On Explicit Difference Schemes for Autonomous Systems

Report for CASC'2019

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Abstract

We will consider finite difference schemes for autonomous systems of ordinary differential equations on algebraic manifolds.

Cases in point.

1. What are autonomous systems of ordinary differential equations on algebraic manifolds? How we can find integral manifolds using CAS?
2. How we can construct difference schemes preserving exactly the integral manifold? What properties do these schemes have? Why such schemes are useful?
3. When do explicit difference schemes preserving the integral manifold exist? When no? Why?

An autonomous system of differential equations

Consider an autonomous system of differential equations in an affine space of dimension r

$$\frac{dx_1}{dr} = f_1(x_1, \dots, x_n), \dots, \frac{dx_n}{dr} = f_n(x_1, \dots, x_n)$$

or, for the sake of brevity,

$$\frac{dx}{dt} = f(x). \tag{1}$$

Here $x = (x_1, \dots, x_r)$ is a point of an affine space,

$$f = (f_1, \dots, f_r)$$

is a list of rational functions from the field $\mathbb{Q}(x)$.

Integral manifolds

Definition

An algebraic manifold V will be called integral for system (1) if every integral curve of this system that has at least one common point with the manifold V belongs to this manifold entirely.

Example

The Darboux polynomial for system (1) is a polynomial g, for which it is possible to specify a polynomial h, such that

$$\frac{dg}{dt} = \sum_{i=1}^{r} f_i \frac{\partial g}{\partial x_i} = hg.$$

Therefore, the hypersurface $g(x) = 0$ in the affine space is an integral manifold for system (1).

Using CAS for searching of integral manifolds

Problem

Given an autonomous system (1)*, clarify whether an algebraic integral exists. If the answer is positive, present such an integral.*

Problem

Given an autonomous system (1)*, clarify whether a Darboux polynomial exists. If the answer is positive, present such a polynomial.*

In all known algorithms for solution of these problems a user must give a boundary for degree of required integral or Darboux polynomial [Chèze G., 2011].

Lagutinski method for searching of integral manifolds

Most general method for finding of integral and Darboux polynomial was suggested by M.N. Lagutinski in 1914 and rediscovered by J.-M. Strelcyn in 1990s.
Our realization of Lagutinski method was presented at PCA'2016 in St. Petersburg.

- Version for CAS Sage (Malykh M.D., Yu Ying) is available at my site `malykhmd.neocities.org`,
- Version for Math Partner (Malashonok G.I.) is available at `mathpar.cloud.unihub.ru`

Autonomous systems on algebraic manifolds

The search for the solutions of system (1) belonging to a known integral manifold will be referred to as a problem of autonomous system integration on the manifold.

Example

The motion of a top is described by six variables, which satisfy a system of six autonomous equations with quadratic right-hand side

$$
\begin{aligned}
A\dot{p} &= (B - C)qr + Mg(y_0\gamma'' - z_0\gamma'), \dots \\
\dot{\gamma} &= r\gamma' - q\gamma'', \dots
\end{aligned}
$$

There are only three algebraic integrals of motions. Therefore, this system of differential equations should be considered not in the entire six-dimensional space, but in a three-dimensional manifold embedded in it.

The finite difference method

The system of differential equations (1) is replaced with an algebraic system of equations that describe a transition from the value x of the solution at a certain moment of time t to the approximate value $\hat{x}$ of the solution at the moment of time $t + \Delta t$.

Example

The explicit Euler scheme

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

describes such a transition and yields for $x(t + \Delta t)$ the approximate value $\hat{x}$.

Below we consider x and $\hat{x}$ as points of two adjacent layers, and the difference scheme as a system of equations specifying the transition from one layer to another.

The conservation of integral manifolds

The popular difference schemes (like Euler, Runge-Kutta) don't conserve integral manifolds: from $x \in V$ it does not follow that $\hat{x} \in V$.

Popular idea

Since for the exact solution $x(t + \Delta t) \in V$, the deviation of the points of an approximate solution from the manifold V can be used as an estimate for the error of the numerical method.

Example

In the problem of top rotation, this means considerable violation of fundamental laws of mechanics, e.g., introduces "numerical" dissipation into a dissipation-free system. It is particularly annoying when the geometric constraints are affected, e.g., a sum of direction cosine squares becomes not equal to 1. The interpretation of this result is not understandable.

