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Oscillatory Störmer–Cowell methods ☆

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Abstract

We consider explicit methods for initial-value problems for special second-order ordinary differential equations where the right-hand side does not contain the derivative of y and where the solution components are known to be periodic with frequencies ω_j lying in a given nonnegative interval $[\underline{\omega}, \overline{\omega}]$. The aim of the paper is to exploit this extra information and to modify a given integration method in such a way that the method parameters are "tuned" to the interval $[\underline{\omega}, \overline{\omega}]$. Such an approach has already been proposed by Gautschi in 1961 for linear multistep methods for first-order differential equations in which the dominant frequencies ω_j are a priori known. In this paper, we only assume that the interval $[\underline{\omega}, \overline{\omega}]$ is known. Two "tuning" techniques, respectively based on a least squares and a minimax approximation, are considered and applied to the *classical* explicit Störmer–Cowell methods and the recently developed *parallel* explicit Störmer–Cowell methods.

MSC: 65L06

Keywords: Numerical analysis; Periodic problems; Störmer–Cowell methods; Parallelism

1. Introduction

We consider explicit methods for nonstiff initial-value problems (IVPs) for the special second-order ordinary differential equation (ODE)

$$\frac{d^2y}{dt^2} = f(y), \quad y, f \in \mathbb{R}^d, \quad t_0 \leqslant t \leqslant t_{\text{end}}, \tag{1.1}$$

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where the right-hand side does not contain the derivative of y. On a set of subintervals, the solution of this IVP can be piecewise approximated by a sum of complex exponential functions like

$$y(t) \approx \gamma_0 + \gamma_1 e^{i\omega_1 t} + \gamma_2 e^{i\omega_2 t} + \cdots + \gamma_s e^{i\omega_s t}, \tag{1.2}$$

where the vectors γ_j and the frequencies ω_j are such that the approximation error is small in some sense. These frequencies ω_j will be referred to as *dominant* frequencies. For a given subinterval and tolerance, many trigonometric approximations like (1.2) are possible, and for a given s the approximation error can be made smaller as the length of the subinterval decreases. We are particularly interested in the case where the solution of (1.1) can be approximated such that in all subintervals (i) the values of $||\gamma_j||_\infty$ are of modest magnitude and (ii) the frequencies ω_j are located in a given, relatively small, nonnegative interval $[\underline{\omega}, \overline{\omega}]$ (in Section 2.3.1, we shall show that this is not an exceptional situation). The aim of the paper is to exploit this extra information on the solution by modifying a given integration method for (1.1) in such a way that the method parameters are "tuned" to the interval $[\underline{\omega}, \overline{\omega}]$. A related approach has already been proposed by Gautschi in 1961 [2]. He considered linear multistep methods for first-order ODEs whose solutions are known to have a priori given, dominant frequencies ω_j, and he "tuned" the linear multistep coefficients to these dominant frequencies. However, instead of assuming that the location of the dominant frequencies is given, we only assume that the interval $[\underline{\omega}, \overline{\omega}]$ is available. By using a minimax technique, we will "tune" the coefficients of the integration method to this interval. The tuning will of course be more effective as $\overline{\omega} - \underline{\omega}$ is smaller.

In [5] we applied the minimax approach to linear multistep methods for first-order ODEs. In this paper, we analyse this approach for two families of second-oder ODE methods, viz. the *classical* explicit Störmer–Cowell methods (see e.g. [3, p. 422]) and the *parallel* explicit Störmer–Cowell methods developed in [4]. In addition, we show that in general the minimax approach is superior to a tuning technique based on least squares minimization. The minimax and least-squares versions of the Störmer–Cowell methods will be called *oscillatory* Störmer–Cowell methods.

2. The numerical schemes

The methods studied in this paper are of the explicit general linear method (GLM) form

$$\boldsymbol{Y}_{n+1} = (R \otimes I)\boldsymbol{Y}_n + h^2(S \otimes I)\boldsymbol{F}(\boldsymbol{Y}_n), \quad n = 0, 1, \ldots . \tag{2.1}$$

Here R and S are k-by-k matrices with $k \geqslant 2$, $\otimes$ the Kronecker product, h denotes the stepsize $t_{n+1} - t_n$, and each of the k components $y_{n+1,j}$ of the kd-dimensional solution vector $\boldsymbol{Y}_{n+1}$ represents a numerical approximation to $y(t_n + a_j h)$. The vector $\boldsymbol{a} := (a_j)$ is called the *abscissa vector*, the quantities $\boldsymbol{Y}_n$ the *stage vectors* and their components y_{nj} the *stage values*. Furthermore, for any vector $\boldsymbol{Y}_n = (y_{nj})$, $\boldsymbol{F}(\boldsymbol{Y}_n)$ contains the righthand side values $(f(y_{nj}))$. The abscissae a_j are assumed to be distinct with $a_k = 1$.

The GLM (2.1) is completely determined by the matrices $\{R, S\}$ and the starting vector $\boldsymbol{Y}_0 \approx (y(t_0 + (a_j - 1)h))$. Thus, given $\{\boldsymbol{Y}_0, R, S\}$, (2.1) defines the sequence of vectors $\boldsymbol{Y}_1, \boldsymbol{Y}_2, \ldots$. Evidently, each step requires the evaluation of the k right-hand side functions $f(y_{nj})$, but they can be evaluated in parallel, so that effectively the GLM requires only one right-hand side function per step.

2.1. The local error

The local error is defined by the residue upon substitution of the exact solution into the GLM. The rate by which the residue tends to zero as $h \to 0$ determines the *order of consistency*. We shall call the GLM (and the stage vector $\boldsymbol{Y}_{n+1}$) *consistent of order* q if the residue upon substitution of the exact solution values $\boldsymbol{y}(t_n + a_j h)$ into (2.1) is of order h^{q+2}. The value of q is often called the *stage order*. Given the vector $\boldsymbol{a}$, the consistency condition leads to a set of order conditions to be satisfied by the matrices R and S. In addition, in order to have convergence, the GLM has to satisfy the *necessary* condition of *zero-stability*, that is, the matrix R should have its eigenvalues on the unit disk and the eigenvalues of modulus one should have multiplicity not greater than two.

From the consistency definition given above, the order conditions follow immediately. For simplicity of notation, we assume that the ODE is a scalar equation. Here, and in the sequel of this paper, we will use the componentwise definition of functions of vectors, that is, for any function g and vector $\boldsymbol{v}$, we define $g(\boldsymbol{v}) := (g(v_j))$. Then, substituting the exact solution into (2.1), we define the local error

$$\begin{aligned} \varepsilon(t,h) &:= R\boldsymbol{Y}(t) + h^2 S\boldsymbol{F}(\boldsymbol{Y}(t)) - \boldsymbol{Y}(t+h) \\ &= \left(\left(R + h^2\frac{\mathrm{d}^2}{\mathrm{d}t^2}S\right)\exp\left(\boldsymbol{b}h\frac{\mathrm{d}}{\mathrm{d}t}\right) - \exp\left(\boldsymbol{a}h\frac{\mathrm{d}}{\mathrm{d}t}\right)\right)\boldsymbol{y}(t) = \phi\left(h\frac{\mathrm{d}}{\mathrm{d}t}\right)\boldsymbol{y}(t), \end{aligned} \tag{2.2}$$

where $\boldsymbol{b} := \boldsymbol{a} - \boldsymbol{e}$, $\boldsymbol{e}$ being the vector with unit entries, $\boldsymbol{Y}(t)$ denotes the vector containing the exact stage values, and

$$\phi(z) := (R + z^2 S)\exp(\boldsymbol{b}z) - \exp(\boldsymbol{a}z). \tag{2.3}$$

Let us expand ϕ in the Taylor series

$$\begin{aligned} &\phi(z) = \boldsymbol{c}_{-2} + \boldsymbol{c}_{-1}z + \cdots + z^{q+2}\boldsymbol{c}_q + \cdots, \\ &\boldsymbol{c}_{-2} := R\boldsymbol{e} - \boldsymbol{e}, \qquad \boldsymbol{c}_{-1} := R\boldsymbol{b} - \boldsymbol{a}, \qquad \boldsymbol{c}_j := \frac{1}{(j+2)!}(R\boldsymbol{b}^{j+2} - \boldsymbol{a}^{j+2}) + \frac{1}{j!}S\boldsymbol{b}^j, \quad j \geqslant 0. \end{aligned} \tag{2.4}$$

Furthermore, let us choose the matrix R such that $\boldsymbol{c}_{-2} = \boldsymbol{c}_{-1} = \boldsymbol{0}$. By defining the matrices

$$\begin{aligned} &C := (\boldsymbol{c}_0, \ldots, \boldsymbol{c}_{k-1}), \qquad U_{\boldsymbol{v}} := \left(\frac{1}{2!}\boldsymbol{v}^2, \ldots, \frac{1}{(k+1)!}\boldsymbol{v}^{k+1}\right), \\ &X := \left(\boldsymbol{e}, \boldsymbol{b}, \frac{1}{2!}\boldsymbol{b}^2, \ldots, \frac{1}{(k-1)!}\boldsymbol{b}^{k-1}\right) \end{aligned} \tag{2.5a}$$

we find that the matrix S and the error matrix C are related by the formula

$$SX - C = U_{\boldsymbol{a}} - RU_{\boldsymbol{b}}. \tag{2.5b}$$

The conventional way of constructing IVP solvers chooses distinct abscissae a_j (so that X is non-singular) and defines S by (2.5b) with $C = \mathrm{O}$ yielding methods with stage order $q = k$. By a judicious choice of $\boldsymbol{a}$ one may increase the order of accuracy at the step points t_n to obtain step point order $p > q$ (superconvergence at the step points).

