Title: Computational Proofs in Dynamics

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Dynamics

The origins of dynamics lie in the study of solutions of initial value problems for systems of differential equations. The seminal work of Poincaré in the late 1800s made clear that given the complexity of these systems they could best be understood by studying the qualitative structure of sets of solutions. The explosion of interest starting in the 1960s in nonlinear systems is due to the advent of the computer that allows researchers to easily observe the breadth of dynamic behavior that can be realized. Typically, the computer is the only tool for studying specific systems, and thus the ability to provide computational proofs concerning the existence and structure of the qualitative properties of dynamical systems has particular relevance.

To put the computational challenges in perspective we begin by describing the mathematical framework for the qualitative theory of dynamics. Solutions to an ordinary differential equation $\dot{x} = V(x, \lambda)$ defined on a state space X and parameter space Λ are described via a *flow*, which is a continuous function $\varphi\colon \mathbb{R} \times X \times \Lambda \to X$ satisfying $\varphi(0, x, \lambda) = x$ and $\varphi(s, \varphi(t, x, \lambda), \lambda) = \varphi(s + t, x, \lambda)$. Since parameters are typically assumed to be fixed, given $\lambda \in \Lambda$ one restricts attention to $\varphi_\lambda(t, x) := \varphi(t, x, \lambda)$. Observe that if one samples at fixed rate of time $T > 0$, then the dynamics appears as if it is generated by a continuous parameterized family of maps $f_\lambda(\cdot) := \varphi_\lambda(T, \cdot)\colon X \to X$. From a computational perspective this latter approach is often more useful and thus we use this framework for most of our presentation. If the dynamics is generated by a partial or functional differential equation then in general one cannot expect $f_\lambda\colon X \to X$ to be invertible. In practice this has limited conceptual consequences, but can significantly increase the technical challenges, thus we assume that f is a homeomorphism.

A set $S \subset X$ is *invariant* under f if $f(S) = S$. These are the fundamental objects of study. While general invariant sets are too complicated to be classified, there are well understood invariant sets which can be used to describe many aspects of the dynamics. A point $x \in X$ is a *fixed point* if $f(x) = x$. It is a *periodic point* if there exits $N > 0$ such that $f^N(x) = x$. The associated invariant set $\{f^n(x) \mid n = 1, \ldots, N\}$ is called a *periodic orbit*. Similarly, $x \in X$ is a *heteroclinic point* if $\lim_{n\to\pm\infty} f^n(x) = y^\pm$ where $y^\pm$ are distinct fixed points. If $y^+ = y^-$, then x is a *homoclinic point*. Again, the complete set $\{f^n(x) \mid n \in \mathbb{Z}\}$ is a *heteroclinic* or *homoclinic orbit*.

Because they are both mathematically tractable and arise naturally *invariant manifolds* play an important role. For example, periodic orbits for flows form invariant circles and integrable Hamiltonian systems give rise to invariant tori. If $\bar{x}$ is a *hyperbolic* fixed point; that is the spectrum of $Df(\bar{x})$ does not intersect the unit circle in the the complex plane, then the sets $W^s(\bar{x}) := \{x \in X \mid \lim_{n\to\infty} f^n(x) = \bar{x}\}$ and $W^u(\bar{x}) := \{x \in X \mid \lim_{n\to-\infty} f^n(x) = \bar{x}\}$ are immersed manifolds called the *stable* and *unstable manifolds*, respectively. The concept of stable and unstable manifolds extends to hyperbolic invariant sets [41].

Cantor sets also play an important role. *Subshifts on finite symbols* arise as explicit examples of invariant sets with complicated dynamics. For a positive integer K, let $\Sigma = \{k \mid k = 0, \ldots, K-1\}^{\mathbb{Z}}$ with the product topology and consider the dynamical system generated by $\sigma\colon \Sigma \to \Sigma$ given by $\sigma(\mathbf{a})_j = a_{j+1}$. Observe that if A be a $K \times K$ matrix with $0, 1$ entries and $\Sigma_A := \left\{\mathbf{a} = \{a_j\} \in \Sigma \mid A_{a_j, a_{j+1}} \neq 0\right\}$, then Σ_A is an invariant set for σ. If the spectral radius $\rho(A)$ of the matrix A is greater than one then the invariant set Σ_A is said to be *chaotic*. In particular, it can be shown that Σ_A contains infinitely many periodic, heteroclinic, and homoclinic orbits and furthermore one can impose a metric d on Σ compatible with the product topology such that given distinct elements $\mathbf{a}, \mathbf{b} \in \Sigma_A$ there exists $n \in \mathbb{Z}$ such that $d(\sigma^n(\mathbf{a}), \sigma^n(\mathbf{b})) \geq 1$. *Topological entropy* provides a measure of how chaotic an invariant set is. In the case of subshift dynamics the entropy is given by $\ln(\rho(A))$.

