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Numerical Continuation of Connecting Orbits of Maps in MATLAB

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We present new or improved methods to continue heteroclinic and homoclinic orbits to fixed points in iterated maps and to compute their fold bifurcation curves, corresponding to the tangency of the invariant manifolds. The proposed methods are applicable to general n-dimensional maps and are implemented in MATLAB. They are based on the continuation of invariant subspaces (CIS) algorithm, which is presented in a novel way. The systems of defining equations include the Riccati equations appearing in CIS for bases of the generalized stable and unstable eigenspaces. We use the bordering techniques to continue the folds, and provide full algorithmic details on how to treat the Jacobian matrix of the defining system as a sparse matrix in MATLAB.

For a special – but important in applications – case $n = 2$ we describe the first MATLAB implementation of known algorithms to grow one-dimensional stable and unstable manifolds of the fixed points of noninvertible maps.

The methods are applied to study heteroclinic and homoclinic connections in the generalized Hénon map.

1 Introduction

The accurate computation of orbits connecting fixed points of an iterated map, and the study of associated topological properties have long been recognized as a very important problem both in the theory of nonlinear dynamical systems and in a variety of applied problems, e.g. in models for economical, biological, and physical phenomena. Indeed, as discovered by Poincaré and Birkhoff, such orbits may generate rich dynamics. For example, an orbit that connects a

hyperbolic fixed point to itself (a homoclinic orbit) generically implies the existence of an infinite number of periodic orbits nearby, see [24, 30, 31] and tutorial presentations in [17,26,32]. As discovered in [9,10,16], the appearance of a pair of such homoclinic orbits is accompanied by an infinite sequence of fold and period-doubling bifurcations of periodic orbits, for more details see [25,27], as well as [22]. Moreover, since a homoclinic orbit of a planar map belongs to the intersection of the stable and the unstable invariant curves of a saddle fixed point, such orbits can be involved in the destruction of a closed invariant curve which is born, for example, at a Neimark-Sacker bifurcation [23, 28, 29]. This destruction mechanism has been studied in [1, 4].

Numerical methods for bifurcation analysis of maps have received considerable attention recently and are supported by existing software. Location, analysis, and continuation of fixed-point and cycle bifurcations are implemented, e.g. in CONTENT [13] and CL_MATCONTM [15]. Algorithms for the computation of the one-dimensional manifolds are implemented in DSTOOL [8, 20] and DYNAMICS [34, 35], while those for the continuation of homoclinic orbits and their tangencies using the projection asymptotic boundary conditions [2] are implemented in an AUTO-driver [33].

In this paper, we present new or improved methods to continue heteroclinic and homoclinic orbits to fixed points in iterated maps and to compute the tangencies of their invariant manifolds. In contrast with [33], the projection asymptotic boundary conditions are formulated using the *continuation of invariant subspaces* method [7], which we present in a novel way, using only linear algebra arguments. Moreover, in our approach the Riccati equation is included into the defining system and the continuation of the tangencies is based on the bordering technique. We revisit known algorithms to grow stable and unstable invariant 1D manifolds of cycles in a 2D map without using its inverse [8, 20]. We discuss the implementation of all mentioned above methods in MATLAB as a part of CL_MATCONTM. In particular, we provide full algorithmic details on how to treat the Jacobian matrix of the defining system as a sparse matrix in MATLAB. Therefore CL_MATCONTM becomes a unique integrated toolbox for the numerical bifurcation analysis of maps and difference equations, that covers both local and global phenomena. To illustrate its strength, we compute heteroclinic and homoclinic connections in the generalized Hénon map.

We consider the J-th iterate of a smooth map at some parameter as follows:

$$x \mapsto f^J(x,\alpha) = \underbrace{f(f(f(\cdots f}_{J \text{ times}}(x,\alpha),\alpha),\alpha),\alpha), \quad f : \mathbb{R}^n \times \mathbb{R}^{n_\alpha} \to \mathbb{R}^n. \qquad (1)$$

A sequence $(x_k)_{k\in\mathbb{Z}}$ is called a *connecting orbit* of the map $f^J(\cdot,\alpha)$ at $\alpha=\bar{\alpha}$ if

$$\begin{aligned} \lim_{k\to-\infty} x_k &= x_{-\infty}, \\ f^J(x_k,\bar{\alpha}) &= x_{k+1}, \quad \text{for all} \quad k\in\mathbb{Z}, \\ \lim_{k\to+\infty} x_k &= x_{+\infty}. \end{aligned} \tag{2}$$

Due to the continuity, points $x_{\pm\infty}$ are *fixed points* of $f^J(\cdot,\bar{\alpha})$. A connecting orbit is called *homoclinic* if $x_{-\infty}=x_{+\infty}$ and *heteroclinic* otherwise. From a geometrical point of view, the connecting orbit lies in the intersection of the unstable manifold $W^u_{-\infty}$ of $x_{-\infty}$ and the stable manifold $W^s_{+\infty}$ of $x_{+\infty}$. A connecting orbit is *regular* if $x_{-\infty}$ and $x_{+\infty}$ are hyperbolic and the stable manifold $W^u_{-\infty}$ and the unstable manifold $W^s_{+\infty}$ have transversal intersections at x_k for all $k\in\mathbb{Z}$.

Degenerate cases occur when either one of its fixed points becomes nonhyperbolic or the connecting orbit loses transversality. In the former case the unstable and center-stable manifolds have a transversal intersection, which produces a connecting orbit with a singular endpoint. In the simplest case there is precisely one multiplier 1 or -1, or one conjugate pair of multipliers of $f^J(x,\alpha)$ on the unit circle. This gives us the *saddle-fold, saddle-flip, saddle-Neimark-Sacker* connecting orbits, respectively, see e.g. [3,18]. We will not treat such cases and deal only with the latter case, i.e. the case of nontransversality.

The corresponding numerical problem, for a regular heteroclinic connection between hyperbolic fixed points x_1 and x_N of (1), is that of finding a solution $(x_k)_{k=1,2,\ldots,N}$ of the following system [2]:

$$\begin{aligned} x_1 &= f^J(x_1,\alpha), \\ x_{k+1} &= f^J(x_k,\alpha), \quad k=2,\ldots,N-2, \\ x_N &= f^J(x_N,\alpha), \end{aligned} \tag{3}$$

such that $(x_k)_{k=2,\ldots,N-1}$ leave x_1 along its unstable manifold and approach x_N along its stable manifold. These requirements are then substituted by *projection boundary conditions* which place x_2 and x_{N-1} into the corresponding tangent spaces, i.e. unstable and stable invariant subspaces of the Jacobian matrices of f^J at x_1 and x_N, respectively [2].

2 Continuation of heteroclinic connections

We use an improved algorithm [2] for locating and continuing connecting orbits, which is based on an algorithm for the continuation of invariant subspaces

(CIS) [5,7]. Assume the eigenvalues of the Jacobian matrices $(f^J(x_1,\alpha))_x$ and $(f^J(x_N,\alpha))_x$, where the subscript denotes differentiation, are ordered, respectively, as follows:

$$|\lambda_n^U| \leq \ldots \leq |\lambda_{n_U+1}^U| < 1 < |\lambda_1^U| \leq \ldots \leq |\lambda_{n_U}^U|,$$

$$|\lambda_1^S| \leq \ldots \leq |\lambda_{n_S}^S| < 1 < |\lambda_{n_S+1}^S| \leq \ldots \leq |\lambda_n^S|.$$

The algorithm requires the evaluation of various projections associated with the eigenspaces of $(f^J(x_1,\alpha))_x$ and $(f^J(x_N,\alpha))_x$. These projections are constructed using the real Schur factorizations.

$$(f^J(x_1,\alpha))_x = Q^{(1)}R^{(1)}[Q^{(1)}]^T, \quad (f^J(x_N,\alpha))_x = Q^{(N)}R^{(N)}[Q^{(N)}]^T,$$

where $Q^{(1)}, R^{(1)}, Q^{(N)}$ and $R^{(N)}$ are $n \times n$-matrices.

The first factorization has been chosen so that the first n_U columns $q_1^U, \ldots, q_{n_U}^U$ of $Q^{(1)}$ form an orthonormal basis of the right invariant subspace S_1 of $(f^J(x_1,\alpha))_x$, corresponding to $\lambda_1^U, \ldots, \lambda_{n_U}^U$ and the remaining $n - n_U$ columns $q_{n_U+1}^U, \ldots, q_n^U$ of $Q^{(1)}$ form an orthonormal basis of the orthogonal complement $S_1^\perp$. Similarly, the first n_S columns $q_1^S, \ldots, q_{n_S}^S$ of $Q^{(N)}$ form an orthonormal basis of the right invariant subspace S_N of $(f^J(x_N,\alpha))_x$, corresponding to $\lambda_1^S, \ldots, \lambda_{n_S}^S$ and the remaining $n - n_S$ columns $q_{n_S+1}^S, \ldots, q_n^S$ of $Q^{(N)}$ form an orthonormal basis of the orthogonal complement $S_N^\perp$.

When dealing with heteroclinic connections, we want to find a sequence of points $(x_k)_{k=1,\ldots,N}$ satisfying:

- Stationary state conditions for the initial fixed point:

$$f^J(x_1,\alpha) - x_1 = 0; \tag{4}$$

- The iteration conditions

$$f^J(x_k,\alpha) - x_{k+1} = 0, \quad k = 2,3,\ldots,N-2; \tag{5}$$

- Stationary state conditions for the final fixed point:

$$f^J(x_N,\alpha) - x_N = 0; \tag{6}$$

- The left projection boundary conditions

$$(x_2 - x_1)^T q_{n_{U+i}}^U = 0, \quad i = 1,\ldots,n-n_U; \tag{7}$$

- The right projection boundary conditions

$$(x_{N-1} - x_N)^T q^S_{n_{S+i}} = 0, \quad i = 1, \ldots, n - n_S. \tag{8}$$

A regular zero of a system of equations (4), (5), (6), (7), and (8) corresponds to an approximation of a transversal heteroclinic orbit with hyperbolic fixed points. Thus, a zero for this system can be continued in one parameter, for example, using the standard pseudo-arclength continuation algorithm [19].