Infinitely small dt in classical mechanics

The laws of classical mechanics are formulated for infinitely small dt, although in reality this quantity should be rather large to neglect quantum mechanical effects [Feynman]. However, the transition from a continuous equation of motion

$$\frac{dp}{dt} = -\frac{\partial H}{\partial x}(x, p), \quad \frac{dx}{dt} = \frac{\partial H}{\partial p}(x, p)$$

to a finite-difference one

$$\frac{\hat{p} - p}{\Delta t} = -\frac{\partial H}{\partial x}(x, p), \quad \frac{\hat{x} - x}{\Delta t} = \frac{\partial H}{\partial p}(x, p)$$

leads to the violation of the energy conservation law

$$H(\hat{x}, \hat{p}) = H(x, p).$$

We want to show that there are such scheme which more convenient to modeling in classical mechanics.

Conservative difference schemes

Definition

A difference scheme for system (1) on the manifold V is called conservative, if it assigns to a general point $x \in V$ a point $\hat{x}$ that also belongs to this manifold. In this case, we will speak that the difference scheme conserves the manifold V exactly.

Questions:

1. Such schemes exist?
2. If yes, what are their properties?
3. Haw we can construct such schemes?

We can construct simple examples when such scheme exist using the midpoint scheme.

The midpoint scheme

By mean value theorem, for any function G there exists a point c in (a, b) such that

$$G(b) - G(a) = G'(c) \cdot (b - a),$$

but in general we can't find such a value of c. If G is quadratic function then $c = \frac{b+a}{2}$.

Theorem (Cooper, 1987)

The midpoint scheme

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

conserves all quadratic integrals of the autonomous system (1).

Ex. 1. The harmonic oscillator

Consider a standard model described the motion of linear oscillator

$$\frac{dx}{dt} = -y, \quad \frac{dy}{dt} = x,$$

There is only one algebraic integral

$$x^2 + y^2 = C.$$

Thus the midpoint scheme

$$\hat{x} - x = -(\hat{y} + y)\frac{\Delta t}{2}, \quad \hat{y} - y = (\hat{x} + x)\frac{\Delta t}{2}$$

conserves the integral manifold $x^2 + y^2 = C$.

Ex. 1. The properties of the approximate solutions

Let's take a point (x_0, y_0) on the plane xy and calculate partial solution (x_0, y_0), $(x_1, y_1), \dots,$ by the midpoint scheme

$$x_{N+1} - x_N = -(y_{N+1} + y_N)\frac{\Delta t}{2}, \quad y_{N+1} - y_N = (x_{N+1} + x_N)\frac{\Delta t}{2}$$

For any integer N the calculation with the step

$$\Delta t = 2 \tan \frac{\pi}{N} \in \overline{\mathbb{Q}}$$

give a periodic series, that is

$$x_N = x_0, \quad y_N = y_0.$$

Thus:

1. the approximate trajectory on xy plane is closed and
2. the approximate solution is periodic functions of t with period

$$N\Delta t = 2N \tan \frac{\pi}{N} \to 2\pi \quad (N \to \infty)$$

The first important observation

In example 1, the verbal description of the exact solution and the approximate one found in this way will be identical:

- one conservation law is valid, for the energy;
- the trajectories on xy plane are closed curves;
- the variable x periodically oscillates with constant amplitude.

Observation

It is difficult, if possible at all, to detect qualitative differences between the exact and approximate solutions, and only quantitative discrepancies due to the precision of the period calculation are seen at large values of t.

For ex., the difference between approximate and exact periods is equal to

$$2N \tan \frac{\pi}{N} - 2\pi = \frac{2\pi^3}{3} \frac{1}{N^2} + \dots$$

Ex. 2. The elliptic oscillator

By definition, the Jacobi elliptic functions

$$p = \mathrm{sn}\ t, \quad q = \mathrm{cn}\ t, \quad r = \mathrm{dn}\ t$$

are the solutions of the nonlinear system

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

with initial conditions

$$p = 0,\ q = r = 1 \text{ at } t = 0.$$

This autonomous system possesses two quadratic integrals of motion

$$p^2 + q^2 = \text{const} \quad \text{and} \quad k^2 p^2 + r^2 = \text{const}. \tag{3}$$

The elliptic modulus k will be fixed below and, thus, the second argument of Jacobi functions will not be indicated.

