

NEW NUMERICAL INTEGRATORS BASED ON SOLVABILITY AND SPLITTING

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...approach suggested by

Arieh Iserles

Outline of the talk



1. Some (well known) Lie group methods for linear problems (Fer and Magnus expansions).
2. Schemes based on triangular matrices (splitting + solvability).
3. Some methods and practical issues in their construction

1 Lie group methods (linear problems)

Let us consider a linear matrix ODE evolving in a Lie group $\mathcal{G}$

$$Y' = A(t)Y, \quad Y(t_0) = Y_0 \in \mathcal{G}$$

(0)

with $A : [t_0, \infty[\times \mathcal{G} \longrightarrow \mathfrak{g}$ smooth enough.

$\mathfrak{g}$: Lie algebra associated with $\mathcal{G}$

Examples of $\mathcal{G}$: $SL(n)$, $O(n)$, $SU(n)$, $Sp(n)$, $SO(n)$, ...

$$Y(t) \in \text{Lie group } \mathcal{G} \text{ if } A(t) \in \text{Lie algebra } \mathfrak{g}$$

* There are several schemes preserving this feature (Magnus, Fer, Cayley,...)

1.1 Magnus expansion

For the equation

$$Y' = A(t)Y, \quad Y(t_0) = I,$$

* **Magnus** (1954) proposed

$$Y(t) = e^{\Omega(t)}, \quad \Omega(t) = \sum_{k=1}^{\infty} \Omega_k(t) \quad (1)$$

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with $\log(Y(t))$ satisfying

$$\Omega' = d \exp_{\Omega}^{-1} A(t) = \sum_{k=0}^{\infty} \frac{B_k}{k!} \operatorname{ad}_{\Omega}^k A(t), \quad \Omega(t_0) = 0, \quad (2)$$

1.1 Magnus expansion (II)

Here

$$\mathrm{ad}_{\Omega}^0 A = A$$

$$\mathrm{ad}_{\Omega}^k A = [\Omega, \mathrm{ad}_{\Omega}^{k-1} A]$$

$$[\Omega, A] \equiv \Omega A - A \Omega$$

and B_k are Bernoulli numbers.

1.1 Magnus expansion (III)

First terms in the expansion ($A_i \equiv A(t_i)$):

$$\Omega_1(t) = \int_{t_0}^t A(t_1) dt_1$$

$$\Omega_2(t) = \frac{1}{2} \int_{t_0}^t dt_1 \int_{t_0}^{t_1} dt_2 [A_1, A_2]$$

$$\Omega_3(t) = \frac{1}{6} \int_{t_0}^t dt_1 \int_{t_0}^{t_1} dt_2 \int_{t_0}^{t_2} dt_3 ([A_1, [A_2, A_3]] + [A_3, [A_2, A_1]])$$

$e^{\Omega(t)} \in \mathcal{G}$ even if the series Ω is truncated

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$e^{\Omega(t)} \in \mathcal{G}$ even if the series Ω is truncated

* Expansion widely used in Quantum Mechanics, NMR spectroscopy, infrared divergences in QED, control theory,...

1.1 Magnus expansion (IV)



Magnus as a numerical integration method (Iserles & Nørsett, 1997)

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(Moler & Van Loan, Celledoni & Iserles,...)

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Two critical factors in the computational cost of the resulting algorithms:

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(2) Number of commutators involved in the expansion

To reduce this number is particularly useful the concept of **graded free Lie algebra** (Munthe-Kaas, Owren 1999)

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As a result,

- * Numerical schemes based on Magnus up to order 8 have been constructed involving the minimum number of commutators in terms of quadratures and/or univariate integrals.
- * Efficient in applications

1.2 Other schemes



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* Referred erroneously in the (mathematical physics) literature (e.g., Wilcox 1967), but ...

