Simultaneous preservation of two or more geometric properties, Network wide training course 6

Elena Celledoni

February 5, 2021

1 Simultaneous preservation of two or more geometric properties

1.1 Energy-momentum methods

The energy momentum methods are discrete gradient methods which also preserve the components of the angular momentum for certain special problems. The following exercise gives an example of a energy-momentum method introduced by Simo, Tarnow and Wong in 1992 [30].

Exercise 1.1 *Consider the Hamiltonian*

$$H(q,p) = \frac{1}{2m}p^T p + U(q)$$

where p *and* q *are vectors of* $\mathbf{R}^3$ *and describe the motion of a particle of mass* m *in space. We assume*

$$U(q) = V(\|q\|).$$

The corresponding Hamiltonian system takes the form

$$\begin{cases} \dot{q} = \frac{1}{m}p, \\ \dot{p} = -\nabla U(q), \end{cases} \tag{1}$$

and $\nabla U(q) = V'(\|q\|)\frac{q}{\|q\|}$. *We consider the following modification of the midpoint rule*

$$\begin{bmatrix} \frac{q_{n+1}-q_n}{h} \\ \frac{p_{n+1}-p_n}{h} \end{bmatrix} = \begin{bmatrix} O & I \\ -I & O \end{bmatrix} \cdot \begin{bmatrix} \kappa\,\nabla U(\frac{q_{n+1}+q_n}{2}) \\ \frac{1}{m}\frac{p_{n+1}+p_n}{2} \end{bmatrix}$$

where κ *is a scalar.*

1. *Prove that the equation* (1) *has the components of* $q \times p$ *as invariants*[1].
2. *Prove that for an appropriate choice of the scalar factor* κ *(a function of* q_n, p_n, q_{n+1}, p_{n+1}*),*

$$\bar{\nabla} H := \begin{bmatrix} \kappa\,\nabla U(\frac{q_{n+1}+q_n}{2}) \\ \frac{1}{m}\frac{p_{n+1}+p_n}{2} \end{bmatrix}$$

is a discrete gradient and therefore the method is energy preserving.

[1] $q \times p$ is the angular momentum of the particle.

3. Prove that the method preserves angular momentum, i.e.

$$q_{n+1} \times p_{n+1} = q_n \times p_n, \quad n = 1, 2, \dots$$

Proof.

1. We have
$$\frac{d}{dt}(q \times p) = \dot{q} \times \dot{p} + q \times \dot{p} = \frac{1}{m} p \times p - \frac{V'(\|q\|)}{\|q\|} q \times q = 0.$$

2. We start imposing the first property of discrete gradients on $\bar{\nabla} H$. Let $y_n := [q_n^T p_n^T]^T$ then we want to determine κ so that
$$(y_{n+1} - y_n)^T \bar{\nabla} H = H(y_{n+1}) - H(y_n).$$
We expand the left hand side and obtain
$$\kappa\, (q_{n+1} - q_n)^T \nabla U(\frac{q_{n+1} + q_n}{2}) + (p_{n+1} - p_n)^T (\frac{p_{n+1} + p_n}{2}) =$$
$$\frac{1}{2} p_{n+1}^T p_{n+1} - p_n^T p_n + \kappa\, (q_{n+1} - q_n)^T \nabla U(\frac{q_{n+1} + q_n}{2})$$
and choosing
$$\kappa = \frac{U(q_{n+1}) - U(q_n)}{(q_{n+1} - q_n)^T \nabla U(\frac{q_{n+1}+q_n}{2})}$$
we obtain
$$(y_{n+1} - y_n)^T \bar{\nabla} H = \frac{1}{2} p_{n+1}^T p_{n+1} - p_n^T p_n + U(q_{n+1}) - U(q_n) = H(y_{n+1}) - H(y_n).$$
So that the first condition for discrete gradients is satisfied.
Assume $T(p) = \frac{1}{2m} p^T p$. To prove the second condition for discrete gradients consider
$$\lim_{y' \to y} \bar{\nabla} H(y, y')$$
this is
$$\lim_{q' \to q} \kappa\, \nabla U(\tfrac{q'+q}{2}) = \lim_{q' \to q} \frac{U(q') - U(q)}{(q'-q)^T \nabla U(\frac{q'+q}{2})} \nabla U(\tfrac{q'+q}{2})$$
$$\lim_{p' \to p} \tfrac{1}{m} \tfrac{p'+p}{2} = \tfrac{p}{2m} = \nabla T(p)$$
Taylor expanding $U(q')$ around $\frac{q+q'}{2}$ we get
$$U(q') = U(\frac{q+q'}{2}) + \frac{q'-q}{2}^T \nabla U(\frac{q+q'}{2}) + \frac{1}{2}(\frac{q'-q}{2})^T U''(\frac{q+q'}{2})(\frac{q'-q}{2}) + \mathcal{O}(\|q'-q\|^3),$$
and similarly expanding $U(q)$ around $\frac{q+q'}{2}$ we obtain
$$U(q) = U(\frac{q+q'}{2}) - \frac{q'-q}{2}^T \nabla U(\frac{q+q'}{2}) + \frac{1}{2}(\frac{q'-q}{2})^T U''(\frac{q+q'}{2})(\frac{q'-q}{2}) + \mathcal{O}(\|q'-q\|^3),$$
so
$$U(q') - U(q) = (q'-q)^T \nabla U(\frac{q+q'}{2}) + \mathcal{O}(\|q'-q\|^3)$$

