THE ROLE OF GEOMETRY IN COMPUTATIONAL DYNAMICS

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ABSTRACT. This paper is an informal discussion of how geometry and numerical analysis are intertwined in the computational study of dynamical systems and their bifurcations. We use the example of determining the phase portrait of planar vector fields to illustrate the more general and philosophical attitudes that constitute our main thesis. Few mathematical details are included.

1. Introduction

There are two fundamental aspects of dynamical systems theory that lead us to reliance upon computers. First, "most" nonlinear vector fields cannot be integrated explicitly, so numerical methods are absolutely essential to obtain quantitative information about the solutions to particular systems. This is usually done through the iterative computation of approximate solutions by numerical integration algorithms. Second, computers work well for simulating trajectories of vector fields of modest complexity. Modern workstations have an architecture that emphasizes very rapid floating point calculations on data that is stored in cache memories of moderate size. This is well matched to obtaining maximal performance from application of a numerical integration algorithm as long as the size of a system allows the data and inner loop of of an algorithm to be stored in cache memory. Even without worrying about data locality, computers have increased their speed enormously over the past decade.

Numerical integration is not a panacea for the investigation of dynamical systems that occur as "real world" examples. There are many problems involving dynamical systems that are not easily solved by numerical integration. Here we focus upon the mathematical problem of providing proofs for the qualitative structure of phase portraits of dynamical systems. Traditional computational theories have regarded questions of dynamical systems largely as analytic problems. However, there are fundamental limitations on error estimation for numerical computation of trajectories for dynamical systems. Naive error estimation applied to an iterative method for computing trajectories yields an exponential growth in the estimates. Moreover, the finite precision with which calculations are performed results in a trade-off between truncation and round off errors that is due to the increasing length of a computation with reductions in step sizes.

There are alternate strategies to error estimation of trajectory computations for the rigorous analysis of dynamical systems properties. In particular, geometric approaches can be productively combined with computation to address some questions about dynamical systems. We shall make this argument in a specific context in which the geometry is relatively simple, namely the study of planar vector fields. We draw heavily upon the work of Salvador Malo [5, 3] in the discussion.

2. Hilbert's XVI Problem

Of the problems posed by Hilbert at the beginning of the century, the sixteenth remains of one of the few that has been resistant to solution. The problem asks for a bound on the number of limit cycles of a polynomial vector field

$$\dot{x} = P(x, y) \qquad \dot{y} = Q(x, y)$$

as a function of the degrees of the polynomials P, Q. The problem remains unsolved for polynomials of any degree $d > 1$. One of the difficulties associated with Hilbert's sixteenth problem is the lack of principles that allow one to deduce information about the phase portrait of a vector field from its analytic expression. There are perturbation methods that can be used to study vector fields that are close to integrable ones with families of periodic orbits and ones that are close to bifurcations of a specific codimension. For structurally stable systems, numerical integration and root finding frequently produce a correct phase portrait with minimal effort. On the other hand, proving that the computed pictures produce the correct phase portrait for a system has been a difficult task, usually involving lengthy analytic arguments for each example or class of examples. Our goal is to create computer algorithms that automate these analytic arguments. We illustrate how transversality is used by describing how to prove the existence of a hyperbolic periodic orbit in a planar vector field.

The strategy that we adopt is based upon transversality. For planar vector fields, the Poincaré-Bendixon Theorem can be used to prove the existence of a periodic orbit [1]. If a vector field X enters an annulus A and does not leave, there is either an equilibrium point or a periodic orbit in A. Verification of the fact that X enters A at all points of its boundary does not require integration of the vector field. Instead, one needs a representation of the boundary of A for which it is possible to prove that the vector field points into A at all points of this boundary. Location of the equiibrium points of X is a matter of solving polynomial equations, and Bezout's Theorem tells us that the number of complex equilibrium points is generically the product of the degrees of P and Q. Thus the existence of a hyperbolic periodic orbit of X can be proved by finding an annulus that contains the periodic orbit but no equilibrium points and has the property that the vector field enters (or leaves) the annulus at all points of its boundary.

