The Fer expansion and time symmetry: a Strang-type approach

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Abstract

We introduce a symmetric version of the Fer expansion for the solution of the ODE $y' = \gamma(t,y)y$. We show that the scheme are time symmetric for linear problems, and, because of the symmetry of the scheme, one gets order $2p+2$ whereby the classical Fer expansion would display order $2p+1$ only. This reduces significantly the computational cost of the classical Fer expansion. We prove the convergence of the proposed symmetric schemes and obtain an estimate of the radius of convergence. We present some numerical methods of this type and test them on a linear and a nonlinear problem. The numerical experiment confirm that the proposed methods are time-symmetric to machine accuracy for linear problem, while, for nonlinear problem, they are not time symmetric but obey time-symmetry to a higher order of accuracy.

1 The classical Fer expansion

We consider the differential equation

$$y' = \gamma(t,y)y, \qquad y(0) = y_0, \tag{1.1}$$

where $y \in \mathbb{R}^{n\times n}$ and $\gamma(t,y)$ is a $n \times n$ matrix function of y and, possibly, of the time t. Of particular relevance is the case when y evolves on a matrix Lie group G, in which case $\gamma \in \mathfrak{g}$, the Lie algebra of G (see [14, 13, 10, 19] and references therein), in which case it is useful that also (numerical) approximations of the exact solution $y(t)$ remain on the same Lie group G. Such Lie-group approximations can be obtained by means of the Fer expansion [19, 20], the Magnus expansion and many more exponential expansions.

In particular, the Fer expansion consists of writing the solution $y(t)$ of (1.1) as the product of infinite exponentials, i.e.

$$y(t) = \lim_{m\to\infty} \mathrm{e}^{\sigma_0}\mathrm{e}^{\sigma_1}\cdots\mathrm{e}^{\sigma_m} y_0, \tag{1.2}$$

a procedure that is equivalent to the following algorithm: Write $y(t) = \mathrm{e}^{\sigma_0} r_1(t) y_0$, where σ_0 is the integral of a known function, that we choose to be

$$\sigma_0(t) = \int_0^t \gamma(s,y)\,\mathrm{d}s \tag{1.3}$$

(note the dependence of the exact solution y of (1.1)).

We derive the differential equation obeyed by the *first residual* r_1: from

$$\gamma \mathrm{e}^{\sigma_0} r_1 y_0 = \mathrm{dexp}_{\sigma_0}\gamma \mathrm{e}^{\sigma_0} r_1 y_0 + \mathrm{e}^{\sigma_0} r_1' y_0$$

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we obtain

$$r_1' = \gamma_1 r_1, \quad \gamma_1 = \mathrm{Ad}_{\exp(-\sigma_0)}(\gamma - \mathrm{dexp}_{\sigma_0}\gamma) r_1$$

(see Section 2 for a definition of the functions Ad and dexp). Since r_1' obeys a differential equation of the same type as (1.1), the same splitting is applied to r_1,

$$r_1' = \mathrm{e}^{\sigma_1} r_2, \qquad \sigma_1 = \int_0^t \gamma_1(s)\,\mathrm{d}s,$$

and the procedure is hence iterated to obtain (1.2). In particular, if (1.1) is linear, then all the differential equations $r_i' = \gamma_i r_i$ are also linear, since the γ_i's are independent of the r_i's.

A Fer expansion can be truncated after $M+1$ terms,

$$y^{[M]}(t) = \mathrm{e}^{\sigma_0} \cdots \mathrm{e}^{\sigma_M} y_0, \tag{1.4}$$

and it is well known [5, 8, 20] that such an approximation is of the order $p = 2^{M+2} - 2$, i.e. is exponential in the number of factors employed in the expansion.

One major drawback of a truncated Fer expansion of the form (1.4) is that it generally loses eventual 'time-symmetry' properties of the underlying solution. This becomes apparent already when we consider two exponential factors.

Time-symmetry of Magnus-type methods for linear problem has been proved by Iserles *et al.* in [11]. Although in some application time-symmetry is not vital for a good numerical solution, the analysis shows that time-symmetry can be employed to reduce the complexity of the underlying numerical methods, since it helps in reducing the order conditions and the commutators therein, which usually constitute the bottle-neck of the numerical computation, together with the evaluation of exponentials.

1.1 Time-symmetry for linear problems: A numerical experiment

Let us consider the differential equation

$$y' = \gamma(t) y,$$

to which we wish to apply a Fer-type method and a Magnus-type method based on Gauss–Legendre quadrature points.

For the Fer-type scheme, we consider the numerical approximations obtained as

$$y_{n+1} = \exp\Big(\tfrac{h}{2}(\gamma_1 + \gamma_2)\Big) \exp\Big(- h^2 \tfrac{\sqrt{3}}{12}[\gamma_1, \gamma_2]\Big) y_n, \quad n = 0, 1, 2 \ldots, \tag{1.5}$$

where

$$\gamma_i = \gamma(t_n + c_i h), \quad i = 1, 2, \qquad c_1 = \frac{1}{2} - \frac{\sqrt{3}}{6}, \quad c_2 = \frac{1}{2} + \frac{\sqrt{3}}{6},$$

c_1, c_2 being the nodes of Gaussian quadrature that yield order $p = 4$. However, since we have not included the terms that arise from the order-four trees, we expect the scheme (1.5) to have order three only. To render (1.5) of effective order four, we should need to incorporate the order-four conditions,

$$y_{n+1} = \exp\Big(\tfrac{h}{2}(\gamma_1 + \gamma_2)\Big) \exp\Big(- h^2 \tfrac{\sqrt{3}}{12}[\gamma_1, \gamma_2] + h^3[\tfrac{139}{2861}\gamma_1 + \tfrac{217}{9201}\gamma_2, [\gamma_1, \gamma_2]]\Big) y_n, \quad n = 0, 1, 2 \ldots,$$

This means more commutators and a higher computational cost.

The corresponding Magnus method, based on the same nodes, is

$$y_{n+1} = \exp(\tfrac{h}{2}(\gamma_1 + \gamma_2) - h^2 \tfrac{\sqrt{3}}{12}[\gamma_1, \gamma_2]) y_n, \tag{1.6}$$

and also here we have not included the order-four conditions. However the scheme (1.6) is time symmetric [11]. Time-symmetry implies that the error must expand in even powers of the stepsize [6], which, in the case of the method (1.6), is equivalent to say that the method possesses order four instead of order three only.

To illustrate the two different behaviours (of two very similar numerical methods), we choose the function γ as

$$\gamma(t) = \sin(t) \begin{pmatrix} 0 & 2 & -3 \\ -2 & 0 & 1 \\ 3 & -1 & 0 \end{pmatrix} + \log(1+t) \begin{pmatrix} 0 & t & 5t \\ -t & 0 & -2\cos(t) \\ -5t & 2\cos(t) & 0 \end{pmatrix}. \tag{1.7}$$

and arbitrary 3×3 orthogonal initial condition y_0. We integrate with constant stepsize h from time $t = 0$ to time $t = T = Nh$, obtaining a numerical approximation y_N. Then we integrate between $t = Nh$ and $t = 0$ with stepsize $-h$ and initial condition y_N, denoting by $\tilde{y}_0$ the result obtained in this manner. A time symmetric method produces $\tilde{y}_0 = y_0$, while, if the method is not time symmetric, we would observe $\|\tilde{y}_0 - y_0\| = \mathcal{O}(h^p)$, p being the order of the method in consideration.

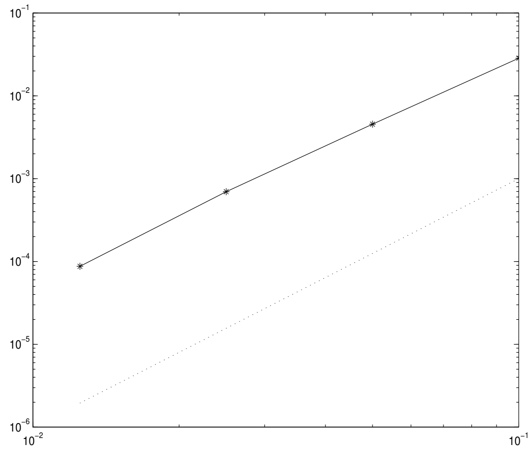


Figure 1: Error in time symmetry $\|\tilde{y}_0 - y_0\|$ versus stepsize for the function $\gamma(t)$ as in (1.7) (logarithmic scale). The method under consideration is (1.5) (asterisks joined by solid line), the asterisks corresponding to the samples of the error for $h = \frac{1}{10}, \frac{1}{20}, \ldots, \frac{1}{80}$. The dotted line indicates the slope of h^3. Here, the interval of integration is $[0, 10]$.

Figure 1.1 clearly displays that the method (1.5) is not time symmetric and possesses order three only, since the $\log \|\tilde{y}_0 - y_0\|$, as a function of h, is parallel to the $\log h^3$ line.

Figure 2 displays the time-symmetry error for the Magnus-type method (1.6), which is now of the order of machine rounding error. It is because of this time-symmetry that the numerical method (1.6) possesses order four instead of order three only, at the 'same' computational cost of the order-three scheme (1.5).

It should be noted, however, that there is no evidence that the Magnus-type methods are time-symmetric for nonlinear equations: In Section 3 we will consider a nonlinear problem for which the corresponding Magnus-type method is not time-symmetric, although it displays a better time-symmetry retention.

Motivated by the experiment above, in this paper we wish to introduce a new type of Fer expansion, which is symmetric in its composition of exponentials.

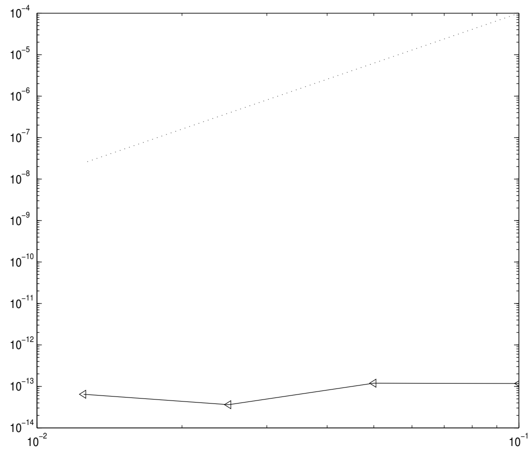


Figure 2: Error in time symmetry $\|\tilde{y}_0 - y_0\|$ versus stepsize for the function $\gamma(t)$ as in (1.7) (logarithmic scale). The method under consideration is (1.6) (triangles joined by solid line), the triangles corresponding to the samples of the error for $h = \frac{1}{10}, \frac{1}{20}, \ldots, \frac{1}{80}$. The dotted line indicates the slope of h^4. Also in this case, $T = 10$.

The paper is organized as follows: In Section 2 we will introduce a symmetric version of the Fer expansion (1.2). We obtain a sequence of differential equations for the residuals, which, however, differently from the case of the classical Fer expansion, are not linear any longer even if (1.1) is linear. We prove that the symmetric Fer expansion has the same rate of convergence as the classical Fer expansion, and, because of the Strang-type splitting, it has even order and is time-symmetric for linear problems. This is an improvement on the complexity of the numerical schemes, since it allows us to use less commutator, whose numerical evaluation is often a consistent part of the bottle-neck of the calculation. We also investigate the radius of convergence, which we find to be very similar to the one of the classical Fer expansion.

In Section 3 we introduce some numerical schemes and we display their time-symmetry features on differential equation of the form (1.1), considering a linear and a nonlinear example. The methods introduced (as well as the Magnus-type methods in [10, 19, 20]) are time-symmetric for linear problems, but not for nonlinear ones, although in the latter case they display a better time-symmetry than expected.

