A general framework for the numerical solution of second order ODEs

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Abstract

In this paper the authors consider the family of General Linear Methods (GLMs) for special second order Ordinary Differential Equations (ODEs) of the type $y'' = f(y(t))$, recently introduced with the aim to provide an unifying formulation for numerical methods solving such problems and achieve a general strategy for the analysis of the minimal demandings in terms of accuracy and stability to be asked for, such as consistency, zero-stability and convergence. They emphasize the generality of this approach, by showing that the family of GLMs for second order ODEs recovers classical numerical formulae known in the literature and allows to easily obtain new methods by proving their convergence in a simple, straightforward way.

Keywords: Second order Ordinary Differential Equations, General Linear Methods, Nyström methods, MEBDF methods

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1. Introduction

We focus our attention on the numerical solution of special second order Ordinary Differential Equations (ODEs)

$$\begin{cases} y''(t) = f(y(t)), \quad t \in [t_0, T], \\ y(t_0) = y_0 \in \mathbb{R}^d, \\ y'(t_0) = y'_0 \in \mathbb{R}^d, \end{cases} \tag{1.1}$$

where the function $f : \mathbb{R}^d \to \mathbb{R}^d$ is smooth enough for the Hadamard well-posedness of the differential problem. Problem (1.1) could certainly be trans-

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formed into an equivalent system of first order ODEs, but the consequent augmentation of the dimensionality deters such an approach, in favour of the direct integration of the second order system.

In the recent paper [9], a general framework for the numerical solution of special second order ODE-based problems (1.1) has been introduced. The principal initial aim was that of assessing an unifying formulation for numerical methods solving such problems and provide a general strategy for the analysis of the minimal demandings of accuracy and stability to be asked for, such as consistency, zero-stability and convergence. Following contributions on the topic have been devoted to introducing a general theory to study the order of convergence of such methods [8] and the linear stability properties [10], leading to new examples of P-stable methods improving classical ones.

The main aim of this paper is to effectively use the derived theory, showing that it is a useful tool not only for the analysis of the properties of methods, but also for deriving new methods. First we emphasize the generality of this approach, by showing that the family of GLMs for second order ODEs properly contains many classical numerical formulae known in the literature, and the analysis of their properties can be correctly done through the usage of the developed theory. Moreover we show that it is possible to easily obtain new methods and prove their convergence in a simple way.

The treatise is organized as follows: for the sake of completeness, Section 2 recalls the formulation of GLMs for (1.1) and the notions of consistency, zero-stability and convergence defined in the general setting of GLMs; the representation of classical methods regarded as GLMs is reported in Section 3, and we prove for the first time their convergence properties by employing the GLM machinary. Section 5 is devoted to the introduction and convergence analysis of a new family of methods for the numerical solution of (1.1), which provides the extension of the modified extended BDF formulae introduced by Cash [3, 4, 14] for first order ODEs. Some conclusions are given in Section 5.

2. Basic tools

2.1. Representation of General Linear Methods

In this section, we recall the formulation of GLMs for second order ODEs (1.1) introduced in [9]. To this purpose, we define the following supervectors

$$y^{[n-1]} = \begin{bmatrix} y_1^{[n-1]} \\ y_2^{[n-1]} \\ \vdots \\ y_r^{[n-1]} \end{bmatrix} \in \mathbb{R}^{rd},\ y'^{[n-1]} = \begin{bmatrix} {y'}_1^{[n-1]} \\ {y'}_2^{[n-1]} \\ \vdots \\ {y'}_{r'}^{[n-1]} \end{bmatrix} \in \mathbb{R}^{r'd},\ Y^{[n]} = \begin{bmatrix} Y_1^{[n]} \\ Y_2^{[n]} \\ \vdots \\ Y_s^{[n]} \end{bmatrix} \in \mathbb{R}^{sd}.$$

The vector $y^{[n-1]}$ is denoted as *input vector* of the external stages, and contains all the informations we aim to transfer advancing from point t_{n-1} to t_n of the grid. The vector $y'^{[n-1]}$ involves previous approximations to the first derivative of the solution computed in previous step points, while the values $Y_j^{[n-1]}$, denoted as *internal stage* values, provide an approximation to the solution in the internal points $t_{n-1} + c_j h$, $j = 1, 2, \ldots, s$.

