On computer experiments with reversible difference schemes in Sage

PCA'2024

Mark Gambaryan, Mikhail Malykh, and **Lubov' Lapshenkova**

Peoples' Friendship University of Russia, Moscow, Russia

April 17 2024, ver. April 15, 2024

This work is supported by the Russian Science Foundation (grant no. 20-11-20257).

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 equation (1).

The t-symmetry

Since schemes are algebraic equations, we want to construct the schemes that preserve the algebraic properties of the original system of odes.

Definition

We will say that the difference scheme

$$g_i(\mathfrak{x}, \hat{\mathfrak{x}}, \Delta t) = 0, \quad i = 1, \ldots, n, \tag{3}$$

has t-symmetry if the system of Equations (3) is equivalent to the system

$$g_i(\hat{\mathfrak{x}}, \mathfrak{x}, -\Delta t) = 0, \quad i = 1, \ldots, n.$$

Integrals

Definition

The difference scheme

$$g_i(\mathfrak{x}, \hat{\mathfrak{x}}, \Delta t) = 0, \quad i = 1, \ldots, n, \tag{4}$$

will be said to preserve the expression $h(\mathfrak{x}, \Delta t)$ if it follows from Equations (4) that

$$h(\hat{\mathfrak{x}}, \Delta t) = h(\mathfrak{x}, \Delta t).$$

We call that the scheme

- conserves an integral of the system of odes if the expression h does not depend on Δt.
- inherits an integral $g(\mathfrak{x})$ of the system of odes if the expression $h(\mathfrak{x}, \Delta t)$ tends to the expression $g(\mathfrak{x})$ when $\Delta t \to 0$.

Example 1

The midpoint scheme

$$\hat{\mathfrak{x}} - \mathfrak{x} = \mathfrak{f}\left(\frac{\hat{\mathfrak{x}} + \mathfrak{x}}{2}\right)\Delta t, \tag{5}$$

and the trapezoid scheme

$$\hat{\mathfrak{x}} - \mathfrak{x} = \frac{\mathfrak{f}(\hat{\mathfrak{x}}) + \mathfrak{f}(\mathfrak{x})}{2}\Delta t \tag{6}$$

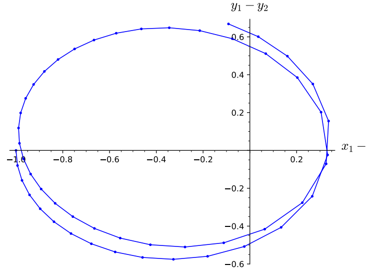
have t-symmetry. The first of them preserves the linear and quadratic integrals exactly [Cooper, 1990], the second inherits such an integral [Malykh, 2022].

Embarrassment

The preservation of all algebraic integrals and t-symmetry does not guarantee the preservation of other algebraic properties.

Example (Konyaeva, 2024)

There is a scheme that conserves all 10 motion integrals in the 2-body problem [Baddur et al., 2021], but the points of the approximate trajectory do not lie on the conical sections.



Reversible schemes

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.

This is a natural property for dynamical systems in classical mechanics, where a given initial value $\mathfrak{x}$ corresponds to one single final value $\hat{\mathfrak{x}}$, and a given final value $\hat{\mathfrak{x}}$ to one initial value $\mathfrak{x}$.
We believe, that the «reversibility» is more significant than conservativity.

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 depending 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 approximated 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

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

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-Lotka system and explain the successes of the method to the inheritance of the symplectic structure

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

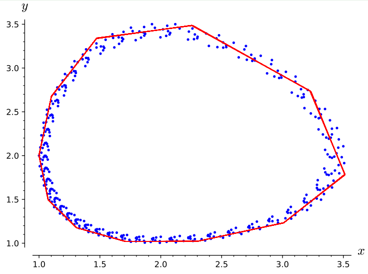
Ref.: J.M. Sanz-Serna // Applied Numerical Mathematics 16 (1994) 245-250.

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

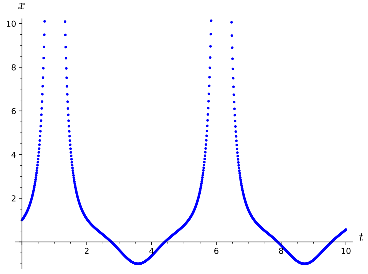
Points at infinity

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)

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

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



The approximate solutions describe correct the behavior at infinity.