In Section 4 we discuss the complexity of the proposed methods with respect to the classical Fer expansion. At a price of extra matrix multiplications (that is proportional to the number of exponentials) we obtain significant savings on the number of commutators, whose number is instead exponential with respect to the order of the method.

Finally, in Section 4 we present some conclusions and sketch some ideas and work in progress.

2 A symmetric Fer expansion

In this section we focus first on the linear version of (1.1),

$$y' = \gamma(t)y, \tag{2.1}$$

and we wish to devise a symmetric version of the Fer expansion (1.2). To this purpose, we look for an expansion of the exact solution $y(t)$ of the form

$$y(t) = \lim_{m\to\infty} \overbrace{\mathrm{e}^{\sigma_0}\mathrm{e}^{\sigma_1}\cdots\mathrm{e}^{\sigma_1}\mathrm{e}^{\sigma_0}}^{2m+1 \text{ terms}} y_0. \tag{2.2}$$

A first obvious manner of obtaining an expression of the form (2.2) is to write the exact solution y of (1.1) as

$$y(t) = \mathrm{e}^{\sigma_0} r_1 \mathrm{e}^{\sigma_0} y_0, \tag{2.3}$$

where, in analogy with the standard one-sided Fer expansion, we choose

$$\sigma_0 = \frac{1}{2}\int_0^t \gamma(s)\,\mathrm{d}s. \tag{2.4}$$

By differentiation of (2.3), one readily obtains the differential equation obeyed by r_1, i.e.

$$r_1' = \mathrm{e}^{-\sigma_0}\Big(\gamma - \mathrm{dexp}_{\sigma_0}(\sigma_0')\Big)\mathrm{e}^{-\sigma_0} r_1 - r_1 \mathrm{dexp}_{\sigma_0}(\sigma_0'), \qquad \sigma_0' = \frac{1}{2}\gamma. \tag{2.5}$$

We recall that, given $\alpha \in \mathfrak{g}$ and $x \in G$, the following fundamental identity

$$\mathrm{Ad}_{\mathrm{e}^\alpha}(x) = \mathrm{e}^\alpha x \mathrm{e}^{-\alpha} = \exp(\mathrm{ad}_\alpha)(x) = \sum_{k=0}^\infty \frac{1}{k!}\mathrm{ad}_\alpha^k(x), \tag{2.6}$$

holds (see for instance [2]), whereby

$$\mathrm{ad}_\alpha^0(x) = x, \quad \mathrm{ad}_\alpha^{i+1} = \mathrm{ad}_\alpha \circ \mathrm{ad}_\alpha^i(x) = [\alpha, \mathrm{ad}_\alpha^i(x)], \quad i = 0,1,2\ldots.$$

Another fundamental formula that will be used time and again in the sequel is

$$\mathrm{dexp}_\alpha = \frac{\mathrm{e}^z - 1}{z}\Big|_{z=\mathrm{ad}} = \sum_{k=0}^\infty \frac{1}{(k+1)!} z^k\Big|_{z=\mathrm{ad}_\alpha}. \tag{2.7}$$

so that

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{e}^{\alpha(t)} = \mathrm{dexp}_\alpha(\alpha')\mathrm{e}^{\alpha(t)}.$$

Furthermore, the dexp operator can be inverted,

$$\mathrm{dexp}_\alpha^{-1} = \frac{z}{\mathrm{e}^z - 1}\Big|_{z=\mathrm{ad}_\alpha} = \sum_{k=0}^\infty \frac{B_k}{k!} z^k\Big|_{z=\mathrm{ad}_\alpha}, \tag{2.8}$$

where the B_k are the *Bernoulli numbers* (cfr. [1]).

Having said this, we observe a fundamental difference between the original problem (2.1) and the differential equation (2.5) for r_1: the in the first one, γ depends on time only, while the second can be written as $r_1' = \gamma_1 r_1$ at the price that γ_1 now depends on r_1. Set now

$$\gamma_1 = \mathrm{e}^{-\sigma_0}\Big(\gamma - \mathrm{dexp}_{\sigma_0}(\sigma_0')\Big)\mathrm{e}^{\sigma_0} - r_1 \mathrm{dexp}_{\sigma_0}(\sigma_0') r_1^{-1}, \qquad \sigma_0' = \frac{1}{2}\gamma, \tag{2.9}$$

and let

$$r_1 = \mathrm{e}^{\sigma_1} r_2 \mathrm{e}^{\sigma_1}, \qquad \sigma_1 = \frac{1}{2}\int_0^t \gamma_1(s, r_1(s))\,\mathrm{d}s.$$

The procedure can be iterated for $i = 2, 3, \ldots$, so that

$$\begin{aligned} r_i' &= \gamma_i r_i, \qquad r_i = \mathrm{e}^{\sigma_i} r_{i+1} \mathrm{e}^{\sigma_i}, \qquad \sigma_i = \frac{1}{2}\int_0^t \gamma_i(s, r_i(s))\,\mathrm{d}s, \\ \gamma_i &= \mathrm{e}^{-\sigma_{i-1}}\Big(\gamma_{i-1} - \mathrm{dexp}_{\sigma_{i-1}}(\tfrac{1}{2}\gamma_{i-1})\Big)\mathrm{e}^{\sigma_{i-1}} - r_i \mathrm{dexp}_{\sigma_{i-1}}(\tfrac{1}{2}\gamma_{i-1}) r_i^{-1}. \end{aligned}$$

where the γ_i's satisfy a formula similar to (2.9), so that *formally* (2.2) holds.

2.1 Order analysis of the symmetric Fer expansion

In order to analyze the convergence of the symmetric Fer expansion introduced above, we define the *discrepancy* of y and $y^{[M]} = \exp(\sigma_0)\cdots\exp(2\sigma_M)\cdots\exp(\sigma_0)y_0$, as the function $d : G \times G \to \mathfrak{g}$ such that

$$d(y, y^{[M]}) = \log(y\,(y^{[M]})^{-1}) = \log(\mathrm{e}^{\sigma_0}\cdots\mathrm{e}^{\sigma_M} r_M \mathrm{e}^{-\sigma_M}\cdots\mathrm{e}^{-\sigma_0}) \tag{2.10}$$

[9]. The above logarithm is defined by writing its argument as a single exponential (for instance by means of the BCH formula) and taking as a result the exponent itself.

A useful formula for evaluating (2.10) is a Lie-group analogous of (2.7),

$$\mathrm{e}^{\sigma_1}\mathrm{e}^{\sigma_2}\mathrm{e}^{-\sigma_1} = \mathrm{e}^{\exp(\sigma_1)\sigma_2\exp(-\sigma_1)} = \mathrm{e}^{\exp(\mathrm{ad}_{\sigma_1})(\sigma_2)}. \tag{2.11}$$

The proof is quite simple: set $x = \mathrm{e}^{\sigma_1}$, then $\mathrm{e}^{-\sigma_1} = x^{-1}$ and

$$\mathrm{e}^{x\sigma_2 x^{-1}} = \sum_{k=0}^{\infty}\frac{1}{k!}(x\sigma_2 x^{-1})^k = x\sum_{k=0}^{\infty}\frac{1}{k!}\sigma_2^k x^{-1} = x\exp(\sigma_2)x^{-1}.$$

Let us consider first the case when $M = 0$, so that the departure

$$d(y, y^{[0]}) = \log(y\,(y^{[0]})^{-1}) = \log(\mathrm{e}^{\sigma_0} r_1 \mathrm{e}^{-\sigma_0}) = \log(\mathrm{e}^{\exp(\mathrm{ad}_{\sigma_0})(\tilde\sigma_1)}) = \exp(\mathrm{ad}_{\sigma_0})(\tilde\sigma_1) \in \mathfrak{g},$$

where we have set $r_1 = \mathrm{e}^{\tilde\sigma_1}$ and we have made use of (2.11). Here $\tilde\sigma_1 \in \mathfrak{g}$ is the solution of the differential equation

$$\tilde\sigma_1' = \mathrm{dexp}_{\tilde\sigma_1}^{-1}\Big(\mathrm{e}^{-\sigma_0}(\gamma - \tfrac12\mathrm{dexp}_{\sigma_0}(\gamma))\mathrm{e}^{\sigma_0} - \tfrac12\mathrm{e}^{\tilde\sigma_1}\mathrm{dexp}_{\sigma_0}(\gamma)\mathrm{e}^{-\tilde\sigma_1}\Big), \quad \tilde\sigma_1(0) = O. \tag{2.12}$$

Let us assume next that $\gamma(t) = \mathcal{O}(1)$, hence $\sigma_0(t) = \frac12\int_0^t\gamma(s)\,\mathrm{d}s = \mathcal{O}\big(\frac{t}{2}\big)$. As a first step, we would like to remove the dependence of $\mathrm{dexp}_{\tilde\sigma_1}^{-1}$ on $\mathrm{e}^{\tilde\sigma_1}$ in the second term of (2.12). To this purpose, recall that $\mathrm{e}^{\tilde\sigma_1}\mathrm{dexp}_{\sigma_0}(\gamma)\mathrm{e}^{-\tilde\sigma_1} = \mathrm{Ad}_{\exp\tilde\sigma_1}(\mathrm{dexp}_{\sigma_0}(\gamma)) = \exp(\mathrm{ad}_{\tilde\sigma_1})(\mathrm{dexp}_{\sigma_0}(\gamma))$, hence

$$\mathrm{dexp}_{\tilde\sigma_1}^{-1}\circ\exp(\mathrm{ad}_{\tilde\sigma_1}) = \frac{z}{\mathrm{e}^z - 1}\mathrm{e}^z\Big|_{z=\mathrm{ad}_{\tilde\sigma_1}} = \sum_{k=0}^{\infty}\frac{(-1)^k B_k}{k!}\mathrm{ad}_{\tilde\sigma_1}^k,$$

where the B_k's are again the Bernoulli numbers. We recall that all the odd Bernoulli numbers are zero except for the first one, $B_1 = \frac12$.

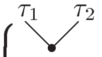
Next, denote

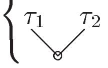
$$\gamma_{1,1}(t) = \mathrm{e}^{-\sigma_0}(\gamma - \mathrm{dexp}_{\sigma_0}(\tfrac12\gamma))\mathrm{e}^{\sigma_0}.$$

One has

$$\begin{aligned}
\gamma_{1,1}(t) &= \sum_{k=0}^{\infty}\frac{(-1)^k}{k!}\mathrm{ad}_{\sigma_0}^k(\gamma) - \frac12\sum_{k=0}^{\infty}\frac{(-1)^k}{(k+1)!}\mathrm{ad}_{\sigma_0}^k(\gamma)\\
&= \frac12\sum_{k=0}^{\infty}\frac{(-1)^k(2k+1)}{(k+1)!}\mathrm{ad}_{\sigma_0}^k(\gamma)\\
&= \frac12\Big(\gamma - \frac32[\sigma_0,\gamma] + \frac56[\sigma_0,[\sigma_0,\gamma]] - \frac{7}{24}[\sigma_0,[\sigma_0,[\sigma_0,\gamma]] + \cdots\Big),
\end{aligned}$$

which one can express in terms of the *order trees* introduced in [10] and [19, 20]. Here, we will follow [19, 20], and use therefore bi-coloured trees. These are used to express terms which are obtained by integrating and commuting γ, and the rules are as follows: 1) γ is represented by $\bullet$, 2) given a tree τ consisting of integrals and commutators of γ, the integral of this tree is obtained by adding a white root to the tree, i.e. $\int \tau \equiv$  , 3) the commutators of τ_1 and τ_2 (both representing trees in terms of integrals and commutators of γ) is obtained by joining τ_1 and τ_2 with a black root, if none of the two is the integral of the other, while they are joined by a white root if one of the trees is the integral of the other, i.e.