Our formulation of GLMs for second order ODEs then involves nine coefficient matrices $\mathbf{A} \in \mathbb{R}^{\mathbf{s}\times\mathbf{s}}$, $\mathbf{P} \in \mathbb{R}^{\mathbf{s}\times\mathbf{r}'}$, $\mathbf{U} \in \mathbb{R}^{\mathbf{s}\times\mathbf{r}}$, $\mathbf{C} \in \mathbb{R}^{\mathbf{r}'\times\mathbf{s}}$, $\mathbf{R} \in \mathbb{R}^{\mathbf{r}'\times\mathbf{r}'}$, $\mathbf{W} \in \mathbb{R}^{\mathbf{r}'\times\mathbf{r}}$, $\mathbf{B} \in \mathbb{R}^{\mathbf{r}\times\mathbf{s}}$, $\mathbf{Q} \in \mathbb{R}^{\mathbf{r}\times\mathbf{r}'}$, $\mathbf{V} \in \mathbb{R}^{\mathbf{r}\times\mathbf{r}}$, which are put together in the following partitioned $(s + r' + r) \times (s + r' + r)$ matrix

$$\left[\begin{array}{c|c|c} \mathbf{A} & \mathbf{P} & \mathbf{U} \\ \hline \mathbf{C} & \mathbf{R} & \mathbf{W} \\ \hline \mathbf{B} & \mathbf{Q} & \mathbf{V} \end{array}\right], \tag{2.2}$$

which is denoted as the Butcher tableau of the GLM. Using these notations, a GLM for second order ODEs can then be expressed as follows

$$\begin{aligned} Y^{[n]} &= h^2(\mathbf{A} \otimes \mathbf{I})F^{[n]} + h(\mathbf{P} \otimes \mathbf{I})y'^{[n-1]} + (\mathbf{U} \otimes \mathbf{I})y^{[n-1]}, \\ hy'^{[n]} &= h^2(\mathbf{C} \otimes \mathbf{I})F^{[n]} + h(\mathbf{R} \otimes \mathbf{I})y'^{[n-1]} + (\mathbf{W} \otimes \mathbf{I})y^{[n-1]}, \\ y^{[n]} &= h^2(\mathbf{B} \otimes \mathbf{I})F^{[n]} + h(\mathbf{Q} \otimes \mathbf{I})y'^{[n-1]} + (\mathbf{V} \otimes \mathbf{I})y^{[n-1]}, \end{aligned} \tag{2.3}$$

where $\otimes$ denotes the usual Kronecker tensor product, $\mathbf{I}$ is the identity matrix in $\mathbb{R}^{d\times d}$ and $F^{[n]} = [f(Y_1^{[n]}), f(Y_2^{[n]}), \ldots, f(Y_s^{[n]})]^T$.

It is evident from (2.3) that, when the method does not explicitly depend on the first derivative approximations, the matrices $\mathbf{P}, \mathbf{Q}, \mathbf{C}, \mathbf{R}, \mathbf{W}$ do not provide any contribution in the computation of the numerical solution to the problem. In this case, we will always use the reduced tableau

$$\left[\begin{array}{c|c} \mathbf{A} & \mathbf{U} \\ \hline \mathbf{B} & \mathbf{V} \end{array}\right], \tag{2.4}$$

to figure out the *hybrid* formulation

$$\begin{aligned} Y^{[n]} &= h^2(\mathbf{A} \otimes \mathbf{I})F^{[n]} + (\mathbf{U} \otimes \mathbf{I})y^{[n-1]}, \\ y^{[n]} &= h^2(\mathbf{B} \otimes \mathbf{I})F^{[n]} + (\mathbf{V} \otimes \mathbf{I})y^{[n-1]}. \end{aligned} \tag{2.5}$$

2.2. Consistency, stability, convergence

We now recall the basic definitions of consistency, zero-stability and convergence introduced in [9] which, define, as well known in the literature (refer, for instance, to the monographs [2, 13, 17]), the minimal requirements of accuracy and stability for the numerical solution of ODEs.

Definition 2.1. *A GLM (2.3) is preconsistent if there exist vectors* $\mathbf{q}_0$*,* $\mathbf{q_1}$ *and* $\mathbf{q}_1'$ *such that*

$$\mathbf{U}\mathbf{q}_0 = e, \quad \mathbf{W}\mathbf{q}_0 = 0, \quad \mathbf{V}\mathbf{q}_0 = \mathbf{q}_0,$$

$$\mathbf{P}\mathbf{q_1}' + \mathbf{U}\mathbf{q_1} = \mathbf{c}, \quad \mathbf{R}\mathbf{q_1}' + \mathbf{W}\mathbf{q_1} = \mathbf{q_1}', \quad \mathbf{Q}\mathbf{q_1}' + \mathbf{V}\mathbf{q_1} = \mathbf{q}_0 + \mathbf{q_1},$$

where $\mathbf{c}$ *is the vector of nodes associated to* (2.3).

Definition 2.2. *A preconsistent GLM (2.3) is consistent if there exist vectors* $\mathbf{q_2}$ *and* $\mathbf{q_2}'$ *such that*

$$\mathbf{C}e + \mathbf{R}\mathbf{q_2}' + \mathbf{W}\mathbf{q_2} = \mathbf{q_1}' + \mathbf{q_2}', \quad \mathbf{B}e + \mathbf{Q}\mathbf{q_2}' + \mathbf{V}\mathbf{q_2} = \frac{\mathbf{q}_0}{2} + \mathbf{q_1} + \mathbf{q_2}.$$

Definition 2.3. *A GLM (2.3) is zero-stable if there exist two real constants* C *and* D *such that*

$$\|\mathbf{M}_0^m\| \leq mC + D, \quad \forall m = 1, 2, \ldots, \tag{2.6}$$

being $\mathbf{M}_0$ *the block matrix*

$$\mathbf{M}_0 = \begin{bmatrix} \mathbf{R} & \mathbf{W} \\ \mathbf{Q} & \mathbf{V} \end{bmatrix}$$

A criterion equivalent to condition (2.6) is given in the following theorem, contained in [9].