Kahan's method for Hamiltonian systems

1. Geometric properties of Kahan's method 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).

Elliptic oscillators

Definition

Dynamical system with quadratic right-side will be called as elliptic oscillator if points of orbits $O(\mathfrak{x})$ lie on a curve of a genus 1 (elliptic curve) almost for any election of the point $\mathfrak{x} \in \mathbb{P}_n$.

Almost all investigated examples are elliptic oscillators.

- 2d Hamiltonian systems with cubic Hamiltonian. Celledoni's result gives us a pencil of invariant cubics, investigated by Suris et al. in 2019.
- Euler-Poinsot case of the top moving. There are two pencils of invariant surfaces in pqr space [Hirota and Kimura, 2000]. Cross-sections of two surfaces are invariant curves of genus 1.
- Jacobi oscillator as a variant of previous example, more convenient for calculations, PCA'2023.

Refs.: 1.) Suris et al. // Proc. R. Soc. A. 2019. 475: 20180761; 2.) Malykh et al. // Mathematics 2024, 12 (1), 167

Elliptic oscillators

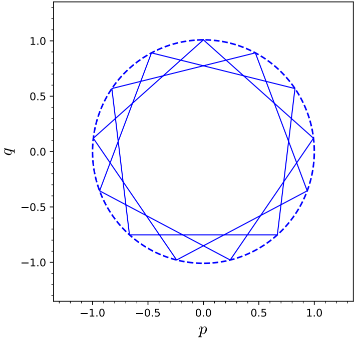
The discrete theory repeats the continuous theory completely:

1. the difference scheme can be represented using quadrature

$$\int_{\mathfrak{x}}^{\hat{\mathfrak{x}}} v(\mathfrak{x})dx_1 = \Delta u(\Delta t),$$

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

2. the approximate solution can be represented using an elliptic function of a discrete argument.



Using quadrature, we can pick a step Δt so that $O(\mathfrak{x})$ is a periodic sequence.

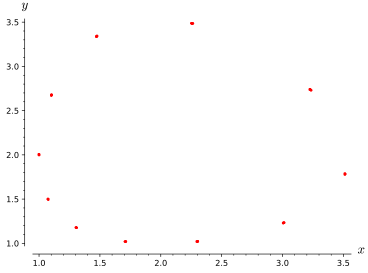
Ref: Malykh et al. // Zapiski sem. POMI. 2023

Non-elliptic oscillators

Example (Volterra-Lotka system)

The invariant curves for Volterra-Lotka system are transcendental, thus the orbits for any small step $\Delta t > 0$ can't lie on algebraic curves.

We can't pick a step Δt so that $O(\mathfrak{x})$ is a periodic sequence, but it seems that this is possible under $\Delta t = 0.30083$.
Thus the scheme can't described as a quadrature.



Non algebraic invariant curves for Cremona transformations was introduced in usage by Rerikh in 1980.
Ref: Rerikh // Translated from Teoreticheskaya i Matematicheskaya Fizika, No. 2, pp. 251-260, 1982.

Closure of the set $O(\mathfrak{x})$

Let us denote the closure of the set $O(\mathfrak{x})$ in $\mathbb{P}_n$ by $Z(\mathfrak{x})$. This set is obviously invariant under the transformation C.

The equality $Z(\mathfrak{x}) = Z(\mathfrak{x}')$ means that the different integral curves $O(\mathfrak{x})$ and $O(\mathfrak{x}')$ are close to each other, and, therefore, they should not be distinguished.

In simple cases, this set turns out to be an algebraic curve, and, therefore, the approximate solutions turn out to be periodic. In more complex cases, this set is neither algebraic nor one-dimensional, we cannot even rule out that its dimension may be fractal.

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.

Appelroth variables

Let f_i be polynomials and

$$m = \max_i \operatorname{degree}(f_i)$$

Let $z_1, \dots$ be monomials, which degree are less than m. Then

$$\frac{dx_p}{dt} = \sum_{i,j} a_{ij}^{(p)} x_i z_j + \sum_j b_j^{(p)} z_j + \sum_j c_j^{(p)} x_j + d^{(p)},$$

i.e. $\dot{x}_p$ is quadratic with respect to $x_1, \dots, z_1, \dots$. If $m_1 + \dots + m_n < m$, then

$$\frac{dx_1^{m_1} \dots x_n^{m_n}}{dt} = m_1 x_1^{m_1 - 1} \dots x_n^{m_n} \left(\sum_{i,j} a_{ij}^{(1)} x_i z_j + \dots \right) + \dots,$$

i.e. $\dot{z}_q$ is quadratic with respect to $x_1, \dots, z_1, \dots$ also.