In the computational process the conditions in (7) and (8) imply that we need to access the unstable and stable eigenspaces of the linearization of the map (1) at the fixed points x_1 and x_N at each step of the continuation, respectively. It is not efficient to recompute these spaces from scratch in each continuation step. In the next section we explain an algorithm for continuing the invariant subspaces S_1 and S_2 effectively. Contrary to [5,7], our algorithm is purely based on linear algebra arguments.

2.1 *Continuation of invariant subspaces*

Let $A(\alpha) \in \mathbb{R}^{n\times n}$ denote $(f^J(x_1, \alpha))_x$. The basic continuation algorithm requires at each pseudo-arclength continuation step the computation of the orthogonal complement of the right invariant (unstable) n_U-dimensional subspace $S(\alpha)$ of $A(\alpha)$. In general, the function $A(\alpha)$ is smooth in α, and it is important that $S(\alpha)$ is smooth as well, as otherwise convergence difficulties can be expected. We show how to constructively obtain smooth bases for the unstable eigenspace and its orthogonal complement.

Continuation of invariant subspaces was introduced in [5]. We formulate it in a novel way, using only linear algebra arguments. To justify our construction, we recall that in our continuation procedure we parametrize a solution branch in terms of so called pseudo-arclength; let s denote the pseudo-arclength variable. Thus, both fixed points x_1 and x_N as well as the parameter(s) α are smooth functions of s. The matrix-valued function $A : \alpha \in \mathbb{R}^{n_\alpha} \to \mathbb{R}^{n\times n}$ can thus be viewed as a smooth function of $s \in \mathbb{R}$. As a consequence, we consider the continuation of invariant subspaces with respect to the scalar pseudo-arclength variable s. For this reason, we use the notation $A(s)$ for $A(\alpha)$.

We first consider x_1 and its unstable eigenspace. Suppose that initially we have the (real) block Schur factorization

$$A(0) = Q(0)R(0)Q^T(0), \quad Q(0) = [Q_1(0) \;\; Q_2(0)], \tag{9}$$

where $A(0), R(0)$ and $Q(0)$ are $n \times n$-matrices, $Q(0)$ is orthogonal, $Q_1(0)$ has

dimensions $n \times n_U$ and $R(0)$ is block upper triangular

$$R(0) = \begin{bmatrix} R_{11}(0) & R_{12}(0) \\ 0 & R_{22}(0) \end{bmatrix}, \tag{10}$$

where $R_{11}(0)$ and $R_{22}(0)$ are $n_U \times n_U$- and $(n - n_U) \times (n - n_U)$-matrices, respectively; $R_{ii}(0), i = 1, 2$, are not required to be triangular. The columns of $Q_1(0)$ span the unstable invariant subspace $S(0)$ of $A(0)$, and the columns of $Q_2(0)$ span the orthogonal complement $S^{\perp}(0)$. We want to obtain a block Schur factorization for the matrix $A(s)$, close to $A(0)$.

Suppose that the matrix $A(s)$ has two groups of eigenvalues, $\Lambda_1(s)$ (with modulus > 1) and $\Lambda_2(s)$ (with modulus < 1), which stay disjoint for all s around 0. Then, in a neighborhood of $s = 0$, we need a smooth factorization

$$A(s) = Q(s)R(s)Q^T(s), \quad Q(s) = [Q_1(s) \;\; Q_2(s)], \tag{11}$$

where $R(s)$ is in block Schur form

$$R(s) = \begin{bmatrix} R_{11}(s) & R_{12}(s) \\ 0 & R_{22}(s) \end{bmatrix}. \tag{12}$$

Here, R_{11} has eigenvalues $\Lambda_1(s)$ and R_{22} has eigenvalues $\Lambda_2(s)$. As shown in [6], it is always possible to obtain a smooth path of block Schur factorizations that satisfies (11) and (12). However, this smooth path is usually not unique.

Thus we can write

$$Q(s) = Q(0)U(s), \quad \text{with} \;\; U(0) = I, \tag{13}$$

so that we only need to compute the $n \times n$-matrix $U(s)$. We partition $U(s)$ in blocks of the same size as $R(0)$ in (10):

$$U(s) = [U_1(s) \;\; U_2(s)] = \begin{bmatrix} U_{11}(s) & U_{12}(s) \\ U_{21}(s) & U_{22}(s) \end{bmatrix}, \tag{14}$$

so that $U_{11}(s)$ and $U_{22}(s)$ are $n_U \times n_U$- and $(n - n_U) \times (n - n_U)$-matrices, respectively.

We now show that we can always assume that $U_{11}(s)$ and $U_{22}(s)$ are symmetric positive-definite by redefining $Q(s)$ and $R(s)$ if necessary and that this defines $Q(s)$ and $R(s)$ in a unique way.

PROPOSITION: *Suppose $Q(0)$ and $R(0)$ are chosen such that (9) and (10) hold. Then for all s sufficiently close to 0 there exist a unique orthogonal matrix $Q(s) = [Q_1, Q_2]$ of size $n \times n$ such that the columns of Q_1 span the*

unstable invariant subspace of $A(s)$ and the columns of Q_2 span the orthogonal complement of the unstable eigenspace, and a unique block triangular matrix

$$R(s) = \begin{bmatrix} R_{11}(s) & R_{12}(s) \\ 0 & R_{22}(s) \end{bmatrix} \tag{15}$$

of size $n \times n$ where R_{11} has eigenvalues $\Lambda_1(s)$ with modulus > 1 and R_{22} has eigenvalues $\Lambda_2(s)$ with modulus < 1, such that

$$A(s)Q(s) = Q(s)R(s) \tag{16}$$

and

$$Q^{-1}(0)Q(s) = \begin{bmatrix} U_{11}(s) & U_{12}(s) \\ U_{21}(s) & U_{22}(s) \end{bmatrix}, \tag{17}$$

where the blocks U_{11} and U_{22} are symmetric positive definite (SPD).

Proof Suppose that $Q(s)$ and $R(s)$ satisfy (15) and (16). Let $Q^{'}(s)$ and $R^{'}(s)$ be any other pair that satisfies (15) and (16). Then we must have

$$Q^{'}(s) = Q(s)T(s) = Q(s) \begin{bmatrix} T_1 & 0 \\ 0 & T_2 \end{bmatrix}, \tag{18}$$

where T is orthogonal, and also block diagonal.

Suppose also that in

$$Q^{-1}(0)Q^{'}(s) = \begin{bmatrix} U_{11}^{'} & U_{12}^{'} \\ U_{21}^{'} & U_{22}^{'} \end{bmatrix} \tag{19}$$

both $U_{11}^{'}$ and $U_{22}^{'}$ are SPD. By (18) and (19), we have

$$Q^{-1}(0)Q^{'}(s) = Q^{-1}(0)Q(s) \begin{bmatrix} T_1 & 0 \\ 0 & T_2 \end{bmatrix} = \begin{bmatrix} U_{11}^{'} & U_{12}^{'} \\ U_{21}^{'} & U_{22}^{'} \end{bmatrix}, \tag{20}$$

or, equivalently,

$$Q^{-1}(0)Q(s) = \begin{bmatrix} U_{11}^{'}T_1^{-1} & U_{12}^{'}T_2^{-1} \\ U_{21}^{'}T_1^{-1} & U_{22}^{'}T_2^{-1} \end{bmatrix}. \tag{21}$$

According to the polar decomposition of matrices [11], §4.2.10, A_1 and A_2, the upper left and lower right blocks of $Q^{-1}(0)Q(s)$ respectively, are uniquely presented as a product of an SPD matrix and an orthogonal matrix. This implies that T_1 and T_2 are uniquely defined. □

Since $U(0) = I$, there is an open interval about 0, call it I_0, where we can require that U_1 has the structure

$$U_1(s) = \begin{bmatrix} I \\ U_{21}(s)U_{11}^{-1}(s) \end{bmatrix} U_{11}(s). \tag{22}$$

Next, for all $s \in I_0$, we define

$$Y_U(s) = U_{21}(s)U_{11}^{-1}(s). \tag{23}$$

The orthogonality relation $U_1^T U_1 = I$ implies:

$$U_1^T(s)U_1(s) = U_{11}^T(s)U_{11}(s) + U_{21}^T(s)U_{21}(s) = I. \tag{24}$$

Using (24), we obtain

$$\begin{aligned} I + Y_U^T Y_U &= I + U_{11}^{-T}(s)U_{21}^T(s)U_{21}(s)U_{11}^{-1}(s) \\ &= I + U_{11}^{-T}(s)\left[I - U_{11}^T(s)U_{11}(s)\right]U_{11}^{-1}(s) \\ &= I + U_{11}^{-T}(s)U_{11}^{-1}(s) - I \\ &= U_{11}^{-T}(s)U_{11}^{-1}(s). \end{aligned}$$

Now because U_{11} is symmetric positive definite, U_{11}^{-1} is the unique square root of $I + Y_U^T Y_U$. This implies that we can rewrite (22) in terms of Y_U and choose U_{11} symmetric, to obtain

$$U_1 = \begin{bmatrix} I \\ Y_U \end{bmatrix} (I + Y_U^T Y_U)^{-\frac{1}{2}}. \tag{25}$$

Similarly, using $U_2^T U_2 = I$ and $U_1^T U_2 = 0$ for U_2, so that eventually we obtain for every $s \in I_0$,

$$U(s) = \begin{bmatrix} \begin{pmatrix} I \\ Y_U \end{pmatrix} (I + Y_U^T Y_U)^{-\frac{1}{2}} & \begin{pmatrix} -Y_U^T \\ I \end{pmatrix} (I + Y_U Y_U^T)^{-\frac{1}{2}} \end{bmatrix}. \tag{26}$$

Hence, the columns of

$$Q_U(0)\begin{bmatrix} I \\ Y_U \end{bmatrix} \tag{27}$$

form a base for the unstable eigenspace at x_1 and the columns of

$$Q_U^{\perp}(s) = Q_U(0)\begin{bmatrix} -Y_U^T \\ I \end{bmatrix} \tag{28}$$

form a base for the orthogonal complement of the unstable eigenspace. We note that these bases are in general not orthogonal.

