On difference schemes that inherit algebraic properties of dynamical systems

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Dynamic systems

One of the main continuous models is a dynamic system described by an autonomous system of ordinary differential equations, that is, a system of equations of the form

$$\frac{dx_i}{dt} = f_i(x_1, \ldots, x_m), \quad i = 1, 2, \ldots m, \tag{1}$$

where t is an independent variable commonly interpreted as time, $x_1, \ldots, x_m$ are the coordinates of a moving point or several points. In practice, the right-hand sides f_i are often rational or algebraic functions of coordinates $x_1, \ldots, x_m$ or can be reduced to such form by a certain change of variables.

Finite difference method

Within the framework of the finite difference method the system of differential equations is replaced with the system of algebraic equations

$$g_i(x, \hat{x}, \Delta t) = 0, \quad i = 1, \ldots, m. \qquad (2)$$

In this case, x is interpreted as the value of the solution at the time t, and $\hat{x}$ as the solution at the time $t + \Delta t$.

Example

- Euler scheme $\hat{x} - x = f(x)\Delta t$,
- midpoint scheme $\hat{x} - x = f\left(\frac{\hat{x}+x}{2}\right)\Delta t$,
- trapezoid scheme $\hat{x} - x = \frac{f(\hat{x})+f(x)}{2}\Delta t$, ...

Newton's equations as difference equations

In the course of searching for numerical methods for integrating dynamical systems, a very interesting construction was found — a difference scheme of a dynamical system that preserves all algebraic integrals of motion.
Attempts have been made for a long time to consider Newton's equations as difference equations:

$$m\frac{d^2x}{dt^2} = F(x) \quad \to \quad m\frac{\Delta^2 x}{\Delta t^2} = F(x).$$

See, for ex., [Feynman, ch. 2, §3].
However with the standard discretization such a representation faces a violation of the fundamental conservation laws.

Difference model of the dynamical system

The scheme is a difference model of the dynamical system, if

1. the schema has same discrete symmetries as the original problem, including t-symmetry

   $$dt \to -dt, \quad x \to \hat{x}, \quad \hat{x} \to x$$

   and bodies permutations in many body problem.
2. the schema preserves all algebraic integral in some sense, for ex., like

   $$g(x) = \text{const} \quad \to \quad g(\hat{x}) = g(x)$$
3. approximate solution inherits qualitative properties of exact solution like periodicity.

Euler scheme does not inherit any properties of the initial differential problem.

Midpoint scheme vs. trapezoid scheme

For ode $\dot{x} = f(x)$ there are two schemes with t-symmetry:

- midpoint scheme

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

- trapezoid scheme

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

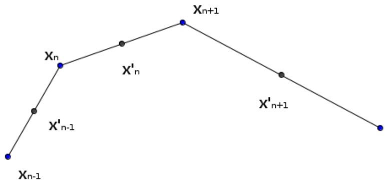
The midpoint scheme is the simplest from trapezoid schemes.

Theorem (Cooper, 1989)

The midpoint scheme preserves linear and quadratic integrals.

Principle of duality

Let $x_0, x_1, x_2, \ldots$ be approximate solution calculated by midpoint scheme. Then midpoints $x'_0, x'_1, x'_2, \ldots$ of segments of broken line $x_0 x_1 x_2 \ldots$ are approximate solution calculated by symmetric scheme.



Theorem (Yu Ying et al., DCM & ACS, 2021)

Trapezoid scheme inherits linear and quadratic integrals of the dynamical system, difference analogue for the integral $g(x)$ will be

$$g\left(x - f(x)\frac{dt}{2}\right).$$

Ex. Linear oscillator

The linear oscillator

$$\dot{x} = -y, \quad \dot{y} = x$$

has an integral $x^2 + y^2 = \text{const}$. Midpoint solution $(x_0, y_0), (x_1, y_1), \dots$ is a broken line, its vertexes lie at circle with radius R. Dual trapezoid solution $(x_0', y_0'), (x_1', y_1'), \dots$ is a broken line, its vertexes lie at circle with radius r. They will be right polygon iff

$$r/R = \cos\frac{\pi}{N}, \quad N \in \mathbb{N}.$$

This approximate solution is periodic sequence with period N iff the step Δt is a root of the equation

$$1 + dt^2/4 = \cos^2\frac{\pi}{N}, \quad N \in \mathbb{N}.$$

See: [Gerdt V.P. et al., DCM & ACS, 2019]

Ex. Jacobi oscillator

The dynamical system

$$\dot{p} = qr,\ \dot{q} = -pr,\ \dot{r} = -k^2pq,$$

integrable in terms of elliptic Jacobi functions and has two quadratic integrals.

