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Invariantization of Numerical Schemes Using Moving Frames

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Abstract.

This paper deals with a geometric technique to construct numerical schemes for differential equations that inherit Lie symmetries. The moving frame method enables one to adjust existing numerical schemes in a geometric manner and systematically construct proper invariant versions of them. Invariantization works as an adaptive transformation on numerical solutions, improving their accuracy greatly. Error reduction in the Runge-Kutta method by invariantization is studied through several applications including a harmonic oscillator and a Hamiltonian system.

AMS subject classification (2000): 65L12, 70G65.

Key words: Invariant scheme, Lie symmetry, geometric integration.

1 Introduction

During the past decade, there have been increasing efforts to implement more accurate numerical schemes in consideration of qualitative characteristics of the underlying systems. Such schemes inherit from their original systems structural properties exactly, i.e. within round-off error, many of which are of significance in physical phenomena. Examples include preservation of the Hamiltonian or Poisson structure [1, 10, 13, 17, 20], first integrals or conservation laws [31, 35, 37, 49, 50], and symmetry structures [7, 8, 14, 28, 29, 30, 39, 51]. Some variational integrators adopt the variational character of Lagrangian and canonical Hamiltonian systems [3, 4, 38, 41]. This approach, now termed *geometric integration*, has made a notable success in many applications across science and engineering: from celestial mechanics [32, 53] to molecular dynamics [33], from complex systems [2] to multi scale systems [27] and from quantum mechanics [52] to elastodynamics [49]. One can find more details and extensive references in several recent books and survey articles [7, 21, 24, 36, 40].

In this paper, we introduce a novel method to generate invariant schemes, meaning numerical schemes that preserve Lie symmetries of the system of differential equations. The method serves not only for preservation of symmetries of the system but also for reduction of error. Discrete symmetries on a lattice space can be determined for difference equations [22, 34]. To obtain invariant numerical schemes for a given differential equation, Dorodnitsyn's approach [14, 15] is to first find a complete set of functionally independent difference invariants, and

then use them to construct a numerical approximation on an appropriate mesh. However, even once a set of invariants is found, there still leaves the problem of how to assemble them into a stable and accurate numerical scheme on an appropriate mesh.

Moving frames, as developed by Fels and Olver in [16], are powerful tools to investigate group actions and their invariants. The moving frame method provides an algorithmic way to find complete sets of invariants for general group actions. The resulting invariantization process will convert an arbitrary function, differential equation, or numerical scheme into an invariant version thereof. The method has applications in a wide range of areas including geometry, computer vision, classical invariant theory, the calculus of variations and numerical analysis [5, 6, 45]. Using moving frames, we invariantize existing numerical schemes so that the schemes carry symmetry structures of differential equations. Invariantization enables delicate manipulations of numerical schemes in a geometric manner, without any need to compute the difference invariants. By invariantization, we are also able to utilize a wide range of numerical techniques that have already been developed.

In a practical sense, invariantization of a given numerical scheme is an adaptive transformation on numerical solutions at each integration step. Invariantization by symmetry transformations allows us to transform the points at each step along the orbits of the symmetry group to a region where the numerical scheme works better. Figure 1.1 illustrates this idea. N stands for a given numerical scheme that evaluates the solution value at x_{i+1} from its value at x_i.

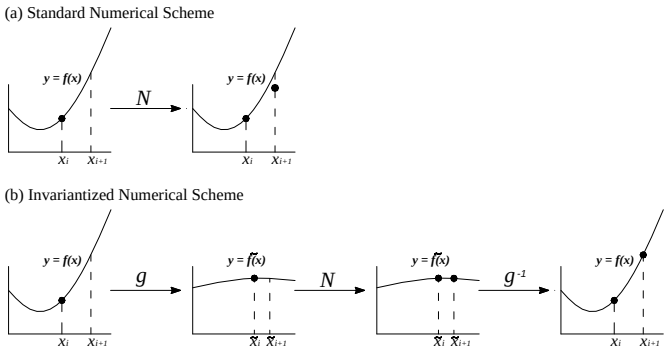

Figure 1.1: Basic idea of invariantization of numerical scheme

If the graph of the solution varies rapidly between the points, the scheme may result in poor performance, as sketched in (a). This situation may be avoided by applying a symmetry transformation, which maps the solution of the differential equation to another solution. In many cases, we select the symmetry transformation g wisely so that, between the points, the solution is mapped to another nicer solution that is well approximated by the numerical scheme. In practice, the symmetry transformation g can be interpreted as a local substitution, or

an adaptive mapping that updates the numerical scheme N at each step. The good choice of g usually depends on a position of the points being evaluated, and therefore changes from point to point. In the moving frame theory this procedure can be viewed as invariantization on a joint product space.

The idea of solving a transformed system in a more convenient form and transforming its result back has actually been widely adopted in numerical analysis. Local substitution can reduce the amount of computation for a linear system that has to be solved by preconditioning [26] or reducing its dimension [9]. Numerical schemes can inherit some geometric properties, such as first integrals, symmetries and symplectic structure from their original systems, by composition with proper transformations [20, 39, 47]. One of the common strategies for exponential integrators, numerical integrators for ordinary differential equations on curved manifolds, is to map them locally to a flat vector space and applying classical methods thereon. When combining with transformations, exponential integrators can decrease computational cost [12] and successfully deal with highly oscillatory equations [25]. These are just a few examples where the transformation technique has been applied. Compared to the above transformations, the symmetry transformations have a distinct feature that aides in direct error reduction: The symmetry transformations leave the equations *exactly* the same, and therefore the control of error becomes much easier. Also, for high order methods, the accuracy is well preserved under the inverse transformations since exact solutions are mapped to other exact solutions under symmetry transformations.

The invariantization technique can be applied to any numerical method based on finite differences for both ordinary differential equations (ODEs) and partial differential equations (PDEs). In [30], an invariantized Crank-Nicolson method is applied to Burgers' equation and successfully removes undesirable numerical oscillation occurring in a sharp transition layer. In this work we mainly focus on ODEs with nonlinear symmetry transformations, since most of traditional numerical schemes are already invariant with respect to affine symmetries [46]. The idea of invariantization of numerical schemes first appeared in [44] in the form of an invariantization of multi-step methods for difference equations.

