Geometric Integration via Multi-space

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August 20, 2004

Abstract

We outline a general construction of symmetry-preserving numerical schemes for ordinary differential equations. The method of invariantization is based on the equivariant moving frame theory applied to prolonged symmetry group actions on multi-space, which has been proposed as the proper geometric setting for numerical analysis. We explain how to invariantize standard numerical integrators such as the Euler and Runge–Kutta schemes. In favorable situations, the resulting symmetry-preserving geometric integrators offer significant advantages.

1 Introduction.

In modern numerical analysis, the development of schemes that incorporate additional structure enjoyed by the problem being approximated has become become increasingly active in recent years, [14]. The class of geometric numerical methods include symplectic integrators, [8], energy conserving methods, [18], and Lie group methods, [15, 17]. The focus of this paper is on symmetry-preserving numerical approximation schemes for differential equations, as developed by Shokin, [24], Dorodnitsyn, [11], Axford and Jaegers, [16], and Budd and Collins, [3], and others.

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Supported in part by NSF Grant DMS 01–03944

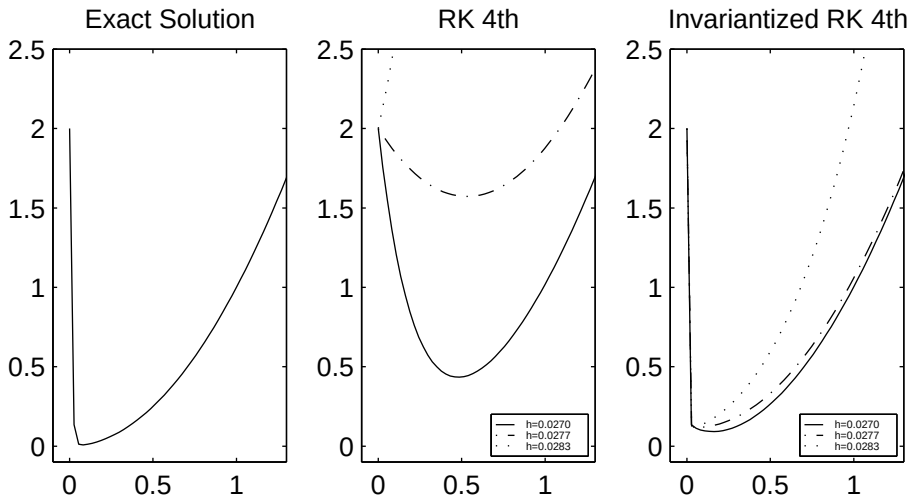

Figure 1: The equation $y' + 100y = 100x^2 + 2x$

In [22], the second author proposed a new foundation for geometric numerical analysis, called multi-space. A direct implementation of the equivariant moving frame algorithms, [12, 21], in multi-space leads to the systematic construction of invariant numerical approximations to differential invariants and invariant differential equations. As we demonstrate here, the invariantization process based on the moving frame can be applied to numerical integration schemes for ordinary differential equations. Invariantized numerical algorithms based on symmetry groups of the differential equation can greatly reduce the numerical error. Figure 1 shows how the performance of the Runge–Kutta method is improved through invariantization by the symmetry group of an elementary first order equation; additional examples can be found in the final section of the paper.

Instead of pursuing the exact symmetry group for a difference equation, we start from the fact that the continuous symmetry group of a given differential equation also applies to its numerical scheme roughly. In practice, the symmetry groups of a differential equation are found by the usual Lie infinitesimal prolongation algorithm, [20]. For the moving frame procedure, one must determine the corresponding finite group transformations by exponentiating the infinitesimal generators. We will not dwell on the determination of symmetry groups, but will concentrate on their application to geometric numerical integration of the underlying differential equation.

2 Geometry of Numerical Methods.

In this section, we outline the basic construction of multi-space for curves, which correspond to functions of a single independent variable, and hence satisfy ordinary differential equations. The more difficult case of higher dimensional submanifolds, corresponding to functions of several variables that satisfy partial differential equations, remains to be completely developed; the proposed construction requires a new approach to multi-dimensional interpolation theory, [23].

Let M be an m-dimensional manifold M; in all examples, $M = \mathbb{R}^m$ is ordinary Euclidean space. Let $\pi\colon \mathrm{J}^n \to M$ denote the n–th order jet space for curves $C \subset M$, defined as the space of equivalence classes of curves under the equivalence relation of n–th order contact at a single point. We let $\mathrm{j}_n C|_z$ denote the n-jet or equivalence class of the curve C at the point $z \in C$.

If we introduce local coordinates $z = (x, y) = (x, y^1, \dots, y^q)$, where $q = m-1$, then a curve $C = \{y = f(x)\}$ defined by a smooth function $f\colon I \to M$ defined on an interval $I \subset \mathbb{R}$ will be called a *graph*. The corresponding jet coordinates of $\mathrm{j}_n C|_z$ at $z = (x, f(x)) \in C$ are the value of x and all the derivatives $y_i^{(k)} = f_i^{(k)}(x)$ for $i = 1, \dots, q$, $k = 0, 1, 2, \dots, n$.

Numerical finite difference approximations to the derivatives of a function $y = f(x)$ rely on its values $y_0 = f(x_0), \dots, y_n = f(x_n)$ at several distinct points $z_i = (x_i, y_i) = (x_i, f(x_i))$ on the curve. Thus, discrete approximations to jet coordinates on J^n are functions $F(z_0, \dots, z_n)$ defined on the *joint space*

$$M^{\diamond(n+1)} = \{\, (z_0, \dots, z_n) \mid \ z_i \neq z_j \text{ for all } i \neq j \,\} \subset M^{\times(n+1)}$$

which is the off-diagonal part of the Cartesian product consisting of all distinct $(n+1)$-tuples of points in M. As the points come together, the limiting value of $F(z_0, \dots, z_n)$ will be governed by the derivatives of the appropriate order governing the direction of convergence, i.e., the jet of the curve at the point of coalescence. Our goal is to construct a space that incorporates both the jet space J^n and the joint space $M^{\diamond(n+1)}$ in a consistent manner.

Definition 1 An $(n+1)$-*pointed manifold* is an object $\mathbf{M} = (z_0, \dots, z_n; M)$ consisting of a smooth manifold M and $n+1$ not necessarily distinct points $z_0, \dots, z_n \in M$.

Let $\mathcal{C}^{(n)}$ denote the set of all $(n+1)$-pointed curves $\mathbf{C} = (z_0, \dots, z_n; C)$ contained in M. We define an equivalence relation on $\mathcal{C}^{(n)}$ that generalizes the jet equivalence relation of n–th order contact at a single point.