Theorem 2.4.
The following statements are equivalent:

(i) $\mathbf{M}_0$ *satisfies the bound (2.6);*
(ii) the roots of the minimal polynomial of the matrix $\mathbf{M}_0$ *lie on or within the unit circle and the multiplicity of the zeros on the unit circle is at most two;*
(iii) there exist a matrix B *similar to* $\mathbf{M}_0$ *such that*

$$\sup_m \{\|B^m\|_\infty, \ m \geq 1\} \leq m + 1.$$

As usual in the numerical integration of ODEs, consistency and zero-stability are necessary and sufficient conditions for the convergence of the method (for the notion of convergence specialized to GLMs (2.3), again see [9]). This is proved in the following theorem given in [9].

Theorem 2.5. *A GLN method* (2.3) *is convergent if and only if it is consistent and zero-stable.*

3. Classical methods regarded as GLMs

The family of GLMs for second order ODEs properly contains as special cases all the numerical methods for second order ODEs already introduced in the literature. This is made clear in the following examples, where we recast classical families of methods as GLMs.

3.1. Linear multistep methods

Linear multistep methods for second order ODEs [13, 15], defined by

$$y_n = \sum_{j=1}^{k} \alpha_j y_{n-j} + h^2 \sum_{j=0}^{k} \beta_j f(y_{n-j}), \tag{3.7}$$

can be regarded as GLMs with $r = 2k$, $s = 1$, $Y^{[n]} = [y_n]$,

$$y^{[n-1]} = [y_{n-1} \quad y_{n-2} \quad \dots \quad y_{n-k} \quad h^2 f(y_{n-1}) \quad h^2 f(y_{n-2}) \quad \dots \quad h^2 f(y_{n-k})]^T,$$

and in correspondence to the reduced tableau (2.4)

$$\left[\begin{array}{c|c} \mathbf{A} & \mathbf{U} \\ \hline \mathbf{B} & \mathbf{V} \end{array}\right] = \left[\begin{array}{c|cccccccc} \beta_0 & \alpha_1 & \dots & \alpha_{k-1} & \alpha_k & \beta_1 & \dots & \beta_{k-1} & \beta_k \\ \hline \beta_0 & \alpha_1 & \dots & \alpha_{k-1} & \alpha_k & \beta_1 & \dots & \beta_{k-1} & \beta_k \\ 0 & 1 & \dots & 0 & 0 & 0 & \dots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \dots & 1 & 0 & 0 & \dots & 0 & 0 \\ 1 & 0 & \dots & 0 & 0 & 0 & \dots & 0 & 0 \\ 0 & 0 & \dots & 1 & 0 & 1 & \dots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \dots & 1 & 0 & 1 & \dots & 1 & 0 \end{array}\right],$$

with $\mathbf{c} = [1]$. A famous example of linear multistep method is the Numerov method (see, for instance, [13, 16])

$$y_n = 2y_{n-1} - y_{n-2} + h^2 \left(\frac{1}{12} f(t_n, y_n) + \frac{5}{6} f(t_{n-1}, y_{n-1}) + \frac{1}{12} f(t_{n-2}, y_{n-2}) \right), \tag{3.8}$$

which is an order four method corresponding to the GLM with $r = 4$, $s = 1$, $Y^{[n]} = [y_n]$,

$$y^{[n-1]} = \left[y_{n-1} \quad y_{n-2} \quad h^2 f(y_{n-1}) \quad h^2 f(y_{n-2}) \right]^T,$$

and reduced tableau (2.4)

$$
\left[\begin{array}{c|c} \mathbf{A} & \mathbf{U} \\ \hline \mathbf{B} & \mathbf{V} \end{array}\right] = \left[\begin{array}{c|cccc} \frac{1}{12} & 2 & -1 & \frac{5}{6} & \frac{1}{12} \\ \hline \frac{1}{12} & 2 & -1 & \frac{5}{6} & \frac{1}{12} \\ 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \end{array}\right].
$$

