INVARIANTIZATION OF NUMERICAL SCHEMES USING MOVING FRAMES

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Abstract. This paper deals with the algorithm that invariantizes the existing numerical schemes of differential equations with respect to their symmetry group using the moving frame method. The Invariantization work as an adaptive transformation on the solutions and provides much better circumstance for the numerical scheme. Error reduction of numerical schemes such as the Runge-Kutta method by invariantization is studied and some applications in ordinary differential equations are illustrated by examples including a harmonic oscillator and a Hamiltonian system.

1. Introduction

Symmetry has long been recognized as the key to the study of differential equations. It has a remarkable range of applications including simplification of equations by symmetry reduction and determination of conservation laws by Noethers Theorem. Recently, there is a growing interest in the applications of symmetries of differential equations to their numerical solutions. Several different approaches are being pursued, closely related to an extension of Lie group theory to difference equations.

One natural approach is to determine symmetries for given difference equations and simplify the equations using them [16, 17, 21]. In order to obtain symmetries that coincide with Lie symmetries in the continuous limit, one needs to significantly modify the Lie techniques used in the continuous case. Another approach is to discretize differential equations in a way that preserves some of the symmetries [4, 9, 10]. Given a differential equation, one constructs a difference equation and a mesh in such a manner as to be compatible with the original symmetry group. It is found [23, 26] that composition of numerical schemes by manipulation from automorphism point of view can make some geometric integrators, including one that preserves time-reversal symmetry.

The goal of this paper is to introduce a novel method, invariantization of numerical schemes, which serves not only for preservation of symmetries of the system but also for reduction of the error. Applying the moving frame method to the existing numerical schemes, one can easily get an invariant numerical scheme without computation to find difference invariants. Invariantization also enables delicate manipulations of numerical schemes in geometric manner and therefore control of the error. We are able to utilize a wide range of numerical techniques that have been already developed.

In a practical sense, invariantization is an adaptive transformation on numerical solutions at each step of numerical schemes. The invariantization by the symmetry transformation allows us to transform the points at each step along the orbits of the symmetry group to the proper places where the numerical scheme works better. Figure 1 illustrates this idea. N stands for a given numerical scheme that evaluates x_{i+1} from x_i. If the

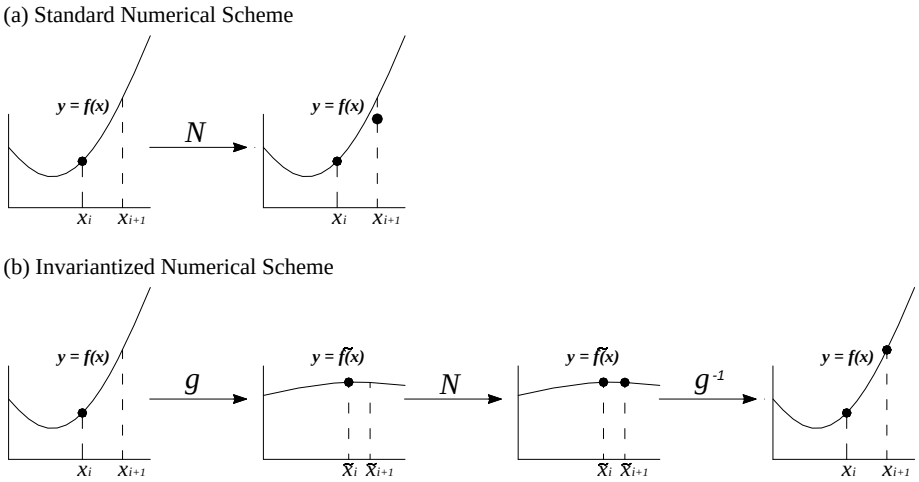

FIGURE 1. Basic idea of invariantization of numerical scheme

graph of solution varies rapidly or is highly oscillatory near the points, the scheme may result in poor performance like (a). This situation can be avoided by applying symmetry transformations, which map a solution of the differential equation to another one. In many cases we can pick the transformation g wisely so that the pair of points is mapped into another nicer solution that cooperates well with the numerical scheme. The transformation g practically means local substitution that updates numerical schemes N at each step. The good choice of g usually depends on the position of the points being evaluated, and therefore changes at steps. In the moving frame theory this procedure can be dealt as the invariantization on the joint 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 it [20] or reducing its dimension [5]. Numerical scheme can inherit some geometric properties such as first integrals, symmetries and symplectic structure from their original systems by composition with proper transformations[14, 23, 28]. One of the common strategies for integration of ordinary differential equations on manifolds is mapping the system locally to other equations on a vector space and applying classical methods. Combining with transformation, exponential integrators can decrease computational cost [8] and deal with highly oscillatory equations [19]. These are just a few of examples of where the transformation technique is applied. Compared to the above transformations, the symmetry transformations have a distinctive feature that serves for direct error reduction: The symmetry transformations leave the equations *exactly* the same, and therefore the control of error becomes much easier. Also, the accuracy are well preserved in the inverse transformation for high order methods, since exact solutions are mapped to other exact solutions under the symmetry transformation.

The invariantization technique can be applied to any numerical methods based on finite difference scheme for both ordinary differential equations (ODEs) and partial differential equations (PDEs). In this paper we mainly focus on ODEs with nonlinear symmetry

transformations, since most of traditional numerical schemes are already invariant with respect Affine symmetry [26]. The idea of invariantization of numerical schemes first appeared in [25] 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 the differential equation

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

It has a 1-parameter symmetry group G whose infinitesimal generator and finite transformation are $X = e^x \frac{\partial}{\partial y}$, $\varepsilon \cdot (x, y) = (x, y + \varepsilon e^x)$ for all $\varepsilon \in \mathbf{R}$ respectively. We suppose the point $(x_i, y_i) = (x_i, y(x_i))$ is the initial condition, and y_{i+1} is the next point generated by the Euler method for fixed x_{i+1}. Let us set the transformed points $(\tilde{x}, \tilde{y}) = \varepsilon \cdot (x, y)$ and the step size $h = x_{i+1} - x_i = \tilde{x}_{i+1} - \tilde{x}_i$. The Euler method is $y_{i+1} = y_i + h\dot{y}(x_i) = y_i + hy_i = (1 + h)y_i$. If we apply the method to the transformed pair of the points, $(\tilde{x}_i, \tilde{y}_i)$ and $(\tilde{x}_{i+1}, \tilde{y}_{i+1})$, we obtain $\tilde{y}_{i+1} = (1 + h)\tilde{y}_i$ or,