Definition 2 Two $(n+1)$-pointed curves

$$\mathbf{C} = (z_0, \dots, z_n; C), \qquad \widetilde{\mathbf{C}} = (\widetilde{z}_0, \dots, \widetilde{z}_n; \widetilde{C}),$$

have *n–th order multi-contact* if and only if

$$z_i = \widetilde{z}_i, \quad \text{and} \quad \mathrm{j}_{\#i-1} C|_{z_i} = \mathrm{j}_{\#i-1} \widetilde{C}|_{z_i}, \quad \text{for each} \quad i = 0, \dots, n,$$

where $\#i = \#\{\, j \,|\, z_j = z_i \,\}$ denotes the number of points which coincide with the i–th one.

The n–th order *multi-space*, denoted $M^{(n)}$ is the set of equivalence classes of $(n+1)$-pointed curves in M under the equivalence relation of n–th order multi-contact. The equivalence class of an $(n+1)$-pointed curves $\mathbf{C}$ is called its n–th order *multi-jet*, and denoted $\mathbf{j}_n\mathbf{C} \in M^{(n)}$.

In particular, if the points on $\mathbf{C} = (z_0, \dots, z_n; C)$ are all distinct, then $\mathbf{j}_n\mathbf{C} = \mathbf{j}_n\widetilde{\mathbf{C}}$ if and only if $z_i = \widetilde{z}_i$ for all i, which means that $\mathbf{C}$ and $\widetilde{\mathbf{C}}$ have all $n+1$ points in common. Therefore, we can identify the subset of multi-jets of multi-pointed curves having distinct points with the off-diagonal Cartesian product space $M^{\diamond(n+1)} \subset \mathrm{J}^n$. On the other hand, if all $n+1$ points coincide, $z_0 = \dots = z_n$, then $\mathbf{j}_n\mathbf{C} = \mathbf{j}_n\widetilde{\mathbf{C}}$ if and only if $\mathbf{C}$ and $\widetilde{\mathbf{C}}$ have n–th order contact at their common point $z_0 = \widetilde{z}_0$. Therefore, the multi-space equivalence relation reduces to the ordinary jet space equivalence relation on the set of coincident multi-pointed curves, and in this way $\mathrm{J}^n \subset M^{(n)}$. These two extremes do not exhaust the possibilities, since one can have some but not all points coincide. Intermediate cases correspond to *multi-jet spaces*

$$\begin{aligned} &\mathrm{J}^{k_1} \diamond \cdots \diamond \mathrm{J}^{k_i} \\ &\qquad \equiv \Big\{ (z_0^{(k_1)}, \dots, z_i^{(k_i)}) \in \mathrm{J}^{k_1} \times \cdots \times \mathrm{J}^{k_i} \,\Big|\, z_\nu = \pi(z_\nu^{(k_\nu)}) \text{ are distinct} \Big\}, \end{aligned} \tag{1}$$

where $\sum k_\nu = n$; see [10, 22] for details.

Theorem 3 *If M is a smooth m-dimensional manifold, then its n–th order multi-space $M^{(n)}$ is a smooth manifold of dimension $(n+1)m$, which contains the joint space $M^{\diamond(n+1)}$ as an open, dense submanifold, and the n–th order jet space J^n as a smooth submanifold.*

Just as the local coordinates on J^n are provided by the coefficients of Taylor polynomials, the local coordinates on $M^{(n)}$ are provided by the coefficients of

interpolating polynomials, and are most conveniently written in terms of the classical divided differences of numerical interpolation theory, [9]. In terms of the local coordinates on M, an $(n+1)$-*pointed graph* consists of the graph of a smooth function $y = f(x)$ together with $(n+1)$ points $z_i = (x_i, f(x_i))$ thereon. Again, it is worth emphasizing that we allow some or all of the *mesh points* $x_0, \dots, x_n \in \mathbf{R}$ to coincide. The multi-jets of $(n+1)$-pointed graphs will form an open, dense submanifold $M^{(n)}_\Gamma \subset M^{(n)}$. The missing part $M^{(n)} \setminus M^{(n)}_\Gamma$ consists of multi-jets of $(n+1)$-pointed curves with either vertical tangents at repeated points, or having two or more distinct points lying on the same vertical line $\{x = c\}$.

We define the classical *divided differences* $[\, z_0 z_1 \dots z_k \,]$ by the standard recursive rule, namely $[\, z_j \,] = y_j$ and

$$[\, z_0 z_1 \dots z_{k-1} z_k \,] = \frac{[\, z_0 z_1 z_2 \dots z_{k-2} z_k \,] - [\, z_0 z_1 z_2 \dots z_{k-2} z_{k-1} \,]}{x_k - x_{k-1}} \,. \tag{2}$$

The divided differences are well-defined provided no two points lie on the same vertical line.

Remark: The more usual divided difference notation $[\, y_0 y_1 \dots y_k \,]$ is ambiguous since it assumes that the mesh $x_0, \dots, x_n$ is fixed throughout. Because we are regarding the independent and dependent variables on the same footing — and, indeed, are allowing changes of variables that mix up the two — it is important to adopt an unambiguous divided difference notation here.

Divided differences are initially defined only for distinct points z_k. Requiring the points to lie on a smooth curve (graph) allows us to extend the definitions to cases when two or more points are coincident. To emphasize that the resulting "confluent divided differences" depend on the underlying curve (or function) we sometimes write $[\, z_0 z_1 \dots z_k \,]_C$ instead of $[\, z_0 z_1 \dots z_k \,]$.

Definition 4 Given an $(n+1)$-pointed graph $\mathbf{C} = (z_0, \dots, z_n; C)$, its divided differences are defined by $[\, z_j \,]_C = f(x_j)$, and

$$[\, z_0 z_1 \dots z_{k-1} z_k \,]_C = \lim_{z \to z_k} \frac{[\, z_0 z_1 z_2 \dots z_{k-2} z \,]_C - [\, z_0 z_1 z_2 \dots z_{k-2} z_{k-1} \,]_C}{x - x_{k-1}}. \tag{3}$$

When taking the limit, the point $z = (x, f(x))$ must lie on the curve C, and take limiting values $x \to x_k$ and $f(x) \to f(x_k)$.

In the non-confluent case $z_k \neq z_{k-1}$ we can replace z by z_k directly in the difference quotient (3) and so ignore the limit. On the other hand, when all $k+1$ points coincide, the k–th order confluent divided difference converges to

$$[\, z_0 \dots z_0 \,] = \frac{f^{(k)}(x_0)}{k!}\,. \tag{4}$$

The classical Newton interpolation formula, [9], can be stated as follows.

