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Solving ODEs numerically while preserving a first integral

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Abstract

We give general algorithms for the numerical integration of ordinary differential equations (ODEs) that possess a first integral $I(x)$. Our discrete algorithms preserve the integral I exactly. Our method works both for dissipative and for all Hamiltonian ODEs. For non-Hamiltonian systems a sufficient (but not necessary) condition for our method to work is that $|\nabla I| \neq 0$ on the isosurface we are integrating on.

1. Introduction

In recent years much effort has been devoted to the construction of numerical integration schemes for ordinary differential equations (ODEs) in such a way that some *qualitative* property of the ODE is exactly preserved.

This has resulted in symplectic integrators for Hamiltonian ODEs [1–3], volume-preserving integrators for divergence-free ODEs [4–6], and symmetry-preserving integrators for ODEs with symmetries and/or time-reversing symmetries [7–9]. In this Letter we are interested in the numerical integration of an ODE that possesses a first integral, and we explicitly give numerical integration methods that preserve this first integral. Special cases of this problem have been studied before. We mention the work by Cooper on preserving quadratic integrals [10], the work by Itoh and Abe [2] on preserving energy in Hamiltonian systems [11], and the work by Greenspan and collaborators on preserving the first integrals of the n-body problems of celestial mechanics [12]. We stress that our method as described in this Letter is not restricted to such special cases, and in particular is not restricted to Hamiltonian systems (although Hamiltonian systems are included as a very special case). In this Letter our treatment is confined to preserving *one* first integral. The simultaneous preservation of two or more first integrals will be treated in a future paper [13].

2. Integral-preserving integrators

Consider the autonomous ODE

$$\frac{dx}{dt} = f(x), \quad x \in \mathbb{R}^n, \tag{1}$$

where f is a function from $\mathbb{R}^n$ to $\mathbb{R}^n$. We are interested in the case that the ODE (1) has a first integral I,

$$\frac{dI(x)}{dt} = 0, \tag{2}$$

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[2] We mention these authors in particular because their integrators have the nice property of being free of singularities.

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where I is a function from $\mathbb{R}^n$ to $\mathbb{R}$ (in the sequel we will assume that f and I possess suitable regularity properties). In general it is of course impossible to solve the initial value problem for the ODE (1) analytically. We therefore pose the following problem: *Find a discrete approximation to the ODE (1) that preserves the first integral $I(x)$ exactly.* In this paper this problem is solved [3].

Our solution proceeds in four steps:

(i) We rewrite the ODE (1) in the form of a "skew-gradient system", i.e.

$$\frac{\mathrm{d}x}{\mathrm{d}t} = S(x) \cdot \nabla I(x), \tag{3}$$

where $S(x)$ is some skew-symmetric matrix (i.e. $S^t = -S$) [4]. This can always be done (generally in infinitely many different ways) subject to a mild technical condition. Below we will give an explicit construction of $S(x)$ for a given vectorfield $f(x)$ and integral $I(x)$.

(ii) We use (3) to split [5] the n-dimensional vectorfield into essentially two-dimensional vectorfields that all possess the original integral I.

(iii) We integrate each two-dimensional (2D) vectorfield, using a discrete approximation that preserves the integral I exactly.

(iv) We construct an n-dimensional integrator for the ODE (1) by composition of the two-dimensional integrators obtained in (iii). Since each 2D integrator preserves I, so does the ensuing n-dimensional integrator.