$[\tau_1, \tau_2] =$  if $\tau_1 \neq \int \tau_2, \tau_2 \neq \int \tau_1$,

 otherwise.

The advantage of using bi-coloured trees instead of th single-coloured trees of Iserles *et al.* [10], consists in the fact that the order in t of each tree is exactly the number of white vertices. Thus, we have

$$\gamma_{1,1}(t) = \tfrac{1}{2}\gamma - \tfrac{3}{4}[\sigma_0, \gamma] + \tfrac{5}{12}[\sigma_0, [\sigma_0, \gamma]] + \cdots$$

$$\mathcal{O}(1) + \mathcal{O}\big(t^2\big) + \mathcal{O}\big(t^3\big) + \text{h.o.t.}$$

Let us come back to (2.12). After further algebraic manipulations, one has

$$\tilde{\sigma}_1' = \sum_{k=0}^{\infty} \frac{B_k}{k!} \mathrm{ad}_{\tilde{\sigma}_1}^k(\gamma_{1,1}) - \frac{1}{2}\sum_{k=0}^{\infty} \frac{(-1)^k B_k}{k!} \mathrm{ad}_{\tilde{\sigma}_1}^k(\mathrm{dexp}_{\sigma_0}(\gamma)),$$

so that, given that only the first odd Bernoulli number is different from zero, we can group all the terms that include even Bernoulli numbers and consider the terms including B_1 separately. We have

$$\tilde{\sigma}_1' = \gamma_{1,1} - \frac{1}{2}\mathrm{dexp}_{\sigma_0}(\gamma) + B_1[\tilde{\sigma}_1, \gamma_{1,1}] + \sum_{k=1}^{\infty} \frac{B_{2k}}{(2k)!} \mathrm{ad}_{\tilde{\sigma}_1}^{2k}(\gamma_{1,1} - \frac{1}{2}\mathrm{dexp}_{\sigma_0}(\gamma)).$$

Denote next

$$\gamma_{1,2} = \gamma_{1,1} - \frac{1}{2}\mathrm{dexp}_{\sigma_0}(\gamma) = \frac{1}{2}\sum_{k=0}^{\infty} \frac{(-1)^k(2k+1)-1}{(k+1)!} \mathrm{ad}_{\sigma_0}^k(\gamma) = \frac{1}{2}\sum_{k=1}^{\infty} \frac{(-1)^k(2k+1)-1}{(k+1)!} \mathrm{ad}_{\sigma_0}^k(\gamma),$$

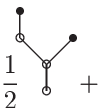
since the term corresponding to $k = 0$ in the expansion above vanishes, therefore

$$\gamma_{1,2} = -[\sigma_0, \gamma] + \frac{1}{3}[\sigma_0, [\sigma_0, \gamma]] - \frac{1}{6}[\sigma_0, [\sigma_0, [\sigma_0, \gamma]]] + \cdots,$$

(note that the first term is $\mathcal{O}\big(t^2\big)$). Hence, we obtain the following expression for $\tilde{\sigma}_1'$, which now is only in terms of the $\mathrm{ad}_{\tilde{\sigma}_1}^k$'s, namely

$$\tilde{\sigma}_1' = \gamma_{1,2} + B_1[\tilde{\sigma}_1, \gamma_{1,1}] + \sum_{k=1}^{\infty} \frac{B_{2k}}{(2k)!} \mathrm{ad}_{\tilde{\sigma}_1}^{2k}(\gamma_{1,2}) \tag{2.13}$$

Next, we solve for $\tilde{\sigma}_1$ employing the technique of Picard's iterations to find that

$\tilde{\sigma}_1 = -\frac{1}{2}$  $+ \text{h.o.t.},$

which gives

$$d(y, y^{[0]}) = \tilde{\sigma}_1 + [\sigma_0, \tilde{\sigma}_1] + \cdots = \mathcal{O}\big(t^3\big),$$

hence $y^{[0]}$ is an order-two approximant to y. And, up to this point, there is nothing surprising, since $y^{[0]}$ corresponds to the first exponential approximation obtained with the Fer expansion, which is well known to be of order two.

It is therefore interesting to see what happens when we consider the next approximation $y^{[1]}$, i.e. when $M = 1$ and

$$d(y, y^{[1]}) = \log(\mathrm{e}^{\sigma_0}\mathrm{e}^{\sigma_1} r_2 \mathrm{e}^{-\sigma_1}\mathrm{e}^{-\sigma_0}) = \exp(\mathrm{ad}_{\sigma_0})\big(\exp(\mathrm{ad}_{\sigma_1}(\tilde\sigma_2))\big).$$

Recall that, by the end of last section, we have found

$$\gamma_1 = \mathrm{e}^{-\sigma_0}(\gamma - \mathrm{dexp}(\tfrac{1}{2}\gamma))\mathrm{e}^{\sigma_0} - r_1 \mathrm{dexp}_{\sigma_0}(\tfrac{1}{2}\gamma) r_1^{-1},$$

whereby the first term is a linear part, that we have called $\gamma_{1,1}$, while the second term is nonlinear, since it contains $r_1 = \exp(\frac{1}{2}\int\gamma_1) r_2 \exp(\frac{1}{2}\int\gamma_1)$. The expression for $r_1 = \mathrm{e}^{\tilde\sigma_1}$ has been already evaluated ($\tilde\sigma_1$ is the exact solution of (2.12)), hence, substitution in γ_1 results in

$$\gamma_1 = \gamma_{1,1} - \mathrm{e}^{\tilde\sigma_1}\mathrm{dexp}_{\sigma_0}(\tfrac{1}{2}\gamma)\mathrm{e}^{-\tilde\sigma_1}$$

(note that the difference between γ_1 and the $\tilde\sigma_1'$ above consists in the missing $\mathrm{dexp}_{\tilde\sigma_1}^{-1}$ operator in front of the right-hand side). Setting $r_2 = \mathrm{e}^{\tilde\sigma_2}$, one finds that

$$\tilde\sigma_2' = \mathrm{dexp}_{\tilde\sigma_2}^{-1}\Big(\mathrm{e}^{-\sigma_1}(\gamma_1 - \tfrac{1}{2}\mathrm{dexp}_{\sigma_1}(\gamma_1))\mathrm{e}^{\sigma_1} - \frac{1}{2}\mathrm{e}^{\tilde\sigma_2}\mathrm{dexp}_{\sigma_1}(\gamma_1)\mathrm{e}^{-\tilde\sigma_2}\Big), \qquad \sigma_1 = \frac{1}{2}\int_0^t \gamma_1. \tag{2.14}$$

At this point, we need to estimate γ_1, whereby

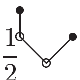
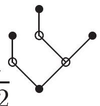
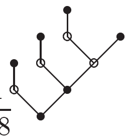
$$\gamma_1 = \gamma_{1,1} - \frac{1}{2}\mathrm{e}^{\tilde\sigma_1}\mathrm{dexp}_{\sigma_0}(\gamma)\mathrm{e}^{-\tilde\sigma_1}.$$

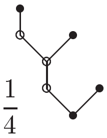
Proceeding very similarly to what already done before, we obtain

$$\gamma_1 = \frac{1}{2}\sum_{k=1}^{\infty}\frac{(-1)^k(2k+1)-1}{(k+1)!}\mathrm{ad}_{\sigma_0}^k(\gamma) - \frac{1}{2}\sum_{k=1}^{\infty}\frac{1}{k!}\mathrm{ad}_{\tilde\sigma_1}^k(\mathrm{dexp}_{\sigma_0}(\gamma)),$$

which, in terms of commutators and then of order trees, can be represented as

$$\gamma_1 = -[\sigma_0,\gamma] + \frac{1}{3}[\sigma_0,[\sigma_0,\gamma]] - \frac{1}{6}[\sigma_0,[\sigma_0,[\sigma_0,\gamma]]] + \cdots - \frac{1}{2}[\tilde\sigma_1,\gamma] + \text{h.o.t.}$$

$= -\frac{1}{2}$  $+ \frac{1}{12}$  $- \frac{1}{48}$  $+ \cdots$

$- \frac{1}{4}$  $+ \cdots.$

Similarly, we set

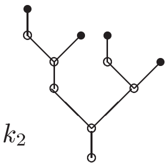
$$\begin{aligned}
\gamma_{2,1} &= \mathrm{e}^{-\sigma_1}(\gamma_1 - \frac{1}{2}\mathrm{dexp}_{\sigma_1}(\gamma_1))\mathrm{e}^{\sigma_1} \\
&= \frac{1}{2}(\gamma_1 - \frac{3}{2}[\sigma_1,\gamma_1] + \frac{5}{6}[\sigma_1,[\sigma_1,\gamma_1]] + \cdots), \\
\gamma_{2,2} &= \gamma_{2,1} - \frac{1}{2}\mathrm{dexp}_{\sigma_1}(\gamma_1),
\end{aligned}$$

to obtain that

$$\tilde{\sigma}_2' = \gamma_{2,2} + B_1[\tilde{\sigma}_2, \gamma_{2,1}] + \sum_{k=1}^{\infty} \frac{B_{2k}}{(2k)!} \mathrm{ad}_{\tilde{\sigma}_2}^{2k}(\gamma_{2,2})$$

that once again we solve by Picard iteration, to find

$$\tilde{\sigma}_2 = \int_0^t \gamma_{2,2} + \mathrm{h.o.t.} = k_2$$



$$+ \mathrm{h.o.t.},$$

from which we deduce that $\tilde{\sigma}_2$ is $\mathcal{O}(t^7)$. Hence, as for the classical Fer expansion, with two steps, one gets order up to six.

The general procedure: Recall that, for $i = 2, 3, \ldots$,

$$\begin{array}{l} r_i' = \gamma_i r_i, \qquad r_i = \mathrm{e}^{\sigma_i} r_{i+1} \mathrm{e}^{\sigma_i}, \qquad \sigma_i = \frac{1}{2}\int_0^t \gamma_i(s, r_i(s))\,\mathrm{d}s, \\ \gamma_i = \mathrm{e}^{-\sigma_{i-1}}(\gamma_{i-1} - \mathrm{dexp}_{\sigma_{i-1}}(\frac{1}{2}\gamma_{i-1}))\mathrm{e}^{\sigma_{i-1}} - r_i \mathrm{dexp}_{\sigma_{i-1}}(\frac{1}{2}\gamma_{i-1}) r_i^{-1}. \end{array} \tag{2.15}$$

We assume that $r_i = \mathrm{e}^{\tilde{\sigma}_i}$, whereby $\tilde{\sigma}_i$ is the solution of the Lie-algebra differential equation

$$\begin{array}{rcl} \tilde{\sigma}_i' &=& \mathrm{dexp}_{\tilde{\sigma}_i}^{-1}\Big(\mathrm{e}^{-\sigma_{i-1}}(\gamma_{i-1} - \mathrm{dexp}_{\sigma_{i-1}}(\frac{1}{2}\gamma_{i-1}))\mathrm{e}^{\sigma_{i-1}} - \mathrm{e}^{\tilde{\sigma}_i}\mathrm{dexp}_{\sigma_{i-1}}(\frac{1}{2}\gamma_{i-1})\mathrm{e}^{-\tilde{\sigma}_i} \\ \tilde{\sigma}_i(0) &=& O. \end{array} \tag{2.16}$$

The above differential equation can be simplified to

$$\begin{array}{rcl} \tilde{\sigma}_i' &=& \gamma_{i,2} + B_1[\tilde{\sigma}_i, \gamma_{i,1}] + \displaystyle\sum_{k=1}^{\infty} \frac{B_{2k}}{(2k)!} \mathrm{ad}_{\tilde{\sigma}_i}^{2k}(\gamma_{i,2}) \\ &=& \Big(\dfrac{z}{\mathrm{e}^z - 1} + \dfrac{1}{2}z\Big)\Big|_{z=\mathrm{ad}_{\tilde{\sigma}_i}}(\gamma_{i,2}) + B_1[\tilde{\sigma}_i, \gamma_{i,1}], \end{array}$$

where

$$\begin{array}{rcl} \gamma_{i,2} &=& \dfrac{1}{2}\displaystyle\sum_{k=1}^{\infty} \frac{(-1)^k(2k+1) - 1}{(k+1)!} \mathrm{ad}_{\sigma_{i-1}}^k(\gamma_{i-1}), \\ \gamma_{i,1} &=& \dfrac{1}{2}\displaystyle\sum_{k=1}^{\infty} \frac{(-1)^k(2k+1)}{(k+1)!} \mathrm{ad}_{\sigma_{i-1}}^k(\gamma_{i-1}). \end{array}$$

Solving by Picard iteration, we find

$$\tilde{\sigma}_i = \int_0^t \gamma_{i,2}\,\mathrm{d}t + \mathrm{h.o.t.}.$$

Theorem 2.1 *The truncated symmetric Fer expansion*

$$y^{[M]} = \mathrm{e}^{\sigma_0}\mathrm{e}^{\sigma_1}\cdots\mathrm{e}^{2\sigma_M}\cdots\mathrm{e}^{\sigma_1}\mathrm{e}^{\sigma_0} y_0,$$

has order $p_M = 2^{M+2} - 2$.

