On the construction of discrete gradients

Elizabeth L. Mansfield

School of Mathematics, Statistics and Actuarial Science,

University of Kent, Canterbury, CT2 7NF, U.K. *

G. Reinout W. Quispel

Department of Mathematics, and ARC Centre of Excellence

for Mathematics and Statistics of Complex Systems,

La Trobe University, Victoria 3086, Australia†

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Abstract

Discrete gradients are used to guarantee preservation of a first integral in a numerical approximation of a differential system. We propose a new method that constructs discrete gradients, potentially an infinite set of them, including the known families.

1 Context and Background

Geometric integration concerns the discretisation of differential equations in such a way that some geometric or physical property is preserved *exactly*, that is, without round off error. Some general references on geometric integration are (Leimkuhler and Reich, 2004; Hairer, Lubich and Wanner, 2006; Quispel and McLachlan, 2006).

* *Email address:* `E.L.Mansfield@kent.ac.uk`

† *Email address:* `R.Quispel@latrobe.edu.au`

Discrete gradients arise in one particular area of geometric integration, that of integral preserving integrators (IPIs). IPIs are numerical integration algorithms that preserve exactly one or more first integrals of a differential equation. Such integrals include, but are not resticted to, energy, momentum and angular momentum, and the differential equations include Hamiltonian as well as non Hamiltonian ones. IPIs can be applied to ordinary differential equations, (ODEs) (McLachlan, Quispel and Robidoux , 1999; McLaren and Quispel, 2004; Quispel and McLaren, 2008) as well as to semi-discretised partial differential equations (Matsuo, 2007; Celledoni *et al*).

The basic steps in constructing an IPI for an ODE that possesses a first integral $V(x)$ is as follows:

1. Write the ODE in the following form:

$$\dot{\mathsf{x}} = S(\mathsf{x})\nabla V(\mathsf{x}) \tag{1.1}$$

   where $S(\mathsf{x})$ is a skew symmetric matrix, $\dot{\mathsf{x}} = \mathrm{d}\mathsf{x}/\mathrm{d}t$ and $\mathsf{x} = (\mathsf{x}_1, \mathsf{x}_2, \ldots, \mathsf{x}_n)$. This can be done for a generic integral V (McLachlan, Quispel and Robidoux, 1999).

2. Discretise Equation (1.1) as follows:

$$\frac{\mathsf{x}' - \mathsf{x}}{h} = \widetilde{S}(\mathsf{x}, \mathsf{x}')\overline{\nabla}(V)(\mathsf{x}, \mathsf{x}'), \tag{1.2}$$

   where, by a slight abuse of notation, x denotes the numerical approximation to $\mathsf{x}(nh)$ and x' to $\mathsf{x}\,((n+1)h)$. Here $\widetilde{S}(\mathsf{x}, \mathsf{x}')$ is any skew symmetric matrix that approaches $S(\mathsf{x})$ in the continuum limit as $\mathsf{x}' \to \mathsf{x}$ and the time step $h \to 0$, and where

$$\begin{aligned} (\mathsf{x}' - \mathsf{x}) \cdot \overline{\nabla}(V) &= V(\mathsf{x}') - V(\mathsf{x}) \\ \overline{\nabla}(V)(\mathsf{x}, \mathsf{x}) &= \nabla V(\mathsf{x}) \end{aligned} \tag{1.3}$$

Substituting Equation (1.1) into the first of Equation (1.3), it can be seen that $V(\mathsf{x}') = V(\mathsf{x})$, that is, the integral V is preserved. All that remains is to find an expression for a discrete gradient $\overline{\nabla}(V)$ satisfying Equations (1.3), the solutions to which are far from unique.

Several discrete gradients have been found in the literature (Harten, Lax and van Leer, 1983; Itoh and Abe, 1988; Gonzales, 1996) and it may be fair to say that their derivations have been *ad hoc*. In this paper, we propose a systematic method to derive discrete gradients.

2 Discrete gradients; definition, examples and applications

Definition 2.1. Given a differentiable function V on $\mathbb{R}^n$, a *discrete gradient* is a vector-valued function $\overline{\nabla}(V) = \overline{\nabla}(V)(\mathbf{x}', \mathbf{x})$ which satisfies

$$\begin{aligned}(\mathbf{x}' - \mathbf{x}) \cdot \overline{\nabla}(V) &= V(\mathbf{x}') - V(\mathbf{x}) \\ \overline{\nabla}(V)(\mathbf{x}, \mathbf{x}) &= \nabla V(\mathbf{x}),\end{aligned}$$

where $\mathbf{x} = (x_1, x_2, \ldots, x_n)$.

