Integral–preserving Integrators

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Many systems of differential equations possess so–called geometric properties, for example one or more first integrals, symplectic structure, volume preservation, and others. Numerical solution of such systems is usually best effected using a geometric integrator, i.e. one that can preserve this property exactly (i.e. up to round–off accuracy) [1, 2, 3].

In this extended abstract we are particulary interested in integral–preserving integrators (IPIs) which are designed to provide exact preservation of any first integral possessed by a system of ordinary differential equations (ODEs), e.g. momentum, angular momentum, energy, etc. We concentrate here on IPIs using so–called discrete gradients [4, 5, 6, 7, 8].

Consider thus an ODE

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

which possesses a first integral $I(x)$, i.e.

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

provided x satisfies (1).

Under conditions that are generally satisfied, (1) and (2) are equivalent to the existence of a skew matrix $S(x)$ such that (1) can be rewritten*

$$\frac{dx}{dt} = S(x)\nabla I(x). \tag{3}$$

An IPI for (3) is given by

$$\frac{x'-x}{h} = \bar{S}(x,x')\bar{\nabla} I(x,x'). \tag{4}$$

Here h denotes the time step, and

$$x := x(nh), \quad x' := x((n+1)h),$$

and $\bar{S}$ and $\bar{\nabla}$ denote a "discrete skew matrix" resp a "discrete gradient".

Discrete gradients must satisfy

$$I(x') - I(x) =: \bar{\nabla} I(x,x') \cdot (x'-x)$$

Discrete skew matrices must be skew, otherwise the only conditions on $\bar{S}$ and $\bar{\nabla}$ are that they must be consistent, i.e. in the limit $h \to 0$, i.e. $x' \to x$, they must go to S resp. ∇.

*Note that in general $S(x)$ does **not** satisfy the Jacobi identity.

It follows that $\bar{S}$ and $\bar{\nabla}$ are not at all unique. Many examples of discrete gradients have been constructed [5, 6], here we give two in $\mathbb{R}^2$:

$$\bar{\nabla}_1 I(x,x') := \begin{pmatrix} \frac{I(x_1',x_2)-I(x_1,x_2)}{x_1'-x_1} \\ \\ \frac{I(x_1',x_2')-I(x_1',x_2)}{x_2'-x_2} \end{pmatrix}$$

Here $x =: (x_1, x_2),\ x' =: (x_1', x_2')$.

A second example is given by

$$\bar{\nabla}_2 I(x,x') := \frac{\bar{\nabla}_1 I(x,x') + \bar{\nabla}_1 I(x',x)}{2}$$

In general, the above will give a numerical integration method of first–order accuracy.

There are various ways to obtain IPIs of higher order of accuracy. One method that we have developed constructs a method of order $n+1$ from a method of order n. For the sake of simplicity we here only give the construction of a second–order IPI from a first–order one:

Let $\dfrac{x'-x}{h} = S_1 \bar{\nabla} I(x,x')$ be a first–order IPI, with $S_1 := S = S(x)$, then a second–order IPI is given by

$$\frac{x'-x}{h} = S_2 \bar{\nabla} I(x,x'),$$

where

$$S_2 := S + h\left(\mathrm{SQS} + \frac{1}{2}C\right).$$

Here C and Q are skew matrices given by:

$$C^{ij} := \frac{\partial S^{ij}}{\partial x_m} S^{ml} \frac{\partial I}{\partial x_l}$$

and

$$Q := \frac{1}{2}(B^T - B),$$

where B is defined by

$$\bar{\nabla} =: \nabla I + B(x)\cdot(x'-x) + O\left(\|x'-x\|^2\right)$$

Similarly one obtains higher–order IPIs.

Concluding, we remark that

(1) Multiple integrals are preserved similarly.
(2) We are currently studying N–dimensional systems with $N-1$ integrals.
(3) Some generalizations of the above ideas to PDEs exist.

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References

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