Thus, we need to find the matrix $Y_U \in \mathbb{R}^{(n-n_U)\times n_U}$ in (26). For any given $s \in I_0$, define $\hat{R}_{11}, \hat{R}_{12}, E_{21}$ and $\hat{R}_{22}$ by

$$Q^T(0)A(s)Q(0) = \begin{bmatrix} \hat{R}_{11} & \hat{R}_{12} \\ E_{21} & \hat{R}_{22} \end{bmatrix}, \tag{29}$$

where $\hat{R}_{11}$ is of size $n_U \times n_U$ and $\hat{R}_{22}$ is an $(n-n_U)\times(n-n_U)$ matrix.

By (11) and (12) we obtain the invariant subspace relation

$$Q_2^T(s)A(s)Q_1(s) = 0. \tag{30}$$

Now we substitute $Q(s)$ given by (13) and (26) and $A(s)$ obtained from (29) into (30)

$$[-Y_U \quad I]\, Q^T(0)Q(0)\begin{bmatrix} \hat{R}_{11} & \hat{R}_{12} \\ E_{21} & \hat{R}_{22} \end{bmatrix} Q^T(0)Q(0)\begin{bmatrix} I \\ Y_U \end{bmatrix} = 0 \tag{31}$$

to obtain the following *algebraic Riccati equation* for Y_U :

$$F(Y_U) = 0, \quad F(Y_U) := \hat{R}_{22}Y_U - Y_U\hat{R}_{11} + E_{21} - Y_U\hat{R}_{12}Y_U. \tag{32}$$

We now look at x_N. In the same way we can compute a right invariant (stable) n_S-dimensional subspace $S(\alpha)$ of $A(\alpha)$. First, we consider $Q(\alpha) = [Q_1(\alpha) \quad Q_2(\alpha)] \in \mathbb{R}^{n\times n}, Q_1(\alpha) \in R^{n\times n_S}, Q_2(\alpha) \in R^{n\times(n-n_S)}$ so that $Q_1(\alpha)$ spans $S(\alpha)$ and $Q_2(\alpha)$ spans the orthogonal complement $S^{\perp}(\alpha)$.

Using the same procedure as used in the computation of the unstable subspace for x_1, we can obtain the relations

$$Q(s) = Q(0)U(s), \quad \text{with} \quad U(0) = I, \tag{33}$$

and

$$U(s) = \left[\begin{pmatrix} I \\ Y_S \end{pmatrix} (I + Y_S^T Y_S)^{-\frac{1}{2}} \quad \begin{pmatrix} -Y_S^T \\ I \end{pmatrix} (I + Y_S Y_S^T)^{-\frac{1}{2}} \right], \tag{34}$$

and eventually the algebraic Riccati equation for Y_S

$$F(Y_S) = 0, \quad F(Y_S) := \hat{R}_{22} Y_S - Y_S \hat{R}_{11} + E_{21} - Y_S \hat{R}_{12} Y_S \tag{35}$$

to compute the stable invariant subspace and its orthogonal complement for x_N. Solving (35) for Y_S of size $(n-n_S) \times n_S$, enables us to compute the span of the stable invariant subspace of x_N and its orthogonal complement. If $Q_S(0)$ is the orthogonal matrix from the starting heteroclinic orbit, related to the stable invariant subspace, then a basis for the stable eigenspace in the new step at x_N is given by the columns of

$$Q_S(0) \begin{bmatrix} I \\ Y_S \end{bmatrix}. \tag{36}$$

A basis for the orthogonal complement of the subspace in the new step $Q_S^{\perp}$, is given by the columns of

$$Q_S^{\perp}(s) = Q_S(0) \begin{bmatrix} -Y_S^T \\ I \end{bmatrix}. \tag{37}$$

These bases are in general not orthogonal.

2.2 *Implementation*

We now discuss the implementation of the algorithm in Cl_MatContM to continue the heteroclinic connection from the fixed point x_1 to the fixed point x_N.

- *Continuation variables*
  The continuation variables are stored in a K-vector, where $K = Nn + (n - n_U)n_U + (n - n_S)n_S + 1$, containing:
  - A n-vector with the coordinates of the initial fixed point.
  - $(N-2)$ n-vectors with the coordinates of the mesh points $x_2, \ldots, x_{N-1}$.
  - A n-vector x_N with the coordinates of the final fixed point.
  - The vector Y_U^v, i.e. columnwise vectorized Y_U.
  - The vector Y_S^v, i.e. columnwise vectorized Y_S.
  - An active parameter *ap*, i.e. α_a.

- *Defining system*
  The defining systems consists of $Nn+(n-n_U)n_U+(n-n_S)n_S$ equations:
  - The initial fixed point constraint $f^J(x_1,\alpha)-x_1=0$.
  - The constraints $f^J(x_{j-1},\alpha)-x_j=0,\quad j=3,\ldots,N-1$.
  - The final fixed point constraint $f^J(x_N,\alpha)-x_N=0$.
  - The rowwise vectorized Riccati equation (32) for Y_U.
  - The rowwise vectorized Riccati equation (35) for Y_S.
  - The initial boundary conditions (7).
  - The final boundary conditions (8).
- *Initialization*
  To implement the algorithm in CL_MatContM [14], we need to initialize the connecting orbit, i.e. we set the problem parameter vector α, mesh points $x_1,\ldots,x_N$, compute $Q_1(0)$ and $Q_2(0)$ corresponding to x_1 and x_N by (9) and initialize the vector $Y_U=0$ and $Y_S=0$ corresponding to the unstable and stable eigenspaces of x_1 and x_N of sizes $((n-n_U)\times n_U)$ and $((n-n_S)\times n_S)$, respectively. We also set a global structure *hetds* containing the following fields:
  - Dimension of the state space (`hetds.nphase`).
  - Number of mesh points, including the two fixed end points (`hetds.npoints`).
  - The iteration number of the map J (`hetds.niteration`).
  - Mapfile where the map is defined (`hetds.mapfile`).
  - Vector of starting values of parameters and index of the active parameter (`hetds.`P_0 and `hetds.ActiveParams`).
  - Dimensions of the stable and unstable manifolds (`hetds.nu` and `hetds.ns`).
  - The matrices Q_U and Q_S, bases for unstable and stable subspaces respectively (`hetds.`Q_U and `hetds.`Q_S).
- *Adaptation*
  At each continuation point a basis for the unstable eigenspace of x_1 is given by $hetds.Q_U\begin{bmatrix} I \\ Y_U \end{bmatrix}$ and for its orthogonal complement by $hetds.Q_U\begin{bmatrix} -Y_U^T \\ I \end{bmatrix}$. However, these bases are not orthogonal. To restore orthogonality we must adapt Q_U from time to time. The base Q_U can be adapted using the *singular value decomposition* (SVD)

$$[U,S,V]=svd\left(hetds.Q_U\begin{bmatrix} I \\ Y_U \end{bmatrix}\right), \tag{38}$$

  where U and V are unitary matrices of sizes $n\times n$ and $n_U\times n_U$, respectively, and S is a diagonal matrix of size $n\times n_U$. An adapted orthogonal base of the unstable subspace is given by U. Then, the vector Y_U is set to zero.

By using a similar procedure we can adapt the matrices Q_S and Y_S.

2.3 *Computing the Jacobian matrix*

To continue a connecting orbit, we need to compute the Jacobian matrix of the corresponding defining system. The Jacobian matrix can be computed by a finite difference approximation or by symbolic derivatives. However, continuation that uses finite differences is much slower in comparison with the symbolic Jacobian.

To compute the Jacobian matrix, we first initialize the Jacobian matrix J as a zero sparse matrix of size $k\times(k+1)$, where $k = Nn+(n-n_U)n_U+(n-n_S)n_S$. We then compute the nonzero entries of J by taking the derivatives of the system of defining equations with respect to the continuation variables.

- For the constraints in (4) we set $J(1:n,1:n) = A(x_1) - I$ where $A(x_1)$ is the Jacobian of (1) at x_1 and I is an identity matrix of size n. For derivatives of (4) w.r.t. the control parameter we set

$$J(1:n,k+1) = (A_\alpha)_1(:,\text{hetds.ActiveParams}),$$

  where $(A_\alpha)_1$ is the Jacobian of f^J w.r.t. the parameter at x_1.
- For the $(N-3)$ constraints defined in (5), we get for $j = 3,\dots,N-1$, $J((j-2)n+1:(j-1)n,(j-2)n+1:(j-1)n) = A(x_{j-1})$ and $J((j-2)n+1:(j-1)n,(j-1)n+1:jn) = -I$.

