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Order conditions for ARKN methods solving oscillatory systems ☆

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ABSTRACT

For the perturbed oscillators in one-dimensional case, J.M. Franco designed the so-called *Adapted Runge–Kutta–Nyström* (ARKN) methods and derived the sufficient order conditions as well as the necessary and sufficient order conditions for ARKN methods based on the B-series theory [J.M. Franco, Runge–Kutta–Nyström methods adapted to the numerical integration of perturbed oscillators, Comput. Phys. Comm. 147 (2002) 770–787]. These methods integrate exactly the unperturbed oscillators and are highly efficient when the perturbing function is small. Unfortunately, some critical mistakes have been made in the derivation of order conditions in that paper. On the basis of the results from that paper, Franco extended directly the ARKN methods and the corresponding order conditions to multidimensional case where the perturbed function f does not depend on the first derivative y' [J.M. Franco, New methods for oscillatory systems based on ARKN methods, Appl. Numer. Math. 56 (2006) 1040–1053]. In this paper, we present the order conditions for the ARKN methods for the general multidimensional perturbed oscillators where the perturbed function f may depend on only y or on both y and y'.

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1. Introduction

Oscillatory phenomena are frequently encountered in pure and applied mathematics and in applied sciences such as mechanics, physics, astronomy, and molecular biology and engineering. A lot of theoretical and numerical researches have been done on the modeling and simulation of these oscillations. Among typical topics is the numerical integration of non-stiff second-order initial value problems of the form

$$\begin{cases} y''(t)+\omega^2 y(t) = f(y(t), y'(t)), & t\in[t_0,T],\\ y(t_0)=y_0, \qquad y'(t_0)=y'_0, \end{cases} \tag{1}$$

where the main frequency w may be known or accurately estimated and the perturbing force has the form $f(y,y')=\varepsilon g(y,y')$, with $\varepsilon \ll 1$ a small parameter. In his pioneer and fruitful paper [1], Franco reformed the update of classical Runge–Kutta–Nyström (RKN) methods proposed the so-called ARKN methods (RKN methods adapted to perturbed oscillators (1) as in (3) below) and presented the corresponding order conditions based on the theory of Nyström trees. An advantage of ARKN methods is that their updates take into account the special structure of Eq. (1) brought by the term $\omega^2 y$ so that they naturally integrate the unperturbed problem $y''+\omega^2 y = 0$ exactly. For work following [1] we refer the reader to [2–7]. However, in [1], the order conditions are incorrect so that the direct generalization of ARKN methods from one-dimensional case to multidimensional case in [4] is not reliable. In fact, τ in Theorems 3.2 and 3.3 should be the Nyström tree corresponding to an elementary differential $\mathcal{F}(y,y')$ of the function $\tilde{f}(y,y') := f(y,y')-\omega^2 y$ and not of the function $f(y,y')$. Furthermore, the paper [4] does not explicitly give a general ARKN scheme for systems of perturbed oscillators even though a family of three-stage ARKN-based methods of order 4 for systems are proposed and analyzed.

The purpose of this paper is to give a standard form of the multidimensional ARKN integrators for systems of second order oscillatory equations and to derive the related order conditions in a correct way based on the B-series theory.

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The rest of the paper is organized as follows. In Section 2, we restate the basic idea and order conditions of ARKN methods for one-dimensional oscillatory problems. Section 3 extends these methods to the multidimensional case. The order conditions for multidimensional ARKN methods are derived in Section 4. Section 5 is devoted to conclusions.

2. One-dimensional ARKN methods and the corresponding order conditions

In this section, we briefly review the formulation of ARKN methods for the initial value problem (1) in one-dimensional case. Applying the well-known variation-of-constants formula to Eq. (1) gives the following integral equations

$$\begin{aligned} y(t_n+h) &= \phi_0(\nu^2)y(t_n) + h\phi_1(\nu^2)y'(t_n) + \frac{1}{\omega}\int_{t_n}^{t_n+h}\psi(z)\sin\big(\omega(t_{n+1}-z)\big)\,\mathrm{d}z, \\ y'(t_n+h) &= \phi_0(\nu^2)y'(t_n) - \omega\nu\phi_1(\nu^2)y(t_n) + \int_{t_n}^{t_n+h}\psi(z)\cos\big(\omega(t_{n+1}-z)\big)\,\mathrm{d}z, \end{aligned} \tag{2}$$

where $\nu = h\omega$, $\phi_0(\nu^2) := \cos(\nu)$, $\phi_1(\nu^2) := \frac{\sin(\nu)}{\nu}$ and $\psi(z) := f(y(z), y'(z))$. Approximating the integrals in these equations by some quadrature formulas results in Franco's definition of ARKN methods.