2.2. Störmer–Cowell methods

The definition of the classical explicit k-step Störmer–Cowell (SC) methods with (step point) order $p = k$ can be found in e.g. [3, p. 422]. These methods fit into the GLM format (2.1) with

$$\boldsymbol{a} = (2-k, 3-k, \ldots, -1, 0, 1)^{\mathrm{T}}, \qquad R = \begin{pmatrix} \mathbf{0} & \boldsymbol{I} \\ 0 & \boldsymbol{r}^{\mathrm{T}} \end{pmatrix}, \qquad S = \begin{pmatrix} \mathrm{O} \\ \boldsymbol{s}^{\mathrm{T}} \end{pmatrix}, \qquad \boldsymbol{r} = (0, \ldots, 0, -1, 2)^{\mathrm{T}}, \tag{2.6a}$$

where the vector $\boldsymbol{s}$ is determined by substituting (2.6a) into (2.5b) and setting $C = \mathrm{O}$. Because the (shifted) abscissae b_j are distinct, X is invertible, and since $\boldsymbol{s}^{\mathrm{T}} = \boldsymbol{e}_k^{\mathrm{T}} S$, it follows from (2.5b) that

$$\boldsymbol{s}^{\mathrm{T}} = \boldsymbol{e}_k^{\mathrm{T}}(U_a - RU_b)X^{-1}. \tag{2.6b}$$

Note that $\boldsymbol{y}_{nj} = \boldsymbol{y}_{n-1,j+1}$ for $j = 1, \ldots, k-1$, so that the first $k-1$ components $\boldsymbol{f}(\boldsymbol{y}_{nj})$ of $\boldsymbol{F}(\boldsymbol{Y}_n)$ are available from the preceding step. Hence, (2.6) defines a classical linear multistep-type method with only one new right-hand side evaluation per step.

In [4] we derived *parallel* Störmer–Cowell (PSC) methods by allowing S to be a full matrix satisfying (2.5b) with $C = \mathrm{O}$, and by defining R according to the (zero-stable) matrix

$$R = (\mathbf{0}, \ldots, \mathbf{0}, \boldsymbol{e} - \boldsymbol{r}, \boldsymbol{r}), \qquad \boldsymbol{r} = \boldsymbol{e} - \frac{\boldsymbol{a}}{a_{k-1} - 1} \tag{2.7a}$$

(note that the consistency conditions $\boldsymbol{c}_{-2} = \boldsymbol{c}_{-1} = \mathbf{0}$ are now automatically satisfied). Since the (shifted) abscissae b_j are distinct, S can be defined by

$$S = (U_a - RU_b)X^{-1} \tag{2.7b}$$

to obtain PSC methods with stage order $q = k$. However, in [4] it was shown that the abscissa vector $\boldsymbol{a}$ can be chosen such that the step-point order $p > k$. In addition, in a few cases it is possible to choose $\boldsymbol{a}$ such that instead of k computational stages only $k-1$ computational stages are involved, that is, only $k-1$ distinct right-hand side functions, and hence only $k-1$ processors, are needed per step. For future reference, Table 1 lists the abscissa vector $\boldsymbol{a}$, the number of computational stages k^* and the order p.

Table 1
Abscissa vector $\boldsymbol{a}$, computational stages k^*, and step-point order p for PSC methods

k	k^*	p	$\boldsymbol{a}$					
4	4	5	$\frac{57+\sqrt{229}}{20}$	$\frac{57-\sqrt{229}}{20}$	$\frac{3}{2}$	1		
5	4	6	$\frac{146-\sqrt{163}}{66}$	$\frac{146+\sqrt{163}}{66}$	$\frac{1}{2}$	$\frac{3}{2}$	1	
6	6	8	1.22047388499174955077317629 5	1.78574817943822242665089811 5				
			2.08280190133990556788442891 9	2.35740460565869388326292524 2	$\frac{3}{2}$	1		
7	6	9	1.22366067273036013403372307 0	1.78314152665176136229310202 1				
			2.08550243286155484559219203 2	2.35984980836284552448224743 6	$\frac{1}{2}$	$\frac{3}{2}$	1	
8	7	10	1.22516824834210228704446788 4	1.78608615201785326002175468 9				
			2.07208031244751681867238199 8	2.34769190490729875418306514 1	$\frac{59}{20}$	$\frac{1}{2}$	$\frac{3}{2}$	1

2.3. Oscillatory Störmer–Cowell methods

Suppose that the components of the exact solution $y(t)$ are expanded piecewise on subintervals with respect to the eigenfunctions $\{\exp(\lambda t)\colon \lambda \in \mathbb{C}\}$ of the operator $\mathrm{d}/\mathrm{d}t$. Then, it follows from (2.2) that the local error $\varepsilon(t,h)$ can be expanded in the functions $\{\phi(h\lambda)\exp(\lambda t)\colon \lambda \in \mathbb{C}\}$, i.e.

$$\varepsilon(t,h) \approx \gamma_1\phi(h\lambda_1)\mathrm{e}^{\lambda_1 t} + \gamma_2\phi(h\lambda_2)\mathrm{e}^{\lambda_2 t} + \cdots + \gamma_s\phi(h\lambda)\mathrm{e}^{\lambda_s t}, \quad \lambda_j \in \mathbb{C}_0, \tag{2.2'}$$

where the γ_j are the coefficient vectors and $\mathbb{C}_0$ denotes the set in the complex plane containing the s parameters λ_j needed in the expansion of the components of $y(t)$. Expansion (2.2′) shows that the magnitude of the local error can be minimized by minimizing the function $\phi(z)$ in the domain $h\mathbb{C}_0$. In this paper, we consider the case where $\mathbb{C}_0 = [\mathrm{i}\underline{\omega}, \mathrm{i}\overline{\omega}]$, that is $y(t)$ can be approximated piecewise by trigonometric formulas of form (1.2). The oscillatory Störmer–Cowell methods (briefly OSC methods) and the parallel OSC methods (POSC methods) constructed in this section use the same matrix R and the same abscissa vector $\boldsymbol{a}$ as defined in (2.6a) and in {(2.7a), Table 1} , respectively. However, the matrix S will be chosen such that in some sense the function $\phi(z)$ is minimized on $[ih\underline{\omega}, ih\overline{\omega}]$. Before discussing this minimization, we consider the piecewise trigonometric approximation of functions in more detail.

