On the Order of General Linear Methods

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Abstract

General linear (GL) methods are numerical algorithms used to solve ODEs [1]. The standard order conditions analysis involves the GL matrix itself and a starting procedure; however, a finishing method ($\mathbb{F}$) is required to extract the actual ODE solution. The standard order analysis and stability are sufficient for the convergence of any GL method. Nonetheless, using a simple GL scheme we show that the order definition may be too restrictive. In this note we explore the order conditions for GL schemes and propose a new definition for characterizing the order of GL methods, which is focused on the final result – the outcome of $\mathbb{F}$ – and can provide more effective algebraic order conditions.

1 Background

In this work we consider the following autonomous initial value problem

$$y'(x) = f\left(y(x)\right)\,,\ x_0 \le x \le x_F\,,\ y(x_0) = y_0\,, \tag{1}$$

where $y \in \mathbb{R}^N$, $f : \mathbb{R}^N \to \mathbb{R}^N$. The solution of (1) can be computed using general linear (GL) methods [1; 2; 3], which can be viewed as generalizations of the classical Runge-Kutta (RK) and linear multistep (LM) methods.

The r-value s-stage GL methods are first described in their current form by Burrage and Butcher [2] and represented compactly (with a harmless abuse of notation) by the following linear scheme:

$$\begin{bmatrix} Y \\ y_i^{[n]} \end{bmatrix} = \begin{bmatrix} A & U \\ B & V \end{bmatrix} \begin{bmatrix} hF \\ y_i^{[n-1]} \end{bmatrix} = \mathbb{M} \begin{bmatrix} hF \\ y_i^{[n-1]} \end{bmatrix}\,, \tag{2}$$

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where $A = [a_{ij}]$, $B = [b_{ij}]$, $U = [u_{ij}]$, $V = [v_{ij}]$ are method-specific coefficients; $Y_i \in \mathbb{R}^{sN}$ are the internal stage values; $F_i = f(Y_i) \in \mathbb{R}^{sN}$ are the internal stage derivatives, $i = 1 \dots s$; $y^{[n-1]}$, $y^{[n]} \in \mathbb{R}^{rN}$ are the input and output values, $0 \le n \le M$, respectively; and h is the discretization step, $h = (x_F - x_0)/M$.

The standard algebraic order analysis for GL methods is done with respect to $\mathbb{M}$ and a starting procedure that generates $y^{[0]}$; however, a finishing procedure ($\mathbb{F}$) is required to compute the final result. The standard consistency analysis along with stability are sufficient for the convergence of any GL scheme. Nonetheless, in some cases they may be too restrictive. In this note we redefine the concept of order for GL methods and argue that it be analyzed with respect to the final result – the outcome of $\mathbb{F}$.

The initial input vector can be generated through a "starting procedure," $\mathbb{S} = \left\{S_i : \mathbb{R}^N \to \mathbb{R}^N\right\}_{i=1\dots r}$, represented by generalized RK methods [1, Chp. 53]:

$$S_i = \begin{array}{c|c} c^{(i)} & \mathcal{A}^{(i)} \\ \hline b_0^{(i)} & \left(b^{(i)}\right)^T \end{array}, \qquad \begin{array}{l} Y^{(i)} = \mathbb{1} y(x_0) + h\mathcal{A}^{(i)} F^{(i)} \\ S_i = b_0^{(i)} y(x_0) + h \left(b^{(i)}\right)^T F^{(i)} \end{array}, \tag{3}$$

where $\mathbb{1}$ is a vector of ones. The final solution is typically obtained by applying a "finishing procedure," $\mathbb{F} : \mathbb{R}^N \to \mathbb{R}^N$ to the last output vector. We denote by GL process the GL method applied n times and described by $\mathbb{S}\mathbb{M}^n\mathbb{F}$. We illustrate this process in Fig. 1.

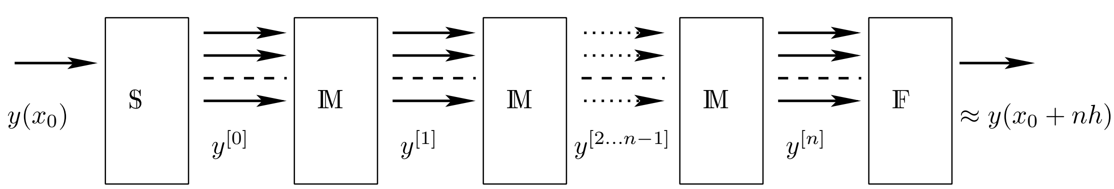

Fig. 1. Graphic representation of the general linear process: $\mathbb{S}\mathbb{M}^n\mathbb{F}$.

Remark 1 The GL process net input and output elements are represented by the initial condition, $y(x_0)$, and the final solution, y_M, respectively. This fact is used to motivate a modified definition for the order of GL methods.

2 The Order of General Linear Methods

Butcher [4] introduced an abstract representation of derivatives occurring in the Taylor expansion of (1). The derivatives are represented by *rooted tree* structures [4; 5], and can be used to algebraically characterize the order conditions for GL methods. Let $\mathbb{T}$ denote the set of rooted trees and consider mappings of type $\Phi : \mathbb{T} \to \mathbb{R}$ that are called *elementary weight functions* which associate a scalar to each element of $\mathbb{T}$.

