an a posteriori analysis very similar to that already discussed for periodic orbits. The discussion will be driven by several application problems including connecting orbits in the Lorenz system and existence of standing and traveling waves.

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

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1 Introduction

The qualitative theory of dynamical systems deals with the global orbit structure of nonlinear models. Owing to Poincare, this goal is reframed in terms of invariant sets. Questions concerning the existence, location, intrinsic geometric and topological properties, and internal dynamics of invariant sets are at the core of dynamical systems theory. In fact, as has already been discussed in this lecture series, Conley's fundamental theorem makes precise the claim that invariant sets *and the connections between them* completely classify the dynamics.

Another theme of this course is that problems in nonlinear analysis are often recast as solutions of functional equations, that these functional equations can be approximately solved by numerical methods, and that approximate solutions lead to mathematically rigorous results via a-posteriori analysis. The present lecture explores this theme in the context of connecting orbits for differential equations. We begin with a brief discussion discrete time dynamical systems, which motivates the more detailed material in the remainder of the notes.

Studying linear and nonlinear stability of invariant sets, i.e. their local stable/unstable manifolds, is the first step in understanding connecting orbits. Our approach to stable/unstable manifolds is based on the Parameterization Method, a functional analytic framework for simultaneous study of both the embedding and the internal dynamics of the invariant manifolds. The core of the parameterization method is the derivation of certain invariance, or infinitesimal conjugacy equations, which are solved numerically to obtain chart or covering maps for the desired invariant manifold. Then, since the Parameterization Method is based on the study of operator equations it is also amiable to the kind of a-posteriori analysis discussed in the notes for the introductory lecture by J.B. van den Berg [1].

Once local invariant manifolds are understood the next step is to connect them. For discrete time dynamical systems this step is quite natural, as the evolution of the system is governed by a known map. Continuous time dynamical systems require a little more work as the evolution of the system is only implicitly defined the differential equation. We briefly review the boundary value formulation for connecting orbits between equilibrium and periodic orbits of differential equations. These boundary value problems are analyzed using computer assisted techniques of proof as discussed in [1], though we only skim the details here and refer the interested reader to the literature on validated numerics for initial value problems. The main focus of these notes is on computation and validation for the stable/unstable manifolds themselves.

Remark 1.1 (Brief remarks on the literature). The reader interested in numerical methods for dynamical systems will find the notes of Carles Simo [14] illuminating. We mention also that the seminal work of Lanford, Eckman, Koch, and Wittwer on the Feigenbaum conjectures (work which arguably launched the field of computer assisted analysis in dynamical systems theory) is based on the study of a certain conjugacy equation (in this case the Cvitanović renormalization operator) via computer assisted means [15, 16]. The reader interested in rigorous numerics for the computer assisted study of connecting orbits (and the related study of topological horse shoes) will be interested in the work of [17] for planar diffeomorphisms, and should of course see the work of [18, 19, 20, 21]. We also mention that the seminal work of Warwick Tucker on the computer assisted solution of Smale’s 14-th problem (existence of the Lorenz attractor) makes critical use of a normal form for the dynamics at the origin of the system. This norm form was computed numerically, and validated numerical bounds obtained by studying a conjugacy equation as referred to above [22, 23].

The original references for the parameterization method, namely [24, 25, 26] for invariant manifolds associated with fixed points, and [27, 28, 29] for invariant manifolds associated with invariant circles, have since launched a small industry. We mention briefly the appearance of KAM theories without action angle variables for area preserving and conformally symplectic systems [30, 31], manifolds associated with invariant tori in Hamiltonian systems [32], phase resetting curves and isochrons [33], quasi-periodic solutions of PDEs [34], and manifolds of mixed-stability [35]. Moreover even more applications are discussed in the references of these papers. We also mention the recent book by Alex Haro, Marta Candell, Jordi-Luis Figueras, and J.M. Mondelo [36].

The references discussed in the preceding paragraphs are by no means a thorough bibliography of the field of computer assisted proof in dynamical systems, and fail to even scratch the surface of the literature on numerical methods for dynamical systems theory. Indeed, the field has exploded in the last decades and any short list of references cannot hope to hit even the high points. We have referred only to the works most closely related to the present discussion. The interested reader will find more complete coverage of the literature in the works cited throughout this lecture.

2 The Parameterization Method

The Parameterization Method is a functional analytic framework for studying invariant manifolds. The method has its roots in the work of Poincaré, and congealed into a mature mathematical theory in a series of papers by de la Llave, Fontich, Cabre, and Haro [24, 25, 26, 27, 28, 29]. An excellent historical overview is found in (CITATION).

The basic idea underpinning the Parameterization Method is simple and is, loosely speaking, based on two observations. First, the dynamical systems notion of equivalence is *conjugacy*. Conjugacy is a notion expressing the fact that one dynamical system embeds in another. For example in differential equations a conjugacy is a mapping which maps orbits in a toy or model system to orbits in the full system of interest. This embedding is now thought of as an unknown, in which case we think of conjugacy as an equation describing the unknown. The second observation is this: once a conjugacy is framed as an equation, it is now amenable to analysis using all the tools of both classical nonlinear and numerical analysis.

We will illustrate the flexibility and utility if these ideas in a number of examples, focusing on computational issues. But first we recall a few ideas concerning formal power series.

2.1 Formal series solutions for stable/unstable manifolds

In this section we illustrate computational aspects and applications of the parameterization method. More precisely we give a number of examples of solving conjugacy equations. The examples are based on power series representations of the unknown functions/invariant objects, so that it is worth reviewing the basic calculus of multivariate power series.

2.1.1 Manipulating power series: automatic differentiation and all that

Consider two power series $P, Q: \mathbb{C}^m \rightarrow \mathbb{C}$

$$P(\sigma) = \sum_{|\alpha|=0}^{\infty} p_{\alpha} \sigma^{\alpha}, \quad \text{and} \quad Q(\sigma) = \sum_{|\alpha|=0}^{\infty} q_{\alpha} \sigma^{\alpha}.$$

Here $\alpha = (\alpha_1, \dots, \alpha_m) \in \mathbb{N}^m$ is an m -dimensional multi-index, $|\alpha| = \alpha_1 + \dots + \alpha_m$ is the order of the multi-index, $p_{\alpha}, q_{\alpha} \in \mathbb{C}$ for all $\alpha \in \mathbb{N}^m$, $\sigma = (\sigma_1, \dots, \sigma_m) \in \mathbb{C}^m$, and $\sigma^{\alpha} := \sigma_1^{\alpha_1} \dots \sigma_m^{\alpha_m}$.

In this chapter we are not concerned with issues of convergence, i.e. we treat P and Q as *formal power series*. We denote by $\mathcal{V}$ the space of all formal power series and note that $\mathcal{V}$ is a vector space. Indeed let $P, Q \in \mathcal{V}$ and $c \in \mathbb{C}$. The sum and scalar product on $\mathcal{V}$ are defined term-by-term as

$$(P + Q)(\sigma) = \sum_{|\alpha|=0}^{\infty} (p_{\alpha} + q_{\alpha}) \sigma^{\alpha},$$

and

$$(cP)(\sigma) = \sum_{|\alpha|=0}^{\infty} cp_{\alpha} \sigma^{\alpha}.$$

The product of two power series is defined via the *Cauchy product*, i.e.

$$(P \cdot Q)(\sigma) = \sum_{|\alpha|=0}^{\infty} (p * q)_{\alpha} \sigma^{\alpha},$$

where

$$(p * q)_\alpha = \sum_{\beta_1=0}^{\alpha_1} \cdots \sum_{\beta_m=0}^{\alpha_m} p_{\alpha_1-\beta_1, \dots, \alpha_m-\beta_m} q_{\beta_1, \dots, \beta_m}.$$

We define formal derivatives on $\mathcal{V}$ via term by term differentiation. For example

$$\frac{\partial}{\partial \sigma_j} P(\sigma) := \sum_{\alpha_1=0}^{\infty} \cdots \sum_{\alpha_j=0}^{\infty} \cdots \sum_{\alpha_m=0}^{\infty} (\alpha_j + 1) p_{\alpha_1, \dots, \alpha_j+1, \dots, \alpha_m} \sigma^\alpha.$$

Two power series $P, Q \in \mathcal{V}$ are equal if and only if their coefficients are equal at all orders. This fact can be used to define other operations on formal series. For example, Q is the *multiplicative inverse* of P if $Q(\sigma)P(\sigma) = 1$, where 1 denotes the series with first order coefficient one and all other coefficients zero. Then in order to work out the coefficients of Q in terms of the coefficients of P , we assume for example that $p_{00} \neq 0$, and write

$$\begin{aligned} (Q \cdot P)(\sigma) &= \left(\sum_{|\alpha|=0}^{\infty} q_\alpha \sigma^\alpha \right) \left(\sum_{|\alpha|=0}^{\infty} p_\alpha \sigma^\alpha \right) \\ &= \sum_{|\alpha|=0}^{\infty} \left(\sum_{\beta_1=0}^{\alpha_1} \cdots \sum_{\beta_m=0}^{\alpha_m} q_{\alpha_1-\beta_1, \dots, \alpha_m-\beta_m} p_{\beta_1, \dots, \beta_m} \right) \sigma^\alpha \\ &= p_{00} q_\alpha + \sum_{|\alpha|=1}^{\infty} \left(\sum_{\beta_1=0}^{\alpha_1} \cdots \sum_{\beta_m=0}^{\alpha_m} q_{\alpha_1-\beta_1, \dots, \alpha_m-\beta_m} p_{\beta_1, \dots, \beta_m} \right) \sigma^\alpha \\ &= 1. \end{aligned}$$

Since the coefficients on both sides of the equation must be equal, we “match like powers” of σ and have

$$p_{0, \dots, 0} q_{0, \dots, 0} = 1,$$

and

$$p_{0, \dots, 0} q_\alpha = - \sum_{\beta_1=0}^{\alpha_1} \cdots \sum_{\beta_m=0}^{\alpha_m} q_{\alpha_1-\beta_1, \dots, \alpha_m-\beta_m} p_{\beta_1, \dots, \beta_m}.$$

Isolating q_α gives

$$q_\alpha = \begin{cases} \frac{1}{p_{0, \dots, 0}} & \text{if } \alpha = (0, \dots, 0) \\ \frac{-1}{p_{0, \dots, 0}} (p * q)_\alpha & \text{otherwise} \end{cases}.$$

Other operations on power series, like composition with the elementary functions of mathematical physics, are computed using *automatic differentiation*.

Examples of automatic differentiation in one dimension: Consider a power series of one variable

$$P(\sigma) = \sum_{n=0}^{\infty} p_n \sigma^n,$$

and assume (for example) that we want to exponentiate P as a power series. More precisely we want to find a power series

$$Q(\sigma) = \sum_{n=0}^{\infty} q_n \sigma^n,$$

so that

$$Q(\sigma) = e^{P(\sigma)}.$$

In other words we want to work out the coefficients q_n in terms of the known coefficients p_n .

The idea is to exploit:

- That differentiation terms composition of scalar functions into multiplication of scalar functions via the chain rule.
- That the exponential function itself solves a simple, linear, differential equation.

So, differentiating $Q(\sigma)$ with respect to σ gives

$$Q'(\sigma) = e^{P(\sigma)} P'(\sigma) = Q(\sigma) P'(\sigma),$$

or, on the level of power series

$$\sum_{n=0}^{\infty} (n+1)q_{n+1}\sigma^n = \left(\sum_{n=0}^{\infty} q_n\sigma^n \right) \left(\sum_{n=0}^{\infty} (n+1)p_{n+1}\sigma^n \right) = \sum_{n=0}^{\infty} \left(\sum_{k=0}^n (n-k+1)p_{n-k+1}q_k \right) \sigma^n.$$

Then, upon matching like powers of σ we have that

$$(n+1)q_{n+1} = \sum_{k=0}^n (n-k+1)p_{n-k+1}q_k.$$

Finally, by reindexing and isolating q_n we have that

$$q_n = \frac{1}{n} \sum_{k=0}^{n-1} (n-k)p_{n-k}q_k.$$

Many other examples can be worked out in this way. For example let

$$Q(\sigma) = P(\sigma)^\alpha,$$

with $\alpha \in \mathbb{C}$. Then by the chain rule

$$Q'(\sigma) = \alpha P(\sigma)^{\alpha-1} P'(\sigma),$$

or

$$P(\sigma)Q'(\sigma) = \alpha Q(\sigma)P'(\sigma).$$

Computing Cauchy products and matching like powers leads to

$$q_n = \frac{1}{np_0} \sum_{k=0}^{n-1} (n\alpha - k(\alpha+1))p_{n-k}q_k.$$

Many other examples can be computed similarly.

Remark 2.1 (Computational efficiency of automatic differentiation). The trick described above is often referred to as automatic differentiation for power series, though the ideas go back centuries. The miricale of automatic differentiation is that it reduces the cost of function composition to the cost of a Cauchy product, as long as one of the functions is itself the solution of a simple differential equation. Note that this includes all the usual functions of elementary calculus, as well as others like Bessel functions and elliptic integrals. The down side is that automatic differentiation requires us to keep track of both the variables p_n and q_n . In many applications however memory is not the primary computational constraint.

The radial gradient and automatic differentiation for multivariate series: In two or more dimensions we require a modification of the tricks above. The idea is to exploit the so called *radial gradient*. More precisely Suppose that

$$P(\sigma_1, \sigma_2) = \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} p_{mn} \sigma_1^m \sigma_2^n,$$

and that we want to compute

$$Q(\sigma_1, \sigma_2) = e^{P(\sigma_1, \sigma_2)} = \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} q_{mn} \sigma_1^m \sigma_2^n.$$

Then we consider the radial gradient given by the expression

$$\nabla Q(\sigma_1, \sigma_2) \begin{pmatrix} \sigma_1 \\ \sigma_2 \end{pmatrix} = \left(\sigma_1 \frac{\partial}{\partial \sigma_1} + \sigma_2 \frac{\partial}{\partial \sigma_2} \right) Q(\sigma_1, \sigma_2) = \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} (m+n) q_{mn} \sigma_1^m \sigma_2^n.$$

At the same time, after using the chain rule, we have that the radial gradient is also given by

$$\begin{aligned} \nabla Q(\sigma_1, \sigma_2) \begin{pmatrix} \sigma_1 \\ \sigma_2 \end{pmatrix} &= \nabla \left(e^{P(\sigma_1, \sigma_2)} \right) \begin{pmatrix} \sigma_1 \\ \sigma_2 \end{pmatrix} \\ &= e^{P(\sigma_1, \sigma_2)} \nabla P(\sigma_1, \sigma_2) \begin{pmatrix} \sigma_1 \\ \sigma_2 \end{pmatrix} \\ &= Q(\sigma_1, \sigma_2) \left(\sigma_1 \frac{\partial}{\partial \sigma_1} + \sigma_2 \frac{\partial}{\partial \sigma_2} \right) P(\sigma_1, \sigma_2) \\ &= \left(\sum_{m=0}^{\infty} \sum_{n=0}^{\infty} q_{mn} \sigma_1^m \sigma_2^n \right) \left(\sum_{m=0}^{\infty} \sum_{n=0}^{\infty} (m+n) p_{mn} \sigma_1^m \sigma_2^n \right) \\ &= \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} \left(\sum_{j=0}^m \sum_{k=0}^n (j+k) q_{m-j, n-k} p_{jk} \right) \sigma_1^m \sigma_2^n, \end{aligned}$$

Matching like powers gives

$$(m+n) q_{mn} = \sum_{j=0}^m \sum_{k=0}^n (j+k) q_{m-j, n-k} p_{jk},$$

or

$$q_{mn} = q_{00} p_{mn} + \frac{1}{(m+n)} \sum_{j=0}^m \sum_{k=0}^n \hat{\delta}_{jk}^{mn} (j+k) q_{m-j, n-k} p_{jk},$$

with

$$\hat{\delta}_{jk}^{mn} := \begin{cases} 0 & \text{if } j = m \text{ and } k = n \\ 0 & \text{if } j = 0 \text{ and } k = 0 \\ 1 & \text{otherwise} \end{cases}$$

So given the coefficients of P we can compute the coefficients of Q at the cost of a Cauchy product, just as in the one dimensional case.

To do $P(\sigma_1, \sigma_2)^\alpha$, consider

$$P(\sigma_1, \sigma_2) = \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} p_{mn} \sigma_1^m \sigma_2^n,$$

and that we want to compute

$$Q(\sigma_1, \sigma_2) = P(\sigma_1, \sigma_2)^\alpha = \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} q_{mn} \sigma_1^m \sigma_2^n.$$

Again, the radial gradient of Q is

$$\nabla Q(\sigma_1, \sigma_2) \begin{pmatrix} \sigma_1 \\ \sigma_2 \end{pmatrix} = \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} (m+n) q_{mn} \sigma_1^m \sigma_2^n.$$

and is also given by

$$\begin{aligned} \nabla Q(\sigma_1, \sigma_2) \begin{pmatrix} \sigma_1 \\ \sigma_2 \end{pmatrix} &= \nabla P(\sigma_1, \sigma_2)^\alpha \begin{pmatrix} \sigma_1 \\ \sigma_2 \end{pmatrix} \\ &= \alpha P(\sigma_1, \sigma_2)^{\alpha-1} \nabla P(\sigma_1, \sigma_2) \begin{pmatrix} \sigma_1 \\ \sigma_2 \end{pmatrix}. \end{aligned}$$

Now, multiply both sides by P get

$$P(\sigma_1, \sigma_2) \nabla Q(\sigma_1, \sigma_2) \begin{pmatrix} \sigma_1 \\ \sigma_2 \end{pmatrix} = \alpha Q(\sigma_1, \sigma_2) \nabla P(\sigma_1, \sigma_2) \begin{pmatrix} \sigma_1 \\ \sigma_2 \end{pmatrix}$$

or

$$\left(\sum_{m=0}^{\infty} \sum_{n=0}^{\infty} p_{mn} \sigma_1^m \sigma_2^n \right) \left(\sum_{m=0}^{\infty} \sum_{n=0}^{\infty} (m+n) q_{mn} \sigma_1^m \sigma_2^n \right) = \left(\sum_{m=0}^{\infty} \sum_{n=0}^{\infty} \alpha q_{mn} \sigma_1^m \sigma_2^n \right) \left(\sum_{m=0}^{\infty} \sum_{n=0}^{\infty} (m+n) p_{mn} \sigma_1^m \sigma_2^n \right)$$

and taking Cauchy products gives

$$\sum_{m=0}^{\infty} \sum_{n=0}^{\infty} \sum_{j=0}^m \sum_{k=0}^n (j+k) p_{m-j, n-k} q_{jk} \sigma_1^m \sigma_2^n = \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} \sum_{j=0}^m \sum_{k=0}^n \alpha (j+k) q_{m-j, n-k} p_{jk} \sigma_1^m \sigma_2^n.$$

Matching like powers we have

$$\sum_{j=0}^m \sum_{k=0}^n (j+k) p_{m-j, n-k} q_{jk} = \sum_{j=0}^m \sum_{k=0}^n \alpha (j+k) q_{m-j, n-k} p_{jk},$$

or

$$(m+n) p_{00} q_{mn} + \sum_{j=0}^m \sum_{k=0}^n \hat{\delta}_{jk}^{mn} (j+k) p_{m-j, n-k} q_{jk} = \alpha (m+n) q_{00} p_{mn} + \sum_{j=0}^m \sum_{k=0}^n \hat{\delta}_{jk}^{mn} \alpha (j+k) q_{m-j, n-k} p_{jk}.$$

Isolating q_{mn} gives

$$q_{mn} = \alpha p_{00}^{\alpha-1} p_{mn} + \frac{1}{(m+n) p_{00}} \sum_{j=0}^m \sum_{k=0}^n \hat{\delta}_{jk}^{mn} (j+k) (\alpha q_{m-j, n-k} p_{jk} - p_{m-j, n-k} q_{jk}).$$

2.1.2 A first example: linearization of an analytic vector field in one complex variable

Perhaps the simplest example which illustrate the idea of the parameterization method is to consider a single first order ODE in one complex variable. So, suppose that $U \subset \mathbb{C}$ is an open set and that $F: U \rightarrow \mathbb{C}$ is complex analytic. We study the differential equation

$$\frac{d}{dz}u(z) = F(u(z)). \quad (1)$$

Assume that that $z_0 \in U$ is an equilibrium solution, i.e. that

$$F(z_0) = 0, \quad \text{and} \quad \frac{d}{dz}F(z_0) = \lambda.$$

A basic dynamical question is: can we, at z_0 , analytically conjugate nonlinear differential equation to the linear differential equation $\sigma' = \lambda\sigma$? An equivalent question is to look for an analytic function P having that $P(0) = z_0$ and satisfying the invariance equation

$$\lambda\sigma P'(\sigma) = F(P(\sigma)), \quad (2)$$

for all σ in some neighborhood of z_0 ?

It turns out that the answer is yes, assuming that z_0 is hyperbolic, i.e. that

$$\text{real}(\lambda) \neq 0.$$

When λ purely imaginary the answer is subtle, involving number theoretic properties of λ , and KAM type arguments (REFERENCES). For the present discussion we put aside issues of convergence and focus on computing a polynomial approximation of P .

