Revised exponentially fitted Runge-Kutta-Nyström methods

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Abstract

It is the purpose of this paper to revise the exponential fitting technique for the numerical solution of special second order ordinary differential equations (ODEs) $y'' = f(x, y)$, with oscillatory or periodic solutions, by Runge-Kutta-Nyström methods. Due to the multistage nature of these methods, the proposed technique takes into account the contribution to the error arising from the computation of the internal stages. The benefit on the accuracy of the overall numerical scheme is visible in the presented numerical evidence.

Key words: Second order ordinary differential equations, Runge-Kutta-Nyström methods, exponential fitting.

1. Introduction

The paper is focused on the numerical solution of Hadamard well-posed special second order ordinary differential equations (ODEs)

$$y'' = f(x, y), \quad y'(x_0) = y'_0, \quad y(x_0) = y_0 \in \mathbb{R}, \tag{1.1}$$

assumed to exhibit an a priori known periodic/oscillatory behaviour. Classical numerical methods for ODEs may not be well-suited to follow a prominent periodic or oscillatory behaviour because, in order to accurately follow the oscillations, a very small stepsize would be required with corresponding deterioration of the numerical performances, especially in terms of efficiency. For this reason, many classical numerical methods have been adapted in order to efficiently approach oscillatory problems. One of the possible ways to proceed in this direction is obtained by imposing that a numerical method exactly integrates (within the round-off error) problems of type (1.1) whose solution can be expressed as linear combination of functions other than polynomials: this is the spirit of the exponential fitting technique (EF, see [20, 21] and references therein), where the adapted numerical method is developed in order to be exact on problems whose solution is linear combination of

$$\{1, x, \dots, x^K, \exp(\pm\mu x), x\exp(\pm\mu x), \dots, x^P \exp(\pm\mu x)\},$$

where K and P are integer numbers.

The methods we consider in this paper belong to the class of explicit Runge-Kutta-Nyström methods (compare [2, 15] and references therein)

$$\begin{aligned} Y_i &= y_n + c_i h y'_n + h^2 \sum_{j=1}^{i-1} a_{ij} f(x_n + c_j h, Y_j), \quad i = 1, 2, \dots, s, \\ y'_{n+1} &= y'_n + h \sum_{i=1}^{s} b'_i f(x_n + c_i h, Y_i), \qquad y_{n+1} = y_n + h y'_n + h^2 \sum_{i=1}^{s} b_i f(x_n + c_i h, Y_i), \end{aligned} \tag{1.2}$$

and we aim to derive a suited EF adaptation of these methods, which takes into account their multistage nature. In the context of Runge-Kutta and Runge-Kutta-Nyström methods, exponentially-fitted methods have already been considered, for instance, by Franco [13, 14], Simos [27, 28], Vanden Berghe [29], Van de Vyver [30] while their trigonometrically-fitted version has been developed by Paternoster in [22]; mixed-collocation based Runge–Kutta–Nyström methods have been introduced by Coleman and Duxbury in [3].

The standard EF technique [20] disregards the contribution of the error in the internal stages Y_i (given by the first equation in (1.2)) to the error of the overall numerical scheme. Here, following the spirit of [5, 18], we explain how to derive EF-based methods which also take into account the error provided by the internal stages computation, which cumulates to the truncation error of the overall scheme.

2. Revised operators

A fundamental role in the standard construction of EF-based explicit RKN methods (compare [20] and references therein) is played by the following $s+2$ functional operators

$$\mathcal{L}_i[h,\mathbf{a}]y(x) = y(x+c_ih) - y(x) - c_ihy'(x) - h^2\sum_{j=1}^{i-1} a_{ij}y''(x+c_jh), \quad i=1,\dots,s, \tag{2.1}$$

$$\mathcal{L}^{(1)}[h,\mathbf{b}']y(x) = hy'(x+h) - hy'(x) - h^2\sum_{i=1}^{s} b_i'y''(x+c_ih), \tag{2.2}$$

$$\mathcal{L}[h,\mathbf{b}]y(x) = y(x+h) - y(x) - hy'(x) - h^2\sum_{i=1}^{s} b_iy''(x+c_ih), \tag{2.3}$$

associated to (1.2). In standard derivations of EF Runge-Kutta methods, the elements b_i and b_i' are computed under the tacit assumption that the error in the internal stages is completely neglected, i.e. $Y_i = y(x_n+c_ih)$. Our aim is now that of deriving EF-based methods where the influence of the errors

$$\varepsilon_i = Y_i - y(x_n+c_ih), \qquad i=1,2,\dots,s, \tag{2.4}$$

associated to the internal stages is also taken into account.

