Numerical Methods on (and off) Manifolds

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Abstract. It is often known from theoretical analysis that the exact solution of an ordinary differential system lies on a specific differentiable manifold and there are important advantages in retaining this feature under discretization. In this paper we examine whether the correct manifold is retained by a class of discretization methods that includes explicit multistep and multiderivative schemes. We obtain a necessary and sufficient condition for the retention of invariance under discretization. In particular, we prove that no such method can be expected to stay on a quadratic manifold. More specifically, given such a method and an arbitrary quadratic manifold $\mathcal{N}$, there exists an ordinary differential equation whose exact solution lies on $\mathcal{N}$, yet its discretization by the underlying method departs from the manifold.

1 Numerical Methods and Differentiable Manifolds

This paper addresses itself to a topic of an increasing interest in the numerical community, the discretization of ordinary differential equations (ODEs) on differentiable manifolds. Suppose that it is known that the solution of the ODE system

$$\boldsymbol{y}' = \boldsymbol{f}(t, \boldsymbol{y}) \quad t \geq 0, \qquad \boldsymbol{y}(0) = \boldsymbol{y}_0 \in \mathcal{U} \subseteq \mathbb{R}^d, \tag{1}$$

where $\boldsymbol{f} \in C[\mathbb{R} \times \mathbb{R}^d \to \mathbb{R}^d]$, lies for all $t \geq 0$ on the differentiable manifold $\mathcal{M}(\boldsymbol{y}_0)$. In other words, the equation (1) defines a foliation of $\mathcal{U}$ into invariant manifolds. This is often a crucially important information, since invariance corresponds to the satisfaction of conservation laws by (1).

To establish common terminology, we let

$$\mathcal{M} = \bigcup_{x \in \mathcal{U}} \mathcal{M}(\boldsymbol{x})$$

and say that a numerical method is $\mathcal{M}$-*invariant* if, whenever the ODE (1) possesses a solution on $\mathcal{M}(\boldsymbol{y}_0)$, so does the method.[1]

Traditionally, there has been little interest in the numerical community in investigating how well is invariance retained under discretization. The prevailing attitude was (and often still is) that the ultimate goal of numerical analysis is to devise, programme and analyse general algorithms, that can cater to the

[1] There should be no confusion with the entirely different concept of G-invariance of the action of a Lie group G on a manifold.

widest-possible range of ODEs, rather than affording special attention to specific equations or classes of equations [7]. This paradigm has been increasingly challenged in the last few years. A new school of thought, sometimes termed *geometric integration* or *qualitative numerical analysis* [7], aims to blend analytic and numerical means: the goal is not computation *per se* but the understanding of the ODE (1) and its behaviour. With growing attention being paid to the question of invariance, several general techniques have been proposed for invariant integration:

