Fourier-Taylor Parameterization of Unstable Manifolds for Parabolic Partial Differential Equations: Formalism, Implementation and Rigorous Validation

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May 26, 2016

Abstract

In this paper we study high order expansions of chart maps for local finite dimensional unstable manifolds of hyperbolic equilibrium solutions of scalar parabolic partial differential equations. Our approach is based on studying an infinitesimal invariance equation for the chart map that recovers the dynamics on the manifold in terms of a simple conjugacy. We develop formal series solutions for the invariance equation and efficient numerical methods for computing the series coefficients to any desired finite order. We show, under mild non-resonance conditions, that the formal series expansion converges in a small enough neighborhood of the equilibrium. An a-posteriori computer assisted argument proves convergence in larger neighborhoods. We implement the method for a spatially inhomogeneous Fisher's equation and numerically compute and validate high order expansions of some local unstable manifolds for morse index one and two. We also provide a computer assisted existence proof of a saddle-to-sink heteroclinic connecting orbit.

Keywords: Parametrization method, invariant manifolds, computer-assisted proof, contraction mapping, connecting orbit

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1 Introduction

Global analysis of nonlinear parabolic PDEs, from the dynamical systems point of view, begins by studying phase space landmarks such as stationary and periodic solutions. Once the existence, stability, and analytic properties of these are catalogued, one wants to understand how the landmarks fit together and organize the phase space. Classical dynamical systems theory for parabolic PDEs tells us that the phase space is organized by global invariant objects such as heteroclinic connecting orbits and inertial manifolds, and a necessary first step toward understanding these is to study the unstable manifolds of the landmarks. These unstable manifolds are necessarily finite dimensional, as the semi-flow generated by a parabolic PDE is compact.

The present work deals with the numerical approximation of unstable manifolds of equilibrium solutions of scalar parabolic PDE. Our approach is based on the parameterization method of [12, 13, 14], which provides a general functional analytic framework for studying *non-resonant* invariant manifolds in Banach spaces. We refer also to the overview in [34], where the Parameterization Method for parabolic PDE is discussed in great generality (indeed this reference suggests the approach of the present work). The idea is to formulate a functional equation whose solutions are chart maps for the unstable manifold. As suggested in [34], we exploit an infinitesimal conjugacy equation which depends explicitly on the form of the PDE but does not involve the flow. Because the parameterization satisfies a conjugacy, our method recovers the dynamics on the manifold in addition to the embedding. We develop a formal series solution of the conjugacy equation, and implement a numerical scheme for computing the coefficients of the series to any desired order.

High order approximations are useful for studying the unstable manifold far from its equilibrium. Yet numerically evaluating a high order expansion far from the equilibrium raises concerns about accuracy. The main result of the present work is a computer assisted argument which provides mathematically rigorous error bounds for high order approximations. The argument does not require restricting the approximation to a small neighborhood of the equilibrium. Rather, we develop a-posteriori tools which use in a fundamental way that the numerical representation of the manifold approximately solves a functional equation.

The problem is infinite dimensional, and in order for our argument to succeed it is critical that we manage a number of errors introduced by the finite dimensional truncations. In the present work this truncation error analysis is facilitated by two observations. First, the compactness/smoothing properties of the parabolic PDE allow us to control the spatial/spectral truncation. Indeed the computer assisted proofs implemented in Section 4 make substantial use of the fact that the PDE is formulated on a geometrically simple domain, where the eigenexpansion of the differential operator is given explicitly in terms of Fourier (cosine) series. Second, the Parameterization Method admits certain free parameters (namely the scalings of the unstable eigenvectors) in the formulation of conjugacy equation, and these scalings control the decay rate of the formal series coefficients. We exploit this control over the decay to insure that the truncated series expansion satisfies some prescribed error tolerance. The second consideration is fundamental to the Parameterization Method, and has nothing to do with the particular eigenbasis for the PDE or even the fact that we consider parabolic problems.

Remark 1.1 (Computer assisted proof for equilibria of PDEs)**.** Establishing existence and stability of stationary solutions to PDEs is a subtle business. When the nonlinearities are strong and the PDE is far from a perturbative regime, it may be impossible to carry out this analysis analytically. Numerical simulations provide valuable insight into the dynamics of PDEs, and in recent years substantial effort has gone into developing computer assisted methods of proof which validate simulation results.

A thorough review of the literature on computer assisted proof for of PDEs would lead us far afield of the present discussion. We refer to the works of [99, 98, 94, 3, 5, 7, 77, 76, 66, 28, 87, 10, 56] for fuller discussion of computer assisted proof for equilibrium solutions of PDEs, and also [89, 64, 75, 5, 24] for more discussion of techniques for validated computation of eigenvalue/eigenvector pairs for infinite dimensional problems. Let us also mention the review articles of [85, 73, 59] and the book of [83] for broader overview of the field. While the list of references given above is far from exhaustive (in particular the list ignores the growing literature on computer assisted proof for periodic orbits of PDEs), it is our hope that these works and the references discussed therein could help the interested reader wade into the literature.

Remark 1.2 (Computer assisted proof for unstable manifolds in finite dimensions)**.** It must also be noted that the present work builds on a growing body of literature devoted to validated numerical methods for studying stable/unstable manifolds of equilibrium solutions for finite dimensional vector fields. A thorough review is beyond the scope of the present work, and we direct the reader to [6, 2, 96, 93, 86, 57, 21, 19, 68, 79, 11, 20] for more complete discussion of the literature. This list ignores works devoted to validated numerical methods for stable/unstable manifolds of discrete time dynamical systems and also validated methods for computing other types of invariant manifolds (for example invariant tori and their stable/unstable manifolds). Again, we refer to the review articles mentioned in Remark 1.1.

1.1 A family of examples

In order to minimize the proliferation of notational difficulties, we consider a fixed specific class of scalar parabolic equations.

More precisely, assume the PDE is of the form

$$u_t = Au + \sum_{n=1}^{s} c_n(x)u^n, \quad u = u(x,t) \in \mathbb{R}, \quad (x,t) \in I \times \mathbb{R}_+ \tag{1}$$

where $I \subset \mathbb{R}$ is a compact interval, A is a parabolic differential operator, s is the order of the nonlinearity and $c_n(x)$ are the smooth coefficient functions possibly depending on the spatial variable x. Using an orthonormal basis corresponding to the eigenfunctions of A for the particular domain and boundary conditions we translate (1) into a countable system of ODEs.

The resulting system of ODEs, projected onto the eigenbasis, is of the form

$$a_k'(t) = \mu_k a_k + \sum_{n=1}^{s} \sum_{\substack{\sum k_i = k \\ k_i \in \mathbb{Z}}} (c_n)_{|k_1|} a_{|k_2|} \cdots a_{|k_{n+1}|} \stackrel{\text{def}}{=} g_k(a) \quad k \geq 0 \tag{2}$$

where μ_k are the eigenvalues of L and $a = (a_k)_{k \geq 0}$ are the expansion coefficients of u in the respective eigenbasis. We use the shorthand notation $a' = g(a)$ for (2). To define the unstable manifold we are interested in, assume $\tilde{a}$ to be given such that $g(\tilde{a}) = 0$. Its unstable manifold is given by

$$W^u(\tilde{a}) = \{a_0 : \exists \text{ solution } a(t) \text{ of } (2) \ : a(0) = a_0 \quad \lim_{t \to -\infty} a(t) = \tilde{a}\}. \tag{3}$$

It is a classical fact that for scalar parabolic PDEs of the form (1), $W^u(\tilde{a})$ is a finite dimensional manifold [81].

As a concrete application consider the boundary value problem for the following reaction diffusion equation on a one-dimensional bounded spatial domain with Neumann boundary conditions:

$$\begin{aligned} u_t &= u_{xx} + \alpha u(1 - c_2(x)u), \quad (x,t) \in [0, 2\pi] \times \mathbb{R}, \\ u_x(0,t) &= u_x(2\pi, t) = 0 \quad \forall t \geq 0 \end{aligned} \tag{4}$$

Here $\alpha > 0$ is a real parameter and $c_2(x) > 0$ is a spatial inhomogeneity. We consider both the case $c_2(x) = 1$ and $c_2(x)$ non-constant, specifically a Poission kernel. For notational convenience we drop the index 2 and refer to the spatial inhomogeneity as $c(x)$. Moreover the parameter α has the role of an eigenvalue parameter to consider different dimension configuration of the unstable manifolds at hand. The equation is known as Fisher's equation, or as the Kolmogorov-Petrovsky-Piscounov equation, and has applications in mathematical ecology, genetics, and the theory of Brownian motion [40, 1, 65].

1.2 Methodology of the present work: sketch of the approach

Let $\tilde{a}$ be an equilibrium solution of (2) with known Morse index and eigendata. More precisely suppose that $Dg(\tilde{a})$ has exactly d unstable eigenvalues $\tilde{\lambda}_j$. In the present work we assume that the unstable eigenvalues are real, and that each has multiplicity one. Then let $\tilde{\xi}_j$, $1 \le j \le d$ denote an associated choice of unstable eigenvectors, i.e. assume that

$$D g(\tilde{a})\tilde{\xi}_j = \tilde{\lambda}_j \tilde{\xi}_j \quad j = 1, \ldots, d. \tag{5}$$

In practice the first order data is not explicitly given, and we perform a sequence of preliminary computer assisted proofs in order to verify that the assumptions are satisfied. We refer the reader again to the references mentioned in Remark 1.1 above, and also to Sections 2.1 and 4 of the present work for more refined discussion of these preliminary considerations.

We are now ready to give an informal description of the Parameterization Method for unstable manifolds. See also [34]. Let

$$\mathbb{B}_1 := \{(\theta_1, \ldots, \theta_d) \in \mathbb{R}^d \colon |\theta_j| < 1, 1 \le j \le d\}.$$

We seek solutions of the functional equation

$$g(P(\theta_1, \ldots, \theta_d)) = \tilde{\lambda}_1 \theta_1 \frac{\partial}{\partial \theta_1} P(\theta_1, \ldots, \theta_d) + \ldots + \tilde{\lambda}_d \theta_d \frac{\partial}{\partial \theta_d} P(\theta_1, \ldots, \theta_d), \tag{6}$$

for all $\theta = (\theta_1, \ldots, \theta_d) \in \mathbb{B}_1$ satisfying the linear constraints

$$P(0) = \tilde{a} \tag{7a}$$

$$\frac{\partial}{\partial \theta_j} P(0) = \tilde{\xi}_j, \quad \text{for } 1 \le j \le d. \tag{7b}$$

Note that Equation (6) is actually a Banach spaced valued partial differential equation (or a system of infinitely many scalar partial differential equations when the Banach space is a sequence space). We refer to Equation (6) as *the invariance equation*, and note that it is expressed more concisely as

$$(g \circ P)(\theta) = DP(\theta) A_u \theta. \tag{8}$$

Here A_u is the $d \times d$ diagonal matrix of unstable eigenvalues. Equation (8) makes it clear that the vector field g is tangent to the image of P, i.e. P parameterizes an invariant manifold. Indeed we have the following lemma, which makes precise the claim that P recovers the dynamics on the manifold.

Lemma 1.3. *Assume that P solves* (6) *and satisfies the first order constraints of* (7)*. Then for every $\theta \in \mathbb{B}_1$ the function*

$$a(t) = P(\exp(A_u t)\theta) \tag{9}$$

solves $a' = g(a)$ for all $t \in (-\infty, T(\theta))$ for a positive time $T(\theta)$. In particular $\lim_{t \to -\infty} a(t) = \tilde{a}$.

The proof is obtained by direct computation using that $\text{real}(\lambda_i) > 0$ for $i = 1, \ldots, d$ (see Lemma 2.1 in [84] and Lemma 2.6 in [79] for elementary proofs in finite dimensional contexts).

In order to obtain an approximate solution of Equation (6) we adopt the power series ansatz

$$P(\theta) = \sum_{|m|=0}^{\infty} p_m \theta^m. \tag{10}$$

Here $m \in \mathbb{N}^d$ is a multi-index, $\theta^m := \theta_1^{m_1} \cdots \theta_d^{m_d}$, and $|m| = m_1 + \ldots + m_d$. Plugging (10) into (6) and matching like powers of θ leads to a system of infinitely many coupled nonlinear equations for the Taylor coefficients $\{p_m\}_{m\in\mathbb{N}^d}$. The details are given in Section 3.3, in particular see Equation (40).

Truncating leads to a system of finitely many coupled nonlinear scalar equations which are solved (for example) by a numerical Newton method, leading to approximate Taylor coefficients $\{\bar{p}_m\}_{|m|=0}^M$ where $p_m \in \mathbb{R}^K$ for each $0 \le |m| \le M$. The numerical procedure is discussed in Section 3.4, with application in Section 4. After this computation we have a finite dimensional approximate parametrization of the form

$$P^{MK}(\theta) = \sum_{m\in\mathcal{F}_M} \bar{p}_m \theta^m. \tag{11}$$

Remark 1.4 (Rescalings)**.** The choice of domain $\mathbb{B}_1$ deserves some explanation. We will see in Section 3 that solutions of Equation (6) are unique up to the choice of the eigenvectors $\xi_1, \ldots, \xi_j$, so that rescaling the eigenvectors leads to parameterizations of larger or smaller local portions of the unstable manifold. On the other hand, one can imagine controlling the size of the local portion by fixing the scalings of the eigenvectors (say with unit norm) and varying instead the size of the domain of P. The two approaches are dynamically equivalent. Nevertheless rescaling the eigenvectors allows us to control also the decay rate of the Taylor coefficients of P, and this stabilizes the problem numerically. Hence we fix once and for all the domain $\mathbb{B}_1$, and ask in a particular problem "what is the best choice of the scalings for the eigenvectors?" The answer depends on the problem at hand and is only answered after some numerical calculations. We return to this question in Section 4.

We now come to the question: how good is this approximation? Define the defect or *a-posteriori error* for the problem by

$$\epsilon_{MN} := \sup_{\theta\in\mathbb{B}_1} \|g[P^{MN}(\theta)] - DP^{MN}(\theta)A_u\theta\|,$$

in an appropriate norm to be specified later (in practice we also "pre-condition" the defect with a smoothing approximate inverse. See Section 2.1). Our task is to establish sufficient conditions, depending on g, $\tilde{a}$, $\tilde{\lambda}_1, \ldots, \tilde{\lambda}_d$, P^{MN}, and the underlying Banach space, so that $\epsilon_{MN} \ll 1$ implies the existence of a true solution P of Equation (6) on $\mathbb{B}_1$. In fact our argument will show that

$$\sup_{\theta\in\mathbb{B}_1} \|P(\theta) - P^{MK}(\theta)\| \le r_P, \tag{12}$$

where P is the true solution of Equation (6), and the explicit value of r_P (which depends on the defect) comes out of our argument. It is critical that we formulate sufficient conditions which can be checked via carefully managing floating point computations. Floating point checks of the hypotheses employ *interval arithmetic* in order to guarantee that we obtain mathematically rigorous results [74, 80, 83].

In order to formulate the sufficient conditions just discussed we implement a computer assisted a-posteriori scheme which has its roots in the the seminal work of [60, 32] on the Feigenbaum conjectures. We study the equation

$$f(P(\theta)) = (g\circ P)(\theta) - DP(\theta)A_u\theta = 0,$$

via a modified Newton-Kantorovich argument. More precisely, we show that the "Newton-like" operator

$$T(P) := P - Af(P),$$

is a contraction on a ball of radius r_P in the Banach space about the approximation solution P^{MN}. Here A is a problem dependent approximate inverse of $Df(P^{MN})$, which we choose based on both numerical and analytic considerations. The argument is formalized in Section 2.1, with implementation discussed in Section 4.

1.3 Discussion

In practice we learn that the argument outlined in Section 1.2 succeeds or fails only after attempting the a-posteriori validation, and these attempts are computationally expensive. With this in mind we include the a-priori Theorem 3.2 in Section 3.1. The theorem says that, given some mild non-resonance conditions between the unstable eigenvalues (assumptions which are made precise in Definition 3.1) there exist choices of eigenvectors so that Equation (6) has a solution. The solution is unique up to the choice of the eigenvectors, but a-priori may parameterize only a small portion of the local unstable manifold near the equilibrium. Our Theorem is an infinite dimensional generalization of the results in Section 10 of [14].

The proof of the Theorem 3.2 assures existence only for a small enough choice of the scalings of the unstable eigenvectors. On the other hand, in Section 3.1 we see that the size of the local manifold parameterized by P is determined in a rather explicit way by the size of these scalings. In applications we would like to choose the eigenvector scalings as large as possible, so that we learn more about the unstable manifold far from the equilibrium solution. This desire must be weighed against the fact that for larger choices of the scalings we risk loosing control of the convergence of the series.

Viewed in this light, the tools of the present work provide a mathematically rigorous computer assisted method for pushing the existence results as far as possible in specific applications. Since the desired parameterization exists in a small enough neighborhood of the equilibrium solution by Theorem 3.2, our argument has a "continuation" flavor (the continuation parameters being the eigenvector scalings, which in turn govern the size of the local unstable manifold in phase space). The novelty is that we care only about rigorous results at the end of the continuation. We argue in Sections 3 and 4 that expensive validation computations can be postponed until we are all but certain the computer aided proof will succeed. These considerations are also discussed at length for finite dimensional vector fields in [11].

Remark 1.5 (Extensions of the a-priori results)**.** A word about the technical assumptions of Theorem 3.2. In addition to the non-resonance conditions postulated in Definition 3.1, Theorem 3.2 postulates that each of the unstable eigenvalues is real and that each has multiplicity one. Moreover we assume that the nonlinearity is given by an analytic function.

We remark that these assumptions are technically convenient, and should not be interpreted as fundamental restrictions. For example real invariant manifolds associated with complex conjugate eigenvalues are treated exactly as discussed in [61]. Indeed it is possible to remove completely the non-resonance and multiplicity conditions, as long as there are "spectral gaps" (eigenvalues bounded away from the imaginary axis). The necessary modification is to conjugate the parameterization to a polynomial, rather than a linear vector field. The reader interested in this technical extension could consult the work of [79] for the case of finite dimensional vector fields, and the work of [12] for the case of infinite dimensional maps.

One can also ease the regularity requirements, and assume only that the nonlinearities are only C^k rather than analytic as in [12, 13]. This however changes substantially the flavor of the validation scheme developed here, which exploits analyticity in a fundamental way. More precisely, the analyticity of the nonlinearity allows us to look for analytic parameterizations, which in turn allows us to study the Taylor coefficients in a Banach space of rapidly decaying infinite sequences. If instead we expand the manifold as a finite Taylor polynomial plus a unknown remainder function, then the a-posteriori analysis for the remainder function must be carried out in function space.

