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Improved High Order Integrators Based on Magnus Expansion

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IMPROVED HIGH ORDER INTEGRATORS BASED ON MAGNUS EXPANSION

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Abstract

We build high order efficient numerical integration methods for solving the linear differential equation $\dot{X} = A(t)X$ based on Magnus expansion. These methods preserve qualitative geometric properties of the exact solution and involve the use of single integrals and fewer commutators than previously published schemes. Sixth- and eighth-order numerical algorithms with automatic step size control are constructed explicitly. The analysis is carried out by using the theory of free Lie algebras.

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1 Introduction

The aim of this paper is to construct efficient numerical integration algorithms for solving the initial value problem defined by the linear differential equation

$$\frac{dX}{dt} = A(t)X, \qquad X(t_0) = I. \tag{1}$$

Here $A(t)$ stands for a sufficiently smooth matrix or linear operator to ensure the existence of solution. As is well known, (1) governs the evolution of a great variety of physical systems. In particular, the time evolution of any quantum mechanical system is described by an equation of this type.

From the general theory of ordinary differential equations, if A is a continuous n-by-n matrix of (complex) functions on a real t interval the matrix differential equation (1) may be considered to be associated with the linear homogeneous system of the n-th order

$$\frac{d\mathbf{u}}{dt} = A(t)\,\mathbf{u}, \qquad \mathbf{u}(t_0) = \mathbf{u}_0 \tag{2}$$

with $\mathbf{u} \in \mathbb{C}^n$, in the sense that

$$\mathbf{u}(t) = X(t,t_0)\,\mathbf{u}_0 \tag{3}$$

is a solution of (2) if $X(t,t_0)$ satisfies (1).

In recent years there has been an increasing interest in designing numerical schemes for solving differential equations that preserve geometric and qualitative properties of the exact solution. For example, in classical Hamiltonian dynamics there are a large number of references on symplectic integration algorithms (see [22] for a review). More generally, the numerical integration of differential equations in Lie groups in such a way that characteristic properties, associated with the algebraic structure of the system, are preserved has received considerable attention [7, 11]. The fundamental motivation for using this kind of schemes rather than general algorithms can be stated as follows: "... an algorithm which transforms properly with respect to a class of transformations is more basic than one that does not. In a sense the invariant algorithm attacks the problem and not the particular representation used..." ([10], cited by [5]).

It has been known for a long time that the solution of (1) can locally be written in the form [15]

$$X(t,t_0) = e^{\Omega(t,t_0)}, \tag{4}$$

where Ω is obtained as an infinite series

$$\Omega(t,t_0) = \sum_{k=1}^{\infty} \Omega_k(t,t_0). \tag{5}$$

Equations (4) and (5) constitute the so-called Magnus expansion of the solution $X(t,t_0)$. Explicit formulae for Ω_k of all orders have been given recently in [11] by using graph theory techniques, although expressions for $k \leq 5$ were already available in terms of nested commutators of $A(t)$ and multivariate integrals [20, 14, 16, 21]. What is more significant for our purposes, a recursive procedure has been designed for the generation of Ω_k [14] that allows also to enlarge the t-domain of convergence of the expansion [2].

An important advantage of the Magnus expansion is that, even if the series (5) is truncated, it still preserves intrinsic geometric properties of the exact solution. For instance, if equation (1) refers to the quantum mechanical evolution operator, the approximate analytical solution obtained by Magnus expansion is still unitary no matter where the series (5) is truncated. More generally, if (1) is considered on a Lie group G, $e^{\Omega(t,t_0)}$ stays on G for all t, provided $A(t)$ belongs to the Lie algebra associated with G.

In this paper we design a whole family of new high order numerical integrators for eq. (1) by appropriately truncating the Magnus series (5) and replacing the multivariate integrals appearing in Ω_k by single analytical integrals and conveniently chosen quadrature formulae. The approach we follow is different from that used by Iserles and Nørsett in their pioneering work [11]. As a result, the time-symmetric algorithms we obtain are optimal with respect to the number of commutators involved, and can be easily implemented with a variable step size control device still retaining important structural properties of the original dynamical system.

The plan of the paper is as follows. In section 2 we introduce the recurrence relation used for constructing explicitly the Magnus expansion and the new approximation schemes, establish the convergence of the series (5), show the equivalence of this procedure with the graph-theoretical approach and analyze the time-symmetry of the expansion. In section 3 we obtain new approximation schemes of order four, six and eigth to the Magnus expansion involving exclusively single analytical integrals with just one, four and ten commutators, respectively. These methods can be used both in perturbative analyses and as numerical integrators if the univariate integrals are evaluated exactly. In section 4 we discuss some issues related to the implementation of the new schemes as practical integration algorithms: we propose two families of such algorithms based on different symmetric quadrature rules, design some hybrid methods involving analytical integrals and quadratures, and present a new way of implementing step size control. Finally, section 5 contains our conclusions.

2 A review of the Magnus series expansion

2.1 The recurrence

Magnus procedure for solving (1) is to consider the representation $X = e^{\Omega}$. If this is substituted in the equation, the following nonlinear differential equation for Ω is obtained [15, 14, 23]

$$\dot{\Omega} = \sum_{j=0}^{\infty} \frac{B_j}{j!} (\mathrm{ad}_{\Omega})^j A, \qquad \Omega(t_0 = 0) = 0. \tag{6}$$

Here the dot stands for time derivative, B_j are Bernoulli numbers [1], and we introduce the adjoint operator: $\mathrm{ad}_{\Omega}^{0} A = A$, $\mathrm{ad}_{\Omega}(A) = [\Omega, A] \equiv \Omega A - A\Omega$, $\mathrm{ad}_{\Omega}^{j} A = \mathrm{ad}_{\Omega}(\mathrm{ad}_{\Omega}^{j-1} A)$.