Let $t \in \mathbb{T}$, then $r(t)$ denotes the *order* of t and $\gamma(t)$ the *density* of t. It is also useful to consider $E^{(\theta)} : \mathbb{T} \to \mathbb{R}$, the "exact solution operator" of differential equation (1), which represents the *elementary weights for the exact solution* at θh. If $\theta = 1$, then $E^{(1)}(t) = E(t) = 1/\gamma(t)$, and in general $E^{(\theta)}(t) = \theta^{r(t)}/\gamma(t)$. All these concepts are defined in [1].

The order of GL methods is characterized by the following definition.

Definition 1 [1, 530B] Consider a general linear method $\mathbb{M}$ and a non-degenerate starting method $\mathbb{S}$ [i.e., $\exists\, i\,,\ b_0^{(i)} \neq 0$]. The method $\mathbb{M}$ has order p relative to $\mathbb{S}$ if the results found from $\mathbb{S}\mathbb{M}$ and $E\mathbb{S}$ agree within $\mathcal{O}\left(h^{p+1}\right)$.

In practice the order is analyzed algebraically by introducing a mapping ξ_i : $\mathbb{T} \to \mathbb{R}$: $\xi_i(\emptyset) = b_0^{(i)}$, $\xi_i(t) = \Phi^{(i)}(t)$, where $\Phi^{(i)}(t)$, $i = 1 \ldots r$ results from (3) and $\emptyset$ represents the "empty tree." Then for the general linear method (A, U, B, V) one has:

$$\eta(t) = A\eta D(t) + U\xi(t)\,, \qquad \widehat{\xi}(t) = B\eta D(t) + U\xi(t)\,, \tag{4}$$

where η, ηD are mappings from $\mathbb{T}$ to scalars that correspond to the internal stages and stage derivatives, and $\widehat{\xi}$ represents the output vector. The exact weights are obtained from $E\xi(t)$. The order of the GL method can be determined by a direct comparison between $\widehat{\xi}(t)$ and $E\xi(t)$.

For a p^{th}-order GL method, Def. (1) requires that all the output vector elementary weights be exact within order p; i.e., $E\xi(t) = \widehat{\xi}(t)$, $\forall t\,,\ r(t) \le p$. This fact follows from Theorem 532A [1]. However, this requirement may not be necessary for all GL schemes and in order to illustrate this aspect we consider the following example [1]:

$$\left[\mathcal{A}, b^T, c\right] = \begin{array}{c|cccc} 0 & 0 & & & \\ -\frac{1}{2} & -\frac{1}{2} & 0 & & \\ \frac{1}{2} & \frac{3}{4} & -\frac{1}{4} & 0 & \\ 1 & -2 & 1 & 2 & 0 \\ \hline & \frac{1}{6} & 0 & \frac{2}{3} & \frac{1}{6} \end{array}\,, \quad \mathbb{M} = \left[\begin{array}{ccc|cc} 0 & 0 & 0 & 1 & 0 \\ \frac{3}{4} & 0 & 0 & 1 & -\frac{1}{4} \\ -2 & 2 & 0 & 1 & 0 \\ \hline \frac{1}{6} & \frac{2}{3} & \frac{1}{6} & 1 & 0 \\ 0 & 1 & 0 & 0 & 0 \end{array}\right]\,, \quad \begin{array}{l} S_1 = \begin{array}{c|c} 0 & 0 \\ \hline 1 & 0 \end{array} \\[2ex] S_2 = \begin{array}{c|cc} 0 & 0 & 0 \\ -\frac{1}{2} & -\frac{1}{2} & 0 \\ \hline 0 & 0 & 1 \end{array} \end{array}\,, \tag{5}$$

where a fourth order RK method $\left[\mathcal{A}, b^T, c\right]$ is expressed as a GL method with the input/output vector $y^{[n]}$ given by an approximation to $y(x_n)$ and $f(y(x_n - \frac{1}{2}))$. The finishing procedure is obtained by the group inverse of

S_1: $\mathbb{F} = S_1^{-1} = S_1$. Clearly S_1 reproduces $y_1^{[0]}$ exactly; however, S_2 yields an approximation of $f(y(-\frac{1}{2}))$ that has the weights accurate for all $t \in \mathbb{T}$ only within $r(t) \leq 2$; i.e., a second order approximation. By employing (4), it follows that $\mathbb{SM}$ and $E\mathbb{S}$ agree within $p = 4$ in the first component and $p = 2$ in the second one, and thus according to Def. 1 the entire method is only second order. In this case, Def. 1 is sufficient but not necessary if the action of $\mathbb{F}$ is considered. To this end we propose the following definition for the order of GL methods.

