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A scalpel, not a sledgehammer: Qualitative approach to numerical mathematics

Arieh Iserles and Antonella Zanna

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Department of Applied Mathematics and Theoretical Physics
Silver Street
Cambridge
England CB3 9EW

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Arieh Iserles[1] and Antonella Zanna[2]

1 A new paradigm for numerical analysis

The classical approach to numerical calculations emphasizes the role of general computational tools that can cater for a wide range of situations. Thus, the quest is for a method for 'all' initial value problems for ordinary differential equations or for 'all' parabolic reaction-diffusion equations or for 'all' algebraic eigenvalue problems. The merit of this 'broad-aperture' outlook is clear, since it means that a relatively modest compendium of computational tools can cater for a wide variety of situations. Most users of numerical mathematics might be specialists in their own domains of expertise but are mostly of a limited numerical (and pure-mathematical) knowledge and experience. Hence the attraction of tools that can be employed to a variety of situations and that do not require profound numerical or mathematical knowledge.

Yet, a different paradigm has evolved in the last few years. It is our intention in this paper to explain briefly why this alternative outlook, while not obviating the quest for general computational tools, has important attractions from theoretical and practical points of view alike.

The classical view of 'doing mathematics' separates the analytical and the numerical. The research into qualitative attributes of mathematical systems and into their numerical realizations is separated both in time – the qualitative research usually precedes the computational stage – and in space: different professionals, are likely to take part in both efforts, often with poor cross-disciplinary communication channels. To coin a phrase, numerical calculation often commences at the exact moment when mathematical analysis finally gives up in despair. *We believe that this attitude is wrong.* At their best, mathematical analysis and computation should coexist in a symbiotic relationship: while computation tells the analyst what to prove, analysis tells the scientific computational professional what to calculate!

[1]Department of Applied Mathematics and Theoretical Physics, University of Cambridge, Cambridge.

[2]Newnham College, University of Cambridge, Cambridge.

Insofar as numerical analysis is concerned, the above sentiment means that *known qualitative information about the system in question should be embedded whenever possible into the numerical method.* Therefore, instead of a quest for general tools, qualitative numerical analysis seeks algorithms that cater for small collections of problems that share similar attributes. Moreover, it does not accept that a fault line runs between analysis and computation.

We hasten to reiterate that the classical, generalist approach has its place and we have no intention of overturning it branch and root. However, the emerging body of results in qualitative numerical analysis makes, we believe, a compelling case for more attention being paid also to this approach.

In the sequel of this paper we restrict our exposition to the numerical solution of initial value problems for ordinary differential equations. This is motivated not just by our personal interest but mainly by the significant body of results that has emerged in this area during the last decade.

'Qualitative behaviour' of ordinary differential equations is typically associated either with their asymptotic attributes or with their invariants. Asymptotic behaviour of numerical methods has attracted a great deal of attention since the pioneering work of Dahlquist in the Sixties. The recent emphasis on techniques from the theory of nonlinear dynamical systems has led to an impressive understanding and it has been comprehensively surveyed in [19]. Henceforth we restrict our attention to the retention of invariants under discretization.

We refer the reader to [14, 21] for any unfamiliar concepts from differential topology, differential geometry and theory of Lie groups.

2 Numerical methods

Two general families of numerical algorithms are most popularly applied to the computation of a ordinary differential system

$$\boldsymbol{y}' = \boldsymbol{f}(t, \boldsymbol{y}), \quad t \geq 0, \qquad \boldsymbol{y}(0) = \boldsymbol{y}_0 \in \mathbb{R}^d, \tag{2.1}$$

namely a *multistep* (s-step) method

$$\sum_{k=0}^{s} \alpha_k \boldsymbol{y}_{n+k} = h \sum_{k=0}^{s} \beta_k \boldsymbol{f}((n+k)h, \boldsymbol{y}_{n+k}), \qquad n \in \mathbb{Z}^+, \tag{2.2}$$