When the Magnus series $\Omega = \sum_{j=1}^{\infty} \Omega_j$ is substituted into equation (6) one gets [14]

$$\Omega_n(t) = \sum_{j=0}^{n-1} \frac{B_j}{j!} \int_0^t S_n^{(j)}(\tau) d\tau, \qquad n \geq 1 \tag{7}$$

with the functions $S_n^{(j)}$ satisfying the recurrence relation

$$\begin{aligned} S_1^{(0)} &= A; \qquad S_n^0 = 0, \qquad n > 1 \\ S_n^{(j)} &= \sum_{m=1}^{n-j} \left[\Omega_m, S_{n-m}^{(j-1)} \right], \qquad 1 \leq j \leq n-1 \end{aligned} \tag{8}$$

so that they have the generic structure

$$S_n^{(j)} = \sum \; [\Omega_{i_1}, [\ldots [\Omega_{i_k}, A] \ldots]] \tag{9}$$

with the sum extended over all $i_1, \ldots, i_k$ such that $i_1 + \cdots + i_k = n - 1$. From this recurrence we get

$$\begin{aligned} \Omega_1(t) &= \int_0^t A(t_1) dt_1 \\ \Omega_2(t) &= \frac{1}{2} \int_0^t dt_1 \int_0^{t_1} dt_2 [A(t_1), A(t_2)] \\ \Omega_3(t) &= \frac{1}{6} \int_0^t dt_1 \int_0^{t_1} dt_2 \int_0^{t_2} dt_3 ([A(t_1), [A(t_2), A(t_3)]] + [A(t_3), [A(t_2), A(t_1)]]), \end{aligned} \tag{10}$$

etc. In general, Ω_k is a k-multivariate integral involving a linear combination of k nested commutators of A evaluated at different times t_i, $i = 1, \ldots, k$.

It is important to emphasize that if (8) is substituted in (7) we are able to obtain bounds on the functions $\Omega_n(t)$ and, consequently, an estimate on the convergence t-domain of the expansion. More specifically, if the matrix $A(t)$ is bounded and $\|A(t)\|$ is a piecewise continuous function, then absolute convergence of Magnus series is ensured for t values which satisfy [2]

$$K(t) \equiv \int_0^t \|A(\tau)\| \, d\tau < \xi \equiv 1.086869. \tag{11}$$

2.2 Connection with the graph-theoretical formalism

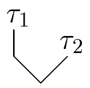
The first analysis of Magnus expansion as a numerical method for integrating matrix differential equations was given by Iserles and Nørsett [11], their point of departure being the correspondence between the terms in Magnus expansion and a subset of binary rooted trees. Thus, by using graph theory, they present a recursive rule of the generation of the different terms and a procedure for reducing the number of commutators and quadratures involved. For completeness, in the sequel we establish the equivalence of the recurrence (7) and (8) with the graph theoretical approach.

In essence, the idea of Iserles and Nørsett is to associate each term in the expansion with a rooted tree, according to the following prescription.

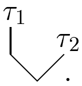
Let us define

$$\mathcal{T}_0 = \{\, \bullet \,\}, \qquad \text{where} \qquad A(t) \rightsquigarrow \bullet\,,$$

and recursively

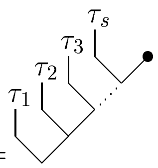
$$\mathcal{T}_m = \Big\{$$  $$:\ \tau_1 \in \mathcal{T}_{k_1},\ \tau_2 \in \mathcal{T}_{k_2},\ k_1 + k_2 = m-1 \Big\}.$$

Then, given two expansion terms H_{τ_1} and H_{τ_2}, which have been associated with $\tau_1 \in \mathcal{T}_{k_1}$ and $\tau_2 \in \mathcal{T}_{k_2}$, respectively ($k_1 + k_2 = m-1$), we associate

$$H_\tau(t) = \left[\int_0^t H_{\tau_1}(\xi) d\xi, H_{\tau_2}(t) \right] \qquad \text{with} \qquad \tau =$$  .

These composition rules establish a one-to-one relationship between a rooted tree $\tau \in \mathcal{T} \equiv \cup_{m\geq 0} \mathcal{T}_m$, and a matrix function $H_\tau(t)$ involving A, multivariate integrals and commutators.

It turns out that every $\tau \in \mathcal{T}_m$, $m \geq 1$, can be written in a unique way as

$\tau =$ 

or $\tau = a(\tau_1, \tau_2, \ldots, \tau_s)$. Then Magnus expansion can be expressed in the form

$$\Omega(t) = \sum_{m=0}^{\infty} \sum_{\tau \in \mathcal{T}_m} \alpha(\tau) \int_0^t H_\tau(\xi) d\xi, \tag{12}$$

with $\alpha(\,\bullet\,) = 1$ and

$$\alpha(\tau) = \frac{B_s}{s!} \prod_{l=1}^{s} \alpha(\tau_l),$$

so that

$$\sum_{m=0}^{\infty} \sum_{\tau \in \mathcal{T}_m} \alpha(\tau) H_\tau(t) = \sum_{s=1}^{m} \frac{B_s}{s!} \sum_{\substack{k_1,\ldots,k_s \\ k_1+\cdots+k_s = m-s}} \sum_{\tau_i \in \mathcal{T}_i} \alpha(\tau_1) \cdots \alpha(\tau_s) H_{a(\tau_1,\ldots,\tau_s)}.$$

Thus, by comparing (7) and (12) we have

$$\Omega_m(t) = \sum_{\tau \in \mathcal{T}_{m-1}} \alpha(\tau) \int_0^t H_\tau(\xi) d\xi = \sum_{j=1}^{m-1} \frac{B_j}{j!} \int_0^t S_m^{(j)}(\xi) d\xi$$

and finally

$$S_m^{(j)} = \sum_{\substack{k_1,\dots,k_j \\ k_1+\dots+k_j=m-1-j}} \sum_{\tau_i \in \mathcal{T}_i} \alpha(\tau_1)\cdots\alpha(\tau_j) H_{a(\tau_1,\dots,\tau_j)}.$$

In other words, each term $S_n^{(j)}$ in the recurrence (8) carries on a complete set of binary trees. Thus, the use of (7) and (8) can be particularly well suited when high orders of the expansion are considered, for two reasons: (i) the enormous number of trees involved and (ii) in (12) many terms are redundant, and a careful graph theoretical analysis is needed to deduce which terms have to be discarded [11].