Lemma 5 *Let $x_0, \dots, x_n \in \mathbf{R}$ be mesh points, and let $a_0, \dots, a_n \in \mathbf{R}^q$. Define the $(n+1)$-pointed graph $\mathbf{C} = (z_0, \dots, z_n; C)$ where C denotes the graph of the polynomial*

$$\begin{aligned} p_n(x) = a_0 + a_1\,(x - x_0) + a_2\,(x - x_0)(x - x_1) + \cdots \\ + a_n\,(x - x_0)(x - x_1)\cdots(x - x_{n-1}), \end{aligned} \tag{5}$$

and $z_k = (x_k, p_n(x_k)) \in C$ for $k = 0, \dots, n$. Then the divided differences for $\mathbf{C}$ are equal to

$$[\, z_0 z_1 \dots z_k \,]_C = a_k, \qquad k = 0, \dots, n. \tag{6}$$

Theorem 6 *Two $(n+1)$-pointed graphs $\mathbf{C}, \widetilde{\mathbf{C}}$ have n–th order multi-contact if and only if they have the same divided differences:*

$$[\, z_0 z_1 \dots z_k \,]_C = [\, z_0 z_1 \dots z_k \,]_{\widetilde{C}}, \qquad k = 0, \dots, n.$$

In particular, $\widetilde{\mathbf{C}} = (z_0, \dots, z_n; \widetilde{C})$ will have n–th order multi-contact with the polynomial curve given by (5) if and only if $\widetilde{C}$ is the graph of a function of the form

$$y = f(x) = p_n(x) + (x - x_0)(x - x_1)\cdots(x - x_n)\,h(x), \tag{7}$$

where $h(x)$ is smooth.

Local coordinates on the multi-graph subset $M^{(n)}_\Gamma \subset M^{(n)}$ consist of the independent variables along with all the divided differences

$$\begin{aligned} x_0, \dots, x_n, \qquad & y^{(0)} = y_0 = [\, z_0 \,]_C, \quad y^{(1)} = [\, z_0 z_1 \,]_C, \\ & y^{(2)} = 2\,[\, z_0 z_1 z_2 \,]_C, \quad \dots \quad y^{(n)} = n!\,[\, z_0 z_1 \dots z_n \,]_C, \end{aligned} \tag{8}$$

prescribed by $(n+1)$-pointed graphs $\mathbf{C} = (z_0, \dots, z_n; C)$. The $n!$ factor is included so that $y^{(n)}$ agrees with the derivative coordinate when restricted

to J^n, cf. (4). The proof that the change of divided difference coordinates is smooth on the overlap of coordinate charts proceeds indirectly; see [22] for details.

A smooth function $\Delta\colon \mathrm{J}^n \to \mathbf{R}$ on (an open subset of) the jet space, written $\Delta(x, y, \dots, y^{(n)})$, is known as a *differential function*. These include individual derivatives, as well as more complicated combinations such as the the Euclidean curvature and torsion, general differential invariants, etc. Any system of differential equations (or, even more generally, a system of differential algebraic equations) is (locally) defined by the vanishing of one or more differential functions:

$$\Delta_1(x, y^{(n)}) = \cdots = \Delta_k(x, y^{(n)}) = 0. \tag{9}$$

To implement a numerical solution to the system (9) by finite difference methods, one relies on suitable discrete approximations to each of its defining differential functions Δ_ν, and this requires extending the differential functions from the jet space to the associated multi-space, in accordance with the following definition.

Definition 7 Let M be a Riemannian manifold with metric $\|\cdot\|$. Suppose $N \subset M$ is a closed submanifold and $H\colon N \to \mathbf{R}$ a smooth function on N. We call $F\colon M \to \mathbf{R}$ a *k–th order extension* of H if for each compact $K \subset M$ there exists a constant $C > 0$ so that

$$| F(x_1) - H(x_2) | \le C \, \| x_1 - x_2 \|^k, \qquad x_1 \in K, \tag{10}$$

where $x_2 \in N$ is the closest point on N to x_1.

Definition 8 An *$(n+1)$-point numerical approximation of order k* to a differential function $\Delta\colon \mathrm{J}^n \to \mathbf{R}$ is a k–th order extension $N_\Delta\colon M^{(n)} \to \mathbf{R}$ of Δ to multi-space, based on the inclusion $\mathrm{J}^n \subset M^{(n)}$.

Let us convince the reader that Definition 8 is a legitimate geometric reformulation of standard numerical approximation ideas. The simplest illustration of Definition 8 is provided by the divided difference coordinates (8). Each divided difference $y^{(n)}$ forms an $(n+1)$-point numerical approximation to the n–th order derivative coordinate on J^n. The order of the approximation is $k = 1$. More generally, any differential function $\Delta(x, y, y^{(1)}, \dots y^{(n)})$ can immediately be given an $(n+1)$-point numerical approximation $N_\Delta = \Delta(x_0, y^{(0)}, y^{(1)}, \dots y^{(n)})$ by replacing each derivative by a k–th order divided difference approximation.

3 Invariantization.

The equivariant approach to moving frames developed in [12, 21] provides a general procedure for *invariantizing* functions, forms, tensors, differential operators, algorithms, etc. for completely general group actions. Our goal is to use invariantization to algorithmically construct invariant numerical approximations to differential invariants and invariant differential equations.

Definition 9 Given an r–dimensional Lie group G acting smoothly on a manifold M, a *moving frame* is a smooth, G-equivariant map $\rho\colon M \to G$.

The group G acts on itself by left or right multiplication. Classical moving frames, [7, 13], which are all included in this general definition, rely on the left action, but, in practice, the right versions are often easier to compute, and will be the version of choice here. Right-equivariance requires

$$\rho(g \cdot z) = \rho(z) \cdot g^{-1} \qquad \text{for all} \qquad z \in M, \quad g \in G.$$

The classical left-equivariant moving frame $\widetilde{\rho}(z) = \rho(z)^{-1}$ may be simply obtained by applying the group inversion.

Theorem 10 *A moving frame exists in a neighborhood of a point $z \in M$ if and only if G acts freely and regularly near z.*

Freeness requires that every point $z \in M$ has trivial isotropy, meaning $g \cdot z = z$ if and only if $g = e$, and so the group orbits are all of dimension $r = \dim G$. Regularity requires that the orbits form a regular foliation; see [12] for details.

The practical implementation of the moving frame construction is based on Cartan's method of *normalization*, [7, 12], which relies on the choice of a (local) 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.

Theorem 11 *If G acts freely, regularly on M, and $\mathcal{K} \subset M$ is a cross-section to the group orbits, then the map $\rho\colon M \to G$ that sends $z \in M$ to the unique group element $g = \rho(z)$ that maps z to the cross-section, $g \cdot z = \rho(z) \cdot z \in \mathcal{K}$, defines a right moving frame.*

One usually chooses a local coordinate cross-section

$$\mathcal{K} = \{\, z_1 = c_1, \dots, z_r = c_r \},$$

where the first r, say, of the coordinates $z = (z_1, \dots, z_m)$ on M are set equal to suitably chosen constants. If we write out the local coordinate formulae $\widetilde{z} = w(g, z) = g \cdot z$ for the group transformations, then the corresponding right moving frame $g = \rho(z)$ is obtained by solving the *normalization equations*

$$w_1(g, z) = c_1, \qquad \dots \qquad w_r(g, z) = c_r, \tag{11}$$

for the group parameters $g = (g_1, \dots, g_r)$ in terms of $z = (z_1, \dots, z_m)$. When we substitute the moving frame expressions $g = \rho(z)$ into the transformation formulae, the resulting functions $I_\nu(z) = w_\nu(\rho(z), z)$ are easily seen to be G-invariant. The first r coincide with the normalization constants, $I_1(z) = c_1, \dots, I_r(z) = c_r$, while the remaining $m-r$ provide a system of fundamental invariants for the group action.