and a *Runge–Kutta* (ν-stage) scheme

$$\begin{aligned}
\boldsymbol{\varphi}_\ell &= \boldsymbol{y}_n + h\sum_{j=1}^{\nu} a_{\ell,j}\boldsymbol{k}_j, \qquad \ell = 1,2,\ldots,\nu,\\
\boldsymbol{k}_\ell &= \boldsymbol{f}((n+c_\ell)h, \boldsymbol{\varphi}_\ell),\\
\boldsymbol{y}_{n+1} &= \boldsymbol{y}_n + h\sum_{\ell=1}^{\nu} b_\ell \boldsymbol{k}_\ell, \qquad n \in \mathbb{Z}^+.
\end{aligned} \tag{2.3}$$

Here $\boldsymbol{y}_m \approx \boldsymbol{y}(mh)$, while $h > 0$ is a given *step-length.* Note that each multistep method can be characterized in terms of the vectors $\boldsymbol{\alpha} = (\alpha_k)$, $\boldsymbol{\beta} = (\beta_k)$, while a Runge–Kutta method is determined by the *RK matrix* $A = (A_{\ell,j})$, the *RK weights* $\boldsymbol{b} = (b_\ell)$ and the *RK nodes* $\boldsymbol{c} = (c_\ell) = A\mathbf{1}$. We recall that an important attribute of any numerical method for (2.1) is its *order,* namely $p \in \mathbb{Z}^+$ such that $\boldsymbol{y}_{n+k} = \boldsymbol{y}((n+k)h)$, $k = 0,1,\ldots,s-1$ ($s = 1$ for (2.3)), implies that $\boldsymbol{y}_{n+s} = \boldsymbol{y}((n+s)h) + \mathcal{O}(h^{p+1})$. Every Runge–Kutta method of order $p \geq 1$ uniformly converges to the exact solution in a compact interval when $h \to 0$, while the convergence of (2.2) requires an extra condition, namely that all the zeros of the polynomial $\sum_{k=0}^{s} \alpha_k w^k$ reside in $|w| \leq 1$ and the zeros on $|w| = 1$ are simple.

We refer the reader to [15] for a comprehensive review of methods (2.2) and (2.3). The purpose of this section is just to establish the formalism for our exposition in the sequel.

3 Quadratic conservation laws

Let us suppose that there exists $S \in \mathrm{M}_d[\mathbb{R}]$, the set of all $d \times d$ real matrices, such that the exact solution of (2.1) obeys the *quadratic conservation law*

$$\boldsymbol{y}^T(t)S\boldsymbol{y}(t) \equiv \boldsymbol{y}_0^T S\boldsymbol{y}_0, \qquad t \geq 0. \tag{3.1}$$

It is trivial to verify that the necessary and sufficient condition for (3.1) is $\boldsymbol{x}^T S\boldsymbol{f}(t,\boldsymbol{x}) \equiv 0$ for all $t \geq 0$ and $\boldsymbol{x} \in \mathbb{R}^d$.

A quadratic conservation law often encapsulates important qualitative information about the solution of (2.1) and its retention under discretization (that is, $\boldsymbol{y}_n^T S\boldsymbol{y}_n \equiv \boldsymbol{y}_0^T S\boldsymbol{y}_0$, $n \in \mathbb{Z}^+$) is the first specific problem of the present paper.

Theorem 1 (Cooper, [9]) *The Runge–Kutta scheme* (2.3) *always renders correctly the quadratic conservation law* (3.1) *subject to the condition* $M = O$*, where* $M = (m_{i,j}) \in \mathrm{M}_\nu$,

$$m_{i,j} = b_i a_{i,j} + b_j a_{j,i} - b_i b_j, \qquad i,j = 1,2,\ldots,\nu. \tag{3.2}$$