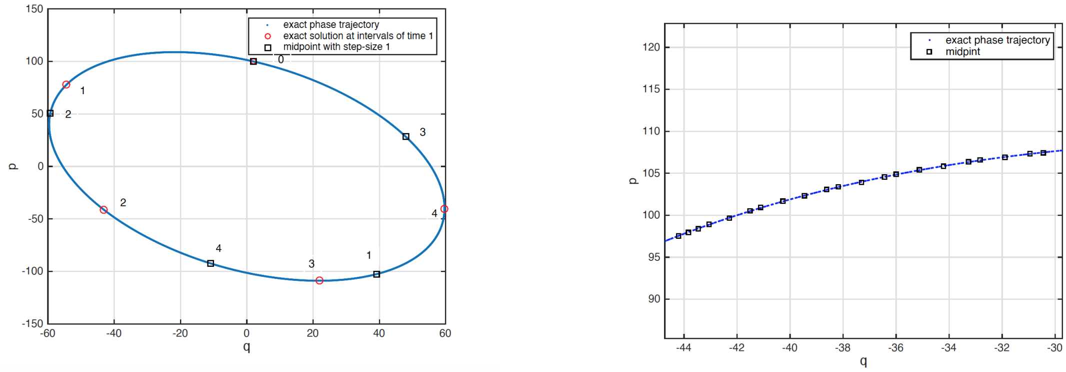

Figure 1: Left, phase space plot of a linear Hamiltonian system. $H(p,q) = \frac{1}{2}y^T Ay$, with $y = [q,p]^T \in \mathbf{R}^2$ and $A_{1,2} = A_{2,1} = 2$, $A_{1,1} = 10$, $A_{2,2} = 3$. Left: comparison of the midpoint time integrator with step-size $\Delta t = 1$ (black squares) and the exact solution (red circles). They both evolve on the same trajectory but with different speeds (the midpoint rule is slower). The numbers on the figure denote the number of performed steps of the midpoint rule and the corresponding value of the exact solution at time $t_n = n \cdot \Delta t$, $n = 0, 1, 2, 3, 4$. Right detail close to the trajectory (comparison of midpoint time integration black squares and the exact trajectory, step-size $\Delta t = 0.5$ integration on the time interval $[0, 200]$).

and

$$\lim_{q' \to q} \frac{U(q') - U(q)}{(q'-q)^T \nabla U(\frac{q'+q}{2})} \nabla U(\frac{q'+q}{2}) = \lim_{q' \to q} \left(1 + \frac{\mathcal{O}(\|q'-q\|^3)}{(q'-q)^T \nabla U(\frac{q'+q}{2})}\right) \nabla U(\frac{q'+q}{2}) = \nabla U(q).$$

We can then conclude that

$$\lim_{y' \to y} \bar{\nabla} H(y, y') = \nabla H(y).$$

3. Is left as an exercise.

■

See [18]. For a class of energy-momentum integrators and integral preserving integrators applied to the Kepler problem see [17].