Definition 2.1. An s-stage ARKN method for the numerical integration of the IVP (1) is given by the following scheme

$$\begin{cases} g_i = y_n + hc_i y'_n + h^2\sum_{j=1}^s \bar{a}_{ij}(f(g_j, g'_j) - \omega^2 g_j), \quad i = 1,\dots,s, \\ g'_i = y'_n + h\sum_{j=1}^s a_{ij}(f(g_j, g'_j) - \omega^2 g_j), \quad i = 1,\dots,s, \\ y_{n+1} = \phi_0(\nu^2)y_n + \phi_1(\nu^2)hy'_n + h^2\sum_{i=1}^s \bar{b}_i(\nu^2)f(g_i, g'_i), \\ y'_{n+1} = \phi_0(\nu^2)y'_n - \omega\nu\phi_1(\nu^2)y_n + h\sum_{i=1}^s b_i(\nu^2)f(g_i, g'_i). \end{cases} \tag{3}$$

This scheme can also be expressed in the Butcher tableau as

$$\begin{array}{c|cc} c & A & \bar{A} \\ \hline & b^T(\nu^2) & \bar{b}^T(\nu^2) \end{array} = \begin{array}{c|cccccc} a_{1s} & & & & \bar{a}_{11} & \dots & \bar{a}_{1s} \\ \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ c_s & a_{s1} & \dots & a_{ss} & \bar{a}_{s1} & \dots & \bar{a}_{ss} \\ \hline & b_1(\nu^2) & \dots & b_s(\nu^2) & \bar{b}_1(\nu^2) & \dots & \bar{b}_s(\nu^2) \end{array}.$$

The method (3) has *order* p, if for sufficiently smooth problems (1) the conditions

$$e_{n+1} := y_{n+1} - y(t_n+h) = \mathcal{O}(h^{p+1}) \quad \text{and} \quad e'_{n+1} := y'_{n+1} - y'(t_n+h) = \mathcal{O}(h^{p+1}) \tag{4}$$

are satisfied simultaneously, where $y(t_n+h)$ and $y'(t_n+h)$ are the exact solution of (1) and its derivative at t_n+h, respectively, and y_{n+1} and y'_{n+1} are the one step numerical results obtained by the method from the exact starting values $y_n = y(t_n)$ and $y'_n = y'(t_n)$ (the local assumptions). The paper [7] gives the correct order conditions for ARKN methods as follows.

Theorem 2.1. *The following are sufficient conditions for an ARKN method to be of order p:*

$$\bar{b}(\nu^2)^T\Phi(\tau) = \frac{\rho(\tau)!}{\gamma(\tau)}\phi_{\rho(\tau)+1}(\nu^2), \quad \rho(\tau) = 1,\dots,p-1, \tag{5}$$

$$b(\nu^2)^T\Phi(\tau) = \frac{\rho(\tau)!}{\gamma(\tau)}\phi_{\rho(\tau)}(\nu^2), \quad \rho(\tau) = 1,\dots,p, \tag{6}$$

where τ is the Nyström tree corresponding to an elementary differential $\mathcal{F}(y, y')$ of the function $\tilde{f}(y, y') := f(y, y') - \omega^2 y$ at (y_n, y'_n), $\phi_j(\nu^2) = \sum_{k=0}^{\infty}\frac{(-1)^k}{(j+2k)!}\nu^{2k}$, $j = 2, 3, \dots,$ the functions $\rho(\tau)$, $\alpha(\tau)$, $\gamma(\tau)$ and $\Phi(\tau)$ are defined in [8].

Theorem 2.2. *An ARKN method is of order p if and only if*

$$\bar{b}(\nu^2)^T\Phi(\tau) - \frac{\rho(\tau)!}{\gamma(\tau)}\phi_{\rho(\tau)+1}(\nu^2) = \mathcal{O}(h^{p-\rho(\tau)}), \quad \rho(\tau) = 1,\dots,p-1, \tag{7}$$

$$b(\nu^2)^T\Phi(\tau) - \frac{\rho(\tau)!}{\gamma(\tau)}\phi_{\rho(\tau)}(\nu^2) = \mathcal{O}(h^{p+1-\rho(\tau)}), \quad \rho(\tau) = 1,\dots,p, \tag{8}$$

where τ is the Nyström tree corresponding to an elementary differential $\mathcal{F}(y, y')$ of the function $\tilde{f}(y, y') := f(y, y') - \omega^2 y$ at (y_n, y'_n).

3. Multidimensional version of ARKN methods

Now we move on to the integration of systems of second order ordinary differential equations in the form

$$\begin{cases} y'' + Ky = f(y(t), y'(t)), \\ y(t_0) = y_0, \\ y'(t_0) = y'_0, \end{cases} \tag{9}$$

where $K \in R^{m\times m}$ is a symmetric positive semi-definite matrix (stiffness matrix) that implicitly contains the main frequencies of the problem, $f(y, y') : R^m \times R^m \to R^m$, $y_0 \in R^m$, $y'_0 \in R^m$. Here we restrict ourselves to the autonomous case for, if $f = f(t, y, y')$ explicitly contains t, we can extend y by one dimension and turn the system equivalently into the following autonomous one

$$\begin{pmatrix} t \\ y \end{pmatrix}'' = -\begin{pmatrix} 0 & 0 \\ 0 & K \end{pmatrix}\begin{pmatrix} t \\ y \end{pmatrix} + \begin{pmatrix} 0 \\ f(t, y, y') \end{pmatrix}.$$

This kind of problems usually arise when, for example, the method of lines is applied to linear wave equations, where spatial derivatives are approximated by appropriate finite difference formulas. This converts each partial differential equation (PDE) into a set of coupled linear ordinary differential equations (ODEs) in time. Although the problem (9) is a special case of the general class of second order initial value problems of the form

$$\begin{cases} y'' = g(y, y'), \\ y(t_0) = y_0, \\ y'(t_0) = y'_0 \end{cases} \tag{10}$$

and quite a lot of discussions are available for the integration of (10), most authors are not able to make full use of the special information transpired from Eq. (9). Franco [4] was the first attempt to extend his ARKN methods in [1] for scalar equations to the systems (9) with the perturbed function f not depending on the first derivative y'. But both the order conditions and analysis for stability and phase properties of the methods are based on the one-dimensional theory. This is not satisfactory.