To date, there have been three main families of examples.

Example 2.2. [Harten, Lax and van Leer, 1983] Suppose we are given a domain $\Omega \subset \mathbb{R}^n$ with co-ordinates $(x_1, \ldots, x_n)$, and V a scalar function on Ω with gradient

$$\nabla V = (V_1, \ldots V_n), \qquad V_i = \frac{\partial}{\partial x_i} V.$$

Suppose further that $\mathbf{x}$, $\mathbf{x}' \in \Omega$ are such that the straight line path from $\mathbf{x}$ to $\mathbf{x}'$ is contained in Ω. Then we define

$$\overline{\nabla} V(\mathbf{x}, \mathbf{x}') := (\overline{V}_1, \ldots, \overline{V}_n), \qquad \overline{V}_i := \int_0^1 V_i((1 - \xi)\mathbf{x} + \xi \mathbf{x}')\, \mathrm{d}\xi. \tag{2.1}$$

Then we have

$$\begin{aligned}\textstyle\sum_1^n (\overline{\nabla} V)_i(\mathbf{x}, \mathbf{x}') \cdot ({x'}_i - x_i) &= \textstyle\int_0^1 \sum_1^n V_i((1 - \xi)\mathbf{x} + \xi \mathbf{x}')({x'}_i - x_i)\, \mathrm{d}\xi \\ &= \textstyle\int_0^1 \frac{\mathrm{d}}{\mathrm{d}\xi} V((1 - \xi)\mathbf{x} + \xi \mathbf{x}')\, \mathrm{d}\xi \\ &= V(\mathbf{x}') - V(\mathbf{x})\end{aligned} \tag{2.2}$$

and

$$\lim_{\mathbf{x} \longrightarrow \mathbf{x}'} \overline{\nabla} V(\mathbf{x}, \mathbf{x}') = \nabla V(\mathbf{x}).$$

Example 2.3. [Itoh and Abe, 1988] constructed families of discrete gradients in terms of difference quotients. One example in $\mathbb{R}^2$ is, for $\mathbf{x} = (x, y)$,

$$\overline{\nabla} V(\mathbf{x}', \mathbf{x}) = \begin{pmatrix} \dfrac{V(x', y) - V(x, y)}{x' - x} \\[2ex] \dfrac{V(x', y') - V(x', y)}{y' - y} \end{pmatrix}.$$

For a third family of discrete gradients, see (Gonzalez, 1996).

Discrete gradients can be used, for example, to ensure conservation of energy in numerical approximations of Hamiltonian systems. If the Hamiltonian system and its approximation are

$$\dot{\mathsf{x}} = J\nabla H(\mathsf{x}), \qquad \frac{\mathsf{x}' - \mathsf{x}}{h} = J\overline{\nabla} H(\mathsf{x}', \mathsf{x}),$$

where h is the timestep and

$$J = \begin{pmatrix} 0 & I_n \\ -I_n & 0 \end{pmatrix},$$

then since J is skew-symmetric, we have both

$$\frac{\mathrm{d}H}{\mathrm{d}t} = \nabla H \cdot \dot{\mathsf{x}} = 0$$

and

$$H(\mathsf{x}') - H(\mathsf{x}) = \overline{\nabla} H \cdot (\mathsf{x}' - \mathsf{x}) = 0.$$

A theorem of (Ge and Marsden, 1988) states that: "Let H be a hamiltonian which has no other conserved quantities other than functions of H... If the numerical approximation is both symplectic and conserves H exactly, then it is the time advance map for the exact Hamiltonian system up to a reparametrization of time... For system with integrals, this result can be applied to the induced algorithm on the symplectic or Poisson reduced spaces...". This result should not be misunderstood as saying that algorithms that conserve all integrals do not exist. Indeed, McLachlan, Quispel and Robidoux (1999) show how to preserve *all* known integrals of an ordinary differential system using discrete gradients.

Example 2.4. The rigid body system reduces to

$$\dot{\mathsf{x}} = \mathsf{x} \times \nabla H$$

where $\mathsf{x} = (x, y, z) \in \mathbb{R}^3$ and $H(\mathsf{x}) = x^2/a^2 + y^2/b^2 + z^2/c^2$. There are two conserved quantities, namely

$$R = x^2 + y^2 + z^2, \qquad H = x^2/a^2 + y^2/b^2 + z^2/c^2.$$

Since $\mathsf{x} = \frac{1}{2}\nabla(R)$, the approximate scheme

$$\mathsf{x}' - \mathsf{x} = \tfrac{1}{2}h\overline{\nabla}R(\mathsf{x}', \mathsf{x}) \times \overline{\nabla}H(\mathsf{x}', \mathsf{x})$$

where $\overline{\nabla}R$ is a discrete gradient of R and $\overline{\nabla}H$ a discrete gradient of H, guarantees the two conserved quantities:

$$R(\mathsf{x}') - R(\mathsf{x}) = 0, \qquad H(\mathsf{x}') - H(\mathsf{x}) = 0.$$

3 Construction of discrete gradients

The construction of families of discrete gradients from given types of approximation data for functions, rests on the following observation.