2.3.1. Trigonometric approximations

We start with the more general approximation problem, where we are given a function y and an approximation g_s to y satisfying $s+1$ distinct collocation conditions $y(\tau_m) = g_s(\tau_m)$, $m = 1,\ldots,s+1$, with $t^* \leqslant \tau_m \leqslant t^* + h$. Since the $(s+1)$-point polynomial interpolation formula interpolating the function $\delta_s(t) := y(t) - g_s(t)$ at the (distinct) points τ_m is identically zero, we obtain the approximation error

$$\delta_s(t) := y(t) - g_s(t) = \frac{1}{(s+1)!}\pi_{s+1}(t)(y^{(s+1)}(\theta(t)) - g_s^{(s+1)}(\theta(t))), \quad t^* \leqslant t \leqslant t^* + h, \tag{2.8}$$

where $\pi_{s+1}(t) := (t-\tau_1)(t-\tau_2)\cdots(t-\tau_{s+1})$, $\theta = \theta(t)$ assumes values in $[t^*, t^*+h]$. By observing that choosing the points τ_m equal to the zeros of the first-kind Chebyshev polynomial shifted to the subinterval $[t^*, t^*+h]$, that is,

$$\tau_m := t^* + \frac{1}{2}h\left(1 + \cos\left(\frac{2m-1}{2(s+1)}\pi\right)\right), \quad m = 1,\ldots,s+1 \tag{2.9}$$

minimizes the maximum of the polynomial $\pi_{s+1}(t)$ in the interval $[t^*, t^*+h]$, it follows from formula (2.8) that we may expect that this choice reduces the magnitude of $\delta_s(t)$. It is easily verified that in the case (2.9) we obtain $\pi_{s+1}(t) = 2^{-2s-1}h^{s+1}T_{s+1}(2h^{-1}(t-t^*)-1)$. Thus, we have the following result:

Theorem 2.1. *Let τ_m be given by (2.9) and let $g_s(t)$ be a function satisfying the collocation conditions $y(\tau_m) = g_s(\tau_m)$, $m = 1,\ldots,s+1$. If $y - g_s$ is $s+1$ times differentiable in $[t^*, t^*+h]$, then*

$$y(t) = g_s(t) + \delta_s(t), \qquad |\delta_s(t)| \leqslant \frac{h^{s+1}}{2^{2s+1}(s+1)!}|y^{(s+1)}(\theta_1) - g_s^{(s+1)}(\theta_2)|, \quad t^* \leqslant t \leqslant t^* + h,$$

where θ_1 and θ_2 are in $[t^*, t^*+h]$.

By means of this theorem we can obtain insight into the trigonometric approximation (1.2). Let $y(t)$ denote a component of the ODE solution $y(t)$ and let us assume that in (1.2) the vectors

Table 2
Maximal approximation errors for $y(t) = t\cos(t^2)$ on [0,1]

s	$\bar{\alpha}$	$[\underline{\omega}, \overline{\omega}]$	$h=1$	$h=\frac{1}{2}$	$h=\frac{1}{4}$	$h=\frac{1}{8}$	$h=\frac{1}{16}$	p
2	3	[2.0, 3.0]	1.5	2.1	2.9	3.8	4.7	3.0
4	3	[2.0, 3.3]	3.1	4.8	6.2	7.5	9.0	5.0
6	5	[2.0, 3.6]	4.5	6.2	8.2	10.3		7.0

$\gamma_0, \gamma_1, \gamma_3, \ldots$ are real and the vectors $\gamma_2, \gamma_4, \gamma_6, \ldots$ are purely imaginary. Then, we can write (1.2) for the component $y(t)$ in the form

$$y(t) \approx g_s(t), \qquad g_s(t) := \alpha_0 + \alpha_1 \cos(\omega_1 t) + \alpha_2 \sin(\omega_2 t) + \cdots + \alpha_{s-1} \cos(\omega_{s-1} t) + \alpha_s \sin(\omega_s t), \tag{1.2'}$$

where all coefficients α_j are real. In each subinterval $[t_n, t_n + h]$ we require that the coefficients α_j are such that $y(\tau_m) = g_s(\tau_m)$ for the $s+1$ points τ_m defined by (2.9) with $t^* = t_n$. In this way, we obtain a piecewise trigonometric approximation of the solution component $y(t)$. In each subinterval, the accuracy of this approximation is determined by Theorem 2.1. This theorem implies that for any given set of frequencies ω_j for which the linear system for the coefficients α_j is nonsingular, the approximation error $\delta(t) = O(h^{s+1})$ in each subinterval. However, large values of $g_s^{(s+1)}(\theta_2)$ may result in large-order constants. From (1.2') we see that given the frequency interval $[\underline{\omega}, \overline{\omega}]$, the frequencies ω_j should be such that the magnitude of the coefficients α_j is as small as possible. In order to see whether it is possible to combine coefficients of modest magnitude with frequencies in a given interval, we determined for a number of given functions, piecewise trigonometric approximations by minimizing the maximal value of $|\delta_s(t)|$ over the ω_j with the constraints $\max_j ||\alpha_j||_\infty \leqslant \bar{\alpha}$ and $\underline{\omega} \leqslant \omega_j \leqslant \overline{\omega}$. A typical situation is shown by the piecewise trigonometric approximation of the function $y(t) = t\cos(t^2)$ on the interval $[0, 1]$. This function oscillates with increasing frequency and amplitude. Table 2 lists the number of correct digits Δ (i.e. the maximal absolute error is written as $10^{-\Delta}$), the constraint on α, a suitable frequency interval, and the observed order of accuracy p. Note that the order of accuracy p is in agreement with Theorem 2.1.

This example illustrates that the representation of oscillatory functions by means of formulas of the form (1.2) with relatively small frequency bands and modest coefficients is quite accurate.

Next, we consider the minimization of $\phi(z)$ in the interval $[ih\underline{\omega}, ih\overline{\omega}]$. In the case of the SC methods only the last component of $\phi(z)$ is relevant, so that only this component needs to be considered. In the case of the PSC methods, all components $\phi_j(z)$ play a role and could be minimized separately on intervals $[ih\underline{\omega}, ih\overline{\omega}]$ depending on j. However, for simplicity, we shall only consider the case where all components are minimized on the same interval $[ih\underline{\omega}, ih\overline{\omega}]$.

If the *location* of the frequencies ω_j is known in advance and if there are sufficiently many free parameters available, then we obtain a perfect tuning of the method by choosing S such that the quantities $\phi_j(ih\omega_1), \ldots, \phi_j(ih\omega_s)$ vanish. This is precisely the approach of Gautschi [2] in his oscillatory linear multistep methods for first-order ODEs with a priori given frequencies.

In this paper, our starting point is that only the *interval* $[\underline{\omega}, \overline{\omega}]$ is known. Then, the most natural option seems to be the minimization of the L_2-norm of $\phi_j(z)$ on the interval $[ih\underline{\omega}, ih\overline{\omega}]$. However, we will show that the system of equations defining the matrix S becomes highly ill-conditioned if the length of the interval $[ih\underline{\omega}, ih\overline{\omega}]$ is small. Another option (already applied in [5] in the case

of linear multistep methods for first-order ODEs) chooses as many zeros of $\phi_j(z)$ as possible in the interval $[ih\underline{\omega}, ih\overline{\omega}]$ in such a way that the maximum norm of $\phi_j(z)$ on the interval $[ih\underline{\omega}, ih\overline{\omega}]$ is minimized. For a given interval $[ih\underline{\omega}, ih\overline{\omega}]$ this minimax approach yields a system for S that is much better conditioned than in the case of the least-squares approach. However, again we are faced with ill-conditioning if $h(\overline{\omega} - \underline{\omega})$ is small. In such cases, one may decide to use a Taylor expansion of $\phi(z)$ at the centre of the interval $[ih\underline{\omega}, ih\overline{\omega}]$ (see Section 2.3.4).

Evidently, for $h \to 0$, the matrix S resulting from the least squares and minimax options converges to the matrix S defining the Störmer–Cowell-type methods discussed in the preceding section. Likewise, the error matrix C defined in (2.5a) converges to O.

The least squares and minimax approach applied to Störmer–Cowell-type methods will be discussed in more detail in the next subsections.

2.3.2. *The least-squares approach*

The least-squares approach minimizes the L_2-norm of $\phi_j(z)$ on the interval $[ih\underline{\omega}, ih\overline{\omega}]$, i.e. it minimizes the components of

$$\int_{h\underline{\omega}}^{h\overline{\omega}} |\phi(\mathrm{i}x)|^2 \,\mathrm{d}x = \int_{h\underline{\omega}}^{h\overline{\omega}} \{(x^2 S\cos(\boldsymbol{b}x) - \chi(x))^2 + (x^2 S\sin(\boldsymbol{b}x) - \sigma(x))^2\} \,\mathrm{d}x, \tag{2.10}$$

$$\chi(x) := R\cos(\boldsymbol{b}x) - \cos(\boldsymbol{a}x), \qquad \sigma(x) := R\sin(\boldsymbol{b}x) - \sin(\boldsymbol{a}x).$$

Minimization of the components of the integral expression (2.10) yields for S the condition

$$SW = V, \quad V = (\boldsymbol{v}_1, \ldots, \boldsymbol{v}_k), \qquad W = (\boldsymbol{w}_1, \ldots, \boldsymbol{w}_k), \tag{2.11}$$

$$\boldsymbol{v}_j := \int_{h\underline{\omega}}^{h\overline{\omega}} x^2(\cos(b_j x)\chi(x) + \sin(b_j x)\sigma(x)) \,\mathrm{d}x,$$

$$\boldsymbol{w}_j := \int_{h\underline{\omega}}^{h\overline{\omega}} x^4(\cos(b_j x)\cos(\boldsymbol{b}x) + \sin(b_j x)\sin(\boldsymbol{b}x)) \,\mathrm{d}x = \int_{h\underline{\omega}}^{h\overline{\omega}} x^4\cos((b_j\boldsymbol{e} - \boldsymbol{b})x) \,\mathrm{d}x. \tag{2.12}$$

