SOLVING ODE's NUMERICALLY WHILE PRESERVING ALL FIRST INTEGRALS

G.R.W. QUISPEL[1,2] and H.W. CAPEL[3]

Abstract.

Using Discrete Gradient Methods (Quispel & Turner, J. Phys. **A29** (1996) L341-L349) we construct integration methods that solve ordinary differential equations numerically while preserving all their first integrals (i.e. constants of the motion) exactly.

[1] Department of Mathematics, La Trobe University, Bundoora, Melbourne, 3083, Australia.

[2] E-mail: R.Quispel@Latrobe.edu.au

[3] Instituut voor Theoretische Fysica, Universiteit van Amsterdam, Valckenierstraat 65, 1018XE, Amsterdam, The Netherlands.

Introduction

In the past, the numerical analysis of ordinary differential equations (ODE's) has focused, on **all-purpose** methods, i.e. integration methods that are applicable to all ODE's. Examples are Runge-Kutta methods and Linear Multistep methods.

In recent years, however, there has been great interest in **special-purpose** methods, designed to exactly preserve the mathematical properties of various special classes of ODE's. This has led to symplectic integrators for Hamiltonian ODE's [1], volume-preserving integrators for divergence-free ODE's [2,3], symmetry-preserving integrators for ODE's possessing some symmetry group [4,5], and isospectral integrators for isospectral ODE's [6,7].[1]

In this paper, we construct integral-preserving integrators (IPI's) for ODE's possessing an arbitrary number of first integrals (i.e. conserved quantities).[2] In the next section we define skew gradient systems, and show they are equivalent to dynamical systems possessing first integrals. This equivalence is then the crucial ingredient for constructing IPI's.

Necessary and sufficient conditions for a dynamical system to possess m first integrals

We first consider ordinary differential equations

Theorem 1. *The autonomous ODE*

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

has m first integrals $I_i(x),\ i = 1, \ldots, m$, if and only if eq.(1) can be written as a skew gradient system

$$\frac{dx}{dt} = S(x).\frac{DI_1}{Dx}(x)\frac{DI_2}{Dx}(x)\ldots\frac{DI_m}{Dx}(x). \tag{2}$$

Here S is some completely skew-symmetric $(m+1)$-tensor (i.e. $S_{i_1,\ldots,i_j,\ldots,i_k,\ldots,i_{m+1}} = -S_{i_1,\ldots,i_k,\ldots,i_j,\ldots,i_{m+1}}$, for all $j,k = 1,\ldots,m+1$), that is

[1] For a review of all these methods see ref. 8.
[2] The case of 1 first integral was treated in refs. 9 and 10.

contracted with the m (continuous) gradients in $\mathbb{R}^n$ denoted by[3]

$$\frac{DI_i}{Dx} := \begin{pmatrix} \frac{DI_i}{Dx_1}(x) \\ \vdots \\ \frac{DI_i}{Dx_n}(x) \end{pmatrix}, \qquad i = 1, \dots, m. \tag{3}$$

Contracting both the l.h.s. and the r.h.s. of eq. (2) with $\frac{DI_j}{Dx}$, and using the skew symmetry of the tensor S it follows easily that I_j is an integral of the skew gradient system, proving the implication in theorem (1) in one direction. The essential part of the proof of the implication in theorem 1 in the other direction is the construction of a skew $(m+1)$-tensor S for given vectorfield F and integrals $I_1, \dots, I_m$. Such a construction is given below in equations (8-10).

Theorem 1 also carries over to the discrete case:

Theorem 2. *Let a 'discrete gradient' $\triangle I/\triangle x$ be any vector satisfying the discrete identity*[4]

$$(x' - x) \cdot \frac{\triangle I}{\triangle x}(x, x') = I(x') - I(x). \tag{4}$$

Then the (implicit) mapping $x \to x'$ given by

$$x' - x = \phi(x, x'), \tag{5}$$

has m first integrals $I_i(x), i = 1, \dots, m$, if and only if eq. (5) can be written as a skew discrete-gradient system:

$$x' - x = \tilde{S}(x, x') \cdot \frac{\triangle I_1}{\triangle x}(x, x') \frac{\triangle I_2}{\triangle x}(x, x') \dots \frac{\triangle I_m}{\triangle x}(x, x'). \tag{6}$$

Here $\tilde{S}$ is some completely skew-symmetric $(m+1)$-tensor. The proof of theorem 2 is analogous to the proof of theorem 1 and will be omitted.

Discrete-gradient methods for integral-preserving integration.