An important special case of quadratic conservation laws is represented by *orthogonal flows*

$$Y' = F(t,Y)Y, \quad t \geq 0, \qquad Y(0) = Y_0 \in \mathrm{O}_d[\mathbb{R}], \tag{3.3}$$

where $F : \mathrm{O}_d[\mathbb{R}] \to \mathrm{o}_d[\mathbb{R}]$. Here $\mathrm{O}_d[\mathbb{R}]$ is the manifold (Lie group) of $d \times d$ real orthogonal matrices, while $\mathrm{o}_d[\mathbb{R}]$ is the set of $d \times d$ real skew-symmetric matrices (the Lie algebra of $\mathrm{O}_d[\mathbb{R}]$). It is easy to verify that $Y(t) \in \mathrm{O}_d[\mathbb{R}]$, $t \geq 0$. Orthogonality being a quadratic conservation law (in the underlying Frobenius inner product), we can deduce from Theorem 1 that, subject to $M = O$, this crucial structural feature of orthogonal flows survives under discretization by a Runge–Kutta method. This has been independently proved by Dieci, Russell and Van Vleck [11], while Calvo, Iserles and Zanna showed that the condition $M = O$ is necessary (as well as sufficient) [4]. These results can be also extended with ease to flows on the *Stiefel manifold.*

The behaviour of multistep methods in the present context is radically different.

Theorem 2 (Calvo, Iserles & Zanna, [7]) *For every multistep method* (2.2) *there exists a system* (2.1) *with a quadratic invariant which is not rendered correctly by the numerical solution.*

The above two theorems present a compelling argument in favour of Runge–Kutta methods, insofar as correct rendition of invariants is at issue. We therefore concentrate on such methods in the sequel.

An alternative route to the maintenance of invariants under discretization is represented by *projective* methods. Thus, in the case of orthogonal flows we may solve (3.3) with an arbitrary method, subsequently projecting the result on $\mathrm{O}_d[\mathbb{R}]$, e.g. with a polar factorization. Projective methods for orthogonal flows have been presented in [11] and general issues of projection are debated in [2].

4 Hamiltonian equations

A Hamiltonian system of ordinary differential equations can be written in the form

$$\begin{array}{rcl} \dfrac{\mathrm{d}\boldsymbol{p}}{\mathrm{d}t} &=& -\dfrac{\partial H(\boldsymbol{p},\boldsymbol{q})}{\partial \boldsymbol{q}}, \\ \dfrac{\mathrm{d}\boldsymbol{q}}{\mathrm{d}t} &=& \dfrac{\partial H(\boldsymbol{p},\boldsymbol{q})}{\partial \boldsymbol{p}}, \end{array} \quad t \geq 0, \qquad \begin{array}{l} \boldsymbol{p}(0) = \boldsymbol{p}_0, \\ \boldsymbol{q}(0) = \boldsymbol{q}_0. \end{array} \tag{4.1}$$

The vectors $\boldsymbol{p}, \boldsymbol{q} \in \mathbb{R}^d$ denote generalized momenta and generalized positions, respectively, in a mechanical system. Hamiltonian equations are ubiquitous in many branches of applied mathematics and physical sciences and they exhibit a significant number of important features. Arguably, the most important invariant associated with isospectral flows is their *symplecticity,* namely the conservation of the alternating differential form $\mathrm{d}\boldsymbol{p} \wedge \mathrm{d}\boldsymbol{q}$. Among the consequences of symplecticity are the conservation of all Poincaré invariants and the existence of invariant tori [1].

Although symplectic discretizations based on generating functions (and primitive by modern standards) have been available since early Eighties, the real breakthrough arrived with the simultaneous discovery of symplectic Runge–Kutta methods by F. Lasagni, J.M. Sanz-Serna and Y.B. Suris in 1988.

