Automatic classification of global dynamics in multi-parameter systems

Paweł Pilarczyk

Between Theory and Applications – Mathematics in Action
Będlewo, May 25–30, 2015

Abstract

This document contains a concise introduction to the computational method developed by the author with his collaborators for automatic classification of global dynamics in multi-parameter dynamical systems with discrete or continuous time.

1 Introduction

A dynamical system is a mathematical concept for describing an object varying in time, using a fixed rule that depends on the current state of the object (and not on its past). Dynamical systems can be used to describe a variety of phenomena, such as the growth of a population or spreading of an infectious disease.

In this concise note, I am going to introduce a framework for automatic classification of global dynamics in a dynamical system depending on a few parameters (such as fertility rates or disease transmission rates). A set-oriented topological approach is used, based on Conley's idea of a Morse decomposition (see [5]), combined with rigorous numerics, graph algorithms, and computational algebraic topology. This approach allows to effectively compute outer estimates of all the recurrent dynamical structures encountered in the system (such as equilibria or periodic solutions), as perceived at a prescribed resolution. It thus provides an automatic computational method for concise and comprehensive classification of all the dynamical phenomena found across the given parameter ranges. The method is mathematically rigorous (a.k.a. computer-assisted proof), and has a potential for wide applicability thanks to the mild assumptions on the system.

The method was introduced in [1], where an application to a 2-dimensional discrete-time dynamical system is thoroughly discussed. Additional description of the method and other applications are provided in [2]. This method was applied to some nonlinear population models [1, 2], to a population model with harvesting [8], to a theoretical physics model of plasma confinement transitions [17], to an epidemic model of infectious disease spreading in two locations connected by transportation [7], and some other dynamical systems [2]. In each of the applications, the method provided additional information that complemented analytical results and numerical simulations.

2 Preliminaries

Let $\mathbb{T} = \mathbb{Z}$ or $\mathbb{T} = \mathbb{R}$. Let $\varphi\colon \mathbb{R}^n \times \mathbb{T} \ni (x, t) \mapsto \varphi_t(x) \in \mathbb{R}^n$ be a *dynamical system*; that is, for all x, t_1, t_2, we have $\varphi(x, 0) = x$ and $\varphi(\varphi(x, t_1), t_2) = \varphi(x, t_1 + t_2)$. If $\mathbb{T} = \mathbb{R}$ then we call φ a *continuous-time dynamical system* (or a *flow* for short), and if $\mathbb{T} = \mathbb{Z}$ then we call it a *discrete-time dynamical system*.

Note that in the case of discrete time, if the dynamics is induced by a map that is not invertible then backward orbits need not be always defined. Formally, such a system is called a *semidynamical system*, but in order to simplify the terminology and avoid some technical difficulties, this note is written for dynamical systems, even though the theory and algorithms discussed here apply also to semidynamical systems.

A set S is called an *invariant set* with respect to φ if $\varphi(S, \mathbb{T}) = S$. The *invariant part* of a set N, denoted Inv$N$, is the largest, in terms of inclusion, invariant set contained in N. The set N is called an *isolating neighborhood* if N is compact and Inv$N \subset$ int$N$, where int$N$ denotes the interior of N. S is called an *isolated invariant set* if $S =$ Inv$N$ for some isolating neighborhood N.

A *Morse decomposition* (see [5]) of an isolated invariant set X (note that X may be the entire phase space) with respect to φ is a finite collection of disjoint isolated invariant subsets $S_1, \ldots, S_q$ of X (called *Morse sets*) with a strict partial ordering $\prec$ on the index set $\{1, \ldots, q\}$ such that for every $x \in X \setminus (S_1 \cup \cdots \cup S_q)$ and for every orbit $\{\gamma_t\}_{t\in\mathbb{T}}$ such that $\gamma_0 = x$ there exist indices $i \prec j$ such that $\gamma_t \to S_i$ as $t \to \infty$ and $\gamma_t \to S_j$ as $t \to -\infty$.

A *rectangular set* is a product of compact intervals. Given a rectangular set $R = [a_1, a_1 + \delta_1] \times \cdots \times [a_n, a_n + \delta_n] \subset \mathbb{R}^n$ and integer numbers $s_1, \ldots, s_n > 0$, we call the following set an $s_1 \times \cdots \times s_n$ *uniform rectangular grid in* R:

$$\mathcal{G}_{s_1,\ldots,s_n}(R) := \left\{ \prod_{i=1}^{n} [a_i + \frac{j_i}{s_i}\delta_i, a_i + \frac{j_i+1}{s_i}\delta_i] : \right. \\ \left. j_i \in \{0,\ldots,s_i-1\}, i \in \{1,\ldots,n\} \right\}$$

The individual boxes in the grid are indexed by the n-tuples $(j_1,\ldots,j_n)$.