Theorem 12 *If $g = \rho(z)$ is the moving frame solution to the normalization equations* (11)*, then $I_{r+1}(z) = w_{r+1}(\rho(z), z), \dots, I_m(z) = w_m(\rho(z), z)$ form a complete system of functionally independent invariants for the group action.*

The moving frame construction includes an added bonus — a canonical way to associate an invariant with any function.

Definition 13 The *invariantization* of a scalar function $F\colon M \to \mathbf{R}$ with respect to a right moving frame ρ is the the invariant function $I = \iota(F)$ defined by $I(z) = F(\rho(z) \cdot z)$.

In other words, given a function $F(z_1, \dots, z_m)$, its invariantization is the invariant function $\iota(F) = F(I_1, \dots, I_m) = F(c_1, \dots, c_r, I_{r+1}(z), \dots, I_m)$. Geometrically, invariantization amounts to restricting the function to the cross-section and then requiring that the induced invariant be constant along the group orbits. In particular, if $I(z)$ is an invariant, then $\iota(I) = I$. Therefore, invariantization defines a canonical projection, depending on the moving frame, from functions to invariants.

Example 14 Let G be the one-parameter Lie group acting on $\mathbf{R}^3$ as

$$(x_1, x_2, x_3) \quad \longmapsto \quad \left(x_1, \, \frac{x_2}{1 - \varepsilon e^{-x_1} x_2}, \, \frac{x_3 - \varepsilon e^{-x_1} {x_2}^2}{(1 - \varepsilon e^{-x_1} x_2)^2} \right) .$$

Choosing the cross-section $\widetilde{x}_3 = 0$ and solving for the group parameter ε gives the moving frame

$$\varepsilon = \rho(x_1, x_2, x_3) = \frac{x_3 e^{x_1}}{x_2^2}.$$

The resulting fundamental invariants are

$$(I_1, I_2, I_3) = \rho(x_1, x_2, x_3) \cdot (x_1, x_2, x_3) = \left(x_1, \, \frac{{x_2}^2}{x_2 - x_3}, \, 0 \right).$$

Invariantization of a function $F(x_1, x_2, x_3)$ is then given by

$$\iota[\, F(x_1, x_2, x_3) \,] = F(I_1, I_2, I_3) = F\left(x_1, \, \frac{{x_2}^2}{x_2 - x_3}, \, 0 \right).$$

4 Multi-Invariants.

Let G be an r-dimensional Lie group which acts smoothly on M. Since G evidently maps multi-pointed curves to multi-pointed curves while preserving the multi-contact equivalence relation, there is an induced action on the multi-space $M^{(n)}$ called its n–th *multi-prolongation* and denoted by $G^{(n)}$. On the jet subset $\mathrm{J}^n \subset M^{(n)}$ the multi-prolonged action reduced to the usual jet space prolongation of our transformation group, [20]. On the other hand, on the off-diagonal part $M^{\diamond(n+1)} \subset M^{(n)}$ the action coincides with the $(n+1)$-fold Cartesian product action of G on $M^{\times(n+1)}$, [21].

Recall that a *differential invariant* is a function $I\colon \mathrm{J}^n \to \mathbf{R}$ which is invariant under the prolonged action of G on the jet space J^n. Similarly, a *joint invariant* is a function $J\colon M^{\times(n+1)} \to \mathbf{R}$ on the Cartesian product space which is invariant under the product action of G, cf. [21]. In this vein, we define a *multi-invariant* to be a function $K\colon M^{(n)} \to \mathbf{R}$ on multi-space which is invariant under the multi-prolonged action of $G^{(n)}$. The restriction of a multi-invariant K to jet space will be a differential invariant, $I = K \,|\, \mathrm{J}^n$, while restriction to the joint space $M^{\diamond(n+1)}$ will define a joint invariant $J = K \,|\, M^{\diamond(n+1)}$. Smoothness of K will imply that the joint invariant J is an *invariant numerical approximation to the differential invariant* I. Moreover, every invariant finite difference numerical approximation to the differential invariant I arises in this manner. Thus, the theory of multi-invariants *is* the theory of invariant numerical approximations! The basic

idea of replacing differential invariants by joint invariants forms the foundation of Dorodnitsyn's approach to invariant numerical algorithms, [11], and also the invariant numerical approximations of differential invariant signatures in computer vision, [2, 5, 6, 21]. Furthermore, the restriction of a multi-invariant to any intermediate multi-jet subspace, as in (1), will define a joint differential invariant, [21] — also known as a semi-differential invariant in the computer vision literature, [10, 19]. Thus, multi-invariants also include invariant semi-differential approximations to differential invariants as well as joint invariant numerical approximations to differential invariants and semi-differential invariants — all in one seamless geometric framework.

Multi-invariants can be systematically constructed by applying the moving frame method to the multi-prolonged group action. Any equivariant *multi-frame* $\rho^{(n)}\colon M^{(n)} \to G$ will evidently restrict to a classical moving frame $\rho^{(n)}\colon \mathrm{J}^n \to G$ on the jet space along with a compatible product frame $\rho^{\diamond(n+1)}\colon M^{\diamond(n+1)} \to G$. In local coordinates, we use $\widetilde{z}_k = (\widetilde{x}_k, \widetilde{y}_k) = g\cdot z_k$ to denote the transformation formulae for the individual points on a multi-pointed curve. The multi-prolonged action on the divided difference coordinates gives

$$\begin{aligned} \widetilde{x}_0, \dots, \widetilde{x}_n, \qquad & \widetilde{y}^{(0)} = \widetilde{y}_0 = [\,\widetilde{z}_0\,], \qquad \widetilde{y}^{(1)} = [\,\widetilde{z}_0\widetilde{z}_1\,], \\ & \widetilde{y}^{(2)} = 2\,[\,\widetilde{z}_0\widetilde{z}_1\widetilde{z}_2\,], \qquad \dots \qquad \widetilde{y}^{(n)} = n!\,[\,\widetilde{z}_0, \dots, \widetilde{z}_n\,], \end{aligned} \tag{12}$$

where the prolongation formulae are most easily computed via the difference quotients

$$[\,\widetilde{z}_0\widetilde{z}_1\dots\widetilde{z}_{k-1}\widetilde{z}_k\,] = \frac{[\,\widetilde{z}_0\widetilde{z}_1\widetilde{z}_2\dots\widetilde{z}_{k-2}\widetilde{z}_k\,] - [\,\widetilde{z}_0\widetilde{z}_1\widetilde{z}_2\dots\widetilde{z}_{k-2}\widetilde{z}_{k-1}\,]}{\widetilde{x}_k - \widetilde{x}_{k-1}}\,, \tag{13}$$

with $[\,\widetilde{z}_j\,] = \widetilde{y}_j$, and then taking appropriate limits to cover the case of coalescing points.

