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A class of implicit peer methods for stiff systems

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ABSTRACT

We present a class of s-stage implicit two step peer methods for the solution of stiff differential equations using the function values from the previous step in addition to the new function values. This allows to increase the order to $p = s$ and to ensure zero-stability straightforwardly. Corresponding s-stage methods for $s \leq 6$ of order $p = s$ with optimal zero stability are presented and their stability is discussed. Under special conditions, we prove that an optimally zero-stable subclass of these methods is superconvergent of order $p = s + 1$ for variable step sizes. Numerical tests and comparison with `ode15s` show the high potential of this class of implicit peer methods.

1. Introduction

Implicit peer methods for the solution of stiff initial value problems

$$y'(t) = f(t, y(t)), \quad t_0 \leq t \leq t_e, \qquad y(t_0) = y_0 \tag{1}$$

where $f : \mathbb{R} \times \mathbb{R}^n \to \mathbb{R}^n$ were introduced in [1] in the form

$$Y_{m,i} = \sum_{j=1}^{s} b_{ij} Y_{m-1,j} + h_m \sum_{j=1}^{i} g_{ij} f(t_{m,j}, Y_{m,j}), \tag{2}$$

where $t_{m,i} = t_m + c_i h_m$. These methods were studied in a series of papers and adapted to special properties like parallelism or application with Krylov techniques for high dimensional problems e.g. [2–8].

Important properties of (2) are the lack of order reduction for very stiff problems and $M(\infty) = 0$, $M(z)$ the stability matrix, implying $L(\alpha)$-stability for $A(\alpha)$-stable methods. On the other hand the order is restricted to $p = s - 1$ and the construction of zero-stable methods is not trivial. By a special strategy in [4] optimally zero-stable methods of order $p = s - 1$ were constructed.

In this paper, we consider s-stage implicit peer methods for stiff differential equations using in addition the function values from the previous step. This implies the loss of $M(\infty) = 0$ but allows to increase the order to $p = s$ and makes the construction of optimally zero-stable methods rather simple. On the other hand the new methods require more memory which can be important when solving large-scale MOL problems. We will consider the following class of peer methods:

$$Y_{m,i} = \sum_{j=1}^{s} b_{ij} Y_{m-1,j} + h_m \sum_{j=1}^{s} a_{ij} f(t_{m-1,j}, Y_{m-1,j}) + h_m \sum_{j=1}^{i} g_{ij} f(t_{m,j}, Y_{m,j}). \tag{3}$$

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Adding also the new stage values would give no additional information, see [9]. The stage solutions $Y_{m,i}$ are approximations to the exact solution $y(t_m + c_i h_m)$, $i = 1, 2, \ldots, s$. We always assume that the nodes c_i are pairwise distinct. The coefficients a_{ij}, b_{ij} and g_{ij} with $g_{ii} = \gamma > 0$ can be collected in matrices $A_m(a_{ij})$, $B_m = (b_{ij})$, $G_m = (g_{ij}) \in \mathbb{R}^{s\times s}$. G_m is a lower triangular matrix, so the methods are diagonally-implicit. If G_m is a diagonal matrix, then we have a parallel peer method [1]. A compact representation of the method (for simplicity for scalar equations) is as follows:

$$Y_m = B_m Y_{m-1} + h_m A_m F(t_{m-1}, Y_{m-1}) + h_m G_m F(t_m, Y_m), \tag{4}$$

where

$$Y_m = \begin{pmatrix} Y_{m,1} \\ Y_{m,2} \\ \vdots \\ Y_{m,s} \end{pmatrix} \in \mathbb{R}^{sn} \qquad F(t_m, Y_m) = \begin{pmatrix} f(t_{m,1}, Y_{m,1}) \\ f(t_{m,2}, Y_{m,2}) \\ \vdots \\ f(t_{m,s}, Y_{m,s}) \end{pmatrix} \in \mathbb{R}^{sn}.$$

Note that the coefficients will depend on the step size ratio $\sigma_m = h_m/h_{m-1}$ in general, in order to get high order methods due to their two-step formulation. Furthermore for the computation of Y_1 we need starting values Y_0.

In Section 2, we derive order conditions and consider stability properties. In Section 3 we prove that a special subclass of methods is superconvergent of order $p = s + 1$ and some special methods for $s = 3, 4, 5, 6$ will be presented in Section 4, their coefficients are given in the Appendix. In Section 5, we will compare our methods with peer methods of the form (2) and with the MATLAB code `ode15s` [10] on test problems from literature.

2. Order conditions and stability

Order conditions can be derived by substituting the exact solution into the method and making a Taylor expansion of the residual Δ_{mi}. We obtain

$$\Delta_{mi} = \Big(1 - \sum_{j=1}^{s} b_{ij}\Big) y(t_m) + \sum_{k=1}^{p} \left(c_i^k - \sum_{j=1}^{s} b_{ij} \frac{(c_j-1)^k}{\sigma_m^k} - k \sum_{j=1}^{s} a_{ij} \frac{(c_j-1)^{k-1}}{\sigma_m^{k-1}} - k \sum_{j=1}^{i} g_{ij} c_j^{k-1} \right) \frac{h_m^k}{k!} y^{(k)}(t_m) + \mathcal{O}(h_m^{p+1}). \tag{5}$$

Definition 1. The implicit peer method (3) is consistent of order p if $\Delta_{mi} = \mathcal{O}(h_m^{p+1})$ for $i = 1, \ldots, s$, for $h_m \to 0$.

Note that in contrast to Runge–Kutta methods the stage order of peer methods is equal to the order of consistency.

From (5) follows

Theorem 1. *If the coefficients of the method (3) satisfy the conditions $AB(l) = 0$ for all $l = 0, \ldots, p$, where*

$$AB_i(l) = c_i^l - \sum_{j=1}^{s} b_{ij} \frac{(c_j-1)^l}{\sigma_m^l} - l \sum_{j=1}^{s} a_{ij} \frac{(c_j-1)^{l-1}}{\sigma_m^{l-1}} - l \sum_{j=1}^{i} g_{ij} c_j^{l-1}, \quad i = 1, \ldots, s, \tag{6}$$

then method (3) is consistent of order p.

Condition $AB(0) = 0$ is the preconsistency condition $B\mathbb{1} = \mathbb{1}$. In the following we will consider constant coefficient matrices B and G. With the notations

$$V_0 = \begin{pmatrix} 1 & c_1 & \cdots & c_1^{s-1} \\ \vdots & \vdots & \ddots & \vdots \\ 1 & c_s & \cdots & c_s^{s-1} \end{pmatrix}, \qquad V_1 = \begin{pmatrix} 1 & \cdots & (c_1-1)^{s-1} \\ \vdots & \ddots & \vdots \\ 1 & \cdots & (c_s-1)^{s-1} \end{pmatrix}$$

and $D = \mathrm{diag}(1, \ldots, s)$, $S_m = \mathrm{diag}(1, \sigma_m, \ldots, \sigma_m^{s-1})$, $C = \mathrm{diag}(c_i)$ we can characterize methods of order $p = s$. From Theorem 1 follows immediately

Corollary 1. *Let c_i be pairwise distinct and B and G be constant matrices. Then method (3) is consistent of order $p = s$ if $B\mathbb{1} = \mathbb{1}$ and*

$$A_m = (CV_0 - GV_0 D) D^{-1} S_m V_1^{-1} - \frac{1}{\sigma_m} B(C - I) V_1 D^{-1} V_1^{-1}. \tag{7}$$