SENSITIVITY ANALYSIS OF STABLE AND UNSTABLE MANIFOLDS: THEORY AND APPLICATION

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ABSTRACT. We study stable and unstable manifolds of a hyperbolic equilibrium of an autonomous system of ordinary differential equations under change of parameters. Perturbation theory of orbits lying in the stable and unstable manifolds is developed. Both theoretical and numerical aspects are addressed. As an application, a new method of computing connecting orbits is presented. As a numerical example, we compute a traveling wave (represented by a heteroclinic orbit) in a specific system of four viscous conservation laws.

1. INTRODUCTION

In this paper we consider stable and unstable manifolds of hyperbolic equilibria for multi-parameter systems of ordinary differential equations. These manifolds play very important role in the theory of ordinary and partial differential equations for the analysis of structure and bifurcation of phase portraits, the construction of basins of attraction, the study of chaotic behavior, the construction of traveling wave solutions etc., see [12, 20, 22, 23]. The aim of this paper is to create a constructive multi-parameter perturbation theory for stable and unstable manifolds, which can be useful both for analytical and numerical analysis, especially for computing connecting orbits.

The paper is organized as follows. Section 2 contains basic notions and definitions. Section 3 provides a theoretical basis for the sensitivity analysis. Perturbation of an orbit on the stable or unstable manifold is expressed in terms of fundamental matrices of the linearized system. Explicit formulae for decomposing the perturbation in normal and tangent directions to the manifold are derived.

The numerical analysis given in Section 4 is divided into two parts: local computation near the equilibrium (on the semi-infinite interval $-\infty < t < T$) and numerical computation far from the equilibrium ($t > T$). There are a number of numerical methods for computing local stable and unstable manifolds, see [5, 13, 16, 21]. We also mention the numerical packages AUTO [8], DsTool [11], and P4 [2] for investigating ordinary differential equations. In this paper, we suggest a very simple and classical linearization approach for local approximation and for sensitivity analysis of the manifold. To estimate the calculation error, explicit second order accurate formulae are derived. The advantages of this approach are its considerable simplicity for numerical implementation together with fine error control.

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In Section 5, we consider an application of the previous results to the problem of computing connecting orbits, either homoclinic or heteroclinic. The sensitivity analysis describes the behaviour of an orbit on the stable or unstable manifold under change of parameters. This information is used in a flexible numerical method that is user-driven in the computation process. The resulting method of finding connecting orbits is numerically stable and has high convergence speed. For other methods addressing this problem, see [4, 7, 9, 15, 18]. As an example, we compute a traveling wave (heteroclinic orbit) for a specific system of four viscous conservation laws, where the wave speed is taken as a parameter.

2. Stable and unstable manifolds

Let us consider a nonlinear autonomous system of ordinary differential equations

$$\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x}), \tag{2.1}$$

where $\mathbf{x} \in \mathbb{R}^m$ is a point in state space, $\mathbf{f} \in C^2$ is a smooth function with values in $\mathbb{R}^m$, and the dot represents the derivative with respect to $t \in \mathbb{R}$. An equilibrium $\mathbf{x}_0$ of system (2.1) is determined by the condition

$$\mathbf{f}(\mathbf{x}_0) = \mathbf{0}, \tag{2.2}$$

which implies that $\mathbf{x}(t) \equiv \mathbf{x}_0$ is a solution.

Let us denote by

$$\mathbf{F}_0 = \left(\frac{d\mathbf{f}}{d\mathbf{x}}\right)_{\mathbf{x}_0} \tag{2.3}$$

the $m \times m$ Jacobian matrix of the function $\mathbf{f}(\mathbf{x})$ evaluated at the equilibrium $\mathbf{x} = \mathbf{x}_0$. We assume that the matrix $\mathbf{F}_0$ is nonsingular and has k eigenvalues with positive real part, $m-k$ eigenvalues with negative real part, and no eigenvalues on the imaginary axis. In this hyperbolic case, there is a k-dimensional unstable manifold $\mathcal{M}_u(\mathbf{x}_0)$ in state space formed by solutions (orbits) of system (2.1) "starting" at $\mathbf{x}_0$, i.e., satisfying the condition

$$\mathbf{x}(t) \to \mathbf{x}_0 \quad \text{as} \quad t \to -\infty. \tag{2.4}$$

The $(m-k)$-dimensional stable manifold $\mathcal{M}_s(\mathbf{x}_0)$ contains solutions "ending" at $\mathbf{x}_0$ ($\mathbf{x}(t) \to \mathbf{x}_0$ as $t \to +\infty$). Both unstable and stable manifolds are smooth [12].

Now we analyze the unstable manifold $\mathcal{M}_u(\mathbf{x}_0)$. All the results can be used for the stable manifold $\mathcal{M}_s(\mathbf{x}_0)$ because $\mathcal{M}_s(\mathbf{x}_0)$ is the unstable manifold for the system obtained through reversal $t \to -t$:

$$\dot{\mathbf{x}} = -\mathbf{f}(\mathbf{x}). \tag{2.5}$$

Let $\mathbf{x}(t)$ be a solution of system (2.1) lying in the unstable manifold $\mathcal{M}_u(\mathbf{x}_0)$. A nearby solution $\tilde{\mathbf{x}}(t)$ lying in $\mathcal{M}_u(\mathbf{x}_0)$ can be expressed in the form

$$\tilde{\mathbf{x}}(t) = \mathbf{x}(t) + \varepsilon \mathbf{y}(t) + o(\varepsilon), \tag{2.6}$$

where ε is a small real perturbation parameter. Substituting (2.6) into equations (2.1) and (2.4), the first order terms in ε yield the system of linear homogeneous equations

$$\dot{\mathbf{y}} = \mathbf{F}(t)\mathbf{y}, \tag{2.7}$$

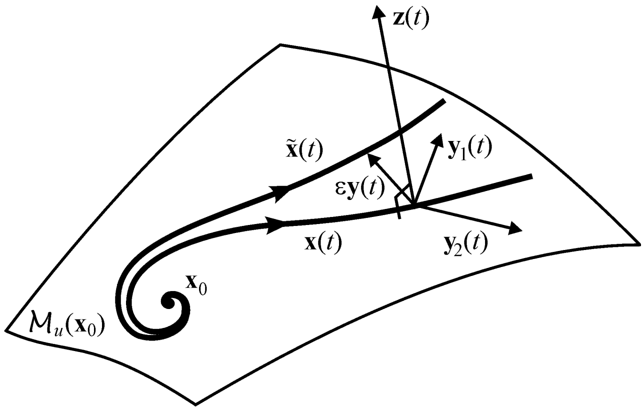

FIGURE 1. Orbits lying in the unstable manifold.

where

$$\mathbf{F}(t) = \left(\frac{d\mathbf{f}}{d\mathbf{x}}\right)_{\mathbf{x}(t)} \tag{2.8}$$

is the Jacobian matrix evaluated at $\mathbf{x} = \mathbf{x}(t)$, and $\mathbf{y}(t)$ satisfies the condition

$$\mathbf{y}(t) \to \mathbf{0} \quad \text{as} \quad t \to -\infty. \tag{2.9}$$

System (2.7), (2.9) represents the linearization of equations (2.1), (2.4) near the solution $\mathbf{x}(t)$.

Since $\mathbf{F}(t) \to \mathbf{F}_0$ as $t \to -\infty$ and the matrix $\mathbf{F}_0$ has k eigenvalues with positive real part, equations (2.7), (2.9) have k linearly independent solutions $\mathbf{y}_1(t), \ldots, \mathbf{y}_k(t)$. Using these solutions, we construct an $m \times k$ fundamental matrix $\mathbf{Y}(t) = [\mathbf{y}_1(t), \ldots, \mathbf{y}_k(t)]$, which generates an arbitrary solution of system (2.7), (2.9) in the form

$$\mathbf{y}(t) = \mathbf{Y}(t)\boldsymbol{\xi}, \tag{2.10}$$

where $\boldsymbol{\xi} \in \mathbb{R}^k$ is a constant vector. Substituting (2.10) into (2.6), we find the following representation for orbits in the unstable manifold $\mathcal{M}_u(\mathbf{x}_0)$ near the orbit $\mathbf{x}(t)$:

$$\tilde{\mathbf{x}}(t) = \mathbf{x}(t) + \varepsilon \mathbf{Y}(t)\boldsymbol{\xi} + o(\varepsilon), \tag{2.11}$$

see Fig. 1. The columns of the matrix $\mathbf{Y}(t)$ span the tangent space of the unstable manifold at the point $\mathbf{x} = \mathbf{x}(t)$.

