Extracting Qualitative Dynamics from Numerical Experiments [1]

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Extended Abstract

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1 INTRODUCTION

One central problem in Qualitative Physics is the qualitative prediction of long-time behavior of physical dynamic systems. The machinery developed for qualitative reasoning – qualitative state vector, quantity space, and limit analysis – are largely applicable to systems which are piecewise well-approximated by low-order linear systems or by first order nonlinear differential equations [3,4,13,12,9]. Nonlinear systems, in general, exhibit a far richer spectrum of dynamical behavior. Simple equilibrium points, periodic and quasiperiodic motion, limit cycles, chaotic motion as unpredictable as a sequence of coin tosses – these are some of the behavior found in a typical nonlinear system.

In this research, I therefore propose to look at dynamical systems – those typically encountered in Physics – to provide a new source of examples for investigation into the fundamental issues of descriptive language, style of reasoning, and representation techniques in qualitative reasoning about nonlinear dynamical systems. Specifically, I will consider two-dimensional discrete dynamical systems defined by area-preserving maps containing a single control parameter. The study of area-preserving map – transformation of the plane which preserves area – began with the venerable problem of the stability of the solar system. I choose to investigate this simplest non-trivial type of conservative system because many important problems in physics – the restricted 3-body problem, orbits of particles in accelerators, and two coupled nonlinear oscillators, just to mention a few – can be reduced to the study of area-preserving maps.

2 THE TASK

Given an one-parameter area-preserving map defining a discrete dynamical system, I am interested in describing the the complete qualitative dynamics of a nonlinear system over a large region of the phase space and parameter space. This is a fairly common problem in the physics literature. A good illustration of this task is provided by Henon's well-known paper, "Numerical Study of Quadratic Area-Preserving Mappings" [7]. The goal of Henon's paper is to provide a description of the main properties of the *quadratic map*:

$$\begin{aligned} x_{n+1} &= x_n \cos\alpha - (y_n - x_n^2)\sin\alpha \\ y_{n+1} &= x_n \sin\alpha + (y_n - x_n^2)\cos\alpha \end{aligned} \tag{1}$$

where x and y are the state variables, and α is the control parameter. The main results of Henon's paper are shown in Figures 1(a)-(f), which display the output of many numerical simulations.