  For derivatives of (5) w.r.t. the control parameter we set

$$J((j-2)n+1:(j-1)n,k+1) = (A_\alpha)_j(:,\text{hetds.ActiveParams}),$$

  where $j = 3,\dots,N-1$ and $(A_\alpha)_j$ is the Jacobian w.r.t. the control parameter at x_j.
- For the final fixed point constraint (6), J is computed as: $J((N-2)n+1:(N-1)n,(N-1)n+1:Nn) = A(x_N) - I$. For derivatives of (6) w.r.t. the control parameter we set $J((N-2)n+1:(N-1)n,k+1) = (A_\alpha)_N(:,\text{hetds.ActiveParams})$, where $(A_\alpha)_N$ is the Jacobian of f^J w.r.t. the parameter at x_N.
- Now we compute the entries of J corresponding to (32) at x_1. First we consider the derivatives with respect to the components of Y_U. For simplicity of the computations we divide (32) into 3 terms $D_1 = \hat{R}_{22}Y_U$, $D_2 = -Y_U\hat{R}_{11}$, $D_3 = -Y_U\hat{R}_{12}Y_U$.
  - We start with D_1 whose derivatives with respect to the components of Y_U are written into a block matrix of size $((n-n_U)\times n_U)\times((n-n_U)\times n_U)$. D_1 is an $(n-n_U)\times n_U$ matrix with general form $(D_1)_{(j,i)} =$

$\sum_{l=1}^{n-n_U}(\hat{R}_{22})_{(j,l)}(Y_U)_{(l,i)}$, $j = 1,\ldots,n-n_U$, $i = 1,\ldots,n_U$. Hence all nonzero derivatives arise from the fact that the derivative of $(D_1)_{(j,i)}$ with respect to $(Y_U)_{(s,i)}$ is $(\hat{R}_{22})_{(j,s)}$, $0 \le s \le n-n_U$. Now if $l = n(N-1)$ and $h = Nn$, then

- $(D_1)_{(j,i)}$ is at row position $r_p = l + i + (j-1)n_U$.
- $(Y_U)_{(s,i)}$ is at column position $c_p = h + s + (i-1)(n-n_U)$.

Therefore we set

$$J(r_p, c_p) := (\hat{R}_{22})_{(j,s)},$$

whenever $1 \le j \le n-n_U$, $1 \le i \le n_U$ and $1 \le s \le n-n_U$.

- D_2 is an $(n-n_U)\times n_U$ matrix with general form

$$(D_2)_{(j,i)} = -\sum_{l=1}^{n_U}(Y_U)_{(j,l)}(\hat{R}_{11})_{(l,i)}, \quad j = 1,\ldots,n-n_U, \quad i = 1,\ldots,n_U.$$

Hence all nonzero derivatives arise from the fact that the derivative of $(D_2)_{(j,i)}$ with respect to $(Y_U)_{(j,s)}$ is $(-\hat{R}_{11})_{(s,i)}$, $1 \le s \le n_U$. Now if $l = n(N-1)$ and $h = Nn$, then

- $(D_2)_{(j,i)}$ is at row position $r_p = l + i + (j-1)n_U$.
- $(Y_U)_{(j,s)}$ is at column position $c_p = h + j + (s-1)(n-n_U)$.

Therefore we update

$$J(r_p, c_p) := J(r_p, c_p) - (\hat{R}_{11})_{(s,i)},$$

whenever $1 \le j \le n-n_U$, $1 \le i \le n_U$ and $1 \le s \le n_U$.

- $D_3 = -Y_U\hat{R}_{12}Y_U$ is an $(n-n_U)\times n_U$ matrix. We introduce $D_{31} = -Y_U\hat{R}_{12}$ and $D_{32} = -\hat{R}_{12}Y_U$. With this notation, we have $D_3^{'} = D_{31}Y_U^{'} + Y_U^{'}D_{32}$ where the apostrophe denotes derivation with respect to an unspecified component of Y_U.

  First we consider $D_{31}Y_U^{'}$ that is a $(n-n_U)\times n_U$ matrix with the general form $(D_{31}Y_U^{'})_{(j,i)} = \sum_{l=1}^{n-n_U}(D_{31})_{(j,l)}(Y_U^{'})_{(l,i)}$. This contributes to the derivative with respect to $(Y_U)_{(r,s)}$ if $i = s$ with the term $(D_{31})_{(j,r)}$. Now if $l = n(N-1)$ and $h = Nn$, then

  - $(D_{31}Y_U^{'})_{(j,i)}$ is at row position $r_p = l + i + (j-1)n_U$;
  - $(Y_U)_{(r,i)}$ is at column position $c_p = h + r + (i-1)(n-n_U)$.

  Therefore we update $J(r_p,\ c_p) := J(r_p,\ c_p) + (D_{31})_{(j,r)}$, whenever $1 \le j \le n-n_U$, $1 \le i \le n_U$ and $1 \le r \le n-n_U$.

  Now we consider $Y_U^{'}D_{32}$ that is a $(n-n_U)\times n_U$ matrix with general form $(Y_U^{'}D_{32})_{(j,i)} = \sum_{l=1}^{n_U}(Y_U^{'})_{(j,l)}(D_{32})_{(l,i)}$. This contributes to the derivative with respect to $(Y_U)_{(r,s)}$ if $r = j$ with the term $(D_{32})_{(s,i)}$.

Now if $l = n(N-1)$ and $h = Nn$, then

- $(Y_U^{'} D_{32})_{(j,i)}$ is at row position $r_p = l + i + (j-1)n_U$;
- $(Y_U)_{(j,s)}$ is at column position $c_p = h + j + (s-1)(n - n_U)$.

Therefore we update

$$J(r_p,\ c_p) := J(r_p,\ c_p) + (D_{32})_{(s,i)},$$

whenever $1 \le j \le n - n_U$, $1 \le i \le n_U$ and $1 \le s \le n_U$.

- We compute the derivatives of $F(Y_U)$ in (32) with respect to the components of x_1. If $1 \le i \le n$, then the derivative of $Q^T(0)A(s)Q(0)$ w.r.t. $x_{(1,i)}$ is given by $D_i = Q^T(0)hess(:,:,i)Q(0)$ where $hess$ is the Hessian of f^J. Then $D_{1i} = D_i(1 : n_U,\ 1 : n_U)$, $D_{2i} = D_i(1 : n_U,\ n_U + 1 : n)$, $D_{3i} = D_i(n_U + 1 : n,\ 1 : n_U)$ and $D_{4i} = D_i(n_U + 1 : n,\ n_U + 1 : n)$ are derivatives of $\hat{R}_{11}$, $\hat{R}_{12}$, E_{21} and $\hat{R}_{22}$, w.r.t. $x_{(1,i)}$, respectively. Derivatives of $F(Y_U)$ w.r.t. $x_{(1,i)}$ are hence given by

$$(F(Y_U))_{x_{(1,i)}} = D_{1i}Y_U - Y_U D_{2i} + D_{3i} - Y_U D_{4i} Y_U.$$

All nonzero derivatives arise from the fact that the derivative of $(F(Y_U))_{(j,s)}$ w.r.t. to $x_{(1,i)}$ is

$$(D_{1i})_{(j,:)}(Y_U)_{(:,s)} - (Y_U)_{(j,:)}(D_{2i})_{(:,s)} + (D_{3i})_{(j,s)} - (Y_U)_{(j,:)}(D_{4i}Y_U)_{(:,s)}.$$

Now if $l = n(N-1)$, then

- $(F(Y_U))_{(j,s)}$ is at row position $r_p = l + s + (j-1)n_U$;
- $x_{(1,i)}$ is at column position $c_p = i$.

Therefore we set

$$\begin{aligned} J(r_p,\ c_p) &:= (D_{1i})_{(j,:)}(Y_U)_{(:,s)} - \\ &(Y_U)_(j,:)(D_{2i})_{(:,s)} + (D_{3i})_{(j,s)} - (Y_U)_{(j,:)}(D_{4i}Y_U)_{(:,s)}, \end{aligned}$$

whenever where $j = 1, \ldots, n - n_U,\ \ s = 1, \ldots, n_U,\ i = 1, \ldots, n$.

- We now compute the derivatives of $F(Y_U)$ in (32) with respect to the control parameter α_a. The derivative of $Q^T(0)A(s)Q(0)$ w.r.t. the control parameter is given by $D = Q^T(0)hessp(:,:,\text{ActiveParams})Q(0)$ where $hessp$ is the Hessian of f^J w.r.t. α_a. Then $D_1 = D(1 : n_U,\ 1 : n_U)$, $D_2 = D(1 : n_U,\ n_U + 1 : n)$, $D_3 = D(n_U + 1 : n,\ 1 : n_U)$ and $D_4 = D(n_U + 1 : n,\ n_U + 1 : n)$ are derivatives of $\hat{R}_{11}$, $\hat{R}_{12}$, E_{21} and $\hat{R}_{22}$, w.r.t. α_a, respectively.

  Derivatives of $F(Y_U)$ w.r.t. the control parameter are hence given by

$$(F(Y_U))_{\alpha_a} = D_1 Y_U - Y_U D_2 + D_3 - Y_U D_4 Y_U.$$

All nonzero derivatives arise from the fact that the derivative of $(F(Y_U))_{(j,s)}$ w.r.t to α_a is

$$(D_1)_{(j,:)}(Y_U)_{(:,s)} - (Y_U)_(j,:)(D_2)_{(:,s)} + (D_3)_{(j,s)} - (Y_U)_{(j,:)}(D_4Y_U)_{(:,s)}.$$

Now if $l = n(N-1)$, then

- $(F(Y_U))_{(j,s)}$ is at row position $r_p = l + s + (j-1)n_U$;
- α_a is at column position $c_p = k + 1$.

Therefore we set

$$J(r_p,\ c_p) := (D_1)_{(j,:)}(Y_U)_{(:,s)} - (Y_U)_(j,:)(D_2)_{(:,s)} + (D_3)_{(j,s)} - (Y_U)_{(j,:)}(D_4Y_U)_{(:,s)},$$

whenever where $j = 1, \ldots, n - n_U, \quad s = 1, \ldots, n_U$.