Step (i): write the ODE in the form $\mathrm{d}x/\mathrm{d}t = S \cdot \nabla I$. Combining (1) and (2) it follows that

$$f \cdot \nabla I = 0. \tag{4}$$

We now want to find a skew-symmetric matrix S such that

$$S \cdot \nabla I = f. \tag{5}$$

Below we will see that the skew symmetry of S makes possible an integral-preserving splitting of the vectorfield. (Actually, this skew symmetry turns out to be even more fundamental, cf. Ref. [22].) For given f and ∇I, Eq. (5) is a system of linear equations for the entries of the matrix S. For dimension $n \geqslant 3$ this system of equations is under-determined. It is easy to check that a particular solution S^{P} to Eq. (5) is given by

$$S^{\mathrm{P}}_{i,j} = \frac{f_i(\partial I/\partial x_j) - f_j(\partial I/\partial x_i)}{\sum_{k=1}^{n}(\partial I/\partial x_k)^2}. \tag{6}$$

The general solution of (5) follows by adding this particular solution to the solution S^{H} of the homogeneous equation,

$$S^{\mathrm{H}} \cdot \nabla I = 0. \tag{7}$$

Assuming $\partial I/\partial x_j$ is not identically zero [6] for any j, the solution of (7) is given by

$$S^{\mathrm{H}}_{i,j} = \alpha_{i,j} \prod_{k}^{*} \left(\frac{\partial I}{\partial x_k}\right), \tag{8}$$

where the product symbol $\prod_k^*$ means $k \neq i$, $k \neq j$, i.e. k takes on the values $1, \dots, i-1, i+1, \dots, j-1, j+1, \dots, n$. The coefficient functions $\alpha_{i,j}(x)$ in (8) can be chosen arbitrarily for $1 \leqslant i < j < n$. The remaining $\alpha_{i,j}$ are then given by

$$\alpha_{i,n}(x) = -\sum_{j=1}^{n-1} \alpha_{i,j}(x), \quad i = 1, \dots, n-1,$$
$$\alpha_{j,i}(x) = -\alpha_{i,j}(x). \tag{9}$$

The general solution S^{G} to (5) is then obtained as the sum of the particular solution (6) and the homogeneous solution (8), (9), i.e.

$$S^{\mathrm{G}} = S^{\mathrm{P}} + S^{\mathrm{H}}.$$

Step (ii): Splitting into 2D vector fields all possessing the integral I. For convenience we use here the equivalence of the ODE (1) with the vectorfield [7]

$$v := \sum_i f_i \frac{\partial}{\partial x_i} = \sum_{i<j} v_{i,j}, \tag{10}$$

[3] A sufficient, but not necessary, condition for our method to work is that $|\nabla I| \neq 0$ on the isosurface we are integrating on.

[4] Note that Eq. (3) is in general *not* Hamiltonian, see example III of Section 3.

[5] A general discussion of splitting methods is given in Ref. [14].

[6] The case that $\partial I/\partial x_j$ is identically zero for some j is treated in Section 4.

[7] The interchangability of (the words) vectorfields and differential operators is explained e.g. in Ref. [18].

where the vector fields $v_{i,j}$ are defined by

$$v_{i,j} := S_{i,j}\frac{\partial I}{\partial x_j}\frac{\partial}{\partial x_i} + S_{j,i}\frac{\partial I}{\partial x_i}\frac{\partial}{\partial x_j}. \quad (11)$$

Using the skew symmetry of S, these vectorfields $v_{i,j}$ can be rewritten,

$$v_{i,j} = S_{i,j}\left(\frac{\partial I}{\partial x_j}\frac{\partial}{\partial x_i} - \frac{\partial I}{\partial x_i}\frac{\partial}{\partial x_j}\right). \quad (12)$$

From (12) it follows immediately that each vectorfield $v_{i,j}$ possesses the original integral I, i.e.

$$v_{i,j}I(x) = S_{i,j}\left(\frac{\partial I}{\partial x_j}\frac{\partial I}{\partial x_i} - \frac{\partial I}{\partial x_i}\frac{\partial I}{\partial x_j}\right) = 0. \quad (13)$$

(It is for this reason that we have insisted that the matrix S in (3) must be skew symmetric.)

Note that the above leads to a splitting into a maximum of $\binom{n}{2}$ vectorfields.

