Lecture 1

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Up to ca 1985-1990 the main concern when solving ODEs was

1. Design methods which were accurate on finite time intervals $0 \le t \le T$
2. By accurate to make the global error as small as possible, e.g. trying to minimize quantities such as

$$\max_n \|y_n - y(t_n)\|, \quad 0 \le n \le T/h$$

   where

$$\begin{aligned} t_n = nh \ & \text{and } h \text{ is the stepsize of the method} \\ y(t_n) \ & \text{is the exact solution at } t = t_n \\ y_n \ & \text{is the numerical approximation } y_n \approx y(t_n) \end{aligned}$$

3. From this point of view one developed Runge–Kutta methods, linear multistep methods, Taylor series methods etc

The central ideas for constructing methods were

1. The concept of order of consistency, i.e. consider largest p such that
$$y_n - y(t_n) = \mathcal{O}(h^p)$$
2. Ensure stability in some suitable form, to somehow control the growth of the numerical solution (many definitions and approaches have been proposed over the years)
3. The concept of stiffness was introduced and gave guidelines for the use of explicit vs implicit integrators

Structure preservation is typically considered whenever

- An important structure can be identified in the exact solution (exact flow of the ODE vector field)
- The same structure makes sense also for the numerical integrator

Structure-preserving discretization of differential equations means to enforce the numerical method to inherit a given structure from the exact solution of the differential equation

In this course we shall learn

1. Which structures are useful to preserve in differential equations (what do we mean by structure)
2. How to design or identify numerical methods which preserve such structure
3. Which are the benefits of preserving structure

1. The most famous "structure" in geometric integration is probably the symplectic form. We shall learn that the class of ODEs called Hamiltonian problems have the property that the exact solution preserves such a symplectic form. We shall see that methods which preserve the same form can be defined
2. Volume preservation. Hamiltonian problems preserve the standard volume form. In general, vector fields which are divergence free has exact solutions which preserve volume. Can integrators preserve volume?
3. Preservation of first integrals. E.g. the exact solution of Hamiltonian problems preserve the Hamiltonian function (the energy). This means

$$\frac{\mathrm{d}}{\mathrm{d}t}H(y(t)) = \nabla H(y(t)) \cdot \dot{y}(t) = 0$$

The numerical counterpart is

$$H(y_n) = H(y_0) = C, \qquad \text{for all } n \in \mathbb{N}$$

4. Lie group structure. A Lie group is a manifold with a group structure. The exact solution of many ODE systems is naturally described by the action of a Lie group. A numerical solution may be constructing by using the same group action. More later.

5. Reversibility. Let ρ be an invertible map on the "solution space" (phase space). A differential equation $\dot{y} = f(y)$ is ρ-reversible if

$$D\rho \circ f = -f \circ \rho$$

Write $y(t) = \varphi_t(y_0)$. The solution of ρ-reversible methods satisfies

$$\rho \circ \varphi_t = \varphi_t^{-1} \circ \rho$$

Numerical methods ϕ_h which do the same are called ρ-reversible methods. These are related to symmetric methods

This picture is stolen from the book by Hairer, Lubich and Wanner.

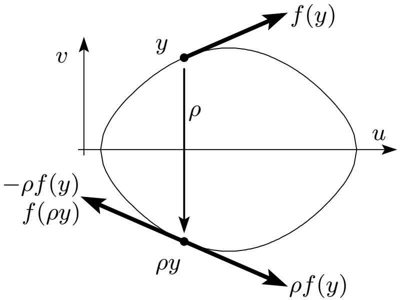


Fig. 1.1. Reversible vector field (left picture) and reversible map (right picture)

