UNIVERSITY OF CAMBRIDGE

Numerical Analysis Reports

Linear ODEs in Lie groups

A. Iserles & S.P. Nørsett

DAMTP 1997/NA9
May 1997

Department of Applied Mathematics and Theoretical Physics
Silver Street
Cambridge
England CB3 9EW

Linear ODEs in Lie groups

Arieh Iserles
DAMTP, University of Cambridge
Silver Street, Cambridge CB3 9EW, England
email: A.Iserles@damtp.cam.ac.uk

and

Syvert P. Nørsett
Institutt for matematiske fag, Norges teknisk-naturvitenskapelige universitet
N-7034 Trondheim, Norway
Syvert.Norsett@math.ntnu.no

Keywords: Lie groups, Lie algebras, numerical methods, rooted trees, multivariate quadrature.

ABSTRACT

The solution of $Y' = A(t)Y, Y(0) = Y_0$, where Y is in a matrical Lie group G and $A(t)$ is in the Lie algebra of G, is discussed in this article. The basis of our approach are generalized iterated commutators. In that manner we can approximate the solution to an arbitrarily high order. The exact solution is given as an infinite series of commutators and order conditions are studied by using binary trees. An important part of our method is a surprising result on multivariate quadrature of multilinear forms over certain simplices, that allows us to decrease the number of function evaluations. The cost of the method can be further decreased by combinatorial considerations.

INTRODUCTION

In this paper we intend to discuss the *Lie type equation*

$$Y'(t) = A(t, Y(t))Y(t), \quad t \geq 0, \qquad Y(0) = Y_0 \in G \tag{1}$$

Here G is a Lie group and $A(t, Y(t)))$ is a mapping from $\mathbb{R}^+ \times G$ to g, the Lie algebra associated with G. Since every connected and simply-connected finite-dimensional Lie group is isomorphic to a subgroup of a matricial Lie group, we henceforth assume that G is a matricial Lie group. Obviously we can solve (1) by a classical method, e.g. a linear multistep method or a Runge–Kutta scheme. However, it has been pointed out by Iserles [6] that the approximations obtained by these methods do not stay on general nonlinear manifolds (except for some Runge–Kutta schemes that retain quadratic conservation laws). Hence there is a need for new methods which ensure that the numerical discretization stays on the correct manifold, thereby retaining an important structural feature of the underlying differential system. In recent years there has emerged a growing interest in this problem and it is illustrated by the papers of Crouch & Grossman [3], Munthe-Kaas [9], Owren & Martinsen [10] and Zanna [11].

A major feature of all these methods is that the numerical solution is evaluated locally in the tangent space, being subsequently mapped to the underlying manifold. In the context of Lie groups, the tangent space is the Lie algebra g and the required mapping (for matricial Lie groups) is the matrix exponential.

This brief review is based in the main on the recent paper of the authors [7] and it represents very recent results and work that is largely in progress.

ITERATED COMMUTATORS

The theme of this paper is the linear equation

$$Y'(t) = A(t)Y(t), \quad t \geq 0, \quad Y(0) = Y_0 \in G, \tag{2}$$

although our results are relevant to the more general problem (1). Note that, even if the equation is linear, classical methods do not fulfil our goal of staying on the manifold.
The technique of *iterated commutators* was discussed in a paper by Iserles [5] from 1984. If the system is scalar then the exact solution of (2) is trivially

$$Y(t) = \mathrm{e}^{\int_0^t A(\tau)\mathrm{d}\tau} Y_0.$$

This motivates the representation (in the general matrix case) of the solution as a product of matrix exponentials. The basic idea starts by setting

$$\tilde{Y}(t) := \mathrm{e}^{-\int_0^t A(\tau)\mathrm{d}\tau} Y(t), \qquad t \geq 0.$$

The matrix function $\tilde{Y}(t)$ also satisfies a linear differential equation , specifically

$$\tilde{Y}' = \tilde{A}(t)\tilde{Y} \quad t \geq 0, \qquad \tilde{Y}(0) = Y_0,$$

where

$$\tilde{A}(t) = \sum_{k=1}^{\infty} \frac{k}{(k+1)!} \mathrm{ad}^k \left(A(t), \int_0^t A(\tau)\mathrm{d}\tau \right).$$

Here

$$\mathrm{ad}^k(P,Q) = \begin{cases} P, & k = 0, \\ [\mathrm{ad}^{k-1}(P,Q), Q], & k \in \mathbb{N}. \end{cases}$$

