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A strategy for selecting the frequency in trigonometrically-fitted methods based on the minimization of the local truncation errors and the total energy error

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Abstract Trigonometrically-fitted methods have been largely used for solving second-order differential problems, and particularly for solving the radial Schrödinger equation (see for instance Alolyan and Simos in J Math Chem 50:782–804, 2012; Simos in J Math Chem 34:39–58, 2003, 44:447–466, 2008; Vigo-Aguiar and Simos in J Math Chem 29:177–189, 2001, 32:257–270, 2002 and the references therein contained). It is well-known that for periodic or oscillatory problems, trigonometrically fitted methods are more efficient than non-fitted methods. A large number of different approaches have been considered in the scientific literature to obtain analytical approximations to the frequency of oscillation in case of periodic solutions, which are valid for a large range of amplitudes of oscillation. However, these techniques have been limited to obtaining only one or two iterates because of the great amount of algebra involved. In this paper we consider the use of a trigonometrically fitted method to obtain numerical approximations for the solutions. This yields very acceptable results provided that the approximation of the parameter of the method is done with great accuracy. Many trigonometrically fitted methods have been reported in the literature, but there is no decisive way to obtain the optimal frequency value. We present a strategy for the choice of the parameter value in the adapted method, based on the minimization of the sum of the total energy error and the local truncation errors in the solution and in the derivative. We include an example solved numerically that confirms the good performance of the strategy adopted.

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1 Introduction

Many nonlinear phenomena can be described in terms of nonlinear oscillators. Perhaps one of the best known nonlinear systems is the simple pendulum (a particle of mass m attached to a wall by a string moving on a surface without friction), in which for small angle oscillations the periodic motion is harmonic; nevertheless, for large oscillations the period depends on the amplitude [6].

Nonlinear oscillators appear in quantum mechanics, biology, optics, and of course, in classical mechanics. Recently, a lot of work has been devoted to obtaining approximate analytical solutions to nonlinear oscillators, and their periods of vibration. Most of the procedures consist of transforming the given second order initial-value problem into an infinite sequence of linear inhomogeneous second-order initial-value problems. A survey of the these approaches with many references can be found in [7]. However, for most cases the application of these methods leads to very complicated sets of algebraic equations with highly complex nonlinearity. In this paper we consider the use of trigonometrically fitted methods for solving this kind of problem, but in the sense that an appropriate strategy is used to obtain the value of the parameter involved with great accuracy.

Let us consider a nonlinear oscillator whose trajectory $x(t)$ is a solution of Newton's equation of motion given in the form

$$\ddot{x} = -\nabla(V(x)) \tag{1}$$

where the potential-energy function $V(x)$ satisfies the condition that $f(x) = \dfrac{-d\,V(x)}{dx}$ for a conservative force $f(x)$. As is usual in classical mechanics, the dot stands for the derivative with respect to time. In the formulation of the above differential equation some constants could appear, but we set them equal to one. This does not change the essential features of the solutions in any way (see [8]). The solutions of this equation may show different types of behavior. In the case of bounded motion, assuming that the equilibrium position takes place at $x = 0$, the amplitude is the largest distance from this equilibrium position. If $f(x)$ does not have a dominant term proportional to x, then the equation in (1) is called "truly nonlinear oscillator" (see [8]).

An important feature in the case of a periodic solution of a nonlinear oscillator is the period: that is, the smallest real value $T > 0$ for which $x(t) = X(t + T)$. It is important to note here that the frequency of the adapted method (the parameter ω that will appear later) is in general different from the angular frequency of the motion $\Omega = \frac{2\pi}{T}$ (see [9]). In this context, the accurate determination of the appropriate value for ω is highly desirable.