Note that from a geometric perspective, Equation (2) asks that the push forward of the vector field $\lambda\sigma$ under P is tangent to (in fact equal to) the vector field f restricted to the image of P . This condition guarantees that P takes solution curves of the equation $\sigma' = \lambda\sigma$ to solution curves of $u' = F(u)$. We revisit this claim in greater generality in Section (REFERENCE). For the moment we are more concerned with computational aspects of the question.

Let

$$F(z) = \sum_{n=1}^{\infty} a_n(z - z_0)^n,$$

be the power series expansion of f at the equilibrium z_0 . Note that $a_0 = 0$ as $F(z_0) = 0$. Since we are interested in P analytic we make the power series *ansatz*

$$P(\sigma) = \sum_{n=0}^{\infty} p_n \sigma^n.$$

and try to work out the unknown coefficients. Note that, since we want $P(0) = z_0$ we have that $p_0 = z_0$.

One sees that

$$\lambda\sigma P'(\sigma) = \sum_{n=0}^{\infty} \lambda n p_n \sigma^n,$$

and lets

$$Q(\sigma) = \sum_{n=1}^{\infty} q_n \sigma^n = F(P(\sigma)).$$

Then, matching like powers of σ we obtain the deceptively simple looking recursion relations

$$n\lambda p_n = q_n. \quad (3)$$

Note that for $n = 1$ we have that

$$\lambda p_1 = q_1 = (F(P(0)))' = F'(P(0))P'(0) = F'(z_0)p_1 = \lambda p_1.$$

In other words, p_1 is completely arbitrary. However, for $n \geq 2$ the q_n depend on the coefficients of P in a rather involved way.

Indeed it turns out that the coefficients p_n are formally well defined to all orders and that at each fixed order $n \geq 2$ the coefficient p_n depends only on the lower order terms $p_0, \dots, p_{n-1}$. The argument establishing this fact is a bit of a technical diversion, but is worth including as it motivates the formalism employed throughout the remainder of the Section.

First, note that by Taylor's theorem

$$P(\sigma) = \sum_{n=0}^{\infty} p_n \sigma^n = \sum_{n=0}^{\infty} \frac{1}{n!} \frac{d^n}{d\sigma^n} P(0) \sigma^n,$$

and

$$f(P(\sigma)) = \sum_{n=1}^{\infty} q_n \sigma^n = \sum_{n=0}^{\infty} \left(\frac{1}{n!} \frac{d^n}{d\sigma^n} (F(P(0))) \right) \sigma^n,$$

so that

$$\frac{d^n}{d\sigma^n} P(0) = n! p_n.$$

To treat the composition term we recall the *Faà di Bruno* formula, which says that for differentiable functions f and g , the n -th derivative of the composition is

$$\frac{d^n}{dx^n} f(g(x)) = \sum_{k=1}^n f^{(k)}(g(x)) B_{n,k}(g'(x), g''(x), g^{(n-k+1)}(x)), \quad (4)$$

where $f^{(m)}, g^{(m)}$ denote m -th derivatives. Here $B_{n,k}$ are the bell polynomials defined by

$$B_{n,k}(u_1, \dots, u_{n-k+1}) = \sum \frac{n!}{\alpha!} \left(\frac{u_1}{1!} \right)^{\alpha_1} \cdots \left(\frac{u_{n-k+1}}{(n-k+1)!} \right)^{\alpha_{n-k+1}}, \quad (5)$$

where the sum is over all multi-indices $\alpha = (\alpha_1, \dots, \alpha_{n-k+1}) \in \mathbb{N}^{n-k+1}$ which simultaneously satisfy that

$$\alpha_1 + \dots + \alpha_{n-k+1} = k,$$

and that

$$\alpha_1 + 2\alpha_2 + \dots + (n-k+1)\alpha_{n-k+1} = n.$$

We are interested in the dependance of $(f(g(x)))^n$ on $g^n(x)$. Inspection of Equation (4) shows that g^{n-k+1} equals g^n if and only if $k = 1$. Then the sums with $k = 2, \dots, n$ contain only derivatives g of order lower than n .

Further inspection of the $k = 1$ term shows that

$$f'(g(x)) B_{n,1}(g'(x), \dots, g^{(n-k+1)}(x)) = f'(g(x)) g^n(x).$$

To see this, consider again Equation (5) with $k = 1$, and note that

$$\alpha_1 + \dots + \alpha_{n-k+1} = \alpha_1 + \dots + \alpha_n = 1,$$

if and only if exactly one of the indices is 1 and the remaining indices are zero. Similarly, when $k = 1$ we have that

$$\alpha_1 + 2\alpha_2 + \dots + (n - k + 1)\alpha_{n-k+1} = \alpha_1 + 2\alpha_2 + \dots + n\alpha_n = n,$$

if and only if $\alpha_1 = \alpha_2 = \dots = \alpha_{n-1} = 0$ and $\alpha_n = 1$. Taking these constraints into consideration we see that $\alpha = (0, \dots, 1) \in \mathbb{N}^n$ is the only multi-index involved in the sum, so that

$$B_{n,1}(u_1, \dots, u_n) = \sum \frac{n!}{\alpha!} \left(\frac{u_1}{1!}\right)^{\alpha_1} \dots \left(\frac{u_n}{n!}\right)^{\alpha_n} = \frac{n!}{0! \dots 0! 1!} \left(\frac{u_1}{1!}\right)^0 \dots \left(\frac{u_n}{n!}\right)^1 = u_n,$$

and indeed

$$B_{n,1}(g'(x), \dots, g^n(x)) = g^n(x),$$

as claimed.

Now, taking $x = 0$, $g(0) = P(0) = z_0$, and $f(g(0)) = F(P(0)) = F(z_0)$ gives

$$\begin{aligned} \frac{d^n}{d\sigma^n}(F(P(0))) &= F(P(0)) \frac{d^n}{dz^n} P(0) + \sum_{k=2}^n R_k^n(P(0)) \\ &= F'(P(0)) \frac{d^n}{dz^n} P(0) + \sum_{k=2}^n R_k^n(P(0)) \\ &= n! F'(z_0) p_n + \sum_{k=2}^n R_k^n(P(0)) \\ &= n! \lambda p_n + \sum_{k=2}^n R_k^n(P(0)), \end{aligned}$$

The terms $R_k^n(P(0))$ involve derivatives of F of order two or more, and derivatives of P of order strictly less than n . Of course the derivatives of F in these formulae are evaluated at $P(0) = z_0$, and derivatives of P are evaluated at 0: but derivatives evaluated at these points are just the Taylor coefficients of f and P . Then, in fact the $R_k(P(0))$ depend only on the Taylor coefficients $a_1, \dots, a_{n-1}$ and $p_0, \dots, p_{n-1}$ as desired.

Then we have that

$$q_n = \frac{1}{n!} \frac{d^n}{d\sigma^n}(f(P(0))) = \lambda p_n + \frac{1}{n!} \sum_{k=1}^{N_n} R_k^n(P(0)),$$

so that the recursion relations of Equation (3) are

$$n\lambda p_n = \lambda p_n + \frac{1}{n!} \sum_{k=1}^{N_n} R_k^n(P(0)),$$

or

$$p_n = \frac{1}{\lambda(n-1)} s_n, \tag{6}$$

when $n \geq 2$. We refer to Equation (6) as the *homological equations* for P . Here s_n depends recursively on $p_0, \dots, p_{n-1}$. In specific examples it is usually better to work out the form of s_n from scratch, exploiting the specific form of the problem. Note that $p_0 = z_0$ and that p_1 is arbitrary.

Even though the argument above is rarely of value in actual computations, it shows that the coefficients of $P(\sigma)$ are formally well defined to all orders and that each coefficient depends only on lower order terms. The argument above insures that in practice we will be able to computer these coefficients recursively.

Consider for example the complex logistic equation

$$u(z)' = cu(z) - u(z)^2, \quad (7)$$

i.e. Equation (1) with

$$F(z) = cz - z^2 = z(c - z),$$

and

$$F'(z) = c - 2z.$$

The equilibria occur at $z = 0$ and $z = c$. Lets focus on the case of $z_0 = c$. Then $\lambda = F'(c) = c - 2c = -c$. Assume that λ does not lie on the imaginary axis

The linearized dynamics are given by $\sigma' = \lambda\sigma$, so that $\sigma(t) = \sigma_0 e^{\lambda t}$ is the linearized flow. We would like to analytically conjugate Equation (7) to the linear flow at $z_0 = c$. In this setting Equation (2) becomes

$$\sigma \lambda P'(\sigma) = cP(\sigma) - P(\sigma)^2.$$

Since we are interested in P analytic we make the power series *ansatz*

$$P(\sigma) = \sum_{n=0}^{\infty} p_n \sigma^n.$$

and try to work out the unknown coefficients. We have that

$$\sum_{n=0}^{\infty} n \lambda p_n \sigma^n = \sum_{n=0}^{\infty} \left(c p_n - \sum_{k=0}^n p_{n-k} p_k \right) \sigma^n.$$

Matching like powers of σ gives the recursion relations

$$\begin{aligned} n \lambda p_n &= c p_n - \sum_{k=0}^n p_{n-k} p_k \\ &= c p_n - 2 p_0 p_n - \sum_{k=1}^{n-1} p_{n-k} p_k \\ &= c p_n - 2 c p_n - \sum_{k=1}^{n-1} p_{n-k} p_k \\ &= -c p_n - \sum_{k=1}^{n-1} p_{n-k} p_k \\ &= \lambda p_n - \sum_{k=1}^{n-1} p_{n-k} p_k \end{aligned}$$

or

$$p_n = \frac{-1}{\lambda(n-1)} \sum_{k=1}^{n-1} p_{n-k} p_k. \quad (8)$$

when $n \geq 2$. Recall that $p_0 = z_0 = c$ and that p_1 is arbitrary.

Of course Equation (8) describes p_n in exactly the fashion anticipated by the homological equations of Equation (6). The advantage being that Equation (8) reveals the explicit form of the dependence of p_n on lower order terms, while in Equation (8) this dependence is still locked up in the notoriously complicated Faà di Bruno formula.

It is worth remarking that this deceptively simple example tells more or less the entire story, thanks to automatic differentiation. For example take

$$u'(z) = cu(z) - e^{u(z)},$$

i.e. Equation (1) with

$$F(z) = cz - e^z.$$

Assume that $z_0 \in \mathbb{C}$ has $F(z_0) = 0$ and that $\lambda = F'(z_0)$ has non-zero real part. Then Equation (2) becomes

$$\sigma \lambda P'(\sigma) = cP(\sigma) - e^{P(\sigma)},$$

and letting

$$P(\sigma) = \sum_{n=0}^{\infty} p_n \sigma^n,$$

and

$$Q(\sigma) = \sum_{n=0}^{\infty} q_n \sigma^n,$$

one recalls from Section (REFERENCE) that $q_0 = e^{p_0} = e^{z_0}$, and that for $n \geq 1$

$$\begin{aligned} q_n &= \frac{1}{n} \sum_{k=0}^{n-1} (n-k) p_{n-k} q_k \\ &= q_0 p_n + \frac{1}{n} \sum_{k=1}^{n-1} (n-k) p_{n-k} q_k. \end{aligned}$$

Then, matching like powers in Equation (2.1.2) leads to

$$n \lambda p_n = c p_n - q_0 p_n - \frac{1}{n} \sum_{k=1}^{n-1} (n-k) p_{n-k} q_k.$$

The interested reader can now check that the homological equations are

$$\begin{pmatrix} p_n \\ q_n \end{pmatrix} = \begin{pmatrix} \frac{-1}{\lambda(n-1)} \sum_{k=1}^{n-1} \frac{(n-k)}{n} p_{n-k} q_k \\ q_0 p_n + \frac{1}{n} \sum_{k=1}^{n-1} (n-k) p_{n-k} q_k \end{pmatrix}.$$

Other problems involving elementary functions are worked out similarly.

We return to Equation (7), with an eye to numerical considerations. The main point to be made, and one which appears again and again when the parameterization method is

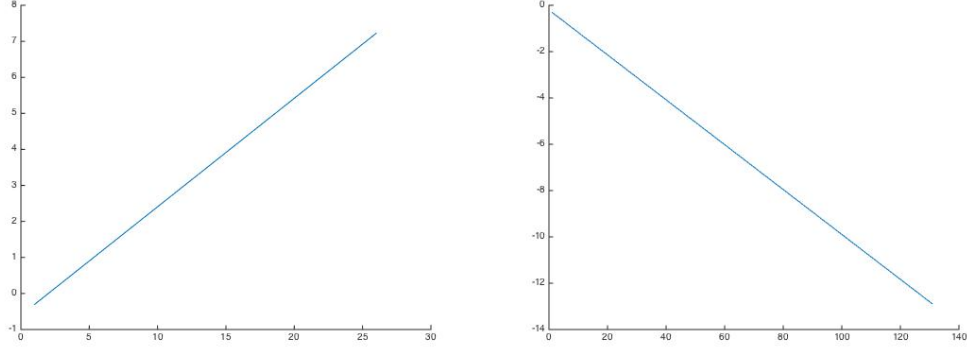


Figure 1: **Dependence of the coefficient decay on the scaling of p_1 : ...**

used to compute stable/unstable manifolds, is that the freedom of choice in the first order Taylor coefficient of P is useful for stabilizing numerics.

To illustrate this point take $c = 1/2$, so that $p_0 = c = 0.5$, and use Equation (8) we then compute the coefficient of P for all $2 \leq n \leq N$, and obtain the polynomial approximation

$$P^N(\sigma) = \sum_{n=0}^N p_n \sigma^n.$$

For example choosing $p_1 = 1$ and $N = 25$ we obtain the Taylor coefficients with magnitudes whose base ten logarithms are illustrated in the left Frame of Figure 1. Note then that the coefficients grow exponentially fast, and that $|p_{25}| \approx 10^7$. From a theoretical point of view there is no problem with this at all. It only suggests that the radius of convergence of the P is something less than one. However from a numerical point of view it is undesirable to work with polynomials whose coefficients are very large.

The problem is overcome by adjusting the scaling of P . Consider the problem again with $c = 1/2$ but this time choosing $p_1 = 0.4$ and $N = 130$. The base ten logarithms of the magnitudes of the resulting Taylor coefficients are shown in the right frame of Figure 1. This time we see that the coefficients decay exponentially fast and there are no large coefficients. The last coefficient has magnitude on the order of machine epsilon. Then it is reasonable to hope that the radius of convergence of the series is at least one.

In order to see that P^N gives results are dynamically meaningful, i.e. that we obtain (at least approximately) the desired conjugacy, choose $\sigma_0 = -1$ (a point on the boundary of the interval $[-1, 1]$) and compute

$$z_1 = P^N(\sigma_0) = \sum_{n=0}^{150} p_n \sigma_0^n = 0.277777777777834$$

as well as

$$z_2 = P^N(e^{\lambda T} \sigma_0) = 0.336649436264490$$

with $T = 1$. Then we integrate the initial condition z_1 numerically for $T = 1$ time units in order to simulate the flow. We obtain that the difference between z_2 and the numerical flow is smaller than 4.2×10^{-14} , a discrepancy of about 200 multiples of machine epsilon.

We remark that checking the conjugacy error with $T = 2, \dots, 10$ produces errors no worse than this, i.e. $T = 1$ is not “cherry picked”. It is also worth remarking that repeating the experiment with $N = 120$ yields conjugacy errors on the order of 10^{-13} , i.e. we actually see a difference using this many terms.

2.1.3 Stable/unstable manifolds for equilibrium solutions of ordinary differential equations

A more important, but only somewhat more complicated class of problems is to consider nonlinear stability in the vicinity of an equilibrium point of a vector field. So, suppose that $f: \mathbb{R}^n \rightarrow \mathbb{R}^n$ is a (real analytic) vector field and that $p_0 \in \mathbb{R}^n$ is a hyperbolic fixed point of f with, let us say, $m \leq n$ -stable eigenvalues. Let $\lambda_1, \dots, \lambda_m \in \mathbb{C}$ denote the stable eigenvalues of $Df(p_0)$ and $\xi_1, \dots, \xi_m \in \mathbb{R}^n$ be associated eigenvectors. We are interested in the m -dimensional local stable manifold attached to p_0 .

The parameterization method studies the *infinitesimal invariance equation*

$$\frac{\partial}{\partial \sigma_1} P(\sigma_1, \dots, \sigma_m) + \dots + \frac{\partial}{\partial \sigma_m} P(\sigma_1, \dots, \sigma_m) = f(P(\sigma_1, \dots, \sigma_m)). \quad (9)$$

As we will see in Section (CITATION), if $P: (-1, 1)^m \rightarrow \mathbb{R}^n$ is a solution of Equation (9) subject to the first order constraints

$$P(0, \dots, 0) = p_0, \quad \text{and} \quad \frac{\partial}{\partial \sigma_j} P(0, \dots, 0) = \xi_j,$$

for $1 \leq j \leq m$, then P parameterizes a local stable manifold patch at p_0 . Indeed, P is a solution of Equation (9) if and only of

$$\Phi(P(\sigma_1, \dots, \sigma_m), t) = P(e^{\lambda_1 t} \sigma_1, \dots, e^{\lambda_m t} \sigma_m), \quad (10)$$

i.e. P recovers the dynamics on the manifold via this conjugacy. The geometric meaning of Equation (10) is illustrated in Figure

Consider for example the Lorenz system defined by the vector field $f: \mathbb{R}^3 \rightarrow \mathbb{R}^3$ given by the formula

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

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

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

Choose one of the three fixed points above 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 stable). The invariance equation reduces to

$$\lambda \sigma \frac{\partial}{\partial \theta} P(\sigma) = f[P(\sigma)],$$

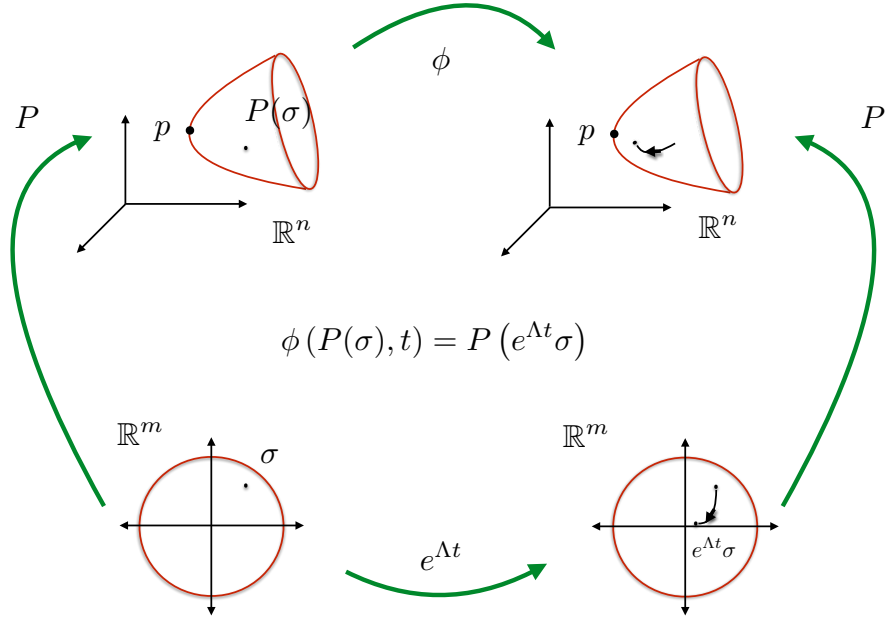


Figure 2: ...

and we look for a power series solution

$$P(\sigma) = \sum_{n=0}^{\infty} \begin{pmatrix} p_n^1 \\ p_n^2 \\ p_n^3 \end{pmatrix} \sigma^n.$$

Imposing the first order constraints leads to

$$p_0 = \hat{p}, \quad \text{and} \quad p_1 = \xi.$$

Then

$$\lambda \sigma \frac{\partial}{\partial \sigma} P(\sigma) = \sum_{n=0}^{\infty} n \lambda \begin{pmatrix} p_n^1 \\ p_n^2 \\ p_n^3 \end{pmatrix} \sigma^n,$$

and

$$f(P(\sigma)) = \sum_{n=0}^{\infty} \begin{pmatrix} \sigma(p_n^2 - p_n^1) \\ \rho p_n^1 - p_n^2 - \sum_{k=0}^n p_{n-k}^1 p_k^3 \\ -\beta p_n^3 + \sum_{k=0}^n p_{n-k}^1 p_k^2 \end{pmatrix} \sigma^n.$$

Matching like powers gives

$$n \lambda \begin{pmatrix} p_n^1 \\ p_n^2 \\ p_n^3 \end{pmatrix} = \begin{pmatrix} \sigma(p_n^2 - p_n^1) \\ \rho p_n^1 - p_n^2 - \sum_{k=0}^n p_{n-k}^1 p_k^3 \\ -\beta p_n^3 + \sum_{k=0}^n p_{n-k}^1 p_k^2 \end{pmatrix},$$

for all $n \geq 2$. Isolate the terms of order n on the left and we have

$$\begin{pmatrix} \sigma(p_n^2 - p_n^1) - n\lambda p_n^1 \\ \rho p_n^1 - p_n^2 - p_0^1 p_n^3 - p_0^3 p_n^1 - n\lambda p_n^2 \\ -\beta p_n^3 + p_0^1 p_n^2 + p_0^2 p_n^1 - n\lambda p_n^3 \end{pmatrix} = \begin{pmatrix} 0 \\ \sum_{k=1}^{n-1} p_{n-k}^1 p_k^3 \\ -\sum_{k=1}^{n-1} p_{n-k}^1 p_k^2 \end{pmatrix}.$$

When expressed in matrix form the above system of equations is

$$[Df(p_0) - n\lambda \text{Id}] p_n = s_n, \quad (11)$$

where $p_n = (p_n^1, p_n^2, p_n^3)^T$ and

$$s_n := \begin{pmatrix} 0 \\ \sum_{k=1}^{n-1} p_{n-k}^1 p_k^3 \\ -\sum_{k=1}^{n-1} p_{n-k}^1 p_k^2 \end{pmatrix}.$$

The main observation is that Equation (11) is a linear equation in p_n , and the right hand side 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, so that $n\lambda < \lambda < 0$ is never an eigenvalue when $n \geq 2$. Solving Equation (11) recursively leads to Taylor coefficients for P to any finite order. Let

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

denote the N -th order approximation obtained by solving Equation (11) for $2 \leq n \leq N$ be our approximation of the stable/unstable manifold.