If A(t)=$\mathcal{O}(1)$ then $\tilde{A}(t) = \mathcal{O}(t^2)$. Therefore

$$\mathrm{e}^{\int_0^t A(\tau)\mathrm{d}\tau} Y_0 = Y(t) + \mathcal{O}(t^3).$$

Continuing this procedure by induction, we obtain

$$\begin{aligned} \mathrm{e}^{\int_0^t A(\tau)\mathrm{d}\tau} \mathrm{e}^{\int_0^t \tilde{A}(\tau)\mathrm{d}\tau} Y_0 &= Y(t) + \mathcal{O}(t^7), \\ \mathrm{e}^{\int_0^t A(\tau)\mathrm{d}\tau} \mathrm{e}^{\int_0^t \tilde{A}(\tau)\mathrm{d}\tau} \mathrm{e}^{\int_0^t \tilde{\tilde{A}}(\tau)\mathrm{d}\tau} Y_0 &= Y(t) + \mathcal{O}(t^{15}) \end{aligned}$$

and, in general, the order after q iterations is $2^{q+1} - 2$.

MAGNUS SERIES

As already noted in the previous section, the solution of equation (2) in the general case cannot be written as a single matrix exponential of a single integral. However, Hausdorff [4] found that one can write it as a single matrix exponential of a function,

$$Y(t) = \mathrm{e}^{\sigma(t)} Y_0 \qquad \text{where} \qquad \sigma(t) \in g.$$

Here σ is the solution of the implicit, nonlinear equation

$$\sum_{k=0}^{\infty} \frac{(-1)^k}{(k+1)!} \mathrm{ad}^k(\sigma', \sigma) = a, \quad t \geq 0, \qquad \sigma(0) = 0.$$

Fortunately this odd-looking equation was rendered into a considerably more user-friendly form by Wilhelm Magnus [8],

$$\sigma' = a + \frac{1}{2}\mathrm{ad}(a,\sigma) + \sum_{k=1}^{\infty} \frac{B_{2k}}{(2k)!}\mathrm{ad}^{2k}(a,\sigma),$$

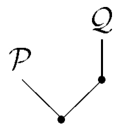
where B_ℓs are the *Bernoulli numbers.* Furthermore Magnus observed that

$$\begin{aligned}
\sigma(t) \;=\; & \int_0^t A(\tau)\mathrm{d}\tau \\
& + \frac{1}{2}\int_0^t \left[A(\tau), \int_0^\tau A(\xi)\mathrm{d}\xi\right] \mathrm{d}\tau \\
& + \frac{1}{4}\int_0^t \left[A(\tau), \int_0^\tau \left[A(\xi), \int_0^\xi A(\zeta)\mathrm{d}\zeta\right] \mathrm{d}\xi\right] \mathrm{d}\tau \\
& + \frac{1}{12}\int_0^t \left[\left[A(\tau), \int_0^\tau A(\xi)\mathrm{d}\xi\right], \int_0^\tau A(\zeta)\mathrm{d}\zeta\right] \mathrm{d}\tau \\
& + \cdots.
\end{aligned}$$

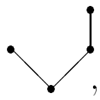
Note that all the individual terms live in g, hence so does their linear combination.
However, Magnus provides neither a formula (or a constructive algorithm) for the evaluation of the full expansion nor analyses the speed of convergence and the order of a truncated approximation.

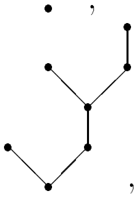
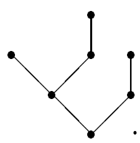
BINARY TREES AND ORDER RESULTS

Graph theory proved itself as an incisive tool in order analysis of classical Runge–Kutta methods [1]. It is equally useful, in a different setting, in the context of Magnus series. Indeed, the main step allowing us to derive the full expansion of σ in a constructive manner is the association between individual terms and certain binary trees. We henceforth present the expansion of σ', rather than of σ, since it leads to simpler notation.
The two operations featuring in the Magnus expansion are *integration* and *commutation.* We associate them with an operation on binary trees: integration with the addition of a root and commutation with a linkage of two sub-trees by a common root. More formally, all terms (except for the first) in the Magnus series are of the form $[P, \int Q]$, where also P and Q are terms in the expansion. Suppose that P and Q have been already associated with the binary trees $\mathcal{P}$ and $\mathcal{Q}$, respectively. Then

$[P, \int Q] \quad \sim$ 

We commence the recursive procedure by associating A with the unique tree of order one. The first few terms and the corresponding trees are thus

$A \;\sim$, $[A, \int A] \;\sim$  ,

$[A, \int[A, \int A]] \;\sim$  , $[[A, \int A], \int A] \;\sim$  .

