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ORIGINAL PAPER

Parameter estimation in exponentially fitted hybrid methods for second order differential problems

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Abstract In this work we deal with exponentially fitted methods for the numerical solution of second order ordinary differential equations, whose solutions are known to show a prominent exponential behaviour depending on the value of an unknown parameter to be suitably determined. The knowledge of an estimation to the unknown parameter is needed in order to apply the numerical method, since its coefficients depend on the value of the parameter. We present a strategy for the practical estimation of the parameter, which is also tested on some selected problems.

Keywords Second order ordinary differential equations · Molecular dynamics · Exponential fitting · Two-step hybrid methods · Parameter estimation

1 Introduction

It is the purpose of this paper to analyse the family of two-step hybrid methods

$$
\begin{aligned}
Y_i^{[n]} &= (1+c_i)y_n - c_i y_{n-1} + h^2 \sum_{j=1}^{s} a_{ij} f(Y_j^{[n]}), \quad i = 1, \ldots, s, \\
y_{n+1} &= 2y_n - y_{n-1} + h^2 \sum_{i=1}^{s} b_i f(Y_i^{[n]}),
\end{aligned}
\tag{1}
$$

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introduced by Coleman in [5] for the numerical solution of initial value problems based on second order ordinary differential equations (ODEs)

$$\begin{cases} y'' = f(x, y), \\ y'(x_0) = y_0', \\ y(x_0) = y_0, \end{cases} \tag{2}$$

under the assumption that the function $f:[x_0, X] \times \mathbb{R}^d \to \mathbb{R}^d$ is smooth enough to guarantee the existence and uniqueness of the solution. Although problem (2) can be regarded as a doubled dimensional system of first order ODEs, it is more natural and efficient to deal with its second order formulation and apply suited numerical methods to approximate its solution.

1.1 The problem: reasons of interest

Second order ODEs (2), especially when their solutions exhibit a prominent periodic or oscillatory behaviour, have a special interest in many applications (see for instance [24] and the references therein contained), such as molecular dynamics (compare [1,3,13,11]). For instance, problems of type (2) provide the equations of motion of atomic systems, as it is briefly described here for a linear molecule. In this case, the angular velocity ω^s and the torque τ^s are both perpendicular to the molecular axis at all times: therefore, denoting by $\mathbf{e}^s$ the unit vector along the axis, we have

$$\tau^s = \mathbf{e}^s \times \mathbf{g}^s,$$

where $\mathbf{g}^s = \sum_a d_a \mathbf{f}_a^s$ is the resultant of the intermolecular forces. Then, the equation of rotational motion can now be written as (see Singer et al. 1997)

$$\ddot{\mathbf{e}}^s = \mathbf{g}^{\perp}/I + \lambda \mathbf{e}^s, \tag{3}$$

where $\mathbf{g}^{\perp} = \mathbf{g}^s - (\mathbf{g}^s \cdot \mathbf{e}^s)\mathbf{e}^s$ and I is the moment of inertia. The two terms in the right hand side of (3) are the force $\mathbf{g}^{\perp}$ responsible for the rotation of the molecule and the force $\lambda \mathbf{e}^s$ along the bond which constraints the bond length to be a constant of the motion. The radial Schrödinger equation [19]

$$y'' + (E - V(x))y = 0, \quad x > 0,$$

is also a second order problem (2) of interest in molecular dynamics. It depends on the value E, which is a real number denoting the energy of the system, while $V(x)$ is a given potential. This equation, which is at the base of nonrelativistic quantum mechanics, provides the description of various effects in nuclear, atomic and molecular physics (compare [20]). An example is given by the radial part of the Schrödinger equation for the hydrogen atom [2]

$$-\frac{\hbar}{2\mu r^2}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)+\left(\frac{\hbar l(l+1)}{2\mu r^2}-\frac{e^2}{4\pi\epsilon_0 r}-E\right)R(r)=0,$$

where $\hbar$ is the Planck constant, μ is the reduced mass of the electron, r is the atomic radius, $R(r)$ is the radial wave function, e is the electron charge and ϵ_0 is the vacuum permittivity. The solution of this equation is

