

Construction of approximate solutions for rigorous numerics of symmetric homoclinic orbits

By

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§ 1. Introduction

In the paper [5], the author proposed a new rigorous numerical method to prove the existence of symmetric homoclinic orbits in an S -reversible system (definition of the reversibility is given in Section 2):

$$(1.1) \quad \frac{dx}{dt} = f(x), \quad f(Sx) = -Sf(x), \quad x \in \mathbf{R}^N.$$

Here we assume that the vector field f is smooth and has a hyperbolic fixed point at the origin. Let us suppose that we have an approximate numerical homoclinic solution

$$(1.2) \quad \{(\xi^i, t_i) \mid \xi^i \in \mathbf{R}^N, t_i \in \mathbf{R}, i = 0, 1, \dots, K, \text{ and } t_i < t_{i+1}\},$$

which is usually obtained by numerical simulations. In this setting, he gives a rigorous numerical method to prove the existence of symmetric homoclinic orbits of (1.1) in a neighborhood of the numerical solution (1.2). We refer to the original paper [5] for the background and motivations of this work.

In the method, it is essential to show the following two steps based on the exponential dichotomy property: (i) the existence of orbits on the stable manifold of the origin in a neighborhood of an approximate solution $w(t)$, $t \in \mathbf{R}$, which is determined by (1.2), (ii) the intersection of the stable manifold and the S -invariant subspace. It is remarked in the paper that we need to construct a suitable approximate solution $w(t)$ in the sense of $C^r(\mathbf{R})$, $r \geq 1$, since the fundamental matrix solution of the variational equation with respect to $w(t)$ is affected by the hyperbolicity in a neighborhood of the origin and it makes difficult numerical verifications of the above two steps.

In this paper, we consider how to practically construct a good approximate solution $w(t)$ for the rigorous numerical method [5] in detail. First of all, it is shown that we

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need a very accurate approximate numerical solution (1.2) in order to obtain appropriate polynomial interpolations. A multiple precision arithmetic in numerical computations, for example [4], becomes necessary for this purpose. Then we compare several techniques to obtain approximate numerical homoclinic solutions such as the spectral method, the Chebyshev method, the finite difference method, and the shooting method. We conclude that the shooting method is the most adequate technique for our purpose. The subjects in this paragraph are discussed in Section 4. The algorithm proposed in [5] is summarized in Section 2 with a numerical example in Section 3 in order for this paper to be self-contained.

There are several other rigorous numerical methods to show the existence of homoclinic and heteroclinic orbits in dynamical systems. Oishi [10] proposes a method in which we transform the original problem into a boundary value problem and study a corresponding contraction mapping principle. Wilczak and Zgliczyński [12] use topological arguments based on covering relations. On the other hand, since our method is based on the rigorous numerics of Melnikov functions, the method may be also applied to the stability analysis of traveling pulses in reaction diffusion equations with one space dimension [7]. Namely, it may be possible that we verify not only the existence of a traveling pulse, which corresponds to a homoclinic or heteroclinic orbit in the moving coordinate, but also its stability simultaneously. This potential to the stability analysis seems remarkable comparing to the above mentioned rigorous numerical methods.

§ 2. Algorithm

The algorithm proposed in the paper [5] consists of the following four steps for the numerical verifications of homoclinic orbits:

- Step 1. Construction of an approximate solution
- Step 2. Enclosure of a fundamental matrix solution
- Step 3. Characterization of orbits on the stable manifold
- Step 4. Analysis for an intersection of the stable and unstable manifolds

The basic strategy is to rigorously perform the techniques in the Melnikov theory by using an approximate numerical homoclinic solution (1.2) and an exponential dichotomy property. We refer to the paper [8] for a comparison to the original Melnikov type argument. In this section, we explain the algorithm in [5] in order for this paper to be self-contained.

We impose the following hypotheses on the dynamical system (1.1):

- (H1): We assume $N = 2n$ and S -reversibility. That is to say, the vector field satisfies $f(Sx) = -Sf(x)$ for a linear map $S: \mathbf{R}^{2n} \rightarrow \mathbf{R}^{2n}$ with $S^2 = I_{2n}$. Here I_{2n}

is the identity map on \mathbf{R}^{2n} .