The derivatives that correspond to (35) can be obtained similarly as those of (32).

- We consider conditions (7) which consists of $(n - n_U)$ equations of the form

$$B_i = \sum_{k=1}^{n} (x_2 - x_1)_{(1,k)} (q^U_{(n_U+i)})_k = 0, \quad i = 1, \ldots, n - n_U.$$

- All nonzero derivatives of B_i w.r.t. $x_{(1,s)}$ are of the form $-(q_{(n_U+i)})_s$. Now if $l = n(N-1) + n_U(n - n_U) + n_S(n - n_S)$, then
  - $B_{(1,i)}$ is at row position $l + i$;
  - $x_{(1,s)}$ is at column position s.

  Therefore we set

$$J(l + i, s) := -(q^U_{(n_U+i)})_{(s)},$$

  whenever $1 \le i \le n - n_U$ and $1 \le s \le n$.

- All nonzero derivatives of B_i w.r.t. $x_{(2,s)}$ are of the form $(q^U_{(n_U+i)})_{(s)}$. Now if $l = n(N-1) + n_U(n - n_U) + n_S(n - n_S)$, then
  - B_i is at row position $l + i$;
  - $x_{(2,s)}$ is at column position $n + s$.

  Therefore we set

$$J(l + i, n + s) := (q^U_{(n_U+i)})(s),$$

  whenever $1 \le i \le n - n_U$ and $1 \le s \le n$.

- We now compute derivatives of (7) w.r.t. the components of Q_U. The equations (7) have the following form

$$B_i = (x_2 - x_1)^T q^U_{n_U+i} = 0, \text{for } \; i = 1, \ldots, n - n_U. \tag{39}$$

Here $q^U_{n_U+i}$ are precisely the columns of $Q_U(0) \begin{bmatrix} -Y_U^T \\ I \end{bmatrix}$. Therefore it is best to introduce the new vector $H = (x_2 - x_1)^T Q(0)$. With this notation the i-th equation becomes

$$-\sum_{j=1}^{n_U} H_j (Y_U^T)_{ji} + \text{terms without components of } Y_U = 0.$$

This means that the i-th equation has derivatives with respect to $(Y_U)_{ji}$ equal to $-H_j$ $(i = 1 \ldots, n - n_U, \;\; j = 1, \ldots, n_U)$.
Let $l = n(N-1) + n_U(n - n_U) + n_S(n - n_S)$, $h = nN$. Then the i-th equation is at column position $l + i$. The variable $(Y_U)_{ji}$ is at column position $h + j + (n - n_U)(i - 1)$. So we have to set

$$J(l + i, \;\; h + j + (n - n_U)(i - 1)) := -H_j, \;\; \text{for the relevant } i, j.$$

The derivatives that corresponds to (8) can be computed as those that correspond to (7).

3 Continuation of homoclinic connections

Assume that the eigenvalues of $(f^J(x_1, \alpha))_x$ are ordered as follows:

$$|\lambda_1| \leq \ldots \leq \; |\lambda_m| < 1 < |\lambda_{m+1}| \leq \ldots \leq |\lambda_n|.$$

The procedure to continue a homoclinic connection to x_1 is similar to the procedure used in Section 2. The algorithm now requires the evaluation of two projections associated with the eigenspaces of $(f^J(x_1, \alpha))_x$. These projections are constructed using the real Schur factorizations

$$(f^J(x_1, \alpha))_x = Q^{(1)} R^{(1)} [Q^{(1)}]^T, \quad (f^J(x_1, \alpha))_x = Q^{(N)} R^{(N)} [Q^{(N)}]^T,$$

where $Q^{(1)}, R^{(1)}, Q^{(N)}$, and $R^{(N)}$ are $n \times n$-matrices. The first factorization has been chosen so that the first m columns $q^S_1, \ldots, q^S_m$ of $Q^{(1)}$ form an orthonormal basis of the right invariant subspace S_1 of $(f^J(x_1, \alpha))_x$, corresponding to

$\lambda_1, \ldots, \lambda_m$ and the remaining $n-m$ columns $q^U_{m+1}, \ldots, q^U_n$ of $Q^{(1)}$ form an orthonormal basis of $S_1^{\perp}$. Similarly, the first $l = n-m$ columns $q^U_1, \ldots, q^U_l$ of $Q^{(N)}$ form an orthonormal basis of the right invariant subspace U_1 of $(f^J(x_1, \alpha))_x$, corresponding to $\lambda_{m+1}, \ldots, \lambda_n$ and the remaining $n-l-m$ columns $q^U_{l+1}, \ldots, q^U_n$ of $Q^{(1)}$ form an orthonormal basis of $S_N^{\perp}$.

When dealing with homoclinic connections, we want to find a sequence of points $(x_k)_{k=1,\ldots,N-1}$ satisfying

- Stationary state condition

$$f^J(x_1, \alpha) - x_1 = 0; \tag{40}$$

- The iteration conditions

$$f^J(x_k, \alpha) - x_{k+1} = 0, \quad k = 2, 3, \ldots, N-2; \tag{41}$$

- The left projection boundary conditions

$$(x_2 - x_1)^T q^U_{n_U+i}(\alpha) = 0, \quad i = 1, \ldots, n - n_U; \tag{42}$$

- The right projection boundary conditions

$$(x_{N-1} - x_1)^T q^S_{n_S+i}(\alpha) = 0, \quad i = 1, \ldots, n - n_S. \tag{43}$$

A regular zero of a system of equations (40), (41), (42) and (43) corresponds to a transversal homoclinic orbit to a hyperbolic fixed point. Thus, a zero for this system can be continued in one parameter.

The equations (42) and (43) imply that we should have the stable and unstable eigenspaces of the map (1) at the fixed points x_1 available at each step of the continuation. Using the same procedure, as in the computation of the unstable subspace for x_1, we can obtain relations analogous to (13), (26) and (32) to compute the stable invariant subspace and its orthogonal complement at x_1.

4 Invariant manifolds of planar maps

Our main motivation for computing stable and unstable manifolds of a saddle point is the role they play in the computation of connecting orbits. Intersections of stable and unstable manifolds give rise to homoclinic or heteroclinic tangles. Stable and unstable manifolds are global objects that cannot be found analytically and, hence, must be computed numerically. These manifolds must

be grown from local knowledge, for example from linear information near a fixed point.

We concentrate here on the simplest case of *planar maps* when these manifolds are one-dimensional. Most algorithms use the idea of computing the manifold by starting from a local approximation near the saddle point. The map that arises in a particular application does not necessarily have an explicit inverse or may not even be invertible, meaning that there may be several branches of inverses. Consequently, the standard algorithms requiring the inverse cannot be used to compute stable manifolds of saddle points in this case.

First we present a known algorithm to compute the stable manifold of a saddle point of a planar map, without requiring any knowledge of its inverse map, either explicitly or approximately. In particular, the algorithm can also be used in the case where the map is noninvertible, so that multiple pre-images may exist. Then we focus on the computation of the unstable manifolds.

We recall some definitions, mostly to fix the notation. We consider (1) when $n = 2$ and assume that f has a fixed point $x_0 = f^J(x_0)$ and that f is differentiable in a neighborhood of x_0, but may not have a single-valued inverse. The fixed point x_0 of f is a saddle if the Jacobian matrix $(f^J(x_0))_x$ has one stable eigenvalue λ_s and one unstable eigenvalue λ_u. The stable manifold theorem [26] guarantees that there exist local stable and unstable manifolds $W^s_{loc}(x_0)$ and $W^u_{loc}(x_0)$ tangent at x_0 to the stable and unstable eigenspaces $E^s(x_0)$ and $E^u(x_0)$, respectively. The global stable manifold $W^s(x_0)$ of x_0 is defined as the set of points that converge to x_0 under forward iteration of f,

$$W^s(x_0) = \left\{ x \in \mathbb{R}^2 : f^J(x) \to x_0 \ \text{ as } \ J \to \infty \right\}. \tag{44}$$

Similarly, the global unstable manifold $W^u(x_0)$ of x_0 consists of points that converge to x_0 under backward iteration of the invertible map f. In terms of forward iterates, this is defined as

$$W^u(x_0) = \left\{ x \in \mathbb{R}^2 : \exists \left\{ q_k \right\}, q_0 = x \text{ and } f^J(q_{k+1}) = q_k, \text{ and } \lim_{k\to\infty} q_k = x_0 \right\}. \tag{45}$$

The stable manifold $W^s(x_0)$ is often defined as the union of the successive pre-images of $W^s_{loc}(x_0)$. However, if multiple inverses exist, then all pre-images, even if disjoint from the main branch, are part of the stable manifold. Hence, thus defined, the stable manifold may or may not be simply connected in phase space.

