Efficient detection of periodic orbits in high dimensional systems

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Received 30 June 2005, revised 30 June 2005, accepted 30 June 2005

Key words unstable periodic orbits, Kuramoto-Sivashinsky equation.
Subject classification 04A25

This paper is concerned with developing a method for detecting unstable periodic orbits (UPOs) by stabilising transformations. Here the strategy is to transform the system of interest in such away that the orbits become stable. However, the number of such transformations becomes overwhelming as we move to higher dimensions [5, 16, 17]. We have recently proposed a set of stabilising transformations which is constructed from a small set of already found UPOs [1]. The real value of the set is that its cardinality depends on the dimension of the unstable manifold at the UPO rather than the dimension of the system. Here we extend this approach to high dimensional systems of ODEs and apply it to the model example of a chaotic spatially extended system – the Kuramoto-Sivashinsky equation.

1 Introduction

The following work is concerned with the detection of UPOs for large systems of ODEs of the form

$$\frac{dx}{dt} = f(x), \tag{1}$$

with $x \in \mathbb{R}^N$ and $f(x) \in \mathbb{R}^N$. Often Eq. (1) is the result of a spatial discretisation of a parabolic PDE. In this way dynamical system results can be applied to extended systems which exhibit chaos. Over the past twenty years the periodic orbit theory (POT) has been developed and successfully applied to low dimensional systems. Many dynamical invariants such as natural measure, Lyapunov exponents, fractal dimensions and entropies [14] can be determined via cycle expansions. It is an open question whether or not the POT has anything to say for spatially extended systems. It is thus an important numerical task to find UPOs for such systems in an attempt to answer this question. The model example of a spatiotemporally chaotic system is the Kuramoto-Sivashinsky equation (KSE), which was first studied in the context of reaction-diffusion equations by Kuramoto and Tsuzuki [11], whilst Sivashinsky derived it independently as a model for thermal instabilities in laminar flame fronts [20]. It is one of the simplest interesting PDEs to exhibit chaos and we have chosen it as a test case for the work that follows.

The problem of finding UPOs is essentially a root finding problem, thus a popular approach is to use some variant of Newton's method. Indeed, Zoldi and Greenside have reported the detection of 127 distinct UPOs for the KSE [23]. Here they solve for the discretised system using simple shooting with a damped Newton method to update each step. Another recent assault on the KSE by Cvitanović and Lan use variational methods [3, 12]. Here a suitable cost function is constructed so that its minimization leads to the detection of a UPO. The main problem however is that Newton type methods suffer from two major drawbacks: firstly, the basin size is essentially restricted to the linear neighborhood of any particular UPO and secondly, the method has no way of differentiating between true roots and local minima of the cost function. The latter drawback is one which increases significantly with dimension due to the complicated topology of multi-dimensional flows.

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The method of detecting UPOs by stabilising transformations [1, 5, 15, 16, 17] aims at transforming the system in such a way that its UPOs become stable. Unlike in the Newton-type methods, the transformations are linear and thus do not suffer from spurious convergence. When faced with the task of finding UPOs of a discrete system

$$x_{j+1} = F(x_j), \quad F : \mathbb{R}^N \to \mathbb{R}^N, \tag{2}$$

one can look instead at the related flow

$$\frac{dx}{ds} = g(x), \tag{3}$$

where $g(x) = F^p(x) - x$. It is straightforward to see that the period$-p$ points of the map are equilibrium points for the associated flow. With this setup we are able to stabilise all UPOs x^* of Eq. (2) such that all the eigenvalues of the Jacobian $DF^p(x^*)$ have real part smaller then one. In order to stabilise all possible UPOs we study the following flow

$$\frac{dx}{ds} = Cg(x), \tag{4}$$

where $C \in \mathbb{R}^{N \times N}$ is a constant matrix introduced in order to stabilise UPOs with the Jacobians that have eigenvalues with real parts greater than one. Given a set $\{C\}$ of such matrices, we have a family of differential equations which need to be solved in order to find all UPOs of Eq. (2). One example of such a set was proposed by Schmelcher and Diakonos (SD) [16]. It is the set $\mathcal{C}_{\text{SD}}$ of orthogonal matrices such that only one entry $\{\pm 1\}$ per row or column is nonzero. It has been verified that the set $\mathcal{C}_{\text{SD}}$ stabilise all hyperbolic fixed points for $N \leq 2$, and numerical evidence suggests the result holds for $N > 2$, but, thus far, no proof has been presented. However, if we wish to extend the stabilising transformation approach to higher dimensions, the set $\mathcal{C}_{\text{SD}}$ cannot be applied directly, since its size increases very rapidly with system dimension ($|\mathcal{C}_{\text{SD}}| = 2^N N!$).

