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

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Abstract

We develop a method for computing polynomial approximations of unstable manifolds at equilibrium solutions of parabolic PDEs. These polynomials have a finite number of variables, even though they map into an infinite dimensional state space. We implement this method numerically, and develop explicit a-posteriori error bounds. By combining the a-posteriori error estimates with careful management of floating point round-off errors we obtain mathematically rigorous error bounds on the truncation and discretization errors associated with our polynomial approximation. We illustrate the method with applications to Fisher's equation.

1 Introduction and setup

Analysis of nonlinear, dissipative, parabolic PDEs from the dynamical system point of view begins with the analysis of stationary and periodic solutions, and is followed by investigation of their stability. After completing this local analysis, we might ask how these landmark solutions fit together. This question leads to the study of connecting orbits. An essential ingredient in the analysis of connecting orbits is control over the unstable manifolds. Since a parabolic PDE generates a compact flow, the linearized dynamics have only a finite number of unstable directions, and such equations admit only finite dimensional unstable manifolds. The present work develops a method for computing polynomial approximations of unstable manifolds at equilibrium solutions of parabolic PDEs. These polynomials have a finite number of variables, even though they map into an infinite dimensional state space. We implement this method numerically, and develop explicit a-posteriori error bounds. By combining the a-posteriori error estimates with careful management of floating point round-off errors we obtain mathematically rigorous error bounds on the truncation and discretization errors associated with our polynomial approximation.

We emphasize that for infinite dimensional dynamical systems the initial analysis of the equilibrium solution is in general far from trivial. Already the stability analysis 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 difficult if not impossible to carry out this analysis analytically. Numerical simulations provide valuable insight into the dynamics of PDEs, and

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in recent years a great deal of effort has gone into developing methods for computer assisted proofs which provide mathematically rigorous validation of simulation results.

A thorough review of the literature on computer assisted proof for dynamics of PDEs would lead us far afield of the present discussion, however the interested reader might consult [70, 69, 66, 3, 5, 7, 54, 53, 46, 21, 59, 9, 39] for fuller discussion of equilibria solutions of PDEs, and also [61, 44, 51, 5, 18] for more complete discussion of techniques for validated computation of solutions of eigenvalue/eigenvector problems for infinite dimensional problems. While the list is far from exhaustive, these works and the references discussed therein provide a helpful introduction to the literature on computer assisted analysis of equilibrium solutions for PDEs.

The approach of the present work is based on the parameterization method of [10, 11, 12], which is a general functional analytic framework for studying *non-resonant* invariant manifolds of fixed points and equilibria of dynamical systems defined on Banach spaces. It is well established that the parameterization method leads to efficient numerical algorithms for computing many different species of invariant manifolds, and that it also provides a convenient setting for a-posteriori error analysis. Another feature of the parameterization method is that one obtains explicitly the dynamics on the manifold, in addition to obtaining information about the embedding. We refer the interested reader to the works of [32, 33, 35, 38, 15, 16, 26, 37, 13, 14, 47, 16], and to the further references cited therein. Our approach builds on various successful applications of the parametrization method to finite dimensional ODEs [58, 48, 42, 8, 55] and infinite dimensional maps [50]. The recent book of [31] contains a much more complete discussion of the parameterization method and its applications. See also [49, 40, 6, 2, 17, 65, 52], and the discussion in these for a more complete picture of the literature on validated numerics for stable/unstable manifolds of finite dimensional dynamical systems, and also the work of [28, 27] for more discussion of the use of the parameterization method in infinite dimensional settings.

The techniques developed in the present work apply in principle to a large class of problems. The main properties we need to exploit are the following:

(I) The eigenfunctions of the linear part of the partial differential equation comprise a countable basis for the Banach space of solutions.

(II) The flow generated by partial differential equation is "smoothing", i.e. the problem is reasonably compact (this is why in our discussion we focus on parabolic equations).

(III) Solutions of the partial differential equation have known a-priori regularity in the spatial variables.

In practice we use assumption (I) in order to recast the PDE as a system of infinitely many scalar ODEs, i.e. in the present work we deal only with spectral projections. Assumption (II) can be restated as asking that the semi-group generated by the linearized partial differential operator is compact. In particular we want that the the linearized flow at an equilibrium solution of the PDE has spectrum composed of discrete eigenvalues which accumulate only at the origin. This insures that the Morse-index of the equilibrium is finite, i.e. that there are only a finite number of unstable eigendirections at the equilibrium. Restricting to a finite dimensional unstable manifold seems to be necessary in order to satisfy the non-resonance requirements of the parameterization method. Finally, assumption (III) asks for some a-priori knowledge of the regularity of solutions (or at least the regularity of solutions on the unstable manifold). Admittedly this last condition is vague. In practice we ask for enough a-priori regularity to guarantee that the infinite sequence of scalar coefficients of the eigenfunction expansion of a solution on the unstable manifold decay at a rate which can

be characterized by some (Banach) sequence space norm. This allows our problem to be cast as an ODE on a weighted ℓ^p space with $1 \leq p \leq \infty$ (in fact weighted sequence spaces with $p = 1$ or $p = \infty$ are typical). In the present work we focus on exponential weights (analytic regularity) but in the literature discussed above algebraic weights are also used (C^k regularity).

In principle the assumptions above are met for problems posed on compact spatial domains in $\mathbb{R}^N$ with smooth boundaries and smooth boundary conditions or more generally for problems posed on smooth compact manifolds. In the present work, in order to minimize the proliferation of notational difficulties, we consider a fixed specific class of parabolic equations (and for the discussion of the numerical implementation we restrict our attention even further to a class of PDEs with logistic nonlinearity).

More precisely, assume the PDE is of the form

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

where $I \subset \mathbb{R}$ is a compact interval, L 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 L 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 residing in a weigthed l^1 space, that we denote by Y^ν and endow with the natural norm $|\cdot|_\nu$ to be specified more precisely later. We use the shorthand notation $a' = g(a)$ for (2). To define the unstable manifold we are interested in, assume $\hat{a}$ to be given such that $g(\hat{a}) = 0$. Its unstable manifold is given by

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

It is a classical fact that for equations of type (1) this is a finite dimensional manifold [56]. We aim at computing a parametrization map $P : \mathbb{C}^d \supset \mathbb{B}_1 \to Y^\nu$, where $\mathbb{B}_1$ is the unit polydisc and d is the dimension of the manifold.