Step (iii): Integral-preserving integration of 2D vectorfields. The vectorfield $v_{i,j}$ (12) is equivalent to the following essentially two-dimensional ODE,

$$\frac{dx_i}{dt} = S_{i,j}(x)\frac{\partial I}{\partial x_j}, \quad \frac{dx_j}{dt} = -S_{i,j}(x)\frac{\partial I}{\partial x_i},$$
$$\frac{dx_k}{dt} = 0, \quad k \neq i,j. \quad (14)$$

A first-order integral-preserving integrator $\phi_{i,j}$ for the "two-dimensional" ODE is given by $\phi_{i,j}(x,\tau) = x'$, where

$$x'_i = x_i + \tau\tilde{S}_{i,j}(x,x',\tau)\frac{I(x'_i,x'_j) - I(x'_i,x_j)}{x'_j - x_j},$$
$$x'_j = x_j - \tau\tilde{S}_{i,j}(x,x',\tau)\frac{I(x'_i,x_j) - I(x_i,x_j)}{x'_i - x_i},$$
$$x'_k = x_k, \quad k \neq i,j \quad (15)$$

(cf. Ref. [15]).

A second-order integral-preserving integrator for the "two-dimensional" ODE (14) is given by $\psi_{i,j}(x,\tau) = x'$, where

$$x'_i = x_i + \tfrac{1}{2}\tau\hat{S}_{i,j}(x,x',\tau) \times \frac{I(x'_i,x'_j) - I(x'_i,x_j) + I(x_i,x'_j) - I(x_i,x_j)}{x'_j - x_j},$$
$$x'_j = x_j - \tfrac{1}{2}\tau\hat{S}_{i,j}(x,x',\tau) \times \frac{I(x'_i,x'_j) - I(x_i,x'_j) + I(x'_i,x_j) - I(x_i,x_j)}{x'_i - x_i},$$
$$x'_k = x_k, \quad k \neq i,j. \quad (16)$$

In these expressions for the integrators (15) and (16) we have used the shorthand notation

$$I(x'_i,x'_j) := I(x_1,\dots,x_{i-1},x'_i,x_{i+1},\dots,x_{j-1}, x'_j,x_{j+1},\dots,x_n),$$
$$I(x'_i,x_j) := I(x_1,\dots,x_{i-1},x'_i,x_{i+1},\dots,x_n),$$
$$I(x_i,x'_j) := I(x_1,\dots,x_{j-1},x'_j,x_{j+1},\dots,x_n),$$
$$I(x_i,x_j) := I(x_1,\dots,x_n), \quad (17)$$

and $\tilde{S}_{i,j}$ and $\hat{S}_{i,j}$ are approximations to $S_{i,j}$, i.e. they satisfy respectively

$$\tilde{S}_{i,j}(x,x',\tau) = S_{i,j}(x) + \mathcal{O}(\tau), \quad (18)$$

and

$$\hat{S}_{i,j}(x,x',\tau) = \hat{S}_{i,j}(x',x,-\tau) := S_{i,j}(x) + \mathcal{O}(\tau). \quad (19)$$

(This freedom in the choice of $\tilde{S}_{i,j}$ and $\hat{S}_{i,j}$ is sometimes useful.)

It is not difficult to check that both integrators (15) and (16) preserve the integral I, i.e. they satisfy

$$I(x') = I(x). \quad (20)$$

The integrator $\psi_{i,j}$ moreover satisfies

$$\psi_{i,j}(x,\tau) = \psi_{i,j}^{-1}(x,-\tau), \quad (21)$$

which makes it suitable as a building block for constructing integrators of arbitrary order, using Yoshida's method [1,16].

Step (iv): Construction of an n-dimensional integral-preserving integrator from 2D integrators. Here we will give two ways to construct n-dimensional integral-preserving integrators for the ODE (1). These integrators are constructed from the "two-dimensional" integral-preserving integrators $\phi_{i,j}$ resp. $\psi_{i,j}$ given in Eqs. (15) and (16).