Let us also mention that, following the work of [12, 13, 14], it might be possible to extend the methods of the present work to problems with continuous spectrum such, as PDEs on unbounded domains. The extensions remarked upon above are not considered further in the present work.

Remark 1.6 (Extension of the formal series results: non-polynomial nonlinearities and systems of scalar parabolic PDE)**.** While Theorem 3.2 is formulated for general analytic nonlinearities, the formal solution of Equation (6) developed in Section 3.3 is derived under the further assumption of polynomial nonlinearity. This is not as restrictive as it might seem upon first glance, as transcendental nonlinearities given by elementary functions can be treated using methods of automatic differentiation.

A thorough discussion of automatic differentiation as a tool for semi-numerical computations and computer assisted proof is beyond the scope of the present work, and we refer the interested reader to the books [58, 83] and also to the work of [43, 63] as an entry point to the literature. In terms of the present discussion the relevant point is that automatic differentiation allows us to develop formal series evaluation of non-polynomial nonlinearities by appending additional differential equations. When the nonlinearity is among the so called "elementary functions of mathematical physics" the appended equation is polynomial, and we end up with a system of scalar parabolic PDEs with polynomial nonlinearities.

Extending the methods of the present work to such systems will make an interesting topic for a future study. Such a study might treat automatic differentiation and non-polynomial nonlinearities as an application, but could also discuss unstable manifolds for systems of reaction diffusion equations in general. These topics are not pursued further in the present work.

Remark 1.7 (Spectral versus finite element bases)**.** A more fundamental limitation of the present work is that, when it comes to the implementation details in Section 4, we restrict our attention to the case of spectral bases for the spatial dimension of the PDE. This allows us to exploit a sequence space analysis which is very close to the underlying numerical methods, and which for example avoids the use of Sobolev inequalities and interpolation estimates. However such sequence space implementation is only possible on simple domains where the eigenfunction expansion of the linear part of the PDE is explicitly known.

An useful and nontrivial extension of the techniques of the present work would be to implement an a-posteriori argument for the Parameterization Method for unstable manifolds of parabolic PDEs using finite element basis. In such a scheme the sequence space calculus exploited in the present work would be replaced classical Sobolev theory. We believe that this extension is both natural and plausible, and for this reason we frame the a-priori existence results and discussion of formal series in Section 3 in the setting of a general Banach algebra.

Remark 1.8 (The role of a-priori spatial regularity)**.** It is worth noting that, strictly speaking, we do not need to know a-priori the regularity of the unstable manifold: rather this is a convenience. Indeed, if our method succeeds then we obtain regularity results a-posteriori. In practice it is helpful to have an "educated guess" concerning the regularity of the manifold, as this informs the choice of norm in which to frame the computer assisted proof. For more nuanced discussion of computer assisted proof in sequence spaces associated with functions in weaker regularity classes we refer to [62].

This suggests another interesting direction of future study, namely to extend the methods of the present work to infinite dimensional settings such as state dependent delays, where even the a-priori existence of solutions is often in question. More discussion of the computer as a tool for studying breakdown of regularity of invariant objects can be found in the works of [15, 47, 36, 35].

Remark 1.9 (Implementation)**.** We provide full implementation details for the example of a spatially inhomogeneous Fisher equation. The implementation is discussed in Section 4, and involves the derivation of a number of problem dependent estimates. These estimates are then used in order to show that the Newton like operator is a contraction in a neighborhood of our numerical approximation.

We choose not to suppress the derivation of these bounds for two reasons. The first is that their inclusion gives the present work a degree of plausible reproducibility. Indeed the estimates in Section 4 can be viewed (more or less) as pseudo-code for the computer programs which validate our approximation of the unstable manifold. The second reason is that including a few pages of estimates makes entirely transparent the role played by the computer in our arguments. One sees that (after the initial stage of numerical approximation) the computer is primarily used to add and multiply long lists of floating point numbers. If the results satisfy certain completely explicit inequalities then we have our proof.

Remark 1.10 (Computer assisted existence proofs for connecting orbits of parabolic PDEs)**.** As already suggested in the introduction, our primary motivation for validated computation of local unstable manifolds is our interest in global dynamics, for example heteroclinic connecting orbits between equilibrium solutions of parabolic PDE. In order to demonstrate that the methods of the present work are of value in this context, we prove in Section 4.3 the existence of a saddle-to-sink connecting orbit for a Fisher equation. More precisely we establish the existence of an orbit which connects an equilibrium solution of finite non-zero Morse index to a fully stable equilibrium solution.

Nevertheless, we want to be clear that the computer assisted existence proof in Section 4.3 is a "proof of concept", and there remains much work to be done if one wants to develop general computer assisted analysis for transverse connecting orbits for PDEs. In particular, the computations in Section 4.3 establish connections only for orbits asymptotic to a sink, i.e. we compute explicit lower bounds on the size of an absorbing neighborhood of the stable equilibrium state, and then we simply check that our parameterized local manifold enters this neighborhood.

In general one has to contend with saddle-to-saddle connections, in which case a more subtle analysis of the (non-zero co-dimension) stable manifold is needed. The non-resonance conditions required for the Parameterization Method seem to rule out the study of finite co-dimension manifolds in infinite dimensional problems. Nevertheless, error bounds for the stable manifold could be obtained by implementing the geometric methods of [96, 22, 95, 27], or adapting the functional analytic approach of [30] to the setting of parabolic PDEs. We refer to the work of [30] for more discussion of computer assisted existence proofs for saddle-to-saddle connections in infinite dimensions (though [30] treats explicitly only the case of infinite dimensional maps).

We also remark that in general it is not enough to establish the existence of a "short-connection" as we do in Section 4.3. By a short connection we mean a connecting orbit which is described using only parameterizations of the local stable and unstable manifolds (this terminology is discussed further in [61]). Instead, the typical situation is that the rigorously validated local unstable and stable manifolds do not intersect. In this case a computer assisted existence proof for a connecting orbit requires the solution of a two point boundary value problem whose solution is an orbit segment beginning on the unstable and ending on the stable manifold. We refer to the works of [92, 91, 90, 25, 82, 3, 6, 53, 61, 88, 86] for more discussion of computer assisted proof of saddle-to-saddle connections in finite dimensional problems.

Finally we direct the interested reader to the work of [95, 27], where another approach to computer assisted proof for connecting orbits in parabolic PDE is given. The computer aided proofs of connecting orbits in the references just cited are similar in spirit to those developed in the present work, with at least one important difference. While the authors of the work just cited also follow trajectories on a local unstable manifold until they enter a trapping region of a sink, the orbit is propagated via mathematically rigorous numerical integration of the PDE. Then their approach could be used to study substantially longer connecting orbits than those obtained with our proof of concept in Section 4.3. More thorough discussion of rigorous integration of PDEs can be found in the works of [97, 26, 4].

At the same time, we remark that the authors of [95, 27] represent the unstable manifold locally using a linear approximation and obtain validated error bounds on this approximation via geometric arguments based on cone conditions. An interesting avenue of future study might be to combine the high order methods of the present work with methods for rigorous numerical integration of parabolic PDEs as developed in [95, 27, 97, 26, 4] in order to prove the existence of connecting orbits in more challenging applications.

The paper is organized as follows. First in Section 2.2 we discuss the Banach spaces we will be working on. In Section 2.1 we discuss the method we use to validate the solution to a zero finding problem $f(x) = 0$ together with the analysis of the linear eigendata of $Df(x)$. Specifically in Section 2.1 we discuss the radii polynomial method from [28]. In Section 2.3 we demonstrate how to make sure the accurate Morse index of $Df(x)$ is obtained given an approximate derivative $A^\dagger$ whose spectrum is understood completely. In Section 3.4 we describe how to setup a zero finding problem whose solution corresponds to the power series coefficients of a parametrization of the unstable manifold of a hyperbolic fixed point. In Section 4 we showcase our method in examples. We discuss Fisher's equation from (4). In Section 4.1 we describe how to compute and validate the first order data at an equilibrium in the specific example, including the validation of the eigendata and the Morse index. In Section 4.2 we compute a one and two dimensional unstable manifold for a non-trivial equilibrium and the origin respectively. In Section 4.3 we discuss the computer-assisted proof of a short connecting orbit from a fixed point of Morse index 1 to Morse index 0.

All computer programs used to obtain the results in this work are freely available at the papers home page [78].

2 Background

2.1 A-posteriori analysis for nonlinear operators

Let X and X' be Banach spaces and $f\colon X \to X'$ be a smooth map. Throughout the sequel we are interested in the zero finding problem

$$f(x) = 0.$$

Suppose we have in hand an approximate solution $\bar{x}$. In our context $\bar{x}$ is usually the result of a numerical computation. Our goal is to prove that there exists a true solution nearby.

To this end let A be an injective (one-to-one) bounded linear operator having that

$$Af(x), ADf(x) \in X$$

for all $x \in X$. Heuristically we think of A as being a smoothing approximate inverse for $Df(\tilde{x})$. In other words, we ask neither that $f(x)$ is a self map or that $Df(x)$ is a bounded linear operator. Rather, we allow that f and $Df(x)$ may be unbounded operators and that A "smooths" f and Df, bringing the composition back into X.

Now we define the Newton-like operator

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

and note that the fixed points of T are in one-to-one correspondence with the zeros of f. We use the Banach Fixed Point Theorem on a ball of radius r around an approximate solution $\bar{x}$ to show that that T has a unique fixed point in said ball.

Our approach follows that of [94], in that we consider the radius r as one of our unknowns, and find a suitable range of radii such that T is a contracting selfmap on the corresponding balls (rather than guessing a value for the radius r and applying the Newton-Kantorovich Theorem). This is referred to by some authors as the radii-polynomial approach, and in addition to the work just cited we refer the interested reader also to the work of [28, 87] and the references discussed therein.

Definition 2.1. Y, Z-bounds and the radii polynomial
Recall the fixed point operator T specified in (44) corresponding to the zero finding map (41). Assume an approximate zero $\bar{x}$ to be given. Let us define the following bounds $Y \in \mathbb{R}$ and $Z(r) \in \mathbb{R}[r]$:

1. the Y-bound $Y \in \mathbb{R}$ measuring the residual:
$$\|T(\bar{x}) - \bar{x}\| \leq Y \tag{13}$$

2. the r-dependent Z-bound measuring the contraction rate on a ball of (variable) radius r:
$$\sup_{u,v \in \mathbb{B}_1} \|DT(\bar{x} + ru)rv\| \leq Z(r) \tag{14}$$

Define the polynomial
$$\beta(r) = Y + Z(r) - r. \tag{15}$$

The benefit of Definition 2.1 is the following Lemma.

Lemma 2.2. *Assume an approximate zero $\bar{x}$ of f defined in* (41) *to be given. If $\beta(r) < 0$ with β defined in* (15) *for a positive radius $r_{\bar{x}}$, then T given by* (44) *is a contraction on $\mathbb{B}_{r_{\bar{x}}}(\bar{x})$. Hence there is a unique zero $\tilde{x}$ with $\tilde{x} \in \mathbb{B}_{r_{\bar{x}}}(\bar{x})$.*

A proof of this lemma has appeared in many places. See for example [28]. The decisive feature of the condition $\beta(r) < 0$ in our context is that after deriving explicit expressions for the bounds in (13) and (14) are it can be checked rigorously by a computer using interval arithmetic.

2.2 Norms and spaces

We are interested in solutions of PDEs whose spectral representation have coefficients with very rapid decay. To be more precise let us consider

$$\ell^1_\nu = \left\{ a = (a_k)_{k \geq 0}, a_k \in \mathbb{R} : \quad |a|_\nu \stackrel{\text{def}}{=} |a_0| + 2\sum_{k=1} |a_k|\nu^k < \infty \right\}. \tag{16}$$

Denote the induced operator norm by $|\cdot|_{\ell^1_\nu}$. Note that if $\nu > 1$ and $a \in \ell^1_\nu$ the function

$$u(x) = a_0 + 2\sum_{k=1}^{\infty} a_k \cos(kx),$$

is real analytic and extends to a periodic and analytic function on the complex strip of width $\log(\nu)$. Moreover we have that

$$\|u\|_{C^0([0,2\pi])} := \sup_{x\in[0,2\pi]} |u(x)| \leq |a|_\nu,$$

i.e. the ℓ^1_ν norm provides bounds on the supremum norm of the corresponding analytic function.

ℓ^1_ν is a Banach algebra under the discrete convolution operation $a * b$ given by

$$(a*b)_k = \sum_{\substack{k_1+k_2=k \\ k_i\in\mathbb{Z}}} a_{|k_1|}b_{|k_2|}. \tag{17}$$

with $a, b \in \ell^1_\nu$. For later use we define the notation a^{*n} for $\underbrace{a*\cdots*a}_{n \ \text{times}}$.

When we consider unstable manifolds for PDEs we are interested in analytic functions taking their values in ℓ^1_ν as just defined. Such functions have convergent power series representations of the form

$$P(\theta, x) = \sum_{|m|=0}^{\infty} \left(p_{m0} + 2\sum_{n=1}^{\infty} p_{mk}\cos(kx) \right) \theta^m, \tag{18}$$

where $m = (m_1, \ldots, m_d) \in \mathbb{N}^d$ is a d-dimensional multi-index, $\theta = (\theta_1, \ldots, \theta_d) \in \mathbb{C}^d$ and $\{p_{mk}\}_{m\in\mathbb{N}^d k\in\mathbb{N}}$ is a sequence of *Fourier-Taylor* coefficients (more specifically *cosine-Taylor* coefficients in this case).

We shorten this notation and write $\{p_m\}_{m\in\mathbb{N}^d}$, where for each $m \in \mathbb{N}^d$ we have $p_m \in \ell^1_\nu$. Then we are led to consider the multi-sequence space

$$X^{\nu,d} = \left\{ p = (p_m)_{m\in\mathbb{N}^d} : p_m \in \ell^1_\nu \text{ and } \|p\|_\nu \overset{\text{def}}{=} \sum_{|m|=0}^{\infty} |p_m|_\nu < \infty \right\}, \tag{19}$$

of power series coefficients in (10). We will drop the superscript d whenever the dimension of the unstable manifold at hand is clear from the context. We note that if $p \in X^\nu$ then the function $P(\theta, x)$ defined in Equation (18) is periodic and analytic in the variable x on the complex strip with width $\log(\nu)$, and is analytic on the d-dimensional unit polydisk $\mathbb{B}_1 \subset \mathbb{C}^d$ given by

$$\mathbb{B}_1 := \left\{ \theta = (\theta_1, \ldots, \theta_d) \in \mathbb{C}^d : \max_{1\leq j\leq d} |\theta_j| < 1 \right\}.$$

Moreover we have that

$$\sup_{\theta\in D} \sup_{x\in[0,2\pi]} |P(\theta, x)| \leq \|p\|_\nu,$$

i.e. the norm on X^ν bounds the supremum norm of P.

The space X^ν inherits a Banach algebra structure from the multiplication operator in the function space representation.

Definition 2.3. Let two sequences $p, q \in X^{\nu,d}$ be given. Define $*_{TF} : X^{\nu,d} \times X^{\nu,d} \to X^{\nu,d}$ by

$$(p *_{TF} q)_m = \sum_{l\preceq m} p_l * q_{m-l}, \tag{20}$$

where $l \preceq m$ means $l_i \leq m_i$ for all $i = 1, \ldots, d$. Set $p^{*_{TF}n} \overset{\text{def}}{=} \underbrace{p *_{TF} \cdots *_{TF} p}_{n \ \text{times}}$.

The well-definedness of this operation follows from the following lemma.

Lemma 2.4. *Let $p, q \in X^{\nu,d}$ be given. Then*

$$\|p *_{TF} q\|_\nu \leq \|p\|_\nu \|q\|_\nu. \tag{21}$$

In particular $(X^\nu, *_{TF})$ is a Banach algebra.

Recall that if $F\colon X \to Y$ is a mapping between Banach spaces and $x \in X$ then we say that F is *Fréchet differentiable at x* if there exists a bounded linear operator $A\colon X \to Y$ so that

$$\lim_{\|h\| \to 0} \frac{\|F(x+h) - F(x) - Ah\|_Y}{\|h\|_X} = 0.$$

Recall that the operator A, if it exists, is unique. When there is such an A we write $DF(x) := A$. Since ℓ^1_ν and X^ν are both commutative Banach algebras we recall the following general facts from the calculus of Banach algebras. Let $(X, *)$ be a commutative Banach algebra. It is a straightforward exercise to prove the following:

- For any fixed $a \in X$ the map $L\colon X \to X$ defined by $L(x) = a * x$ is a bounded linear operator, hence it is Fréchet differentiable with $DL\, h = a * h$ for all $h \in X$.
- The monomial operator $F\colon X \to X$ defined by $F(x) = x * x$ is Fréchet differentiable with $DF(x)h = 2x * h$ for any $h \in X$.
- Applying this rule inductively gives that the nonlinear map $G\colon X \to X$ defined by $G(x) = x^{*n}$ is Fréchet differentiable with $DG(x)h = nx^{*n-1}h$ for all $h \in X$.

2.3 Computer assisted verification of the unstable eigenvalue count for a bounded perturbation of an eventually diagonal linear operator

In the sequel we are interested in counting the number of unstable eigenvalues of certain linear operators which arise as small, infinite dimensional, perturbations of some finite dimensional matrices. The following spectral perturbation lemma is formulated in a fashion which is especially well suited to our computational needs. Similar results have appeared in [32, 7, 69]. See also Remark 1.1. The approach described in this section takes rather explicit advantage of the sequence space structure of the problem. In particular we study a class of linear operators which have a "infinite matrix" representation. First some notation.

Suppose that $A, Q, Q^{-1}\colon \ell^1_\nu \to \ell^1_\nu$ are bounded linear operators. Assume that A is compact and that $\{\lambda_j\}_{j=0}^\infty$ are the eigenvalues of A. Suppose that for some $m \geq 0$ the eigenvalues satisfy

$$0 < \text{ real}(\lambda_m) \leq \ldots \leq \text{real}(\lambda_0),$$

i.e. that there are $m+1$ unstable eigenvalues. Assume that for all $j \geq m+1$ we have

$$\text{real}(\lambda_j) < 0,$$

i.e. the remaining eigenvalues are stable.

Then A has no eigenvalues on the imaginary axis, i.e. A is hyperbolic. Moreover we assume that the stable spectrum of A is contained in some cone in the left half plane. More precisely, suppose that there is $\mu_0 > 0$ so that

$$\mu_0 := \sup_{j \geq 0} \sqrt{1 + \left(\frac{\text{imag}(\lambda_j)}{\text{real}(\lambda_j)}\right)^2} < \infty.$$

Note that, since A is compact, the λ_j accumulate only at zero and the spectrum of A is comprised of the union of these eigenvalues and the origin in $\mathbb{C}$.