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

in terms of the original points. Using the fact that $y = \dot{y} = \ddot{y} = \cdots$ and the Taylor expansion at x_0, we have

$$y_{i+1} = y(x_{i+1}) - (y_i + \varepsilon e^{x_i}) \left(\frac{h^2}{2!} + \frac{h^3}{3!} + \dots \right)$$

So far, this is nothing more than the Euler method with error $O(h^2)$. Now suppose we actually transform (x_i, y_i) to $(\tilde{x}_{i+1}, \tilde{y}_{i+1}) = (x_i, 0)$. That is, we set $\varepsilon = -y_i/e^{x_i}$. Then all error terms are cancelled and we have exactly $y_{i+1} = y(x_{i+1})$. Again, note that our choice of transformation parameter ε depended on x_i, y_i and x_{i+1} and varies at steps. In this simple example the Euler method yields an exact solution after an appropriate symmetry transformation. However, the accuracy of the invariant scheme greatly depends on the choice of ε.

2. Invariantization of Numerical Schemes by Moving Frames

Denote $z = (x, y) \in M = \mathbf{R} \times \mathbf{R}^n$ where x is the independent variable and y the dependent. In our applications we focus on a normal ordinary differential equation

$$\dot{y} = f(x, y). \tag{2.1}$$

To deal with distinct points on the graph, we introduce the *joint product* of M

$$M^{\diamond k} = \{ (z_1; \dots; z_k) \,|\, z_i \in M, z_i \neq z_j \text{ for all } i \neq j \}$$

which is the off-diagonal part of the Cartesian product. Every action of group G on M naturally extends to the *product action* of $g \in G$ on $M^{\diamond k}$ as

$$g \cdot z = g \cdot (z_1; \dots; z_k) = (g \cdot z_1; \dots; g \cdot z_k) \text{ for } z \in M^{\diamond k}.$$

By numerical schemes we mean here a real-valued function N on $M^{\diamond k}$ such that $N(z) = O(H)$ whenever z is on a solution of the differential equation, where H is a step size function of which arguments are differences between independent variables of $z_1, \cdots, z_k$.

Let G be a Lie group acting on M. We say that a real-valued function f is an *invariant* if $f(g \cdot z) = f(z)$ for all $g \in G$ and $z \in M$. The *g-transformation* of numerical scheme of N is defined as

$$N^g(z) = N(g \cdot z).$$

Proposition 2.1. *Let N be the numerical scheme for a differential equation and G be symmetry group of the equation. Then N^g is also a numerical scheme for the equation for all $g \in G$.*

Example 2.1. Transformation of the Euler method
Let G be the 1-parameter symmetry group acting on $\mathbf{R}^2$ in the example of (1.1). We can extend the action of $\varepsilon \in G$ on $(\mathbf{R}^2)^{\diamond 2}$ as

$$\begin{aligned} \varepsilon \cdot z &= \varepsilon \cdot (z_i;\, z_{i+1}) \\ &= (\varepsilon \cdot z_i;\, \varepsilon \cdot z_{i+1}) \\ &= (x_i, y_i + \varepsilon e^{x_i};\, x_{i+1}, y_{i+1} + \varepsilon e^{x_{i+1}}). \end{aligned} \tag{2.2}$$

The Euler method for (2.1) is

$$N(z_i;\, z_{i+1}) = y_{i+1} - y_i + (x_{i+1} - x_i) f(x_i, y_i) \text{ with } H = (x_{i+1} - x_i)^2,$$

and its ε-transformed version is

$$\begin{aligned} N^\varepsilon(z_i;\, z_{i+1}) &= N(\varepsilon \cdot (z_i;\, z_{i+1})) \\ &= N(x_i, y_i + \varepsilon e_i^x;\, x_{i+1}, y_{i+1} + \varepsilon e_{i+1}^x) \\ &= (y_{i+1} + \varepsilon e^{x_{i+1}}) - (y_i + \varepsilon e^{x_i}) - (x_{i+1} - x_i) f(x_i, y_i). \end{aligned} \tag{2.3}$$

Our main concern is not just invariantization, but also invariantization reducing error in numerical schemes. It turned out that the moving frame methods are very effective at the manipulation of numerical schemes for this purpose. Moving frames, which Fels and Olver recently developed in [11, 12], are a powerful tool to investigate invariants of group actions. The moving frames methods provide an algorithmic way to invariantize a given function and to find complete set of invariants for general group actions.

Definition 2.1. 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 existence of a moving frame requires freeness of the underlying group action.

Theorem 2.2. *A moving frame exists if and only if the action of the group is free and regular.*

Suppose G acts effectively on M. Except for few exceptional cases, for most group actions including all those arising in known applications, it is true that the product action is free and regular on an open subset of $M^{\times k}$ for $k \gg 0$ sufficiently large. Consequently, the moving frame method is applicable to such a joint space. The practical construction of a moving frame can be done by taking a cross-section K to the orbits of G on M. Normalization equations from a cross-section $\tilde{z} = g \cdot z$ with $\tilde{z} \in K$ implicitly defines $g \in G$ as a function of $z \in M$. One solves this and obtains a moving frame $g = \rho(z)$. Once a moving frame is found, it is easy to make an invariant from a given function.

Definition 2.3. The *invariantization* of a scalar function $F : M \to G$ with respect to a right moving frame ρ is the invariant function $I = \iota(F)$ defined by $I(z) = F(\rho(z) \cdot z)$.

It is notable that the components of $\rho(z) \cdot z$ naturally provides a complete set of invariants since they are the invariantization of the coordinate functions. We refer the reader to [11] for more detail.

Example 2.2. For the transformation (2.2), let us choose a cross-section $\widetilde{y}_i = 0$. Then the corresponding moving frame is

$$\varepsilon = \rho(z) = -y_i/e^{x_i}$$

where $z = (x_i, y_i;\, x_{i+1}, y_{i+1})$ in the joint space $(\mathbf{R}^2)^{\diamond 2}$. One can observe that the components of $\rho(z) \cdot z = (x_i, 0;\, x_{i+1}, y_{i+1} - y_i e^{x_{i+1}-x_i})$ are the joint invariants.