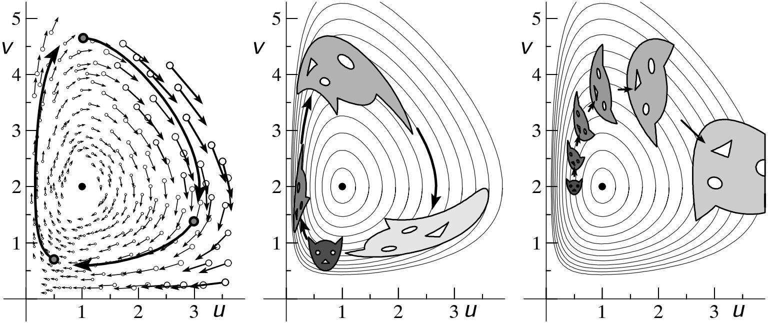
- $u(t)$ number of predators
- $v(t)$ number of prey

$$\dot{u} = u(v - 2)$$
$$\dot{v} = v(1 - u)$$

In general, autonomous ODE systems can be written in the form

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

- y is a point in phase space
- $f(y)$ is a vector field (velocity or tangent at y)
- flow: $\varphi_t : y_0 \mapsto y(t)$ if $y(0) = y_0$



v
u
1
2
3
4
5

$$\dot{u} = u(v-2), \qquad \dot{v} = v(1-u)$$

Divide by each other and separate variables, then

$$0 = \frac{1-u}{u}\dot{u} - \frac{v-2}{v}\dot{v} = \frac{\mathrm{d}}{\mathrm{d}t} I(u,v)$$

with invariant or first integral

$$I(u,v) = \ln u - u + 2\ln v - v$$

- Every solution lies on a level curve of I
- level curves are closed, thus all solutions are periodic

autonomous problem $y' = f(y)$

- explicit Euler method:

$$y_{n+1} = y_n + hf(y_n)$$

- implicit Euler method:

$$y_{n+1} = y_n + hf(y_{n+1})$$

- implicit midpoint rule:

$$y_{n+1} = y_n + hf\left(\frac{y_n + y_{n+1}}{2}\right)$$

Discrete or numerical flow $\Phi_h : y_n \mapsto y_{n+1}$

$$\dot{u} = f(u, v), \qquad \dot{v} = g(u, v)$$

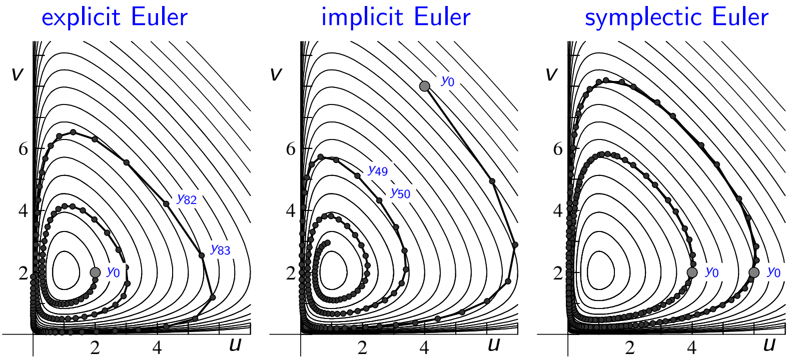
combine explicit and implicit Euler yields symplectic Euler

$$u_{n+1} = u_n + hf(u_n, v_{n+1})$$
$$v_{n+1} = u_n + hg(u_n, v_{n+1})$$

or

$$u_{n+1} = u_n + hf(u_{n+1}, v_n)$$
$$v_{n+1} = u_n + hg(u_{n+1}, v_n)$$

Method 1 is explicit if $f(u, v) = f(u)$ and $g(u, v) = g(v)$
Method 2 is explicit if $f(u, v) = f(v)$ and $g(u, v) = g(u)$


explicit Euler
implicit Euler
symplectic Euler
v
6
4
2
2
4
u
y_0
y_{82}
y_{83}
y_{49}
y_{50}

The collected energy of the planets

$$H(p,q) = \frac{1}{2}\sum_{i=0}^{5}\frac{1}{m_i}p_i^\top p_i - g\sum_{i=1}^{5}\sum_{j=0}^{i-1}\frac{m_i m_j}{\|q_i - q_j\|}$$

- astronomical units (1 A.U. = 149 597 870 km)
- masses relative to mass of sun
- $m_0 = 1.00000597682$ (account for inner planets)
- $g = 2.95\ldots10^{-4}$ gravitational constant
- initial positions and initial velocity from Sept. 5, 1994, 0h00

Numerical tests – outer solar system