The following simple example shows how this method improves the existing numerical algorithms. Consider an elementary ODE

$$\dot{y} = y. \tag{1.1}$$

It admits a one-parameter symmetry group G, whose symmetry transformations are

$$(x, y) \mapsto (\tilde{x}, \tilde{y}) = (x, y + \varepsilon e^x) \tag{1.2}$$

for a parameter $\varepsilon \in \mathbf{R}$. Assume that $(x_i, y_i) = (x_i, y(x_i))$ is the currently computed solution value and y_{i+1} is the numerical approximation to the solution at the following mesh point. Let us apply the Euler method to a transformed point $(\tilde{x}, \tilde{y})$,

$$\tilde{y}_{i+1} = \tilde{y}_i + (\tilde{x}_{i+1} - \tilde{x}_i)\, \tilde{y}_i$$

$$= (1 + \tilde{x}_{i+1} - \tilde{x}_i)\, \tilde{y}_i.$$

Transforming back by the inverse symmetry transformation, we find

$$y_{i+1} + \varepsilon e^{x_{i+1}} = (1 + x_{i+1} - x_i)(y_i + \varepsilon e^{x_i}) \tag{1.3}$$

in terms of the original points. As long as ε remains as a constant, (1.3) is nothing more than a numerical scheme with error $O(h^2)$. However, for reasons to be clarified in the following sections, suppose we choose $\varepsilon = -y_i/e^{x_i}$. This removes the right hand side of (1.3) and leads to the "invariantized" scheme

$$y_{i+1} = y_i e^{x_{i+1} - x_i}. \tag{1.4}$$

One can easily prove that this scheme is exact, namely, $y_{i+1} = y(x_{i+1})$. Although our success can be immediately explained by observing that the scheme (1.4) has the form of the general solution of (1.1), this simple example shows how symmetry transformations can be used to improve an existing scheme. Note again that transformation parameter ε depends on x_i, y_i and x_{i+1} and varies at steps. Finding an appropriate choice of ε is an essential part of the invariantization process induced by the method of moving frames.

2 Invariant Numerical Schemes

In order to define what is meant by an "invariant numerical scheme", we begin by introducing an extended space on which we can give a formal definition of a numerical scheme. The formalization will also helps us understand how invariantization is accomplished by the moving frame method that we will introduce in the next section.

Let $z = (x, y) \in M = \mathbf{R}^p \times \mathbf{R}^q$, where x is the independent variable and y the dependent variable. Also let $\Delta = 0$ be a differential equation defined over M. We focus on a normal ordinary differential equation $\dot{y} = f(x, y)$, namely

$$\Delta = \dot{y} - f(z) = 0, \tag{2.1}$$

where $z = (x, y) \in M = \mathbf{R} \times \mathbf{R}^q$.

Finite difference numerical schemes are based on the evaluation of function at several distinct points lying on the graph of a solution over a chosen set of mesh points. Thus, to deal with distinct points on the graphs of solutions, we introduce the *joint product* of M

$$M^{\diamond n} = \{\, (z_1; \ldots; z_n) \,|\, z_i \in M, z_i \neq z_j \text{ for all } i \neq j\}.$$

We say a collection of n points $\mathbf{z} = (z_1; \cdots; z_n) \in M^{\diamond n}$ is *exact* for the differential equation $\Delta = 0$ if there exists an exact solution whose graph contains $z_1, \cdots, z_n$.

Example 2.1. For the equation $\dot{y} = y$ in (1.1), the collection of three points

$$\mathbf{z} = \Big((0, -1); (1, -e); (2, -e^2) \Big) \in M^{\diamond 3}$$

is exact, because all of the three points are on a graph of an exact solution, namely $y = -e^x$.

The motivation to introduce the notion of exactness is to generalize consistency and convergence of finite different schemes in a geometrical sense and establish invariantization of them on a theoretical base. Let N be a map $N : M^{\diamond n} \mapsto \mathbf{R}^n$. The implicit expression $N(\mathbf{z}) = 0$ is called a (implicit) numerical approximation for $\Delta = 0$, if $N(\mathbf{z})$ is approximately zero whenever $\mathbf{z}$ is exact for $\Delta = 0$. Here the approximate equality should be specified by an asymptotic upper bound with respect to the step sizes in the scheme. More precise definition of numerical schemes requires a further condition on stencil and its coalescent limit. See [29].

Example 2.2. The Euler scheme for the equation (2.1) is a one-step scheme, which works on a collection of two consecutive points $\mathbf{z} = (z_i; z_{i+1}) \in M^{\diamond 2}$, via

$$N(\mathbf{z}) = y_{i+1} - y_i - (x_{i+1} - x_i) f(z_i). \tag{2.2}$$

Similarly, the two-step Adam-Bashforth method [19] uses

$$N(\mathbf{z}) = y_{i+2} - y_i - \frac{3h}{2} f(z_{i+1}) + \frac{h}{2} f(z_i)$$

with $\mathbf{z} = (z_i; z_{i+1}; z_{i+2}) \in M^{\diamond 3}$.

Let G be a Lie group acting on M. We say that a function f is an *invariant* if $f(g \cdot z) = f(z)$ for all $g \in G$ and $z \in M$. The action of G on M easily extends to a *product action* of G on $M^{\diamond n}$:

$$g \cdot \mathbf{z} = g \cdot (z_1; \ldots; z_n) = (g \cdot z_1; \ldots; g \cdot z_n) \text{ for } \mathbf{z} \in M^{\diamond n}, g \in G. \tag{2.3}$$

Let $\Delta = 0$ be a differential equation on $z = (x_1, \cdots, x_p, y_1, \cdots, y_q) \in M$ where x_i and y_i are independent and dependent variables, respectively. If every element of G maps solutions of $\Delta = 0$ to other solutions, G is called a symmetry group of Δ [42]. Note that this symmetry transformation acts on the independent and dependent variables at the same time, and therefore the graph of solutions are transformed to others point-wise. This implies that $\Delta(g \cdot z) = 0$ coincides with $\Delta(z) = 0$, or in other words, the zero level set of Δ is invariant.

Now suppose N defines a numerical scheme for $\Delta = 0$. We say the numerical scheme N is invariant if the system of equations $N(\mathbf{z}) = 0$ is invariant under the product action, i.e.,

$$N(g \cdot \mathbf{z}) = 0 \iff N(\mathbf{z}) = 0\,,$$

for all $g \in G$.

