Singly diagonally implicit multivalue collocation methods

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***Abstract*—The purpose of this work is to derive a family of multivalue collocation methods for the numerical solution of ordinary differential equations. The methods are characterized by a lower triangular coefficient matrix of the nonlinear system for the computation of the stages, with all equal diagonal entries. Such structure can be exploited in order to obtain an efficient implementation. The constructed methods are A-stable and have a uniform order of convergence.**

***Index Terms*—Multivalue methods, Collocation, General Linear Methods.**

I. Introduction

In this paper, we consider multivalue collocation numerical methods for the solution of Ordinary Differential Equations (ODEs):

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

$f : \mathbb{R}^k \to \mathbb{R}^k$. Such methods have been introduced in [32] and are able to avoid the order reduction phenomenon which typically arises when collocation based Runge-Kutta methods are applied to stiff systems [37]. As a matter of fact, these methods have uniform order of convergence on the whole integration interval together with high stability properties.

Multivalue collocation methods require the solution of mk simultaneous nonlinear equations at each time step, where k is the dimension of system (1) and m is the number of stages. The coefficient matrix of such system is typically a full matrix. With the aim of reducing the computational effort, in [10] multivalue almost collocation methods with a lower triangular coefficient matrix have been introduced. A lower triangular matrix allows to solve the equations in m successive stages, with only a k-dimensional system to be solved at each stage. It is the purpose of this work to construct singly diagonally implicit multivalue collocation based methods, i.e. methods for which the coefficient matrix is lower triangular and all the elements on the diagonal are equal. This structure allows to further decrease the computational cost because, in solving the nonlinear systems by means of Newton-type iterations, it is possible to use repeatedly the stored LU factorization of the Jacobian. This approach hase been expoited in [28] and [7] in the context of two-step almost collocation for ODEs and Volterra Integral Equations, respectively.

Two-step almost collocation methods have been introduced in [23] for the numerical solution of ODEs and are derived from collocation methods by relaxing some interpolation/collocation conditions in order to achieve A-stability together with high uniform order of convergence. Such ideas have been further investigated in [25], [26], [43] for ODEs and in [2], [3], [12], [16], [17] for Volterra integral and integro-differential equations. Two step collocation methods have been also analyzed for the numerical solution of fractional differential equations. General linear methods (GLMs) for the numerical solution of second order differential equations, as well as P-stable methods, have been investigated in [47]. As regards the nonlinear stability properties of GLMs for ODEs, it has beel subject of several papers, see for instance [11], [13], [39], [40].

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II. Multivalue collocation methods

Consider the uniform grid $t_n = t_0 + nh, n = 0, 1, ..., N, Nh = T - t_0$. Collocation methods approximate the solution of (1) by means of a piecewise collocation polynomial:

$$y(t_n + \theta h) \approx P_n(t_n + \theta h), \quad \theta \in [0, 1],$$

with

$$P_n(t_n + \theta h) = \sum_{i=1}^{r} \alpha_i(\theta) y_i^{[n]} + h \sum_{i=1}^{m} \beta_i(\theta) f(P_n(t_n + c_i h)), \tag{2}$$

where $\{\alpha_i(\theta), \beta_j(\theta), i = 1, ..., r, j = 1, ..., m\}$ are functional the basis of the method, and in the following have been chosen as polynomials of degree less or equal to r. We impose the following interpolation conditions:

$$P_n(t_n) = y_1^{[n]}, \quad P_n'(t_n) = y_2^{[n]}, \quad ... \quad P_n^{(r-1)}(t_n) = y_{r-1}^{[n]},$$

and collocation conditions

$$P_n'(t_n + c_i h) = f(P_n(t_n + c_i h)), \quad i = 1, 2, .., m.$$

As a consequence, by using the Nodrdsiek form for the external stages

$$y^{[n]} = \begin{bmatrix} y_1^{[n]} \\ y_2^{[n]} \\ \vdots \\ y_r^{[n]} \end{bmatrix} \approx \begin{bmatrix} y(x_n) \\ hy'(x_n) \\ \vdots \\ h^{r-1}y^{r-1}(x_n) \end{bmatrix}, \qquad (3)$$

multivalue collocation methods can be expressed in the general linear method (GLM) form:

$$\begin{aligned} Y_i^{[n]} &= h\sum_{j=1}^{m} a_{ij} f\left(Y_j^{[n]}\right) + \sum_{j=1}^{r} u_{ij} y_j^{[n-1]}, \quad i = 1,2,...,m, \\ y_i^{[n]} &= h\sum_{j=1}^{m} b_{ij} f\left(Y_j^{[n]}\right) + \sum_{j=1}^{r} v_{ij} y_j^{[n-1]}, \quad i = 1,2,...,r, \end{aligned} \qquad (4)$$

