On the algebraic properties of difference approximations of Hamiltonian systems

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Difference schemes

The finite difference method proposes replacing the system of **differential equations**

$$\frac{dx_i}{dt} = f_i(x_1, \dots, x_n), \quad i = 1, \dots, n,$$

or, for short,

$$\frac{d\mathfrak{x}}{dt} = \mathfrak{f}(\mathfrak{x}), \tag{1}$$

with a system of **algebraic equations**

$$g_i(\mathfrak{x}, \hat{\mathfrak{x}}, \Delta t) = 0, \quad i = 1, \dots, n, \tag{2}$$

relating the value $\mathfrak{x}$ of the solution at some moment in time t with the value $\hat{\mathfrak{x}}$ of the solution at the moment in time $t + \Delta t$.
The system of the algebraic equation (2) itself will be called **a difference scheme** for a system of **the differential equations** (1).

Discrete models

In mechanics, both old and new, the quantity dt has often been treated as a finite increment, and it was implied that Newton's equations were actually difference equations [Feynman].

Example

The explicit Euler scheme

$$\hat{\mathfrak{x}} - \mathfrak{x} = \mathfrak{f}(\mathfrak{x})\Delta t$$

for linear oscillator preserves the energy $H = x^2 + y^2$ only at $\Delta t \to 0$.

Classic difference schemes (explicit Runge-Kutta schemes) have few of algebraic properties (lack of them). We describe properties of **discrete models** by looking back at continuous models.

Midpoint scheme

In 1990, the concept of geometric integrators arose: we construct schemes that inherit certain **algebraic properties** of the original continuous model.
On the midpoint scheme

$$\hat{\mathfrak{x}} - \mathfrak{x} = \mathfrak{f}\left(\frac{\hat{\mathfrak{x}} + \mathfrak{x}}{2}\right)\Delta t$$

we can tell that

- it is t-symmetric,
- it is symplectic,
- it preserves quadratic integrals (Cooper's theorem).

Systems with quadratic Hamiltonian

The midpoint scheme perfectly imitates a Hamiltonian system

$$\frac{dx}{dt} = \frac{\partial H}{\partial y}, \quad \frac{dy}{dt} = -\frac{\partial H}{\partial x} \tag{3}$$

with a **quadratic Hamiltonian** H, for example, a harmonic oscillator with Hamiltonian $H = x^2 + y^2$.

- According to Cooper's theorem, the energy integral is preserved exactly on the scheme, and the approximate solution itself is a sequence of points $\mathfrak{x}_n = (x_n, y_n)$ of the circle $x^2 + y^2 = C$.
- Each step of the approximate solution is a rotation by an angle

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

which does not depend on n.

Systems with cubic Hamiltonian

If the Hamiltonian is a **cubic polynomial**, then the exact solution to the continuous model lies on a third degree curve

$$H(x, y) = c,$$

whose genus is 1. Thus the quadrature

$$\int \frac{dx}{H_y(x, y)} = t + C$$

on the curve H is elliptic integral of the 1st kind.
If the invariant curve is closed, the functions $x(t), y(t)$ are elliptic, one of the periods is real and we see periodic movement along the oval on the phase plane xy.

Midpoint scheme for systems with cubic Hamiltonian

In the 1990s, we there was a thought that sympletic structure preservation would lead to an imitation of a continuous model in the non-linear case. The midpoint scheme is symplictic Runge-Kutta scheme, i.e.

$$d\hat{x} \wedge d\hat{y} = dx \wedge dy.$$

However, now the energy integral is not conserved, but inherit in a very tricky formulation.

Theorem (J. M. Sanz-Serna and M.P. Calvo, 1994)

For any $k \in \mathbb{N}$, there exists a polynomial $H_k(x, y, \Delta t)$ such that

- H_k *goes to* H *at* $\Delta t \to 0$,
- $H_k(\hat{x}, \hat{y}, \Delta t) = H_k(x, y, \Delta t) + O(\Delta t^k)$.

Thus, in computer experiments, it seems that approximate solution lies on closed curve $H_k(x, y) = c$ at sufficiently large k.

Problem of the extra roots

If $\mathfrak{f}$ is not linear function of $\mathfrak{x}$, than equations

$$\hat{\mathfrak{x}} - \mathfrak{x} = \mathfrak{f}\left(\frac{\hat{\mathfrak{x}} + \mathfrak{x}}{2}\right)\Delta t$$

define a multiple-valued correspondence between $\mathfrak{x}$ and $\hat{\mathfrak{x}}$ spaces. Multiple values of $\hat{\mathfrak{x}}$ correspond to the same value $\mathfrak{x}$ and vice versa. The geometric meaning of the extra roots is not clear. In numerical analysis, they are discarded.