3.2. Runge-Kutta-Nyström methods

Runge-Kutta-Nyström methods (see [13])

$$
\begin{aligned}
Y_i &= y_{n-1} + c_i h y_{n-1}' + h^2 \sum_{j=1}^{s} a_{ij} f(Y_j), \quad i = 1, ..., s, \\
h y_n' &= h y_{n-1}' + h^2 \sum_{j=1}^{s} b_j' f(Y_j), \qquad (3.9) \\
y_n &= y_{n-1} + h y_{n-1}' + h^2 \sum_{j=1}^{s} b_j f(Y_j),
\end{aligned}
$$

provide an extension to second order ODEs (1.1) of Runge–Kutta methods (see, for instance, [1, 18]) and involve the dependence on the approximation to the first derivative in the current grid point. Such methods can be recast as GLMs (2.3) with $r = 1$, in correspondence to the tableau (2.2)

$$
\left[\begin{array}{c|c|c} \mathbf{A} & \mathbf{P} & \mathbf{U} \\ \hline \mathbf{C} & \mathbf{R} & \mathbf{W} \\ \hline \mathbf{B} & \mathbf{Q} & \mathbf{V} \end{array}\right] = \left[\begin{array}{c|c|c} A & \mathbf{c} & \mathbf{e} \\ \hline \mathbf{b}'^T & 1 & 0 \\ \hline \mathbf{b}^T & 1 & 1 \end{array}\right],
$$

where $\mathbf{e}$ is the unit vector in $\mathbb{R}^s$, and to the input vectors $y^{[n-1]} = [y_{n-1}]$, $y'^{[n-1]} = [y'_{n-1}]$.

3.3. Coleman hybrid methods

We now consider the following class of methods

$$
\begin{aligned}
Y_i &= (1 + c_i) y_{n-1} - c_i y_{n-2} + h^2 \sum_{j=1}^{s} a_{ij} f(Y_j), \quad i = 1, ..., s, \qquad (3.10) \\
y_n &= 2y_{n-1} - y_{n-2} + h^2 \sum_{j=1}^{s} b_j f(Y_j),
\end{aligned}
$$

introduced by Coleman in [5], which are denoted as two-step hybrid methods. Such methods (3.10) can be regarded as GLMs corresponding to the reduced tableau (2.4)

$$\left[\begin{array}{c|c}\mathbf{A} & \mathbf{U}\\ \hline \mathbf{B} & \mathbf{V}\end{array}\right] = \left[\begin{array}{c|cc} A & \mathbf{e}+\mathbf{c} & -\mathbf{c}\\ \hline \mathbf{b}^T & 2 & -1\\ \mathbf{0} & 1 & 0\end{array}\right]$$

and characterized by the input vector $y^{[n-1]} = [y_{n-1} \quad y_{n-2}]^T$.

3.4. Two-step Runge-Kutta-Nyström methods

Another interesting class of numerical methods for second order ODEs is given by the family of two-step Runge-Kutta-Nyström methods [6]

$$\begin{aligned}
Y_i^{[n-1]} &= y_{n-2} + hc_i y'_{n-2} + h^2 \sum_{j=1}^{s} a_{ij} f(Y_j^{[n-1]}), \quad i = 1, \dots, s,\\
Y_i^{[n]} &= y_{n-1} + hc_i y'_{n-1} + h^2 \sum_{j=1}^{s} a_{ij} f(Y_j^{[n]}), \quad i = 1, \dots, s,\\
hy'_n &= (1-\theta)hy'_{n-1} + \theta h y'_{n-2} + h^2 v'_j f(Y_j^{[n-1]}) + h^2 w'_j f(Y_j^{[n]}), \qquad (3.11)\\
y_n &= (1-\theta)y_{n-1} + \theta y_{n-2} + h\sum_{j=1}^{s} v'_j y'_{n-2} + h\sum_{j=1}^{s} w'_j y'_{n-1}\\
&\quad + h^2 \sum_{j=1}^{s} v_j f(Y_j^{[n-1]}) + h^2 \sum_{j=1}^{s} w_j f(Y_j^{[n]}).
\end{aligned}$$

Such methods depend on two consecutive approximations to the solution and its first derivative in the grid points, but also on two consecutive approximations to the stage values (i.e. the ones related to the points $t_{n-2} + c_i h$ and the ones corresponding to the points $t_{n-1} + c_i h$, $i = 1, 2, \dots, s$). Two-step Runge-Kutta-Nyström methods can be represented as GLMs (2.3) with $r = s + 2$ and $r' = 2$ through the tableau (2.2)

$$\left[\begin{array}{c|c|c}\mathbf{A} & \mathbf{P} & \mathbf{U}\\ \hline \mathbf{C} & \mathbf{R} & \mathbf{W}\\ \hline \mathbf{B} & \mathbf{Q} & \mathbf{V}\end{array}\right] = \left[\begin{array}{c|cc|ccc} A & \mathbf{c} & \mathbf{0} & \mathbf{e} & \mathbf{0} & \mathbf{0}\\ \hline \mathbf{w}'^T & (1-\theta) & \theta & 0 & 0 & \mathbf{v}'^T\\ \mathbf{0} & 1 & 0 & 0 & 0 & \mathbf{0}\\ \hline \mathbf{w}^T & \mathbf{w}'^T\mathbf{e} & \mathbf{v}'^T\mathbf{e} & (1-\theta) & \theta & \mathbf{v}^T\\ \mathbf{0} & 0 & 0 & 1 & 0 & \mathbf{0}\\ \mathbf{I} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0}\end{array}\right],$$

in correspondence of the input vectors $y^{[n-1]} = [y_{n-1} \quad y_{n-2} \quad h^2 f(Y^{[n-1]})]^T$, $y'^{[n-1]} = [y'_{n-1} \quad y'_{n-2}]^T$.