For high dimensional systems with relatively few unstable directions, the method of stabilising transformations can be applied efficiently by restricting our attention to the unstable part of Eq. (2). Indeed, by constructing transformations which only alter the stability of the flow in Eq. (4) in the unstable subspace of DF^p, it is possible to reduce the number of transformations considerably. The authors have recently proposed a new set of matrices $\mathcal{C}$ based on the properties of a small already detected set of UPOs. Here the cardinality is $|\mathcal{C}| = 2^{n_u}$, where n_u is the dimension of the unstable manifold at x^*. This is the key to extending these ideas to spatially extended systems, since often in practice the systems of interest are such that $n_u \ll N$. For example, after a finite difference discretisation of the KSE [23] with resulting system of size $N = 100$, only four of the corresponding Lyapunov exponents are positive. Thus at each seed we would have only $|\mathcal{C}| = 16$ matrices as opposed to $|\mathcal{C}_{\text{SD}}| = 2^{99}99!$ if we used the SD matrices [1].

2 Subspace decomposition

In what follows we take our leave from the subspace iteration methods [13, 19], where the idea is to split the phase space into an unstable subspace $\mathbb{P}$

$$\mathbb{P} \quad = \quad \text{Span}\{\mathbf{u}_i \in \mathbb{R}^N | DF^p(x^*)\mathbf{u}_i = \lambda_i \mathbf{u}_i, |\lambda_i| > 1\}, \tag{5}$$

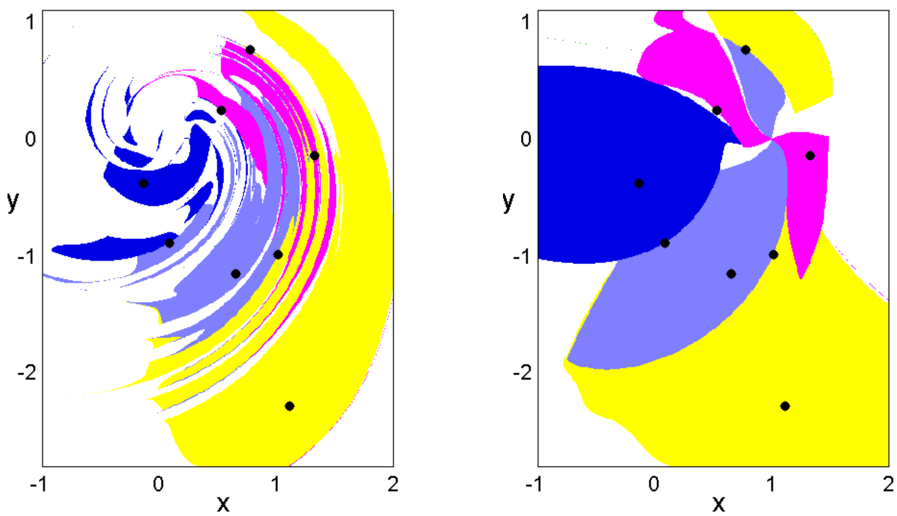
and its orthogonal complement $\mathbb{Q}$, so that any $x \in \mathbb{R}^N$ can be uniquely represented as $x = x_p + x_q$, where $x_p \in \mathbb{P}$ and $x_q \in \mathbb{Q}$. By decomposing Eq. (2) onto the respective spaces it is possible to apply Newton's method on the unstable subspace and fixed point iteration to its complement. As long as $n_u \ll N$ where n_u is the dimension of $\mathbb{P}$, this gives an efficient solver. However, primary concern of the work in [13, 19] is the continuation of branches of periodic orbits, where it is assumed that a reasonable approximation to a UPO is known. This is not a luxury which we share and we shall need to accommodate this into our extension of the method to Eq. (4).

