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Search for efficient general linear methods for ordinary differential equations

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ABSTRACT

We analyze implicit general linear methods with s internal stages and $r = s + 1$ external stages of order $p = s + 1$ and stage order $q = s$ or $q = s + 1$. These methods might eventually lead to more efficient formulas than the class of DIMSIMs and the class of general linear methods with inherent Runge–Kutta stability. We analyze also error propagation and estimation of local discretization errors. Examples of such methods which are A- and L-stable are derived up to the stage order $q = 3$ or $q = 4$ and order $p = 4$.

1. Introduction

Consider the initial-value problem for ordinary differential equations (ODEs)

$$y'(t) = f\big(y(t)\big), \qquad y(t_0) = y_0, \tag{1.1}$$

$t \in [t_0, T]$, where the function $f : \mathbb{R}^m \to \mathbb{R}^m$ is sufficiently smooth and $y_0 \in \mathbb{R}^m$ is a given initial value. For the numerical solution of (1.1) we consider the class of general linear methods (GLMs) with s internal stages and r external stages which, on the uniform grid $t_n = t_0 + nh,\ n = 0, 1, \ldots, N,\ Nh = T - t_0$, are defined by

$$\begin{aligned} Y_i^{[n]} &= h\sum_{j=1}^{s} a_{ij} f(Y_j^{[n]}) + \sum_{j=1}^{r} u_{ij} y_j^{[n-1]}, \quad i = 1, 2, \ldots, s, \\ y_i^{[n]} &= h\sum_{j=1}^{s} b_{ij} f(Y_j^{[n]}) + \sum_{j=1}^{r} v_{ij} y_j^{[n-1]}, \quad i = 1, 2, \ldots, r, \end{aligned} \tag{1.2}$$

$n = 1, 2, \ldots, N$. Here $Y_i^{[n]}, i = 1, 2, \ldots, s$, are approximations of stage order q to $y(t_{n-1} + c_i h)$, and $y_i^{[n]}, i = 1, 2, \ldots, r$, are approximations of order p to the linear combinations of the derivatives of y at the grid point t_n. This will be made more precise in the next section.

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The class of GLMs (1.2) include many methods as special cases, compare [1–3]. In particular, these methods include the class of diagonally implicit multistage integration methods (DIMSIMs) introduced in [4] and further investigated in [5–10, 3,11], two-step Runge–Kutta (TSRK) methods introduced in [12] and further investigated in [13–19,3,20–23], peer methods investigated in [24–28], the so-called GLMs with inherent Runge–Kutta stability (IRKS) investigated in [29,30,3,31,32], and GLMs with quadratic stability investigated in [33–36].

Putting

$$Y^{[n]} = \begin{bmatrix} Y_1^{[n]} \\ \vdots \\ Y_s^{[n]} \end{bmatrix}, \qquad f(Y^{[n]}) = \begin{bmatrix} f(Y_1^{[n]}) \\ \vdots \\ f(Y_s^{[n]}) \end{bmatrix}, \qquad y^{[n]} = \begin{bmatrix} y_1^{[n]} \\ \vdots \\ y_r^{[n]} \end{bmatrix},$$

$$\mathbf{A} = \left[a_{ij}\right] \in \mathbb{R}^{s\times s}, \qquad \mathbf{U} = \left[u_{ij}\right] \in \mathbb{R}^{s\times r}, \qquad \mathbf{B} = \left[b_{ij}\right] \in \mathbb{R}^{r\times s}, \qquad \mathbf{V} = \left[v_{ij}\right] \in \mathbb{R}^{r\times r},$$

the method (1.2) can be written in the vector form

$$\begin{aligned} Y^{[n]} &= h(\mathbf{A}\otimes\mathbf{I})f(Y^{[n]}) + (\mathbf{U}\otimes\mathbf{I})y^{[n-1]}, \\ y^{[n]} &= h(\mathbf{B}\otimes\mathbf{I})f(Y^{[n]}) + (\mathbf{V}\otimes\mathbf{I})y^{[n-1]}, \end{aligned} \tag{1.3}$$

$n = 1, 2, \ldots, N$. Here, $\mathbf{I}$ is the identity matrix of dimension m and '$\otimes$' stand for Kronecker product of matrices. This method is characterized by four integers: the order of the method p, the stage order q, the number of external stages r, and the number of internal stages s.