Consider the equation

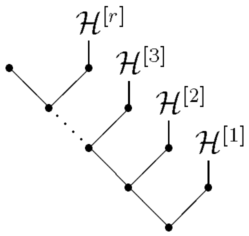
$$\sigma' = \sum_{k=0}^{\infty} f_k \mathrm{ad}^k(a,\sigma), \quad t \geq 0, \qquad \sigma(0) = 0, \tag{3}$$

where $f_0 = 1$ and $\sum_0^\infty f_k z^k$ is analytic at the origin. We expand

$$\sigma = \sum_{n=1}^{\infty} \sum_{m \in C_n} \alpha_m H_m, \tag{4}$$

where $H_m \sim \mathcal{H}_m$, say, and the inner summation is carried over the set C_n of all binary trees $\mathcal{H}_m$ (*modulo* equivalences) of order n.

Substitution of the above form of σ into (3) leads, after some manipulation, to a recursive formula for the determination of the coefficients α_m. Specifically, each $\mathcal{H}$ can be written in a unique way as

$\mathcal{H} =$ 

where $\mathcal{H}^{[k]}$, $k = 1, 2, \ldots, r$, are lower-order trees with the coefficients $\alpha^{[k]}$, $k = 1, 2, \ldots, r$, respectively. In that case the coefficient corresponding to the term $H \sim \mathcal{H}$ is

$$\alpha = f_r \prod_{k=1}^{r} \alpha^{[k]}.$$

Since the coefficient of the first term, A, is unity, we have thus a recursive rule for the evaluation of the Magnus expansion (4).

Each binary tree corresponding to a term in the expansion is of order $1 \bmod 3$ and it is possible to prove that $H \sim \mathcal{H}$, where $\operatorname{ord}\mathcal{H} = 3n + 1$, $n \geq 1$, implies $H(t) = \mathcal{O}(t^{n+1})$. This is a crucial step in proving the local convergence of the Magnus expansion in Iserles & Nørsett [7].

QUADRATURE

On the face of it, the most cost-intensive step in a numerical implementation of a Magnus expansion is the replacement of integrals by quadratures. As is well-known, the approximation of multivariate integrals to high order usually entails a very large number of function evaluations [2]. Fortunately, it is possible to take advantage of the special structure of our problem to reduce drastically the numerical cost.

The domains of integration in Magnus series are simplices $h\mathcal{S}$, where

$$\mathcal{S} = \{(t_1, t_2, \ldots, t_m) \,:\, 0 \leq t_j \leq t_{i_j},\ j = 1, 2, \ldots, m\},$$

where $t_0 = 1$ and $i_j \in \{1, 2, \ldots, j\}$, $j = 1, 2, \ldots, m$. The integrand itself is an m-linear form $\mathcal{L}$, say, acting on the arguments $A(t_1), A(t_2), \ldots, A(t_m)$. We approximate

$$\int_{h\mathcal{S}} \mathcal{L}(A(t_1), A(t_2), \ldots, A(t_m))\mathrm{d}t_m \mathrm{d}t_{m-1} \cdots \mathrm{d}t_1 \approx h^m \sum_{\mathbf{i} \in \Lambda_m^\nu} b_{\mathbf{i}} \mathcal{L}(A(c_{i_1}h), A(c_{i_2}h), \ldots, A(c_{i_\nu})),$$

where $c_1, c_2, \ldots, c_\nu$ are quadrature points in $[0, 1]$ and Λ_m^ν is the set of all combinations of length ν from the set $\{1, 2, \ldots, m\}$.

It has been proved in [7] that, with an appropriate choice of the weights $b_{\mathbf{i}}$ (which can be deduced from the corresponding binary tree), the above quadrature formula is of order $p = \nu + s$, where $s \geq 0$ is the largest integer such that

$$\int_0^1 t^{k-1} \prod_{j=1}^{\nu} (t - c_j)\mathrm{d}t = 0, \qquad k = 1, 2, \ldots, s.$$

Therefore, choosing $c_1, c_2, \ldots, c_\nu$ as Gauss–Legendre points leads to an order-2ν quadrature formula. Note that just ν function evaluations are required to approximate *all* the necessary integrals in the Magnus expansion!