If we define orthogonal projectors P and Q onto the respective subspaces

$$P \quad = \quad V_u V_u^{\mathsf{T}} \quad V_u \in \mathbb{R}^{N \times n_u}, \tag{6}$$

$$Q \quad = \quad I_N - P = V_s V_s^{\mathsf{T}}, \quad V_s \in \mathbb{R}^{N \times N - n_u}, \tag{7}$$

[1] Here we reduce the flow to a Poincaré surface of section in order to obtain a discrete system



(a) Schur decomposition (b) Singular value decomposition

Fig. 1 Basins of attraction for the period-3 orbits of the Ikeda map with parameter values $a = 1.0$, $b = 0.9$, $k = 0.4$ and $\eta = 6.0$. Here we have chosen $\tilde{C} = -1$ since in this example the unstable subspace is $1-$dimensional.

where I_N is the identity matrix and the columns of V_u and V_s are orthonormal vectors that span the spaces $\mathbb{P}$ and $\mathbb{Q}$ respectively, then Eq. (3) can be rewritten as

$$\frac{dp}{ds} = g_u(p,q), \quad (8)$$
$$\frac{dq}{ds} = g_s(p,q), \quad (9)$$

where $g_u = V_u^{\mathsf{T}} g$, $g_s = V_s^{\mathsf{T}} g$, $p = V_u^{\mathsf{T}} x$, $q = V_s^{\mathsf{T}} x$ and $x = V_u p + V_s q$. Thus we have replaced the original Eq. (3) by a pair of coupled equations, Eq. (8) of dimension n_u and Eq. (9) of dimension $N - n_u$. The usefulness of this splitting can be seen in the following lemma [13]

Lemma 2.1 *Let x^* be a fixed point of F^p and let the columns of V_u and V_s consist of the first n_u and remaining $N - n_u$ Schur vectors of $DF^p(x^*)$ ($x^* = V_u^{\mathsf{T}} p^* + V_s^{\mathsf{T}} q^*$). Then all the eigenvalues of*

$$\frac{\partial}{\partial q} g_s(p^*, q^*) = V_s^{\mathsf{T}} D g V_s \quad (10)$$

have negative real part.

From this lemma we see that it is only necessary to apply a stabilising transformation to Eq. (8) in order to converge to the UPO x^*. Therefore in order to stabilise all equilibrium points of Eq. (3) we elect to study:

$$\frac{dp}{ds} = \tilde{C} g_u(p,q), \quad (11)$$
$$\frac{dq}{ds} = g_s(p,q), \quad (12)$$

where $\tilde{C} \in \mathbb{R}^{n_u \times n_u}$ is a constant matrix.

In Lemma 2.1 the Schur decomposition is used in order to construct the projectors P and Q. This is fine for continuation problems since one may assume from the offset that they possess an initial condition x_0 sufficiently close to a UPO such that the Schur decomposition of $DF(x_0)$ gives a good approximation to the eigenspace

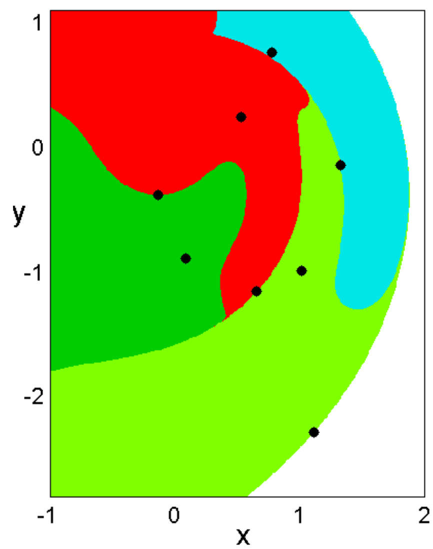


Fig. 2 The basins of attraction for the Ikeda map for the choice of $\tilde{C} = 1$. Fixed points of F^3 with negative unstable eigenvalues are stable stationary solutions of the associated flow, while those with positive eigenvalues are saddles located at the basin boundaries.

of $DF(x^*)$. However it is well known that the eigenvectors of the perturbed Jacobian $DF(x^* + \delta x)$ behave erratically as we increase δx. In order to enlarge the basins of attraction for the UPOs we propose that singular value decomposition (SVD) be used instead. That is we choose an initial condition x_0 and construct the SVD of its preimage i.e. $DF(F^{-1}(x_0)) = USW^{\mathsf{T}}$ (or in the continuous case $D\phi^T(\phi^{-T}(x_0)) = USW^{\mathsf{T}}$ for some time T), the columns of U give the stretching directions of the map at x_0, whilst the singular values determine whether the directions are expanding or contracting. It is these directions which we use to construct the projectors P and Q. Due to the robustness of the SVD we expect the respective basins of attraction to increase [2].

