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A Collocation Multistep Method for Integrating Ordinary Differential Equations on Manifolds

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Abstract: This study 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 $x\text{-}x_{n+k}$, for k - 0,1...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 study an implicit algorithm was formulated and 2 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 Runga-Kutta and other one step methods, in the setting of homogeneous manifolds and lie groups.

Consider the equation below:

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

and in the vectorised form

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

Where, $y'_i\ f_i\ (x, y_1, y_2,..., y_m)$ and $y_i\ (a) = y_i$, i = 1, 2,...m is called a system of ivps.

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

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

Where α_j and β_j, j = 0, 1….., k are given constants that are independent of the differential equation to be solved, the step size h and n i.e., the parameters $\{\alpha_j\}^k_j$ and $\{\beta_j\}^k_{j=0}$ 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.

Calvo *et al.* (1997) showed that the methods in the family defined by Eq. 3 only can retain linear invariants. In this study, 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

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

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

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

Definition

Differential equation on manifolds: Let M be an (n-m) dimensional sub-manifold of R^n.

The problem

$$y = f\,(y) \qquad (5)$$

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is a differential equation on the manifold Eq. 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,

$$\gamma(0) = A, \gamma(0) = V \qquad (6)$$

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 Eq. 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 *et al*. (2002) gave 2 illustrative examples (i.e., 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.

MATERIALS AND METHODS

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

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

Where, the f_i are real analytic functions on $\Re \times M$. The numerical schemes are defined in terms of vector fields with coefficients frozen relative to the frame vector fields, i.e.,

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

The k-step Crouch and Grossman (1993) methods may now be written as:

$$\begin{aligned} u^1_{n+k-1} &= y_{n+k-1,} \\ u^1_{n+k-1}(h, y_{n+k-1}, \ldots, y_n, u^{j+1}_{n+k-1}) &= e^{(h\alpha^j_0 F_{y_{n+k-1}})} * e^{(h\alpha^j_1 F_{y_{n+k-2}})} \\ &* \ldots * e^{(h\alpha^j_{k-1} F_{y_n})} * (u^{j+1}_{n+k-1}), \quad 0 \le j \le 1-1, \\ y_{n+k} &= u^0_{n+k-1}(h, y_{n+k-1,}, \ldots, u^1_{n+k-1}) \end{aligned} \qquad (8)$$

Letting l-2 this scheme becomes:

$$\begin{aligned} y_{n+k} = {} & e^{(h\alpha^0_0 F_{y_{n+k-1}})} * e^{(h\alpha^0_1 F_{y_{n+k-2}})} * \ldots * e^{(h\alpha^0_{k-1} F_{y_n})} \\ & * e^{(h\alpha^1_0 F_{y_{n+k-1}})} * e^{(h\alpha^1_1 F_{y_{n+-2}})} * \ldots * e^{(h\alpha^1_{k-1} F_n)} y_{n+k-1} \end{aligned} \qquad (9)$$

and it is clear that if

$$\alpha_i = \sum_{j=0}^{1-1} \alpha^j_i \quad 0 \le i \le k-1$$

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

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

The k-step Crouch and Grossman (1993) 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.

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

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

$$y' = F\lambda(t, y) = (\lambda \times f(t, y))(y); \; y(0) = \in M \qquad (11)$$

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 Munthe-Kaas (1999) that the solution of Eq. 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 Eq. 12:

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

It is important to note that

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

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 study, we follow the same approach of Crouch and Grossman (1993) and we blend with Hairer *et al.* (2002) to formulate an implicit multistep method following the spirit of Trapezoidal rule which is known to be structure preserving in geometric integration.

RESULTS AND DISCUSSION

The new implicit multistep methods: In this approach, we consider $\beta_k \neq 0$ in Eq. (3), then we:

$$\begin{aligned} u^{l}_{n+k} &= y_{n+k}, \\ u^{l}_{n+k}(h, y_{n+k-1}, \ldots, y_n, u^{j+2}_{n+k}) &= e^{(h\alpha^j_0 F_{y_{n+k-1}})} * e^{(h\alpha^j_1 F_{y_{n+k-2}})} \\ &* \ldots * e^{(h\alpha^j_k F_{y_n})} * (u^{j+1}_{n+k}), \quad 0 \le j \le 1, \\ y_{n+k} &= u^{0}_{n+k-1}(h, y_{n+k-1}, \ldots, y_n, u^{1}_{n+k}) \end{aligned} \quad (15)$$

Letting l = 2, the new scheme becomes

$$\begin{aligned} y_{n+k} &= e^{(h\alpha^0_0 F_{y_{n+k-1}})} * e^{(h\alpha^0_1 F_{y_{n+k-2}})} * \ldots * e^{(h\alpha^0_{k-1} F_{y_n})} \\ &* e^{(h\alpha^1_0 F_{y_{n+k-1}})} * e^{(h\alpha^1_1 F_{y_{n+-2}})} * \ldots * e^{(h\alpha^1_{k-1} F_n)} * e^{(h\alpha^1_k F_{y_n})} y_{n+k} \end{aligned} \quad (16)$$