Proof. By induction. We have $p_0 = 2$. Furthermore, if p_m is the order corresponding to $m+1$ steps, i.e. $\|\sigma_m\| = \mathcal{O}(t^{p_m+1})$, we observe that $\mathcal{O}(\|\tilde{\sigma}_{m+1}\|) = \mathcal{O}(\|\gamma_{m+1,2}\|)+1$. However, $\gamma_{m+1,2} = -[\sigma_m, \gamma_m] + \text{h.o.t.}$, from which we deduce that $\|\gamma_{m+1,2}\| = \mathcal{O}(2p_m+2)$, given that $\sigma_m = \frac{1}{2}\int \gamma_m$. Hence, $p_{m+1} = 2p_m + 2$, a one term recurrence relation that has as a solution $p_m = 2^{m+2}-2$. Thus, the theorem follows from the fact that $\tilde{\sigma}_{m+1}$ is the leading error term. □

Although this might not really appear as an advantage with respect to the classical Fer expansion (we obtain the same type of exponential growth of order, i.e. $p_M = 2^{M+2}-2$ with the disadvantage that we need to employ more exponentials), the benefit are hidden in the intermediate stages of the expansion.

In general, at the $(m+1)$-th stage of the expansion, the function σ_m is not computed to order $2^{m+2}-2$, but to some order between $2^{m+1}-1$ and $2^{m+2}-3$. We claim that if the σ_i's are computed to include all the trees of order $2k-1$, where $2^{m+1}-1 \le 2k-1 \le 2^{m+2}-3$, then the expansion has automatically order $2k$ instead of $2k-1$ only. This is the same phenomenon that was discovered for the Magnus expansion [11].

Theorem 2.2 *Assume that the σ_i's, $i = 0,1,\ldots,M$, are computed to include all the trees of order up to $2k-1$, where $2^M \le k \le 2^{M+1}-1$. Then the expansion* (2.3) *has order $2k$ instead of $2k-1$ only.*

Proof. Follows from the properties of the Strang splitting $\mathrm{e}^{\sigma_0}\mathrm{e}^{\sigma_1}\cdots\mathrm{e}^{2\sigma_M}\cdots\mathrm{e}^{\sigma_1}\mathrm{e}^{\sigma_0}$. □

Hence, for $M=1$, the inclusion of all order trees of order up to $3,5$ respectively, yields methods of order $4,6$; when $M=2$, the inclusion of all trees of order up to $7,9,11,13$, yields order $8,10,12,14$ respectively and so on and so forth.

We show the result in detail in the example below, where we consider the case when $M=1$ and $2k-1=3$.

Example 2.1 Consider the approximation

$$y^{[1]} = \mathrm{e}^{\hat{\sigma}_0}\mathrm{e}^{2\hat{\sigma}_1}\mathrm{e}^{\hat{\sigma}_0}y_0, \tag{2.17}$$

where

$$\hat{\sigma}_0 = \frac{1}{2}\int_0^t \gamma(\tau)\,\mathrm{d}\tau, \qquad \hat{\sigma}_1 = -\frac{1}{4}\int_0^t [\int_0^\tau \gamma(u)\,\mathrm{d}u, \gamma(\tau)]\,\mathrm{d}\tau,$$

are order three truncation of the functions σ_0, σ_1 introduced above. Although from the theory we expect order three (i.e. $\log\left(y(t)(y^{[1]})^{-1}\right) = \mathcal{O}(t^4)$) the approximation possesses effective order four. To this purpose, we analyse

$$\begin{aligned} d(y, y^{[1]}) &= \log\left(\mathrm{e}^{\hat{\sigma}_0}\mathrm{e}^{\hat{\sigma}_1}\mathrm{e}^{\tilde{\sigma}_2}\mathrm{e}^{-\hat{\sigma}_1}\mathrm{e}^{-\hat{\sigma}_0}\right) \\ &= \log\left(\mathrm{e}^{\exp(\mathrm{ad}_{\hat{\sigma}_0})(\exp(\mathrm{ad}_{\hat{\sigma}_1})(\tilde{\sigma}_2))}\right) \\ &= \exp(\mathrm{ad}_{\hat{\sigma}_0})\sum_{k=0}^{\infty}\frac{1}{k!}\mathrm{ad}_{\hat{\sigma}_1}^k(\tilde{\sigma}_2) \\ &= \tilde{\sigma}_2 + [\hat{\sigma}_0, \tilde{\sigma}_2] + \text{h.o.t.} \end{aligned}$$

Let us recall next that $\tilde{\sigma}_2$ is the solution of the differential equation

$$\begin{aligned} \mathrm{dexp}_{\tilde{\sigma}_2}\tilde{\sigma}_2' &= \mathrm{e}^{\hat{\sigma}_1}\left(\mathrm{e}^{-\hat{\sigma}_0}(\gamma - \mathrm{dexp}_{\hat{\sigma}_0}(\hat{\sigma}_0'))\mathrm{e}^{\hat{\sigma}_0} - \mathrm{dexp}_{\hat{\sigma}_1}(\hat{\sigma}_1')\right)\mathrm{e}^{\hat{\sigma}_1} \\ &\qquad \mathrm{e}^{\tilde{\sigma}_2}\left(\mathrm{dexp}_{\hat{\sigma}_1}(\hat{\sigma}_1') + \exp(\mathrm{ad}_{\hat{\sigma}_1})(\mathrm{dexp}_{\hat{\sigma}_0}(\hat{\sigma}_0'))\right)\mathrm{e}^{-\tilde{\sigma}_2}, \\ \tilde{\sigma}_2(0) &= O, \end{aligned}$$

which, making use of the relations $\hat{\sigma}_0' = \frac{1}{2}\gamma$ and $\hat{\sigma}_1' = -\frac{1}{2}[\hat{\sigma}_0, \gamma]$, yields

$$\begin{aligned}
\mathrm{dexp}_{\tilde{\sigma}_2}\tilde{\sigma}_2' &= \mathrm{e}^{-\hat{\sigma}_1}\Big(\mathrm{e}^{-\hat{\sigma}_0}(\gamma - \tfrac{1}{2}\mathrm{dexp}_{\hat{\sigma}_0}(\gamma))\mathrm{e}^{\hat{\sigma}_0} + \tfrac{1}{2}\mathrm{dexp}_{\hat{\sigma}_1}([\hat{\sigma}_0,\gamma])\Big)\mathrm{e}^{\hat{\sigma}_1} \\
&\qquad - \mathrm{e}^{\tilde{\sigma}_2}\Big(- \tfrac{1}{2}\mathrm{dexp}_{\hat{\sigma}_1}([\hat{\sigma}_0,\gamma]) + \exp(\mathrm{ad}_{\hat{\sigma}_1})(\tfrac{1}{2}\mathrm{dexp}_{\hat{\sigma}_0}(\gamma))\Big)\mathrm{e}^{-\tilde{\sigma}_2},
\end{aligned}$$

so that, inverting the $\mathrm{dexp}_{\tilde{\sigma}_2}$, we obtain

$$\begin{aligned}
\tilde{\sigma}_2' &= \mathrm{dexp}_{\tilde{\sigma}_2}^{-1}\Big[\mathrm{e}^{-\hat{\sigma}_1}\Big(\mathrm{e}^{-\hat{\sigma}_0}(\gamma - \tfrac{1}{2}\mathrm{dexp}_{\hat{\sigma}_0}(\gamma))\mathrm{e}^{\hat{\sigma}_0} + \tfrac{1}{2}\mathrm{dexp}_{\hat{\sigma}_1}([\hat{\sigma}_0,\gamma])\Big)\mathrm{e}^{\hat{\sigma}_1} \\
&\qquad - \mathrm{e}^{\tilde{\sigma}_2}\Big(- \tfrac{1}{2}\mathrm{dexp}_{\hat{\sigma}_1}([\hat{\sigma}_0,\gamma]) + \exp(\mathrm{ad}_{\hat{\sigma}_1})(\tfrac{1}{2}\mathrm{dexp}_{\hat{\sigma}_0}(\gamma))\Big)\mathrm{e}^{-\tilde{\sigma}_2}\Big].
\end{aligned}$$

Since all the terms appearing on the right hand side will be k-th order *commutators* of $\tilde{\sigma}_2$ and some other arguments, for the approximation analysis we are really interested in the leading term, obtained for $k = 0$. Therefore, let us analyze the function (of γ, since both $\hat{\sigma}_0$ and $\hat{\sigma}_1$ can be written as combination of integrals and commutators of γ)

$$\begin{aligned}
F(\gamma) &= \mathrm{e}^{-\hat{\sigma}_1}\Big(\mathrm{e}^{-\hat{\sigma}_0}(\gamma - \frac{1}{2}\mathrm{dexp}_{\hat{\sigma}_0}(\gamma))\mathrm{e}^{\hat{\sigma}_0} - \frac{1}{2}\mathrm{dexp}_{\hat{\sigma}_1}([\hat{\sigma}_0,\gamma])\Big)\mathrm{e}^{\hat{\sigma}_1} \\
&\qquad - \frac{1}{2}\mathrm{dexp}_{\hat{\sigma}_1}([\hat{\sigma}_0,\gamma]) - \frac{1}{2}\exp(\mathrm{ad}_{\hat{\sigma}_1})(\mathrm{dexp}_{\sigma_0}(\gamma)).
\end{aligned}$$

Using time and again the same formulae, we find:

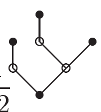
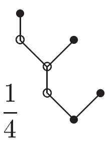
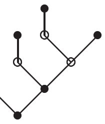
$$\begin{aligned}
F(\gamma) &= \mathrm{e}^{-\hat{\sigma}_1}\Big(\mathrm{e}^{-\hat{\sigma}_0}(\gamma - \tfrac{1}{2}\mathrm{dexp}_{\hat{\sigma}_0}(\gamma))\mathrm{e}^{\hat{\sigma}_0} + \tfrac{1}{2}\mathrm{dexp}_{\hat{\sigma}_1}([\hat{\sigma}_0,\gamma])\Big)\mathrm{e}^{\hat{\sigma}_1} \\
&\qquad + \tfrac{1}{2}\mathrm{dexp}_{\hat{\sigma}_1}([\hat{\sigma}_0,\gamma]) - \tfrac{1}{2}\exp(\mathrm{ad}_{\hat{\sigma}_1})(\mathrm{dexp}_{\hat{\sigma}_0}(\gamma)) \\
&= \frac{1}{2}\sum_{k=0}^{\infty}\frac{1}{k!}\mathrm{ad}_{\hat{\sigma}_1}^{k}\Big(\sum_{j=0}^{\infty}\frac{(-1)^{k+j}(2j+1)-1}{(j+1)!}\mathrm{ad}_{\hat{\sigma}_0}^{j}(\gamma)\Big) + \sum_{k=0}^{\infty}\frac{1}{(2k+1)!}\mathrm{ad}_{\hat{\sigma}_1}^{2k}([\hat{\sigma}_0,\gamma]).
\end{aligned}$$

Recall now that $\gamma = \mathcal{O}(1)\,, \hat{\sigma}_0 = \mathcal{O}(t)$ and $\hat{\sigma}_1 = \mathcal{O}\big(t^3\big)$. Hence, in the first sum, terms of the form $\mathrm{ad}_{\hat{\sigma}_1}^{k}\mathrm{ad}_{\hat{\sigma}_0}^{j}(\gamma) = \mathcal{O}\big(t^{3k+j+1}\big)$, for $j > 1$, which means that we need to consider the following combination of indices:

$$\begin{aligned}
k &= 0 \qquad j = 0, 1, 2, 3, \\
k &= 1 \qquad j = 0
\end{aligned}$$

(given that integration between 0 and t gives an extra order of t). For what the second sum is concerned, note that $\mathrm{ad}_{\hat{\sigma}_1}^{2k}([\hat{\sigma}_0,\gamma]) = \mathcal{O}\big(t^{6k+2}\big)$ hence only the term corresponding to $k = 0$ is worth of consideration. We have:

$$\begin{aligned}
F(\gamma) &= \frac{1}{2}\Big(- 2[\hat{\sigma}_0,\gamma] + \frac{2}{3}[\hat{\sigma}_0,[\hat{\sigma}_0,\gamma]] - \frac{1}{3}[\hat{\sigma}_0,[\hat{\sigma}_0,[\hat{\sigma}_0,\gamma]]] + \cdots - 2[\hat{\sigma}_1,\gamma] + \cdots\Big) \\
&\qquad + \Big([\hat{\sigma}_0,\gamma] + \cdots\Big) \\
&= \frac{1}{3}[\hat{\sigma}_0,[\hat{\sigma}_0,\gamma]] - 2[\hat{\sigma}_1,\gamma] - \frac{1}{6}[\hat{\sigma}_0,[\hat{\sigma}_0,[\hat{\sigma}_0,\gamma]]] + \cdots
\end{aligned}$$

$= \frac{1}{12}$  $- \frac{1}{4}$  $- \frac{1}{48}$  $+ \cdots.$

Note that the first two trees appear (integrated) in the order-four conditions for the Magnus expansion [11, 20] and we already know particular combination yields effective order four instead of three. As a result,

$$\tilde{\sigma}_2 = \int_0^t F(\gamma) + \text{h.o.t.} = \mathcal{O}(t^5)\,,$$

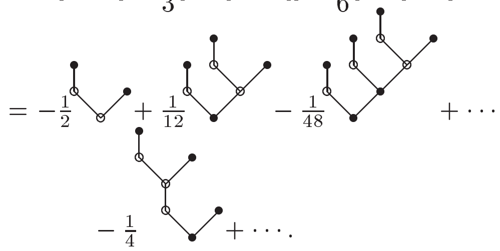
hence the obtained approximation to the solution has order four. We remark that the formulae

$$\begin{aligned} y(t)^{[1]} &= \mathrm{e}^{2(\hat{\sigma}_0+\hat{\sigma}_1)} && \text{(Magnus-type method)},\\ y(t)^{[1]} &= \mathrm{e}^{2\hat{\sigma}_0}\mathrm{e}^{2\hat{\sigma}_1} && \text{(Fer-type method)},\\ y(t)^{[1]} &= \mathrm{e}^{\hat{\sigma}_0}\mathrm{e}^{2\hat{\sigma}_1}\mathrm{e}^{\hat{\sigma}_0} && \text{('symmetric-Fer'-type method)}, \end{aligned}$$

can be obtained one from the other by means of a first approximation of the BCH formula, but the first one possesses order four (like the symmetric Fer formula on the third line) while the second one has order three only. ◇

Recall that

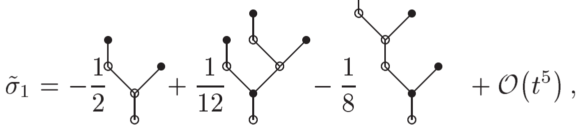
$$\begin{aligned} \gamma_1 &= \frac{1}{2}\sum_{k=1}^{\infty}\frac{(-1)^k(2k+1)-1}{(k+1)!}\mathrm{ad}^k_{\sigma_0}(\gamma) - \frac{1}{2}\sum_{k=1}^{\infty}\frac{1}{k!}\mathrm{ad}^k_{\tilde{\sigma}_1}(\mathrm{dexp}_{\sigma_0}(\gamma))\\ &= -[\sigma_0,\gamma] + \frac{1}{3}[\sigma_0,[\sigma_0,\gamma]] - \frac{1}{6}[\sigma_0,[\sigma_0,[\sigma_0,\gamma]]] + \cdots - \frac{1}{2}[\tilde{\sigma}_1,\gamma] + \text{h.o.t.} \end{aligned}$$



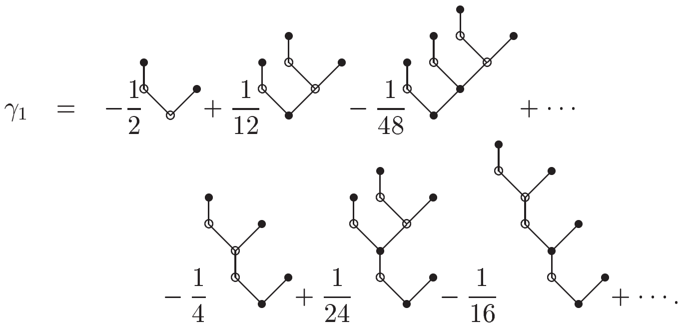
(2.18)

and note that, since $\tilde{\sigma}_1$ is already of order t^3, all the terms of the second sum (except the first one) are of order higher or equal to seven. But the highest order that we can attain with a formula $\exp\sigma_0\exp 2\sigma_1\exp\sigma_0$ is at most six! Hence this implies that we can disregard all the terms except the one corresponding to $k=1$, i.e. $[\tilde{\sigma}_1,\gamma]$.

In order to devise schemes of order higher than four, which we have presented in the example above, we need to an expansion of $\tilde{\sigma}_1$ to higher order. Using a further Picard iteration on (2.13), we obtain



which, substituted back in γ_1, yields



Integration of γ_1 is obtained by adding an extra white root to the collection of trees above: differently from the classical Fer expansion, this symmetric Fer version is nearer to the Magnus expansion, since it requires two trees of order four and three trees of order five.[1]

2.2 The symmetric Fer expansion and time-symmetry

In this section we wish to investigate the time-symmetry properties of the symmetric Fer expansion introduced above.

Definition 2.1 [7] A one-step numerical method $\Psi_h(t_0, h, y_0)$ is said to be *symmetric* if $\Psi(t_0 + h, -h, \Psi(t_0, h, y_0)) = y_0$. $\diamond$

To use a shorter notation, we will write $y_1 = \Psi_h y_0$ for $y_1 = \Psi_h(t_0, h, y_0)$, so that time-symmetry is equivalent to $\Psi_{-h} \circ \Psi_h = \mathrm{Id}$, whereby Id is the identity function. In other words, if we integrate the given ODE between t_0 and $t_1 = t_0 + h$ to obtain a numerical approximation y_1, and then back from t_1 to t_0, we obtain back the initial value (in exact arithmetic).

Symmetric methods are also known sometimes in literature as *self-adjoint* or *time-symmetric* schemes. We will often use all of these terms to indicate that the scheme in consideration obeys the definition above.

Theorem 2.3 *Assume that the σ_i's, $i = 0, 1, \ldots, M$, are computed to include all the trees of order up to k, where $2^{M+1} - 1 \le k \le 2^{M+2} - 2$. Then the expansion (2.3) is time-symmetric when γ is function of time only. Time-symmetry is retained when the integrals are replaced by symmetric quadrature formulae.*

Proof. Assume that $\gamma \equiv \gamma(t)$ so that the problem under consideration is

$$y' = \gamma(t) y, \qquad y(0) = y_0, \quad t \in [0, h].$$

Denote $\hat{\sigma}_i$ the truncation of σ_i to include all the trees of order up to k. Then, since $k \ge 1$,

$$\hat{\sigma}_0(t) = \sigma_0(t),$$

while in general, all the other σ_i are truncated, so that $\hat{\sigma}_i \neq \sigma_i$. In particular,

$$\hat{\sigma}_i(t) = \sum_{\ell=2^{i+1}-1}^{k} \sum_{m_\ell \in \mathcal{F}_\ell} \alpha(m_\ell) \int_0^t H_{m_\ell}(s)\,\mathrm{d}s,$$

whereby $\mathcal{F}_\ell$ is the forest of all order trees of order ℓ; for a given tree in the forest $\mathcal{F}_\ell$, the tree being identified by the index m_ℓ, $\alpha(m_\ell)$ is the corresponding coefficient, and finally H_{m_ℓ} is the integral term associated to it. Then,

$$y_1 = \mathrm{e}^{\hat{\sigma}_0(h)} \cdots \mathrm{e}^{2\hat{\sigma}_M(h)} \cdots \mathrm{e}^{\hat{\sigma}_0} y_0.$$

Next, we use the same formula to solve

$$\tilde{y}' = \gamma(t)\tilde{y}, \qquad \tilde{y}(h) = y_1, \quad t \in [0, h].$$

Fixed a $0 \le t \le h$, by construction

$$\tilde{y}(t) = \mathrm{e}^{\tilde{\sigma}_0(t)} \cdots \mathrm{e}^{2\tilde{\sigma}_M(t)} \cdots \mathrm{e}^{\tilde{\sigma}_0(t)} y_1,$$

[1]Although the order-four trees are the same as in the Magnus expansion, with exactly the same coefficients, we obtain a different collection of order five trees than the Magnus expansion, with different coefficients. This might show that the order five trees are not all independent and that one might have different equivalent combinations.

where now

$$\tilde{\sigma}_i(t) = \sum_{\ell=2^{i+1}-1}^{k} \sum_{m_\ell \in \mathcal{F}_\ell} \alpha(m_\ell) \int_h^t H_{m_\ell}(s)\,\mathrm{d}s,$$

In particular,

$$\tilde{\sigma}_i(0) = \sum_{\ell=2^{i+1}-1}^{k} \sum_{m_\ell \in \mathcal{F}_\ell} \alpha(m_\ell) \int_h^0 H_{m_\ell}(s)\,\mathrm{d}s = -\sum_{\ell=2^{i+1}-1}^{k} \sum_{m_\ell \in \mathcal{F}_\ell} \int_0^h H_{m_\ell}(s)\,\mathrm{d}s = -\hat{\sigma}_i(h),$$

therefore, because of the symmetry of the formula and the sign change, all the exponential terms cancel and we obtain $\tilde{y}(h) = y_0$.