It is not necessary in practice to decompose Eq. (3) in order to to apply the new stabilising transformation. Rather we can express C in terms of $\tilde{C}$ and V_u. To see this we add V_u times Eq. (11) to V_s times Eq. (12) to get

$$\begin{aligned} \frac{dx}{ds} &= V_u \tilde{C} V_u^{\mathsf{T}} g(x) + V_s V_s^{\mathsf{T}} g(x), \\ &= [I_N + V_u(\tilde{C} - I_{n_u})V_u^{\mathsf{T}}]g(x), \end{aligned} \tag{13}$$

where the second line follows from Eq. (7). From this we see that the following choice of C is equivalent to the preceding decomposition

$$C = I_N + V_u(\tilde{C} - I_{n_u})V_u^{\mathsf{T}}. \tag{14}$$

Thus in practice we compute V_u and $\tilde{C}$ at the seed x_0 in order to construct C and then proceed to solve Eq. (4). The advantage of using the SVD rather than the Schur decomposition can be illustrated by the following example. Consider the Ikeda map [8]:

$$F\begin{pmatrix} x_{n+1} \\ y_{n+1} \end{pmatrix} = \begin{pmatrix} a + b(x_n cos(\phi) - y_n sin(\phi)) \\ b(x_n sin(\phi) + y_n cos(\phi)) \end{pmatrix}, \tag{15}$$

where $\phi = k - \eta/(1 + x^2 + y^2)$ and the parameters are chosen such that the map has a chaotic attractor: $a = 1.0$, $b = 0.9$, $k = 0.4$ and $\eta = 6.0$. For this choice of parameters the Ikeda map possesses eight period-3 orbit points (two period-3 orbits and two fixed points, one of which is on the attractor basin boundary). In our experiments

[2] The theory at present holds for Schur decomposition and it is an on going effort to formulate similar ideas for SVD. However numerical experiments using SVD have had considerable success.

we have covered the attractor for Eq. (15) with a grid of initial seeds and solved the associated flow for $p = 3$. This is done twice, firstly in the case where the projections P and Q are constructed via the Schur decomposition and secondly when they are constructed through the SVD. Since all orbits of the Ikeda map are of saddle type, the unstable subspace is one-dimensional and we need only two transformations: $C = 1$ and $C = -1$. Figure 1 shows the respective basins of attraction for the two experiments with $\tilde{C} = -1$. It can be clearly seen that the use of SVD corresponds to a significant increase in basin size compared to the Schur decomposition. Note that with $\tilde{C} = -1$ we stabilise four out of eight fixed points of F^3. The other four are stabilised with $\tilde{C} = 1$. The corresponding basins of attraction are shown in Figure 2. Note that for this choice of stabilising transformation the choice of basis vectors is not important, since Eq. (14) yields $C = I$, so that the associated flow is given by Eq. (3).

3 Stabilising transformations

There are several options for choosing the stabilising transformations $\tilde{C}$. One choice would be to apply the matrices of Schmelcher and Diakonos $\mathcal{C}_{\rm SD}$. With this new setup the numbers would be manageable for systems with up to two or three unstable directions. However numerical experiments have shown that many of the matrices in $\mathcal{C}_{\rm SD}$ are redundant. Thus it is useful to find a minimal subset $\mathcal{C}_{\rm Min} \subset \mathcal{C}_{\rm SD}$ such that all hyperbolic UPOs of a given N-dimensional system are stabilised by at least one of the elements of $\mathcal{C}_{\rm Min}$. Pingel *et al.* provide a non-rigorous approach to this problem in [15]. Here a candidate for the minimal set $\mathcal{C}_{\rm Min}$ is determined via a statistical approach. The idea is to construct a large ensemble of $N \times N$ matrices $\{A_i\}$ whose elements are chosen at random from the unit interval, then apply each of the $2^N N!$ stabilising transformations to each matrix A_i. The set $\mathcal{C}_{\rm Min}$ is then formed by retaining only those transformations which stabilise at least one matrix A_i.