Now let λ_1 and λ_2 have the same stability (both stable or both unstable) and assume that the remaining eigenvalue has opposite stability (unstable or stable). The invariance equation reduces to

$$\lambda_1 \sigma_1 \frac{\partial}{\partial \sigma_1} P(\sigma_1, \sigma_2) + \lambda_2 \sigma_2 \frac{\partial}{\partial \sigma_2} P(\sigma_1, \sigma_2) = f[P(\sigma_1, \sigma_2)],$$

and we look for

$$P(\sigma_1, \sigma_2) = \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} \begin{pmatrix} p_{mn}^1 \\ p_{mn}^2 \\ p_{mn}^3 \end{pmatrix} \sigma_1^m \sigma_2^n.$$

Power matching as above gives

$$[Df(p_0) - (m\lambda_1 + n\lambda_2)\text{Id}] p_{mn} = s_{mn}, \quad (12)$$

where

$$s_{mn} = \begin{pmatrix} 0 \\ \sum_{k=0}^m \sum_{l=0}^n \delta_{kl}^{mn} p_{(m-k)(n-l)}^1 p_{kl}^3 \\ -\sum_{k=0}^m \sum_{l=0}^n \delta_{kl}^{mn} p_{(m-k)(n-l)}^1 p_{kl}^2 \end{pmatrix}.$$

Here $\delta_{kl}^{mn} = 0$ when either $k = 0$ and $l = 0$ or when $k = m$ and $l = n$. Otherwise it is one (so δ_{kl}^{mn} simply extracts terms of order mn from the sum).

Again, if $m\lambda_1 + n\lambda_2 \neq \lambda_{1,2}$ then the matrix is invertible and the formal series solution P is defined to all orders. Then solving the homological equations for all $2 \leq |\alpha| \leq N$ leads to our numerical approximation

$$P^N(\sigma_1, \sigma_2) = \sum_{n=0}^N \sum_{m=0}^n p_{n-m,m} \sigma_1^{n-m} \sigma_2^m.$$

2.1.4 A more realistic example: stable/unstable manifolds in a restricted four body problem

For a less elementary example we consider the following model from celestial mechanics. Consider three particles with masses $m_1, m_2, m_3 > 0$, normalized so that

$$m_1 + m_2 + m_3 = 1.$$

We assume that the particles are located at the vertices of a planar equilateral triangle. These masses are called the primaries. We choose rotating coordinates which fix the barycenter of the triangle is at the origin and cause the x -axis to bisect the triangle. This places the primaries at positions

$$p_1 = (x_1, y_1), \quad p_2 = (x_2, y_2), \quad \text{and} \quad p_3 = (x_3, y_3),$$

with

$$\begin{aligned} x_1 &= \frac{-|K|\sqrt{m_2^2 + m_2m_3 + m_3^2}}{K} \\ y_1 &= 0 \\ x_2 &= \frac{|K|[(m_2 - m_3)m_3 + m_1(2m_2 + m_3)]}{2K\sqrt{m_2^2 + m_2m_3 + m_3^2}} \\ y_2 &= \frac{-\sqrt{3}m_3}{2m_2^{3/2}}\sqrt{\frac{m_2^3}{m_2^2 + m_2m_3 + m_3^2}} \end{aligned}$$

and

$$\begin{aligned} x_3 &= \frac{|K|}{2\sqrt{m_2^2 + m_2m_3 + m_3^2}} \\ y_3 &= \frac{\sqrt{3}}{2\sqrt{m_2}}\sqrt{\frac{m_2^3}{m_2^2 + m_2m_3 + m_3^2}} \end{aligned}$$

where

$$K = m_2(m_3 - m_2) + m_1(m_2 + 2m_3).$$

We are interested in the equations of motion for a fourth, massless particle p with coordinates (x, y) whose trajectory is governed by the gravitational field of the primaries. Define

$$\Omega(x, y) := \frac{1}{2}(x^2 + y^2) + \frac{m_1}{r_1(x, y)} + \frac{m_2}{r_2(x, y)} + \frac{m_3}{r_3(x, y)},$$

where

$$\begin{aligned} r_1(x, y) &:= \sqrt{(x - x_1)^2 + (y - y_1)^2}, \\ r_2(x, y) &:= \sqrt{(x - x_2)^2 + (y - y_2)^2}, \end{aligned}$$

and

$$r_3(x, y) := \sqrt{(x - x_3)^2 + (y - y_3)^2}.$$

Then

$$\frac{\partial}{\partial x}\Omega = \Omega_x(x, y) = x - \frac{m_1(x - x_1)}{r_1(x, y)^3} - \frac{m_2(x - x_2)}{r_2(x, y)^3} - \frac{m_3(x - x_3)}{r_3(x, y)^3},$$

and

$$\frac{\partial}{\partial y} \Omega = \Omega_y(x, y) = y - \frac{m_1(y - y_1)}{r_1(x, y)^3} - \frac{m_2(y - y_2)}{r_2(x, y)^3} - \frac{m_3(y - y_3)}{r_3(x, y)^3},$$

and

We introduce the variables

$$u_1 = x, \quad u_2 = x', \quad u_3 = y, \quad u_4 = y',$$

The vector field in the co-rotating frame is given by

$$\begin{pmatrix} u'_1 \\ u'_2 \\ u'_3 \\ u'_4 \end{pmatrix} = \begin{pmatrix} u_2 \\ 2u_4 + \Omega_x(u_1, u_3) \\ u_4 \\ -2u_2 + \Omega_y(u_1, u_3) \end{pmatrix} =: f(u_1, u_2, u_3, u_4). \quad (13)$$

This time we consider $\bar{p}_0 = (\bar{p}_0^1, \bar{p}_0^2, \bar{p}_0^3, \bar{p}_0^4) \in \mathbb{R}^4$ an equilibrium point with two unstable eigenvalues $\lambda_1, \lambda_2 \in \mathbb{C}$. Choose associated eigenvectors $\xi_1, \xi_2 \in \mathbb{R}^4$. Now we seek a parameterization $P: (-1, 1) \times (-1, 1) \rightarrow \mathbb{R}^4$ satisfying

$$\lambda_1 \sigma_1 \frac{\partial}{\partial \sigma_1} P(\sigma_1, \sigma_2) + \lambda_2 \sigma_2 \frac{\partial}{\partial \sigma_2} P(\sigma_1, \sigma_2) = f(P(\sigma_1, \sigma_2)),$$

with

$$P(0, 0) = \bar{p}_0, \quad \frac{\partial}{\partial \sigma_1} P(0, 0) = \xi_1, \quad \text{and} \quad \frac{\partial}{\partial \sigma_2} P(0, 0) = \xi_2.$$

Let

$$P(\sigma_1, \sigma_2) = \begin{bmatrix} P_1(\sigma_1, \sigma_2) \\ P_2(\sigma_1, \sigma_2) \\ P_3(\sigma_1, \sigma_2) \\ P_4(\sigma_1, \sigma_2) \end{bmatrix}$$

with

$$\begin{aligned} P_1(\sigma_1, \sigma_2) &= \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} a_{mn} \sigma_1^m \sigma_2^n, \\ P_2(\sigma_1, \sigma_2) &= \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} b_{mn} \sigma_1^m \sigma_2^n, \\ P_3(\sigma_1, \sigma_2) &= \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} c_{mn} \sigma_1^m \sigma_2^n, \\ P_4(\sigma_1, \sigma_2) &= \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} d_{mn} \sigma_1^m \sigma_2^n, \end{aligned}$$

and have that

$$a_{00} = \bar{p}_0^1, \quad b_{00} = 0, \quad c_{00} = \bar{p}_0^3, \quad \text{and} \quad d_{00},$$

and that

$$\begin{aligned} a_{10} &= \xi_1^1, & b_{10} &= \xi_1^2, & c_{10} &= \xi_1^3, & d_{10} &= \xi_1^4, \\ a_{01} &= \xi_2^1, & b_{01} &= \xi_2^2, & c_{01} &= \xi_2^3, & d_{01} &= \xi_2^4, \end{aligned}$$

Then

$$\lambda_1 \sigma_1 \frac{\partial}{\partial \sigma_1} P(\sigma_1, \sigma_2) + \lambda_2 \sigma_2 \frac{\partial}{\partial \sigma_2} P(\sigma_1, \sigma_2) = \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} (m\lambda_1 + n\lambda_2) \begin{pmatrix} a_{mn} \\ b_{mn} \\ c_{mn} \\ d_{mn} \end{pmatrix} \sigma_1^m \sigma_2^n.$$

Let

$$(P_1(\sigma_1, \sigma_2) - x_1)^2 + (P_3(\sigma_1, \sigma_2) - y_1)^2 = Q(\sigma_1, \sigma_2) = \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} Q_{mn} \sigma_1^m \sigma_2^n,$$

$$(P_1(\sigma_1, \sigma_2) - x_2)^2 + (P_3(\sigma_1, \sigma_2) - y_2)^2 = R(\sigma_1, \sigma_2) = \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} R_{mn} \sigma_1^m \sigma_2^n,$$

$$(P_1(\sigma_1, \sigma_2) - x_3)^2 + (P_3(\sigma_1, \sigma_2) - y_3)^2 = S(\sigma_1, \sigma_2) = \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} S_{mn} \sigma_1^m \sigma_2^n,$$

Define

$$\hat{\delta}_{jk}^{mn} = \begin{cases} 0 & \text{if } j = m \text{ and } k = n \\ 0 & \text{if } j = 0 \text{ and } k = 0 \\ 1 & \text{otherwise} \end{cases}.$$

Then

$$Q_{00} = (a_{00} - x_1)^2 + (c_{00} - y_1)^2,$$

$$Q_{mn} = 2(a_{00} - x_1)a_{mn} + 2(c_{00} - y_1)c_{mn} + \sum_{j=0}^m \sum_{k=0}^n (a_{m-j, n-k} a_{jk} + c_{m-j, n-k} c_{jk})$$

$$R_{00} = (a_{00} - x_2)^2 + (c_{00} - y_2)^2,$$

$$R_{mn} = 2(a_{00} - x_2)a_{mn} + 2(c_{00} - y_2)c_{mn} + \sum_{j=0}^m \sum_{k=0}^n (a_{m-j, n-k} a_{jk} + c_{m-j, n-k} c_{jk})$$

$$S_{00} = (a_{00} - x_3)^2 + (c_{00} - y_3)^2,$$

$$S_{mn} = 2(a_{00} - x_3)a_{mn} + 2(c_{00} - y_3)c_{mn} + \sum_{j=0}^m \sum_{k=0}^n (a_{m-j, n-k} a_{jk} + c_{m-j, n-k} c_{jk}).$$

We also define

$$T(\sigma_1, \sigma_2) = Q(\sigma_1, \sigma_2)^{-3/2} = \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} T_{mn} \sigma_1^m \sigma_2^n,$$

$$U(\sigma_1, \sigma_2) = R(\sigma_1, \sigma_2)^{-3/2} = \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} U_{mn} \sigma_1^m \sigma_2^n,$$

$$V(\sigma_1, \sigma_2) = S(\sigma_1, \sigma_2)^{-3/2} = \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} V_{mn} \sigma_1^m \sigma_2^n,$$

and have that

$$T_{00} = Q_0^{-3/2} = ((a_0 - x_1)^2 + (c_0 - y_1)^2)^{-3/2}$$

and

$$T_{mn} = \frac{-3}{2} Q_{00}^{-5/2} Q_{mn} + \frac{1}{(m+n)Q_{00}} \sum_{j=0}^m \sum_{k=0}^n \hat{\delta}_{jk}^{mn}(j+k) \left(\frac{-3}{2} T_{m-j,n-k} Q_{jk} - Q_{m-j,n-k} T_{jk} \right)$$

$$U_{00} = R_0^{-3/2} = ((a_0 - x_2)^2 + (c_0 - y_2)^2)^{-3/2}$$

and

$$U_{mn} = \frac{-3}{2} R_{00}^{-5/2} R_{mn} + \frac{1}{(m+n)R_{00}} \sum_{j=0}^m \sum_{k=0}^n \hat{\delta}_{jk}^{mn}(j+k) \left(\frac{-3}{2} U_{m-j,n-k} R_{jk} - R_{m-j,n-k} U_{jk} \right)$$

and finally

$$V_{00} = S_0^{-3/2} = ((a_0 - x_3)^2 + (c_0 - y_3)^2)^{-3/2}$$

and

$$V_{mn} = \frac{-3}{2} S_{00}^{-5/2} S_{mn} + \frac{1}{(m+n)S_{00}} \sum_{j=0}^m \sum_{k=0}^n \hat{\delta}_{jk}^{mn}(j+k) \left(\frac{-3}{2} V_{m-j,n-k} S_{jk} - S_{m-j,n-k} V_{jk} \right).$$

Define

$$\begin{aligned} \bar{s}_{mn}^2 &:= -\frac{3}{2} Q_{00}^{-5/2} (a_{00} - x_1) \sum_{j=0}^m \sum_{k=0}^n \hat{\delta}_{jk}^{mn} (a_{m-j,n-k} a_{jk} + c_{m-j,n-k} c_{jk}) \\ &+ \frac{a_{00} - x_1}{(m+n)Q_{00}} \sum_{j=0}^m \sum_{k=0}^n \hat{\delta}_{jk}^{mn}(j+k) \left(\frac{-3}{2} T_{m-j,n-k} Q_{jk} - Q_{m-j,n-k} T_{jk} \right) + \sum_{j=0}^m \sum_{k=0}^n \hat{\delta}_{jk}^{mn} a_{m-j,n-k} T_{jk}, \\ \hat{s}_{mn}^2 &:= -\frac{3}{2} R_{00}^{-5/2} (a_{00} - x_2) \sum_{j=0}^m \sum_{k=0}^n \hat{\delta}_{jk}^{mn} (a_{m-j,n-k} a_{jk} + c_{m-j,n-k} c_{jk}) \\ &+ \frac{a_{00} - x_2}{(m+n)R_{00}} \sum_{j=0}^m \sum_{k=0}^n \hat{\delta}_{jk}^{mn}(j+k) \left(\frac{-3}{2} U_{m-j,n-k} R_{jk} - R_{m-j,n-k} U_{jk} \right) + \sum_{j=0}^m \sum_{k=0}^n \hat{\delta}_{jk}^{mn} a_{m-j,n-k} U_{jk} \\ \tilde{s}_{mn}^2 &:= -\frac{3}{2} S_{00}^{-5/2} (a_{00} - x_3) \sum_{j=0}^m \sum_{k=0}^n \hat{\delta}_{jk}^{mn} (a_{m-j,n-k} a_{jk} + c_{m-j,n-k} c_{jk}) \\ &+ \frac{a_{00} - x_3}{(n+m)S_{00}} \sum_{j=0}^m \sum_{k=0}^n \hat{\delta}_{jk}^{mn}(j+k) \left(\frac{-3}{2} V_{m-j,n-k} S_{jk} - S_{m-j,n-k} V_{jk} \right) + \sum_{j=0}^m \sum_{k=0}^n \hat{\delta}_{jk}^{mn} a_{m-j,n-k} V_{jk}, \\ \bar{s}_{mn}^4 &:= -\frac{3}{2} Q_{00}^{-5/2} (c_{00} - y_1) \sum_{j=0}^m \sum_{k=0}^n \hat{\delta}_{jk}^{mn} (a_{m-j,n-k} a_{jk} + c_{m-j,n-k} c_{jk}) \\ &+ \frac{c_{00} - y_1}{(m+n)Q_{00}} \sum_{j=0}^m \sum_{k=0}^n \hat{\delta}_{jk}^{mn}(j+k) \left(\frac{-3}{2} T_{m-j,n-k} Q_{jk} - Q_{m-j,n-k} T_{jk} \right) + \sum_{j=0}^m \sum_{k=0}^n \hat{\delta}_{jk}^{mn} c_{m-j,n-k} T_{jk}, \\ \hat{s}_{mn}^4 &:= -\frac{3}{2} R_{00}^{-5/2} (c_{00} - y_2) \sum_{j=0}^m \sum_{k=0}^n \hat{\delta}_{jk}^{mn} (a_{m-j,n-k} a_{jk} + c_{m-j,n-k} c_{jk}) \end{aligned}$$

$$\begin{aligned}
& + \frac{c_{00} - y_2}{(m+n)R_{00}} \sum_{j=0}^m \sum_{k=0}^n \hat{\delta}_{jk}^{mn}(j+k) \left(\frac{-3}{2} U_{m-j,n-k} R_{jk} - R_{m-j,n-k} U_{jk} \right) + \sum_{j=0}^m \sum_{k=0}^n \hat{\delta}_{jk}^{mn} c_{m-j,n-k} U_{jk} \\
& \quad \tilde{s}_n^4 := -\frac{3}{2} S_{00}^{-5/2} (c_{00} - y_3) \sum_{j=0}^m \sum_{k=0}^n \hat{\delta}_{jk}^{mn} (a_{m-j,n-k} a_{jk} + c_{m-j,n-k} c_{jk}) \\
& + \frac{c_{00} - y_3}{(m+n)S_{00}} \sum_{j=0}^m \sum_{k=0}^n \hat{\delta}_{jk}^{mn}(j+k) \left(\frac{-3}{2} V_{m-j,n-k} S_{jk} - S_{m-j,n-k} V_{jk} \right) + \sum_{j=0}^m \sum_{k=0}^n \hat{\delta}_{jk}^{mn} c_{m-j,n-k} V_{jk}.
\end{aligned}$$

The homological equations for $p_{mn} = (a_{mn}, b_{mn}, c_{mn}, d_{mn})$ are

$$[Df(\bar{p}_0) - (m\lambda_1 + n\lambda_2)\text{Id}] p_{mn} = H_{mn},$$

where

$$H_{mn} = \begin{pmatrix} 0 \\ h_{mn}^2 \\ 0 \\ h_{mn}^4 \end{pmatrix},$$

with

$$h_{mn}^2 = m_1 \bar{s}_{mn}^2 + m_2 \hat{s}_{mn}^2 + m_3 \tilde{s}_{mn}^2,$$

and

$$h_{mn}^4 = m_1 \bar{s}_{mn}^4 + m_2 \hat{s}_{mn}^4 + m_3 \tilde{s}_{mn}^4.$$

Remark 2.2. Several technical details deserve remark.

- (Complex conjugate eigenvalues) When there are complex conjugate eigenvalues in fact none of the preceding discussion changes. The only modification is that, if we choose complex conjugate eigenvectors, then the coefficients will appear in complex conjugate pairs, i.e.

$$p_{mn} = \overline{p_{mn}}.$$

Then taking the complex conjugate variables gives the parameterization of the real invariant manifold,

$$\hat{P}(\sigma_1, \sigma_2) := P(\sigma_1 + i\sigma_2, \sigma_1 - i\sigma_2),$$

where P is the formal series defined in the preceding discussion. For more details see also [42, 4, 5].

- (Resonance and non-resonance) When the eigenvalues are resonant, i.e. when there is a fixed pair $(\hat{m}, \hat{n}) \in \mathbb{N}^2$ so that

$$\hat{m}\lambda_1 + \hat{n}\lambda_2 = \lambda_j,$$

for either $j = 1$ or $j = 2$, then all is not lost. In this case we cannot conjugate analytically to the diagonalized linear vector field. However by modifying the model vector field to include a polynomial term which “kills” the resonance the formal computation goes through. The theoretical details are in [24], and numerical implementation with computer assisted error bounds are discussed and implemented in [40].