(H2): Eigenvalues of the linearized matrix $f_x(0)$ at the origin are given by

$$\{\pm\lambda_i \mid i = 1, \dots, n, \operatorname{Re}\lambda_i > 0, \lambda_1 < \operatorname{Re}\lambda_j (j \geq 2)\}.$$

From the reversibility, we can show that if λ is an eigenvalue then so is $-\lambda$. Therefore hypothesis (H2) actually imposes $0 < \lambda_1 \in \mathbf{R}$ and $\lambda_1 < \operatorname{Re}\lambda_j, j = 2, \dots, n$.

A homoclinic orbit $h(t)$ in the reversible system (1.1) is called symmetric if $h(-t) = Sh(t)$ for all t . Since we only deal with symmetric homoclinic orbits in this paper, we prepare a numerical homoclinic solution (1.2) as the following form

$$(2.1) \quad \{(\xi^i, t_i) \mid i = 0, \pm 1, \dots, \pm K, \xi^{-i} = S\xi^i, t_{-i} = -t_i, \xi^{\pm K} \approx 0\}.$$

It should be noted that ξ^0 is selected at a point on the S -invariant subspace $\operatorname{Fix}(S) := \{x \in \mathbf{R}^{2n} \mid Sx = x\}$ (see Fig. 1). Under this situation, we explain each step of the algo-

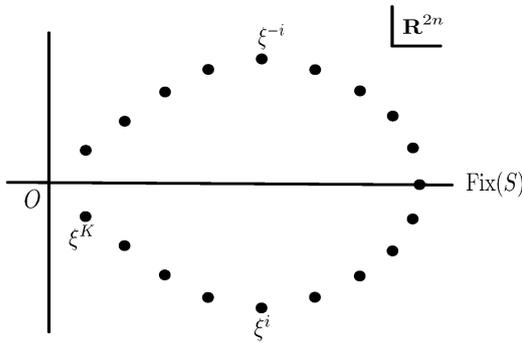


Fig. 1: numerical homoclinic solution

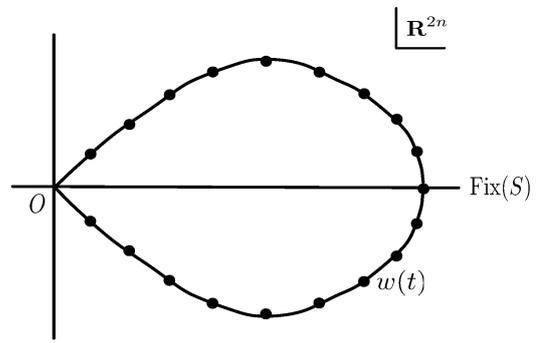


Fig. 2: approximate solution $w(t)$

rithm in detail.

§ 2.1. Step 1: Construction of an approximate solution

In this step, we construct an approximate solution $w(t) \in \mathbf{R}^{2n}, t \in \mathbf{R}$, as a continuous curve by a given numerical homoclinic solution (2.1). A basic strategy for the construction is given as follows (see Fig. 2):

- $w(t_i) := \xi^i$
- Polynomial interpolation for each time interval $[t_i, t_{i+1}]$, $i = 0, \dots, K - 1$
- $w(t) := \xi^K e^{-\lambda_1(t-t_K)}, t \geq t_K$
- $w(t) := Sw(-t), t \leq 0$

Namely, we adopt a polynomial interpolation for each time interval in the finite time region $[0, t_K]$, and we put an exponential decay property for $t \in [t_K, \infty)$. Here, let us note that the decay rate is determined by λ_1 . This is because a homoclinic orbit generically decays along the stable subspace given by the eigenvector of $-\lambda_1$ [3].

In practical numerical verifications, we shall put some additional information on coefficients of polynomial interpolations. For example, we can determine a polynomial interpolation by specifying its differential coefficients at each end point $t = t_i$. These derivative information will be given in such a way that an operator introduced in Step 3 becomes contractive. We will discuss this subject in Section 2.3 in detail.

§ 2.2. Step 2: Enclosure of a fundamental matrix solution

First of all, let us recall an exponential dichotomy property [2] on an ordinary differential equation

$$(2.2) \quad \dot{x} = A(t)x, \quad x \in \mathbf{R}^n, \quad t \in I,$$

where I is an interval in \mathbf{R} . Let $X(t)$ be its fundamental matrix solution.