Given that the focus of dynamics is on invariant sets and their structure, the appropriate comparison of different dynamical systems is as follows. Two maps $f\colon X \to X$ and $g\colon Y \to Y$ generate *topologically conjugate* dynamical systems if there exists a homeomorphism $h\colon X \to Y$ such that $h \circ f = g \circ h$. Returning to the context of a parameterized family of dynamical systems $\lambda_0 \in \Lambda$ is a *bifurcation point* if for any neighborhood U of λ_0 there exists $\lambda_1 \in U$ such that f_{λ_1} is not conjugate to f_{λ_0}, i.e. the set of invariant sets of f_{λ_1} differs from that of f_{λ_0}. Our understanding of bifurcations arises from *normal forms*; polynomial approximations of the dynamics from which one can extract the conjugacy classes of dynamics in a neighborhood of the bifurcation point.

The presence of chaotic invariant sets has profound implications for computations. In particular, arbitrarily small perturbations, e.g. numerical errors, lead to globally distinct trajectories. Nevertheless for some chaotic systems one can show that numerical trajectories are *shadowed* by true trajectories, that is there are true trajectories that lie within a given bound of the numerical trajectory. From the perspective of applications and computations an even more profound realization is the fact that there exist parameterized families of dynamical systems for which the set of bifurcation points form a Cantor set of positive measure. This implies that invariant sets associated to the dynamics of the numerical scheme used for computations cannot be expected to converge to the invariant sets of the true dynamics.

A-Posteriori Functional Analytic Methods

Newton's method is a classical tool of numerical analysis for finding approximate solutions to $F(x) = 0$. The Newton-Kantorovich theorem provides sufficient a-posteriori conditions to rigorously conclude the existence of a true solution within an explicit bound of the approximate solution. INTLAB is a Matlab toolbox that using interval arithmetic can rigorously carry out these types of computations for $x \in \mathbb{R}^n$ [65; 64]. Since fixed points and periodic points of a map $f\colon X \to X$ can be viewed as zeros of an appropriate function, this provides an archetypical approach to computational proofs in dynamics: establish the equivalence between an invariant set and a solution to an operator equation, develop an efficient numerical method for identifying an approximate solution, and prove a theorem–that can be verified by establishing explicit bounds–that guarantees a rigorous solution in a neighborhood of the approximate solution.

Even in rather general settings this philosophy is not new. As an example, observe that $x(t)$ is a τ-periodic solution of the differential equation $\dot{x} = V(x)$ if and only if x is a solution of the operator equation $\Phi[x] = 0$ where $\Phi[x](t) = \int_0^\tau V[x(t)]\, dt$. Representing x in Fourier space and using theoretical and computer assisted arguments to verify functional analytic bounds allows one to rigorously conclude the existence of the desired zero. This was done as early as 1963 [17]. By now there are a significant number of results of this nature, especially with regard to fixed points for PDEs [57; 61].

The field of computer assisted proof in dynamical systems arguably came into its own through the study of the *Feigenbaum conjecture*; a large class of unimodal differentiable mappings $\phi\colon [-1,1] \to \mathbb{R}$ exhibit an infinite sequence of period doubling bifurcations and the values of the bifurcation points are governed by a universal constant δ [36]. This conjecture is equivalent to the statement that the doubling operator $T[\phi](x) = -\frac{1}{a}\phi \circ \phi(-ax)$ has a hyperbolic fixed point $\bar{\phi}$, and that the Frechet derivative at the fixed point $DT[\bar{\phi}]$ has a single unstable eigenvalue with value δ [22; 21]. A good approximation of the fixed point and the unstable eigenvalue was determined using standard numerical methods. Newton-Kantorovich was then used conclude the existence and bounds of a true fixed point and unstable eigenvalue, where the latter computations are done using upper and lower bounds to control for the errors arising from the finite dimensional truncation and the finite precision of the computer [47; 48].