1. *Serendipitous methods:* Existing numerical methods which can be shown to respect specific manifolds. In particular, Runge–Kutta methods of certain type always stay on the symplectic group $\mathrm{Sp}(2d)$ [11], the orthogonal group $\mathrm{O}(d, \mathbb{R})$ and the unitary group $\mathrm{U}(d, \mathbb{C})$ [2, 7].
2. *Projective methods:* An obvious idea (yet, with nontrivial ramifications) is to solve (1) with an arbitrary numerical method, subsequently projecting the result on $\mathcal{M}(\boldsymbol{y}_0)$. Although this approach is sometimes infeasible or inordinately expensive – symplectic [11] and isospectral [2] flows are two important examples – it often offers a cheap and affordable means of retaining invariance. There exists an intimate connection between projective methods and differential-algebraic equations [1, 6].
3. *Rigid frame methods:* In a pioneering paper, Crouch and Grossman generalized conventional Runge–Kutta methods from Euclidean space to the setting of differentiable manifolds by correcting in a local rigid frame of $\mathcal{M}(\boldsymbol{y}_0)$ [4]. This approach has been recently extended by Marthinsen and Owren [8] but its main shortcoming is that the complexity of order analysis grows very fast, limiting its present scope. Moreover, the method requires the explicit knowledge of the tangent space $T\mathcal{M}(\boldsymbol{y}_0)$ at each solution point – an easy commodity in a Lie group but much less so in a general manifold.
4. *Tangent space methods:* Unlike the former class, these methods operate exclusively in the tangent space and restrict themselves to linear space operations and to commutation, subsequently returning to $\mathcal{M}(\boldsymbol{y}_0)$ by means of the exponential map. Runge–Kutta methods of this kind have been recently introduced by Munthe-Kaas [9, 10] and they are particularly effective in a Lie group setting. A very interesting class of explicit algorithms that always respect a Lie group by correcting in a Lie algebra with a numerical equivalent of the Lie reduction method has been recently introduced by Zanna [12, 13].
5. *Diffeomorphism methods:* A simple idea has been presented in [3]. The manifold $\mathcal{M}(\boldsymbol{y}_0)$ might sometimes have complicated geometry, yet be of a simple diffeotype. In particular, it might be diffeomorphic to a manifold that can be respected under discretization. In that case [3] advocates subjecting (1) to the same diffeomorphism, solving in the 'simpler' manifold and mapping the numerical solution back to $\mathcal{M}(\boldsymbol{y}_0)$.

The purpose of this paper is to explore the potential and the limitations of a 'serendipitous' method. In other words, we consider the scope for the conservation of manifolds by conventional numerical schemes. We have already proved, together with Mari Paz Calvo and Antonella Zanna, that no nonconfluent Runge–Kutta methods are assured of staying on manifolds that are level sets of r-degree tensors with $r \geq 3$ [3]. Here we address ourselves to explicit multistep-multiderivative methods, which fall outside the Runge–Kutta formalism. We prove in the sequel that such methods are, if at all, even less suitable in the integration of ODEs on manifolds and no such method can be invariant on a quadratic manifold.

By showing the limitations of 'serendipity', this paper, together with [3], provides motivation and philosophical underpinning to the ongoing search for new types of numerical ODE methods.

2 Taylor-type Discretization Methods

We assume in the sequel that the function $\boldsymbol{f}$ is analytic, hence so is the exact solution of (1). Analyticity of $\boldsymbol{f}$ implies that we can repeatedly differentiate (1), thereby explicitly expressing arbitrarily high derivatives of $\boldsymbol{y}(t)$,

$$\boldsymbol{y}^{(\ell)} = \boldsymbol{g}_\ell(t, \boldsymbol{y}), \qquad t \geq 0, \quad \ell \in \mathbb{Z}^+,$$

where

$$\boldsymbol{g}_0(t,\boldsymbol{y}) = \boldsymbol{y}, \quad \boldsymbol{g}_1(t,\boldsymbol{y}) = \boldsymbol{f}(t,\boldsymbol{y}), \quad \boldsymbol{g}_2(t,\boldsymbol{y}) = \frac{\partial \boldsymbol{f}(t,\boldsymbol{y})}{\partial t} + \frac{\partial \boldsymbol{f}(t,\boldsymbol{y})}{\partial \boldsymbol{y}} \boldsymbol{f}(t,\boldsymbol{y}), \quad \ldots.$$

We say that a discretization method at step $n \in \mathbb{Z}^+$ is of a *Taylor type* if, perhaps after some algebraic manipulation, it can be written in the form

$$\boldsymbol{y}_{n+1} = \sum_{\ell=0}^{\infty} c_{n,\ell} h^\ell \boldsymbol{g}_\ell(nh, \boldsymbol{y}_n), \tag{2}$$

where $\boldsymbol{y}_n \approx \boldsymbol{y}(nh)$, $h > 0$, and the coefficients $\{c_{n,\ell}\}$ are independent of the ODE (1). In order to make (2) consistent with the differential equation, we stipulate that $c_{n,0} = c_{n,1} = 1$.