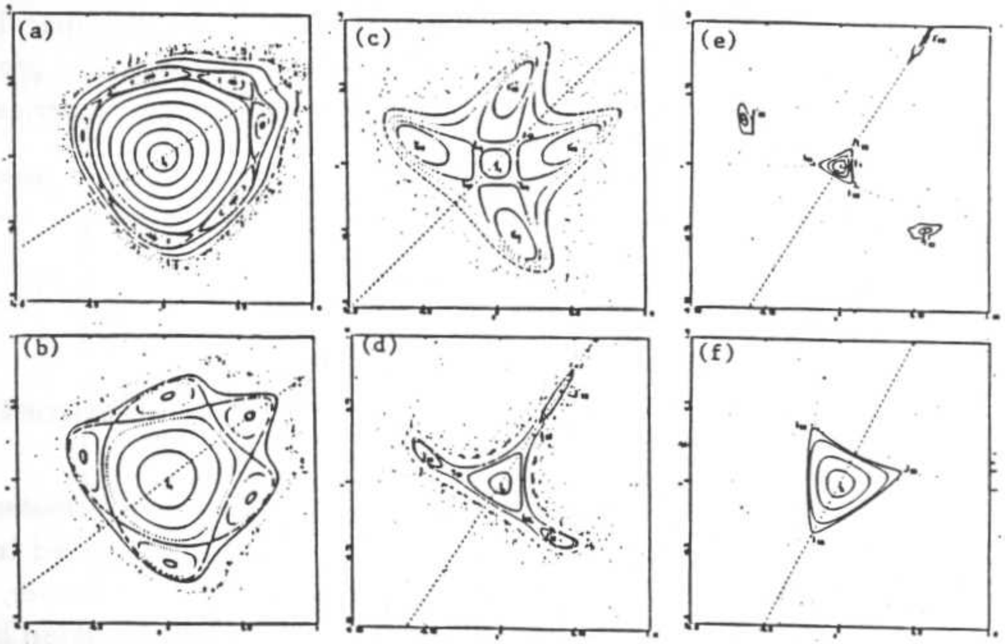

Figure 1: *A partial list of phase portraits from numerical experiments.* (a) $\alpha = 1.16$ (b) $\alpha = 1.33$ (c) $\alpha = 1.58$ (d) $\alpha = 2.0$ (e) $\alpha = 2.04$ (f) $\alpha = 2.21$. *Dashed line: axis of symmetry.*

To illustrate the vocabularies that a physicist uses to describe the qualitative behavior of nonlinear systems, we examine the following description of one of the phase portraits obtained from the results of numerical experiments with the *quadratic map* (see next section):

> *Figure 1a represents a number of trajectories (sequences of points) for* $\cos\alpha =$ 0.4 ... *a regular structure in a neighborhood of the elliptic fixed point at the origin, and farther away a chaotic zone. In many places the plotted points are so dense that they give the illusion of a continuous curve. Near the origin, the "curves" are almost circular. As we move outward, the curves become distorted. Just inside the outermost regular curve lies a chain of six closed curves, or "chain of islands". Successive points of a trajectory jump from one island to another by application of the mapping. Finally, as the curves become more distorted, there is a sudden break-up and the set of points no longer lies on a curve, but seems rather to fill a two-dimensional region.*

What is striking in this description is that the language is entirely geometric: it contains terms like *fixed point, continuous curve, chain of islands, two-dimensional region* etc. A goal of this research is to develop a clear understanding of the geometric language displayed in the above description. In particular, I want to understand how representation and reasoning techniques based on the geometric language can be used as a basis for a program to perform automatic numerical experiment control and interpretation.

3 WHAT IS THE KNOWLEDGE

3.1 Qualitative Dynamics and their Geometry

Restricted to a constant energy surface, a conservative system of two degrees of freedom has a 3-dimensional phase space. A torus is called **invariant** if an orbit starting at a point on the surface of the torus stays on it forever. Qualitatively, three special types of motion are important: (1) **periodic motion** lying on an invariant torus, (2) **quasiperiodic motion** that densely covers an invariant torus, and (3) **chaotic motion** that wanders in a 3-dimensional volume of the phase space.

If we take a 2-dimensional cross-section of the 3-dimensional flow, we have the following correspondence between special types of motion and their geometrical manifestations on the cross-section:

periodic motion	$\Longleftrightarrow$	periodic points
quasiperiodic motion	$\Longleftrightarrow$	invariant curve
chaotic motion	$\Longleftrightarrow$	chaotic region

3.2 Bifurcations: Qualitative changes in the phase portrait

Two phase portraits are **qualitatively equivalent** if there exists a homeomorphism between them which preserves fixed points, periodic points, invariant curves, and their stability. **Bifurcation** is said to occur when the dynamical system goes through a qualitative change in its phase portrait as the control parameter is varied. I will focus on one important type of bifurcation: appearance and disappearance of periodic orbits.

Meyer [10] gives a complete classification of the generic bifurcations of periodic points for one-parameter area-preserving maps. There are five types of generic bifurcation: (1) extremal, (2) transitional, (3) phantom 3-kiss, (4) phantom 4-kiss, and (5) emission. Because of space limitation, I only discuss the case of *phantom 3-kiss* as an illustration of what the bifurcation geometry is, and how it can help solve the control and interpretation problem.