2.1.5 Stable/unstable manifolds for periodic solutions of ordinary differential equations

Utility of the parameterization method is not limited to the study of stable/unstable manifolds of equilibria. The method can also be used to compute invariant manifolds associated with periodic orbits. Suppose for example that $\gamma: [0, T] \mathbb{R}^n$ is a smooth periodic orbit for the (real analytic) vector field $f: \mathbb{R}^n \rightarrow \mathbb{R}^n$, i.e. suppose that

$$\gamma(0) = \gamma(T),$$

and that

$$\frac{d}{dt}\gamma(t) = f(\gamma(t)).$$

The stability of the periodic orbits is determined by its Floquet exponents. A thorough review of Floquet theory would be beyond the scope of the present discussion. Suffice to say, $\lambda \in \mathbb{C}$ is a stable Floquet exponent for γ , and $\xi: [0, 2T] \rightarrow \mathbb{R}^n$ is the parameterization of an associated stable normal bundle for γ , if ξ is smooth and $2T$ periodic, and the pair solve the eigenvalue problem

$$\frac{d}{dt}\xi(t) + \lambda\xi(t) - Df(\gamma(t))\xi(t) = 0, \quad (14)$$

for all $t \in [0, 2T]$.

Suppose now that $\gamma(t)$ has $m < n$ stable Floquet exponents $\lambda_1, \dots, \lambda_m \in \mathbb{C}$ and let $\xi_1, \dots, \xi_m: [0, 2T] \rightarrow \mathbb{R}^n$ be associated stable normal bundles. (Stability for Floquet exponents means that the real part of the exponent is strictly less than zero). We are interested in the local stable manifold attached to γ and tangent to the span of $\xi_1(t), \dots, \xi_m(t)$ for each $t \in [0, 2T]$.

In this case the parameterization method seeks a covering map $P: [0, 2T] \times (-1, 1)^m \rightarrow \mathbb{R}^n$ satisfying the invariance equation

$$\frac{\partial}{\partial t}P(t, \sigma_1, \dots, \sigma_m) + \frac{\partial}{\partial \sigma_1}P(t, \sigma_1, \dots, \sigma_m) + \dots + \frac{\partial}{\partial \sigma_m}P(t, \sigma_1, \dots, \sigma_m) = f(P(t, \sigma_1, \dots, \sigma_m)), \quad (15)$$

subject to the first order constraints

$$P(t, 0, \dots, 0) = \gamma(t), \quad \text{and} \quad \frac{\partial}{\partial \sigma_j}P(t, 0, \dots, 0) = \xi_j(t),$$

for all $t \in [0, 2T]$.

It can be shown that P , satisfying the first order constraints, is a solution of Equation (15) if and only if P satisfies the flow conjugacy

$$\Phi(P(s, \sigma_1, \dots, \sigma_m), t) = P(s + t, e^{\lambda_1 t} \sigma_1, \dots, e^{\lambda_m t} \sigma_m). \quad (16)$$

for all $s \in [0, 2T]$ and all $t \geq 0$. From this it follows that P parameterizes a local stable manifold for γ . Then, as in the equilibrium case, we recover the dynamics on the manifold in addition to the embedding. The geometric meaning of Equation (16) is illustrated in Figure 16.

Suppose now that we wish to numerically approximate P . Since P is analytic, periodic in t , and satisfies first order constraints in $\sigma_1, \dots, \sigma_m$, the *Fourier-Taylor ansatz*

$$\begin{aligned} P(t, \sigma_1, \dots, \sigma_m) &= \sum_{\alpha_1=0}^{\infty} \dots \sum_{\alpha_m=0}^{\infty} \sum_{n \in \mathbb{Z}} p_{\alpha_1, \dots, \alpha_m, n} e^{2\pi i \omega_k t} \sigma_1^{\alpha_1} \dots \sigma_m^{\alpha_m} \\ &= \sum_{|\alpha|=0}^{\infty} \sum_{k \in \mathbb{Z}} p_{\alpha, n} e^{2\pi i \omega_k t} \sigma^\alpha, \end{aligned}$$

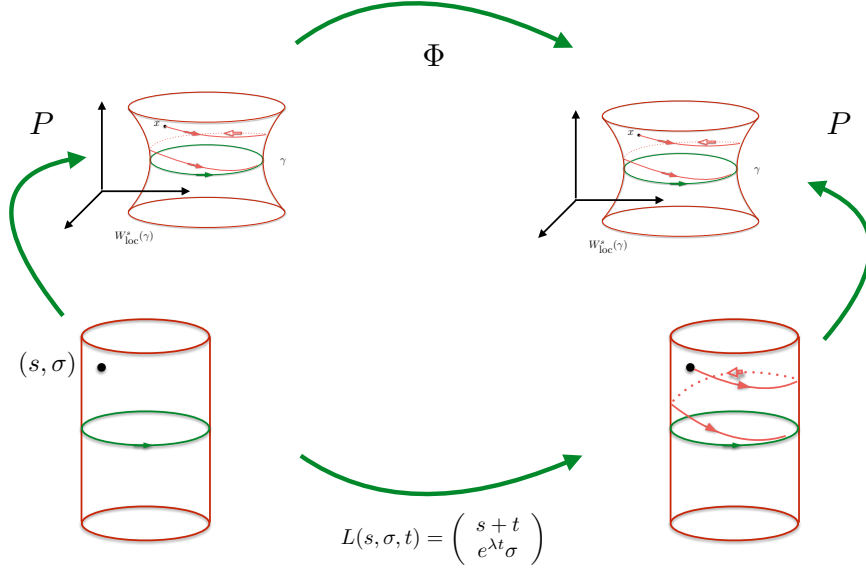


Figure 3: ...

is appropriate. Here the last line exploits the multi-index notation for power series.

Now one inserts the Fourier-Taylor ansatz into the invariance equation (15), expands the nonlinearities using Cauchy products or automatic differentiation, and matches like powers of $\sigma = (\sigma_1, \dots, \sigma_m)$ to obtain the appropriate homological equations. It is illuminating to examine these ideas further in the context of a specific example.

So, returning to the Lorenz equation suppose that $\gamma: [0, T] \rightarrow \mathbb{R}^3$ is a periodic solution with a single real stable Floquet exponent $\gamma < 0$, and let $\xi: [0, T] \rightarrow \mathbb{R}^3$ denote the associated stable normal bundle. Let

$$\gamma(t) = \sum_{k \in \mathbb{Z}} \gamma_k e^{2\pi i \omega k t}, \quad \text{and} \quad \xi(t) = \sum_{k \in \mathbb{Z}} \xi_k e^{2\pi i \omega k t},$$

denote the Fourier series of this data.

In this case we want to solve the equation

$$\frac{\partial}{\partial t} P(t, \sigma) + \lambda \sigma \frac{\partial}{\partial \sigma} P(t, \sigma) = f(P(t, \sigma)),$$

where $t \in [0, T]$ and $\sigma \in (-1, 1)$. For the moment we suppress the Fourier series notation and write

$$P(t, \sigma) = \sum_{n=0}^{\infty} p_n(t) \sigma^n,$$

and have

$$\frac{\partial}{\partial t} P(t, \sigma) + \lambda \sigma \frac{\partial}{\partial \sigma} P(t, \sigma) = \sum_{n=0}^{\infty} \left(\frac{d}{dt} p_n(t) + n \lambda p_n(t) \right) \sigma^n,$$

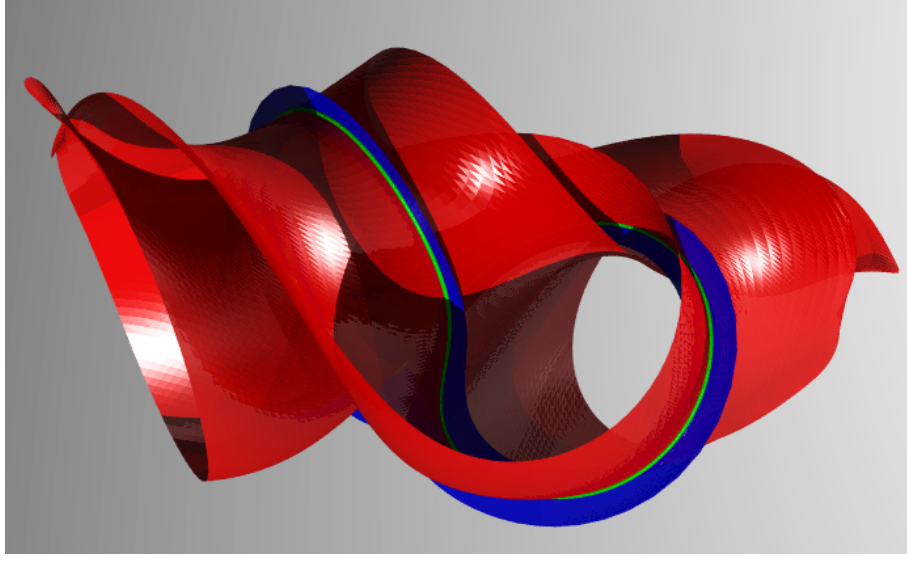


Figure 4: ...

on the left and

$$f(P(t, \sigma)) = \sum_{n=0}^{\infty} \begin{pmatrix} \sigma p_n^2(t) - \sigma p_n^1(t) \\ \rho p_n^1(t) - p_n^2(t) - \sum_{j=0}^n p_{n-j}^1(t) p_j^3(t) \\ -\beta p_n^3(t) + \sum_{j=0}^n p_{n-j}^1(t) p_j^2(t) \end{pmatrix} \sigma^n,$$

on the right. Matching like powers and isolating the n -th order term (a computation which goes almost exactly as the one illustrated in section (REFERENCE)) leads to the homological equations

$$\frac{d}{dt} p_n(t) + n\lambda p_n(t) - Df(\gamma(t))p_n(t) = S_n(t), \quad (17)$$

where

$$S_n(t) = \begin{pmatrix} 0 \\ -\sum_{j=1}^{n-1} p_{n-j}^1(t) p_j^3(t) \\ \sum_{j=1}^{n-1} p_{n-j}^1(t) p_j^2(t) \end{pmatrix}.$$

In other words, we obtain that each coefficient $p_n(t)$ for $n \geq 2$ solves a linear ordinary differential equation with T -periodic data. These equations are solved recursively in Fourier space to obtain an approximation of P to as many Fourier and Taylor modes as we wish.

Figure 4 illustrates a pair of local stable/unstable manifolds computed using the method sketched above. The reader interested in the details may be interested in consulting (CITATION). In that reference efficient numerical solution of the homological equations in Fourier space is accomplished using a change of coordinates which exploits a numerically computed Floquet normal form.

Remark 2.3 (First order Fourier data and homological equations). Note that it is already a nontrivial problem to obtain the Fourier expansions of the periodic orbit and its normal bundles. We note that this can be done using methods similar to those being discussed here. Namely one expands the differential equation or the eigenvalue problem in terms

of the unknown Fourier series and tries to work out the unknown coefficients by power matching.

In the case of Fourier series we cannot solve order by order as in the Taylor case, because the discrete convolution product (analog of the Cauchy product of power series) couples every term to every other. Instead one truncates to a finite Fourier series and applies a numerical solver to the resulting system of scalar algebraic equations.

Such methods are discussed in much greater detail, even with computer assisted methods for obtaining mathematically rigorous error bounds, in the notes of (JP and JB). The methods discussed in those lectures can easily be applied to the (linear!) homological equations discussed above. Therefore in the present discussion we simply assume that we are able to solve Fourier equations. The interested reader may also want to consult (CITATIONS).

2.1.6 Unstable manifolds for equilibrium solutions of partial differential equations

The utility of the parameterization method is not limited to finite dimensional dynamical system. For example the method is used to study unstable manifolds associated with steady state solutions of parabolic partial differential equations.

Proceeding somewhat informally, let $\Omega \subset \mathbb{R}^n$ be an open set and consider the parabolic reaction diffusion equation

$$\frac{\partial}{\partial t} u(x, t) = \Delta u(x, t) + F(u(x, t)). \quad (18)$$

Here $u: \Omega \times [0, \infty) \rightarrow \mathbb{R}$, $x \in \Omega$, $t \in [0, \infty)$ and $F: \mathbb{R} \rightarrow \mathbb{R}$ is a smooth function (in fact let's assume that it is analytic).

The problem is well-posed if we impose an initial and boundary conditions. Suppose for example we require that

$$u(x, 0) = u_0(x),$$

with $u_0: \Omega \rightarrow \mathbb{R}$ in an appropriate Sobolev space, and the Neumann boundary conditions

$$\frac{\partial}{\partial \eta} u(x, t) = 0,$$

for all $t \geq 0$ and $x \in \partial\Omega$. Here $\partial/\partial\eta$ is the normal derivative and $\partial\Omega$ denotes the boundary of the domain. Then Equation (18) generates a (compact) semiflow on a Sobolev space. We denote the Sobolev space by $\mathcal{X}$ and the semiflow by $\Phi^+: \mathcal{X} \times \mathbb{R}^+ \rightarrow \mathcal{X}$.

Suppose that $\hat{u}_0 \in \mathcal{X}$ is a hyperbolic fixed point for Equation (18), i.e. that $\hat{u}_0$ satisfies the boundary conditions, has

$$\Delta \hat{u}_0(x) + F(\hat{u}_0(x)) = 0,$$

at least in a weak sense. In this context, hyperbolicity means that the spectrum of the linear operator $L := \Delta + DF(\hat{u}_0)$ (subject to the boundary conditions) does not accumulate at the imaginary axis. Here L is typically an unbounded, densely defined linear operator on $\mathcal{X}$. Note in fact that L is sectorial, hence the spectrum is pure point and accumulates only at minus infinity.

Then L has at most finitely many unstable eigenvalues each with finite multiplicity. We assume for the sake of simplicity that L has exactly m unstable eigenvalues $\lambda_1, \dots, \lambda_m \in \mathbb{C}$, and that $\xi_1, \dots, \xi_m: \Omega \rightarrow \mathbb{R}$ are associated eigenfunctions. More precisely suppose that

the λ_j have positive real part, that each has multiplicity exactly one, that the pair (λ_j, ξ_j) (weakly) solves the eigenvalue problem

$$\Delta \xi_j(x) + F(\hat{u}_0(x)) \xi_j(x) - \lambda_j \xi_j(x) = 0,$$

for each $1 \leq j \leq m$, and that each ξ_j satisfies the boundary conditions.

The classical stable/unstable manifolds theorems extend to the situation just described (see for example REFERENCE), hence there exists a local stable/unstable manifolds attached to $\hat{u}_0$. We will describe briefly the use of the parameterization method to approximation the local unstable manifold.

We will look for a function $P: (-1, 1)^m \rightarrow \mathcal{X}$ having that

$$\sum_{j=1}^m \lambda_j \sigma_j \frac{\partial}{\partial \sigma_j} P(x, \sigma_1, \dots, \sigma_m) = \Delta P(x, \sigma_1, \dots, \sigma_m) + F(P(x, \sigma_1, \dots, \sigma_m)), \quad (19)$$

where for each fixed $(\sigma_1, \dots, \sigma_m) \in (-1, 1)^m$, the function $P(x, \sigma_1, \dots, \sigma_m)$ satisfies the boundary conditions. We impose also the first order constraints

$$P(x, 0, \dots, 0) = \hat{u}_0(x), \quad \text{and} \quad \frac{\partial}{\partial \sigma_j} P(x, 0, \dots, 0) = \xi_j(x),$$

for all $x \in \Omega$ and $1 \leq j \leq m$.

We make the power series ansatz

$$P(x, \sigma) = \sum_{|\alpha|=0}^{\infty} p_{\alpha}(x) \sigma^{\alpha},$$

where each $p_{\alpha}: \Omega \rightarrow \mathbb{R}$ is in $\mathcal{X}$ (hence each satisfies the boundary conditions).

Consider for example the Fisher equation

(20)

2.1.7 Unstable manifolds for equilibrium and periodic solutions of delay differential equations

2.2 Equilibrium solutions for vector fields on $\mathbb{R}^n$ (slight return): beyond formalism

2.2.1 Justification of the invariance equation

2.2.2 Non-resonant eigenvalues: existence

2.2.3 Rescaling the eigenvectors: uniqueness

2.2.4 Homological equations: the polynomial case

2.2.5 Homological equations: Faa Di Bruno formula and the general case

2.3 Further reading

3 Taylor methods and computer assisted proof

3.1 Analytic functions of several complex variables

Let $m \in \mathbb{N}$ and $z = (z_1, \dots, z_m) \in \mathbb{C}^m$. We endow $\mathbb{C}^m$ with the norm

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

where $|z_j| = \sqrt{\text{real}(z_j)^2 + \text{imag}(z_j)^2}$ is the usual complex absolute value. Let $r > 0$ and $z_0 = (z_1^0, \dots, z_m^0) \in \mathbb{C}^m$. The set

$$D_r^m(z_0) := \{z = (z_1, \dots, z_m) \in \mathbb{C}^m : |z_j - z_j^0| < r \text{ for all } 1 \leq j \leq m\},$$

is called the *polydisk* of radius r centered at $z_0 \in \mathbb{C}^m$. When d, m, r , and z_0 are understood we sometimes abbreviate to $D := D_r^m(z_0)$.

Let $U \subset \mathbb{C}^m$ be an open set and $z \in U$. A continuous function $f: U \rightarrow \mathbb{C}$ is said to be holomorphic at z if for each $1 \leq j \leq m$ the complex partial derivative

$$\frac{\partial}{\partial z_j} f(z) := \lim_{h \rightarrow 0} \frac{f(z_1, \dots, z_j + h, \dots, z_m) - f(z_1, \dots, z_j, \dots, z_m)}{h},$$

exists and is finite. In other words, f is holomorphic at z if it is holomorphic in the one dimensional sense separately in each variable with the others fixed. We say that f is holomorphic on the open set $\Omega \subset \mathbb{C}^m$ if f is holomorphic at z for each $z \in \Omega$.

A fundamental result from the theory of functions of one complex variable is that a function is holomorphic if and only if it is analytic. For functions of several complex variables this is still the case that, i.e. we have that $f: \Omega \rightarrow \mathbb{C}^m$ is holomorphic if and only if f has a convergent power series representation about each point in Ω . To be more precise, let $\alpha = (\alpha_1, \dots, \alpha_m) \in \mathbb{N}^m$ denote an m -dimensional multi-index, $|\alpha| := \alpha_1 + \dots + \alpha_m$ denote the “norm” or “order” of the multi-index, and $(z - z_0)^\alpha := (z_1 - z_1^0)^{\alpha_1} \dots (z_m - z_m^0)^{\alpha_m}$ to denote $(z - z_0) \in \mathbb{C}^m$ raised to the α -power. A continuous function $f: \Omega \rightarrow \mathbb{C}$ is analytic if and only if for each $z_0 \in \Omega$ there is an $r > 0$ and a multi-indexed sequence of complex numbers $\{a_\alpha\}_{\alpha \in \mathbb{N}^m} \subset \mathbb{C}$ so that $D_r^m(z_0) \subset \Omega$ and

$$f(z) = \sum_{\alpha_1=0}^{\infty} \dots \sum_{\alpha_m=0}^{\infty} a_{\alpha_1, \dots, \alpha_m} (z_1 - z_1^0)^{\alpha_1} \dots (z_m - z_m^0)^{\alpha_m}.$$

with the series converging absolutely and uniformly for all $z \in D_r^m(z_0)$. We often employ the convenient short hand

$$\sum_{|\alpha|=0}^{\infty} a_\alpha (z - z_0)^\alpha := \sum_{\alpha_1=0}^{\infty} \dots \sum_{\alpha_m=0}^{\infty} a_{\alpha_1, \dots, \alpha_m} (z_1 - z_1^0)^{\alpha_1} \dots (z_m - z_m^0)^{\alpha_m}.$$

As in the one dimensional case the power series coefficients – or *Taylor coefficients* – are determined by certain Cauchy integrals. More precisely, suppose that $f: \Omega \rightarrow \mathbb{C}$ is analytic and $\overline{D_r^m(z_0)} \subset \Omega$. Then the α -th Taylor coefficient of the power series expansion of f at z_0 is given by the iterated line integral

$$a_\alpha := \frac{1}{(2\pi i)^m} \int_{|z_1 - z_1^0|=r} \dots \int_{|z_m - z_m^0|=r} \frac{f(z_1, \dots, z_m)}{(z_1 - z_1^0)^{\alpha_1+1} \dots (z_m - z_m^0)^{\alpha_m+1}} dz_1 \dots dz_m,$$

where the curves $|z_j - z_j^0| = r$, $1 \leq j \leq m$ are parameterized with with positive orientation, i.e. each curve has winding number $+1$ about z_j^0 . Just as in the one dimensional case, the function f is uniquely determined by its Taylor coefficients and in particular if Ω is connected then these coefficients are all zero if and only if f is identically zero on Ω .

Define $\alpha! := \alpha_1! \dots \alpha_m!$ and let

$$\frac{\partial^{|\alpha|}}{\partial z^\alpha} f(z_0) := \frac{\partial^{\alpha_1 + \dots + \alpha_m}}{\partial z_1^{\alpha_1} \dots \partial z_m^{\alpha_m}} f(z_0),$$

denote the α -th partial derivative of f at z_0 . In analogy with the one dimensional case we have that if f is analytic on Ω then so is the function $\partial^{|\alpha|}/\partial z^\alpha f$ for every $\alpha \in \mathbb{N}^m$. Moreover, the power series of the partial derivatives are given by “term-by-term” differentiation of the power series for f and we have the expression

$$a_\alpha = \frac{1}{\alpha!} \frac{\partial^{|\alpha|}}{\partial z^\alpha} f(z_0),$$

for the Taylor series coefficients. We also have the following Cauchy estimates.