Ex. 2. The midpoint scheme for the elliptic oscillator

By Cooper theorem the midpoint scheme

$$\begin{cases} 4(\hat p - p) = (\hat q + q)(\hat r + r)\Delta t \\ 4(\hat q - q) = -(\hat p + p)(\hat r + r)\Delta t \\ 4(\hat r - r) = -k^2(\hat p + p)(\hat q + q)\Delta t \end{cases}$$

conserves these integrals exactly. These equations are nonlinear with respect to $\hat p, \hat q, \hat r$.

- For numerical calculation of approximate solutions we have to solve nonlinear system of algebraic equations on each step.
- For investigation of qualitative properties of approximate solutions we have to use the elimination technique for many variables.

The comparison of standard solvers for the solution of the system (2) in terms of preservation of integrals of the motion is presented in the talk of Yu. A. Blinkov and V.P. Gerdt at PCA'2019.

The second important observation

Observation

For linear differential equations, the midpoint scheme is described by a system of linear algebraic equations for $\hat{x}$ and therefore, it is easy to organize the transition from layer to layer.
On the contrary, in the case of nonlinear equations, this scheme is described by a system of nonlinear equations, the solution of which is the main difficulty in practical application of such schemes.

The numerical solution of systems of nonlinear equations is always associated with a number of complexities, therefore, there is no universal numerical method for solving such systems [Numerical Recipes].

Explicit schemes

Definition

A difference scheme describing the transition from layer to layer by a system of linear algebraic equations for $\hat{x}$ is called explicit.

Of course, from the point of view of this definition, the implicit Euler scheme

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

for a linear differential equation is explicit, and for a nonlinear one, it is implicit. In the following, we consider nonlinear equations, so this difference is not fundamental.

The main problem

Problem

Given an autonomous system (1) *and its integral manifold* V*, clarify whether an explicit difference scheme exists that approximates this system and exactly preserves the integral manifold. If the answer is positive, present such a difference scheme.*

Solving this problem have to use theorems from algebraic geometry and calculation in computer algebra systems.

We believe that in future solving of differential equations will consist of two stages:

1. generation of the finite difference scheme with given properties in CAS,
2. numerical calculation of partial solutions by this scheme.

About explicit conservative schemes for ex. 2

Theorem

Suppose that there is an explicit conservative scheme for the system

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

on the integral curve

$$V: \quad p^2 + q^2 = 1 \quad \text{and} \quad k^2p^2 + r^2 = 1.$$

Then

$$\int_{(p,q,r)}^{(\hat{p},\hat{q},\hat{r})} \frac{dp}{qr} = \beta(\Delta t), \tag{4}$$

where β is an analytic function of Δt.

The proof is closely related to algebraic geometry.

Algebraic background: genus

In algebraic geometry, curves are characterized by an integer non-negative number called the genus. Modern computer algebra systems, including Maple and Sage, can calculate this number for a given curve.
The genus of the curve

$$V: \quad p^2 + q^2 = 1 \quad \text{and} \quad k^2p^2 + r^2 = 1.$$

is equal to 1, thus the curve is birational equivalent to an elliptic curve.

Algebraic background: differential

Since only one of the variables p, q, r is independent on the curve V, an Abelian differential can always be written as $H(p,q,r)dp$, where H is a rational function on V. The integral

$$\int H(p,q,r)dp$$

without non-integrable singularity at any point of V (even at infinity) is called an integral of the 1st kind. The set of such integrals is a linear space and its dimension is equal to the genus.

On elliptic curve, there is a single Abelian integral of the 1st kind up to a multiplicative constant. In our case this is

$$\int \frac{dp}{qr}.$$

The sketch of the proof of the theorem

1. For the explicit conservative scheme:
   1. $\hat{p}, \hat{q}, \hat{r}$ are rational functions on the curve V (due to the scheme is explicit),
   2. if $x = (p, q, r) \in V$, then $\hat{x} = (\hat{p}, \hat{q}, \hat{r}) \in V$ (due to the scheme is conservative).
2. The integral

$$\int\limits_{o}^{(\hat{p},\hat{q},\hat{r})} \frac{dp}{qr},$$

with any choice of the upper limit, remains finite, and, therefore, is an integral of the first kind, that is

$$\int\limits_{o}^{\hat{x}} \frac{dp}{qr} = \alpha(\Delta t) \int\limits_{o}^{x} \frac{dp}{qr} + \beta(\Delta t).$$