In view of the importance of the algebraic order theory for the construction of ARKN methods, we, instead, present the order conditions of ARKN methods for the system (9) based on the B-series theory. Let

$$u(t) = \left[y(t)^T, y'(t)^T\right]^T, \qquad u_0 = \left[y_0^T, y_0'^T\right]^T,$$
$$G\big(u(t)\big) = \left[0, f\big(u(t)\big)^T\right]^T = \left[0, f\big(y(t)^T, y'(t)\big)^T\right]^T,$$

and

$$W = \begin{pmatrix} O & I_m \\ -K & O \end{pmatrix}.$$

Then the initial value problem (9) can be rewritten in a more compact form as

$$\begin{cases} u'(t) = Wu(t) + G(u(t)), \\ u(t_0) = u_0, \end{cases} \tag{11}$$

which is a system of first order nonhomogeneous differential equations, where W is a $2m \times 2m$ constant matrix. From the well-known variation-of-constants formula, the solution at $t \geqslant t_0$ of system (11) has the form

$$u(t) = \exp\big((t - t_0)W\big)u_0 + \int_{t_0}^{t} \exp\big((t - \xi)W\big)G\big(u(\xi)\big)\,\mathrm{d}\xi. \tag{12}$$

Here and in the sequel, the integral of a matrix function is understood as componentwise. Define

$$\phi_0(K) := \sum_{k=0}^{\infty} \frac{(-1)^k K^k}{(2k)!}, \qquad \phi_1(K) := \sum_{k=0}^{\infty} \frac{(-1)^k K^k}{(2k+1)!}.$$

Then we have the following formulas for the exact solution of the system (9) and its derivative.

Theorem 3.1. *If $K \in R^{m\times m}$ is a symmetric positive semi-definite matrix and $f : R^m \times R^m \to R^m$ is continuous in (9), then the solution of (9) and its derivative satisfy the following equations*

$$\begin{cases} y(t) = \phi_0((t - t_0)^2 K)y_0 + (t - t_0)\phi_1((t - t_0)^2 K)y'_0 + \int_{t_0}^{t} (t - \xi)\phi_1((t - \xi)^2 K)\hat{f}(\xi)\,\mathrm{d}\xi, \\ y'(t) = -(t - t_0)K\phi_1((t - t_0)^2 K)y_0 + \phi_0((t - t_0)^2 K)y'_0 + \int_{t_0}^{t} \phi_0((t - \xi)^2 K)\hat{f}(\xi)\,\mathrm{d}\xi \end{cases} \tag{13}$$

for any real number $t_0, t \in (-\infty, +\infty)$, where $\hat{f}(\xi) = f(y(\xi), y'(\xi))$.

Proof. It is easy to see that

$$W^2=\begin{pmatrix}-K & O\\ O & -K\end{pmatrix},\qquad W^3=\begin{pmatrix}O & -K\\ K^2 & O\end{pmatrix},$$
$$W^4=\begin{pmatrix}K^2 & O\\ O & K^2\end{pmatrix},\qquad W^5=\begin{pmatrix}O & K^2\\ -K^3 & O\end{pmatrix}.$$

An argument by induction yields that for every nonnegative integer k

$$W^k=(-1)^{\lfloor k/2\rfloor}\begin{pmatrix}\frac{1+(-1)^k}{2}K^{\lfloor k/2\rfloor} & \frac{1-(-1)^k}{2}K^{\lfloor k/2\rfloor}\\ -K\frac{1-(-1)^k}{2}K^{\lfloor k/2\rfloor} & \frac{1+(-1)^k}{2}K^{\lfloor k/2\rfloor}\end{pmatrix},$$

where $\lfloor k/2\rfloor$ stands for the integer part of $k/2$. Then

$$\begin{aligned}\exp\big((t-t_0)W\big)&=\begin{pmatrix}I_m-\frac{(t-t_0)^2K}{2!}+\frac{(t-t_0)^4K^2}{4!}+\cdots & (t-t_0)I_m-\frac{(t-t_0)^3K}{3!}+\frac{(t-t_0)^5K^2}{5!}+\cdots\\ -(t-t_0)K+\frac{(t-t_0)^3K^2}{3!}-\frac{(t-t_0)^5K^3}{5!}+\cdots & I_m-\frac{(t-t_0)^2K}{2!}+\frac{(t-t_0)^4K^2}{4!}+\cdots\end{pmatrix}\\ &=\begin{pmatrix}\phi_0((t-t_0)^2K) & (t-t_0)\phi_1((t-t_0)^2K)\\ -(t-t_0)K\phi_1((t-t_0)^2K) & \phi_0((t-t_0)^2K)\end{pmatrix}\end{aligned}$$