Now suppose that A factors as

$$A = Q\Sigma Q^{-1},$$

where for all $h \in \ell_\nu^1$ we define

$$(\Sigma h)_k = \lambda_k h_k,$$

i.e. suppose that A is diagonalizable. Note that Σ is a compact operator. Consider the operator Σ^{-1} given by

$$(\Sigma^{-1} h)_k = \frac{h_k}{\lambda_k},$$

for $k \geq 0$. The operator is formally well defined as the assumption that all the λ_j have non-zero real part implies in particular that $\lambda_j \neq 0$ for all $j \geq 0$. Moreover the operator Σ^{-1} has exactly m unstable eigenvalues $1/\lambda_j$ for $0 \leq j \leq m$, and the stable spectrum is contained in the same cone as the stable spectrum of A. Note however that Σ^{-1} need not be a bounded linear operator on ℓ_ν^1. Nevertheless one checks that

$$\Sigma\Sigma^{-1} = \mathrm{I} \qquad \text{and} \qquad \Sigma^{-1}\Sigma = \mathrm{I},$$

on ℓ_ν^1. In the applications below Σ^{-1} will be a densely defined operator on ℓ_ν^1.

Consider now the operator

$$B = Q\Sigma^{-1}Q^{-1}.$$

B is formally well-defined (in fact has the same domain as Σ^{-1}) and has

$$AB = \mathrm{I}, \qquad \text{and} \qquad BA = \mathrm{I},$$

on ℓ_ν^1. Moreover, if Σ^{-1} is densely defined so is B. The eigenvalues of B are precisely $\frac{1}{\lambda_k}$ and in particular B has exactly the $m+1$ unstable eigenvalues $\frac{1}{\lambda_j}$ for $0 \leq j \leq m$. We are interested in bounded perturbations of B, and have the following Lemma.

Lemma 2.5. *Suppose that $A, Q, Q^{-1} \colon \ell_\nu^1 \to \ell_\nu^1$, $\{\lambda_j\}_{j=0}^\infty \subset \mathbb{C}$ and $\mu_0 > 0$ are as discussed above, and that $B = Q\Sigma^{-1}Q^{-1}$ is a (possibly only densely defined) linear operator on ℓ_ν^1. Let $H \colon \ell_\nu^1 \to \ell_\nu^1$ be a bounded linear operator and let M be the (densely defined) linear operator*

$$M = B + H.$$

Assume that $\epsilon > 0$ is a positive real number with

$$\|I - AM\|_{B(\ell_\nu^1)} \leq \epsilon,$$

and

$$\|Q\|_{B(\ell_\nu^1)} \|Q^{-1}\|_{B(\ell_\nu^1)} \mu_0 \epsilon < 1.$$

Then M has exactly m unstable eigenvalues.

Proof. The result and its proof are similar to Lemma E.1 of [69]. Indeed, we will construct a homotopy from A to B just as in Lemma E.1. Repeating the argument of Step 1 of the proof of Lemma E.1, one sees that A and B have the same Morse index as soon as we can show that no eigenvalues cross the imaginary axis during the homotopy.

We begin by noting that for all $\mu \in \mathbb{R}$ the operator

$$B - i\mu \mathrm{I},$$

is boundedly invertible, as $i\mu$ is not in the spectrum of B. Similarily, we have that the operator

$$\mathrm{I} - \mu i A = Q(\mathrm{I} - \mu i \Sigma)Q^{-1},$$

is boundedly invertible. To see this note that

$$(\mathrm{I} - \mu i A)^{-1} = Q(\mathrm{I} - \mu i \Sigma)^{-1}Q^{-1},$$

where

$$[(\mathrm{I} - \mu i \Sigma)^{-1}h]_k = \frac{1}{1 - \mu i \lambda_k} h_k$$

for all $k \geq 0$, and since λ_k is never purely imaginary this denominator is never zero. Indeed for each j the worst case scenario is that $\mu = \mathrm{imag}(\lambda_j^{-1})$, so that

$$\sup_{j\geq 0} \left| \frac{1}{1 - \mu i \lambda_j} \right| \leq \sup_{j\geq 0} \left| \frac{\lambda_j^{-1}}{\lambda_j^{-1} - i\mu} \right|$$

$$\begin{aligned}
&\leq \sup_{j\geq 0} \left| \frac{\lambda_j^{-1}}{\lambda_j^{-1} - i\,\mathrm{imag}(\lambda_j^{-1})} \right| \\
&= \sup_{j\geq 0} \left| \frac{\lambda_j^{-1}}{\mathrm{real}(\lambda_j^{-1})} \right| \\
&= \sup_{j\geq 0} \sqrt{1 + \left(\frac{\mathrm{imag}(\lambda_j^{-1})}{\mathrm{real}(\lambda_j^{-1})} \right)^2} \\
&= \sup_{j\geq 0} \sqrt{1 + \left(\frac{\mathrm{imag}(\lambda_j)}{\mathrm{real}(\lambda_j)} \right)^2} \\
&= \mu_0,
\end{aligned}$$

as $\mathrm{Arg}(\lambda_j^{-1}) = -\mathrm{Arg}(\lambda_j)$. From this we obtain that

$$\|(\mathrm{I} - \mu i A)^{-1}\|_{B(\ell^1_\nu)} \leq \|Q\|_{B(\ell^1_\nu)} \|Q^{-1}\|_{B(\ell^1_\nu)} \sup_{j\geq 0} \left| \frac{1}{1 - i\mu\lambda_j} \right| \leq \|Q\|_{B(\ell^1_\nu)} \|Q^{-1}\|_{B(\ell^1_\nu)} \mu_0.$$

Note that

$$\|AH\| = \|A(M - B)\| = \|AM - AB\| = \|\mathrm{I} - AM\| \leq \epsilon < 1,$$

by hypothesis.

We now consider the homotopy

$$C_t = B + tH,$$

for $t \in [0, 1]$ and note that $C_0 = B$ and $C_1 = M$. Again, we take $\mu \in \mathbb{R}$ and consider the resolvent operator

$$\begin{aligned}
C_t - i\mu\mathrm{I} &= B - i\mu\mathrm{I} + tH \\
&= (B - i\mu\mathrm{I}) \left[\mathrm{I} + t(B - i\mu\mathrm{I})^{-1}H\right] \\
&= (B - i\mu\mathrm{I}) \left[\mathrm{I} + t(B - i\mu\mathrm{I})^{-1}BAH\right] \\
&= (B - i\mu\mathrm{I}) \left[\mathrm{I} + t(\mathrm{I} - i\mu A)^{-1}AH\right].
\end{aligned}$$

Note that for all $t \in [0,1]$ we have

$$\|t(\mathrm{I} - i\mu A)^{-1} A H\| \leq \|Q\|_{B(\ell^1_\nu)} \|Q^{-1}\|_{B(\ell^1_\nu)} \mu_0 \|AH\| \leq \|Q\|_{B(\ell^1_\nu)} \|Q^{-1}\|_{B(\ell^1_\nu)} \mu_0 \epsilon < 1,$$

by hypothesis. By the Neumann theorem, $C_t - i\mu\mathrm{I}$ is boundedly invertible for all $\mu \in \mathbb{R}$ and all $t \in [0,1]$. Then the resolvent is boundedly invertible throughout the homotopy, which implies that no eigenvalues cross the imaginary axis. Then the number of unstable eigenvalues is constant throughout the homotopy, i.e. B and M have exactly m unstable eigenvalues as claimed. $\square$

3 Parameterization Method for unstable manifolds of parabolic PDE

Since its introduction in [12, 13, 14, 45, 46], a small industry has grown up around the Parameterization Method and its applications. A proper review of the literature would make an excellent subject for an entire manuscript, and is certainly beyond the scope of the present work. A wonderful survey of the subject, with many applications and thorough discussion of the literature, is found in the book of [44].

The modest aim of the present discussion is to give the reader the flavor of the activity in this area. More importantly, we hope to indicate that the Parameterization Method is a much more general tool than the present work, viewed in isolation, would suggest. Here follows a brief (and by no means definitive) survey of some of problems which have been addressed using the method. The list is organized by topic with corresponding citations. The interested reader will be lead to many additional techniques and applications by consulting the references of the works cited here.

- *Stable/unstable manifolds for non-resonant fixed points/equilibria:* theory for maps on Banach spaces [12, 13], parabolic fixed points [8], numerical implementation for maps and ODEs [67, 71, 71, 11, 43], validated numerical methods for maps and ODEs [72, 79, 86, 79].

- *Stable/unstable bundles and manifolds for invariant tori:* discrete time [49, 48, 18, 36, 50, 37], Hamiltonian ODEs and PDEs [54, 38]

- *Stable/unstable manifolds of periodic orbits for ODEs:* theory and numerical implementation [14, 55, 41, 23].

- *KAM without action angle variables:* [55] invariant tori for symplectic maps [29], invariant tori for non-autonomous Hamiltonian systems [17], invariant tori in dissipative systems [16], mixed stability invariant manifolds associated with fixed points in symplectic/volume preserving maps [31].

- *Map Lattices:* stable/unstable manifolds for invariant tori [39], almost-periodic breathers and their stable/unstable manifolds [9].

- *Invariant tori for state dependent delay equations:* C^k/hyperbolic case [51], Analytic/KAM case [52].

- *Invariant manifolds for dissipative infinite dimensional dynamical systems:* parabolic PDEs [34], compact maps [69].

3.1 A-priori existence for solutions of Equation (6): a non-resonant unstable manifold theorem for parabolic PDE

Let X be a Banach algebra and let A be a closed, densely defined, with compact resolvent. Then A generates a compact semigroup, which we denote by e^{At}, $t \geq 0$. An explicit formula for the exponential can be obtained as a line integral of the resolvent operator in the complex plane. While we make no explicit use of this representation in the present work, it is important to us that an estimate of the form

$$\|e^{At}\|_{B(X)} \leq Me^{\mu_* t},$$

can be obtained from this line integral representation. The explicit values of the constants will not matter to us in the sequel. However we will exploit the fact that if A is sectorial with spectrum in the open left half plane then $\mu_* < 0$. Such an operator will be called dissipative. The material above is standard in the theory of analytic semi-groups and parabolic PDEs. See for example [42, 33].

Now let $G\colon X \to X$ be a Fréchet differentiable map. In fact we will be interested in the convergence of certain formal series, so we assume in addition that G is analytic. Consider the differential equation

$$x' = Ax + G(x) \tag{22}$$

Suppose that $\tilde{x} \in X$ is a hyperbolic stationary solution of Equation (22), i.e. that $A + DG(\tilde{x})$ has no eigenvalues on the imaginary axis. Since $DG(\tilde{x})$ is a bounded linear operator the operator $A + DG(\tilde{x})$ remains sectorial, and again generates a compact semigroup. Then $A + DG(\tilde{x})$ has at most finitely many unstable eigenvalues of finite multiplicity. We denote these eigenvalues by $\lambda_1, \ldots, \lambda_d$ and suppose for the sake of simplicity (this is the case studied in the sequel) that they are real and distinct, i.e. of multiplicity one. Then there are eigenvectors $\xi_1, \ldots, \xi_d$ which we choose to have unit norm (we will rescale them by explicit constants below).

After an affine change of variables we can arrange that $\tilde{x} = 0$ and that the equation becomes

$$x' = Ax + N(x) \stackrel{\text{def}}{=} F(x), \tag{23}$$

with

$$A = \begin{pmatrix} A_u & 0 \\ 0 & A_s \end{pmatrix},$$

where

$$A_u = \begin{pmatrix} \lambda_1 & \ldots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \ldots & \lambda_d \end{pmatrix}$$

and A_s is a dissipative operator, i.e. there are $M, \mu_* > 0$ so that

$$\|e^{A_s t}\|_{B(X)} \leq Me^{-\mu_* t},$$

for all $t \geq 0$. Moreover the semigroup $e^{A_s t}$ is compact. The function N, is analytic in a neighborhood of the origin and is zero to second order, and we write

$$N(x) = \sum_{j=2}^{\infty} n_j x^{*j}, \tag{24}$$

with coefficients $n_j \in X$. Since N is analytic on the disk there exists an $R > 0$ so that

$$\sum_{j=2}^{\infty} \|n_j\| R^{|m|} < \infty.$$

Definition 3.1 (Resonance of order m)**.** We say that the complex numbers $\lambda_1, \ldots, \lambda_d$ have a resonance of order $(m_1, \ldots, m_d) = m \in \mathbb{N}^d$ if

$$m_1\lambda_1 + \ldots + m_d\lambda_d = \lambda_j,$$

for some $1 \leq j \leq d$ and some $|m| \geq 2$. We say that $\lambda_1, \ldots, \lambda_d$ are non-resonant if there is no resonance of order m for any order $|m| \geq 2$.

If we consider $\lambda_1, \ldots, \lambda_d$ a finite collection of unstable eigenvalues, then there are only finitely many opportunities for resonances between these (as for $|m|$ large enough the product on the left has magnitude larger than any unstable eigenvalue). Then, despite first impressions, Definition 3.1 imposes only a finite number of constraints.

Define the linear approximation

$$P_1(\theta_1, \ldots, \theta_d) = \tilde{x} + s_1\xi_1\theta_1 + \ldots + s_d\xi_d\theta_d.$$

where the $s_1, \ldots, s_d$ are arbitrary non-zero real numbers (these numbers can be thought of as "tuning" the scalings of the eigenvectors, as we choose the ξ_j to have unit norm). We have the following unstable manifold theorem.

Theorem 3.2 (Existence of a conjugating chart map for the unstable manifold)**.** *Suppose that the unstable spectrum of $DF(\tilde{x})$ consists of only the unstable eigenvalues $\lambda_1, \ldots, \lambda_d$. Assume that each of these is real and has finite multiplicity one. Assume in addition that $\lambda_1, \ldots, \lambda_d$ are non-resonant in the sense of Definition 3.1. Then there is a $\delta > 0$ so that if*

$$\max_{1 \leq j \leq d} |s_j| \leq \delta,$$

then there exists a unique $P \colon B_1 \to X$ satisfying the first order constraints

$$P(0) = \tilde{x}, \qquad \text{and} \qquad \frac{\partial}{\partial \theta_j} P(0) = s_j \xi_j, \tag{25}$$

and having that P is a solution of the invariance equation

$$F(P(\theta)) = DP(\theta) A_u \theta \tag{26}$$

on B_1. In particular $P[B_1]$ is a local unstable manifold at $\tilde{x}$.

To solve (26) we introduce some notation. Let $\pi_u, \pi_s \colon X \to X$ be the spectral projections associated with A_u and A_s and let $X_u := \pi_u(X)$, $X_s = \pi_s(X)$. Then for any $x \in X$ we can write $x = (x_1, x_2)$ with $x_1 = \pi_u(x) \in X_u$ and $x_2 = \pi_s(x) \in X_s$. Indeed, we can further decompose X_u by noting that each of the eigenvalues λ_j, $1 \leq j \leq d$ has an associated spectral projection operator $\pi_j \colon X \to X$. Define the linear subspaces $X_j = \pi_j(x)$ and note that $X_u = X_1 \oplus \ldots \oplus X_d$. Moreover, since ξ_j spans X_j we have that each $x_j \in X_j$ can be written uniquely as $x_j = c_j\xi_j$ for some scalar c_j.

Define

$$\mu^* = \min_{1 \leq j \leq d} \text{real}(\lambda_j),$$

and note that this is $\mu^* = \min_{1 \le j \le d} \lambda_j$ as the unstable eigenvalues are assumed to be real.

We look for a solution of Equation (26) in the form

$$P(\theta) = P_1(\theta) + H(\theta),$$

where $H(0) = \partial H / \partial \theta_j(0) = 0$ for $1 \le j \le d$. Note that in this context the left hand side of Equation (26) becomes

$$\begin{aligned} F(P) &= F(P_1 + H) \\ &= AP_1 + AH + N(P_1 + H) \end{aligned}$$

while the right hand side is

$$\begin{aligned} DP(\theta)A_u\theta &= DP_1(\theta)A_u\theta + DH(\theta)A_u\theta \\ &= \lambda_1\theta_1 s_1 \xi_1 + \ldots + \lambda_d \theta_d s_d \xi_d + DH(\theta)A_u\theta. \end{aligned}$$

We note that

$$\begin{aligned} AP_1(\theta) &= s_1\theta_1 A\xi_1 + \ldots + s_d\theta_d A\xi_d \\ &= \lambda_1\theta_1 s_1\xi_1 + \ldots + \lambda_d\theta_d s_d \xi_d, \end{aligned}$$

as λ_1, ξ_j are eigenvalue/eigenvector pair for A. After cancelation of these terms on the left and the right, Equation (26) becomes

$$DH(\theta)A_u\theta - AH(\theta) = N(P_1(\theta) + H(\theta)). \tag{27}$$

The left hand side of this expression defines a boundedly invertible linear operator on a suitable space of functions, as the next lemma shows. For $P \colon B_1 \to X$ analytic define the norm

$$\|P\|_1 := \sum_{|m|=0}^{\infty} \|p_m\|$$

where $p_m \in X$ for each $m \in \mathbb{N}^d$. Note that

$$\sup_{\theta \in B_1} \|P(\theta)\| \le \|P\|_1,$$

where the norm on the left is the norm on X and the inequality holds even in the case that one is infinite. We employ the $\| \cdot \|_1$ norm below (and throughout the remainder of the paper) in spite of the fact that this is less fine than the supremum norm, due to the fact that it makes numerical calculations and some formal manipulations easier. Define

$$\mathcal{H} = \left\{ H \in C^\omega(B_1, X) \,|\, H(0) = \frac{\partial H}{\partial \theta_j}(0) = 0, \text{ and } \|H\|_1 < \infty \right\}.$$

Lemma 3.3. *Suppose that the unstable eigenvalues $\lambda_1, \ldots, \lambda_d$ are non-resonant in the sense of Definition 3.1. Then the linear operator given by*

$$\mathcal{L}[H](\theta) = DH(\theta)A_u\theta - AH(\theta),$$

is boundedly invertible on $\mathcal{H}$.

Proof. Let $E \in \mathcal{H}$. Taking the spectral projections we write

$$E(\theta) = \begin{pmatrix} E_u(\theta) \\ E_s(\theta) \end{pmatrix},$$

where $E_u = E_1 + \ldots E_d$. Consider the projected equations

$$DH_u(\theta)A_u\theta + A_uH_u(\theta) = E_u(\theta), \tag{28}$$

and

$$DH_s(\theta)A_u\theta + A_sH_s(\theta) = E_s(\theta). \tag{29}$$

We begin by solving Equation (28) term by term in the sense of power series.