1. The midpoint scheme preserves the quadratic integrals exactly.
2. The trapezoid scheme preserves the quadratic integrals, but the integral

$$p^2 + q^2 = \text{const}$$

turning into the polynomial

$$(p^2 + q^2)\left(1 + \frac{r^2dt^2}{4}\right).$$

Usage for numerical integration

Against use of conservative schemes for numerical integration, two fundamental considerations come to mind:

- In the case of non-integrable systems, while remaining on the integral manifold, we can decline far from the exact solution. Thus conservation laws cease to be indexers of error but it is not guarantee of success.
- All conservative schemes are implicit thus at any step we have to solve a system of nonlinear algebraic equations. This is hard job, thus the methods is not effective.

Note

Buono and Mastroserio in 2002 proposed a construction which looks like explicit RK scheme and preserves integrals. Although it is not even difference scheme, this method is very effective for numerical integration. See: [Zhang, 2020].

One step of midpoint scheme (theory)

Input: 1.) right-hand sides of equations f, 2.) initial conditions, 3.) list of quadratic integrals $g_1, \dots, g_r$, 4.) time step dt.
Output: values of $x_1, \dots x_n$ at the moment of time, differing from the initial one by dt.
In theory we have to solve the system of nonlinear equations

$$\hat{x} = x + f\left(\frac{\hat{x} + x}{2}\right) dt.$$

We try to solve it in CAS analytically, but this system is reduced to equation of the 5th degree in the simplest nonlinear case of elliptic oscillator. Thus we will use iterative numerical method to solve this system.
See: [Gerdt V.P. et al., DCM & ACS, 2019]

Many body problem

Question

How we can construct various such conservative difference schemes for the most famous family of dynamical systems, the many-body problem?

The classical problem of n bodies consists in finding solutions to an autonomous system of ordinary differential equations

$$m_i \ddot{\vec{r}}_i = \sum_{j=1}^{n} \gamma \frac{m_i m_j}{r_{ij}^3} (\vec{r}_j - \vec{r}_i) \,, \quad i = 1, \ldots, n \tag{3}$$

Here $\vec{r}_i$ is the radius vector of the i-th body, m_i is its masses, r_{ij} is the distance between the i-th and j-th bodies, and γ is the gravitational constant.

Algebraic integrals

Bruns [Whittaker, § 164] proved that every algebraic integral of motion in this system is expressed algebraically in terms of the 10 classical integrals.
The energy

$$\sum_{i=1}^{n} \frac{m_i}{2} |\vec{v}_i|^2 - \gamma \sum_{i,j} \frac{m_i m_j}{r_{ij}}$$

is not quadratic function thus midpoint scheme does not preserve energy integral.
The first finite-difference scheme for the many-body problem, preserving all classical integrals of motion, was proposed in 1992 by Greenspan and independently in somewhat different form by Simo and González.

Our idea

The simplest way to construct conservative schemes is to introduce additional variables with respect to which all algebraic integrals of the many-body problem are expressed in terms of linear and quadratic integrals.
The beginning of our study was laid by the description of a regularizing transformation, which was proposed by Burdet and Heggie, in the book by Marchal.
In other hand, the introduction of additional variables in the construction of difference schemes is known as the scalar auxiliary variable approach (SAV), proposed by Jie Shen et al.