and (12) becomes

$$\begin{aligned}\begin{pmatrix}y(t)\\ y'(t)\end{pmatrix}&=\begin{pmatrix}\phi_0((t-t_0)^2K) & (t-t_0)\phi_1((t-t_0)^2K)\\ -(t-t_0)K\phi_1((t-t_0)^2K) & \phi_0((t-t_0)^2K)\end{pmatrix}\begin{pmatrix}y_0\\ y'_0\end{pmatrix}\\ &\quad+\int_{t_0}^{t}\begin{pmatrix}\phi_0((t-\xi)^2K) & (t-\xi)\phi_1((t-\xi)^2K)\\ -(t-\xi)K\phi_1((t-\xi)^2K) & \phi_0((t-\xi)^2K)\end{pmatrix}\begin{pmatrix}0\\ f(y(\xi),y'(\xi))\end{pmatrix}\mathrm{d}\xi\\ &=\begin{pmatrix}\phi_0((t-t_0)^2K)y_0+(t-t_0)\phi_1((t-t_0)^2K)y'_0\\ \phi_0((t-t_0)^2K)y'_0-(t-t_0)K\phi_1((t-t_0)^2K)y_0\end{pmatrix}+\begin{pmatrix}\int_{t_0}^{t}(t-\xi)\phi_1((t-\xi)^2K)\hat f(\xi)\,\mathrm{d}\xi\\ \int_{t_0}^{t}\phi_0((t-\xi)^2K)\hat f(\xi)\,\mathrm{d}\xi\end{pmatrix}.\end{aligned}$$

This is exactly the vector form of (13). The proof is complete. □

Consequently, if $y(t_n)$ and $y'(t_n)$ are prescribed, it follows from (13) that

$$\begin{cases}y(t_n+h)=\phi_0(V)y(t_n)+h\phi_1(V)y'(t_n)+\int_{t_n}^{t_n+h}(t_{n+1}-\xi)\phi_1((t_{n+1}-\xi)^2K)\hat f(\xi)\,\mathrm{d}\xi,\\ y'(t_n+h)=-hK\phi_1(V)y(t_n)+\phi_0(V)y'(t_n)+\int_{t_n}^{t_n+h}\phi_0((t_{n+1}-\xi)^2K)\hat f(\xi)\,\mathrm{d}\xi,\end{cases}\tag{14}$$

where $V=h^2K$. Formulas (14) can also be written as

$$\begin{cases}y(t_n+h)=\phi_0(V)y(t_n)+h\phi_1(V)y'(t_n)+h^2\int_0^1(1-z)\phi_1((1-z)^2V)\hat f(t_n+hz)\,\mathrm{d}z,\\ y'(t_n+h)=-hK\phi_1(V)y(t_n)+\phi_0(V)y'(t_n)+h\int_0^1\phi_0((1-z)^2V)\hat f(t_n+hz)\,\mathrm{d}z\end{cases}\tag{15}$$

according to the change of variable $\xi=t_n+hz$.

In order to obtain a numerical integrator for (9) we approximate the integrals in (15) by some higher order quadrature formulas. This leads to the following family of schemes for the systems of oscillatory second order ordinary differential equations (9).

Definition 3.1. An s-stage ARKN method for numerical integration of the oscillatory system (9) is defined as

$$\begin{cases}Y_i=y_n+hc_iy'_n+h^2\sum_{j=1}^{s}\bar a_{ij}(f(Y_j,Y'_j)-KY_j),\quad i=1,\dots,s,\\ Y'_i=y'_n+h\sum_{j=1}^{s}a_{ij}(f(Y_j,Y'_j)-KY_j),\quad i=1,\dots,s,\\ y_{n+1}=\phi_0(V)y_n+h\phi_1(V)y'_n+h^2\sum_{i=1}^{s}\bar b_i(V)f(Y_i,Y'_i),\\ y'_{n+1}=\phi_0(V)y'_n-hK\phi_1(V)y_n+h\sum_{i=1}^{s}b_i(V)f(Y_i,Y'_i).\end{cases}\tag{16}$$

Here, the weight functions $b_i:V\in\mathbb{R}^{m\times m}\to b_i(V)$ and $\bar b_i:V\in\mathbb{R}^{m\times m}\to\bar b_i(V)$, $i=1,\dots,s$ in the updates are functions of V with $V=h^2K$. The scheme (16) can also be denoted by the Butcher tableau as

$$\begin{array}{c|cc}c & A & \bar A\\ \hline & b^T(V) & \bar b^T(V)\end{array}\;=\;\begin{array}{c|ccc ccc}c_1 & a_{11} & \dots & a_{1s} & \bar a_{11} & \dots & \bar a_{1s}\\ \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots\\ c_s & a_{s1} & \dots & a_{ss} & \bar a_{s1} & \dots & \bar a_{ss}\\ \hline & b_1(V) & \dots & b_s(V) & \bar b_1(V) & \dots & \bar b_s(V)\end{array}.$$

It is convenient to express the equations of (16) in block-matrix notation in terms of Kronecker products

$$\begin{cases} Y = e \otimes y_n + hc \otimes y'_n + h^2(\bar{A} \otimes I_m)(f(Y, Y') - (I_s \otimes K)Y), \\ Y' = e \otimes y'_n + h(A \otimes I_m)(f(Y, Y') - (I_s \otimes K)Y), \\ y_{n+1} = \phi_0(V)y_n + h\phi_1(V)y'_n + h^2\bar{b}^T(V)f(Y, Y'), \\ y'_{n+1} = \phi_0(V)y'_n - hK\phi_1(V)y_n + hb^T(V)f(Y, Y'), \end{cases} \tag{17}$$

where $e = (1, 1, \dots, 1)^T$ is an $s \times 1$ vector, and the block vectors are defined by

$$Y = \begin{bmatrix} Y_1 \\ \vdots \\ Y_s \end{bmatrix}, \qquad Y' = \begin{bmatrix} Y'_1 \\ \vdots \\ Y'_s \end{bmatrix}, \qquad f(Y, Y') = \begin{bmatrix} f(Y_1, Y'_1) \\ \vdots \\ f(Y_s, Y'_s) \end{bmatrix}.$$