Note that W is symmetric, so that its computation requires the evaluation of only $k(k+1)/2$ entries. For the OSC methods we only have to minimize the last component of (2.10), so that we find for $\boldsymbol{s}$ the equation $\boldsymbol{s}^{\mathrm{T}} W = \boldsymbol{e}_k^{\mathrm{T}} V$. On substituting $b_j = j - k$ it follows that the values $\boldsymbol{e}_k^{\mathrm{T}}\boldsymbol{v}_j$ can be written as

$$\boldsymbol{e}_k^{\mathrm{T}}\boldsymbol{v}_j = \int_{h\underline{\omega}}^{h\overline{\omega}} x^2\{2\cos(b_j x) - \cos((b_j - 1)x) - \cos((b_j + 1)x)\} \,\mathrm{d}x.$$

For the POSC methods we obtain by substituting $b_{k-1} = \frac{1}{2}$, $b_k = 0$ that $\boldsymbol{w}_j$ is again given by (2.12) and that

$$\boldsymbol{v}_j = \int_{h\underline{\omega}}^{h\overline{\omega}} x^2\{(\boldsymbol{e} - \boldsymbol{r})\cos\left(\left(b_j - \frac{1}{2}\right)x\right) + \boldsymbol{r}\cos(b_j x) - \cos((b_j\boldsymbol{e} - \boldsymbol{a})x)\} \,\mathrm{d}x.$$

In order to evaluate the expressions for $\boldsymbol{v}_j$ and $\boldsymbol{w}_j$ analytically we use the integration formulae

$$I_m := \int_{\underline{x}}^{\overline{x}} x^m \cos(cx) \,\mathrm{d}x = c^{-m-1}(F_m(c\overline{x}) - F_m(c\underline{x})), \quad m = 2, 4 \tag{2.13}$$

with

$$F_2(u) = (u^2 - 2)\sin(u) + 2u\cos(u), \quad F_4(u) = (u^4 - 12u^2 + 24)\sin(u) + (4u^3 - 24u)\cos(u).$$

If $c(\overline{x} - \underline{x})$ is small, then these formulas may be inaccurate and it is preferable to use the following expansions that are valid for $|c\overline{x}| < 1$:

$$\begin{aligned} I_2 &= \overline{x}^3 \left(\frac{1}{3}\theta_3 - \frac{1}{5.2!}\theta_5(c\overline{x})^2 + \frac{1}{7.4!}\theta_7(c\overline{x})^4 - \frac{1}{9.6!}\theta_9(c\overline{x})^6 + \frac{1}{11.8!}\theta_{11}(c\overline{x})^8 - \cdots \right), \\ I_4 &= \overline{x}^5 \left(\frac{1}{5}\theta_5 - \frac{1}{7.2!}\theta_7(c\overline{x})^2 + \frac{1}{9.4!}\theta_9(c\overline{x})^4 - \frac{1}{11.6!}\theta_{11}(c\overline{x})^6 + \frac{1}{13.8!}\theta_{13}(c\overline{x})^8 - \cdots \right), \end{aligned} \tag{2.13'}$$

where $\theta_j := 1 - \underline{x}^j \overline{x}^{-j}$.

In order to compare the behaviour of the function $\phi(z)$ associated with the least-squares approach and the function $\tilde{\phi}(z)$ associated with the conventional approach (where the components of $\tilde{\phi}(z)$ have all their zeros at the origin), we have plotted the quotients

$$\theta_{\mathrm{OSC}}(x) := \left| \frac{\phi_k(\mathrm{i}x)}{\tilde{\phi}_k(\mathrm{i}x)} \right|, \quad \theta_{\mathrm{POSC}}(x) := \left\| \frac{\phi(\mathrm{i}x)}{\tilde{\phi}(\mathrm{i}x)} \right\|_\infty \tag{2.14}$$

as a function of x, respectively for the OSC and POSC methods. The least-squares approach is more effective than the conventional approach if $\theta(x) < 1$. Figs. 1a and b, respectively, present plots for the OSC and POSC methods of order $p = 6$ on the interval $h\underline{\omega} \leqslant x \leqslant h\overline{\omega}$ with $h\underline{\omega} = 0.8$ and $h\overline{\omega} = 1$ (dashed line). This behaviour of $\theta(x)$ is typical for a whole range of $h\underline{\omega}$ and $h\overline{\omega}$ values, and shows that the least-squares approach yields in the interval $h\underline{\omega} \leqslant x \leqslant h\overline{\omega}$ a substantially smaller local error than the conventional approach. Note that the $\theta(x)$ values are smaller in the SC case than in the PSC case. This is due to the fact that in the PSC case all components of $\phi(\mathrm{i}x)/\tilde{\phi}(\mathrm{i}x)$ are taken into account. Furthermore, Figs. 2a and b show on the whole interval $0 \leqslant x \leqslant h\overline{\omega}$ the behaviour of the functions $\{|\phi_k(\mathrm{i}x)|, |\tilde{\phi}_k(\mathrm{i}x)|\}$ and $\{||\phi(\mathrm{i}x)||_\infty, ||\tilde{\phi}(\mathrm{i}x)||_\infty\}$, respectively, for the OSC and POSC methods (dashed and dashed-dotted lines). From these figures it follows that an underestimation of the interval of dominant frequencies is always (albeit slightly) better than the conventional approach, whereas overestimation may easily be worse than the conventional approach.

A computational drawback of the least-squares approach is the poor condition of the system defining S because W converges to a singular matrix as $h\overline{\omega}$ becomes smaller. In fact, it follows from the definition of W and (2.13') that $W = \frac{1}{5}(h\overline{\omega})^5\theta_5(\boldsymbol{e}, \ldots, \boldsymbol{e}) + \mathrm{O}((h\overline{\omega})^7)$.

2.3.3. The minimax approach

The condition of the system defining S can be improved by requiring that the components $|\phi_j(\mathrm{i}x)|$ possess zeros in the interval $h\underline{\omega} \leqslant x \leqslant h\overline{\omega}$. If $|\phi_j(z)|$ would be a polynomial of degree $2r$ in z, then its maximum norm on the interval $[\mathrm{i}h\underline{\omega}, \mathrm{i}h\overline{\omega}]$ would be minimized if we identify the zeros of $|\phi_j(z)|$ with the zeros of the corresponding minimax polynomial on $[\mathrm{i}h\underline{\omega}, \mathrm{i}h\overline{\omega}]$. Such minimax polynomials have r double zeros given by (cf. [5])

$$z_m = \mathrm{i}x_m, \qquad x_m := \frac{1}{2}h\left(\underline{\omega} + \overline{\omega} + (\overline{\omega} - \underline{\omega})\cos\left(\frac{2m-1}{2r}\pi\right)\right), \quad m = 1, \ldots, r. \tag{2.15a}$$

This leads us to require

$$\phi(\mathrm{i}x_m) = (R - x_m^2 S)\exp(\mathrm{i}\boldsymbol{b}x_m) - \exp(\mathrm{i}\boldsymbol{a}x_m) = \boldsymbol{0}, \quad m = 1, \ldots, r, \tag{2.15b}$$