Since E is analytic we can write

$$E(\theta) = \sum_{|m|=2}^{\infty} e_m\theta^m,$$

for some $e_m \in X$, where the series converges absolutely and uniformly for all $\theta \in B_1$, and in fact

$$\sum_{|m|=2}^{\infty} \|e_m\| = \|E\|_1 < \infty,$$

as $E \in \mathcal{H}$. Taking projections, we write

$$E_u(\theta) = E_1(\theta) + \ldots + E_d(\theta),$$

where

$$E_j(\theta) = \sum_{|m|=2}^{\infty} e_m^j\theta^m = \sum_{|m|=2}^{\infty} b_m^j\xi_j\theta^m,$$

with $e_m^j = \pi_j(e_m)$ and $e_m^j = b_m^j\xi_j$ for some unique scalars b_m^j.

Proceeding formally, we look for $H_u \colon B_1 \to X_u$ in the form

$$H_u(\theta) = H_1(\theta) + \ldots + H_d(\theta),$$

where $H_j \colon B_1 \to X_j$ is given by

$$H_j(\theta) = \sum_{|m|=0}^{\infty} c_m^j\xi_j\theta^m,$$

for some unknowns scalar coefficients c_m^j. Projecting Equation (28) onto X_j for $1 \leq j \leq d$, and noting that A_u is a diagonal matrix leads to the equations

$$DH_j(\theta)A_u\theta + \lambda_jH_j(\theta) = E_j(\theta),$$

so, upon making the power series substitutions, we have that

$$\sum_{|m|=2}^{\infty} (m_1\lambda_1 + \ldots m_d\lambda_d - \lambda_j)c_m^j\xi_j\theta^m = \sum_{|m|=2}^{\infty} b_m^j\xi_j\theta^m.$$

Matching like powers of θ leads to

$$(m_1\lambda_1 + \ldots m_d\lambda_d - \lambda_j)c_m^j\xi_j = b_m^j\xi_j,$$

from which we conclude that

$$c_m^j = \frac{1}{m_1\lambda_1 + \ldots m_d\lambda_d - \lambda_j} b_m^j,$$

for all $1 \le j \le d$ and $|m| \ge 2$.

Motivated by the discussion above we define the linear solution operators

$$\mathfrak{L}_j^{-1}[E](\theta) = \sum_{|m|=2}^{\infty} \frac{1}{m_1\lambda_1 + \ldots + m_d\lambda_d - \lambda_j}\, \pi_j(e_m)\theta^m, \qquad 1 \le j \le d,$$

for $1 \le j \le d$. Note that that $\mathfrak{L}_j^{-1}$ are well defined as the $\lambda_1, \ldots, \lambda_d$ are non-resonant. Defining

$$C_j = \max_{|m|\ge 2} |m_1\lambda_1 + \ldots + m_d\lambda_d - \lambda_j|^{-1},$$

we see that the solution operators are bounded on $\mathcal{H}$ as

$$\begin{aligned}
\|\mathfrak{L}_j^{-1}[E_u](\theta)\|_1 &= \sum_{|m|=2}^{\infty} \frac{1}{|m_1\lambda_1 + \ldots + m_d\lambda_d - \lambda_j|} \|\pi_j(e_m)\| \\
&\le C_j \sum_{|m|=2}^{\infty} \|\pi_j\|\|e_m\| \\
&\le C_j \|\pi_j\|\|E\|_1,
\end{aligned}$$

which is bounded due to the fact that the spectral projections are bounded linear operators and $E \in \mathcal{H}$. Now let $H_j := \mathfrak{L}_j^{-1}[E]$ for $1 \le j \le d$, and $H_u = H_1 + \ldots + H_d$. Then $DH_j \in \mathcal{H}$ for each $1 \le j \le d$, and working the argument backwards shows that H_u is indeed a solution of Equation (28).

In order to solve Equation (29), consider the change of variables

$$\theta \to e^{\lambda t}\theta,$$

with $\theta \in B_1$ fixed, and define

$$x(t) = H_s(e^{\lambda t}\theta), \qquad \text{and} \qquad p(t) = E_s(e^{\lambda t}\theta).$$

Suppose that $x(t)$ is a solution of the differential equation

$$x' - A_s x = p, \tag{30}$$

for all $t \le 0$. Then $x(0)$ is a solution Equation (29). But solutions of Equation (30) are given by Duhamel's formula. More precisely, we begin by multiplying both sides by $e^{-A_s t}$ and integrating form t_0 to t_1 to obtain

$$e^{-A_s t_1} x(t_1) - e^{-A_s t_0} x(t_0) = \int_{t_0}^{t_1} e^{-A_s t} E_s(e^{\lambda t}\theta)\, dt. \tag{31}$$

Assuming that $H_s \in \mathcal{H}$ (so that H is zero to second order) we have that

$$\begin{aligned}
\lim_{t_0 \to -\infty} e^{-A_s t_0} x(t) &= \lim_{t_0 \to \infty} e^{A_s t_0} x(-t_0) \\
&= \lim_{t_0 \to \infty} e^{A_s t_0} H_s(e^{-\lambda t_0}\theta) \\
&= 0
\end{aligned}$$

as

$$
\begin{aligned}
\|e^{A_s t_0} H_s(e^{-\lambda t_0}\theta)\| &\leq \|e^{A_s t_0}\| \|H_s(e^{-\lambda t_0}\theta\| \\
&\leq M e^{-\mu_* t_0} \left(e^{-\mu^* t_0}\right)^2 \|H_s\| \\
&\leq M e^{-(\mu_* + 2\mu^*) t_0} \|H_s\|
\end{aligned}
$$

and $\|H_s\| < \infty$. Then taking $t_0 \to -\infty$ in Equation (31) and $t_1 = 0$ gives

$$
x(0) = \int_{-\infty}^{0} e^{-A_s t} E_s(e^{\lambda t}\theta)\, dt = \int_0^\infty e^{A_s t} E_s(e^{-\lambda t}\theta)\, dt,
$$

after switching the limits of integration and changing $t \to -t$.

Motivated by this discussion we define the linear solution operator

$$
\mathfrak{L}_s^{-1}[E_s](\theta) := \int_0^\infty e^{A_s t} \pi_s \left[E(e^{-\lambda t}\theta)\right]\, dt.
$$

Let $H_s := \mathfrak{L}_s^{-1}[E_s]$, and note that

$$
\|H_s\| \leq \frac{M}{2\mu^* + \mu_*} \|E_s\|,
$$

as the integrand satisfies

$$
\|e^{A_s t} E_s(e^{-\lambda t}\theta)\| \leq M e^{-\mu_* t} e^{-2\mu^* t} \|E_s\|,
$$

i.e. the operator is well defined and bounded. Moreover we see that H_s is analytic by Morera's Theorem. To see that H_s is zero to second order we differentiate under the integral and note that $E_s(0) = 0$ and $\partial E_s / \partial \theta_j(0) = 0$ for $1 \leq j \leq d$. To see that $\|H_s\|_1 < \infty$ we expand E_s as a power series inside the formula for $\mathfrak{L}_s^{-1}[E_s]$ and, after exchanging the sum and the integral, bound $\|H_s\|_1$ in terms of $\|E_s\|_1$. We then check by differentiating that H_s so defined solves the desired equation. □

Proof of Theorem 3.2. Let

$$
\max_{1 \leq j \leq d} |s_j| = s.
$$

Then for any $H \in \mathcal{H}$ with $\|H\| \leq r$ we have that

$$
\sup_{\theta \in B_1} \|P_1(\theta) + H(\theta)\| \leq s + r.
$$

Suppose now that $\lambda_1, \ldots, \lambda_d$ are non-resonant and choose $s, r > 0$ so that

$$
s + r < R, \tag{32}
$$

where R is the radius of convergence of the series expansion of N. Then the nonlinear operator $\Phi \colon \mathcal{H} \to \mathcal{H}$ given by

$$
\Phi[H](\theta) = \mathfrak{L}^{-1}\left[N(P_1(\theta) + H(\theta))\right],
$$

is well defined for any s, r satisfying the Equation (32). Note also that $N(P_1 + H(\theta))$, is a composition of analytic functions, hence is analytic on B_1. Then $N \circ (P_1 + H) \in \mathcal{H}$ as is seen by evaluating $N(P_1(\theta) + H(\theta))$ and its first partials at $\theta = 0$.

The rest of the argument hinges on the fact that H is a fixed point of Φ if and only if H is a solution of Equation (27), if and only if $P = P_1 + H$ is a solution of Equation (6). In order to establish that Φ has a fixed point we employ the contraction mapping theorem. For the remainder of the argument we suppose that $s, r > 0$ satisfy Equation (32).

First, note that since N is zero to second order at the origin there are $M_1, M_2 > 0$ so that

$$\|N(x)\| \leq M_1 \|x\|^2,$$

and

$$\|DN(x)\|_{B(X)} \leq M_2 \|x\|,$$

for all $x \in X$ with $\|x\| < R$. (Explicit constants can be obtained for example by adapting the argument of Lemma 2.5 of [70]).

Then for any $H \in \mathcal{H}$ with $\|H\| \leq r$ we have

$$\begin{aligned} \|\Phi[H]\| &\leq \|\mathfrak{L}^{-1} N[P_1 + H]\| \\ &\leq \|\mathfrak{L}^{-1}\| M_1 (s + r)^2. \end{aligned}$$

Also note that if $\|H\| \leq r$ then we have that Φ is Fréchet differentiable at H with

$$D\Phi[H]v = \mathfrak{L}^{-1} DN(P_1 + H)v,$$

for $v \in \mathcal{H}$, and the bound

$$\|D\Phi[H]\| \leq \|\mathfrak{L}^{-1}\| M_2 (s + r).$$

Now choose $H_1, H_2 \in \mathcal{H}$ with $\|H_1\|, \|H_2\| \leq r$. We have that

$$\|\Phi[H_1] - \Phi[H_2]\| \quad \leq \quad \sup_{H \leq r} \|D\Phi[H]\| \|H_1 - H_2\|$$

$$\|\mathfrak{L}^{-1}\| M_2 (s + r) \|H_1 - H_2\|.$$

Suppose that $\delta > 0$ is small enough that

$$2\delta < R,$$

$$\|\mathfrak{L}^{-1}\| M_1 4\delta^2 \leq \frac{\delta}{2},$$

and

$$2\|\mathfrak{L}^{-1}\| M_2 \delta < 1.$$

Then for any choice of $s_1, \ldots, s_d, r > 0$ so that

$$s, r \leq \frac{\delta}{2},$$

we have that Φ is a contraction on the complete metric space

$$U_r = \{H \in \mathcal{H} \,|\, \|H\| \leq r\}.$$

Now the contraction mapping theorem implies that there exists a unique $\tilde{H} \in U_r$ so that $\Phi[\tilde{H}] = \tilde{H}$. It follows that

$$P(\theta) = P_1(\theta) + \tilde{H}(\theta),$$

satisfies Equation (6). Since P_1 satisfies the constraints of Equation (7) and $\tilde{H}$ is zero to second order at zero, we have that P satisfies the first order constraints as well. Then by Lemma 1.3, the image of P is the desired local unstable manifold. $\square$

Remark 3.4 (Uniqueness)**.** The solution of Equation (6) obtained in the proof of Theorem 3.2 is up to the choice of the eigenvectors and their scalings. In other words we obtain parameterizations of larger or smaller local unstable manifolds by choosing larger or smaller scalings $s_1, \ldots, s_d$. The non-uniquness is exploited in numerical computations, and in theoretical considerations of the decay rates of the Taylor coefficients of H.

3.2 Non-uniqueness and Taylor coefficient decay: rescaling the unstable eigenvectors

Suppose that $s_j = 1$ for $j = 1, \ldots, d$ in (25) are the scalings for the eigenvectors and that $P \colon B_1 \subset \mathbb{R}^d \to X$ is a corresponding analytic solution of Equation (26). Now let $s_1, \ldots, s_d > 0$, $s_j \neq 1$, $j = 1, \ldots, d$ and consider the function

$$\hat{P}(\theta_1, \ldots, \theta_d) = P(s_1\theta_1, \ldots, s_d\theta_d),$$

defined for $\theta_j s_j \leq 1$. Note that

$$\hat{P}(0) = \tilde{x},$$

and that

$$\frac{\partial \hat{P}}{\partial \theta_j}(0) = s_j \frac{\partial P}{\partial \theta_j}(0) = s_j \xi_j,$$

so that $\hat{P}$ satisfies the first order constraints of Equation (25), a scaled version (7). Moreover we have that

$$\begin{aligned}
F[\hat{P}(\theta_1, \ldots, \theta_d)] &= F[P(s_1\theta_1, \ldots, s_d\theta_d)] \\
&= \lambda_1(s_1\theta_1)\frac{\partial}{\partial \theta_1} P(s_1\theta_1, \ldots, s_d\theta_d) + \ldots + \lambda_d(s_d\theta_d)\frac{\partial}{\partial \theta_d} P(s_1\theta_1, \ldots, s_d\theta_d) \\
&= \lambda_1\theta_1 \frac{\partial}{\partial \theta_1} \hat{P}(s_1\theta_1, \ldots, s_d\theta_d) + \ldots + \lambda_d\theta_d \frac{\partial}{\partial \theta_d} \hat{P}(s_1\theta_1, \ldots, s_d\theta_d).
\end{aligned}$$

In other words $\hat{P}$ is a solution of Equation (26) corresponding the the rescaled choice of eigenvectors. Since the solution of Equation (26) is unique up to this choice of scalings we see that all solutions of Equation (26) are obtained in this manor.

Remark 3.5 (Rescaling and Taylor coefficient decay rates)**.** Consider the power series expansion

$$P(\theta) = \sum_{|m|=0}^{\infty} p_m \theta^m,$$

and a choice of scalings $s_1, \ldots, s_d \neq 0$. Then the rescaled solution $\hat{P}$ has power series given by

$$\begin{aligned}
\hat{P}(\theta) &= P(s_1\theta_1, \ldots, s_d\theta_d) \\
&= \sum_{|m|=0}^{\infty} p_m s_1^{m_1} \ldots s_d^{m_d} \theta^m,
\end{aligned}$$

i.e. given the Taylor coefficient sequence $\{p_m\}_{|m|=0}^{\infty}$ of one solution of Equation (26), the power series coefficients $\{\hat{p}_m\}_{|m|=0}^{\infty}$ of all other solutions of Equation (26) are obtained by the transformation

$$\hat{p}_m = s_1^{m_1} \ldots s_d^{m_d} p_m. \tag{33}$$

This is a useful observation. For example given the Taylor coefficients of one solution P, Equation (33) can be used to obtain a solution with more desirable decay rates (faster or slower decay).

3.3 Formalism and homological equations

We now return to Equation (23) under the assumptions given in the beginning of Section 3.1. Using the assumption that $(X, *)$ is a Banach algebra leads to an elegant formalism for Equation (6). We begin by developing a few formulas.

First consider

$$P(\theta) = \sum_{|m|=0}^{\infty} p_m \theta^m, \tag{34}$$

the power series of some analytic function $P\colon B_1 \to X$, and let $Q_2\colon X \to X$ be the quadratic function defined by

$$Q_2(a) = c * a * a,$$

where $c \in X$ is fixed.

A power series for the composition $Q_2 \circ P\colon B_1 \to X$ is given by

$$\begin{aligned} Q_2(P(\theta)) &= c * P(\theta) * P(\theta) \\ &= c * \left(\sum_{|m|=0}^{\infty} p_m \theta^m \right) * \left(\sum_{|m|=0}^{\infty} p_m \theta^m \right) \\ &= \sum_{|m|=0}^{\infty} \sum_{m_1+m_2=m} c * p_{m_1} * p_{m_2} \theta^m \end{aligned}$$

Let $(Q_2 \circ P)_m \in X$ denote the power series coefficients of the analytic function $Q_2 \circ P$. Matching like powers of θ leads to

$$(Q_2 \circ P)_m = \sum_{m_1+m_2=m} c * p_{m_1} * p_{m_2} = 2c * p_0 * p_m + \sum_{m_1+m_2=m} \delta^m_{m_1,m_2} c * p_{m_1} * p_{m_2},$$

where

$$\delta^m_{m_1,m_2} := \begin{cases} 0 & \text{if} \quad m_1 = m \quad \text{or} \quad m_2 = m \\ 1 & \text{otherwise} \end{cases}.$$

We write

$$p_m \diamond p_m := \sum_{m_1+m_2=m} \delta^m_{m_1,m_2} c * p_{m_1} * p_{m_2},$$

to denote the sum over terms with no p_m dependance. Noting that

$$2c * p_0 * p_m = DQ_2(p_0) p_m,$$

we define the operator

$$\tilde{Q}_2(P)_m := c * p_m \diamond p_m,$$

and have the formula

$$(Q_2 \circ P)_m = DQ_2(p_0)\, p_m + \tilde{Q}_2(P)_m, \tag{35}$$

where $\tilde{Q}_2(P)_m$ depends on neither p_m nor p_0.

More generally let $Q_n \colon X \to X$ be the monomial defined by

$$Q_n(a) = c * a^{*n},$$

and consider the analytic function $Q_n \circ P \colon B_1 \to X$. A nearly identical computation to the one given above shows that the m-th coefficient of the power series expansion of $Q_n \circ P$ is given by

$$(Q_n \circ P)_m = DQ_n(p_0)p_m + \tilde{Q}_n(P), \tag{36}$$

where

$$DQ_n(p_0)p_m = np_0^{*n-1} * p_m,$$

and we define

$$\tilde{Q}_n(P)_m = \sum_{m_1+\ldots+m_n=m} \delta^m_{m_1,\ldots,m_n} p_{m_1} * \ldots * p_{m_n}, \tag{37}$$

with

$$\delta^m_{m_1,\ldots,m_n} = \begin{cases} 0 & \text{if } m_j = m \text{ for some } 1 \leq j \leq n \\ 1 & \text{otherwise} \end{cases}.$$

We extend this formalism to the special case of $n = 1$ by letting $Q_1 \colon X \to X$ be

$$Q_1(a) := c * a,$$

with $c \in X$ fixed. The formula

$$Q_1(P(\theta))_m = DQ_1(p_0)p_m + \tilde{Q}_1(P)_m,$$

holds in this case as well once we note that

$$DQ_1(p_0)p_m = c * p_m,$$

and define $\tilde{Q}_1(P)_m = 0$ for all $m \in \mathbb{N}^d$.

Assume in (23) is given by a polynomial. This is also the case we study in the example described in (2) in the introduction. That is we can write the vector field as

$$F(x) = Ax + \sum_{n=1}^{s} c_n * x^{*_n},$$

where for $1 \leq n \leq s$ the $c_n \in X$ are fixed. We seek a solution of Equation (26) under these conditions.