The retention of time-symmetry when the integrals are replaced by symmetric quadrature formulas follows by standard arguments (see for instance [7]. □

In passing, we note that Theorem 2.2 can be obtained as a corollary of Theorem 2.3 above, since time-symmetry implies that the error of the numerical integrator Ψ expands in odd powers of h [7].

Time-symmetry for linear problems is a consequence of the fact that, when (1.1) is linear, all its solution can be found simply by multiplying the initial condition y_0 on the left by the *fundamental solution*. This is not true in the case of nonlinear equations, hence we cannot expect, by the arguments used above, that the methods discussed here are time-symmetric in this latter case.

2.3 On the convergence radius of the symmetric Fer expansion

Lemma 2.4 *Given a sequence of real numbers* $\{\alpha_n\}_{n=0}^{\infty}$, $|\alpha_n| < 1$, *the infinite product*

$$\lim_{n\to\infty} \prod_{k=0}^{n} (1+\alpha_k) \tag{2.19}$$

converges provided that

$$\sum_{n=0}^{\infty} \alpha_n \tag{2.20}$$

converges. In particular, provided that (2.20) *converges,*

$$\prod_{n=0}^{\infty} \mathrm{e}^{\alpha_n} = \exp\Big(\sum_{n=0}^{\infty} \alpha_n\Big).$$

Proof. We take the logarithm of (2.19),

$$\log \lim_{n\to\infty} \prod_{k=0}^{n} (1+\alpha_k) = \lim_{n\to\infty} \sum_{k=0}^{n} \log(1+\alpha_k) \le \lim_{n\to\infty} \sum_{k=0}^{n} \log \mathrm{e}^{\alpha_k} = \lim_{n\to\infty} \sum_{k=0}^{n} \alpha_k.$$

Thus, if (2.20) is obeyed, (2.19) is bounded by a converging series, hence it converges. The second part is a trivial consequence of the above. □

For the symmetric Fer expansion,

$$y = \mathrm{e}^{\sigma_0} \cdots \mathrm{e}^{\sigma_0} y_0,$$

we have

$$\|y\| \le \mathrm{e}^{\|\sigma_0\|} \cdots \mathrm{e}^{\|\sigma_0\|} \|y_0\| = \exp\Big(2 \sum_{0}^{\infty} \|\sigma_i\|\Big) \|y_0\|.$$

Hence, the symmetric Fer expansion converges uniformly for all $t \in [0,T]$, provided that

$$\lim_{m\to\infty} \sum_{i=0}^{m} \|\sigma_i\|$$

converges.

We recall the conditions for convergence for the classical Fer expansion (1.2). Let $\mu > 0$ be the least constant such that

$$\|[\gamma_1,\gamma_2]\| \le \mu\|\gamma_1\|\|\gamma_2\|, \qquad \forall \gamma_1,\gamma_2 \in \mathfrak{g}. \tag{2.21}$$

Theorem 2.5 *[16] The Fer expansion* (1.2) *converges uniformly in the interval* $[0,T]$*, provided that*

$$\int_0^T \|\gamma\|\,\mathrm{d}t \le \frac{1.720817\ldots}{\mu}. \tag{2.22}$$

A similar result holds for the symmetric Fer expansion (2.3):

Theorem 2.6 *The symmetric Fer expansion* (2.3) *converges uniformly in the interval* $[0,T]$*, provided that*

$$\int_0^T \|\gamma\|\,\mathrm{d}t \le \frac{1.4713\ldots}{\mu}. \tag{2.23}$$

Proof. Recall that

$$\begin{aligned} \sigma_i(t) &= \frac{1}{2}\int_0^t \gamma_i(\tau)\,\mathrm{d}\tau, &(2.24)\\ \gamma_i(\tau) &= \mathrm{e}^{-\sigma_{i-1}}\Big(\gamma_{i-1} - \mathrm{dexp}_{\sigma_{i-1}}(\tfrac{1}{2}\gamma_{i-1})\Big)\mathrm{e}^{\sigma_{i-1}} - \mathrm{e}^{\tilde\sigma_i}\mathrm{dexp}_{\sigma_{i-1}}(\tfrac{1}{2}\gamma_{i-1})\mathrm{e}^{-\tilde\sigma_i}, &(2.25)\end{aligned}$$

where $\tilde\sigma_i$ is the solution of the differential equation

$$\begin{aligned} \tilde\sigma_i' &= \mathrm{dexp}^{-1}_{\tilde\sigma_i}\{\mathrm{e}^{-\sigma_{i-1}}\Big(\gamma_{i-1} - \mathrm{dexp}_{\sigma_{i-1}}(\tfrac{1}{2}\gamma_{i-1})\Big)\mathrm{e}^{\sigma_{i-1}} - \mathrm{e}^{\tilde\sigma_i}\mathrm{dexp}_{\sigma_{i-1}}(\tfrac{1}{2}\gamma_{i-1})\mathrm{e}^{-\tilde\sigma_i}\} \quad (2.26)\\ &= \gamma_{i,2} + B_1[\tilde\sigma_i,\gamma_{i,1}] + \sum_{k=1}^{\infty}\frac{B_{2k}}{(2k)!}\mathrm{ad}^{2k}_{\tilde\sigma_i}(\gamma_{i,2})\\ &= \Big(\frac{z}{\mathrm{e}^z-1}+\frac{1}{2}z\Big)\Big|_{z=\mathrm{ad}_{\tilde\sigma_i}}(\gamma_{i,2}) + B_1[\tilde\sigma_i,\gamma_{i,1}],\end{aligned}$$

where

$$\begin{aligned} \gamma_{i,2} &= \frac{1}{2}\sum_{k=1}^{\infty}\frac{(-1)^k(2k+1)-1}{(k+1)!}\mathrm{ad}^k_{\sigma_{i-1}}(\gamma_{i-1}), &(2.27)\\ \gamma_{i,1} &= \frac{1}{2}\sum_{k=1}^{\infty}\frac{(-1)^k(2k+1)}{(k+1)!}\mathrm{ad}^k_{\sigma_{i-1}}(\gamma_{i-1}). &(2.28)\end{aligned}$$

It follows that

$$\tilde\sigma_i = \int_0^t \Big[\Big(\frac{z}{\mathrm{e}^z-1}+\frac{1}{2}z\Big)\Big|_{z=\mathrm{ad}_{\tilde\sigma_i}}(\gamma_{i,2}) + B_1[\tilde\sigma_i,\gamma_{i,1}]\Big]\,\mathrm{d}s,$$

hence, making use of the triangle inequality and of (2.21), we find

$$\|\tilde\sigma_i\| \le \int_0^t \sum_{k=0}^{\infty}\frac{|B_{2k}|}{(2k)!}(\mu\|\tilde\sigma_i\|)^{2k}\|\gamma_{i,2}\|\,\mathrm{d}s + \frac{1}{2}\int_0^t \mu\|\tilde\sigma_i\|\|\gamma_{i,1}\|\,\mathrm{d}s. \tag{2.29}$$

Note that

$$\sum_{k=0}^{\infty} \frac{|B_{2k}|}{(2k)!} z^{2k} = 2 - \frac{x}{2}\cot(\frac{x}{2}), \qquad |x| < 2\pi,$$

hence,

$$\|\tilde{\sigma}_i\| \leq \int_0^t g_1(\mu\|\tilde{\sigma}_i\|)\|\gamma_{i,2}\| \, \mathrm{d}s + \frac{1}{2}\int_0^t g_2(\mu\|\tilde{\sigma}_i\|)\|\gamma_{i,1}\| \, \mathrm{d}s,$$

where

$$g_1(x) = 2 - \frac{x}{2}\cot(\frac{x}{2}), \quad g_2(x) = x,$$

for x in $[0, 2\pi)$. We observe that $\gamma_{i,1}, \gamma_{i,2}$ do not depend on $\tilde{\sigma}_i$, while they depend on σ_{i-1} and γ_{i-1}. Furthermore, because of (2.27) and (2.28),

$$\begin{aligned} \|\gamma_{i,2}\| &\leq \sum_{k=1} \frac{1}{k!}(\mu\|\sigma_{i-1}\|)^k \|\gamma_{i-1}\| \leq \mathrm{e}^{\mu\|\sigma_{i-1}\|}\|\gamma_{i-1}\|, \\ \|\gamma_{i,1}\| &\leq \mathrm{e}^{\mu\|\sigma_{i-1}\|}\|\gamma_{i-1}\| - 1 < \mathrm{e}^{\mu\|\sigma_{i-1}\|}\|\gamma_{i-1}\|, \end{aligned}$$

hence

$$\|\tilde{\sigma}_i\| \leq \int_0^t (g_1(\mu\|\tilde{\sigma}_i\|) + \frac{1}{2}\mu\|\tilde{\sigma}_i\|)\mathrm{e}^{\mu\|\sigma_{i-1}\|}\|\gamma_{i-1}\| \, \mathrm{d}s,$$

whereby $\exp(\mu\|\sigma_{i-1}\|)\|\gamma_{i-1}\| = v(s)$ is a positive function which does not depend on $\tilde{\sigma}_i$. Now we can apply Lemma 1 in [12], to obtain

$$\|\tilde{\sigma}_i\|(t) \leq \frac{1}{\mu} G^{-1}\Big(\mu \int_0^t v(s) \, \mathrm{d}s\Big), \tag{2.30}$$

(we observe that $\tilde{\sigma}_i$ obeys a convergence condition similar to the case of the Magnus expansion [12]), where

$$G(x) = \int_0^x \frac{1}{g(s)} \, \mathrm{d}s, \quad g(z) = 2 + \frac{z}{2}\Big(1 - \cot(\frac{z}{2})\Big), \quad 0 \leq z < 2\pi.$$

which, in Taylor expansion at $x = 0$, yields

$$\begin{aligned} G(x) \;\; = \;\; & x - \frac{1}{4}x^2 + \frac{1}{18}x^3 - \frac{1}{96}x^4 + \frac{1}{900}x^5 + \frac{1}{4320}x^6 \\ & - \frac{43}{211680}x^7 + \frac{3}{35840}x^8 - \frac{209}{8164800}x^9 + \mathcal{O}(x^{10}) \, . \end{aligned}$$

The graph of $G(x)$ is displayed in Figure 3 below. We observe that, by (2.24) and a change of variable,

$$\mu \int_0^t v(s) \, \mathrm{d}s = \mu \int_0^t \mathrm{e}^{\mu\|\sigma_{i-1}\|}\|\gamma_{i-1}\| \, \mathrm{d}s = \mu \int_0^{\|\sigma_{i-1}(t)\|} 2\mathrm{e}^{\mu x} \, \mathrm{d}x = 2(\mathrm{e}^{\mu||\sigma_{i-1}(t)||} - 1),$$

hence, in order to have $\mu\|\tilde{\sigma}_i\| < 2\pi$, we must require that

$$G(\mu\|\tilde{\sigma}_i\|) \leq 2(\mathrm{e}^{\mu||\sigma_{i-1}(t)||} - 1) < G(2\pi) = \int_0^{2\pi} \frac{\mathrm{d}s}{g(s)} \approx 2.1737\ldots$$

(since G is strictly non decreasing), hence,

$$\|\sigma_{i-1}\| \leq \frac{0.73565\ldots}{\mu}.$$

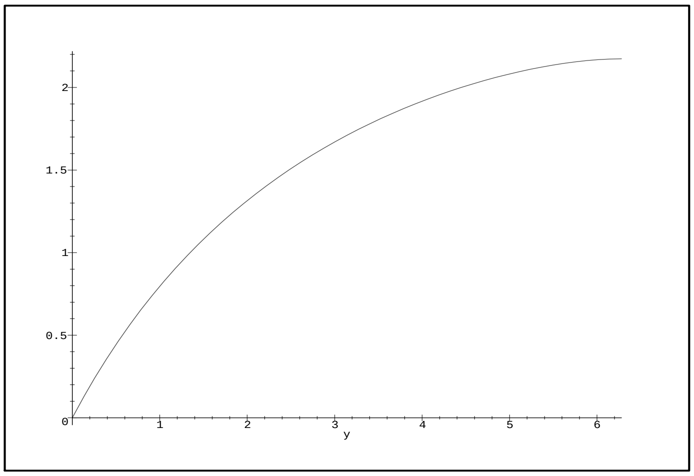


Figure 3: The plot of $G(x)$, for $x \in [0, 2\pi)$. See text for details.