4.1 *Computing a stable manifold*

To compute the one-dimensional stable manifold of a saddle point of a planar map, we use the *Search Circle* (SC) algorithm proposed in [8]. We assume that f is orientation preserving; otherwise we consider its second iterate. We briefly explain this algorithm that extends the one-dimensional manifold in steps by adding new points according to the local curvature properties of the manifold, and finds a new point close to the last computed point that maps under f to a piece of the manifold that was already computed. SC produces a piecewise linear approximation W^s_{pl} of $W^s(x_0)$ by computing an ordered list of points $M = \{p_0, p_1, \ldots, p_n\}$ at varying distance from each other. The first point p_1 is taken a small distance $\delta > 0$ from $p_0 = x_0$ along $E^s(x_0)$. The distance between consecutive points is adjusted according to the curvature of the manifold. To ensure an acceptable resolution of the curve according to pre-specified accuracy parameters, we monitor α_k, the angle between p_{k-1}, p_k and p_{k+1}, and the product $\alpha_k\Delta_k$. The α_k is approximated by

$$\alpha_k = 2\sin^{-1}\left(\frac{\|\bar{p} - p_{k-1}\|}{2\|p_k - p_{k-1}\|}\right) \approx \frac{\|\bar{p} - p_{k-1}\|}{\|p_k - p_{k-1}\|}, \tag{46}$$

where

$$\bar{p} = p_k + \frac{\|p_k - p_{k-1}\|}{\|p_k - p_{k+1}\|}(p_k - p_{k+1}) \tag{47}$$

is the point on the line through p_k and p_{k+1} that lies at the same distance from p_k as p_{k-1}. We check the conditions

$$\alpha_k < \alpha_{max} \tag{48}$$

$$\alpha_k\Delta_k < (\alpha\Delta)_{max} \tag{49}$$

Condition (48) ensures that the resolution of the curve is maintained and condition (49) controls the local interpolation error. The new point p_{k+1} is accepted if it satisfies the above criteria. If one of the criteria is not satisfied, then we replace Δ_k by $\frac{1}{2}\Delta_k$ and repeat the procedure to find a new candidate for p_{k+1}. We set $\Delta_{k+1} = 2\Delta_k$ if both $\alpha_k > \alpha_{min}$ and $\alpha_k\Delta_k > (\alpha\Delta)_{min}$ for a user-specified choice of parameters α_{min} and $(\alpha_k\Delta_k)_{min}$. This ensures that the number of points used to approximate the manifold is in some sense optimized for the required accuracy constraints, see [21] for more details.

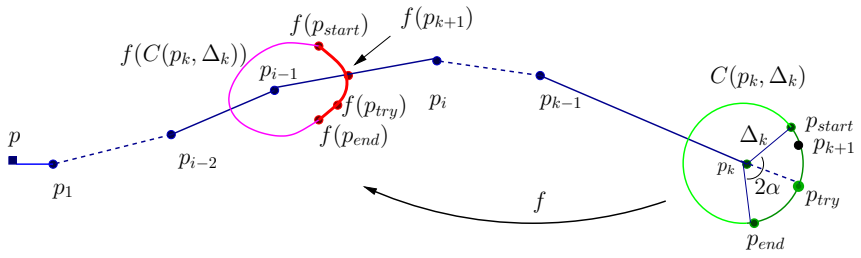

Figure 1. A graphical illustration of the SC algorithm. A new point p_{k+1} is found on the circle $C(p_k, \Delta_K)$ centered at p_k with radius Δ_k such that $f(p_{k+1})$ lies on a previously computed part of $W^S(x_0)$.

A pseudo-code representation of how the branch is grown can be found in [8]. A graphical illustration of the SC algorithm is given in Figure 1.

4.2 *Computing an unstable manifold*

We use the algorithm for computing the global one-dimensional unstable manifold of a saddle point of a map proposed in [20]. To keep the exposition simple, we consider a planar *diffeomorphism* and suppose f is orientation-preserving, otherwise we consider its second iterate. Let x_0 be a saddle point of f. The unstable manifold of x_0 can now be defined as

$$W^u(x_0) = \left\{x \in \mathbb{R}^2 : f^{-J}(x) \to x_0 \quad \text{as} \quad J \to \infty\right\}. \tag{50}$$

now Note that, since f is invertible, the stable manifold $W^s(x_0)$ is simply the unstable manifold of f^{-1} at x_0. The unstable manifold theorem [26] guarantees the existence of the local unstable manifold

$$W^u_{loc}(x_0) = \left\{x \in W^u(x_0) : f^{-n}(x) \in U \quad \text{for all} \quad n \in \mathbb{N}\right\}. \tag{51}$$

in a suitable neighborhood U of x_0. Furthermore, it states that $W^u_{loc}(x_0)$ is tangent to the unstable eigenspace $E^u(x_0)$ corresponding to λ^U.

Similar to the algorithm that is used for computing the stable manifold, the idea is to grow the manifold independently of the dynamics in steps as a list of ordered points. At each step a new point is added at a prescribed distance Δ_k from the last point. New points are found as f-images of suitable points from the part already computed. The algorithm starts with a linear approximation of the local manifold and grows the manifold up to a prespecified arclength l with a speed depending on the local curvature of the manifold.

We now briefly describe a single step of the algorithm and suppose that the piecewise-linear approximation W^u_{pl} of the manifold defined by points $M =$

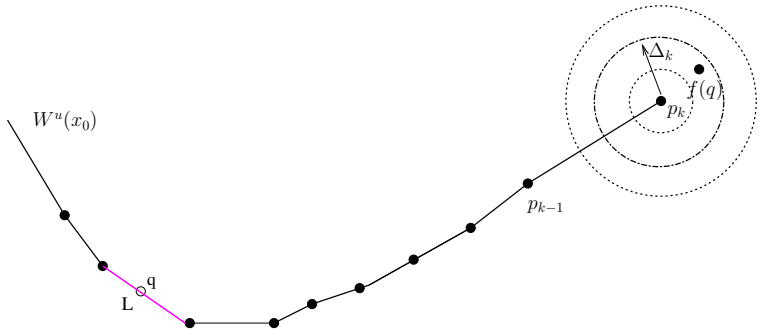

Figure 2. The next point $p_{k+1} = f(q)$ is chosen at approximate distance Δ_k from p_k.

$\{p_0, p_1, \ldots, p_k\}$ is already computed, where $p_0 = x_0$ and the point p_1 is taken at a small distance δ from x_0 in the unstable eigenspace $E^u(x_0)$. The next point p_{k+1} should have the property that the line segment $[p_k, p_{k+1}]$ accurately approximates $W^u(x_0)$. In order to achieve a good approximation, the distance Δ_k between p_k and p_{k+1} must be adjusted from step to step according to the curvature of the manifold.

We want to find p_{k+1} in a small annulus around the circle at p_k with radius Δ_k. To this end, we search in $W^u_{pl}(x_0)$ a line L that is mapped by f to a curve which intersects the circle with center p_k and radius Δ_k. We start with the line segment in $W^u_{pl}(x_0)$ that contains the preimage of p_k and move linearly through $W^u_{pl}(x_0)$. Once L is found, we use bisection to find a point $q \in L$ such that

$$(1 - \epsilon)\Delta_k < \|f(q) - p_k\| < (1 + \epsilon)\Delta_k$$

The point $p_{k+1} = f(q)$ is a candidate for the next point in M, see Figure 2. If Δ_k is acceptable ,then $p_{k+1} = f(q)$ is added to M, $[p_k, p_{k+1}]$ is added to $W^u_{pl}(x_0)$, and the step is completed. However, if Δ_k was too large then we reject $f(q)$, half the estimate Δ_k, and repeat the procedure. This algorithm is presented in the pseudo-code in [21].

5 Continuation of heteroclinic and homoclinic tangencies

Let $F(X, \alpha) = 0$ be the defining system of the heteroclinic connection introduced in Section 2.2, then a heteroclinic tangency satisfies the following

limit-point conditions:

$$\begin{cases} F(X,\alpha) = 0, \\ \det(F_X(X,\alpha)) = 0, \end{cases} \tag{52}$$

which is a system of $K_1 = n(N-1) + n_U(n-n_U) + n_S(n-n_S) + 2n - n_U - n_S + 1$ equations in an $K_2 = (nN + n_U(n-n_U) + n_S(n-n_S) + n_\alpha)$-dimensional space. We recall that $X = (x_1, \ldots, x_N, Y_U, Y_S, \alpha)$.

If $n_U + n_S = n$ and $n_\alpha = 2$, then (52) defines a generic continuation problem. This system is natural from a theoretical perspective but may lead to numerical scaling problems. If the Jacobian has eigenvalues of large magnitude, then these eigenvalues contribute to the determinant (which is the product of all eigenvalues) and may make it difficult to satisfy the defining equations to a desired tolerance. The larger the system, the worse this problem becomes. Thus there are circumstances in which it is desirable to seek alternate defining equations that avoid calculation of the determinant. Bordered matrices allow us to find a substitute function of the determinant.

We define a curve of heteroclinic tangencies by the following system

$$\begin{cases} F(X,\alpha) = 0, \\ g(X,\alpha) = 0, \end{cases} \tag{53}$$

where $g(X,\alpha)$ is computed as the last component of the solution vector in the K_1-dimensional *bordered system*:

$$\begin{pmatrix} F_X(X,\alpha) & b \\ c^T & 0 \end{pmatrix} \begin{pmatrix} v \\ g \end{pmatrix} = \begin{pmatrix} 0_{(K_1-1)} \\ 1 \end{pmatrix}, \tag{54}$$

for suitable vectors $b, c \in \mathbb{R}^{K_1-1}$.

If c is close to the nullvector of $F_X(X,\alpha)$ and b is close to the nullvector of $F_X^T(X,\alpha)$, then the matrix

$$M = \begin{pmatrix} F_X(X,\alpha) & b \\ c^T & 0 \end{pmatrix} \tag{55}$$

is nonsingular at (X,α) and (54) has a unique solution. In practical computations, c and b are approximations of the null vectors of $F_X(X,\alpha)$ and $F_X^T(X,\alpha)$, respectively.

In the continuation of heteroclinic tangencies b and c are computed in the curve initializer `init_HetT_HetT` and stored in the fields `hetTds.b` and `hetTds.c` of the global variable *hetTds*.

The vectors b and c must be adapted during the continuation of heteroclinic tangencies to keep the matrix M nonsingular. Towards this end we use the SVD decomposition $[U, S, V] = svd(full(F_X(X, \alpha)))$ where U, V are orthogonal matrices and S is a diagonal matrix, and $F_X(X, \alpha) = USV^T$. Using the fact that c is a normalized right nullvector of F_X we have:

$$F_X(X, \alpha)c = USV^T c = 0.$$

By the orthogonality of U, we get $SV^T c = 0$. The only possibility for the null vector of S is $V^T c = [0, \ldots, 0, 1]^T$. Sine V is an orthogonal matrix, we finally obtain: $c = V[0, \ldots, 0, 1]^T$. That means c is the last column of V.