The simplest integral-preserving integrator for the ODE (1) is

$$\phi(x,\tau) := \prod_{i<j} \phi_{i,j}(x,\tau), \tag{22}$$

where the two-dimensional maps $\phi_{i,j}$ are given by (15). The product in (21) denotes composition in arbitrary order (e.g. $\phi(\tau) = \phi_{1,2}(\tau) \circ \phi_{1,3}(\tau) \circ \cdots \circ \phi_{1,n}(\tau) \circ \phi_{2,3}(\tau) \circ \phi_{2,4}(\tau) \circ \cdots \circ \phi_{n-1,n}(\tau)$). Since each of the $\phi_{i,j}$ preserves the integral I, so does ϕ.

A second integral-preserving integrator for the ODE(1) is given by the symmetric product

$$\psi(x,\tau) := \psi_{1,2}(\tfrac{1}{2}\tau) \circ \cdots \circ \psi_{n-2,n}(\tfrac{1}{2}\tau) \circ \psi_{n-1,n}(\tau) \circ \psi_{n-2,n}(\tfrac{1}{2}\tau) \circ \cdots \circ \psi_{1,2}(\tfrac{1}{2}\tau), \tag{23}$$

where the two-dimensional maps $\psi_{i,j}$ are given by (16). The advantage of the integrator (22) is that it is second order, it also satisfies the property (21).

Moreover, if all $\psi_{i,j}$ possess a certain group of symmetries and time-reversing symmetries, then so does ψ (cf. Ref. [9]).

There are of course other ways to construct n-dimensional integrators from the two-dimensional maps $\phi_{i,j}$ and $\psi_{i,j}$ (e.g. $\phi(\frac{1}{2}\tau) \circ \phi^{-1}(-\frac{1}{2}\tau)$, where $\phi(\tau)$ is given by (22), cf. Ref. [8]) but we leave this to the interested reader.

3. Some examples

To illustrate our method, in this section we give several examples of ODEs possessing an integral I, and explicitly rewrite them in the form (3)

$$\frac{dx}{dt} = S(x) \cdot \nabla I,$$

which is suitable for our construction of integral-preserving integrators to work. In the following examples, a convenient choice for the skew-symmetric matrix S is obtained by inspection rather than using the general formulae of Section 2.

(I) A Lotka–Volterra system [17].

$$\frac{dx_1}{dt} = e^{x_3}, \quad \frac{dx_2}{dt} = e^{x_1} + e^{x_3}, \quad \frac{dx_3}{dt} = Be^{x_1} + e^{x_2}, \tag{24}$$

where B is a parameter. The ODE (24) has the integral

$$I = e^{x_2 - x_1} + B(x_2 - x_1) - x_3. \tag{25}$$

The ODE (24) can be rewritten in the form (3) as follows,

$$\begin{pmatrix} \frac{dx_1}{dt} \\ \frac{dx_2}{dt} \\ \frac{dx_3}{dt} \end{pmatrix} = \begin{pmatrix} 0 & 0 & -e^{x_3} \\ 0 & 0 & -e^{x_1} - e^{x_3} \\ e^{x_3} & e^{x_1} + e^{x_3} & 0 \end{pmatrix} \cdot \nabla I. \tag{26}$$

(II) A second example in $\mathbb{R}^3$.

$$\frac{dx_1}{dt} = -\tfrac{1}{2}x_1x_2 + x_1x_3 - x_1 + x_2x_3, \quad \frac{dx_2}{dt} = x_1x_2 - x_2x_3 - x_2, \quad \frac{dx_3}{dt} = 2x_1x_3 + x_2x_3. \tag{27}$$

This ODE has the integral

$$I = x_3 \exp(2x_1 + x_2 - x_3). \tag{28}$$

The ODE (27) can be rewritten in the form (3) as follows,

$$\begin{pmatrix} \frac{dx_1}{dt} \\ \frac{dx_2}{dt} \\ \frac{dx_3}{dt} \end{pmatrix} = \exp(-2x_1 - x_2 + x_3) \times \begin{pmatrix} 0 & -\frac{1}{2}x_1x_2 + x_2 & -\frac{1}{2}x_1x_2 - x_1 \\ \frac{1}{2}x_1x_2 - x_2 & 0 & x_1x_2 - x_2 \\ \frac{1}{2}x_1x_2 + x_1 & -x_1x_2 + x_2 & 0 \end{pmatrix} \cdot \nabla I. \tag{29}$$

