

Full Length Research Paper

A collocation multistep method for integrating ordinary differential equations on manifolds

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This paper concerns a family of generalized collocation multistep methods that evolves the numerical solution of ordinary differential equations on configuration spaces formulated as homogeneous manifolds. Collocating the general linear method at $x = x_{n+k}$ for $k = 0, 1, \dots, s$, we obtain the discrete scheme which can be adapted to homogeneous spaces. Varying the values of k in the collocation process, the standard Munthe-Kass ($k = 1$) and the linear multistep methods ($k = s$) are recovered. Any classical multistep methods may be employed as an invariant method and the order of the invariant method is as high as in the classical setting. In this paper an implicit algorithm was formulated and two approaches presented for its implementation.

Key words: Collocation, multistep methods, homogeneous manifolds, implicit methods, invariant methods, differential equations on manifolds, geometric integration.

INTRODUCTION

Geometric integration and in particular integration methods on lie groups and homogeneous spaces, has received much attention the last few years. Most of the development has been related to generalization of Runge-Kutta and other one step methods, in the setting of homogeneous manifolds and lie groups. Consider the equation below

$$\sum_{i=0}^k a_i(x) \frac{d^{k-i} y}{dx^{k-i}} = f(x); \quad y(a) = \eta \quad (1)$$

and in the vectorised form

$$\underline{y}'(x) = \underline{f}(x, \underline{y}(x)); \quad \underline{y}(a) = \underline{\eta} \quad (2)$$

where

$$y'_i = f_i(x, y_1, y_2, \dots, y_m) \quad \text{and} \quad y_i(a) = y_i, \quad i = 1, 2, \dots, m.$$

is called a system of ivps.

The general k -step method (classical multistep method) for solving (1)-(2) above may be written in the form

$$\sum_{j=0}^k \alpha_j y_{n+j} = h \sum_{j=0}^k \beta_j f_{n+j} \quad (3)$$

where α_j and β_j , $j = 0, 1, \dots, k$ are given constants that are independent of the differential equation to be solved, the step size h and n , that is, the parameters $\{\alpha_j\}_{j=0}^k$ and $\{\beta_j\}_{j=0}^k$ defines the particular method. It may be assumed that $\alpha_k = 1$. If $\beta_k = 0$ then the method is explicit whilst if $\beta_k \neq 0$ then a non-linear equation must be solved to determine y_{n+k} and the method is termed implicit. Iserles, (1997) and Budd and Iserles (1999) showed that the methods in the family defined by equation (3) only can retain linear invariants. In this paper, a reformation of the multistep methods in the setting of lie groups and homogeneous spaces is considered and it shows that the method respects the configuration space of the problem when implemented in a correct way.

Definition 1

A manifold

In a neighborhood of $a \in R^n$ a manifold is given by

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$$M = \{y \in U : g(y) = 0\} \tag{4}$$

When $g : U \rightarrow R^n$ is differentiable, $g(a) = 0$ and $g'(a)$ has full rank m .

Definition 2

Differential equation on manifolds

Let M be an $(n-m)$ dimensional sub-manifold of R^n . The problem

$$\dot{y} = f(y) \tag{5}$$

is a differential equation on the manifold (1.4) satisfying $f(y) \in T_a M$ for all $y \in M$

$T_a M = \{V \in R^n\}$ there exist a differentiable path $\gamma : (-\epsilon, \epsilon) \rightarrow R^n$ with $\gamma(t) \in M$ for all t ,

$$\gamma(0) = a, \dot{\gamma}(0) = V \tag{6}$$

Differential equations on manifolds arise in a variety of applications, and their numerical treatment has been the subject of many research reports. A naïve approach for the numerical solution of a differential equation on manifold M would be to apply a method to the problem (5) without taking care of the manifold M , and to hope that the solution stays close to the manifold. A foremost requirement on a numerical integrator is that the numerical approximation lies exactly on the manifold. But, if the exact flow on the manifold has certain geometric properties, it is natural to ask for numerical methods that preserve them. Hairer (2002) gave 2 illustrative examples (that is, the mathematical pendulum problem and the Toda Lattice problem) which show that the trapezoidal method preserves the structures of the original equations. He later presented the projection methods using one step numerical integrators, thus yielding the approach of geometric integration. See also Calvo et al. (2007), for more details.