Appelroth variables

Example

$$\frac{dx_1}{dt} = x_1^2 + x_2^2, \quad \frac{dx_2}{dt} = x_1^3 + x_2.$$

Here

$$m = 3, \text{ and } z_1 = x_1^2,\ z_2 = x_1 x_2,\ z_3 = x_2^2.$$

New system is

$$\begin{cases} \frac{dx_1}{dt} = z_1 + z_3, \quad \frac{dx_2}{dt} = x_1 z_1 + x_2, \quad \frac{dz_1}{dt} = 2x_1(z_1 + z_3), \\ \frac{dz_2}{dt} = z_1^2 + z_2 + x_2(z_1 + z_3), \quad \frac{dz_3}{dt} = 2z_1 z_2 + 2z_3. \end{cases}$$

It has an integral variety

$$z_1 = x_1^2,\ z_2 = x_1 x_2,\ z_3 = x_2^2.$$

Quadratization and discretization

Any dynamical system

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

with polynomial right-side can be integrated by reversible scheme in two steps:

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

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

This can be illustrated by a simple example.

Example

$$\frac{dx}{dt} = x^3, \quad x(0) = 1.$$

The exact solution

$$x = \frac{1}{\sqrt{1-2t}}$$

has a branch point at $t = 1/2$.
The additional variable is $z = x^2$ and thus the quadratizated system is

$$\frac{dx}{dt} = xz, \quad \frac{dz}{dt} = 2z^2$$

on the integral variety

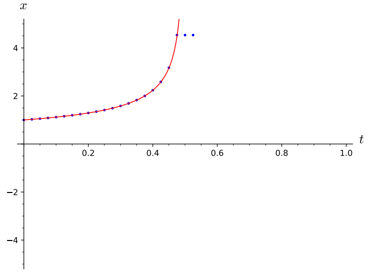
$$z = x^2$$

Branch point

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

Example

Before the point $t = 1/2$ the exact and approximate solutions are coincide. After this point the exact solution in imaginary, but the approximate is real.



Integral variety

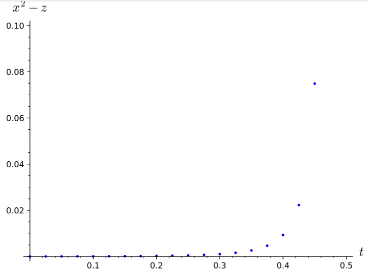
The integral that connect old and additional variables is not preserved by reversible schemes.

Example

Before the point $t = 1/2$ the expression

$$x^2 - z$$

is equal to 0 on exact solution and is small on approximate solution, but its value at $t = 1/2$ is very large (about 10^{29}).



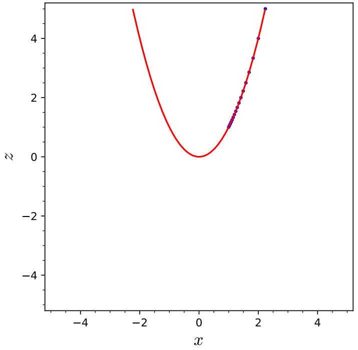
Appelroth's theorem and integrals of Kahan scheme

Example

The points of the orbit $O((1,1))$ lie almost on the curve

$$x^2 = z$$

at $t < 1/2$, but after this value of t they lie on another curve.



After quadratization we take the dynamical system with algebraic integrals, which can't preserved because the approximate solution can be continued beyond the branch point.

Effective quadratization

Appelroth's quadratization give us a lot of new variables. Sometimes the number of variables entered can be reduced.

Definition

The quadratization is called effective if there are not quadratization with fewer additional variables exists for given system.

In 2021 Pogudin et al. developed an algorithm for efficient quadratization and implemented it in the form of a library **qbee**. Any dynamical system with polynomial right-side can be integrated by reversible scheme in two steps:

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

Ref.: `https://github.com/AndreyBychkov/QBee`

Example

Let's move on to Example

$$\begin{cases} \dot{x_1} = {x_2}^4, \\ \dot{x_2} = {x_1}^2. \end{cases}$$

This system has an algebraic integral

$$\frac{{x_1}^3}{3} = \frac{{x_2}^5}{5} + C.$$

At this curve the solution described by quadrature

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

Example

Quadratized system is stated below:

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

Program specifications

Problem

Pogudin's algorythm implementations in Qbee by Bychkov are made using SymPy library.