Definition 2.1. The equation (2.2) is said to have an exponential dichotomy on I if there exist positive constants M , α , and a projection matrix P such that the following inequalities

$$(2.3) \quad \begin{aligned} |X(t)PX(s)^{-1}| &\leq Me^{-\alpha(t-s)}, & \text{if } s \leq t \text{ and } s, t \in I \\ |X(t)(I-P)X(s)^{-1}| &\leq Me^{-\alpha(s-t)}, & \text{if } t \leq s \text{ and } s, t \in I \end{aligned}$$

are satisfied.

We consider the variational equation

$$(2.4) \quad \dot{x} = A(t)x, \quad A(t) = f_x(w(t))$$

with respect to the approximate solution $w(t)$. Then, due to [1] and [8], the following property holds for (2.4).

Lemma 2.2. *The variational equation (2.4) has an exponential dichotomy on $\mathbf{R}_+ = [0, \infty)$ with the projection matrix*

$$(2.5) \quad P = \begin{pmatrix} I_n & 0 \\ 0 & 0 \end{pmatrix}.$$

In this step, we explicitly construct an enclosure of the fundamental matrix solution which satisfies the exponential dichotomy property on \mathbf{R}_+ with the projection matrix (2.5).

It should be noted that, from the asymptotic behavior of $A(t)$, there exist fundamental solutions $\varphi_i(t)$, $i = \pm 1, \pm 2, \dots, \pm n$, of (2.4) such that the following property holds (e.g., [1]):

$$(2.6) \quad \lim_{t \rightarrow \infty} \varphi_i(t)e^{-\lambda_i(t-t_K)} = p_i \quad \lim_{t \rightarrow \infty} \varphi_{-i}(t)e^{\lambda_i(t-t_K)} = Sp_i.$$

Here p_i is an eigenvector for the eigenvalue λ_i and, from the reversibility, Sp_i corresponds to an eigenvector for the eigenvalue $-\lambda_i$. Then, it is easily shown that the fundamental matrix solution determined by $X(t) = [\varphi_{-1}(t) \cdots \varphi_{-n}(t) \varphi_1(t) \cdots \varphi_n(t)]$ attains the exponential dichotomy property on \mathbf{R}_+ with (2.5). Hence, for the enclosure of $X(t)$, it suffices to enclose all fundamental solutions $\varphi_i(t), i = \pm 1, \dots, \pm n$, which satisfy (2.6) on \mathbf{R}_+ . In what follows, by dividing into the asymptotic part $[t_K, \infty)$ and the finite interval part $[0, t_K]$, we construct these enclosures on both parts, respectively.

We first explicitly construct the successive approximations $\varphi_i^{(j)}(t), j = 0, 1, \dots$, of the fundamental solutions $\varphi_i(t), i = \pm 1, \dots, \pm n$, for $t \in [t_K, \infty)$ by using the similar manner discussed in Chapter 3 of [1]. Namely, we successively derive approximate solutions $\varphi_i^{(j)}(t)$ by taking $\varphi_i^{(0)}(t) = p_i e^{\lambda_i(t-t_K)}$ and $\varphi_{-i}^{(0)}(t) = Sp_i e^{-\lambda_i(t-t_K)}$ as initial approximate solutions. It can be proved that, for each eigenvalue, there exist functions $\varphi_i(t), i = \pm 1, \dots, \pm n$, to which the sequences of the approximate solutions converge, and these functions satisfy (2.4) and (2.6). Moreover, it is important that the error bound between the approximate solution $\varphi_i^{(j)}(t)$ and $\varphi_i(t)$ can be explicitly derived for each j . Therefore, it enables us to enclose the fundamental solution $\varphi_i(t)$ for $t \in [t_K, \infty)$ by using the approximate solution $\varphi_i^{(j)}(t)$ and its error bound.

Next, let us enclose the fundamental solutions in the finite interval part by using Lohner's method [9], which is one of the numerical verification techniques to enclose solutions of initial value problems for a finite time interval in ordinary differential equations. We take the enclosure of $\varphi_i(t_K)$ as the set of initial values and solve (2.4) from $t = t_K$ to $t = 0$ by Lohner's method.

§ 2.3. Step 3: Characterization of orbits on the stable manifold

In this step we characterize orbits on the stable manifold of the origin in a neighborhood of $w(t)$. For this purpose, let us introduce a new variable $v := x - w$. Then the differential equation (1.1) is transformed into

$$(2.7) \quad \begin{aligned} \dot{v} &= A(t)v + g(t, v) \\ g(t, v) &:= -\dot{w}(t) + f(w(t) + v) - A(t)v. \end{aligned}$$

We should note that, due to the hyperbolicity of the origin and the asymptotic behavior of $w(t)$, if $v(t)$ is a solution of (2.7) such that $\sup_{t \in \mathbf{R}_+} |v(t)| < \epsilon$ for a sufficiently small ϵ , then $x(t) = w(t) + v(t)$ stays on the stable manifold of the origin.

