

Linear multistep methods and global Richardson extrapolation

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ABSTRACT

In this work, we study the application the classical Richardson extrapolation (RE) technique to accelerate the convergence of sequences resulting from linear multistep methods (LMMs) for solving initial-value problems of systems of ordinary differential equations numerically. The advantage of the LMM-RE approach is that the combined method possesses higher order and favorable linear stability properties in terms of A - or $A(\alpha)$ -stability, and existing LMM codes can be used without any modification.

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1. Introduction

Richardson extrapolation (RE) [1,2] is a classical technique to accelerate the convergence of numerical sequences depending on a small parameter, by eliminating the lowest order error term(s) from the corresponding asymptotic expansion. When the sequence is generated by a numerical method solving the initial-value problem

$$y'(t) = f(t, y(t)), \quad y(t_0) = y_0, \quad (1)$$

the parameter in RE can be chosen as the discretization step size $h > 0$. The application of RE to sequences generated by one-step — e.g., Runge–Kutta-methods is described, for example, in [3,4]. In [5], global (also known as passive) or local (active) versions of RE are implemented with Runge–Kutta sequences. These combined methods can find applications in air pollution problems [6] or in machine learning [7], for example.

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In this paper, we analyze the application of global Richardson extrapolation (GRE) to sequences generated by linear multistep methods (LMMs) approximating the solution of (1). We will refer to a k -step LMM as the underlying LMM, and its recursion has the usual form

$$\sum_{j=0}^k \alpha_j y_{n+j} = \sum_{j=0}^k h \beta_j f_{n+j}, \quad (2)$$

where $f_m := f(t_m, y_m)$, and the numbers $\alpha_j \in \mathbb{R}$ and $\beta_j \in \mathbb{R}$ ($j = 0, \dots, k$) are the given method coefficients with $\alpha_k \neq 0$. The LMM is implicit, if $\beta_k \neq 0$.

In Section 2, given an underlying LMM, we define its extrapolated version, referred to as LMM-GRE, and investigate its convergence. Then, we carry out linear stability analysis for the LMM-GREs. In Section 2.4, we focus on the BDF family as underlying LMMs due to their good stability properties, although the results from Sections 2.1–2.3 are clearly applicable to other LMM families as well. The numerical experiments in Section 3 demonstrate the expected convergence order — here, we use several different types of LMMs with GRE to solve (1).

As a conclusion of this study, we see that

- (i) to implement a LMM-GRE, existing LMM codes can directly be used, thanks to the simple linear combination appearing in definition (3); moreover,
- (ii) the higher computational cost of a LMM-GRE is compensated by its higher convergence order and favorable linear stability properties.

Remark 1.1. In [5, Section 3.4], the authors comment on the possible combination of LMMs and *local* Richardson extrapolation. Working out the necessary details and convergence theorems for this case could be the subject of a future study.

2. Results for LMM-GREs

2.1. Definition

Let us assume that the function f in (1) is sufficiently smooth, hence the initial-value problem has a unique smooth solution y , and we seek its approximation on an interval $[t_0, t_{\text{final}}]$. To this end, we apply a k -step LMM to (1) on a uniform grid $\{t_n\}$ to generate the sequence $y_n(h)$ according to (2). Here, $h := t_{n+1} - t_n > 0$ is the step size (or grid length), and $y_n(h)$ is supposed to approximate the exact solution at t_n , that is, $y_n(h) \approx y(t_n)$. We assume that the LMM is of order $p \geq 1$.

The idea of classical RE is to take a suitable linear combination of two approximations, one generated on a coarser grid and one on a finer grid, to obtain a better approximation of the solution y of (1). Here, we will only consider its simplest form and define

$$r_n(h) := \frac{2^p}{2^p - 1} \cdot y_{2n}\left(\frac{h}{2}\right) - \frac{1}{2^p - 1} \cdot y_n(h), \quad (3)$$

that is, the coarser and finer grids have grid lengths h and $h/2$, respectively. Since the sequence $y_n(h)$ on the coarser grid and the sequence $y_{2n}(\frac{h}{2})$ on the finer grid are computed independently (their linear combination is formed only in the last step), we refer to this procedure as *global* (or *passive*) *extrapolation*, or, in short, LMM-GRE.

