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Geometric Integration by Playing with Matrices

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Abstract. We show that many Runge-Kutta methods derived in the framework of *Geometric Integration* can be elegantly formalized by using special matrices defined by a suitable polynomial basis.

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INTRODUCTION

Geometric Integration deals with the numerical solution of differential problems, whose associated vector field has relevant geometric properties. It is then of interest to be able to reproduce such properties in the discrete vector field induced by a numerical method. The most famous instance of problem dealt within geometric integration is given by Hamiltonian problems, i.e., problems in the form,

$$y' = J\nabla H(y), \qquad y(t_0) = y_0 \in \mathbb{R}^{2m}, \tag{1}$$

where J is a constant, orthogonal, and skew-symmetric matrix. Such problems have been actively investigated in the last thirty years. However, the very first significant attempt of performing geometrical integration can be led back to the early works of G. Dahlquist, leading to the linear stability analysis of the methods, where the asymptotic stability of equilibria is asked to be reproduced by the numerical methods.

Coming back to problem (1), the scalar function $H(y)$ is called the *Hamiltonian* of the problem and its value is constant during the motion, i.e., $H(y(t)) \equiv H(y_0),\ \forall t \geq t_0$, for the solution $y(t)$ of (1). Often, the Hamiltonian H is also called the *energy*, since for isolated mechanical systems it has the physical meaning of total energy. Consequently, *energy conservation* is an important feature in the simulation of such problems. The energy conservation property of (1) may be shown to derive from the *symplecticity* of the associated flow. This is no longer true in the discrete setting.

Concerning the numerical integration of (1), two main lines of investigation have been the definition and the study of *symplectic* methods and *energy-conserving* methods, respectively. This reflects the fact that the symplecticity of the map associated with (1) and energy conservation are the most relevant features characterizing a Hamiltonian system.

Symplectic methods are obtained by imposing that the discrete map, associated with a given numerical method, is symplectic, as is the continuous one. Since for the continuous map symplecticity implies energy-conservation, then one expects that something similar happens for the discrete map as well. As a matter of fact, under suitable assumptions, it can be proved that, when a symplectic method is used with a constant step-size, the numerical solution satisfies a perturbed Hamiltonian problem, thus providing a quasi-conservation property over "exponentially long times" [1]. Even though this is an interesting feature, nonetheless, it constitutes a somewhat weak stability result since, in general, it doesn't extend to infinite intervals. Consequently, it makes sense to directly looking for *energy-conserving* methods, able to exactly satisfy the conservation property of the Hamiltonian along the numerical trajectory.

The very first attempts to face this problem were based on projection techniques coupled with standard non conservative numerical methods. However, it is well-known that this approach suffers from many drawbacks, in that this is usually not enough to correctly reproduce the dynamics (see, e.g., [18, p. 111]).

A completely new approach is represented by *discrete gradient methods*, which are based upon the definition of a discrete counterpart of the gradient operator, so that energy conservation of the numerical solution is guaranteed at each step and for any choice of the integration step-size [16, 24].

A different approach is based on the concept of *time finite element methods*, where one finds local Galerkin approximations on each subinterval of a given mesh of size h for the equation (1). This, in turn, has led to the definition

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of energy-conserving Runge–Kutta methods [2, 3, 26].

A partially related approach is given by *discrete line integral methods* [20, 21, 22], where the key idea is to exploit the relation between the method itself and the *discrete line integral*, i.e., the discrete counterpart of the the line integral in conservative vector fields. This, in turn, allows exact conservation for polynomial Hamiltonians of arbitrarily high-degree, resulting in the class of methods later named *Hamiltonian Boundary Value Methods (HBVMs)*, which have been developed in a series of papers [5, 6, 4, 7, 8, 9, 10, 11].

Another approach, strictly related to the latter one, is given by the *Averaged Vector Field* method [25, 14] and its generalizations [17], which have been also analysed in the framework of B-series [15] (i.e., methods admitting a Taylor expansion with respect to the step-size).