3. Rotated Vector Fields and Interval Arithmetic: Malo's Thesis

Salvador Malo [5] has implemented a simple version of this process and applied it to polynomial vector fields. There are two aspects to the problem: choosing an annulus A and showing that the vector field enters or leaves the annulus at all points of its boundary. He uses annuli that have piecewise linear boundaries. The verification that the vector field enters the annulus A is reduced to proving that certain polynomials do not vanish on specific intervals. Specifically, if $\phi(s) = \mathbf{u} + s\mathbf{v}$, $s \in [a, b]$ is a segment of the boundary of the annulus, then we must prove that the polynomial $\mathbf{v} \times X(\phi(s))$ does not change sign for $s \in [a, b]$. This computation is carried out by interval arithmetic in a straightforward fashion. The application of this computation to each segment of the boundary of A is used to prove that X does not both enter and leave A.

The novel part of the implementation lies mainly in the strategy used to identify an annulus that whose boundary is transverse to the flow. to do so, the properties of *rotated* vector fields are used. Consider the one parameter family of vector fields $X_\theta = R_\theta \circ X$, where R_θ is rotation by the angle θ. The equilibrium points of X remain fixed under rotation, and X_θ is transverse to X at all other points. Duff [2] proved that hyperbolic periodic orbits of X_θ shrink and expand monotonically under rotation. In particular, if Γ is a hyperbolic periodic orbit of X, then there is an $\epsilon > 0$ and a continuous family of periodic orbits Γ_θ with $-\epsilon < \theta < \epsilon$ and $\Gamma = \Gamma_0$. The Γ_θ are disjoint and either expand or contract as θ increases. Thus we can use periodic orbits of rotated vector fields to form the boundary of an annulus that contains the periodic orbit Γ.

The use of periodic orbits of rotated vector fields to obtain an annulus with boundary transverse to X works well numerically. We compute periodic orbits of $X_{\pm\epsilon}$ with a numerical integration algorithm. Discrete versions of these trajectories are used to form the boundary of an annulus that contains the periodic orbit Γ. This construction works well on numerical examples that would clearly be difficult to work with analytically. For example, Malo [5] proves that in the system $\dot{z} = \lambda z + a|z|^2 z + b\bar{z}^3$ (with z, λ, a, b complex) arising in the study of fourth order resonant Hopf bifurcation from a periodic orbit, that there are parameter values with a pair of concentric limit cycles.

Transversality techniques are used by Malo to produce proofs for the non-existence of limit cycles as well as existence proofs. Once again appeal is made to topological arguments in the proof. A limit cycle must contain equilibrium points in its interior. If two equilibrium points have a trajectory that connects the two equilibria, then no periodic orbit can separate the two equilibria. By using estimates of the size of a neighborhood contained in the domain of attraction of a sink, together with rotated vector fields, it is possible to prove the existence of a trajectory with a specified initial condition that reaches a sink. A region is identified with boundary a piecewise smooth triangle so that one vertex is at the given initial point, the vector field points inward on the boundaries of the two adjacent sides, and the opposite side lies in the domain of attraction of the sink. Of course, these techniques can be applied in backwards as well as in forward time. Information about the α and ω limit sets of the stable and unstable manifolds of a saddle can be obtained with similar calculations.

4. Uniqueness of Limit Cycles

The phase portrait for a structurally stable planar vector field is determined by

- the number and type of equilibrium points
- the number of periodic orbits and their stability
- the α and ω limit sets of the stable and unstable manifolds of the saddle points in the system.

The methods discussed above are sufficient to determine all aspects of this structure except the determination of the number of periodic orbits. For this purpose, we need the means of proving the uniqueness of periodic orbits in annuli. Around each periodic orbit, we not only need to find an annulus with boundary transverse to the vector field, we also need to prove that there is only one periodic orbit in the annulus. If the divergence of the vector field does not change sign in the annulus, then Dulac's criterion [1] finishes this step in the proof. However if the limit cycle intersects the zero set of the divergence of X, then additional numerical computations are required to establish uniqueness of the limit cycle. We outline an approach to these computations that appears feasible, but has not yet been implemented.

We want to describe an algorithm that gives a constructive procedure for estimating properties of the return map defined in a neighborhood of a periodic orbit. Let $\gamma(s)$, $s \in S^1$, be a C^2 curve parametrized by arc length that approximates a periodic orbit of the vector field X. (We think of γ as a spline approximation to a numerically computed trajectory of X that has been reparametrized.) Let $\nu(s)$ be the unit normal to γ and let $\Psi(r,s) = \gamma(s)+r\nu(s)$. The map Ψ^{-1} is a coordinate system on a tubular neighborhood of γ for which the "radial" curves are normal lines to γ. To make calculation with interval arithmetic easier, we may assume that the curve γ is piecewise polynomial. This assumption implies that Ψ is also a piecewise polynomial map. Expressed in terms of the (r,s) coordinates, X will be given by the expression $\tilde{X}(r,s) = (D\Psi_{(r,s)})^{-1}X(\Psi(r,s))$. This is a piecewise rational expression, with the denominator of the rational expression coming from $det((D\Psi_{(r,s)}))$ when computing the inverse of $(D\Psi_{(r,s)})$. Moreover, the s component of $\tilde{X}$ is non-zero, so we can reparametrize $\tilde{X}$ to yield a vector field Y which has the form