To lower the implementation costs of GLMs (1.3) we will assume that the coefficient matrix $\mathbf{A}$ is lower triangular with the same element $\lambda > 0$ on the diagonal. This corresponds to implicit methods. To guarantee that the GLM (1.3) is zero-stable we will always assume that the coefficient matrix $\mathbf{V}$ has the form

$$\mathbf{V} = \left[\begin{array}{c|c} 1 & v^T \\ \hline 0 & V \end{array}\right],$$

where $v \in \mathbb{R}^{r-1}$ and the matrix $V \in \mathbb{R}^{(r-1)\times(r-1)}$ is strictly upper triangular. Then the spectrum $\sigma(\mathbf{V})$ of the matrix $\mathbf{V}$ is equal to $\sigma(\mathbf{V}) = \{1, 0\}$, where 0 is the eigenvalue of multiplicity $r-1$, and the matrix $\mathbf{V}$ is power-bounded. This is sufficient to guarantee zero-stability of GLM (1.3).

Applying (1.3) to the linear test equation $y' = \xi y,\ t \geq 0,\ \xi \in \mathbb{C}$, leads to the vector recurrence relation $y^{[n]} = \mathbf{M}(z)y^{[n-1]},\ n = 1, 2, \ldots,$ where $z = h\xi$, and $\mathbf{M}(z)$ is the stability matrix defined by $\mathbf{M}(z) = \mathbf{V} + z\mathbf{B}(\mathbf{I} - z\mathbf{A})^{-1}\mathbf{U}$. We also define the stability function $p(w, z)$ of (1.3) as the characteristic polynomial of $\mathbf{M}(z)$, i.e,. $p(w, z) = \det\big(w\mathbf{I} - \mathbf{M}(z)\big)$. This is a rational function and to analyze stability properties of GLMs (1.3) it will be more convenient to work instead with the polynomial $(1 - \lambda z)^s p(w, z)$. This polynomial will be denoted by the same symbol $p(w, z)$. It follows from the structure of the coefficient matrix $\mathbf{V}$ that the stability polynomial $p(w, z)$ has the form:

$$p(w, z) = (1 - \lambda z)^s w^r - p_{r-1}(z)w^{r-1} + \cdots + (-1)^{r-1}p_1(z)w + (-1)^r p_0(z), \tag{1.4}$$

where

$$p_{r-1}(z) = 1 + \sum_{j=1}^{s} p_{r-1,j}z^j \quad \text{and} \quad p_i(z) = \sum_{j=1}^{s} p_{i,j}z^j, \quad i = 0, 1, \ldots, r-2.$$

The coefficients p_{ij} depend on coefficients of the method.

It is the purpose of this paper to analyze implicit GLMs (1.3) with $p = r = s + 1$ and $q = s$ or $q = s + 1$. This choice of p, q, r, and s leads to more efficient GLMs than the formulas investigated before in the literature on the subject, where it was usually assumed that $p = q = r = s$ or $p = q = r - 1 = s - 1$. The former choice corresponds to the class of DIMSIMs investigated in [4–10,3,11], and the latter choice corresponds to GLMs with IRKS investigated in [29,30,3,31,32]. Moreover, the choice $p = r = s + 1$ permits Nordsieck representation of (1.3) which will be discussed in detail in the next section. This representation is convenient in implementation of GLMs (1.3) since it facilitates efficient stepsize and order changing strategies in numerical algorithms based on these methods.

2. Derivation of stage order and order conditions

To formulate stage order and order conditions for the GLM (1.3) we follow the standard approach (compare [4,5,3]) and assume that the components $y_i^{[n-1]}$ of the input vector for the step from t_{n-1} to t_n approximate the linear combinations of the scaled derivatives $h^k y^{(k)}(t_{n-1})$ up to the order $p = s + 1$, i.e.,

$$y_i^{[n-1]} = \sum_{k=0}^{s+1} q_{ik}h^k y^{(k)}(t_{n-1}) + O(h^{s+2}), \tag{2.1}$$