Example 2.3. Let G be a 1-parameter Lie group acting on $\mathbf{R}^3$ as

$$\varepsilon \cdot (x, y, z) = (\tilde{x}, \tilde{y}, \tilde{z}) = \left(\frac{x}{1 - \varepsilon x},\ \frac{y}{1 - \varepsilon x},\, \varepsilon(y - xz) + z \right) \quad \text{for } \varepsilon \in G.$$

Setting a cross-section $\tilde{z} = 0$ gives the moving frame $\rho(x, y, z) = \frac{z}{xz - y}$. Observe that $\rho(x, y, z) \cdot (x, y, z) = \left(\frac{x(y-xz)}{y},\, y - xz,\, 0 \right)$ are the invariants.

Suppose G is a symmetry group for a given differential equation and ρ is a moving frame for G. The invariantization of the numerical scheme N with respect to the moving frame ρ is

$$\iota(N)(z) = N^{\rho(z)}(z) = N(\rho(z) \cdot z).$$

As mentioned before, most standard schemes are invariant under time translation, space translation and scaling. Therefore we only need to focus on other more complicated symmetries in invariantization. Also, the fact that invariantization is decided by the cross-section implies we have families of infinitely many invariant schemes in most cases. In the following example, the procedure of invariantizing numerical schemes is explained and also the importance of choice of moving frames is shown by comparison of two different invariantized schemes.

Example 2.4. Invariatization of the Euler method.
The equation

$$\dot{y} = xy + 1 \tag{2.4}$$

has a 1-parameter symmetry group whose infinitesimal generator is $X = e^{\frac{x^2}{2}} \frac{\partial}{\partial y}$. Its prolonged generator and the corresponding transformation are, respectively,

$$\mathbf{pr}^{(2)} X = e^{\frac{x^2}{2}} \frac{\partial}{\partial y} + x e^{\frac{x^2}{2}} \frac{\partial}{\partial \dot{y}} + (e^{\frac{x^2}{2}} + x^2 e^{\frac{x^2}{2}}) \frac{\partial}{\partial \ddot{y}},$$

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

To construct the first invariant scheme (type I), let us set a cross section as $\widetilde{\ddot{y}} = 0$ for normalization. This gives the prolonged moving frame

$$\varepsilon(z) = -\frac{e^{-\frac{1}{2}x^2}\ddot{y}}{x^2+1}$$

or

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

as $\ddot{y} = y + x\dot{y} = (x^2+1)y + x$. Now the invariantized Euler method for (2.4) can be obtained by plugging ε to (2.3). Another way to understand the invariantization is using a local substitution. Applying the moving frame ε to $z = (z_i;\, z_{i+1}) = (x_i, y_i;\, x_{i+1}, y_{i+1})$ we have

$$\begin{aligned}\varepsilon(z)\cdot z &= \varepsilon(z_i)\cdot(z_i;\, z_{i+1})\\ &= (\varepsilon(z_i)\cdot z_i;\, \varepsilon(z_i)\cdot z_{i+1})\\ &= \left(x_i, -\frac{x_i}{x_i^2+1}\,;\, x_{i+1}, y_{i+1} - \alpha y_i - \frac{\alpha x_i}{x_i^2+1}\right)\end{aligned}$$

where α is $e^{-\frac{1}{2}({x_{i+1}}^2 - {x_i}^2)}$. The invariantization is a local change of variables in the Euler method as

$$\begin{aligned}&(x_i,\, y_i\,;\; x_{i+1},\, y_{i+1}) \longmapsto\\ &\left(x_i, -\frac{x_i}{x_i^2+1}\,;\; x_{i+1},\, y_{i+1} - \alpha y_i + -\frac{\alpha x_i}{x_i^2+1}\right).\end{aligned}$$

This substitutions seem complicated but are actually easily implementable using the moving frame. The step size remains the same under the transformation, so the error reduces from $O(h^2)$ to $O(h^3)$. The second invariantization (type II) is done in the same way, but with normalization $\widetilde{\ddot{y}} = 100$. The numerical solutions from the Euler method, the type I invariant method and the type II are shown in Figure 2. (a),(b) and (c), respectively.

From Example 2.4 we can see that there are infinite choices for the moving frames and each of them decides the corresponding symmetric integrator. It must be noted that the result from type II is poorer than that of the standard Euler method, even though the scheme preserves symmetry of the equation (2.4). This implies that preservation of symmetries is not enough to gain high accuracy and must be accompanied by careful design of the schemes.

However, there is not much surprise at the excellent performance of the type I scheme either. This is because the invariantization in the example actually increased the number of stages by requiring the value of the second derivative, which is higher than the order of the Euler method. The true benefit of invariantization appears when applied to numerical schemes of second order or higher, such as the Runge-Kutta method.

3. Invariantization of the Runge-Kutta method

The invariantizations shown in the previous examples bring up the issues about how we can choose a proper section for a general case and what amount of error reduction we can expect from that. We have learned that normalizing the second derivative to

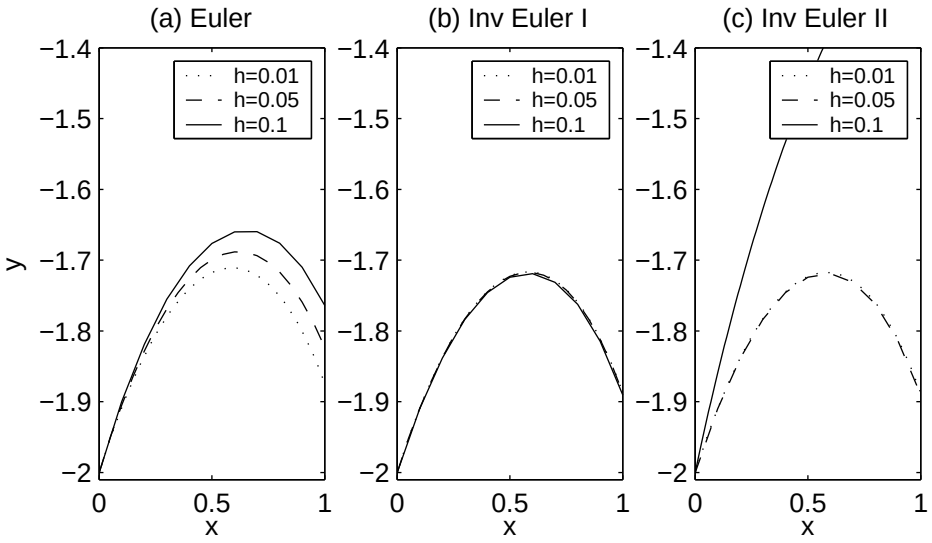

FIGURE 2. Invariantized Euler methods

zero is the best strategy for the Euler method. The situation becomes much complicated when we adopt numerical schemes of higher order. The number of terms that we need to deal with for the error analysis undergoes combinatorial explosion as the order increases and we unavoidably face the huge complexity of the error. While there have been many researches on error estimation related to the adaptive step size control, not much has been done for the structural analysis of the error that enables direct error manipulation. Because of such difficulty, we will mainly resort to quantitative methods which is based on the plausible assumption,