The first step of our method is to find an equilibrium solution $\hat{a}$ of (2) together with its Morse index and eigendata. More precisely we compute $\hat{a}$ such that $g(\hat{a}) = 0$ together with the d unstable eigenvalues $\hat{\lambda}_i$ and eigenvectors $\hat{\xi}_i \in Y^\nu$, such that

$$Dg(\hat{a})\hat{\xi}_i = \hat{\lambda}_i \hat{\xi}_i \quad i = 1, \ldots, d. \tag{4}$$

We use the hat notation to stress that the quantity at hand comes out of a computer-assisted proof for the zero-finding problem $g(\hat{a}) = 0$ that we solve via a Newton-like fixed point operator. This means that $\hat{a}$ is only known to us as a numerical approximation endowed with explicit error norm. As this will be the basis for many crucial arguments in the paper let us explain the philosophy. We compute a numerical approximate zero $\tilde{a}$ and

construct the operator $T(x) = x - Ag(x)$, where A is an approximate inverse of $Dg(\tilde{a})$. Via showing that T is a contraction on a ball of appropriate radius $r_{\tilde{a}}$ around the approximate zero $\tilde{a}$ we obtain the existence of a genuine zero $\hat{a}$ in this ball. In particular we get that $\hat{a} = \tilde{a} + a^{\infty}$ with $|a^{\infty}|_{\nu} \leq r_a$. Concerning the eigenvalue problem we take three additional steps. First by construction of our method we can solve the eigenvalue problem (4) for $A^{\dagger} \approx A^{-1}$ explicitly. In addition we can show that $A^{\dagger}$ and $Dg(\hat{a})$ have the same Morse index. To get an exclosure of the eigenvalues and eigenvectors of the form $\hat{\lambda}_i = \tilde{\lambda}_i + \lambda_i^{\infty}$ with $|\lambda_i^{\infty}| \leq r_{\tilde{\lambda}_i}$ and $\hat{\xi}_i = \tilde{\xi}_i + \xi_i^{\infty}$ with $|\xi_i^{\infty}|_{\nu} \leq r_{\tilde{\xi}_i}$ for $i = 1, \ldots, d$ we interpret the eigenvalue equations (4) as (nonlinear) zero finding problems in the unknowns (λ_i, ξ_i) and apply the fixed point approach to $g_i^{eig} = Dg(\hat{a})\xi_i - \lambda_i \xi_i$ using as approximate solution the numerical unstable eigendata $(\tilde{\lambda}_i, \tilde{\xi}_i)$ from $Dg(\tilde{a})$. Note that by completing this three step process we in particular exclude spurious eigendata. See Section 3.1 for more details.

The next step is to use this linear data to compute a parametrization map P for the finite dimensional unstable manifold in the infinite dimensional phase space Y^{ν}. The foundation of our method is the parametrization method developed in [10, 11, 12].

More precisely we compute the map $P : \mathbb{B}_1 \to Y^{\nu}$ as solution of the functional equation

$$g(P(\theta)) = DP(\theta)\Lambda\theta \quad \forall \theta \in \mathbb{B}_1, \tag{5}$$

together with the linear constraints

$$P(0) = \hat{a} \tag{6a}$$

$$DP(0) = [\hat{\xi}_1, \ldots, \hat{\xi}_d], \tag{6b}$$

where $\Lambda \in \mathbb{C}^{d,d}$ is the diagonal matrix with the eigenvalues $\hat{\lambda}_i$ on the diagonal. Under the non-resonance assumptions

$$m_1\hat{\lambda}_1 + \cdots + m_d\hat{\lambda}_d \stackrel{\text{def}}{=} m \cdot \hat{\lambda}_d \neq \hat{\lambda}_i \quad \forall m \in \mathbb{N}^d, |m| \geq 2, \forall i = 1, \ldots, d \tag{7}$$

the map P can be written as a convergent power series. We use the notation $|m| = m_1 + \cdots + m_d$. Note that the resonance assumption can be dropped by using the techniques of [55], but for the clarity of exposition we restrict to the non-resonant case in this paper. Also the eigenvalues will be real in the applications we consider but with the techniques from [55] the setup can be adapted. Let us state the significance of the above functional equation more precisely.

Lemma 1.1. *Assume that P solves (5) and (6) then for every $\theta \in \mathbb{B}_1$ the function*

$$a(t) = P(\exp(\Lambda t)\theta) \tag{8}$$

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

The proof is obtained by direct computation using that $\text{real}(\lambda_i) < 0$ for $i = 1, \ldots, d$. Hence we can set out to solve (5) via a power series ansatz of the form

$$P(\theta) = \sum_{|m|=0}^{\infty} p_m \theta^m \tag{9}$$

with multiindices $m \in \mathbb{N}^d$, $\theta^m = \theta_1^{m_1} \cdots \theta_d^{m_d}$ and $p_m = (p_m)_{k \geq 0} \in l^1_{\nu}$ for all $k \in \mathbb{N}^d$. Plugging (9) into (5) we obtain an equivalent zero finding problem $f(p) = f_m(p)_{m \in \mathbb{N}^d} = 0$

for the power series coefficients $p = (p_m)_{m\in\mathbb{N}^d}$. Note that for each index m we demand $f_m(p) = 0 \in Y^\nu$. To obtain a numerical approximate solution $\tilde{p}$ we truncate the map f to a finite dimensional map $f^{MK} : \mathbb{R}^{(|M|+1)(K+1)} \to \mathbb{R}^{(|M|+1)(K+1)}$ by restricting m to $\mathcal{F}_M = \left\{m \in \mathbb{N}^d : m_i \leq M_i \ \forall i = 1, \ldots, d\right\}$ and truncating $p_m \in l^1_\nu$ at order $K > 0$ and compute an approximate zero $\tilde{p} \in \mathbb{R}^{(|M|+1)(K+1)}$. From this we obtain an approximate parametrization of the form

$$P^{MK}(\theta) = \sum_{m\in\mathcal{F}_M} \tilde{p}_m \theta^m. \tag{10}$$

The rigorous a-posteriori validation of the approximate solution $\tilde{p}$ uses the Newton-like fixed point approach applied to the zero finding problem $f(p) = 0$. As a result we obtain an explicit error bound of the form

$$\sup_{\theta\in\mathbb{B}_1} |P(\theta) - P^{MK}(\theta)|_\nu \leq r_P, \tag{11}$$

where we make the norm $\|\cdot\|$ more precise below. Let us summarize the inputs and outputs of our method:

Input

- Approximate equilibrium $\tilde{a}$ of $a' = g(a)$ with g defined in (2)
- Approximate eigendata $(\tilde{\lambda}_i, \tilde{\xi}_i)$, $i = 1, \ldots \tilde{d}$, where $\tilde{d}$ is the approximate Morse index

Output

- Error bound: r_a and the proof that $\tilde{d}$ is the true Morse index, we write $\tilde{d} = d$.
- Error bounds r_{λ_i}, r_{ξ_i} for $i = 1, \ldots, d$ for the eigenvalues and eigenvectors.
- Approximate parametrization P^{MK} together with error bound r_P fulfilling (11).