Example 2.3. Let us show the scheme (1.4) is invariant under the group action (1.2). The corresponding joint product action on $M^{\diamond 2}$ is

$$\begin{aligned} g \cdot \mathbf{z} &= (\tilde{x}_i, \tilde{y}_i; \tilde{x}_{i+1}, \tilde{y}_{i+1}) \\ &= (\, x_i, y_i + \varepsilon e^{x_i} \,; x_{i+1}, y_{i+1} + \varepsilon e^{x_{i+1}}) \text{ for } \varepsilon \in \mathbf{R}. \end{aligned} \tag{2.4}$$

The scheme (1.4) can be rewritten in an implicit form $N(\mathbf{z}) = y_{i+1} - y_i e^{x_{i+1} - x_i}$. One can show

$$N(g \cdot \mathbf{z}) = \tilde{y}_{i+1} - \tilde{y}_i e^{\tilde{x}_{x+1} - \tilde{x}_1}$$

$$
\begin{aligned}
&= y_{i+1} + \varepsilon e^{x_{i+1}} - (y_i + \varepsilon e^{x_i}) e^{x_{i+1}-x_i} \\
&= y_{i+1} - y_i e^{x_{i+1}-x_i} \\
&= N(\mathbf{z})
\end{aligned}
$$

and therefore $N(\mathbf{z}) = 0$ implies $N(g \cdot \mathbf{z}) = 0$, proving invariance.

3 Invariantization of Numerical Schemes by Moving Frames

Now we review the Fels-Olver moving frame method and study its application to numerical schemes [16, 43]. In this section, for more clear and general explanation, we adopt coordinates $z = (x_1, \cdots, x_m) \in M$, $m = p + q$, ignoring the difference between the independent and dependent variables. Let G be an r-dimensional Lie group acting on M.

DEFINITION 3.1. *A* (right) moving frame *is a map* $\rho : M \to G$ *such that* $\rho(g \cdot z) = \rho(z) g^{-1}$ *for all* $g \in G$.

The following result characterizes when a moving frame exists.

THEOREM 3.1. *A moving frame exists if and only if the action of the group is free and regular.*

We say that a group action is *free* if the only group element that fixes any point z in M is the identity. Regularity requires that the group orbits form a regular foliation; see [42, 16] for details. Essentially all group actions arising in applications are regular and so we need not be concerned with it here.

The implementation of the moving frame construction is based on Cartan's method of *normalization* [11, 16], which relies on the choice of a cross-section to the r-dimensional group orbits, i.e. a submanifold having the complementary dimension $m - r$ that intersects each orbit once and transversally.

The practical construction of a moving frame can be done by the following algorithmic procedure [5].

- Step 1: Write down the explicit formulas for the group action $g \cdot z = \tilde{z}$ in the given coordinates.

$$
\left\{
\begin{array}{rl}
\alpha_1(\varepsilon_1, \cdots, \varepsilon_r, x_1, \cdots, x_m) = & \tilde{x}_1 \\
\vdots & \\
\alpha_m(\varepsilon_1, \cdots, \varepsilon_r, x_1, \cdots, x_m) = & \tilde{x}_m
\end{array}
\right. \tag{3.1}
$$

  where $g = (\varepsilon_1, \cdots, \varepsilon_r)$ are the group parameters.

- Step 2: Choose the $r = \dim G$ normalization equations which define a cross-section transversal to the orbits of the group actions on M.

$$
\left\{
\begin{array}{rl}
\beta_1(x_1, \cdots, x_m) = & 0 \\
\vdots & \\
\beta_r(x_1, \cdots, x_m) = & 0
\end{array}
\right. \tag{3.2}
$$

- Step 3: Replace x_i in (3.2) by $\tilde{x}_i$ as in (3.1). The resulting system

$$\begin{cases} \beta_1(\tilde{x}_1, \cdots, \tilde{x}_m) = & 0 \\ \qquad\qquad \vdots & \\ \beta_r(\tilde{x}_1, \cdots, \tilde{x}_m) = & 0 \end{cases} \tag{3.3}$$

  is solved for $g = (\varepsilon_1, \cdots, \varepsilon_r)$ in terms of z. The solution $g = \rho(z)$ is a moving frame. Note that setting the cross-section in Step 2 guarantees solvability of this system.

Since the only restriction is that the normalization equations have to be set as a cross-section to the orbits of the group action, there is great amount of flexibility in constructing a moving frame.

Once a moving frame is constructed, there is a natural way to associate an invariant to any given function.

DEFINITION 3.2. *The* invariantization *of a scalar function $F\colon M \to \mathbf{R}$ with respect to a right moving frame ρ is the invariant function $\iota(F)$ defined by $\iota(F)(z) = F(\rho(z) \cdot z)$. In particular, if F is invariant, then $\iota(F) = F$.*

If a moving frame is obtained by normalization of the first r coordinates, i.e., $x_i = c_i \in \mathbf{R}$, $i = 1, \cdots, r$, in (3.2), then invariantization of the remaining coordinates, $\iota(x_{r+1}), \cdots, \iota(x_m)$, provides a complete set of $(m - r)$ functionally independent invariants for the group action [43].

EXAMPLE 3.1. Let $G = \mathbf{R}$ be a one-parameter Lie group acting on $\mathbf{R}^3$ as

$$(x_1, x_2, x_3) \mapsto (\tilde{x}_1, \tilde{x}_2, \tilde{x}_3) = \left(\frac{x_1}{1 - \varepsilon x_1}, \ \frac{x_2}{1 - \varepsilon x_1}, \varepsilon(x_2 - x_1 x_3) + x_3 \right) \quad \text{for } \varepsilon \in G.$$

Choosing the cross-section defined by a normalization equation $x_3 = 0$, we derive

$$\begin{aligned} & \tilde{x}_3 = 0 \\ \Rightarrow \ & \varepsilon(x_2 - x_1 x_3) + x_3 = 0 \\ \Rightarrow \ & \varepsilon = \frac{x_3}{x_1 x_3 - x_2} \end{aligned}$$

which defines the corresponding moving frame $\rho(x, y, z)$. Observe that $\rho(x_1, x_2, x_3) \cdot (x_1, x_2, x_3) = \left(\frac{x_1(x_2 - x_1 x_3)}{x_2}, \ x_2 - x_1 x_3, \ 0 \right)$ are the invariants under the action of G.

Now, suppose G is a symmetry group for a given differential equation $\Delta = 0$. Let $\rho : M^{\diamond n} \to G$ be a moving frame on the joint product space, obtained by the proceeding algorithm. The invariantization of the numerical scheme N with respect to the moving frame ρ is defined as $\iota(N)$ or, explicitly

$$N(\rho(\mathbf{z}) \cdot \mathbf{z}) = 0. \tag{3.4}$$

Is (3.4) still a numerical scheme for $\Delta = 0$? The property of symmetry groups gives an immediate positive answer.