$$R_{nl}(r)=-\left[\frac{(n-l-1)!}{2n[(n+l)!]^3}\right]^{1/2}\left(\frac{2}{na_0}\right)l+3/2r^l\exp\left(-\frac{r}{na_0}\right)L_{n+l}^{2l+1}\left(\frac{2r}{na_0}\right),$$

where $0\leq l\leq n-1$, a_0 is the Bohr radius and the functions $L_{n+l}^{2l+1}\left(\frac{2r}{na_0}\right)$ are the associated Laguerre functions. The hydrogen atom eigenvalues are

$$E_n=-\frac{e^2}{8\pi\epsilon_0 a_0 n^2},\quad n=1,2,\ldots$$

We observe that the solutions of the hydrogen Schrödinger equation are of exponential type: this behaviour or, more in general, a behaviour described by an exponential of real or complex argument, is quite typical in second order problems (2) of interest in the applications.

1.2 The method: a family of special purpose formulae

It is worthy to mention that classical numerical methods for ODEs are not able to efficiently follow a prominent exponential, periodic or oscillatory behaviour of the solutions, because a small stepsize would be needed to accurately catch the oscillations in the solution. On the contrary, the usage of *special purpose* numerical formulae, i.e. formulae suited to solve a particular family of problems whose solution is linear combination of a selected set of functions, allows to obtain an accurate solution with larger stepsizes than those needed when we apply classical formulae (see [18] and the references therein contained).

In order to obtain special purpose formulae we should impose that a certain numerical method exactly integrates (within the round-off error) problems of type (2) whose solution can be expressed as linear combination of functions other than polynomials. For instance, assuming that the solution of the problem is spanned by the functional basis

$$\{1,x,\ldots,x^K,\exp(\pm\mu x),x\exp(\pm\mu x),\ldots,x^P\exp(\pm\mu x)\},\tag{4}$$

where K and P are integer numbers, we obtain formulae based on the so-called *exponential fitting* (EF, see [18]), i.e. formulae exactly integrating (within round-off errors) problems whose solution is linear combination of (4). An extensive bibliography concerning the EF technique can be found in the monograph [18] (also see [12,21,22,26,27] about EF-based methods for the solution of ODEs).

The coefficients of classical formulae are constant matrices and vectors, while, on the contrary, the coefficients of EF formulae are matrices and vectors depending on the value of a parameter to be suitably determined. This parameter depends on the solution of the problem and its behaviour: for instance, it could be the value of the frequency of the oscillations when the solution is oscillatory, or the argument of the exponential function describing the exponential decay of a certain phenomenon modelled by (2). The authors have recently introduced in [7] the family of EF-based methods (1), assuming that the parameter is known in advance (also see [8,9,28]).

A rigorous theory for the exact computation of the parameter has not yet been developed. However, some attempts have been done in the literature (see, for instance, [17,23,25] and references therein contained) in order to provide an accurate estimation of the parameter, generally based on the minimization of the leading term of the local discretization error. We aim to provide in this paper an analogous strategy to determine an approximation to the parameter of EF methods (1), in such a way that its performances are not compromised by the missing of the exact value of the parameter.

The paper is organized as follows: Sect. 2 reports the constructive strategy introduced in [7] to derive EF-based formulae within the class (1); Sect. 3 is devoted to the presentation of the parameter estimation technique, while Sect. 4 provides some numerical tests. Some conclusions and further developments of this research are reported in Sect. 5.

2 Exponentially fitted two-step hybrid methods

In this section we recall the constructive technique introduced in [7] to derive EF-based methods within the class (1). This strategy is based on the *six-step flow chart* introduced by Ixaru and Vanden Berghe in [18] for the derivation of EF-based formulae approaching many problems of Numerical Analysis (e.g. interpolation, numerical quadrature and differentiation, numerical solution of ODEs) especially when their solutions show a prominent periodic/oscillatory behaviour.