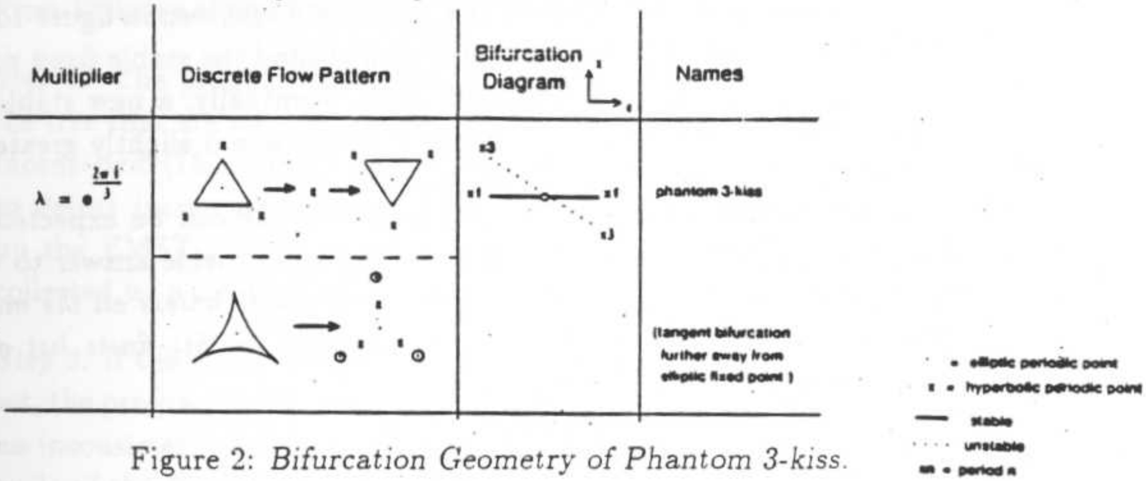

Figure 2: *Bifurcation Geometry of Phantom 3-kiss.*

Phantom 3-kiss occurs when the multiplier λ of the map is a cube root of unity. The region of stability of the elliptic fixed point shrinks to zero as the hyperbolic points of an unstable period-3 cycle "kiss" at the origin. After the "kiss", the fixed point turns elliptic again, and a new unstable period-3 cycle is emitted. Note the change in orientation of the *triangular* region around the elliptic point. The phantom 3-kiss is often preceded by extremal bifurcations in a region a bit further away from the original elliptic fixed point, resulting in the formation of a pair of elliptic and hyperbolic period-3 points.

4 APPROACH TO THE CONTROL PROBLEM

The **Control Problem** consists of three sub-problems: (1) How to start the numerical experiment? (2) How to decide what experiment to try next? and (3) How to decide when to terminate the experiments?

Elliptic fixed points are good places to start. We expect that the orbits near an elliptic fixed point, where the linear terms of the map dominate, will be mostly invariant curves. Knowing the generic bifurcation patterns is valuable for controlling numerical experiments. Once a given flow pattern is found to match some parts in our library of bifurcation geometries, it will give us strong evidence that the corresponding bifurcation exists, and we should be able to locate the rest of the flow patterns as given by the generic bifurcation. The pre-stored knowledge about these bifurcations gives us the complete information about what geometric objects, and approximately where in the control parameter space to look for.

To take an example, consider the *phantom 3-kiss* seen in figure 1d. According to the bifurcation pattern, the regular region around the stable fixed point will shrink in size, becoming an unstable fixed point; eventually, a new stable fixed point is born. So, we should expect to see figure 1f at some α slightly greater than two.

Besides imposing a strong constraint on what can be expected to happen in the phase portrait, the generic bifurcations also provide answer to the problem of termination: *a simulation experiment is incomplete unless all the major qualitative features in the phase portrait can be explained by this finite list of local generic bifurcations.*

5 SOLVING THE INTERPRETATION PROBLEM

The **Interpretation Problem** consists of the following sub-problems:

1. *Orbit Type.* How can one recognize the orbit type – a 0-dimensional finite point set whose elements are encountered repeatedly, a 1-dimensional smooth curve, or a 2-dimensional region – of a set of iterates?
2. *Clustering.* How can one determine the number of islands in an island chain? This number gives the period of the enclosing periodic point.
3. *Area and Centroid.* How can one estimate the centroid and area enclosed by the curve? The centroid is a good approximation of the location of the enclosing periodic point. The area gives a measure of saliency of the island chain.
4. *Shape.* How can one recognize the shape of the curve?