Now we are ready to estimate $\|\sigma_i\|$,

$$\|\sigma_i\| \le \frac{1}{2}\int_0^t \|\gamma_i\|\,\mathrm{d}s \le \int_0^t \|\gamma_{i,1}\| + \frac{1}{2}\|\sum_{k=0}^{\infty}\frac{1}{k!}\mathrm{ad}_{\tilde\sigma_i}^k \sum_{\ell=0}^{\infty}\frac{1}{(\ell+1)!}\mathrm{ad}_{\sigma_{i-1}}^{\ell}(\gamma_{i-1})\|\,\mathrm{d}s,$$

and, in a procedure very similar to the one followed above, we find

$$\|\sigma_i\| \le \frac{1}{2}\int_0^t \left[\mathrm{e}^{\mu\|\sigma_{i-1}\|} + \frac{1}{2}\mathrm{e}^{\mu\|\tilde\sigma_i\|}\frac{\mu\|\sigma_{i-1}\|}{\mathrm{e}^{\mu\|\sigma_{i-1}\|}-1}\right]\|\gamma_{i-1}\|\,\mathrm{d}s.$$

We observe that $G(x) \le \log(2x+1)$. Hence, $x = G^{-1}(y) \le (\mathrm{e}^y - 1)/2$. We use this bound to estimate $\|\tilde\sigma_i\|$, and finally we obtain a relation of the form

$$\|\sigma_i\| \le \frac{1}{2\mu}F(\mu\sigma_{i-1}),$$

whereby

$$F(x) = \int_0^x \left(\mathrm{e}^x + \frac{1}{2}\mathrm{e}^{(\mathrm{e}^x-1)/2}\frac{x}{\mathrm{e}^x-1}\right)\mathrm{d}x \approx \frac{3}{2}x + \frac{1}{2}x^2 + \frac{29}{144}x^3 + \frac{5}{96}x^4 + \mathcal{O}(x^5).$$

Let $\bar x$ be such that

$$F(x) \le 2x, \qquad \forall x \le \bar x, \quad \bar x \approx 0.73843\ldots.$$

Then, provided that $\mu\|\sigma_{i-1}\| < 0.73565\ldots < 0.73843\ldots$,

$$\|\sigma_i\|/\|\sigma_{i-1}\| \le \frac{1}{2}\frac{F(\mu\|\sigma_{i-1}\|)}{\mu\|\sigma_{i-1}\|} < 1,$$

and, because of the comparison test, the series converges. Hence, convergence is guaranteed for all $t \in [0, T]$ for which $\int_0^t \|\gamma\| < 1.4713\ldots/\mu$. □

Thus, the radius of convergence of the symmetric Fer expansion introduced above is at least $1.4713\ldots/\mu$, which however is smaller than $1.720813\ldots/\mu$, the radius for the Fer expansion as derived by [16]. We should also mention that the bounds used in the proof above are not 'optimal' and could be improved, for instance one could find a better estimate for the inverse of the function G, or, more importantly, a sharper bound for $\|\tilde\sigma_i\|$.

3 Some numerical schemes

The construction of the numerical schemes for the symmetric Fer expansion introduced above is a procedure very similar to the case of the standard Fer and Magnus expansions. Assuming that $\gamma(t_n)$ or an approximation to it, say γ_n, is known, we replace the function $\gamma(t)$ by its interpolant at some given nodes $t_n + c_1 h, \ldots, t_n + c_\nu h$, where h is the stepsize of integration, $h = t_{n+1} - t_n$. Such interpolating polynomial is substituted on the leaves of the relevant order trees of expansion (see Section 2), and, by the linearity of the commutator operator, we obtain the integration weights. We refer the reader to [10, 20, 19], where the procedure is described in detail.

Here, we consider the method (2.13) introduced in Example 2.1, which we have proved to be of order four. We choose the Gauss-Legendre quadrature nodes $c_1 = \frac{1}{2} - \frac{\sqrt{3}}{6}, c_2 = \frac{1}{2} + \frac{\sqrt{3}}{6}$, to obtain

$$\begin{aligned}
\hat{\sigma}_0 &= \frac{1}{2}\int_{t_n}^{t_{n+1}} \gamma(\tau)\,\mathrm{d}\tau \approx \frac{1}{2}\Big(\frac{h}{2}(\gamma(t_n + c_1 h) + \gamma(t_n + c_2 h))\Big) = \frac{h}{4}(\gamma_1 + \gamma_2)\\
\hat{\sigma}_1 &= -\frac{1}{4}\int_0^t [\int_0^\tau \gamma(u)\,\mathrm{d}u, \gamma(\tau)]\,\mathrm{d}\tau \approx -\frac{\sqrt{3}}{24} h^2[\gamma_1, \gamma_2],
\end{aligned}$$

where γ_i denotes $\gamma(t_n + c_i h), i = 1, 2$. The numerical approximation looks like

$$y_{n+1} = \exp\Big(\frac{h}{4}(\gamma_1 + \gamma_2)\Big)\exp\Big(-\frac{\sqrt{3}}{12}h^2[\gamma_1, \gamma_2]\Big)\exp\Big(\frac{h}{4}(\gamma_1 + \gamma_2)\Big) y_n, \qquad n = 0, 1, 2, \ldots. \tag{3.1}$$

We evaluate the time symmetry error of the above schemes for the function γ as in (1.7). The plot is displayed in Figure 4.

A nonlinear version of the scheme (3.1) is

$$\begin{aligned}
Y_i &= \exp(\tfrac{h}{2}\textstyle\sum_{j=1}^2 a_j^i \gamma_j)\exp\Big(h^2 \Delta^i_{1,2}[\gamma_1, \gamma_2]\Big)\exp(\tfrac{h}{2}\textstyle\sum_{j=1}^2 a_j^i \gamma_j) y_n,\\
\gamma_i &= \gamma(t_n + c_i h), \qquad i = 1, 2\\
y_{n+1} &= \exp(\tfrac{h}{4}(\gamma_1 + \gamma_2))\exp\Big(-\tfrac{\sqrt{3}}{12}h^2[\gamma_1, \gamma_2]\Big)\exp(\tfrac{h}{4}(\gamma_1 + \gamma_2)) y_n,
\end{aligned} \tag{3.2}$$

where

$$(a_j^i) = \begin{pmatrix} \frac{1}{4} - \frac{\sqrt{3}}{6} & \frac{1}{4} \\ \frac{1}{4} & \frac{1}{4} + \frac{\sqrt{3}}{6} \end{pmatrix}, \qquad \Delta^1_{1,2} = \frac{5}{72} - \frac{\sqrt{3}}{24}, \Delta^2_{1,2} = -\frac{5}{72} - \frac{\sqrt{3}}{24}$$

The time-symmetry error of the method (3.1) is displayed in Figure 5 below, for the problem

$$y' = \gamma(y) y, \qquad y(0) = y_0, \quad t \in [0, 10],$$

where now $y \in \mathbb{R}^3$ and $\gamma : \boldsymbol{y} \in \mathbb{R}^3 \to \mathfrak{so}(3)$ is the map

$$\gamma(y) = -\begin{pmatrix} 0 & v_3 & -v_2 \\ -v_3 & 0 & v_1 \\ v_2 & -v_1 & 0 \end{pmatrix}.$$

It is clear that the nonlinear method (3.2) is not time-symmetric for nonlinear problems, but has better time-symmetry than expected (we would expect the time-symmetry error to be $\mathcal{O}(h^4)$ while it is $\mathcal{O}(h^5)$). Exactly the same behaviour is displayed in Figure 6 below, by the Magnus-type method for nonlinear problems [19, 20]

$$\begin{aligned}
Y_i &= \exp\Big(h\textstyle\sum_{j=1}^2 a_j^i \gamma_j + h^2 \Delta^i_{1,2}[\gamma_1, \gamma_2]\Big) y_n,\\
\gamma_i &= \gamma(t_n + c_i h), \qquad i = 1, 2\\
y_{n+1} &= \exp\Big(\tfrac{h}{2}(\gamma_1 + \gamma_2) - \tfrac{\sqrt{3}}{12}h^2[\gamma_1, \gamma_2]\Big) y_n,
\end{aligned} \tag{3.3}$$

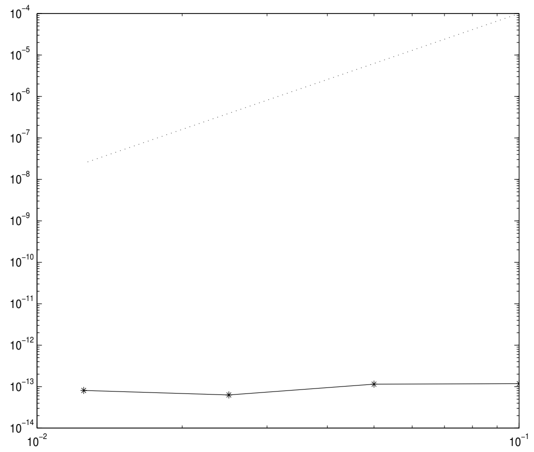


Figure 4: Time symmetry error of the method (3.1) for γ as in (1.7). The dotted line represents the slope of h^4. Compare with Figure 1-2

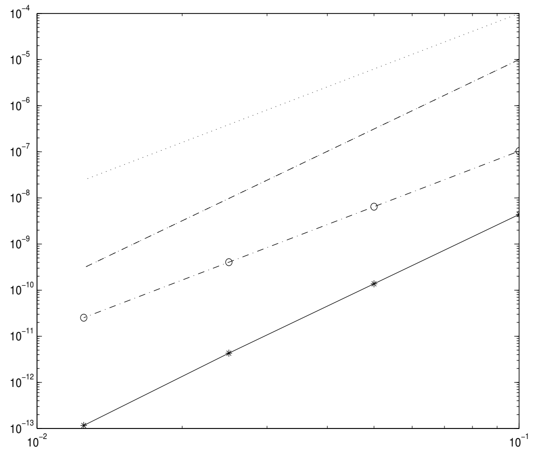


Figure 5: Time-symmetry error (asterisks joined by solid line) for the nonlinear method (3.2) when applied to nonlinear problems. The circles joined by dash-dotted line represent the norm of the error at $t = 10$. The dotted line is the slope of h^4, while the dashed line represents the slope of h^5. The method displays order four in approximation and order five in time-symmetry.

where the a_j^i's and the $\Delta_{1,2}^i$ are the same coefficients as above.