Since, under the hypotheses of Theorem 3.2, there exists an analytic solution of Equation (26), we look for $P \colon B_1 \to X$ a satisfying the *ansatz* of Equation (34). Imposing the first order constraints given in Equation (25) gives that the first order coefficients of the power series solution are given by

$$p_0 = \tilde{x} \quad \text{and} \quad p_{e_j} = s_j \xi_j \qquad \text{for } 1 \leq j \leq d,$$

where e_j, $1 \leq j \leq d$ is the standard basis for the multi-indices $m \in \mathbb{N}^d$ with $|m| = 1$. Considering the left hand side of Equation (26) subject to the power series ansatz leads to

$$\begin{aligned} F(P(\theta)) &= AP(\theta) + \sum_{n=1}^{s} c_n * (P(\theta))^{*n} \\ &= AP(\theta) + \sum_{n=1}^{s} (Q_n \circ P)(\theta), \end{aligned}$$

and after matching like powers of θ we see that the m-th power series coefficient of $F \circ P$ is given by

$$(F \circ P)_m = Ap_m + \sum_{n=1}^{s} DQ_n(p_0)p_m + \sum_{n=1}^{s}(\tilde{Q}_n \circ P)_m = Dg(p_0)p_m + \sum_{n=1}^{s} \tilde{Q}_n(P)_m. \quad (38)$$

Similarly the right hand side of Equation (26) is, in light of the power series ansatz, given by

$$\lambda_1\theta_1 \frac{\partial}{\partial\theta_1} P(\theta) + \ldots + \lambda_d\theta_d \frac{\partial}{\partial\theta_1} P(\theta) = \sum_{|m|=0}^{\infty} (m_1\lambda_1 + \ldots + m_d\lambda_d)p_m\theta^m. \quad (39)$$

Equating like powers of θ in Equation (38) and Equation (39) gives that for each $m \in \mathbb{N}^d$ with $|m| \geq 2$ the coefficient $p_m \in X$ is a solution of the equation

$$[DG(p_0) - (m_1\lambda_1 + \ldots + m_d\lambda_d)\mathrm{Id}]p_m = -\sum_{n=1}^{s} \tilde{Q}_n(P)_m, \quad (40)$$

where the right hand side is in X and depends on neither p_m nor p_0.

Equation (40) gives one equation for each m, and we refer to these as the *homological equations* for P. We note that since $p_0 = \tilde{x}$, the linear operator A_m defined by

$$A_m = DF(p_0) - (\lambda_1 + \ldots + \lambda_d)\mathrm{Id},$$

is a boundedly invertible linear operator on X assuming that

$$m_1\lambda_1 + \ldots + m_d\lambda_d \notin \mathrm{spec}(DF(\tilde{x})).$$

But $m_1, \ldots, m_d \geq 0$ and the $\lambda_1, \ldots, \lambda_d$ are positive real numbers, so that $m_1\lambda_1 + \ldots + m_d\lambda_d \in (0, \infty)$ for all $|m| \geq 2$. Since $\lambda_1, \ldots, \lambda_d$ are the only elements of the unstable spectrum of $DF(\tilde{x})$ we have that A_m is an isomorphism as long as

$$m_1\lambda_1 + \ldots + m_d\lambda_d \neq \lambda_j$$

for $1 \leq j \leq d$, i.e. as long as the unstable eigenvalues are non-resonant in the sense of Definition 3.1. Then the homological equations are uniquely and recursively solvable to all orders, and P is formally well defined and unique in the sense of power series (once the (scaled) eigenvectors $\xi_1, \ldots, \xi_d$ are fixed).

3.4 Zero finding problem and the Newton-like operator for the unstable manifold

In this section we interpret (40) as a zero finding problem for the Taylor coefficients of the unstable manifold parameterization. That is, we define a map f such that P given by (34) solves (26) together with (25) if and only of $f(p) = 0$, where p is the sequence of coefficient sequences of P.

To begin consider the set of all infinite sequences $p = \{p_m\}_{m \in \mathbb{N}^d}$ with $p_m \in X$. The sequence space is endowed with the norm

$$\|p\|_1 := \sum_{|m|=0}^{\infty} \|p_m\|,$$

where the norm inside the sum is the X norm. Note that if $\{p_m\}_{m\in\mathbb{N}^d}$ are the Taylor coefficients of an analytic function on $\mathbb{B}_1$ then this is the $\mathcal{H}$ norm defined in Section 3.1. Let

$$\ell_d^1(X) := \{\{p_m\}_{m\in\mathbb{N}^d}\,,\ p_m \in X :\ \|p\|_1 < \infty\}\,,$$

and note that this is a Banach space.

Zero finding map Returning to the discussion of formal series in Section 3.3, and in particular by considering again the formulas developed in Equations (38) and (39), we define the map $b\colon \ell_d^1(X) \to \ell_d^1(X)$ component wise by

$$b_m(p) := Dg(p_0)p_m + \sum_{n=1}^{s} \tilde{Q}_n(p)_m,$$

where $\tilde{Q}_n$ is as defined in Equation (37). We now have the following.

Definition 3.6. Let an equilibrium $\tilde{x}$ of (23) together with eigenvalues λ_i and eigenvectors ξ_i for $i = 1, \ldots, d$ be given. Define the map on $\ell_d^1(X)$ by

$$f_m(p) = \begin{cases} p_0 - \tilde{x} & m = 0 \\ p_{e_i} - \xi_i & m = e_i \\ (\lambda\cdot m)p_m - b_m(p) & |m| \geq 2 \end{cases} \tag{41}$$

where $\lambda \cdot m \overset{\text{def}}{=} \sum_{i=1}^{d} \lambda_i m_i$.

The following Lemma is an immediate consequence of the above definitions.

Lemma 3.7. *Suppose that $p \in \ell_d^1(X)$ has $f(p) = 0$, where f is given by* (41)*. Then $P : \mathbb{B}_1 \to \ell_\nu^1$ given by* (34) *solves* (26) *together with* (25)*.*

Remark 3.8. The scalings of the eigenvectors are free in the definition of the map. In practice we choose the scalings as discussed in Section 4.

3.5 Fixed point operator in the Fourier-Taylor basis

We now specify the operators A and $A^\dagger$ as promised in Section 2.1. Here the map f corresponds to the invariance equation (6), where g is given by the infinite dimensional ODE system for the eigenbasis coefficients as specified in (2). Therefore we specialize to the case of a Fourier-Taylor base so that, combining the notation of Section 2.2 and 3.4, we let of $X = \ell_\nu^1$ so that $\ell_d^1(X) = X^\nu$.

We define the finite dimensional truncation of f, which we denote by f^{MK}. Let us set for $M \in \mathbb{N}^d$ and $K > 0$ the set

$$\mathcal{I}_{MK} = \{(m,k) : m \preceq M \quad k \leq K\}$$

and the projection $\Pi_{MK} : X^\nu \to \mathbb{R}^{(|M|+1)(K+1)}$ by $\Pi_{MK}p = (p_{mk})_{(m,k)\in\mathcal{I}_{MK}} \overset{\text{def}}{=} p^{MK}$. We identify $\mathbb{R}^{(|M|+1)(K+1)}$ as a subspace of X^ν by seeing an element as a sequence of sequences, where each sequence entry p_{mk} vanishes for either $k > K$ or $m \succ M$. We denote this operation formally by the immersion $\tau : \mathbb{R}^{(|M|+1)(K+1)} \to X^\nu$. Here $m \succ M$ means $m_i > M_i$ for at least one $i = 1, \ldots, d$. Then we assume a splitting of the map f in the form

$$f(p) = \tau(f^{MK}(p^{MK})) + f^\infty(p), \tag{42}$$

where $f^{MK} : \mathbb{R}^{(|M|+1)(K+1)} \to \mathbb{R}^{(|M|+1)(K+1)}$ is the map we implement numerically on the computer. In the following we will drop the immersion τ whenever it is simplifying the notation. Assume we compute an approximate zero $\bar{p} \in X^\nu$ of f, that is $f^{MK}(\bar{p}^{MK}) \approx 0 \in \mathbb{R}^{(|M|+1)(K+1)}$. To define the Newton-like fixed point operator we need an approximate inverse of $Df(\bar{p})$.

Definition 3.9. 1. The following operator is an approximate inverse of $Df(\bar{p})$. Let $A^{MK} \approx Df^{MK}(\bar{p})^{-1}$ and set

$$(Ap)_{mk} = \begin{cases} (A^{MK}p^{MK}))_{mk} & (m,k) \in \mathcal{I}_{MK} \\ p_{mk} & |m| \leq 1 \text{ and } k > K \\ \frac{1}{(\tilde{\lambda}\cdot m)-\mu_k} p_{mk} & (m,k) \notin \mathcal{I}_{MK} \text{ and } |m| > 1 \end{cases} \tag{43}$$

2. If A is injective, then fixed points of

$$T : X^\nu \to X^\nu, \quad Tp = p - Af(p) \tag{44}$$

correspond to zeros of f.

We also specify the operator $A^\dagger \approx A^{-1}$:

$$(A^\dagger p)_{mk} = \begin{cases} (Df^{MK}(\bar{p})p^{MK})_{mk} & (m,k) \in \mathcal{I}_{MK} \\ p_{mk} & |m| \leq 1 \text{ and } k > K \\ (\tilde{\lambda} \cdot m - \mu_k) p_{mk} & (m,k) \notin \mathcal{I}_{MK} \text{ and } |m| > 1 \end{cases} . \tag{45}$$

4 Applications

Consider Fisher's equation with Neumann boundary conditions as specified in (4). Because we impose Neumann boundary conditions we expand $u(x,t)$ in a Fourier cosine series and obtain the infinite system of ODEs for the real Fourier coefficients $a = (a_k)_{k \geq 0}$

$$a_k'(t) = (\alpha - k^2)a_k(t) + \sum_{\substack{k_1+k_2+k_3=k \\ k_i \in \mathbb{Z}}} c_{|k_1|}a_{|k_2|}a_{|k_3|} \stackrel{\text{def}}{=} g_k(a) \tag{46}$$

where $c = (c_k)_{k \geq 0}$ is the sequence of real Fourier coefficients of $c(x)$.

4.1 Validated computation of the first order data

In order to build a high order approximation of the unstable manifold of an equilibrium $\tilde{a}$ of (46) we need a validated representation of $\tilde{a}$ and also its eigendata. In the following paragraphs we discuss how this is achieved. All of the computer programs discussed in this Section are available for download at [78].

Equilibrium solution: We look for an equilibrium solution $\tilde{a}$ of Equation (46), that is we demand $g(\tilde{a}) = 0$. The map is well defined as long as $1 < \bar{\nu} < \nu$, but unbounded for $\bar{\nu} = \nu$. In fact g is Frechet differentiable with differential $Dg(a)\colon \ell^1_\nu \to \ell^1_{\bar{\nu}}$ given by

$$[Dg(a)h]_k = (\alpha - k^2)h_k - 2\alpha(c * a * h)_k, \qquad k \geq 0,$$

for $a, h \in \ell^1_\nu$. Let us specify the operator A and $A^\dagger$ in this specific context. We choose $K > 0$, and define the projection $g^K : \mathbb{R}^{K+1} \to \mathbb{R}^{K+1}$ by

$$g^K(a^K) := (\alpha - k^2)a_k - \alpha(c^K * a^K * a^K)^K_k,$$

where

$$(c^K * a^K * a^K)^K_k \stackrel{\text{def}}{=} \sum_{\substack{k_1+k_2+k_3=k \\ -K \le k_1,k_2,k_3 \le K}} c_{|k_1|} a_{|k_2|} a_{|k_3|},$$

is the truncated cubic discrete convolution.

Remark 4.1. Note that even though the nonlinearity is only quadratic (as a function of $a \in \ell^1_\nu$) from a numerical point of view the nonlinearity requires computation of the full cubic discrete convolution. For this we use the fast Fourier transform built into the IntLab library. The reader interested in the details can find the map implemented in the program

`fisherMapII_cos_intval.m`.

Similarly the Jacobian matrix is computed using the FFT and standard shift operations. Our implementation is in the program

`fisherMapII_Differential_cos_intval.m`

Now, if $\bar{a}^K$ is an approximate solution of $g^K = 0$ then we let A^K be a numerical approximate inverse of the matrix $Dg^K(\bar{a}^K)$, i.e. suppose that A^K is an invertible matrix with

$$\|\mathrm{Id} - A^K Dg^K(\bar{a}^K)\| \ll 1.$$

Define the linear operators A and $A^\dagger$ by

$$(A^\dagger h)_n = \begin{cases} (Dg^K(\bar{a}^K)h^K)_k & \text{if } 0 \le k \le K \\ (\alpha - k^2)h_k & \text{if } k \ge K+1 \end{cases} \tag{47}$$

and

$$(Ah)_k = \begin{cases} (A^K h^K)_k & \text{if } 0 \le k \le K \\ \frac{1}{\alpha - k^2} h_k & \text{if } k \ge K+1 \end{cases}. \tag{48}$$

Let $\bar{a} \in \ell^1_\nu$ denote the inclusion of $\bar{a}^K$ into ℓ^1_ν. For the sake of completeness we include the following Lemma providing the Y- and Z- bounds fulfilling (13) and (14). The proof is a computation similar to those in Section 5 of [56], and is discussed in detail in [62]. The MatLab program

`fisherEquilibriumAnalyticProof.m`

implements the computations which check that the hypotheses of Lemma 4.2 are satisfied.

Lemma 4.2. *Suppose that $\sqrt{\alpha} < K+1$ and that $c = c^K + c^\infty \in \ell^1_\nu$. Let*

$$Y_0 := |A^K g^K(\bar{a})|_\nu + \alpha |A^K|_{\ell^1_\nu} |\bar{a}|^2_\nu |c^\infty|_\nu + \alpha \frac{|c^\infty|_\nu |\bar{a}|^2_\nu}{(K+1)^2 - \alpha} + 2 \sum_{k=K+1}^{3K} \alpha \frac{|(c^K * \bar{a}^K * \bar{a}^K)_k|}{k^2 - \alpha} \nu^k,$$

$$Z_0 := |Id - A^K Dg^K(\bar{a}^K)|_{\ell^1_\nu},$$

$$Z_1 := 2\alpha \sum_{k=0}^{K} |A_{0k}^K| \beta_k + 4\alpha \sum_{n=1}^{K} \left(\sum_{k=0}^{K} |A_{nk}^K| \beta_k \right) \nu^n + \frac{2\alpha}{(K+1)^2 - \alpha} |c|_\nu |\bar{a}|_\nu,$$

where

$$\beta_k := \max_{K+1 \le j \le 2K-k} \frac{|(c^K * \bar{a}^K)_{j+k}|}{2\nu^j} + \max_{K+1 \le j \le 2K+k} \frac{|(c^K * \bar{a}^K)_{j-k}|}{2\nu^j},$$

and

$$Z_2 = 2\alpha \max\left(|A^K|_{B(\ell_\nu^1)}, 1\right) \max\left(|c|_\nu, 1\right).$$

Then the constants

$$Y = Y_0,$$

and

$$Z(r) = Z_2 r - (1 - Z_0 - Z_1),$$

satisfy (13) *and* (14)*. In particular, if* $r > 0$ *is a positive constant with*

$$Z(r)r + Y_0 < 0,$$

then there is a unique $\tilde{a} \in B_r(\bar{a}) \subset \ell_\nu^1$ *so that* $g(\tilde{a}) = 0$*.*

Validated computation of eigenvalue/eigenvector pairs: Suppose now that $\tilde{u}$ is any equilibrium solution of Fisher's equation with Neumann boundary conditions. Linearizing about $\tilde{u}$ leads to the eigenvalue problem

$$\frac{d^2}{dx^2}\xi + \alpha\xi - 2\alpha c\tilde{u}\xi = \lambda\xi, \qquad \xi'(0) = \xi'(\pi) = 0.$$

Letting $\tilde{a}$ denote the sequence of cosine series coefficients for $\tilde{u}$ leads to the Fourier space formulation

$$(\alpha - k^2)\xi_k - 2\alpha(c * \tilde{a} * \xi)_k = \lambda\xi_k, \qquad \text{for } k \ge 0,$$

for the cosine series coefficients of ξ. We note that this is the precisely the eigenvalue problem

$$Dg(\tilde{a})\xi = \lambda\xi,$$

in the sequence space, in direct analogy with the case of a finite dimensional vector field.

As per the philosophy of the present work, we solve the eigenvalue problem via a zero finding argument. Since a scalar multiple of an eigenvector is again an eigenvector it is necessary to append some scalar constraint in order to isolate a unique solution of the eigenvalue/eigenvector problem. We choose $s \in \mathbb{R}$ and look for a solution $\xi \in \ell_\nu^1$ having $\xi_0 = s$. (The choice of phase condition is a convenience. Other phase conditions such as $|\xi|_\nu = 1$ or $\xi(0) = s$ would work as well, and can be incorporated by making only minor modifications to the mappings defined below).

Define the mappings $h\colon \ell_\nu^1 \to \mathbb{R}$ by

$$\tau(\xi) := \xi_0 - s,$$

and $h\colon \mathbb{R} \times \ell_\nu^1 \to \ell_\nu^1$ by

$$h(\lambda, \xi)_k := (\mu - k^2)\xi_k - 2\mu(c * \tilde{a} * \xi)_k - \lambda\xi_k, \qquad k \ge 0.$$

We then define the mapping $H\colon \mathbb{R} \times \ell_\nu^1 \to \mathbb{R} \times \ell_\nu^1$ by

$$H(\lambda, \xi) := \begin{pmatrix} \tau(\xi) \\ h(\lambda, \xi) \end{pmatrix}$$

A zero of H is an eigenvalue/eigenvector pair for the operator $Dg(\tilde{a})$. In turn λ is an eigenvalue for the PDE with eigenfunction given by

$$\xi(x) = \xi_0 + 2\sum_{k=1}^{\infty} \xi_k \cos(kx).$$

We note that the mapping H is nonlinear due to the coupling term $\lambda\xi_k$ (i.e. we consider λ and ξ as simultaneous unknowns).