METHODS

Explicit multistep algorithms based on rigid frames were proposed by Crouch and Grossman (1993). This method assume that smooth vector fields E_1, \dots, E_d on a differentiable manifold M are available such that the differential equation can be written in the form:

$$\dot{y} = F(y) = \sum_{i=1}^d f_i(y) E_i, \quad y \in M \tag{7}$$

Where the f_i are real analytic functions on $\mathfrak{R} \times M$.

The numerical schemes are defined in terms of vector fields with coefficients frozen relative to the frame vector fields, that is,

$$F_p = \sum_{i=1}^d f_i(p) E_i$$

The k -step Crouch-Grossman methods may now be written as:

$$\begin{aligned} u_{n+k-1}^l &= y_{n+k-1}, \\ u_{n+k-1}^l(h, y_{n+k-1}, \dots, y_n, u_{n+k-1}^{j+1}) &= e^{(h\alpha_0^l F_{y_{n+k-1}})} * e^{(h\alpha_1^l F_{y_{n+k-2}})} * \dots * e^{(h\alpha_{k-1}^l F_{y_n})} * (u_{n+k-1}^{j+1}), \quad 0 \leq j \leq l-1, \\ y_{n+k} &= u_{n+k-1}^0(h, y_{n+k-1}, \dots, u_{n+k-1}^1). \end{aligned} \tag{8}$$

Letting $l = 2$, this scheme becomes

$$y_{n+k} = e^{(h\alpha_0^1 F_{y_{n+k-1}})} * e^{(h\alpha_1^1 F_{y_{n+k-2}})} * \dots * e^{(h\alpha_{k-1}^1 F_{y_n})} * e^{(h\alpha_0^2 F_{y_{n+k-1}})} * \dots * e^{(h\alpha_{k-1}^2 F_{y_n})} y_{n+k-1} \tag{1.9}$$

and it is clear that if $\alpha_i = \sum_{j=0}^{l-1} \alpha_i^j$ $0 \leq i \leq k-1$ this

algorithm reduces to the classical Adams Bashforth method in the Euclidean case:

$$y_{n+k} = y_{n+k-1} + h \sum_{i=0}^{k-1} \alpha_i F(y_{n+k-1-i}) \tag{10}$$

The k -step Crouch-Grossman method evolves the numerical approximation by composing flows of vector fields on M . Computing flows of vector fields are very time consuming operations and it may be advantageous to consider methods that combined frozen vector fields and compute the flow of the resulting vector field at the end of each step only. Lopez (1997), discussed the analogous on matrix manifolds.

Munthe-Kass et al (1999) improved on this by making an assumption that there exists a Lie algebra g with a Lie bracket $[.,.]$, a left Lie algebra action defined as follows:

Let $\Lambda : G \times M \rightarrow M$ be a left Lie group action. We get a left Lie algebra action $\lambda : g \times M \rightarrow M$. by $\lambda(v, p) = \Lambda(e^{(v)}, p)$, where $g \rightarrow G$ is the matrix exponential when G is a matrix group.

A function $f : \mathfrak{R} \times M \rightarrow g$ such that the ordinary differential equation for $y(t) \in M$ can be written in the form:

$$y' = F_\lambda(t, y) = (\lambda * f(t, y))(y); \quad y(0) = p \in M. \tag{11}$$

Equation (11) is the canonical form of an ordinary differential equation on manifold. We assume that $y_0 \in M$ and it follows that $y' \in TM_y$, where TM_y is the tangent space of M at $y \in M$.

It is proved in H. Munthe-Kass (1999), that the solution of (11) is given for sufficiently small t , as $y(t) = \lambda(u(t), p)$, with $y(0)=p$, where $u(t) \in g$ satisfies the differential equation

$$u' = \bar{f}(u) = d \exp_u^{-1}(f(t, \lambda(u, p))); \quad u(0) = 0 \in g \quad (12)$$

It is important to note that

$$\Lambda(e^{(u_1)}, \Lambda(e^{(u_2)})) = \Lambda(e^{(u_1)} \cdot e^{(u_2)}, p) = \Lambda(e^{(B(u_1, u_2))}) \quad (13)$$

and hence

$$\lambda(u_1, \lambda(u_2, p)) = \lambda(B(u_1, u_2), p) \quad (14)$$

Where B is the Baker-Campbell-Hausdorff formula.