3 The Case of a Discrete-Time Dynamical System

Consider an m-parameter family of discrete-time (semi)dynamical systems in $\mathbb{R}^n$:

$$\varphi\colon \mathbb{R}^n \times \mathbb{R}^m \times \mathbb{Z} \ni (x,p,t) \mapsto \varphi_t^p(x) \in \mathbb{R}^n.$$

Let $B \subset \mathbb{R}^n$ and $P \subset \mathbb{R}^m$ be rectangular sets.

The computational method introduced in [1] provides a finite resolution description of global dynamics exhibited by the system across the provided ranges P of the parameters. In particular, the family of sets $N_1,\ldots,N_q \subset B$ is constructed with some strict partial ordering $\prec$ on $\{1,\ldots,q\}$, such that for each $p \in \hat{p}$, each set N_i, $i = 1,\ldots,q$, is an isolating neighborhood in B, and whenever a possibility of the existence of an orbit from N_i to N_j is detected, the relation $N_j \prec N_i$ is set to hold true. The family $\{S_i := \text{Inv}N_i : i = 1,\ldots,q\}$ forms a Morse decomposition of $\text{Inv}B$ with respect to φ^p with the ordering $\prec$, where $\varphi^p = \varphi(\cdot,p,\cdot)$ indicates the dynamical system φ with the parameter fixed to p. The sets N_i are constructed as unions of closed boxes with respect to the $d_1 \times \cdots \times d_n$ uniform rectangular grid in B. The union $N_1 \cup \cdots \cup N_q$ contains all the chain recurrent dynamics present in B. The collection $N_1,\ldots,N_q$ is called a *numerical Morse decomposition*, and the isolating neighborhoods $N_1,\ldots,N_q$ are called *numerical Morse sets*. Note that if N_i touches the boundary of B for some i then it is not known if N_i is an isolating neighborhood in the entire phase space X, so caution should be taken when drawing conclusions from such a construction.

A numerical Morse decomposition can be schematically depicted as a directed graph whose vertices correspond to the Morse sets and edges indicate possible connecting orbits between them. In order to simplify such a representation, one can plot the transitive reduction of this graph, as it is typically done in the presentation of the results.

The *Conley index*, introduced by Conley [5] for flows, and generalized, e.g., by Mrozek [12] and Szymczak [19] to discrete semidynamical systems induced by continuous maps, is a topological invariant that provides information about isolated invariant sets. Its homological version is algorithmically computable (to certain extent) from an isolating neighborhood and an outer estimate of the map, like those computed by the method being described. This index takes into account the *exit set* of an isolating neighborhood N, that is, the part of the forward image of N that sticks out of N, and thus reflects the stability of what N contains.

The knowledge of the Conley index of an isolating neighborhood N allows to draw conclusions on the invariant part of N. In particular, if the index of N is nontrivial then $\mathrm{Inv}N \neq \emptyset$. The index can also be used to prove the existence of periodic orbits or more complicated dynamics.

The Conley index and the relation of the forward image of N with respect to N can be used to classify each computed isolating neighborhood N on the basis of its stability. We say that an isolating neighborhood N is *attracting* if the forward image of N is entirely contained in N. One can prove that then N contains a local attractor, which justifies this terminology. Otherwise, if the forward image of N is not fully contained in N, we say that N is *unstable*. If N has the Conley index of a hyperbolic fixed point with d-dimensional unstable manifold then we say that N *is of the type* of the corresponding point. For a typical system, it is likely that N indeed contains an equilibrium of the expected stability, but—since the Conley index is a purely topological tool and does not provide information about derivatives—the dynamics in N may turn out to be much more complicated than seen from outside (that is, from the perspective of the isolating neighborhood). If $N \subset \mathbb{R}^n$ is of the type of a fixed point with n-dimensional unstable manifold then we say that N is *repelling*. Obviously, other types of indices are possible; for example, the index of a periodic trajectory differs from the index of any fixed point.

Since detailed introduction to the Conley index is beyond the scope of this note and requires certain knowledge of algebraic topology, we refer the reader to [5, 12, 19] for more details on the Conley index, and to [6, 10, 18] and references therein for discussion of some technical aspects of the method for the computation of this index implemented in the software used in the software provided at [16].

