On the algebraic properties of difference approximations of Hamiltonian systems

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Abstract. We consider difference approximations of dynamic systems with a polynomial Hamiltonian that define birational correspondences between the initial and final positions of the system.

1. Introduction

One of mathematical models most widespread in celestial mechanics is a dynamic system described by a Hamiltonian system of ordinary differential equations. In applications, the Hamiltonian is often a polynomial or an algebraic function of coordinates $q_1, \ldots, q_n$ and momenta $p_1, \ldots p_n$. As a rule, from physical reasons a few integrals of motion are known, but they are not sufficient to reduce the system of differential equations to Abel quadratures.

Unable to reduce the system to quadratures, we are forced to solve it numerically. Having solved the many-body problem using the explicit Runge-Kutta method, we can only sadly watch as the mechanical energy of the system changes, and closed trajectories turn out to be open.

In the 1990s, the concept of geometric integrators emerged, i.e. numerical methods that in some sense inherit the analytical properties of the original Hamiltonian system. Historically, the first approach to designing difference schemes was proposed, in which the transition from one time layer to another is carried out using a canonical transformation. Such difference schemes were called symplectic. The simplest example of a symplectic scheme is the midpoint scheme.

This scheme perfectly imitates a Hamiltonian system with a quadratic Hamiltonian, for example, a harmonic oscillator with Hamiltonian $H = p^2+q^2$. According to Cooper's theorem, the energy integral is preserved exactly in the scheme, and the approximate solution itself is a sequence of points $\mathfrak{r}_n = (p_n, q_n)$ of the circle

$p^2 + q^2 = C$. Each step of the approximate solution is a rotation by an angle

$$\Delta u = \int_{\mathfrak{x}_n}^{\mathfrak{x}_{n+1}} \frac{dq}{\sqrt{C - q^2}},$$

which does not depend on n [1]. Thus, even in calculations with a very coarse time step, energy is conserved exactly, and the motion occurs along closed trajectories.

However, in the nonlinear case, the conservation of symplecticity does not entail the inheritance of other properties of the original Hamiltonian system. What principles should be used as the basis for the design of difference schemes that imitate Hamiltonian systems with a polynomial Hamiltonian?

2. Conservative schemes

The obvious approach is to abandon symplecticity in favor of the exact preservation of all algebraic integrals.

In [2] we introduced additional variables for the many-body problem, namely distances and reciprocal distances between bodies, and wrote down a system of differential equations with respect to the coordinates, velocities, and the additional variables. In this case, the system lost its Hamiltonian form, but all the classical integrals of motion of the many-body problem under consideration, as well as new integrals describing the relationship between the coordinates of the bodies and the additional variables are described by linear or quadratic polynomials in these new variables. Therefore, any symplectic Runge–Kutta scheme preserves these integrals exactly.

Ten classical integrals are sufficient to reduce the two-body problem to quadratures. However, as our computer experiments have shown, preserving them in the difference scheme is not sufficient for the points of the approximate solution to lie on an ellipse (or at least on a closed curve). Thus, preserving the integrals of motion also does not entail inheriting other properties of the original Hamiltonian system.

3. Kahan's Method and the Cubic Hamiltonian

From general considerations, it follows that any mechanical system should define a one-to-one correspondence between the initial and final positions of the system. In order to construct a difference scheme that imitates this property, we can try to approximate the original Hamiltonian system by equations that define a birational correspondence between the points $\mathfrak{x}$ and $\hat{\mathfrak{x}}$.

It is easy to see that this can always be done for systems with a cubic Hamiltonian, using a method that arose in the field of solitonics [3]; some authors associate it with the name of W. Kahan, others with the names of Hirota and Kimura

[4, 5]. We came to it when searching for a discrete analogue of the Painlevé theory [6, n. 3.2].

A Hamiltonian system with a cubic Hamiltonian is reduced to a quadrature

$$\int \frac{dq}{H_p} = t,$$

and the differential dq/H_p is an integral of the first kind on the elliptic curve $H(p,q) = C$, which is inverted in elliptic functions. After the Kahan discretization, the energy integral is inherited [4] and therefore the points of the approximate solution also lie on some elliptic curve, and the scheme itself can be written as a quadrature

$$\Delta u = \int_{\mathfrak{x}_n}^{\mathfrak{x}_{n+1}} v dq,$$

where vdq is again an elliptic integral of the first kind [7]. Thus, the Kahan difference scheme inherits both the form of the trajectory (a closed elliptic curve), and the quadrature, and even the possibility of representing the solution as a meromorphic function of time [7]. The symplectic structure is not preserved exactly, but is inherited [4]. Thus, Kahan's method allows imitating an elliptic oscillator to the same extent as the midpoint scheme allows imitating a linear oscillator.

The subtlety is that when designing the difference scheme we have included a property that is not present in the original Hamiltonian system, but which should be present in any mechanical system from general considerations. The point is that in the nonlinear case the general solution of the elliptic oscillator defines a birational transformation on the integral curve $H(p,q) = C$, which does not extend to a birational transformation of the entire phase space pq. Using Kahan's method we approximate this solution by a birational transformation of the entire space, for which we correct the integral curve, preserving its genus. Thus, Kahan's scheme imitates the elliptic oscillator, but does not reproduce its properties exactly. This makes it extremely difficult to find such schemes.

4. Appelroth Method and polynomial Hamiltonian

Transferring the developed technique to the case of equations with a polynomial right-hand side does not cause significant difficulties, since back at the beginning of the 20th century G.G. Appelroth [8] proposed a method that allows, by increasing the number of unknowns, to reduce a system with a polynomial right-hand side to a system with a quadratic right-hand side. This procedure was later called quadratization [9].

Computer experiments have shown that the relationships between new and old variables, which are valid for the exact solution, are no longer valid for the approximate solution, which is especially noticeable near moving singular points of the solution.

5. Discussion

Designing schemes that imitate systems with polynomial Hamiltonians raises a question that lies at the interface between algebra and physics: should the correspondence between the initial and final positions of the system be a one-to-one correspondence? Since Jacobi, we have known that the quadrature

$$\int \frac{dq}{H_p} = t$$

does not allow q to be represented as a single-valued analytic function of t if the genus of the curve $H(p, q) = C$ exceeds 1. However, we can approximate the solution of such a system using Cremona transformations by combining the methods of Appelroth and Kahan. Thus, the analytic properties of the difference approximation are simpler than those of the original Hamiltonian model. Does this mean that such models are better than continuous ones?

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