Two–Step Hybrid Collocation Methods for $y'' = f(x, y)$

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Abstract

We consider a new class of two–step collocation methods for the numerical integration of second order Initial Value Problems having periodic or oscillatory solutions. We describe the constructive technique, discuss the order of the resulting methods and analyse their stability properties.

Keywords: ordinary differential equations, general linear methods, two-step collocation methods, hybrid methods, linear stability analysis.

1 Introduction

It is the purpose of this paper to construct a new class of two–step collocation methods for the numerical integration of second order Initial Value Problems

$$\begin{cases} y'' = f(x, y), \\ y'(x_0) = y_0', \\ y(x_0) = y_0 \end{cases} \tag{1.1}$$

having periodic or oscillatory solutions. Even if (1.1) can be transformed into a first order system of double dimension, the development of numerical methods for its direct integration seems more natural and efficient. One–step collocation methods for the problem (1.1) already appeared in the literature (see for instance [3, 11, 18]). Two–step collocation methods for first order ODEs have already been considered in [7, 12], but not yet in the context of special second order ODEs. In the construction of two–step collocation methods for this type of problems, different possibilities can be taken into account. First we have to choose if we want to approximate, in addition to the solution in the step points, also the derivative of the solution, as for instance Runge–Kutta–Nyström methods do in the one step case. Then we can use also stage values which are associated to the previous step points, in order to highten the order of the resulting method, without hightening the computational cost too much, as done for instance in [10]. The methods we have considered are of the following type

$$Y_i^{[n]} = u_i y_{n-1} + (1 - u_i) y_n + h^2 \sum_{j=1}^{m} a_{ij} f(x_n + c_j h, Y_j^{[n]}), \tag{1.2}$$

$$y_{n+1} = \theta y_{n-1} + (1 - \theta) y_n + h^2 \sum_{j=1}^{m} w_j f(x_n + c_j h, Y_j^{[n]}). \tag{1.3}$$

They belong to the class of two–step hybrid methods introduced by Coleman in [2]. We derive the parameters of the methods by using a collocation technique based on algebraic polynomials,

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then we handle the study of order and stability properties of the resulting methods. The development of classical collocation methods (i.e. methods based on algebraic polynomials) is the first necessary step in order to construct collocation methods whose collocation function is expressed as linear combination of different functions, e.g. trigonometric polynomials, mixed or exponential basis (see, for instance, [3, 8]).

2 Derivation of methods

We compute the parameters of the methods extending the technique introduced by Hairer and Wanner in [7] in the first order case. In order to derive two–step collocation methods of the form (1.2), (1.3), we compute a polynomial (the so–called *collocation polynomial*) satisfying the following $m+2$ conditions

$$\begin{aligned} P(x_{n-1}) &= y_{n-1}, \qquad P(x_n) = y_n, && (2.1)\\ P''(x_n + c_j h) &= f(x_n + c_j h, P(x_n + c_j h)), \qquad j = 1, \dots, m. && (2.2) \end{aligned}$$

which allow us to derive a polynomial of degree at most $m+1$. We express the collocation polynomial as linear combination of polynomials of degree at most $m+1$:

$$P(x_n + th) = \varphi_1(t) y_{n-1} + \varphi_2(t) y_n + h^2 \sum_{j=1}^{m} \chi_j(t) P''(x_n + c_j h), \tag{2.3}$$

where $t = \frac{x - x_n}{h} \in [0, 1]$. In order to satisfy (2.1), (2.2), we impose the following set of conditions on the basis functions:

$$\begin{array}{ccccc} \varphi_1(-1) = 1, & \varphi_2(-1) = 0, & \chi_j(-1) = 0, & \varphi_1(0) = 0, & \varphi_2(0) = 1, \\ \chi_j(0) = 0, & \varphi_1''(c_i) = 0, & \varphi_2''(c_i) = 0, & \chi_j''(c_i) = \delta_{ij}, & \end{array} \tag{2.4}$$