2.2. Convergence

Lemma 2.1. *Under the above assumptions on the function f in (1) and on the LMM, further, if the starting values $y_j(h)$ and $y_j(\frac{h}{2})$ ($j = 1, 2, \dots, k-1$) of the LMM are $\mathcal{O}(h^{p+1})$ -close to the corresponding exact solution*

values, then the sequence $r_n(h)$ converges to the exact solution y of (1), and the order of convergence is at least $p + 1$.

Proof. The proof relies on the fact that – under the assumptions of the lemma – the global error $y_n(h) - y(t_n)$ of a LMM possesses an asymptotic expansion in h . More precisely, according to, e.g., [8, Section 6.3.4], there exist a function \mathbf{e} and a constant $C_{k,p}$ such that

$$y_n(h) - y(t_n) = C_{k,p} \cdot h^p \cdot \mathbf{e}(t_n) + \mathcal{O}(h^{p+1}) \quad \text{as } h \rightarrow 0^+, \quad (4)$$

for any $n \in \mathbb{N}$ for which $t_n \in [t_0, t_{\text{final}}]$. Here, the function \mathbf{e} depends only on f in (1) (and not on the chosen LMM), while the error constant $C_{k,p}$ depends only on the k -step LMM (and not on (1) or on h). Then, by applying (4) on a grid with grid length $h/2$ and focusing on the same (i.e., h -independent) grid point $t_n = t^*$, we have

$$y_{2n}\left(\frac{h}{2}\right) - y(t^*) = C_{k,p} \cdot \left(\frac{h}{2}\right)^p \cdot \mathbf{e}(t^*) + \mathcal{O}(h^{p+1}). \quad (5)$$

Combining (3)–(5), we easily see that $r_n(h) - y(t^*) = \mathcal{O}(h^{p+1})$ as $h \rightarrow 0^+$. \square

2.3. Linear stability analysis

Let us now recall the definition of the region of absolute stability of a LMM — here, this region will be denoted by \mathcal{S}_{LMM} . It is known (see [9] or [10, Section 2.3]) that \mathcal{S}_{LMM} can be characterized by the following boundedness condition. Let us fix some $h > 0$ and $\lambda \in \mathbb{C}$ such that for $\mu := h\lambda$ one has $\alpha_k - \mu\beta_k \neq 0$. Suppose that the LMM (2), with step size h and starting values y_0, y_1, \dots, y_{k-1} , applied to the usual scalar linear test equation

$$y'(t) = \lambda y(t), \quad y(t_0) = y_0 \quad (6)$$

generates the sequence y_n ($n \in \mathbb{N}$). Then $\mu \in \mathcal{S}_{\text{LMM}} \subset \mathbb{C}$ if and only if the sequence y_n is bounded for any choice of the starting values y_0, y_1, \dots, y_{k-1} .

Remark 2.2. Considering the differential equation (6), if $\mu \in \mathbb{C}$ is chosen such that $\alpha_k - \mu\beta_k = 0$, then the order of the recursion generated by the LMM becomes strictly less than k , hence the starting values y_0, y_1, \dots, y_{k-1} could not be chosen arbitrarily (see also [10, Remark 2.7]).

We define the region of absolute stability, $\mathcal{S}_{\text{GRE}} \subset \mathbb{C}$, of the combined LMM-GRE method (3) analogously to that of the underlying LMM. Let us apply (3) to the scalar linear test Eq. (6) with some $h > 0$ and $\lambda \in \mathbb{C}$. Then \mathcal{S}_{GRE} is defined to be

the set of numbers $\mu := h\lambda$ for which the sequence $r_n(h)$ is bounded (in $n \in \mathbb{N}$) for any choice of the starting values of the sequence $y_n(h)$ and for any choice of the starting values of the sequence $y_m(\frac{h}{2})$, but excluding the values of μ for which $\alpha_k - \mu\beta_k = 0$ or $\alpha_k - \frac{\mu}{2}\beta_k = 0$.

Now we can relate the stability region of the combined method to that of the underlying LMM as follows. For a set $S \subset \mathbb{C}$, we define $2S := \{2z : z \in S\}$.

Lemma 2.3. *We have the inclusions (i) $\mathcal{S}_{\text{LMM}} \cap (2\mathcal{S}_{\text{LMM}}) \subseteq \mathcal{S}_{\text{GRE}}$, and (ii) $\mathcal{S}_{\text{GRE}} \subseteq \mathcal{S}_{\text{LMM}}$.*

Proof. Suppose that $h > 0$ and $\lambda \in \mathbb{C}$ have been chosen such that $h\lambda \in \mathcal{S}_{\text{LMM}} \cap (2\mathcal{S}_{\text{LMM}})$, and we apply the LMM-GRE method with this step size h to (6) with this λ . Then both sequences $y_n(h)$ and $y_m(\frac{h}{2})$ are bounded for any choice of their respective k starting values. Hence the sequence $r_n(h)$, as their linear combination, is also bounded. This proves (i).