Let $B(\mathbf{R}_+)$ be the set of all continuous and bounded functions from \mathbf{R}_+ to \mathbf{R}^{2n} . This function space becomes a Banach space under the norm defined by $\|v\| := \sup_{t \in \mathbf{R}_+} |v(t)|$. Then, the following lemma holds due to the exponential dichotomy.

Lemma 2.3. ([8]) *The differential equation (2.7) is equivalent to*

$$(2.8) \quad v(t) = X(t)P \left\{ X(0)^{-1}v(0) + \int_0^t X(s)^{-1}g(s, v)ds \right\} - \int_t^\infty X(t)(I - P)X(s)^{-1}g(s, v)ds$$

on $B(\mathbf{R}_+)$.

We now define an operator on $B(\mathbf{R}_+)$ which depends on a parameter $\eta \in \mathbf{R}^{2n}$ as follows:

$$(2.9) \quad (T_\eta(v))(t) := X(t)P \left\{ X(0)^{-1}\eta + \int_0^t X(s)^{-1}g(s, v)ds \right\} - \int_t^\infty X(t)(I - P)X(s)^{-1}g(s, v)ds$$

Note that a fixed point $v = T_\eta(v)$ becomes a solution of (2.7) and η controls the initial value of the fixed point. In addition, we can also show that $T_\eta : B(\mathbf{R}_+) \rightarrow B(\mathbf{R}_+)$ from the exponential dichotomy.

Let $B_M(\mathbf{R}_+) := \{v \in B(\mathbf{R}_+) \mid \|v\| \leq M\}$ be the closed ball with the radius M . Then, by using the similar arguments in [13], we can prove the following proposition about the shadowing of orbits converging to the origin.

Proposition 2.4. *Suppose $Y, Z > 0$ are taken for $\eta \in \mathbf{R}^{2n}$ and $\epsilon > 0$ such that*

$$\|T_\eta(0)\| \leq Y, \quad \sup_{w_1, w_2 \in B_\epsilon(\mathbf{R}_+)} \|T'_\eta(w_1)w_2\| \leq Z.$$

If $Y + Z < \epsilon$, then there exists the unique fixed point v_η of T_η in $B_{Y+Z}(\mathbf{R}_+)$.

Let us note that Y and Z appearing in the proposition can be explicitly calculated for each ϵ and η , and hence this proposition enables us to study the existence of the fixed point of T_η . In fact, by the explicit form of $w(t)$ and $X(t)$ treated in Step 1 and Step 2, we can estimate $T_\eta(0)$ and $T'_\eta(w_1)w_2$ for a given $B_\epsilon(\mathbf{R}_+)$. Namely, we derive these estimates by numerical verifications for $[0, t_K]$, and by the asymptotic forms of $w(t)$ and the enclosure of $X(t)$ for $[t_K, \infty)$, respectively.

In addition, let us remark that, if there exist Y, Z , and ϵ satisfying the sufficient condition $Y + Z < \epsilon$ for any η in some subset $D \subset \mathbf{R}^{2n}$, the stable manifold of the origin in a neighborhood of $w(0)$ can be described by $w(0) + v_\eta(0)$ for $\eta \in D$, where v_η expresses the unique fixed point of T_η . Thus, in the practical numerical verification, we try to construct a suitable subset $D \subset \mathbf{R}^{2n}$ given by the product of intervals such that the sufficient condition is satisfied for any $\eta \in D$, and characterize the stable manifold. This stable manifold will be finally analyzed to show the existence of symmetric homoclinic orbits in the next step.

Before discussing Step 4, let us briefly summarize the relationship of the contractiveness of T_η , the choice of the approximate solution $w(t)$, and ϵ . In general, it is

obvious that we can not expect T_η to be contractive. One of the reasons is that, since the fundamental matrix solution $X(t)$ possesses the exponential dichotomy property, the fundamental solutions $\varphi_{-i}(t), i = 1, 2, \dots, n$, grows exponentially as t decreases from t_K . This causes Y and Z to be large unless $g(s, v)$ and $g_v(s, w_1)w_2, w_1, w_2 \in B_\epsilon(\mathbf{R}_+)$, are sufficiently small, where $g_v(s, v)$ denotes the derivative of $g(s, v)$ with respect to v . Hence, let us here explain how we guarantee the contractiveness of the operator T_η by controlling $g(s, v)$ and $g_v(s, v)$.