Taken together, theorems 1 and 2 suggest the following two steps for constructing integral-preserving integrators (IPI's):

---

[3]For later convenience we use the notation DI_i/Dx_j for partial derivatives rather than the more common notation $\partial I_i/\partial x_j$.

[4]This definition is due to Gonzalez [11]

Step (i)

Write the ODE in skew gradient form

$$\frac{dx}{dt} = S(x) \cdot \frac{DI_1}{Dx}(x) \ldots \frac{DI_m}{Dx}(x). \tag{7}$$

There are infinitely many choices for the tensor S such that eq. (7) is equivalent to eq. (1). One can either choose a sufficiently regular S that one is given or that one has found heuristically (e.g. for Nambu systems [12, 13] S is given), or as a default one can choose

$$S_{i_0,\ldots,i_m}(x) = \frac{D_{i_0,\ldots,i_m}(x)}{d(x)}, \tag{8}$$

where the determinant D is given by

$$D_{i_0,\ldots,i_m} = \begin{vmatrix} f_{i_0} & DI_1/Dx_{i_0} & \ldots & DI_m/Dx_{i_0} \\ \vdots & \vdots & & \vdots \\ f_{i_m} & DI_1/Dx_{i_m} & \ldots & DI_m/Dx_{i_m} \end{vmatrix}, \tag{9}$$

and the normalization factor d is given by

$$d(x) = \sum_{n \geqslant j_1 > j_2 \cdots > j_m \geqslant 1} \begin{vmatrix} DI_1/Dx_{j_1} & \ldots & DI_m/Dx_{j_1} \\ \vdots & & \vdots \\ DI_1/Dx_{j_m} & \ldots & DI_m/Dx_{j_m} \end{vmatrix}^2 \tag{10}$$

Substituting the $(m+1)$-tensor S into eq. (7) and contracting it with the m gradients of I_1 to I_m, it is not difficult to retrieve the ODE (1).

STEP (ii). Integrate the skew gradient system (7), using an integral-preserving discrete-gradient method:

$$\frac{x' - x}{\tau} = S(x) \cdot \frac{\triangle I_1}{\triangle x}(x, x') \ldots \frac{\triangle I_m}{\triangle x}(x, x'). \tag{11}$$

Here the discrete gradient $\triangle I_i / \triangle x$ is any vector satisfying eq. (4), i.e. any vector of the form

$$\frac{\triangle I}{\triangle x}(x, x') = a(x, x') - (x' - x)\frac{(x' - x).a(x, x') + I(x) - I(x')}{(x' - x) \cdot (x' - x)}, \tag{12}$$

where $a(x, x')$ is any vector that (in order to be consistent) is close to the continuous gradient DI/Dx, i.e.

$$a(x, x') = \frac{DI}{Dx} + O(\tau) \tag{13}$$

and τ denotes the discrete timestep.

A simple choice satisfying eq. (13) is:

$$a_1(x, x') = \frac{DI}{Dx}(x) \tag{14}$$

Another choice is (cf. [14])

$$a_2(x, x') := \begin{pmatrix} \frac{I(x_1', x_2, x_3, \ldots, x_n) - I(x_1, x_2, x_3, \ldots, x_n)}{x_1' - x_1} \\ \frac{I(x_1', x_2', x_3, \ldots, x_n) - I(x_1', x_2, x_3, \ldots, x_n)}{x_2' - x_2} \\ \vdots \\ \frac{I(x_1', x_2', \ldots, x_{n-1}', x_n') - I(x_1', x_2', \ldots, x_{n-1}', x_n)}{x_n' - x_n} \end{pmatrix} \tag{15}$$

(substituting (15) into eq. (12) gives $\frac{\triangle I}{\triangle x} = a_2(x, x')$).

Higher-order discrete gradient methods for integral-preserving integration

The first-order method (11) defines a map $\phi_\tau : x \to x'$. A second-order method ψ_τ may be obtained by a Scovel projection [15]

$$\psi_\tau := \phi_{\tau/2} \circ \phi_{-\tau/2}^{-1} \tag{16}$$

The resulting ψ_τ has time-symmetry

$$\psi_\tau = \psi_{-\tau}^{-1}, \tag{17}$$

and can thus be used to construct IPI's of arbitrary order using the Yoshida method [16, 17].