The usage of previous stage values has also been used in the context of Parallel-Iterated Pseudo Two-Step Runge-Kutta-Nyström methods

$$\begin{aligned}
V_n &= y_{n-1}\mathbf{e}_v + hy'_{n-1}c_v + h^2\mathbf{A}_{vv}f(V_{n-1}) + h^2\mathbf{A}_{vw}f(W_{n-1}),\\
W_n &= y_{n-1}\mathbf{e}_w + hy'_{n-1}c_w + h^2\mathbf{A}_{wv}f(V_n) + h^2\mathbf{A}_{ww}f(W_n),\\
hy'_n &= hy'_{n-1} + h^2\mathbf{d}_v^T f(V_n) + h^2\mathbf{d}_w^T f(W_n),\\
y_n &= y_{n-1} + hy'_{n-1} + h^2\mathbf{b}_v^T f(V_n) + h^2\mathbf{b}_w^T f(W_n),
\end{aligned}$$

introduced by Cong [7]. Also these methods can be reformulated as GLMs with $r = 2s + 1$ and $r' = 1$, in correspondence to the tableau (2.2)

$$\left[\begin{array}{c|c|c} \mathbf{A} & \mathbf{P} & \mathbf{U} \\ \hline \mathbf{C} & \mathbf{R} & \mathbf{W} \\ \hline \mathbf{B} & \mathbf{Q} & \mathbf{V} \end{array}\right] = \left[\begin{array}{cc|c|ccc} \mathbf{0} & \mathbf{0} & \mathbf{c}_v & \mathbf{e}_v & \mathbf{A}_{vv} & \mathbf{A}_{vw} \\ \mathbf{A}_{wv} & \mathbf{A}_{ww} & \mathbf{c}_w & \mathbf{e}_w & \mathbf{0} & \mathbf{0} \\ \hline \mathbf{d}_v^T & \mathbf{d}_w^T & 1 & \mathbf{0} & \mathbf{0} & 0 \\ \hline \mathbf{b}_v^T & \mathbf{b}_w^T & 1 & 1 & \mathbf{0} & \mathbf{0} \\ \mathbf{I} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{I} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \end{array}\right],$$

and the vectors $Y^{[n]} = [V_n \quad W_n]^T$, $y^{[n-1]} = [y_{n-1} \quad h^2 f(V_{n-1}) \quad h^2 f(W_{n-1})]^T$ and $y'^{[n-1]} = [y'_{n-1}]$.

3.5. Recovering the convergence of classical methods

Using the GLM formalism, according to the definitions recalled in Section 2, we can easily prove consistency, zero-stability and thus convergence of the classical numerical methods considered in Sections 3.1, 3.2, 3.3 and 3.4.

- The Numerov method (3.8) is consistent with preconsistency and consistency vectors

  $$\mathbf{q}_0 = [1 \quad 1 \quad 0 \quad 0]^T, \quad \mathbf{q_1} = [0 \quad -1 \quad 0 \quad 0]^T, \quad \mathbf{q_2} = [0 \quad 1/2 \quad 1 \quad 1]^T.$$

  The minimal polynomial associated to the zero-stability matrix of the Numerov method (3.8) is

  $$p(\lambda) = \lambda^2(\lambda - 1)^2,$$

  which satisfies the requirement (*ii*) in Theorem 2.4, i.e. the Numerov method is zero-stable;

- in the case of Runge–Kutta–Nyström methods (3.9), preconsistency and consistency vectors assume the forms

$$\mathbf{q}_0 = [1], \quad \mathbf{q_1} = \mathbf{q_2} = [0], \quad \mathbf{q}'_1 = [1], \quad \mathbf{q}'_2 = [0],$$

  and the minimal polynomial of the zero-stability matrix is

$$p(\lambda) = (\lambda - 1)^2,$$

  which satisfies the requirement (ii) in Theorem 2.4;

- Coleman hybrid methods (3.10) are consistent with preconsistency and consistency vectors

$$\mathbf{q}_0 = [1 \quad 1]^T, \quad \mathbf{q_1} = [0 \quad -1]^T, \quad \mathbf{q_2} = [0 \quad 1/2]^T.$$

  Moreover, the minimal polynomial associated to their zero-stability is

$$p(\lambda) = (\lambda - 1)^2,$$

  then they provide a family of zero-stable methods;

- two-step Runge–Kutta–Nyström methods (3.11) are consistent with preconsistency and consistency vectors

$$\begin{aligned}
\mathbf{q}_0 &= [1 \quad 1 \quad 0 \quad \dots \quad 0 \quad 0]^T \in \mathbb{R}^{s+2},\\
\mathbf{q_1} &= [0 \quad -1 \quad 0 \quad \dots \quad 0 \quad 0]^T \in \mathbb{R}^{s+2},\\
\mathbf{q_2} &= [0 \quad 1/2 \quad 1 \quad \dots \quad 1 \quad 1]^T \in \mathbb{R}^{s+2},\\
\mathbf{q_1}' &= [1 \quad 1]^T, \quad \mathbf{q_2}' = [0 \ -1]^T.
\end{aligned}$$

  The minimal polynomial of their zero-stability matrix is

$$p(\lambda) = \lambda^2(\lambda^2 - (1 - \theta)\lambda - \theta)$$

  and, therefore, such methods are zero-stable if and only if $-1 < \theta \leq 1$: this restriction on θ recovers the classical result on the zero-stability of two-step Runge–Kutta–Nyström methods (refer to [19]).