Since system (2.1), (2.4) is autonomous, a solution of equations (2.1), (2.4) $\mathbf{x}(t)$ has the property that $\tilde{\mathbf{x}}(t) = \mathbf{x}(t+\tau)$, obtained through phase shift, is a solution too. Taking small τ, we find

$$\tilde{\mathbf{x}}(t) = \mathbf{x}(t) + \tau \frac{d\mathbf{x}}{dt} + o(\tau) = \mathbf{x}(t) + \tau \mathbf{f}(\mathbf{x}(t)) + o(\tau), \tag{2.12}$$

which implies that $\mathbf{y}(t) = \mathbf{f}(\mathbf{x}(t))$ is a solution of the linearized system (2.7), (2.9).

3. SENSITIVITY TO PERTURBATION OF PARAMETERS

Let us assume that the function $\mathbf{f}(\mathbf{x}, \mathbf{p})$ in system (2.1) depends smoothly on a vector of parameters $\mathbf{p} \in \mathbb{R}^n$, and $\mathbf{x}_0$ is an equilibrium of the system for a given value of $\mathbf{p} = \mathbf{p}_0$, i.e., $\mathbf{f}(\mathbf{x}_0, \mathbf{p}_0) = 0$. Let us consider a perturbation of the parameter vector in the form

$$\mathbf{p} = \mathbf{p}_0 + \varepsilon\mathbf{e}, \tag{3.1}$$

where $\mathbf{e}$ is a direction vector with unit norm. The corresponding perturbation of the equilibrium takes the form

$$\tilde{\mathbf{x}}_0 = \mathbf{x}_0 + \varepsilon\mathbf{y}_0 + o(\varepsilon), \tag{3.2}$$

where the vector $\mathbf{y}_0$ can be found from the equation $\mathbf{f}(\mathbf{x}, \mathbf{p}) = \mathbf{0}$ as follows

$$\mathbf{y}_0 = -\mathbf{F}_0^{-1}\mathbf{G}_0\mathbf{e}. \tag{3.3}$$

Here

$$\mathbf{F}_0 = \left(\frac{\partial \mathbf{f}}{\partial \mathbf{x}}\right)_{\mathbf{x}_0, \mathbf{p}_0}, \quad \mathbf{G}_0 = \left(\frac{\partial \mathbf{f}}{\partial \mathbf{p}}\right)_{\mathbf{x}_0, \mathbf{p}_0} \tag{3.4}$$

are $m \times m$ and $m \times n$ matrices, respectively, evaluated at $\mathbf{x} = \mathbf{x}_0$ and $\mathbf{p} = \mathbf{p}_0$. Recall that the matrix $\mathbf{F}_0$ is nonsingular by the hyperbolicity assumption.

The perturbation of the parameter vector leads also to a perturbation of the unstable manifold. Let $\mathbf{x}(t)$ be an orbit lying in $\mathcal{M}_u(\mathbf{x}_0)$. Then the orbit $\tilde{\mathbf{x}}(t)$ lying in the perturbed unstable manifold $\mathcal{M}_u(\tilde{\mathbf{x}}_0)$ can be expressed as

$$\tilde{\mathbf{x}}(t) = \mathbf{x}(t) + \varepsilon\mathbf{y}(t) + o(\varepsilon). \tag{3.5}$$

Substituting expressions (3.1)–(3.3) and (3.5) into equations (2.1), (2.4), the first order terms in ε yield the variational linear system

$$\dot{\mathbf{y}} = \mathbf{F}(t)\mathbf{y} + \mathbf{G}(t)\mathbf{e}, \tag{3.6}$$

$$\mathbf{y}(t) \to \mathbf{y}_0 = -\mathbf{F}_0^{-1}\mathbf{G}_0\mathbf{e} \quad \text{as} \quad t \to -\infty, \tag{3.7}$$

where

$$\mathbf{F}(t) = \left(\frac{\partial \mathbf{f}}{\partial \mathbf{x}}\right)_{\mathbf{x}(t), \mathbf{p}_0}, \quad \mathbf{G}(t) = \left(\frac{\partial \mathbf{f}}{\partial \mathbf{p}}\right)_{\mathbf{x}(t), \mathbf{p}_0} \tag{3.8}$$

are $m \times m$ and $m \times n$ matrices, respectively, evaluated at $\mathbf{x} = \mathbf{x}(t)$ and $\mathbf{p} = \mathbf{p}_0$.

The general solution of equations (3.6), (3.7) can be represented as a sum of a particular solution and the general solution of the corresponding homogeneous system (2.7), (2.9). Taking the latter from (2.10), we find

$$\mathbf{y}(t) = \mathbf{Y}_p(t)\mathbf{e} + \mathbf{Y}(t)\boldsymbol{\xi}, \tag{3.9}$$

where the $m \times n$ matrix $\mathbf{Y}_p(t)$ is a particular solution of the system

$$\dot{\mathbf{Y}}_p = \mathbf{F}(t)\mathbf{Y}_p + \mathbf{G}(t), \tag{3.10}$$

$$\mathbf{Y}_p(t) \to \mathbf{Y}_0 = -\mathbf{F}_0^{-1}\mathbf{G}_0 \quad \text{as} \quad t \to -\infty. \tag{3.11}$$

Theorem 3.1. *Let $\mathbf{x}(t)$ be a solution of system (2.1) lying in the unstable manifold $\mathcal{M}_u(\mathbf{x}_0)$ for the parameter vector $\mathbf{p}_0$. Then nearby solutions $\tilde{\mathbf{x}}(t)$ in $\mathcal{M}_u(\tilde{\mathbf{x}}_0)$ for the perturbed parameter vector $\mathbf{p} = \mathbf{p}_0 + \varepsilon\mathbf{e}$ can be represented in the form*

$$\tilde{\mathbf{x}}(t) = \mathbf{x}(t) + \varepsilon\big(\mathbf{Y}_p(t)\mathbf{e} + \mathbf{Y}(t)\boldsymbol{\xi}\big) + o(\varepsilon), \tag{3.12}$$

where $\boldsymbol{\xi} \in \mathbb{R}^k$ is an arbitrary constant vector. The sum $\mathbf{x}(t) + \varepsilon\mathbf{Y}_p(t)\mathbf{e}$ is the approximation of a particular solution in the perturbed unstable manifold $\mathcal{M}_u(\tilde{\mathbf{x}}_0)$, and the additional term $\varepsilon\mathbf{Y}(t)\boldsymbol{\xi}$ describes nearby orbits of this particular solution in $\mathcal{M}_u(\tilde{\mathbf{x}}_0)$; see Fig. 2.

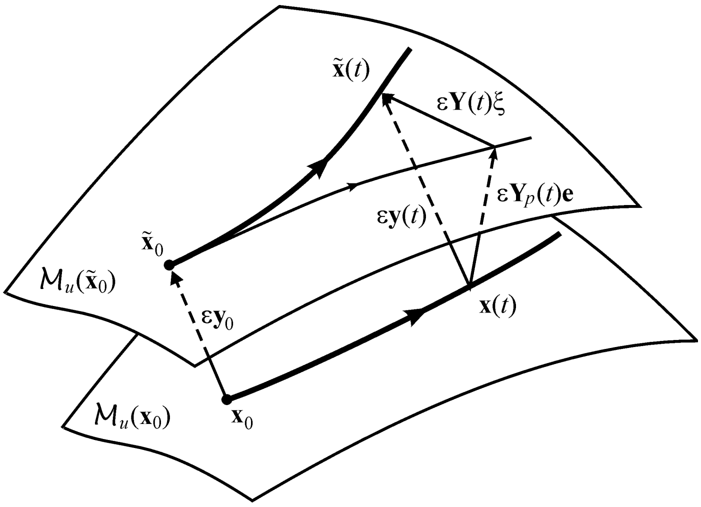

FIGURE 2. Perturbation of an orbit lying in the unstable manifold under change of parameters.