In the special case where the perturbed function does not depend on the first derivative y', the ARKN method (16) reduces to

$$\begin{cases} Y_i = y_n + hc_i y'_n + h^2 \sum_{j=1}^s \bar{a}_{ij}(f(Y_j) - KY_j), \quad i = 1, \dots, s, \\ y_{n+1} = \phi_0(V)y_n + h\phi_1(V)y'_n + h^2 \sum_{i=1}^s \bar{b}_i(V)f(Y_i), \\ y'_{n+1} = \phi_0(V)y'_n - hK\phi_1(V)y_n + h\sum_{i=1}^s b_i(V)f(Y_i), \end{cases} \tag{18}$$

which can also be expressed in the Butcher tableau as

$$\begin{array}{c|c} c & \bar{A} \\ \hline & \bar{b}^T(V) \\ \hline & b^T(V) \end{array} \quad = \quad \begin{array}{c|ccc} c_1 & \bar{a}_{11} & \dots & \bar{a}_{1s} \\ \vdots & \vdots & \ddots & \vdots \\ c_s & \bar{a}_{s1} & \dots & \bar{a}_{ss} \\ \hline & \bar{b}_1(V) & \dots & \bar{b}_s(V) \\ \hline & b_1(V) & \dots & b_s(V) \end{array}.$$

As a simple example, the trapezoidal discretization of the integrals in the formulas (15) with a fixed step size h gives

$$\begin{cases} y_{n+1} = \phi_0(V)y_n + h\phi_1(V)y'_n + \frac{1}{2}h^2\phi_1(V)f(t_n, y_n, y'_n), \\ y'_{n+1} = -hK\phi_1(V)y_n + \phi_0(V)y'_n + \frac{1}{2}h(\phi_0(V)f(t_n, y_n, y'_n) + f(t_{n+1}, y_{n+1}, y'_{n+1})). \end{cases} \tag{19}$$

If the perturbed function f does not depend on the first derivative y', formulas (19) reduce to the explicit scheme

$$\begin{cases} y_{n+1} = \phi_0(V)y_n + h\phi_1(V)y'_n + \frac{1}{2}h^2\phi_1(V)f(t_n, y_n), \\ y'_{n+1} = -hK\phi_1(V)y_n + \phi_0(V)y'_n + \frac{1}{2}h(\phi_0(V)f(t_n, y_n) + f(t_{n+1}, y_{n+1})). \end{cases} \tag{20}$$

For a theoretical analysis of formulas (20) and its application to oscillatory systems of differential equations, see Hairer and Lubich [9].

In practical computation, instead of applying the formulas (19) and (20) directly, we take the following schemes

$$\begin{cases} y_{n+1} = Qy_n + hy'_n + \frac{1}{2}h^2 f(t_n, y_n, y'_n), \\ y'_{n+1} = -hKy_n + Qy'_n + \frac{1}{2}h(Qf(t_n, y_n, y'_n) + f(t_{n+1}, y_{n+1}, y'_{n+1})), \end{cases} \tag{21}$$

and

$$\begin{cases} y_{n+1} = Qy_n + hy'_n + \frac{1}{2}h^2 f(t_n, y_n), \\ y'_{n+1} = -hKy_n + Qy'_n + \frac{1}{2}h(Qf(t_n, y_n) + f(t_{n+1}, y_{n+1})), \end{cases} \tag{22}$$

which are obtained by taking the second order and first order truncations of $\phi_0(V)$ and $\phi_1(V)$, respectively, in the formulas (19) and (20), with $Q = I_m - \frac{h^2}{2}K$.

4. Order conditions for multidimensional ARKN methods

The definition of the order of a multidimensional ARKN method is the same in form as Eqs. (4), except that the errors e_{n+1} and e'_{n+1} are understood as vectors.

It is easy to verify that the formulas (19), (20), (21) and (22) are all of order two.

The aim of this section is to present a correct derivation of order conditions for ARKN methods for perturbed oscillators in multidimensional case based on the B-series theory and Nyström trees. For this purpose, we need to move the term Ky in Eq. (9) to the right-hand side of the equation, namely, in the autonomous case, the equation of the problem (9) should be read as $y'' = \tilde{f}(y, y') = f(y, y') - Ky$.

Define the ϕ-functions apart from ϕ_0 and ϕ_1 as follows:

$$\phi_j(K) := \sum_{k=0}^{\infty} \frac{(-1)^k K^k}{(2k+j)!}, \quad j = 2, 3, \dots. \tag{23}$$