2.3 Time-symmetry of the expansion

The linear differential equation

$$\dot{X} = A(t)X, \qquad X(t_0) = X_0 \tag{13}$$

is time-symmetric, in the sense that, for every $t_f \geq t_0$, integrating (13) from $t = t_0$ to $t = t_f$, followed by the integration of

$$\dot{Y} = -A(t_0 + t_f - t)Y, \qquad Y(t_0) = X(t_f) \tag{14}$$

in the same range, bring us back to the initial condition X_0. If we denote by $\Lambda(t_f, t_0)$ the Magnus expansion of (14), then time-symmetry implies that

$$\Omega(t_f, t_0) + \Lambda(t_f, t_0) = 0$$

and, since all the terms Ω_k are independent,

$$\Omega_k(t_f, t_0) = -\Lambda_k(t_f, t_0) \qquad \text{for all } k.$$

Observe that $\Lambda(t_f, t_0)$ has exactly the same structure as $\Omega(t_f, t_0)$ but reversing the sign of A and interchanging t_0 and t_f.

To take advantage of the time-symmetry, let us write the solution of (13) at the final time $t_f = t_0 + h$ as

$$X(t_{1/2} + \frac{h}{2}) = \exp\left(\Omega(t_{1/2} + \frac{h}{2}, t_{1/2} - \frac{h}{2})\right) X(t_{1/2} - \frac{h}{2}), \tag{15}$$

where $t_{1/2} = (t_0 + t_f)/2$. Then

$$X(t_{1/2} - \frac{h}{2}) = \exp\left(-\Omega(t_{1/2} + \frac{h}{2}, t_{1/2} - \frac{h}{2})\right) X(t_{1/2} + \frac{h}{2}). \tag{16}$$

On the other hand, the solution at t_0 can be written as

$$X(t_{1/2} - \frac{h}{2}) = \exp\left(\Omega(t_{1/2} - \frac{h}{2}, t_{1/2} + \frac{h}{2})\right) X(t_{1/2} + \frac{h}{2}), \tag{17}$$

so that, by comparing (16) and (17),

$$\Omega(t_{1/2} - \frac{h}{2}, t_{1/2} + \frac{h}{2}) = -\Omega(t_{1/2} + \frac{h}{2}, t_{1/2} - \frac{h}{2}) \tag{18}$$

and so Ω does not contain even powers of h. If $A(t)$ is an analytic function and a Taylor series centered around $t_{1/2}$ is considered, then each term in Ω_k is an odd function of h and, in particular, $\Omega_{2i+1} = O(h^{2i+3})$ for $i \geq 1$. This fact has been noticed in [13] and [19].

3 Approximation schemes based on Magnus expansion

3.1 General considerations

The usual procedure for implementing Magnus expansion as a practical integration algorithm involves three steps. First, the Ω series is truncated at an appropriate order. Second, the multivariate integrals in Ω are replaced by conveniently chosen quadratures. Third, the exponential of the resulting approximation to the matrix Ω is computed.

Concerning the first aspect, it is clear from (18) that, for achieving a $2n$-th ($n > 1$) order integration method only terms up to Ω_{2n-2} in the Ω series are required [11, 4].

On the other hand, Iserles and Nørsett [11] have demonstrated how Ω_k, $k > 1$, can be approximated in terms of nested commutators of $A(t_{i_k})$ at different nodes $t_{i_k} \in [t_0, t_0 + h]$, h being the time step size:

$$\Omega_k = h^k \sum_{1 \leq i_1, i_2, \ldots, i_k \leq N} \beta_{i_1 i_2 \cdots i_k} \, [A(t_{i_1}), [A(t_{i_2}), \ldots, A(t_{i_k})]] + O(h^{2n+1}). \tag{19}$$

Then, in terms of function evaluations, the cost of all the multivariate quadratures needed to approximate Magnus expansion to given order is the same as the cost of the single quadrature formula for Ω_1.

The coefficients $\beta_{i_1 i_2 \cdots i_k}$ in (19) have to satisfy an extraordinarily large system of linear equations for $n \geq 3$ and consequently the number of commutators required grows rapidly with the order, this fact being the bottleneck for the practical utility of this class of methods.

Different strategies have been analyzed to reduce the total number of commutators, including the use of time-symmetry and the concept of a graded free Lie algebra [19]. The usual approach consists in constructing an interpolating approximation $\tilde{A}$ of the matrix A based on Gauss-Legendre points and then compute the truncated Magnus expansion for $\tilde{A}$. This process can be implemented in a symbolic computation package [17, 19]. As a result, methods of order 4, 6 and 8 using Gauss-Legendre quadratures have been obtained with 2, 7 and 22 independent terms. In the case of the 4-th and 6-th order schemes, these terms are combined in such a way that the actual number of commutators reduces to 1 and 5, respectively [19].

A different procedure for obtaining integration methods based on Magnus expansion was proposed in [3, 4]. The idea is to apply directly the recurrence (7)-(8) to a Taylor series expansion of the matrix $A(t)$ and then to reproduce the resulting expression of Ω with a linear combination of nested commutators involving A evaluated at certain quadrature points. In this way, some 4-th and 6-th order methods with one and seven commutators were designed, both with Gauss-Legendre and Newton-Cotes quadrature rules [3, 4].

Here we pursue this strategy and, by a careful analysis of the different terms of the expansion concerning its behaviour with respect to time-symmetry, we obtain approximation schemes of order 6 and 8 involving the evaluation of only 4 and 10 commutators, respectively. The new methods are expressed in terms of single analytical integrals, so that they can be used either as numerical schemes for carrying out the integration of (1) or as analytical approximations to the exact solution in perturbative analyses. In the first case the integrals are usually discretised with symmetric quadrature rules.