Another possibility which has been successfully used by the authors in low dimensional systems ($N \leq 6$), is to construct stabilising transformations from the Jacobians of already found UPOs. Recall that any non-singular $N \times N$ matrix can be uniquely represented as a product

$$G = QB\,, \tag{16}$$

where Q is an orthogonal matrix and B is a symmetric positive definite matrix. Now for $N > 2$, we can always use the polar decomposition to construct a transformation that will stabilise a given fixed point. Indeed, if a fixed point x^* of an N-dimensional flow has a non-singular matrix $G \equiv Dg(x^*)$, then we can calculate the polar decomposition $G = QB$ and define

$$C = -Q^{\mathsf{T}}\,, \tag{17}$$

which will stabilise x^*. Moreover, as we have shown in our recent work [1], the same matrix C will also stabilise other UPOs with stability properties similar to those of x^*. In the scheme where already detected periodic orbits are used as seeds to detect other orbits [5], we can use C in Eq. (17) as a stabilising matrix for the seed x^* in order to detect other UPOs in its vicinity.

In the current work we use the following set $\tilde{\mathcal{C}} = \mathrm{diag}(\pm 1, \pm 1, \ldots, \pm 1)$ with cardinality $|\tilde{\mathcal{C}}| = 2^{n_u}$, which, according to our numerical experiments, is sufficient to stabilise most of the UPOs that have eigenvalues with both positive and negative real parts. Note that, as can be seen from Eq. (13), for every -1 in $\tilde{C}$, the transformation represents a Householder reflection in the plane normal to the corresponding vector v_u. Therefore, if an eigenvector corresponding to a positive eigenvalue is close to v_u, the transformation is likely to produce an associated flow with a negative eigenvalue along the corresponding direction. A more rigorous treatment of this argument is currently under investigation.

4 Implementation

A typical approach in the determination of UPOs for flows is via a Poincaré surface of section (PSS). By "clever" placement of an $N-1$ dimensional manifold in the phase space, the problem is reduced to a discrete map defined via intersections with the manifold. However, a correct choice of PSS is a challenging problem in itself. Due to the complex topology of a high dimensional phase space, the successful detection of UPOs will be highly dependent upon the choice of PSS. When the choice of a suitable PSS is not obvious *a priori* we found it preferable to work with the full flow, adding an auxiliary equation to determine the integration time T.

Let $x \mapsto \phi^T(x)$ define the flow map of the solution of Eq. (1). Similar to Eq. (4), we define the associated flow as follows:

$$\frac{dx}{ds} = C(\phi^T(x) - x). \tag{18}$$

The additional equation for T is defined in the following form

$$\frac{dT}{ds} = -\alpha f(\phi^T(x)) \cdot (\phi^T(x) - x), \tag{19}$$

such that T is always changing in the direction that decreases the distance $|\phi^T(x) - x|$. Here $\alpha > 0$ is a constant that controls the relative convergence speed of Eq. (19).

4.1 Numerical results

We have chosen the KSE for our numerical experiments. It is the simplest example of spatiotemporal chaos and has been studied in a similar context in [4, 12, 23], where the detection of many UPOs have been reported. We work with the KSE in the form

$$u_t = (u^2)_x - u_{xx} - \nu u_{xxxx}, \tag{20}$$

where $x \in [0, 2\pi]$ is the spatial coordinate, $t \in \mathbb{R}^+$ is the time and the subscripts x, t denote differentiation with respect to space and time. The viscosity parameter $\nu > 0$ determines the amount of dissipation present within the system. For values of $\nu > 1$ we have that $u(x, t) = 0$ is the global attractor for the system and the resulting long time dynamics are trivial. However, as ν is decreased the system undergoes a sequence of bifurcations leading to complicated dynamics (see for example [10]).