We will now construct a Newton-like operator in order to study the equation $H(\lambda, \xi) = 0$. First we note that

$$D_\lambda \tau(\xi) = 0, \qquad D_\xi h(\xi) = e_0,$$

where $(e_0)_k = 1$ if $k = 0$ and is zero otherwise, that

$$D_\xi h(\lambda, \xi)v = \left[Dg(\tilde{a}) - \lambda \mathrm{Id}\right] v,$$

and that

$$D_\lambda H(\lambda, \xi) = -\xi.$$

In block form we write

$$DH(\lambda, \xi)(w, v) = \begin{pmatrix} 0 & e_0 \\ -\xi & Dg(\tilde{a}) - \lambda \mathrm{Id} \end{pmatrix} \begin{bmatrix} w \\ v \end{bmatrix},$$

where $w \in \mathbb{R}$ and $v \in \ell^1_\nu$. Consider the projected map $h^K : \mathbb{R}^{K+2} \to \mathbb{R}^{K+1}$ defined by

$$h^K(\lambda, \xi^K)_k := (\alpha - k^2)\xi^K_k - 2\alpha(c^K * \bar{a}^K * \xi^K)^K_k - \lambda\xi^K \qquad 0 \le n \le N \tag{49}$$

and define the total projection map $H^K : \mathbb{R}^{K+2} \to \mathbb{R}^{K+2}$ by

$$H^K(\lambda, \xi^K) = \begin{pmatrix} \xi_0 - s \\ h^K(\lambda, \xi^K) \end{pmatrix}.$$

Suppose now that $(\bar{\lambda}, \tilde{\xi}^K)$ is an approximate solution of $G^K = 0$.

Remark 4.3. In applications we choose a numerical eigenvalue/eigenvector pair $(\bar{\lambda}, \bar{\xi}^K)$ for the matrix $Dg^K(\bar{a}^K)$. We are free to solve the finite dimensional eigenvalue/eigenvector problem using any convenient linear algebra package. For an illustation of the type of validation result we obtain is given in Figure 1.

Let B^K be a $K{+}2 \times K{+}2$ matrix which is obtained as a numerical inverse of $DH^K(\bar{\lambda}, \tilde{\xi}^K)$. We partition B^K as

$$B^K = \begin{pmatrix} B^K_{11} & B^K_{12} \\ B^K_{21} & B^K_{22} \end{pmatrix},$$

where $B^K_{11} \in \mathbb{R}$ is the first entry of B^K , $B^K_{12} \in \left(\mathbb{R}^{K+1}\right)^*$ is the remainder of the first row of B^K, $B^K_{21} \in \mathbb{R}^{K+1}$ is the remainder of the first column of B^K and B^K_{22} is the remaining $K + 1 \times K + 1$ matrix block. The linear operators $B, B^\dagger$ are defined respectively by

$$B^\dagger := \begin{pmatrix} B^\dagger_{11} & B^\dagger_{12} \\ B^\dagger_{21} & B^\dagger_{22} \end{pmatrix},$$

where the sub-operators are $B^\dagger_{11} : \mathbb{R} \to \mathbb{R}$ defined by

$$B^\dagger_{11} := 0,$$

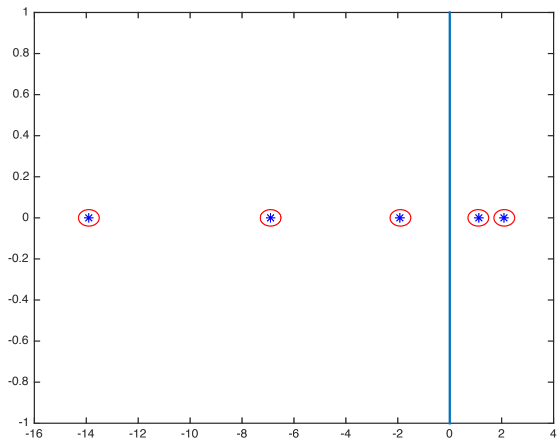

Figure 1: This is an illustration of the type of result our eigenvalue validation method yields. The blue crosses indicate the numerical eigenvalues $\bar{\lambda}$ of the finite dimensional matrix $Dg^K(\bar{a}^K)$. The red circles centered at the crosses indicate where true eigenvalues of $Dg(\tilde{a})$, that is the linearization of the *infinite dimensional* map g at the *precise* equilibrium $\tilde{a}$, can be found. It remains to be checked that the number of positive eigenvalues of $Dg(\tilde{a})$ is the same as the one of $A^\dagger$ in (47), or A in (48) equivalently. This is subject of Lemma 4.5.

$B_{12}^\dagger \colon \ell_\nu^1 \to \mathbb{R}$ defined by

$$B_{12}^\dagger(v)_k = v_k$$

$B_{21}^\dagger \colon \mathbb{R} \to \ell_\nu^1$ defined by

$$B_{21}^\dagger(w) := \begin{cases} -\tilde{\xi}_k w & 0 \le k \le K \\ 0 & k \ge K+1 \end{cases}$$

and $B_{22}^\dagger \colon Y^{\nu'} \to \ell_\nu^1$ defined by

$$B_{22}^\dagger(v)_k := \begin{cases} \left[Dh^K(\bar{\lambda}, \tilde{\xi}^K)v^K\right]_k & 0 \le k \le K \\ (\alpha - k^2)v_k & k \ge K+1 \end{cases},$$

and

$$B := \begin{pmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{pmatrix},$$

and $B_{11} \colon \mathbb{R} \to \mathbb{R}$ defined by

$$B_{11} := B_{11}^K,$$

$B_{12} \colon \ell_\nu^1 \to \mathbb{R}$ defined by

$$B_{12}(v) := \sum_{k=0}^{K} (B_{12}^K)_k v_k,$$

$B_{21} \colon \mathbb{R} \to \ell_\nu^1$ defined by

$$B_{21}(w) := \begin{cases} \left(B_{21}^K w\right)_k & 0 \le k \le K \\ 0 & k \ge K+1 \end{cases}$$

and $B_{22}\colon \ell^1_\nu \to \ell^1_\nu$ defined by

$$B_{22}(v)_k := \begin{cases} \left[B_{22}^K v^K\right]_k & 0 \le k \le K \\ (\alpha - k^2)^{-1} v_k & k \ge K+1 \end{cases} .$$

Define the space

$$\mathcal{X}_\nu := \mathbb{R} \times \ell^1_\nu.$$

We write $x = (\lambda, \xi)$ for an element of $\mathcal{X}_\nu$. We employ the product space norm on $\mathcal{X}_\nu$ so that

$$\|x\| = \|(\lambda, \xi)\| := \max\left(|\lambda|, |\xi|_\nu\right).$$

Then we write

$$H(x) = H(\lambda, \xi),$$

and for $y = (w, v) \in \mathcal{X}_\nu$ we have for example that

$$B\, y := \begin{pmatrix} B_{11} w + B_{12} v \\ B_{21} w + B_{22} v \end{pmatrix},$$

(and similarly for $Dh(\tilde{x})y$ and $B^\dagger y$). Define the Newton-like operator $\hat{T}\colon \mathcal{X}_\nu \to \mathcal{X}_\nu$ by

$$T(x) = x - BH(x). \tag{50}$$

The following lemma gives sufficient conditions that T is a contraction in a neighborhood of the approximate solution. The standard proof is a computation similar (for example) to that carried out explicitly in Section 5 of [56].

Lemma 4.4. *Suppose that $K + 1 > \sqrt{\alpha}$, and for each $0 \le k \le K$ define the quantities*

$$\hat{\alpha}_k := \sup_{K+1 \le n \le 2K-k} \frac{\left|(c^K * a^K)_{k+n}\right|}{2\nu^n},$$

and

$$\hat{\beta}_k := \sup_{K+1 \le n \le 2K+k} \frac{\left|(c^K * a^K)_{n-k}\right|}{2\nu^n}.$$

Let b_{ij} denote the entries of the $K+1 \times K+1$ matrix B_{22}^K. Then the constants

$$\hat{Y}_0^1 := \left|B_{11}^K\right| \left|\tilde{\xi}_0^K - s\right| + \sum_{k=0}^K \left|(B_{12}^K)_k\right| \left|h^K(\bar{\lambda}, \tilde{\xi}^K)_k\right| + 2\alpha |B_{12}^K|_{(\ell_\nu)^*} |\tilde{\xi}|_\nu \left(|c^K|_\nu |a^\infty|_\nu + |c^\infty|_\nu |\tilde{a}|_\nu\right),$$

$$\begin{aligned} \hat{Y}_0^2 \quad := \quad & \left|B_{21}^K\right|_\nu \left|\tilde{\xi}_0^K - s\right| + |B_{22}^K h^K(\bar{\lambda}, \tilde{\xi})|_\nu + 2\alpha |B_{22}^N|_{B(\ell_\nu)} |\tilde{\xi}|_\nu \left(|c^K|_\nu |a^\infty|_\nu + |c^\infty|_\nu |\tilde{a}|_\nu\right) \\ + \quad & 2 \sum_{k=K+1}^{3K} 2\alpha \frac{\left|\left(c^K * \bar{a}^K * \tilde{\xi}^K\right)_k\right|}{k^2 - \alpha} \nu^k + 2\alpha \frac{|\tilde{\xi}|_\nu \left(|c^K|_\nu |a^\infty|_\nu + |c^\infty|_\nu |\bar{a}|_\nu\right)}{(K+1)^2 - \alpha}, \end{aligned}$$

$$\begin{aligned} \hat{Z}_1^2 \quad := \quad & 2\alpha \max_{0 \le k \le K} |b_{0k}| (|c^K|_\nu |a^\infty|_\nu + |c^\infty|_\nu |\bar{a}|_\nu) + 2\alpha \sum_{k=0}^K |b_{0k}| (\hat{\alpha}_k + \hat{\beta}_k) \\ + \quad & 2\alpha \sum_{k=1}^K \left(\max_{0 \le n \le K} |b_{kn}| (|c^K|_\nu |a^\infty|_\nu + |c^\infty|_\nu |\bar{a}|_\nu) + 2 \sum_{n=0}^K |b_{kn}| (\hat{\alpha}_k + \hat{\beta}_k) \right) \nu^k \\ + \quad & \frac{2\alpha}{(K+1)^2 - \alpha} \left(|c|_\nu |\tilde{a}|_\nu + |\bar{\lambda}|\right), \end{aligned}$$

$$\hat{Z}_0^1 := \left|\left(Id_{\mathbb{R}^{K+2}} - B^K DH^K(\tilde{x}^K)\right)_{11}\right| + \left|\left(Id_{\mathbb{R}^{K+2}} - B^K DH(\tilde{x}^K)\right)_{12}\right|_{(\ell_\nu)^*},$$

$$\hat{Z}_0^2 := \left|\left(Id_{\mathbb{R}^{K+2}} - B^K DH^K(\tilde{x}^K)\right)_{21}\right|_\nu + \left|\left(Id_{\mathbb{R}^{K+2}} - B^K DH^K(\tilde{x}^K)\right)_{22}\right|_{B(\ell_\nu)},$$

$$\hat{Z}_1^1 := 0,$$

$$\hat{Z}_2^1 := 0, \qquad \textit{and} \qquad \hat{Z}_2^2 := \|B\|,$$

satisfy (13) *and* (14)*, i.e. the polynomials*

$$p_1(r) := Z_2^1 r^2 - (1 - Z_1^1 - Z_0^1) + Y_0^1,$$

and

$$p_2(r) := Z_2^2 r^2 - (1 - Z_1^2 - Z_0^2) + Y_0^2,$$

are radii-polynomials for the eigenvalue/eigenvector problem. In particular, if r is a positive constant having $p_1(r), p_2(r) > 0$ then there exists a unique pair $(\hat{\xi}, \hat{\lambda})$ so that $\hat{\xi} \in B_r(\tilde{\xi}) \subset \ell_\nu^1$ and $|\hat{\lambda} - \bar{\lambda}| \leq r$ having that the pair solve the equation $\hat{G} = 0$, i.e. they are an eigenvalue/eigenvector pair for Fisher's equation.

Correct eigenvalue count for the equilibrium: Now suppose that $\tilde{a} \in \ell_\nu^1$ is as in the previous sections, so that $g(\bar{a}) = 0$. Let $A\colon \ell_\nu^1 \to \ell_\nu^1$ be the linear operator defined by Equation (48). Moreover suppose that the $K+1 \times K+1$ matrix A^K is diagonalizable, with eigenvalues $\lambda_0, \ldots, \lambda_K \in \mathbb{C}$, and eigenvectors $\xi_0, \ldots, \xi_K \in \mathbb{C}^{K+1}$. Letting $Q^K = [\xi_0, \ldots, \xi_K]$ and Σ^K be the diagonal matrix of eigenvalues we have that

$$A^K = Q^K \Sigma^K Q^{-K},$$

where $Q^{-K} := (Q^K)^{-1}$.

Suppose that all of the eigenvalues have non-zero real part, that exactly $m > 0$ are unstable, and that $\sqrt{\alpha} < K + 1$. Define the operators $Q, Q^{-1}, \Sigma\colon \ell_\nu^1 \to \ell_\nu^1$ by

$$(Qh)_k := \begin{cases} [Q^K h^K]_k & 0 \leq k \leq K \\ h_k & k \geq K+1 \end{cases},$$

$$(Q^{-1}h)_k := \begin{cases} [Q^{-K} h^K]_k & 0 \leq k \leq K \\ h_k & k \geq K+1 \end{cases},$$

and

$$(\Sigma h)_k := \begin{cases} [\Sigma^K h^K]_k & 0 \leq k \leq K \\ \frac{h_k}{\alpha - k^2} & k \geq K+1 \end{cases}.$$

Then note that

- Σ is well defined,
- A and Σ have the same spectrum,
- the spectrum of Σ and hence of A is

$$\mathrm{spec}(A) = \{\lambda_0, \ldots, \lambda_K\} \cup \bigcup_{k=K+1}^{\infty} \frac{1}{\alpha - k^2} \cup \{0\},$$

- Σ is a compact,
- $A = Q\Sigma Q^{-1}$.
- The operator $B = Q\Sigma^{-1}Q^{-1}$ is unbounded but densely defined, due to the algebraic growth of the eigenvalues $\alpha - k^2$. Since the eigenvalues approach $-\infty$, we have that B generates a compact semi-group.

The following lemma provides sufficient conditions that the matrix A^K gives the correct unstable eigenvalue count for the infinite dimensional linearized problem. The MatLab program

`fisher_validateEigCount.m`

performs the computations which check the hypotheses of Lemma 4.5.

Lemma 4.5. *Let Y_0, Z_0, Z_1 and Z_2 be the positive constants defined in Lemma 4.2, and suppose that A, Q, Q and $\{\lambda_0, \ldots, \lambda_K\}$ are as discussed above. Define*

$$\mu_0 := \max_{0 \leq j \leq K} \sqrt{1 + \left(\frac{\text{imag}(\lambda_j)}{\text{real}(\lambda_j)} \right)^2},$$

and suppose that $r > 0$ has that

$$Z_2 r^2 - (1 - Z_0 - Z_1)r + Y_0 < 0.$$

Define

$$\epsilon := Z_2 r + Z_1 + Z_0,$$

and assume that

$$\|Q^K\| \|Q^{-K}\| \mu_0 \epsilon < 1.$$

Then $Dg(\tilde{a})$ has exactly m unstable eigenvalues.

Proof. Note that

$$DT(x) = \mathrm{I} - ADg(x),$$

and inspection of Equation (14) implies that

$$\|\mathrm{I} - ADg(x)\| \leq Z_2 r + Z_1 + Z_0 \leq \epsilon,$$

for all $x \in B_r(\tilde{x})$, in particular this inequality holds at $x = \tilde{x}$. Then the operators A, $B = Q\Sigma^{-1}Q^{-1}$, and $M = B + H$ (with $H = Dg(\tilde{x}) - B$) satisfy the hypothesis of Lemma 2.5 with

$$M = Dg(\tilde{x}),$$

so that we have that correct eigenvalue count as claimed. □

Example numerical computation of the linear data with a non-constant spatial inhomogeneity: Consider Fisher's equation with $\alpha = 2.1$ and the spatial inhomogeneity given by a Poission kernel

$$c(x) = 1 + 2 \sum_{k=1}^{\infty} r^k \cos(kx), \tag{51}$$

with $r = 1/5$. As a matter of fact the Fourier coefficients $c_k = r^k$ are in ℓ^1_ν whenever $r\nu < 1$. We also have explicit control over the norm $|c|_\nu = \frac{2}{1-rv} - 1$. To deal with the inhomogeneity $c(x)$ we split its sequence of Fourier coefficients into the form $c = \bar{c} + c^\infty$, where we have precise control over $|c^\infty|_\nu$. The Matlab script `a_validateLinearData_paperVersion` carries out all the necessary computations to validate the equilibrium together with its stability data and is available at [78].

The numerically computed equilibrium solution $\bar{a}^2$ and its approximate unstable eigenfunction $\bar{\xi}$ are illustrated in Figure 4. We refer to this solution as nontrivial and give it the number 2 as there are two explicit equilibria given by the constant zero solution and the function $\frac{1}{c(x)}$.

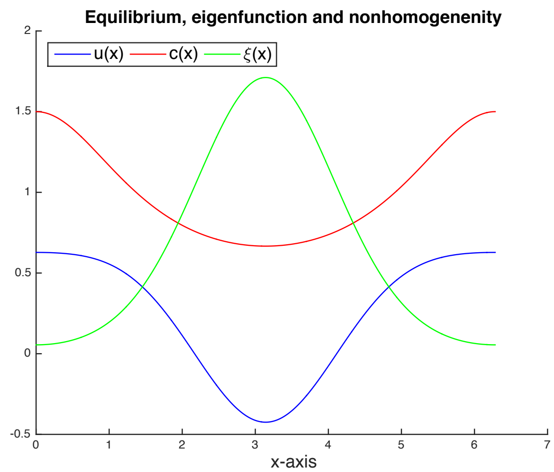

Figure 2: Linear data for the Fisher equation with $\alpha = 2.1$. The red curve illustrates the spatial inhomogeneity with $c(x)$ a Poisson kernel with parameter $r = 1/5$. The blue curve illustrates the numerically computed non-trivial equilibrium solution $\bar{a}^2$. The greed curve illustrates the numerically computed unstable eigenfunction $\bar{\xi}$. The data is validated in ℓ^1_ν with $\nu = 1.001$ and C^0 errors less than 5×10^{-13}.

We approximate the system using $K = 20$ cosine modes, i.e. the numerical computations are carried out in $\mathbb{R}^{21}$. We choose $\nu = 1.1$ and use the MatLab programs discussed in the preceding paragraphs to validate the results. We obtain that there exists a true analytic equilibrium solution for the problem whose C^0 distance from the numerical approximation is less than $r_0 = 2.1 \times 10^{-14}$. Similarly, we obtain that the equilibrium has exactly one unstable eigenvalue

$$\lambda_u = 2.194489888429804 \pm 3.5 \times 10^{-13},$$

and obtain validated error bounds on the eigenfunction of the same order.