System with quadratic polynomial integrals

Theorem

The system

$$\dot{\vec{r}}_i = \vec{v}_i, \quad m_i \dot{\vec{v}}_i = \sum_{j=1}^{n} \gamma \frac{m_i m_j \rho_{ij}}{r_{ij}^2} (\vec{r}_j - \vec{r}_i), \quad i = 1, \ldots, n$$

$$\dot{r}_{ij} = \frac{1}{r_{ij}} (\vec{r}_i - \vec{r}_j) \cdot (\vec{v}_i - \vec{v}_j), \quad i, j = 1, \ldots, n;\ i \neq j$$

$$\dot{\rho}_{ij} = -\frac{\rho_{ij}}{r_{ij}^2} (\vec{r}_i - \vec{r}_j) \cdot (\vec{v}_i - \vec{v}_j), \quad i, j = 1, \ldots, n;\ i \neq j$$

has 10 classical integrals, which are linear or quadratic with respect new variables, and the additional integrals $r_{ij}\rho_{ij} = \text{const}$ and

$$r_{ij}^2 - (x_i - x_j)^2 - (y_i - y_j)^2 - (z_i - z_j)^2 = \text{const}.$$

Conservative schemes for N body problem

Since all classical integrals of the many-body problem, as well as the additional integrals, are quadratic in their variables, any symplectic Runge-Kutta difference scheme, including the simplest midpoint one, preserves all these integrals.

The midpoint scheme written for the system with additional variables, preserves all its algebraic integrals exactly and is invariant under permutations of bodies and time reversal.

It is not difficult to create high-order schemes which preserve all integrals of motion in the many-body problem, which is one of major advantages of the proposed approach to constructing conservative difference schemes.

Proofs of Ths. see in: Gerdt V.P. et al. // ArXiv. 2007.01170.

Computer experiments with plane three-body problem

We wrote our implementation of the midpoint method in CAS Sage and applied it to the study of the dimensionless problem of the motion of three bodies of equal mass with $m_i = \gamma = 1$ on a plane. We compared three methods to solve the problem:

1. the explicit Runge-Kutta method (standard method), which does not preserve the integrals of motion,
2. the midpoint method written to the system without introducing additional variables, which preserve all quadratic integrals,
3. the midpoint method written to the system with introducing additional variables, which preserve all integrals.

Test problem

Initial condition

$$x_1 = 0,\ x_2 = 1,\ x_3 = 2,$$

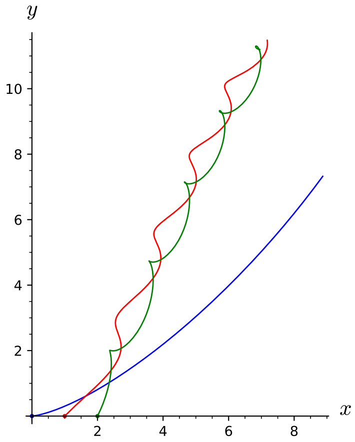
$$y_1 = 0,\ y_2 = 0,\ y_3 = 0$$

and

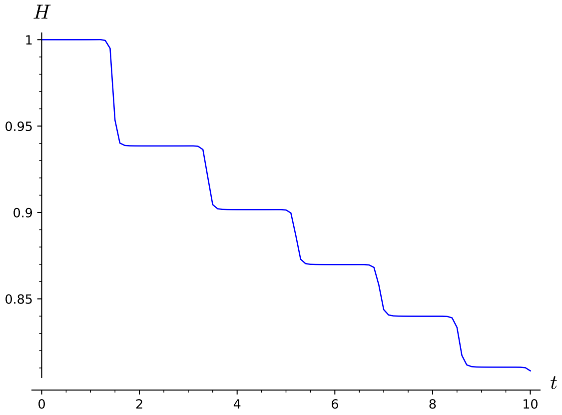
$$u1 = 0,\ u_2 = 1,\ u_3 = 1,$$

$$v_1 = 0,\ v_2 = 1,\ v_3 = 2.$$

General description: two bodies move nearby, forming cuspids and small loops.



Test problem: rk4 vs. our method



The energy does not preserve, although rk4 method describe loops on trajectories correctly.

Reversibility

Definition

By reversibility, we should understand the possibility to uniquely determine the final data $\hat{x}$ from the initial data x and vice versa using the system

$$g_i(x, \hat{x}, \Delta t) = 0, \quad i = 1, \dots, m,$$

for any fixed value of the step Δt.

Since g_i are polynomials, this means that $\hat{x}$ must be a rational function of x, and x must be a rational function of $\hat{x}$.

Example

Euler scheme $\hat{x} - x = f(x)\Delta t$ written for linear dynamical system is reversible.

Cremona transformations

We will consider $x, \hat{x}$ as two points of the projective space $\mathbb{P}_m$ and say that the difference scheme

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

is invertible if for any fixed value of Δt this scheme defines a Cremona transformation.