Our setup will be close to that found in [12]. Thus in what follows we assume periodic boundary conditions: $u(x, t) = u(x + 2\pi, t)$, and restrict our search to the subspace of antisymmetric solutions i.e. $u(2\pi - x, t) = -u(x, t)$. Due to the periodicity of the solution we can solve Eq. (20) using the psuedo-spectral method [7, 21]. Representing the function $u(x, t)$ in terms of its Fourier modes:

$$\hat{u}(k, t) = \frac{1}{2\pi} \int_0^{2\pi} u(x, t) e^{-ikx} dx, \quad u(x, t) = \sum_{k \in \mathbb{Z}} \hat{u}(k, t) e^{ikx}, \tag{21}$$

we arrive at the following system of ODEs:

$$\hat{u}_t(k, t) = (k^2 - \nu k^4)\hat{u}(k, t) + ik\widehat{u^2}(k, t). \tag{22}$$

Since KSE has a rapidly decaying Fourier spectrum we can restrict the system to a finite number of modes N and use the discrete Fourier transform instead of Eq. (21).

The search for UPOs is conducted within a rectangular region containing the chaotic invariant set. Initial seeds are obtained by integrating a random point within the region for some transient time. In order to build the stabilising transformations it is necessary to approximate the local stretching rates at the seed. Thus we solve the variational form [2] in addition to the flow each time we determine an initial seed.

Our experiments thus far have been carried out using Matlab. We use an exponential time differencing method (ETDRK4) due to Kassam and Trefethen [9] in order to solve the KSE and variational equations. Note that the method uses a fixed step-size ($h = 0.002$ in our calculations) thus it is necessary to use an interpolation scheme in order to integrate up to arbitrary times. In our work we have used cubic interpolation [22]. Since the resulting associated flow is typically stiff, we use Matlab routine `ode15s` [18]. In our calculations we have chosen the viscosity parameter $\nu = 0.015$, our system size is $N = 32$ and the positive constant $\alpha = 0.1$ in Eq. (19). Typically the associated flow converges to a UPO within approximately 150 integration steps with accuracy of about 10^{-7}. If the flow does not converge within 300 integration steps, we have found it more efficient to terminate the solver and re-start with a different stabilising transformation or a new seed. In our numerical experiments, about half