They do not allow to investigate the algebraic properties of the midpoint scheme. This scheme is probably poor in **algebraic properties**.

Reversible schemes

Newton's equations must define a one-to-one correspondence between the initial and final positions of a dynamical system. Difference schemes define a correspondence between the initial and final positions of the system, which is described by algebraic equations. Such a correspondence will be one-to-one if and only if it is birational.

Definition

We call a difference scheme **reversible** if it specifies a birational map between an n-dimensional $\mathfrak{x}$-space and an n-dimensional $\hat{\mathfrak{x}}$-space.

We believe, that the «reversibility» is more significance than conservativity or symplectivity.

Approximate solutions by reversible scheme

Definition

The birational map of projective space is called **the Cremona transformation**.

Let a transition from layer t to layer $t + \Delta t$ be described by the Cremona transformation C depeesnding on Δt:

$$\hat{\mathfrak{x}} = C\mathfrak{x}.$$

Definition

By the approximate solution released from the point $\mathfrak{x}$, we mean the sequence

$$O(\mathfrak{x}) = \{C^m\mathfrak{x},\, m \in \mathbb{Z}\},$$

i.e., the orbit of Cremona transformation C.

Construction of reversible schemes

Any dynamical system with a quadratic right-hand side

$$\frac{d\mathfrak{x}}{dt} = \mathfrak{f}(\mathfrak{x})$$

can be approximation by the equation

$$\hat{\mathfrak{x}} - \mathfrak{x} = \mathfrak{F}\Delta t,$$

which is linear with respect to $\mathfrak{x}$ and $\hat{\mathfrak{x}}$. Thus $\hat{\mathfrak{x}}$ is a rational function of $\mathfrak{x}$ and vice verse $\mathfrak{x}$ is a rational function of $\hat{\mathfrak{x}}$.

Example

$$\frac{dx}{dt} = 1 + x^2 \quad \rightarrow \quad \hat{x} - x = (1 + x \cdot \hat{x})\Delta t.$$

An unconventional integrator of W. Kahan

Firstly, indicated method to construct reversible schemes was presented by William "Velvel" Kahan in 1993 at conference in Ontario.

> *I have used these unconventional methods for 24 years without quite understanding why they work so well as they do, when they work. That is why I pray that some reader of these notes will some day explain the methods' behavior to me better than I can, and perhaps improve them.*

In 1994 Sanz-Serna applied the method to Volterra-Latka system and explain the successes of the method to the inheritance of the symplectic structure

$$\frac{dx \wedge dy}{xy}.$$

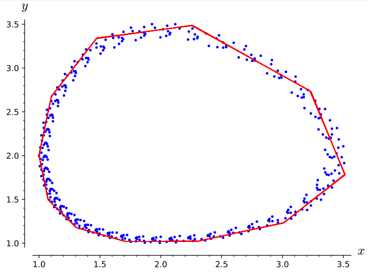
Ref.: J.M. Sanz-Serna // Applied Numerical Mathematics 16 (1994) 245-250.

Invariant curves

In two dimensional case, the points of the approximate solution lie on some curve even at big step Δt.

Example (Volterra-Lotka system)

$$\begin{cases} \dfrac{dx}{dt} = -x(y-2), \\ \dfrac{dy}{dt} = (x-2)y, \\ x(0) = 1, \quad y(0) = 2 \end{cases}$$



Two solutions were found at $\Delta t = 0.30083$

blue by the Runge-Kutta scheme and

red by the reversible scheme

Kahan's method for Hamiltonian systems

1. Geometric properties of Kahan's method are restricted to quadratic vector fields.
2. For the systems with cubic hamiltonian, Kahan's method conserved the modified Hamiltonian

$$H + \frac{\Delta t}{3} \nabla H^T \left(E - \frac{\Delta t}{2} \frac{\partial \mathfrak{f}}{\partial \mathfrak{x}} \right)^{-1} \mathfrak{f}$$

3. For the systems with cubic Hamiltonian, Kahan's method preserves the measure

$$\frac{dx_1 \wedge dx_2 \cdots \wedge dx_n}{\det \left(E - \frac{\Delta t}{2} \frac{\partial \mathfrak{f}}{\partial \mathfrak{x}} \right)}$$

Ref.: E. Celledoni et al // J. Phys. A: Math. Theor. 46 (2013) 025201

Method of Hirota and Kimura

- In 2000, reversible scheme was written by Hirota and Kimura for odes, describing the motion of the top. For 2 classical cases, modified integrals was written. The expressions for two integral for Euler-Poinsot case are the same which we presented at PCA'2022.
- In 2010, Suris et al. indicated that the scheme of Hirota and Kimura define Cremona transformation between the layers.
- In 2019, Suris et al. described the method of Hirota and Kimura for finding the integrals. It is, of course, the variation around Lagutinski method (1912).