We associate to (1) the following $s+1$ linear operators

$$\begin{aligned}
\mathcal{L}[h,\mathbf{b}]y(x) &= y(x+h)-2y(x)+y(x-h)-h^2\sum_{i=1}^{s} b_i y''(x+c_i h)\\
\mathcal{L}_i[h,\mathbf{a}]y(x) &= y(x+c_i h)-(1+c_i)y(x)+c_i y(x-h)\\
&\quad -h^2\sum_{j=1}^{s} a_{ij} y''(x+c_j h),\quad i=1,\dots,s,
\end{aligned}$$

and proceed as follows:

– step (i) We compute the *starred classical moments* (see [18]) by using formulae

$$\begin{aligned}
L^*_m(\mathbf{b}) &= h^{-(m+1)}\mathcal{L}[h;\mathbf{b}]x^m,\quad m=0,1,2,\dots,\\
L^*_{im}(\mathbf{a}) &= h^{-(m+1)}\mathcal{L}_i[h;\mathbf{a}]x^m,\quad i=1,\dots,s,\ m=0,1,2,\dots
\end{aligned}$$

– step (ii) *Compatibility analysis*. We examine the algebraic systems

$$L^*_m(\mathbf{b}) = 0, \quad m = 0, 1, \ldots, M' - 1, \tag{5}$$
$$L^*_{im}(\mathbf{a}) = 0, \quad i = 1, \ldots, s, \;\; m = 0, 1, \ldots, M - 1, \tag{6}$$

to find out the maximal values of M and M' for which the above systems are compatible. Assuming $s = 2$, we proved in [7] that such values are $M = M' = 4$.

– step (iii) *Computation of the G functions*. In order to derive EF methods, we need to compute the so-called *starred exponential moments* (see [18], p. 42), i.e.

$$E^*_0(\pm z, \mathbf{b}) = \exp(\pm\mu x)\mathcal{L}[h, \mathbf{b}]\exp(\pm\mu x), \tag{7}$$
$$E^*_{0i}(\pm z, \mathbf{a}) = \exp(\pm\mu x)\mathcal{L}_i[h, \mathbf{a}]\exp(\pm\mu x), \quad i = 1, \ldots, s. \tag{8}$$

Once computed the reduced exponential moments, we derive the following set of functions:

$$G^+(Z, \mathbf{b}) = \frac{1}{2}\Big(E^*_0(z, \mathbf{b}) + E^*_0(-z, \mathbf{b})\Big),$$
$$G^-(Z, \mathbf{b}) = \frac{1}{2z}\Big(E^*_0(z, \mathbf{b}) - E^*_0(-z, \mathbf{b})\Big),$$
$$G^+_i(Z, \mathbf{a}) = \frac{1}{2}\Big(E^*_{0i}(z, \mathbf{a}) + E^*_{0i}(-z, \mathbf{a})\Big), \quad i = 1, \ldots, s,$$
$$G^-_i(Z, \mathbf{a}) = \frac{1}{2z}\Big(E^*_{0i}(z, \mathbf{a}) - E^*_{0i}(-z, \mathbf{a})\Big), \quad i = 1, \ldots, s,$$

where $Z = z^2$. In our case, the G functions take the following form

$$G^+(Z, \mathbf{b}) = 2\eta_{-1}(Z) - 2 - Z\sum_{j=1}^{s} b_j\eta_{-1}(c_j^2 Z),$$
$$G^-(Z, \mathbf{b}) = -Z\sum_{j=1}^{s} b_j c_j \eta_0(c_j^2 Z),$$
$$G^+_i(Z, \mathbf{a}) = \eta_{-1}(c_i^2 Z) + c_i\eta_{-1}(Z) - 2(1 + c_i) - Z\sum_{j=1}^{s} a_{ij}\eta_{-1}(c_j^2 Z),$$
$$G^-_i(Z, \mathbf{a}) = c_i\eta_0(c_i^2 Z) - c_i\eta_0(Z) - 2(1 + c_i) - Z\sum_{j=1}^{s} c_j a_{ij}\eta_0(c_j^2 Z).$$

We observe that the above expressions depend on the functions $\eta_{-1}(Z)$ and $\eta_0(Z)$ (compare [16,18]), which are defined as follows

$$\eta_{-1}(Z) = \frac{1}{2}[\exp(Z^{1/2}) + \exp(-Z^{1/2})] = \begin{cases} \cos(|Z|^{1/2}) & \text{if } \; Z \leq 0, \\ \cosh(Z^{1/2}) & \text{if } \; Z > 0, \end{cases}$$

and

$$\eta_0(Z) = \begin{cases} \dfrac{1}{2Z^{1/2}}[\exp(Z^{1/2}) - \exp(-Z^{1/2})] & \text{if } \ Z \neq 0, \\ 1 & \text{if } \ Z = 0, \end{cases}$$
$$= \begin{cases} \sin(|Z|^{1/2})/|Z|^{1/2} & \text{if } \ Z < 0, \\ 1 & \text{if } \ Z = 0, \\ \sinh(Z^{1/2})/Z^{1/2} & \text{if } \ Z > 0. \end{cases}$$