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

Indeed, this assumption is just a verbal description of Figure 1.

For a nth order numerical scheme, the method suggested here is to remove a substantial number of the terms from the $(n+1)$th order error by locally normalizing the first or second derivatives to zero. We mainly focus on the Runge-Kutta method (RK) in this paper, which is the one of the most widely used one-step multi-stage method. With help of a computer algebra tool, we can easily enumerate the error terms of the RK for the general cases. For example, the fifth order error from the fourth order RK for a first order

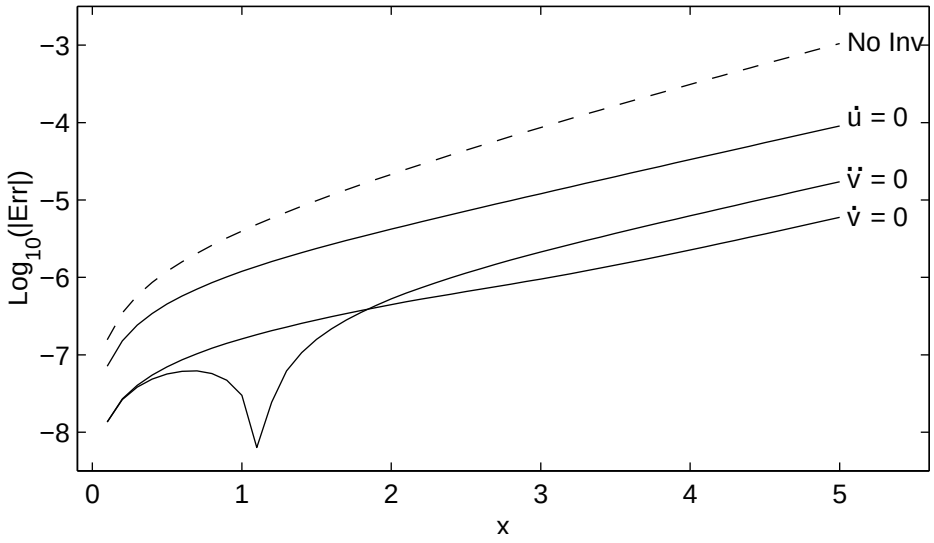

FIGURE 3. $\ddot{y} - y + \sin(y - \dot{y}) = 1$, $y(0) = \dot{y}(0) = 1$.

differential equation is,

$$\begin{aligned} E_5 = \frac{1}{5760}\,(\, & 3f_{xxxx} + 12ff_{xxxy} - 12f_xf_{xxy} + 18f^2f_{xxyy} + 12f_{xx}f_{xy} \\ & + 24f{f_{xy}}^2 - 24ff_xf_{xyy} + 12f^3f_{xyyy} + 8f_{xxx}f_y + 12ff_{xxy}f_y \\ & - 24f_xf_{xy}f_y - 12f_{xx}{f_y}^2 - 48ff_{xy}{f_y}^2 + 48f_x{f_y}^3 + 48f{f_y}^4 \\ & - 36{f_x}^2f_{yy} + 12ff_{xx}f_{yy} + 36f^2f_{xy}f_{yy} - 96ff_xf_yf_{yy} \\ & - 72f^2{f_y}^2f_{yy} + 12f^3{f_{yy}}^2 - 12f^2f_xf_{yyy} - 4f^3f_yf_{yyy} + 3f^4f_{yyyy}\,). \end{aligned}$$

More than 70% of terms have $\dot{y} = f$ as a factor if counted uniformly. It is observed that for the high order RKs that the ratio of those terms in the error rises and approaches to 1 as the order of the methods increases. This implies that the local error of the high order methods is very sensitive to the value of the first derivative. Therefore, invariantization with $\tilde{y}_x = 0$ brings much more improvement when we use the higher order schemes.

Through the examples in the rest of the paper, except the Hamiltonian system with the exact solution, we use the pseudo error. The pseudo error is defined as difference from a numerical solution with much smaller step size. We mostly compare the results from $h = 0.1$ with those from $h = 0.001$.

Example 3.1. $\ddot{y} - y + \sin(y - \dot{y}) = 1$.
The corresponding system is

$$\begin{aligned} \dot{u} &= f(u, v) = v \\ \dot{v} &= g(u, v) = u - \sin(u - v) + 1 \end{aligned}$$

The system is autonomous and admits a 1-parameter symmetry generator, $X = e^x\frac{\partial}{\partial u}$ and the transformation $(x, u, v, \dot{v}) \mapsto (x, u + \varepsilon e^x, v + \varepsilon e^x, \dot{v} + \varepsilon e^x)$. Using computer algebra tools, we can check that this system has 106 terms and 694 terms in the fifth order error