3.2 The new approximation schemes

As stated above, to take advantage of the time-symmetry property we consider a Taylor expansion of $A(t)$ around $t_{1/2} = t_0 + \frac{h}{2}$,

$$A(t) = \sum_{i=0}^{\infty} a_i \left(t - t_{1/2}\right)^i, \tag{20}$$

where $a_i = \frac{1}{i!} \frac{d^i A(t)}{dt^i}\Big|_{t=t_{1/2}}$, and then compute the corresponding expression for the terms $\Omega_k(t_0 + h, t_0)$ in the Magnus expansion. This has been done by programming the recurrence (7)-(8) in *Mathematica*, after taking into account the existing linear relations between different nested commutators due to the Jacobi identity.

For order 8, the final expressions for Ω_k, $k = 1, \ldots, 6$ obtained by our code are

$$\begin{aligned}
\Omega_1 &= h a_0 + h^3 \frac{1}{12} a_2 + h^5 \frac{1}{80} a_4 + h^7 \frac{1}{448} a_6 \\
\Omega_2 &= h^3 \frac{-1}{12}[a_0, a_1] + h^5 \Big(\frac{-1}{80}[a_0, a_3] + \frac{1}{240}[a_1, a_2] \Big) + \\
& \quad h^7 \Big(\frac{-1}{448}[a_0, a_5] + \frac{1}{2240}[a_1, a_4] - \frac{1}{1344}[a_2, a_3] \Big) \\
\Omega_3 &= h^5 \Big(\frac{1}{360}[a_0, a_0, a_2] - \frac{1}{240}[a_1, a_0, a_1] \Big) + h^7 \Big(\frac{1}{1680}[a_0, a_0, a_4] - \\
& \quad \frac{1}{2240}[a_0, a_1, a_3] + \frac{1}{6720}[a_1, a_1, a_2] + \frac{1}{6048}[a_2, a_0, a_2] - \frac{1}{840}[a_3, a_0, a_1] \Big)
\end{aligned}$$

Method of order	$s=4$	$s=6$	$s=8$	$s=10$
Dimension of $\mathfrak{g}$	7	22	70	225
Magnus (t_0)	6	20	66	216
Magnus ($t_{1/2}$)	3	9	27	80
# commutators	1	4	10	

Table 1: *Number of terms appearing in the Magnus expansion for achieving methods of order s. The actual number of commutators of the new schemes is given in the last row.*

$$\begin{aligned}
\Omega_4 &= h^5 \frac{1}{720}[a_0,a_0,a_0,a_1] + h^7\Big(\frac{1}{6720}[a_0,a_0,a_0,a_3] - \frac{1}{7560}[a_0,a_0,a_1,a_2] + \\
&\quad \frac{1}{4032}[a_0,a_2,a_0,a_1] + \frac{11}{60480}[a_1,a_0,a_0,a_2] - \frac{1}{6720}[a_1,a_1,a_0,a_1]\Big) \\
\Omega_5 &= h^7\Big(\frac{-1}{15120}[a_0,a_0,a_0,a_0,a_2] - \frac{1}{30240}[a_0,a_0,a_1,a_0,a_1] + \\
&\quad \frac{1}{7560}[a_1,a_0,a_0,a_0,a_1]\Big) \qquad (21) \\
\Omega_6 &= h^7 \frac{-1}{30240}[a_0,a_0,a_0,a_0,a_0,a_1]
\end{aligned}$$

Here we denote $[a_{i_1},a_{i_2},\ldots,a_{i_{l-1}},a_{i_l}] \equiv [a_{i_1},[a_{i_2},[\ldots,[a_{i_{l-1}},a_{i_l}]\ldots]]]$. As is well known, the matrices $q_i \equiv a_{i-1}h^i$, $i=1,2,\ldots,s$ can be considered as the generators of a graded free Lie algebra with grades $1,2,\ldots,s$ [19]. In Table 1 we show the dimension of the graded free Lie algebra $\mathfrak{g}$ involved in the process of obtaining a s-th order integration method from Magnus expansion, computed according to Munthe-Kaas and Owren [19]. We also include the *actual* number of terms appearing in the Magnus expansion when a Taylor series of $A(t)$ around $t=t_0$ (second row) and $t=t_{1/2}$ (third row) is considered. It is worth noticing how the time-symmetry reduces significantly the dimension and thus the number of determining equations to be satisfied by the integration algorithms.

Let us now introduce the univariate integrals

$$B^{(i)} = \frac{1}{h^{i+1}} \int_{-h/2}^{h/2} t^i A\left(t+\frac{h}{2}\right) dt, \qquad i=0,1,2,\ldots \qquad (22)$$

When the Taylor series (20) is inserted into (22) we get

$$\begin{aligned}
B^{(0)} &= a_0 + \frac{1}{12}h^2 a_2 + \frac{1}{80}h^4 a_4 + \frac{1}{448}h^6 a_6 + \cdots \\
B^{(1)} &= \frac{1}{12}h a_1 + \frac{1}{80}h^3 a_3 + \frac{1}{448}h^5 a_5 + \cdots \qquad (23) \\
B^{(2)} &= \frac{1}{12}a_0 + \frac{1}{80}h^2 a_2 + \frac{1}{448}h^4 a_4 + \frac{1}{2304}h^6 a_6 + \cdots
\end{aligned}$$

and so on. In general, $B^{(2i)}(-h) = B^{(2i)}(h)$ (containing only elements a_{2j}) and $B^{(2i+1)}(-h) = -B^{(2i+1)}(h)$ (containing only a_{2j+1}). We observe then that the expressions of Ω_k, as collected in (21), can be rewritten in terms of the $B^{(i)}$ with a very simple change of variables. For instance, the second order approximation to the solution is given by

$$e^{\Omega} = e^{ha_0} + O(h^3) = e^{hB^{(0)}} + O(h^3)$$

whereas a 4-th order scheme is obtained

$$e^{\Omega} = e^{\Omega_1+\tilde{\Omega}_2} + O(h^5)$$

when

$$\boxed{\begin{array}{rcl} \Omega_1 &=& hB^{(0)} \\ \tilde{\Omega}_2 &=& -h^2[B^{(0)}, B^{(1)}] \end{array}} \tag{24}$$

In general, to achieve a $2n$-th order approximation to Ω it is only necessary to consider single integrals $B^{(i)}$ up to $i = n-1$.