We next compute the p-th derivatives $G^{\pm(p)}$ and $G_i^{\pm(p)}$, taking into account the formula for the p-th derivative of $\eta_k(Z)$ (see [18])

$$\eta_k^{(p)}(Z) = \frac{1}{2^p}\eta_{k+p}(Z),$$

and obtaining

$$G^{+(p)}(Z, \mathbf{b}) = \frac{1}{2^{p-1}}\eta_{p-1}(Z) - \sum_{j=1}^{s} b_j \frac{d^p}{dZ^p}\Big(Z\eta_{-1}(c_j^2 Z)\Big),$$
$$G^{-(p)}(Z, \mathbf{b}) = -\sum_{j=1}^{s} b_j c_j \frac{d^p}{dZ^p}\Big(Z\eta_{-1}(c_j^2 Z)\Big),$$
$$G_i^{+(p)}(Z, \mathbf{a}) = \frac{c_i^{2p}}{2^p}\eta_{p-1}(c_i^2 Z) + \frac{c_i}{2^p}\eta_{p-1}(Z) - \sum_{j=1}^{s} a_{ij} \frac{d^p}{dZ^p}\Big(Z\eta_{-1}(c_j^2 Z)\Big),$$
$$G_i^{-(p)}(Z, \mathbf{a}) = \frac{c_i^{2p+1}}{2^p}\eta_{p}(c_i^2 Z) - \frac{c_i}{2^p}\eta_{p}(Z) - \sum_{j=1}^{s} a_{ij} c_j \frac{d^p}{dZ^p}\Big(Z\eta_{0}(c_j^2 Z)\Big).$$

– step (iv) *Definition of the function basis*. We next decide the shape of the function basis to take into account: as a consequence, the corresponding method will exactly integrate (i.e. the operator $\mathcal{L}[h, \mathbf{b}]y(x)$ annihilates in correspondence of the function basis) all those problems whose solution is linear combination of the basis functions. In the exponential fitting framework, the function basis (also known as *fitting space*) is a set of M functions of the type

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

where K and P are integer numbers satisfying the relation

$$K + 2P = M - 3. \tag{9}$$

Let us next consider the set of M' functions

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

annihilating the operators $\mathcal{L}_i[h, \mathbf{a}]y(x)$, $i = 1, 2, \ldots, s$ and assume that $K' = K$ and $P' = P$, i.e. the external stage and the internal ones are exact on the same function basis.

– step (v) *Determination of the coefficients*. After a suitable choice of K and P, we next solve the following algebraic systems

$$G^{\pm(p)}(Z, \mathbf{b}) = 0, \quad p = 0, \ldots, P,$$
$$G_i^{\pm(p)}(Z, \mathbf{a}) = 0, \quad i = 1, \ldots, s, \;\; p = 0, \ldots, P,$$

and derive the coefficient of the corresponding EF-based method.

– step (vi) *Error analysis*. According to the used procedure [18], the general expression of the local truncation error for an EF method with respect to the basis of functions (16) takes the form

$$lte^{EF}(x) = (-1)^{P+1}h^M \frac{L^*_{K+1}(\mathbf{b}(Z))}{(K+1)Z^{P+1}} D^2(D^2 - \mu^2)y(x), \tag{10}$$

with K, P and M satisfying the condition (9). For the sake of completeness, we remark that this expression of the local truncation error can be derived by using the approach of Coleman and Ixaru [6], who provided an adaptation of the theory by Ghizzetti and Ossicini (1970) to the case of EF-based formulae. This approach consists in regarding the error associated to an EF-based formula as

$$E[y] = L[y](\xi)\int_{-h}^{h} \Phi(x)dx,$$

where $\xi \in (-h, h)$ and, in our case, $L[y] = D^{k+1}(D - \mu)^{P+1}y(x)$. We observe that the kernel $\Phi(x)$ is an even function in the null space of L.