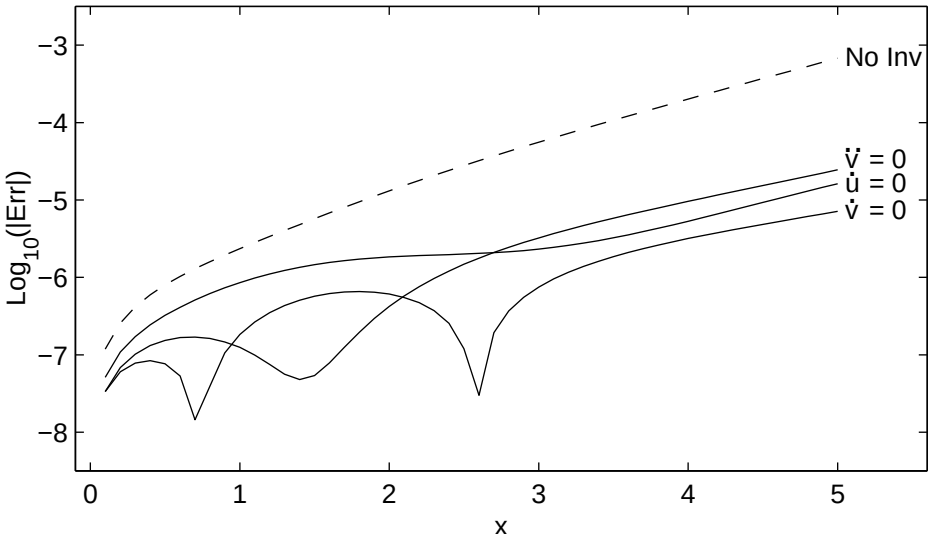

FIGURE 4. $\ddot{y} + x\dot{y} - (x+1)y = \sin(x)$, $y(0) = \dot{y}(0) = 1$.

in the RK for u and v respectively.

$$E_5^u = \frac{1}{2880}\,(\, f{g_u}^2 + fgg_{uu} + \cdots 106 \text{ terms} \cdots + g^2 g_y g_{vv} + g^3 g_{vvv}\,)$$
$$E_5^v = \frac{1}{2880}\,(\, g{g_u}^2 + g^2 g_{uu} + \cdots 694 \text{ terms} \cdots - g^3 g_v g_{vvv} - g^4 g_{vvvv}\,).$$

There are 71 terms and 539 terms respectively that have g as a factor in them. Therefore setting $\widetilde{v} = 0$ gives 67% and 78% reduction of the error terms in ${E^u}_5, {E^v}_5$ respectively. The corresponding moving frame for the cross-section is $\varepsilon = -e^{-x}(u - \sin(u-v) + 1)$ and the transformation

$$\begin{aligned}\varepsilon \cdot (x, u, v, \dot{v}) &= (\tilde{x}, \tilde{u}, \tilde{v}, \tilde{\dot{v}}) \\ &= (x, \sin(u-v) - 1,\ -(u-v) + \sin(u-v) - 1, 0).\end{aligned}$$

Now the corresponding invariantized RK can be obtained by substitution at each step,

$$(x_i, u_i, v_i; x_{i+1}, u_{i+1}, v_{i+1}) \mapsto (x_i, u_i - \alpha, v_i - \alpha; x_{i+1}, u_{i+1} - \beta\alpha, v_{i+1} - \beta\alpha).$$

where $\alpha = u_i - \sin(u_i - v_i) + 1$ and $\beta = e^{x_{i+1} - x_i}$. Refer to Figure 3 to see the results of the invariantized RK with different cross-sections that outperforms the standard one.

Example 3.2. $\ddot{y} + x\dot{y} - (x+1)y = \sin x$
This linear differential equation is converted to the equivalent dynamical system,

$$\begin{aligned}\dot{u} &= f(x, u, v) = v \\ \dot{v} &= g(x, u, v) = (x+1)u - xv + \sin x.\end{aligned}$$

The system has the same symmetry as the previous example. Quantitative error analysis shows that the errors of the system are 226 and 487 terms for u and v respectively, as

$$E_5^u = \frac{1}{2880}\,(\,g_{xxx} + gg_{xu} + \cdots 226 \text{ terms} \cdots + fg_u{g_v}^2 + g{g_v}^3\,)$$
$$E_5^v = \frac{1}{2880}\,(\,g_{xxxx} + fg_{xxxu} + \cdots 487 \text{ terms} \cdots + fg_u{g_v}^3 + g^4 g_{vvvv}\,).$$

Among them 84 in ${E^u}_5$ and 108 in ${E^v}_5$ terms have $\dot{v}$ as a factor. Therefore if we set $\widetilde{\dot{v}} = g = 0$, 37% and 22% of the terms vanish respectively. These percentages seem too small for us to expect error reduction. This cross-section gives the moving frame $\varepsilon = -e^{-x}((x+1)u - xv + \sin x)$ and the transformation

$$\begin{aligned}\varepsilon \cdot (x, u, v, \dot{v}) &= (\tilde{x}, \tilde{u}, \tilde{v}, \tilde{\dot{v}}) \\ &= (x, -x(u-v) - \sin x,\ -(x+1)(u-v) - \sin x, 0).\end{aligned}$$

However, from the simple analysis of the given equation we observe that $u - v$ converges rapidly to zero while $|u|, |v|$ increase to infinity as time goes on. Therefore we have two additional approximate normalizations $\tilde{u} \approx -\sin x$, $\tilde{v} \approx -\sin x$ under the setting $\widetilde{\dot{v}} = g = 0$. This implies more that 70% of the error terms are transformed to zero or almost zero. Now we obtain the corresponding invariantized RK by substitution at each step,

$$(x_i, u_i, v_i; x_{i+1}, u_{i+1}, v_{i+1}) \mapsto (x_i, u_i - \alpha, v_i - \alpha; x_{i+1}, u_{i+1} - \beta\alpha, v_{i+1} - \beta\alpha).$$

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

Figure 4 shows the results from the RK and the invariantized RKs with the different cross-sections. The one from $\dot{v} = 0$ is the best on the whole, which is also confirmed by the quantitative error analysis.

Adding even one dependent variable greatly raises the complexity and lowers the density of the first derivatives in the errors. If a given system is non-autonomous and of three dependent variables, the invariantizations into one cross-section usually do not make much change. However, this situation can be improved if we can utilize more symmetry transformations of the system. The following example is about an interesting synergy of two symmetry transformations.