Theorem 3 [18] *The Runge–Kutta method* (2.3) *is symplectic if $M = O$, the matrix M having been defined in* (3.2)*.*

An important caveat is associated with the implementation of symplectic Runge–Kutta methods. It is an act of faith in the numerical community that realistic implementation of algorithms for initial value problems requires variable step sizes. Specifically, the local error is monitored in each step and the size of the next step is chosen to minimize the computational cost, consistently with user-provided error tolerance [15]. (The description of numerical methods in Section 2 in a constant step-size formalism is exclusively for the sake of an ease of exposition.) However, symplecticity requires that the step-size remains constant throughout the whole integration and, as soon as variable step-size is allowed, all its benefits are lost.

An important benefit of symplecticity is that the error in the numerical time-stepping scheme accumulates in a linear fashion [18]. However, similar behaviour is displayed when, instead of $\mathrm{d}\,\mathrm{I} \wedge \mathrm{d}\,\mathrm{II}$ one conserves the Hamiltonian energy $H(\mathrm{I}, \mathrm{II})$ [12]. The situation is further complicated because the only 'method' that renders correctly both the symplectic invariant and the Hamiltonian energy is the exact solution of (4.1) [13]. The jury is still out on the question of what is the most appropriate invariant that should be retained in the discretization of Hamiltonian systems.

5 Isospectral flows

It is relatively straightforward to prove that flows of the form

$$L' = [B(L), L] = B(L)L - LB(L), \quad t \geq 0, \qquad L(0) = L_0 \in \mathrm{M}_d[\mathbb{R}], \quad (5.1)$$

where $B \in \mathrm{Lip}[\mathrm{M}_d[\mathbb{R}] \to \mathrm{M}_d[\mathbb{R}]]$, is *isospectral.* This means that the eigenvalues of $L(t)$ are invariant, hence $\sigma(L(t)) \equiv \sigma(L_0)$. Moreover, provided that $L_0 \in \mathrm{S}_d[\mathbb{R}]$, the set of all $d \times d$ symmetric real matrices, and $B : \mathrm{S}_d[\mathbb{R}] \to \mathrm{o}_d[\mathbb{R}]$, it is true that $L(t) \in \mathrm{S}_d[\mathbb{R}]$, $t \geq 0$.

Isospectral flows feature in a large number of applications. Examples include the motion of a lattice of particles under near-neighbour exponential interaction (Toda flows), the interaction of two motions of a lattice (Kac–van Moerbeke flows), applications to a range of problems in numerical algebra [8] and in linear programming [3] etc. The retention of the isospectral invariant under discretization is often of crucial importance: an extreme case is when specific isospectral flows (e.g. QR flows or double-bracket flows [3, 8]) are used to calculate eigenvalues of L_0 or to compute inverse eigenvalue problems [8].

Let $\{L_n\}_{n\in\mathbb{Z}^+}$ be a sequence of approximants to the solution of (5.1) at the points $\{nh\}_{n\in\mathbb{Z}^+}$ and denote the eigenvalues of L_n by $\{\lambda_{n,\ell}\}_{\ell=1}^d$. In an appropriate ordering, isospectrality is tantamount to $\lambda_{n,\ell} \equiv \lambda_{0,\ell}$ for all $\ell = 1, 2, \ldots, d$ and $n \in \mathbb{Z}^+$. This, in turn, is equivalent to

$$\mathrm{tr}\, L_n^k = \sum_{\ell=1}^{d} \lambda_{n,\ell}^k \equiv \text{const}, \qquad n \in \mathbb{Z}^+,\ k = 1, 2, \ldots, d. \tag{5.2}$$

For every $k \in \mathbb{Z}^+$ and $c_k \in \mathbb{R}$ consider the manifold $\mathcal{M}_k(c_k) := \{L \in \mathrm{M}_d[\mathbb{R}] : \mathrm{tr}\, L^k = c_k\}$. The condition (5.2) can be rendered in the form

$$L_n \in \bigcap_{k=1}^{d} \mathcal{M}_k(c_k).$$

for $c_k = \mathrm{tr}\, L_0^k$, $k = 1, 2, \ldots, d$. This motivates our interest in Runge–Kutta methods (2.3) that stay on manifolds $\mathcal{M}_k$.