We consider the local error associated to the external approximation y_{n+1} in (1.2)

$$\mathcal{L}^R[h,\mathbf{b}]y(x)\Big|_{x=x_n} = y(x_n+h) - y(x_n) - hy'(x_n) - h^2\sum_{i=1}^{s} b_i^R f(x_n+c_ih, Y_i), \tag{2.5}$$

where the superscript R denotes that we are considering *revised* EF methods. Taking into account that

$$y''(x_n+c_ih) = f(x_n+c_ih, Y_i+\varepsilon_i) = f(x_n+c_ih, Y_i) + \varepsilon_i f_y(x_n+c_ih, Y_i) + O(\varepsilon_i^2) \tag{2.6}$$

we obtain the revised operators

$$\mathcal{L}^{(1),R}[h,\mathbf{b}]y'(x)\Big|_{x=x_n} = y'(x+h) - y'(x) - h\sum_{i=1}^{s} b_i'^R\left(y''(x_n+c_ih) - f_y(x_n+c_ih, Y_i)\varepsilon_i\right), \tag{2.7}$$

$$\mathcal{L}^R[h,\mathbf{b}]y(x)\Big|_{x=x_n} = y(x_n+h) - y(x_n) - hy'(x) - h^2\sum_{i=1}^{s} b_i^R\left(y''(x_n+c_ih) - f_y(x_n+c_ih, Y_i)\varepsilon_i\right), \tag{2.8}$$

which, unlike (2.2) and (2.3), explicitly depend on the errors ε_i associated to the computation of the internal stages Y_i. Hereinafter $f_y^{(i)}$ is the short-hand notation for $f_y(x_n+c_ih,\ Y_i)$.

3. Construction of a family of methods

Let us now consider, as a case study, the practical derivation of revised EF formulae (1.2) with $s=2$, by assuming as fitting spaces the

$$\hat{\mathcal{F}} = \{1, e^{\pm\mu x}\}, \qquad \mathcal{F} = \{1, e^{\mu x}\}, \tag{3.1}$$

which are respectively associated to the external and internal stages computation: i.e. the external value is exact on the linear space generated by $\hat{\mathcal{F}}$, while the internal stages approximations are exact on the linear space spanned by $\mathcal{F}$. We observe that, in the choice of the fitting spaces (3.1), we have totally neglected the presence of monomials (which are typically at the basis of classical continuous methods [15, 1]), in order to derive methods which are more exponentially fitted, thus more suited to integrate differential problems with non-polynomial solutions.

In order to compute the unknown coefficients a_{21}, $b_1{}'$, $b_2{}'$, b_1 and b_2, we proceed as follows:

- we annihilate the operator (2.1) on $\mathcal{F}$ and, due to the invariance in translation [20], we restrict to $x = 0$, i.e. we compute the solution of
$$\mathcal{L}_2{}^R[h, \mathbf{b}]e^{\mu x}\Big|_{x=0} = 0,$$
obtaining
$$a_{21}(z) = \frac{e^{c_2 z} - c_2 z - 1}{z^2}.$$
We observe that the obtained $a_{21}(z)$ corresponds to $\varphi_2(c_2 z)$, a function commonly used in the context of exponential integrators (compare [16]);

- we compute the error ε_2, needed to compute the revised operators (2.7) and (2.8). We observe that the basis functions of $\mathcal{F}$ in (3.1) are solutions of the reference differential equation
$$y'' \pm \mu y' = 0,$$
thus, the leading term of the error in the computation of Y_2 is given by
$$\varepsilon_2 = Y_2 - y(x_n + c_2 h) = h^2 \alpha(z)(y''(x) \pm \mu y'(x)), \tag{3.2}$$
where α is the stage error constant associated to Y_2. Following the procedure used in [5, 18], we compute α as solution of the linear equation
$$\mathcal{L}_2[h, \mathbf{a}]x^2\Big|_{x=0} = \varepsilon_2\Big|_{y(x)=x^2,\ x=0},$$
obtaining
$$\alpha(z) = \frac{c_2^2 - 2a_{21}(z)}{2}; \tag{3.3}$$