Then the asymptotic expansions of the true solution the problems (9) and its derivative in powers of h are given, respectively, by

$$y(t_n+h)=\phi_0(V)y_n+h\phi_1(V)y'_n+\sum_{j=0}^{\infty}h^{j+2}\phi_{j+2}(V)\hat{f}_n^{(j)},$$

$$y'(t_n+h)=\phi_0(V)y'_n-hK\phi_1(V)y_n+\sum_{j=0}^{\infty}h^{j+1}\phi_{j+1}(V)\hat{f}_n^{(j)},$$

where $\hat{f}_n^{(j)}=\frac{\mathrm{d}^j}{\mathrm{d}z^j}\hat{f}_n(z)|_{z=t_n}$ is the j-th derivative of $\hat{f}(z)$ at $z=t_n$. In order to prove the first of the two expansions, we take $t_0=t_n$, $t=t_n+h$ in Eqs. (14), utilize the series expansions of $\hat{f}(\xi)$, ϕ_1 in the integrands to get

$$\begin{aligned}y(t_n+h)&=\phi_0(V)y_n+h\phi_1(V)y'_n+\int_{t_n}^{t_n+h}(t_n+h-\xi)\phi_1\big((t_n+h-\xi)^2K\big)\hat{f}(\xi)\,\mathrm{d}\xi\\&=\phi_0(V)y_n+h\phi_1(V)y'_n+\int_0^1(1-z)h^2\phi_1\big((1-z)^2h^2K\big)\hat{f}(t_n+zh)\,\mathrm{d}z\\&=\phi_0(V)y_n+h\phi_1(V)y'_n+\int_0^1(1-z)\phi_1\big((1-z)^2V\big)\sum_{j=0}^{\infty}\frac{h^{j+2}}{j!}z^j\hat{f}_n^{(j)}\,\mathrm{d}z\\&=\phi_0(V)y_n+h\phi_1(V)y'_n+\sum_{j=0}^{\infty}\sum_{k=0}^{\infty}h^{j+2}(-1)^k\left(\int_0^1\frac{(1-z)^{2k+1}z^j}{(2k+1)!j!}\,\mathrm{d}z\right)V^k\hat{f}_n^{(j)}\\&=\phi_0(V)y_n+h\phi_1(V)y'_n+\sum_{j=0}^{\infty}\sum_{k=0}^{\infty}h^{j+2}(-1)^k\frac{1}{(2k+j+2)!}V^k\hat{f}_n^{(j)}\\&=\phi_0(V)y_n+h\phi_1(V)y'_n+\sum_{j=0}^{\infty}h^{j+2}\phi_{j+2}(V)\hat{f}_n^{(j)}.\end{aligned}$$

Likewise the second expansion is obtained. For $j\geqslant 2$, $\hat{f}_n^{(j)}$ can be expressed by the B-series

$$\hat{f}_n^{(j)}=\big(\tilde{f}(y,y')+Ky\big)^{(j)}\big|_{h=0}=\sum_{\rho(\tau)=j+1}\alpha(\tau)\mathcal{F}(\tau)(y_n,y'_n)+K\sum_{\rho(\tau)=j-1}\alpha(\tau)\mathcal{F}(\tau)(y_n,y'_n),$$

where τ is the Nyström tree associated with an elementary differential $\mathcal{F}(\tau)(y_n,y'_n)$ of the function $\tilde{f}(y,y')=f(y,y')-Ky$ at (y_n,y'_n), the order of τ is denoted by $\rho(\tau)$, and $\alpha(\tau)$ is the number of possible monotonic labellings of τ. Then we have

$$\begin{aligned}y(t_n+h)&=\phi_0(V)y_n+h\phi_1(V)y'_n+\sum_{j=0}^{\infty}h^{j+2}\phi_{j+2}(V)\hat{f}_n^{(j)}\\&=\phi_0(V)y_n+h\phi_1(V)y'_n+\sum_{j=0}^{\infty}h^{j+2}\phi_{j+2}(V)\sum_{\rho(\tau)=j+1}\alpha(\tau)\mathcal{F}(\tau)(y_n,y'_n)\\&\quad+h^2K\phi_2(V)y_n+h^3K\phi_3(V)y'_n+K\sum_{j=2}^{\infty}h^{j+2}\phi_{j+2}(V)\sum_{\rho(\tau)=j-1}\alpha(\tau)\mathcal{F}(\tau)(y_n,y'_n).\end{aligned}$$

On the other hand, we know from [8, II.14] that

$$(Y_i)^{(q+1)}\big|_{h=0}=(q+1)\sum_{\rho(\tau)=q}\gamma(\tau)\sum_{j=1}^{s}\bar{a}_{ij}\Phi_j(\tau)\alpha(\tau)\mathcal{F}(\tau)(y_n,y'_n),$$

where $\gamma(\tau)$ is the density of the Nyström tree τ and $\Phi_j(\tau)$, $j=1,\dots,s$, are weight functions as defined in [8]. Then we expand the numerical solution as

$$\begin{aligned}y_{n+1}&=\phi_0(V)y_n+h\phi_1(V)y'_n+h^2\sum_{i=1}^{s}\bar{b}_i(V)\big(f(Y_i,Y'_i)-KY_i\big)+h^2\sum_{i=1}^{s}\bar{b}_i(V)KY_i\\&=\phi_0(V)y_n+h\phi_1(V)y'_n+\sum_{j=0}^{\infty}\frac{h^{j+2}}{(j+1)!}\sum_{\rho(\tau)=j+1}\gamma(\tau)\big(\Phi(\tau)^T\otimes I_m\big)\bar{b}(V)\alpha(\tau)\mathcal{F}(\tau)(y_n,y'_n)\\&\quad+h^2K\big(e^T\otimes I_m\big)\bar{b}(V)y_n+h^3K\big(c^T\otimes I_m\big)\bar{b}(V)y'_n\\&\quad+K\sum_{j=2}^{\infty}\frac{h^{j+2}}{(j-1)!}\sum_{\rho(\tau)=j-1}\gamma(\tau)\big(\big(\bar{A}\Phi(\tau)\big)^T\otimes I_m\big)\bar{b}(V)\alpha(\tau)\mathcal{F}(\tau)(y_n,y'_n).\end{aligned}$$