In the following, I will show how these four problems can be solved by applying techniques from computational geometry and computer vision. Euclidean minimal spanning tree (EMST) [11], and scale space image [14] – these are the two important data structures used by the interpretation program. The main processing steps are as follows.

- *Step 1.* The program computes a EMST from the input point set using the Prim-Dijkstra algorithm.
- *Step 2.* The program detects clusters in the EMST by looking for edges in the tree that are significantly longer than nearby edges. Such edges are called *inconsistent* [15]. The criterion of edge inconsistency suggested by Zahn is used to detect inconsistent edges. Inconsistent edges are then deleted, breaking up the EMST into connected sub-components. These sub-components are collected by a depth-first tree walk.
- *Step 3.* If the clustering procedure detects inconsistent edges in a given point set, the program concludes the point set represents an island chain. If, instead, no inconsistent edge is found, then the program examines the degree at each node of the EMST. For a smooth curve, the EMST consists of two terminal nodes of degree one; the rest, degree two. For a point set that fills an area, its corresponding EMST consists of many nodes having degree three or higher.
- *Step 4.* To compute the area and centroid of the region bounded by a curve, the program generates an ordered sequence of points from the EMST, and spline-interpolates the sequence to obtain a smooth curve. The smooth curve is encoded using chain coding [5]. Straightforward algorithms are then applied to compute the area and centroid.
- *Step 5.* A curve is parametrized by $C(s) = (x(s), y(s))$ where s is the arc length along the curve. The two functions x(s) and y(s) are computed from the chain code representation. Then, x(s) and y(s) are smoothed by the Gaussian and its first two derivatives of multiple spatial scales. Finally, the zero-crossings of the curvature function $\kappa(s)$, and the signs of $\dot{\kappa}(s)$ are computed to determine the locations and type of the extrema.

Appendix

The appendix is included as a reminder for some of the concepts and definitions of Dynamical Systems Theory. It should not be necessary for most of the reviewers to labor through this section.

A dynamical system consists of two parts: (1) the system state, and (2) the evolution law. The **system state** at any time t_0 is a minimum set of values of variables $\{x_1, \ldots, x_n\}$ which, along with the input to the system for $t \geq t_0$, is sufficient to determine the behavior of the system for all time $t \geq t_0$. The variables which define the system state are called **state variables**. The conceptual n-dimensional space with the n state variables as basis vectors is called the **phase space**. A **state vector** is a set of state variables considered as a vector in the phase space. As the system evolves with time, the state vector traces out a path in the phase space; the path is called an **orbit** or a **trajectory**. Finally, a **phase portrait** is a partition of the phase space into orbits.

The **evolution law** determines how the state vector evolves with time. In a finite dimensional discrete time system, the evolution law is given by difference equations. The difference equation is specified by a function $f : X \rightarrow X$ where X is the phase space of the discrete system. The function f which defines a discrete dynamical system is called a **mapping**, or a **map**, for short. The **multipliers** of the map f are the eigenvalues of the Jacobian of f. An **area-preserving map** is a map whose Jacobian has a unit determinant.

The set of iterates of f, $\{ f^n(x) \mid n \in Z \}$, is called the **orbit of x relative to f**; it captures the **history** of x as f is iterated.

Two types of point have the simplest histories – fixed point, and periodic point. The point x is a **fixed point** of f if f(x) = x. A fixed point x is called **stable**, or **elliptic**, if all the multipliers of f at x lie on the unit circle; it is called **unstable**, or **hyperbolic**, otherwise. The point x is a **periodic point** of period n if $f^n(x) = x$. The least positive n for which $f^n(x) = x$ is called the period of x. The set of all iterates of a periodic point forms a **periodic orbit**.

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