PROPOSITION 3.2. *Let N be a numerical scheme for $\Delta = 0$, G a symmetry group, and $\rho : M^{\diamond n} \to G$ a moving frame. Then the scheme $\iota(N)$ invariantized by ρ is also a numerical scheme for $\Delta = 0$.*

EXAMPLE 3.2. In the example of the equation (1.1), the normalization $y = 0$ leads to $\varepsilon = -y/e^x$, which serves to define the corresponding moving frame. Note that any moving frame $\rho\colon M \to G$ can be extended to a moving frame $\hat{\rho}\colon M^{\diamond n} \to G$ defined by (2.3). From now on, we will denote the extended moving frame as ρ too, when there is no possibility for confusion. In this case, ρ on $M^{\diamond 2}$ can be obtained from (2.4) with $\varepsilon = -y_i/e^{x_i}$. Substituting for ε in the transformed formulas, we have

$$\begin{aligned}\rho(\mathbf{z}) \cdot \mathbf{z} &= (\, \tilde{x}_i,\, \tilde{y}_i;\, \tilde{x}_{i+1},\, \tilde{y}_{i+1}\,) \\ &= (\, x_i,\, 0\,;\, x_{i+1},\, y_{i+1} - y_i e^{x_{i+1}-x_i}\,).\end{aligned}$$

The nonconstant entries are a complete set of joint invariants. Now, invariantization of the Euler scheme (2.2) is obtained as

$$\begin{aligned}N(\rho(\mathbf{z}) \cdot \mathbf{z}) &= \tilde{y}_{i+1} - \tilde{y}_i - (\tilde{x}_{i+1} - \tilde{x}_i) f(\tilde{z}_i) \\ &= \tilde{y}_{i+1} - \tilde{y}_i - (\tilde{x}_{i+1} - \tilde{x}_i)\tilde{y}_i \\ &= (y_{i+1} - y_i e^{x_{i+1}-x_i}) - 0 - (x_{i+1} - x_i)\, 0 \\ &= y_{i+1} - y_i e^{x_{i+1}-x_i},\end{aligned}$$

which is the same as (1.4).

The fact that invariantization is prescribed by the choice of normalization equations defining a cross-section means that there are large families of invariant schemes. We need to choose them carefully since not every invariantized numerical scheme works better than the original one. Our main concern is not merely invariantization, but also invariantization reducing error in numerical schemes. It turned out that the moving frame method is very effective at the manipulation of numerical schemes for this purpose. To find an appropriate cross-section, one often takes into consideration the jet space, an extended space of M including derivatives of the dependent variables up to a certain order.

EXAMPLE 3.3. The equation

$$\dot{y} = xy + 1 \tag{3.5}$$

admits the one-parameter symmetry group

$$(x, y) \mapsto (\tilde{x}, \tilde{y}) = (\, x\,,\, y + \varepsilon e^{\frac{x^2}{2}}\,). \tag{3.6}$$

By the chain rule, the corresponding prolonged action on the second order jet space is

$$(x, y, \dot{y}, \ddot{y}) \mapsto (\tilde{x}, \tilde{y}, \widetilde{\dot{y}}, \widetilde{\ddot{y}}) = \left(\, x\,,\, y + \varepsilon e^{\frac{x^2}{2}}\,,\, \dot{y} + \varepsilon x e^{\frac{x^2}{2}}\,, \ddot{y} + \varepsilon(e^{\frac{x^2}{2}} + x^2 e^{\frac{x^2}{2}})\right)$$

Let us choose the normalization equation $\ddot{y} = 0$ or,

$$\widetilde{\ddot{y}} = \ddot{y} + \varepsilon(e^{\frac{x^2}{2}} + x^2 e^{\frac{x^2}{2}}) = 0,$$

which fixes the group parameter ε to be

$$\varepsilon = -\frac{\ddot{y}}{e^{\frac{x^2}{2}} + x^2 e^{\frac{x^2}{2}}}\,.$$

Note that this parameter gives the moving frame over M as

$$\varepsilon = -e^{-\frac{1}{2}x^2}\left(y + \frac{x}{x^2+1}\right) \tag{3.7}$$

where we use the equation to replace

$$\ddot{y} = y + x\dot{y} = (x^2+1)y + x.$$

With this result, we move on to the joint product space $M^{\diamond 2}$ and replace (x, y) by (x_i, y_i) in (3.7). Thus,

$$\begin{aligned}\rho(\mathbf{z})\cdot\mathbf{z} &= (\,\tilde{x}_i,\,\tilde{y}_i;\,\tilde{x}_{i+1},\,\tilde{y}_{i+1}\,)\\ &= \left(x_i, -\frac{x_i}{x_i^2+1}\,;\, x_{i+1}, y_{i+1} - \alpha y_i - \frac{\alpha y_i}{x_i^2+1}\right) \quad \text{where } \alpha = e^{-\frac{1}{2}({x_{i+1}}^2 - {x_i}^2)}.\end{aligned}$$

The corresponding invariantized Euler method for (3.5) is therefore

$$\begin{aligned}N(\rho(\mathbf{z})\cdot\mathbf{z}) &= \tilde{y}_{i+1} - \tilde{y}_i - (\tilde{x}_{i+1} - \tilde{x}_i) f(\tilde{z}_i)\\ &= \tilde{y}_{i+1} - \tilde{y}_i - (\tilde{x}_{i+1} - \tilde{x}_i)(\tilde{x}_i\tilde{y}_i + 1)\\ &= \left(y_{i+1} - \alpha y_i - \frac{\alpha x_i}{x_i^2+1}\right) - \left(-\frac{x_i}{x_i^2+1}\right)\\ &\quad - (x_{i+1} - x_i)\left(x_i\left(-\frac{x_i}{x_i^2+1}\right) + 1\right)\\ &= y_{i+1} - \alpha y_i - \frac{\alpha x_i - 2x_i + x_{i+1}}{x_i^2+1}.\end{aligned} \tag{3.8}$$

This scheme has error of order $O(h^3)$, which can be confirmed by observing that the transformation puts the second derivative to zero without changing the step size. This error reduction does not happen if we use other normalizations than $\ddot{y} = 0$ to construct the moving frames.

Figure 3.1 compares the results from the standard Euler method and two invariantized schemes. The invariant scheme (3.8) is marked as Inv Euler I in (b). We can see that its performance is much better than that of the original one in (a). On the contrary, another invariant scheme, which is constructed in the same way but by use of the normalization equation $\ddot{y} = 100$, shows a poor result in (c). This implies again that high accuracy is gained not solely by preservation of symmetries but also by being accompanied by a careful choice of invariantization.