Every method (2.3) retains a linear invariant, hence conservation of $\mathcal{M}_1$ is assured. Insofar as $\mathcal{M}_2$ is concerned, this is a quadratic conservation law, therefore Theorem 1 proves that $M = O$ is sufficient for its retention. Moreover, it is possible to construct an isospectral problem (5.1) for which $M = O$ is necessary as well for the retention of the quadratic invariant [4].

In the case of the third integral of motion, $\mathcal{M}_3$, it has been proved in [4] that the departure of an arbitrary Runge–Kutta method from the manifold can be written in the form

$$\alpha h^2 + \beta h^3 + \mathcal{O}(h^3),$$

where $\alpha = 0$ for *all* problems of the form (5.1) if and only if $M = O$, while $\beta = 0$ for *all* problems (5.1) if and only if $N = O$, where

$$\begin{aligned} n_{i,j,k} := {} & b_i a_{i,j} a_{i,k} + b_j a_{j,i} a_{j,k} + b_k a_{k,i} a_{k,j} \\ & - b_i b_j a_{i,k} - b_j b_k a_{j,i} - b_k b_i a_{k,j} + b_i b_j b_k, \qquad i, j, k = 1, 2, \ldots, \nu. \end{aligned}$$

Theorem 4 (Calvo, Iserles & Zanna, [4]) *No Runge–Kutta method of order $p \geq 1$ can conserve the isospectrality of the system (5.1) for $d \geq 3$.*

Proof Choose $s \in \{1, 2, \ldots, \nu\}$ such that $b_s \neq 0$ (since $p \geq 1$, necessarily $\sum_{\ell=1}^{\nu} b_\ell = 1$, hence such an s exists). Letting $i = j = k = s$,

$$\begin{aligned} m_{s,s} &= 0 \qquad \Rightarrow \qquad 2\frac{a_{s,s}}{b_s} + 1 = 0, \\ n_{s,s,s} &= 0 \qquad \Rightarrow \qquad 3\left(\frac{a_{s,s}}{b_s}\right)^2 - 3\frac{a_{s,s}}{b_s} + 1 = 0. \end{aligned}$$

It is trivial to verify that the last two identities are contradictory. Therefore, $M = O$ is incompatible with $N = O$ and we deduce that the third integral of motion is not retained by producing for every Runge–Kutta method an example of an isospectral flow for which both $M = O$ and $N = O$ are necessary. $\Box$

The design of isospectral solvers requires the abandonment of classical numerical methods. Instead, we have proposed in [4] to use a theorem of Flaschka that, provided U is the solution of the system

$$U' = B(L(t + nh))U, \quad t \geq 0, \qquad U(0) = I, \tag{5.3}$$

we can obtain the solution of (5.1) at $t = (n + 1)h$ from the formula

$$L((n + 1)h) = U(h)L(nh)U^{-1}(h). \tag{5.4}$$

We henceforth assume that $L_0 \in \mathrm{S}_d[\mathbb{R}]$ and $B : \mathrm{S}_d[\mathbb{R}] \to \mathrm{o}_d[\mathbb{R}]$. Therefore (5.3) is an orthogonal flow and the inverse in (5.4) can be replaced by a transpose. The outcome is

$$U' = B(UL(nh)U^T)U, \quad t \geq 0, \qquad U(0) = I. \tag{5.5}$$

To prevent the loss of isospectrality, we must discretize (5.5) with a time-stepping method that retains orthogonality. According to Theorems 1–2, for Runge–Kutta methods a necessary and sufficient condition for this is $M = O$. An implementation of such methods is discussed in [4].