Suppose the scalar function $V : \mathbb{R}^n \to \mathbb{R}$, and $\mathsf{x}', \mathsf{x} \in \mathbb{R}^n$ are given. If $\widetilde{V} : \mathbb{R}^n \to \mathbb{R}$ satisfies both

$$\widetilde{V}(\mathsf{x}') = V(\mathsf{x}'), \qquad \widetilde{V}(\mathsf{x}) = V(\mathsf{x}), \tag{3.1}$$

then for any discrete gradient $\overline{\nabla}\widetilde{V}$ of $\widetilde{V}$ we have

$$(\mathsf{x}' - \mathsf{x})\overline{\nabla}\widetilde{V} = V(\mathsf{x}') - V(\mathsf{x}).$$

Theorem 3.1. Suppose that $\widetilde{V} = \widetilde{V}_{(\mathsf{x}', \mathsf{x})}$ is constructed from V according to some algorithmic function approximation process that includes as part of the input, specific points x' and x, such that the Equations (3.1) hold. Then a discrete gradient for $\widetilde{V}$ yields a discrete gradient for V.

Proof: By construction, V and $\widetilde{V}$ agree at the two points x' and x. If we take the discrete gradient of V at the point $(\mathsf{x}'\mathsf{x})$ to be $\overline{\nabla}\widetilde{V}$, we have

$$\begin{aligned}
(\mathsf{x}' - \mathsf{x}) \cdot \overline{\nabla}V &= (\mathsf{x}' - \mathsf{x}) \cdot \overline{\nabla}\widetilde{V} \\
&= \widetilde{V}(\mathsf{x}') - \widetilde{V}(\mathsf{x}) \\
&= V(\mathsf{x}') - V(\mathsf{x}).
\end{aligned}$$

Further for $\mathsf{x}' \neq \mathsf{x}$,

$$\frac{V(\mathsf{x}') - V(\mathsf{x})}{\mathsf{x}' - \mathsf{x}} = \frac{\widetilde{V}(\mathsf{x}') - \widetilde{V}(\mathsf{x})}{\mathsf{x}' - \mathsf{x}},$$

defined component wise. Taking the limit $\mathsf{x}' \to \mathsf{x}$ on both sides yields $\overline{\nabla} V(\mathsf{x}, \mathsf{x}) = \nabla \widetilde{V}(\mathsf{x}) = \nabla V(\mathsf{x})$. $\square$

If we take the "prototypical" discrete gradient to be the average value of the gradient as given in Equation (2.1) then we obtain the following theorem.

Theorem 3.2. Let $V : \mathbb{R}^n \to \mathbb{R}$ be given. Suppose for any two points x' and x, we have that

(i) there exists an open set $\Omega \subset \mathbb{R}^n$, such that the straight line $(1-\lambda)\mathsf{x} + \lambda\mathsf{x}'$, $0 \leq \lambda \leq 1$ is contained wholly within Ω, and

(ii) there exists $\widetilde{V} = \widetilde{V}_{(\mathsf{x}',\mathsf{x})} : \Omega \to \mathbb{R}$, depending on x' and x, satisfying the Equations (3.1).

Then a discrete gradient for V is given by

$$\overline{\nabla} V(\mathsf{x}', \mathsf{x}) = \left(\overline{V}_1, \ldots, \overline{V}_n\right)$$

where

$$\overline{V}_i = \int_0^1 \frac{\partial \widetilde{V}}{\partial x_i}((1-\lambda)\mathsf{x} + \lambda\mathsf{x}')\, \mathrm{d}\lambda.$$

We will call this the *average value discrete gradient defined by the approximation* $\widetilde{V}$. We now give three examples.

Example 3.3. If for all $(\mathsf{x}', \mathsf{x})$ we take $\widetilde{V}_{(\mathsf{x}',\mathsf{x})} = V$, we obtain the average value discrete gradient of (Harten, Lax and van Leer, 1983), Example 2.2.