* proposed (as an exercise!) by R. Bellman, 'Introduction to Matrix Analysis', 1960, page 204:

"The solution of $dX/dt = Q(t)X$, $X(0) = I$, can be put in the form $e^P e^{P_1} \dots e^{P_n} \dots$, where $P = \int_0^t Q(s)ds$, and $P_n = \int_0^t Q_n ds$, with

$$Q_n = e^{-P_{n-1}} Q_{n-1} e^{P_{n-1}} + \int_0^{-1} e^{sP_{n-1}} Q_{n-1} e^{-sP_{n-1}} ds$$

The infinite product converges if t is sufficiently small."

(See also Mathematical Reviews 21 2771, review done by R. Bellman)

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- * used as an (analytic) procedure in perturbation theory in Quantum Mechanics by Klarsfeld & Oteo (1989), but...
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- * This class of methods can actually be built from Magnus.
- * They require the computation of several matrix exponentials.

1.3 Methods based on the Cayley transform

Let us suppose that $Y' = A(t)Y$ is defined in a J -orthogonal Lie group,

$$O_J(n) = \{A \in GL_n(\mathbb{R}) : A^T J A = J\},$$

J : constant matrix

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J : constant matrix

Examples: orthogonal group ($J = I$), symplectic group, Lorentz group ($J = \text{diag}(1, -1, -1, -1)$).

Solution:

$$Y(t) = \left(I - \frac{1}{2}C(t) \right)^{-1} \left(I + \frac{1}{2}C(t) \right)$$

1.3 Methods based on the Cayley transform (II)

with $C(t) \in \mathfrak{o}_J(n)$ satisfying (Iserles 2001)

$$\frac{dC}{dt} = A - \frac{1}{2}[C, A] - \frac{1}{4}CAC, \quad t \geq t_0, \quad C(t_0) = 0.$$

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In fact, one can also combine Magnus with Padé to avoid the use of matrix exponentials in J -orthogonal groups!

* It is possible to construct methods which are more efficient than those based on the Cayley transform (Blanes, C., Ros 2002).

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- * These methods require the evaluation of one or several matrix exponentials

⇒ They are expensive when n is very large

- * In some cases, if the exponential is approximated by rational functions the method does not preserve the Lie group structure,

in particular, when $\mathcal{G} = \text{SL}(n)$

⇒ Another class of methods is required.

2 Solvability + splitting

The procedure

For the linear system

$$Y' = A(t)Y, \quad Y(0) = I,$$

we denote $Y_0 \equiv Y$, $A_0 \equiv A$ and suppose that

$$A_0(t) = A_{0+}(t) + A_{0-}(t),$$

where

$A_{0+} \in \nabla_n$ is strictly upper-triangular

$A_{0-} \in \tilde{\Delta}_n$ is weakly lower-triangular.

2 Solvability + splitting (II)

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More specifically, we propose the following factorization:

$$Y_0(t) = L_0(t)U_0(t)Y_1(t)$$

such that

$$L'_0 = A_{0-}(t)L_0, \quad L_0(0) = I$$

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$$Y_0(t) = L_0(t)U_0(t)Y_1(t)$$

such that

$$L_0' = A_{0-}(t)L_0, \quad L_0(0) = I$$

Observe then that $L_0(t)$ can be obtained by quadratures and $L_0(t) \in \tilde{\Delta}_n$.

2 Solvability + splitting (III)

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$$C_0 = L_0^{-1} A_{0+} L_0$$

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which can also be split as

$$C_0(t) = C_{0+}(t) + C_{0-}(t),$$

where

$C_{0+} \in \tilde{\nabla}_n$ is weakly upper-triangular

$C_{0-} \in \Delta_n$ is strictly lower-triangular.

2 Solvability + splitting (IV)

Next we choose U_0 as the solution of

$$U_0' = C_{0+}(t)U_0, \quad U_0(0) = I$$

so that $U_0(t)$ can also be obtained by quadratures.

2 Solvability + splitting (IV)

Next we choose U_0 as the solution of

$$U_0' = C_{0+}(t)U_0, \quad U_0(0) = I$$

so that $U_0(t)$ can also be obtained by quadratures.