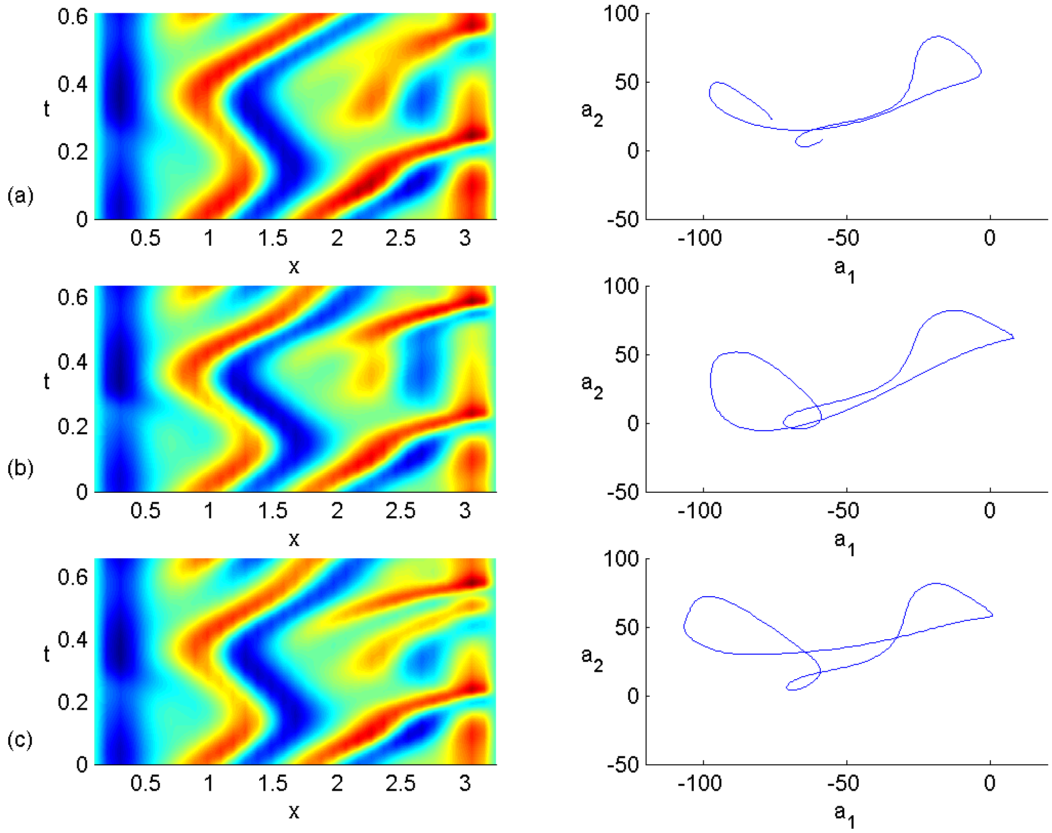


Fig. 3 Illustration of two UPOs of KSE detected from a single seed. We show both a level plot for the solutions and a projection onto the first two Fourier components where a $= \mathrm{Im}(\hat{u})$ denotes the fact that we restrict our search to the space of odd solutions: (a) Seed with time $T = 0.6110$, (b) a periodic solution of length $T = 0.6352$ detected with stabilising transformation $\tilde{C} = I_3$ and (c) a periodic solution of length $T = 0.6619$ detected with stabilising transformation $\tilde{C} = \mathrm{diag}(1, -1, 1)$.

of the seeds yielded UPOs, often converging to several different UPOs from the same seed, depending on the stabilising transformation used.

Figure 3 shows one of such cases, where Eqs. (18) and (19) are solved from the same seed for each of the 2^{n_u} stabilising transformations ($n_u = 3$ in this example), with two of them converging to two different UPOs. Figure 3a shows the level plot of the initial condition and a projection onto the first two Fourier components. Figures 3b and 3c show two unstable spatiotemporally periodic solutions which were detected from this initial condition, the first of period $T = 0.6352$ was detected using $\tilde{C} = I_3$, whilst the second of period $T = 0.6619$ was detected using $\tilde{C} = \mathrm{diag}(1, -1, 1)$. The ability to detect several orbits from one seed increases the efficiency of the algorithm.

5 Conclusions and further work

We have presented a scheme for detecting UPOs in high dimensional chaotic systems based upon the stabilising transformations proposed in [5, 16]. Due to the fact that one often wishes to study low dimensional dynamics embedded in a high dimensional phase space, it is possible to increase the efficiency of the stabilising transformations approach by restricting the construction of such transformations only to the low-dimensional unstable subspace. Following the approach often adopted in subspace iteration methods [13], we construct a decomposition of the tangent space into unstable and stable orthogonal subspaces. We find that the use of SVD to approximate the appropriate subspaces is preferable to that of Schur decomposition, which is usually employed within the subspace iteration approach. As illustrated with the example of the Ikeda map, the decomposition based on SVD is less susceptible to variations in the properties of the tangent space away from a seed and thus produce larger basins of attraction for stabilised periodic orbits. Within the low-dimensional unstable subspace, the number of useful stabilising transformations is relatively small, so it is possible to apply the full set of SD matrices. In fact, we have found that the subset of diagonal matrices of ± 1 is capable of locating a large number of UPOs, although more analysis will be carried out in the future to determine if it is possible to detect all types of UPOs with this subset.

The proposed method for detecting UPOs in high-dimensional dynamical systems has been tested on a 32-dimensional system of ODEs representing odd solutions of the Kuramoto-Sivashinsky equation in the weakly turbulent regime. We have been able to detect many UPOs using only the standard set of linear algebra tools and a stiff ODE solver available within the Matlab environment.

In conclusion, we have presented an extension of the stabilising transformations approach for locating periodic orbits in high-dimensional dynamical systems. Future work will concentrate on rigorous mathematical analysis of this approach in order to determine the range of its applicability. We will also work on the development, within the stabilising transformations approach, of an efficient strategy for systematic detection of periodic orbits in high-dimensional systems.

Acknowledgements We would like to thank Alexander Gorban for a fruitful discussion about the properties of tangent spaces. This work is supported by the EPSRC grant GR/S98986/01.

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