Consequently, the local error of y_{n+1} can be expressed by

$$\begin{aligned}
e_{n+1} &= y_{n+1} - y(t_n + h) \\
&= \sum_{j=0}^{\infty} h^{j+2} \sum_{\rho(\tau)=j+1} \left(\frac{\gamma(\tau)}{\rho(\tau)!} \big(\Phi(\tau)^T \otimes I_m\big)\bar{b}(V) - \phi_{\rho(\tau)+1}(V) \right) \alpha(\tau)\mathcal{F}(\tau)(y_n, y'_n) \\
&\quad + h^2 K\big(\big(e^T \otimes I_m\big)\bar{b}(V) - \phi_2(V)\big) y_n + h^3 K\big(\big(c^T \otimes I_m\big)\bar{b}(V) - \phi_3(V)\big) y'_n \\
&\quad + K \sum_{j=2}^{\infty} h^{j+2} \sum_{\rho(\tau)=j-1} \left(\frac{\gamma(\tau)}{\rho(\tau)!} \big(\big(\bar{A}\Phi(\tau)\big)^T \otimes I_m\big)\bar{b}(V) - \phi_{\rho(\tau)+3}(V) \right) \alpha(\tau)\mathcal{F}(\tau)(y_n, y'_n).
\end{aligned}$$

Similarly, we have

$$\begin{aligned}
y'(t_n + h) &= \phi_0(V) y'_n - hK\phi_1(V) y_n + \sum_{j=0}^{\infty} h^{j+1} \phi_{j+1}(V) \sum_{\rho(\tau)=j+1} \alpha(\tau)\mathcal{F}(\tau)(y_n, y'_n) \\
&\quad + hK\phi_1(V) y_n + h^2 K\phi_2(V) y'_n + K \sum_{j=2}^{\infty} h^{j+1} \phi_{j+1}(V) \sum_{\rho(\tau)=j-1} \alpha(\tau)\mathcal{F}(\tau)(y_n, y'_n),
\end{aligned}$$

and

$$\begin{aligned}
y'_{n+1} &= \phi_0(V) y'_n - hK\phi_1(V) y_n + h \sum_{i=1}^{s} b_i(V)\big(f(Y_i, Y'_i) - KY_i\big) + h \sum_{i=1}^{s} b_i(V) K Y_i \\
&= \phi_0(V) y'_n - hK\phi_1(V) y_n + \sum_{j=0}^{\infty} \frac{h^{j+1}}{(j+1)!} \sum_{\rho(\tau)=j+1} \gamma(\tau)\big(\Phi(\tau)^T \otimes I_m\big) b(V) \alpha(\tau)\mathcal{F}(\tau)(y_n, y'_n) \\
&\quad + hK\big(e^T \otimes I_m\big) b(V) y_n + h^2 K\big(c^T \otimes I_m\big) b(V) y'_n \\
&\quad + K \sum_{j=2}^{\infty} \frac{h^{j+1}}{(j-1)!} \sum_{\rho(\tau)=j-1} \gamma(\tau)\big(\big(\bar{A}\Phi(\tau)\big)^T \otimes I_m\big) b(V) \alpha(\tau)\mathcal{F}(\tau)(y_n, y'_n).
\end{aligned}$$

Then we get the local error of y'_{n+1} as

$$\begin{aligned}
e'_{n+1} &= y'_{n+1} - y'(t_n + h) \\
&= \sum_{j=0}^{\infty} h^{j+1} \sum_{\rho(\tau)=j+1} \left(\frac{\gamma(\tau)}{\rho(\tau)!} \big(\Phi(\tau)^T \otimes I_m\big) b(V) - \phi_{\rho(\tau)}(V) \right) \alpha(\tau)\mathcal{F}(\tau)(y_n, y'_n) \\
&\quad + hK\big(\big(e^T \otimes I_m\big) b(V) - \phi_1(V)\big) y_n + V\big(\big(c^T \otimes I_m\big) b(V) - \phi_2(V)\big) y'_n \\
&\quad + K \sum_{j=2}^{\infty} h^{j+1} \sum_{\rho(\tau)=j-1} \left(\frac{\gamma(\tau)}{\rho(\tau)!} \big(\big(\bar{A}\Phi(\tau)\big)^T \otimes I_m\big) b(V) - \phi_{\rho(\tau)+2}(V) \right) \alpha(\tau)\mathcal{F}(\tau)(y_n, y'_n).
\end{aligned}$$

The above analysis proves the following theorem.