for $i, j = 1, \dots, m$. The coefficients of the unknown basis functions

$$\{\varphi_1(t),\ \varphi_2(t),\ \chi_j(t),\ j = 1,\ 2,\ \dots,\ m\}$$

are given by the solutions of $m+2$ linear systems having the following coefficient matrix

$$H = \begin{pmatrix} 1 & -1 & 1 & \dots & (-1)^i & \dots & (-1)^{m+1} \\ 1 & 0 & 0 & \dots & 0 & \dots & 0 \\ 0 & 0 & 2 & \dots & i(i-1)c_1^{i-2} & \dots & (m+1)mc_1^{m-1} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 2 & \dots & i(i-1)c_m^{i-2} & \dots & (m+1)mc_m^{m-1} \end{pmatrix},$$

which is a nonsingular matrix (apart for some exceptional values of the collocation abscissa) because of Vandermonde type (see [14]). After computing the basis functions, the class of methods takes the following form

$$\begin{aligned} Y_i^{[n]} &= \varphi_1(c_i) y_{n-1} + \varphi_2(c_i) y_n + h^2 \sum_{j=1}^{m} \chi_j(c_i) P''(x_n + c_j h), && (2.5)\\ y_{n+1} &= \varphi_1(1) y_{n-1} + \varphi_2(1) y_n + h^2 \sum_{j=1}^{m} \chi_j(1) P''(x_n + c_j h). && (2.6) \end{aligned}$$

For brevity we drop the expression of the parameters of the resulting methods. The coefficients of the methods (2.5), (2.6) with number of stages up to 4 can be provided by the authors.

3 Order conditions

We now derive order conditions, by considering $P(x_n+th)$ as an uniform approximation of $y(x_n+th)$ on the whole integration interval.

Theorem 3.1
Assume that the function f is sufficiently smooth. Then the method (2.5), (2.6) has uniform order p if the following conditions are satisfied:

$$1-\varphi_1(t)-\varphi_2(t)=0, \tag{3.1}$$

$$t+\varphi_1(t)=0, \tag{3.2}$$

$$\frac{t^k}{k!}-\varphi_1(t)\frac{(-1)^k}{k!}-\sum_{j=1}^{m}\chi_j(t)\frac{(c_j)^{k-2}}{(k-2)!}=0. \tag{3.3}$$

$k=2,\ldots,p, \quad t\in[0,1]$.

Proof: We consider the local discretization error

$$\xi(x_n+th)=y(x_n+th)-\varphi_1(t)y(x_n-h)-\varphi_2(t)y(x_n)-h^2\sum_{j=1}^{m}\chi_j(t)y''(x_n+c_jh), \tag{3.4}$$

and expand $y(x_n+th)$, $y(x_n-h)$, $y''(x_n+c_jh)$ in Taylor series around the point x_n, obtaining

$$\begin{aligned}\xi(x_n+th) &= y(x_n)+thy'(x_n)+\ldots+\frac{(th)^p}{p!}y^{(p)}(x_n)+\\ &- \varphi_1(t)[y(x_n)-hy'(x_n)+\ldots+\frac{(-1)^ph^p}{p!}y^{(p)}(x_n)]-\varphi_2(t)y(x_n)\\ &- h^2\sum_{j=1}^{m}\chi_j(t)[y''_n+c_jhy'''(x_n)+\ldots+\frac{(c_jh)^{p-2}}{(p-2)!}y^{(p)}(x_n)]+O(h^{p+1}).\end{aligned}$$

We then compare the coefficients of the same power of h, achieving the thesis.

$\diamondsuit$

Theorem 3.1 allows us to prove that every two–step collocation method of the type (2.5), (2.6) has order $p=m$ on the whole integration interval, and this is result is in keeping with [2]. In the context of General Linear Methods [1, 9], the condition (3.1) is the so-called *preconsistency condition*, while the (3.2) is the *consistency condition*. In order to be the method preconsistent and consistent, it must be $\varphi_1(t)=-t$ and $\varphi_2(t)=1+t$, i.e. the methods (1.2), (1.3) exactly fall in the class of Coleman hybrid methods [2], as $\theta=-1$ and $u_i=c_i$, $i=1,...,m$.