3.1. **Orthogonal decomposition of sensitivity.** Let us consider the linear homogeneous differential equation

$$\dot{\mathbf{z}} = -\mathbf{F}^T(t)\mathbf{z} \tag{3.13}$$

with solutions $\mathbf{z}(t)$ satisfying the condition

$$\mathbf{z}(t) \to \mathbf{0} \quad \text{as} \quad t \to -\infty, \tag{3.14}$$

where $\mathbf{F}^T$ denotes matrix (2.8) transposed. Since $-\mathbf{F}^T(t) \to -\mathbf{F}_0^T$ as $t \to -\infty$ and the matrix $\mathbf{F}_0$ has $m-k$ eigenvalues with negative real part, system (3.13), (3.14) has $m-k$ linearly independent solutions $\mathbf{z}_1(t), \ldots, \mathbf{z}_{m-k}(t)$. We take these solutions as columns of an $m \times (m-k)$ real matrix $\mathbf{Z}(t) = [\mathbf{z}_1(t), \ldots, \mathbf{z}_{m-k}(t)]$. The matrices $\mathbf{Y}(t)$ and $\mathbf{Z}(t)$ satisfy the orthogonality condition

$$\mathbf{Z}^T(t)\mathbf{Y}(t) = \mathbf{0}, \tag{3.15}$$

which can be verified by differentiating (3.15) with respect to t and using the equations

$$\dot{\mathbf{Y}} = \mathbf{F}(t)\mathbf{Y}, \quad \dot{\mathbf{Z}} = -\mathbf{F}^T(t)\mathbf{Z} \tag{3.16}$$

with solutions satisfying the conditions

$$\mathbf{Y}(t) \to \mathbf{0}, \quad \mathbf{Z}(t) \to \mathbf{0} \quad \text{as} \quad t \to -\infty. \tag{3.17}$$

System (3.13), (3.14) is called the adjoint of (2.7), (2.9). The columns of the matrices $\mathbf{Y}(t)$ and $\mathbf{Z}(t)$ form a basis in $\mathbb{R}^m$ depending smoothly on t. This basis is appropriate to represent the columns of the unknown matrix $\mathbf{Y}_p(t)$ as

$$\mathbf{Y}_p(t) = \mathbf{Y}(t)\mathbf{C}_y(t) + \mathbf{Z}(t)\mathbf{C}_z(t), \tag{3.18}$$

where $\mathbf{C}_y(t)$ and $\mathbf{C}_z(t)$ are $k \times n$ and $(m-k) \times n$ matrices, respectively, depending smoothly on t. The latter matrices can be found explicitly utilizing the following theorem.

Theorem 3.2. *Any solution $\mathbf{Y}_p(t)$ of system (3.10), (3.11) can be represented in the form (3.18) through the matrices*

$$\begin{aligned} \mathbf{C}_y(t) &= \mathbf{C}_{yT} + \int_T^t \left(\mathbf{Y}^T\mathbf{Y}\right)^{-1}\mathbf{Y}^T\left((\mathbf{F}+\mathbf{F}^T)\mathbf{Z}\mathbf{C}_z + \mathbf{G}\right)d\tau, \\ \mathbf{C}_z(t) &= \left(\mathbf{Z}^T(t)\mathbf{Z}(t)\right)^{-1}\int_{-\infty}^t \mathbf{Z}^T\mathbf{G}d\tau, \end{aligned} \tag{3.19}$$

where $\mathbf{C}_{yT}$ is an arbitrary constant $k \times n$ matrix, and T is an arbitrary number.

Proof. Substituting expression (3.18) into equation (3.10) and using equations (3.16), we obtain

$$\mathbf{Y}\dot{\mathbf{C}}_y + \mathbf{Z}\dot{\mathbf{C}}_z = (\mathbf{F}+\mathbf{F}^T)\mathbf{Z}\mathbf{C}_z + \mathbf{G}. \tag{3.20}$$

Pre-multiplying (3.20) by $\mathbf{Z}^T$, using equation (3.16) for the matrix $\mathbf{Z}$ and condition (3.15), we find

$$\frac{d}{dt}(\mathbf{Z}^T\mathbf{Z}\mathbf{C}_z) = \mathbf{Z}^T\mathbf{G}. \tag{3.21}$$

Integrating this relation in the interval $(-\infty, t]$ and pre-multiplying the result by $[\mathbf{Z}^T(t)\mathbf{Z}(t)]^{-1}$, we obtain the second expression in (3.19). Condition (3.17) for the matrix $\mathbf{Z}(t)$ was used here.

Pre-multiplying (3.20) by $(\mathbf{Y}^T\mathbf{Y})^{-1}\mathbf{Y}^T$ and using condition (3.15), we get

$$\dot{\mathbf{C}}_y = (\mathbf{Y}^T\mathbf{Y})^{-1}\mathbf{Y}^T\left((\mathbf{F}+\mathbf{F}^T)\mathbf{Z}\mathbf{C}_z + \mathbf{G}\right). \tag{3.22}$$

Integrating (3.22) in the interval $[T, t]$ yields the first formula in (3.19). The constant matrix $\mathbf{C}_{yT} = \mathbf{C}_y(T)$ yields the matrix $\mathbf{Y}(t)\mathbf{C}_{yT}$ in (3.18), whose columns are solutions of the homogeneous system (2.7), (2.9). □

Theorem 3.2 says that an orbit lying in the perturbed unstable manifold takes the form

$$\tilde{\mathbf{x}}(t) = \mathbf{x}(t) + \varepsilon\big(\mathbf{Y}(t)(\mathbf{C}_y(t)\mathbf{e}+\boldsymbol{\xi}) + \mathbf{Z}(t)\mathbf{C}_z(t)\mathbf{e}\big) + o(\varepsilon). \tag{3.23}$$

Taking into account the orthogonality condition (3.15), we see that expression (3.23) decomposes explicitly the orbit perturbation into tangent and normal directions to the unstable manifold, represented by the terms $\varepsilon\mathbf{Y}(t)(\mathbf{C}_y(t)\mathbf{e}+\boldsymbol{\xi})$ and $\varepsilon\mathbf{Z}(t)\mathbf{C}_z(t)\mathbf{e}$, respectively.

Remark 3.3. The unstable manifold $\mathcal{M}_u(\mathbf{x}_0)$ of a non-hyperbolic equilibrium $\mathbf{x}_0$ is tangent to the invariant subspace of the matrix $\mathbf{F}_0$ corresponding to eigenvalues with positive real part [12]. The above results remain valid for a non-hyperbolic equilibrium, if the nature of the perturbation is such that the dimension of the unstable manifold does not change under perturbation of parameters, and the dependence of the unstable manifold on parameters remains smooth. Notice that this happens only in specific situations. Nevertheless, this nongeneric situation appears in the study of traveling waves, see [20], as well as in the study of boundaries between structurally stable phase portrait regions in parameter space, see [19].

Remark 3.4. Let $\mathbf{x}(t)$ be a homoclinic or heteroclinic orbit, i.e., it lies in the intersection of stable and unstable manifolds of the same or two distinct equilibria. Then the formulae in Theorems 3.1 and 3.2 allow evaluating the distance between the stable and unstable manifolds due to perturbation of parameters. These formulae yield a constructive generalization of the Melnikov theory to multi-dimensional and multi-parameter autonomous systems, as well as giving additional important information on the manifolds behavior. For other generalizations of the Melnikov method we refer to [3, 17, 24].

4. Numerical evaluation of sensitivity

We need to compute an orbit lying in the unstable manifold in a semi-infinite interval $-\infty < t \leq t_0$. For numerical calculation of the orbit and its sensitivity it is convenient to divide this interval into two parts. In the first interval $-\infty < t \leq T$ we approximate the orbit using local information on the nature of the equilibrium. Then, we use a numerical integration method in the second interval $T \leq t \leq t_0$, where initial conditions at $t = T$ are taken from the local approximation.