McLaren and Quispel (2004) discussed using the discrete gradient method, and by bootstrapping repeatedly the order of accuracy can be improved and the first integrals can be preserved.

In this paper, we follow the same approach of Crouch-Grossman (1993) and we blend with Hairer (2002) to formulate an implicit multistep method following the spirit of trapezoidal rule which is known to be structure preserving in geometric integration.

RESULTS

The new implicit multistep methods

In this approach we consider $\beta_k \neq 0$ in (1.3), then we

$$u_{n+k}^l = y_{n+k},$$

$$u_{n+k}^j(h, y_{n+k-1}, \dots, y_n, u_{n+k}^{j+2}) = e^{(h\alpha_k^j F_{y_{n+k-1}})} * e^{(h\alpha_k^j F_{y_{n+k-2}})} * \dots * e^{(h\alpha_k^j F_{y_n})} * (u_{n+k}^{j+1}), \quad 0 \leq j \leq l, y_{n+k}, \quad \omega_k^{(n)} \quad \text{and} \quad f_{n+k} = f(t_{n+k}, y_{n+k}), \quad \text{for} \quad \beta \neq 0$$

$$y_{n+k} = u_{n+k-1}^0(h, y_{n+k-1}, \dots, y_n, u_{n+k}^1). \quad (15)$$

Letting $l = 2$, the new scheme becomes

$$y_{n+k} = e^{(h\alpha_k^2 F_{y_{n+k-1}})} * e^{(h\alpha_k^2 F_{y_{n+k-2}})} * \dots * e^{(h\alpha_k^2 F_{y_n})} * e^{(h\alpha_k^1 F_{y_{n+k-1}})} * e^{(h\alpha_k^1 F_{y_{n+k-2}})} * \dots * e^{(h\alpha_k^1 F_{y_n})} * e^{(h\alpha_k^0 F_{y_n})} y_{n+k} \quad (16)$$

Hence we have that if $\alpha_i = \sum_{j=0}^l \alpha_i^j$ $0 \leq i \leq k$ this

algorithm reduces to the classical Adams Moulton implicit method in the Euclidean case:

$$y_{n+k} = y_{n+k-1} + h \sum_{i=0}^k \alpha_i F(y_{n+i}) \quad (17)$$

To solve the problem (11) using a multistep method, there to transform the previous information in the $k-1$ steps to the new coordinate system in each step so as to preserve the geometric structures.

In the spirit of Munthe-Kass et al. (1999), if we let t_i to be equidistant time points and $y_i \approx y(t_i)$. At step n of the new algorithm the r.h.s. y_{n+k} is obtained, by using a coordinated chart centered at $p = y_{n+k-1}$. Let $\omega_i^{(n)} \in g$ be the points corresponding to $y_{n+i} \in G$ at step n , that is,

$$\lambda_{y_{n+k-1}}(\omega_i^{(n)}) = y_{n+i} \quad \text{for} \quad i = 0, 1, 2, \dots, k-1 \quad (18)$$

If $f_i = f(t_i, y_i)$ and $\omega_i^{(n)}$ are known for $i = 0, \dots, k-1$, then y_{n+k} can be found by the following multistep algorithm:

$$\bar{f}_i^{(n)} = d \exp_{\omega_i^{(n)}}^{-1}(f_{n+i}) \quad (19)$$

$$\sum_{i=0}^k \alpha_i \omega_i^{(n)} = h \sum_{i=0}^k \beta_i \bar{f}_i^{(n)} \quad (20)$$

$$y_{n+k} = \lambda_{y_{n+k-1}}(\omega_k^{(n)}) \quad (21)$$

Using the following transformation for

$$\omega_i^{(n)} = B(\omega_{i-1}^{(n+1)}, -\omega_k^{(n)}) \quad \text{we have}$$

$$\omega_{i-1}^{(n+1)} = B(\omega_i^{(n)}, -\omega_k^{(n)}) \quad (22)$$

which gives the solution of (11) from time t_{n+k-1} to t_{n+k} defining an equation system for the unknowns

$$y_{n+k}, \quad \omega_k^{(n)} \quad \text{and} \quad f_{n+k} = f(t_{n+k}, y_{n+k}), \quad \text{for} \quad \beta \neq 0 \quad (23)$$

Theorem (1)

If $(y_{n+i}, f(t_{n+i}, y_{n+i})) \in M \times g$, $i = 0, \dots, k-1$, then the Algorithm (19) - (22) generates an element $y_{n+k} \in M$. If the classical multistep method defined by the coefficients α_i and β_i , $i = 0, \dots, k$ is of order q , then the order of approximation of y_{n+k} to $y(t_{n+k})$ is q .