To compute a multi-frame, we need to normalize by choosing a cross-section to the group orbits in $M^{(n)}$, which amounts to setting $r = \dim G$ of the transformed divided difference coordinates (12) equal to suitably chosen constants. An important observation is that in order to obtain the limiting differential invariants, we must require our local cross-section to pass through the jet space, and define, by intersection, a cross-section for the prolonged action on J^n. This compatibility constraint implies that we are only allowed to normalize the first lifted independent variable $\widetilde{x}_0 = c_0$. If we try to normalize $\widetilde{x}_1$ then we must either set $\widetilde{x}_1 = c_0 = \widetilde{x}_0$, and the cross-section would only be valid for coincident points $\widetilde{z}_1 = \widetilde{z}_0$ which would prevent us from extending

it to the non-coincident case required for constructing invariant numerical approximations, or set $\widetilde{x}_1 = c_1 \neq c_0$, and this would prevent the points $\widetilde{z}_0$ and $\widetilde{z}_1$ from coalescing, so our moving frame could not be restricted to the jet subspace.

With the aid of the multi-frame, the most direct construction of the requisite multi-invariants and associated invariant numerical differentiation formulae is through the invariantization of the original finite difference quotients (2). Substituting the multi-frame formulae for the group parameters into the lifted coordinates (12) provides a complete system of multi-invariants on $M^{(n)}$; this follows immediately from Theorem 12. We denote the fundamental multi-invariants by

$$H_i = \iota(x_i), \qquad\qquad K^{(n)} = \iota(y^{(n)}), \tag{14}$$

where ι denotes the invariantization map associated with the multi-frame. The fundamental differential invariants for the prolonged action of G on J^n can all be obtained by restriction, so that $I^{(n)} = K^{(n)} \,|\, \mathrm{J}^n$. On the jet space, the points are coincident, and so the multi-invariants H_i will all restrict to the *same* differential invariant $c_0 = H = H_i \,|\, \mathrm{J}^n$ — the normalization value of $\widetilde{x}_0$. On the other hand, the fundamental joint invariants on $M^{\diamond(n+1)}$ are obtained by restricting the multi-invariants $H_i = \iota(x_i)$ and $K_i = \iota(y_i)$. The multi-invariants can computed by using a multi-invariant divided difference recursion

$$\begin{aligned} &[\, I_j \,] = K_j = \iota(y_j), \\ &[\, I_0 \dots I_k \,] = \iota(\, [\, z_0 z_1 \dots z_k \,] \,) = \frac{[\, I_0 \dots I_{k-2} I_k \,] - [\, I_0 \dots I_{k-2} I_{k-1} \,]}{H_k - H_{k-1}}, \end{aligned} \tag{15}$$

and then relying on continuity to extend the formulae to coincident points. The multi-invariants

$$K^{(n)} = n! \, [\, I_0 \dots I_n \,] = \iota(\, y^{(n)} \,) \tag{16}$$

define the fundamental first order invariant numerical approximations to the differential invariants $I^{(n)}$.

Given a G-invariant differential equation

$$\Delta(x, y, \dots . y^{(n)}) = 0, \tag{17}$$

we can invariantize the left hand side to rewrite the differential equation in terms of the fundamental differential invariants:

$$\iota(\Delta(x, y, \dots . y^{(n)})) = \Delta(H_0, I^{(0)}, \dots, I^{(n)}) = 0.$$

The invariant finite difference approximation to the differential equation is then obtained by replacing the differential invariants $I^{(k)}$ by their multi-invariant counterparts $K^{(k)}$:

$$\Delta(H_0, K^{(0)}, \dots, K^{(n)}) = 0. \tag{18}$$

Example 15 The action of the proper Euclidean group SE(2) on $M = \mathbf{R}^2$ given by

$$(\widetilde{x}, \widetilde{y}) = g \cdot (x, y) = (x \cos\varepsilon - y \sin\varepsilon + a, x \sin\varepsilon + y \cos\varepsilon + b) \tag{19}$$

forms the foundation of the Euclidean geometry of planar curves. The multi-prolonged action is locally free on $M^{(n)}$ for $n \geq 1$, and we can thereby determine a first order multi-frame and use it to completely classify Euclidean multi-invariants. The first order transformation formulae are

$$\begin{aligned} \widetilde{x}_0 &= x_0 \cos\varepsilon - y_0 \sin\varepsilon + a, & \widetilde{y}_0 &= x_0 \sin\varepsilon + y_0 \cos\varepsilon + b, \\ \widetilde{y}_1 &= x_1 \cos\varepsilon - y_1 \sin\varepsilon + a, & \widetilde{y}^{(1)} &= \frac{\sin\varepsilon + y^{(1)} \cos\varepsilon}{\cos\varepsilon - y^{(1)} \sin\varepsilon}, \end{aligned} \tag{20}$$

where $u^{(1)} = [\, z_0 z_1 \,]$. Normalization based on the cross-section $\widetilde{x}_0 = \widetilde{y}_0 = \widetilde{y}^{(1)} = 0$ results in the right moving frame

$$\begin{aligned} a &= -x_0 \cos\varepsilon + y_0 \sin\varepsilon = -\frac{x_0 + y^{(1)}\, y_0}{\sqrt{1 + (y^{(1)})^2}}, \\ b &= -x_0 \sin\varepsilon - y_0 \cos\varepsilon = \frac{x_0\, y^{(1)} - y_0}{\sqrt{1 + (y^{(1)})^2}}, \end{aligned} \qquad \tan\varepsilon = -y^{(1)}. \tag{21}$$

(For simplicity, we will ignore the ambiguity of adding a multiple of π to the angular coordinate; see [21] for complete details.) Substituting the moving frame formulae (21) into the lifted divided differences results in a complete system of (oriented) Euclidean multi-invariants. These are easily computed by beginning with the fundamental joint invariants

$$\begin{aligned} H_k = \iota(x_k) &= \frac{(x_k - x_0) + y^{(1)}\,(y_k - y_0)}{\sqrt{1 + (y^{(1)})^2}} = (x_k - x_0)\, \frac{1 + [\, z_0 z_1 \,]\, [\, z_0 z_k \,]}{\sqrt{1 + [\, z_0 z_1 \,]^2}}, \\ K_k = \iota(y_k) &= \frac{(y_k - y_0) - y^{(1)}\,(x_k - x_0)}{\sqrt{1 + (y^{(1)})^2}} = (x_k - x_0)\, \frac{[\, z_0 z_k \,] - [\, z_0 z_1 \,]}{\sqrt{1 + [\, z_0 z_1 \,]^2}}. \end{aligned}$$