- we finally evaluate the revised operators in correspondence to the elements of $\mathcal{F}$ in (3.1). Since $\mathcal{L}^R[h, \mathbf{b}]1 = 0$, we derive $b_1^R(z)$ and $b_2^R(z)$ as solution of the linear system
$$\begin{cases} \mathcal{L}^R[h, \mathbf{b}]e^{\mu x}\Big|_{x=0} = 0, \\ \mathcal{L}^R[h, \mathbf{b}]e^{-\mu x}\Big|_{x=0} = 0, \end{cases}$$
obtaining
$$b_1^R(z, f_y) = \frac{2\mu^2 e^{c_2 z}(z - \sinh(z)) + \beta(z, f_y)(e^z - z - 1)}{\beta(z, f_y) z^2}, \qquad b_2^R(z, f_y) = \frac{2\mu^2(\sinh(z) - z)}{\beta(z, f_y) z^2},$$
with $\beta(z, f_y) = 2\left(\mu^2 - f_y\right)\sinh(c_2 z) + f_y(c_2 z(c_2 z + 2) - 2\cosh(c_2 z) + 2)$. In analogous way, we compute $b_1'^R(z)$ and $b_2'^R(z)$ as solution of the linear system
$$\begin{cases} \mathcal{L}^{(1),R}[h, \mathbf{b}]e^{\mu x}\Big|_{x=0} = 0, \\ \mathcal{L}^{(1),R}[h, \mathbf{b}]e^{-\mu x}\Big|_{x=0} = 0, \end{cases}$$

obtaining

$$b_1'^R(z, f_y) = \frac{(e^z - 1)\left(\mu^2 e^{(2c_2-1)z} - \mu^2 e^{(2c_2-1)z+z} + \gamma(z, f_y)\right)}{\gamma(z, f_y)z}, \qquad b_2'^R(z, f_y) = \frac{(e^z - 1)^2 \mu^2 e^{(c_2-1)z}}{\gamma(z, f_y)z},$$

with $\gamma(z, f_y) = e^{2c_2 z}\left(\mu^2 - 2f_y\right) + f_y e^{c_2 z}(c_2 z(c_2 z + 2) + 2) - \mu^2$.

4. Numerical experiments

We now provide a numerical evidence to highlight the behaviour of EF-revised methods with respect to the analogous standard ones. The computations have been performed on a node with CPU Intel Xeon 6 core X5690 3,46GHz, belonging to the E4 multi-GPU cluster of the Department of Mathematics of the University of Salerno.

It is evident that, in order to effectively apply the methods derived in Section 3, it is necessary to provide an accurate estimation of the parameter μ (compare [8, 9, 17, 19, 26]). To this purpose, we approximate the value of the parameter related to the solution computed in the n-th step point by the formula

$$\mu_n = \pm\frac{y''(x_n)}{y'(x_n)}. \tag{4.1}$$

We observe that this value annihilates the leading term of the local truncation error which, due to choice (3.1) of the fitting space $\mathcal{F}$, is equal to the reference differential equation

$$(D^{(2)} \pm \mu D)y(x) = 0$$

times a constant term.

Due to the nature (1.1) of the operator under investigation and supposing that the problem is autonomous, we have

$$y''(x_n) = f(y(x_n)),$$

thus

$$\mu_n = \pm\frac{f(y_n)}{y'_n}, \tag{4.2}$$

where y_n and y_n' are the approximations to the solution of (1.1) and its first derivative carried out by the RKN method (1.2) in the n-th step point.

We first consider the Prothero-Robinson problem

$$\begin{cases} y''(x) = -\left(y(x) - e^{-\mu x}\right) + \mu^2 e^{-\mu x}, & x \in [0, 1], \\ y'(0) = -\mu, \qquad y(0) = 1, \end{cases} \tag{4.3}$$

whose exact solution $y(x) = e^{-\mu x}$ belongs to the fitting space, thus the derived methods are able to solve this problem exactly. In Table 4, we report the global errors in the final step points, obtained in correspondence of several fixed values of the stepsize and the abscissa c_2. We observe that both the revised and the standard versions exactly compute the solution of problem (within round-off error), as expected. In addition, the revised method is able to achieve a better accuracy than the standard one, with the same computational cost. In Table 4 we report the minima and maxima approximated values of the parameter μ, computed by (4.2).

We next consider the undamped Duffing problem

$$\begin{cases} y''(x) = -(1 + y^2)y + (\cos(x) + \epsilon\sin(10x))^3 - 99\epsilon\sin(10x), & x \in [0, 100], \\ y'(0) = 10\epsilon, \qquad y(0) = 1, \end{cases} \tag{4.4}$$

with $\epsilon = 10^{-3}$, whose exact solution $y(x) = \cos(x) + \epsilon\sin(10x)$ does not belong to the chosen fitting space. The results, reported in Table 4, show a better performance of the revised method with respect to the standard one.

