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An unconventional symplectic integrator of W. Kahan

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This paper is dedicated to Professor Robert Vichnevetsky to honor him on the occasion of his 65th birthday

Abstract

Among other unconventional numerical methods, W. Kahan has suggested a discretization of a simple Lotka–Volterra system with the property that the computed points do not spiral. We explain this behaviour by showing that Kahan's method is symplectic with respect to a noncanonical symplectic structure.

1. Introduction

Among other "unconventional" numerical methods, W. Kahan [1] considers the scheme

$$\frac{X-x}{\Delta t} = \frac{\alpha}{2}(X+x) + \frac{\beta}{2}(Xy+xY), \tag{1}$$

$$\frac{Y-y}{\Delta t} = \frac{\gamma}{2}(Y+y) + \frac{\delta}{2}(Xy+xY), \tag{2}$$

which approximates the system of differential equations

$$\frac{\mathrm{d}x}{\mathrm{d}t} = \alpha x + \beta xy, \tag{3}$$

$$\frac{\mathrm{d}y}{\mathrm{d}t} = \gamma y + \delta xy. \tag{4}$$

In (1)–(2), Δt is the time step, (x, y) the current solution value and (X, Y) the solution value at the next time level. What makes (1)–(2) unconventional is the treatment of the quadratic xy term in (3)–(4): the standard trapezoidal rule discretizes this as $\frac{1}{2}XY + \frac{1}{2}xy$ and the midpoint rule as $\frac{1}{2}(X+x) \cdot \frac{1}{2}(Y+y)$. Both conventional discretizations are quadratic in the new solution (X, Y). Since (1)–(2) is *linear* in (X, Y), it is possible to express X and Y in closed form as

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(rational) functions of (x, y) and therefore the implementation of the scheme does not require the solution of nonlinear algebraic equations.

The coordinate axes $x=0$ and $y=0$ are invariant for (3)–(4); this implies that a solution $(x(t), y(t))$ that is positive at some time $t=t_0$ cannot leave the orthant $x>0$, $y>0$. In the remainder of the paper we only consider solutions of (3)–(4) in this orthant. Kahan focuses on the case

$$\alpha < 0, \qquad \beta > 0, \qquad \gamma > 0, \qquad \delta < 0, \tag{5}$$

that yields a simplified predator (x) and pray (y) Lotka–Volterra system. Then $x = -\alpha/\beta > 0$, $y = -\gamma/\delta > 0$ is an equilibrium; all other solutions describe closed trajectories which surround the equilibrium in the phase orthant of the variables (x, y). Of course, these trajectories represent periodic fluctuations in the numbers of individuals in the x, y species. The most remarkable feature of the unconventional scheme (1)–(2) is that it produces solution values that stay on closed curves; almost any other integrator one may try produces points that either spiral in towards the equilibrium point or spiral out of the equilibrium point. Our aim is to explain this behaviour. It turns out that a key feature of (1)–(2) is that it is symplectic with respect to a nonstandard structure [3]. While many schemes are now available which are symplectic with respect to the standard or canonical symplectic structure [3], the scheme (1)–(2) is one of the few examples known to me of a noncanonical symplectic scheme. This makes (1)–(2) unconventional in a second sense!

2. Hamiltonian problems

We begin by looking at the system (3)–(5). For systems of differential equations in the plane, the situation where all trajectories in phase plane are closed curves is *nongeneric*, i.e., atypical. If a system is in this situation, then any small perturbation of the right-hand side typically changes the closed curves into spirals. The effect of numerical integration amounts to changing the system being solved into a nearby system (see, e.g., [3, Chapter 10]). This explains why numerical integrators for (3)–(5) typically spiral.

On the other hand, there is a class of systems in the plane where closed curves are typical. This is the class of (canonical or standard) Hamiltonian problems

$$\frac{\mathrm{d}x}{\mathrm{d}t} = -\frac{\partial H}{\partial y}, \tag{6}$$

$$\frac{\mathrm{d}y}{\mathrm{d}t} = +\frac{\partial H}{\partial x}, \tag{7}$$

The trajectories of (6)–(7) are the level sets of the Hamiltonian function $H = H(x, y)$. If all trajectories of (6)–(7) are closed, then all nearby Hamiltonian systems also have closed trajectories. (The term "nearby Hamiltonian systems" refers to systems that are of the form (6)–(7) with the Hamiltonian function $H = H(x, y)$ replaced by a function $\tilde{H} = \tilde{H}(x, y)$ close to H.)

Is (3)–(5) a Hamiltonian system? In other words, is it possible to write (3)–(4) in the form (6)–(7) for some function H? The answer is no: for a planar system $\mathrm{d}x/\mathrm{d}t = f(x, y)$,

$dy/dt = g(x, y)$ to be Hamiltonian (see, e.g., [3, Chapter 2]), it is necessary and sufficient that the vector field (f, g) be divergence free, $\partial f/\partial x + \partial g/\partial y = 0$, a condition that (3)–(5) does not satisfy.