The combination of t-symmetry and reversibility means that the difference scheme defines a one-parameter family of Cremona transformations $\mathcal{C}$, such that

$$\hat{x} = \mathcal{C}(\Delta t)x$$

and

$$\mathcal{C}(\Delta t)^{-1} = \mathcal{C}(-\Delta t).$$

Reversibility in mechanics

Let us consider the following Painlevé initial problem

$$\frac{dx}{dt} = f(x), \quad x|_{t=t_0} = x_0 \tag{4}$$

on the segment $[t_0, t_0 + \Delta t]$ of the real axis t.
For some values of t_0, the procedure for analytic continuation of the solution obtained in the Cauchy theorem along a segment does not encounter singular points other than poles, and in this case the final value of $x(t_0 + \Delta t)$ is uniquely determined by the initial value of x_0. However, if the path encounters a branch point, then the final value depends on the way it is passed. Therefore, $x(t_0 + \Delta t)$ is a multivalued function of the initial value x_0.

Painlevé property

If a dynamical system has the global reversibility property, then it also has the Painlevé property.

Definition

A dynamical system has the Painlevé property, if the singular points of the solution are not branch points.

Example

Classical completely integrable models, including pendulums and tops, are integrable in elliptic functions and, as can be seen from the solution, have the Painlevé property.

One-dimensional case

In the one-dimensional case ($n = 1$), only the Riccati equation has the Painlevé property

$$\frac{dx}{dt} = a + bx + cx^2 \tag{5}$$

for any, including zero values of constants a, b, c. Moreover, the initial problem defines a Möbius transformation on the projective line.

It is not difficult to construct a difference scheme that inherits this property:

$$\hat{x} - x = \left(a + b\frac{x + \hat{x}}{2} + cx\hat{x} \right) \Delta t \tag{6}$$

Riccati equation

Since any birational transformation on a projective line is a Möbius one, it is easy to prove the converse.

Theorem (Malikh M.D., 2019)

In the one-dimensional case, an invertible difference scheme can be constructed only for the Riccati equation

Ref.: E. A. Ayryan et al. On Difference Schemes Approximating First-Order Differential Equations and Defining a Projective Correspondence Between Layers. Journal of Mathematical Sciences 240 (2019), 634–645. DOI: 10.1007/s10958-019-04380-0

Many dimensional case

For $n > 1$, the continuous and discrete case lose their similarity.

1. For any dynamical system with a quadratic right-hand side, a t-symmetric reversible difference scheme can be constructed:

$$\hat{x}_i - x_i = F_i(x, \hat{x})\Delta t, \quad i = 1, \ldots, n, \tag{7}$$

where F_i is obtained from f_i by replacing monomials: x_j with $(\hat{x}_j + x_j)/2$, $x_j x_k$ with $(\hat{x}_j + x_j)(\hat{x}_k + x_k)/4$, and x_j^2 with $x_j \hat{x}_j$.

2. Only a few dynamical systems with a quadratic right-hand side possess the Painlevé property.

Systems with a quadratic right-hand side

The dynamical system describing the rotation of a rigid body around a fixed point always has a quadratic right-hand side and has the Painlevé property only in 4 special cases found by S.V. Kovalevskaya.

Theorem (Appelroth, 1911)

Any dynamical system can be reduced algebraically to a system with a quadratic right-hand side.

There are effective algorithms for monomial quadratization for ODE systems [Bychkov A., Pogudin G., 2020].

Periodicity of approximate solutions

The approximate solution is a sequence $x_0, x_1, \dots,$ each next element of which is obtained from the previous one by applying the Cremona transformation $\mathcal{C}$:

$$x_{x+1} = \mathcal{C} x_n$$

This sequence will have period n, if $x_n = x_0$, i.e., if x_0 is a fixed point of $\mathcal{C}^n$.

Calculation of the step when a period and an initial value are given

Problem

Let a positive integer n and an initial value $x_0 \in \mathbb{Q}^m$ be given. We want to calculate the step Δt at which the sequence has a period n.