To showcase our method we the following boundary value problem for the following reaction diffusion equation on a one-dimensional bounded spatial domain with Neumann boundary conditions:

$$\begin{aligned} u_t &= u_{xx} + \alpha u(1 - c_2(x)u), \quad (x,t) \in [0, 2\pi] \times \mathbb{R}, \\ u_x(0,t) &= u_x(2\pi, t) = 0 \quad \forall t \geq 0 \end{aligned} \tag{12}$$

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. For notational convenience we drop the index 2 and refer to the spatial inhomogeneity as $c(x)$. 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 [30, 1, 45].

Remark 1.2 (Further comments on regularity)**.** It is worth noting that, strictly speaking, we do not need to know a-priori the regularity of the solutions: rather this is a convenience. Indeed, if our method succeeds then we obtain regularity results for the unstable manifold a-posteriori. In practice however it is helpful to have at least a reasonable "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 this point we refer to [43]. Fuller discussion of the computer as a tool for studying breakdown of regularity of invariant objects can be found in the works of [13, 34, 25, 24].

Remark 1.3 (Extension to finite element bases)**.** An important extension of the methods of the present work would be to develop a numerical implementation and a-posteriori theory for computing unstable manifolds for PDEs using the Parameterization Method in a finite element basis. Such a scheme would have to abandon the "sequence space calculus" exploited in the present work. Nevertheless we believe that this extension can succeed by considering the so called *homological equations* for the jets of the parameterization "term by term", as was done in [58, 48] for ordinary differential equations. In order to validate the error bounds one would then have to study a PDE for the "tail" of the parameterization (projection onto the orthogonal complement of the span of the finite elements), probably in some Sobolev space. The so called "N-tail" approach of the references just mentioned, and also the discussion of error bounds in [12], suggest that this analysis could be framed in a fairly classical perturbative framework. Nevertheless the program just mentioned is a non-trivial extension of the techniques developed in the present work, and these more speculative developments will wait for a separate future work.

Remark 1.4 (Computer assisted existence proofs for connecting orbits of parabolic PDEs)**.** As mentioned before, our main motivation for validated computation of local unstable manifolds is that they can be used in order to study heteroclinic connecting orbits. Indeed, in Section 5.3 we use the parameterization of the unstable manifold (combined with the validated error bounds obtained using the techniques of Section 4) in order to prove, with computer assistance, the existence of some saddle-to-sink connecting orbits: i.e. orbits which connect an equilibrium solution of finite non-zero Morse index to a fully stable equilibrium solution. We remark that the proofs given in Section 5.3 are included primarily to substantiate our claim that the tools developed in the present work can be of value in computer assisted existence proofs for connecting orbits of PDEs.

Nevertheless, we want to be clear that the computations in Section 5.3 have a strong "proof of concept" flavor, and there remains much work to be done in order to develop a satisfactory general computational theory for computer assisted proof of connecting orbits for PDEs. This assessment is largely due to the fact that in the present work we establish connections only for orbits asymptotic to a sink, i.e. we computing explicit lower bounds on the size of an absorbing neighborhood of the stable equilibrium solution, and then we simply check that our parameterized local manifold enters this neighborhood. Yet 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. Here we refer to the work of [22] for a more complete discussion of computer assisted existence proofs for saddle-to-saddle connections in infinite dimensions (yet we also note that [22] 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 in Section 5.3. By a short connection we mean a connecting orbit which is described only using local stable and unstable manifolds. 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 will require some mathematically rigorous "integration" in order to flow from the local unstable to the local stable manifolds. We refer to the works of [64, 63, 62, 19, 57, 3, 6, 36, 42, 60, 58] for a number of methods which overcome this difficulty, and provide successful computer assisted proof of saddle-to-saddle connections for finite dimensional ODEs.

Finally we mention that the work of [67] develops a computer assisted existence proof for saddle-to-sink connecting orbits for PDEs in a similar spirit to the one given in the present work. In this reference an orbit on a local unstable manifold is integrated rigorously until the orbit enters a trapping region of a sink. The unstable manifold is represented using the linear approximation, and validated error bounds are obtained by combining topological covering arguments with cone conditions. The method developed in the present work (when combined with a rigorous integration scheme for PDEs and a rigorous approximation scheme for the stable manifold) could be a powerful tool as part of a general scheme for computer assisted proof of connecting orbits for PDEs. For more discussion of rigorous integration of PDEs we refer the interested reader to the works of [68, 20, 4].

The paper is organized as follows. First in Section 2 we discuss the Banach spaces we will be working on. Furthermore in Section 3 we explain our validation method and also how we verify the Morse index. In Section 4 we explain how to set up the zero finding problem whose solutions correspond to the Taylor coefficients of a parametrization for the unstable manifold. In Section 5 we describe the application of our method to Fisher's equation. All computer programs used to obtain the results in this work are available on request.

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

$$Y^\nu = \left\{ a = (a_k)_{k\geq 0}, a_k \in \mathbb{R} : \quad |a|_\nu \stackrel{\text{def}}{=} |a_0| + 2\sum_{k=1} |a_k|\nu^k < \infty \right\}. \tag{13}$$

Denote the induced operator norm by $|\cdot|_{B(Y^\nu)}$. Note that if $\nu > 1$ and $a \in Y^\nu$ 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 radius $\log(\nu)$ about the real axis. Moreover we have that

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

i.e. the Y^ν norm provides bounds on the supremum norm of the corresponding analytic function.

Y^ν is a Banach algebra under the discrete convolution operation $a * b$ given by

$$(a*b)_k = \sum_{\substack{k_1+k_2=k \\ k_i\in\mathbb{Z}}} a_{|k_1|} b_{|k_2|}. \tag{14}$$

with $a, b \in Y^\nu$. 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 Y^ν as just defined. Such functions have convergent power series representations of the form

$$P(\theta, x) = \sum_{|m|=0}^{\infty} \left(p_{m0} + 2\sum_{k=1}^{\infty} p_{mk} \cos(kx) \right) \theta^m, \tag{15}$$

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 $p_m \in Y^\nu$. Then we are led to consider the multi-sequence space

$$X^{\nu,d} = \left\{ p = (p_m)_{m \in \mathbb{N}^d} : p_m \in Y^\nu \text{ and } \|p\|_\nu \stackrel{\text{def}}{=} \sum_{|m|=0}^{\infty} |p_m|_\nu < \infty \right\}, \tag{16}$$

of power series coefficients in (9). 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 (15) is periodic and analytic in the variable x on the complex strip about the real axis of width $\log(\nu)$, and is analytic on the d-dimensional unit polydisk $\mathbb{B}_1 \subset \mathbb{C}^d$ given by

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

Moreover we have that

$$\sup_{\theta \in \mathbb{B}_1} \sup_{x \in [0, 2\pi]} |P(\theta, x)| \le \|p\|_\nu,$$