$$\begin{aligned} \dot{r} &= g(r,s) \\ \dot{s} &= 1 \end{aligned}$$

The function g is also piecewise rational.

If γ is a sufficiently good approximation to a periodic orbit of X, then the periodic orbit will be in the image of Ψ, and will project monotonically onto the s axis. The curves parallel to the r axis map into themselves under the flow of Y since $\dot{s} = 1$. Thus, the return map Θ of a cross-section $s = s_0$ is just the time T map of the flow of Y, and

$$\Theta(r) = \int_0^T g(\rho(s), s)ds$$

with $(\rho(s), s)$ the trajectory with initial condition r. To assess the potential existence of another periodic orbit near γ, we compute

$$I(\sigma) = \int_0^T \frac{\partial g(\sigma(s), s)}{\partial r} ds$$

over curves in a neighborhood of γ. Since

$$\int\int \frac{\partial g(\sigma(s), s)}{\partial r} dA$$

is the rate of change of area under the flow of Y, the existence of multiple periodic orbits implies that $I(\sigma)$ vanishes on some closed curve σ in an annulus bounded by periodic orbits. We use this fact to formulate a test to prove that such curves do not exist. Fix an annulus defined by $|r| < \epsilon$ where we shall test for the existence of periodic orbits. Compute rigorous upper and lower bounds for g along radial segments with constant s in this annulus. For curves σ with derivatives lying in the computed range of values of g, establish bounds for $I(\sigma)$ by using interval versions of algorithms for evaluating integrals. If these bounds maintain a constant sign, then there cannot be two periodic orbits in the annulus. For the algorithm to produce the existence of a unique limit cycle in the annulus, ϵ must be large enough that we can prove existence of a limit cycle in the annulus with rotated vector fields, but small enough that the $I(\sigma)$ maintain a constant sign. Successful implementation of this algorithm would complete the construction of a practical toolkit for the verification of correctness of phase portraits for structurally stable planar vector fields defined by expressions that can be computed with interval arithmetic.

5. Concluding Remarks

We would like to extend the rigorous analysis described above to more problems involving qualitative properties of dynamical systems. For example, consider the analysis of bifurcations in families of planar vector fields as well as establishing the structure of individual phase portraits. It seems feasible to use similar ideas to prove that a specified family is stable and does not contain degenerate bifurcations. To carry out this task, rigorous evaluation of higher derivatives along trajectories is required. We discuss the rigorous determination of saddle-nodes of periodic orbits as an example. Let X_λ be a one parameter family of vector fields. Suppose that there are parameter values $\lambda_0 < \lambda_1$ and an annulus A such that X_λ has no equilibrium points in A and is transverse to its boundary for $\lambda_0 < \lambda < \lambda_1$, X_{λ_0} has a pair of periodic orbits in A and trajectories of X_{λ_1} connect the two boundary components of A. These assumptions can all be verified using the techniques described above. They imply the existence of a bifurcation of periodic orbits occurs for some $\lambda_0 < \lambda < \lambda_1$. This bifurcation is a saddle-node if two non-degeneracy conditions are met by the return map: the first derivative with respect to the parameter and the second derivative with respect to the coordinate on the cross section should not vanish. These calculations can be performed in the coordinate system described above as integrals of the appropriate derivatives of the vector field along the periodic orbit. Though the periodic orbit is not known precisely, interval computations can provide rigorous estimates that hold on all curves in a C^1 neighborhood of the periodic orbit.

The computational complexity of determining the qualitative structure of vector fields increases rapidly with dimension. Nonetheless, we suggest that the use of more geometry in the development of algorithms for computing properties about dynamical systems will be productive and worthwhile. We point to the discussion of computation of two dimensional stable and unstable manifolds of equilibrium points for flows in [4] as an illustration of the efficacy of geometric approaches to computations of dynamical system structure.

6. References

References

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