Let us first discuss how to make Y small. Since Y is obtained by an upper estimate of

$$(2.10) \quad (T_\eta(0))(t) = X(t)P \left\{ X(0)^{-1}\eta + \int_0^t X(s)^{-1}g(s, 0)ds \right\} - \int_t^\infty X(t)(I - P)X(s)^{-1}g(s, 0)ds$$

for $\eta \in D$ and D is usually taken as a small subset in \mathbf{R}^{2n} , if we have small $g(t, 0)$, then we can derive small Y . Here $g(t, 0)$ is given from (2.7) as

$$(2.11) \quad g(t, 0) = f(w(t)) - \dot{w}(t).$$

As is mentioned right after Proposition 2.4, $|T_\eta(0)(t)|$ is estimated for $[0, t_K]$ by the numerical verification. Especially, the rigorous calculations of the integral parts are performed for each time step $[t_i, t_{i+1}], i = 0, \dots, K - 1$. Hence, if $g(t, 0)$ is small for each time step, then the estimates of the integrals become small.

Let us note that, by Taylor's theorem, $g(t, 0), t \in [t_i, t_{i+1}]$, can be expressed as

$$g(t, 0) = g(t_i) + \frac{dg}{dt}(t_i, 0)(t - t_i) + \dots + \frac{d^{m-1}g}{dt^{m-1}}(t_i, 0) \frac{(t - t_i)^{m-1}}{(m-1)!} + \frac{d^m g}{dt^m}(t_\theta, 0) \frac{(t - t_i)^m}{m!},$$

where $t_\theta \in [t_i, t_{i+1}]$. From this expression, if

$$(2.12) \quad \frac{d^k g}{dt^k}(t_i, 0) = 0, \quad k = 0, 1, \dots, m - 1$$

holds, then $g(t, 0)$ satisfies

$$(2.13) \quad g(t, 0) \in \frac{1}{m!} \frac{d^m g}{dt^m}([t_i, t_{i+1}], 0)[0, (t_{i+1} - t_i)^m].$$

It means that $g(t, 0)$ can be suppressed by the m -th order of the time step.

Now, as we explained in Step 1, the coefficients of the polynomial interpolations for $w(t)$ are adjusted so as to satisfy (2.12). Namely, we successively determine the differential coefficients $\frac{d^{k+1}w}{dt^{k+1}}(t_i)$ by (2.11) in such a way that (2.12) holds, and obtain the polynomial interpolation for each time step $[t_i, t_{i+1}]$. In Section 4, an example where $w(t)$ is $C^1(\mathbf{R})$ and $m = 3$ is treated. From this process, we can expect to obtain small Y , if we set sufficiently small time steps. Let us comment that this process corresponds to

adding the derivative information to $w(t)$ in order to approximate the true homoclinic orbit.

Next we consider the estimate of Z . In this case, since $(T'_\eta(w_1)w_2)(t)$ is given as

$$(T'_\eta(w_1)w_2)(t) = \int_0^t X(t)PX(s)^{-1}g_v(s, w_1)w_2 ds - \int_t^\infty X(t)(I - P)X(s)^{-1}g_v(s, w_1)w_2 ds,$$

$$w_1, w_2 \in B_\epsilon(\mathbf{R}_+),$$

we wish to have small $g_v(t, w_1)w_2$ for $w_1, w_2 \in B_\epsilon(\mathbf{R}_+)$. Here, let us consider a formal expansion of $g_v(t, w_1)w_2$ at $w(t)$. Then the following estimate holds:

$$\begin{aligned} g_v(t, w_1(t))w_2(t) &= f_x(w(t) + w_1(t))w_2(t) - Aw_2(t) \\ &= f_{xx}(w(t))w_2(t)w_1(t) + \cdots + \frac{1}{(n-1)!}f_{nx}(w(t))w_2(t)w_1(t)^{n-1} + \cdots \\ &\subset f_{xx}(w(t))[-\epsilon^2, \epsilon^2] + O(\epsilon^3) \end{aligned}$$

It means that $g_v(t, w_1)w_2$ can be estimated by the second order with respect to ϵ .