The process for obtaining higher order approximations can be optimized to reduce the total number of commutators appearing in Ω_k (last row of Table 1) with an appropriate choice of linear combinations of the single integrals $B^{(i)}$. We illustrate the procedure by constructing schemes of order six and eight which preserve time-symmetry. We denote by $\tilde{\Omega}_i$ the corresponding approximations to Ω_i up to the order considered.

Sixth-order. The most general time-symmetric form for Ω_2 is

$$\tilde{\Omega}_2 = h^2[B^{(1)}, b_1B^{(0)} + b_2B^{(2)}]. \tag{25}$$

The coefficients b_1, b_2 are obtained by solving a linear system of three equations. In fact, only two of them are independent, so that the solution is $b_1 = 3/2$, $b_2 = -6$. For Ω_3 another linear system of two equations has to be solved, and this can be done with

$$\tilde{\Omega}_3 = c_1h^3[B^{(0)}, [B^{(0)}, B^{(2)}]] + c_2h[B^{(1)}, \tilde{\Omega}_2], \tag{26}$$

where $c_1 = 1/2$, $c_2 = 3/5$ and $\tilde{\Omega}_2$ is evaluated according to (25). Finally, the unique equation arising in Ω_4 can be solved if we take

$$\tilde{\Omega}_4 = d\,h^2[B^{(0)}, [B^{(0)}, \tilde{\Omega}_2]] \tag{27}$$

with $d = -1/60$. This can be seen by noticing that $\tilde{\Omega}_2 \propto h^3[a_0, a_1] + O(h^5)$ and $[B^{(0)}, [B^{(0)}, \cdot]]$ gives $[a_0, [a_0, \cdot]]$. In summary, the 6-th order approximation can be written as

$$\boxed{\begin{array}{rcl} \Omega_1 &=& hB^{(0)} \\ \tilde{\Omega}_2 &=& h^2[B^{(1)}, \frac{3}{2}B^{(0)} - 6B^{(2)}] \\ \tilde{\Omega}_3 + \tilde{\Omega}_4 &=& h^2[B^{(0)}, [B^{(0)}, \frac{1}{2}hB^{(2)} - \frac{1}{60}\tilde{\Omega}_2]] + \frac{3}{5}h[B^{(1)}, \tilde{\Omega}_2] \end{array}} \tag{28}$$

thus requiring the computation of only four different commutators.

Eighth-order. To reproduce the six commutators of Ω_2 we consider the combination

$$\begin{aligned} \tilde{\Omega}_2 &= h^2([b_1 B^{(0)} + b_2 B^{(2)}, B^{(3)}] + [b_3 B^{(0)} + b_4 B^{(2)}, -uB^{(1)} + B^{(3)}]) \\ &\equiv h^2(R_{21} + R_{22}). \end{aligned} \tag{29}$$

As a matter of fact, only the four parameters b_i are needed to get the coefficients in (21). The constant u has been introduced to satisfy some of the equations appearing in Ω_3 without increasing the total number of commutators. More specifically, the three equations corresponding to $[a_0, a_0, a_2]$, $[a_0, a_0, a_4]$, $[a_2, a_0, a_2]$ (containing only even subindices) can be solved with

$$R_{31} \equiv [c_1 B^{(0)} + c_2 B^{(2)}, [B^{(0)}, B^{(2)}]], \tag{30}$$

whereas for the remaining four equations we need, in particular,

$$R_{32} \equiv [B^{(3)}, c_3 R_{21} + c_4 R_{22}], \tag{31}$$

with solution

$$c_1 = \frac{19}{28}, \quad c_2 = -\frac{15}{7}, \quad c_3 = \frac{20}{7}, \quad c_4 = 10, \quad u = \frac{5}{28} \tag{32}$$

and thus

$$\tilde{\Omega}_3 = h^3(R_{31} + R_{32}).$$

For this particular value of u we get

$$b_1 = -\frac{38}{5}, \quad b_2 = 24, \quad b_3 = \frac{63}{5}, \quad b_4 = -84. \tag{33}$$

With respect to Ω_4, the equations corresponding to $[a_1, a_0, a_0, a_2]$, $[a_1, a_1, a_0, a_1]$ can be solved with

$$R_{41} \equiv [B^{(3)}, d_1 R_{31} + d_2 R_{32}] \tag{34}$$

and the remaining four equations are satisfied through the combination

$$\begin{aligned} R_{42} + R_{43} \equiv\ & [c_1 B^{(0)} + c_2 B^{(2)}, [B^{(0)}, d_3 R_{21} + d_4 R_{22}]] + \\ & [d_5 B^{(0)} + d_6 B^{(2)}, [B^{(2)}, R_{21}]] \end{aligned} \tag{35}$$

where the form of R_{42} has been chosen so as to evaluate R_{31} and R_{42} together. The coefficients are given by

$$d_1 = d_2 = \frac{20}{7}, \quad d_3 = \frac{61}{588}, \quad d_4 = -\frac{1}{12}, \quad d_5 = -\frac{6025}{4116}, \quad d_6 = \frac{2875}{343}, \tag{36}$$

and then

$$\tilde{\Omega}_4 = h^4(R_{41} + R_{42} + R_{43}).$$

Finally, for Ω_5 and Ω_6 we take

$$\begin{aligned}\tilde{\Omega}_5+\tilde{\Omega}_6 &= h^5([B^{(0)},[B^{(0)},e_1(R_{31}+hR_{42})+e_2R_{32}+hfR_{43}]]+\\ &\quad [B^{(3)},d_1R_{42}+e_3R_{43}]) \;\equiv\; h^5(R_{51}+R_{52})\end{aligned} \tag{37}$$

in order to reduce the number of commutators. The coefficients are

$$e_1=-\frac{1}{42},\quad e_2=\frac{1}{126},\quad e_3=\frac{820}{189},\quad f=-\frac{1}{42}. \tag{38}$$