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

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

Definition 2.1. 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

$$(p *_{TF} q)_m = \sum_{l \preceq m} p_l * q_{m-l}, \tag{17}$$

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

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

Lemma 2.2. *Let $p, q \in X^{\nu,d}$ be given. Then*

$$\|p *_{TF} q\|_\nu \le \|p\|_\nu \|q\|_\nu. \tag{18}$$

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

3 A-posteriori analysis for nonlinear operators

To compute and validate the equilibrium $\hat{a} \in Y^\nu$, the eigenvalues and eigenvectors $(\hat{\lambda}_i, \hat{\xi}_i) \in \mathbb{C} \times Y^\nu$ for $i = 1, \ldots, d$ and the parametrization coefficients $p \in X^{\nu,d}$ we solve zero finding problems. In order to derive explicit a-posteriori error bounds on approximate solutions we follow an approach based on [21]. We point out that similar approaches were used as early as the work of Lanford on the computer assisted proof of the Feigenbaum conjectures [41]. See also work of [29, 23] on computer assisted analysis of fixed points of renormalization operators and the work of [66] on computer assisted analysis of fixed point problems arising from the study of ordinary and partial differential equations.

3.1 The method of radii polynomials

In this section we set the general framework for this procedure. Think of f as being a nonlinear operator defined on Y^ν or $X^{\nu,d}$ and study the zero finding problem

$$f(x) = 0, \qquad x \in Y^\nu, X^{\nu,d}.$$

Assume that we have found an approximate solution $\tilde{x}$. In our context this is done numerically by considering a finite dimensional projection of the zero finding problem. Our goal is to prove that there exists a true solution nearby.

To this end let A be an injective bounded linear operator having that

$$Af(x), ADf(x) \in Y^\nu, X^{\nu,d},$$

for all $x \in Y^\nu, X^{\nu,d}$. Note we do not ask that $f(x)$ is a self map or that $Df(x)$ is a bounded linear operator into $Y^\nu, X^{\nu,d}$. Rather, A may "smooth" f and Df, bringing them back into the original domain. Heuristically we think of A as being an approximate inverse for $Df(\tilde{x})$ in a sense to be made precise below, and which must ultimately be checked in any computer assisted proof.

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, due to the assumption that A is an injection. The approach discussed here is to use the Banach Fixed Point Theorem on a ball of radius r around an approximate solution $\tilde{x}$, and derive sufficient conditions that T is a contraction on this ball. These sufficient conditions must be checkable by finite computations. Rather than guessing a value for the radius r and applying the Newton-Kantorovich Theorem, 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. For more details on this approach we refer to the work of [21, 59].

Definition 3.1. **Y, Z-bounds and the radii polynomial**
Recall the fixed point operator T specified in (27) corresponding to the zero finding map (24). Assume an approximate zero $\tilde{p}$ 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:

$$\|T(\tilde{x}) - \tilde{x}\| \leq Y \tag{19}$$

2. the r-dependent Z-bound measuring the contraction rate on a ball of (variable) radius r:

$$\sup_{\|u\|,\|v\|=1} \|DT(\tilde{x} + ru)rv\| \leq Z(r) \tag{20}$$

We define the radii polynomial to be

$$\beta(r) = Y + Z(r) - r. \tag{21}$$

$\|\cdot\|$ will be either $\|\cdot\|_\nu$ or $|\cdot|_\nu$.

The benefit of Definition 3.1 is the following Lemma.

Lemma 3.2. *Assume an approximate zero $\tilde{x}$ of f defined in (24) to be given. If $\beta(r) < 0$ with β defined in (21) for a positive radius $r_{\tilde{p}}$, then T given by (27) is a contraction on $\mathbb{B}_{r_{\tilde{x}}}(\tilde{x})$. Hence there is a unique zero $\hat{x}$ with $\hat{x} \in \mathbb{B}_{r_{\tilde{x}}}(\tilde{x})$.*

A proof of this lemma has appeared in many places. See for example [21]. The decisive feature of the condition $\beta(r) < 0$ in our context is that after deriving explicit expressions for the bounds in (19) and (20) are it can be checked rigorously by a computer using interval arithmetic.

Remark 3.3. *(Eventually diagonal approximate derivative and inverse)*

1. *In a later section we will also use an operator $A^\dagger \approx Df(\tilde{x})$ which fulfills $AA^\dagger \approx Id$. We will specify both A and $A^\dagger$ in more detail later.*
2. *What is important is to note that A has the structure*

$$A = \begin{pmatrix} A^F & 0 \\ 0 & A^\infty \end{pmatrix} \tag{22}$$

with A^F being a matrix and A^∞ a diagonal operator. Similarly for $A^\dagger$. We refer to this structure as eventually diagonal. We come back to this in the next section

In the context of computing a high order parametrization of the unstable manifold it will be important to not only have the existence of zero $\hat{x}$ with explicit error bounds but we will also need the eigendata of $Df(\hat{x})$. The following results show that we can use the explicit information about $A^\dagger$ to obtain this.

3.2 Computer assisted verification of the unstable eigenvalue count for a bounded perturbation of a 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. We remark that similar results have appeared in [23, 7, 50].

First some notation. Suppose that $A, Q, Q^{-1} \colon Y^\nu \to Y^\nu$ 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

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

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

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

i.e. the remaining eigenvalues are stable. We use the terminology (un)stable spectrum respectively.

Then A has no eigenvalues on the imaginary axis, i.e. A. 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

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

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 $h \in Y^\nu$ 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 Y^ν. Nevertheless one checks that

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

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

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 Y^ν. 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 3.4. *Suppose that $A, Q, Q^{-1} \colon Y^\nu \to Y^\nu$, $\{\lambda_j\}_{j=0}^\infty \subset \mathbb{C}$ 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 Y^ν. Let $H \colon Y^\nu \to Y^\nu$ 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

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

and

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

Then M has exactly m unstable eigenvalues.

Proof. 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

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

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

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

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

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

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. □

4 Zero finding problem and fixed point operator for the unstable manifold

In this section we specify the zero finding problem together with the associated fixed point operator we use in order to compute and validate the sequence of power series coefficients for P solving (5) and (6). That is first we define a map $f : X^{\nu,d} \to X^{\nu',d}$ such that P given by (9) solves (5) together with (6) if and only of $f(p) = 0$, where p is the sequence of coefficient sequences of P. Then we specify the operators A and $A^\dagger$ explained in Section 3.1 which are used to define and analyze the fixed point operator.

Zero finding map To this end we compute an expansion of $g(P(\theta))$. Recall (2) for the definition of the vectorfield g and note that we can rewrite g_k in the form

$$g_k(a) = \mu_k a_k + \sum_{n=1}^{s} (c_n * a^{*n})_k.$$

We are now able to write the composition $g(P(\theta))$ in the following compact form.