Theorem 4.1. *The sufficient conditions for an ARKN method to be of order p are given by*

$$\big(\Phi(\tau)^T \otimes I_m\big)\bar{b}(V) = \frac{\rho(\tau)!}{\gamma(\tau)} \phi_{\rho(\tau)+1}(V), \quad \rho(\tau) = 1, \ldots, p-1, \tag{24}$$

$$\big(\big(\bar{A}\Phi(\tau)\big)^T \otimes I_m\big)\bar{b}(V) = \frac{\rho(\tau)!}{\gamma(\tau)} \phi_{\rho(\tau)+3}(V), \quad \rho(\tau) = 1, \ldots, p-3, \tag{25}$$

$$\big(\Phi(\tau)^T \otimes I_m\big) b(V) = \frac{\rho(\tau)!}{\gamma(\tau)} \phi_{\rho(\tau)}(V), \quad \rho(\tau) = 1, \ldots, p, \tag{26}$$

$$\big(\big(\bar{A}\Phi(\tau)\big)^T \otimes I_m\big) b(V) = \frac{\rho(\tau)!}{\gamma(\tau)} \phi_{\rho(\tau)+2}(V), \quad \rho(\tau) = 1, \ldots, p-2, \tag{27}$$

where τ is the Nyström tree associated with an elementary differential $\mathcal{F}(\tau)(y_n, y'_n)$ of the function $\tilde{f}(y, y') = f(y, y') - Ky$ at (y_n, y'_n).

These conditions can be simplified as follows.

Theorem 4.2. *The conditions (24) of Theorem 4.1 imply conditions (25) and conditions (26) imply conditions (27).*

Proof. Let $\hat{\tau}$ be a Nyström tree of order $\rho(\hat{\tau}) \leqslant p-3$ and denote by τ the Nyström tree of order $\rho(\tau) = \rho(\hat{\tau})+2$ obtained by connecting the root of $\hat{\tau}$ to a meagre vertex and then to a new (fat) root. From the definitions of functions ρ, γ and Φ [8], it follows that

$$\gamma(\tau) = \big(\rho(\hat{\tau})+2\big)\big(\rho(\hat{\tau})+1\big)\gamma(\hat{\tau}), \quad \text{and} \quad \Phi(\tau) = \bar{A}\Phi(\hat{\tau}).$$

The conditions (24) assure that

$$\begin{aligned}
&\big(\big(\bar{A}\Phi(\hat{\tau})\big)^T \otimes I_m\big)\bar{b}(V) - \frac{\rho(\hat{\tau})!}{\gamma(\hat{\tau})}\phi_{\rho(\hat{\tau})+3}(V) \\
&\quad = \big(\big(\bar{A}\Phi(\hat{\tau})\big)^T \otimes I_m\big)\bar{b}(V) - \frac{\rho(\hat{\tau})+2}{\rho(\hat{\tau})+2}\cdot\frac{\rho(\hat{\tau})+1}{\rho(\hat{\tau})+1}\cdot\frac{\rho(\hat{\tau})!}{\gamma(\hat{\tau})}\phi_{\rho(\hat{\tau})+3}(V) \\
&\quad = \big(\Phi(\tau)^T \otimes I_m\big)\bar{b}(V) - \frac{\rho(\tau)!}{\gamma(\tau)}\phi_{\rho(\tau)+1}(V) = 0, \quad \rho(\hat{\tau}) = 1,\ldots,p-3.
\end{aligned}$$

Similarly, conditions (26) can deduce conditions (27). The proof is complete. □

From Theorems 4.1 and 4.2 we arrive at the conclusive theorem of this paper.

Theorem 4.3. *The necessary and sufficient conditions for an ARKN method to be of order* p *are given by*

$$\begin{aligned}
&\big(\Phi(\tau)^T \otimes I_m\big)\bar{b}(V) - \frac{\rho(\tau)!}{\gamma(\tau)}\phi_{\rho(\tau)+1}(V) = \mathcal{O}\big(h^{p-\rho(\tau)}\big), \quad \rho(\tau) = 1,\ldots,p-1, \\
&\big(\Phi(\tau)^T \otimes I_m\big)b(V) - \frac{\rho(\tau)!}{\gamma(\tau)}\phi_{\rho(\tau)}(V) = \mathcal{O}\big(h^{p+1-\rho(\tau)}\big), \quad \rho(\tau) = 1,\ldots,p,
\end{aligned}$$

where τ *is the Nyström tree associated with an elementary differential* $\mathcal{F}(\tau)(y_n, y'_n)$ *of the function* $\tilde{f}(y,y') = f(y,y') - Ky$ *at* (y_n, y'_n).

5. Conclusions and discussions

Sections 3 and 4 successfully generalize Franco's ARKN methods in [1] for scalar perturbed oscillators to oscillatory systems. Unlike the methods proposed by García et al. [10], the multidimensional ARKN methods (16) also share the favorable property that they integrate exactly the unperturbed oscillators $y'' + Ky = 0$ and the coefficients in the update depend on the matrix of principal frequencies. The order conditions have a similar form to those conditions for the classical RKN methods after introducing the ϕ-functions.

Finally, given an ARKN method of order p for the system of oscillatory second order ordinary differential equations (9), we can adopt some variations in actual applications in order to avoid the evaluation of the functions $\phi_0(V)$ and $\phi_1(V)$. We can follow Franco's advice to use in the updates some polynomials $P_0(V^2)$ and $P_1(V^2)$ (for example, the Taylor polynomials of $\phi_0(V)$ and $\phi_1(V)$) in place of the functions $\phi_0(V)$ and $\phi_1(V)$, respectively, with P_0 and P_1 satisfying

$$\phi_0(V) = P_0\big(V^2\big) + \mathcal{O}\big(h^{q+1}\big), \qquad \phi_1(V) = P_1\big(V^2\big) + \mathcal{O}\big(h^q\big), \tag{28}$$

with $V = h^2K$ and $q \geqslant p$ (see [4]). The weight functions $b_i(V)$ and $\bar{b}_i(V)$ should also be replaced by some appropriate orders of truncations of their Taylor series.

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