However (3)–(4) is not far away from being Hamiltonian; it becomes Hamiltonian after the change of variables $\xi = \log x$ and $\eta = \log y$. To see this note that (3)–(4) is of the form

$$\frac{dx/dt}{x} = -m(y),$$

$$\frac{dy/dt}{y} = +n(x),$$

which in terms of the new variables becomes

$$\frac{d\xi}{dt} = -m(\exp(\eta)), \tag{8}$$

$$\frac{d\eta}{dt} = +n(\exp(\xi)), \tag{9}$$

a system whose right-hand side is obviously divergence-free in the (ξ, η) plane. The corresponding Hamiltonian function is not difficult to find; it is given by

$$\mathscr{H}(\xi, \eta) = N(\exp(\xi)) + M(\exp(\eta)),$$

where $N(x)$ and $M(y)$ are antiderivatives (integrals) of the functions $n(x)/x$ and $m(y)/y$ respectively. The trajectories of (8)–(9) lie in level curves of $\mathscr{H}$ in the (ξ, η) plane and hence the trajectories of the original system (3)–(4) lie in level curves of the function

$$H(x, y) = \mathscr{H}(\log x, \log y) = N(x) + M(y). \tag{10}$$

There is a second connection between (3)–(4) and the theory of Hamiltonian systems. If $\sigma(x, y)$ is a fixed function that does not vanish in the region of interest, then the *noncanonical* or *nonstandard* Hamiltonian system with Hamiltonian function $H(x, y)$ is, by definition,

$$\frac{dx}{dt} = -\frac{1}{\sigma(x, y)} \frac{\partial H}{\partial y}, \tag{11}$$

$$\frac{dy}{dt} = +\frac{1}{\sigma(x, y)} \frac{\partial H}{\partial x}. \tag{12}$$

For $\sigma \equiv 1$ we recover the canonical case (6)–(7). It is trivial to check that solutions of (11)–(12) have the conserved quantity $H(x(t), y(t)) = \text{constant}$, and hence the corresponding trajectories lie on level sets of H. With this terminology, it is easily seen that (3)–(4) is the noncanonical Hamiltonian system associated with $\sigma(x, y) = 1/(xy)$ and the Hamiltonian function $H(x, y)$ in (10). To sum up, (3)–(4) is a *noncanonical* Hamiltonian problem that can be brought into *canonical* form by a change of variables.

Comment. All planar systems that become canonical Hamiltonian after a change of variables $\xi = \xi(x, y)$ and $\eta = \eta(x, y)$ are noncanonical Hamiltonian with σ given by the determinant of the Jacobian matrix $\partial(\xi, \eta)/\partial(x, y)$. The Hamiltonian $H(x, y)$ for the noncanonical formulation is $\mathscr{H}(\xi(x, y), \eta(x, y))$, where $\mathscr{H}$ is the Hamiltonian function for the canonical formulation in the variables ξ and η. The proofs of these facts are elementary.

Before discussing numerical methods, we need to point out how to characterize planar Hamiltonian problems in terms of their flows. The flow ϕ_t of a system of differential equations $dx/dt = f(x, y)$, $dy/dt = g(x, y)$ is the map given by $(x, y) \mapsto (X, Y)$, where (X, Y) is the value at time t of the solution of the system that takes the initial value (x, y) at time $t = 0$. By Liouville's theorem, the flow ϕ_t of a system preserves area if and only if the associated vector field (f, g) is divergence free. In turn, and as mentioned above, $\nabla \cdot (f, g) = 0$ is equivalent to the differential system being canonical Hamiltonian. We conclude that a planar system is canonical Hamiltonian if and only if its flow ϕ_t is, for all values of t, an area-preserving mapping. In terms of differential forms, canonical Hamiltonian systems are characterized by the conservation of the form $dx \wedge dy$ that provides the "element" of oriented area in the plane. This fact is often expressed by saying that the flow of a standard Hamiltonian system is a symplectic transformation with respect to the canonical symplectic structure given by $dx \wedge dy$.

Noncanonical Hamiltonian systems (11)–(12) are characterized by the conservation of the form $\sigma\, dx \wedge dy$, that represents an element of area weighted with an (x, y)-dependent weight function $\sigma(x, y)$. Note that

$$\sigma\, dx \wedge dy = d\xi \wedge d\eta,$$

because, as mentioned before, σ is the Jacobian determinant of the change of variables. Therefore the weighted area of a set in (x, y) plane is, as expected, the same as the standard area of the transformed set in (ξ, η) variables. The flow of a nonstandard Hamiltonian system is a symplectic transformation with respect to the noncanonical or nonstandard symplectic structure given by $\sigma\, dx \wedge dy$.

3. Numerical methods

A one-step numerical method for a system of differential equations $dx/dt = f(x, y)$, $dy/dt = g(x, y)$ is given by my a mapping $(X, Y) = \psi_{\Delta t}(x, y)$ that specifies how the numerical solution is advanced over a time interval of length Δt. Since for the true solution $(X, Y) = \phi_{\Delta t}(x, y)$, the mapping $\psi_{\Delta t}$ should approximate the flow $\phi_{\Delta t}$ of the system being integrated.