2 A formula for the period

In order to determine whether a given differential problem has periodic solutions or not, it is convenient to reformulate the differential equation in (1) as an equivalent system of two first-order equations

$$\dot{x} = y, \qquad \dot{y} = f(x) \tag{2}$$

where the variables x and y define the phase-space. The equilibrium solutions are of the form

$$x(t) = \bar{x}, \qquad y(t) = 0$$

where $\bar{x}$ are constant solutions of $f(x) = 0$. If we consider initial values $x(0) = x_0$, $y(0) = y_0$, for $t \geq 0$ the points $(x(t), y(t))$ describe a trajectory in the phase-space, with $x(t)$ and $y(t)$ the corresponding solutions of the IVP with equations in (2). The closed curves in the phase-space plane correspond to periodic solutions. The differential equation of the trajectories is easily deduced from (2) and is (see [8])

$$\frac{dy}{dx} = \frac{f(x)}{y}.$$

Taking initial conditions $x(0) = A$, $y(0) = 0$, after integrating we obtain the first integral

$$\frac{1}{2} y^2 + V(x) = V(A) = K$$

where the constant total energy function is given by $H(x, y) = \frac{1}{2} y^2 + V(x)$.

In the case of a periodic motion, considering the values on the trajectory with $y = 0$, which prove to be the two values x_+ and x_- for which $V(x_+) = V(x_-) = K$, the period of the motion is given by (see [10])

$$T = \sqrt{2} \int_{x_-}^{x_+} \frac{dx}{\sqrt{K - V(x)}} \tag{3}$$

and thus the angular frequency is $\Omega = \dfrac{2\pi}{T}$. In a few cases it is possible to solve the integral analytically and thus obtain the exact period, but in most cases only an approximate solution can be found.

For solving the integral in (3) numerically it is appropriate to make a change of the variable, setting

$$x = \frac{x_+ + x_-}{2} + \frac{x_+ - x_-}{2} \cos\theta$$

which transforms the above integral into a new one over the interval $[0, \pi]$. In general the resulting integral must be solved numerically, for which there are many highly effective quadrature formulas.

3 Trigonometrically-fitted methods

One of the most useful procedures for the construction of numerical methods that approximate the solution of second-order initial-value problems is the adaptation technique (of which the most used are exponentially or trigonometrically fitted). In particular, when the solution exhibits periodic or oscillatory behavior the trigonometrically fitted methods are much more efficient than non-fitted methods, with similar costs.

These trigonometrically fitted methods are obtained by demanding that they be exact for any linear combination of the functions

$$\{1, t, t^2, \ldots, \cos(\omega t), \sin(\omega t), \ldots\}.$$

Methods of this type have recently been developed by Simos and Vigo-Aguiar [11], Franco [12] and Fang and Wu [13].

In all of the above-cited papers the value for the frequency ω that appears in the numerical methods is chosen close to the exact frequency of the true solution (the angular frequency Ω) or it is assumed that the frequency value is known in advance. In fact, for the simplest orbital problem, $\ddot{x} + \Omega^2 x = 0$, by taking $\omega = \Omega$ the trigonometrically-fitted methods are exact, which means that the errors are due only to roundoff considerations. But as ω departs farther from the exact value (even for small deviations), the results become worse than those for the corresponding non-fitted methods. The question of how to choose the frequencies on the trigonometrically-fitted (and exponentially-fitted) techniques is a very difficult task. In [9] there is an empirical study showing the strong dependence of the frequency ω on different parameters. For solving the initial-value problem corresponding to the differential equation in (1) we shall consider a two-step trigonometrically-fitted method given by the two formulae

$$x_{n+1} = x_n + h\dot{x}_n + \alpha_{-1}\ddot{x}_{n-1} + \alpha_0\ddot{x}_n \tag{4}$$

$$\dot{x}_{n+1} = \dot{x}_n + \beta_{-1}\ddot{x}_{n-1} + \beta_0\ddot{x}_n + \beta_1\ddot{x}_{n+1} \tag{5}$$

where the coefficients are given by

$$\alpha_{-1} = \frac{1 - h\omega\csc(h\omega)}{\omega^2} \qquad \alpha_0 = \frac{h\omega\left(\csc(h\omega) - \tan\left(\frac{h\omega}{2}\right)\right) + 1 - 2\cos(h\omega)}{\omega^2}$$

$$\beta_{-1} = \frac{h\omega - 2\tan\left(\frac{h\omega}{2}\right)}{2\omega - 2\omega\cos(h\omega)} \qquad \beta_0 = \frac{h\omega\cos(h\omega) - \sin(h\omega)}{\omega(\cos(h\omega) - 1)}$$

$$\beta_1 = \frac{2\sin(h\omega) - h\omega - 2\tan\left(\frac{h\omega}{2}\right)}{2\omega(\cos(h\omega) - 1)}$$