(III) All autonomous Hamiltonian and Poisson systems. Poisson systems are described by ODEs of the form [18]

$$\frac{dx}{dt} = J(x) \cdot \nabla H(x), \tag{30}$$

where the matrix J is skew symmetric, but moreover must satisfy the "Jacobi identity":

$$\sum_{\ell=1}^{n} \left(J_{i,\ell} \frac{\partial}{\partial x_\ell} J_{j,k} + J_{k,\ell} \frac{\partial}{\partial x_\ell} J_{i,j} + J_{j,\ell} \frac{\partial}{\partial x_\ell} J_{k,i} \right) \equiv 0, \quad i,j,k = 1,\ldots,n. \tag{31}$$

Because of the skew symmetry of J the Hamiltonian H in (30) is conserved, and all Poisson systems (30), (31) are automatically in the right form (3) for our method to work (it is not even necessary for $|\nabla H|$ to be unequal to zero). In case the matrix J is of maximal rank, the system (30), (31) is called Hamiltonian. In the special case that, moreover,

$$J = \begin{pmatrix} & & 1 & \\ & & & \ddots & \\ & & & & 1 \\ -1 & & & & \\ & \ddots & & & \\ & & -1 & & \end{pmatrix}, \tag{32}$$

our method reduces to that of Itoh and Abe [8] [11].

Note that in examples I and II, the Jacobi identity is not satisfied (although Eq. (26) *is* divergence free).

(IV) The Landau–Lifshitz spin chain.

$$\frac{\mathrm{d}\boldsymbol{s}_n}{\mathrm{d}t} = \boldsymbol{s}_n \times \boldsymbol{\omega}_n, \quad \boldsymbol{s}_n \in \mathbb{R}^3, \quad n = 1, \dots, N,$$

where

$$\boldsymbol{\omega}_n := J\boldsymbol{s}_{n+1} + J\boldsymbol{s}_{n-1} + D\boldsymbol{s}_n,$$

and periodic boundary conditions are imposed. This system has the integral

$$I = \sum_{n=1}^{N} \boldsymbol{s}_n^2,$$

and can be written in the skew-gradient form (3) as follows [9],

$$\frac{\mathrm{d}s_{n,\alpha}}{\mathrm{d}t} = \sum_{m=1}^{N} \sum_{\beta=1}^{3} S_{n,\alpha;m,\beta} s_{m,\beta},$$

where

$$S_{n,\alpha;m,\beta} = -\delta_{m,n} \varepsilon_{\alpha,\beta,\gamma} \omega_{n,\gamma}.$$

Here δ is the Kronecker delta and ε is the Levi–Civita tensor.

[8] Note that in general it is impossible to preserve the symplectic structure and the Hamiltonian simultaneously, see Ref. [19].

[9] A more conventional splitting based on the Hamiltonian $H = \sum(\boldsymbol{s}_n J \boldsymbol{s}_{n+1} + \boldsymbol{s}_n D \boldsymbol{s}_n)$ can also be obtained [20].

In this example, all 2D vectorfields obtained after splitting have a similar structure, e.g.

$$\frac{\mathrm{d}s_{n,1}}{\mathrm{d}t} = \omega_{n,3} s_{n,2}, \quad \frac{\mathrm{d}s_{n,2}}{\mathrm{d}t} = -\omega_{n,3} s_{n,1}.$$

This ODE can be integrated exactly,

$$\begin{pmatrix} s'_{n,1} \\ s'_{n,2} \end{pmatrix} = \begin{pmatrix} \cos(\omega_{n,3}\tau) & \sin(\omega_{n,3}\tau) \\ -\sin(\omega_{n,3}\tau) & \cos(\omega_{n,3}\tau) \end{pmatrix} \begin{pmatrix} s_{n,1} \\ s_{n,2} \end{pmatrix}.$$

As a bonus, this will lead to an integrator which is volume-preserving and explicit, and which preserves each integral s_n^2 separately.