From the above argument, since the right hand side of the sufficient condition in Proposition 2.4 is given by ϵ (linear), we can expect the contractiveness of the operator (2.9) by taking small time steps and ϵ .

§ 2.4. Step 4: Analysis for an intersection of the stable and unstable manifolds

This is the final step of the algorithm, and we investigate an intersection of the stable and unstable manifolds of the origin. Here we explicitly use the reversibility of the vector field $f(x)$, which makes easy the analysis for an intersection of the stable and unstable manifolds. Therefore, let us first briefly recall some of the fundamental properties of reversible systems (e.g., see [11]).

Suppose a dynamical system $\dot{x} = f(x)$ is S -reversible, i.e., $f(Sx) = -Sf(x)$. It is obvious that, if $x(t)$ is a solution, so is $Sx(-t)$. Thus, $x(0) \in \text{Fix}(S)$ leads to $x(t) = Sx(-t)$ from the uniqueness of the initial value. Let $x = 0$ be a fixed point and $W^s(0), W^u(0)$ be the stable and unstable manifolds of the origin, respectively. Then, if $x(0) \in \text{Fix}(S) \cap W^s(0)$, then $x(0) \in W^u(0)$ by $\lim_{t \rightarrow -\infty} x(t) = \lim_{t \rightarrow -\infty} Sx(-t) = 0$. Namely, it becomes the symmetric homoclinic orbit.

From these properties, we can verify the existence of symmetric homoclinic orbits by investigating an intersection of the stable manifold constructed in Step 3 and $\text{Fix}(S)$ without explicitly deriving the unstable manifold. This is the reason that we only treated \mathbf{R}_+ so far. Moreover, it is known that symmetric homoclinic orbits in reversible systems are structurally stable [6]. Hence, it is not necessary to deal with the analysis as bifurcation problems.

Now we consider how to verify an intersection of the stable manifold and $\text{Fix}(S)$. Suppose that we succeeded in verifying the fixed points of (2.9) for η belonging to some subset D . In order to show $x_\eta(0) = w(0) + v_\eta(0) \in \text{Fix}(S)$, it is sufficient to check that there exists $\eta \in D$ such that $v_\eta(0) \in \text{Fix}(S)$, since $w(0) = \xi^0 \in \text{Fix}(S)$. Therefore, for analyzing $v_\eta(0)$, let us introduce the following decomposition

$$\mathbf{R}^{2n} = \text{Fix}(S) \oplus V, \quad V := \{x \in \mathbf{R}^{2n} \mid Sx = -x\}$$

and the projection $Q : \mathbf{R}^{2n} \rightarrow \text{Fix}(S)$.

Here we define the following operator

$$\begin{aligned} E &: \text{Fix}(S) \oplus V \rightarrow V, \\ E(\eta_1, \eta_2) &:= (I - Q)\tilde{E}(\eta_1, \eta_2), \quad (\eta_1, \eta_2) \in \text{Fix}(S) \oplus V, \\ (2.14) \quad \tilde{E}(\eta_1, \eta_2) &:= v_\eta(0) = X(0) \left(PX(0)^{-1}\eta - \int_0^\infty (I - P)X(s)^{-1}g(s, v_\eta)ds \right), \end{aligned}$$

where $\eta_1 = Q\eta$, $\eta_2 = (I - Q)\eta$. From this definition, $\eta \in D$ satisfying $E(\eta_1, \eta_2) = 0$ leads to $v_\eta(0) \in \text{Fix}(S)$. Therefore, we finally transform the operator E into some fixed point form on D in order to study the existence of its fixed point by numerical verifications.

In fact, from (2.14), let us define

$$R := \frac{\partial}{\partial \eta_2} \{(I - Q)X(0)PX(0)^{-1}\eta\}$$

as an approximate matrix to $\frac{\partial}{\partial \eta_2} E(\eta_1, \eta_2)$ and introduce the following Newton type operator as a fixed point form of $E(\eta_1, \eta_2) = 0$:

$$(2.15) \quad F(\eta_1, \eta_2) := R^{-1} \{R\eta_2 - E(\eta_1, \eta_2)\}.$$

It is obvious that $F(\eta_1, \eta_2) = \eta_2$ is equivalent to $E(\eta_1, \eta_2) = 0$ and the fixed point of F can be easily studied by numerical verification techniques, since F is an operator on the finite dimensional space.