A useful example of an such a method is an isospectral modification of the well-known *implicit midpoint rule*

$$L_{n+1} = L_n + h[B(L_{n+1/2}), L_{n+1/2}], \quad n \in \mathbb{Z}^+,$$

where $L_{n+1/2} = \frac{1}{2}(L_n + L_{n+1})$, which reads

$$L_{n+1} = L_n + h[B(L_{n+1/2}), L_{n+1/2}] + \tfrac{1}{4}h^2 B(L_{n+1/2})(L_{n+1} - L_n)B(L_{n+1/2}).$$

A major disadvantage of orthogonal methods is that $M = O$ implies that the underlying scheme is necessarily implicit. Of course, unless we replace the inverse by a transpose, we might use any viable time-stepping algorithm to advance (5.3), since (5.4) is a similarity transformation and isospectrality is assured. Unfortunately, unless the underlying method conserves orthogonality, this procedure is bound to render the solution sequence $\{L_n\}_{n\in\mathbb{N}}$ nonsymmetric. Sometimes this does not matter but, if symmetry is at issue, we propose in [6] an approach which, while falling short of eliminating the symmetry error altogether, decreases it a great deal.

Consider the systems

$$\begin{aligned} U' &= B(UL(nh)U^{-1})U, \quad t \geq 0, \qquad U(0) = I \\ L_{n+1} &= U(h)L(nh)U^{-1}(h) \end{aligned} \tag{5.6}$$

and

$$\begin{aligned} V' &= -VB(V^{-1}L(nh)V), \quad t \geq 0, \qquad V(0) = I, \\ L_{n+1} &= V^{-1}(h)L(nh)V(h). \end{aligned} \tag{5.7}$$

Note that, while (5.6) is nothing else but (5.3),(5.4), the system (5.7) corresponds to an equation for $V = U^{-1}$. As long as we are using an orthogonal solver, there is not much to choose between the two systems. However, this is no longer true when a general method, e.g. an explicit Runge–Kutta method, is implemented. Given an order-p method, either (5.6) or (5.7) results in $L_n - L_n^T = \mathcal{O}(h^{p+1})$, $n \in \mathbb{N}$. However, using (5.6) for *odd* n and (5.7) for *even* n yields $L_n - L_n^T = \mathcal{O}(h^{p+2})$, $n \in \mathbb{N}$ [6].

6 Numerical methods on differentiable manifolds

We have seen in the last three sections several examples of ordinary differential systems (2.1) whose solution lies on a specific manifold. This motivates our interest in numerical methods with solutions on more general differentiable manifolds. Suppose thus that for every $\boldsymbol{y}_0 \in \mathcal{U} \subseteq \mathbb{R}^d$ the solution $\boldsymbol{y}(t)$

of (2.1) lies on the differentiable manifold $\mathcal{M}(\boldsymbol{y}_0)$. We say that a numerical method is $\mathcal{M}$-invariant, where $\mathcal{M}$ is the foliation of $\mathcal{U}$ into the manifolds $\mathcal{M}(\boldsymbol{y}_0)$, if $\boldsymbol{y}_n \in \mathcal{M}(\boldsymbol{y}_0)$ for all $n \in \mathbb{Z}^+$.

We have already seen in Section 3 that multistep methods fail to stay on manifolds described by 2-tensors, while in Section 5 we have demonstrated that Runge–Kutta methods depart from a manifold described by 3-tensors. The proof of the following, more general, theorem will feature in a forthcoming paper.

Theorem 5 (The 'Cheesecutter Theorem', Calvo, Iserles & Zanna, [7]) *Suppose that there exist $\boldsymbol{y}_0 \in \mathcal{U}$ and a two-dimensional section $\mathcal{K}$ through the manifold $\mathcal{M}(\boldsymbol{y}_0)$ such that $\mathcal{K}$ is a level set of the function ρ. Unless ρ obeys the partial differential equation*

$$\rho_y^3 \rho_{xxx} - 3\rho_x \rho_y^2 \rho_{xxy} + 3\rho_x^2 \rho_y \rho_{xyy} - \rho_x^3 \rho_{yyy} = 0, \tag{6.1}$$

for every Runge–Kutta method (2.3) there exists an ordinary differential system, invariant on $\mathcal{M}$, for which the Runge–Kutta method is not $\mathcal{M}$-invariant.