Lemma 3.1 (Cauchy Estimates). *Suppose that f is analytic on an open set $\Omega \subset \mathbb{C}$, and that there are $z_0 \in \Omega$ and $R > 0$ such that*

$$\overline{D_R^m(z_0)} \subset \Omega.$$

Then

$$|a_\alpha| \leq \frac{1}{R^{|\alpha|}} \sup_{z \in D_R^m(z_0)} |f(z)|.$$

It follows, just as in the one dimensional case that

$$\sum_{|\alpha|=0}^{\infty} |a_\alpha| \nu^{|\alpha|} < \frac{M}{(1 - \frac{\nu}{R})^m} < \infty,$$

where M is any bound on $|f(z)|$ in $\overline{D_R^m(z_0)}$ and $0 < \nu < R$.

There is also a Cauchy product in the setting of several complex variables. More precisely, suppose that $\Omega \subset \mathbb{C}^m$ is an open set, that $z_0 \in \Omega$, and that $f, g: \Omega \rightarrow \mathbb{C}$ are analytic. Let

$$f(z) = \sum_{|\alpha|=0}^{\infty} a_\alpha (z - z_0)^\alpha, \quad \text{and} \quad g(z) = \sum_{|\alpha|=0}^{\infty} b_\alpha (z - z_0)^\alpha,$$

denote the power series expansions of f and g at z_0 , and assume that these series converge absolutely and uniformly on some poly-disk $D_r^m(z_0) \subset \mathbb{C}$. Then the pointwise product $f \cdot g$ is analytic on Ω and has power series expansion at z_0 given by

$$(f \cdot g)(z) = \sum_{|\alpha|=0}^{\infty} c_\alpha (z - z_0)^\alpha, \tag{21}$$

where

$$c_\alpha = \sum_{\beta_1=0}^{\alpha_1} \cdots \sum_{\beta_m=0}^{\alpha_m} a_{\alpha_1-\beta_1, \dots, \alpha_m-\beta_m} b_{\beta_1, \dots, \beta_m}.$$

The power series defined by the right hand side of Equation (21) is called the multivariable Cauchy product of two power series (or just the Cauchy product). The Cauchy product converges absolutely and uniformly at least on the poly-disk $D_r^m(z_0)$.

Finally we define the function spaces used in this Chapter. Let $\Omega \subset \mathbb{C}^m$ be an open set and $f: \Omega \rightarrow \mathbb{C}$ be a function. The norm

$$\|f\|_{C^0(\Omega, \mathbb{C})} := \sup_{z \in \Omega} |f(z_1, \dots, z_m)|,$$

is referred to as the supremum norm, or “norm of uniform convergence” on Ω . We often abbreviate this simply to $\|f\|_\infty$ when there is no cause for confusion. Let

$$C^\omega(\Omega, \mathbb{C}) := \{f: \Omega \rightarrow \mathbb{C} : f \text{ is analytic on } \Omega, \text{ and } \|f\|_\infty < \infty\},$$

denote the set of bounded analytic functions on Ω . As in the one dimensional case we have that if $f, \{f_n\}_{n=0}^\infty: \Omega \rightarrow \mathbb{C}$ are functions and the $\{f_n\}_{n=0}^\infty$ are analytic on Ω , then

$$\lim_{n \rightarrow \infty} \|f - f_n\|_\infty = 0,$$

implies that f is analytic, i.e. $C^\omega(\Omega, \mathbb{C})$ is a Banach space when endowed with the $\|\cdot\|_\infty$ norm. In fact $C^\omega(\Omega, \mathbb{C})$ is a Banach algebra when endowed with pointwise multiplication of functions.

3.2 Banach algebras of infinite sequences

Define $\mathcal{S}_m$ to be the collection of all complex m -dimensional multi-indexed sequences $\{a_\alpha\}_{\alpha \in \mathbb{N}^m}$. For $a = \{a_\alpha\}_{\alpha \in \mathbb{N}^m} \in \mathcal{S}_m$ and $\nu > 0$ define the norm

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

and let

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

This defines a Banach space structure.

Suppose that f is analytic at $z_0 \in \mathbb{C}^m$. We define the *Taylor transform* of f at z_0 to be the resulting sequence of Taylor coefficients. More formally define the map $\mathcal{T}_{z_0}$ which associates to the f its sequence of Taylor coefficient $\{a_\alpha\}_{\alpha \in \mathbb{N}^m}$. Here the power series expansion is taken at z_0 . We have that

$$\|f\|_\infty \leq \|\mathcal{T}(f)\|_\nu,$$

even when one of the two is infinite. So, let $a = \{a_\alpha\}_{\alpha \in \mathbb{N}^m} \in \ell_{\nu, m}^1$. The function $f(z)$ defined by

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

has $f \in C^\omega(D_\nu^m)$. Conversely, if $f: D_r^m \rightarrow \mathbb{C}$ is analytic then

$$\mathcal{T}(f) \in \ell_\nu^1,$$

for all $0 < \nu < r$. As in the one dimensional case we have that the Taylor transform is a well defined mapping from $C^\omega(D_r^m(z_0), \mathbb{C})$ into $\ell_{\nu, m}^1$ for any $0 < \nu < r$, that the mapping is one-to-one, and bounded with bounded inverse.

One easily checks that $\ell_{\nu, m}^1$ inherits a Banach algebra structure from pointwise multiplication of functions through the Taylor transform. This fact is critical in nonlinear analysis. More precisely, given $a, b \in \ell_\nu^1$ we define the binary operator $*$: $\ell_\nu^1 \times \ell_\nu^1 \rightarrow \mathbb{S}_d$ by

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

We refer to $*$ as the *Cauchy product*, and have that

•

$$\|a * b\|_\nu \leq \|a\|_\nu \|b\|_\nu,$$

for all $a, b \in \ell_\nu^1$, i.e. $*$ actually takes values in ℓ_ν^1 , making it a Banach algebra.

- For all $f, g \in C^\omega(D_r^d)$,

$$\mathcal{T}(fg) = \mathcal{T}(f) * \mathcal{T}(g),$$

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

Finally we note that, just as in the one variable case, differentiation is not a bounded operation on $C^\omega(D_r^m(z_0), \mathbb{C})$ and hence does not induce a bounded linear map on $\ell_{\nu,m}^1$. But, just as before, we recover boundedness by giving up domain. More precisely we have the following Lemma, whose proof we leave as an exercise.

Lemma 3.2 (Cauchy Bounds in Several Complex Variables). *Let $\nu > 0$, $z_0 \in \mathbb{C}^m$ and $a = \{a_\alpha\}_{\alpha \in \mathbb{N}^m} \in \ell_{\nu,m}^1$. Define $f: D_\nu^m(z_0) \rightarrow \mathbb{C}$*

$$f(z) := \sum_{|\alpha|=0}^{\infty} a_\alpha (z - z_0)^\alpha.$$

Let $0 < \sigma \leq 1$ and

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

Then

$$\sup_{z \in D_{\tilde{\nu}}^m(z_0)} \left| \frac{\partial}{\partial z_j} f(z) \right| \leq \frac{1}{\nu \sigma} \|a\|_{\nu,m}^1.$$

In the validated numerical arguments to follow it makes sense to split $\ell_{\nu,m}^1$ into a finite dimensional vector space where we can do numerical computations, and an infinite dimensional space of “tails” in which we must do some analysis. To this end, define the Banach spaces

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

and

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

Note that

$$\ell_{\nu,m}^1 = X_{\nu,m}^N \oplus X_{\nu,m}^\infty,$$

and each $a \in \ell_{\nu,m}^1$ has a unique representation

$$a = a^N + h,$$

with $a^N \in X_{\nu,m}^N$ and $h \in X_{\nu,m}^\infty$. (It might be natural to write h^∞ to denote elements of X^∞ but the “infinity” superscript becomes cumbersome).

The Cauchy product is the fundamental nonlinear operation appearing in the discussion of validated Taylor methods to follow. The following considerations will simplify our discussion of truncation error analysis. Note that in the case of the Lorenz system as well as the case of the restricted four body problem (after automatic differentiation), we encounter only quadratic nonlinearities. Hence we focus only on the quadratic case now.

Let $a, b \in \ell_{\nu, m}^1$ and $a = a^N + u$ and $b = b^N + v$ with $a^N, b^N \in X_{\nu, m}^N$ and $u, v \in X_{\nu, m}^\infty$. Consider the convolution

$$a * b = (a^N + u) * (b^N + v) = (a^N * b^N) + (a^N * v) + (b^N * u) + (u * v).$$

Note that if $b = a$ this reduces to

$$(a * a) = (a^N * a^N) + 2(a^N * v) + (v * v).$$

For the applications to follow it is desirable to define the two additional binary operators $\hat{*}, \tilde{*}: \ell_{\nu, m}^1 \oplus \ell_{\nu, m}^1 \rightarrow \ell_{\nu, m}^1$ given by

$$(a \hat{*} b)_\alpha = \sum_{\beta_1=0}^{\alpha_1} \dots \sum_{\beta_m=0}^{\alpha_m} \hat{\delta}_\beta^\alpha a_{\alpha_1-\beta_1, \dots, \alpha_m-\beta_m} b_{\beta_1, \dots, \beta_m}, \quad (22)$$

and

$$(a \tilde{*} b)_\alpha = \frac{1}{|\alpha|} \sum_{\beta_1=0}^{\alpha_1} \dots \sum_{\beta_m=0}^{\alpha_m} \hat{\delta}_\beta^\alpha |\beta| a_{\alpha_1-\beta_1, \dots, \alpha_m-\beta_m} b_{\beta_1, \dots, \beta_m}, \quad (23)$$

for $|\alpha| > 0$ and $(a \tilde{*} b)_0 = 0$. Here, for $\alpha, \beta \in \mathbb{N}^m$ with $0 \leq |\beta| \leq |\alpha|$ we define

$$\hat{\delta}_\beta^\alpha := \begin{cases} 0 & \text{if } \beta_j = 0 \text{ for } 1 \leq j \leq m \\ 0 & \text{if } \beta_j = \alpha_j \text{ for } 1 \leq j \leq m, \\ 1 & \text{otherwise} \end{cases}$$

i.e. $\hat{\delta}_\beta^\alpha$ is zero if β is the zero multi-index, or if $\beta = \alpha$, but is one otherwise. Note that if δ_β^α is the traditional *Kronecker delta* then $\hat{\delta}_\beta^\alpha = 1 - \delta_\beta^\alpha$. Note that

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

i.e. that $(a \hat{*} b)_\alpha$ is the α term of the Cauchy product with all dependance on a_α and b_α removed. Similar for $(a \tilde{*} b)$.

Note that for these operators we have the estimates

$$\|a \hat{*} b\|_{\nu, m}^1 \leq \left(\sum_{|\alpha|=1}^\infty |a_\alpha| \nu^{|\alpha|} \right) \left(\sum_{|\alpha|=1}^\infty |b_\alpha| \nu^{|\alpha|} \right), \quad (24)$$

and

$$\|a \tilde{*} b\|_{\nu, m}^1 \leq \left(\sum_{|\alpha|=1}^\infty |a_\alpha| \nu^{|\alpha|} \right) \left(\sum_{|\alpha|=1}^\infty |b_\alpha| \nu^{|\alpha|} \right). \quad (25)$$

For the first of these we define the sequences

$$\hat{a} = \begin{cases} 0 & \text{if } \alpha = 0 \\ a_\alpha & \text{otherwise} \end{cases}, \quad \text{and} \quad \hat{b} = \begin{cases} 0 & \text{if } \alpha = 0 \\ b_\alpha & \text{otherwise} \end{cases},$$

and note that

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

For the second bound, let $|a|, |b| \in \ell_{\nu, m}^1$ denote the sequences whose terms are given by the absolute values of the terms of a and b . Then

$$\begin{aligned}
\|a \tilde{*} b\|_{\nu, m}^1 &= \sum_{|\alpha|=0}^{\infty} \left| \frac{1}{|\alpha|} \sum_{\beta_1=0}^{\alpha_1} \cdots \sum_{\beta_m=0}^{\alpha_m} \hat{\delta}_{\beta}^{\alpha} |\beta| a_{\alpha_1-\beta_1, \dots, \alpha_m-\beta_m} b_{\beta_1, \dots, \beta_m} \right| \nu^{|\alpha|} \\
&\leq \sum_{|\alpha|=0}^{\infty} \sum_{\beta_1=0}^{\alpha_1} \cdots \sum_{\beta_m=0}^{\alpha_m} \hat{\delta}_{\beta}^{\alpha} \frac{|\beta|}{|\alpha|} |a_{\alpha_1-\beta_1, \dots, \alpha_m-\beta_m}| |b_{\beta_1, \dots, \beta_m}| \nu^{|\alpha|} \\
&\leq \sum_{|\alpha|=0}^{\infty} \sum_{\beta_1=0}^{\alpha_1} \cdots \sum_{\beta_m=0}^{\alpha_m} \hat{\delta}_{\beta}^{\alpha} |a_{\alpha_1-\beta_1, \dots, \alpha_m-\beta_m}| |b_{\beta_1, \dots, \beta_m}| \nu^{|\alpha|} \\
&\leq \| |a| \tilde{*} |b| \|_{\nu, m}^1 \\
&\leq \left(\sum_{|\alpha|=1}^{\infty} |a_{\alpha}| \nu^{|\alpha|} \right) \left(\sum_{|\alpha|=1}^{\infty} |b_{\alpha}| \nu^{|\alpha|} \right),
\end{aligned}$$

as desired.

Now, with $a^N, b^N \in X_{\nu, m}^N$ fixed, we define the operators $\hat{C}, \tilde{C}: X_{\nu, m}^N \oplus X_{\nu, m}^N \rightarrow X_{\nu, m}^{\infty}$, $\hat{L}, \tilde{L}: X_{\nu, m}^N \oplus X_{\nu, m}^{\infty} \rightarrow X_{\nu, m}^{\infty}$ and $\hat{N}, \tilde{N}: X_{\nu, m}^{\infty} \oplus X_{\nu, m}^{\infty} \rightarrow X_{\nu, m}^{\infty}$ by

$$\hat{C}(a^N, b^N)_{\alpha} = \begin{cases} 0 & \text{for } 0 \leq |\alpha| \leq N \\ (a^N \hat{*} b^N)_{\alpha} & \text{for } N+1 \leq |\alpha| \leq 2N, \\ 0 & \text{otherwise} \end{cases} \quad (26)$$

$$\tilde{C}(a^N, b^N)_{\alpha} = \begin{cases} 0 & \text{for } 0 \leq |\alpha| \leq N \\ (a^N \tilde{*} b^N)_{\alpha} & \text{for } N+1 \leq |\alpha| \leq 2N, \\ 0 & \text{otherwise} \end{cases} \quad (27)$$

$$\hat{L}(a^N, v)_{\alpha} = \begin{cases} 0 & \text{for } 0 \leq |\alpha| \leq N \\ (a^N \hat{*} v)_{\alpha} & |\alpha| \geq N+1 \end{cases}, \quad (28)$$

$$\tilde{L}(a^N, v)_{\alpha} = \begin{cases} 0 & \text{for } 0 \leq |\alpha| \leq N \\ (a^N \tilde{*} v)_{\alpha} & |\alpha| \geq N+1 \end{cases}, \quad (29)$$

$$\hat{N}(u, v)_{\alpha} = \begin{cases} 0 & \text{for } 0 \leq |\alpha| \leq N \\ (u \hat{*} v)_{\alpha} & |\alpha| \geq N+1 \end{cases}, \quad (30)$$

and

$$\tilde{N}(u, v)_{\alpha} = \begin{cases} 0 & \text{for } 0 \leq |\alpha| \leq N \\ (u \tilde{*} v)_{\alpha} & |\alpha| \geq N+1 \end{cases}, \quad (31)$$

Now for $|\alpha| \geq N+1$ the tail terms of the binary operators have

$$\begin{aligned}
(a \hat{*} b)_{\alpha} &= \hat{C}(a^N, b^N)_{\alpha} + \hat{L}(a^N, v)_{\alpha} + \hat{L}(b^N, u)_{\alpha} + \hat{N}(u, v)_{\alpha}, \\
(a \tilde{*} b)_{\alpha} &= \tilde{C}(a^N, b^N)_{\alpha} + \tilde{L}(a^N, v)_{\alpha} + \tilde{L}(b^N, u)_{\alpha} + \tilde{N}(u, v)_{\alpha}, \\
(a \hat{*} a)_{\alpha} &= \hat{C}(a^N, a^N)_{\alpha} + 2\hat{L}(a^N, u)_{\alpha} + \hat{N}(u, u).
\end{aligned}$$

and

$$(a \tilde{*} a)_{\alpha} = \tilde{C}(a^N, a^N)_{\alpha} + 2\tilde{L}(a^N, u)_{\alpha} + \tilde{N}(u, u).$$

The following Lemma records some useful bounds.

Lemma 3.3. Fix $a^N, b^N \in X_{\nu, m}^N$. We have the bounds

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

and

$$\|\tilde{N}(u, v)\|_{X_{\nu, m}^\infty} \leq \|u\|_{\nu, m}^1 \|v\|_{\nu, m}^1.$$

Proof. For $a^N, b^N \in X_{\nu, m}^N$ fixed simply note that

$$\begin{aligned}\|\hat{C}(a^N, b^N)\|_{X^\infty} &= \sum_{|\alpha|=N+1}^{\infty} |C(a^N, b^N)_\alpha| \nu^{|\alpha|} \\ &= \sum_{|\alpha|=N+1}^{2N} |(a^N \hat{*} b^N)_\alpha| \nu^{|\alpha|},\end{aligned}$$

just by the definition of $\hat{C}(a^N, b^N)$, and similarly for the $\tilde{C}(a^N, b^N)$ estimate.

Now, take $a^N \in X_{\nu, m}^N$ and $v \in X_{\nu, m}^\infty$. Then

$$\begin{aligned}\|\hat{L}(a^N, v)\|_{X^\infty} &= \sum_{|\alpha|=N+1}^{\infty} |(L(a^N, v))_\alpha| \nu^{|\alpha|} \\ &= \sum_{|\alpha|=N+1}^{\infty} |(a^N \hat{*} v)_\alpha| \nu^{|\alpha|} \\ &\leq \sum_{|\alpha|=0}^{\infty} |(a^N * v)_\alpha| \nu^{|\alpha|} \\ &= \|a^N \hat{*} v\|_{\nu, m}^1 \\ &\leq \left(\sum_{|\alpha|=1}^N |a_\alpha^N| \nu^{|\alpha|} \right) \|v\|_{X^\infty},\end{aligned}$$

exploiting the product estimate for the operator $\hat{*}$, the fact that a^N is zero at orders above N , and the fact that v is zero at orders below $N+1$. Again, the $\tilde{L}$ estimate is similar.

Finally if $u, v \in X_{\nu, m}^\infty$ then $\|\hat{N}(u, v)\|_{X_{\nu, m}^\infty} \leq \|u\|_{\nu, m}^1 \|v\|_{\nu, m}^1$, just by the Banach algebra estimate for the Cauchy product. The $\tilde{N}$ estimate is similar. $\square$

Holding $a^N \in X_{\nu,m}^N$ fixed, and considering the action of the derivatives of $\hat{L}, \tilde{L}, \hat{N}, \tilde{N}$ on $h \in X_{\nu,m}^\infty$, we see that

$$D\hat{L}(a^N, v)h = \hat{L}(a^N, h),$$

$$D\tilde{L}(a^N, v)h = \tilde{L}(a^N, h),$$

as $\hat{L}, \tilde{L}$ are linear in v . Similarly

$$D_u \hat{N}(u, v)h = \hat{N}(h, v),$$

$$D_u \tilde{N}(u, v)h = \tilde{N}(h, v),$$

$$D_v \hat{N}(u, v)h = \hat{N}(u, h),$$

$$D_v \tilde{N}(u, v)h = \tilde{N}(u, h),$$

and also

$$D\hat{N}(u, u)h = 2\hat{N}(u, h),$$

and

$$D\tilde{N}(u, u)h = 2\tilde{N}(u, h),$$

by the Banach algebra properties of $\ell_{\nu,m}^1$. Bounds on the derivatives follow immediately.