Lemma 4.1. *Assume P is of the form (9). Then*

$$g(P(\theta)) = \sum_{|m|=0} b_m \theta^m$$

with

$$b_{mk}(p) = \mu_k p_k + \sum_{n=0}^{s} (c_n * p_m^{*_{TF}n})_k \quad |m| \geq 0, \quad k \geq 0. \tag{23}$$

Proof. This follows inductively from the observation that for every fixed $\theta \in \mathbb{B}_1$

$$P(\theta) * P(\theta) = \sum_{|m|=0}^{\infty} (p *_{TF} p)_m \theta^m.$$

□

Now we can define the zero finding map in the following way.

Definition 4.2. Let an equilibrium $\hat{a}$ of (2) together with eigenvalues $\hat{\lambda}_i$ and eigenvectors $\hat{\xi}_i$ for $i = 1, \ldots, d$ be given. Then P of the form (9) solves (5) together with (6) if and only if $f(p) = 0 \in X^{\nu,d}$ with

$$f_m(p) = \begin{cases} p_0 - \hat{a} & m = 0 \\ p_{e_i} - \hat{\xi}_i & m = e_i \\ (\hat{\lambda} \cdot m) p_m - b_m(p) & |m| \geq 2 \end{cases} \tag{24}$$

where $\hat{\lambda} \cdot m \overset{\text{def}}{=} \sum_{i=1}^{d} \hat{\lambda}_i m_i$ and $b_m(p) = (b_{mk}(p))_{k \geq 0} \in Y^\nu$ is given by (23) for each $|m| \geq 0$. We also define the map $b : X^{\nu,d} \to X^{\nu,d}$ by $b(p) = (b_m(p))_{m \in \mathbb{N}^d}$.

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

Lemma 4.3. *Let $p \in X^{\nu,d}$ be given such that $f(p) = 0$, where f is given by (24). Then $P : \mathbb{B}_1 \to Y^\nu$ given by (9) solves (5) together with (6).*

Fixed point operator To define the fixed point operator we first define a finite dimensional truncation of f, that 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 $\Pi_{MK} p = (p_{mk})_{(m,k)\in\mathcal{I}_{MK}} \stackrel{\text{def}}{=} p^{MK}$. 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

$$f(p) = \tau(f^{MK}(p^{MK})) + f^\infty(p), \tag{25}$$

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 an approximate zero $\tilde{p} \in X^\nu$ of f to be computed, that is $f^{MK}(\tilde{p}^{MK}) \approx 0 \in \mathbb{R}^{(|M|+1)(K+1)}$. To define the Newton-like fixed point operator we need an approximate inverse of $Df(\tilde{p})$.

Definition 4.4. 1. The following operator is an approximate inverse of $Df(\tilde{p})$. Let $A^{MK} \approx Df^{MK}(\tilde{p})^{-1}$ and set

$$(Ap)_{mk} = \begin{cases} (A^{MK} p^{MK}))_{mk} & (m,k) \in \mathcal{I}_{MK} \\ p_{mk} & |m| \leq 1 \text{ and } k > K \\ \frac{1}{(\hat{\lambda}\cdot m) - \mu_k} p_{mk} & (m,k) \notin \mathcal{I}_{MK} \text{ and } |m| > 1 \end{cases} \tag{26}$$

2. If A is injective, then fixed points of

$$T : X^\nu \to X^\nu, \quad Tp = p - Af(p) \tag{27}$$

correspond to zeros of f.

We also specify the operator $A^\dagger \approx A^{-1}$ from Remark 3.3:

$$(A^\dagger p)_{mk} = \begin{cases} (Df^{MK}(\tilde{p}) p^{MK})_{mk} & (m,k) \in \mathcal{I}_{MK} \\ p_{mk} & |m| \leq 1 \text{ and } k > K \\ (\hat{\lambda}\cdot m - \mu_k) p_{mk} & (m,k) \notin \mathcal{I}_{MK} \text{ and } |m| > 1 \end{cases}. \tag{28}$$

5 Applications

Consider Fisher's equation with Neumann boundary conditions as specified in (12). 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 $a = (a_k)_{k\geq 0}$

$$a_k'(t) = (\alpha - k^2) a_k(t) + \sum_{\substack{k_1+k_2+k_3=k \\ k_i \in \mathbb{Z}}} c_{|k_1|} a_{|k_2|} a_{|k_3|} \stackrel{\text{def}}{=} g_k(a) \tag{29}$$

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

5.1 Validated computation of the first order data

In order to build a high order approximation of the unstable manifold of an equilibrium $\hat{a}$ of (29) we need a validated representation of $\hat{a}$ 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 [**?**].

Equilibrium solution: We look for an equilibrium solution $\hat{a}$ of Equation (29), that is we demand $g(\hat{a}) = 0$. 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 $Dg(a)\colon Y^\nu \to Y^{\bar{\nu}}$ given by

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

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

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

where

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

is the truncated cubic discrete convolution.

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

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

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

$$(A^\dagger h)_n = \begin{cases} (Dg^K(\tilde{a}^K)h^K)_k & \text{if } 0 \leq k \leq K \\ (\alpha - k^2)h_k & \text{if } k \geq K+1 \end{cases} \tag{30}$$

and

$$(Ah)_k = \begin{cases} (A^K h^K)_k & \text{if } 0 \leq k \leq K \\ \frac{1}{\alpha - k^2}h_k & \text{if } k \geq K+1 \end{cases}. \tag{31}$$

Let $\tilde{a} \in Y^\nu$ denote the inclusion of $\tilde{a}^K$ into Y^ν. For the sake of completeness we include the following Lemma providing the Y- and Z- bounds fulfilling (19) and (20). The proof is a computation similar to those in Section 5 of [39], and is discussed in detail in [43]. The MatLab program implementing the computations which check that the hypotheses of Lemma 5.1 are satisfied is available on request.

Lemma 5.1. *Suppose that* $\sqrt{\alpha} < K+1$ *and that* $c = c^K + c^\infty \in Y^\nu$. *Let*

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

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

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

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

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

Then the constants

$$Y = Y_0,$$

and

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

satisfy (19) *and* (20)*. In particular, if* $r > 0$ *is a positive constant with*

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

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

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

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

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

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

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

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

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 as solution $\xi \in Y^\nu$ 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 $h\colon Y^\nu \to \mathbb{R}$ by

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

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

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

We then define the mapping $H\colon \mathbb{R} \times Y^\nu \to \mathbb{R} \times Y^\nu$ 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 $Dg(\hat{a})$. 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

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

and that

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

In block form we write

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

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

$$h^K(\lambda, \xi^K)_k := (\alpha - k^2)\xi^K_k - 2\alpha(c^K * \tilde{a}^K * \xi^K)^K_k - \lambda\xi^K \qquad 0 \le n \le N \tag{32}$$

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

Remark 5.2. In applications we choose a numerical eigenvalue/eigenvector pair $(\tilde{\lambda}, \tilde{\xi}^K)$ for the matrix $Dg^K(\tilde{a}^K)$. We are free to solve the finite dimensional eigenvalue/eigenvector problem using any convenient linear algebra package.