Definition 2 Consider a general linear method $\mathbb{M}$, a non-degenerate starting method $\mathbb{S}$, and a finishing method $\mathbb{F}$. The method $\mathbb{M}$ has order p relative to $\mathbb{S}$ and $\mathbb{F}$ if the results found from $\mathbb{SM}^n\mathbb{F}$ and E^n agree within $\mathcal{O}\left(h^{p+1}\right)$, with $n = 1\,,\ 2\,, \ldots\,,$ sufficiently small.

Remark 2 The focus of Def. 2 is on the final outcome of the GL methods. In practice one is typically interested in the solution of (1) as obtained from $\mathbb{F}$ and not on the other solution components resulting in the output vector (i.e., $\mathbb{SM}^M$). It is hence sensible to include the finishing method in the order analysis.

Remark 3 The definition requires the verification of $\mathbb{F}$ applied after $1\,,\ 2\,, \ldots$ steps of $\mathbb{M}$. This constraint is needed to ensure that non-vanishing $E\xi(t) - \widehat{\xi}(t)$, $r(t) \leq p$ do not affect the output of $\mathbb{F}$ after taking a few steps.

Remark 4 It can be easily checked that a GL method with starting and finishing procedures that satisfy Def. 1 also verify Def. 2. In this sense the proposed definition is less strict.

We now return to the GL method example (5) and explain why the proposed definition is appropriate in this instance. The starting procedure yields ξ_1 with accurate weights within $r(t) \leq 4$ and ξ_2 accurate within $r(t) \leq 2$. By applying $\mathbb{M}$ once, and using (4) one obtains $\widehat{\xi}_1$ accurate within $r(t) \leq 4$, and $\widehat{\xi}_2$ accurate within $r(t) \leq 2$; however, the finishing method extracts only the first component which is accurate up to order four, and thus the method is fourth order accurate according to Def. 2 for $n = 1$. The next step is to analyze the case for $n = 2$.

Consider that we take an additional step with $\mathbb{M}$ and let the inputs be the ones resulting from $\mathbb{SM}$. The $\widehat{\xi}$ weights produced by $\mathbb{SM}$ have the same error structure as the ones generated by $\mathbb{S}$: Spurious weights for ξ_2 are present for trees that are $3 \leq r(t) \leq 4$, and are now propagated through $\mathbb{M}$ again. By using (4) one finds accurate $\widehat{\xi}_1$, $r(t) \leq 4$ and $\widehat{\xi}_2$, $r(t) \leq 2$. Now by applying $\mathbb{F}$ one obtains fourth order again according to Def. 2. This analysis can be continued to obtain the same conclusions for $n \geq 2$.

Method (5) is fourth order accurate according to the classical RK theory which also results from the analysis done on its equivalent GL representation by using the proposed Def. 2; however, the standard Def. 1 only agrees to order two.

Remark 5 One needs to address the propagation of the elementary weights through the GL process in order to have an accurate algebraic characterization for the order conditions by using (4). This aspect poses an inherent difficulty in characterizing the algebraic order conditions for any given GL method.

We give the following proposition as a practical companion to Def. 2.

Proposition 1 Consider a GL method $\mathbb{M}$ with starting $\mathbb{S}$ and finishing $\mathbb{F}$ procedures and let $t^{[p]} \in \mathbb{T}$ be all the rooted trees with $r(t^{[p]}) \leq p$. The ($\mathbb{M}$, $\mathbb{S}$, $\mathbb{F}$) GL process is at least of order p if the elementary weights obtained through (4) after $n = 1\,, 2\,, \ldots$ steps of the GL process defined by $\mathbb{S}\mathbb{M}^n\mathbb{F}$ agree with the ones obtained from the exact solution for all $t^{[p]}$.

Proof The proof adopts the philosophy of the proposed definition (Def. 2) and follows from Theorem 532A (T532A) introduced by Butcher [1]. T532A describes the relation between the Taylor expansion of $E\mathbb{S} - \mathbb{S}\mathbb{M}$ and the elements of (4):

$$\varepsilon(t) = E\xi(t) - B\eta D(t) - V\xi(t); \quad E\mathbb{S} - \mathbb{S}\mathbb{M} = \sum_{t,\, r(t)>p} \frac{\varepsilon(t)}{\sigma(t)} h^{r(t)} F(t)(y(x_0))\,,$$

where $F(t)$ is the *elementary differential* and $\sigma(t)$ the symmetry of t. The proof follows then by using the same arguments as in T532A, but now consider the more involved expressions resulting from the full GL process ($\mathbb{S}\mathbb{M}^M\mathbb{F}$) and using (4). $\square$

3 Discussion

In this manuscript we propose a new definition for the order conditions of general linear methods. In some cases this definition leads to a more accurate algebraic characterization of the order conditions than the standard one given in [1, 530B]. However, the new approach may be more difficult to be applied in practice.

The proposed definition focuses on the GL method output rather than on the starting procedure and one GL step. A proposition is given to address its practical aspect. Furthermore, an example is used to illustrate an instance when the standard definition is less appropriate, and explains the necessity of using this new approach. Nonetheless, an algebraic criterion for order conditions depends on the structure of the GL method coefficients and how lower order intermediate approximations propagate to the final solution. It is thus very difficult to broaden this algebraic approach to any GL process. This is however not in the scope of this note.

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Note