It is easy to show that Y_1 satisfies

$$Y_1' = A_1(t)Y_1, \quad Y_1(0) = I,$$

with

$$A_1 = U_0^{-1}C_{0-}U_0.$$

2 Solvability + splitting (V)

This gives a single step of the *solvable cycle*, which we repeat with A_1 .

$$A_1 = A_{1+} + A_{1-}, \quad A_{1+} \in \nabla_n, \quad A_{1-} \in \tilde{\Delta}_n$$

$$Y_1 = L_1 U_1 Y_2$$

$$L'_1 = A_{1-} L_1, \quad L_1(0) = I$$

etc.

2 Solvability + splitting (VI)

In this way one has the following algorithm:

$$Y \equiv Y_0 = L_0 U_0 L_1 U_1 \cdots L_k U_k Y_{k+1}$$

with $(k = 0, 1, 2, \dots)$

$$A_k = A_{k+} + A_{k-}, \quad A_{k+} \in \nabla_n, \quad A_{k-} \in \tilde{\Delta}_n$$

$$L'_k = A_{k-} L_k, \quad L_k(0) = I$$

$$C_k \equiv L_k^{-1} A_{k+} L_k = C_{k+} + C_{k-}$$

$$C_{k+} \in \tilde{\nabla}_n, \quad C_{k-} \in \Delta_n$$

$$U'_k = C_{k+} U_k, \quad U_k(0) = I$$

2 Solvability + splitting (VII)

and finally

$$A_{k+1} \equiv U_k^{-1} C_{k-} U_k, \quad Y'_{k+1} = A_{k+1} Y_{k+1}$$

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In what follows we will analyse the main features of this procedure as a *numerical integrator*.

2.1 Order of the method



Suppose that $A(t) = \varepsilon(a_0 + a_1t + a_2t^2 + \dots)$ for some parameter $\varepsilon > 0$.

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Then

$$A_{j-} = t^{n_j} \varepsilon^{n_j} (\varepsilon \alpha_1 + t(\varepsilon \alpha_2 + \varepsilon^2 \alpha_3) + O(t^2))$$

$$A_{j+} = t^{m_j} \varepsilon^{m_j} (\varepsilon \beta_1 + t(\varepsilon \beta_2 + \varepsilon^2 \beta_3) + O(t^2))$$

for $j = 1, 2, \dots$, so that

$$L_j(t) = I + \frac{1}{n_j + 1} (t\varepsilon)^{n_j+1} \alpha_1 + \frac{1}{n_j + 2} t^{n_j+2} \varepsilon^{n_j} (\varepsilon \alpha_2 + \varepsilon^2 \alpha_3) + \dots$$

$$U_j(t) = I + \frac{1}{m_j + 1} (t\varepsilon)^{m_j+1} \beta_1 + \frac{1}{m_j + 2} t^{m_j+2} \varepsilon^{m_j} (\varepsilon \beta_2 + \varepsilon^2 \beta_3) + \dots$$

2.1 Order of the method (II)

Furthermore,

$$n_{j+1} = n_j + m_j + 1$$

$$m_{j+1} = n_j + 2m_j + 2 \quad j = 1, 2, \dots$$

2.1 Order of the method (II)

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$$m_{j+1} = n_j + 2m_j + 2 \quad j = 1, 2, \dots$$

j	n_j	m_j
1	1	2
2	4	7
3	12	20
4	33	54
5	88	143

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(1) This algorithm could be useful for problems of the form

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$$Y' = (B_0 + \varepsilon B_1)Y$$

if the system $Y' = B_0 Y$ can be solved exactly.

(2) The order of approximation is...

2.1 Order of the method (IV)

$Y_0 \approx L_0 U_0$	is order	1
$Y_0 \approx L_0 U_0 L_1$		2
$Y_0 \approx L_0 U_0 L_1 U_1$		4
$Y_0 \approx L_0 U_0 L_1 U_1 L_2$		7
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...if we can compute L_k and U_k up to this order...