4 Linear Stability Analysis

We now examine the linear stability of the obtained methods by using the procedure from [15, 17, 18]. We apply the class of methods (1.2), (1.3), to the test problem

$$y''=-\omega^2y, \qquad \omega\in\mathbf{R}$$

obtaining

$$Y_i^{[n]} = u_iy_{n-1}+(1-u_i)y_n-z^2\sum_{j=1}^{m}a_{ij}Y_j^{[n]}, \tag{4.1}$$

$$y_{n+1} = \theta y_{n-1}+(1-\theta)y_n-z^2\sum_{j=1}^{m}w_jY_j^{[n]}, \tag{4.2}$$

where $z^2 = \omega^2 h^2$. In matrix notation,

$$Y^{[n]} = u y_{n-1} + \widetilde{u} y_n - z^2 A Y^{[n]}, \tag{4.3}$$

$$y_{n+1} = \theta y_{n-1} + (1-\theta) y_n - z^2 w^T Y^{[n]}, \tag{4.4}$$

where $Y^{[n]} = (Y_i^{[n]})_{i=1}^m$, $u = (u_i)_{i=1}^m$, $\widetilde{u} = (1-u_i)_{i=1}^m$, $w = (w_i)_{i=1}^m$, $A = (a_{ij})_{i,j=1}^m$. The following expression for the stage values holds:

$$Y^{[n]} = Q[u y_{n-1} + \widetilde{u} y_n], \tag{4.5}$$

where $Q = [I + z^2 A]^{-1}$ and I is the identity matrix of dimension m. If we substitute this expression in (4.4), the following recurrence relation arises:

$$y_{n+1} = [\theta - z^2 w^T Q u] y_{n-1} + [1 - \theta - z^2 w^T Q \widetilde{u}] y_n, \tag{4.6}$$

that is

$$\begin{bmatrix} y_{n+1} \\ y_n \end{bmatrix} = \begin{bmatrix} M_{11}(z^2) & M_{12}(z^2) \\ 1 & 0 \end{bmatrix} \begin{bmatrix} y_n \\ y_{n-1} \end{bmatrix}, \tag{4.7}$$

where

$$M_{11}(z^2) = 1 - \theta - z^2 w^T Q \widetilde{u}, \qquad M_{12}(z^2) = \theta - z^2 w^T Q u.$$

The so-called stability matrix [17, 18] takes the form

$$M(z^2) = \begin{bmatrix} M_{11}(z^2) & M_{12}(z^2) \\ 1 & 0 \end{bmatrix}. \tag{4.8}$$

From [17, 18], we consider the following definitions.

Definition 1 *$(0, \beta^2)$ is a stability interval for the method (1.2), (1.3) if, for $z^2 \in (0, \beta^2)$, it is*

$$\rho(M(z^2)) < 1,$$

where $\rho(M(z^2))$ is the spectral radius of $M(z^2)$.

Definition 2 *The method (1.2), (1.3) is* **A**–*stable if $(0, \beta^2) = (0, +\infty)$.*

Definition 3 *$(0, H_0^2)$ is a periodicity interval if, for $z^2 \in (0, H_0^2)$ the roots $r_1(z^2)$, $r_2(z^2)$ of the stability polynomial $\pi(\lambda) = \det[M(z^2) - \lambda I]$ are complex conjugate and $|r_1(z^2)| = |r_2(z^2)| = 1$.*

Definition 4 *The method (1.2), (1.3) is* **P**–*stable if its periodicity interval is $(0, +\infty)$.*

According to def. 1, in order to reach A–stability, it must be $\rho(M(z^2)) < 1$, i.e. both the eigenvalues $\lambda_1(z^2)$, $\lambda_2(z^2)$ of $M(z^2)$ must satisty the condition $|\lambda_1(z^2)| < 1$, $|\lambda_2(z^2)| < 1$, for any value of z^2. For $m = 1$, through an analytical study of the stability matrix (4.8), it is possible to prove the following result which characterises A–stable methods.