If we have been able to find a skew tensor S without singularities, one can also obtain the time-symmetry (16) by using time-symmetric expressions for both the skew matrix $\tilde{S}$ and the discrete gradient in eq. (6). For example, for $\tilde{S}$ one may then take

$$\tilde{S}(x, x') := S\left(\frac{x + x'}{2}\right). \tag{18}$$

Similarly, one can take

$$a_3(x, x') = \frac{DI}{Dx}\left(\frac{x + x'}{2}\right) \tag{19}$$

in (12) (this discrete gradient is due to Gonzalez), or more generally

$$a_4(x,x') = \frac{\hat{a}(x,x') + \hat{a}(x',x)}{2}, \tag{20}$$

where $\hat{a}$ is any vector satisfying (13).

A numerical example

To illustrate our method we have chosen a Hamiltonian ODE in $\mathbb{R}^4$ with two integrals (i.e. $n = 4, m = 2$), studied by Hall and by Grammaticos et al. [18, 19]

$$\begin{aligned}
\frac{dx_1}{dt} &= p_1 \\
\frac{dx_2}{dt} &= p_2 \\
\frac{dp_1}{dt} &= -2x_1x_2 - ax_1 \\
\frac{dp_2}{dt} &= -16x_2^2 - x_1^2 - 16ax_2.
\end{aligned} \tag{21}$$

The integrals are

$$\begin{aligned}
I_1 &= \frac{1}{2}p_1^2 + \frac{1}{2}p_2^2 + \frac{16}{3}x_2^3 + x_1^2x_2 + \frac{a}{2}(x_1^2 + 16x_2^2) \qquad (22)\\
I_2 &= p_1^4 + (2ax_1^2 + 4x_1^2x_2)p_1^2 - \frac{4}{3}x_1^3p_1p_2 - \frac{4}{3}ax_1^4x_2 - \frac{4}{3}x_1^4x_2^2 - \frac{2}{9}x_1^6 + a^2x_1^4
\end{aligned}$$

In figure 1 we plot the value of the integral I_1 as a function of (numerical) time t, for three fourth-order numerical integration methods.[5] RK4 and LM4 are standard Runge-Kutta and Linear Multistep methods (see ref. 10 for more details), and QT4 is a discrete-gradient method. The value of the integral is seen to diverge for both standard methods, in contrast to the Discrete Gradient method. We hope to carry out a more detailed error analysis and more extended comparisons with other methods in the future.

Figure in here

[5] A similar picture is obtained for the other integral, I_2.

Singular points of the level sets belong to invariant sets

Differentiating the equation

$$I_i(x') = I_i(x) \qquad\qquad i = 1, \ldots, m. \tag{23}$$

with respect to x we obtain

$$\frac{DI_i}{Dx}(x')\frac{Dx'}{Dx} = \frac{DI_i}{Dx}(x) \tag{24}$$

Hence

$$\left[\sum_i a_i \frac{DI_i}{Dx}(x')\right]\frac{Dx'}{Dx} = \sum_i a_i \frac{DI_i}{Dx}(x). \tag{25}$$

Since the Jacobian matrix Dx'/Dx is nonsingular for sufficiently small τ, it follows that

$$\sum_i a_i \frac{DI_i}{Dx}(x') = 0 \Leftrightarrow \sum_i a_i \frac{DI_i}{Dx}(x) = 0. \tag{26}$$

It follows that for an integral-preserving map, any set of points x satisfying

$$\sum_i a_i \frac{DI_i}{Dx}(x) = 0 \tag{27}$$

is an invariant set.

The denominator $d(x)$ of S in eq. (8) is zero precisely if and only if the gradients of the integrals I_i are dependent. The above result implies that we can excise any such points from our phase space with impunity if we wish to use the tensor S given by eq. (8) in our integration scheme.

Concluding remarks

1. Discrete gradient systems are very suitable for applying splitting methods (A good reference on splitting methods is [20]). For instance split the vectorfield in eq. (7) in the following way:

$$v = \sum_{i_0<i_1<\cdots<i_m} v_{i_0,i_1,\ldots,i_m} \tag{28}$$

with

$$v_{i_0,i_1,\ldots,i_m} := \sum_{\pi} S_{i_0,i_1,\ldots,i_m}(x)\frac{DI_1}{Dx_i}(x)\ldots\frac{DI_m}{Dx_{i_m}}(x)\frac{\partial}{\partial x_{i_0}}, \tag{29}$$

where the sum in (29) is over all permutations of $i_0, i_1, \ldots, i_m$. Each vectorfield $v_{i_0,i_1,\ldots,i_m}$ preserves all m integrals, i.e. the splitting (28) is integral preserving. The integrators for these vectorfields will in general be less implicit, which may lead to increased efficiency.