An obvious example of a Taylor-type method (2) is the truncated Taylor expansion

$$\boldsymbol{y}_{n+1} = \sum_{\ell=0}^{q} \frac{1}{\ell!} h^\ell \boldsymbol{g}_\ell(nh, \boldsymbol{y}_n), \qquad n \in \mathbb{Z}^+.$$

For a more interesting example let us consider the *explicit multistep* scheme

$$\boldsymbol{y}_{n+1} + \sum_{k=0}^{m} a_k \boldsymbol{y}_{n-m+k} = h \sum_{k=0}^{m} b_k \boldsymbol{f}((n-m+k)h, \boldsymbol{y}_{n-m+k}), \qquad n \geq m. \tag{3}$$

As usual with multistep methods, we need to provide *starting values* $\boldsymbol{y}_k$, $k = 1, 2, \ldots, m$, in addition to the initial value $\boldsymbol{y}_0$. Let us assume that the starting values are exact, hence $\boldsymbol{y}_k = \boldsymbol{y}(kh)$, $k = 0, 1, \ldots, m$, and consider (3) for $n = m$. Therefore, expanding in Taylor series,

$$\begin{aligned}
\boldsymbol{y}_{m+1} &= -\sum_{k=0}^{m} a_k \boldsymbol{y}(kh) + h \sum_{k=0}^{m} b_k \boldsymbol{y}'(kh) \\
&= -\sum_{\ell=0}^{\infty} \frac{(-1)^\ell}{\ell!} \left[\sum_{k=0}^{m} a_k (m-k)^\ell \right] \boldsymbol{g}_\ell(mh, \boldsymbol{y}(mh)) h^\ell \\
&\quad - \sum_{\ell=1}^{\infty} \frac{(-1)^\ell}{(\ell-1)!} \left[\sum_{k=0}^{m} (m-k)^{\ell-1} b_k \right] \boldsymbol{g}_\ell(mh, \boldsymbol{y}(mh)) h^\ell .
\end{aligned}$$

Similar expansion applies to the explicit multistep-multiderivative scheme

$$\boldsymbol{y}_{n+1} = \sum_{k=0}^{m} \sum_{\ell=0}^{q} \alpha_{k,\ell} h^\ell \boldsymbol{g}((n-m+k)h, \boldsymbol{y}_{n-m+k}), \qquad n \geq m, \tag{4}$$

whereby

$$c_{m,\ell} = \sum_{j=(\ell-q)_+}^{\ell} \frac{(-1)^j}{j!} \sum_{k=0}^{m} (m-k)^j \alpha_{k,\ell-j}, \qquad \ell \in \mathbb{Z}^+ .$$

There is nothing special about a constant step-size h and our formalism can easily accomodate variable step sequences.

Note that a scheme may well be of a Taylor type for just some values of n: both (3) and (4) are of Taylor type just for $n = m$. Yet, this is sufficient for the purpose of the present paper.

3 A Necessary Condition for $\mathcal{M}$-invariance

Given a differentiable manifold $\mathcal{M}(\boldsymbol{x})$, embedded in $\mathbb{R}^d$, it is well known that there exists a smooth function $\rho = \rho(\,\cdot\,, \omega) : \mathbb{R}^m \to \mathbb{R}$ such that the manifold coincides with the variety

$$\mathcal{M}_\omega = \{ \boldsymbol{x} \in \mathbb{R}^d \,:\, \rho(\boldsymbol{x}) = 0 \}$$

[5]. Therefore we can rewrite the foliation from Sect. 1 in the form

$$\mathcal{M} = \bigcup_{\omega \in \Omega} \mathcal{M}_\omega$$

for some parameter set Ω. We henceforth stipulate that each ρ is an analytic function of $\boldsymbol{x}$ within the domain of interest.