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- (2) Solve explicitly the systems $L'_k = A_{k-} L_k$ and $U'_k = C_{k+} U_k$

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- (1) Does the approximate solution evolve in the Lie group if A is in the Lie algebra, i.e., is it a Lie group method?
- (2) Solve explicitly the systems $L'_k = A_{k-} L_k$ and $U'_k = C_{k+} U_k$
- (3) Approximate efficiently the (multiple) integrals involved.

3 Practical issues

(1) Preservation of the Lie-group structure

If $A(t) \in \mathfrak{sl}(n)$, the algorithm provides by construction approximations to $Y(t)$ in $SL(n)$.

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Proof. $A_k = A_{k+} + A_{k-}$, with $A_{k+} \in \nabla_n$, $A_{k-} \in \tilde{\Delta}_n$. In fact A_{k-} belongs to a solvable subalgebra of $\mathfrak{sl}(n)$. Therefore the solution of

$$L'_k = A_{k-} L_k, \quad L_k(0) = I$$

$L_k(t) \in SL(n)$ (in fact, a solvable subgroup of).

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$$L'_k = A_{k-} L_k, \quad L_k(0) = I$$

$L_k(t) \in SL(n)$ (in fact, a solvable subgroup of).

$\text{Tr}(A_{k+}) = 0$, and the trace is invariant under similarity, so that

$$\text{Tr}(C_k) = \text{Tr}(L_k^{-1} A_{k+} L_k) = \text{Tr}(A_{k+}) = 0 \Rightarrow C_k \in \mathfrak{sl}(n)$$

3 Practical issues (II)

Next, $C_k = C_{k+} + C_{k-}$, with $C_{k+} \in \tilde{\nabla}_n$, $C_{k-} \in \Delta_n$ and U_k , solution of

$$U'_k = C_{k+} U_k, \quad U_k(0) = I$$

belongs to $SL(n)$. Finally

$$A_{k+1} \equiv U_k^{-1} C_{k-} U_k \in \mathfrak{sl}(n)$$

and the process is repeated. □

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Other properties (i.e., orthogonality) are preserved only up to the order of the method.

3 Practical issues (III)

(2a) Explicit solution of $L'_k = A_{k-} L_k$

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Consider $k = 0$ and denote $A_0(t) = (a_{ij})$, $i, j = 1, \dots, n$, $L_0(t) = (L_{ij})$,
 $j \leq i$

$$A_{ii}(t) \equiv \int_0^t a_{ii}(t_1) dt_1.$$

Then the solution of $L'_0 = A_{0-}(t)L_0$, $L_0(0) = I$ is

$$L_{ii}(t) = e^{A_{ii}(t)}, \quad i = 1, \dots, n \quad (3)$$

$$L_{ij}(t) = e^{A_{ii}(t)} \int_0^t e^{-A_{ii}(t_1)} \left(\sum_{k=j}^{i-1} a_{ik}(t_1) L_{kj}(t_1) \right) dt_1$$

$i = 2, \dots, n$, $j = 1, \dots, i-1$.

3 Practical issues (IV)

(2b) Explicit solution of $U'_k = C_{k+} U_k$

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Consider $k = 0$ and denote $C_0(t) = (c_{ij})$, $i, j = 1, \dots, n$, $U_0(t) = (U_{ij})$,
 $j \geq i$

$$C_{ii}(t) \equiv \int_0^t c_{ii}(t_1) dt_1.$$

Then the solution of $U'_0 = C_{0+}(t)U_0$, $U_0(0) = I$ is

$$U_{ii}(t) = e^{C_{ii}(t)}, \quad i = 1, \dots, n \quad (4)$$

$$U_{ij}(t) = e^{C_{ii}(t)} \int_0^t e^{-C_{ii}(t_1)} \left(\sum_{k=i+1}^j c_{ik}(t_1) U_{kj}(t_1) \right) dt_1$$

$$i = 1, \dots, n-1, j = i+1, \dots, n.$$

3 Practical issues (V)

⇒ Explicit expressions for the elements of L_k and U_k in terms of multivariate integrals.