For a canonical Hamiltonian system (6)–(7), the flow $\phi_{\Delta t}$ is area-preserving and it makes sense to use numerical methods for which $\psi_{\Delta t}$ also preserves area, i.e, preserves the form $dx \wedge dy$. Those numerical methods are called canonical; many of them have been devised [3]. If a planar canonical Hamiltonian system (6)–(7) that has a stable equilibrium point surrounded by closed curves (i.e., a centre) is integrated by a canonical method, then the computed points do not spiral. This is guaranteed by the KAM theory [2]. Hence, to perform a nonspiralling integration of (3)–(5), we could switch to variables $\xi = \log x$ and $\eta = \log y$ and then use one of the available canonical integrators to advance the solutions of the resulting system for (ξ, η). Mathematically (but not computationally) this is equivalent to integrating (3)–(5) in the (x, y)

variables by means of the scheme resulting from changing variables in the (ξ, η)-scheme. For instance, the canonical midpoint rule for (8)–(9) gives rise to the scheme

$$\frac{\log X - \log x}{\Delta t} = -m\left(\exp\left(\frac{\log Y + \log y}{2}\right)\right),$$

$$\frac{\log Y - \log y}{\Delta t} = +n\left(\exp\left(\frac{\log X + \log x}{2}\right)\right).$$

This example proves that (x, y)-schemes derived from conventional canonical (ξ, η)-schemes are likely to be wildly nonlinear.

Is it possible to derive nonspiralling (x, y)-schemes without going through a (ξ, η)-scheme? According to the discussion of the preceding section, the sought (x, y)-scheme has to preserve the form $\sigma \, \mathrm{d}x \wedge \mathrm{d}y$, $\sigma = 1/(xy)$. This is precisely what Kahan's scheme (1)–(2) achieves, as the following theorem shows.

Theorem 1. *If A, B, C and D are real constants, the transformation defined by*

$$X - x = A(X + x) + B(Xy + xY), \tag{13}$$

$$Y - y = C(Y + y) + D(Xy + xY), \tag{14}$$

preserves the form $(xy)^{-1} \, \mathrm{d}x \wedge \mathrm{d}y$, *i.e.*,

$$\frac{1}{xy}(\mathrm{d}x \wedge \mathrm{d}y) \equiv \frac{1}{XY}(\mathrm{d}X \wedge \mathrm{d}Y). \tag{15}$$

Proof. A direct proof, using the explicit expression of (X, Y) as functions of (x, y) is possible but lengthy. We give a shorter alternative. Differentiate (13)–(14) and rearrange to get

$$(1 - A) \, \mathrm{d}X - By \, \mathrm{d}X - Bx \, \mathrm{d}Y = (1 + A) \, \mathrm{d}x + BY \, \mathrm{d}x + BX \, \mathrm{d}y,$$

$$(1 - C) \, \mathrm{d}Y - Dy \, \mathrm{d}X - Dx \, \mathrm{d}Y = (1 + C) \, \mathrm{d}y + DY \, \mathrm{d}x + DX \, \mathrm{d}y.$$

Now take the wedge product of these equations to obtain

$$\begin{aligned}&[(1 - A)(1 - C) - (1 - A)Dx - (1 - C)By] \, \mathrm{d}X \wedge \mathrm{d}Y \\ &\quad = [(1 + A)(1 + C) + (1 + A)DX - (1 + C)BY] \, \mathrm{d}x \wedge \mathrm{d}y.\end{aligned} \tag{16}$$

On the other hand, we rewrite (13)–(14) as

$$(1 - A)X - BXy = (1 + A)x + BxY,$$

$$(1 - C)Y - DxY = (1 + C)y + DXy.$$

Multiplication of these equations leads to

$$\begin{aligned}&[(1 - A)(1 - C) - (1 - A)Dx - (1 - C)By]XY \\ &\quad = [(1 + A)(1 + C) + (1 + A)DX - (1 + C)BY]xy,\end{aligned}$$

a result that, along with (16), implies (15). □

A couple of final comments. Since (1)–(2) is reversible (selfadjoint), it may be composed with itself to give rise to symplectic schemes of arbitrarily high order as explained in [1] or [3]. On the other hand, the technique used in (1)–(2) to deal with the xy term can be applied to any quadratic term in any differential system [1]. If $\boldsymbol{z}$ is the vector of independent variables, a quadratic nonlinearity is of the form $\boldsymbol{F}(\boldsymbol{z}, \boldsymbol{z})$ for a suitable bilinear symmetric operator. Kahan's unconventional discretization, $\boldsymbol{F}(\boldsymbol{Z}, \boldsymbol{z})$ is linear in the advanced solution vector $\boldsymbol{Z}$. The conventional midpoint $\boldsymbol{F}(\frac{1}{2}(\boldsymbol{Z}+\boldsymbol{z}), \frac{1}{2}(\boldsymbol{Z}+\boldsymbol{z}))$ and trapezoidal $\frac{1}{2}(\boldsymbol{F}(\boldsymbol{Z}, \boldsymbol{Z})+\boldsymbol{F}(\boldsymbol{z}, \boldsymbol{z}))$ discretizations are both quadratic in $\boldsymbol{Z}$ and therefore result in nonlinear algebraic equations to be solved at each step.

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