$\mathcal{M}$-invariance of a numerical method is equivalent to the statement that

$$\rho(\boldsymbol{y}_n, \omega) = 0, \qquad n \in \mathbb{Z}^+, \quad \omega \in \Omega,$$

where ω is such that $\rho(\boldsymbol{y}_0, \omega) = 0$. Substituting (2) into this identity (letting $c_\ell = c_{n,\ell}$ and suppressing the dependence of ρ on ω for the sake of clarity) we have

$$\begin{aligned}
\rho(\boldsymbol{y}_{n+1}) &= \rho\left(\boldsymbol{y}_n + \sum_{\ell=1}^{\infty} c_\ell \boldsymbol{g}_\ell\right) \\
&= \rho(\boldsymbol{y}_n) + \sum_{m=1}^{\infty} \frac{1}{m!} \sum_{\ell_1,\ldots,\ell_m=1}^{\infty} c_{\ell_1} \cdots c_{\ell_m} h^{\ell_1+\cdots+\ell_m} \\
&\quad \times \sum_{\alpha_1,\ldots,\alpha_m=1}^{d} \rho_\alpha g_{\ell_1,\alpha_1} \cdots g_{\ell_m,\alpha_m},
\end{aligned}$$

where $\boldsymbol{g}_\ell = \boldsymbol{g}_\ell(nh, \boldsymbol{y}_n)$, the scalar $g_{\ell,\beta}$ is the βth coordinate of $\boldsymbol{g}_\ell$, $1 \le \beta \le d$, and

$$\rho_\alpha = \frac{\partial^{\alpha_1+\cdots+\alpha_m}}{\partial x_{\ell_1}^{\alpha_1} \cdots \partial x_{\ell_m}^{\alpha_m}} \rho(\boldsymbol{y}_n).$$

Therefore, changing the order of summation,

$$\begin{aligned}
&\rho(\boldsymbol{y}_{n+1}) - \rho(\boldsymbol{y}_n) \\
&= \sum_{m=1}^{\infty} \frac{1}{m!} \sum_{r=m}^{\infty} h^r \sum_{\substack{\ell_1+\cdots+\ell_m=r \\ \ell_1,\ldots,\ell_m \ge 1}} \left(\prod_{k=1}^{m} c_{\ell_k}\right) \sum_{\alpha_1,\ldots,\alpha_m=1}^{d} \rho_\alpha \prod_{j=1}^{m} g_{\ell_j,\alpha_j} \\
&= \sum_{r=1}^{\infty} h^r \sum_{m=1}^{r} \frac{1}{m!} \sum_{\substack{\ell_1+\cdots+\ell_m=r \\ \ell_1,\ldots,\ell_m \ge 1}} \left(\prod_{k=1}^{m} c_{\ell_k}\right) \sum_{\alpha_1,\ldots,\alpha_m=1}^{d} \rho_\alpha \prod_{j=1}^{m} g_{\ell_j,\alpha_j}.
\end{aligned} \tag{5}$$

Next, we examine the derivatives of ρ. We have

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}t}\rho(\boldsymbol{y}_n) &= \sum_{\alpha} \rho_\alpha y'_\alpha, \\
\frac{\mathrm{d}^2}{\mathrm{d}t^2}\rho(\boldsymbol{y}_n) &= \sum_{\alpha} \rho_\alpha y''_\alpha + \sum_{\alpha,\beta} \rho_{\alpha\beta} y'_\alpha y'_\beta, \\
\frac{\mathrm{d}^3}{\mathrm{d}t^3}\rho(\boldsymbol{y}_n) &= \sum_{\alpha} \rho_\alpha y'''_\alpha + 3\sum_{\alpha,\beta} \rho_{\alpha\beta} y'_\alpha y''_\beta + \sum_{\alpha,\beta,\gamma} \rho_{\alpha\beta\gamma} y'_\alpha y'_\beta y'_\gamma, \\
\frac{\mathrm{d}^4}{\mathrm{d}t^4}\rho(\boldsymbol{y}_n) &= \sum_{\alpha} \rho_\alpha y^{(iv)}_\alpha + 4\sum_{\alpha,\beta} \rho_{\alpha\beta} y'_\alpha y'''_\beta + 3\sum_{\alpha,\beta} \rho_{\alpha\beta} y''_\alpha y''_\beta + 6\sum_{\alpha,\beta,\gamma} \rho_{\alpha\beta\gamma} y'_\alpha y'_\beta y''_\gamma \\
&\quad + \sum_{\alpha,\beta,\gamma,\delta} \rho_{\alpha\beta\gamma\delta} y'_\alpha y'_\beta y'_\gamma y'_\delta,
\end{aligned}$$