Let B^K be a $K+2 \times K+2$ matrix which is obtained as a numerical inverse of $DH^K(\tilde{\lambda}, \tilde{\xi}^K)$. 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 $B^\dagger_{11} \colon \mathbb{R} \to \mathbb{R}$ defined by

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

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

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

$B_{21}^{\dagger}\colon \mathbb{R} \to Y^{\nu}$ 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 $B_{22}^{\dagger}\colon Y^{\nu'} \to Y^{\nu}$ defined by

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

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

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

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

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

$B_{21}\colon \mathbb{R} \to Y^{\nu}$ 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 $B_{22}\colon Y^{\nu} \to Y^{\nu}$ 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

$$T(x) = x - BH(x). \tag{33}$$

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 [39]. The MatLab program implementing the computations which check the hypotheses of Lemma 5.3 is available on request.

Lemma 5.3. *Suppose that $K+1>\sqrt{\alpha}$, and for each $0\leq k\leq K$ define the quantities*

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

and

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

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

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

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

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

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

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

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

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

satisfy (19) *and* (20)*, 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 $\hat{\xi}\in B_r(\tilde{\xi})\subset Y^\nu$ and $|\hat{\lambda}-\tilde{\lambda}|\leq r$ 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 $\hat{a} \in \ell^1_\nu$ is as in the previous sections, so that $g(\hat{a}) = 0$. Let $A\colon \ell^1_\nu \to \ell^1_\nu$ be the linear operator defined by Equation (31). 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 $Q, Q^{-1}, \Sigma\colon \ell^1_\nu \to \ell^1_\nu$ by

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

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

and

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

Then note that

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

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

- 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 which checks the hypotheses of Lemma 5.4 is available on request.

Lemma 5.4. *Let Y_0, Z_0, Z_1 and Z_2 be the positive constants defined in Lemma 5.1, and suppose that A, Q, Q and $\{\lambda_0, \ldots, \lambda_K\}$ are as discussed above. Define*

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

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

Proof. Note that

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

and inspection of Equation (20) 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 $x = \hat{x}$. Then the operators A, $B = Q\Sigma^{-1}Q^{-1}$, and $M = B + H$ (with $H = Dg(\hat{x}) - B$) satisfy the hypothesis of Lemma 3.4 with

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

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

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

$$c(x) = 1 + 2\sum_{n=1}^{\infty} r^n \cos(x),$$

with $r = 1/5$. The numerically computed equilibrium solution and unstable eigenfunction are illustrated in Figure 1.

We approximate the system using $N = 25$ cosine modes, i.e. the numerical computations are carried out in $\mathbb{R}^{26}$. We choose $\nu = 1.001$ 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.

5.2 Parameterization of the Unstable Manifold for $c(x) = 1$

First let us give a concrete formula for $b : X^{\nu,d} \to X^{\nu,d}$ as specified in (23):

$$b_{mk} = (-k^2 + \alpha)p_{mk} - \alpha(p^{*T_F 2})_{mk}, \quad |m| \geq 0, k \geq 0, \tag{34}$$

where $d = 1$ in the following. We start by considering a one-dimensional unstable manifold at a nontrivial equilibrium. 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 5.1.

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

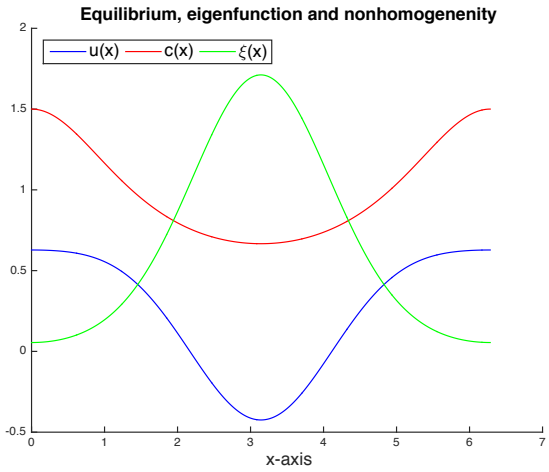

Figure 1: Linear data for the Fisher equation with $\alpha = 2.1$. The red curve illustrates the spatial inhomogeneity with $c(x)$ a Poisson kernel with parameter $r = 1/5$. The blue curve illustrates the numerically computed non-trivial equilibrium solution. The greed curve illustrates the numerically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

$\alpha > 0$, that is $Dg(\hat{a}^1)$ only has negative eigenvalues. It turns out that in this parameter regime there is also a third fixed point $\hat{a}^2$ that has a 1D unstable manifold. We first describe the details of our method for this manifold and indicate the changes for the two-dimensional manifold.

1D unstable manifold at a nontrivial equilibrium The methods from Section 5.1 provide us with the exact linear data $\hat{a}$, $\hat{\lambda}$ and $\hat{\xi}$ in the form:

$$\hat{a}^2 = \tilde{a}^2 + a^\infty \quad \text{with} \quad |a^\infty|_\nu \leq r_{\tilde{a}^2} \tag{35a}$$

$$\hat{\xi} = \tilde{\xi} + \xi^\infty \quad \text{with} \quad |\xi^\infty|_\nu < r_{\tilde{\xi}} \quad \text{for a given} \quad \nu > 1 \tag{35b}$$

$$\hat{\lambda} = \tilde{\lambda} + \lambda^\infty, \quad \text{with} \quad |\lambda^\infty| < r_{\tilde{\lambda}}, \tag{35c}$$

where we recall that $Dg(\hat{a})\hat{\xi} = \hat{\lambda}\hat{\xi}$. In addition by checking condition from Lemma 5.4 we ensure that the $\hat{\lambda}$ indeed is the only positive eigenvalue of $Dg(\hat{a})$.

In order to derive the bounds from Definition 3.1 we first need to make precise how we split the map f from 4.2 into the form (25).