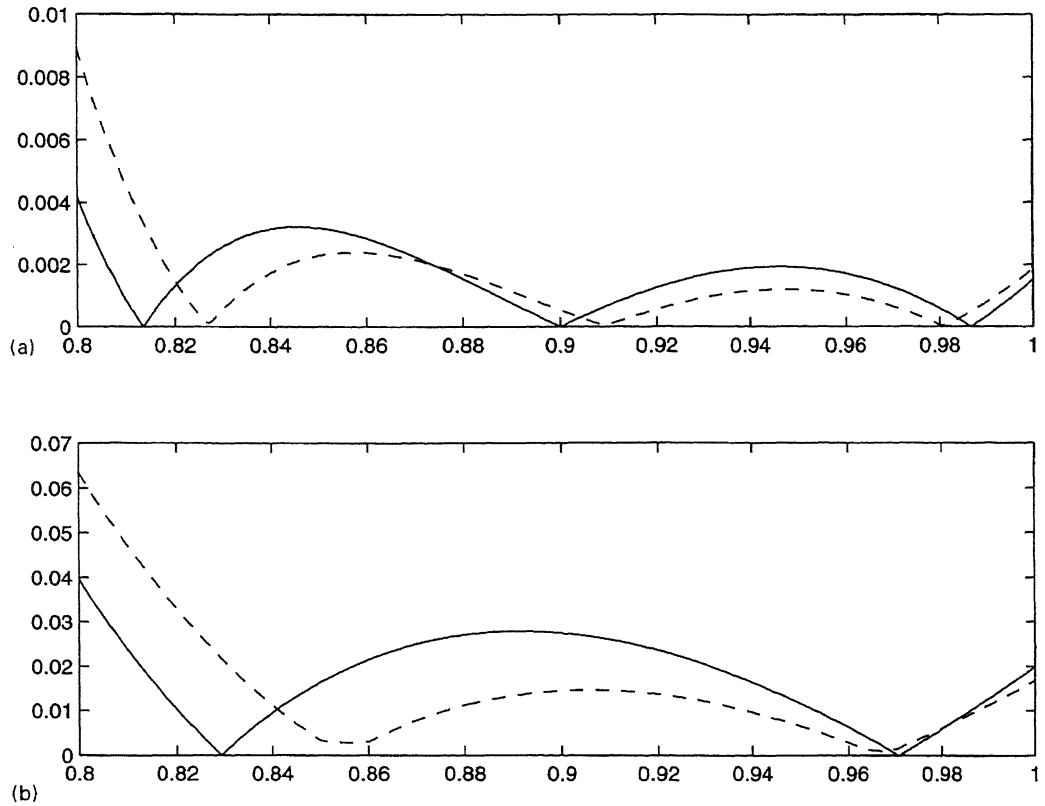

Fig. 1. (a) Plots of the quotients (2.14) on [0.8,1] for OSC methods. (b) Plots of the quotients (2.14) on [0.8,1] for POSC methods.

where r is determined by the number of free parameters available in the function ϕ. Thus, we have to solve the equations

$$\begin{aligned} x_m^2 S\cos(\boldsymbol{b}x_m) &= R\cos(\boldsymbol{b}x_m) - \cos(\boldsymbol{a}x_m),\\ x_m^2 S\sin(\boldsymbol{b}x_m) &= R\sin(\boldsymbol{b}x_m) - \sin(\boldsymbol{a}x_m), \end{aligned} \qquad m = 1,\dots,r. \tag{2.16a}$$

If k is even, we may set $r = k/2$, so that the matrix S is completely determined by (2.16a). If k is odd, we set $r = (k-1)/2$ and we add the consistency condition $c_0 = \mathbf{0}$, i.e.

$$2S\boldsymbol{e} = \boldsymbol{a}^2 - R\boldsymbol{b}^2, \quad k \text{ odd}. \tag{2.16b}$$

Let us introduce the k-by-k matrices V_v and W:

$$\begin{aligned} V_v &:= (-x_1^{-2}\cos(\boldsymbol{v}x_1),\dots,-x_r^{-2}\cos(\boldsymbol{v}x_r),-x_1^{-3}\sin(\boldsymbol{v}x_1),\dots,-x_r^{-3}\sin(\boldsymbol{v}x_r)), \quad k \text{ even},\\ V_v &:= (\boldsymbol{v}^2,-x_1^{-2}\cos(\boldsymbol{v}x_1),\dots,-x_r^{-2}\cos(\boldsymbol{v}x_r),-x_1^{-3}\sin(\boldsymbol{v}x_1),\dots,-x_r^{-3}\sin(\boldsymbol{v}x_r)), \quad k \text{ odd},\\ W &:= (\cos(\boldsymbol{b}x_1),\dots,\cos(\boldsymbol{b}x_r),\ x_1^{-1}\sin(\boldsymbol{b}x_1),\dots,x_r^{-1}\sin(\boldsymbol{b}x_r)), \quad k \text{ even},\\ W &:= (2\boldsymbol{e},\cos(\boldsymbol{b}x_1),\dots,\cos(\boldsymbol{b}x_r),\ x_1^{-1}\sin(\boldsymbol{b}x_1),\dots,x_r^{-1}\sin(\boldsymbol{b}x_r)), \quad k \text{ odd}. \end{aligned} \tag{2.17a}$$

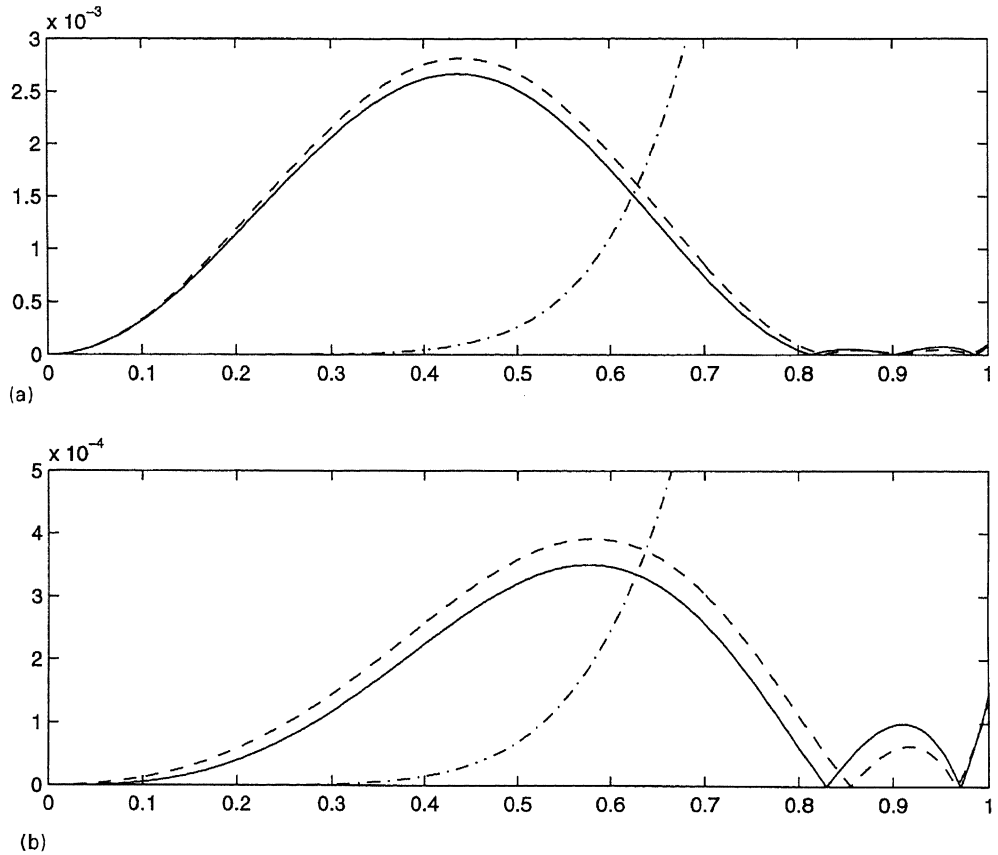

Fig. 2. (a) Plots of the max norm of (2.3) in [0,i] for OSC and SC (dash-dotted curve) methods. (b) Plots of the max norm of (2.3) on [0,i] for POSC and PSC (dash-dotted curve) methods.

Then conditions (2.16) can be expressed as $SW = V := V_a - RV_b$, leading to a family of OSC and POSC methods by defining

$$S = VW^{-1}, \qquad V := V_a - RV_b. \tag{2.17b}$$

Again the condition of the matrix W becomes worse if $h\underline{\omega}$ and $h\overline{\omega}$ are both small. However, the condition is much better than in the case of the least squares approach. For example, for k even we have that $W = (\boldsymbol{e},\ldots,\boldsymbol{e},\boldsymbol{b},\ldots,\boldsymbol{b}) + \mathrm{O}(h^2)$, so that only $k/2$ columns of W are approximately equal, whereas in the least-squares approach k columns of W are approximately equal.

The solid lines in Figs. 1 and 2 represent the minimax analogues of the least-squares plots.