For the left nullvector b, we have

$$b^T F_X(X, \alpha) = b^T USV^T = 0.$$

By the orthogonality of V, we get $b^T US = 0$. The only possibility for the null vector of S is $b^T U = [0, \ldots, 0, 1]$. Since U is an orthogonal matrix, we finally obtain: $b = U[0, \ldots, 0, 1]^T$. That means b is the last column of U.

By now it is fairly clear that homoclinic tangencies can be computed in essential the same way.

6 Examples and applications

We consider the generalized Hénon map (GHM)

$$F : \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} \mapsto \begin{pmatrix} x_2 \\ \alpha - \beta x_1 - x_2^2 + R x_1 x_2 + S x_2^3 \end{pmatrix}, \tag{56}$$

which appears in numerous theoretical studies of homoclinic bifurcations, see [12]. In what follows we set $S = 0$.

6.1 *Heteroclinic connection*

For $\alpha = 0.3$, $\beta = -1.057$, and $R = -0.5$, F has two fixed points, namely

$$X_0 = (0.4666170238049, 0.4666170238049),$$
$$X_1 = (-0.4286170238049, -0.4286170238049),$$

with multipliers -1.662111803, $.4955692430$ at X_0 and multipliers 1.784113932, $-.7125713719$ at X_1. Since F is now orientation-reversing, we

will consider the second iterate F^2 to compute heteroclinic connections and, in particular, $\lambda_2^U = 2.762615646$.

We use the algorithm for computing the unstable manifold as described in Section 4.2, to construct the one-dimensional manifold of the saddle point X_0, by calling the newly implemented MATLAB function *Umanifold.m*. To this end, first we set `amax, amin, dmax, dmin, damax, damin, dk` and `epsb` corresponding to α_{max} , α_{min}, Δ_{max}, Δ_{max}, $(\Delta\alpha)_{max}$, $(\Delta\alpha)_{min}$,Δ_k and ϵ_b, respectively, as described in §4.2. The input commands are:

```
epsb=1e-10; Arc=8.6; dk=1e-3; amax=0.6; amin=0.2;
dmin=0.001; damax=0.07; damin=1e-4; dmax=0.2;
p0=[0.46661702380495;0.46661702380495];
p=[0.3;-1.057;-0.5;0];%alpha,beta,R,S
lambda=2.76261564458262; del=1e-2;
v=[0.51553133957551;-0.85687072415592];
M1=Umanifold(p0,Arc,amax,amin,dmax,dmin,damax,damin,
       dk,p,epsb,lambda,del,v);
for i=1:size(M1,2) hold on, plot(M1(1,i),M1(2,i),'r.'), end

del=-1e-4;
M2=Umanifold(p0,Arc,amax,amin,dmax,dmin,damax,damin,
       dk,p,epsb,lamb,del,v);
for i=1:size(M2,2) hold on, plot(M2(1,i),M2(2,i),'r.'), end

plot(0.46661702380495,0.46661702380495,'--sk')
```

where p_0 represents the saddle point X_0, p is the vector of parameters (α, β, R, S), λ is the unstable multiplier of F_x at X_0 and Arc is the total length of the unstable manifold to be computed. The plot of the two unstable manifolds was given in Figure 3. The elapsed time to compute 215200 points was 1470 seconds on a AMD Athlon XP 2800+ processor. We note that a continuation run to compute 100 period-2 cycles of F takes about 2.4 seconds.

We now use the algorithm for computing the stable manifold as described in Section 4.1, to obtain the stable manifold of X_1. The commands are:

```
epsb=1e-7; Arc=5; dk=1e-4; amax=0.5; amin=0.2;
dmin=0.01; damax=0.7; damin=1e-3 ;dmax=1e-2;
p0=[-0.42861702380495;-0.42861702380495];
p=[0.3;-1.057;-0.5;0];%alpha,beta,R,S
p1=p0-1e-3*[-0.81439328674458;0.58031334165721];%p0-1e-3*v
M1=Smanifold(p0,p1,Arc,amax,amin,dmax,dmin,damax,damin,
       dk,p,epsb,n);
for i=1:size(M1,2) hold on, plot(M1(1,i),M1(2,i),'k.'), end
```

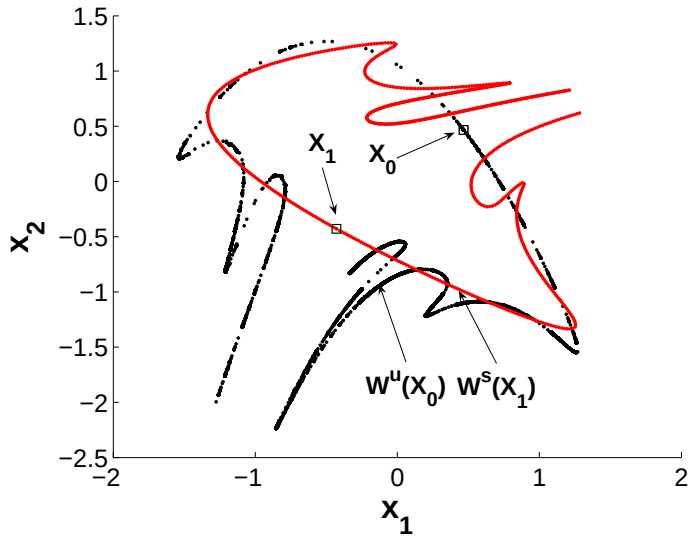

Figure 3. The transversal intersection of unstable and stable manifolds of F at X_0 and X_1, respectively.

```
p1=p0+1e-3*[-0.81439328674458;0.58031334165721];%p0+1e-3*v
M2=Smanifold(p0,p1,Arc,amax,amin,dmax,dmin,damax,damin, dk,p,epsb,n);
for i=1:size(M2,2) hold on, plot(M2(1,i),M2(2,i),'k.'), end
plot(-0.42861702380495;-0.42861702380495,'--sk')
```

The plot of the two stable manifolds is given in Figure 3. The elapsed time to compute 92000 points was 560 seconds.

We will now continue w.r.t. parameter β the heteroclinic orbit in CL_MATCONTM, using the transversal intersection of invariant manifolds at X_0 and X_1, as an initial approximation. The set of intersection points $\{x_5, x_6, \ldots, x_{10}\}$ from Figure 4 is an initial approximation. To get a more accurate heteroclinic orbit we extend it by adding more points. To this end, we use iterations of F^{-1} and F and project the resulting points on $E^u(x_0)$ and $E^s(x_1)$, respectively.

We start from x_5 and compute the point $F^{-1}(x_5)$. By projecting the resulting point on $E^u(x_0)$, we compute x_4 as an approximation of a new intersection point of $W^u(x_0)$ and $W^s(x_1)$. We then apply F^{-1} on x_4 and by projecting the new point on $E^u(x_0)$ we compute x_3. We proceed with the same steps to compute the points x_2 and x_1.

We now use the same procedure by applying F on x_{10}. By projecting the resulting point on $E^s(x_1)$ we compute x_{11} as an approximation of an intersec-

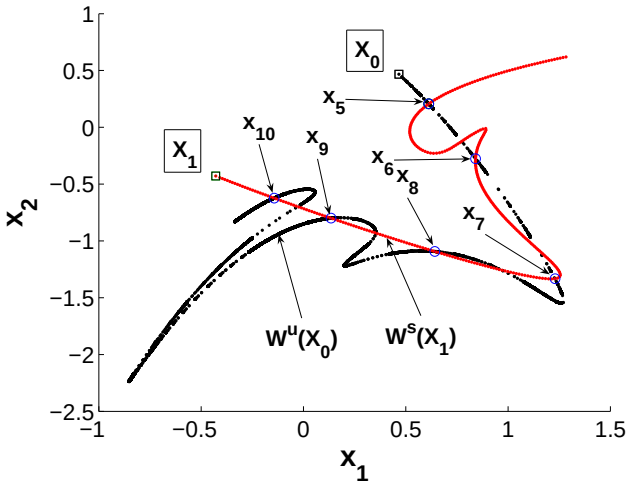

Figure 4. The transversal intersection of the unstable and stable manifolds of F at X_0 and X_1, respectively.

tion point of $W^u(x_0)$ and $W^s(x_1)$. We repeat the same steps to compute the points $x_{12}, x_{13}, \ldots, x_{16}$.