4.1. First order approximation of an orbit near an equilibrium.

A first order approximation of an orbit $\mathbf{x}(t)$ lying in the unstable manifold $\mathcal{M}_u(\mathbf{x}_0)$ can be found using the equations

$$\Delta\dot{\mathbf{x}} = \mathbf{F}_0\Delta\mathbf{x}, \quad \Delta\mathbf{x} = \mathbf{x} - \mathbf{x}_0, \tag{4.1}$$

$$\Delta\mathbf{x}(t) \to \mathbf{0} \quad \text{as} \quad t \to -\infty, \tag{4.2}$$

which are the linearization of system (2.1), (2.4) near the equilibrium $\mathbf{x}_0$. Solutions of equations (4.1), (4.2) are determined by the unstable invariant subspace of the matrix $\mathbf{F}_0$. This subspace can be found in a convenient and numerically stable way by the real Schur decomposition [10]:

$$\mathbf{S} = \mathbf{U}^{-1}\mathbf{F}_0\mathbf{U}, \tag{4.3}$$

where $\mathbf{S}$ is a real Schur canonical form of the matrix $\mathbf{F}_0$ (block-upper-triangular real matrix with diagonal blocks corresponding to real eigenvalues or complex-conjugate pairs of eigenvalues), and $\mathbf{U}$ is an orthogonal real matrix. It is always possible to order the diagonal blocks in $\mathbf{S}$ so that

$$\mathbf{S} = \begin{pmatrix} \mathbf{S}_u & \mathbf{S}' \\ \mathbf{0} & \mathbf{S}_s \end{pmatrix}, \tag{4.4}$$

where $\mathbf{S}_u$ and $\mathbf{S}_s$ are $k \times k$ and $(m-k) \times (m-k)$ block-upper-triangular matrices having eigenvalues with positive and negative real parts, respectively. We partition the orthogonal matrix $\mathbf{U} = [\mathbf{U}_u, \mathbf{U}_s]$ according to (4.4). The matrices $\mathbf{U}_u$ and $\mathbf{U}_s$ satisfy the orthogonality conditions

$$\mathbf{U}_u^T\mathbf{U}_u = \mathbf{I}_k, \quad \mathbf{U}_u^T\mathbf{U}_s = \mathbf{0}, \quad \mathbf{U}_s^T\mathbf{U}_s = \mathbf{I}_{m-k}, \tag{4.5}$$

where $\mathbf{I}_k$ is the $k \times k$ identity matrix. Using equations (4.3)–(4.5), we find that

$$\mathbf{F}_0\mathbf{U}_u = \mathbf{U}_u\mathbf{S}_u, \quad \mathbf{F}_0^T\mathbf{U}_s = \mathbf{U}_s\mathbf{S}_s^T. \tag{4.6}$$

Then, a solution of the equations (4.1), (4.2) is given explicitly in the form

$$\Delta\mathbf{x} = \mathbf{U}_u \exp(\mathbf{S}_u(t-T))\,\boldsymbol{\eta}, \tag{4.7}$$

where $\boldsymbol{\eta} \in \mathbb{R}^k$ is an arbitrary constant vector, and $T \in \mathbb{R}$ is an arbitrary number. Expression (4.7) provides the first order approximation

$$\mathbf{x}_{app}(t) = \mathbf{x}_0 + \mathbf{U}_u \exp(\mathbf{S}_u(t-T))\,\boldsymbol{\eta} \tag{4.8}$$

of an orbit lying in $\mathcal{M}_u(\mathbf{x}_0)$ in the neighborhood of $\mathbf{x}_0$. At the end of the approximation interval we have

$$\mathbf{x}_{app}(T) = \mathbf{x}_0 + \mathbf{U}_u\boldsymbol{\eta}. \tag{4.9}$$

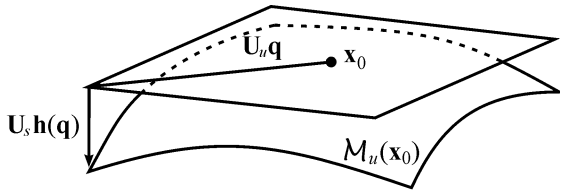

FIGURE 3. Local representation of the unstable manifold.

The accuracy of the approximation depends on the vector $\boldsymbol{\eta}$. It can be estimated using the second order approximation of the unstable manifold.

4.2. **Second order approximation of the unstable manifold.** The columns of the matrices $\mathbf{U}_u$ and $\mathbf{U}_s$ span the tangent and orthogonal subspaces of the unstable manifold $\mathcal{M}_u(\mathbf{x}_0)$ at $\mathbf{x}_0$, respectively. This decomposition allows representing the unstable manifold in the vicinity of $\mathbf{x}_0$ as

$$\mathcal{M}_u(\mathbf{x}_0) = \{\mathbf{x}(\mathbf{q}) = \mathbf{x}_0 + \mathbf{U}_u\mathbf{q} + \mathbf{U}_s\mathbf{h}(\mathbf{q}) \mid \mathbf{q} \in \mathbb{R}^k\}, \tag{4.10}$$

where $\mathbf{h}(\mathbf{q})$ is the unique smooth function in the vicinity of $\mathbf{q} = \mathbf{0}$ with values in $\mathbb{R}^{m-k}$, see Fig. 3. The tangency condition ensures that the function $\mathbf{h}(\mathbf{q})$ satisfies

$$\mathbf{h}(\mathbf{0}) = \mathbf{0}, \quad \left(\frac{d\mathbf{h}}{d\mathbf{q}}\right)_{\mathbf{0}} = \mathbf{0}. \tag{4.11}$$

The tangent space of $\mathcal{M}_u(\mathbf{x}_0)$ at the point $\mathbf{x}(\mathbf{q})$ has the form

$$T_{\mathbf{x}(\mathbf{q})}\mathcal{M}_u(\mathbf{x}_0) = \{\mathbf{U}_u d\mathbf{q} + \mathbf{U}_s\frac{d\mathbf{h}}{d\mathbf{q}}\,d\mathbf{q} :\ d\mathbf{q} \in \mathbb{R}^k\}, \tag{4.12}$$

where $d\mathbf{h}/d\mathbf{q}$ is the $(m-k)\times k$ Jacobian matrix of the mapping $\mathbf{h}(\mathbf{q})$ evaluated at $\mathbf{x}(\mathbf{q})$. Since $\mathcal{M}_u(\mathbf{x}_0)$ is an invariant manifold with respect to the vector field $\mathbf{f}(\mathbf{x},\mathbf{p}_0)$, we have

$$\mathbf{f}(\mathbf{x}(\mathbf{q}),\mathbf{p}_0) \in T_{\mathbf{x}(\mathbf{q})}\mathcal{M}_u(\mathbf{x}_0). \tag{4.13}$$

Using condition (4.13) and expression (4.12), we find

$$\mathbf{f}(\mathbf{x}(\mathbf{q}),\mathbf{p}_0) = \mathbf{U}_u d\mathbf{q} + \mathbf{U}_s\frac{d\mathbf{h}}{d\mathbf{q}}\,d\mathbf{q}. \tag{4.14}$$

Pre-multiplying equation (4.14) by $\mathbf{U}_u^T$ and using properties (4.5), we obtain

$$d\mathbf{q} = \mathbf{U}_u^T\mathbf{f}(\mathbf{x}(\mathbf{q}),\mathbf{p}_0). \tag{4.15}$$

Pre-multiplying equation (4.14) by $\mathbf{U}_s^T$ and using expressions (4.5), (4.10), and (4.15), we get [16]:

$$\mathbf{U}_s^T\mathbf{f}(\mathbf{x}_0 + \mathbf{U}_u\mathbf{q} + \mathbf{U}_s\mathbf{h}(\mathbf{q}),\mathbf{p}_0) = \frac{d\mathbf{h}}{d\mathbf{q}}\mathbf{U}_u^T\mathbf{f}(\mathbf{x}_0 + \mathbf{U}_u\mathbf{q} + \mathbf{U}_s\mathbf{h}(\mathbf{q}),\mathbf{p}_0). \tag{4.16}$$

Notice that (4.16) is a system of first order partial differential equations for $\mathbf{h}(\mathbf{q})$.