The expression of the local truncation error (10) is our starting point to estimate the unknown parameter μ.

3 Parameter selection

Step (vi) of the constructive procedure described above provided us the expression of the local truncation error (10), with K, P and M satisfying the condition $K + 2P = M - 3$. For instance, assuming $K = 1$, $P = 0$ and $M = 4$, we obtain

$$lte^{EF}(x) = -h^2 \frac{L^*_2(\mathbf{b}(Z))}{2\mu^2} D^2(D^2 - \mu^2)y(x). \tag{11}$$

We aim to estimate the value of the parameter μ that annihilates or minimizes the leading term of (10), by solving the equation

$$D^2(D^2 - \mu_j^2)y(x_j) = 0, \tag{12}$$

where μ_j is an approximation to the unknown parameter μ in the point x_j of the grid.

We observe that the values

$$\mu_j = \pm\sqrt{\frac{y^{(iv)}(x)}{y''(x)}}\Bigg|_{x=x_j}, \quad \mu_j = \pm y''(x)\Bigg|_{x=x_j},$$

are solutions of (12). More generally, it can be shown that for any integer K and P, the value

$$\mu_j = \pm y''(x)\Bigg|_{x=x_j}$$

satisfies the reference differential equation

$$D^{K+1}(D^2 - \mu^2)^{P+1}y(x) = 0, \tag{13}$$

in every point of the grid. This situation is formalized in the following result.

Proposition 1 *For any grid point x_j, $\mu_j = \pm y''(x_j)$ is solution of* (13) with multiplicity $P+1$, $P \geq 0$.

Proof Equation (13) can be regarded in the form

$$D^{K+1}\left(\sum_{i=0}^{P+1}(-1)^i\binom{P+1}{i}D^{P+1-i}\mu_j^i\right)y(x_j) = 0.$$

Therefore, in correspondence of $\mu_j = y''(x_j)$, we obtain

$$D^{K+2P+3}\left(\sum_{i=0}^{P+1}(-1)^i\binom{P+1}{i}\right)y(x_j) = 0,$$

which is always satisfied because

$$\sum_{i=0}^{P+1}(-1)^i\binom{P+1}{i} = (1+(-1))^{P+1} = 0.$$

□

These preliminary remarks confirm that Eq. (13) leads to different choices to estimate the unknown parameter and, the more P is high, the more the number of possible choices increases. In order to establish a suitable strategy for the derivation of an appropriate and reliable estimation to the unknown parameter, we follow the lines drawn in [15] in the case of two-point boundary value problems. In particular, we first analyze the solutions of (13) when the solution $y(x)$ belongs to the fitting space: for instance, we assume that

$$y(x) = x^q e^{\mu x}.$$

Then, the following result holds.

Theorem 1 *Let us assume that* $y(x) = x^q e^{\mu x}$ *is solution to the differential problem* (2). Then,

$$\nu^2 = \mu^2$$

is a root of $D^{K+1}(D^2 - \mu^2)^{P+1} y(x)$ with multiplicity $P - q + 1$.

Proof In correspondence of $y(x) = x^q e^{\mu x} = D_\mu^q e^{\mu x}$, the reference differential equation (13) assumes the form

$$D_\mu^q D_x^{K+1} (D_x^2 - \nu^2)^{P+1} e^{\mu x} = 0$$

or, equivalently,

$$D_\mu^q \mu^{K+1} (\mu^2 - \nu^2)^{P+1} e^{\mu x} = 0.$$

By using the Leibniz rule for higher derivatives, the previous formula can be expressed in the form

$$\sum_{n=0}^{q} \sum_{r=0}^{q-n} \binom{q}{n} \binom{q-n}{r} \beta_{n,r} \mu^{K+1-q+n+r} (\mu^2 - \nu^2)^{P+1-r} x^n e^{\mu x} = 0, \tag{14}$$

with

$$\beta_{n,r} = \frac{(K+1)!}{(K+1+n+r-q)!} \cdot \frac{(P+1)!}{(P+1-r)!}.$$

The thesis is obtained by observing that the left hand side of (14) has a common factor $(\mu^2 - \nu^2)^{P-q+1}$. □