Corollary 3.4. *Fix $a^N, b^N \in X_{\nu,m}^N$. Then*

$$\|D\hat{L}(a^N, v)\|_{B(X_{\nu,m}^\infty)} \leq \sum_{|\alpha|=1}^N |a_\alpha| \nu^{|\alpha|},$$

$$\|D\tilde{L}(a^N, v)\|_{B(X_{\nu,m}^\infty)} \leq \sum_{|\alpha|=1}^N |a_\alpha| \nu^{|\alpha|},$$

$$\|D_u \hat{N}(u, v)\|_{B(X_{\nu,m}^\infty)} \leq \|v\|_{\nu,m}^1,$$

$$\|D_u \tilde{N}(u, v)\|_{B(X_{\nu,m}^\infty)} \leq \|v\|_{\nu,m}^1,$$

$$\|D_v \hat{N}(u, v)\|_{B(X_{\nu,m}^\infty)} \leq \|u\|_{\nu,m}^1,$$

$$\|D_v \tilde{N}(u, v)\|_{B(X_{\nu,m}^\infty)} \leq \|u\|_{\nu,m}^1,$$

and

$$\|D\hat{N}(u, u)\|_{B(X_{\nu,m}^\infty)} \leq 2\|u\|_{\nu,m}^1,$$

$$\|D\tilde{N}(u, u)\|_{B(X_{\nu,m}^\infty)} \leq 2\|u\|_{\nu,m}^1.$$

Remark 3.5. Note that in the estimates above, the quantity

$$\|\hat{a}^N\|_{\nu,m}^1 = \sum_{|\alpha|=1}^N |a_\alpha^N| \nu^{|\alpha|},$$

is made as small as we wish, by taking ν small enough. This is due to the removal of the constant term from the norm.

3.3 Validated numerics for local Taylor methods

The observation driving our computer assisted error analysis is that, *the recursion relations give rise to a fixed point problem for the unknown Taylor series, and the fixed point operator becomes a contraction if we take the projection dimension high enough*. Rather than proving this maxim in general, we will illustrate its use in a number of example problems. We exploit the following lemma, which encodes convenient sufficient conditions for application of the Banach fixed point theorem.

Lemma 3.6. *Let X be a Banach space, $x_0 \in X$ and suppose that for some $r_* > 0$, $T: \overline{B_{r_*}(x_0)} \rightarrow X$ is a Fréchet differentiable mapping. Let Y_0 be a positive constant so that*

$$\|T(x_0) - x_0\| \leq Y_0,$$

and assume that there are positive constants Z_1, Z_2 so that for all $0 < r \leq r_*$ we have that

$$\|DT(x) - DT(x_0)\| \leq Z_1 + Z_2r,$$

with $x \in \overline{B_r(x_0)}$.

Then, for any $0 < r \leq r_*$ so that

$$Z_2r^2 - (1 - Z_1)r + Y_0 \leq 0, \tag{32}$$

there is unique $\hat{x} \in \overline{B_r(x_0)}$ so that $T(\hat{x}) = \hat{x}$.

Proof. Note that $\overline{B_r(x_0)}$ is a complete metric space. For $x \in \overline{B_r(x_0)}$ consider

$$\begin{aligned} \|T(x) - x_0\| &\leq \|T(x) - T(x_0)\| + \|T(x_0) - x_0\| \\ &\leq \sup_{z \in \overline{B_r(x_0)}} \|DT(z)\| \|x - x_0\| + Y_0 \\ &\leq (Z_1 + Z_2r) \|x - x_0\| + Y_0 \\ &\leq Z_2r^2 + Z_1r + Y_0 \\ &\leq r, \end{aligned}$$

by the hypothesis given in Equation (32). Then T maps $\overline{B_r(x_0)}$ into itself.

Now choose $x, y \in \overline{B_r(x_0)}$, and consider

$$\begin{aligned} \|T(x) - T(y)\| &\leq \sup_{z \in \overline{B_r(x_0)}} \|DT(z)\| \|x - y\| \\ &\leq (Z_1 + Z_2r) \|x - y\|. \end{aligned}$$

From Equation (32) we have that

$$Z_2r^2 + Z_1r + Y_0 \leq r,$$

or

$$Z_2r + Z_1 + \frac{Y_0}{r} \leq 1.$$

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

$$Z_2r + Z_1 < 1,$$

so that T is a contraction mapping on $\overline{B_r(x_0)}$. □

3.3.1 A first example: one scalar equation in a single complex variable

Recall that in Section 2.1.2 we studied the analytic linearization problem for a single first order analytic differential equation in one complex variable. For the example of the logistic nonlinearity we found that the linearizing change of coordinates has Taylor coefficient given by

$$p_0 = z_0,$$

where z_0 is the equilibrium point,

$$p_1 = s,$$

with $s \in \mathbb{C}$ an arbitrary scaling, and

$$p_n = \frac{-1}{\lambda(n-1)} \sum_{k=1}^{n-1} p_{n-k} p_k. \quad (33)$$

for $n \geq 2$. Suppose we compute the coefficients p_n for $0 \leq n \leq N$ using Equation (33) and that we choose a numerical radius of validity $\nu > 0$. Then, ideally speaking, we would like to prove that for some $r > 0$ we have the bound

$$\sup_{|\sigma| \leq \nu} |P^N(\sigma) - P(\sigma)| \leq r.$$

In fact, by choosing s appropriately we can arrange that the coefficients $\{p_n\}_{n=0}^\infty$ decay rapidly enough that we simply take $\nu = 1$.

Following the sketch outlined in the previous section, define the mapping $\Psi: \ell^1 \rightarrow \ell^1$ by

$$\Psi(p)_n = \begin{cases} z_0 & \text{if } n = 0 \\ s & \text{if } n = 1 \\ \frac{-1}{\lambda(n-1)} \sum_{k=1}^{n-1} p_{n-k} p_k & \text{for } n \geq 2 \end{cases}. \quad (34)$$

Clearly, $\hat{p} = \{\hat{p}_n\}_{n=0}^\infty$ are the Taylor coefficients of the desired parameterization if and only if $\hat{p}$ is a fixed point of Ψ . Moreover, if $\hat{p}$ is a fixed point of Ψ and $\hat{p} \in \ell^1$ then the parameterization

$$P(\sigma) = \sum_{n=0}^{\infty} \hat{p}_n \sigma^n,$$

is analytic on the unit disk.

Let $X_{1,1}^N, X_{1,1}^\infty$ be as defined in Section 3.2 (noting that in this case the multi-indices are one dimensional i.e. $m = 1$, and that we have also fixed $\nu = 1$). Then Ψ has the projections

$$\Psi(a) = \Psi^N(a^N) + T(h, a^N),$$

where

$$\Psi^N(a^N)_n = \begin{cases} z_0 & \text{if } n = 0 \\ s & \text{if } n = 1 \\ \frac{-1}{\lambda(n-1)} \sum_{k=1}^{n-1} a_{n-k}^N a_k^N & \text{for } 2 \leq n \leq N \\ 0 & \text{for } n \geq N+1 \end{cases},$$

and

$$T(h, a^N)_n = \begin{cases} 0 & \text{if } 0 \leq n \leq N \\ \frac{-1}{\lambda(n-1)} \sum_{k=1}^{n-1} a_{n-k} a_k & \text{for } 2 \leq n \leq N \end{cases},$$

where $a = a^N + h$. Exploiting the operators $\hat{C}$, $\hat{L}$, and $\hat{N}$ defined in Section 3.2, we rewrite T as

$$\begin{aligned} T(h, a^N)_n &= \frac{-1}{\lambda(n-1)} \left(\hat{C}(a^N, a^N)_n + 2\hat{L}(a^N, h)_n + \hat{N}(h, h)_n \right) \\ &= \frac{-1}{\lambda(n-1)} \left(\sum_{k=1}^{n-1} a_{n-k}^N a_k^N + 2 \sum_{k=1}^{n-1} a_{n-k}^N h_k + \sum_{k=1}^{n-1} h_{n-k} h_k \right), \end{aligned}$$

for $n \in \mathbb{N}$.

The key is to observe that by computing exactly the coefficient up to order N , we obtain an exact fixed point of the operator Ψ^N (exactly in the sense of interval arithmetic, i.e. up to interval enclosures). These coefficients can be computed exactly (up to interval enclosures) simply iterative evaluating the recursion relations. We denote the sequence of coefficients so computed by $\bar{a}^N \in X_{1,1}^N$.

Once we have in hand the unique fixed point $\bar{a}^N \in X_{1,1}^N$ of Ψ^N , what remains is to find a fixed point of $T(h, \bar{a}^N)$, where we now think of the second argument $\bar{a}^N$ as being fixed. Define the map $T(\cdot, \bar{a}^N): X_{1,1}^\infty \rightarrow X_{1,1}^\infty$ by

$$T(h, \bar{a}^N)_n = \frac{-1}{\lambda(n-1)} \left(\hat{C}(\bar{a}^N, \bar{a}^N)_n + 2\hat{L}(\bar{a}^N, h)_n + \hat{N}(h, h)_n \right), \quad (35)$$

for $n \in \mathbb{N}$. One now checks that the Fréchet derivative of $T(h, \bar{a}^N)$ with respect to h , and acting on a vector $v \in X_{1,1}^\infty$ is given by

$$[DT(h, \bar{a}^N)v]_n = \frac{-1}{\lambda(n-1)} \left(2\hat{L}(\bar{a}^N, v)_n + 2\hat{N}(h, v)_n \right), \quad (36)$$

for $n \in \mathbb{N}$.

The following lemma facilitates our computer assisted error analysis, and follows directly from the estimates of Section 3.2.

Lemma 3.7 (The Y and Z bounds). *Fix $\bar{a}^N \in X_{1,1}^N$ and let $T(\cdot, \bar{a}^N): X_{1,1}^\infty \rightarrow X_{1,1}^\infty$ be as defined in Equation (35). Define the constants*

$$Y_0 := \frac{1}{|\lambda|} \sum_{n=N+1}^{2N} \frac{1}{n-1} \left| \sum_{k=1}^{n-1} \bar{a}_{n-k}^N \bar{a}_k^N \right|,$$

$$Z_1 := \frac{2}{|\lambda|N} \sum_{n=1}^N |\bar{a}_n^N|,$$

and

$$Z_2 := \frac{2}{|\lambda|N}.$$

Then

$$\|T(0, \bar{a}^N)\|_{X_{1,1}^\infty} \leq Y_0.$$

and

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

Proof. The proof is just a matter of applying the bounds derived in Lemmas 3.3 and 3.4 to the expressions for T and DT given in Equations (35) and (36), and taking into account the fact that $m = \nu = 1$ in the present set up. $\square$

Example: validated numerics for the complex logistic equation

3.3.2 A second example: system of scalar equations in two complex variables and stable/unstable manifolds for Lorenz

Recall that the power series coefficients for the Parameterization of a two dimensional stable/unstable manifold for the Lorenz system were found to be solutions of the homological equations

$$[Df(p_0) - (m\lambda_1 + n\lambda_2)\text{Id}]p_{mn} = s_{mn}, \quad (37)$$

where p_0 is the desired fixed point of the Lorenz equations (either the origin or one of “the eyes”)

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

are the Taylor coefficients of the parameterization of the local manifold, and

$$s_{mn} = \begin{pmatrix} 0 \\ \sum_{k=0}^m \sum_{l=0}^n \delta_{kl}^{mn} a_{(m-k)(n-l)} c_{kl} \\ -\sum_{k=0}^m \sum_{l=0}^n \delta_{kl}^{mn} a_{(m-k)(n-l)} b_{kl} \end{pmatrix} = \begin{pmatrix} 0 \\ (a \hat{*} c)_{mn} \\ -(a \hat{*} b)_{mn} \end{pmatrix},$$

using the notation of Section 3.2.

Suppose now that $Df(p_0)$ is diagonalizable, and that the eigenvalues $\lambda_1, \lambda_2, \lambda_3 \in \mathbb{C}$, and the associated eigenvectors are known $\xi_1, \xi_2, \xi_3 \in \mathbb{R}^3$ are known (at least up to interval enclosures). Then we will 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. Letting

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

denote the diagonal matrix of eigenvalues, and assuming that λ_1, λ_2 are stable and λ_3 is unstable, we have that

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

from which we obtain that

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

Here

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

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

$$A_{mn} = \begin{pmatrix} A_{mn}^{11} & A_{mn}^{12} & A_{mn}^{13} \\ A_{mn}^{21} & A_{mn}^{22} & A_{mn}^{23} \\ A_{mn}^{31} & A_{mn}^{32} & A_{mn}^{33} \end{pmatrix} = Q(\Lambda - (m\lambda_1 + n\lambda_2)\text{Id})^{-1}Q^{-1},$$

and note that

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

where

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

Here $K_{mn} \rightarrow 0$ as $(m+n) \rightarrow \infty$, and none of the denominators is zero by the assumption that the eigenvalues are non-resonant (an assumption which holds at all equilibria of the Lorenz system, for the classical parameter values).

We now consider the problem in the “Taylor transform” domain. Note that our sequences have $m = 2$ dimensional multi-indices and that, by exploiting the free choice of eigenvector scalings, we are able to take $\nu = 1$. More precisely we look for Taylor coefficients in the space $\ell_{1,2}^1$. We start by defining the “diagonal” bounded linear operators $A^{12}, A^{13}, A^{22}, A^{23}, A^{32}, A^{33}: \ell_{1,2}^1 \rightarrow \ell_{1,2}^1$ by

$$A^{jk}(a)_{mn} = A_{mn}^{jk} a_{mn},$$

for $j = 1, 2, 3$, and $k = 2, 3$ for all $(m, n) \in \mathbb{N}^2$.

Now 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

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

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

$$\Psi(a, b, c)_{mn} = \begin{pmatrix} \Psi(a, b, c)_{mn}^1 \\ \Psi(a, b, c)_{mn}^2 \\ \Psi(a, b, c)_{mn}^3 \end{pmatrix}, \quad (38)$$

with

$$\Psi(a, b, c)^j = A^{j2}(a \hat{*} c) - A^{j3}(a \hat{*} b),$$

for $j = 1, 2, 3$. 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.

Let $X_{1,2}^N$ and $X_{1,2}^\infty$ be as defined in Section 3.2. Then Ψ has the decomposition

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

where $\Psi^N: (X_{1,2}^N)^3 \rightarrow (X_{1,2}^N)^3$ and $T: (X_{1,2}^\infty)^3 \oplus (X_{1,2}^N)^3 \rightarrow (X_{1,2}^\infty)^3$. Here the components of Ψ^N are just the homological equations for $0 \leq m+n \leq N$. Suppose that $\bar{a}^N, \bar{b}^N, \bar{c}^N \in X_{1,2}^N$ are obtained by solving these homological equations exactly (at least in the sense of interval arithmetic). Since solving the recursion relations to N -th order gives the fixed point of Φ^N , we need only prove the existence of a fixed point of $T(\cdot, \cdot, \cdot, \bar{a}^N, \bar{b}^N, \bar{c}^N)$ with the $X_{1,2}^N$ data considered as fixed.

In this case $T: (X_{1,2}^\infty)^3 \rightarrow (X_{1,2}^\infty)^3$ is given by

$$T(u, v, w, \bar{a}^N, \bar{b}^N, \bar{c}^N) = \begin{pmatrix} T(u, v, w, \bar{a}^N, \bar{b}^N, \bar{c}^N)^1 \\ T(u, v, w, \bar{a}^N, \bar{b}^N, \bar{c}^N)^2 \\ T(u, v, w, \bar{a}^N, \bar{b}^N, \bar{c}^N)^3 \end{pmatrix}, \quad (39)$$

where, using the notation of Section 3.2, we have

$$\begin{aligned} T(u, v, w, \bar{a}^N, \bar{b}^N, \bar{c}^N)^j &= A^{j2} (C(\bar{a}^N, \bar{c}^N) + L(\bar{a}^N, w) + L(\bar{c}^N, u) + N(u, w)) \\ &\quad - A^{j3} (C(\bar{a}^N, \bar{b}^N) + L(\bar{a}^N, v) + L(\bar{b}^N, u) + N(u, v)). \end{aligned}$$

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

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

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

$$\begin{aligned} D_1 T^j(u, v, w, \bar{a}^N, \bar{b}^N, \bar{c}^N)h &= A^{j2} (L(\bar{c}^N h) + N(h, w)) - A^{j3} (L(\bar{b}^N, h) + N(h, v)) \\ D_2 T^j(u, v, w, \bar{a}^N, \bar{b}^N, \bar{c}^N)h &= -A^{j3} (L(\bar{a}^N, h) + N(u, h)), \end{aligned}$$

and

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

for $j = 1, 2, 3$.

We would like to show that T is a contraction in some small neighborhood of $(0, 0, 0) \in (X_{1,2}^\infty)^3$. Since we adopted the max norm on the product space the norm of the matrix DT is bound by the max of the sums of the row entries. Then, recalling the bounds of Lemma (REFERENCE), we have the following.

Lemma 3.8. *Let*

$$K^N := \|Q\| \|Q^{-1}\| \max_{1 \leq j \leq 3} \sup_{m+n \geq N+1} \frac{1}{|m\lambda_1 + n\lambda_2 - \lambda_j|},$$

and define

$$\begin{aligned} Y_0 &:= 2K^N \left(\sum_{m+n=N+1}^{2N} |(a^N \hat{*} b^N)_{mn}| + |(a^N \hat{*} c^N)_{mn}| \right), \\ Z_1 &:= K^N \left(2 \sum_{1 \leq m+n \leq N} |\bar{a}_{mn}^N| + \sum_{1 \leq m+n \leq N} (|\bar{b}_{mn}^N| + |\bar{c}_{mn}^N|) \right), \end{aligned}$$

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

$$\sup_{(a,b,c) \in B_r(0)} \|DT(a, b, c)\|_{B((X_{1,2}^\infty)^3)} \leq Z_1 + Z_2 r.$$

Proof. First consider, for $j = 1, 2, 3$ and $k = 2, 3$, the operators A^{jk} restricted to $X_{1,2}^\infty$. We have that

$$\begin{aligned} \|A^{ji}\|_{B(X_{1,2}^\infty)} &:= \sup_{\|h\|_{X_{1,2}^\infty}=1} \|A^{ij}h\|_{X_{1,2}^\infty} \\ &= \sup_{\|h\|_m^1=1} \sum_{m+n=N+1}^{\infty} |A_{mn}^{ij} h_{mn}| \\ &\leq \sup_{\|h\|_{1,2}^1=1} \sum_{m+n=N+1}^{\infty} \frac{\|Q\| \|Q^{-1}\|}{|m\lambda_1 + n\lambda_2 - \lambda_j|} |h_{mn}| \\ &\leq K^N. \end{aligned}$$

Then

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

Now let $u, v, w \in X_{1,2}^\infty$ all with norm less than or equal to r . Considering the derivative in light of the estimates in Lemma (REFERENCE) one has that

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

□

Example: validated numerics for the Lorenz manifolds

3.3.3 The more realistic example: stable/unstable manifolds of equilibrium configurations in the four body problem

Let Σ denote the 4×4 diagonal matrix of eigenvalues and

$$Q = [\xi_1, \xi_2, \xi_3, \xi_4],$$

denote the matrix of eigenvectors, and Q^{-1} be its inverse. Define

$$\begin{aligned}
\Sigma_{mn} &= \Sigma - (m\lambda_1 + n\lambda_2)\text{Id}_4 \\
&= \begin{pmatrix} \lambda_1 - (m\lambda_1 + n\lambda_2) & 0 & 0 & 0 \\ 0 & \lambda_2 - (m\lambda_1 + n\lambda_2) & 0 & 0 \\ 0 & 0 & \lambda_3 - (m\lambda_1 + n\lambda_2) & 0 \\ 0 & 0 & 0 & \lambda_4 - (m\lambda_1 + n\lambda_2) \end{pmatrix},
\end{aligned}$$

where λ_1, λ_2 are the stable (or respectively unstable) eigenvalues, and the matrices

$$A_{mn} = \begin{pmatrix} A_{mn}^{11} & A_{mn}^{12} & A_{mn}^{13} & A_{mn}^{14} \\ A_{mn}^{21} & A_{mn}^{22} & A_{mn}^{23} & A_{mn}^{24} \\ A_{mn}^{31} & A_{mn}^{32} & A_{mn}^{33} & A_{mn}^{34} \\ A_{mn}^{41} & A_{mn}^{42} & A_{mn}^{43} & A_{mn}^{44} \end{pmatrix} = Q \Sigma_{mn}^{-1} Q^{-1}.$$

with

$$\begin{pmatrix} F_{mn}^1(a, b, c, d, q, r, s, T, U, V) \\ F_{mn}^2(a, b, c, d, q, r, s, T, U, V) \\ F_{mn}^3(a, b, c, d, q, r, s, T, U, V) \\ F_{mn}^4(a, b, c, d, q, r, s, T, U, V) \end{pmatrix} = Q \Sigma_{mn}^{-1} Q^{-1} H_{mn},$$

and

$$H_{mn} = \begin{pmatrix} 0 \\ h_{mn}^2 \\ 0 \\ h_{mn}^4 \end{pmatrix},$$

with

$$h_{mn}^2 = m_1 \bar{s}_{mn}^2 + m_2 \hat{s}_{mn}^2 + m_3 \tilde{s}_{mn}^2,$$

and

$$h_{mn}^4 = m_1 \bar{s}_{mn}^4 + m_2 \hat{s}_{mn}^4 + m_3 \tilde{s}_{mn}^4.$$

Then for $1 \leq j \leq 4$ we write

$$F^j(a, b, c, d, q, r, s, T, U, V)_{mn} = A_{mn}^{j2} h_{mn}^2 + A_{mn}^{j4} h_{mn}^4,$$

where

$$\bar{s}^2 = -\frac{3}{2} Q_{00}^{-5/2} (a_{00} - x_1) (a \hat{*} a + c \hat{*} c) - \frac{(a_{00} - x_1)}{Q_{00}} \left(\frac{3}{2} T \tilde{*} Q + Q \tilde{*} T \right) + a \hat{*} T,$$

$$\hat{s}^2 = -\frac{3}{2} R_{00}^{-5/2} (a_{00} - x_2) (a \hat{*} a + c \hat{*} c) - \frac{(a_{00} - x_2)}{R_{00}} \left(\frac{3}{2} U \tilde{*} R + R \tilde{*} U \right) + a \hat{*} U,$$

$$\tilde{s}^2 = -\frac{3}{2} S_{00}^{-5/2} (a_{00} - x_3) (a \hat{*} a + c \hat{*} c) - \frac{(a_{00} - x_3)}{S_{00}} \left(\frac{3}{2} V \tilde{*} S + S \tilde{*} V \right) + a \hat{*} V,$$

$$\bar{s}^4 = -\frac{3}{2} Q_{00}^{-5/2} (c_{00} - y_1) (a \hat{*} a + c \hat{*} c) - \frac{(a_{00} - x_1)}{Q_{00}} \left(\frac{3}{2} T \tilde{*} Q + Q \tilde{*} T \right) + c \hat{*} T,$$

$$\hat{s}^4 = -\frac{3}{2} R_{00}^{-5/2} (c_{00} - y_2) (a \hat{*} a + c \hat{*} c) - \frac{(a_{00} - x_2)}{R_{00}} \left(\frac{3}{2} U \tilde{*} R + R \tilde{*} U \right) + c \hat{*} U,$$

and

$$\tilde{s}^4 = -\frac{3}{2} S_{00}^{-5/2} (c_{00} - y_3) (a \hat{*} a + c \hat{*} c) - \frac{(a_{00} - x_3)}{S_{00}} \left(\frac{3}{2} V \tilde{*} S + S \tilde{*} V \right) + c \hat{*} V.$$