Taking the derivative $\partial^2/\partial q_i\partial q_j$ of both sides of equation (4.16) at $\mathbf{q} = \mathbf{0}$ and using equalities (2.2), (4.6), and (4.11), we find

$$\mathbf{S}_s\mathbf{h}_{ij} + \mathbf{f}_{ij} = [\mathbf{h}_{i1},\ldots,\mathbf{h}_{ik}][\mathbf{S}_u]_j + [\mathbf{h}_{j1},\ldots,\mathbf{h}_{jk}][\mathbf{S}_u]_i, \tag{4.17}$$

where $[\mathbf{S}_u]_i$ is the ith column of the matrix $\mathbf{S}_u$, and the vectors $\mathbf{h}_{ij},\ \mathbf{f}_{ij} \in \mathbb{R}^{m-k}$ are

$$\mathbf{h}_{ij} = \frac{\partial^2 \mathbf{h}}{\partial q_i \partial q_j}, \quad \mathbf{f}_{ij} = \mathbf{U}_s^T \sum_{v,w=1}^{m} \frac{\partial^2 \mathbf{f}}{\partial x_v \partial x_w} \mathbf{U}_u(v,i)\mathbf{U}_u(w,j), \tag{4.18}$$

with derivatives evaluated at $\mathbf{q} = \mathbf{0}$ and $\mathbf{x} = \mathbf{x}_0$; $\mathbf{U}_u(v,i)$ denotes the (v,i)th element of the matrix $\mathbf{U}_u$. Introducing the $(m-k) \times k^2$ matrices

$$\begin{aligned} \mathbf{H} &= [\mathbf{h}_{11}, \dots, \mathbf{h}_{1k}, \mathbf{h}_{21}, \dots, \mathbf{h}_{2k}, \dots, \mathbf{h}_{k1}, \dots, \mathbf{h}_{kk}], \\ \mathbf{F} &= [\mathbf{f}_{11}, \dots, \mathbf{f}_{1k}, \mathbf{f}_{21}, \dots, \mathbf{f}_{2k}, \dots, \mathbf{f}_{k1}, \dots, \mathbf{f}_{kk}], \end{aligned} \tag{4.19}$$

we write equation (4.17) in the form

$$\mathbf{S}_s \mathbf{H} - \mathbf{H}\mathbf{R} = -\mathbf{F}, \tag{4.20}$$

where $\mathbf{R}$ is the $k^2 \times k^2$ matrix

$$\mathbf{R} = \begin{pmatrix} \mathbf{S}_u & & \\ & \ddots & \\ & & \mathbf{S}_u \end{pmatrix} + \begin{pmatrix} [\mathbf{S}_u]_1 & & & & [\mathbf{S}_u]_k & & \\ & \ddots & & \cdots & & \ddots & \\ & & [\mathbf{S}_u]_1 & & & & [\mathbf{S}_u]_k \end{pmatrix} \tag{4.21}$$

with blank entries filled by zeros.

Equation (4.20) represents a system of linear equations for the elements of $\mathbf{H}$. A system of this type is called the Sylvester equation for the matrix $\mathbf{H}$ [10]. Such a system has a unique solution, since there is a unique function $\mathbf{h}(\mathbf{q})$ parameterizing the unstable manifold (4.10). The solution of the Sylvester equation can be found numerically using standard codes, for example, LAPACK [1]. Having found the matrix $\mathbf{H}$, we use its columns $\mathbf{h}_{ij}$ to approximate $\mathbf{h}(\mathbf{q})$ as

$$\mathbf{h}(\mathbf{q}) = \frac{1}{2} \sum_{i,j=1}^{k} \mathbf{h}_{ij} q_i q_j + o(\|\mathbf{q}\|^2). \tag{4.22}$$

Theorem 4.1. *The second order approximation of the unstable manifold in the neighborhood of the equilibrium* $\mathbf{x}_0$ *has the form*

$$\mathcal{M}_u(\mathbf{x}_0) = \{\mathbf{x}(\mathbf{q}) = \mathbf{x}_0 + \mathbf{U}_u\mathbf{q} + \frac{1}{2}\mathbf{U}_s \sum_{i,j=1}^{k} \mathbf{h}_{ij} q_i q_j + o(\|\mathbf{q}\|^2) \mid \mathbf{q} \in \mathbb{R}^k\}. \tag{4.23}$$

Notice that the second order analysis of individual orbits in the unstable manifold is unnecessary for our purposes.

4.3. **Error analysis.** The second order term in (4.23) is orthogonal to the first order term $\mathbf{U}_u\mathbf{q}$ and, therefore, it provides a good quantitative estimate for the error in (4.8) as follows

$$\|\mathbf{x}(t) - \mathbf{x}_{app}(t)\| = \left\| \frac{1}{2}\mathbf{U}_s \sum_{i,j=1}^{k} \mathbf{h}_{ij} q_i q_j \right\| + o(\|\mathbf{q}\|^2), \tag{4.24}$$

where $\mathbf{x}_{app}(t) = \mathbf{x}_0 + \mathbf{U}_u\mathbf{q}$ with $\mathbf{q} = \exp(\mathbf{S}_u(t-T))\,\boldsymbol{\eta}$, and $\mathbf{x}(t)$ is the unstable manifold exact orbit nearest to $\mathbf{x}_{app}(t)$. At the end of the approximation interval $t = T$ we find

$$\|\mathbf{x}(T) - \mathbf{x}_{app}(T)\| = \left\| \frac{1}{2}\mathbf{U}_s \sum_{i,j=1}^{k} \mathbf{h}_{ij} \eta_i \eta_j \right\| + o(\|\boldsymbol{\eta}\|^2), \tag{4.25}$$

where η_i is the ith component of the vector $\boldsymbol{\eta}$. If the error (4.25) exceeds a prescribed bound, we can take a lower value of T' of T (i.e. $T' < T$), thereby shortening the approximate part of the orbit $\mathbf{x}(t)$. Then, the approximate solution (4.8) is defined in the interval $-\infty < t < T'$ and is written as

$$\mathbf{x}_{app}(t) = \mathbf{x}_0 + \mathbf{U}_u \exp(\mathbf{S}_u(t-T))\,\boldsymbol{\eta} = \mathbf{x}_0 + \mathbf{U}_u \exp(\mathbf{S}_u(t-T'))\,\boldsymbol{\eta}', \tag{4.26}$$

where

$$\boldsymbol{\eta}' = \exp(\mathbf{S}_u(T'-T))\,\boldsymbol{\eta}. \tag{4.27}$$

If T' is low enough, the new vector $\boldsymbol{\eta}'$ provides tighter estimate for error (4.25).

4.4. **Orbit sensitivity near the equilibrium.** Let us consider a perturbation of the parameter vector $\mathbf{p} = \mathbf{p}_0 + \varepsilon\mathbf{e}$. Near the equilibrium, the variational equations (3.6), (3.7) can be approximated by

$$\dot{\mathbf{y}} = \mathbf{F}_0\mathbf{y} + \mathbf{G}_0\mathbf{e}, \tag{4.28}$$

$$\mathbf{y}(t) \to \mathbf{y}_0 \quad \text{as} \quad t \to -\infty, \tag{4.29}$$

where $\mathbf{F}_0$ and $\mathbf{G}_0$ are the limits of $\mathbf{F}(t)$ and $\mathbf{G}(t)$ as $t \to -\infty$. The general solution of system (4.28), (4.29) is

$$\mathbf{y} = \mathbf{y}_0 + \mathbf{U}_u \exp(\mathbf{S}_u(t-T))\,\boldsymbol{\xi}, \tag{4.30}$$

where $\boldsymbol{\xi} \in \mathbb{R}^k$ is an arbitrary constant vector, and $T \in \mathbb{R}$ is an arbitrary number. Recall that the vector $\mathbf{y}_0$, determined by formula (3.3), describes the perturbation of the equilibrium. Using expression (4.8), we find the first order approximation of the orbit (3.5) on the perturbed unstable manifold $\mathcal{M}_u(\tilde{\mathbf{x}}_0)$ as

$$\begin{aligned} \tilde{\mathbf{x}}_{app}(t) &= \mathbf{x}_{app}(t) + \varepsilon\left(\mathbf{y}_0 + \mathbf{U}_u \exp(\mathbf{S}_u(t-T))\,\boldsymbol{\xi}\right) \\ &= \tilde{\mathbf{x}}_{0,app} + \mathbf{U}_u \exp(\mathbf{S}_u(t-T))(\boldsymbol{\eta} + \varepsilon\boldsymbol{\xi}), \end{aligned} \tag{4.31}$$

where

$$\tilde{\mathbf{x}}_{0,app} = \mathbf{x}_0 + \varepsilon\mathbf{y}_0 = \mathbf{x}_0 + \mathbf{Y}_0\Delta\mathbf{p}, \quad \Delta\mathbf{p} = \varepsilon\mathbf{e}, \tag{4.32}$$

is the approximation of the perturbed equilibrium $\tilde{\mathbf{x}}_0$.