Considering Δt as a symbolic variable, we calculate $\mathcal{C}^n x_0$. We get m rational functions from $\mathbb{Q}(dt)$. Equating them to x_0, we obtain m of algebraic equations, the common roots of which are the required step values.
Generally speaking, several equations for one variable may not have common roots, but they have common roots in all our examples.

Examples

We have considered three examples:

1. a linear oscillator that can be easily investigated analytically,
2. $\wp$-oscillator
$$\dot{x} = y, \quad \dot{y} = 6x^2 - a, \tag{8}$$
which is integrable in terms of Weierstrass elliptic functions.
3. Jacobi oscillator, i.e., dynamical system
$$\dot{p} = qr, \, \dot{q} = -pr, \, \dot{r} = -k^2 pq, \tag{9}$$
which is integrable in terms of elliptic Jacobi functions.

We chose different initial data and considered n in the interval from 2 to 10. The degrees of polynomials, the common roots of which give the desired step values, increase exponentially with n, which significantly limited our ability to increase n.

Example 2. $\wp$-oscillator

For the $\wp$-oscillator with $a = \frac{1}{2}$ under the initial conditions $(x_0, y_0) = (1, 2)$, there are no values of step Δt for which the solution has a period $n = 2, 3, 6$. For $n = 4$ the step is independent of the starting point. The table contains all the matched positive values for Δt found for n in the top ten.

n	Δt
2	$\emptyset$
3	$\emptyset$
4	1.074
5	6.908
6	$\emptyset$
7	$0.556, 5.870, 7.759$
8	$0.535, 1.074, 6.843$
9	$0.504, 9.187$
10	$0.471, 0.559, 6.777, 6.908$

Example 3. Jacobi oscillator

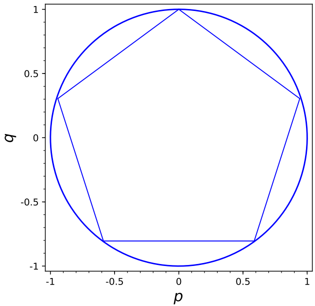
For the Jacobi oscillator with $k = \frac{1}{5}$ under the initial conditions

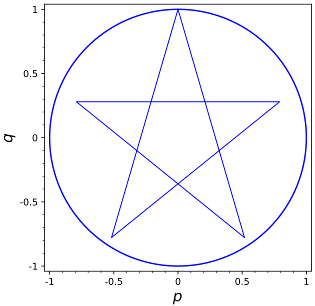
$$p = 0, \quad q = 1, \quad r = 0,$$

there are positive values of step Δt for any periods $n > 2$.

n	Δt
2	$\emptyset$
3	3.609
4	2.041
5	$1.47,\ 6.86$
6	$1.17,\ 3.60$
7	$0.97,\ 2.57,\ 10.85$
8	$0.83,\ 2.04,\ 5.18$
9	$0.73,\ 1.70,\ 3.60,\ 16.23$

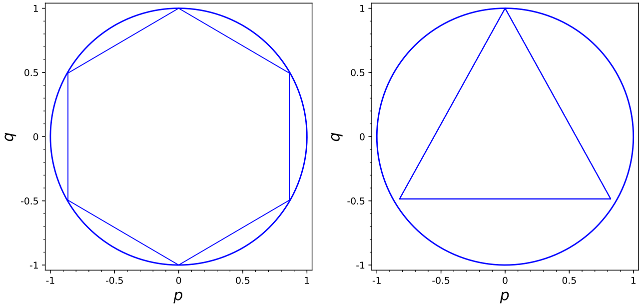
Example 3. Jacobi oscillator, $n = 5$





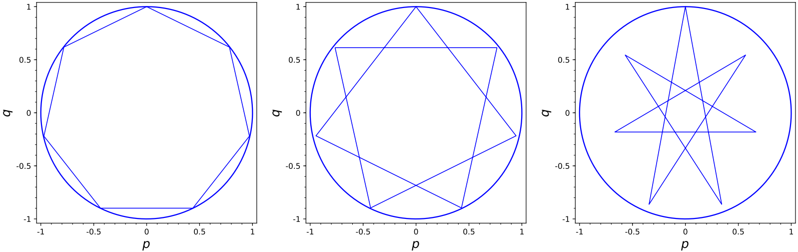
Approximate solution has the period $n = 5$ at two values of the step. In the plane pq, at the first value of the step, an almost regular pentagon is obtained and at the second value we obtain a pentagram.

