Solving Numerically Hamiltonian Systems

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1. Introduction

This is a short summary of my oral presentation at the Zurich International Congress of Mathematicians. The presentation was aimed at providing an easy introduction to the field of symplectic numerical integrators for Hamiltonian problems. Some sacrifices in rigor and precision were deliberately made.

We are concerned with initial value problems for systems of ordinary differential equations

$$\frac{dy}{dt} = f(y), \quad 0 \leq t \leq T, \qquad y(0) = \alpha \in \mathcal{R}^D, \tag{1}$$

where f is a smooth function. The basic theory of numerical methods for (1) has been known for more than thirty years, see e.g. [8]. This theory, in tandem with practical experimentation, has led to the development of general software packages for the efficient solution of (1). It is perhaps remarkable that both the theory and the packages do not take into account any structure the problem may have and work under virtually no assumption on the (smooth) vector field f. This contributes to the elegance of the theory and to the versatility of the software.

However, it is clear that a method that can solve "all" problems is bound to be inefficient in some problems. Stiff problems [9], frequent in many applications, provide an example of problems of the format (1) where general packages are very inefficient. Accordingly, a special theory and special software have been created to cope with stiff problems.

Are there other classes of problems of the form (1) that deserve a separate study? In recent years much work has been done on special methods for *Hamiltonian problems.* Of course, Hamiltonian problems [11] play a crucial role as mathematical models of situations where dissipative effects are absent or may be ignored. Most special methods for Hamiltonian problems are *symplectic* methods; other possibilities, not discussed here, include reversible and energy-conserving methods [16]. Early references on symplectic integration are Channell [4], Feng [5], and Ruth [12]. In the last ten years the growth of the "symplectic" literature has been impressive, both in mathematics and in the various application fields. The monograph [16] contains over a hundred references from the mathematical literature. The second edition of the excellent treatise by Hairer, Nørsett, and Wanner [8] includes a section on symplectic integration.

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In the talk I presented several examples, taken from mathematics [16], astronomy [20], and molecular dynamics [6] that illustrated the practical advantages of symplectic integrators when compared with general software.

2. Symplecticness

For our purposes here, a Hamiltonian problem is a problem of the form (1) where the dimension D is even, $D = 2d$, and the components f_i of f are given by

$$f_i = -\frac{\partial H}{\partial y_{d+i}}, \quad f_{d+i} = +\frac{\partial H}{\partial y_i}, \quad i = 1, \ldots, d, \tag{2}$$

for a suitable real-valued function $H = H(y)$ (the Hamiltonian). It is standard notation to set $p_i = y_i$, $q_i = y_{d+i}$, $i = 1, \ldots, d$, and then the Hamiltonian system with Hamiltonian function H reads

$$\frac{dp_i}{dt} = -\frac{\partial H}{\partial q_i}, \quad \frac{dq_i}{dt} = +\frac{\partial H}{\partial p_i}, \quad i = 1, \ldots, d. \tag{3}$$

Whether a system of the form (1) with $D = 2d$ is Hamiltonian or otherwise can be decided [1] by the symplecticness of its flow. Recall that, for each real t, the t-flow ϕ_t of the differential system in (1) is the mapping in $\mathcal{R}^D$ that maps each $\alpha \in \mathcal{R}^D$ into the value $y(t)$ at time t of the solution y of the initial value problem (1). A symplectic transformation Φ in $\mathcal{R}^{2d}$ is a transformation that preserves the differential form

$$\omega = dp_1 \wedge dq_1 + \cdots + dp_d \wedge dq_d.$$

When $d = 1$ preservation of ω is simply preservation of oriented area: a smooth Φ is symplectic if and only if for each oriented domain D in $\mathcal{R}^2$, $\Phi(D)$ possesses the same area and orientation as D. For $d > 1$, preservation of ω means preservation of the sum of the two-dimensional oriented areas of the projections onto the planes (p_i, q_i), $i = 1, \ldots, d$, of oriented two-dimensional surfaces D in $\mathcal{R}^{2d}$.

For each t, the flow ϕ_t of (3) is a symplectic transformation. Conversely if (1) (with $D = 2d$) is such that, for each t, ϕ_t is symplectic then (1) is a Hamiltonian problem, in the sense that a scalar function H may be found such that (2) holds. The conclusion is that the symplecticness of the flow characterizes Hamiltonian problems. In fact, all qualitative properties of the solutions of Hamiltonian systems derive from the symplecticness of the flow.

When solving (1) with a one-step numerical method, the true flow $\phi_{\Delta t}$ is replaced by a computable approximation $\psi_{\Delta t}$. For instance, for the standard Euler rule $\psi_{\Delta t}(y) = y + \Delta t f(y)$. For an order r method $\psi_{\Delta t}$ is an $O(\Delta t^{r+1})$ perturbation of $\phi_{\Delta t}$ as $\Delta t \to 0$. The numerical approximation y^n at time $t_n = n\Delta t$, $n = 1, 2, \ldots$, is computed by iterating the map $\psi_{\Delta t}$, i.e. $y^{n+1} = \psi_{\Delta t}(y^n)$, $n = 0, 1, \ldots$. Then $y^n - y(n\Delta t)$ is $O(\Delta t^r)$ as $\Delta t \to 0$, uniformly in bounded intervals of the variable $t = n\Delta t$.