USEFUL MATRICES IN GEOMETRIC INTEGRATION

Even though most of the following arguments can be extended to more general settings [11], we here consider the polynomial basis given by the Legendre polynomials, shifted on the interval $[0,1]$, and scaled so that they are orthonormal:

$$\int_0^1 P_i(c)P_j(c)\mathrm{d}c = \delta_{ij}, \qquad \forall i,j \geq 0, \tag{2}$$

with δ_{ij}, the Kroneckher symbol. Consequently, they are defined by the following recurrence:

$$\begin{aligned} P_0(\tau) &\equiv 1, \qquad P_1(\tau) = \sqrt{3}\,(2\tau-1)\,, \\ P_{j+1}(\tau) &= \left[\frac{2j+1}{j+1}\sqrt{\frac{2j+3}{2j+1}}\right](2\tau-1)P_j(\tau) - \left[\frac{j}{j+1}\sqrt{\frac{2j+3}{2j-1}}\right]P_{j-1}(\tau), \quad j \geq 1. \end{aligned} \tag{3}$$

They satisfy, for $c \in [0,1]$:

$$\int_0^c P_0(\tau)\mathrm{d}\tau = \xi_1 P_1(c) + \frac{1}{2}P_0(c), \qquad \int_0^c P_j(\tau)\mathrm{d}\tau = \xi_{j+1}P_{j+1}(c) - \xi_j P_{j-1}(c), \quad j \geq 1, \tag{4}$$

where

$$\xi_j = \left(2\sqrt{4j^2-1}\right)^{-1}, \quad j \geq 1. \tag{5}$$

Then, let us introduce, for $r \geq 1$, the matrices (see (3))

$$\mathscr{P}_r = \begin{pmatrix} P_0(c_1) & \dots & P_{r-1}(c_1) \\ \vdots & & \vdots \\ P_0(c_k) & \dots & P_{r-1}(c_k) \end{pmatrix}, \quad \mathscr{I}_r = \begin{pmatrix} \int_0^{c_1} P_0(x)\mathrm{d}x & \dots & \int_0^{c_1} P_{r-1}(x)\mathrm{d}x \\ \vdots & & \vdots \\ \int_0^{c_k} P_0(x)\mathrm{d}x & \dots & \int_0^{c_k} P_{r-1}(x)\mathrm{d}x \end{pmatrix} \in \mathbb{R}^{k\times r}, \tag{6}$$

for a given set of abscissae $0 \leq c_1 < \cdots < c_k \leq 1$, and (see (5))

$$X_r = \begin{pmatrix} \frac{1}{2} & -\xi_1 & & \\ \xi_1 & 0 & \ddots & \\ & \ddots & \ddots & -\xi_{r-1} \\ & & \xi_{r-1} & 0 \end{pmatrix} \in \mathbb{R}^{r\times r}, \qquad \widehat{X}_r = \begin{pmatrix} \frac{1}{2} & -\xi_1 & & \\ \xi_1 & 0 & \ddots & \\ & \ddots & \ddots & -\xi_{r-1} \\ & & \xi_{r-1} & 0 \\ & & & \xi_r \end{pmatrix} \in \mathbb{R}^{r+1\times r}. \tag{7}$$

We observe that, by virtue of (4), one has

$$\mathscr{I}_r = \mathscr{P}_{r+1}\widehat{X}_r, \qquad r \geq 1. \tag{8}$$

Finally, let us define the diagonal matrix

$$\Omega = \mathrm{diag}(b_1,\dots,b_k) \in \mathbb{R}^{k\times k},$$

where the $\{b_i\}$ are the quadrature weights defined at the abscissae $\{c_i\}$. From (2) it follows that $\mathscr{P}_r^T\Omega\mathscr{P}_r = I_r$, the identity matrix of dimension r, provided that the order of the quadrature is at least $2r$ (that is, exact for polynomials of degree at most $2r-1$). In particular, we shall hereafter assume that the abscissae are placed at the Gauss-Legendre points in $[0,1]$, so that the order of the quadrature is $2k$.