Examples of invariant sets that can be formulated as the zero of a typically infinite dimensional operator include stable and unstable manifolds of fixed points and equilibria [13; 14], invariant tori in Hamiltonian systems [52], hyperbolic invariant tori and their stable and unstable manifolds [40], existence of heteroclinic and homoclinic orbits [12; 11], and shadowing orbits for systems with exponential dichotomies [60]. Thus for all these problems there are numerical methods that can be used to find approximate solutions. Furthermore, for parameterized families continuation methods can be use to identify smooth branches of approximate zeros [45]. In tandem with non-trivial analytic estimates, this has been successfully exploited to obtain computational proofs in a variety of settings: universal properties of area-preserving maps [34], KAM semi-conjugacies for elliptic fixed points [51], relativistic stability of matter against collapse of a many-body system in the Born-Oppenheimer approximation [35], computation of stable and unstable manifolds for differential equations [9; 42], existence of connecting orbits for differential equations and maps [9; 25; 24], existence of chaotic dynamics for maps and differential equations [69; 6; 7], equilibria and periodic solutions of PDEs [28; 5; 4], and efficient computation of one parameter branches of equilibria and periodic orbits for families of PDEs and FDEs [29; 37; 8; 7; 49].

A-Posteriori Topological Methods

An alternative approach to extracting the existence and structure of invariant sets is to localize them in phase space and then deduce their existence using a topological argument. The common element of this approach is to replace the study of $f\colon X \to X$ by that of an *outer approximation*, a multivalued map $F\colon X \rightrightarrows X$ whose images are compact sets that satisfy the property that for each $x \in X$, $f(x) \in \operatorname{int} F(x)$ where int denotes interior. This implies that precise information about the nonlinear dynamics is lost–at best one has information about neighborhoods of orbits–however this is the maximal direct information one can expect using a numerical approximation. The central concept in this approach is the following. A compact set $N \subset X$ is an *isolating neighborhood* under f if $\operatorname{Inv}(N, f)$, the maximal invariant set in N under f, is contained in the interior of N. The theoretical underpinnings for these methods go back to [23; 54; 33], where, for example, the existence of the stable and unstable manifolds of a hyperbolic fixed point is proven by studying iterates of an isolating neighborhood using the contractive and expansive properties guaranteed by the hyperbolicity. The first rigorous computational proof using these types of ideas was the demonstration of the existence of chaotic dynamics in Hamiltonian systems [19].

To indicate the breadth of this approach we provide a few examples of computational implementations. By definition a homoclinic point to a hyperbolic fixed point $\bar{x}$ corresponds to an intersection point of the stable $W^s(\bar{x})$ and unstable $W^s(\bar{x})$ manifolds of $\bar{x}$. If this intersection is transverse, then there exists an invariant set which is conjugate to subshift dynamics with positive entropy [68]. This suggests the following computational strategy: find a hyperbolic fixed point $\bar{x}$; compute geometric enclosures of $W^s(\bar{x})$ and $W^s(\bar{x})$; verify the transverse intersection; and if one wants a lower bound on the associated entropy, use the identified homoclinic points to construct the appropriate subshift dynamics. Beginning with the work of [58], this approach has been applied repeatedly. The accuracy of the bound on entropy is limited by the enclosure of $W^s(\bar{x})$ and $W^s(\bar{x})$. An efficient implementation of higher order Taylor methods [10] that leads to high precision outer approximations was used to attain the best current lower bounds on the entropy of the Henon map at the classical parameter values [59].

A constraint for this strategy is the rapid growth in cost of approximating invariant manifolds as a function of dimension. This can be avoided by isolating only the invariant set of interest using *covering relations*; parallelograms which are properly aligned under the differential of the map. While applications of this idea to planar maps appear as early as [67], a general theory along with efficient numerical implementation has been developed by [16; 76; 39]. In conjunction with rigorous tools for integrating differential equations [15] this method has found wide application including proofs of the existence of heteroclinic and homoclinic connecting orbits and chaotic dynamics in celestial mechanics [74; 73], uniformly hyperbolic invariant sets for differential equations [72], and particular orbits in PDEs [75].