2. A second feature of discrete gradient methods is their generality. They include all integral-preserving one-step methods (e.g. projection methods and energy-momentum methods). The advantage of this generality is that the freedom in choosing the tensor $\tilde{S}$ or the discrete gradient can be used to decrease the implicitness of the algorithm. One can also use this freedom to try to preserve some other property (e.g. symmetry) of the system. The task of finding the appropriate tensor $\tilde{S}$ for this purpose is, however, nontrivial.

Acknowledgements.

G.R.W.Q. is very grateful to the Australian Academy of Science for support under the Royal Society Exchange Program. We are indebted to G.S. Turner for producing Figure 1, and to La Trobe University for a Central Large Research Grant supporting this work. We are also indebted to J.A.G. Roberts for pointing out that singular points of the level sets form invariant sets.

References

[1] M. Sanz-Serna and M.P. Calvo, *Numerical Hamiltonian Problems*, Chapman Hall (1994).

[2] Feng Kang and Wang Dao-Liu, Dynamical systems and geometric construction of algorithms, in *Contemporary Mathematics* **163**, eds. Z. Shi and C. Yang, 1994.

[3] G.R.W. Quispel, Volume-preserving integrators, *Phys. Lett. A* 206 (1995), 26-30.

[4] D. Stoffer, Variable steps for reversible integration methods, *Computing* **55** (1995), 1-22.

[5] R.I. McLachlan, G.R.W. Quispel and G.S. Turner, Numerical integrators that preserve symmetries and reversing symmetries, *SIAM J. Num. Anal.* (accepted for publication).

[6] M.P. Calvo, A. Iserles and A. Zanna, Runge-Kutta methods for orthogonal and isospectral flows, preprint. DAMTP 1996/NA08.

[7] G.R.W. Quispel and R.I. McLachlan, in preparation.

[8] R.I. McLachlan and G.R.W. Quispel, Generating functions for dynamical systems with symmetries, differential invariants and first integrals, submitted to *Physica D.*

[9] G.R.W. Quispel and H.W. Capel, Solving ODE's numerically while preserving a first integral, *Phys. Lett.* **218A** (1996) (223-228).

[10] G.R.W. Quispel and G.S. Turner, Discrete gradients for solving ODE's numerically while preserving a first integral, *J. Phys. A* **29** (1996) L341-L349.

[11] O. Gonzalez, Time integration and discrete Hamiltonian systems, *J. Nonlinear Sci.*

[12] Y. Nambu, Generalized Hamiltonian dynamics, *Phys. Rev.* D7 (1973) 2405-2412.

[13] L. Takhtajan, On the foundation of generalized Nambu mechanics, *Comm. Math. Phys.* **100** (1994) 295-315.

[14] T. Itoh and K. Abe, Hamiltonian-conserving discrete canonical equations based on variational difference quotients, *J. Comput. Phys.* **77** (1988), 85.

[15] J.C Scovel, Symplectic numerical integration of Hamiltonian systems, in *The Geometry of Hamiltonian systems*, pp. 463-496, ed. T. Ratiu, MSRI Publ. 22, Springer, New York, 1991.

[16] H. Yoshida, Construction of higher order symplectic integrators, *Phys. Lett.* **150A** (1990) 262-268.

[17] M.-Z.Qin and W.-J.Zhu, Construction of higher order symplectic schemes by composition, *Computing* **47** (1992) 309-321.

[18] L.S. Hall, A theory of exact and approximate configurational invariants, *Physica* **8D** (1983) 90.

[19] B. Grammaticos, B. Dorizzi and R. Padjen, Painlevé property and integrals of motion for the Hénon-Heiles system, *Phys. Lett. A* **89** (1982) 111.

[20] R.I. McLachlan, On the numerical integration of ordinary differential equations by symmetric composition methods, *SIAM J.Sci. Com.* **16** (1995) 151-168.

Figure 1.

This figure illustrates that conventional integration methods (RK4 and LM4) do not preserve first integrals. It shows the numerial value of the integral I_1, as a function of time $t = n\tau$, for the $4D$ test system (21) (with $a = 0.1$). It compares the standard 4th order Runge-Kutta method (RK4; $\tau = 0.000017$), the 4th order Adams-Bashforth method (LM4; $\tau = 0.000015$) and a 4th order Discrete Gradient Method (QT4; $\tau = 0.0001$). (Timesteps τ have been adjusted such that the amount of numerical work done by the three methods is equivalent.)