Energy-conserving methods: HBVMs

By using the above notation, let us consider the k-stage Runge-Kutta method defined by the following Butcher tableau,

$$\frac{\boldsymbol{c} \;\big|\; \mathscr{I}_s \mathscr{P}_s^T \Omega}{\;\big|\; \boldsymbol{b}^T}, \qquad s \le k. \tag{9}$$

It defines a HBVM(k,s) method [5, 7, 10]. For $k = s$ it becomes the well known s-stage Gauss method, which is symplectic and conserves quadratic Hamiltonians. For all $k > s$, the method is no more symplectic but turns out to have order $2s$ and exactly conserves polynomial Hamiltonians of degree no larger than

$$\nu = \lceil \frac{2k}{s} \rceil.$$

Clearly, this implies a *practical* conservation for all suitably regular Hamiltonians, by taking k large enough [5, 7, 11]. This, in turn, doesn't increase the computational cost of the method too much since the Butcher matrix in (9) has rank s, for all $k \ge s$, since, by virtue of (8),

$$\mathscr{I}_s \mathscr{P}_s^T \Omega = \mathscr{P}_{s+1} \widehat{X}_s \mathscr{P}_s^T \Omega, \tag{10}$$

so that, by virtue of (2), and considering that matrix X_s in (7) is nonsingular,

$$\mathscr{P}_s^T \Omega \left(\mathscr{P}_{s+1} \widehat{X}_s \mathscr{P}_s^T \Omega \right) = [I_s \; \mathbf{0}] \widehat{X}_s \mathscr{P}_s^T \Omega = X_s \mathscr{P}_s^T \Omega.$$

Consequently, $k - s$ stages can be cast as linear combinations of *s fundamental stages* [5, 7, 10] (see also [9]).

Symplectic low-rank Runge-Kutta methods

By considering, instead of (9)–(10), the k-stage Runge-Kutta method defined by the Butcher tableau,

$$\frac{\boldsymbol{c} \;\big|\; \mathscr{P}_s X_s \mathscr{P}_s^T \Omega}{\;\big|\; \boldsymbol{b}^T}, \qquad s \le k, \tag{11}$$

one obtains methods which are symplectic. Indeed (see, e.g., [18]), from (7) one easily verifies that

$$\Omega \left(\mathscr{P}_s X_s \mathscr{P}_s^T \Omega \right) + \left(\mathscr{P}_s X_s \mathscr{P}_s^T \Omega \right)^T \Omega = \boldsymbol{b}\boldsymbol{b}^T. \tag{12}$$

Again, for $k = s$ one obtains the s-stage Gauss method. For $k > s$ one obtains *symplectic low-rank Runge-Kutta (SLIRK) methods*, which proved to be very suited for efficiently solving stochastic Hamiltonian problems with additive noise [13].

EQUIP methods

A further approach is obtained by considering $k = s$, and observing that, for any skew-symmetric matrix $W \in \mathbb{R}^{s \times s}$, one has (compare with (12))

$$\Omega \left(\mathscr{P}_s (X_s + W) \mathscr{P}_s^T \Omega \right) + \left(\mathscr{P}_s (X_s + W) \mathscr{P}_s^T \Omega \right)^T \Omega = \boldsymbol{b}\boldsymbol{b}^T.$$

Consequently, the s-stage Runge-Kutta method

$$\frac{\boldsymbol{c} \;\big|\; \mathscr{P}_s (X_s + W) \mathscr{P}_s^T \Omega}{\;\big|\; \boldsymbol{b}^T} \tag{13}$$

turns out to be symplectic, thus conserving all quadratic invariants. By following an approach similar to that used in [23], in [12] it is shown that by taking matrix W in the form

$$W = \alpha(\boldsymbol{e}_2 \boldsymbol{e}_1^T - \boldsymbol{e}_1 \boldsymbol{e}_2),$$

with $\boldsymbol{e}_i \in \mathbb{R}^s$ the i-th unit vector, it is possible to choose, at each step of integration, α such that energy conservation is gained. Moreover, in so doing the original order $2s$ of the underlying Gauss method (obtained for $\alpha = 0$) is retained by the new method which has been, therefore, named an *energy and quadratic invariant preserving (EQUIP)* method.

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