To prove (ii), let us choose $h > 0$ and $\lambda \in \mathbb{C}$ such that $h\lambda \in \mathcal{S}_{\text{GRE}}$. Then the sequence $r_n(h)$ is bounded. By choosing every starting value 0, we can have that the sequence $y_m(\frac{h}{2})$ is identically 0. Hence $r_n(h) = -\frac{1}{2^p-1} \cdot y_n(h)$, so the sequence $y_n(h)$ is also bounded. Therefore $h\lambda \in \mathcal{S}_{\text{LMM}}$. \square

Remark 2.4. The reasoning in the above proof of (ii) could not be applied to prove $\mathcal{S}_{\text{GRE}} \subseteq 2\mathcal{S}_{\text{LMM}}$: although the boundedness of $r_n(h)$ implies (via a special choice of the starting values of the sequence $y_n(h)$) that the sequence $y_{2n}(\frac{h}{2})$ is also bounded, this alone would be insufficient to guarantee the boundedness of the sequence $y_m(\frac{h}{2})$ ($m \in \mathbb{N}$).

To conclude this section, we give a sufficient condition for the stability regions \mathcal{S}_{LMM} and \mathcal{S}_{GRE} to coincide. As it is well-known, all practically relevant LMMs are zero-stable [11].

Lemma 2.5. Assume that the underlying LMM is zero-stable, and \mathcal{S}_{LMM} is convex. Then $\mathcal{S}_{\text{GRE}} = \mathcal{S}_{\text{LMM}}$.

Proof. Zero-stability implies that $0 \in \mathcal{S}_{\text{LMM}}$, so from the convexity of \mathcal{S}_{LMM} we have that $\mathcal{S}_{\text{LMM}} \subseteq 2\mathcal{S}_{\text{LMM}}$. But this means that $\mathcal{S}_{\text{LMM}} \cap (2\mathcal{S}_{\text{LMM}}) = \mathcal{S}_{\text{LMM}}$, so from Lemma 2.3 we get that $\mathcal{S}_{\text{GRE}} = \mathcal{S}_{\text{LMM}}$. \square

Remark 2.6. By analyzing the root-locus curve [9] of the underlying LMM as a parametric curve, it can be proved that \mathcal{S}_{LMM} is convex, for example, for the Adams–Bashforth method with $k = 2$ steps, or for the Adams–Moulton method with $k = 2$ steps. However, for the Adams–Bashforth method with $k = 3$ steps, \mathcal{S}_{LMM} is not convex.

2.4. BDFk-GRE methods

We obtain an efficient family of LMM-GRE methods if the underlying LMM is a k -step BDF method (referred to as a BDFk-method) with some $1 \leq k \leq 6$ (recall that for zero-stability we need $k \leq 6$). It is known that a BDFk-method has order $p = k$, see [9].

Suppose that the sequences $y_n(h)$ and $y_{2n}(\frac{h}{2})$ in (3) are generated by a BDFk-method, and the starting values for both sequences are $(k+1)^{\text{st}}$ -order accurate. Then, due to Lemma 2.1, the sequence $r_n(h)$ with $p := k$ converges to the solution of (1) with order $k+1$.

To measure the size of the region of absolute stability of the BDFk-GRE methods, one can invoke the concepts of A -stability and $A(\alpha)$ -stability [9]. It is easily seen that scaling the region of absolute stability of the underlying method \mathcal{S}_{LMM} by a factor of 2 preserves the $A(\alpha)$ -stability angles (see [10, Figure 1] for an illustration). Hence, due to Lemma 2.3, the BDFk-GRE method has the same $A(\alpha)$ -stability angle as that of the underlying BDFk-method.

In Table 1, we present the order of convergence and the $A(\alpha)$ -stability angles for the BDFk-GRE methods. (For the exact values of the angles α , see, e.g., [10, Table 1].) The BDFk-GRE methods are particularly suitable for stiff problems.