Algebraic form of the scheme

Using the addition theorem for elliptic functions, the relation

$$\int_{(p,q,r)}^{(\hat{p},\hat{q},\hat{r})} \frac{dp}{qr} = \beta(\Delta t),$$

can be rewritten in algebraic form as

$$\hat{p} = \frac{p \ \mathrm{cn}\ \beta \ \mathrm{dn}\ \beta - \mathrm{sn}\ \beta \, qr}{1 - k^2 p^2 \, \mathrm{sn}^2 \, \beta}$$

$$\hat{q} = \frac{q \ \mathrm{cn}\ \beta - \mathrm{sn}\ \beta \ \mathrm{dn}\ \beta \, pr}{1 - k^2 p^2 \, \mathrm{sn}^2 \, \beta}$$

and

$$\hat{r} = \frac{r \ \mathrm{dn}\ \beta - k^2 \, \mathrm{sn}\ \beta \ \mathrm{cn}\ \beta \, pq}{1 - k^2 p^2 \, \mathrm{sn}^2 \, \beta}.$$

Thus $\mathrm{sn}\, \beta$ must be an algebraic function.

Using the condition of the approximation

The explicit conservative scheme exists iff we can choose β so that the difference scheme approximates the original differential equation, i.e.,

$$\beta = \Delta t + \mathcal{O}(\Delta t^2),$$

and that the equations describing the transition from layer to layer depend on Δt algebraically.
This can be achieved by taking

$$\mathrm{sn}\ \beta = \Delta t, \quad \mathrm{cn}\ \beta = \sqrt{1-\Delta t^2}, \quad \mathrm{dn}\ \beta = \sqrt{1-k^2\Delta t^2}.$$

The explicit conservative schemes for ex. 2

Theorem

The scheme

$$\hat p = \frac{p\ \mathrm{cn}\ \beta\ \mathrm{dn}\ \beta - \mathrm{sn}\ \beta\, qr}{1 - k^2 p^2\, \mathrm{sn}^2\, \beta}$$

$$\hat q = \frac{q\ \mathrm{cn}\ \beta - \mathrm{sn}\ \beta\ \mathrm{dn}\ \beta\, pr}{1 - k^2 p^2\, \mathrm{sn}^2\, \beta},$$

$$\hat r = \frac{r\ \mathrm{dn}\ \beta - k^2\, \mathrm{sn}\ \beta\ \mathrm{cn}\ \beta\, pq}{1 - k^2 p^2\, \mathrm{sn}^2\, \beta},$$

where

$$\mathrm{sn}\ \beta = \Delta t, \quad \mathrm{cn}\ \beta = \sqrt{1 - \Delta t^2}, \quad \mathrm{dn}\ \beta = \sqrt{1 - k^2 \Delta t^2},$$

is an explicit conservative schemes for ex. 2.

This is exactly Gudermann's method for calculation of the elliptic functions. We check this scheme in num. experiments Sage.

The periodicity of an approximate solution

Let's take a point $x^{(0)} = (0,1,1)$ in the space pqr and calculate partial solution $x^{(0)}, x^{(1)}, \dots$ by the scheme

$$\int_{(p,q,r)}^{(\hat{p},\hat{q},\hat{r})} \frac{dp}{qr} = \beta(\Delta t).$$

The equation

$$p^{(N)} = p^0, \quad q^{(N)} = q^{(0)}, \quad r^{(N)} = r^{(0)}$$

is equivalent to

$$N\beta = \int_{(0,1,1)}^{(0,1,1)} \frac{dp}{qr} = \oint \frac{dp}{qr} = 4K.$$

or

$$\Delta t = \operatorname{sn} \frac{4K}{N} \in \overline{\mathbb{Q}}.$$

The first important observation again

In example 2, the verbal description of the exact solution and the approximate one found in this way will be identical:

- one conservation law is valid, for the energy;
- the trajectories on pqr space are closed curves;
- the variable p periodically oscillates with constant amplitude.

Observation

It is difficult, if possible at all, to detect qualitative differences between the exact and approximate solutions, and only quantitative discrepancies due to the precision of the period calculation are seen at large values of t.

For ex., the difference between approximate and exact periods is equal to

$$N \,\mathrm{sn}\, \frac{4K}{n} - 4K = -\frac{k^2+1}{6}\frac{4^3K^3}{N^2} + \mathcal{O}\left(\frac{1}{N^4}\right)$$

The barrier for existence of explicit conservative schemes

Whether there is always a scheme that approximates the system and exactly preserves the integral manifold?

Theorem

Let the autonomous system have an integral curve of the genus ρ.