As an example of this procedure, herewith fourth-order formulae for the first four integrals in the Magnus expansion:

$$
\begin{aligned}
\int_0^h A(t_1)\mathrm{d}t_1 &\approx \tfrac{1}{2}h(A_1 + A_2), \\
\int_0^h \int_0^{t_1} [A(t_1), A(t_2)]\mathrm{d}t_2\mathrm{d}t_1 &\approx -\tfrac{\sqrt{3}}{6}h^2[A_1, A_2], \\
\int_0^h \int_0^{t_1} \int_0^{t_1} [A(t_1), [A(t_2), A(t_3)]]\mathrm{d}t_3\mathrm{d}t_2\mathrm{d}t_1 &\approx h^3[(\tfrac{3}{80} - \tfrac{\sqrt{3}}{48})A_1 - (\tfrac{3}{80} + \tfrac{\sqrt{3}}{48})A_2, [A_1, A_2]], \\
\int_0^h \int_0^{t_1} \int_0^{t_1} [[A(t_1), A(t_2)], A(t_3)]\mathrm{d}t_3\mathrm{d}t_2\mathrm{d}t_1 &\approx h^3[(\tfrac{3}{80} + \tfrac{\sqrt{3}}{16})A_1 - (\tfrac{3}{80} - \tfrac{\sqrt{3}}{16})A_2, [A_1, A_2]].
\end{aligned}
$$

Here

$$A_1 = A((\tfrac{1}{2} - \tfrac{\sqrt{3}}{6})h), \qquad A_2 = A((\tfrac{1}{2} + \tfrac{\sqrt{3}}{6})h).$$

Assembling the above quadratures results in a fourth-order method for the linear equation (2) which respects arbitrary Lie-group structure,

$$
\begin{aligned}
A_1 &= A(t_n + (\tfrac{1}{2} - \tfrac{\sqrt{3}}{6})h), \qquad A_2 = A(t_n + (\tfrac{1}{2} + \tfrac{\sqrt{3}}{6})h), \\
\Sigma &= \tfrac{1}{2}h[A_1 + A_2] - \tfrac{\sqrt{3}}{12}h^2[A_1, A_2] + \tfrac{1}{80}h^3[A_1 - A_2, [A_1, A_2]], \\
Y_{n+1} &= \mathrm{e}^{\Sigma}Y_n.
\end{aligned}
\tag{5}
$$

Higher-order quadrature requires the evaluation of a considerably larger number of commutators. However, using techniques from combinatorics and the theory of Lie algebras, it is possible to reduce greatly the computational cost [7].

NUMERICAL RESULTS

The fourth-order method (5) was applied in [7] to a number of linear equations (2). Predictably, it conserves Lie structure, e.g. of equations in $\mathrm{SL}_m[\mathbb{R}]$ and in $\mathrm{SU}_m[\mathbb{C}]$. Perhaps more intriguing is, however, the remarkably good performance of (5) when applied to the Airy equation $y'' + ty = 0$, $0 \le t \le 100$, vastly superior to classical fourth-order methods.

The implementation of (5) with variable steps and local error control is a subject to ongoing research by the authors, together with Arne Marthinsen.

REFERENCES

[1] J.C. Butcher, "The Numerical Analysis of Ordinary Differential Equations", John Wiley, New York (1987).

[2] R. Cools, *Constructing cubature formulae: the science behind the art,* Acta Numerica **6** (1997), 1–54.

[3] P. Crouch, R. Grossman, *Numerical integration of ordinary differential equations on manifolds,* J. Nonlinear Sc. **3** (1993), 1–33.

[4] F. Hausdorff, *Die symbolische Exponentialformel in der Gruppentheorie,* Berichte der Sächsischen Akademie der Wissenschaften (Math. Phys. Klasse) **58** (1906), 19–48.

[5] A. Iserles, *Solving linear ordinary differential equations by exponentials of iterated commutators,* Numer. Math. **45** (1984), 183–199.

[6] A. Iserles, *Numerical methods on (and off) manifolds,* in "Foundations of Computational Mathematics" (F. Cucker & M. Shub, eds), Springer-Verlag, New York (1997), 180–189.

[7] A. Iserles, S.P. Nørsett, *On the solution of linear differential equations in Lie groups,* DAMTP Tech. Report 1997/NA3, University of Cambridge (1997).

[8] W. Magnus, *On the exponential solution of differential equations for a linear operator,* Comm. Pure & Appl. Maths **7** (1954), 649–673.

[9] H. Munthe-Kaas, *Runge–Kutta methods on Lie groups,* Dept of Informatics Tech. Rep. 122, University of Bergen (1997).

[10] B. Owren, A. Marthinsen, *Integration methods based on rigid frames,* Norwegian University of Science & Technology Tech. Report (1997).

[11] A. Zanna, *The method of iterated commutators for ordinary differential equations on Lie groups,* Tech. Rep. DAMTP 1996/NA12, University of Cambridge (1996).