μ	h	$c_2 = 1/2$ S	SA	R	RA	$c_2 = 3/4$ S	SA	R	RA
1	1/512	1.0e-10	5.5e-16	2.0e-13	7.2e-16	2.3e-10	6.7e-16	8.6e-14	7.2e-16
	1/1024	1.3e-11	4.4e-16	1.1e-14	4.4e-16	2.9e-11	3.9e-16	4.9e-15	3.9e-16
	1/2048	1.6e-12	5.0e-16	1.2e-15	4.9e-16	3.6e-12	5.0e-16	6.6e-16	4.9e-16
	1/4096	2.0e-13	4.4e-16	4.4e-16	4.4e-16	4.5e-13	4.4e-16	4.4e-16	4.4e-16
2	1/512	5.68e-07	1.1e-15	3.0e-13	3.3e-16	1.4e-09	9.9e-16	1.0e-12	3.0e-16
	1/1024	1.42e-07	1.3e-15	2.0e-14	1.8e-15	1.7e-10	1.3e-15	6.6e-14	1.3e-15
	1/2048	3.55e-08	1.1e-15	2.4e-15	5.8e-16	2.2e-11	7.8e-16	6.0e-15	7.8e-16
	1/4096	8.89e-09	2.8e-16	2.5e-16	2.8e-16	2.7e-12	3.3e-16	1.1e-16	3.6e-16

Table 1: Numerical results originated from the application of standard and revised EF methods to problem (4.3). S and SA (R and RA) denote the errors for the standard (revised) version, without and with approximation of parameter μ, respectively.

μ	h	SA $\min(\mu_n)$	$\max(\mu_n)$	RA $\min(\mu_n)$	$\max(\mu_n)$
1	1/4	0.999999999934466	1.0000000000000000	1.0000000000000000	1.000000694302470
	1/8	0.999999999999546	1.0000000000000000	1.0000000000000000	1.000000018623597
	1/16	0.999999999999996	1.0000000000000000	1.0000000000000000	1.000000000529162
	1/32	0.999999999999999	1.0000000000000000	1.0000000000000000	1.000000000015725
2	1/4	2.0000000000000000	1.999999981300431	2.0000000000000000	2.000074030808046
	1/8	2.0000000000000000	1.999999999851776	2.0000000000000000	2.000002393779446
	1/16	2.0000000000000000	1.999999999998860	2.0000000000000000	2.000000073872768
	1/32	2.0000000000000000	1.999999999999991	2.0000000000000000	2.000000002275468

Table 2: Minimum and maximum value of approximated paramater μ_n on problem (4.3) for $c_2 = 1/2$, various stepsize h and real value of μ.

5. Conclusions

We have introduced a revised technique for the computation of the coefficients of EF-based RKN methods (1.2), which takes into account the multistage nature of the methods under investigations, by considering the contributions of the stage errors in the overall numerical scheme. The methods depend on the values of parameters to be suitably determined: the proposed strategy, consisting in applying Equation (4.2) at each step, does not require the computation of further function evaluations The numerical experiments have underlined the superiority of the revised EF methods with respect to the standard ones and accuracy of the parameter estimates. Further developments regard the application of the revised technique to other family of methods, such as two-step hybrid methods [4, 6, 7], two-step Runge-Kutta-Nyström methods [23, 24, 25] and general linear methods [10] for (1.1) and ODEs with discontinuous right-hand side [11, 12].

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μ	h	$c_2 = 1/2$				$c_2 = 1$			
		S	SA	R	RA	S	SA	R	RA
$10i$	1/2048	9.2e-05	3.5e-06	9.2e-05	1.7e-06	2.6e-04	3.4e-02	2.6e-04	1.7e-05
	1/4096	2.6e-05	3.4e-05	2.6e-05	2.3e-07	5.8e-05	1.2e-05	5.7e-05	5.0e-07
	1/8192	6.7e-06	2.4e-08	6.7e-06	2.2e-08	1.4e-05	1.9e-06	1.4e-05	9.3e-07
	1/16384	1.7e-06	5.1e-07	1.7e-06	3.2e-09	3.4e-06	5.8e-08	3.4e-06	6.7e-09
i	1/2048	2.4e-06	2.8e-06	2.3e-06	1.8e-06	4.3e-06	3.4e-02	4.7e-06	1.9e-05
	1/4096	6.0e-07	3.3e-05	5.9e-07	2.2e-07	1.1e-06	1.2e-05	1.1e-06	4.3e-07
	1/8192	1.5e-07	1.4e-08	1.4e-07	2.3e-08	2.9e-07	1.9e-06	2.9e-07	9.2e-07
	1/16384	3.7e-08	5.3e-07	3.7e-08	3.4e-09	7.3e-08	5.8e-08	7.4e-08	6.9e-09

Table 3: Numerical results originated from the application of standard and revised EF methods on problem (4.4). S and SA (R and RA) denote the errors for the standard (revised) version, without and with approximation of parameter μ, respectively.

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