Exponential integrators of Rosenbrock-type

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(joint work with Julia Schweitzer)

1. Introduction

We consider a system of ordinary differential equations in autonomous form

$$y'(t) = f(y), \qquad y(t_0) = y_0, \tag{1}$$

assuming that the linearisation $J = Df(y)$ is uniformly sectorial in a neighbourhood of the exact solution. Consequently, there exist constants C and ω (both independent of y) such that

$$\left\| \mathrm{e}^{tJ} \right\| \le C\, \mathrm{e}^{\omega t}, \qquad t \ge 0. \tag{2}$$

Typical examples are abstract nonlinear parabolic equations, see [4], and their spatial discretisations.

Recently, we studied a class of explicit exponential Runge–Kutta methods for similar problems, see [2]. Due to the involved structure of the order conditions, however, it seems to be difficult to construct reliable and efficient error estimates for these methods. Moreover, in contrast to classical time integrators, exponential Runge–Kutta methods are *not invariant* under linearisation. This results in an error behaviour similar to classical W-methods, see [1]. Therefore, one has to expect large errors whenever the linear part is not well chosen.

2. Method class

Motivated by the observations just mentioned, we propose to linearise the right-hand side of (1) in each step, as it is done in classical Rosenbrock methods. Thus we write

$$y' = J_n y + g_n(y), \qquad J_n = Df(y_n), \quad g_n(y) = f(y) - J_n y. \tag{3}$$

Here, y_n is the numerical approximation to $y(t_n)$.

Applying then an exponential Runge–Kutta method to (3) gives the following s-stage exponential Rosenbrock-type scheme

$$Y_{ni} = \mathrm{e}^{c_i h J_n} y_n + h \sum_{j=1}^{i-1} a_{ij}(hJ_n)\, g_n(Y_{nj}), \tag{4a}$$

$$y_{n+1} = \mathrm{e}^{hJ_n} y_n + h \sum_{i=1}^{s} b_i(hJ_n)\, g_n(Y_{ni}). \tag{4b}$$

For a variable step size implementation of (4), we base the step size selection on a local error control. For that purpose, we consider the embedded error estimator

$$\widehat{y}_{n+1} = \mathrm{e}^{hJ_n} y_n + h \sum_{i=1}^{s} \widehat{b}_i(hJ_n)\, g_n(Y_{ni}) \tag{5}$$

and take the difference $\|y_{n+1} - \widehat{y}_{n+1}\|$ as error estimate.

3. Stiff order conditions

As usual in exponential integrators, the functions

$$\varphi_k(hJ) = h^{-k} \int_0^h \mathrm{e}^{(h-\tau)J} \frac{\tau^{k-1}}{(k-1)!}\, \mathrm{d}\tau, \qquad k \geq 1$$

play an important role. For sectorial operators J, the bound (2) shows that these functions are well defined and bounded on compact time intervals.

It is shown in [3] that the stiff order conditions for an exponential Rosenbrock-type method are given as:

No.	Order	Order Condition
1	1	$\sum_{i=1}^{s} b_i(hJ) = \varphi_1(hJ)$
2	2	$\sum_{j=1}^{i-1} a_{ij}(hJ) = c_i\varphi_1(c_i hJ), \quad 2 \leq i \leq s$
3	3	$\sum_{i=2}^{s} b_i(hJ)c_i^2 = 2\varphi_3(hJ)$
4	4	$\sum_{i=2}^{s} b_i(hJ)c_i^3 = 6\varphi_4(hJ)$

The first, third, and fourth order condition are just the (exponential) quadrature conditions, the second one is the well-known $C(1)$ condition, generalised to the operator case.

It is worth noting that the exponential Euler method applied to (3) is second-order accurate. It has one stage ($s = 1$) with weight $b_1(hJ) = \varphi_1(hJ)$ and consequently satisfies the first two order conditions.

4. Examples

From the above order conditions, it is straightforward to construct pairs of embedded methods up to order 4. We consider two examples. The method `exprb32` is a third-order method with a second-order error estimator (the exponential Euler method). Its coefficients are

$$\begin{array}{c|cc} c_1 & & \\ c_2 & a_{21} & \\ \hline & b_1 & b_2 \\ & \widehat{b}_1 & \end{array} \quad = \quad \begin{array}{c|cc} 0 & & \\ 1 & \varphi_1 & \\ \hline & \varphi_1 - 2\varphi_3 & 2\varphi_3 \\ & \varphi_1 & \end{array}$$

The method `exprb43` is a fourth-order method with a third-order error estimator. Its coefficients are

$$\begin{array}{c|ccc} c_1 & & & \\ c_2 & a_{21} & & \\ c_3 & a_{31} & a_{32} & \\ \hline & b_1 & b_2 & b_3 \\ & \widehat{b}_1 & \widehat{b}_2 & \widehat{b}_3 \end{array} \quad = \quad \begin{array}{c|ccc} 0 & & & \\ \frac{1}{2} & \frac{1}{2}\varphi_1(\frac{1}{2}\,\cdot) & & \\ 1 & 0 & \varphi_1 & \\ \hline & \varphi_1 - 14\varphi_3 + 36\varphi_4 & 16\varphi_3 - 48\varphi_4 & -2\varphi_3 + 12\varphi_4 \\ & \varphi_1 - 14\varphi_3 & 16\varphi_3 & -2\varphi_3 \end{array}$$

5. Stability and Convergence

For proving convergence estimates, the temporal smoothness of the *exact solution* is one of our basic ingredients. Using this property, we establish by Taylor series expansion a recursion for the global errors $E_n = y_n - y(t_n)$ in terms of the defects

$$E_{n+1} = \mathrm{e}^{h_n J_n} E_n + h_n \Delta_n.$$

Here Δ_n depends on E_n and on the defects itself. The stability of this recursion is all-important. It is verified in [3] that there exist constants C and Ω such that

$$\left\| \mathrm{e}^{h_n J_n} \cdots \mathrm{e}^{h_0 J_0} \right\| \;\le\; C\, \mathrm{e}^{\Omega(h_0 + \ldots + h_n)},$$

whenever the involved step sizes are sufficiently small. We emphasise that our proof of this result does *not* require the unrealistic condition $\left\| \mathrm{e}^{h_m J_m} \right\| \le 1$.

A method is said to have *order* p, if it fulfils the stiff order conditions up to order p. For such methods, we have the following convergence result, see [3].

Theorem (Convergence). *Under the above assumptions, for $H > 0$ sufficiently small and $T \ge t_0$, there exists a constant C such that the global error satisfies*

$$\left\| y_n - y(t_0 + nh) \right\| \;\le\; C\, h^p,$$

uniformly for all $0 < h \le H$ and all $n \ge 0$ with $nh \le T - t_0$. The constant C is independent of n and h.

Methods up to order 4 can be constructed easily, see the previous section. For numerical comparisons, we refer to [3].

References

[1] E. Hairer and G. Wanner, *Solving Ordinary Differential Equations II. Stiff and Differential-Algebraic Problems.* 2nd rev. ed., Springer, Berlin, 1996.

[2] M. Hochbruck and A. Ostermann, *Explicit exponential Runge-Kutta methods for semilinear parabolic problems.* SIAM J. Numer. Anal. **43** (2005), 1069–1090.

[3] M. Hochbruck, A. Ostermann, and J. Schweitzer, *Exponential Rosenbrock-type methods.* In preparation.

[4] A. Lunardi, *Analytic Semigroups and Optimal Regularity in Parabolic Problems.* Birkhäuser, Basel, 1995.