Example 3.3. Double invariantization
The system

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

has two symmetry generators

$$X_1 = \sqrt{x}\frac{\partial}{\partial v}, \qquad X_2 = \frac{1}{\sqrt{x}}\frac{\partial}{\partial v}$$

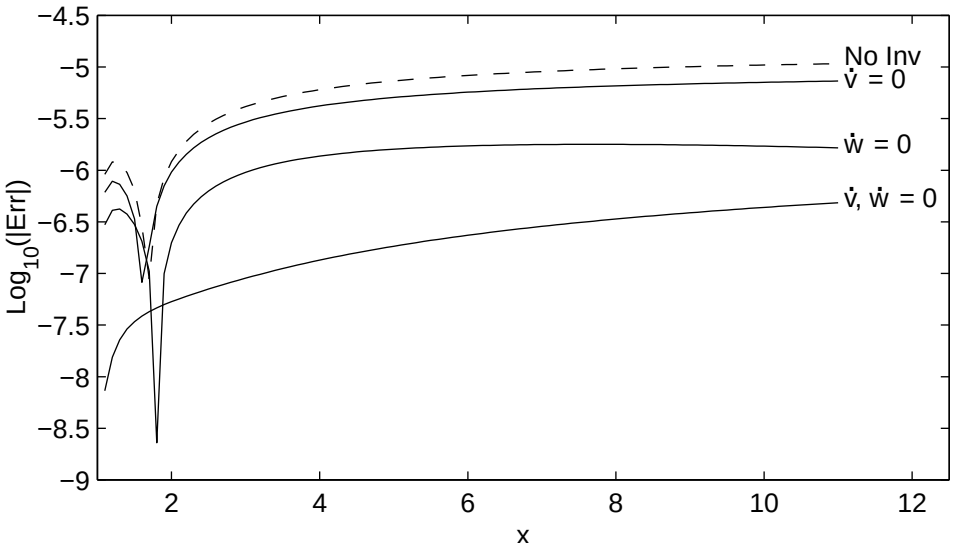

FIGURE 5. The Double Invariantization

and the transformations

$$\varepsilon_1\cdot(x,u,v,w,\dot{w}) = \left(x, u+\varepsilon_1\sqrt{x}, v+\varepsilon_1\frac{1}{2\sqrt{x}}, w-\varepsilon_1\frac{1}{4x\sqrt{x}}, \dot{w}+\varepsilon_1\frac{3}{8x^2\sqrt{x}}\right) \tag{3.1}$$

$$\varepsilon_2\cdot(x,u,v,w,\dot{w}) = \left(x, u+\varepsilon_2\frac{1}{\sqrt{x}}, v-\varepsilon_2\frac{1}{2x\sqrt{x}}, w+\varepsilon_2\frac{3}{4x^2\sqrt{x}}, \dot{w}-\varepsilon_2\frac{15}{8x^3\sqrt{x}}\right). \tag{3.2}$$

Using a symbolic algebra software we can confirm that there are 13,364 terms in the fifth order for each u, v and w in the RK. In this example, since every derivative of u, v is either one or zero, the actual numbers of the terms are are reduced, for example, to 3516 terms in $E^w{}_5$. Suppose we pick $\widetilde{v} = 0$ for a cross-section and the corresponding moving frame $\varepsilon_1 = 4x^2\sqrt{x}w$. This removes 1813 out of 3516 terms in the terms in $E^w{}_5$. The choice of $\widetilde{\dot{w}} = 0$ with the moving frame $\varepsilon_1 = -\frac{8}{3}x^3\sqrt{x}$ works similarly. However, we can build a better transformation by proper combination of the two transformations. Through the successive applications of the two moving frames $\varepsilon_1 = -10x\sqrt{x}w + 4x^2\sqrt{x}\dot{w}$ for (3.1) and $\varepsilon_2 = 2x^2\sqrt{x}w + \frac{4}{3}x^3\sqrt{x}\dot{w}$ for (3.2), every point (x, y) is projected to the intersection of $\widetilde{v} = 0$ and $\widetilde{\dot{w}} = 0$. This implies we invariantize the numerical scheme as

$$(N^{\varepsilon_1})^{\varepsilon_2}(z) = N(\ \varepsilon_2(\varepsilon_1(z)\cdot z)\cdot(\varepsilon_1(z)\cdot z)\ ).$$

This invariantization gets rid of 2916 out of terms from the errors, which is 83% reduction. In Figure 5, one can see the the doubly-invariantized scheme excels other results by far. The initial condition is $y(0) = \dot{y}(0) = -1, \ddot{y}(0) = 1$.

Many geometric integrators, by preserving geometric properties of the solutions, shows the excellent long-term behavior [15, 29]. It turned out that the invatiantization technique also enhance the long term stability of the standard schemes considerably.

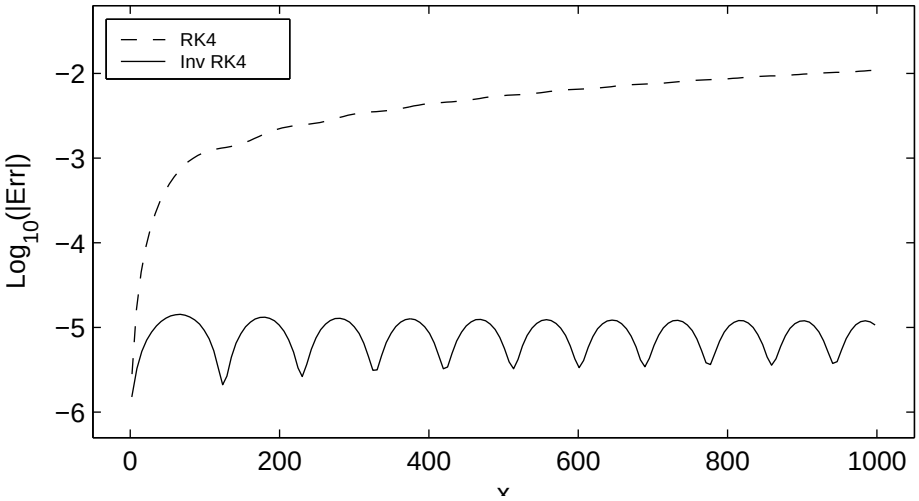

FIGURE 6. Long term integration of harmonic oscillator

Example 3.4. Driven Harmonic oscillator.
The equation

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

describes a driven harmonic oscillator, one of whose examples is the inductor-capacitor circuit. Recall that resonance occurs when $\alpha = 1$. Here we use $\alpha = 0.99$, which yields solutions close to resonance but still bounded. Since this is linear constant-coefficient equation, its symmetry generators are easily found as

$$X_1 = \sin x \frac{\partial}{\partial y}, \qquad X_2 = \cos x \frac{\partial}{\partial y}.$$

As in the previous example, we can doubly invariantize the RK setting $\widetilde{\dot{y}} = 0$ and $\widetilde{\ddot{y}} = 0$. Time interval $h = 0.1$ is used up to $x = 1000$. Figure 8 shows that the invariantized scheme produces much better results in the long term-integration. Since the errors oscillate fast around zero with varying amplitudes, we only compare their amplitudes as representative values in the figure. On the contrary to the standard scheme case, 10,000 repetition of applications hardly ruins the quality of the solution of the invariantized scheme.