The multi-invariants are obtained by forming divided difference quotients

$$[\, I_0 I_k \,] = \frac{K_k - K_0}{H_k - H_0} = \frac{K_k}{H_k} = \frac{(x_k - x_1)[\, z_0 z_1 z_k \,]}{1 + [\, z_0 z_k \,]\,[\, z_0 z_1 \,]}\,,$$

where, in particular, $I^{(1)} = [\, I_0 I_1 \,] = 0$. The second order multi-invariant

$$\begin{aligned} I^{(2)} &= 2\,[\, I_0 I_1 I_2 \,] = 2\,\frac{[\, I_0 I_2 \,] - [\, I_0 I_1 \,]}{H_2 - H_1} \\ &= \frac{2\,[\, z_0 z_1 z_2 \,]\sqrt{1 + [\, z_0 z_1 \,]^2}}{(\,1 + [\, z_0 z_1 \,]\,[\, z_1 z_2 \,]\,)(\,1 + [\, z_0 z_1 \,]\,[\, z_0 z_2 \,]\,)} \\ &= \frac{y^{(2)}\sqrt{1 + (y^{(1)})^2}}{\Big[\, 1 + (y^{(1)})^2 + \tfrac{1}{2} y^{(1)} y^{(2)} (x_2 - x_0) \,\Big]\,\Big[\, 1 + (y^{(1)})^2 + \tfrac{1}{2} y^{(1)} y^{(2)} (x_2 - x_1) \,\Big]} \end{aligned}$$

provides a Euclidean–invariant numerical approximation to the Euclidean curvature:

$$\lim_{z_1, z_2 \to z_0} I^{(2)} = \kappa = \frac{y^{(2)}}{(1 + (y^{(1)})^2)^{3/2}}\,.$$

Similarly, the third order multi-invariant

$$I^{(3)} = 6\,[\, I_0 I_1 I_2 I_3 \,] = 6\,\frac{[\, I_0 I_1 I_3 \,] - [\, I_0 I_1 I_2 \,]}{H_3 - H_2}$$

will form a Euclidean–invariant approximation for the normalized differential invariant $\kappa_s = \iota(y_{xxx})$, the derivative of curvature with respect to arc length, [5, 12]. Higher order invariant numerical approximations can be obtained by invariantization of the higher order divided difference approximations. The moving frame construction has a significant advantage over the infinitesimal approach used by Dorodnitsyn, [11], in that it does not require the solution of partial differential equations in order to construct the multi-invariants.

5 Invariantization of Numerical Schemes.

Given a symmetry group of an ordinary differential equation, we can apply the invariantization procedure to standard numerical integration schemes such as the Euler and the Runge–Kutta methods to derive invariantized numerical scheme that respects the symmetries. Invariantization under a well-chosen group has the effect of transforming the points at each step along

the orbits of the symmetry group to the proper place where the numerical scheme works better. Since it is the symmetry group that acts on the points, the numerical scheme remains valid after the transformation. In this way we invariantize existing numerical schemes, not necessarily changing the mesh. The invariantization also can be applied to numerical methods for both ordinary differential equations and partial differential equations. Moreover this method works efficiently with symmetry groups that are more complicated than the similarity or scaling group.

The following simple example shows how this method improves the existing numerical algorithms. Consider the scalar differential equation

$$y' = y. \tag{22}$$

Linearity implies that it has a one-parameter symmetry group

$$(\widetilde{x}, \widetilde{y}) = \varepsilon \cdot (x, y) = (x, y + \varepsilon e^x) \qquad \text{for all} \qquad \varepsilon \in \mathbf{R}. \tag{23}$$

Let $(x_0, y_0) = (x_0, y(x_0))$ be the initial condition, and $y_1 = y_0 + hy'(x_0) = y_0 + hy_0 = (1 + h)y_0$ the next point generated by the Euler method for fixed x_1. Since G does not act on the independent variable, the step size $h = x_1 - x_0 = \widetilde{x}_1 - \widetilde{x}_0$ is not affected by the group transformations. Thus, the transformed version the Euler method is

$$\widetilde{y}_1 = y_1 + \varepsilon e^{x_1} = (1 + h)(y_0 + \varepsilon e^{x_0}) = (1 + h)\widetilde{y}_0$$

Since $y^{(n)}(x) = y(x)$ for all $n = 1, 2, 3 \ldots$, using the Taylor expansion at x_0, we obtain

$$y_1 = y(x_1) - (y_0 + \varepsilon e^{x_0}) \left(\frac{h^2}{2!} + \frac{h^3}{3!} + \ldots \right)$$

So far, this is nothing more than the Euler method with error $\mathrm{O}(h^2)$. Now suppose we actually transform (x_0, y_0) to $(\widetilde{x}_0, \widetilde{y}_0) = (x_0, 0)$. That is, we set $\varepsilon = -y_0/e^{x_0}$. Then all error terms cancel and we have $y_1 = y(x_1)$ exactly. Note that our choice of transformation parameter ε depended on (x, y). Therefore, in this simple example the Euler method yields an exact solution after an appropriate symmetry transformation.

In general, suppose the function $N_\Delta(z_0, \ldots, z_k)$ on the joint space $M^{\diamond(k+1)}$ defines a numerical integration scheme for a differential equation (17). Given a group transformation g, we define the *g-transformed numerical scheme* as

$$N^g_\Delta(z_0, \ldots, z_k) = N_\Delta(g \cdot z_0, \ldots, g \cdot z_n).$$

If g defines a symmetry of the differential equation, in the sense that it maps solutions to solutions, [20], then it is not hard to see that N_Δ^g is also a numerical scheme for the differential equation.

Example 16 The elementary Euler method for the first order differential equation

$$\Delta(x, y, y') = y' - f(x, y) = 0$$

is given by the function

$$N_\Delta(z_0,\, z_1) = y_1 - y_0 + (x_1 - x_0) f(x_0, y_0), \tag{24}$$

which is defined on the joint space $(\mathbf{R}^2)^{\diamond 2}$. Under the one-parameter group (23), the ε-transformed Euler scheme is

$$\begin{aligned} N_\Delta^\varepsilon(z_0,\, z_1) &= N_\Delta(\varepsilon \cdot z_0, \varepsilon \cdot z_1)) = N_\Delta(x_0, y_0 + \varepsilon e_0^x,\, x_1, y_1 + \varepsilon e_1^x) \\ &= (y_1 + \varepsilon e^{x_1}) - (y_0 + \varepsilon e^{x_0}) - (x_1 - x_0) f(x_0, y_0). \end{aligned} \tag{25}$$

Suppose G is a symmetry group for a differential equation $\Delta = 0$, and let $\rho \colon M^{\diamond(k+1)} \to G$ be a moving frame. The invariantization of the numerical scheme N_Δ with respect to the moving frame ρ is given by

$$I_\Delta(z_0, \dots, z_k) \equiv N_\Delta^{\rho(z)}(z_0, \dots, z_k) = N_\Delta(\rho(z) \cdot z_0, \dots, \rho(z) \cdot z_k).$$

This means that, at each step, we apply the numerical scheme after shifting the points to a fixed cross-section and map the result back to the original location. In particular, the invariantization of (25) using the moving frame $\varepsilon = \rho(z) = -y_0 e^{-x_0}$ is

$$I_\Delta(z) = N_\Delta(\rho(z) \cdot z) = y_1 - y_0 e^{x_1 - x_0} - (x_1 - x_0) f(x_0, y_0).$$

The key to the success of the invariantized numerical scheme lies in the intelligent choice of cross-section for the moving frame. We usually set the dependent variables and/or some of their derivatives to zero. Even though the associated computations can become complicated, the more the symmetry group is prolonged, the more choices we have for a cross-section.