If (1) is a Hamiltonian problem, there is no guarantee that a given numerical method yields a mapping $\psi_{\Delta t}$ that is symplectic. Therefore, in general, numerical methods do not share the property of symplecticness that is the hallmark of

Hamiltonian problems. A numerical method is said to be symplectic, if, whenever it is applied to a Hamiltonian problem (3), it produces a mapping $\psi_{\Delta t}$ that is symplectic for each Δt.

3. Available symplectic methods

The available symplectic methods can be grouped broadly into three classes.

The earliest symplectic methods were based on the fact that symplectic transformations in $\mathcal{R}^{2d}$ can be expressed in terms of the partial derivatives of a real-valued *generating function*. For the true flow $\phi_{\Delta t}$, the generating function is a solution of the Hamilton-Jacobi equation, and by approximately solving the Hamilton-Jacobi equation one constructed the generating function of the numerical method $\psi_{\Delta t}$. The methods obtained in this way require the knowledge of higher derivatives of H and tend to be cumbersome.

Lasagni [10], Suris [19], and I [13] discovered independently that standard classes of methods, like *Runge-Kutta* methods, include schemes that just 'happen' to be symplectic.

The third class of symplectic methods is built around the idea of *splitting*. It is required that the Hamiltonian H of interest may be decomposed as a sum $H = H_1 + \cdots + H_s$ such that the Hamiltonian systems with Hamiltonians H_i may be integrated in closed form, so that the corresponding flows $\phi_{\Delta t, H_i}$, $i = 1, \ldots, s$, are explicitly available. These "fractional" flows are then combined to produce an approximation $\psi_{\Delta t, H}$ to $\phi_{\Delta t, H}$. When $s = 2$, the simplest possibility is to set

$$\psi_{\Delta t, H} = \phi_{\Delta t, H_1} \phi_{\Delta t, H_2}.$$

This provides a first-order method that is symplectic: $\psi_{\Delta t, H}$ is a composition of two Hamiltonian flows, and hence of two symplectic mappings. Higher-order splittings exist; for instance the second-order recipe

$$\psi_{\Delta t, H} = \phi_{\Delta t/2, H_1} \phi_{\Delta t, H_2} \phi_{\Delta t/2, H_1}$$

goes back to Strang [18], and Yoshida [21] has developed a way of constructing splittings of arbitrarily high orders.

4. Discussion

In which way are symplectic methods better than their conventional counterparts? The standard criterion for determining the merit of numerical methods for (1) is as follows. One measures the error $|y^n - y(n\Delta t)|$ (numerical minus exact) at some prescribed time $t = n\Delta t$; method A is then an improvement on method B if A attains a prescribed error size with less work than B. There is some evidence suggesting that symplectic methods may be advantageous when this standard comparison criterion is used. For instance, it is possible to show [3] that, in the integration of the classical two-body problem, symplectic integrators have errors whose leading terms in the asymptotic expansion grow linearly with t; the error in conventional methods grows like t^2.

However the standard criterion described above may not be a sensible choice in many instances. Sometimes numerical integrators are used to get an indication of the long-time behavior of a differential system [14]. When t is large all numerical methods are likely to produce approximations y^n that differ significantly from $y(n\Delta t)$; therefore all methods would be regarded as bad with the standard criterion. This is particularly clear in cases, including chaotic regimes, where neighboring solutions of the system diverge exponentially as t increases and hence numerical errors also increase exponentially. It is then useful to derive new alternative criteria to judge the goodness of numerical methods in long-time integrations, see e.g. [17].

An idea that has recently attracted much attention [16], [2], [15], [7] is that of *backward error analysis.* In numerical analysis, given a problem $\mathcal{P}$ with true solution $\mathcal{S}$ and given an approximate solution $\tilde{\mathcal{S}}$, forward error analysis consists of estimating the distance between $\mathcal{S}$ and $\tilde{\mathcal{S}}$. Traditionally, error analyses in numerical differential equations are forward error analyses. Backward error analysis consists of showing that $\mathcal{S}$ is the exact solution of a problem $\tilde{\mathcal{P}}$ that is close to $\mathcal{P}$. Let $\psi_{t,f}$ be a numerical method of order $r \geq 1$ for the integration of (1). Given any *large* integer N, there is an autonomous vector field $\tilde{f}$, that depends on N and Δt, such that $\psi_{\Delta t,f} - \phi_{\Delta t,\tilde{f}} = O(\Delta t^{N+1})$ as $\Delta t \to 0$. This means that the numerical solution, that is an approximation of order r to the solution of the problem (1) we are trying to solve, is an approximation of order $N >> r$ to the perturbed problem

$$\frac{dy}{dt} = \tilde{f}(y), \quad 0 \leq t \leq T, \qquad y(0) = \alpha \in \mathcal{R}^D. \tag{4}$$

Ignoring $O(\Delta t^N)$ terms, the numerical solution is really solving the modified problem (4). Here $\tilde{f} = f + O(\Delta t^r)$, so that the higher the order of the method, the closer the modified problem is to the true problem (1). In any case, if the discrepancy between f and $\tilde{f}$ is of the same size as the uncertainty in f that results from modelling errors, experimental errors in measuring the constants that may feature in f, etc., then we are sure that there is nothing seriously wrong in solving (1) numerically.

In this connection, it turns out that if the numerical method is symplectic and (1) is Hamiltonian, then (4) is also a Hamiltonian problem. In this sense, a symplectic integrator changes the problem being solved by slightly altering the Hamiltonian function H; a general integrator changes the problem being solved by introducing a non-Hamiltonian perturbation.

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