Definition 5.5. 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

$$f^{MK}(p^{MK})_{mk} = \begin{cases} \tilde{a}_k - (p^{MK})_{0k} & m = 0 \\ \tilde{\xi}_k - (p^{MK})_{1k} & m = 1 \\ (\tilde{\lambda} \cdot m + k^2 - \alpha)(p^{MK})_{mk} + \alpha \left(p^{MK} *_{TF} p^{MK}\right)^{MK}_{mk} & 2 \le m \le M, \\ & 0 \le k \le K \end{cases} \tag{36}$$

and

$$(f^\infty(p))_m = \begin{cases} a^\infty_k - p^\infty_{0k} & m = 0, k \ge 0 \\ \xi^\infty_k - p^\infty_{1k} & m = 1, k \ge 0 \\ (\lambda^\infty \cdot m)(\Pi_{MK} p)_{mk} + (\tilde{\lambda} \cdot m + k^2 - \alpha) p^\infty_{mk} + & \\ \alpha(Id - \Pi_{MK}) \left(p^{MK} *_{TF} p^{MK}\right)_{mk} + & \\ \alpha \left[(2p^{MK} *_{TF} p^\infty)_{mk} + (p^\infty *_{TF} p^\infty)_{mk}\right] & m \ge 2, k \ge 0 \end{cases} . \tag{37}$$

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

The following Theorems summarize the Y-bounds and Z-bounds from Definition 3.1. Note that Theorem 5.6 rigorously controls the numerical residual and Theorem 5.8 controls the contraction rate. The standard proofs are again a computations similar (for example) to that carried out explicitly in Section 5 of [39]. We will split the derivative in the following way:

$$DT(\tilde{p} + ru)rv = (Id - AA^\dagger)rv - A\left[(A^\dagger - Df(\tilde{p} + ru))rv\right]. \tag{38}$$

The motivation for this 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

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

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

$$\Delta_{mk}(u, v) = \left[(A^\dagger - Df(\tilde{p} + ru))rv\right]_{mk}, \tag{39}$$

which will be of the form

$$\Delta = r\Delta^{(1)} + r^2\Delta^{(2)}. \tag{40}$$

Theorem 5.6. *Y-bounds*
Assume truncation dimensions $M > 0$ and $K > 0$ and an approximate zero $\tilde{p}$, with $\Pi_{MK}\tilde{p} = \tilde{p}$ to be given. Define

$$Y^{MK}_m = |(Df^{MK}(\tilde{p})\tilde{p})_{m0}| + 2\sum_{k=1}^{K} |(Df^{MK}(\tilde{p})\tilde{p})_{mk}|\nu^k, \quad m = 0, \ldots, M, \tag{41}$$

and

$$Y^\infty_m = \begin{cases} |(|Df^{MK}(\tilde{p})|\delta^\infty)_{m0}| + 2\sum_{k=1}^{K} |(|Df^{MK}(\tilde{p})|\delta^\infty)_{mk}|\nu^k + & \\ 2\sum_{k=K+1}^{2K} \frac{\alpha|(\tilde{p} * \tilde{p})_{mk}|}{\tilde{\lambda} \cdot m + k^2 - \alpha}\nu^k & m = 0, \ldots M \\ \frac{\alpha|(\tilde{p} *_{TF} \tilde{p})_{m0}|}{\tilde{\lambda} \cdot m} + 2\sum_{k=1}^{2K} \frac{\alpha|(\tilde{p} *_{TF} \tilde{p})_{mk}|}{\tilde{\lambda} \cdot m + k^2 - \alpha} & M + 1 \le m \le 2M, \end{cases} \tag{42}$$

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

$$\delta^\infty_{mk} = \begin{cases} \frac{r_{\tilde{a}}}{\nu^k} & m = 0, 0 \le k \le K \\ \frac{r_{\tilde{\xi}}}{\nu^k} & m = 1, 0 \le k \le K \\ |\tilde{p}_{mk}|\lambda^\infty & 2 \le m \le M, 0 \le k \le K. \end{cases} \tag{43}$$

Then $Y = \sum_{m=0}^{M} \left(Y_m^{MK} + Y_m^\infty\right) + r_{\tilde{a}} + r_{\tilde{\xi}} + \sum_{m=M+1}^{2M} Y_m^\infty$ *fulfills* (19).

As a preparation for the Z-bounds we need the following Lemma.

Lemma 5.7. *Let* $\|v\| \le 1$*, truncation dimensions* $M > 0$ *and* $K > 0$ *and* $\tilde{p} = \Pi_{MK}\tilde{p}$ *be given. Then for every* $l \le M$ *and for each* $0 \le k \le K$ *the following estimate is valid:*

$$|(\tilde{p}_l * v^\infty)_k| \le \max_{j=K+1-k,\dots,K} \frac{|\tilde{p}_{lj}|}{2\nu^{j+k}} \stackrel{\text{def}}{=} h_{lk}(\tilde{p}), \tag{44}$$

where we set the convention $h(l,0) = 0$ *and*

$$v_k^\infty = \begin{cases} 0 & 0 \le k \le K \\ v_k & k \ge K+1 \end{cases}. \tag{45}$$

Proof. The proof follows by using the fact that the dual space of $(Y^\nu)^*$ is given by

$$(Y^\nu)^* = \left\{ (a_k)_{k\ge 0} : \quad \sup_{k\ge 0} \frac{|a_k|}{2\nu^k} < \infty \right\}.$$

□

Theorem 5.8. *Z-bounds*
Assume truncation dimensions $M > 0$ *and* $K > 0$ *and an approximate zero* $\tilde{p}$*, with* $\Pi_{MK}\tilde{p} = \tilde{p}$ *to be given. Define*

$$|\Delta^{(1)}|_{mk} = \begin{cases} 0 & m = 0, 1, k \ge 0 \\ \frac{r_\lambda m}{\nu^k} + \sum_{l=0}^{m} h_{lk}(\tilde{p}) & 2 \le m \le M, 0 \le k \le K \\ 0 & (m \ge M+1, k \ge 0) \vee (0 \le m \le M, k \ge K+1) \end{cases} \tag{46a}$$

$$|\Delta^{(2)}|_{mk} = \begin{cases} 0 & m = 0, 1, k \ge 0 \\ \frac{2\alpha}{\nu^k} & 2 \le m \le M, 0 \le k \le K \\ 0 & (m \ge M+1, k \ge 0) \vee (0 \le m \le M, k \ge K+1) \end{cases} \tag{46b}$$

,

$$\Sigma_{MK}^{(j)} = \sum_{m=0}^{M} \left(|(|A||\Delta^{(i)}|)_0| + \sum_{k=1}^{K} |(|A||\Delta^{(i)}|)_k| \nu^k \right). \tag{47}$$

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

$$\begin{aligned} Z(r) =& r\left(\epsilon + \Sigma_{MK}^{(1)} + 2\alpha\|\tilde{p}\|_\nu \left(\frac{1}{K^2 - \alpha} + \frac{1}{(\tilde{\lambda} + r_\lambda)M - \alpha}\right)\right) \\ &+ r^2\left(\Sigma_{MK}^{(2)} + 2\alpha\left(\frac{1}{K^2 - \alpha} + \frac{1}{(\tilde{\lambda} + r_\lambda)M - \alpha}\right)\right) \end{aligned} \tag{48}$$

fulfills (20).