where $y_\alpha^{(\ell)}$ is the αth component of $\boldsymbol{y}^{(\ell)}(nh)$. With greater generality, it is easy to prove by induction that

$$\frac{\mathrm{d}^r}{\mathrm{d}t^r}\rho(\boldsymbol{y}_n) = \sum_{m=1}^{r} \sum_{\substack{\ell_1+\cdots+\ell_m=r \\ \ell_1,\ldots,\ell_m\geq 1}} s_\ell \sum_{\alpha_1,\ldots,\alpha_m=1}^{d} \rho_\alpha y_{\alpha_1}^{(\ell_1)}\cdots y_{\alpha_m}^{(\ell_m)}, \tag{6}$$

where $s_r = 1$ and the only occurrence of $\boldsymbol{y}^{(r)}$ is for $m = 1$ and $\ell_1 = r$.

Let us suppose that (2) is of order $p \geq 1$, therefore $c_k = 1/k!$, $k = 1, 2, \ldots, p$. We compare (5) with (6), recalling that $\boldsymbol{g}_\ell(nh, \boldsymbol{y}_n) = \boldsymbol{y}^{(\ell)}(nh)$, $\ell \in \mathbb{Z}^+$. Our first observation is that, except for $m = 1$ and $\ell_1 = p + 1$, all the h^{p+1} coefficients in (5) depend solely upon $c_1, \ldots, c_p$ and are independent of c_{p+1}. We consider c_{p+1} as a parameter: had it equalled $1/(p+1)!$, all the h^{p+1} terms in (5) and (6) would have matched perfectly, since (2) would have been of order $p + 1$. Therefore all the terms in the two expansions, except for $m = 1$, $\ell_1 = p + 1$, are identical and we derive explicitly an expression of the leading error term.

Theorem 1. *The departure of a p-order Taylor-like method (2) from the manifold $\mathcal{M}_\omega$ is*

$$\rho(\boldsymbol{y}_{n+1}, \omega) - \rho(\boldsymbol{y}_n, \omega) = \left(c_{p+1} - \frac{1}{(p+1)!}\right) h^{p+1} \sum_{\alpha=1}^{d} \rho_\alpha y_\alpha^{(p+1)} + \mathcal{O}(h^{p+2}). \tag{7}$$

Corollary 2. *The Taylor-like method (2) is $\mathcal{M}$-invariant if and only if for every $\mathcal{M}$-invariant ODE (1) and every $r \in \mathbb{N}$ it is true either that $c_r = 1/r!$ or that*

$$\sum_{\alpha=1}^{d} \rho_\alpha y_\alpha^{(r)} = 0. \tag{8}$$

Corollary 3. *Suppose that there exists an ODE (1) such that $\boldsymbol{y}(t) \in \mathcal{M}_\omega$, $t \geq 0$, and such that*

$$\sum_{\alpha=1}^{d} \rho_\alpha y_\alpha^{(r)} \neq 0, \qquad r \geq 2. \tag{9}$$

Then no Taylor-like method (2) may be $\mathcal{M}$-invariant, except for the exact solution of the ODE.

4 Nonexistence of Quadratically-Invariant Taylor-type Methods

We restrict our attention to nontrivial quadratic manifolds embedded in $\mathbb{R}^2$. Each such manifold can be linearly mapped onto the unit circle $y_1^2 + y_2^2 = 1$ hence, without loss of generality, we consider ODEs in $\mathbb{R}^2$ whose solution obeys $\|\boldsymbol{y}(t)\|_2 \equiv 1$, $t \geq 0$. Quadratic manifolds are significant as the simplest example of a genuinely nonlinear manifold but they are important also for their own sake since they include as special cases orthogonal, unitary, Stiefel and Grassmann manifolds and their retention by physical systems can be often interpreted as conservation of mechanical energy.