4. Concluding remarks

(i) In case the integral $I(x)$ does not depend on each of the variables x_i, the above procedure can be simplified somewhat. Let us assume I depends on only m of the n variables x_i. Without loss of generality we may assume I only depends on $x_1, \dots, x_m$. The vectorfield v can then be split into two parts

$$v = v_1 + v_2, \tag{33}$$

where

$$v_1 := \sum_{i=1}^{m} f_i \frac{\partial}{\partial x_i}, \quad v_2 := \sum_{i=m+1}^{n} f_i \frac{\partial}{\partial x_i}. \tag{34}$$

Each of these vectorfields separately preserves the integral I. The vectorfield v_1 can now be integrated as indicated in Section 2. Since the integral I does not depend on $x_{m+1}, \dots, x_n$, however, the vectorfield v_2 can be integrated using any arbitrary integration method, without the need to use the methods of Section 2. This decreases the maximum number of vectorfields, after splitting, from $\binom{n}{2}$ to $\binom{m}{2} + 1$.

(ii) As mentioned in Footnote 3, a sufficient condition for our integral-preserving integration method to work is that $|\nabla I| \neq 0$. We will now give a second example that shows this condition is sufficient but not necessary.

Consider the ODE

$$\frac{\mathrm{d}x_1}{\mathrm{d}t} = x_2 x_3^2, \quad \frac{\mathrm{d}x_2}{\mathrm{d}t} = x_3,$$
$$\frac{\mathrm{d}x_3}{\mathrm{d}t} = -x_1 x_2 x_3 - x_2^3 - 1. \tag{35}$$

This ODE has the integral

$$I = \tfrac{1}{2}x_1^2 + \tfrac{1}{4}x_2^4 + \tfrac{1}{2}x_3^2 + x_2. \qquad (36)$$

It follows that

$$\nabla I = \begin{pmatrix} x_1 \\ x_2^3 + 1 \\ x_3 \end{pmatrix}, \qquad (37)$$

and hence $|\nabla I| = 0$ for $(x_1, x_2, x_3) = (0, -1, 0)$.

Nevertheless the ODE (35) can be rewritten in the form (3) as follows,

$$\begin{pmatrix} \dfrac{\mathrm{d}x_1}{\mathrm{d}t} \\ \dfrac{\mathrm{d}x_2}{\mathrm{d}t} \\ \dfrac{\mathrm{d}x_3}{\mathrm{d}t} \end{pmatrix} = \begin{pmatrix} 0 & 0 & x_2x_3 \\ 0 & 0 & 1 \\ -x_2x_3 & -1 & 0 \end{pmatrix} \cdot \nabla I, \qquad (38)$$

and can be integrated using the methods of Section 2.

(iii) We note that our method for constructing integral-preserving integrators resembles Feng and Wang's method for constructing volume-preserving integrators [4]. We hope to exploit this similarity in a future paper.

(iv) Non-Hamiltonian skew-gradient systems of the form (3) can also arise in finite-mode truncations of Hamiltonian PDEs [21].

(v) Associated with skew-gradient systems of the form (3), there is also a formulation in terms of a bracket

$$\frac{\mathrm{d}}{\mathrm{d}t} f(x) = \{f, I\}_s,$$

where the bracket is defined by

$$\{f, g\}_s := \sum_{i,j} \frac{\partial f}{\partial x_i} S_{i,j} \frac{\partial g}{\partial x_j}.$$

This bracket satisfies (i) $\{f,g\}_s = -\{g,f\}_s$ (skew symmetry), (ii) $\{f, \phi(g_1, \ldots, g_k)\}_s = \sum_{i=1}^{k} (\partial\phi/\partial g_i)\{f, g_i\}_s$ (Leibnitz rule), but in general the Jacobi identity is not satisfied. It follows that $\tilde{I}(x)$ is an integral of the skew-gradient system (3) iff $\{\tilde{I}, I\}_s = 0$.

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