As a result, the 8-th order approximation can be expressed in terms of only ten commutators. In fact, if we denote

$$\begin{array}{llll} Q_1=R_{21}, & Q_2=R_{22}, & Q_3=R_{31}+hR_{42}, & Q_4=R_{32},\\ Q_5=R_{43}, & Q_6=R_{41}+hR_{52}, & Q_7=R_{51} & \end{array}$$

we have the following algorithm

$$\begin{array}{ll} Q_1=[-\frac{38}{5}B^{(0)}+24B^{(2)},B^{(3)}] & Q_2=[\frac{63}{5}B^{(0)}-84B^{(2)},-\frac{5}{28}B^{(1)}+B^{(3)}]\\ Q_3=[\dfrac{19}{28}B^{(0)}-\dfrac{15}{7}B^{(2)},[B^{(0)},B^{(2)}+h(\dfrac{61}{588}Q_1-\dfrac{1}{12}Q_2)]] & \\ Q_4=[B^{(3)},\frac{20}{7}Q_1+10Q_2] & Q_5=[-\frac{6025}{4116}B^{(0)}+\frac{2875}{343}B^{(2)},[B^{(2)},Q_1]]\\ Q_6=[B^{(3)},\frac{20}{7}(Q_3+Q_4)+\frac{820}{189}hQ_5] & Q_7=-\frac{1}{42}[B^{(0)},[B^{(0)},Q_3-\frac{1}{3}Q_4+hQ_5]] \end{array} \tag{39}$$

and finally

$$\boxed{\begin{aligned}\Omega_1 &= hB^{(0)}\\ \tilde{\Omega}_2 &= h^2(Q_1+Q_2)\\ \tilde{\Omega}_3+\tilde{\Omega}_4+\tilde{\Omega}_5+\tilde{\Omega}_6 &= h^3(Q_3+Q_4)+h^4(Q_5+Q_6)+h^5Q_7\end{aligned}} \tag{40}$$

It is worth noticing that, due to the dependence of the univariate integrals $B^{(i)}$ on h and the structure of the approximations $\tilde{\Omega}_i$, the schemes (24), (28) and (40) are time-symmetric, as we announced previously.

4 Numerical integrators with quadratures

4.1 Numerical algorithms

The new integration methods (24), (28) and (40) can be applied directly in numerical studies of the differential equation (1) only if the components of $A(t)$ are simple enough to evaluate the integrals $B^{(i)}$ exactly. Otherwise, we must replace $B^{(i)}$ by numerical quadratures. This is necessarily so if A is known only numerically. Observe also that with the same basic quadrature we can approximate all the integrals $B^{(i)}$.

In the following we consider two different families of methods based on symmetric quadrature rules: Gauss-Legendre and Newton-Cotes. The numerical schemes obtained with the first one require less evaluations of A per step, although cannot be applied if the matrix $A(t)$ is known only numerically at a fixed number of points. This happens, for instance, when equation (1) is the variational equation corresponding to a given solution $\mathbf{x}(t)$ of a nonlinear system $\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x}, t)$. If $\mathbf{x}(t)$ is determined by a constant step size numerical method such as a symplectic integrator, then the Newton-Cotes formulae constitute the natural election.

Let us denote $A_i \equiv A(t_i + \frac{h}{2})$, the matrix A evaluated at each node of the quadrature rule. Then we approximate the univariate integrals $B^{(j)}$ up to the order considered.

(i) 6-th order method with Gauss-Legendre quadrature. The nodes of the quadrature are given by $t_1 = -vh$, $t_2 = 0$, $t_3 = vh$, with $v = \sqrt{3/20}$. If we introduce the combinations $S_1 = A_1 + A_3$, $S_2 = A_2$, and $R_1 = A_3 - A_1$, then we have

$$B^{(0)} = \frac{1}{18}(5S_1 + 8S_2), \qquad B^{(1)} = \frac{\sqrt{15}}{36}R_1, \qquad B^{(2)} = \frac{1}{24}S_1. \tag{41}$$

(ii) 6-th order method with Newton-Cotes quadrature. Now the nodes of the quadrature for approximating $B^{(i)}$ are $t_i = -\frac{h}{2} + i\frac{h}{4}$, $0 \le i \le 4$. Let us form the combinations $S_1 = A_0 + A_4$, $S_2 = A_1 + A_3$, $S_3 = A_2$ (even functions of h) and $R_1 = A_4 - A_0$, $R_2 = A_3 - A_1$ (odd functions of h). Then

$$\begin{aligned} B^{(0)} &= \frac{1}{90}(7S_1 + 32S_2 + 12S_3) \\ B^{(1)} &= \frac{1}{90}\Big(\frac{7}{2}R_1 + 8R_2\Big) \\ B^{(2)} &= \frac{1}{90}\Big(\frac{7}{4}S_1 + 2S_2\Big) \end{aligned} \tag{42}$$

(iii) 8-th order method with Gauss-Legendre quadrature. In this case, with the same notation, we have the nodes $t_1 = -t_4 = -v_1 h$, $t_2 = -t_3 = -v_2 h$, with

$$v_1 = \frac{1}{2}\sqrt{\frac{3 + 2\sqrt{6/5}}{7}}, \qquad v_2 = \frac{1}{2}\sqrt{\frac{3 - 2\sqrt{6/5}}{7}},$$

whereas the weights are

$$w_1 = \frac{1}{2} - \frac{1}{6}\sqrt{\frac{5}{6}}, \qquad w_2 = \frac{1}{2} + \frac{1}{6}\sqrt{\frac{5}{6}}.$$