Solution

Pogudin's algorythm implemented with Qbee integration into Sage environment.

Program listing

1. Importing all the necessary Python libraries.
2. Entering the stated problem in SymPy specifications.
3. Receiving the quadratized difference scheme:

```
res = quadratize(system)
```

Program listing

Rewriting the quadratization results into the variable as a string:

```
tmp = sys.stdout
eq_system = StringIO()
sys.stdout = eq_system
res.print()
sys.stdout = tmp
eq_system = eq_system.getvalue()
eq_system = eq_system[22:]
```

Program listing

1. Decomposing the string result into the variables.
2. Entering the independent variable and initial parameters values.
3. Using the Cremona transformation to solve the initial problem:

```
pr2 = Initial_problem([eval(dn) for dn in
    derivative_names], [eval(ed) for ed in
    equations_derivatives], [a1,a2,a3,a4,a5], 0.6)
sol2=cremona_scheme(pr2, N=100, field=RR)
```

Program listing

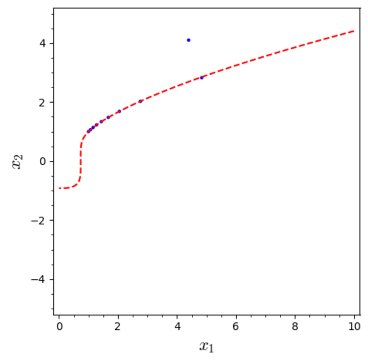
Making a comparison between approximate and exact solution:

```
u=x1**3/3-x2**5/5
pl=sol2.plot(x1,x2,points=True)+implicit_plot(u==u.
    subs([x1==1, x2==1]),(x1,0,10),(x2,-5,5),
color='red', linestyle='--')
pl.show(xmin=0,xmax=10,ymin=-5, ymax=5)
```

Results

Example

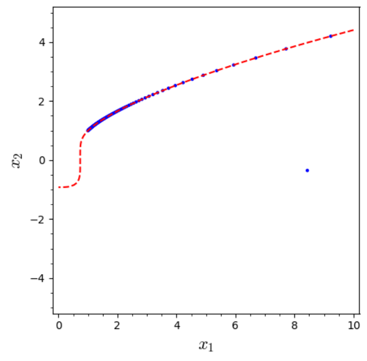
The comparison is made on $N = 10$ dots.
Most of the approximate solution points are coincide with exact solution curve.



Results

Example

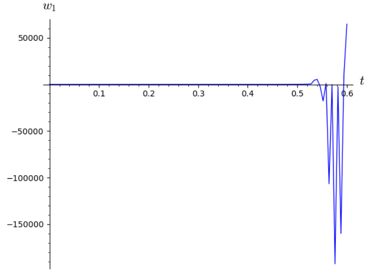
The correlation between x_2 and x_1 $N = 100$ dots accuracy is received.
One of approximate solution dots is out of the exact solution curve because of solution accuracy.



Results

Example

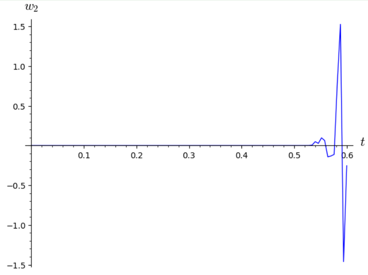
For $N = 10$ the approximate solution on the set segment $[0, t = 0.6]$ mostly coincides with the exact solution.



Results

Example

For $N = 100$ the approximate solution on the set segment $[0, t = 0.6]$ mostly coincides with the exact solution. As it stated before, point $t \approx 0.52$ is the point where the found solutions differ.



Conclusion

1. For dynamical systems with quadratic right-hand side, the difference scheme defining the birational map between layer is known since 1990s.
2. For elliptic oscillators such a scheme inherit almost all properties of dynamical like periodicity.
3. Appelroth's theorem allows you to quadratize a dynamic system with a polynomial right-hand side. Herewith:
   - The integral that connect old and additional variables is not preserved by reversible schemes.
   - The approximate solution passes through the branch point as a pole.
4. Procedures of quadratization and discretization are implemented in Sage.

The End

© 2024, Mikhail Malykh et al. Creative Commons Attribution-Share Alike 3.0 Unported.

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