$n = 0, ..., N$, where m is the number of internal stages, r is the number of external stages, $\mathbf{c} = [c_1, c_2, ..., c_m]^T$ is the abscissa vector and the coefficient matrices are:

$$\begin{aligned} \mathbf{A} &= [\beta_j(c_i)]_{i,j=1,...,m} \in \mathbb{R}^{m\times m}, \\ \mathbf{U} &= [\alpha_j(c_i)]_{i=1,...,m, j=1,...,r} \in \mathbb{R}^{m\times r}, \\ \mathbf{B} &= \left[\beta_j^{(i-1)}(1)\right]_{i=1,...,m, j=1,...,r} \in \mathbb{R}^{r\times m}, \\ \mathbf{V} &= \left[\alpha_j^{(i-1)}(1)\right]_{i,j=1,...,r} \in \mathbb{R}^{r\times r}. \end{aligned}$$

We can observe that the polynomial (2) has globally class C^{r-1} while most interpolants based on Runge-Kutta methods only have global C^1 continuity [34]–[36], [41]. Highly continuous interpolants are very useful in many different situations already shown in the existing literature such as scientific visualization [45], functional differential equations with state-dependent delay [38], numerical solution of differential-algebraic equations and nonlinear equations [44], [50], [51], optimal control problems [48], discontinuous initial value problems [35], [49] or, more in general, whenever a smooth dense output is needed [41], [46].

It has been proved in [32] that a multivalue collocation method given by the approximation $P_n(t_n + \theta h)$ in (2), is an approximation of uniform order p to the solution of problem (1) if and only if the polynomials $\alpha_i(\theta)$ and $\beta_j(\theta)$ in (2) are computed in according to the following conditions:

$$\alpha_1(\theta) = 1 \qquad (5)$$

$$\frac{\theta^\nu}{\nu!} - \alpha_{\nu+1}(\theta) - \sum_{i=1}^{m} \frac{c_i^{\nu-1}}{(\nu-1)!}\beta_i(\theta) = 0, \quad \nu = 1, ..., r-1, \qquad (6)$$

$$\frac{\theta^\nu}{\nu!} - \sum_{i=1}^{m} \frac{c_i^{\nu-1}}{(\nu-1)!}\beta_i(\theta) = 0, \quad \nu = r, ..., p. \qquad (7)$$

The uniform order of convergence for a multivalue collocation method (2) is $m+r-1$ and, in order to obtain A-stability the constraint $r \leq m+1$ must be fulfilled.

We can write order conditions in (5)-(7) in an equivalent discrete form:

$$\begin{gathered} \alpha_j(0) = \delta_{j1}, \ \alpha_j^{(\nu)}(0) = \delta_{j,\nu+1}, \qquad (8) \\ j = 1,2,...,r, \quad \nu = 1,2,...,r-1, \end{gathered}$$

$$\beta_j(0) = \beta_j^{(\nu)}(0) = 0, \quad j = 1,2,...,m, \quad \nu = 1,2,...,r-1, \qquad (9)$$

$$\alpha_j'(c_i) = 0, \quad i = 1,2,...,r, \quad j = 1,2,...,m, \qquad (10)$$

$$\beta_j'(c_i) = \delta_{ij}, \quad i,j = 1,2,...,m, \qquad (11)$$

being δ_{ij} the usual Kronecker delta.

