On the Order of General Linear Methods

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Abstract

General linear (GL) methods are numerical algorithms used to solve ODEs. 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. Specifically, the order for GL methods with low order intermediate components may be underestimated. 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 by using general linear (GL) methods [1; 2; 3], which can be viewed as generalizations of the classical Runge-Kutta (RK) and linear multistep methods.

The r-value s-stage GL methods were first described in their current form by Burrage and Butcher [3] 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, $0 \leq n \leq M$, 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 and stability are sufficient for the convergence of any GL scheme. Nonetheless, in some cases they may be too restrictive. In particular, the convergence order for GL methods that have low order intermediate components may be underestimated. 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]:

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

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 the 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.

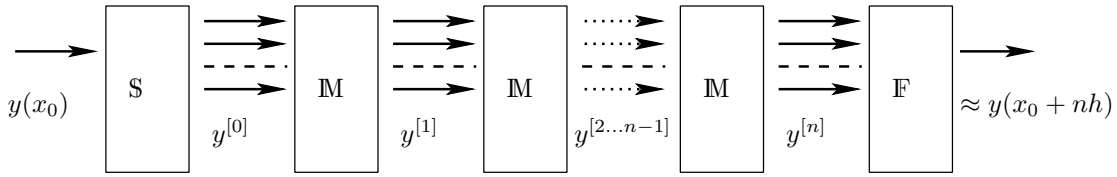

Fig. 1. Graphic representation of the general linear process: $\mathbb{S}\mathbb{M}^n\mathbb{F}$.

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 $\Phi : \mathbb{T} \to \mathbb{R}$, which are called *elementary weight functions* and 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; 6].

The order of GL methods is characterized by the following two definitions.

Definition 1 [1, 530B] Consider a general linear method $\mathbb{M}$ and a nondegenerate 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 $\mathcal{O}\left(h^{p+1}\right)$.

Definition 2 [1, 530C] A general linear method $\mathbb{M}$ has order p if there exists a non-degenerate starting method $\mathbb{S}$ such that $\mathbb{M}$ has order p relative to $\mathbb{S}$.

In practice, the order is analyzed algebraically by introducing a mapping $\xi_i : \mathbb{T} \to \mathbb{R}$: $\xi_i(\emptyset) = b_0^{(i)}$, $\xi_i(t) = \Phi^{(i)}(t)$, 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 and 2 require that all the output vector elementary weights be exact within order p; in other words, $E\xi(t) = \widehat{\xi}(t)$, $\forall t\,,\ r(t) \leq p$. This fact follows from Theorem 532A [1]. However, this requirement may not be necessary for all GL schemes. To illustrate this aspect, we consider the following example:

$$\mathbb{M} = \left[\begin{array}{ccc|cc} 0 & 0 & 0 & 1 & 0 \\ \frac{7}{8} & 0 & 0 & 1 & -\frac{3}{8} \\ -\frac{5}{2} & 2 & 0 & 1 & \frac{3}{2} \\ \hline \frac{1}{6} & \frac{2}{3} & \frac{1}{6} & 1 & 0 \\ -2 & 2 & 0 & 0 & 1 \end{array}\right], \qquad S_1 = \left[\begin{array}{c|c} 0 & 0 \\ \hline 1 & 0 \end{array}\right], \qquad S_2 = \left[\begin{array}{c|cc} 0 & 0 & 0 \\ \hline -\frac{1}{3} & -\frac{1}{3} & 0 \\ \hline 0 & 0 & 1 \end{array}\right], \qquad \mathbb{F} = S_1^{-1} = S_1\,. \tag{5}$$

The input/output vector $y^{[n]}$ represents an approximation to $y(x_n)$ and $f(y(x_n - \frac{1}{3}h))$. Clearly S_1 reproduces $y_1^{[0]}$ exactly; however, S_2 yields an approximation of $f(y(-\frac{1}{3}h))$ that has the weights accurate for all $t \in \mathbb{T}$ only within $r(t) \leq 2$, i.e., a second-order approximation.

By using the algebraic instruments presented in [1][Chp. 532], it can be shown that method (5) with the specified starting and finishing procedures is fourth order accurate. However, by employing (4), it follows that there is no starting procedure $\mathbb{S}$, such that the intermediate values be fourth order accurate. Specifically, $\mathbb{SM}$ and $E\mathbb{S}$ agree within $p = 4$ in the first component and $p = 2$ in the second one ($\widehat{\xi}_2([\tau^2]) \neq E\xi_2([\tau^2])$), and thus according to Def. 1 and 2 the entire method is only of second order. In this case, Def. 1 and 2 are sufficient but not necessary if the action of $\mathbb{F}$ is considered. In other words, Def. 1 and 2 always underestimate the order of convergence for the class of problems represented by this example. To this end we propose the following definition for the order of GL methods.

Definition 3 Consider a general linear method $\mathbb{M}$, a nondegenerate 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 elementary weights found from $\mathbb{SM}^n\mathbb{F}$ and E^n agree within order p for $n = 1, 2, \ldots$.

Remark 2 The focus of Def. 3 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 in 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 nonvanishing error terms $E\xi(t) - \widehat{\xi}(t)$, $r(t) \leq p$ do not affect the output of $\mathbb{F}$.

Remark 4 It can be easily checked that a GL method with starting and finishing procedures that satisfy Def. 1 and 2 also verify Def. 3. 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 more 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. 3 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. 3. This analysis can be continued to obtain the same conclusions for $n \geq 2$.

Method (5) can be shown to be fourth-order accurate, which also results from the analysis done on its equivalent GL representation by using the proposed Def. 3; however, the standard Def. 1 and 2 agree only 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. 3.

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 $\mathbb{SM}^n\mathbb{F}$ agree with the ones obtained from the exact solution for all $t^{[p]}$.

Proof The proof adopts the philosophy of the proposed definition (Def. 3) and follows from Theorem 532A (T532A) introduced by Butcher [1]. T532A describes the relation between the Taylor expansion of $E\mathbb{S} - \mathbb{SM}$ and the elements of (4):

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

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 ($\mathbb{SM}^M\mathbb{F}$) and using (4). $\square$

Due to the fact that in practice the starting and finishing procedures are necessary to obtain the numerical solution, we consider the GL method described by the triplet ($\mathbb{M}$, $\mathbb{S}$, $\mathbb{F}$). In order to guarantee that the GL method is of order p, by using (4), one needs to ensure that possible spurious intermediate lower order solution components $\xi_i(t^{[k]})$, $1 \leq i \leq r$, $1 \leq k \leq p$ do not degrade the order of the method output. In practice a few steps of the GL process are

required to convince oneself that the output of the GL method retains order p.

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 ones given in [1, 530B & 530C]. Specifically, the standard approach may underestimate the convergence order of GL methods that have low order intermediate components.

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, a simple 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 define this algebraic approach more specifically without loosing generality. This is, however, not in the scope of this note.

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Note