Hence, we have that if

$$\alpha_i = \sum_{j=0}^{1} \alpha^j_i \quad 0 \le i \le k$$

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 Eq. 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-Kaas (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 $p = y_{n+k}$. Let $\omega^{(n)} \in g$ be the points corresponding to $y_{n+k} \in G$ at step n, i.e.:

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

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

$$\bar{f}^{(n)}_i = d\exp^{-1}_{\omega^{(n)}_i}(f_{n+1}) \quad (19)$$

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

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

Using the following transformation for $\omega_i^{(n)} = B(\omega_i^{(n+1)}, -\omega_k^{(n)})$, we have

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

which gives the solution of Eq. 11 from time t_{n+k-1}-t_{n+k} defining an equation system for the unknowns:

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

Theorem (1): If $(y_{n+i}, f(t_{n+i}, y_{n+i})) \in M \times g$, i = 0,..., k-l, then the algorithm (1.91-1.22) generates an element $y_{n+k} \in M$. If the classical multistep method defined by the coefficients α_i and β_i, i = 0,..., 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 $\bar{f}^{(n)}_k$, i = 0,... k-1 as well as $\bar{f}^{(n)}_k$ are elements of g. Solution of Eq. 20 yields an element $\omega_i^{(n)} \in g$. The first part of the theorem now follows, since λ_n: g → M ∀ y ∈ M.

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

$$\omega^{(l+1)}_k = h\beta_k d\exp^{-1}_{\omega^{[l]}_k}(f^{[l]}_k) + h\sum_{i=0}^{k-1}\beta_i \tilde{f}^{(n)}_i - \sum_{i=0}^{k-1}\alpha_i \omega^{(n)}_i \quad (24)$$

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

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

$$\begin{aligned}\left\|\omega_k^{(l+1)} - \hat{\omega}_k^{(l+1)}\right\| &= h\beta_k \left\|\tilde{f}(\omega_k^{[l]} - \tilde{f}(\hat{\omega}_k^{[l]})\right\| \\ &\leq h\beta_k L \left\|\omega_k^{[l]} - \hat{\omega}_k^{[l]}\right\|\end{aligned} \quad (25)$$

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

Procedures for implementing the implicit multistep methods on manifolds: Two approaches are proposed here. First, the use of predictor- corrector approach as in Munthe-Kaas (1999). Secondly we shall use the self starting algorithm of Fatokun and Onumanyi (2008) and Fatokun (2007). This is done by using the idea of block methods as illustrated below:

Let

$$\begin{aligned} y(\xi) = \phi_0(\xi)\, y_r + \Psi_0(\xi) z_r + \Psi_1(\xi) z_{r+1} + \\ \Psi_2(\xi) z_{r+3/2} + \Psi_3(\xi) z_{r+2} \end{aligned} \quad (26)$$

The corresponding D (collocation matrix) is given as:

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

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

Where, D is invertible DC = I and hence, we obtain explicitly y (ξ) in Eq. 26 with

$$\phi_0(\xi) = 1$$

$$\psi_0(\chi) = \frac{1}{12h^3}\begin{Bmatrix} -(x-x_r)^4 + 6h(x-x_r)^3 - \\ 13h^2(x-x_r)^2 + 12h^3(x-x_r) \end{Bmatrix}$$

$$\psi_1(\chi) = \frac{1}{6h^3}\left\{3(x-x_r)^4 - 14h(x-x_r)^3 + 18h^2(x-x_r)\right\}$$

$$\psi_2(\chi) = \frac{1}{3h^3}\left\{-2(x-x_r)^4 + 8h(x-x_r)^3 - 8h^2(x-x_r)^2\right\}$$

$$\psi_3(\chi) = \frac{1}{12h^3}\left\{3(x-x_r)^4 - 10h(x-x_r)^3 + 9h^2(x-x_r)^2\right\}.$$

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

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

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

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

Solving the Eq. 28-30, simultaneously as an A-stable integrator for z_{r+1}, $z_{r+2/3}$ and z_{r+2} give the following first derivative FD approximation schemes

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

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

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

Now, we put Eq. 31 and 33, respectively in the following algorithm:

$$\begin{aligned} z_{r+1} = \frac{1}{4h}\left(y_{r+2} + 4y_{r+1} - 5y_r\right) \\ -\frac{1}{2}z_r,\ \text{order } 2, c_3 = \frac{-1}{240} \end{aligned} \quad (34)$$

$$\begin{aligned} z_{r+2} = \frac{2}{h}\left(y_{r+2} - 2y_{r+1} + y_r\right) + z_r \\ \text{order } 2,\ c_3 = \frac{-1}{6} \end{aligned} \quad (35)$$

to obtain the final algorithm to solve Eq. 11.

Numerical experiment: Munthe-Kaas (1999) used an example by Zanna (1999), 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 λ: g $\times$G $\rightarrow$ G, where $\lambda_{(v,p)}$ = exp (v).p. This reduces Eq. 11 to a first order differential Eq. 36:

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

This was conveniently solved as in Munthe-Kaas (1999).

CONCLUSION

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

In a follow-up study, we shall consider some second order differential equations on manifold and use the self-starting approach described in this research. 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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