Proof

We observe that $\omega_i^{(n)}$ and $\bar{f}_i^{(n)}$, $i = 0, \dots, k-1$ as

well as $\tilde{f}_k^{(n)}$ are elements of g . Solution of (20) yields an element $\omega_i^{(n)} \in g$. The first part of the theorem now follows, since $\lambda_y : g \rightarrow M \quad \forall y \in M$.

Using a classical multistep method of order q to integrate (12), we observe that the Baker Campbell-Hausdorff formula B , introduces an order $O(h^{q+1})$ modification of $\omega_i^{(n)}$, $i = 0, \dots, k-2$, and that $d \exp_{\omega_i^{(n)}}^{-1}$ introduces an $O(h^{q+1})$ modification of f_{n+1} , $i = 0, \dots, k-2$, thus the second part of the theorem follows by noting that the pullback vector field \tilde{f} in (12) correct to order q (Munthe-Kass, 1999).

It is a requirement and natural to impose a Lipschitz condition on the problems in order to ascertain the existence of solutions of the problems within the space of consideration. Thus we state the following basic result for the differential equations on manifold M .

Theorem (2)

Assume that the lie algebra g is a Banach space and that \tilde{f} is Lipschitz with constant L . Then the iteration

$$\omega_k^{(l+1)} = h\beta_k d \exp_{\omega_k^{(l)}}^{-1} (f_k^{[l]}) + h \sum_{i=0}^{k-1} \beta_i \tilde{f}_i^{(n)} - \sum_{i=0}^{k-1} \alpha_i \omega_i^{(n)} \tag{24}$$

for the implicit multistep algorithm converges provided that $h\beta_k L < 1$.

Proof

Let $\|\cdot\|_g$ be a norm on g . Consider $\hat{\omega}_k^{(l)}$ defined by the iteration (24) with initial condition $\hat{\omega}_k^{(0)} \neq \omega_k^{(0)}$. Thus we get that:

$$\|\omega_k^{(l+1)} - \hat{\omega}_k^{(l+1)}\| = h\beta_k \|\tilde{f}(\omega_k^{[l]} - \tilde{f}(\hat{\omega}_k^{[l]})\| \leq h\beta_k L \|\omega_k^{[l]} - \hat{\omega}_k^{[l]}\|. \tag{25}$$

Since $h\beta_k L < 1$, this is a contraction and there exists a unique fixed-point of iteration (24) in the complete space g .

Procedures for implementing the implicit multistep methods on manifolds

2 approaches are proposed here. First, the use of predictor-corrector approach as in Munthe-Kass (1999). Secondly we shall use the self starting algorithm of

Onumanyi and Fatokun (2008) and Fatokun (2007). This is done by using the idea of block methods as illustrated below:

Let

$$y(\xi) = \phi_0(\xi)y_r + \Psi_0(\xi)z_r + \Psi_1(\xi)z_{r+1} + \Psi_2(\xi)z_{r+\frac{3}{2}} + \Psi_3(\xi)z_{r+2} \tag{26}$$

The corresponding D (Collocation matrix) is given as

$$\phi_0(x) = 1, \psi_j(x) = \sum_{i=0}^4 \beta_{j,i+1} x^i, j = 0(1)3.$$

$$D = \begin{bmatrix} 1 & x & x^2 & x^3 & x^4 \\ 0 & 1 & 2x_r & 3x_r^2 & 4x_r^3 \\ 0 & 1 & 2x_{r+1} & 3x_{r+1}^2 & 4x_{r+1}^3 \\ 0 & 1 & 2x_{r+\frac{3}{2}} & 3x_{r+\frac{3}{2}}^2 & 4x_{r+\frac{3}{2}}^3 \\ 0 & 1 & 2x_{r+2} & 3x_{r+2}^2 & 4x_{r+2}^3 \end{bmatrix} \tag{27}$$