One of the volatile features of the method is that the Conley index cannot be computed in certain cases, for example, if the constructed isolating neighborhood touches the boundary of B. This is because in a typical situation we may not know if the chosen set B is indeed an isolating neighborhood (and in fact it is not in many cases). Therefore, one can only be sure that $N_i \subset B$ is an isolating neighborhood if actually $N_i \subset \mathrm{int}B$. In fact, this problem is one of the reasons for why the Conley index cannot be computed in many cases, and this happens especially for the origin, which is often an isolating neighborhood but lies at the boundary of B, e.g., in biological models, where it is normally assumed that the size of the population is non-negative.

4 The Case of a Flow

Now consider an m-parameter family of flows on $\mathbb{R}^n$:

$$\varphi \colon \mathbb{R}^n \times \mathbb{R}^m \times \mathbb{R} \ni (x, p, t) \mapsto \varphi_t^p(x) \in \mathbb{R}^n.$$

Let $B \subset \mathbb{R}^n$ and $P \subset \mathbb{R}^m$ be rectangular sets.

In order to apply the method for automatic analysis of global dynamics to a continuous-time dynamical system (a flow) induced by an ODE, it is natural to consider a time-τ map for some fixed $\tau > 0$, and to conduct the computations for the discrete-time dynamical system induced by this map. Namely, let $\tau > 0$, and consider the m-parameter discrete-time dynamical system φ_τ obtained by restriction of φ to $\mathbb{R}^n \times \mathbb{R}^m \times \tau\mathbb{Z}$. Let $d_1, \ldots, d_n$ and $s_1, \ldots, s_m$ be positive integers. For each parameter box $\hat{p} \subset P$ in the $s_1 \times \cdots \times s_m$ uniform rectangular grid in P, and for each box b in the $d_1 \times \cdots \times d_n$ uniform rectangular grid in B, one can use the CAPD software library [4] to compute a rigorous outer estimate for $\varphi(b, \hat{p}, \tau)$. In this way, we apply the computational method introduced in [1] to φ_τ.

The following theorem justifies this approach, as it shows that the results obtained from the computations conducted for the time-τ map are valid for the flow, too.

Theorem 4.1 (see [7, §5.2])**.** *Let φ be a flow on $\mathbb{R}^n$. Let $\tau > 0$. Let $B \subset \mathbb{R}^n$ be an isolating neighborhood with respect to φ_τ. Assume that $N_1, \ldots, N_k \subset B$ are some isolating neighborhoods for φ_τ, with pairwise disjoint interiors. Assume that $\mathbb{M} := \{M_i := \mathit{Inv} N_i \mid i = 1, \ldots, k\}$ is a Morse decomposition of Inv(B, φ_τ) with respect to φ_τ. Then $N_1, \ldots, N_k$ are isolating neighborhoods for φ, and $\mathbb{M}$ is a Morse decomposition of Inv(B, φ) with respect to φ. Moreover, if there exists a connecting orbit in B for φ between some of the Morse sets then there exists a connecting orbit in B for φ_τ between the same Morse sets.*

Note that in this theorem there is no one-to-one correspondence between objects computed for the time-τ map and the flow, it only says about one direction of implication. In particular, an isolating neigborhood for the flow need not be an isolating neighborhood for the time-τ map. Moreover, there might exist a connecting orbit for φ_τ in B with no corresponding connecting orbit for φ in B.

We remark that the Conley indices with respect to the flow φ can be instantly obtained from those computed when considering φ_τ.

Choosing an optimal value of $\tau > 0$ is not a trivial task. In fact, in our approach, we use a heuristic method which chooses a supposedly good $\tau > 0$ by trial and error: τ is initially chosen quite arbitrarily, and then increased if possible or decreased if it yields too high overestimates in the computation of outer enclosures of the images of grid elements by φ_τ.

5 Application of the Method to a Specific System

The input to the rigorous set-oriented numerical method applied to a specific dynamical system consists of the data listed below.

(I1) A procedure for computing outer bounds for images of arbitrary boxes (cartesian products of intervals) under the dynamical system for all the parameters in the ranges provided at the time of the computation. If a formula for the map is known (in the case of a discrete-time dynamical system) then this can be easily done by means of using simple interval arithmetic. If an ODE that generates the flow is known and is given by an elementary formula then one can use a wrapper provided in the software which requires providing the formula for the right-hand side of the ODE.