This result can be exploited to establish a strategy for the approximation of the unkwown parameter in the coefficients of the methods. We denote by $p(\mu_j)$ the value of $D^{K+1}(D^2 - \mu_j^2)^{P+1} y(x_j)$ and apply Theorem 1, i.e. we solve at each time step the nonlinear equations $p(\mu) = 0$, $p'(\mu) = 0$, …, $p^{(P-q+1)}(\mu) = 0$. If there exist a common solution for all these equations which is constant overall the integration interval, then the solution to the problem we are solving belongs to the fitting space and the obtained constant value is chosen as approximation to the unknown parameter μ. On the contrary, if such common solution does not exist and the values of μ_j vary along the integration interval, the solution to the approached differential problem does not belong to the fitting space and the approximation to μ we choose at each time step is the root of smallest modulus among the set of solutions of $p(\mu) = 0$, $p'(\mu) = 0$, ..., $p^{(P-q+1)}(\mu) = 0$, in order to avoid inaccurate results due to numerical instability.

This approach for the estimation of the unknown parameter will next be applied to some test cases reported in Sect. 4.

4 Numerical results

We present the numerical results arising from the implementation of the following methods belonging to the same family (1):

– HYB2, two-step hybrid method (1) having constant coefficients (see [5])

$$\begin{array}{c|cc} \frac{1}{\sqrt{6}} & \frac{1+\sqrt{6}}{12} & \\ -\frac{1}{\sqrt{6}} & -\frac{\sqrt{6}}{12} & \frac{1}{12} \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array} \tag{15}$$

with $s = 2$ and order 4;

– EXP2, one-parameter depending exponentially-fitted method (1), with $s = 2$ and order 2, corresponding to the fitting space (4) with $K = 1$ and $P = 0$, i.e.

$$\{1, x, \exp(\pm\mu x)\}, \tag{16}$$

and depending on the following coefficients

$$\begin{aligned}
b_1 &= \frac{2c_2(\eta_1(Z) - 1)\eta_0(c_2^2 Z)}{-Z(c_1\eta_1(c_2^2 Z)\eta_0(c_1^2 Z) - c_2\eta_1(c_1^2 Z)\eta_0(c_2^2 Z))},\\
b_2 &= \frac{2c_1(\eta_1(Z) - 1)\eta_0(c_1^2 Z)}{Z(c_1\eta_1(c_2^2 Z)\eta_0(c_1^2 Z) - c_2\eta_1(c_1^2 Z)\eta_0(c_2^2 Z))},\\
a_{11} &= \frac{c_1(1 + c_1)(c_1 - 3c_2 - 1)}{6(c_1 - c_2)},\\
a_{12} &= \frac{c_1(1 + 3c_1 + 2c_1^2)}{6(c_1 - c_2)},\\
a_{21} &= \frac{-c_2(1 + 3c_2 + 2c_2^2)}{6(c_1 - c_2)},\\
a_{22} &= \frac{c_2(1 + c_2)(3c_1 - c_2 + 1)}{6(c_1 - c_2)},
\end{aligned}$$

where $c = [c_1, c_2]^T$ is the abscissa vector.

Both methods depend on the same number of internal stages, therefore the computational cost due to the solution of the nonlinear system in the stages is the same and the numerical evidence shows their comparison in terms of accuracy. The methods are implemented with fixed stepsize

$$h = \frac{1}{2^k},$$

where k is a positive integer number. The reported experiments aim to confirm the theoretical expectations regarding the derived methods and to test the strategy of parameter estimation above described. We consider the following problems:

– the scalar linear test equation

$$\begin{cases} y''(x) = \lambda^2 y(x), \\ y(0) = 1, \\ y'(0) = -\lambda, \end{cases} \tag{17}$$

with $\lambda > 0$ and $x \in [0, 1]$, whose exact solution is $y(x) = \exp(-\lambda x)$;

– the linear problem

$$\begin{cases} y''(x) - y(x) = x - 1, \\ y(0) = 2, \\ y'(0) = -2, \end{cases} \tag{18}$$

with $\lambda > 0$ and $x \in [0, 5]$ and exact solution $y(x) = 1 - x + \exp(-x)$, which is linear combination of the basis functions in (16);

– the Prothero-Robinson problem [25]

$$\begin{cases} y''(x) + \nu^2[y(x) - \exp(-\lambda x)]^3 = \lambda^2 y, \\ y(0) = 1, \\ y'(0) = -\lambda, \end{cases} \tag{19}$$

with $x \in [0, 5]$, whose exact solution is $y(x) = \exp(-\lambda x)$.