The restriction to two dimensions does not lead to any loss of generality: Our purpose is to show that no Taylor-like method (2) can be invariant on a Euclidean sphere in $\mathbb{R}^d$, $d \geq 2$. It is enough to prove this result by singling out an ODE that escapes from the sphere through a two-dimensional slice. (In the context of Runge–Kutta methods a similar, albeit more complicated, technique of cutting a manifold into two-dimensional slices has led to the descriptivelly named Cheesecutter Theorem [6].)

We consider the linear system

$$\boldsymbol{y}' = \psi(t) J \boldsymbol{y}, \qquad \text{where} \qquad J = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix} \tag{10}$$

where the analytic function ψ is yet to be determined. We assume that $\|\boldsymbol{y}_0\|_2 = 1$. Since $\boldsymbol{y}^T \boldsymbol{f}(t, \boldsymbol{y}) \equiv 0$ for all $t \geq 0$, $\boldsymbol{y} \in \mathbb{R}^2$, it trivially follows that $\boldsymbol{y}(t)$ indeed lives on the unit circle.[2] Moreover, repeatedly differentiating (10) and using $J^2 = -I$, it is easy to prove by induction that for every $k \in \mathbb{Z}^+$ there exist functions $\mathfrak{p}_k$ and $\mathfrak{q}_k$ such that the kth derivative of $\boldsymbol{y}$ has the form

$$\boldsymbol{g}_k(t, \boldsymbol{y}) = [\mathfrak{p}_k(t) I + \mathfrak{q}_k(t) J] \boldsymbol{y}. \tag{11}$$

These functions obey the differential recurrence relations

$$\begin{aligned} &\mathfrak{p}_0 \equiv 1, && \mathfrak{q}_0 \equiv 0, \\ &\mathfrak{p}_{k+1} = \mathfrak{p}_k' - \psi \mathfrak{q}_k, && \mathfrak{q}_{k+1} = \psi \mathfrak{p}_k + \mathfrak{q}_k', \qquad k \in \mathbb{Z}^+. \end{aligned} \tag{12}$$

Since $\rho(\boldsymbol{x}) = \frac{1}{2}(x_1^2 + x_2^2 - 1)$ and $\boldsymbol{x}^T J \boldsymbol{x} = 0$ for all $\boldsymbol{x} \in \mathbb{R}^2$, we deduce that

$$\sum_{\alpha=1}^{s} \rho_\alpha y_\alpha^{(r)} = \boldsymbol{y}^T \boldsymbol{g}_r(t, \boldsymbol{y}) = \mathfrak{p}_r(t) \|\boldsymbol{y}\|_2^2, \qquad r \in \mathbb{Z}^+.$$

Therefore, *pace* Corollary 3, it is enough to prove that there exists a continuous function ψ such that $\mathfrak{p}_r(0) \neq 0$ for all $r \geq 2$. As a matter of fact, even less is required to prove that no Taylor-type method can be invariant on the unit circle, namely that, given any integer $m \geq 2$, there exists $\psi = \psi_m$ such that $\mathfrak{p}_r(0) \neq 0$ for all $r = 2, 3, \ldots, m$.

Let us examine the first few iterates of (12):

$$\begin{aligned} k = 1: \quad & \mathfrak{p}_2 = -\psi^2, \\ & \mathfrak{q}_2 = \psi'; \\ k = 2: \quad & \mathfrak{p}_3 = -3\psi\psi', \\ & \mathfrak{q}_3 = \psi'' - \psi^3; \end{aligned}$$

[2] For another proof note that ψJ, being skew-symmetric, lives in the Lie algebra of $\mathrm{O}(2, \mathbb{R})$.