In that the invariantized Euler scheme (3.8) actually increases the number of function evaluations since it requires the value of the second derivative, its improved performance might become less attractive. In other words, it is just a two-stage method of order two. Nevertheless, comparison with Heun's method, which

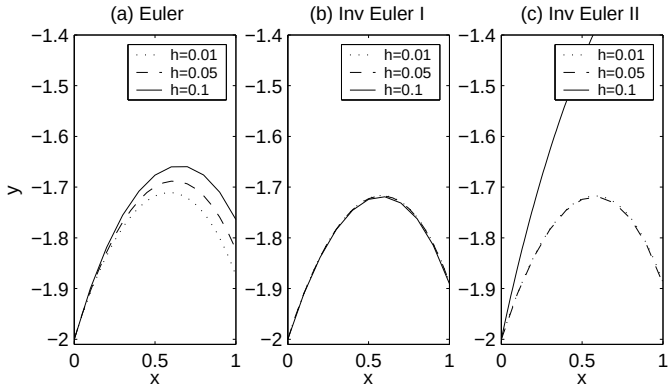

Figure 3.1: Invariantized Euler methods

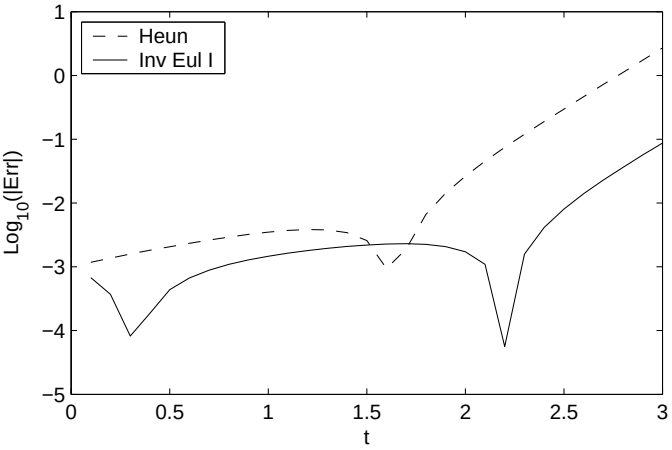

Figure 3.2: Invariantized Euler methods

is another two-stage scheme of order two, reveals that the invariant schemes have additional advantages beyond mere reduction of the order of the scheme.

Heun's method is

$$y_{i+1} = y_i + \frac{x_{i+1} - x_i}{2} (A_1 + A_2)$$

where

$$A_1 = f(x_i, y_i),$$
$$A_2 = f(x_{i+1}, y_i + (x_{i+1} - x_i) A_1).$$

In Figure 3.2, the invariant Euler method yields a better result than Heun's method, although they have error of the same order. This implies that normal-

ization $\ddot{y} = 0$ also has the effect of eliminating a substantial number of third order terms in the error.

4 Invariantization of the Runge-Kutta method

While the optimal normalization for the Euler method, $\ddot{y} = 0$, can be easily confirmed by simple computation, error analysis becomes much complicated when we deal with higher order numerical schemes. The number of terms that we need to handle for the analysis undergoes combinatorial explosion as the order increases, and we unavoidably face a huge complexity in the error formulas. For this reason, we will mainly resort to a quantitative method based on the plausible assumption:

> *On solution curves, numerical schemes generally work better where low order derivatives are zero.*

For a dth order numerical scheme, the method suggested here is to remove a substantial number of the terms from the $(d+1)$th order error by normalizing the first or second derivative to zero. With help of computer algebra, one can enumerate the error terms of Runge-Kutta methods (RK) for general cases. For example, the fifth order error of the fourth order RK for a first order differential equation $\dot{y} = f(x, y)$, $x, y \in \mathbf{R}$ is

$$\frac{1}{5760}\,(\, f_{xxxx} + f f_{xxxy} + \cdots 768 \text{ terms } \cdots - f^3 f_y f_{yyy} + f^4 f_{yyyy}\,). \tag{4.1}$$

It is notable that more than 70% of the terms in (4.1) have $\dot{y} = f$ as a factor if counted uniformly. It is also observed that the ratio of those terms in the error rises and approaches 1 as the order of RK increases. This implies that the local error of high order methods is very sensitive to the size of the first derivative at the point being evaluated. Therefore, we expect that invariantization with $\dot{y} = 0$ will significantly decrease the error, especially when dealing with higher order schemes.

From now on, we denote the standard fourth order Runge-Kutta method implicitly as $N(\mathbf{z}) = 0$, $\mathbf{z} = (z_i; z_{i+1}) \in M^{\diamond 2}$. Also we assume that a moving frame constructed on M (or its prolonged jet space) automatically extends over the joint product space $M^{\diamond 2}$ as

$$\begin{aligned} \rho(\mathbf{z}) \cdot \mathbf{z} &\equiv \rho(z_i) \cdot (z_i; z_{i+1}) \\ &= (\rho(z_i) \cdot z_i; \rho(z_i) \cdot z_{i+1}). \end{aligned}$$

Example 4.1. $\ddot{y} - y + \sin(y - \dot{y}) = 1$. [1]

[1] In the examples in the rest of the paper, except for the Hamiltonian system, pseudo error is used to evaluate the schemes. The pseudo error is defined as the difference between the given numerical solution and a solution computed with much smaller step size. We mostly compare the results from $h = 0.1$ with those from $h = 0.001$.

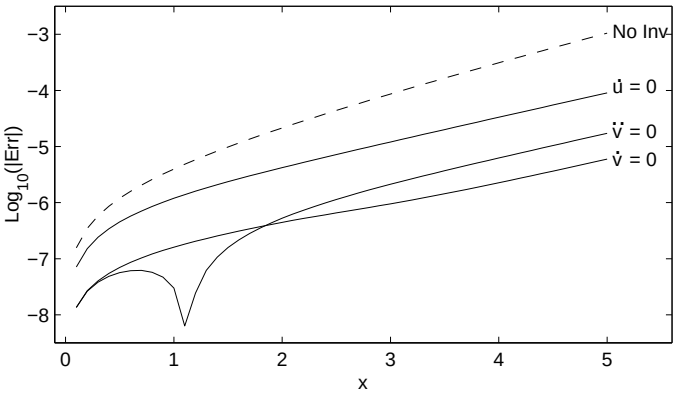

Figure 4.1: $\ddot{y} - y + \sin(y - \dot{y}) = 1$, $y(0) = \dot{y}(0) = 1$.