1.2 Simultaneous preservation of energy and symplecticity

Theorem 1.1 *Let $\dot{y} = J\nabla H(y)$ be a Hamiltonian system with Hamiltonian H and with no other conserved quantities than H. Let Φ_h be a symplectic and energy-preserving method for the Hamiltonian system, then Φ_h reproduces the exact solution up to a time re-parametrization.*

Proof. A reference to the proof of this theorem can be found in [11]. Other versions of this result for B-series methods appeared in [5] see also [14]. ■

A consequence of this theorem is that methods which are simultaneously energy-preserving and symplectic are difficult to obtain unless we look at some special problems.

One class of problems where this is possible is the case of linear Hamiltonian systems, which arise when we consider quadratic Hamiltonian functions. Applying a Runge-Kutta method which preserves quadratic invariants on these problems, we obtain a numerical flow which is symplectic and preserves energy. In Figure 1 we can see the effect of symplectic integration on a linear Hamiltonian system with scalar position and momentum. The symplectic integrator produces a numerical flow that evolves precisely on the correct phase-space trajectory, but at a different speed compared to the exact solution. Methods which reproduce the exact solution a part from a time re-parametrization are of interest also for use on certain completely integrable problems, and techniques to align the time re-parametrized solution with the exact solution have bee studied for example in the case of the Euler equations for the free rigid body, see e.g. [25].

The use of Theorem 1.1 beyond the case of Hamiltonian completely integrable systems, is conjectured to be as hard as reproducing the exact solution.

1.3 Holonomically constrained mechanical systems

We consider a mechanical system with holonomic constraints. The generalized position coordinates are $q \in \mathrm{R}^d$ and the constraint is expressed as $g(q) = 0$ where $g : \mathbf{R}^d \to \mathbf{R}^m$ with $m < d$. We use the setting of Lagrangian mechanics and define the Lagrangian so to incorporate the constraints using Lagrangian multipliers:

$$L(q, \dot{q}) := T(\dot{q}) - U(q) - g(q)^T \lambda,$$

and we have assumed for simplicity that the the kinetic energy does not depend on q and the potential energy does not depend on $\dot{q}$. The vector of Lagrangian multipliers has m components which we denote by $\lambda_1, \dots, \lambda_m$. The Euler Lagrange equations become

$$\begin{aligned} \frac{d}{dt}\frac{\partial L}{\partial \dot{q}} &= \frac{\partial L}{\partial q} \\ g(q) &= 0 \end{aligned}$$

and because of the particular format of our Lagrangian we get

$$\frac{\partial L}{\partial \dot{q}} = M\dot{q},$$

which together with $G(q) = \frac{\partial g}{\partial q}$ leads to

$$\begin{aligned} M\ddot{q} &= -\frac{\partial U}{\partial q} - G(q)^T \lambda, \\ g(q) &= 0. \end{aligned}$$

The Hamiltonian form of the equations is obtained via the Legendre transform

$$p = M\dot{q}$$

and reads

$$\dot{q} = M^{-1} p \tag{2}$$

$$\dot{p} = -\frac{\partial U}{\partial q} - G(q)^T \lambda, \tag{3}$$

$$g(q) = 0. \tag{4}$$

These are indeed the equations of a Hamiltonian system on the manifold

$$\mathcal{Q} := \{q \in \mathrm{R}^d \,|\, g(g) = 0\}.$$

This subset of $\mathbb{R}^d$ is a submanifold provided g is a submersion in $\mathbf{R}^d$, i.e. $G(q)$ has maximum rank for all q. The tangent space of this manifold is

$$T_q\mathcal{Q} := \{v \in \mathrm{R}^d \,|\, G(q)v = 0\}$$

and the corresponding co-tangent space is

$$T_q^*\mathcal{Q} := \{p \in \mathrm{R}^d \,|\, G(q)M^{-1}p = 0\}.$$

The relevant symplectic structure for problems of type (2) is a non-degenerate and closed 2-form on $T^*\mathcal{Q}$ which, as a submanifold of $\mathbb{R}^{2d}$ can be described as

$$T^*\mathcal{Q} := \{(q,p) \in \mathbb{R}^{2d} \,|\, g(q) = 0, \quad G(q)M^{-1}p = 0\}.$$

Symplectic methods for these kind of problems on manifolds have been derived in [29] and [1], and later extended to more general Hamiltonian functions in [16], [15], [28], and [20].