III. Construction of methods

With the aim of constructing methods having singly lower triangular coefficient matrix $\mathbf{A}$, as discussed in [10], we will derive multivalue almost collocation methods, by relaxing some of the conditions (5)-(7). In order to obtain this structured matrix, the functional basis $\{\beta_j(\theta), j = 1, ..., m\}$ must satisfy $\beta_j(c_i) = 0$ for $i > j$, so:

$$\beta_j(\theta) = \omega_j(\theta)\prod_{k=1}^{j-1}(\theta - c_k), \quad j = 1, ..., m, \qquad (12)$$

where $\omega_j(\theta)$ is a polynomial of degree $r - m + 1$:

$$\omega_j(\theta) = \sum_{k=0}^{r-m+1} \mu_k^{(j)}\theta^k, \qquad (13)$$

We want, also, the diagonal elements of the coefficient matrix $\mathbf{A}$ to be the same, so $\beta_1(c_1) = \beta_2(c_2)$.
In the following we will fix $r = m+1$. Moreover, we impose all the conditions (5)-(6) and the parameters $\mu_k^{(j)}$ are free parameters which will be chosen by eventually imposing some of conditions (7) together with A-stability.

The stability matrix of method (4) is

$$\mathbf{M}(z) = \mathbf{V} + z\mathbf{B}(I - z\mathbf{A})^{-1}\mathbf{U}, \qquad (14)$$

where I is the identity matrix in $\mathbb{R}^{m\times m}$.
The method is A-stable if the roots of the stability function:

$$p(\omega, z) = det(\omega I - \mathbf{M}(z)). \qquad (15)$$

are in the unit circle for all $z \in \mathbb{C}$ such that $Re(z) \leq 0$. By the maximum principle, that will happen if the denominator of $p(\omega, z)$ does not have poles in the negative half plane $\mathbb{C}_-$ and if the roots of the $p(\omega, iy)$ are in the unit circle for all $y \in \mathbb{R}$. The last condition can be verified using the Schur criterion [10].

We present an example of A-stable methods with $m = 2$ and $r = 3$, so $\omega_j(\theta)$ are polynomial of degree 2. The order of those methods is 3. So, the collocation polynomial is:

$$\begin{gathered} P_n(t_n + \vartheta h) = y_1^{[n]} + \alpha_2(\vartheta)y_2^{[n]} + \alpha_3(\vartheta)y_3^{[n]} + \\ h\left(\beta_1(\vartheta)f(P(t_n + c_1h)) + \beta_2(\vartheta)f(P(t_n + c_2h))\right). \end{gathered}$$

and the Butcher tableau of the considered methods is the following:

$$\left[\begin{array}{c|c}\mathbf{A} & \mathbf{U} \\ \hline \mathbf{B} & \mathbf{V}\end{array}\right] = \left[\begin{array}{cc|ccc} \beta_1(c_1) & 0 & 1 & \alpha_2(c_1) & \alpha_3(c_1) \\ \beta_2(c_1) & \beta_2(c_2) & 1 & \alpha_2(c_2) & \alpha_3(c_2) \\ \hline \beta_1(1) & \beta_2(1) & 1 & \alpha_2(1) & \alpha_3(1) \\ \beta_1'(1) & \beta_2'(1) & 0 & \alpha_2'(1) & \alpha_3'(1) \\ \beta_1''(1) & \beta_2''(1) & 0 & \alpha_2''(1) & \alpha_3''(1) \end{array}\right]$$

Some values for the free parameters $\mu_k^{(j)}$ have been chosen by imposing the condition (7) for $\nu = r$ and $\beta_1(c_1) = \beta_2(c_2)$

$$\mu_1^{(1)} = -\frac{\mu_0^{(1)}}{c_1} + \frac{c_2^2 \mu_1^{(2)}}{c_1},$$
$$\mu_2^{(1)} = -\frac{1}{3(c_1 - c_2)} - \frac{\mu_0^{(1)}}{c_2^2} - \frac{(c_1 c_2 + c_2^2)\mu_1^{(2)}}{c_1^2},$$
$$\mu_3^{(1)} = -\frac{-2c_1 + c_2}{3c_1^2(c_1 - c_2)} + \frac{\mu_0^{(1)}}{c_1 c_2^2} + \frac{c_2}{c_1^2}\mu_1^{(2)},$$
$$\mu_0^{(2)} = \frac{c_1}{c_2^2}\mu_0^{(1)}, \quad \mu_2^{(2)} = -\frac{c_1}{3(c_1 - c_2)c_2^2} - \frac{c_1}{c_2^4}\mu_0^{(1)} - \frac{\mu_1^{(2)}}{c_2}.$$