4.2 Validated parameterization of the unstable manifold

First let us give a concrete formula for $b : X^{\nu,d} \to X^{\nu,d}$ as specified in (41):

$$b_{mk} = (-k^2 + \alpha)p_{mk} - \alpha(c * (p^{*_{TF}2})_m)_k, \quad |m| \geq 0, k \geq 0, \tag{52}$$

where $d = 1$ or $d = 2$ in the following. We start by considering the one-dimensional unstable manifold at the nontrivial equilibrium considered in the example of the last paragraph of 4.1. In this case we highlight how our analysis works if the fixed point together with the eigenvalues and eigenvectors are only known as numerical values together with bounds on the truncation error obtained by methods described in Section 4.1. This in particular includes checking the Morse index. Then we describe the computation of a two-dimensional manifold at the origin in order to show that our analysis carries over to higher dimensional manifolds.

In the following we choose the parameter $\alpha = 2.1$. The parameter α is an eigenvalue parameter for the zero solution, in the sense that for $(l-1)^2 < \alpha < l^2$ the linearization $Dg(\tilde{a}^0)$ has exactly l unstable eigenvalues. Hence by fixing $\alpha = 2.1$ we obtain a 2D unstable manifold at the origin.

1D unstable manifold at a nontrivial equilibrium From Section 4.1 we are given the exact linear data $\tilde{a}$, $\tilde{\lambda}$ and $\tilde{\xi}$ in the form:

$$\tilde{a}^2 = \bar{a}^2 + a^\infty \quad \text{with} \quad |a^\infty|_\nu \le r_{\bar{a}^2} \tag{53a}$$

$$\tilde{\xi} = \bar{\xi} + \xi^\infty \quad \text{with} \quad |\xi^\infty|_\nu < r_{\tilde{\xi}} \quad \text{for a given} \quad \nu > 1 \tag{53b}$$

$$\tilde{\lambda} = \bar{\lambda} + \lambda^\infty, \quad \text{with} \quad |\lambda^\infty| < r_{\tilde{\lambda}}, \tag{53c}$$

where we recall that $Dg(\tilde{a})\tilde{\xi} = \tilde{\lambda}\tilde{\xi}$. In addition by checking the conditions in Lemma (4.5) we ensure that the $\tilde{\lambda}$ indeed is the only positive eigenvalue of $Dg(\tilde{a})$.

In order to derive the bounds from Definition 2.1 we first need to make precise how we split the map f from 3.6 into the form (42).

Definition 4.6. Assume we are given truncation dimensions $M > 0$ and $K > 0$. Split $p = \Pi_{MK}p + p^\infty$, where $p^\infty = (Id - \Pi_{MK})\,p$. We set

$$f^{MK}(p^{MK})_{mk} = \begin{cases} \bar{a}_k - (p^{MK})_{0k} & m = 0 \\ \bar{\xi}_k - (p^{MK})_{1k} & m = 1 \\ (\bar{\lambda} \cdot m + k^2 - \alpha)p^{MK}_{mk} + \alpha(\bar{c} * \left(p^{MK} *_{TF} p^{MK}\right)^{MK}_m)^K_k & 2 \le m \le M, \\ & 0 \le k \le K \end{cases} \tag{54}$$

and

$$(f^\infty(p))_m = \begin{cases} a^\infty_k - p^\infty_{0k} & m = 0, k \ge 0 \\ \xi^\infty_k - p^\infty_{1k} & m = 1, k \ge 0 \\ (\lambda^\infty \cdot m)(\Pi_{MK}p)_{mk} + (\tilde{\lambda} \cdot m + k^2 - \alpha)p^\infty_{mk} + & \\ \alpha(Id - \Pi_{MK})\left(\bar{c} * (p^{MK} *_{TF} p^{MK})_m\right)_k + & \\ \alpha\left[c * ((2p^{MK} *_{TF} p^\infty)_{mk} + (p^\infty *_{TF} p^\infty)_m)_k\right] & m \ge 2, k \ge 0 \end{cases}. \tag{55}$$

Then $f(p) = f^{MK}(p^{MK}) + f^\infty(p)$.

The following Theorems summarize the Y-bounds and Z-bounds from Definition 2.1. Note that Theorem 4.7 rigorously controls the numerical residual and Theorem 4.9 controls the contraction rate. We will split the derivative in the following way:

$$DT(\bar{p} + ru)rv = (Id - AA^\dagger)rv - A\left[(A^\dagger - Df(\bar{p} + ru))rv\right]. \tag{56}$$

Note that we (for convenience) use a refined definition for $A^\dagger$, where we replace $\mu_k = -k^2$ from (45) by $\mu_k - \alpha$. The motivation for this splitting is that the first term is expected to be small and the second one is convenient to keep under explicit control. To bound the norm we use

$$\|DT(\bar{p}+ru)rv\|_\nu \leq \|(Id - AA^\dagger)rv\|_\nu + \|A\left[(A^\dagger - Df(\bar{p}+ru))rv\right]\|_\nu.$$

To structure later estimates let us define $\Delta \in X^{\nu,1}$

$$\Delta_{mk}(u,v) = \left[(A^\dagger - Df(\bar{p}+ru))rv\right]_{mk}, \tag{57}$$

which will be of the form

$$\Delta = r\Delta^{(1)} + r^2\Delta^{(2)}. \tag{58}$$

Theorem 4.7. *Y-bounds - 1D*
Assume truncation dimensions $M > 0$ and $K > 0$ and an approximate zero $\bar{p}$, with $\Pi_{MK}\bar{p} = \bar{p}$ to be given. Define

$$Y_m^{MK} = |(Df^{MK}(\bar{p})\bar{p})_{m0}| + 2\sum_{k=1}^{K} |(Df^{MK}(\bar{p})\bar{p})_{mk}|\nu^k, \quad m = 0,\dots,M, \tag{59}$$

and

$$Y_m^\infty = \begin{cases} r_{\bar{a}} & m = 0 \\ r_{\bar{\xi}} & m = 1 \\ |(|Df^{MK}(\bar{p})|\delta^\infty)_{m0}| + 2\sum_{k=1}^{K} |(|Df^{MK}(\bar{p})|\delta^\infty)_{mk}|\nu^k + & \\ 2\sum_{k=K+1}^{3K} \dfrac{\alpha|(\bar{c}*(\bar{p}*_{TF}\bar{p})_m)_k|}{\tilde{\lambda}\cdot m + k^2 - \alpha}\nu^k & m = 2,\dots M \\ \frac{\alpha|(\bar{c}*\bar{p}*_{TF}\bar{p})_{m0}|}{\tilde{\lambda}\cdot m} + 2\sum_{k=1}^{3K} \dfrac{\alpha|(\bar{c}*(\bar{p}*_{TF}\bar{p})_m)_k|}{\tilde{\lambda}\cdot m + k^2 - \alpha}\nu^k & M+1 \leq m \leq 2M, \end{cases} \tag{60}$$

where δ^∞ with $\Pi_{MK}\delta^\infty = \delta^\infty$ is given by

$$\delta_{mk}^\infty = \begin{cases} |\bar{p}_{mk}|\lambda^\infty & 2 \leq m \leq M, 0 \leq k \leq K. \end{cases} \tag{61}$$

Then

$$Y = \sum_{m=0}^{M} Y_m^{MK} + \sum_{m=0}^{M} Y_m^\infty + \sum_{m=M+1}^{2M} Y_m^\infty \tag{62}$$

fulfills (13).

Proof. To derive (71) and (72) we notice that $p^\infty = 0$ for $p = \bar{p}$. Hence formula (70) reduces to

$$(f^\infty(\bar{p}))_m = \begin{cases} a_k^\infty & m = 0, k \geq 0 \\ \xi_k^\infty & m = 1, k \geq 0 \\ (\lambda^\infty \cdot m)(\Pi_{MK}\bar{p})_{mk} + & \\ \alpha(Id - \Pi_{MK})\left(\bar{c}*(\bar{p}^{MK} *_{TF} \bar{p}^{MK})_m\right)_k & m \geq 2, k \geq 0 \end{cases}. \tag{63}$$

We see that δ^{∞}_{mk} in (61) is a component-wise bound for the terms in $|(f^{\infty}(\bar{p}))_{mk}|$ with $m \geq 2$ known to use only via error bounds. Next recall that we demand Y to fulfill $\|Af(\bar{p})\|_{\nu} \leq Y$. Note that even though $\bar{p}$ only has finitely many non-zero components, $f(\bar{p})$ does not, due to the linear data being infinite dimensional. Now $Y^{MK}_m + Y^{\infty}_m$ bounds $|(Af(\bar{p}))_m|_{\nu}$ by definition of A in (43) for $m = 0, \ldots, M$ and Y^{∞}_m for $m = M+1, \ldots, 2M$. Then (73) follows from the definition of $\| \cdot \|_{\nu}$. □

As a preparation for the Z-bounds we need the following Lemma, see also [69]. We state the more general version with l being a multi-index as this will be needed later on for higher dimensional manifolds.

Lemma 4.8. *Let $v \in \mathbb{B}_1(0) \subset \ell^1_{\nu}$, truncation dimensions $M \in \mathbb{N}^d$ and $K > 0$ and $\bar{p} = \Pi_{MK}\bar{p} \in X^{\nu}$ be given. Then for every $l \preceq M$ and for each $0 \leq k \leq K$ the following estimate is valid:*

$$|(\bar{c} * \bar{p}_l * v^{\infty})_k| \leq h^1_{lk}(\bar{p}) + h^2_{lk}(\bar{p}), \tag{64}$$

with

$$\max_{j=K+1,\ldots,2K-k} \frac{|(\bar{c} * \bar{p}_l)_{j+k}|}{2\nu^j} \stackrel{\text{def}}{=} h^1_{lk}(\bar{p}) \quad \text{and} \quad \max_{j=K+1,\ldots,2K+k} \frac{|(\bar{c} * \bar{p}_l)_{j+k}|}{2\nu^j} \stackrel{\text{def}}{=} h^2_{lk}(\bar{p}).$$

We set the convention $h(l,0) = 0$ and

$$v^{\infty}_k = \begin{cases} 0 & 0 \leq k \leq K \\ v_k & k \geq K+1 \end{cases}. \tag{65}$$

Proof. See [69]. □

Theorem 4.9. *Z-bounds - 1D*
Assume truncation dimensions $M > 0$ and $K > 0$ and an approximate zero $\bar{p}$, with $\Pi_{MK}\bar{p} = \bar{p}$ to be given. Define

$$|\Delta^{(1)}|_{mk} = \begin{cases} 0 & m = 0,1, k \geq 0 \\ \frac{r_{\lambda} m}{\nu^k} + \sum_{l=0}^{m} h_{lk}(\bar{p}) + m\|p\|_{\nu}|c^{\infty}|_{\nu} & 2 \leq m \leq M, 0 \leq k \leq K \\ 0 & (m \geq M+1, k \geq 0) \vee (0 \leq m \leq M, k \geq K+1) \end{cases} \tag{66a}$$

$$|\Delta^{(2)}|_{mk} = \begin{cases} 0 & m = 0,1, k \geq 0 \\ \frac{2\alpha|c|_{\nu}}{\nu^k} & 2 \leq m \leq M, 0 \leq k \leq K \\ 0 & (m \geq M+1, k \geq 0) \vee (0 \leq m \leq M, k \geq K+1) \end{cases} \tag{66b}$$

,

$$\Sigma^{(j)}_{MK} = \sum_{m=0}^{M} \left(|(|A||\Delta^{(j)}|)_0| + \sum_{k=1}^{K} |(|A||\Delta^{(j)}|)_k|\nu^k \right). \tag{67}$$

and ϵ such that $\sup_{v \in B_1(0)} \|(Id - AA^{\dagger})rv\|_{\nu} \leq \epsilon r$. Then

$$\begin{aligned} Z(r) =& r\left(\epsilon + \Sigma^{(1)}_{MK} + 2\alpha|c|_{\nu}\|\bar{p}\|_{\nu}\left(\frac{1}{K^2-\alpha} + \frac{1}{|(\bar{\lambda}+r_{\lambda})M - \alpha|}\right)\right) \\ &+ r^2\left(\Sigma^{(2)}_{MK} + 2\alpha|c|_{\nu}\left(\frac{1}{K^2-\alpha} + \frac{1}{|(\bar{\lambda}+r_{\lambda})M - \alpha|}\right)\right) \end{aligned} \tag{68}$$

fulfills (14).

Proof. We start by expanding the difference $\Delta = Df(\bar{p}+ru)rv - A^{\dagger}rv$ from equation (58). Using the formula

$$(Df(p)q)_{mk} = \begin{cases} q_0 & m=0, k\geq 0 \\ q_1 & m=1, k\geq 0 \\ (\tilde{\lambda}m + k^2 - \alpha)q_{mk} + 2\alpha(c * (p *_{TF} q)_m)_k & m\geq 2, k\geq 0 \end{cases},$$

we obtain

$$Df(\bar{p}+ru)rv = \begin{cases} rv_0 & m=0, k\geq 0 \\ rv_1 & m=1, k\geq 0 \\ (\tilde{\lambda}m + k^2 - \alpha)rv_{mk} + 2\alpha r(c * (\bar{p} *_{TF} v)_m)_k & m\geq 2, k\geq 0 \\ 2\alpha r^2(c * (u *_{TF} v)_m)_k \end{cases}.$$

Using the refined definition of $A^{\dagger}$ alluded to above (all linear terms cancel) we obtain for Δ

$$\Delta_{mk} = \begin{cases} 0 & m=0,1 \\ (\lambda^{\infty} m)p_{mk} + 2\alpha r(\bar{c} * (\bar{p} *_{TF} v^{\infty})_m)_k & 2\leq m\leq M, 0\leq k\leq K \\ 2\alpha r(c^{\infty} * (\bar{p} *_{TF} v)_m)_k + 2\alpha r^2(c^{\infty} * (u *_{TF} v)_m)_k & \\ 2\alpha r(c * (\bar{p} *_{TF} v)_m)_k + 2\alpha r^2(c^{\infty} * (u *_{TF} v)_m)_k & m > M \vee k > K, \end{cases}$$

where we use the notation v^{∞} from Lemma 4.8. Now using this very Lemma and the decay information on u, v we obtain (74). The proof follows from applying A to Δ, taking the norm $\|\cdot\|_{\nu}$ and using

$$\frac{1}{|\tilde{\lambda}|m + k^2 - \alpha} \leq \begin{cases} \frac{1}{|\tilde{\lambda}(M+1)| - \alpha} & m > M, k\geq 0 \\ \frac{1}{(K+1)^2 - \alpha} & m\geq 0, k > K \end{cases}.$$

□

This provides us with the ingredients to define the radii polynomials by

$$p(r) = Y + Z(r) - r,$$

with Y given by (73) and $Z(r)$ given by (76). The Matlab script

`validateparametrization_c_intval.m`

implements these bounds.

Remark 4.10. *Using a radius r_P such that $Y + Z(r_p) - r_p < 0$ we can now rigorously enclose the image $P(\theta) \in \ell^1_{\nu}$ of every $\theta \in B_1(0)$. More precisely if $\|\tilde{p} - \bar{p}\|_{\nu} < r_P$ then $|P(\theta) - P^{MK}(\theta)|_{\nu} < r_P$. This allows is to bound the distance of $P(\theta)$ to any point using the triangle inequality. This will be used in our connecting orbit proof in Section 4.3.*

Results We take $\nu = 1.1$ and choose truncation dimensions in Fourier direction to be $K = 20$ and in Taylor direction $M = 60$. In Figure 4.2 we illustrate the decay in these two directions. In Figure 4.2 we show an illustration of the manifold in function space and demonstrate the conjugation property of the parametrization map P. The corresponding computations are to befound in `unstable1D_c_intval.m`

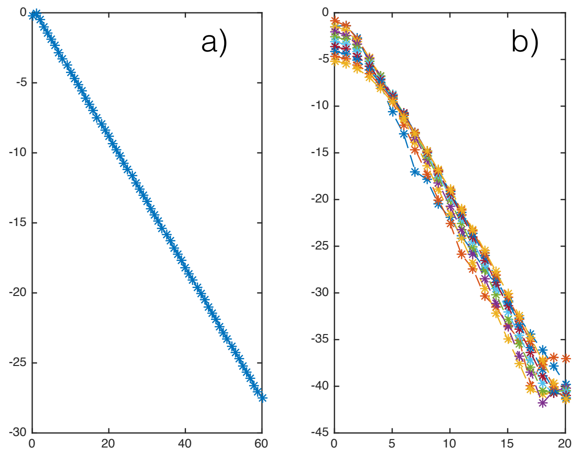

Figure 3: a) We show the decay of $|p_m|_\nu$ with m. b) This illustrates the decay of the individual coefficient sequences $p_m \in \ell^1_\nu$ for $m = 0, \ldots, 60$. Our approach quantifies the truncation error in both directions.

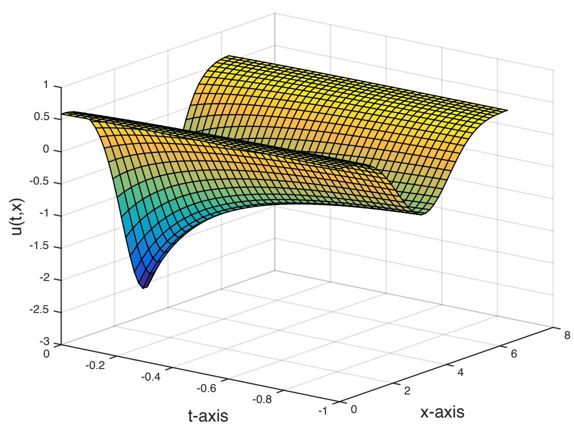

Figure 4: 3D image of the unstable manifold in function space. We use the fact that $a(t) = P(\exp(\tilde{\lambda} t))$ solves (46) backward in time. We integrate the initial condition $P(0.9)$ backward for one time unit. Observe the convergence towards $\tilde{a}^2$.

Two unstable eigenvalues (at the origin): As alluded to above the Morse index of the origin is 2 which is clearly seen from the fact that for $b \in \ell^1_\nu$ we have that $(Dg(0)b)_k = (\alpha - k^2) b_k$ for $k \geq 0$. This implies that the unstable eigenvalues are $\tilde{\lambda}_1 = \alpha$ and $\tilde{\lambda}_2 = \alpha - 1 > 0$ together with the eigenvectors $\tilde{\xi}_1 = (1, 0, 0 \ldots)$ and $\tilde{\xi}_2 = (0, 1, 0, \ldots)$. Note that we still use tildas even though the quantities are not computed by computer-assisted means. Assume an approximate solution $\bar{p}$ corresponding to truncation dimensions $M \in \mathbb{N}^2$ with $M_i > 1$ $(i = 1, 2)$ and $K > 0$ to be given. In Figure 5 we show an illustration of a 2D unstable manifold with truncation dimensions $M = (5, 20)$ and $K = 20$.