Approximations of the fundamental matrix $\mathbf{Y}(t)$ and of the partial solution $\mathbf{Y}_p(t)$, determined by equations (3.16), (3.17) and (3.10), (3.11), are obtained as solutions of the systems

$$\begin{aligned} &\dot{\mathbf{Y}} = \mathbf{F}_0\mathbf{Y}, && \mathbf{Y}(t) \to \mathbf{0} \quad \text{as} \quad t \to -\infty, \\ &\dot{\mathbf{Y}}_p = \mathbf{F}_0\mathbf{Y}_p + \mathbf{G}_0, && \mathbf{Y}_p(t) \to \mathbf{Y}_0 \quad \text{as} \quad t \to -\infty, \end{aligned} \tag{4.33}$$

in the form

$$\begin{aligned} &\mathbf{Y}_{app}(t) = \mathbf{U}_u \exp(\mathbf{S}_u(t-T)), \\ &\mathbf{Y}_{p,app}(t) = \mathbf{Y}_0. \end{aligned} \tag{4.34}$$

4.5. **Numerical computations away from the equilibrium.** For $t > T$ the orbit $\mathbf{x}(t)$ lying in the unstable manifold can be found by numerical integration of equation (2.1) with the initial condition

$$\mathbf{x}(T) = \mathbf{x}_0 + \mathbf{U}_u\boldsymbol{\eta} \tag{4.35}$$

obtained from the approximation (4.9).

Sensitivity of the orbit is determined by the matrices $\mathbf{Y}(t)$ and $\mathbf{Y}_p(t)$, which can be evaluated numerically using equations (3.16) and (3.10). The initial conditions follow from approximations (4.34) as follows

$$\mathbf{Y}(T) = \mathbf{U}_u, \quad \mathbf{Y}_p(T) = \mathbf{Y}_0. \tag{4.36}$$

Solutions lying in the unstable manifold diverge from each other as we move away from the equilibrium. The rate of divergence is different in different directions; it depends on real parts of eigenvalues of the Jacobian matrix $\mathbf{F}(t)$. If the real parts of these eigenvalues differ strongly, the matrix $\mathbf{Y}(t)$ becomes ill-conditioned for large values of t. As a result, the numerical accuracy of the sensitivity estimate may be affected. This loss of accuracy can be minimized by utilizing the QR-decomposition of the matrix $\mathbf{Y}(t)$ as

$$\mathbf{Y}(t) = \mathbf{Q}(t)\mathbf{R}(t), \tag{4.37}$$

where $\mathbf{Q}(t)$ is an $m \times k$ orthogonal matrix satisfying the condition

$$\mathbf{Q}^T(t)\mathbf{Q}(t) = \mathbf{I}_k, \tag{4.38}$$

and $\mathbf{R}(t)$ is an upper-triangular $k \times k$ matrix [10]. The matrices $\mathbf{Q}(t)$ and $\mathbf{R}(t)$ are smooth functions of t.

The QR-decomposition is a practical tool for computing and storing ill-conditioned matrices: the ith column of the orthogonal matrix $\mathbf{Q}$ determines the direction for the difference between the ith column of the matrix under consideration and the linear span of its first $i-1$ columns, while the matrix $\mathbf{R}$ provides coordinates in the basis given by the columns of $\mathbf{Q}$. Working with the matrices $\mathbf{Q}$ and $\mathbf{R}$ instead of the original ill-conditioned matrix decreases the effect of numerical errors.

Substituting expression (4.37) into the first equation in (3.16) and differentiating the orthogonality condition (4.38) with respect to t, we obtain

$$\begin{aligned} \dot{\mathbf{Q}}\mathbf{R} + \mathbf{Q}\dot{\mathbf{R}} &= \mathbf{F}(t)\mathbf{Q}\mathbf{R}, \\ \dot{\mathbf{Q}}^T\mathbf{Q} + \mathbf{Q}^T\dot{\mathbf{Q}} &= \mathbf{0}. \end{aligned} \tag{4.39}$$

The first equality in (4.39) contains $m \times k$ independent equations. The second equality of (4.39) is obtained by differentiating the symmetric $k \times k$ matrix $\mathbf{Q}^T\mathbf{Q}$ and, hence, it contains $k(k+1)/2$ independent equations. The unknowns are $m \times k$ elements of the matrix $\mathbf{Q}$ and $k(k+1)/2$ elements of the upper-triangular matrix $\mathbf{R}$. It can be shown that implicit equations (4.39) can always be solved for derivatives. Hence, the matrices $\mathbf{Q}(t)$ and $\mathbf{R}(t)$ can be found by numerical integration of system (4.39). The initial conditions follow from (4.36) in the form

$$\mathbf{Q}(T) = \mathbf{U}_u, \quad \mathbf{R}(T) = \mathbf{I}_k. \tag{4.40}$$

5. Computation of connecting orbits

Let us consider two equilibria $\mathbf{x}_0^a$ and $\mathbf{x}_0^b$. An orbit tending to $\mathbf{x}_0^a$ as $t \to -\infty$ and tending to $\mathbf{x}_0^b$ as $t \to +\infty$ is called an orbit connecting $\mathbf{x}_0^a$ to $\mathbf{x}_0^b$. A connecting orbit is called heteroclinic if $\mathbf{x}_0^a \neq \mathbf{x}_0^b$ and homoclinic if $\mathbf{x}_0^a = \mathbf{x}_0^b$. The set of orbits connecting $\mathbf{x}_0^a$ to $\mathbf{x}_0^b$ represents the intersection of the unstable manifold $\mathcal{M}_u(\mathbf{x}_0^a)$ with the stable manifold $\mathcal{M}_s(\mathbf{x}_0^b)$. If $\mathcal{M}_u(\mathbf{x}_0^a)$ has dimension k^a and $\mathcal{M}_s(\mathbf{x}_0^b)$ has dimension k^b, then the dimension of the intersection is generically $k^a + k^b - m$, where m is the state space dimension. If $k^a + k^b - m \leq 0$, then connecting orbits may exist only for specific values of the parameter vector.

Let us consider a connecting orbit with a corresponding parameter vector as a curve in state-parameter space. Then a set of connecting orbits (intersection of the unstable and stable manifolds) in state-parameter space has dimension $k^a + k^b - m + n$, where n is the number of parameters. In particular, existence of a connecting orbit for at least one value of the parameter vector requires generically $n > m - k^a - k^b$ parameters. Homoclinic orbits require $n > m - k^a - k^b = 0$ and, hence, parameters are generally necessary to ensure the existence of a homoclinic orbit.