Unfortunately, invariantization by elementary symmetry groups has no effect. Every standard numerical scheme is already invariant with respect to the affine symmetry group $\widetilde{z} = Az + b$ whose infinitesimal generators are

$$\frac{\partial}{\partial x}, \qquad \frac{\partial}{\partial y}, \qquad x\frac{\partial}{\partial x}, \qquad y\frac{\partial}{\partial x}, \qquad x\frac{\partial}{\partial y}, \qquad y\frac{\partial}{\partial y}.$$

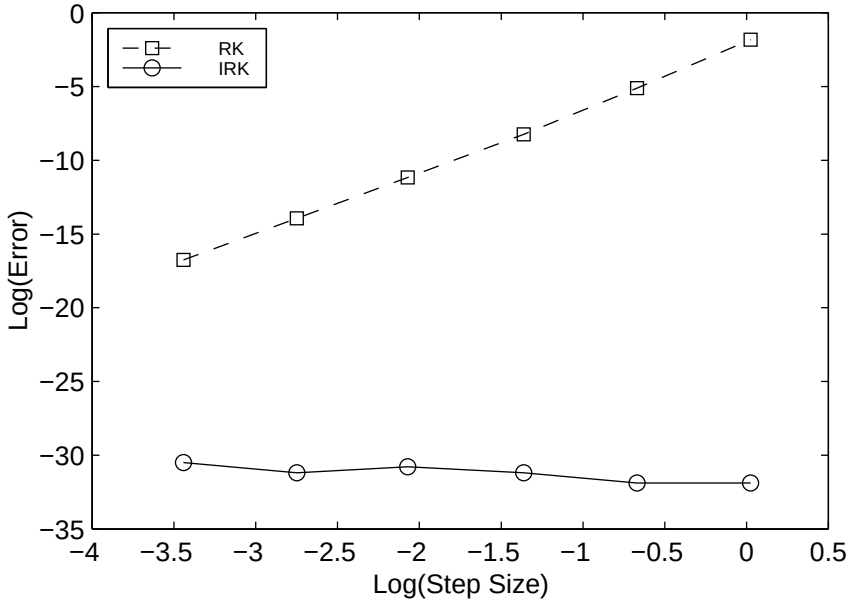

Figure 2: The logistic equation $y' = y(\,1 - \frac{y}{100}\,)$

However, as we will see below, affine symmetries can be still used to enhance the numerical scheme when combined with other nontrivial symmetry groups.

In the following examples, we concentrate on the fourth order Runge–Kutta method (RK) since is the most widely used single-step numerical scheme for ordinary differential equations. Implementation of the resulting invariantized Runge–Kutta schemes (IRK) is straightforward, and requires only a small number of lines to be added to existing numerical codes.

Example 17 The logistic equation

$$y' = y\left(1 - \frac{y}{100}\right). \tag{26}$$

possesses the one-parameter symmetry group with infinitesimal generator $\mathbf{v} = e^{-x}y^2\frac{\partial}{\partial y}$. The corresponding prolonged group transformations are

$$(\widetilde{x}, \widetilde{y}, \widetilde{y'}) = \left(x\,,\, \frac{y}{1 - \varepsilon e^{-x}y}\,,\, \frac{y' - \varepsilon e^{-x}y^2}{(1 - \varepsilon e^{-x}y)^2}\right),$$

which we analyzed in Example 14. Again, setting $\widetilde{y'} = 0$ gives the moving

frame $\rho(x, y, y') = e^x y^{-2} y'$ and therefore

$$\rho(x, y, y') \cdot (x, y, y') = \left(x,\, \frac{y^2}{y - y'},\, 0 \right).$$

Since the standard RK scheme involves $z_0 = (x_0, y_0, y_0')$ and $z_1 = (x_1, y_1, y_1')$, it is defined on the joint space $(\mathrm{J}^1)^{\diamond 2} \simeq (\mathbf{R}^3)^{\diamond 2}$. The previous moving frame is now extended and defined on the joint space as $\rho(z_0,\, z_1) = \rho(z_0)$, i.e., it depends only on the first point. The invariantized numerical scheme $\iota[N_\Delta]$ can be obtained by substitution

$$\begin{aligned} &(x_0,\, y_0,\, y_0';\; x_1,\, y_1,\, y_1') \quad \longmapsto \\ &\qquad \left(x_0,\, \frac{{y_0}^2}{y_0 - y_0'}\,, 0;\; x_1\,,\, \frac{{y_0}^2 y_1}{{y_0}^2 - e^{x_0 - x_1} y_1 y_0'}\,,\, \frac{{y_0}^4 y_1' - e^{x_0 - x_1} {y_0}^2 {y_1}^2 y_0'}{({y_0}^2 - e^{x_0 - x_1} y_1 y_0')^2} \right). \end{aligned}$$

As Figure 2 shows, the performance of invariantized RK overwhelms that of the standard RK.

Example 18 The second order equation

$$y'' = y'^2 \tag{27}$$

admits two independent one-parameter symmetry groups, with generators

$$\mathbf{v}_1 = x^2 \frac{\partial}{\partial x} - x \frac{\partial}{\partial y}, \qquad \mathbf{v}_2 = e^y \frac{\partial}{\partial y}$$

The corresponding prolonged transformations are

$$(x, y, y') \longmapsto \begin{cases} \left(\dfrac{x}{1 - \varepsilon_1 x}\,, y(1 - \varepsilon_1 x)\,, \dfrac{\varepsilon_1 x - 1}{x} + (xy' + 1) \dfrac{(\varepsilon_1 x - 1)^2}{x} \right), \\ \left(x, -\log(e^{-y} - \varepsilon_2),\, \dfrac{e^{-y} y'}{e^{-y} - \varepsilon_2} \right). \end{cases}$$

Even though the second is easier to compute, it is less beneficial since we can make neither $\widetilde{y}$ nor $\widetilde{y}'$ zero by its action. So we use the first. By fixing $\widetilde{y}' = 0$, we obtain the moving frame

$$\rho(x, y, y', y'') = \frac{y'}{xy' + 1}.$$

Figure 3 shows that the invariantized RK excels the RK by far again. It even seems not affected by the step size!