§ 3. Numerical example

In this section, we apply the numerical verification method to a practical problem in order to check the validity of the algorithm. Let us consider the following two dimensional reversible system

$$(3.1) \quad \frac{du}{dt} = f(u), \quad f(u) = \begin{pmatrix} u_2 \\ 4u_1 - 3u_1^2 \end{pmatrix}$$

as an example. Here the vector field is reversible with respect to $S(u_1, u_2) = (u_1, -u_2)$. This dynamical system is obtained from the KdV equation under a moving coordinate and the existence of 1-soliton solutions, which correspond to symmetric homoclinic orbits, is known. Here, by applying Newton's method to (3.1), we prepare a homoclinic numerical solution

$$\{(\xi_1^i, \xi_2^i, t_i) \mid i = 0, \pm 1, \dots, \pm K\},$$

which is shown in Fig. 3. Here we take $K = 6000$, $t_K = 4.0$. In addition, we adopt

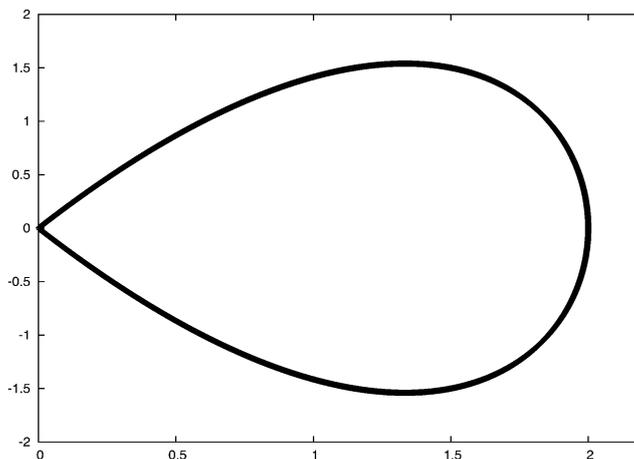


Fig. 3: numerical homoclinic solution for (3.1)

cubic polynomial interpolations for the construction of the approximate solution $w(t)$.

First of all, about the sufficient condition of Proposition 2.4, when we choose $\epsilon = 0.00005$ and $D = [-10^{-10}, 10^{-10}] \times [-10^{-5} \times 10^{-5}]$, we have obtained

$$Y = 0.000013012, \quad Z = 0.000002167$$

for $\eta \in D$, so $Y + Z < \epsilon$ have been verified.

Next, we study an intersection of the stable manifold and $\text{Fix}(S)$ by investigating the fixed point of (2.15) with respect to η_2 . The image of D have been rigorously calculated as follows

$$F(D) \subset [-0.0000050527, 0.0000051626] \subset D_{\eta_2},$$

where $D_{\eta_2} := (I - Q)D$. Due to Brouwer's fixed point theorem, this inclusion shows the existence of the fixed point and, hence the existence of the symmetric homoclinic orbit have been verified by our method.

§ 4. Construction of approximate solutions

In this section, let us explain how to practically construct a suitable approximate solution $w(t)$ for the algorithm. As we discussed in Section 2.3, we determine the

coefficients of polynomial interpolations for $w(t)$ by (2.12) so as to make $|g(t, 0)|$ small for each small interval $[t_i, t_{i+1}]$. For example, let us construct each component of $w(t) = (w_1(t), \dots, w_n(t))$ as $C^1(\mathbf{R})$ and adopt a fifth order polynomial for each small time step $[t_i, t_{i+1}]$ satisfying (2.13) with $m = 3$. We here denote them by

$$w_j(t) = \alpha_{i,j}^{(5)}t^5 + \alpha_{i,j}^{(4)}t^4 + \alpha_{i,j}^{(3)}t^3 + \alpha_{i,j}^{(2)}t^2 + \alpha_{i,j}^{(1)}t + \alpha_{i,j}^{(0)}, \quad t \in [t_i, t_{i+1}].$$

Then, the equations to determine $\alpha_{i,j}^{(l)}, l = 0, 1, \dots, 5, j = 1, \dots, n$, are given by

$$\begin{aligned} w_j(t_i) &= \xi_j^i, & w_j(t_{i+1}) &= \xi_j^{i+1}, & \frac{dw_j}{dt}(t_i) &= f_j(w(t_i)), & \frac{dw_j}{dt}(t_{i+1}) &= f_j(w(t_{i+1})), \\ \frac{d^2w_j}{dt^2}(t_i) &= \frac{df_j}{dt}(w(t_i)), & \frac{d^3w_j}{dt^3}(t_i) &= \frac{d^2f_j}{dt^2}(w(t_i)). \end{aligned}$$