5.1. Approximation of the connecting orbit.

First, we consider heteroclinic orbits, when the equilibria $\mathbf{x}_0^a$ and $\mathbf{x}_0^b$ are different. Let $\mathbf{x}^a(t)$ and $\mathbf{x}^b(t)$ be the orbits belonging to the unstable manifold $\mathcal{M}_u(\mathbf{x}_0^a)$ and to the stable manifold $\mathcal{M}_s(\mathbf{x}_0^b)$, respectively. By Theorem 3.1, under perturbation of the parameter vector $\mathbf{p} = \mathbf{p}_0 + \varepsilon\mathbf{e}$, the orbits $\mathbf{x}^a(t)$ and $\mathbf{x}^b(t)$ change as follows

$$\begin{aligned} \tilde{\mathbf{x}}^a(t) &= \mathbf{x}^a(t) + \mathbf{Y}_p^a(t)\Delta\mathbf{p} + \mathbf{Y}^a(t)\hat{\boldsymbol{\xi}}^a + o(\varepsilon), \\ \tilde{\mathbf{x}}^b(t) &= \mathbf{x}^b(t) + \mathbf{Y}_p^b(t)\Delta\mathbf{p} + \mathbf{Y}^b(t)\hat{\boldsymbol{\xi}}^b + o(\varepsilon), \end{aligned} \tag{5.1}$$

where we introduced the vectors $\Delta\mathbf{p} = \varepsilon\mathbf{e}$, $\hat{\boldsymbol{\xi}}^a = \varepsilon\boldsymbol{\xi}^a$, and $\hat{\boldsymbol{\xi}}^b = \varepsilon\boldsymbol{\xi}^b$. Recall that the analysis of the orbit $\mathbf{x}^b(t)$ is carried out using the system (2.5) obtained by the reversal $t \to -t$, where the solution $\mathbf{x}^b(-t)$ lies in the unstable manifold of the equilibrium $\mathbf{x}_0^b$.

Let us consider a hyperplane

$$\mathbf{n}^T\mathbf{x} + a = 0, \tag{5.2}$$

where $\mathbf{n} \in \mathbb{R}^m$ and $a \in \mathbb{R}$, as a Poincaré section (typically, a finite part of the plane is used), and assume that the orbits $\mathbf{x}^a(t)$ and $\mathbf{x}^b(t)$ intersect this plane on opposite sides at the points $\mathbf{x}_P^a = \mathbf{x}^a(t_P^a)$ and $\mathbf{x}_P^b = \mathbf{x}^b(t_P^b)$; see Fig. 4. We assume that $t_P^a = t_P^b = t_P$, which can always be achieved by phase shift in one of the solutions.

The parameter vector $\mathbf{p}_{new} = \mathbf{p}_0 + \Delta\mathbf{p}$ for which the connecting orbit exists can be approximated using the condition that the perturbed orbits $\tilde{\mathbf{x}}^a(t)$ and $\tilde{\mathbf{x}}^b(t)$ coincide up to a phase shift in t. Without loss of generality, we assume that the perturbed orbits intersect the plane (5.2) at the same value of $t = t_P$. This requirement can be treated as a phase condition. Using the expressions (5.1) in the connection equation $\tilde{\mathbf{x}}^a(t_P) = \tilde{\mathbf{x}}^b(t_P)$ and the intersection condition (5.2) for the first orbit, we obtain the approximate equations

$$\mathbf{x}_P^a + \mathbf{Y}_p^a(t_P)\Delta\mathbf{p} + \mathbf{Y}^a(t_P)\hat{\boldsymbol{\xi}}^a = \mathbf{x}_P^b + \mathbf{Y}_p^b(t_P)\Delta\mathbf{p} + \mathbf{Y}^b(t_P)\hat{\boldsymbol{\xi}}^b, \tag{5.3}$$

$$\mathbf{n}^T(\mathbf{Y}_p^a(t_P)\Delta\mathbf{p} + \mathbf{Y}^a(t_P)\hat{\boldsymbol{\xi}}^a) = 0. \tag{5.4}$$

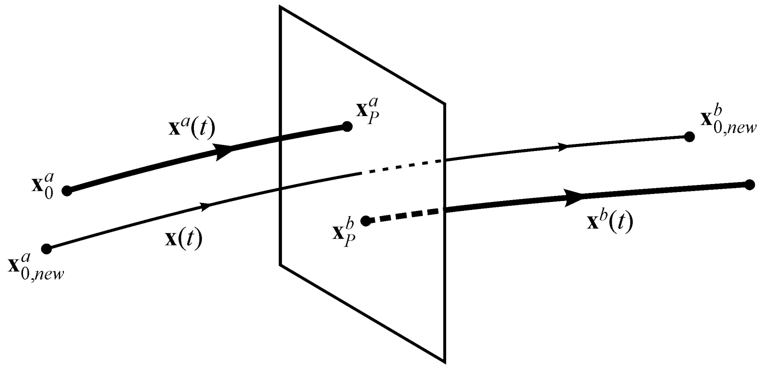

FIGURE 4. Numerical computation of a heteroclinic orbit.

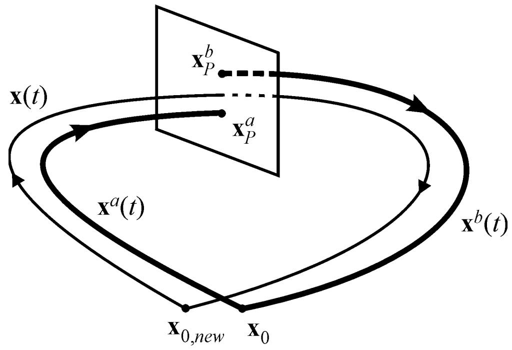

FIGURE 5. Numerical computation of a homoclinic orbit.

Notice that equations (5.3), (5.4) imply the intersection condition (5.2) for the second orbit as well.

System (5.3), (5.4) contains $m+1$ linear equations in $n+k^a+k^b$ unknown components of the vectors $\Delta\mathbf{p}$, $\hat{\boldsymbol{\xi}}^a$, and $\hat{\boldsymbol{\xi}}^b$. Hence, the solution of this system is a hyperplane of dimension $n+k^a+k^b-m-1$. Substituting solutions $\Delta\mathbf{p}$, $\hat{\boldsymbol{\xi}}^a$, and $\hat{\boldsymbol{\xi}}^b$ into expressions (5.1), we obtain the first order approximation of the intersection of $\mathcal{M}_u(\mathbf{x}_0^a)$ and $\mathcal{M}_s(\mathbf{x}_0^b)$ in state-parameter space. If $n=m+1-k^a-k^b$, equations (5.3), (5.4) generically have a unique solution, and there is a single connecting orbit. If $n>m+1-k^a-k^b$, a particular solution is singled out according to user choice of a specific connecting orbit.

In the homoclinic case the equilibria coincide, $\mathbf{x}_0^a=\mathbf{x}_0^b=\mathbf{x}_0$, see Fig. 5. The analysis of this case is identical to that for a heteroclinic orbit.

5.2. **Computer program.** The proposed approach was implemented in a computer program for finding connecting orbits in a multi-parameter autonomous system of ordinary differential equations. The m-dimensional space is visualized through several two-dimensional projections. The program automatically detects equilibria and evaluates orbits on stable and unstable manifolds. A specific orbit can be chosen by providing a reference point, where the orbit is likely to pass. Then this point is projected to the tangent space of the manifold to determine the value of the vector $\boldsymbol{\eta}$, see equation (4.9). The length of the approximate local part of the orbit is corrected to attain a required accuracy, see Subsection 4.3. The Poincaré section is implemented as a convex hull of m points (simplex with m vertices), e.g. it is a segment and triangle in two- and three-dimensional spaces, respectively. Manipulations of orbits and Poincaré section are done automatically as well as interactively using a flexible graphical user interface.

As soon as two orbits are chosen on stable and unstable manifolds intersecting the Poincaré section on opposite sides, Newton's method based on equations (5.3), (5.4) is applied to find a connecting orbit. If the difference $\|\mathbf{x}_P^a - \mathbf{x}_P^b\|$ is large, then a gradient method is used initially. At each iteration step, the vector $\Delta\mathbf{p}$ is used to update the parameter vector, and new reference points for two orbits are found from approximations (5.1). Recall that orbits (5.1) are determined up to phase shifts represented by the terms $c^a\mathbf{f}(\mathbf{x}^a(t))$ and $c^b\mathbf{f}(\mathbf{x}^b(t))$ ($c^a, c^b \in \mathbb{R}$), which are contained in the fundamental matrices $\mathbf{Y}^a(t)$ and $\mathbf{Y}^b(t)$, respectively. In the program, we choose these terms in such a way that the phase shifts at the reference points are minimized.