They may be seen in a simpler form via the transformations

$$\csc(h\omega) = \nu, \qquad 1 - \cos(h\omega) = \mu, \qquad \tan\left(\frac{h\omega}{2}\right) = \tau$$

from which the resulting coefficients become

$$\alpha_{-1} = \frac{1 - h\omega v}{\omega^2} \qquad \alpha_0 = \frac{2\mu - h\omega\tau}{\omega^2} - \alpha_{-1}$$

$$\beta_{-1} = \frac{h\omega - 2\tau}{2\omega\mu} \qquad \beta_0 = \frac{1/v + h\omega(\mu - 1)}{\omega\mu} \qquad \beta_1 = h - \beta_0 - \beta_{-1}.$$

As is commonly used in numerical methods, h denotes the stepsize and x_n is the approximation for $x(t_n)$, where the grid points are $t_n = t_0 + n\,h$. The above method is exact when the solution of the differential equation is in the vector space spanned by

$$\{1, t, \cos(\omega t), \sin(\omega t)\},$$

and the local truncation errors for each of the formulae in (4–5) result respectively in

$$\mathcal{L}(x(t_n); h) = x(t_{n+1}) - x_{n+1} = \frac{1}{8} h^4 \left(x^{(4)}(t_n) + \omega^2 \ddot{x}(t_n) \right) + \mathcal{O}(h^5)$$

$$\mathcal{L}(\dot{x}(t_n); h) = \dot{x}(t_{n+1}) - \dot{x}_{n+1} = -\frac{1}{24} h^4 \left(x^{(5)}(t_n) + \omega^2 x^{(3)}(t_n) \right) + \mathcal{O}(h^5),$$

indicating that the method is of second order accuracy.

Note that the above method is explicit, since for the evaluation of the term $\ddot{x}_{n+1} = f(x_{n+1})$ in the formula (5) we use the value of x_{n+1} which was previously obtained with the formula in (4).

4 Strategy for selecting the frequency

As was shown in [9], choice of the frequency in trigonometrically fitted methods is a fundamental question, especially if long-term prediction is considered. For the harmonic oscillator, the frequency of a trigonometrically fitted method is the same as the angular frequency of the solution of the initial value problem. However, for nonlinear problems the frequency of the method is, in general, different from the frequency of the true solution. The frequency choice is crucial, owing to the extreme sensitivity of the numerical method with regard to this choice.

The strategy adopted is based on the minimization of a function that depends on the local errors and the error of the total energy in an selected interval $[0, t_F]$ where the final point t_F is chosen as N_c times the period: that is, $t_T = N_c \times T$. We consider the function $F(\omega)$ given by

$$F(\omega) = |x(t_F) - x_F| + |\dot{x}(t_F) - \dot{x}_F| + |K - H(x_F, \dot{x}_F)|$$