Then some elementary calculations show that each coefficient is given by the following form

$$(4.1) \quad \alpha_{i,j}^{(l)} = \frac{C_{l,j}(\xi^i, \xi^{i+1})}{(t_{i+1} - t_i)^5},$$

where $C_{l,j}(\xi^i, \xi^{i+1})$ are constants depending on ξ^i, ξ^{i+1} .

It is obvious from (4.1) that we need at least the same accuracy for ξ^i and ξ^{i+1} as $O((t_{i+1} - t_i)^5)$ in order to numerically obtain $\alpha_{i,j}^{(l)}$. Namely, if we set a small time step in order to make $|g(t, 0)|$ small, then it requires us to prepare very accurate approximate numerical solutions ξ^i . The same argument also holds when we increase the degree of polynomial interpolations. This causes the following problems.

- limitations of double precision arithmetic in numerical computations
- choice of numerical methods to obtain an approximate numerical homoclinic solution

We can cope with the first problem by using multiple precision arithmetic softwares (e.g., exflib [4]). By using these softwares, we can easily calculate basic operations of floating point numbers under very high accuracy.

Next, we consider the second problem. Let us recall that ξ^K is expected to be very close to the subspace $\text{Span}\{p_{-1}\}$, since $w(t)$ is constructed by $w(t) = \xi^K e^{-\lambda_1(t-t_K)}, t \geq t_K$ (see Section 2.1), where p_{-1} is an eigenvector with respect to $-\lambda_1$. The distance between ξ^K and $\text{Span}\{p_{-1}\}$ directly affects the estimate of $Y(0)$, especially the estimate of $g(s, 0)$ for $s \geq t_K$ in (2.10) (see the paragraph after Proposition 2.4). Moreover let us note that ξ^0 is assumed to be on $\text{Fix}(S)$. The numerical homoclinic solution $\{(\xi^i, t_i) \mid i = 0, 1, \dots, K\}$ satisfying these two restrictions can be derived by solving the following boundary value problem:

$$\frac{dx}{dt} = f(x), \quad t \in [0, t_K], \quad x(0) \in \text{Fix}(S), \quad x(t_K) \in \text{Span}\{p_{-1}\}.$$

Therefore summarizing the discussion in the last few paragraphs yields the following requirements on $\{(\xi^i, t_i) \mid i = 0, 1, \dots, K\}$.

- (1) it should be a good approximate solution of $\frac{dx}{dt} = f(x)$
- (2) K may be very large
- (3) it satisfies the boundary conditions

Here, let us compare several numerical methods to obtain $\{(\xi^i, t_i) \mid i = 0, 1, \dots, K\}$ satisfying the above three requirements. First of all, the finite difference method is not a good choice because of (2). Similarly, the Chebyshev Series method for boundary value problems does not admit (2). These two methods generally need $K \times K$ matrices for computations. On the other hand, for example, when we derive numerical standing pulse solutions of reaction diffusion equations, which correspond to homoclinic orbits in appropriate settings, the spectral method is often used for computations. By adding some modifications, the spectral method can manage (2). However, it is impossible to treat boundary conditions except for the periodic case.

One possibility which deals with the above three requirements is the shooting method. Let us remark that the computational cost for the shooting method linearly depend on K , so we can take large K . Moreover, the boundary condition $x(0) \in \text{Fix}(S)$ should be satisfied rigorously, but it is practically sufficient that $x(t_K)$ is very close to $\text{Span}\{p_{-1}\}$. Thus, it turns out that, in the practical numerical computations, $x(0) \in \text{Fix}(S)$ is given as initial condition at $t = 0$ and perform the shooting method in order to derive a solution which approximately satisfies $x(t_K) \in \text{Span}\{p_{-1}\}$.

From the arguments in this section, we understood that (i) multiple precision arithmetic and (ii) the shooting method are unavoidable to apply the rigorous numerical method proposed in the paper [5] into a wide class of reversible systems. In fact, we have some examples to which the method in [5] does not work well without (i) or (ii). The practical numerical verifications based on the arguments in this paper are now on the experiments and will be published elsewhere in the near future.

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