Table 1
Convergence order and $A(\alpha)$ -stability angles for the BDFk-GRE methods.

| k | Order | $A(\alpha)$ -stability angle |
|-----|---------|------------------------------|
| 1 | $p = 2$ | 90° , A -stable |
| 2 | $p = 3$ | 90° , A -stable |
| 3 | $p = 4$ | 86.032° |
| 4 | $p = 5$ | 73.351° |
| 5 | $p = 6$ | 51.839° |
| 6 | $p = 7$ | 17.839° |

Notice, in particular, that the BDF2-GRE method is a 3rd-order A -stable method (recall that, due to the classical Dahlquist theorem, no 3rd-order A -stable LMM can exist).

In terms of computational cost, due to the presence of the coarser and finer grids, the sequence $r_n(h)$ in (3) corresponding to a LMM-GRE method is approximately three times as expensive to generate as the sequence $y_n(h)$ corresponding to the underlying LMM. However, the extra computing time is balanced by the higher order and $A(\alpha)$ -stability; the BDF5-GRE method, for example, has order 6, and its $A(\alpha)$ -stability angle is approximately three times as large as the stability angle of the classical 6th-order BDF6-method.

3. Numerical experiments

To verify the rate of convergence of LMM-GREs, we chose some benchmark problems, including a Lotka–Volterra system

$$y_1'(t) = 0.1y_1(t) - 0.3y_1(t)y_2(t), \quad y_2'(t) = 0.5(y_1(t) - 1)y_2(t)$$

for $t \in [0, 62]$ with initial condition $y(0) = (1, 1)^\top$; or the mildly stiff van der Pol equation

$$y_1'(t) = y_2(t), \quad y_2'(t) = 2(1 - y_1^2(t))y_2(t) - y_1(t)$$

for $t \in [0, 20]$ with initial condition $y(0) = (2, 0)^\top$.

As underlying LMMs, we considered the 2nd- and 3rd order Adams–Bashforth (AB), Adams–Moulton (AM), and BDF methods. The AM methods were implemented in predictor–corrector style. For starting methods, we chose the 2nd- and 3rd-order Ralston methods, having minimum error bounds [12]. For the nonlinear algebraic equations arising in connection with implicit LMMs, we use MATLAB's `fsolve` command. Following [13, Appendix A], the fine-grid solutions obtained by the classical 4th-order Runge–Kutta method with 2^{16} grid points are used to measure the global error in maximum norm and to estimate the corresponding convergence order. Table 2 and Fig. 1 illustrate the expected order of convergence for all tested LMM-GREs.

Table 2

The estimated order of convergence for the Lotka–Volterra system for different LMM-GREs with 64, 128, ..., 1024 grid points.

| AB2-GRE | AM2-GRE | BDF2-GRE | AB3-GRE | AM3-GRE | BDF3-GRE |
|---------|---------|----------|---------|---------|----------|
| 3.7674 | 3.3545 | 3.2045 | 4.1864 | 3.7644 | 3.6254 |
| 3.5761 | 3.2095 | 3.1703 | 3.9928 | 3.8903 | 3.7630 |
| 3.1981 | 3.1068 | 3.1340 | 3.9873 | 3.9718 | 3.9411 |
| 3.0297 | 3.0520 | 3.0807 | 3.9975 | 3.9856 | 3.9896 |

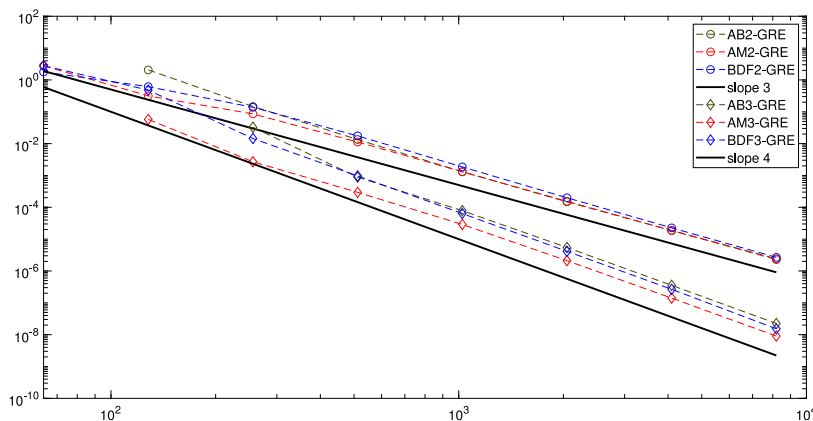


Fig. 1. Results for the van der Pol equation for LMM-GREs, number of grid points versus the global error in maximum norm.

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