4. Modified extended BDF formulae for second order ODEs

Having a general theory for the analysis of the convergence of numerical methods for second order ODEs (1.1) makes life easier when new methods are aimed to be introduced, reducing the proof of convergence to the verification of simple algebraic properties on the coefficients of the methods. Let us analyse this aspect in concrete, by introducing a new family of numerical methods for (1.1) through the GLM machinary. The class of methods we introduce is the family of modified extended backward differentiation formulae (MEBDF) introduced by Cash for the numerical solution of first order ODEs [3, 4, 14]. Such formulae provides improvement to the stability regions of the classical BDF methods and are characterized by the involvement of the knowledge of the solution in a future point. The first introduced modification regards the so-called extended BDF (EBDF) methods of order $p = k + 1$

$$\sum_{j=0}^{k} \alpha_j y_{n+j} = h\beta_k f_{n+k} + h\beta_{k+1} f_{n+k+1}, \tag{4.12}$$

where $f_{n+k} = f(t_{n+k}, y_{n+k})$, $f_{n+k+1} = f(t_{n+k+1}, y_{n+k+1})$. This numerical method is employed as corrector in a predictor corrector scheme which can be summarized as follows:
(i) Compute $\bar{y}_{n+k}$ as the solution of the conventional BDF method

$$\bar{y}_{n+k} + \sum_{j=0}^{k-1} \hat{\alpha}_j y_{n+j} = h\hat{\beta}_k \bar{f}_{n+k}, \tag{4.13}$$

$\bar{f}_{n+k} = f(t_{n+k}, \bar{y}_{n+k})$.
(ii) Compute $\bar{y}_{n+k+1}$ as the solution of the same BDF advanced one step, that is,

$$\bar{y}_{n+k+1} + \hat{\alpha}_{k-1}\bar{y}_{n+k} + \sum_{j=0}^{k-2} \hat{\alpha}_j y_{n+j+1} = h\hat{\beta}_k \bar{f}_{n+k+1}, \tag{4.14}$$

$\bar{f}_{n+k+1} = f(t_{n+k+1}, \bar{y}_{n+k+1})$.
(iii) Discard $\bar{y}_{n+k}$, insert $\bar{f}_{n+k+1}$ into EBDF method (4.12), and solve for y_{n+k}:

$$y_{n+k} + \sum_{j=0}^{k-1} \alpha_j y_{n+j} = h\beta_k f_{n+k} + h\beta_{k+1} \bar{f}_{n+k+1}. \tag{4.15}$$

If the EBDF method (4.12) is of order $k + 1$ and BDF methods (4.13) and (4.14) are of order k, then the overall algorithm (i)-(iii) based on (4.13), (4.14), and (4.15) is of order $k + 1$, as proved in [3].

It was observed by Cash [4] that the disadvantage of the algorithm given above is that stages (i) and (ii) represent nonlinear systems with the same Jacobian $I - h\hat{\beta}_k J$, $J = \partial f/\partial y$, but stage (iii) has a different Jacobian, $I - h\beta_k J$, which requires extra LU decomposition. To remedy this situation, he proposed in [4] an algorithm where the last stage (iii) was replaced by a modified EBDF (MEBDF) method of the form

$$\sum_{j=0}^{k} \alpha_j y_{n+j} = h\hat{\beta}_k f_{n+k} + h(\beta_k - \hat{\beta}_k)\bar{f}_{n+k} + h\beta_{k+1}\bar{f}_{n+k+1}. \tag{4.16}$$

These methods have order $k+1$.

Substituting (4.13) into (4.14), we obtain

$$\bar{y}_{n+k+1} = \hat{\alpha}_{k-1}\hat{\alpha}_0 y_n + \sum_{j=1}^{k-1} \big(\hat{\alpha}_{k-1}\hat{\alpha}_j - \hat{\alpha}_{j-1}\big) y_{n+j} - h\hat{\alpha}_{k-1}\hat{\beta}_k \bar{f}_{n+k} + h\hat{\beta}_k \bar{f}_{n+k+1}. \tag{4.17}$$

Our aim, which is a novelty provided by this paper, is now that of performing a similar numerical scheme for second order ODEs (1.1), which can be summarized as follows

(i) Compute $\bar{y}_{n+k}$ by the following predictor method

$$\bar{y}_{n+k} + \sum_{j=0}^{k-1} \hat{\alpha}_j y_{n+j} = h^2\hat{\beta}_k \bar{f}_{n+k}, \qquad \bar{f}_{n+k} = f(t_{n+k}, \bar{y}_{n+k}). \tag{4.18}$$