Moreover, by defining

$$F^5(a, b, c, d, q, r, s, T, U, V) =$$

$$2(a_{00} - x_1) F^1(a, b, c, d, q, r, s, T, U, V) + 2(c_{00} - y_1) F^3(a, b, c, d, q, r, s, T, U, V) + a \hat{*} a + c \hat{*} c,$$

$$F^6(a, b, c, d, q, r, s, T, U, V) =$$

$$2(a_{00} - x_2) F^1(a, b, c, d, q, r, s, T, U, V) + 2(c_{00} - y_2) F^3(a, b, c, d, q, r, s, T, U, V) + a \hat{*} a + c \hat{*} c,$$

$$F^7(a, b, c, d, q, r, s, T, U, V) =$$

$$2(a_{00} - x_3) F^1(a, b, c, d, q, r, s, T, U, V) + 2(c_{00} - y_3) F^3(a, b, c, d, q, r, s, T, U, V) + a \hat{*} a + c \hat{*} c,$$

$$F^8(a, b, c, d, q, r, s, T, U, V) = \frac{-3}{2} Q_{00}^{-5/2} F^5(a, b, c, d, q, r, s, T, U, V) - \frac{1}{Q_{00}} \left(\frac{-3}{2} T \tilde{*} Q + Q \tilde{*} T \right),$$

$$F^9(a, b, c, d, q, r, s, T, U, V) = \frac{-3}{2} R_{00}^{-5/2} F^6(a, b, c, d, q, r, s, T, U, V) - \frac{1}{R_{00}} \left(\frac{-3}{2} U \tilde{*} R + R \tilde{*} U \right),$$

$$F^{10}(a, b, c, d, q, r, s, T, U, V) = \frac{-3}{2} S_{00}^{-5/2} F^7(a, b, c, d, q, r, s, T, U, V) - \frac{1}{S_{00}} \left(\frac{-3}{2} V \tilde{*} S + S \tilde{*} V \right),$$

and

$$\Psi(a, b, c, d, q, r, s, T, U, V) = \begin{pmatrix} F^1(a, b, c, d, q, r, s, T, U, V) \\ F^2(a, b, c, d, q, r, s, T, U, V) \\ F^3(a, b, c, d, q, r, s, T, U, V) \\ F^4(a, b, c, d, q, r, s, T, U, V) \\ F^5(a, b, c, d, q, r, s, T, U, V) \\ F^6(a, b, c, d, q, r, s, T, U, V) \\ F^7(a, b, c, d, q, r, s, T, U, V) \\ F^8(a, b, c, d, q, r, s, T, U, V) \\ F^9(a, b, c, d, q, r, s, T, U, V) \\ F^{10}(a, b, c, d, q, r, s, T, U, V) \end{pmatrix},$$

we have that the sequences of Taylor coefficients for the desired stable parameterization are given by the fixed point of Ψ .

Define the product spaces

$$\mathcal{X}^N = (X_{\nu,4}^N)^{10},$$

and

$$\mathcal{X}^\infty = (X_{\nu,4}^\infty)^{10},$$

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

Then, as in the previous examples, Ψ is decomposed as

$$\Psi(a, b, c, d, q, r, s, T, U, V) = \Psi^N(a, b, c, d, q, r, s, T, U, V) + T(a, b, c, d, q, r, s, T, U, V).$$

Let $(\bar{a}^N, \bar{b}^N, \bar{c}^N, \bar{d}^N, \bar{q}^N, \bar{r}^N, \bar{s}^N, \bar{T}^N, \bar{U}^N, \bar{V}^N) = \bar{x} \in \mathcal{X}^N$ denote the exact fixed point of Ψ^N , computed using the recursion relations. We seek a fixed point of the map $T(\cdot, \bar{x}): \mathcal{X}^\infty \rightarrow \mathcal{X}^\infty$.

Now, T is given by

$$T(H, \bar{x}) = \begin{pmatrix} T_1(H, \bar{x}) \\ T_2(H, \bar{x}) \\ T_3(H, \bar{x}) \\ T_4(H, \bar{x}) \\ T_5(H, \bar{x}) \\ T_6(H, \bar{x}) \\ T_7(H, \bar{x}) \\ T_8(H, \bar{x}) \\ T_9(H, \bar{x}) \\ T_{10}(H, \bar{x}) \end{pmatrix}$$

where the truncated maps now proliferate substantially.

Define the linear operators $A^{j2}, A^{j4}: X_{\nu,4}^\infty \rightarrow X_{\nu,4}^\infty$ by

$$(A^{jk}h)_{mn} = A_{mn}^{jk} h_{mn},$$

for $j = 1, 2, 3, 4$ and $k = 2, 4$, and the components

$$T_j(H, \bar{x}) = A^{j2} T_{11}(H, \bar{x}) + A^{j4} T_{12}(H, \bar{x}),$$

where

$$T_{11}(H, \bar{x}) = m_1 \bar{T}_{11}(H, \bar{x}) + m_2 \hat{T}_{11}(H, \bar{x}) + m_3 \tilde{T}_{11}(H, \bar{x}),$$

and

$$\begin{aligned} \bar{T}_{11}(H, \bar{x}) = & -\frac{3}{2} Q_{00}^{-5/2} (a_{00} - x_1) \left(\hat{C}(\bar{a}^N, \bar{a}^N) + \hat{C}(\bar{c}^N, \bar{c}^N) + \hat{L}(\bar{a}^N, h_1) + \hat{L}(\bar{c}^N, h_3) + \hat{N}(h_1, h_1) + \hat{N}(h_3, h_3) \right) \\ & - \frac{(a_{00} - x_1)}{Q_{00}} \left(\frac{3}{2} (\tilde{C}(\bar{T}^N, \bar{Q}^N) + \tilde{L}(\bar{T}^N, h_5) + \tilde{L}(\bar{Q}^N, h_8) \tilde{N}(h_5, h_8)) \right) + \\ & (\tilde{C}(\bar{Q}^N, \bar{T}^N) + \tilde{L}(\bar{Q}^N, h_8) + \tilde{L}(\bar{T}^N, h_5) \tilde{N}(h_8, h_5)) + \hat{C}(\bar{a}^N, \bar{T}^N) + \hat{L}(\bar{a}^N, h_8) + \hat{L}(\bar{T}^N, h_1) + \hat{N}(h_1, h_8) \end{aligned}$$

3.3.4 A brief closing example: validated Taylor integrators

4 Connecting Orbits and the Method of Projected Boundaries

We now return to the problem of connecting orbits for differential equations. We are ready to formulate the method of projected boundaries for differential equations.

4.1 Heteroclinic connections between equilibria of vector fields

Let $f: \mathbb{R}^N \rightarrow \mathbb{R}^N$ be a smooth vector field and $p, q \in \mathbb{R}^N$ be hyperbolic equilibria for f . Suppose that $P: D^{m_p} \rightarrow \mathbb{R}^N$ and $Q: D^{m_q} \rightarrow \mathbb{R}^N$ are parameterizations of the local unstable and stable manifolds at p and q respectively. Just as in the case of maps, we say that there is a short connection from p to q (relative to P and Q) if the equation

$$P(\theta) - Q(\phi) = 0,$$

has a solution $(\theta_*, \phi_*) \in D^{m_p} \oplus D^{m_q}$. Note however that in the case of differential equations solutions of this equation cannot be isolated. This is because any infinitesimal flow of an intersection point is again a point of intersection. Then we look for a solution on a fixed sphere in the unstable parameter space.

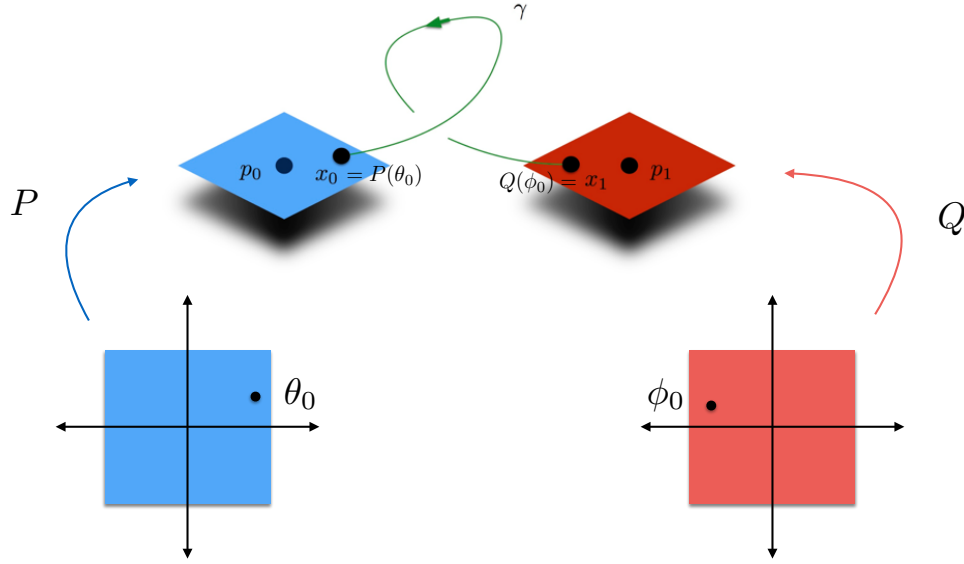


Figure 5: Projected boundaries for flows.

When the images of the local parameterizations P and Q do not intersect then the situation is a little more involved. Let $\Phi: \mathbb{R}^N \times \mathbb{R} \rightarrow \mathbb{R}^N$ denote the flow generated by f .

We define the map

$$F(\theta, \phi, T) = \Phi(P(\theta), T) - Q(\phi),$$

and seek θ_*, ϕ_*, T_* so that

$$F(\theta_*, \phi_*, T_*) = 0.$$

Then the orbit of $P(\theta_*)$ is heteroclinic from p to q . An equivalent operator not involving the flow Φ is given the integrated form, i.e. consider the operator $\mathcal{F}: \mathcal{X} \rightarrow \mathcal{X}$

$$\mathcal{F}(\alpha, \beta, T, x(t)) := \begin{pmatrix} Q(\phi(\beta)) - P(\theta(\alpha)) - \int_0^T f(x(\tau)) d\tau \\ P(\theta(\alpha)) + \int_0^t f(x(\tau)) d\tau - x(t) \end{pmatrix},$$

where $\phi(\beta)$ and $\theta(\alpha)$ are parameterizations of spheres in the parameter spaces of the unstable and stable parameterizations. Then $\mathcal{F}$ maps the space

$$\mathcal{X} := \mathbb{R}^n \oplus C([0, T], \mathbb{R}^N),$$

to itself.

Discretization of $C([0, T], \mathbb{R}^n)$: The function space must be discretized in order to solve the problem numerically. In [54, 4] for example the function space is discretized using piecewise linear splines. Spectral approximation using Chebyshev series is used in [55, 56]. Chebyshev series are “Fourier series for boundary value problems” and are amenable to a sequence space a-posteriori analysis as discussed in the Lecture of J.B. van den Berg [1].

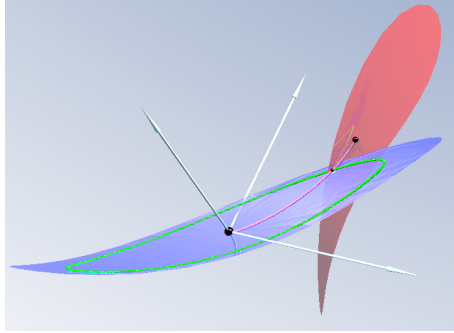


Figure 6: An illustration of a “short connection” for the Lorenz system. The green circle on the blue manifold illustrates the “phase condition” used to isolate the connecting orbit segment.

4.2 Example: Heteroclinic Connections, Patterns, and Traveling Waves

The following application appears in [55], and uses all of the techniques discussed above in order to solve an interesting pattern formation problem for PDEs. The pattern formation model

$$\partial_t U = -(1 + \Delta)^2 U + \mu U - \beta |\nabla U|^2 - U^3 \quad (40)$$

in the plane, i.e., $U = U(t, x) \in \mathbb{R}$, $t \geq 0$, $x \in \mathbb{R}^2$ was introduced in [57]. This equation generalizes the Swift-Hohenberg equation [58]. The additional term $\beta |\nabla U|^2$, reminiscent

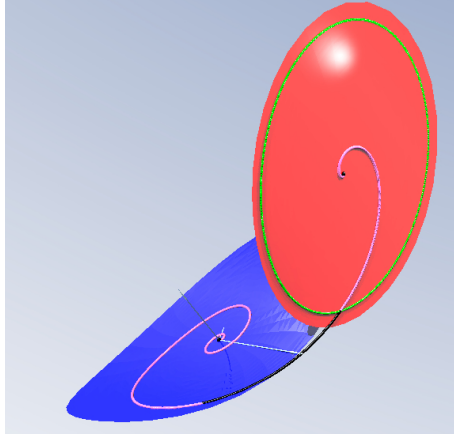


Figure 7: A long connection for Lorenz. Now the phase condition is the green circle on the red manifold. The black curve is the solution of the projected boundary value problem. The boundary value problem is discretized using piecewise linear splines. The pink curves are found using the conjugacy to the linear dynamics in the stable/unstable parameter spaces.

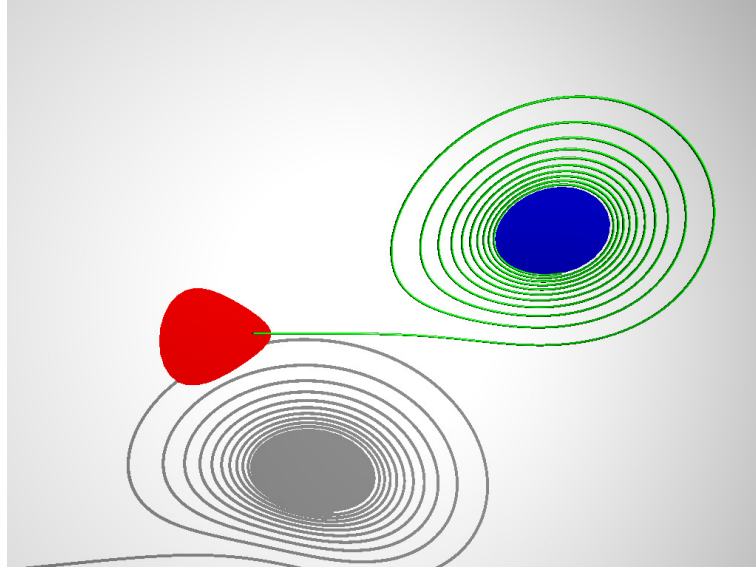


Figure 8: Long connection for the classic parameter values in Lorenz. The boundary value problem is discretized using Chebyshev series.

of the Kuramoto-Sivashinsky equation [51, 52], breaks the up-down symmetry $U \mapsto -U$ for $\beta \neq 0$. The Swift-Hohenberg equation acts as a phenomenological model for pattern formation in Rayleigh-Bénard convection, with $\beta \neq 0$ corresponding to a free boundary at the top of the convection cell, rather than a fixed one for the symmetric case $\beta = 0$ [59]. The parameter μ is related to the distance to the onset of convection rolls. For $\mu < 0$ the trivial equilibrium $U \equiv 0$ is locally stable, whereas for $\mu > 0$ it is unstable.

Depending on the parameter values the dynamics generated by (40) exhibit a variety of patterns besides simple convection rolls (a stripe pattern); in particular, hexagonal spot patterns are observed. In [60] it is shown that stable hexagonal patterns with small amplitude can be found for $\beta < 0$ only. In [57] the interplay between hexagons and rolls near onset (small μ) is examined using a weakly nonlinear analysis. Introducing a small parameter $\epsilon > 0$, the parameters are scaled as

$$\mu = \epsilon^2 \tilde{\mu}, \quad \beta = \epsilon \tilde{\beta}.$$

In the asymptotic regime $\epsilon \ll 1$, one can describe the roll and hexagonal patterns via amplitude equations. The seminal result in [57], based on spatial dynamics and geometric singular perturbation theory, is that heteroclinic solutions of the system

$$\begin{cases} 4B_1'' + \tilde{c}B_1' + \tilde{\mu}B_1 - \tilde{\beta}B_2^2 - 3B_1^3 - 12B_1B_2^2 = 0 \\ B_2'' + \tilde{c}B_2' + \tilde{\mu}B_2 - \tilde{\beta}B_1B_2 - 9B_1^3 - 6B_1^2B_2 = 0 \end{cases} \quad (41)$$

correspond to modulated front solutions, travelling at (rescaled) speed $\tilde{c}$, which corresponds to an asymptotically small velocity $\epsilon\tilde{c}$ in the original spatio-temporal variables. We note that the system (41) also shows up in the analysis of solidification fronts describing crystallization in soft-core fluids.

The variables B_1 and B_2 represent amplitudes of certain wave modes (slowly varying in the original variables). We refer to [57] for the details and the rigorous justification of the derivation. The dynamical system (41) has up to seven stationary points:

$$\begin{array}{ll} (B_1, B_2) = (0, 0) & \text{trivial state} \\ (B_1, B_2) = (B_{\text{rolls}}, 0) & \text{“positive” rolls} \\ (B_1, B_2) = (-B_{\text{rolls}}, 0) & \text{“negative” rolls} \\ (B_1, B_2) = (B_{\text{hex}}^+, B_{\text{hex}}^+) & \text{hexagons} \\ (B_1, B_2) = (B_{\text{hex}}^-, B_{\text{hex}}^-) & \text{“false” hexagons} \\ (B_1, B_2) = (-\tilde{\beta}/3, B_{\text{mm}}^\pm) & \text{two “mixed mode” states.} \end{array} \quad (42)$$

Here $B_{\text{rolls}} = \sqrt{\tilde{\mu}/3}$ and $B_{\text{hex}}^\pm = \frac{-\tilde{\beta} \pm \sqrt{\tilde{\beta}^2 + 60\tilde{\mu}}}{30}$ and $B_{\text{mm}}^\pm = \pm \frac{1}{3} \sqrt{\tilde{\mu} - \tilde{\beta}^2/3}$. Due to symmetry, there are two equilibria corresponding to rolls. We refer to [57] for a full discussion of all states and their stability properties. In this paper we consider the interplay between hexagons and rolls (both positive and negative).

While the weakly nonlinear analysis in [57] provided a vast reduction in complexity from (40) to (41), one outstanding issue remained: the heteroclinic solutions are difficult to analyse rigorously due to the nonlinear nature of the equations (41). In the limit $\tilde{c} \rightarrow \infty$ various connections could be found through a further asymptotic reduction [57], but for finite wave speeds the analysis of (41) was out of reach. In the present paper we introduce a computer-assisted, rigorous method for finding heteroclinic solutions for $\tilde{c} = 0$, i.e. standing waves. In particular we find connections between hexagons and rolls with *zero* propagation speed, i.e., the two patterns coexist.