These techniques can also be applied to detect complicated bifurcations. A family of ODEs in $\mathbb{R}^3$, exhibits a *cocooning cascade of heteroclinic tangencies* (CCHT) centered at λ_*, if there is a closed solid torus T, equilibria $x^\pm \notin T$, and a monotone infinite sequence of parameters λ_n converging to λ_* for which $W^u_{\lambda_*}(x^+)$ and $W^s_{\lambda_*}(x^-)$ intersect tangentially in T and the length of the corresponding heteroclinic orbit within T tends to infinity as $\lim_{n\to\infty}$. For systems with appropriate symmetry a CCHT can be characterized in terms the topologically transverse intersection of stable and unstable manifolds between the fixed points and a periodic orbit [32], and therefore can be detected using the above mentioned techniques. This was used in [46] to obtain tight bounds on parameter values at which the Michelson equation exhibits a CCHT.

Identifying structurally stable parameter values is important. This is associated with hyperbolic invariant sets. Let X be a manifold. If $N \subset X$ is an isolating neighborhood and $\text{Inv}(N, f)$ is chain-recurrent, then to prove that $\text{Inv}(N, f)$ is hyperbolic it is sufficient to show that there is an isolating neighborhood $\bar{N} \subset TX$, the tangent bundle, under $Tf: TX \to TX$ such that $\text{Inv}(\bar{N}, Tf)$ is the zero section over N [66; 20]. This was used by [1] to determine lower bounds on the set of parameter values for which the the Henon map is hyperbolic (see Fig. 1).

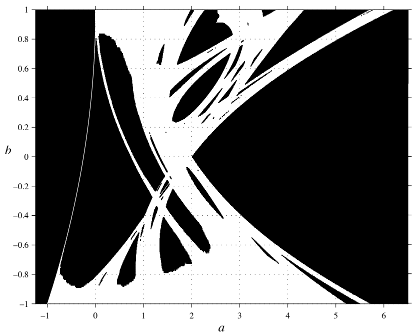

Fig. 1. Black region indicate parameter values at which maximal invariant set of Henon map is hyperbolic.

To efficiently identify isolating neighborhoods it helps to work with a special class of outer approximations. For $f: \mathbb{R}^n \to \mathbb{R}^n$ let $\mathcal{X}$ denote a cubical grid which forms a cover for a compact set $X \subset \mathbb{R}^n$. For each cube $\xi \in \mathcal{X}$, let $\mathcal{F}(\xi) \subset \mathcal{X}$ such that $f(\xi) \subset \text{int}\left(\cup_{\xi' \in \mathcal{F}(\xi)} \xi'\right)$. Observe that $\mathcal{F}$ can be view both as an outer approximation and as a directed graph. The latter perspective is useful since it suggests the use of efficient algorithms from computer science. The construction $\mathcal{X}$ and the search for isolating neighborhoods can be done in an adaptive manner which in some settings implies that computational cost is determined by the dimension of the invariant set as opposed to the ambient space $\mathbb{R}^n$ [31; 43]. A representative of any isolating neighborhood can be identified by this process if the grid and the outer approximation are computed with sufficiently fine resolution [44].

Given an isolating neighborhood N the *Conley index* can be used to characterize the structure of $\text{Inv}(N, f)$. To compute this one needs to construct a pair of compact sets $P = (P_1, P_0)$, called an *index pair*, on which f induces a continuous function $f_{P*}\colon (P_1/P_0, [P_0]) \to (P_1/P_0, [P_0])$ on the quotient space [62]. The induced map on homology $f_{P*}\colon H_*(P_1/P_0, [P_0]) \to H_*(P_1/P_0, [P_0])$ is a representative for the Conley index. Given an outer approximation $\mathcal{F}\colon \mathcal{X} \rightrightarrows \mathcal{X}$ there are efficient directed graph algorithms to construct index pairs. Furthermore, f_{P*} can be computed using $\mathcal{F}$ [43; 56; 18].

The first nontrivial computational use of these ideas was a proof that the Lorenz equations exhibit chaotic subshift dynamics [55]. Since then Conley index technique have been applied in the context of rigorous computations to a variety of problems concerning the existence and structure of invariant sets including chaotic dynamics in the Henon map [30] and the infinite dimensional Kot-Shaffer map [26], homoclinic tangencies in the Hénon map [2], global dynamics of variational PDEs [27; 53], and chaotic dynamics in fast-slow systems [38].