Note that the suggested method is convenient from the point of view of interaction with the user: changes in the parameters lead to prescribed changes in the phase portraits. Other advantages, related to the usage of Newton's and gradient methods, are high convergence speed, simplicity in numerical implementation, and accurate error control. The latter is especially important for application to the stability analysis of traveling waves, see [6]. Limitations are related to the local nature of the method.

5.3. **Example: computation of a traveling wave for a system of four viscous conservation laws.** Let us consider the system of partial differential equation for $\mathbf{w}(x,t)$, $-\infty < x < \infty$, $t \geq 0$ [14]:

$$\frac{\partial \mathbf{w}}{\partial t} + \frac{\partial \tilde{\mathbf{f}}(\mathbf{w})}{\partial x} = \frac{\partial}{\partial x}\left(\mathbf{D}(\mathbf{w})\frac{\partial \mathbf{w}}{\partial x}\right), \tag{5.5}$$

where the $m \times m$ viscosity matrix $\mathbf{D}(\mathbf{w})$ and the m-dimensional flux function $\tilde{\mathbf{f}}(\mathbf{w})$ are smooth functions of $\mathbf{w} \in \mathbb{R}^m$. Traveling waves for system (5.5) are given by heteroclinic orbits $\mathbf{x}(t)$ of the system of ordinary differential equations

$$\mathbf{D}(\mathbf{x})\dot{\mathbf{x}} = -\sigma(\mathbf{x} - \mathbf{x}_0) + \tilde{\mathbf{f}}(\mathbf{x}) - \tilde{\mathbf{f}}(\mathbf{x}_0), \tag{5.6}$$

such that the left state is $\mathbf{x}_0^a = \mathbf{x}_0$; the parameter σ represents the speed of the traveling wave. When the dimension k^a of the unstable manifold $\mathcal{M}_u(\mathbf{x}_0^a)$ and the dimension k^b of the stable manifold $\mathcal{M}_s(\mathbf{x}_0^b)$ are related as $k^a + k^b = m$, a connecting orbit appears at isolated values of σ that need to be determined numerically.

Let us investigate the problem of finding the traveling wave and the corresponding wave speed σ for a particular system of fourth order ($m = 4$), where

$$\mathbf{D}(\mathbf{x}) = \mathbf{I}, \quad \tilde{\mathbf{f}}(\mathbf{x}) = \begin{pmatrix} 0.01x_1 + 0.1x_2 + 0.02x_3 - 0.5x_1^2 + 0.5x_2^2 \\ -0.1x_1 + 0.01x_4 + x_1x_2 \\ -0.02x_2 - 0.12x_3 + 0.01x_4 + 0.2x_3x_4 \\ 0.01x_1 + 0.01x_3 + 0.11x_4 + 0.1x_1x_4 \end{pmatrix}, \tag{5.7}$$

and $\mathbf{x}_0 = (0.13, 0.07, 0.05, 0.02)^T$. The system has a single parameter $p = \sigma$. As an initial value we take $\sigma_0 = -0.01$. The second equilibrium is found numerically as $\mathbf{x}_0^b = (-0.168036, 0.128799, 0.045215, 0.055120)^T$.

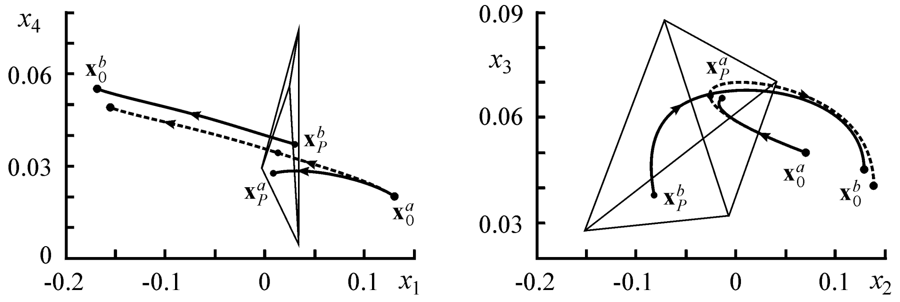

FIGURE 6. Initial orbits $\mathbf{x}^a(t)$ and $\mathbf{x}^b(t)$ (solid lines) and the heteroclinic orbit (dotted line).

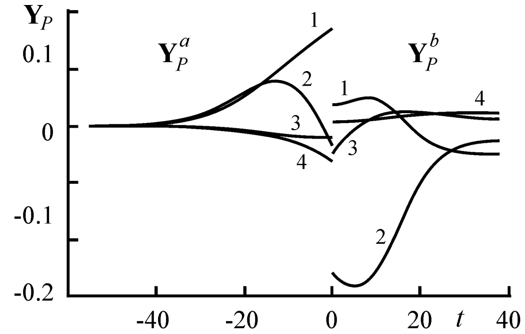

FIGURE 7. Sensitivity analysis of the orbits $\mathbf{x}^a(t)$ and $\mathbf{x}^b(t)$ lying in the unstable and stable manifolds.

The orbits on the stable and unstable manifolds are chosen using the computer program described above. They intersect the Poincaré section, which is given by four points that are vertices of the tetrahedron, see Fig. 6. In this figure the (x_1, x_4) and (x_2, x_3) projections are shown. Sensitivity analysis of these orbits provides the vectors $\mathbf{Y}_p^a(t)$ and $\mathbf{Y}_p^b(t)$ and the 4×2 matrices $\mathbf{Y}^a(t)$ and $\mathbf{Y}^b(t)$ describing the structure of the perturbed manifolds. Fig. 7 shows components of the vectors $\mathbf{Y}_p^a(t)$ and $\mathbf{Y}_p^b(t)$, where $t_P = t_P^a = t_P^b$ is set to zero. These vectors describe specific orbits on the perturbed manifolds. Solving equations (5.3), (5.4) yields the value $\Delta\sigma = -0.011196$, which is used to get a new corrected $\sigma = \sigma_0 + \Delta\sigma = -0.021196$.

Application of Newton's method implemented in the computer program yields a heteroclinic orbit $\mathbf{x}(t)$ after four iterations. All the computations were carried out using the absolute error bound $\varepsilon = 10^{-6}$. Table 1 gives the values of σ together with the distance $||\mathbf{x}_P^b - \mathbf{x}_P^a||$ between two orbits at the Poincaré section found at each iteration step. As a result, we obtain the value $\sigma = -0.025955$ for the wave speed corresponding to the heteroclinic orbit $\mathbf{x}(t)$. Each of the components of $\mathbf{x}(t)$ for $i = 1, 2, 3, 4$ are shown in Fig. 8. The same connecting orbit is given in Fig. 6 by the dotted line.

6. CONCLUSION

In this paper, we developed a constructive perturbation theory for orbits lying in stable and unstable manifolds of equilibria for autonomous systems of ordinary

Iteration number	σ	$\|\mathbf{x}_P^b - \mathbf{x}_P^a\|$
Initial state	-0.01	0.078619
1	-0.021196	0.024450
2	-0.025612	0.002195
3	-0.025954	3.836E-5
4	-0.025955	2.459E-7

TABLE 1. Results of Newton's iteration procedure for calculation of the heteroclinic orbit

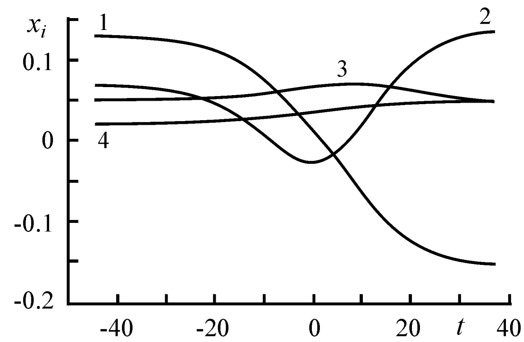

FIGURE 8. Traveling wave (heteroclinic orbit).

differential equations depending on several parameters. The sensitivity analysis with a simple and efficient error control is implemented numerically. As an application, we propose a new method for computing heteroclinic and homoclinic orbits; the method was tested in interactive computer software. The results of this paper are useful for parametric analysis in problems of applied mathematics and natural sciences modeled by systems of ordinary differential equations.

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