$$
\begin{aligned}
k=3: \quad & \mathfrak{p}_4 = -4\psi\psi'' - 3\psi'^2 + \psi^4,\\
& \mathfrak{q}_4 = \psi''' - 6\psi^2\psi';\\
k=4: \quad & \mathfrak{p}_5 = -5\psi\psi''' - 10\psi'\psi'' + 10\psi^3\psi',\\
& \mathfrak{q}_5 = \psi^{(\mathrm{iv})} - 10\psi^2\psi'' - 15\psi\psi'^2 + \psi^5;\\
k=5: \quad & \mathfrak{p}_6 = -6\psi\psi^{(\mathrm{iv})} - 10\psi''^2 - 15\psi'\psi''' + 20\psi^3\psi'' + 45\psi^2\psi'^2 - \psi^6,\\
& \mathfrak{q}_6 = \psi^{(\mathrm{v})} - 15\psi^2\psi''' - 60\psi\psi'\psi'' - 15\psi'^3 + 15\psi^4\psi'.
\end{aligned}
$$

In general, our claim is that for every $k \geq 3$

$$
\begin{aligned}
\mathfrak{p}_k &= -k\psi\psi^{(k-2)} + \cdots, && (13)\\
\mathfrak{q}_k &= \psi^{(k-1)} - \binom{k}{2}\psi^2\psi^{(k-3)} + \cdots, && (14)
\end{aligned}
$$

where the remaining terms in (13) do not include $\psi^{(j)}$ for $j \geq k-2$, while the remaining terms in (14) do not include $\psi^{(j)}$ for $j \geq k-3$. The proof is by induction: We directly verify (13–14) when $k=3$, while for every $k \geq 3$ the recurrences (12) yield

$$
\mathfrak{p}_{k+1} = [-k\psi\psi^{(k-2)} + \cdots]\psi[\psi^{(k-1)} + \cdots] = -(k+1)\psi\psi^{(k-1)} + \cdots
$$

and

$$
\begin{aligned}
\mathfrak{q}_{k+1} &= \psi[-k\psi\psi^{(k-2)} + \cdots] + \left[\psi^{(k)} - \binom{k}{2}\psi^2\psi^{(k-2)} + \cdots\right]\\
&= \psi^{(k)} - \binom{k+1}{2}\psi^2\psi^{(k-2)} + \cdots.
\end{aligned}
$$

Let an integer $m \geq 2$ be given. We choose a function ψ such that $\mathfrak{p}_k(0) \neq 0$, $k = 2,3,\ldots,m$, by specifying its derivatives consecutively. We commence by letting $\psi(0) = 1$. Let us suppose that we have already chosen $\psi(0), \psi'(0), \ldots, \psi^{(k-3)}(0)$ so that $\mathfrak{p}_j(0) \neq 0$, $j = 2,3,\ldots,k-1$. According to (13), it is thus true that $\mathfrak{p}_k(0) = -k\psi(0)\psi^{(k-2)}(0) + \xi_k$, where ξ_k depends (in a nonlinear fashion) exclusively upon $\psi^{(j)}(0)$, $j = 0,1,\ldots,k-3$. We choose an arbitrary $|\psi^{(k-2)}(0)| > |\xi_k|/k$, whence $\mathfrak{p}_k(0) \neq 0$. Finally, we let $\psi^{(k)}(0) = 0$, $k \geq m-1$, to ensure analyticity.

Theorem 4. *No Taylor-type method (2) may be invariant on the unit circle in* $\mathbb{R}^2$, *except for the exact solution of the underlying ODE.*

Proof. Let us suppose that a p-order method (2) is invariant on the unit circle. Note that $c_k = 1/k!$, $k = 0,1,\ldots,p$, and $c_{p+1} \neq 1/(p+1)!$. We consider the linear system (10) where the function ψ is chosen as above so that $\mathfrak{p}_2(0), \mathfrak{p}_3(0), \ldots, \mathfrak{p}_{p+1}(0) \neq 0$. By continuity, there exists $t^* > 0$ such that $\mathfrak{p}_j(t) \neq 0$ for all $j = 2,3,\ldots,p+1$ and $t \in (0,t^*]$. Integrating from the origin with step size $0 < h \leq t^*$, we reach a contradiction with Corollary 2. Hence no such method exists. □