(I2) The ranges of the parameters that are varying in the computations. The cartesian product of these ranges will be further denoted by P.

(I3) The phase space bounding box that contains all the asymptotic dynamics of our interest.

(I4) The resolutions in the parameter space and in the phase space, which are given by the numbers of subintervals into which each of the parameter intervals is going to be subdivided uniformly, and also a subdivision depth $d > 0$ for the phase space. Note that in the software, the phase space is subdivided uniformly into 2^d subintervals in each direction.

In addition to this initial data, there are also several technical parameters, such as a suggestion for τ in case of working with an ODE. All of these technicalities can be easily found in the software available at [16].

The computations can be run at a computer cluster in a convenient way, using a flexible dynamic parallelization scheme introduced in [15], which is built into the software.

The output of the computations consists of the following information:

(O1) Classes of parameters for which the qualitative global dynamics is equivalent. These classes are given as subsets of P, built of the boxes into which P was subdivided.

(O2) For each parameter box, selected information about the computed numerical Morse decomposition: the number of the sets, their sizes (in terms of the number of boxes), their Conley indices (whenever it was possible to compute them), and information on the detected possible connecting orbits.

(O3) [optionally] A 2D projection of the phase space portrait of the sets of which the numerical Morse decomposition is composed. The projection is done onto two preselected variables. This form of output is optional, because the amount of the data can be overwhelming.

References

[1] Z. Arai, W. Kalies, H. Kokubu, K. Mischaikow, H. Oka, P. Pilarczyk, A database schema for the analysis of global dynamics of multiparameter systems, SIAM J. Appl. Dyn. Syst. 8 (2009) 757–789.

[2] J. Bush, M. Gameiro, S. Harker, H. Kokubu, K. Mischaikow, I. Obayashi, P. Pilarczyk, Combinatorial-topological framework for the analysis of global dynamics, Chaos, Vol. 22, No. 4 (2012) 047508.

[3] Computational Homology Project Software, Rutgers University, http://chomp.rutgers.edu/software/.

[4] Computer Assisted Proofs in Dynamics, Jagiellonian University, http://capd.ii.uj.edu.pl/.

[5] C. Conley, Isolated invariant sets and the Morse index, CBMS Regional Conference Series in Math., no. 38, Amer. Math. Soc., Providence, RI (1978).

[6] S. Harker, H. Kokubu, K. Mischaikow, P. Pilarczyk, Inducing a map on homology from a correspondence, Trans. AMS, accepted.

[7] D.H. Knipl, P. Pilarczyk, G. Röst, Rich bifurcation structure in a two-patch vaccination model, SIAM J. Appl. Dyn. Syst., accepted.

[8] E. Liz, P. Pilarczyk, Global dynamics in a stage-structured discrete-time population model with harvesting, J. Theoret. Biol., Vol. 297 (2012) 148–165.

[9] S. Luzzatto, P. Pilarczyk, Finite resolution dynamics, Foundations of Computational Mathematics 11 (2011) 211–239.

[10] K. Mischaikow, M. Mrozek, P. Pilarczyk, Graph approach to the computation of the homology of continuous maps, Foundations of Computational Mathematics 5 (2005) 199–229.

[11] R.E. Moore, Interval analysis, Prentice-Hall, Inc., Englewood Cliffs, N.J. (1966).

[12] M. Mrozek, Leray functor and cohomological Conley index for discrete dynamical systems, Trans. Am. Math. Soc. 318 (1990) 149–178.

[13] M. Mrozek, The Conley index on compact ANR's is of finite type, Results in Mathematics 18 (1990) 306–313.

[14] P. Pilarczyk, Computer assisted method for proving existence of periodic orbits, Topol. Methods Nonlinear Anal. 13 (1999) 365–377.

[15] P. Pilarczyk, Parallelization method for a continuous property, Foundations of Computational Mathematics 10 (2010) 93–114.

[16] P. Pilarczyk, Conley-Morse Graphs Computation Software, http://www.pawelpilarczyk.com/cmgraphs/.

[17] P. Pilarczyk, L. García, B. A. Carreras, I. Llerena, A dynamical model for plasma confinement transitions, J. Phys. A: Math. Theor., Vol. 45, No. 12 (2012) 125502.

[18] P. Pilarczyk, K. Stolot, Excision-preserving cubical approach to the algorithmic computation of the discrete Conley index, Topology Appl. 155 (2008) 1149–1162.

[19] A. Szymczak, The Conley index for discrete semidynamical systems, Topology Appl. 66 (1995) 215–240.