2.3.4. *Small frequency intervals*

If the zeros x_m in the minimax approach are close together, then it seems equally effective to concentrate as many zeros as possible of ϕ at $z_0 = \mathrm{i}x_0 = \mathrm{i}h\omega_0$ with $\omega_0 = (\underline{\omega} + \overline{\omega})/2$. Let us expand

$\phi(z)$ around z_0 (compare (2.4))

$$\begin{aligned}\phi(z) &= \phi(z_0) + (z - z_0)\phi'(z_0) + \frac{1}{2}(z - z_0)^2\phi''(z_0) + \cdots + \frac{1}{m!}(z - z_0)^m\phi^{(m)}(z_0) + \cdots,\\ \phi^{(j)}(z) &= S(z^2\boldsymbol{b}^j + p_j z\boldsymbol{b}^{j-1} + q_j\boldsymbol{b}^{j-2})\exp(\boldsymbol{b}z) + R\boldsymbol{b}^j\exp(\boldsymbol{b}z) - \boldsymbol{a}^j\exp(\boldsymbol{a}z), \quad j \geqslant 0,\end{aligned} \tag{2.18}$$

where $p_{j+1} = p_j + 2$ and $q_{j+1} = p_j + q_j$ with $p_0 = q_0 = 0$. If k is even, then we find

$$\begin{aligned}\operatorname{Re}\phi^{(j)}(z_0) &= S((q_j\boldsymbol{b}^{j-2} - x_0^2\boldsymbol{b}^j)\cos(\boldsymbol{b}x_0) - p_j x_0\boldsymbol{b}^{j-1}\sin(\boldsymbol{b}x_0)) + R\boldsymbol{b}^j\cos(\boldsymbol{b}x_0) - \boldsymbol{a}^j\cos(\boldsymbol{a}x_0),\\ \operatorname{Im}\phi^{(j)}(z_0) &= S(p_j x_0\boldsymbol{b}^{j-1}\cos(\boldsymbol{b}x_0) - (x_0^2\boldsymbol{b}^j - q_j\boldsymbol{b}^{j-2})\sin(\boldsymbol{b}x_0)) + R\boldsymbol{b}^j\sin(\boldsymbol{b}x_0) - \boldsymbol{a}^j\sin(\boldsymbol{a}x_0),\end{aligned} \tag{2.19}$$

where $j = 0, 1, \ldots, (k-2)/2$. Setting $\operatorname{Re}\phi^{(j)}(z_0) = \operatorname{Im}\phi^{(j)}(z_0) = \mathbf{0}$ yields the required system of equations for S. If k is odd, then we add the consistency condition $c_0 = \mathbf{0}$ given by (2.16b) and proceeding as in Section 2.3.3 we can again define appropriate matrices V and W such that $SW = V$. The resulting matrix W is less 'singular' than in the minimax approach. In fact, if k is even, then $W = (-\boldsymbol{e}, -3\boldsymbol{b}, q_j\boldsymbol{b}^{j-2}, -\boldsymbol{b}, 2\boldsymbol{e}, (p_j + q_j)\boldsymbol{b}^{j-1}) + \mathrm{O}(h^2)$ where $j = 2, 3, \ldots, (k-2)/2$, showing that for $k > 6$ it is better conditioned than in the case (2.17a). In our numerical experiments, we define the matrix S in this way as soon as $h(\overline{\omega} - \underline{\omega}) < 0.001$.

2.3.5. Oscillatory methods for arbitrary frequency intervals

Evidently, the oscillatory methods constructed above should be more accurate than the underlying conventional methods provided that the frequency interval $[\underline{\omega}, \overline{\omega}]$ is small. This raises the question what happens if this interval in *not* small. In other words, How robust are the oscillatory methods in nonmodel situations. To answer this question, we look at the local error of the oscillatory methods which is determined by the error matrix C defined in (2.5a). This matrix depends on h and is related to the matrix S by the equation $C(h) = S(h)X - U_a + RU_b$. We restrict our considerations to the matrix $C(h)$ associated with the minimax method. It follows from the minimax equations (2.16a) that $S(h)$ can be expanded in powers of h^2, so that $C(h)$ can also be expanded in powers of h^2. Since $C(0) = S(0)X - U_a + RU_b$ vanishes, we have that $C(h) = \frac{1}{2}h^2C''(0) + \frac{1}{24}h^4C''''(0) + \mathrm{O}(h^6)$. Evidently, the derivatives of $C(h)$ equal those of $S(h)X$, e.g. $C''(0) = S''(0)X$. It is tempting to compute the derivatives of $S(h)$ from the formula $SW = V := V_a - RV_b$ by substituting Taylor expansions of $S(h)$, $V(h)$, and $W(h)$. However, the resulting systems appear to be singular. For example, $S''(0)$ satisfies the equation $W''(0) + S''(0)W(0) = V''(0)$ in which $W(0)$ is a singular matrix. The reason is that a number of entries of $S''(0)$ are zero. Only if we know in advance which entries vanish, we can solve this singular system. An alternative is to look at the function $||\phi(\mathrm{i}x)||_\infty$ in the interval $h\underline{\omega} \leqslant x \leqslant h\overline{\omega}$. From (2.2') it follows that

$$\begin{aligned}||\varepsilon(t,h)||_\infty &\leqslant ||\gamma_1||_\infty||\phi(\mathrm{i}h\omega_1)||_\infty + ||\gamma_2||_\infty||\phi(\mathrm{i}h\omega_2)||_\infty + \cdots + ||\gamma_s||_\infty||\phi(\mathrm{i}h\omega_s)||_\infty\\ &= \gamma(||\phi(\mathrm{i}h\omega_1)||_\infty + ||\phi(\mathrm{i}h\omega_2)||_\infty + \cdots + ||\phi(\mathrm{i}h\omega_s)||_\infty),\end{aligned} \tag{2.20}$$

where γ is a sort of averaged weighted coefficient. Evidently, γ is at most $\max_j ||\gamma_j||_\infty$, but usually much smaller. Thus, the size of $||\varepsilon(t,h)||_\infty$ is largely determined by $||\phi(\mathrm{i}x)||_\infty$, $h\underline{\omega} \leqslant x \leqslant h\overline{\omega}$. In the following, we write $\phi(\mathrm{i}x)$ as $\phi(\mathrm{i}x, h\underline{\omega}, h\overline{\omega})$, because both in the least squares and the minimax case, the function $\phi(\mathrm{i}x)$ is completely defined by $h\underline{\omega}$ and $h\overline{\omega}$. It is now of interest to know how $\phi(\mathrm{i}x, h\underline{\omega}, h\overline{\omega})$ depends on $h\underline{\omega}$ and $h\overline{\omega}$. We shall confine our considerations to the minimax case. Furthermore, since for an arbitrary problem the dominant frequencies may be located anywhere, we

Table 3
Values of $\phi_{\max}$ and ϕ_{aver}

		$k=4$	$k=5$	$k=6$	$k=7$	$k=8$	$k=9$	$k=10$
OSC	$\phi_{\max}$	1.8_{10-2}	1.6_{10-2}	5.2_{10-3}	4.7_{10-3}	1.5_{10-3}	1.4_{10-3}	4.7_{10-4}
	ϕ_{aver}	2.3_{10-3}	1.7_{10-3}	6.7_{10-4}	5.0_{10-4}	1.8_{10-4}	1.4_{10-4}	5.1_{10-5}
POSC	$\phi_{\max}$	6.3_{10-3}	2.2_{10-3}	9.7_{10-5}	3.5_{10-5}	1.4_{10-5}		
	ϕ_{aver}	6.6_{10-4}	2.2_{10-4}	1.2_{10-5}	3.5_{10-6}	1.5_{10-6}		

shall assume them in an interval $[0,\overline{\omega}]$ where $\overline{\omega}$ is a guess for the actual upperbound of the dominant frequencies. We expect that the quotient $Q(x,h\overline{\omega}) := ||\phi(\mathrm{i}x,0,h\overline{\omega})||_\infty / ||\phi(\mathrm{i}x/h\overline{\omega},0,1)||_\infty$ behaves like some power of $h\overline{\omega}$ as $h\overline{\omega}$ tends to zero, independently of x. Therefore, we considered for a number of $h\overline{\omega}$-values the function $\log Q(x,h\overline{\omega})/\log(h\overline{\omega})$. For $h\overline{\omega}\leqslant 1$, we found for each OSC and each POSC method an almost constant value $k+2$. Hence,

$$Q(x,h\overline{\omega}) := \frac{||\phi(\mathrm{i}x,0,h\overline{\omega})||_\infty}{||\phi(\mathrm{i}x/h\overline{\omega},0,1)||_\infty} \approx (h\overline{\omega})^{k+2}, \quad 0\leqslant x\leqslant h\overline{\omega}\leqslant 1. \tag{2.21}$$

On substitution into (2.20), we obtain

$$||\varepsilon(t,h)||_\infty \leqslant \gamma(h\overline{\omega})^{k+2}(||\phi(\mathrm{i}\omega_1\overline{\omega}^{-1},0,1)||_\infty + ||\phi(\mathrm{i}\omega_2\overline{\omega}^{-1},0,1)||_\infty + \cdots + ||\phi(\mathrm{i}\omega_s\overline{\omega}^{-1},0,1)||_\infty). \tag{2.22}$$

This error estimate shows that irrespective the value of $\overline{\omega}$ the oscillatory methods possess stage order at least $q=k$ (just as the underlying conventional methods). The high power of $\overline{\omega}$ in (2.22) looks alarming if $\overline{\omega}$ is large. However, if expansion (1.2) of the solution contains dominant terms of high frequency, then we need anyhow small stepsizes to represent the solution, so that it is reasonable to assume that $h\overline{\omega}\leqslant 1$. In fact, the factor $\overline{\omega}^{k+2}$ will also appear in the first nonzero term of the Taylor expansion of the local error (see Section 2.1).