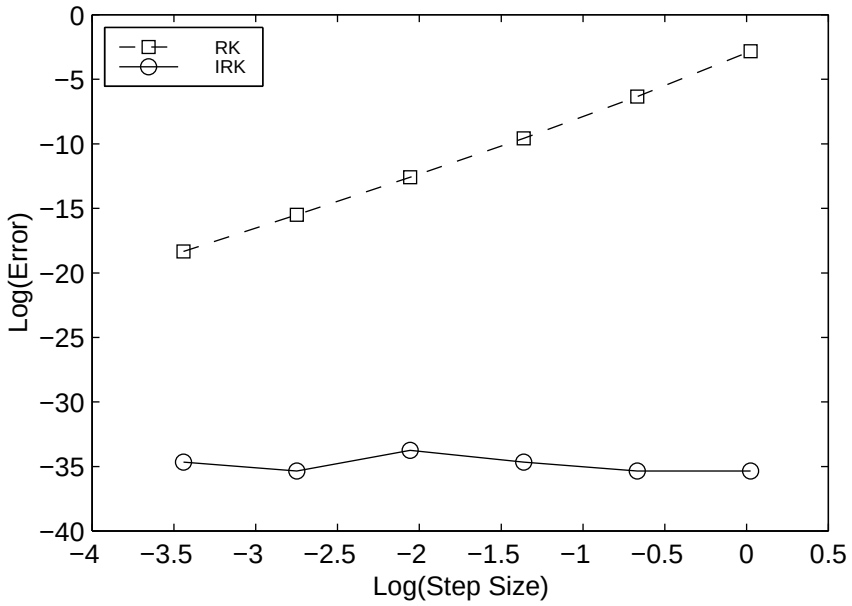

Figure 3: The equation $y'' = y'^2$

Example 19 Ames's equation

$$y'' = -\frac{y'}{x} - e^y \tag{28}$$

is a stiff equation that arises in a wide range of fields, including kinetics and heat transfer, vortex motion of incompressible fluids, and the mass distribution of gaseous interstellar material under influence of its own gravitational fields, [1]; it is also known as the Frank-Kaminetskii equation, the Gelfand equation, and the Barenblatt equation. The infinitesimal generators

$$\mathbf{v}_1 = -x\frac{\partial}{\partial x} + 2\frac{\partial}{\partial y}, \qquad \mathbf{v}_2 = -\frac{1}{2}x\log x\frac{\partial}{\partial x} + (1+\log x)\frac{\partial}{\partial y},$$

induce the prolonged one-parameter symmetry groups

$$(x, y, y') \longmapsto \begin{cases} (e^{-\varepsilon_1}x\,, y + 2\varepsilon_1\,, e^{\varepsilon_1}y'), \\ \left(e^{e^{-\varepsilon_2/2}\log x}\,,\; y + 2\log x(1 - e^{-\varepsilon_2/2}) + \varepsilon_2\,,\; \dfrac{xy' + 2 - 2e^{-\varepsilon_2/2}}{e^{e^{-\varepsilon_2/2}\log x - \frac{1}{2}\varepsilon_2}} \right). \end{cases}$$

The first is a scaling transformation group, which does not change the performance of the original scheme as mentioned above. The difficulty with

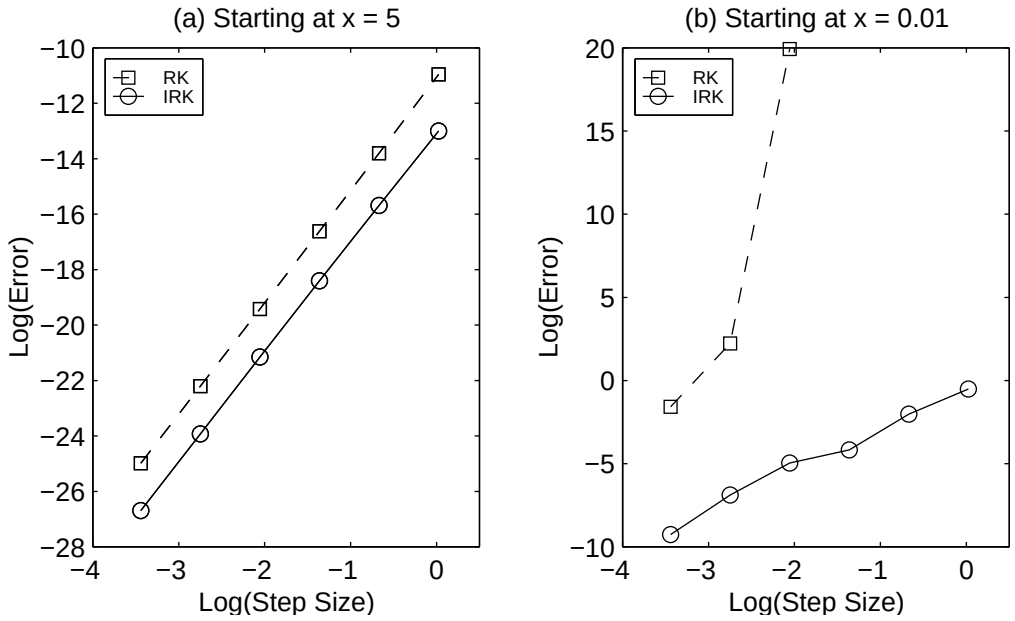

Figure 4: Ames' equation $y'' = -\dfrac{y'}{x} - e^y$

the second one is that we cannot set $\widetilde{y}$ or $\widetilde{y'}$ zero. However, we can build a better transformation by proper combination of the two groups. Let $\rho_1(z_0;\, z_1) = \log x_0$ and $\rho_2(z_0;\, z_1) = -y_0$. Through the successive applications of the two moving frames $\rho_1\rho_2$, every point (x, y) is projected to the cross-section $\widetilde{y} = 0$. The corresponding invariantized numerical scheme is written

$$I_\Delta(z) = (N_\Delta^{\rho_1})^{\rho_2}(z) = N_\Delta(\ \rho_2(\rho_1(z)\cdot z)\cdot(\rho_1(z)\cdot z)\ ).$$

Figure 4(a) is the comparison between the RK and the IRK scheme when they start at $x = 5$. Even in this domain the performance of IRK exceeds RK, but more dramatic difference appears when they apply around $x = 0$, as illustrated in Figure 4(b). This implies that the invariantized Runge–Kutta method successfully avoids the equation's stiffness by preserving the equation's geometric structure.

In conclusion, the geometric foundations of numerical analysis based on multi-space and the moving frame invariantization process leads, in favorable cases, to significant improvements to standard numerical integration schemes for ordinary differential equations with symmetry. Applications of

invariantized schemes to more challenging systems of ordinary differential equations are currently under investigation. The construction of multi-space for functions of several variables and applications to numerical analysis of partial differential equations will be the subject of future research.

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