Conceptually, partitioning a-posteriori methods of computational proofs in dynamics into functional analytic and topological methods is useful, but for applications a combination of these tools is often desirable. For example the proof of the existence of the Lorenz attractor at the classic parameter values [71] is based on a-posteriori topological arguments. However, the construction of the rigorous numerical outer approximation exploits a high order normal form computed at the origin and a-posteriori functional analytic tools are used in order to obtain rigorous bounds on truncation error for the normal form and its derivative.

Global Topological Methods

The underlying strategy for a posteriori analytic and topological techniques is to identify a priori a class of invariant sets, numerically approximate and then rigorously verify the existence. Since it is impossible to enumerate all invariant sets, an algorithmic analysis of arbitrary dynamical systems using a classification based on structural stability is impossible. An alternative approach based on using isolating neighborhoods to characterize the objects of interest in dynamical systems [23] appears to be well suited for rigorous systematic computational exploration of global dynamics. To provide partial justification for this method we return to the setting of an outer approximation $\mathcal{F}$ of f defined on a cubical grid $\mathcal{X}$ covering a compact set $X \in \mathbb{R}^n$. Let $S := \mathrm{Inv}(X, f)$. Viewing $\mathcal{F}$ as a directed graph, there exist efficient algorithms for identifying the strongly connected path components $\{\mathcal{M}(p) \subset \mathcal{X} \mid p \in (\mathsf{P}, <)\}$ [70] where the partial ordering is determined by paths in $\mathcal{F}$. Furthermore the collection of invariant sets $\left\{M(p) := \mathrm{Inv}(\cup_{\xi \in \mathcal{M}(p)} \xi, f)\right\}$ forms a *Morse decomposition* of S under f; a finite collection of mutually disjoint compact invariant subsets of S with the property that if $x \in S \backslash \cup M(p)$ then its forward orbit limits in $M(p)$ and its backward orbit limits in $M(q)$ where $p < q$. Stated differently, this procedure identifies the locations in phase space in which recurrent dynamics can occur and identifies the gradient-like dynamics between these regions. Furthermore, each $\mathcal{M}(p)$ defines an isolating neighborhood for $M(p)$ [44] and thus the Conley index can be used to understand the structure of $M(p)$.

Let $\mathcal{X}^\epsilon$ denote a cubical grid with cubes of diameter $\epsilon > 0$ and set $\mathcal{F}^\epsilon(\xi) := \{\xi' \in \mathcal{X}^\epsilon \mid f(\xi) \cap \xi' \neq \emptyset\}$. This defines $\{\mathcal{M}(p^\epsilon) \subset \mathcal{X}^\epsilon \mid p^\epsilon \in (\mathsf{P}^\epsilon, <^\epsilon)\}$. As is shown in [44] the *chain recurrent set* $R := \cap_n \cup_{p^{\epsilon_n} \in \mathsf{P}^{\epsilon_n}} \mathcal{M}(p^{\epsilon_n})$ is independent of the sequence $\epsilon_n \to 0$. This provides an algorithmic construction of *Conley's Fundamental Decomposition Theorem* [63] that states that R is the minimal invariant subset of S for which there exists a Lyapunov function $V\colon S \to [0, 1]$ with the property that V is constant on R and for every $x \in S \setminus R$, $V(f(x)) < V(x)$.

In the the case of a parameterized family of maps $f\colon X \times \Lambda \to X$ where $\lambda \in \Lambda \subset \mathbb{R}^m$ let $\mathcal{Q}$ be a covering of Λ by compact cubes. For each $Q \in \mathcal{Q}$ define $\mathcal{F}^\epsilon_Q\colon \mathcal{X}^\epsilon \rightrightarrows \mathcal{X}^\epsilon$ by $\mathcal{F}^\epsilon_Q(\xi) := \{\xi' \in \mathcal{X}^\epsilon \mid f(\xi, Q) \cap \xi' \neq \emptyset\}$. Applying the same algorithms as above produces $\left\{\mathcal{M}(p^\epsilon_Q) \subset \mathcal{X}^\epsilon \mid p^\epsilon_Q \in (\mathsf{P}^\epsilon_Q, <)\right\}$ which results in a Morse decomposition and associated Conley indices that are valid for all f_λ, $\lambda \in \Lambda$. This allows for an algorithmic approach to the rigorous analysis of the global dynamics of $f\colon X \times \Lambda \to X$ in both phase space and parameter space. This relatively new approach to computational dynamics of multiparameter systems has been applied to simple population models [3; 50].

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