From the above four examples of the invariantized RKs, it should be noted that this invariantization does not change the number of the stages of the RK, although construction of moving frames often needs computation of the first stage of the RK. Once the RK is invariantized by moving frames, the first stage of the transformed RK is to be zero and therefore the total number of the stages remains the same.

4. Comparison with Other Geometric Integrators

Several types of Lie-symmetric integrators have been developed as mentioned in the introduction, 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. First, we study how symmetry reduction affects the performances of the

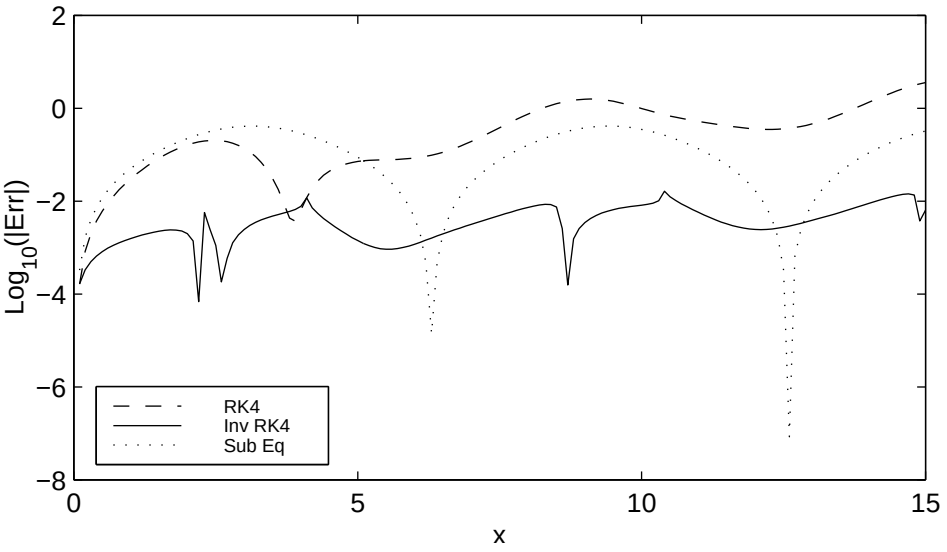

FIGURE 7. Comparison with Symmetry Reduction in $\dot{y} = \sin x\, y + \cos x$.

numerical schemes in comparison to invariantization. Both of them are the same in that they use a symmetry structure of a given differential equation, but symmetry reduction is a global substitution while invariantization is a local one.

Example 4.1. Comparison with symmetry reduction.
Consider the equation

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

This has symmetry generators $X = e^{-\cos x}\frac{\partial}{\partial y}$, which suggests the substitution $u = e^{\cos x}y$. The substituted equation is

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

This equation is simpler than the original one in the view of the number of variables that appear on the right hand side. It is interesting to see the difference of the performances between the RK and the invariantized RK on the original equations, and the RK on the substituted equation. In Figure 7 we can see the invariantized RK works better than both of the RK on the original equation and substituted equation. In the long term, the error of the invariantized RK is observed to slowly rise and converge to that of the RK on substituted one.

It is certain that substitution by the symmetry group does not actually guarantee simpler equations. For the linear equations $\ddot{y} + x\,\dot{y} - (x+1)y = \sin x$ in Example 3.2, the substitution leads to a more complicated one even with the reduction of variables. Refer to Figure 8.

The symplectic integrator is one of the most successful geometric integrators for ODEs[15]. The popularity of a symplectic integrator stems from its area-preservation, time-reversibility and energy conservation in a time-independent Hamiltonian systems. Many of symplectic integrators have been developed based on the RK method. Even though the invariantization method does not use Hamiltonian structure directly, it is interesting to compare two methods as geometric integrators.

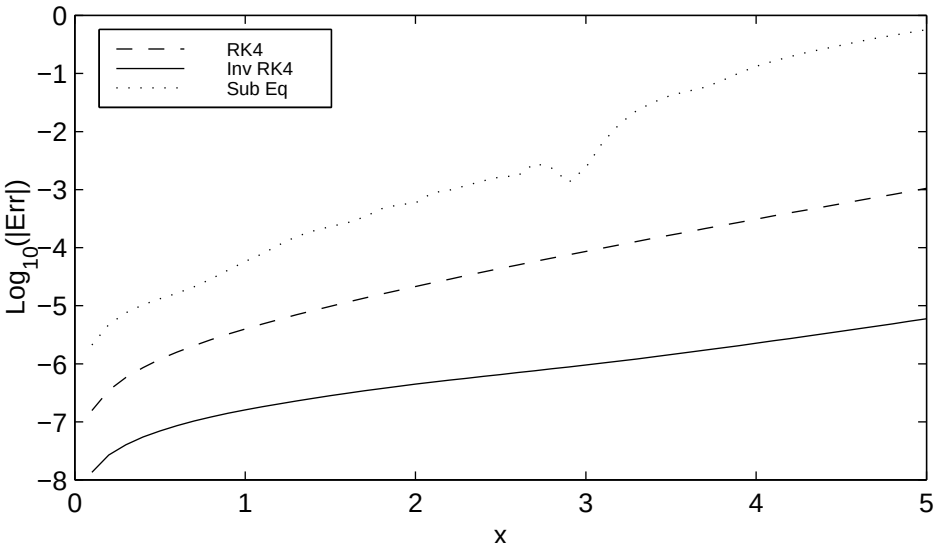

FIGURE 8. Comparison with Symmetry Reduction in $\ddot{y} + x\,\dot{y} - (x+1)y = \sin x$

Example 4.2. Comparison with symplectic integrators.
Suppose we have the Hamiltonian,

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

which leads to the system

$$\begin{aligned} \dot{p} &= -H_q = q^{-3} \\ \dot{q} &= H_p = p. \end{aligned} \tag{4.1}$$