Example 3. Jacobi oscillator, $n = 6$



Approximate solution has the period $n = 6$ at two values of the step. First of them is coincide with the step at $n = 3$ and give us a triangle, the second give a hexagon.

Example 3. Jacobi oscillator, $n = 7$



Approximate solution has the period $n = 7$ at three values of the step.
In all cases, the integral of motion $p^2 + q^2 = 1$ is not exactly conserved.

Example 3. Jacobi oscillator, $n \to \infty$

As n grows, the number of step values at which periodic approximations to the solution of the Cauchy problem are obtained grows. The smallest possible Δt for fixed n corresponds to an almost regular n-gon in the pq plane.
These solutions revert to their original value in times $n\Delta t$, collected in Table. These times seem to form a monotonically decreasing sequence converging to the exact period.

n	$n\Delta t$
3	10.827
4	8.164
5	7.379
6	7.022
7	6.827
8	6.706
9	6.627
∞	6.347

Results of computer experiments

It is convenient to present the results of the experiments carried out in the form of two hypotheses:

1. for any sufficiently large n and any initial conditions, one can specify a finite number of positive values for the step Δt, at which periodic sequences with the period n are obtained,
2. if we associate each n with a minimum period, we get a sequence converging to the period of the exact solution for $n \to \infty$.

By virtue of the first hypothesis, any exact particular solution can be approximated by an approximate solution that inherits the periodic nature of the exact solution, and by virtue of the second hypothesis the approximation step Δt can be taken arbitrarily small and, therefore, approach the exact solution with any given accuracy.

Equiperiodic sets

In the previous Section, we followed one solution, but changed Δt. Let us now look at the behavior of solutions in the phase space, but for a fixed Δt.

Definition

The set in the phase space formed by all the initial data generating approximate solutions with the same period n is algebraic; we will call it an equiperiodic set of the n-th order.

The equiperiodic set E is an invariant set for difference model:

$$x \in E \Rightarrow \hat{x} \in E.$$

It is easy to deduce from the first hypothesis that equiperiodic sets of sufficiently large order are not empty and have codimension 1.

Calculation of equiperiodic sets

Problem

Let a positive integer n and a step Δt be given. We want to calculate the equations described the equiperiodic set of the n-th order.

To find it in the previous algorithm, it is necessary to consider x_0 as a tuple of m symbolic variables. We managed to find these sets only for small n.

Example. $\wp$-oscillator with $a = \frac{1}{2}$

- At $n = 2$ and 3 the equiperiodic sets are empty.
- At $n = 4$ the curve equation degenerates into

$$3\Delta t^4 - 4 = 0,$$

thus the step is independent of the initial data.
- At $n = 5$ the equiperiodic set appears to be an elliptic curve

$$27\Delta t^{10}x - 432\Delta t^8 xy^2 + 432\Delta t^8 x^2 + 1728\Delta t^6 x^3 + 27\Delta t^8$$
$$-432\Delta t^6 y^2 - 936\Delta t^6 x + 168dt^4 + 240\Delta t^2 x - 80 = 0.$$

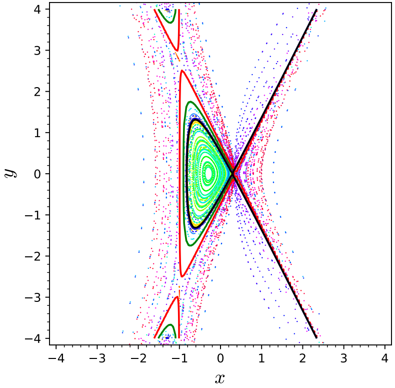
Degrees of the equiperiodic curves

The degrees of $F_n \in \mathbb{Q}[\Delta t][x, y]$ are presented in the table.
Due to the degree grows , the equiperiodic curves do not belong to the same sheaf, linear or irrational.

n	Degre of F_n
4	0
5	3
6	3
7	6
8	6
9	9
10	12

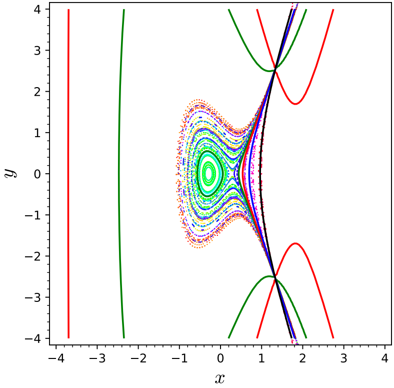
$\wp$-oscillator. Phase diagram, $\Delta t = 1$

Points of approximate solutions generated by the initial values belonging to the square $[-1,1]\times[-1,1]$ with space step $d = 1/5$, colored in HUE, and equiperiodic curves (F_5 in black, F_6 in red, F_7 in blue, F_8 in green).