The system (41) is gradient-like for $\tilde{c} \neq 0$, while it is Hamiltonian for $\tilde{c} = 0$. Hence, for hexagons and rolls to coexist their free energy must be equal, a situation that occurs when $\tilde{\mu} = \frac{7+3\sqrt{6}}{30} \tilde{\beta}^2$. We prove the following theorem, which settles the conjecture in [57] about the coexistence of hexagons and rolls:

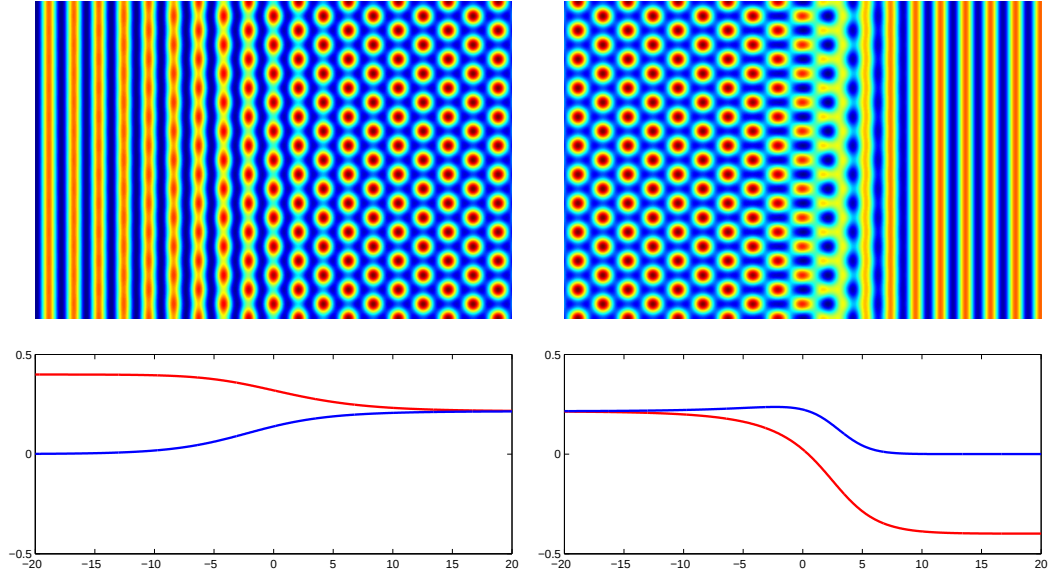


Figure 9: At the bottom are graphs of B_1 (red) and B_2 (blue) representing heteroclinic solutions of (41) that connect the hexagon state to the positive rolls (on the left) and negative rolls (and the right). The parameter values are $\tilde{c} = 0$, $\tilde{\mu} = \frac{7+3\sqrt{6}}{30}$ and $\tilde{\beta} = 1$, corresponding to the assumptions in Theorem 4.1. At the top we illustrate the corresponding stationary patterns of (40). We note that the two phase transitions from rolls to hexagons have distinctive features. On the left, the stripes (“positive” rolls) undergo pearling, which gradually leads to separation into spots (hexagons). On the right, the stripes (“negative” rolls) develop transverse waves, which break up into a block structure that then transforms into hexagonal spots. The figures of the patterns at the top were made using $\epsilon = \frac{1}{3}$. For smaller ϵ the transition between the two states is more gradual.

Theorem 4.1. *For parameter values $\tilde{\mu} = \frac{7+3\sqrt{6}}{30}\tilde{\beta}^2$ and $\tilde{c} = 0$ there exists a heteroclinic orbit of (41) between the hexagons and positive rolls, see (42), as well as a heteroclinic orbit between the hexagons and negative rolls.*

The heteroclinic solutions are depicted in Figure 9, together with the corresponding patterns of the PDE (40). These orbits thus represent two types of stationary domain walls between hexagons and rolls (spots and stripes). While each heteroclinic connection exists on a parabola in the $(\tilde{\beta}, \tilde{\mu})$ parameter plane, a parameter scaling reduces this to a single connecting orbit.

The problem is solved using a scheme very similar to the one illustrated above for the Lorenz system. So, an approximate solution u_{num} , obtained through a numerical calculation. We then construct an operator which has as its fixed points the heteroclinic solutions, and we set out to prove that this operator is a contraction mapping on a small ball around u_{num} in an appropriate Banach space. The ball should be small enough for the estimates to be sufficiently strong to prove contraction, but large enough to include both u_{num} (the center of the ball) and the solution (the fixed point). Qualitatively, considering the numerical approximations of solutions depicted as graphs in Figure 9, we can choose the radius of the ball so small that the solution is guaranteed to lie within the thickness of the lines.

Note: the rigorous justification in [57] of the link between the PDE (40) and the ODE

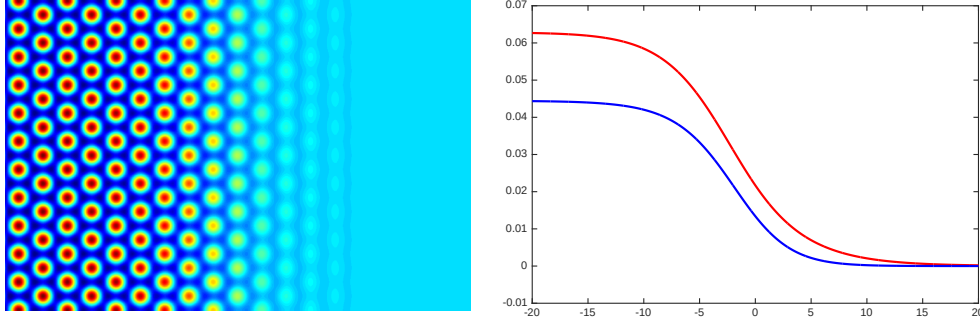


Figure 10: Left: co-existing hexagonal and trivial patterns for $\beta = 1$ and $\mu = -\frac{2}{135}$. Right: corresponding connecting orbit with u and v components in red and blue, respectively.

system (41) focuses on the case of nonzero propagation speed. The case of stationary fronts is only briefly mentioned in [57], since in that case the ODEs can be found more directly by a reduction to a spatial center manifold. In both the zero and nonzero speed setting, the rigorous derivation of (41) relies on a (weakly) nonlinear analysis to justify that one may ignore higher order terms in ϵ . Reciprocally, a heteroclinic solution of (41) is only guaranteed to survive in the full PDE system for small $\epsilon > 0$, if the orbit is a transversal intersection of stable and unstable manifolds. This is clearly *not* the case in (41) for $\tilde{c} = 0$, since the system is Hamiltonian. On the other hand, one should be able to exploit the “robustness” of the solution, which is a by-product of the contraction argument, to justify rigorously that existence of the front extends to the full system for small $\epsilon > 0$. However, since stationary coexistence (i.e. a pinned front) is a co-dimension one phenomenon, this needs to be viewed in the context of embedding the $\tilde{c} = 0$ case into a one parameter family of heteroclinic orbits with wave speed $\tilde{c} = \tilde{c}(\gamma)$. In that setting transversality is recovered.

Finally, to find a connection for $\tilde{c} = 0$ between the hexagons and the trivial state (the appropriate parameter value for coexistence is $\tilde{\mu} = -\frac{2}{135}\tilde{\beta}^2$), one needs to deal with resonances between eigenvalues in the spectrum of the trivial state. The resonance problem is treated in [40], and there the interested reader can find the computer assisted proof of the connection between the hexagons and the trivial state.

4.3 Heteroclinic connections between periodic orbits of vector fields

The method of projected boundaries is extended to connecting orbits between periodic orbits simply by replacing the parameterizations of the local stable/unstable manifolds of the fixed points by the parameterizations of the local stable/unstable manifolds of the periodic orbits.

Consider again $f: \mathbb{R}^N \rightarrow \mathbb{R}^N$ a smooth vector field and suppose that $\gamma_0: [0, T_0] \rightarrow \mathbb{R}^N$ and $\gamma_1: [0, T_1] \rightarrow \mathbb{R}^N$ are a pair of hyperbolic periodic orbits for f . We write

$$\frac{d}{d\theta}\gamma_0(\theta) = f[\gamma_0(\theta)] \quad \text{for all } \theta \in [0, T_0],$$

and

$$\frac{d}{d\phi}\gamma_1(\phi) = f[\gamma_1(\phi)] \quad \text{for all } \phi \in [0, T_1],$$

subject to the constraints

$$\gamma_0(0) = \gamma_0(T_0) \quad \text{and} \quad \gamma_1(0) = \gamma_1(T_1).$$

Suppose in addition that $P: [0, 2T_0] \times D^{m_0} \rightarrow \mathbb{R}^N$ and $Q: [0, 2T_1] \times D^{m_1} \rightarrow \mathbb{R}^N$ are parameterizations of the local unstable and stable manifolds of γ_0 and γ_1 respectively, i.e. we suppose that

$$P(\theta, v) \in W_{\text{loc}}^u(\gamma_0), \quad \text{for all } \theta \in [0, 2T_0], \quad v \in D^{m_0},$$

and

$$Q(\phi, w) \in W_{\text{loc}}^s(\gamma_1), \quad \text{for all } \phi \in [0, 2T_1], \quad w \in D^{m_1}.$$

Finally, assume that

$$(m_0 + 1) + (m_1 + 1) = N + 1,$$

i.e. that the dimension of the unstable manifold of γ_0 plus the dimension of the stable manifold of γ_1 is one more than the dimension of the phase space. This dimension count allows for the possibility of a transverse and isolated heteroclinic orbit from γ_0 to γ_1 .

Just as in the case of maps and equilibria of differential equations, we say that there is a short connection from γ_0 to γ_1 (relative to P and Q) if the equation

$$P(\theta, v) - Q(\phi, w) = 0,$$

has a solution

$$(\theta_*, v_*, \phi_*, w_*) \in [0, 2T_0] \times [0, 2T_1] \times D^{m_0} \times D^{m_1}.$$

Note however that in the case of differential equations solutions of this equation cannot be isolated. This is because any infinitesimal flow of an intersection point is again a point of intersection. Then we look for a solution on a fixed sphere in the unstable parameter space.

Suppose instead that the images of the local parameterizations P and Q do not intersect. Let $\theta(\alpha), \phi(\beta)$ be parameterizations of m_0, m_1 dimensional spheres, and $\Phi: \mathbb{R}^N \times \mathbb{R} \rightarrow \mathbb{R}^N$ denote the flow generated by f . Define the map

$$F(\alpha, \beta, v, w, T) = \Phi(P(\theta(\alpha), v), T) - Q(\phi(\beta), w),$$

and seek $\alpha_*, \beta_*, v_*, w_*, T_*$ so that

$$F(\alpha_*, \beta_*, v_*, w_*, T_*) = 0.$$

Then the orbit of $P(\theta(\alpha_*))$ is heteroclinic from p to q . Note that $F: \mathbb{R}^N \rightarrow \mathbb{R}^N$ is a balanced system of equations. Figure 11 illustrates the geometric idea behind the mapping F .

In some situations it is desirable to study an operator which does not explicitly involve the flow operator, and just as in the case of connections between equilibria we have the integrated form of the operator $\mathcal{F}: \mathcal{X} \rightarrow \mathcal{X}$

$$\mathcal{F}(\alpha, \beta, v, w, T, x(t)) := \begin{pmatrix} Q(\phi(\beta), w) - P(\theta(\alpha), v) - \int_0^T f(x(\tau)) d\tau \\ P(\theta(\alpha), v) + \int_0^t f(x(\tau)) d\tau - x(t) \end{pmatrix},$$

where $\phi(\beta)$ and $\theta(\alpha)$ are parameterizations of spheres in the parameter spaces of the unstable and stable parameterizations. Then $\mathcal{F}$ maps the space

$$\mathcal{X} := \mathbb{R}^{n_0+n_1} \oplus C([0, T], \mathbb{R}^N),$$

to itself.

Discretization of $C([0, T], \mathbb{R}^n)$: The function space must be discretized in order to solve the problem numerically and again splines [54, 4] and Chebyshev series [55, 56] are good options. Sequence space a-posteriori analysis as discussed in the Lecture of J.B. van den Berg [1] can be used to design computer assisted proofs.

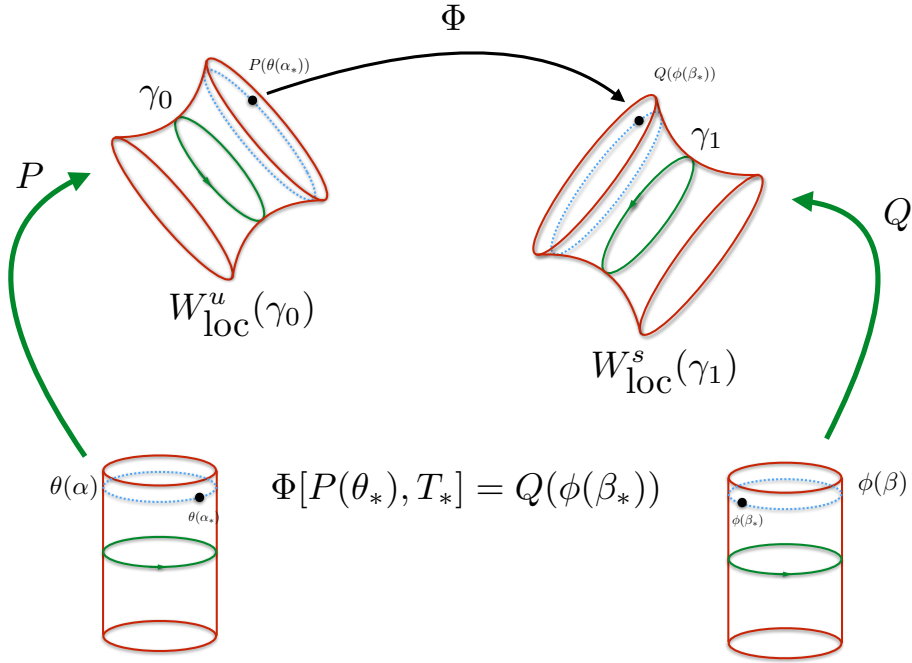


Figure 11: The method of projected boundaries for flows. We fix a boundary sphere on the stable/unstable manifolds and look for a time of flight which takes us from one sphere to another.

4.3.1 Examples

The method described above is useful for computing heteroclinic and homoclinic connecting orbits for differential equations. For example in Figure 12 we see a homoclinic connection orbit for a periodic orbit near the attractor in the Lorenz system. Figure 13 illustrates six different periodic orbits (in blue) and a number of heteroclinic and homoclinic orbits between them. The periodic orbits and their connections fill out the attractor fairly well. The connections are illustrated by a connectivity graph in Figure 14. The A-B symbols code the number of left/right winds around the two “eyes” of the Lorenz attractor. Lastly in Figure 15 we illustrate a homoclinic connecting orbit for the system of ten ODEs associated with the finite dimensional projection of the Kuramoto-Shivinsky equations.

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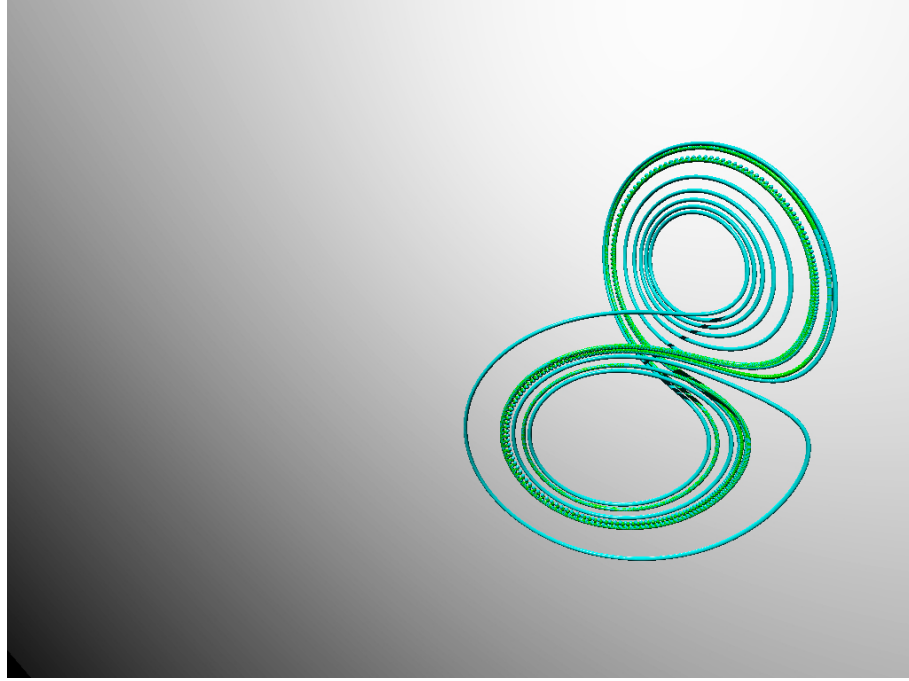


Figure 12: Homoclinic connection for a periodic orbit in the attractor of the Lorenz systems.

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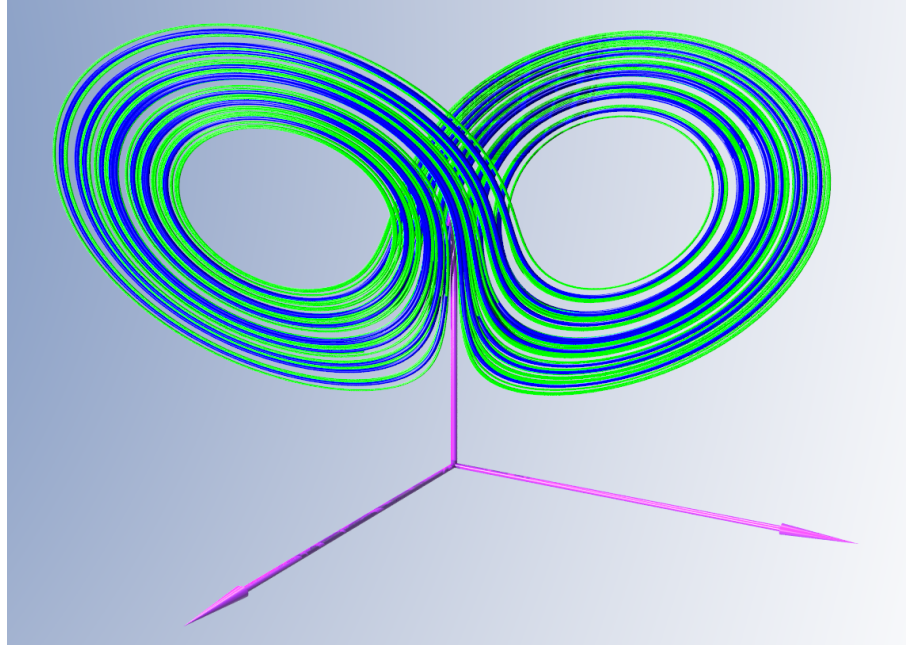


Figure 13: Heteroclinic and homoclinic connection between six different periodic orbits in the attractor of the Lorenz systems.

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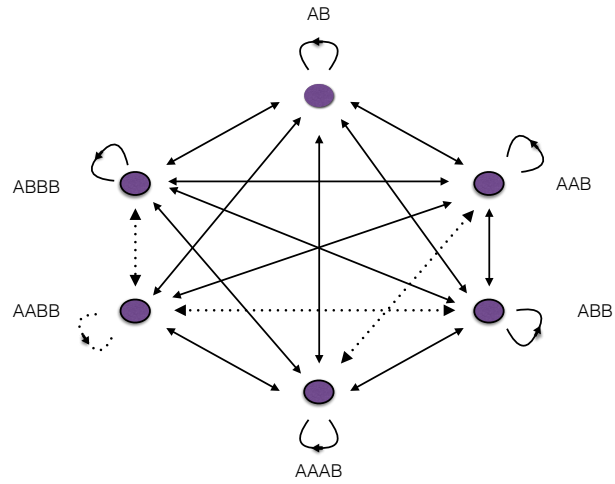


Figure 14: Directed graph depiction of the connections.

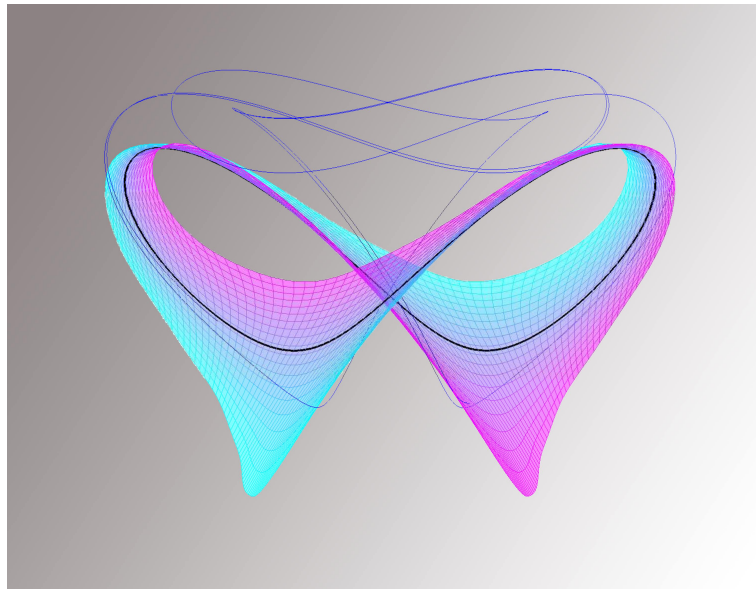


Figure 15: Homoclinic connection for a periodic orbit of the Kuramoto-Shivisinsky PDE, truncated to ten spatial modes.

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