Furthermore, the error estimate (2.22) shows that the function $||\phi(\mathrm{i}x,0,1)||_\infty$, $0\leqslant x\leqslant 1$, plays a central role. This function assumes a maximum at $x=1$, so that

$$||\varepsilon(t,h)||_\infty \leqslant \gamma s(h\overline{\omega})^{k+2}\phi_{\max}, \qquad \phi_{\max} := ||\phi(\mathrm{i},0,1)||_\infty. \tag{2.23a}$$

However, this estimate is too pessimistic, because it assumes that all dominant frequencies are located near $\overline{\omega}$. A more realistic estimate is obtained by replacing the sum in (2.22) by s times the averaged value of $||\phi(\mathrm{i}x,0,1)||_\infty$ in the interval $0\leqslant x\leqslant 1$, i.e. we use the 'approximation'

$$||\varepsilon(t,h)||_\infty \approx \gamma s(h\overline{\omega})^{k+2}\phi_{\text{aver}}, \qquad \phi_{\text{aver}} := \int_0^1 ||\phi(\mathrm{i}x,0,1)||_\infty \,\mathrm{d}x. \tag{2.23b}$$

Table 3 lists the values of $\phi_{\max}$ and ϕ_{aver} for the OSC and POSC methods. The values of ϕ_{aver} are smaller than $\phi_{\max}$ by a factor of about 10.

2.4. Stability

One may wonder how the oscillatory modes affect the stability of the method. We restrict our considerations to the *linear* stability of (2.1). The linear stability is determined by the matrix $M(z) := R + zS$ with $z = h^2\lambda$, λ running through the eigenvalues of the Jacobian matrix of the

Table 4a
Stability boundaries for the case $\underline{\omega} = \overline{\omega}$

$h\underline{\omega} = h\overline{\omega}$	0	0.5	1.0	1.5	2.0	2.2	2.3	3.0	3.9	4.0
POSC (6)	0.85	0.87	0.89	0.97	1.18	1.29	0			
POSC (10)	0.78	0.78	0.78	0.81	0.87	0.89	0.90	1.11	1.45	1.40

Table 4b
Stability boundaries for the case $\underline{\omega} = 0$

$h\overline{\omega}$	0	0.5	1.0	2.0	4.0	6.0	8.0	10.0	11.0	12.0
POSC (6)	0.85	0.86	0.87	0.90	0.98	1.05	1.03	1.10	1.12	0
POSC (10)	0.78	0.78	0.78	0.81	0.85	0.91	0.93	0.55		

righthand side function f of the ODE (1.1). Assuming that (1.1) is linearly stable itself, we only consider negative values of z. Here, the *stability interval* is defined by the interval $-\beta^2 \leqslant z \leqslant 0$, where $M(z)$ has its eigenvalues on the unit disk. The value of β is called the *stability boundary*. As an illustration, we have computed the stability boundaries of the POSC methods with $\underline{\omega} = \overline{\omega}$ and with $\underline{\omega} = 0$. Tables 4a, 4b present values of β for the 6-th order ($k = 5$) and the 10th-order ($k = 8$) POSC methods (these methods are also used in the numerical experiments in Section 3). In all cases, the oscillatory approach slightly stabilizes the PSC method until some maximal value of $h\overline{\omega}$ is reached.

3. Numerical experiments

In this section we compare the performance of the OSC and POSC methods in least squares and minimax mode with the nonoscillatory Störmer–Cowell methods. In the tables of results, we use the following abbreviations:

SC(p) Classical Störmer–Cowell method (2.6) of order $p = k$,
OSC(p) Oscillatory version of the SC(p) method,
PSC(p) Parallel Störmer–Cowell method {(2.7), Table 1} of order p,
POSC(p) Oscillatory version of the PSC(p) method.

If in the examples the exact solutions are known, the starting vector Y_0 was taken from the solution values ($y(t_0 + b_j h)$), otherwise it was computed numerically by a one-step method. We used a few well-known test problems from the literature. The accuracy is defined by the number of correct digits Δ at the end point (the maximal absolute end point error is written as $10^{-\Delta}$). The number of steps taken in the integration interval is denoted by N which is at the same time for all methods the total number of *sequential* right-hand sides needed to perform the integration.

3.1. Problems with one dominant frequency

We start with Bessel's equation [5]

$$\frac{d^2y}{dt^2} = -\left(100 + \frac{1}{4t^2}\right) y, \qquad y(1) = J_0(10), \qquad y'(1) = \frac{1}{2}J_0(10) - 10J_1(10) \tag{3.1}$$

on the interval [1,10] with exact solution $y(t)=\sqrt{t}J_0(10t)$. This equation shows that there is just one frequency $\omega=\sqrt{100+(4t^2)^{-1}}\approx 10$. The oscillatory methods were applied with $[\underline{\omega},\overline{\omega}]=[9.9,10.1]$.

The second test problem is the Orbit problem from the Toronto test set [6] on the interval [0,20] with eccentricity $\varepsilon=0.01$. The solution is known to have one dominant frequency $\omega\approx 1$. The oscillatory methods were applied with $[\underline{\omega},\overline{\omega}]=[0.9,1.1]$. The results in Tables 5a, 5b and 6a, 6b indicate that

(i) The least-squares approach is unreliable, even for relatively large stepsizes, which is due to the bad condition of the W matrix.
(ii) The minimax approach can be used until the 20 decimals accuracy range.
(iii) The minimax approach produces higher accuracies than the conventional approach.

The fact that the minimax method is less effective in the case of the Orbit problem, particularly in the high-accuracy range, can be explained by the fact that for high accuracies, frequencies other than $\omega\approx 1$ start to come into play.

From now on, we do not apply the least-squares strategy because of its erratic performance.

Table 5a
(N,Δ)-values for the Bessel problem on [1,10]; 6th-order methods with $[\underline{\omega},\overline{\omega}]=[9.9,10.1]$

Method	Version	100	200	400	800
SC(6)	Conventional	*	2.3	4.0	5.8
OSC(6)	Least squares	4.7	6.6	8.7	10.6
	Minimax	4.7	6.6	8.7	10.6
PSC(6)	Conventional	1.4	5.9	8.6	9.5
POSC(6)	Least squares	6.4	8.8	10.9	13.2
	Minimax	6.0	8.9	11.0	13.7

Table 5b
(N,Δ)-values for the Bessel problem on [1,10]; 10th-order methods with $[\underline{\omega},\overline{\omega}]=[9.9,10.1]$

Method	Version	100	200	400	800
SC(10)	Conventional	*	*	6.7	9.7
OSC(10)	Least squares	*	*	8.8	11.1
	Minimax	*	*	12.0	14.7
PSC(10)	Conventional	*	8.3	11.6	15.0
POSC(10)	Least squares	*	10.9	11.2	12.1
	Minimax	*	13.3	16.5	19.8

Table 6a
(N,Δ)-values for the Orbit problem on [0,20]; 6th-order methods with $[\underline{\omega},\overline{\omega}]=[0.9,1.1]$

Method	Version	40	80	160	320	640
SC(6)	Conventional	0.4	2.4	5.0	6.8	8.3
OSC(6)	Least squares	1.8	3.6	5.1	6.8	8.6
	Minimax	1.8	3.6	5.1	6.8	8.6
PSC(6)	Conventional	2.5	4.7	6.7	8.8	10.9
POSC(6)	Least squares	3.4	6.1	8.2	10.2	11.5
	Minimax	3.4	6.2	8.1	10.1	12.2

Table 6b
(N, Δ)-values for the Orbit problem on [0,20]; 10th-order methods with $[\underline{\omega}, \overline{\omega}] = [0.9, 1.1]$

Method	Version	40	80	160	320	640
SC(10)	Conventional	*	4.1	7.6	10.1	13.0
OSC(10)	Least squares	*	4.7	3.0	*	*
	Minimax	*	4.7	8.2	10.6	13.5
PSC(10)	Conventional	4.5	9.8	13.0	15.9	18.4
POSC(10)	Least squares	5.4	10.3	*	*	*
	Minimax	5.4	10.8	13.6	16.4	18.8