Where D is invertible $DC = I$ and hence we obtain explicitly $y(\xi)$ in (26) with

$$\begin{aligned} \phi_0(\xi) &= 1 \\ \psi_0(\chi) &= \frac{1}{12h^3} \{-(x-x_r)^4 + 6h(x-x_r)^3 - 13h^2(x-x_r)^2 + 12h^3(x-x_r)\} \\ \psi_1(\chi) &= \frac{1}{6h^3} \{3(x-x_r)^4 - 14h(x-x_r)^3 + 18h^2(x-x_r)\} \\ \psi_2(\chi) &= \frac{1}{3h^3} \{2(x-x_r)^4 + 8h(x-x_r)^3 - 8h^2(x-x_r)^2\} \\ \psi_3(\chi) &= \frac{1}{12h^3} \{3(x-x_r)^4 - 10h(x-x_r)^3 + 9h^2(x-x_r)^2\} \end{aligned}$$

Evaluating $y(\xi)$ at $x = x_{r+1}, x = x_{r+\frac{3}{2}}$ and $x = x_{r+2}$ we obtain three discrete schemes

$$y_{r+1} = y_r + \frac{h}{6} (2z_r + 7z_{r+1} - 4z_{r+\frac{3}{2}} + z_{r+2}), \quad \text{order 4, } c_5 = \frac{-31}{2880} \tag{28}$$

$$y_{r+\frac{3}{2}} = y_r + \frac{3h}{64} (7z_r + 30z_{r+1} - 8z_{r+\frac{3}{2}} + 3z_{r+2}), \quad \text{order 4, } c_5 = \frac{-51}{5120} \tag{29}$$

$$y_{r+2} = y_r + \frac{h}{3} (z_r + 4z_{r+1} + z_{r+2}), \quad \text{order 4, } = \frac{-1}{90}. \tag{30}$$

Solving the equations (28) - (30) simultaneously as an A-stable integrator for $z_{r+1}, z_{r+\frac{3}{2}}$ and z_{r+2} give the following first derivative FD approximation schemes

$$z_{r+1} = \frac{1}{36h} \left(64y_{r+\frac{3}{2}} - 9y_{y+2} - y_{r+1} - 19y_r \right) - \frac{1}{6} z_r, \quad \text{order 4, } c_5 = \frac{-1}{240} \tag{31}$$

$$z_{r+\frac{3}{2}} = \frac{1}{48h} \left(27y_{r+2} + 64y_{y+\frac{3}{2}} - 108y_{r+1} + 17y_r \right) + \frac{1}{8} z_r, \quad \text{order 4, } c_5 = \frac{-3}{640} \tag{32}$$

$$z_{r+2} = \frac{1}{9h} \left(36y_{r+2} - 64y_{y+\frac{3}{2}} + 36y_{r+1} - 8y_r \right) - \frac{1}{3} z_r, \quad \text{order 4, } c_5 = \frac{-1}{60} \tag{33}$$

Now we put (31) and (33) respectively in the following algorithm:

$$z_{r+1} = \frac{1}{4h} (y_{r+2} + 4y_{r+1} - 5y_r) - \frac{1}{2} z_r, \quad \text{order 2, } c_3 = \frac{-1}{24} \tag{1.34}$$

$$z_{r+2} = \frac{2}{h} (y_{r+2} - 2y_{r+1} + y_r) + z_r \quad \text{order 2, } c_3 = \frac{-1}{6}. \tag{35}$$

to obtain the final algorithm to solve (11).

Numerical experiment

Munthe-Kass et al. (1999) used an example by Zanna (1996) which is a first order differential equation on manifold. Let the manifold $M = G$ be a matrix Lie group with lie algebra $(g, [, .])$. The action of the Lie algebra on G is given by $\lambda : g \times G \rightarrow G$, where $\lambda(v, p) = \exp(v).p$. This reduces equation (11) to a first order differential equation

$$y' = f(t, y).y \quad \text{with } y(0) \in G \tag{36}$$

This was conveniently solved as in Munthe-Kass et al. (1999).

CONCLUSION AND DISCUSSION OF RESULTS

We have seen the theoretical framework of integrating differential equations on manifolds. In this paper we consider using implicit algorithms, which theoretically is more accurate than the explicit types described by Munthe-Kass (1999). The geometric integration methods are generally more expensive than the classical methods.

In a follow-up paper, we shall consider some second order differential equations on manifold and use the self-starting approach described in this work. This is hoped to be a breakthrough in the geometric integration approach and giving due respect to the configuration space of the problem as compute the numerical solutions.

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