As regards EXP2 method, we apply the strategy described in Sect. 3 for the estimation of the unknown parameter μ. To achieve this purpose, we consider the reference differential equation

$$p(\mu, x) = D^2(D^2 - \mu^2)y(x) \tag{20}$$

and, according to the Theorem (1), we determine the roots of $p(\mu_n, x_n) = 0$ of multiplicity $1 - q$, where x_n is the current step point. Equation (20) requires the computation of the second and forth derivatives of $y(x)$; we observe that such derivatives can be derived directly from the analytic formulation of the problem, in terms of the partial derivatives of the function f. In fact, $y''(x) = f(x, y(x))$ and

$y^{(iv)}(x) = f_{yy}(x, y(x))(y'(x), y'(x)) + f_y(x, y(x))f(x, y(x))$, where the unkwown value of $y'(x)$ can be approximated by the finite difference

$$y'(x) \approx \frac{y(x+h) - y(x)}{h}.$$

We observe that, in order to avoid further function evaluations, we can replace the values of the derivatives appearing in (20) by the corresponding backward finite differences in the following way

$$y^{(r)}(x_{n+1}) \approx \frac{1}{h^n} \sum_{i=0}^{n} (-1)^i \binom{n}{i} y_{n-i}. \tag{21}$$

The numerical evidence is reported in Tables 1, 2 and 3. The results confirm that EXP2 method is able to exactly solve the above problems within round-off error, since their solutions belong to the linear space generated by (16). The superiority of EXP2 method in terms of accuracy is visible from the experiments, which reveal that it outperforms HYB2 method on the considered test problems. Although EXP2 and HYB2 depend on the same number of stages, i.e. $m = 2$, and HYB2 has higher order of convergence, a larger computational effort is necessary for the latter to obtain the same accuracy of EXP2.

Table 1 Relative errors corresponding to the solution of the problem (17), for different values of λ and k

λ	k	HYB2	EXP2
2	4	1.10e-5	1.09e-14
	5	7.36e-7	8.45e-14
	6	4.76e-8	1.20e-13
3	4	4.19e-4	2.02e-14
	5	2.89e-5	2.29e-13
	6	1.90e-6	4.02e-13
4	4	9.29e-3	9.49e-14
	5	6.65e-4	6.08e-13
	6	4.43e-5	4.96e-12

Table 2 Relative errors corresponding to the solution of the problem (18)

k	HYB2	EXP2
4	2.65e-4	3.34e-16
5	1.96e-5	1.87e-14
6	1.33e-6	5.16e-14

Table 3 Relative errors corresponding to the solution of the problem (19), with $\nu = 1$

k	HYB2	EXP2
4	9.79e-2	2.43e-12
5	5.36e-3	1.79e-12
6	2.96e-4	1.35e-11

5 Conclusions and further developments

We have presented a strategy for the estimation of the parameters involved in the EF adaptation of the two-step hybrid methods (1) for the numerical solution of second order problems (2) whose solution is supposed to be of exponential type. The strategy, based on determining the roots of certain polynomials associated to the truncation error, is tested on some selected problems. The numerical evidence confirm the theoretical expectations on the accuracy of the derived methods and the effectiveness of the parameter estimation technique.

Future works will regard the usage of different basis of functions for the derivation of function fitted formulae belonging to the family (1). In fact, the only employ of nonnegative powers and exponential functions in the chosen functional basis may not be completely satisfactory if the problem under consideration has an asymptotic exponential behavior which is accompanied by a noninteger power of the independent variable for the infinite interval cases. In such cases some other basis of functions must be accordingly constructed. This construction can be based on the informations coming from the asymptotic behavior analysis of the ODE when the independent variable goes to infinity, if the integration interval is entirely or semi infinite. For instance, a different basis set can be performed in a such a way to reproduce the same asymptotic behaviour of the exact solution. If the integration interval is finite, such asymptotic analysis should be provided for both ends of the interval. Moreover, we aim to achieve orders of convergence greater than two, as it has been done for Runge-Kutta methods (compare [4,14]). This may change the values of the parameters depending on the nature of the ODE under consideration [10].

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