5 Implicit Methods

The analysis of this paper does not apply to implicit multistep methods. Yet, there are good reasons to believe that implicitness does not add much insofar as invariance is concerned. Herewith we present a direct, brute-force approach to the retention of quadratic invariance by the *theta method*

$$\boldsymbol{y}_{n+1} = \boldsymbol{y}_n + h[\theta \boldsymbol{f}(nh, \boldsymbol{y}_n) + (1-\theta)\boldsymbol{f}((n+1)h, \boldsymbol{y}_{n+1})], \qquad n \in \mathbb{Z}^+, \qquad (15)$$

where $\theta \in [0,1]$. We note in passing that it is possible to represent (15) as a Runge–Kutta method and apply the analysis from [2]. This shows that, regardless of the choice of θ, the method cannot be invariant on quadratic manifolds. However, the direct proof adds insight. The method of proof in [2], like that in [3] and, indeed, in Sect. 4, rests upon the presence of a counterexample, a specific ODE (1) which is invariant on a manifold yet which cannot be discretized invariantly by the underlying method. An obvious rejoinder to this approach is that the example might be non-generic and it is perhaps possible that, in a well-defined sense, 'most' invariant ODEs can be discretized invariantly. The following proof demonstrates that this is not true.

By following the argument from Sect. 4, we consider invariance on the Euclidean sphere $\|\boldsymbol{y}\|_2 = 1$. We write (15) in the form

$$\boldsymbol{y}_{n+1} - (1-\theta)h\boldsymbol{f}((n+1)h, \boldsymbol{y}_{n+1}) = \boldsymbol{y}_n + \theta h \boldsymbol{f}(nh, \boldsymbol{y}_n)$$

and take the Euclidean norm. Since invariance and (1) imply that $\boldsymbol{y}^T \boldsymbol{f}(t, \boldsymbol{y}) \equiv 0$, the outcome is

$$\|\boldsymbol{y}_{n+1}\|_2^2 + (1-\theta)^2 h^2 \|\boldsymbol{f}((n+1)h, \boldsymbol{y}_{n+1})\|_2^2 = \|\boldsymbol{y}_n\|_2^2 + \theta^2 h^2 \|\boldsymbol{f}(nh, \boldsymbol{y}_n)\|_2^2.$$

Therefore, assuming invariance and considering small $h > 0$ (hence $\boldsymbol{y}_{n+1}$ arbitrarily close to $\boldsymbol{y}_n$) we deduce that $\theta = \frac{1}{2}$ (the *trapezoidal rule*) and

$$\|\boldsymbol{f}((n+1)h, \boldsymbol{y}_{n+1})\|_2 = \|\boldsymbol{f}(nh, \boldsymbol{y}_n)\|_2. \qquad (16)$$

This, however, is impossible for all ODEs invariant on the unit sphere, as can be easily seen in $\mathbb{R}^2$. In that case the most general sphere-invariant system (1) has the form

$$\boldsymbol{f}(t, \boldsymbol{y}) = g(t, \boldsymbol{y}) \begin{bmatrix} y_2 \\ -y_1 \end{bmatrix},$$

where the function $g : \mathbb{R} \times \mathbb{R}^2 \to \mathbb{R}$ is sufficiently smooth but otherwise arbitrary. Since

$$\|\boldsymbol{f}(t, \boldsymbol{y})\|_2 = |g(t, \boldsymbol{y})| \|\boldsymbol{y}\|_2,$$

we deduce from (16) that necessarily

$$|g((n+1)h, \boldsymbol{y}_{n+1})| = |g(nh, \boldsymbol{y}_n)|,$$

in variance with the arbitrariness of the function g. Hence, not even the trapezoidal rule may be invariant on the unit sphere and, by translation, on an arbitrary nontrivial quadratic manifold.

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