A section through a quadratic manifold is a level set of a quadratic function and (6.1) is satisfied. Other solutions of (6.1) can be expressed in terms of Jacobi elliptic functions or associated with solutions of the Burgers equation [7]. Yet, the implication of the theorem is that retention of invariance by Runge–Kutta methods is impossible for all but very special manifolds.

In other words, as long as numerical retention of invariance is at issue, it is advisable to consider non-classical time-stepping algorithms. Such methods have received increasing attention in the last few years. We have already mentioned the method of projections [2]. An alternative is the method of rigid frames in the normal bundle of the underlying manifold, due to Crouch and Grossman [10]. An allied approach, due to Munthe-Kaas, uses pullbacks and Lie-group techniques [16]. Yet another, perhaps intuitively simplest, approach has been introduced by Calvo, Iserles and Zanna in [5]. Henceforth we describe it briefly.

Let us suppose that $f \in C^1[\mathbb{R} \times \mathbb{R}^d \to \mathbb{R}^d]$ and that (2.1) is invariant on a manifold $\mathcal{M}$ which is of the same diffeotype as a 'simpler' manifold $\mathcal{N}$. By 'simpler' we mean that $\mathcal{N}$-invariance is attainable by a known time-stepping algorithm. Suppose further that a global diffeomorphism $\boldsymbol{g} : \mathcal{M} \to \mathcal{N}$ is known. Letting $\boldsymbol{x}(t) = \boldsymbol{g}(\boldsymbol{y}(t))$, $t \geq 0$, we derive a new differential system,

$$\boldsymbol{x}' = \frac{\partial \boldsymbol{g}(\boldsymbol{g}^{-1}\boldsymbol{x})}{\partial \boldsymbol{y}} \boldsymbol{f}(t, \boldsymbol{g}^{-1}(\boldsymbol{x})), \quad t \geq 0, \qquad \boldsymbol{x}(0) = \boldsymbol{g}(\boldsymbol{y}_0). \tag{6.2}$$

Since the solution of (6.2) stays on $\mathcal{N}$, we can discretize it there with our $\mathcal{N}$-invariant numerical method, subsequently mapping $\boldsymbol{y}_n = \boldsymbol{g}^{-1}(\boldsymbol{x}_n)$, $n \in \mathbb{N}$.

For example, the ℓ_r sphere

$$\mathcal{M}(\boldsymbol{y}_0) = \left\{ \boldsymbol{y} \in \mathbb{R}^d \,:\, \sum_{i=1}^{d} |y_i|^r = \sum_{i=1}^{d} |y_{0,i}|^r \right\}, \qquad r \in (1, \infty),$$

can be diffeomorphed onto an ℓ_2 sphere by means of

$$\boldsymbol{g}(\boldsymbol{y}) := \frac{\boldsymbol{y}}{\|\boldsymbol{y}\|}, \qquad \boldsymbol{g}^{-1}(\boldsymbol{x}) = \frac{\boldsymbol{x}}{\|\boldsymbol{x}\|_r}.$$

We recall that, according to Theorem 1, every Runge–Kutta method with $M = O$ is invariant on an ℓ_2 sphere.

Another example is provided by the algebraic variety

$$\mathcal{M}(\boldsymbol{y}_0) = \left\{ \boldsymbol{y} \in \mathbb{R}^d \,:\, \sum_{i=1}^{d} y_i^r = \sum_{i=1}^{d} y_{0,i}^r \right\},$$

where $r \in \mathbb{N}$ is odd. It is trivial to prove that

$$\boldsymbol{g}(\boldsymbol{y}) = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_{d-1} \end{bmatrix}$$

diffeomorphs $\mathcal{M}(\boldsymbol{y}_0)$ onto $\mathbb{R}^{d-1}$. Thereafter invariance can be retained by any consistent discretization.

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