If $S_1 = A_1 + A_4$, $S_2 = A_2 + A_3$, $R_1 = A_4 - A_1$, $R_2 = A_3 - A_2$, then we get

$$\begin{aligned} \begin{pmatrix} B^{(0)} \\ B^{(2)} \end{pmatrix} &= \frac{1}{2}\begin{pmatrix} 1 & 1 \\ v_1^2 & v_2^2 \end{pmatrix}\begin{pmatrix} w_1 S_1 \\ w_2 S_2 \end{pmatrix} \\ \begin{pmatrix} B^{(1)} \\ B^{(3)} \end{pmatrix} &= \frac{1}{2}\begin{pmatrix} v_1 & v_2 \\ v_1^3 & v_2^3 \end{pmatrix}\begin{pmatrix} w_1 R_1 \\ w_2 R_2 \end{pmatrix} \end{aligned} \tag{43}$$

(iv) 8-th order method with Newton-Cotes quadrature. The nodes are $t_i = -\frac{h}{2} + i\frac{h}{6}$, and we form $S_1 = A_0 + A_6$, $S_2 = A_1 + A_5$,$S_3 = A_2 + A_4$, $S_4 = A_3$,

$R_1 = A_6 - A_0$, $R_2 = A_5 - A_1$, $R_3 = A_4 - A_2$. Then

$$\begin{aligned} \begin{pmatrix} B^{(0)} \\ B^{(2)} \end{pmatrix} &= \frac{1}{840} \begin{pmatrix} 1 & 1 & 1 & 1 \\ \frac{1}{4} & \frac{1}{9} & \frac{1}{36} & 0 \end{pmatrix} \begin{pmatrix} 41S_1 \\ 216S_2 \\ 27S_3 \\ 272S_4 \end{pmatrix} \\ \begin{pmatrix} B^{(1)} \\ B^{(3)} \end{pmatrix} &= \frac{1}{840} \begin{pmatrix} \frac{1}{2} & \frac{1}{3} & \frac{1}{6} \\ \frac{1}{8} & \frac{1}{27} & \frac{1}{216} \end{pmatrix} \begin{pmatrix} 41R_1 \\ 216R_2 \\ 27R_3 \end{pmatrix} \end{aligned} \tag{44}$$

The point we want to stress here is that these numerical quadratures do, indeed, approximate the terms Ω_i in the Magnus series up to the required order, although this fact is not always obvious. For instance, the main error term in $B^{(i)}$ provided by (43) and (44) involves the coefficient a_8, a_7, a_6, a_5 for $i = 0, 1, 2, 3$, respectively. One could think, therefore, that the quadrature cannot reproduce correctly the term $[a_0, a_5$ in Ω_2 as given by (21). This is not the case, however, because the sum $Q_1 + Q_2$ in (40) can be written as

$$Q_1 + Q_2 = [5B^{(0)} - 60B^{(2)}, B^{(3)}] + [\frac{63}{5}B^{(0)} - 84B^{(2)}, -\frac{5}{28}B^{(1)}]$$

and the combination $5B^{(0)} - 60B^{(2)}$ does not depend on a_0, so that the coefficient of $[a_0, a_5]$ in $\hat{\Omega}_2$ is determined solely by $B^{(0)}$, $B^{(1)}$ and $B^{(2)}$.

The numerical integration algorithms are obtained by inserting the linear relations (41)-(44) into the schemes (28) and (40), so that the resulting $2n$-th order ($n = 3, 4$) schemes read

$$\begin{aligned} \tilde{\Omega}^{[2n]} &\equiv \sum_{i=1}^{2n-2} \tilde{\Omega}_i \\ X(t_{k+1}) &= \exp(\tilde{\Omega}^{[2n]})\, X(t_k). \end{aligned} \tag{45}$$

Observe that the resulting methods are then expressed in terms of A evaluated at the nodes of the quadrature rule chosen, but the total number of commutators does not change.

4.2 Hybrid methods

For some problems it could be difficult to evaluate exactly the integrals $B^{(i)}$ with $i \geq 1$, but not $B^{(0)}$. In that case, one should consider the possibility of designing new 'hybrid' integration methods which incoporate both $B^{(0)}$ and the function $A(t)$ computed at different terms in order to approximate Ω_i for $i > 1$. The accuracy attained by this class of methods could improve with respect to those obtained in section 4.1 because now Ω_1 is evaluated exactly. In addition, the knowledge of $B^{(0)}$ could be used to reduce the computational cost of computing the matrix A at the quadrature points.

We illustrate these hybrid methods by constructing new 4-th and 6-th order integration schemes.

Fourth-order. From (21) it is clear that

$$\Omega_1 + \Omega_2 = B^{(0)} - \frac{h^3}{12}[a_0, a_1] + O(h^5), \tag{46}$$

so that if we consider $A_0 \equiv A(t_0)$ and $A_1 \equiv A(t_0 + h)$ (thus with only one evaluation per step) we can take the following time-symmetric approximations

$$h^3[a_0, a_1] = h^2[A_0, A_1] + O(h^5) \tag{47}$$

or

$$h^3[a_0, a_1] = h^2[B^{(0)}, A_1 - A_0] + O(h^5). \tag{48}$$

Substituting (47) or (48) in (46) we obtain the desired 4-th order approximation.

Sixth-order. The scheme (28) can be approximated up to the required order if we compute $B^{(1)}$ and $B^{(2)}$ according to (41). This only requires two evaluations of $A(t)$, and the resulting method improves the sixth-order scheme using only Gaussian quadratures.

4.3 Variable step size implementation

In the literature, the usual strategy for constructing variable step size integration algorithms based on Magnus expansion relies on a local error estimate [12].