1. *If the genus is 0, then there is an infinite number of explicit difference schemes that preserve this curve exactly.*
2. *If the genus is 1, then such scheme exists if and only if*

$$\int \frac{dx_1}{f_1}$$

is an integral of the first kind on the curve V.

3. *If the genus is greater than 1, then such a scheme does not exist.*

Examples

1. If the genus is 0, then there is an infinite number of explicit difference schemes that preserve this curve exactly

Example (1)

The genus of the curve $x^2 + y^2 = C$ is equal to 0. There is explicit conservative scheme for the harmonic oscillator.

2. If the genus is 1, then such scheme exists iff $\int \frac{dx_1}{f_1}$ is an integral of the first kind on the curve V.

Example (2)

The genus of an elliptic curve is equal to 1. There is explicit conservative scheme for the elliptic oscillator.

3. If the genus is greater than 1, then such a scheme does not exist.

Algebraic background: algebraic correspondences

Let V and $\hat{V}$ be affine manifolds, embedded in A_r,

$$\xi = (\xi_1, \ldots, \xi_r) \quad \text{and} \quad \hat{\xi} = (\hat{\xi}_1, \ldots, \hat{\xi}_r)$$

being two tuples, each with r symbolic variables.

Definition

The system of algebraic equations

$$g_1(\xi, \hat{\xi}) = 0, \ldots \tag{5}$$

is said to specify an algebraic correspondence of the $(n, \hat{n})$ type between the manifolds V and $\hat{V}$, iff this system possess the following two properties.

Algebraic background: the properties from previous slide

- If ξ is chosen as coordinates of a general point x of the manifold V, then the system

$$g_1(x, \hat{\xi}) = 0, \dots \tag{6}$$

with respect to $\hat{\xi}$ has $\hat{n}$ different roots, lying on the manifold $\hat{V}$ and changing under variation of x.

- If $\hat{\xi}$ is taken to be coordinates of a general point $\hat{x}$ of the manifold $\hat{V}$, then the system

$$g_1(\xi, \hat{x}) = 0, \dots \tag{7}$$

with respect to ξ possesses n different roots, lying on the manifold V and changing under variation of $\hat{x}$.

The idea for the proof of the theorem, the case $\rho > 1$

An explicit difference scheme that preserves the integral curve V defines a correspondence of the type $(n, 1)$ on this curve.
Therefore, by Zeuthen formula we have

$$2(n-1)(\rho-1) \leq 0.$$

The number is $n = 1$ and the explicit scheme defines a birational correspondence.
If such a scheme really existed, then, by giving Δt different values, we would get infinitely many birational transformations on the curve V. However, by virtue of the theorem, first indicated, probably by Picard, the group of birational transformations on an algebraic curve is finite.

The generalization of the results

We assume that an autonomous system on a manifold admits an explicit conservative difference scheme in two cases.

1. First, if this variety is Abelian and the system itself is integrated in Abelian functions, an example of such a system is a top in the Kovalevskaya case, a double pendulum , the Garnier system...
2. Second, if a rational replacement can reduce the original system to a system of the same kind, but of a smaller order.

It should be noted that these cases coincide with such cases when an autonomous system on a manifold is integrable in classical transcendental functions [Painleve, 1897; Umemura, 1990; Malykh, 2015] . Thus there is a connection between finite difference method and analytical theory of differential equations.

Conclusion, 1

Q. How we can find integral manifolds using CAS?

- This question belongs to Computer algebra and now there are several routines for calculations of algebraic integrals and Darboux polynomials.
- There are unsolved problems with finding orders of required polynomials.

We believe that the generalization of Bruns works [Bruns, 1888] give us solution of these problems.

Conclusion, 2

Q. How we can construct difference schemes preserving exactly the integral manifold? What properties do these schemes have? Why such schemes are useful?
We considered two examples when difference schemes preserving exactly the integral manifold. In the examples, the verbal description of the exact solution and the approximate one found in this way will be identical:

- conservation laws are valid;
- the trajectories are closed curves at some values of the step;
- the solution periodically oscillates with constant amplitude.

Conclusion, 3

Q. When do explicit difference schemes preserving the integral manifold exist? When no? Why?

- The problem about constructing explicit difference schemes preserving exactly the integral manifold was formulated and solved for simplest case when integral manifolds are curves.
- The genus of the integral curves is a barrier for constructing such schemes.

The generalization of this ideas requires a development of theory and software for working with algebraic surfaces and manifolds of large dimensions.

The end.

See additional materials on `http://malykhmd.neocities.org`.