It has an exact solution $q = \pm\sqrt{C_1x^2 + 2C_1C_2x + C_1{C_2}^2 + C_1^{-1}}$ for arbitrary C_1, C_2. The system admits the symmetry groups,

$$\begin{aligned} X_1 &= \frac{\partial}{\partial x} \\ X_2 &= x^2\frac{\partial}{\partial x} + xq\frac{\partial}{\partial q} + (q - xp)\frac{\partial}{\partial p} \end{aligned}$$

and the corresponding transformations,

$$\begin{aligned} \varepsilon_1 \cdot (x,q,p) &= (x + \varepsilon_1, q, p) \\ \varepsilon_2 \cdot (x,q,p) &= (\frac{x}{1-\varepsilon_2 x}, \frac{q}{1-\varepsilon_2 x}, p + \varepsilon_2(q - xp)) \end{aligned}$$

as in Example 2.3. We take the cross-section $x = \frac{1}{2}(2 - h + \sqrt{h^2+4})$ and $p = 0$. The first equation is just for fixing the step size at h to avoid confusion in the error analysis. In fact, the transformation of independent variables provides wider choices of the invariantization, which will be dealt in detail in future studies. The numerical scheme is now invariantized

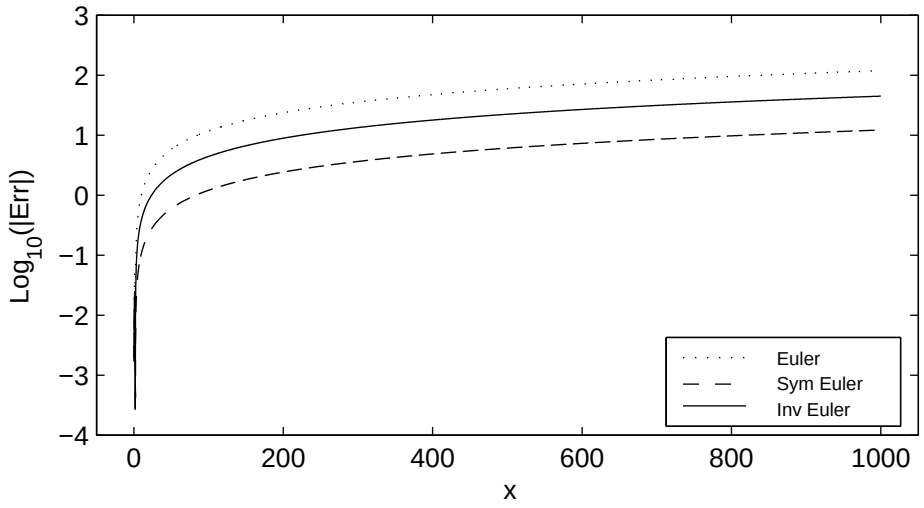

FIGURE 9. Comparison with Symplectic integrator at the first order

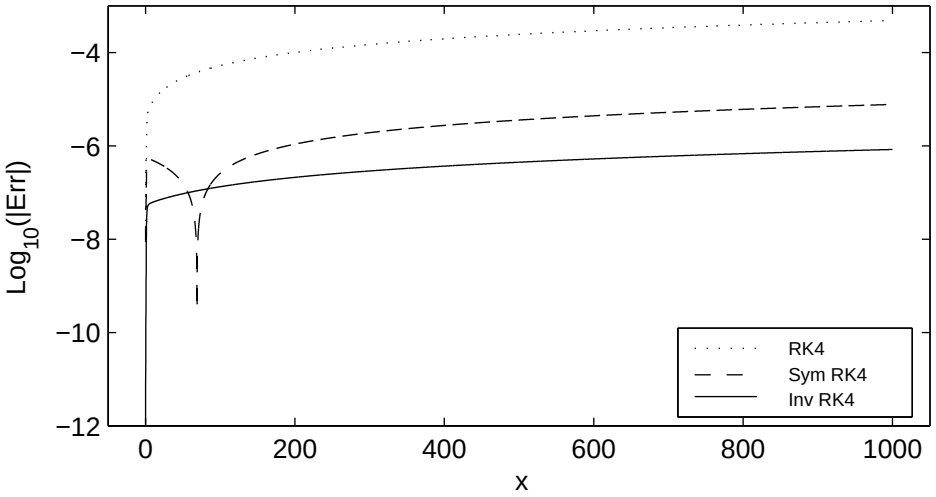

FIGURE 10. Comparison with Symplectic integrator at the fourth order

by the composite of the moving frames $\varepsilon_2 \circ \varepsilon_1$ with

$$\varepsilon_1 = -x + \frac{1}{2}(2 - h + \sqrt{h^2 + 4})$$
$$\varepsilon_2 = \frac{p}{xp - q}.$$

We compare the schemes at the first order (the Euler method) and the fourth (the RK). Even though there is no known explicit symplectic method of the order greater than two for the general Hamiltonian system, many explicit symplectic RKs have been introduced for separable Hamiltonian systems like (4.1). Here we use the symplectic fourth-order RK developed in [7, 13]. The initial condition $q(0) = \sqrt{2}, p(0) = -\frac{1}{\sqrt{2}}$, and the step size $h = 0.05$ are used. Figure 9 compares the errors in the standard method, the symplectic

method and the invariantized one in the long term. Although the invariantized Euler is better than the Euler, it is still behind the symplectic Euler.

This situation changes dramatically when we move on to higher order methods, and the invariantized RK4 excels other two methods as in Figure 10. While the method using the symplectic structure brings almost the same improvement as in the Euler method, the invariantization works much better for the higher order method. The growing dependency of the error terms on the first derivative is responsible for this result.

5. Conclusions

In this paper, we have investigated that the technique of invariantization of numerical schemes for ordinary differential equations. In the practical sense, the procedure of the invariantization is a local substitution at each step in the existing numerical algorithms. Through moving frames one can use the symmetry group of the differential equations to improve the computational performance of the numerical schemes. Our work in this paper suggests that the future study on invariant schemes should focus on implementation in close relation to error reduction.

Beyond the fact that the invariantization method requires only small modification to existing numerical schemes, another appealing point is its generality. Even though 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 based on finite difference schemes such as multi-step methods or numerical methods for for PDEs.

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