The corresponding system

$$\begin{cases} \dot{u} = v \\ \dot{v} = u \ - \sin(u - v) + 1 \end{cases}$$

is autonomous and admits a one-parameter symmetry with a symmetry transformation

$$(x, u, v, \dot{v}) \mapsto (\tilde{x}, \tilde{u}, \tilde{v}, \widetilde{\dot{v}}) = (x, u + \varepsilon e^x, v + \varepsilon e^x, \dot{v} + \varepsilon e^x). \tag{4.2}$$

Let us choose the normalization equation $\dot{v} = 0$. Solving for the group parameter, $\varepsilon = -e^{-x}(u - \sin(u - v) + 1)$, we derive the moving frame for $\mathbf{z} = (x_i, u_i, v_i; x_{i+1}, u_{i+1}, v_{i+1}) \in M^{\diamond 2}$, with

$$\rho(\mathbf{z}) \cdot \mathbf{z} = (x_i, u_i - \alpha, v_i - \alpha; x_{i+1}, u_{i+1} - \beta\alpha, v_{i+1} - \beta\alpha) \tag{4.3}$$

where $\alpha = u_i - \sin(u_i - v_i) + 1$ and $\beta = e^{x_{i+1} - x_i}$. The invariantized RK(IRK) is now $N(\rho(\mathbf{z}) \cdot \mathbf{z}) = 0$ which can be viewed as a substitution of the entries of (4.3) for the inputs of RK, that is,

$$N(\rho(\mathbf{z}) \cdot \mathbf{z}) = 0.$$

In Figure 4.1, we can see the result of IRK with $\dot{v} = 0$ is better than that of RK and the difference between them becomes larger as time processes. The graph also compares the results from other IRKs which are derived by the alternative normalizations: $\dot{u} = 0$, and $\ddot{v} = 0$.

Example 4.2. $\ddot{y} + x\dot{y} - (x + 1)y = \sin x$

This linear differential equation is converted to the equivalent dynamical system,

$$\begin{cases} \dot{u} = v \\ \dot{v} = (\ x + 1)u - xv + \sin x \end{cases}.$$

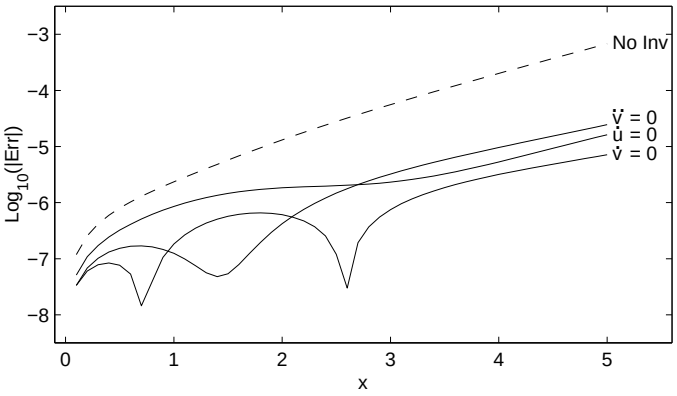

Figure 4.2: $\ddot{y} + x\dot{y} - (x+1)y = \sin(x)$, $y(0) = \dot{y}(0) = 1$.

The system has the same symmetry as (4.2). If one chooses the normalization equation $\dot{v} = 0$, then the parameter becomes $\varepsilon = -e^{-x}((x+1)u - xv + \sin x)$. The corresponding moving frame ρ on $M^{\diamond 2}$ satisfies

$$\rho(\mathbf{z}) \cdot \mathbf{z} = (x_i, u_i - \alpha, v_i - \alpha; x_{i+1}, u_{i+1} - \beta\alpha, v_{i+1} - \beta\alpha),$$

where $\alpha = (x_i + 1)u_i - x_i v_i + \sin x_i$ and $\beta = e^{x_{i+1} - x_i}$.

Figure 4.2 shows the results from RK and IRKs with different normalization equations. The one from $\dot{v} = 0$ is again the best on the whole. This is natural from the fact that the number of terms containing $\dot{v}$ is greater than those containing $\dot{u}$ and $\ddot{v}$ among the fifth-order error terms of the corresponding RK, which can be shown in the Taylor expansion using computer algebra tools.

It is observed that increase in the number of dependent variables weakens the effect of invariantization. If a given system is non-autonomous and of three dependent variables, invariantization under a one-parameter symmetry group usually has little effect. However, this situation can be improved if larger symmetry groups are available for the system.

Example 4.3. The system

$$\begin{cases} \dot{u} = & v \\ \dot{v} = & w \\ \dot{w} = & \dfrac{-12x^2 w - 3xv + \sqrt{4x^2 w + 4xv - u + \log x}}{4x^3} \end{cases}$$

has a two-parameter symmetry group whose symmetry transformations are

$$(x, u, v, w, \dot{w}) \mapsto \left(x, u + \varepsilon_1\sqrt{x}, v + \varepsilon_1 \frac{1}{2\sqrt{x}}, w - \varepsilon_1 \frac{1}{4x\sqrt{x}}, \dot{w} + \varepsilon_1 \frac{3}{8x^2\sqrt{x}}\right),$$
$$(x, u, v, w, \dot{w}) \mapsto \left(x, u + \varepsilon_2 \frac{1}{\sqrt{x}}, v - \varepsilon_2 \frac{1}{2x\sqrt{x}}, w + \varepsilon_2 \frac{3}{4x^2\sqrt{x}}, \dot{w} - \varepsilon_2 \frac{15}{8x^3\sqrt{x}}\right).$$

Since the dimension of the symmetry group is 2, we need to choose a two-dimensional cross-section for normalization. Let us take

$$\dot{v} = 0, \qquad \dot{w} = 0.$$

The corresponding moving frame formulas are

$$\varepsilon_1 = -10x\sqrt{x}w + 4x^2\sqrt{x}\dot{w}, \qquad \varepsilon_2 = 2x^2\sqrt{x}w + \frac{4}{3}x^3\sqrt{x}\dot{w},$$

respectively. Computer algebra confirms that this normalization eliminates 83% of the terms in the fifth order error.

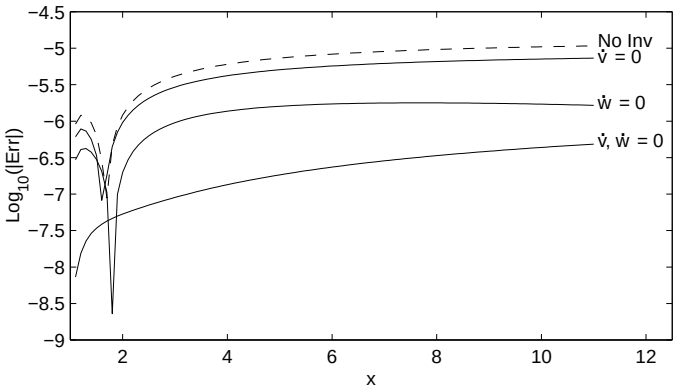

Figure 4.3: Invariantization under two-parameter symmetry group

In Figure 4.3, one can see the the corresponding invariantized scheme excels by far the results based on RK and IRKs with a single normalization. The initial condition used is $u(0) = v(0) = -1, w(0) = 1$.