$\wp$-oscillator. Phase diagram, $\Delta t = \frac{1}{2}$

Points of approximate solutions generated by the initial values belonging to the square $[-1, 1] \times [-1, 1]$ with space step $d = 1/5$, colored in HUE, and equiperiodic curves (F_5 in black, F_6 in red, F_7 in blue, F_8 in green).
It is well seen that most of the diagram points group around these curves.



$\wp$-oscillator. Phase diagram, $\Delta t = 0.471\ldots$

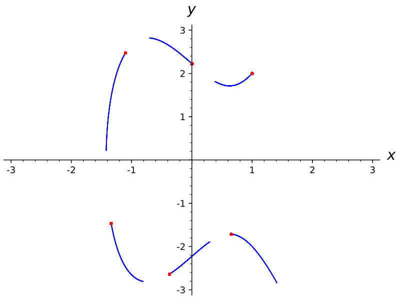
When $\Delta t = 0.471\ldots$, the approximate solution of the initial problem with the condition

$$x = 1, \quad y = 2$$

has the period $n = 10$. Thus the trajectory on xy plane consists from 10 points.
If we perturb the initial condition and take

$$x = 1.0001, \quad y = 2,$$

then the trajectory is infinite set of the points.



These points lie on a curve which repeat the form of F_{10}. Is this curve algebraic?

Differential vs. difference models

Differential model

$$\dot{x} = f(x)$$

has

1. periodic solutions $x(t+T) = x(t)$,
2. algebraic integral, i.e. there is a linear invariant sheaf

$$g(x) + ch(x) = 0,$$

3. the model define a birational transformation on integral manifold

Difference model

$$F(\hat{x}, x, \Delta t) = 0$$

with fixed step Δt has

1. sequence of equiperiodic sets $F_3, F_4, \dots,$
2. they are invariant sets for dynamical system, but they don't form a linear or irrational sheaf.
3. the model define Cremona transformation.

Invertibility vs. exact preservation of all algebraic integrals

The our ultimate goal is to create discrete models that have the most important properties of mechanical models. These include undoubtedly the inheritance of algebraic conservation laws, t-symmetry, reversibility and periodicity.
It is impossible to combine reversibility and exact preservation of all algebraic integrals.

Ref. E. A. Ayryan et al. On Explicit Difference Schemes for Autonomous Systems of Differential Equations on Manifolds. Lecture Notes in Computer Science 11661 (2019), 343–361. DOI: 10.1007/978- 3-030-26831-2_23.

Cremona transformation vs. birational transformation on an integral manifold

The starting point for this article was the observation that dynamical systems with a quadratic right-hand side can be approximated by reversible difference schemes with t-symmetry. The approximate solutions found using these schemes are birational functions of the initial data over the entire phase space. This is surprising since in the continuous case, for this property to appear, one had to restrict the phase space by an algebraic integral manifold.

Historical remark

Hermite believed that the theory of birational transformations of curves would be a section in the theory of the Cremona group, which F. Klein considered an annoying mistake, which he considered necessary to describe in detail in his Lectures on the History of Mathematics.
Now it turns out that Hermite was right after all, and there is a connection between birational transformations on curves and Cremona transformations, which manifests itself in the discretization of dynamical systems.

Results presented in the talk

1. Midpoint scheme and duality to it trapezoid scheme inherit linear and quadratic integrals of the dynamical system. To construct such schemes with non-quadratic integrals (including many-body problem) we can introduce additional variables with respect to which all algebraic integrals are expressed in terms of linear and quadratic integrals. However these schemes aren't reversible.
2. The systems with quadratic right-hand site can be approximates be reversible schemes, preserved algebraic integrals and periodicity in described above general sense.

The End

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