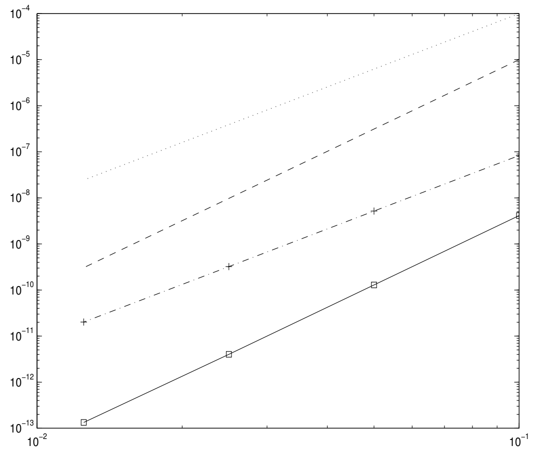


Figure 6: Time-symmetry error (squares joined by solid line) for the nonlinear method (3.3) when applied to nonlinear problems. The pluses joined by dash-dotted line represent the norm of the error at $t = 10$. The dotted line is the slope of h^4, while the dashed line represents the slope of h^5. The method displays order four in approximation and order five in time-symmetry.

The same qualitative behaviour is also displayed by the RKMK-type Lie-group methods [13] based on Gaussian or on symmetric collocation nodes.

4 On the complexity of the symmetric Fer expansion

In this section we wish to discuss the complexity of the symmetric Fer expansion proposed above, when compared to the classical Fer expansion. We need to consider two 'ingredients' in our comparison: the first one is the cost of evaluating the matrix exponential, the second one is the cost of evaluating commutators and performing matrix multiplications.

Since the cost of computing the exponential is quite problem dependent, we will assume that

$$\mathrm{cost}(\mathrm{e}^{\sigma}) = E \equiv E(d), \quad \forall \gamma \in \mathfrak{g},$$

(σ is a $d \times d$ matrix), i.e. it depends on the dimension of the matrix, but it is essentially the same for all matrices in the algebra $\mathfrak{g}$. Thus, two exponentials cost $2E$ and so on and so forth. We do not discuss how to compute the exponential function, while referring the reader to [3] for a deeper treatment of this issue.

With regards to the cost of the commutator, we usually evaluate

$$[\gamma_1, \gamma_2] = \gamma_1\gamma_2 - \gamma_2\gamma_1,$$

so that the cost of the commutator is essentially the cost of matrix multiplications

$$\mathrm{cost}([\gamma_1, \gamma_2]) = d^3.$$

The number of exponential in the expansion is quite easy to evaluate. The evaluation of the number of commutators is a more difficult task. Assume that we have ν nodes: for each order tree appearing in the expansion of the method, we need to evaluate commutators like

$$[\gamma_i, [\gamma_j, \ldots], \gamma_n], \quad i, j, k, \ell, m, n \ldots = 1, \ldots, \nu.$$

To this purpose, we need to establish an ordering of the commutators. We affirm that all commutators can be written using a Hall basis [15], where the terms $\gamma_1, \gamma_2, \ldots$ have all weight equal one. Thus, for each order condition $1 \le k \le p$, (where p is the order of the method), the number of commutators to consider equals the sum of the number of terms in the Hall set with weight exactly k. Such numbers can be evaluated using the *DiffMan* package.[2]

Example 4.1 Let $\nu = 3$, so that we have $\gamma_1, \gamma_2, \gamma_3$ all with weight equal to one. The number of commutators of the form $[\gamma_i, [\gamma_j, \gamma_\ell]]$ is equal to the number of terms in the Hall set with weight equal to three, which is 8.

$$\mathtt{lafcount}(3, [1, 1, 1]) = 8.$$

For a classical Fer order 6 method, we need to consider: $\mathtt{lafcount}(3, [1, 1, 1]) + \mathtt{lafcount}(4, [1, 1, 1]) + \ldots + \mathtt{lafcount}(6, [1, 1, 1]) = 3 + 8 + 18 + 48$. $\diamond$

Since $p = 2\nu$, for the symmetric Fer expansion it is sufficient to count the number of terms in the Hall set with weight $k \le p - 1$.

For what concerns linear problems, the results for methods of order four and six based on Gaussian collocation nodes are shown in Table 1 below.

Order	4	4	6	6
nodes (ν)	2	2	3	3
# exp.	2	2	2	2
# comm.	1+2	1	3 + 8 + 18 + 48	3+8+18
# matr. mult.	2	3	2	3
Total	$5d^3 + 2E$	$4d^3 + 2E$	$79d^3 + 2E$	$32d^3 + 2E$

Table 1: Complexity of the classical Fer (first and third column) and symmetric Fer expansion (second and fourth) based on Gaussian collocation nodes for orders four and six when applied to linear problems.

For nonlinear problems, the count is similar. Assume that the internal stages (for a total of ν stages) are solved for example by fixed point iteration, so that we perform say ℓ iterations. Then, the internal stages of the classical Fer expansion need to be evaluated to order $p - 1$ only [19, 20], while the final stage is evaluated to order $p = 2\nu$. In Figure 7 we plot the difference in the cost of the classical and symmetric Fer scheme when $\nu = 3$, which, assuming that the two schemes require the same number ℓ of nonlinear iteration, is $(-3\ell + 78)d^3$. Clearly, the savings occur especially when the number of nonlinear iterations ℓ is small, and the dimension d of the system is large. In particular, as long as $\ell \le 26$, the symmetric Fer expansion is less expensive: in general, far less numerical fixed point iterations are performed in practical computations. Furthermore, the higher the order of the methods, the greater the savings, because of the growth of the size of the Hall set generated by the γ_i. In passing, we mention that for linear problems it would be possible to apply a transformation of variables to the internal stages in order to operate in a graded free Lie-algebra, and this would further reduce the number of commutators [15]. However, it is not clear how to apply the technique of free Lie algebras to nonlinear problems.

5 Conclusion

In conclusion, we have presented a number of methods that originate from a symmetric version of the Fer expansion. Such methods are based on a Strang-type product of exponentials and,

[2] The DiffMan package can be downloaded at: `www.math.ntnu.no/SYNODE`

Order	4	4
nodes (ν)	2	2
# exp.	$2(\ell\nu+1)$	$2(\ell\nu+1)$
# comm.	$2(\ell\nu+1)+1$	$\ell\nu+1$
# matr. mult.	$2(\ell\nu+1)$	$3(\ell\nu+1)$
Total	$(4\ell\nu+5)d^3+2(\ell\nu+1)E$	$(4\ell\nu+4)d^3+2(\ell\nu+1)E$
Order	6	6
nodes (ν)	3	3
# exp.	$2(\ell\nu+1)$	$2(\ell\nu+1)$
# comm.	$29(\ell\nu+1)+48$	$29(\ell\nu+1)$
# matr. mult.	$2(\ell\nu+1)$	$3(\ell\nu+1)$
Total	$(31\ell\nu+79)d^3+2(\ell\nu+1)E$	$32(\ell\nu+1)d^3+2(\ell\nu+1)E$

Table 2: Complexity of the classical Fer (left column) and symmetric Fer expansion (right column) based on Gaussian collocation nodes for orders four and six when applied to nonlinear problems. Since the methods are implicit, ν is the number of stages, while ℓ is the number of fixed point iterations to solve the nonlinear equations for the internal stages of the methods.

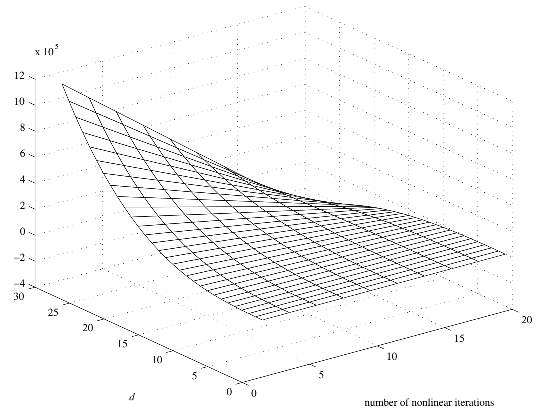


Figure 7: Cost-difference of the classical and symmetric Fer method for three Gaussian nodes

although their analysis is more complicated than that for methods based on the classical Fer expansion, they present a number of advantages. First of all, these methods are time-symmetric for linear problems. This implies that it is possible to simplify the order conditions and reduce the implementation cost. The savings are significant for linear problems, while for nonlinear problems, they depend on the number of fixed point iterations performed. For a small number of fixed point iterations, the new methods are competitive with respect to the old ones, otherwise the cost is very similar. Furthermore, in the case of nonlinear problems, although the methods are not time symmetric, they display a higher degree of time symmetry.

In many applications, for example Hamiltonian problems, it is important to use symplectic methods, since those are the methods that better preserve the qualitative attributes of the solution. In the case when symplecticity is difficult to achieve, time-symmetry is the second best attribute. The methods discussed here are not time-symmetric for nonlinear problem, the main problem being that they employ coordinate charts based on y_n when stepping from y_n to y_{n+1} and charts based on y_{n+1} when instead stepping from y_{n+1} to y_n. This is also the case for the Magnus-type methods in [10, 19, 20] and the RKMK methods in [13]. The 'midpoint' scheme

$$y_{n+1} = \exp(h\gamma_{n+\frac{1}{2}})y_n, \quad \gamma_{n+\frac{1}{2}} = \gamma\Big(\exp(\frac{h}{2}\gamma_{n+\frac{1}{2}})y_n\Big),$$

is the only exception, since, setting $y_{n+\frac{1}{2}} = \exp(\frac{h}{2}\gamma_{n+\frac{1}{2}})y_n$, one could write

$$y_{n+1} = \exp(\frac{h}{2}\gamma_{n+\frac{1}{2}})y_{n+\frac{1}{2}}, \quad y_n = \exp(-\frac{h}{2}\gamma_{n+\frac{1}{2}})y_{n+\frac{1}{2}}.$$

and it is always time-symmetric, both in the linear and nonlinear case [4]. Therefore, if time symmetry is the goal, a better approach would be to consider a coordinate chart centered on a 'midpoint' $y_{n+\frac{1}{2}}$.

A good candidate would be the following variant of the symmetric Fer expansion introduced in this paper. Again, we look for an expansion of the exact solution, depending upon a certain parameter c, of the form

$$y(t) = \mathrm{e}^{\hat\sigma_0}\mathrm{e}^{\hat\sigma_1}\cdots\mathrm{e}^{\sigma_1}\mathrm{e}^{\sigma_0}y_0,$$

where now we set

$$\sigma_0 = \int_0^{ct}\gamma(\tau)\,\mathrm{d}\tau, \quad \hat\sigma_0 = \int_{ct}^{t}\gamma(\tau)\,\mathrm{d}\tau,$$

and, in general

$$\sigma_i = \int_0^{ct}\gamma_i(\tau)\,\mathrm{d}\tau, \quad \hat\sigma_i = \int_{ct}^{t}\gamma_i(\tau)\,\mathrm{d}\tau,$$

where the functions γ_i are to be determined. If $c = \frac{1}{2}$, then our scheme would be centered at the 'midpoint'.

A more general form would be

$$y(t) = \mathrm{e}^{\hat\sigma_0}\mathrm{e}^{\hat\sigma_1}\cdots\mathrm{e}^{\sigma_1}\mathrm{e}^{\sigma_0}y_0,$$

where we are allowed to use a different value $c_i \in [0,1]$ for each $\sigma_i, \hat\sigma_i$,

$$\sigma_i = \int_0^{c_i t}\gamma_i(\tau)\,\mathrm{d}\tau, \quad \hat\sigma_i = \int_{c_i t}^{t}\gamma_i(\tau)\,\mathrm{d}\tau,$$

Note that when $c_i = 0, i = 0, \ldots$ and when $c_i = 1, i = 1, \ldots$, then the above expansion is the classical Fer expansion, while if the $c_i = \frac{1}{2}$, we would obtain the centered version of the scheme. Similarly, one might consider a symmetric version of the Wei and Norman splitting [18]. The analysis of these variants is at the moment work in progress and we expect to report the further results in a future paper.

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