Many geometric integrators, by preserving geometric properties of the solutions, shows excellent long-term behavior [21]. It is observed that the invariantization technique also enhances long-term stability of a standard scheme.

Example 4.4. Driven Harmonic oscillator.
The equation

$$\ddot{y} + y = \sin(x^\alpha)$$

describes a driven harmonic oscillator, one of whose applications is to an inductor-capacitor circuit [48]. Recall that resonance occurs when $\alpha = 1$. Here we set $\alpha = 0.99$, which yields solutions that are close to resonance but remains bounded. Since this is a linear constant-coefficient equation, its symmetry transformations are easily found:

$$(x, u, \dot{u}, \ddot{u}) \mapsto (x, u + \varepsilon_1 \sin x, \dot{u} + \varepsilon_1 \cos x, \ddot{u} - \varepsilon_1 \sin x),$$
$$(x, u, \dot{u}, \ddot{u}) \mapsto (x, u + \varepsilon_2 \cos x, \dot{u} - \varepsilon_2 \sin x, \ddot{u} - \varepsilon_2 \cos x).$$

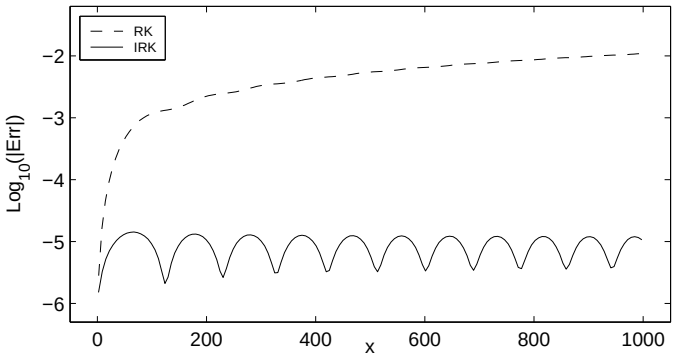

Figure 4.4: Long term integration of harmonic oscillator

As in the previous examples, we invariantize the RK scheme by setting $\dot{u} = 0$ and $\ddot{u} = 0$.

The time step $h = 0.1$ is used and we integrate up to $x = 1000$. Figure 4.4 shows that the invariantized scheme produces a much better result in long term-integration. Since the errors oscillate rapidly around zero with varying amplitudes, we only compare their amplitudes at representative values in the figure. In contrast to the standard scheme case, 10,000 integration steps hardly affects the quality of the numerical solution of IRK.

From the above four examples of IRKs, it should be noted that invariantization does not change the number of evaluation, although construction of the moving frame does require information on derivatives. Once the RK scheme is invariantized by a choice of moving frame, the computation of the first stage is always zero and therefore the total number of evaluations remains the same.

5 Comparison with Other Geometric Integrators

As mentioned in the introduction, several types of Lie-symmetric integrators have been developed but still many of them remain untested on a practical level. In this section the invariantization method is compared with two numerical methods that adopt geometric approaches.

5.1 Symmetry Reduction vs. Invariantization

First, we test how symmetry reduction affects the performance of numerical schemes in comparison to invariantization. Both methods are similar in that they are based on the symmetry structure of the differential equation, but symmetry reduction is a global substitution while invariantization is a local one.

Consider the equation

$$\dot{y} = (\sin x)\, y + \cos x.$$

This equation admits the one parameter symmetry group

$$(x, y, \dot{y}) \mapsto (x, y + \varepsilon e^{-\cos x},\ \dot{y} + \varepsilon \sin x\, e^{-\cos x}),$$

which suggests the substitution $u = e^{\cos x} y$. The reduced equation is

$$\dot{u} = \cos x \, e^{\cos x}.$$

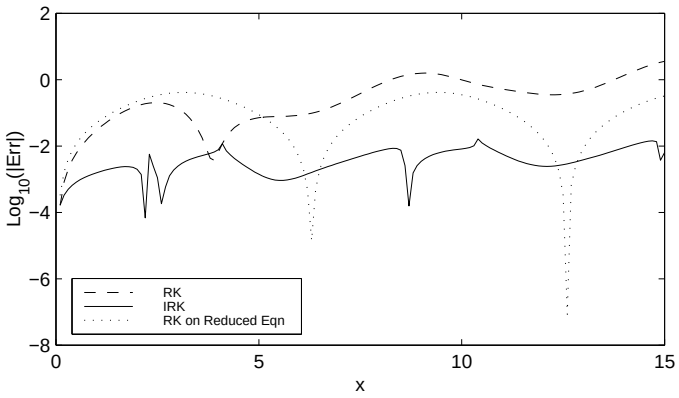

Figure 5.1: Comparison of Symmetry Reduction and Invariantization in $\dot{y} = \sin x \; y + \cos x$.

This equation is simpler than the original one in view of the order. It is interesting to compute the performances of RK and IRK on the original equations, and RK on the reduced equation. In Figure 5.1, we can see IRK works better than both of RKs on the original equation and reduced one. In the long term, the error of IRK is observed to slowly rise and converge to that of RK on the reduced equation.

In fact, reduction by symmetry groups does not always result in simpler equations. For the equations $\ddot{y} + x\,\dot{y} - (x+1)y = \sin x$ in Example 4.2, substitution leads to a more complicated equation of reduced order. Figure 5.2 shows the result of numerical integration.

5.2 Symplectic Integrators vs. Invariant Integrators

Symplectic integrators are one of the most successful classes of geometric integrators for ODEs [1, 10, 13, 17, 20]. The popularity of a symplectic integrator stems from its area-preservation, time-reversibility and energy conservation in a time-independent Hamiltonian system. Many symplectic integrators are based on a RK scheme. Even though the invariantization method does not use Hamiltonian structure directly, it is interesting to compare the two methods as geometric integrators.