Table 7a
Problem (3.2): (N, Δ)-values of for 6th-order methods, $[\underline{\omega}, \overline{\omega}] = [1.5, 3.5]$

		$\varepsilon = 0$		$\varepsilon = \frac{1}{10}$		$\varepsilon = \frac{1}{5}$		$\varepsilon = \frac{1}{3}$	
Method	Version	100	200	100	200	100	200	100	200
SC(6)	Conventional	3.4	5.1	3.4	5.2	3.4	5.3	3.4	5.5
OSC(6)	Minimax	4.8	6.5	4.3	6.0	4.0	5.8	3.8	5.7
PSC(6)	Conventional	6.2	8.3	6.1	8.2	6.0	8.1	6.0	8.0
POSC(6)	Minimax	7.1	9.3	7.1	9.2	7.0	9.2	7.2	9.4

Table 7b
Problem (3.2): (N, Δ)-values of 10th-order methods, $[\underline{\omega}, \overline{\omega}] = [1.5, 3.5]$

		$\varepsilon = 0$		$\varepsilon = \frac{1}{10}$		$\varepsilon = \frac{1}{5}$		$\varepsilon = \frac{1}{3}$	
Method	Version	100	200	100	200	100	200	100	200
SC(10)	Conventional	5.3	8.6	0.7	6.6	0.5	6.3	0.4	6.1
OSC(10)	Minimax	9.8	11.3	1.6	6.7	1.4	6.4	1.4	6.1
PSC(10)	Conventional	10.4	13.8	10.3	13.6	10.6	13.5	8.6	13.8
POSC(10)	Minimax	12.5	15.8	10.7	13.9	10.4	13.7	8.6	14.0

3.2. *Effect of perturbing a periodic problem*

In order to see how the performance of the minimax method changes if an ODE with a fully periodic solution is perturbed, we integrated the IVP

$$\begin{aligned} \frac{d^2y}{dt^2} &= -7y + 3z + \varepsilon \sin^3(y - z), \qquad y(0) = \frac{dy(0)}{dt} = 0, \\ & \qquad\qquad 0 \leqslant t \leqslant 10. \\ \frac{d^2z}{dt^2} &= 2y - 6z + \varepsilon \cos^3(y - z), \qquad z(0) = \frac{dz(0)}{dt} = 1, \end{aligned} \tag{3.2}$$

If $\varepsilon = 0$, then the problem is fully periodic with frequencies $\omega_1 = 2$ and $\omega_2 = 3$. However, if $\varepsilon \neq 0$, then additional frequencies are introduced. We now want to know whether the solution is still approximated piecewise by formulas of the form (1.2) with a relatively small frequency band, say $[\underline{\omega}, \overline{\omega}] = [1.5, 3.5]$. Tables 7a and 7b present results for a few values of ε. These figures show that the two OSC methods and the POSC(10) method 'feel' the introduction of additional frequencies

Table 8
Orbit Problem on [0,20]: (N, Δ)-values for various frequency intervals

Method	Version	40	80	160	320	640
PSC(6)	Conventional	2.5	4.7	6.7	8.8	10.9
POSC(6)	Minimax [0.7,0.9]	3.8	5.7	7.7	9.8	11.9
	Minimax [0.9,1.1]	3.4	6.2	8.1	10.1	12.2
	Minimax [1.5,1.7]	2.1	4.3	6.3	8.4	10.5

as ε increases (the POSC(6) method seems to be insensitive). Apparently, frequencies outside the interval [1.5, 3.5] play a role. Futhermore, like the Orbit problem, these 'outside' frequencies play a more dominant role in the high-accuracy range.

(iv) The minimax approach is more effective in the lower-accuracy range.

3.3. *Influence of wrong frequency estimates*

Suppose that we apply the oscillatory methods with a wrong estimate of the frequency interval for the dominating frequencies. For example, let us compare the results for the orbit problem when integrated with the correct, an underestimated and an overestimated frequency interval. Table 8 confirms our earlier conclusion (see Section 2.3.2):

(v) Underestimation of the interval of dominant frequencies is always better than the conventional approach, whereas overestimation may be worse.

3.4. *Problems with changing frequency*

Next, we consider problems with a changing dominant frequency. One option is to estimate the dominant frequency in each step and to recompute the matrix S. However, this is only justified if the right-hand side function is relatively expensive. If we want to integrate with a fixed S, then we should choose a sufficiently large frequency interval. We illustrate this by means of the nonlinear orbit equation of Fehlberg (cf. [1]):

$$\frac{\mathrm{d}^2y}{\mathrm{d}t^2} = Jy, \qquad J := \begin{pmatrix} -4t^2 & -\dfrac{2}{r(t)} \\ \dfrac{2}{r(t)} & -4t^2 \end{pmatrix}, \qquad r(t) := ||y(t)||_2, \quad \sqrt{\pi/2} \leqslant t \leqslant 10, \tag{3.3}$$

with exact solution $y(t) = (\cos(t^2), \sin(t^2))^{\mathrm{T}}$. This problem has a constant period with respect to the variable t^2, but with respect to t the period is decreasing with t. The decreasing behaviour of the period is also clear from the equation itself. Since $r(t) \approx 1$, it follows from (3.3) that for large values of t the matrix J behaves as a diagonal matrix with diagonal entries $-4t^2$. This indicates that for large t, the frequency behaves as $2t$. Therefore, we applied the oscillatory methods with $[\underline{\omega}, \overline{\omega}] = [2\sqrt{\pi/2}, 20]$. The results are presented in the Tables 9a and 9b from which we conclude:

(vi) Even for larger frequency bands the minimax approach outperforms the conventional approach.

Table 9a
(N, Δ)-values for the Fehlberg problem on $[\sqrt{\pi/2}, 10]$; 6th-order methods with $[\underline{\omega}, \overline{\omega}] = [2\sqrt{\pi/2}, 20]$

Method	Version	160	320	640	1280	2560	5120
SC(6)	Conventional	*	1.7	3.5	5.3	7.2	9.0
OSC(6)	Minimax	1.1	3.0	4.7	6.5	8.3	10.1
PSC(6)	Conventional	2.3	4.2	6.1	8.2	10.3	12.4
POSC(6)	Minimax	3.6	5.5	7.2	9.2	11.3	13.4

Table 9b
(N, Δ)-values for the Fehlberg problem on $[\sqrt{\pi/2}, 10]$; 10th-order methods with $[\underline{\omega}, \overline{\omega}] = [2\sqrt{\pi/2}, 20]$

Method	Version	160	320	640	1280
SC(10)	Conventional	*	3.0	6.0	9.0
OSC(10)	Minimax	*	4.8	7.9	10.7
PSC(10)	Conventional	4.5	7.6	10.9	14.3
POSC(10)	Minimax	5.9	9.0	12.3	15.7

3.5. *Problems with widely spread dominant frequencies*

Finally, we consider the Störmer problem in polar coordinates on the interval [0,0.5] with $u = \pi$ as given in [3, p. 420 (10.11a)]. Piecewise approximation of the solution by formulas of the form (1.2) leads to quite different intervals of dominant frequencies. Hence, the overall frequency band $[\underline{\omega}, \overline{\omega}]$ will be quite large, so that we should not expect a better performance of the oscillatory methods. Surprisingly, the results in Tables 10a and 10b show that for quite arbitrary intervals $[\underline{\omega}, \overline{\omega}]$ the POSC methods are at least competitive with the PSC methods. Thus,

(vii) Even for problems whose solutions possess widely spread frequencies, the oscillatory methods do not perform worse than the conventional methods.

Table 10a
(N, Δ)-values for the Störmer problem on [0, 0.5]; 6th-order methods with various intervals $[\underline{\omega}, \overline{\omega}]$

Method	Version	40	80	160	320	640
PSC(6)	Conventional	0.9	4.6	6.5	8.5	10.5
POSC(6)	Minimax [0,50]	0.9	4.7	6.6	8.5	10.6
	Minimax [0,100]	1.0	5.2	7.1	9.0	11.0
	Minimax [0,200]	1.6	4.4	6.3	8.3	10.3

Table 10b
(N, Δ)-values for the Störmer problem on [0, 0.5]; 10th-order methods with various intervals $[\underline{\omega}, \overline{\omega}]$

Method	Version	40	80	160
PSC(10)	Conventional	0.9	7.0	10.3
POSC(10)	Minimax [0,50]	1.0	7.1	10.4
	Minimax [0,100]	1.0	7.2	10.6
	Minimax [0,200]	0.8	7.5	10.8

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