where $x_F, \dot{x}_F$ are the approximate values obtained with the numerical method at the point t_F, $H(x, y)$ is the total energy function, and $K = H(x_0, \dot{x}_0)$ is the constant value corresponding to the orbit passing through the point $(x_0, \dot{x}_0)$ determined by the initial values. This function measures the sum of the absolute errors in the solution, in the
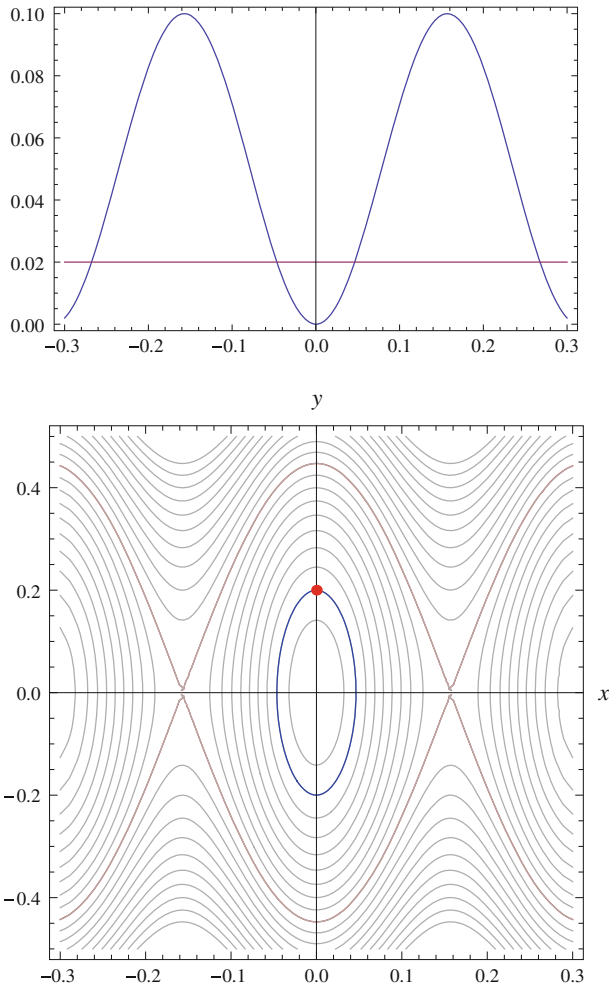
Fig. 1 Potential energy function and phase-plane for the Eq. (6). The *blue line* is the orbit corresponding to $(x_0, \dot{x}_0) = (0, 1/5)$. The *red line* is the separatrix (Color figure online)

derivative and in the total energy at the final point, after performing the integration on $[0, t_F]$.

Using the Golden Section Search technique (see [14]) we obtain the minimum of the function F in a chosen interval enclosing the angular frequency Ω, and this minimum is considered as the optimum value for the parameter, termed ω_{opt}.

5 Numerical example

We illustrate the procedure in the above section considering the problem given by

$$\ddot{x} = -\sin(20x), \quad x(0) = 0, \quad \dot{x}(0) = \frac{1}{5}, t \in [0, 60] \tag{6}$$

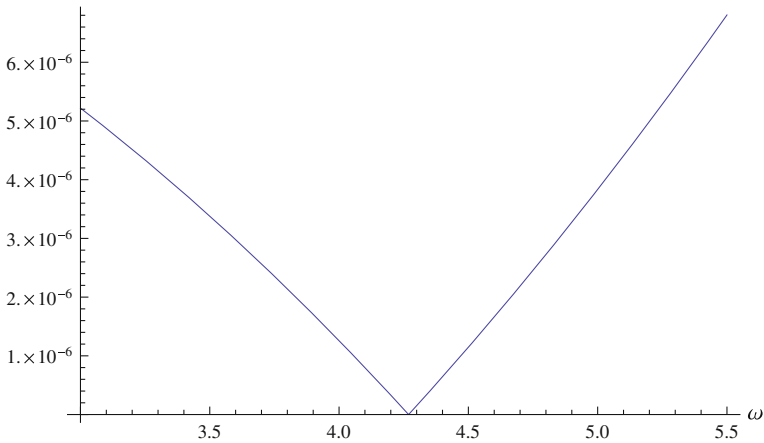**Fig. 2** Typical plot of the function $F(\omega)$ whose minimum ω_{opt} is found using the Golden Section Search technique

Table 1 Maximum absolute errors for the problem in (6) in [0, 60], for different values of the parameter ω using the method in (4–5)

$h = \frac{T}{100} = 0.01484412473422391$	Ω=4.232775875760037	
ω	$Err(x)$	$Err(\dot{x})$
$4.264022254339189(\omega_{opt})$	2.31×10^{-7}	1.01×10^{-6}
Ω	2.71×10^{-5}	1.09×10^{-4}
1	1.75×10^{-3}	7.08×10^{-3}

which is a periodic nonlinear oscillator with angular frequency and period

$$\Omega = 4.232775875760037, \qquad T = 1.4844124734223914. \tag{7}$$

The phase plane is shown in Fig. 1.