Suppose we have a Hamiltonian function

$$H(p,q) = \frac{1}{2}(p^2 + q^{-2}),$$

which leads to the system

$$\left\{ \begin{array}{rcrcr} \dot{p} = & -H_q & = & q^{-3} \\ \dot{q} = & H_p & = & p \end{array} \right. . \tag{5.1}$$

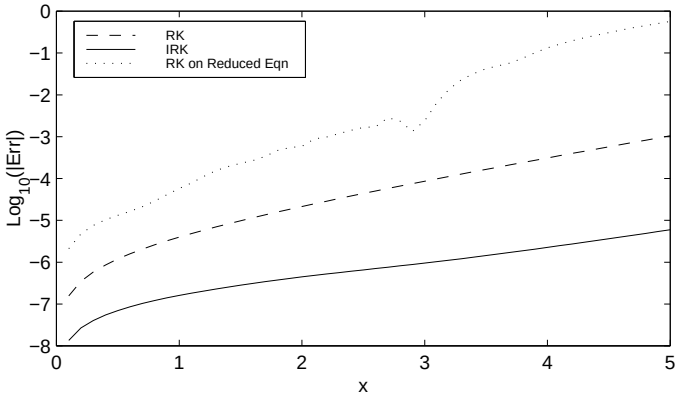

Figure 5.2: Comparison of Symmetry Reduction and Invariantization in $\ddot{y} + x\,\dot{y} - (x+1)y = \sin x$

This has the exact solution

$$q = \pm\sqrt{C_1 x^2 + 2C_1 C_2 x + C_1 {C_2}^2 + C_1^{-1}}$$

for arbitrary C_1, C_2. The system also admits the symmetry transformation

$$(x, q, p) \mapsto \left(\tfrac{x+\varepsilon_1}{1-\varepsilon_2(x+\varepsilon_1)}, \tfrac{q}{1-\varepsilon_2(x+\varepsilon_1)}, p + \varepsilon_2 q - \varepsilon_2 p(x+\varepsilon_1) \right).$$

We take normalization equations

$$\begin{aligned} x &= \frac{q + \sqrt{q^2 + hpq}}{p}, \\ p &= 0. \end{aligned}$$

The first equation is just to fix the step size at h to avoid confusion in error analysis. This intention can be expressed in a neater form, when we set the equivalent normalization on the joint product space, as

$$\begin{aligned} x_{i+1} - x_i &= h \\ p_i &= 0. \end{aligned}$$

Setting the normalization equations on the joint product space, instead of the jet space, is an approach commonly taken in invariantization of PDE schemes [30]. This enables one to deal with changes in independent variables and allow a wider range of choices for invariantization.

A simple computation as in Example 3.1 gives the moving frame

$$\begin{aligned} \varepsilon_1 &= -x + \frac{q + \sqrt{q^2 + hpq}}{p}, \\ \varepsilon_2 &= \frac{p}{\sqrt{q^2 + hpq}}. \end{aligned}$$

We compare schemes of the first order (the Euler method) and of fourth order (RK). Although there is no known explicit symplectic method of order greater than two for general Hamiltonian systems, many explicit symplectic RKs have been introduced for separable Hamiltonian systems like (5.1). Here we use a symplectic fourth-order RK developed in [10, 18]. The initial condition

$$q(0) = \sqrt{2}, \quad p(0) = -\frac{1}{\sqrt{2}},$$

and the step size $h = 0.05$ are used.

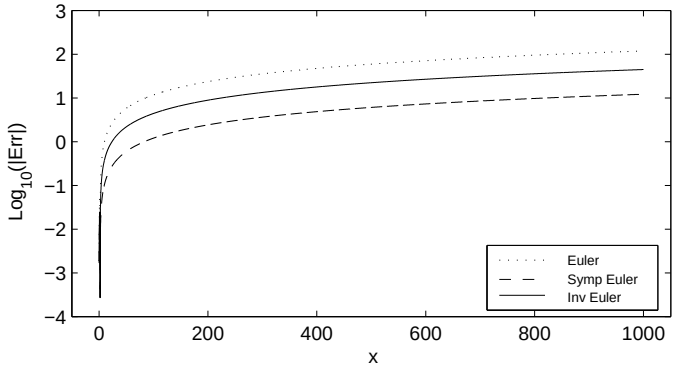

Figure 5.3: Comparison of Symplectic and Invariant integrators at the first order

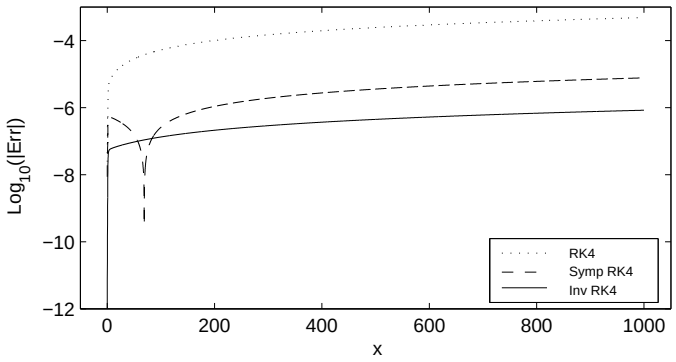

Figure 5.4: Comparison of Symplectic and Invariant integrators at the fourth order

Figure 5.3 compares errors in the standard, symplectic method and invariantized method of the first order in the long term. Although the invariantized Euler method performs better than the Euler method, it is still not as good as the symplectic Euler method.

This situation changes dramatically when we move on to higher order methods, and the invariantized RK4 excels the other two methods, as illustrated in Figure

5.4. While the method based on symplectic structure brings almost the same improvement as in the Euler method, invariantization works much better for the higher order method. The increasing dependency of error terms on the first derivative is responsible for this result.

6 Conclusions

In this paper, we have investigated the technique of invariantization of numerical schemes for differential equations. In a practical sense, the procedure of invariantization is a local substitution at each step in an existing numerical algorithm. Through moving frames, one can exploit the symmetry transformations of the differential equation to adjust computational performance of numerical schemes.

Although the symmetry-preserving property in itself does not guarantee better numerical precision, invariant numerical schemes greatly surpass and complement the original schemes if their defining normalization equations are well chosen. Through various examples in ODEs, we can see that the moving frame method has great potential in constructing invariant schemes and studying their properties.

Invariantization offers many advantages over previous methods based on discrete invariants. Most of all, construction of invariant schemes can be done in a much easier and systematic way through substitution in existing schemes, avoiding complex computation for discrete invariants. Besides the fact that the invariantization method requires only a small modification to the standard numerical schemes, another appealing point is its generality. Although only a few examples of single step methods for ODEs have been dealt in this paper, the invariantization technique can be applied to a wide range of numerical schemes both for ODEs and PDEs. It is worth generalizing the invariantization process to other numerical schemes such as multi-step methods or finite difference schemes for PDEs.

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