The resulting initial approximation is given by

$$C = \{x_1, x_2, x_3, x_4, x_5, x_6, x_7, x_8, x_9, x_{10}, x_{11}, x_{12}, x_{13}, x_{14}, x_{15}, x_{16}\},$$

where

$$\begin{aligned}
x_1 &= (0.4666171; 0.4666171), & x_2 &= (0.519502; 0.376394),\\
x_3 &= (0.483172; 0.439158), & x_4 &= (0.4731169; 0.456962),\\
x_5 &= (0.612300; 0.206700), & x_6 &= (0.841195; -0.276064),\\
x_7 &= (1.229904; -1.332700), & x_8 &= (0.641982; -1.093020),\\
x_9 &= (0.134731; -0.799843), & x_{10} &= (-0.143457; -0.623386),\\
x_{11} &= (-0.333799; -0.495162), & x_{12} &= (-0.380621; -0.462550),\\
x_{13} &= (-0.404242; -0.445916), & x_{14} &= (-0.416213; -0.437437),\\
x_{15} &= (-0.422303; -0.433111), & x_{16} &= (-0.428617; -0.428617).
\end{aligned}$$

The code below is the implementation into CL_MATCONTM:

```
C={x1,x2,x3,x4,x5,x6,x7,x8,x9,x10,x11,x12,x13,x14,x15,x16}
p=[0.3;-1.057;-0.5;0]; ap=[2]; opt = contset;
[x0,v0]=init_HE_HE(@Ghmap,C, p, ap,2);
opt=contset(opt,'MaxNumpoints',30);
opt=contset(opt,'Singularities',1);
```

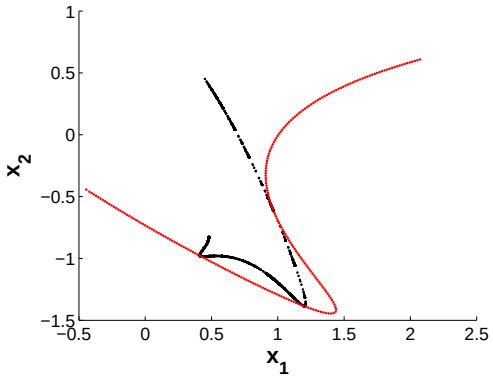

Figure 5. Tangential intersection of the invariant manifolds of (56) for $\alpha = 0.3; \beta = -1.009322; R = -0.5; S = 0$

```
opt=contset(opt,'Backward',1);
[xhet,vhet,shet,hhet,fhet]=cont(@heteroclinic,x0,[],opt);
```

We detect two limit points (LP) on the heteroclinic orbit:

```
label = LP , x = ( 0.450332 0.450332 0.464235 ... -1.009322)
label = LP , x = ( 0.471227 0.471227 0.487755 ... -1.070206)
elapsed time = 1.8 secs
npoints curve = 30
```

In the computed LP points the first 32 components indicate the coordinates of the mesh points $x_1, \ldots, x_{16}$, the following 2 (not shown) indicate Y_U and Y_S in the Riccati equations (32) and (35), respectively, and the last shown component is the value of the control parameter β. A picture of the computed branch of heteroclinic orbits is given in Figure 6.

For the parameter values of the fold points, i.e., $\alpha = 0.3, \beta = -1.009322, R = -0.5$, and $\alpha = 0.3, \beta = -1.070206, R = -0.5$, we have a tangential intersection of the invariant manifolds. A tangential intersection of invariant manifolds is shown in Figure 5.

Next we continue the limit points in two parameters, starting from the *LP* on the heteroclinic connections. This curve is shown in Figure 7. The elapsed time to compute 40 points was about 109 seconds.

6.2 *Homoclinic connection*

Now we consider the parameter values $\alpha = -0.4$, $\beta = 1.03$, and $R = -0.1$. Here F preserves orientation and has a saddle fixed point $X_0 = (-1.62114638486, -1.62114638486)$ with the multipliers 0.2775591559 and

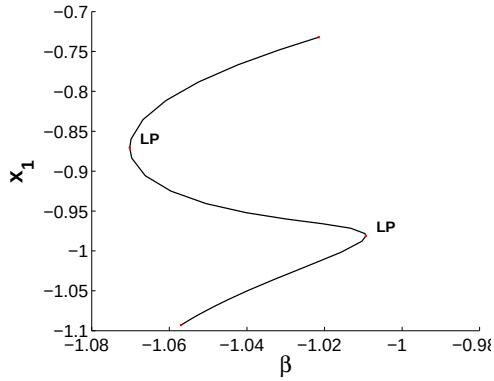

Figure 6. Fold points on the branch of heteroclinic connections of (56)

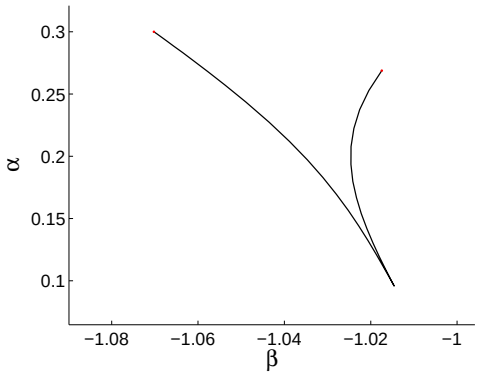

Figure 7. Branch of heteroclinic tangencies of (56)

3.1268482523.

We compute $W^u(X_0)$ and $W^s(X_0)$ and determine their intersection points to be used as initial data for the homoclinic continuation. Figure 8 depicts $W^u(X_0)$ and $W^s(X_0)$ along with their intersection points. We continue the

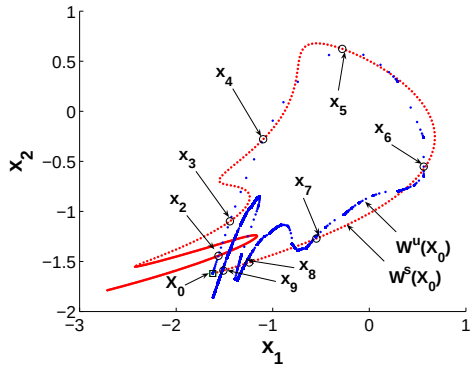

Figure 8. Transversal intersection of the invariant manifolds of (56) for $\alpha = -0.4$, $\beta = 1.03$, $R = -0.1$ and $S = 0$

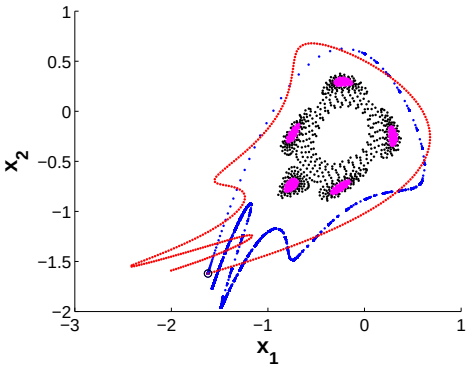

Figure 9. Orbits of (56) for $\alpha = -0.4$, $\beta = 1.03$, $R = -0.1$ and $S = 0$, superposed on Figure 8

homoclinic orbit w.r.t. parameter β in CL_MATCONTM, using the transversal intersection of invariant manifolds at X_0, as an initial approximation. The initial approximation is given by

$$C = \{x_1, x_2, x_3, x_4, x_5, x_6, x_7, x_8, x_9, x_{10}\},$$

where

$$x_1 = (-1.62114638; -1.62114638), \quad x_2 = (-1.56200000; -1.44300000),$$
$$x_3 = (-1.4430000; -1.09878560), \quad x_4 = (-1.09878560; -0.27959456),$$
$$x_5 = (-0.27959456; 0.62285460), \quad x_6 = (0.62285460; -0.48255079),$$
$$x_7 = (-0.48255079; -1.24433961), \quad x_8 = (-1.24433961; -1.51139945),$$
$$x_9 = (-1.51139945; -1.59072793), \quad x_{10} = (-1.59072793; -1.61409646).$$

In Figure 9, obtained by simulations, we present a destructed closed invariant curve for $\alpha = -0.4, \beta = 1.03, R = -0.1$, superposed on Figure 8. This invariant curve is born via the Neimark-Sacker bifurcation and is destructed by approaching the homoclinic tangle.

We detect two limit points (LP):

```
x = ( -1.704631 -1.704631 -1.668284 ... 1.109749 )
x = ( -1.586188 -1.586188 -1.559729 ... 0.996984 )
elapsed time = 1.3 secs
npoints curve = 35
```

In the computed LP points the first 20 components indicate the coordinates of the mesh points $x_1, \ldots, x_{10}$, the following 2 indicate Y_U and Y_S in the Riccati equations (32) and (35), respectively and the last component is the value of the control parameter β. The computed branch of homoclinic connections is presented in Figure 10.

Now we can continue the curve of limit points in two parameters, starting from the *LP* on the homoclinic connections. This curve is given in Figure 11. The elapsed time to compute 53 points was about 42 seconds.

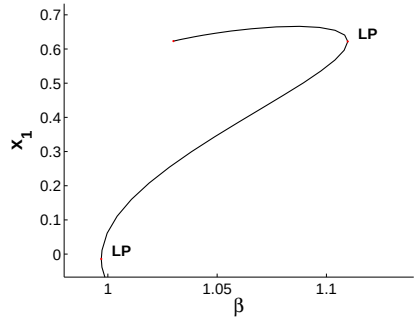

Figure 10. Fold points on the branch of homoclinic connections of (56)

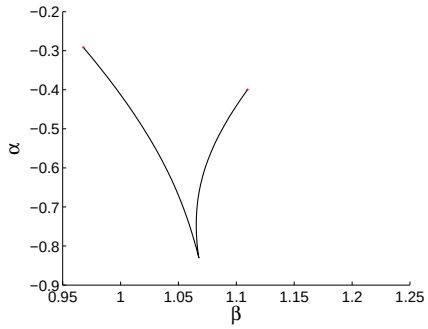

Figure 11. Branch of homoclinic tangencies of (56)

7 Discussion

We have presented new MATLAB tools to continue heteroclinic and homoclinic orbits to fixed points of iterated maps, as well as to compute their fold bifurcation curves, corresponding to the tangencies of the invariant manifolds. The proposed methods work for general n-dimensional maps. For the special, but important in applications, case $n = 2$ we described the first MATLAB implementation of known algorithms to grow one-dimensional stable and unstable manifolds of the fixed points of noninvertible maps.

All algorithms are implemented in CL_MATCONTM, a noninteractive toolbox for the bifurcation analysis of maps in MATLAB. We expect to present an interactive version of this software soon.

Currently, before starting a continuation, the user has to extract manually approximations to the homo-/heteroclinic orbits from the computed stable and unstable manifolds. This procedure has to be automated in the future.

Finally, at least for the one-dimensional unstable manifolds, an algorithm exists that can grow them in n-dimensional maps. This may also be implemented in CL_MATCONTM.

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