To explain how the estimates can be adapted to this setting let us again specify the splitting of the according to (42). Note that we deal with two-dimensional multi-indices for m now but have exact linear data $\tilde{\lambda}, \tilde{\xi}$ for the equlibrium $\tilde{a}$ at the origin at our disposal.

Definition 4.11. Assume we are given truncation dimensions $M \in \mathbb{N}^2$ and $K > 0$. Split $p = \Pi_{MK}p + p^\infty$, where $p^\infty = (Id - \Pi_{MK})\, p$. We set

$$f^{MK}(p^{MK})_{mk} = \begin{cases} -(p^{MK})_{0k} & m = 0 \\ (\tilde{\xi}_i)_k - (p^{MK})_{e_i k} & m = e_i \quad (i = 1,2) \\ (\tilde{\lambda} \cdot m + k^2 - \alpha) p^{MK}_{mk} + \alpha(\left(p^{MK} *_{TF} p^{MK}\right)^{MK}_m)^K_k & |m| \geq 2, m \preceq M \\ & 0 \leq k \leq K \end{cases} \tag{69}$$

and

$$(f^\infty(p))_m = \begin{cases} -p^\infty_{0k} & m = 0, k \geq 0 \\ -p^\infty_{1k} & m = e_i \quad (i = 1,2), k \geq 0 \\ (\tilde{\lambda} \cdot m + k^2 - \alpha) p^\infty_{mk} + & \\ \alpha (Id - \Pi_{MK}) \left((p^{MK} *_{TF} p^{MK} \right)_m)_k + & \\ \alpha \left[((2p^{MK} *_{TF} p^\infty)_{mk} + (p^\infty *_{TF} p^\infty)_m)_k \right] & |m| \geq 2, k \geq 0 \end{cases} . \tag{70}$$

Recall $\tilde{\lambda} \cdot m = \tilde{\lambda}_1 m_1 + \tilde{\lambda}_2 m_2$. Note that in this case we can explicitly check the non-resonance condition from Definition 3.1 by checking that $\frac{\tilde{\lambda}_i}{\tilde{\lambda}_j} \notin \mathbb{N}$ for $i, j = 1, 2$. Then $f(p) = f^{MK}(p^{MK}) + f^\infty(p)$.

Following the same steps as we did in the previous Section we can derive Y- and Z-bounds. We can formulate the corresponding Theorems to 4.7 and 4.9. For the implementation we refer to `validateparametrizationorigin2D.m` to be found at [78]. For a specific example calculation see `manifoldorigin2D.m`, where we compute and validate the unstable manifold for the specific truncation dimension $M = [5, 20]$. We choose $\nu = 1.01$ and obtain a validation radius of $r = 5.978461 \times 10^{-10}$. The results are illustrated in Figure 5.

Theorem 4.12. *Y-bounds - 2D*
Assume truncation dimensions $M \in \mathbb{N}^2$ and $K > 0$ and an approximate zero $\bar{p}$, with $\Pi_{MK}\bar{p} = \bar{p}$ to be given. Define

$$Y^{MK}_m = |(Df^{MK}(\bar{p})\bar{p})_{m0}| + 2 \sum_{k=1}^{K} |(Df^{MK}(\bar{p})\bar{p})_{mk}| \nu^k, \quad m \preceq M, \tag{71}$$

and

$$Y^\infty_m = \begin{cases} 2 \displaystyle\sum_{k=K+1}^{2K} \frac{\alpha |((\bar{p} *_{TF} \bar{p})_m)_k|}{\tilde{\lambda} \cdot m + k^2 - \alpha} \nu^k & |m| \geq 2, m \preceq M \\ \frac{\alpha |(\bar{p} *_{TF} \bar{p})_{m0}|}{\tilde{\lambda} \cdot m} + 2 \displaystyle\sum_{k=1}^{3K} \frac{\alpha |((\bar{p} *_{TF} \bar{p})_m)_k|}{\tilde{\lambda} \cdot m + k^2 - \alpha} \nu^k & M + 1 \preceq m \preceq 2M, \end{cases} . \tag{72}$$

Then

$$Y = \sum_{m_1=0}^{M_1} \sum_{m_2=0}^{M_2} Y^{MK}_m + \sum_{\substack{|m| \geq 2 \\ m \preceq M}} Y^\infty_m + \sum_{\substack{m_1 > M_1 \vee m_2 > M_2 \\ m \preceq 2M}} Y^\infty_m \tag{73}$$

fulfills (13).

Proof. Analogue to Theorem 4.7. $\square$

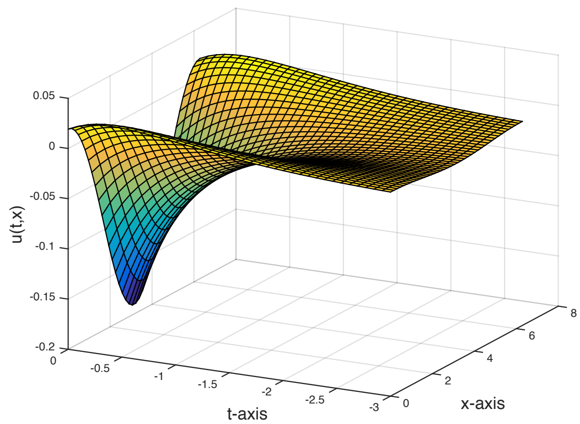

Figure 5: We show the local unstable manifold computed by using that $a(t) = P\left(\exp(\tilde{\Lambda}t)\theta\right)$ is a solution for each $\theta \in \mathbb{B}_1$ $t \leq 0$. Here $\tilde{\Lambda} \in \mathbb{R}^{2,2}$ the diagonal matrix with the unstable eigenvalues $\tilde{\lambda}_{1,2}$ as entries. We integrate P(0.01,0.95) backward for 3 time units and observe the convergence to the stationary solution $\tilde{u} = 0$. We scale the eigenvectors with 0.01 and 0.05 respectively.

Theorem 4.13. *Z-bounds - 2D*
Assume truncation dimensions $M \in \mathbb{N}^2$ and $K > 0$ and an approximate zero $\bar{p}$, with $\Pi_{MK}\bar{p} = \bar{p}$ to be given. Define

$$|\Delta^{(1)}|_{mk} = \begin{cases} 0 & m = 0, e_i (i = 1, 2) \quad k \geq 0 \\ \displaystyle\sum_{l_1=0}^{m_1}\sum_{l_2=0}^{m_2} h_{lk}(\bar{p}) & |m| \geq 2, m \preceq M, 0 \leq k \leq K \\ 0 & (m \geq M + 1, k \geq 0) \vee (0 \leq m \leq M, k \geq K + 1) \end{cases} \tag{74a}$$

$$|\Delta^{(2)}|_{mk} = \begin{cases} 0 & m = 0, e_i (i = 1, 2) \quad k \geq 0 \\ \frac{2\alpha}{\nu^k} & 2 \leq m \leq M, 0 \leq k \leq K \\ 0 & (m \geq M + 1, k \geq 0) \vee (0 \leq m \leq M, k \geq K + 1) \end{cases} \tag{74b}$$

,

$$\Sigma_{MK}^{(j)} = \sum_{m_1=0}^{M_1}\sum_{m_2=0}^{M_2}\left(|(|A||\Delta^{(j)}|)_0| + \sum_{k=1}^{K}|(|A||\Delta^{(j)}|)_k|\nu^k\right). \tag{75}$$

and ϵ such that $\sup_{v \in B_1(0)} \|(Id - AA^\dagger)rv\|_\nu \leq \epsilon r$. Then

$$\begin{aligned} Z(r) =& r\left(\epsilon + \Sigma_{MK}^{(1)} + 2\alpha\|\bar{p}\|_\nu\left(\frac{1}{K^2 - \alpha} + \frac{1}{\min(|\tilde{\lambda}_1|M_1, |\tilde{\lambda}_2|M_2) - \alpha}\right)\right) \\ &+ r^2\left(\Sigma_{MK}^{(2)} + 2\left(\frac{1}{K^2 - \alpha} + \frac{1}{\min(|\tilde{\lambda}_1|M_1, |\tilde{\lambda}_2|M_2) - \alpha}\right)\right) \end{aligned} \tag{76}$$

fulfills (14).

Proof. The proof is similar to the one of Theorem 4.9. $\square$

Lower triangular structure To conclude this section let us remark on some implementation related issues. Recalling (20) to analyze the structure of $(X^{\nu,d}, *_{TF})$ we see that $(p *_{TF} q)_m$ does only depend on terms with $\tilde{m} \preceq m$. This entails that the derivative $\frac{\partial}{\partial p_{\tilde{m}}} f_m \in \mathcal{L}(\ell^1_\nu, \ell^1_{\tilde{\nu}})$ $(1 < \tilde{\nu} < \nu)$ is only non-zero for $\tilde{m} \preceq m$. We refer to this structure as lower triangular structure. We use this structure in our numerical implementation. To explain the idea let us restrict to the case $d = 1$, so there is a canoncial ordering on the indexing set $\mathbb{N}$ for m. Given truncation dimensions $M > 0$ and $K > 0$ the map f^{MK} is a nonlinear map on $\mathbb{R}^{(M+1)(K+1)}$. Its derivative matrix $Df^{MK}(p) \in \mathbb{R}^{(M+1)(K+1),(M+1)(K+1)}$ has the following block structure:

$$Df^{MK}(p) = \begin{pmatrix} B_{00} & 0 & 0 & \\ B_{10} & B_{11} & 0 & 0 \\ \vdots & \vdots & \ddots & 0 \\ B_{M0} & B_{11} & \cdots & B_{MM} \end{pmatrix},$$

with $B_{ij} = \frac{\partial}{\partial p_j} f_i^{MK}(p) \in \mathbb{R}^{K+1,K+1}$. Thus to solve a linear system of the form $Df^{MK}(p)h = b$, with $h, b \in \mathbb{R}^{(M+1)(K+1)}$ we can implement a block backsubstitution algorithm, that necessitates the solution of $M+1$ systems of size $(K+1)$ instead of the solution of one system of size $(M+1)(K+1)$. So the complexity is $O((K+1)^3)$ against $O(((M+1)(K+1))^3)$ In the case that $d > 1$ we see that this translates to the solution of $\prod_{i=1}^d M_i$ systems of size $(K+1)$ making the advantage drawn from this way of implementation even more crucial.

4.3 Computer assisted proof of a heteroclinic connecting orbit

In this section we demonstrate how our technique can be used to prove the existence of a connecting orbit. We restrict our attention to the constant case $c(x) = 1$. In this case the fixed point $\frac{1}{c(x)}$ reduces in Fourier space to $\tilde{a}^1 = (1, 0, 0, \ldots)$. We see directly from the linearization of g around $\tilde{a}^1 = (1, 0, 0, \ldots)$ that $\tilde{a}^1$ is spectrally stable, as all eigenvalues are negative. In addition we can derive nonlinear stability information in terms of an attracting neighborhood of $\tilde{a}^1$, see Lemma 4.14 below.

Lemma 4.14. *The equilibrium point $\tilde{a}^1$ of* (46) *is an attracting fixed point with attracting neighborhood*

$$\mathcal{A} = \left\{ a \in \ell^1_\nu : |a - \tilde{a}^1|_\nu < 1 \right\}. \tag{77}$$

Proof. See Appendix A. $\square$

This provides us with the ingredient to state the following Theorem proving the existence of a connecting orbit from the equilibrium $\tilde{a}^2$ with Morse index 1 to the sink $(1, 0, 0, \ldots)$. Note that we can use Lemma 4.2, 4.4 and 4.5 as well as Theorem 4.7 and 4.9 to compute this equilbirium $\tilde{a}^2$ together with its stability information. This is achieved in the Matlab script `a_validateLinearDatac1_paperVersion.m` at the parameter value $\alpha = 2.1$.

Theorem 4.15. *Let $\nu = 1.1$. Let P be a parametrization of the unstable manifold of $\tilde{a}^2$ with $|DP(0)|_\nu = 0.68194897863182 \pm 10^{-16}$. For $\theta = -0.505050505050505 \pm 10^{-16}$ we have that $P(\theta) \in \mathcal{A}$. Hence there is a connecting orbit from $\tilde{a}^2$ to $\tilde{a}^1$.*

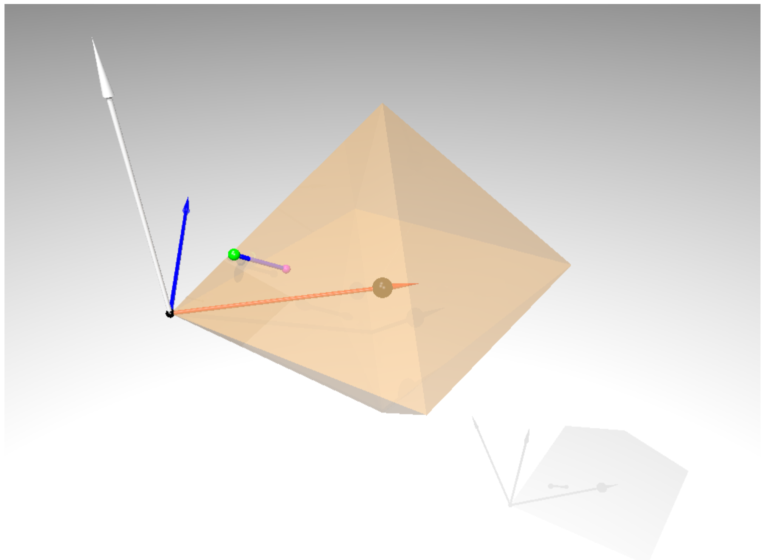

Figure 6: The green dot shows the projection of the non-trivial fixed point $\tilde{a}^2$ to the (a_0, a_1, a_2) coordinate plane. The blue line is the part of the 1D local unstable manifold of $\tilde{a}^2$ that we validate whose endpoint is marked in purple and lies inside the domain of attraction of the sink

Proof. By using the inequality

$$|P(\theta) - \tilde{a}^1|_\nu \leq |P(\theta) - P^{MK}(\theta)|_\nu + |P^{MK}(\theta) - \tilde{a}^1|_\nu \leq r_P + |P^{MK}(\theta) - \tilde{a}^1|_\nu$$

we can rigorously check for any given θ if the true image $P(\theta)$ lies in $\mathcal{A}$. This computation is carried out using Matlab and Intlab in the program. In case of success it follows immediately from Lemma 4.14 that there is a connecting orbit from $\tilde{a}^2$ to $\tilde{a}^1$. The Matlab script `proofconnection.m` available at [78] carries out this check. It is called at the end of the script `unstablec1_intval.m`, which computes and validates the parametrization.

□

5 Acknowledgments

The authors would like to thank Mr. Jonathan Jaquette for suggesting to us the argument given in Appendix A. Conversations with J.B. van den Berg, J.P. Lessard and Rafael de la Llave were also extremely valuable. J.D.M.J. was partially supported by NSF grant DMS-1318172.

A Domain of attraction of $\tilde{a} = (1, 0, 0, \ldots)$

Lemma 4.14 in Section 4.3 states that the equilibrium point $\tilde{a} = (1, 0, 0, \ldots)$ of (46) is an attracting fixed point with attracting neighborhood

$$\mathcal{A} = \left\{ a \in \ell^1_\nu : |a - \tilde{a}|_\nu < 1 \right\}. \tag{78}$$

Proof. Write $a = \tilde{a} + h$. Then $a' = g(a)$ if

$$h'_k = -(k^2 + \alpha)h_k - \alpha(h * h)_k = (Lh)_k + N(h)_k, \quad k \geq 0, \tag{79}$$

where $L = Dg(\tilde{a})$ and $N(h) = g(\tilde{a} + h) - g(\tilde{a}) - Lh$. Denote $h(0) = h_0$ and let $h(t)$ solve (79) with initial condition h_0. We show that if $|h_0|_\nu < 1$, then $\lim_{t\to\infty} |h(t)|_\nu = 0$. Define $\left(\mathrm{e}^{-Lt}h_0\right)_k \overset{\text{def}}{=} \mathrm{e}^{-(k^2+\alpha)t}h_{0k}$. Then

$$|\mathrm{e}^{-Lt}h_0|_\nu \leq \mathrm{e}^{-\alpha t}|h_0|_\nu. \tag{80}$$

Using the variation of constants formula we have

$$h(t) = \mathrm{e}^{-Lt}h_0 + \int_0^t \mathrm{e}^{-L(t-s)}(h * h)(s)ds. \tag{81}$$

Using (80) in (81) we obtain

$$|h(t)|_\nu \leq \mathrm{e}^{-\alpha t}|h_0|_\nu + \int_0^t \mathrm{e}^{-\alpha(t-s)}\alpha \underbrace{|h * h|_\nu}_{\leq |h|_\nu |h|_\nu}(s)ds. \tag{82}$$

Assume $|h_0|_\nu < r < 1$. By continuity of $|h(t)|$ there is a $t_1 > 0$ such that $r \leq \max_{s\in[0,t_1]} \leq \rho_1 < 1$. Then for $t \in [0, t_1]$:

$$\mathrm{e}^{\alpha t}|h(t)|_\nu \leq |h_0|_\nu + \int_0^t \alpha\rho_1 \mathrm{e}^{\alpha s}|h|_\nu(s)ds \tag{83}$$

Using Gronwall's inequality for the function $\mathrm{e}^{\alpha t}|h(t)|_\nu$ we obtain

$$\mathrm{e}^{\alpha t}|h(t)|_\nu \leq |h_0|_\nu \mathrm{e}^{\int_0^t \rho_1 \alpha ds}, \tag{84}$$

hence $|h(t_1)|_\nu \leq |h_0|\mathrm{e}^{-\alpha(1-\rho_1)t_1} < |h_0|_\nu$. Inductively we construct a sequence of times t_k with $\lim_{k\to\infty} t_k = \infty$ and $|h(t_k)| < |h(t_{k-1})|$ for $k \geq 2$. (By continuity of $|h(t)|_\nu$, hence if $t_k \to t^\infty < \infty$, then $|h(t)|_\nu$ would not be continuous in t^∞.) As $(|h(t_k)|_\nu)_{k\in\mathbb{N}}$ is decreasing and bounded from below it converges to $0 \leq \delta < 1$. Assume $\lim_{k\to\infty} |h(t_k)| = \delta > 0$. There exists a $K > 0$ such that $|h(t_k)| < \frac{1-\delta}{2}$ for all $k \geq K$. Then $|h(t)|_\nu \leq |h_0|\mathrm{e}^{-\alpha(1-\rho_K)t} < |h_0|_\nu$ for all $t \geq t_K$. For $t \to \infty$ this yields $\delta < 0$, a contradiction. Hence $\delta = 0$. ☐

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