A prototype method is the RATTLE method which for Hamiltonians of type

$$H(q,p) = \frac{1}{2}p^T M^{-1} p + U(q)$$

has the following form

$$\begin{aligned}
p_{n+\frac{1}{2}} &= p_n - \frac{h}{2}\left(\frac{\partial U}{\partial q}(q_n) + G(q_n)^T\lambda_n\right)\\
q_{n+1} &= q_n + hM^{-1}p_{n+\frac{1}{2}}, \quad 0 = g(q_{n+1})\\
p_{n+1} &= p_{n+\frac{1}{2}} - \frac{h}{2}\left(\frac{\partial U}{\partial q}(q_{n+1}) + G(q_{n+1})^T\mu_n\right), \quad 0 = G(q_{n+1})M^{-1}p_{n+1}
\end{aligned}$$

Theorem 1.2 *RATTLE is symmetric, symplectic and convergent of order* 2.

2 Conjugate symplecticity and conjugate energy preservation

A desired property for (Runge-Kutta) integrators is to be conjugate to symplectic, i.e. symplectic up to an appropriate transformation via another (Runge-Kutta) integrator. There are however few concrete examples of such methods.

Exercise 2.1 *Prove that the trapezoidal rule is conjugate to the midpoint rule.*

Experience shows that the behaviour of integrators which are conjugate to symplectic is virtually the same as symplectic methods. In Figure 2 we report the performance of three methods: the midpoint rule, the trapezoidal rule and the Kahan method. The latter was originally defined for quadratic vector fields, but can also be written as a one step (Runge-Kutta) method and takes the form

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

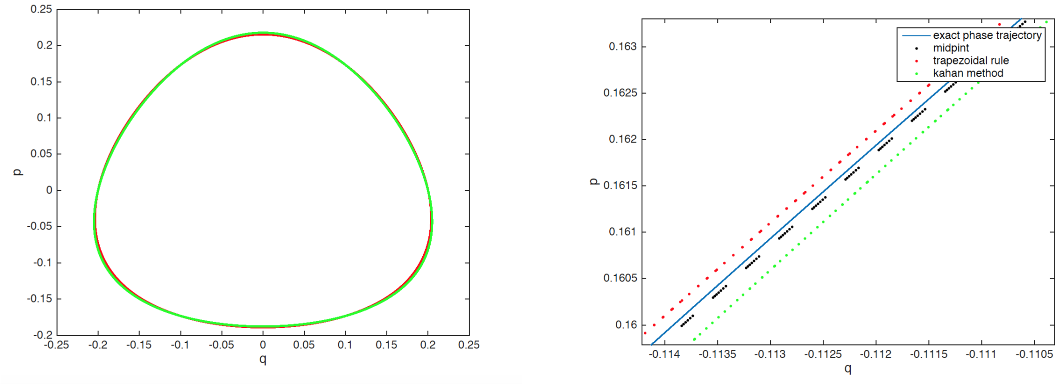

Figure 2: Phase space plot of the Henon Heiles problem $H(q,p) = \frac{1}{2}(q^2+p^2) + q^2p - \frac{1}{3}p^3$ the Hamiltonian vector field is quadratic. Comparison of the midpoint time integrator, the trapezoidal rule and Kahan's method with step-size 0.5, integration on the time interval $[0, 10000]$. Phase space portrait, the tree methods behave similarly, but the symplectic integrator seems to give a smaller error compared to the exact phase space trajectory (blue line). The trapezoidal rule is conjugate to the midpoint rule. The Kahan method preserves a modified energy function and a modified volume form for all Hamiltonian systems with cubic Hamiltonian.

This method, introduced by Kahan, has a number of remarkable properties when applied to quadratic vector fields, especially Hamiltonian ones. When applied to quadratic vector fields it can be written in the form

$$y_{n+1} = y_n + h(I - \frac{h}{2}f'(y_n))^{-1}f(y_n),$$

where f' denotes the Jacobian of f.

It can be shown that Kahan's method preserves a modified volume form and a modified energy whenever applied to quadratic Hamiltonian systems [8]. For this reason in the example of Figure 2, the Henon Heiles problem, which is two dimensional, the modified volume form corresponds to conjugate symplecticity of the method. The energy error remains bounded for the three methods although the error for Kahan's method is larger than for the other two methods. On the other hand Kahan's method preserves exactly a modified energy function whose expression is explicitly known, see [8] for details.

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