There are various generic sources of numerical errors when the Magnus expansion is implemented as a practical numerical integration method for solving equation (1). The first one is associated with the truncation of the Ω series. The second corresponds to the replacement of the multivariate integrals appearing in Ω by appropriate quadrature formulae. The third one is related to the approximation of a matrix exponential, a point not to be diminished. The first two sources of error have been analyzed in [12, 4], whereas the third aspect is discussed in detail in [18, 6, 8].

Once the local error introduced by the approximations is available, standard step size control techniques can be implemented so that the resulting scheme has an automatic step size selection device incorporated in the algorithm.

Alternatively, the local extrapolation procedure can be easily implemented into Magnus based integration schemes. As is well known, in this technique one computes two numerical approximations to the solution, $\mathbf{u}_1$ and $\hat{\mathbf{u}}_1$, with $\mathbf{u}_1$ being of lower order than $\hat{\mathbf{u}}_1$. Then the difference $\mathbf{u}_1 - \hat{\mathbf{u}}_1$ can be used for the purpose of step size selection when the integration is continued with the higher order approximation [9]. Next we illustrate the procedure in the context of Magnus with the 6-th and 8-th order methods built in section 3.

Let us consider the following approximations of order 4 and 6 to the exact solution

$$\mathbf{u}_1 = e^{\tilde{\Omega}^{[4]}}\mathbf{u}_0, \qquad \hat{\mathbf{u}}_1 = e^{\tilde{\Omega}^{[6]}}\mathbf{u}_0, \tag{49}$$

obtained when $\tilde{\Omega}_i$ are taken according to the 6-th order numerical scheme (28) with the appropriate quadratures. Then an estimate of the difference can be done with the Baker-Campbell-Hausdorff formula:

$$\begin{aligned}\hat{\mathbf{u}}_1 - \mathbf{u}_1 &= \left(e^{\tilde{\Omega}^{[6]}} - e^{\tilde{\Omega}^{[4]}}\right)\mathbf{u}_0 = \left(I - e^{\tilde{\Omega}^{[4]}}\, e^{-\tilde{\Omega}^{[6]}}\right)\hat{\mathbf{u}}_1 \\ &= \left(I - \exp(-\tilde{\Omega}_3 - \tilde{\Omega}_4 - \frac{1}{2}[\tilde{\Omega}^{[4]}, \tilde{\Omega}^{[6]}] + O(h^7))\right)\hat{\mathbf{u}}_1 \qquad (50) \\ &= (\tilde{\Omega}_3 + \tilde{\Omega}_4 + \frac{1}{2}[\tilde{\Omega}_1, \tilde{\Omega}_3 + \tilde{\Omega}_4])\hat{\mathbf{u}}_1 + O(h^7),\end{aligned}$$

so that

$$E_r \equiv \|\hat{\mathbf{u}}_1 - \mathbf{u}_1\| = \frac{1}{2}\| \left((\tilde{\Omega}_1 + 2I)V - V\tilde{\Omega}_1\right)\hat{\mathbf{u}}_1\|, \qquad (51)$$

with $V = \tilde{\Omega}_3 + \tilde{\Omega}_4$ evaluated according to (28).

When the 8-th order scheme (40) is considered and a similar approach is followed, then (51) also gives an estimation of the difference between the approximations of order 6 and 8, with $V = \tilde{\Omega}_5 + \tilde{\Omega}_6$. Now V cannot be computed separately from $\tilde{\Omega}_2 + \tilde{\Omega}_3 + \tilde{\Omega}_4$, but instead $V = Q_7 + h\frac{64}{27}[B^{(3)}, Q_5]$. In this case the computation of E_r requires eight matrix-vector products and the evaluation of a norm, but this represents only a small amount of the total computational cost of the method.

When E_r computed at time t_{n+1} is smaller than a prescribed tolerance ε, then the step from t_n to t_{n+1} is accepted and one proceeds to find the approximate solution $\hat{\mathbf{u}}_1$ at t_{n+2}. If $E_r > \varepsilon$ then the approximation at t_{n+1} is rejected and the step from t_n to t_{n+1} is tried again with a smaller step size. In either case, the step size to be employed for a method of order $2m$ is given by [22, 9]

$$h_{n+1} = \alpha \left(\frac{\varepsilon}{E_r}\right)^{1/(2m-1)} h_n, \qquad (52)$$

where α is a safety constant factor.

5 Conclusions

We have analyzed the Magnus expansion as a tool for the numerical integration of linear matrix differential equations. Our point of departure is the recurrence relation (7)-(8) obtained in the treatment of perturbation problems, which has also proved extremely useful for establishing absolute convergence of the Magnus series.

The implementation of Magnus expansion as a numerical integration algorithm involves basically three steps: (i) truncation of the infinite series which gives Ω, (ii) replacement of the multivariate integrals in the approximation $\tilde{\Omega}$ to Ω by single integrals and, when necessary, by numerical quadratures, and (iii) evaluation of the matrix-vector product $e^{\tilde{\Omega}}\mathbf{u}_0$.

By taking into account the time-symmetry of the expansion and a systematic study of the behaviour of each term Ω_i under this symmetry, we have been able to construct 6-th and 8-th order schemes which involve only 4 and 10 different commutators. This represents a meaningful saving with respect to other methods previously available. In this respect, we should remark that $2N^3$ operations are needed for evaluating one commutator, N being the dimension of the matrices involved, whereas in general no more than $15N^2$ floating-point operations are required for computing $e^{\tilde{\Omega}}\mathbf{u}_0$. Thus, reducing to a minimum the number of commutators involved is of the greatest importance.

In addition, we have discussed a certain number of practical issues related to Magnus based numerical integration methods, in particular the use of single analytical integrals for approximating Ω_i up to a given order; the construction of new algorithms from symmetric quadrature rules; the combination of these two approaches to form new hybrid methods, and the implementation of a novel and less costly technique of step size control based on Lie algebraic techniques.

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