Example 3.4. In $\mathbb{R}^2$, suppose the approximation data is the value of V at three points, the given x and x' and any third noncollinear point x''. Set $\widetilde{V}(X, Y) = aX + bY + c$ for arbitrary $(X, Y) \in \mathbb{R}^2$ near x, x' and x'', and solve the equations $\widetilde{V}(\mathsf{x}) = V(\mathsf{x})$, $\widetilde{V}(\mathsf{x}') = V(\mathsf{x}')$ and $\widetilde{V}(\mathsf{x}'') = V(\mathsf{x}'')$ for the three unknown constants a, b and c. It is easy to calculate the average value of the gradient of $\widetilde{V}$ on the straight line between x and x' since $\widetilde{V}$ is linear, and we obtain the discrete gradient defined by $\widetilde{V}$ to be

$$\overline{\nabla} V(\mathsf{x}', \mathsf{x}) = \frac{1}{\Delta}\begin{pmatrix} -V(\mathsf{x})(y''-y') - V(\mathsf{x}')(y-y'') - V(\mathsf{x}'')(y'-y) \\ V(\mathsf{x})(x''-x') + V(\mathsf{x}')(x-x'') + V(\mathsf{x}'')(x'-x) \end{pmatrix}$$

where

$$\mathsf{x} = (x, y), \qquad \mathsf{x}' = (x', y'), \qquad \mathsf{x}'' = (x'', y''), \tag{3.2}$$

and where

$$\Delta = \det \begin{pmatrix} x & y & 1 \\ x' & y' & 1 \\ x'' & y'' & 1 \end{pmatrix}.$$

Indeed, the families of discrete gradients constructed by (Itoh and Abe, 1988), in terms of difference quotients, can all be derived according to Theorem 3.2 from linear approximations of $V : \mathbb{R}^n \to \mathbb{R}$ with the approximation data being the value of V at $n+1$ specific points.

Item (ii) in Theorem 3.2 is achieved in an algorithmic fashion by taking a finite dimensional function space defined in terms of certain moments and function values at given points, that are relevant to the problem at hand. One then takes the *projection* of V to the finite dimensional function space. For example, by taking x and x' to be two vertices of a simplex, approximations of V to any order can be obtained by using standard approximations used in Finite Element Theory.

Example 3.5. For $V : \mathbb{R}^2 \to \mathbb{R}$, suppose the approximation data is the value of V at three points, the given x and x' and any third noncollinear point x'', and in addition the zeroth moment $m_0(V)$ of V along the straight line from x to x', that is, $m_0(V) = \int_0^1 V\left((1-t)\mathsf{x} + t\mathsf{x}'\right) \,\mathrm{d}t$. Take the "shape" of $\widetilde{V}$ to be $\widetilde{V}(X,Y) = aXY + bX + cY + d$ for arbitrary $(X,Y) \in \mathbb{R}^2$ near x, x' and x''. The constants a, b, c and d are solved by setting

$$\begin{aligned} \widetilde{V}(\mathsf{x}) &= V(\mathsf{x}) \\ \widetilde{V}(\mathsf{x}') &= V(\mathsf{x}') \\ \widetilde{V}(\mathsf{x}'') &= V(\mathsf{x}'') \\ m_0(\widetilde{V}) &= m_0(V). \end{aligned}$$

For simplicity take x'' in Equation (3.2) to be $\mathsf{x}'' = (x', y)$, the "corner point". The discrete gradient is then

$$\overline{\nabla} V(\mathsf{x}', \mathsf{x}) = \begin{pmatrix} \dfrac{V(\mathsf{x}) + 3V(\mathsf{x}') + 2V(\mathsf{x}'') - 6m_0(V)}{2(x'-x)} \\ \\ -\dfrac{3V(\mathsf{x}) + V(\mathsf{x}') + 2V(\mathsf{x}'') - 6m_0(V)}{2(y'-y)} \end{pmatrix}.$$

At the present time, we know of no examples of discrete gradients that do not arise by applying Theorem 3.2 to a particular finite dimensional approximation to V. We have already shown this is true for two of the known families. To show it is true for the example due to Gonzalez, one takes as approximation data, in addition to the values $V(\mathsf{x})$ and $V(\mathsf{x}')$, the component of the gradient of V at the point $\frac{1}{2}(\mathsf{x}+\mathsf{x}')$ in the direction normal to $\mathsf{x}'-\mathsf{x}$. However, it is an open problem as to whether *any* discrete gradient can be obtained in this way.

Finally, we note that there is no correlation between the order of the approximation used and the order of the scheme. Indeed, for scalar functions on $\mathbb{R}$, there is only one discrete gradient (Moan, 2003), which is

$$\overline{\nabla}V(x',x) = \frac{V(x')-V(x)}{x'-x}.$$

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