The remaining ones have been chosen by performing the Schur analysis of the stability function (15):

$$\mu_0^{(1)} = 0, \quad \mu_1^{(2)} = 0,$$

so

$$\alpha_2(\vartheta) = \frac{\vartheta^3(c_1^2 + c_1 c_2 - c_2^2) - \vartheta^2 c_1^2(c_1 + c_2) + 3\vartheta c_1^2 c_2^2}{3c_1^2 c_2^2},$$

$$\alpha_3(\vartheta) = \frac{2\vartheta^3(c_1 - c_2) + \vartheta^2 c_1(3c_2 - 2c_1)}{6c_1 c_2)},$$

$$\beta_1(\vartheta) = \frac{\vartheta^2(\vartheta(2c_1 - c_2) - c_1^2)}{3c_1^2(c_1 - c_2)},$$

$$\beta_2(\vartheta) = \frac{\vartheta^2 c_1(c_1 - \vartheta)}{3c_2^2(c_1 - c_2)}. \tag{16}$$

Figure 1 shows the region of A-stability in the (c_1, c_2) plane.

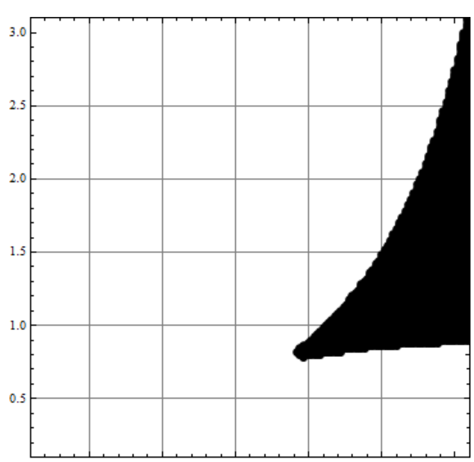

Fig. 1. Region of A-stability in the (c_1, c_2) plane.

As an example, we chose $c_1 = 22/10$ and $c_2 = 9/10$, obtaining:

$$\alpha_2(\vartheta) = \frac{\vartheta\left(15025\vartheta^2 - 37510\vartheta + 29403\right)}{29403},$$

$$\alpha_3(\vartheta) = \frac{\vartheta^2(130\vartheta - 187)}{594},$$

$$\beta_1(\vartheta) = \frac{5}{4719}\vartheta^2(175\vartheta - 242),$$

$$\beta_2(\vartheta) = -\frac{440}{3159}\vartheta^2(5\vartheta - 11).$$

which is the continuous C^2 extension of uniform order $p = 3$ of the A-stable multivalue method:

$$\left[\begin{array}{c|c}\mathbf{A} & \mathbf{U} \\ \hline \mathbf{B} & \mathbf{V}\end{array}\right] =$$

$$= \left[\begin{array}{cc|ccc} \frac{11}{15} & 0 & 1 & \frac{22}{15} & \frac{121}{150} \\ -\frac{351}{4840} & \frac{11}{15} & 1 & \frac{3473}{14520} & -\frac{21}{220} \\ \hline -\frac{335}{4719} & \frac{880}{1053} & 1 & \frac{2306}{9801} & -\frac{19}{198} \\ \frac{205}{4719} & \frac{3080}{3159} & 0 & -\frac{542}{29403} & \frac{8}{297} \\ \frac{2830}{4719} & -\frac{3520}{3159} & 0 & \frac{15130}{29403} & \frac{203}{297} \end{array}\right]$$

IV. Conclusions

In this paper we have derived singly diagonally implicit multivalue almost collocation methods for the numerical solution of ODEs. These method have uniform order of convergence on the whole integration interval, so they do not suffer from order reduction. We have provided examples of A-stable methods with two stages having order 3. Future work will address the construction of methods with diagonal coefficient matrix in order to possibly exploit parallel computation and the application of the same tecnique to other types of problems, such as partial differential equations [4], [27], [30], [31], oscillatory problems [9], [14], [18], [29], [33], [42], integral and fractional equations [1], [2], [5], [6], [8], [19], [20] and stochastic differential equations [15]. In addition, a derivation of algebraically stable high order collocation based multivalue methods [24], the extention to second order problems [22] and the employ of multivalue methods as geometric numerical integrators [21] could be investigate.

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