Theorem 4.1 (One–stage A–stable methods) *For $m = 1$, the method (2.5), (2.6) is A–stable if and only if $c \in (\frac{1}{\sqrt{2}}, 1]$*

Through a numerical search, it is possible to find nonempty periodicity intervals. For instance, in the case $m = 1$, for any $c \in [0, \frac{1}{50})$, the periodicity interval of the resulting methods is $[0, 4]$.

5 Numerical Experiments

The following initial value problem provides an useful illustration of the need of the knowledge of the stability properties in case of stiff systems:

$$y''(t) = \begin{pmatrix} \mu - 2 & 2\mu - 2 \\ 1 - \mu & 1 - 2\mu \end{pmatrix} y(t), \quad y(0) = \begin{pmatrix} 2 \\ -1 \end{pmatrix}, \; y'(0) = \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \tag{5.1}$$

where μ is an arbitrary parameter. The exact solution is $y_1(t) = 2\cos t,\ y_2(t) = -\cos t$, i.e. it is independent on μ. When $\mu = 2500$, then (5.1) is Kramarz's system [11], which is often used in numerical experiments on stiffness in second order ODEs.

The eigenvalues of the coefficient matrix of the system (5.1) are -1 and $-\mu$, so that the analytical solution of the system exhibits the two frequencies 1 and $\sqrt{\mu}$, but the initial conditions eliminate the high frequency component, which corresponds to $\sqrt{\mu}$ when $\mu >> 1$. Notwithstanding this, its presence in the general solution of the system dictates strong restrictions on the choice of the stepsize, so that the system exhibits the phenomenon of *periodic stiffness* [15].

In the usage of a numerical method with constant parameters and having a limited interval of stability $(0, H)$, it is known that the method is stable when $0 < h < \sqrt{H}/\sqrt{\mu}$. As μ increases, the value of h has to be chosen smaller and smaller, to make the computation stable; in this sense the parameter μ is a measure of the stiffness of the system. It is obvious that, for an A–stable method, the choice of the stepsize is governed only by accuracy demands.

Hybrid method, m=1, c=3/4, p=1			
h	fe	cd	ge
0.01	9215	0.6046	0.2485
0.005	18008	0.8930	0.1279
0.0025	33923	1.1877	0.0648
0.00125	61937	1.4856	0.0326
0.000625	109219	1.7850	0.0164
0.0003125	201060	2.0853	0.0082

Hybrid method, m=1, c=1, p=1			
h	fe	cd	ge
0.01	9244	0.4880	0.3250
0.005	18131	0.7723	0.1689
0.0025	34515	1.0649	0.0861
0.00125	64148	1.3617	0.0434
0.000625	115126	1.6606	0.0218
0.0003125	202056	1.9606	0.0109

Radau IIA method, m=1, p=1			
h	fe	cd	ge
0.01	12361	0.4881	0.3250
0.005	24294	0.7724	0.1688
0.0025	46940	1.0650	0.0861
0.00125	88872	1.3617	0.0435
0.000625	165310	1.6606	0.0218
0.0003125	302663	1.9606	0.0109

In the above tables, fe is the counter of function evaluations, cd is the number of correct digits and ge is the norm of the global error in the last step point. The numerical results reveal that two–step collocation methods (2.5), (2.6) show the same behaviour of the indirect collocation Radau IIA method, but with a lower computational cost in a fixed stepsize implementation.

6 Concluding remarks

We have considered the class of collocation methods of the type (2.5), (2.6). As a first step, the collocation function is an algebraic polynomials. It is under development the class of two–

step collocation methods based whose collocation function is expressed as linear combination of trigonometric functions, powers and exponential functions, in order to develop the class of two–step trigonometric collocation, mixed collocation and exponentially-fitted methods [3, 8].

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