Refs.: 1.) Hirota and Kimura // Journal of the Physical Society of Japan Vol. 69, No. 3, March, 2000, pp. 627-630; No. 10, October, 2000, pp. 3193-3199; 2.) Suris et al. // Math. Nachr. 283, No. 11, 1654 – 1663 (2010); 3.) Suris et al. // Experimental Mathematics, 26:3, 324-341 (2019).

Systems with cubic Hamiltonian, external properties

Kahan's scheme perfectly imitates a Hamiltonian system with a cubic Hamiltonian H, for example, a elliptic $\wp$-oscillator.

- According to 1st Celledoni's theorem, the symplectic structure is inherit, i.e.

$$d\hat{x} \wedge d\hat{y} = (1 + O(\Delta t))dx \wedge dy.$$

- According to 2nd Celledoni's theorem, the energy integral is inherit, thus the approximate solution itself is a sequence of points $\mathfrak{x}_n = (x_n, y_n)$ of an elliptic curve $f(x, y, \Delta t) = c$.

Ref.: Suris et al. // Proc. R. Soc. A. 2019. 475: 20180761

Systems with cubic Hamiltonian, quadrature

Consider more closely the narrowing of Cremona map to the invariant curve $f(x, y, \Delta t) = c$.
Using constructions from Picard's theorem, we can prove that the difference scheme can be again represented using quadrature

$$\int_{\mathfrak{x}}^{\hat{\mathfrak{x}}} v(x, y, \Delta t) dx = \Delta u(\Delta t),$$

where $v dx_1$ is an elliptic integral of the 1st kind on invariant curve and, of course,

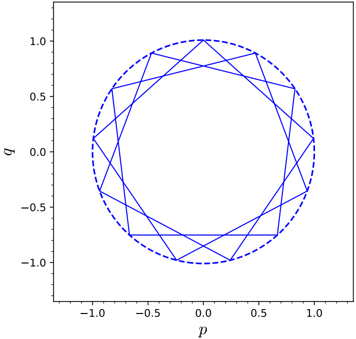
$$v dx \to \frac{dx}{H_y} \quad (\text{at} \Delta t \to 0).$$

Ref.: 1.) Malykh et al. // Mathematics 2024, 12 (1), 167; 2.) Malykh et al. // Zapiski sem. POMI. 2023

Systems with cubic Hamiltonian, internal properties

Consequences of quadrature representation:

1. The approximate solution can be represented using an elliptic function of a discrete argument.
2. We can pick a step Δt so that $O(\mathfrak{x})$ is a periodic sequence.



The reversible difference scheme imitates all the known properties of the system with cubic Hamiltonian.

Popular Q.

What about the convergence and stability of Kahan's scheme? — Kahan's sheme is Runge-Kutta scheme of 2nd order.
If invariant curve is closed, than the approximate solution has the period T, which depends on Δt. This period tends to the exact period at $\Delta t \to 0$, but of course

$$\max_{n \in \mathbb{N}} |x(n\Delta t) - x_n| \not\to 0$$

C-norm is unnatural for this problem.

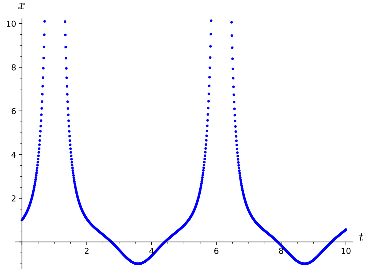
Points at infinity

If at some value k the denominator of the transformation becomes zero, then the point $\mathfrak{x}_{k+1}$ will be infinitely remote. Thus we consider $\mathfrak{x}$ as a point in the projective space $\mathbb{P}_n$.

Example ($\wp$-oscillator)

$$\begin{cases} \dfrac{dx}{dt} = y, \\ \dfrac{d}{dt}y = 6\,x^2 - 1, \\ x(0) = 1, \quad y(0) = 2 \end{cases}$$

The exact solution is periodic and has pols of 2nd degree.



The approximate solutions describe correct the behavior at infinity.

The main difference between discrete and continuous models

Newton's equations must define a one-to-one correspondence between the initial and final positions of a dynamical system.
The system with cubic Hamiltonian define birational transformation on the integral curve $H(x, y) = C$, which cannot be continued to the Cremona transformation of all planes xy (it's Hermite-Klein discussion!).
However, we can approximate the system so that transition from layer to layer is carried out by the Cremona transformation of the entire xy plane.