(ii) Compute $\bar{y}_{n+k+1}$ as the solution of the same predictor, advanced one step

$$\bar{y}_{n+k+1} + \hat{\alpha}_{k-1}\bar{y}_{n+k} + \sum_{j=0}^{k-2} \hat{\alpha}_j y_{n+j+1} = h^2\hat{\beta}_k \bar{f}_{n+k+1}. \tag{4.19}$$

(iii) Employ the following corrector:

$$\sum_{j=0}^{k} \alpha_j y_{n+j} = h^2\hat{\beta}_k f_{n+k} + h^2(\beta_k - \hat{\beta}_k)\bar{f}_{n+k} + h^2\beta_{k+1}\bar{f}_{n+k+1}. \tag{4.20}$$

Following Jackiewicz [17], we regard the numerical scheme based on the formulae (4.18), (4.19), and (4.20) as a GLM in hybrid form (2.5) with $s = 3$, $r = k$, and with the vectors of internal approximations $Y^{[n]}$, $f(Y^{[n]})$, and the vector of external approximations $y^{[n]}$ defined by

$$Y^{[n]} = \begin{bmatrix} \bar{y}_{n+k} \\ \bar{y}_{n+k+1} \\ y_{n+k} \end{bmatrix}, \quad f(Y^{[n]}) = \begin{bmatrix} \bar{f}_{n+k} \\ \bar{f}_{n+k+1} \\ f_{n+k} \end{bmatrix}, \quad y^{[n]} = \begin{bmatrix} y_{n+k} \\ y_{n+k-1} \\ \vdots \\ y_{n+1} \end{bmatrix}, \tag{4.21}$$

and with the coefficient matrices **A**, **U**, **B**, and **V** given by

$$\mathbf{A} = \begin{bmatrix} \hat{\beta}_k & 0 & 0 \\ -\hat{\alpha}_{k-1}\hat{\beta}_k & \hat{\beta}_k & 0 \\ \beta_k - \hat{\beta}_k & \beta_{k+1} & \hat{\beta}_k \end{bmatrix},$$

$$\mathbf{U} = \begin{bmatrix} -\hat{\alpha}_{k-1} & -\hat{\alpha}_{k-2} & \cdots & -\hat{\alpha}_1 & -\hat{\alpha}_0 \\ \hat{\alpha}_{k-1}\hat{\alpha}_{k-1}-\hat{\alpha}_{k-2} & \hat{\alpha}_{k-1}\hat{\alpha}_{k-2}-\hat{\alpha}_{k-3} & \cdots & \hat{\alpha}_{k-1}\hat{\alpha}_1-\hat{\alpha}_0 & \hat{\alpha}_{k-1}\hat{\alpha}_0 \\ -\alpha_{k-1} & -\alpha_{k-2} & \cdots & -\alpha_1 & -\alpha_0 \end{bmatrix},$$

$$\mathbf{B} = \begin{bmatrix} \beta_k - \hat{\beta}_k & \beta_{k+1} & \hat{\beta}_k \\ 0 & 0 & 0 \\ \vdots & \vdots & \vdots \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \ \mathbf{V} = \begin{bmatrix} -\alpha_{k-1} & -\alpha_{k-2} & \cdots & -\alpha_1 & -\alpha_0 \\ 1 & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & \cdots & 1 & 0 \end{bmatrix}.$$

We first analyze the consistency of the numerical scheme, provided by the following theorem.

Theorem 4.1. *A k-step MEBDF method for second order ODEs* (1.1)*, based on the predictor-corrector scheme corresponding to the formulae (4.18), (4.19), and (4.20), is consistent if and only if the following algebraic constraints are* *fulfilled*

$$\sum_{j=0}^{k-1} \hat{\alpha}_j = -1, \tag{4.22}$$

$$\sum_{j=0}^{k-2} \hat{\alpha}_j - \hat{\alpha}_{j+1}\hat{\alpha}_{k-1} = 1 - \hat{\alpha}_{k-1}\alpha_0, \tag{4.23}$$

$$\sum_{j=0}^{k-1} \alpha_j = -1, \tag{4.24}$$

$$\sum_{j=0}^{k-2} (j-k+1)\hat{\alpha}_j = -c_1, \tag{4.25}$$

$$\sum_{j=0}^{k-2} (j-k+1)(\hat{\alpha}_j - \hat{\alpha}_{j+1}\hat{\alpha}_{k-1}) = -c_2, \tag{4.26}$$

$$\sum_{j=0}^{k-1} (j-k+1)\alpha_j = -c_3, \tag{4.27}$$

$$2\beta_k + 2\beta_{k+1} + \sum_{j=0}^{k-1} (j-k+1)\alpha_j = 1. \tag{4.28}$$

Proof. Due to the form (4.21) of the external approximation vector, we easily recognize the following preconsistency and consistency vectors associated to the method

$$q_0 = e, \qquad q_1 = \begin{bmatrix} 0 \\ -1 \\ \vdots \\ -(k-1) \end{bmatrix}, \qquad q_2 = \begin{bmatrix} 0 \\ \frac{1}{2} \\ \vdots \\ \frac{k-1}{2} \end{bmatrix}.$$