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They can be evaluated in sequence as follows:

L_{ii}	$i = 1, \dots, n$	U_{ii}	$i = 1, \dots, n$
$L_{i,i-1}$	$i = 2, \dots, n$	$U_{i,i+1}$	$i = 1, \dots, n-1$
$L_{i,i-2}$	$i = 3, \dots, n$	$U_{i,i+2}$	$i = 1, \dots, n-2$
$\vdots$		$\vdots$	
L_{n1}		U_{1n}	

3 Practical issues (VI)

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Question: Is it possible to approximate *all* the nested integrals with the evaluations required to compute

$$A_{ii} = \int_0^t a_{ii}(t_1) dt_1,$$

i.e., *à la* Magnus?

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YES!

3.1 Example



Illustration: method of order 4 with 2 A evaluations

Step $t = 0 \longmapsto t = h$.

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Step $t = 0 \mapsto t = h$.

1- Approximate $A_{ii}(h)$, $i = 1, \dots, n$ up to order 4

$$\begin{aligned} A_{ii}(h) = \int_0^h a_{ii}(t) dt &= \frac{h}{3} (a_{ii}(0) + 4a_{ii}(h/2) + a_{ii}(h)) + O(h^5) \\ &\equiv \tilde{A}_{ii}(h) + O(h^5) \end{aligned}$$

and $A_{ii}(h/2)$, $i = 1, \dots, n-1$, up to order 3 (necessary to approximate L_{ij}):

$$A_{ii}(h/2) = \frac{h}{24} (5a_{ii}(0) + 8a_{ii}(h/2) - a_{ii}(h)) + O(h^4)$$

3.1 Example (II)

2- $L_{ii}(h) = \exp(\tilde{A}_{ii}(h)) + O(h^5)$ ($i = 1, \dots, n$) and
 $L_{ii}(h/2) = \exp(\tilde{A}_{ii}(h/2)) + O(h^4)$ ($i = 1, \dots, n-1$).

3- Obtain an approximation to $L_{ij}(h)$, $j < i$, of order 4 and $L_{ij}(h/2)$ of order 3

$$L_{ij}(h) = e^{A_{ii}(h)} \int_0^h F_{ij}(t) dt$$

with

$$F_{ij}(t) \equiv e^{-A_{ii}(t)} \sum_{k=j}^{i-1} a_{ik}(t) L_{kj}(t)$$

3.1 Example (III)

Then

$$L_{ij}(h) = e^{\tilde{A}_{ii}(h)} \frac{h}{3} (F_{ij}(0) + 4F_{ij}(h/2) + F_{ij}(h)) + O(h^5)$$

where $F_{ij}(0) = a_{ij}(0)$ and $F_{ij}(h/2)$ and $F_{ij}(h)$ have to be approximated up to order h^3 .

The sequence of computation is $(i = 2, \dots, n)$:

(a) $F_{i,i-1}(h/2) = e^{-\tilde{A}_{ii}(h/2)} a_{i,i-1}(h/2) L_{i-1,i-1}(h/2) + O(h^4)$

(b) $F_{i,i-1}(h) = e^{-\tilde{A}_{ii}(h/2)} a_{i,i-1}(h) L_{i-1,i-1}(h) + O(h^5)$

(c) $L_{i,i-1}(h)$, $i = 2, \dots, n$ up to order 4

3.1 Example (IV)

(d)

$$L_{i,i-1}(h/2) = e^{\tilde{A}_{ii}(h/2)} \frac{h}{24} (5a_{i,i-1}(0) + 8F_{i,i-1}(h/2) - F_{i,i-1}(h)) + O(h^4)$$

(e) $L_{i,i-2}(h)$, $i = 3, \dots, n$, up to order 4 and $L_{i,i-2}(h/2)$ up to order 3

...and so on.