Systems with polynomial Hamiltonian

If the Hamiltonian is a polynomial of degree $r > 3$, then the exact solution to the continuous model lies on an algebraic curve

$$H(x, y) = c,$$

whose genus more than 1. Thus the quadrature

$$\int \frac{dx}{H_y(x, y)} = t + C$$

on the curve H is Abelian integral of the 1st kind.
Integral cannot be inverted and the functions $x(t), y(t)$ aren't meromorphical function of t (Jacobi problem).

Quadratization of dynamical systems

Formally, our method is suitable only for dynamical systems with quadratic right-side.

Theorem (Appelroth, 1902)

Any dynamical system with polynomial right-side can be rewritten as dynamical systems with quadratic right-side in new variables.

Of course, the number of new variables is more than the number of initial variables, i.e. n.
In XXI century the reduction of the given dynamical system to dynamical systems with quadratic right-side was called quadratization.
Ref: Pogudin et al. // Combinatorial Algorithms, 2021, p. 122–136.

Quadratization and discretization

Any system with polynomial Hamiltonian can be integrated by reversible scheme in two steps:

1. the quadratization by Appelroth,
2. the discretization by Kahan.

Although Newton's equations must define a one-to-one correspondence between the initial and final positions of a dynamical system, these equations do not actually define a one-to-one correspondence between the initial and final states of the system. We can impose violently this property on the difference scheme.

Natural questions are:

1. What happens at movable branch points of exact solutions?
2. What happens to the integrals that connect old and additional variables?

Example

Consider the system with Hamiltonian of this system is

$$H = \frac{{x_1}^3}{3} - \frac{{x_2}^5}{5}.$$

The solution is described by the quadrature

$$\int \frac{dx_2}{\sqrt[2/3]{\frac{3}{5}x_2^5 + 3C}} = t + C'.$$

The particular solution of the system (3) with the initial conditions $x_1 = x_2 = 1$ at $t = 0$ has a branching point $t \approx 0.52$.

Quadratisation

After quadratisation we have

$$\begin{cases} \dot{x_1} = w_0 \cdot x_2, \\ \dot{x_2} = {x_1}^2, \\ \dot{w_0} = 2 \cdot w_1 \cdot x_1, \\ \dot{w_1} = {w_0}^2 + 2 \cdot w_2 \cdot x_2, \\ \dot{w_2} = 3 \cdot {w_1}^2. \end{cases} \tag{4}$$

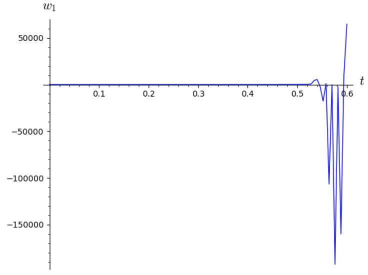
Currently, there are several implementations of quadratization: Qbee by A. Bychkov and BioCham by M. Hemery et all.

Branch point

The approximate solution passes through the branch point as a pole.

Example

Before the branch point the exact and approximate solutions are coincide. After this point the exact solution in imaginary, but the approximate is real.



Integral variety

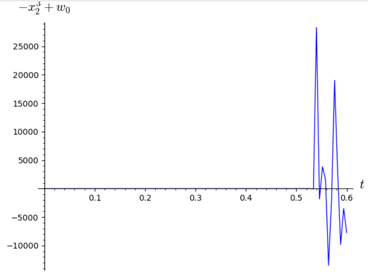
The integral that connect old and additional variables is not preserved by reversible schemes.

Example

Before the branch point the expression

$$w_0 = x_2^3$$

is equal to 0 on exact solution and is small on approximate solution, but its value at the branch point is very large (about 10^{29}).



Can this approach be recommended?

The appropriateness of applying the combined Appelroth-Kahan approach to natural phenomena depends on which properties of these phenomena are important for research and which can be sacrificed.
This approach is good if the one-to-one correspondence between the initial and final positions of the system is most important.

Conclusion

1. The midpoint scheme perfectly imitates a system with a quadratic Hamiltonian H,
2. Kahan's scheme imitates a system with a cubic Hamiltonian H if we replace birational transformations on the curve with Cremona transformations
3. The combined Appelroth-Kahan approach allows to approximate a continuous model with a polynomial Hamiltonian to a discrete model in which there is a one-to-one correspondence between the initial and final positions of the system.

Conclusion

Thus, when constructing difference schemes, we propose to move from the concept of inheritance of algebraic properties of a dynamic system (the idea of geometric integrators) to the concept of violent imposing of such properties, from the concept of mimeting a continuous model of a phenomenon — to the concept of creating a independent discrete model describing the same phenomenon.

The End

Additional materials: https://malykhmd.neocities.org