Numerical example Using the methods from Section 5.1 we compute a non-trivial equilibrium $\hat{a}^2$ for $\nu = 1.5$, where the values for the error bounds in (46) are listed here:

$r_{\tilde{a}^2}$	2.1×10^{-6}
$r_{\tilde{\lambda}}$	1.5×10^{-6}
$r_{\tilde{\xi}}$	1.5×10^{-6}

An illustration of the approximate equilibrium and eigendata is shown in Figure 2. Choosing truncation dimensions $K = 20$ in Fourier space and $M = 60$ for the Taylor modes

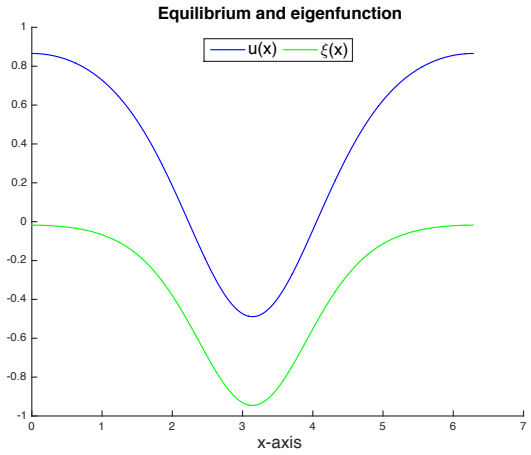

Figure 2: Non-trivial equilbrium $\tilde{a}^2$ (blue) together with a corresponding eigenvector $\tilde{\xi}$ (green).

we obtain a validation radius r_P

$$r_P = 1.5 \times 10^{-04}. \tag{49}$$

That is, defining $p(r) = Y + Z(r) - r$ with Y given by (19) and $Z(r)$ given by (20) we have $p(r_P) < 0$. In particular our corresponding approximate parametrization $P^{MK}(\theta)$ fulfills the uniform bound (11) and we have rigorous control over its image in ℓ_ν. We use this for a computer-assisted proof of a connecting orbit to the sink $\hat{a}^1$.

5.3 Computer assisted proof of a connecting orbit

We see directly form the linearization of g around $\hat{a}^1 = (1, 0, 0, \ldots)$ that $\hat{a}^1$ is spectrally stable, as all eigenvalues are negative. In order to use this fact for a computer-assisted proof of a connecting orbit from the equilibrium whose unstable manifold we computed in Section 5.2 we need nonlinear stability information. The following Lemma provides us with bounds on the attracting neighborhood of $\hat{a}^1$.

Lemma 5.9. *The equilibrium point $\hat{a}^1$ of (29) is an attracting fixed point with attracting neighborhood*

$$\mathcal{A} = \left\{ a \in Y^\nu : |a - \hat{a}^1|_\nu < 1 \right\}. \tag{50}$$

Proof. See Appendix A. □

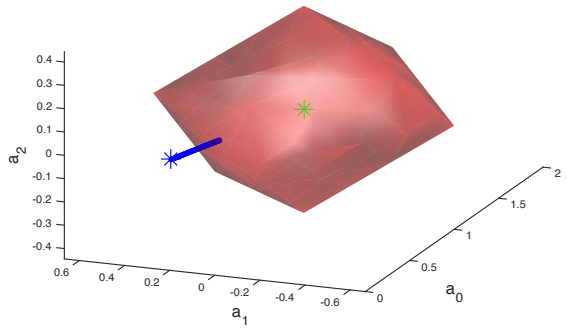

Figure 3: In red a projection on the first three components of the attracting neigborhood of $\hat{a}^2$ (green asterix). In blue also a projection of the unstable manifold of $\hat{a}^1$ (blue asterix).

By using the inequality $|P(\theta) - \hat{a}^1|_\nu \leq r_P + |P^{MK}(\theta) - \hat{a}^1|_\nu$ we can rigorously check for any given θ if the true image $P(\theta)$ lies in $\mathcal{A}$. If this check succeeds it follows immediately that there is a connecting orbit from $\hat{a}^2$ to $\hat{a}^1$.

Lemma 5.10. *Let $\nu = 1.5$. Let P be a parametrization of the unstable manifold of $\hat{a}^2$ with $|DP(0)|_\nu = 0.895212275504314 \pm 10^{-16}$. For $\theta = 0.94$ we have that $P(\theta) \in \mathcal{A}$. Hence there is a connecting orbit from $\hat{a}^2$ to $\hat{a}^1$.*

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

Lemma 5.9 in Section 5.3 states that the equilibrium point $\hat{a} = (1, 0, 0, \ldots)$ of (29) is an attracting fixed point with attracting neighborhood

$$\mathcal{A} = \{a \in Y^\nu : |a - \hat{a}|_\nu < 1\}. \tag{51}$$

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

$$h'_k = -(k^2 + \alpha)h_k - \alpha(h * h)_k \stackrel{\text{def}}{=} (Lh)_k + N(h)_k, \quad k \geq 0, \tag{52}$$

where $L = Dg(\hat{a})$ and $N(h) = g(\hat{a} + h) - g(\hat{a}) - Lh$. Denote $h(0) = h_0$ and let $h(t)$ solve (52) with initial condition h_0. We show that if $|h_0|_\nu < 1$, then $\lim_{t\to\infty} |h(t)|_\nu = 0$. Define $\left(\mathrm{e}^{-Lt}h_0\right)_k \stackrel{\text{def}}{=} \mathrm{e}^{-(k^2+\alpha)t}h_{0k}$. Then

$$|\mathrm{e}^{-Lt}h_0|_\nu \leq \mathrm{e}^{-\alpha t}|h_0|_\nu. \tag{53}$$

Using the variation of constants formula we have

$$h(t) = \mathrm{e}^{-Lt}h_0 + \int_0^t \mathrm{e}^{-L(t-s)}(h * h)(s)ds. \tag{54}$$

Using (53) in (54) we obtain

$$|h(t)|_\nu \leq \mathrm{e}^{-\alpha t}|h_0|_\nu + \int_0^t \mathrm{e}^{-\alpha(t-s)}\alpha \underbrace{|h * h|_\nu}_{\leq |h|_\nu |h|_\nu}(s)ds. \tag{55}$$

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 $t \in [0, t_1]$:

$$e^{\alpha t}|h(t)|_\nu \leq |h_0|_\nu + \int_0^t \alpha\rho_1 e^{\alpha s}|h|_\nu(s)ds \tag{56}$$

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

$$e^{\alpha t}|h(t)|_\nu \leq |h_0|_\nu e^{\int_0^t \rho_1\alpha ds}, \tag{57}$$

hence $|h(t_1)|_\nu \leq |h_0|e^{-\alpha(1-\rho_1)t_1} < |h_0|_\nu$. 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 $|h(t)|_\nu \leq |h_0|e^{-\alpha(1-\rho_K)t} < |h_0|_\nu$ for all $t \geq t_K$. For $t \to \infty$ this yields $\delta < 0$, a contradiction. Hence $\delta = 0$. □

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