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(e) $L_{i,i-2}(h)$, $i = 3, \dots, n$, up to order 4 and $L_{i,i-2}(h/2)$ up to order 3

...and so on.

In this way we have $L_0(h)$ computed up to order $O(h^5)$ and also $L_0(h/2)$ up to order $O(h^4)$ with 2 evaluations of $A(t)$.

3.1 Example (V)

3- Next we compute C_0 :

$$C_0(0) = A_{0+}(0) \quad \text{error } O(h^5)$$

$$C_0(h/2) = L_0^{-1}(h/2)A_{0+}(h/2)L_0(h/2) \quad \text{error } O(h^4)$$

$$C_0(h) = L_0^{-1}(h)A_{0+}(h)L_0(h) \quad \text{error } O(h^5)$$

$$4- C_{ii}(h) = \frac{h}{3} (c_{ii}(0) + 4c_{ii}(h/2) + c_{ii}(h)) + O(h^5)$$

$$C_{ii}(h/2) = \frac{h}{24} (5c_{ii}(0) + 8c_{ii}(h/2) - c_{ii}(h)) + O(h^4)$$

3.1 Example (VI)

5- $U_{i,i+1}(h)$, $i = 1, \dots, n-1$, up to order $O(h^5)$;

$U_{i,i+1}(h/2)$, $i = 1, \dots, n-1$, up to order $O(h^4)$;

$U_{i,i+2}(h)$, $i = 1, \dots, n-2$, up to order $O(h^5)$;

$U_{i,i+2}(h)$, $i = 1, \dots, n-2$, up to order $O(h^4)$;

... and so on.

Thus we compute $U_0(h)$ with error $O(h^5)$ and also $U_0(h/2)$ with error $O(h^4)$.

3.1 Example (VII)

6- A_1 :

$$A_1(0) = C_{0-}(0) \quad \text{error } O(h^5)$$

$$A_1(h/2) = U_0^{-1}(h/2)C_{0-}(h/2)U_0(h/2) \quad \text{error } O(h^4)$$

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... and the process is repeated again for the second cycle

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... and the process is repeated again for the second cycle

$\Rightarrow$ it is possible to construct a method of order 4 with only 2 $A(t)$ evaluations (3 for the first step).

3.2 Other possibilities



One could use other quadrature rules instead, for instance Gauss–Legendre, but...

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Solution: use G–L with matrix evaluations in the previous/next step.

⇒ method of order 4 with 2 evaluations (and 1 in the next step)

3.3 Some methods

Order 4

$$Y \approx L_0 U_0 L_1 U_1$$

* Quadratures NC / GL, 2 matrix evaluations per step

Order 6

$$Y \approx L_0 U_0 L_1 U_1 L_2$$

* order 6 with a 5 points NC quadrature (4 evaluations per step)

* order 7 with a 7 points NC (6 evaluations)

Order 12

$$Y \approx L_0 U_0 L_1 U_1 L_2 U_2$$

* with a 11 points NC (or GL involving several steps).

3.4 Variable step size



Local extrapolation technique is trivial to implement in this setting.

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For instance,

$$Y_1 \equiv L_0 U_0 L_1$$

$$\hat{Y}_1 \equiv L_0 U_0 L_1 U_1 = Y_1 U_1$$

Then

$$\hat{Y}_1 - Y_1 = Y_1 U_1 - Y_1 = Y_1 (U_1 - I)$$

and $\|\hat{Y}_1 - Y_1\|$ can be used as a measure of the error

3.5 Future work



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- * Analyse the convergence of the procedure
- * Consider numerical examples in $SL(n)$ with (very) large n
- * Highly oscillatory problems (with special quadratures)
- * Analyse in practice the preservation of other structures (Blanes & Moan)
- * Try to generalize to nonlinear problems

The End

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