Choosing $N_c = 4$ and an initial searching interval for ω given by [3, 11/2], the minimum of the function $F(\omega)$ using the Golden Section Search technique results in $\omega_{opt} = 4.264022254339189$. Figure 2 shows the plot of the function $F(\omega)$ with the minimum ω_{opt}.

In Table 1 the maximum of the absolute errors for the solution and the derivative, $Err(x)$ and $Err(\dot{x})$ are considered for $h = T/100$. We see that small variations in the parameter lead to very different results in terms of accuracy and that ω_{opt} is the best choice for solving the problem.

We have integrated the above problem using the method in (4–5) taking as the value for the parameter the ω_{opt}. In Fig. 3 we show the absolute error of the solution and the error of the Total Energy for the present method compared with a second order symplectic partitioned Runge–Kutta method using the same number of steps (4044). It is clear that the proposed method performs better than the symplectic partitioned Runge–Kutta method.
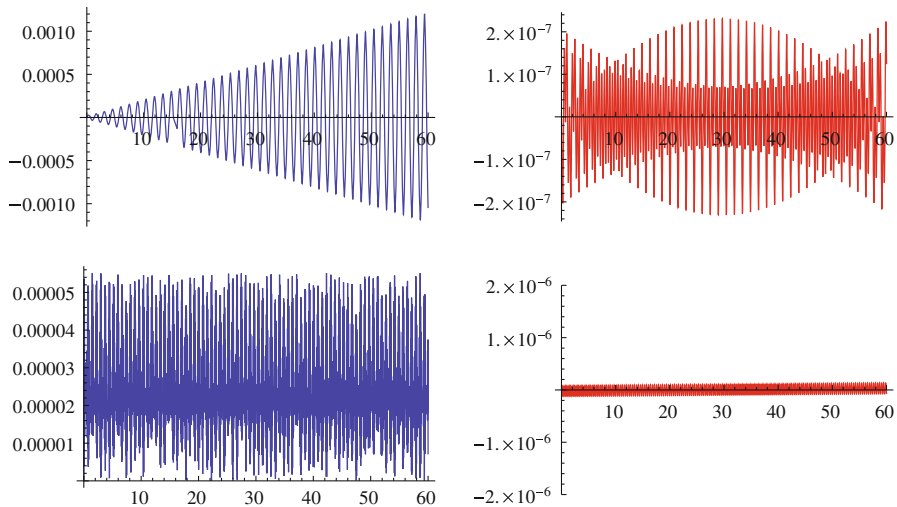
Fig. 3 Absolute error in the solution [*up*] and total energy error [*down*] for the problem in (6). *Left* second order symplectic partitioned R–K method. *Right* method in (4–5). Number of steps: 4044; ω_{opt} : 4.264022254339189

6 Conclusions

In trigonometrically-fitted methods the determination of the parameter (usually known as the frequency of the method) is a critical issue, as was shown in the article by Ramos and Vigo-Aguiar [9]. Knowledge of an estimation of the unknown frequency is needed in order to apply the numerical method efficiently, since its coefficients depend on the value of this parameter. Usually, the value for the frequency ω that appears in trigonometrically-fitted methods is chosen to be equal or close to the angular frequency Ω, but this is not necessarily the best choice, as has been shown in the numerical examples.

In order to provide an estimate of the parameter, some attempts have been made in the literature, based on the minimization of the leading term of the local truncation error (see [15,16]). With this technique an order of accuracy may be gained with respect to the underlying multistep method, but this strategy shows that the frequencies obtained do not reflect the solution itself.

In this paper we apply a trigonometrically-fitted method for solving nonlinear periodic oscillators, and present a strategy for the practical estimation of the parameter, based on the minimization of the sum of the local truncation errors and the total energy error of the system at the final point of a selected interval corresponding to a few times the period. Although here we have presented only a numerical example, the procedure has been tested on different problems, observing its good performance in all cases.

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