Thus, taking into account the above provided GLM formulation of MEBDF methods and Definitions 2.1 and 2.2 of preconsistency and consistency, we get Equations (4.22) to (4.24) from $\mathbf{U}\mathbf{q}_0 = e$ and $\mathbf{V}\mathbf{q}_0 = \mathbf{q}_0$, (4.25) to (4.27) from $\mathbf{U}\mathbf{q_1} = \mathbf{c}$ and $\mathbf{V}\mathbf{q_1} = \mathbf{q}_0 + \mathbf{q_1}$, (4.28) from $\mathbf{B}e + \mathbf{V}\mathbf{q_2} = \frac{\mathbf{q}_0}{2} + \mathbf{q_1} + \mathbf{q_2}$. ∎

Theorem 4.2. *A consistent k-step MEBDF method for second order ODEs* (1.1), *based on the predictor-corrector scheme corresponding to the formulae*

(4.18), (4.19), and (4.20), is zero-stable if

$$\sum_{i=2}^{k-1} i(i-1)\alpha_i + k(k-1) \neq 0,$$

and the roots of the polynomial

$$p_k(t) = \sum_{i=0}^{k-1} \alpha_i t^i + t^k,$$

do not lie outside the unit circle.

Proof. According to Theorem 2.4, the zero-stability of a k-step MEBDF method for second order ODEs (1.1), based on the predictor-corrector scheme corresponding to the formulae (4.18), (4.19), and (4.20), is ensured if the matrix $\mathbf{V}$ satisfies the root condition (ii) given in Theorem 2.4. We observe that $\mathbf{V}$ is a Frobenius companion matrix, thus its eigenvalues are the roots of the polynomial

$$p_k(t) = \sum_{i=0}^{k-1} \alpha_i t^i + t^k.$$

Since the method is consistent, it satisfies condition (4.24) and, as a consequence, $t = 1$ is always a root of the polynomial. This implies that root condition (ii) is fulfilled if the root $t = 1$ is at most a double root, i.e. if

$$p''_k(1) = \sum_{i=2}^{k-1} i(i-1)\alpha_i + k(k-1) \neq 0,$$

which gives the thesis. ■

Due to the general result on convergence given by Theorem 2.5, the results proved in this section provide, together, the convergence analysis of MEBDF methods for second order ODEs (1.1). An example of convergent MEBDF method is given by the following new method

$$\left[\begin{array}{c|c} \mathbf{A} & \mathbf{U} \\ \hline \mathbf{B} & \mathbf{V} \end{array}\right] = \left[\begin{array}{ccc|cc} 1 & 0 & 0 & 2 & -1 \\ 2 & 1 & 0 & 3 & -2 \\ -\beta_3 & \beta_3 & 1 & 2 & -1 \\ \hline -\beta_3 & \beta_3 & 1 & 2 & -1 \\ 0 & 0 & 0 & 1 & 0 \end{array}\right], \tag{4.29}$$

which is consistent (preconsistency and consistency vectors are given by $\mathbf{q}_0 = [1,1]^T$, $\mathbf{q}_1 = [0,-1]^T$, $\mathbf{q}_2 = [0,1/2]^T$) and zero-stable, thus convergent, for any β_3. This is also confirmed by the numerical test reported in Table 4, carried out on the classical test equation

$$y''(x) = -\omega^2 y, \qquad x \in [0, \pi], \tag{4.30}$$

with initial values $y'(0) = 1$, $y(0) = 0$. The exact solution is, therefore, $y(x) = \sin(\omega x)$.

h	$\|err\|_\infty$	p
$\pi/2^5$	9.41e-2	
$\pi/2^6$	4-27e-2	1.14
$\pi/2^7$	2.03e-2	1.07
$\pi/2^8$	9.89e-3	1.04

Table 1: Numerical results originated from the application of the MEBDF method (4.29) with $\beta_3 = 1/2$ to problem (4.30), with $\omega = 1$. h is the employed fixed stepsize, $\|err\|_\infty$ is the infinity norm of the global error, p is the estimated order of convergence.

5. Conclusions

We have focused our attention on the convergence theory of general linear methods (GLMs) for special second order Ordinary Differential Equations (ODEs) of the type $y'' = f(y(t))$, discussing the generality of this approach. Indeed, we have first employed such a theory in order to recover the formulation and convergence properties of several methods for (1.1) introduced in the existing literature. Then, we have specialized the results provided in [9] to the family of modified extended BDF methods, introduced by Cash for first order ODEs and now adapted to second order problems (1.1). The developed theory will profitably be introduced and adapted for the numerical treatment of ODEs with discontinuous right-hand side (see, for instance, [11, 12] and references therein).

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