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Positivity for explicit two-step methods in linear multistep  
and one-leg form

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# Positivity for explicit two-step methods in linear multistep and one-leg form

## ABSTRACT

Positivity results are derived for explicit two-step methods formulated in linear multistep form and in one-leg form. It turns out that the latter formulation allows a slightly larger step size with respect to positivity.

*2000 Mathematics Subject Classification:* 65L06

*1998 ACM Computing Classification System:* G.1.7

*Keywords and Phrases:* Positivity, Multistep Methods, One-Leg Form.

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# POSITIVITY FOR EXPLICIT TWO-STEP METHODS IN LINEAR MULTISTEP AND ONE-LEG FORM

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## Abstract

Positivity results are derived for explicit two-step methods formulated in linear multistep form and in one-leg form. It turns out that the latter formulation allows a slightly larger step size with respect to positivity.

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## 1 Introduction

We consider the initial value problem for a positive system of ordinary differential equations (ODEs) in  $\mathbb{R}^m$

$$\begin{aligned}\mathbf{w}'(t) &= \mathbf{F}(t, \mathbf{w}(t)), \\ \mathbf{w}(0) &= \mathbf{w}_0 \geq 0.\end{aligned}$$

With positivity (actually, non-negativity) we mean that the solution vector  $\mathbf{w}(t) \geq 0, \forall t > 0$  if  $\mathbf{w}_0 \geq 0$ . Here, and in the sequel, such inequalities are to be understood componentwise. For such systems of ODEs we will study whether we can obtain a similar property for the numerical solutions  $\mathbf{W}_n \approx \mathbf{w}(t_n), t_n = n\Delta t, \Delta t$  being the time step. In [4], the related concept of monotonicity with semi-norms for linear multistep methods has been studied. Here we focus on positivity and adapt the results obtained in [4]. In Section 2 we will present an extension in the case of explicit two-step methods with forward Euler start-up (to compute  $\mathbf{W}_1$ ), and we will point out the best method with respect to positivity, i.e.  $\mathbf{W}_n \geq 0$  for  $n \geq 1$ , whenever  $\mathbf{W}_0 \geq 0$ . In Section 3 we consider the corresponding one-leg formulation and show that this allows a slightly larger step size.

## 2 Positivity for linear two-step methods

Consider the following explicit linear two-step scheme

$$\mathbf{W}_{n+2} = \sum_{j=0}^1 \left[ -\alpha_j \mathbf{W}_{n+j} + \beta_j \Delta t \mathbf{F}(t_{n+j}, \mathbf{W}_{n+j}) \right]. \quad (1a)$$

Observe that the freedom in scaling the coefficients has been used to set the coefficient in front of  $\mathbf{W}_{n+2}$  equal to 1. In the one-leg formulation we will use a different scaling.

The scheme (1a) is of second-order accuracy if

$$\alpha_0 = 1 - \xi, \quad \alpha_1 = \xi - 2, \quad \beta_0 = \frac{\xi}{2} - 1, \quad \beta_1 = \frac{\xi}{2} + 1, \quad (1b)$$

where  $\xi$  is a free parameter. We note that the scheme is zero-stable (stable for the trivial equation  $\mathbf{w}'(t) = \mathbf{0}$ , see [5]) if the condition  $-1 \leq \alpha_0 < 1$  is satisfied, i.e. if  $0 < \xi \leq 2$ . In the remainder of this paper we shall always deal with methods that are second-order accurate and zero-stable. In [4], both implicit and explicit methods have been analyzed. In this section we will extend the results obtained in that paper for the explicit methods. For monotonicity results with higher-order methods, we refer to [2, 3].

Following Shu [7], the step in (1a) is written as a linear combination of scaled forward Euler steps yielding

$$\mathbf{W}_{n+2} = -\sum_{j=0}^1 \alpha_j \left[ \mathbf{W}_{n+j} + c_j \Delta t \mathbf{F}(t_{n+j}, \mathbf{W}_{n+j}) \right], \quad c_j = -\frac{\beta_j}{\alpha_j}. \quad (2)$$

We define  $\Delta t_{FE}$  to be the largest time step for which the forward Euler method, starting from a positive value, yields a positive result, i.e.

$$\mathbf{v} + \Delta t \mathbf{F}(t, \mathbf{v}) \geq 0 \quad \text{for all } \mathbf{v} \geq 0, \quad t \geq 0, \quad 0 \leq \Delta t \leq \Delta t_{FE}. \quad (3)$$

Then, if

$$\beta_j \geq 0 \quad \text{and} \quad \alpha_j \leq 0, \quad \text{i.e. } c_j \geq 0, \quad \text{for } j = 0, 1, \quad (4)$$

the terms within the square brackets in (2) are non-negative under the step size restriction  $0 \leq c_j \Delta t \leq \Delta t_{FE}$ ,  $j = 0, 1$ . Therefore,  $\mathbf{W}_{n+2} \geq 0$  for all  $\Delta t \leq \min(\frac{1}{c_0}, \frac{1}{c_1}) \Delta t_{FE}$ , for arbitrary values of  $\mathbf{W}_0, \mathbf{W}_1, \dots, \mathbf{W}_{n+1} \geq 0$ .

However, for the class of explicit second-order two-step methods, condition (4) for  $\beta_0$  leads to  $\xi \geq 2$ . Combining this with the zero-stability requirement  $0 < \xi \leq 2$  gives  $\xi = 2$  as the only possible value. This, however, results in  $c_1 = \infty$  and hence  $\Delta t \leq 0$ . Indeed, for  $\xi = 2$  we obtain

$$\mathbf{W}_{n+2} = \left[ \mathbf{W}_n - \mathbf{W}_{n+1} \right] + \left[ \mathbf{W}_{n+1} + 2\Delta t \mathbf{F}(t_{n+1}, \mathbf{W}_{n+1}) \right].$$

Although the second term gives a positive contribution for  $\Delta t \leq \frac{1}{2} \Delta t_{FE}$ , the first term can be negative for arbitrary positive  $\mathbf{W}_n$  and  $\mathbf{W}_{n+1}$  which may result in  $\mathbf{W}_{n+2} < 0$ .

Fortunately, if we consider appropriate starting conditions, a positive result can be obtained [4, 3]. If  $\mathbf{W}_1$  is obtained by the forward Euler method, i.e.

$$\mathbf{W}_1 = \mathbf{W}_0 + \Delta t \mathbf{F}(t_0, \mathbf{W}_0), \quad (5)$$

we have  $\mathbf{W}_1 \geq 0$  for all  $\Delta t \leq \Delta t_{FE}$  (see (3)). By introducing a non-negative parameter  $\theta$ , which is specified later, and subsequently subtracting and adding  $\theta^j \mathbf{W}_{n+2-j}$ ,  $j = 1, 2, \dots, n+1$ , in (1a), in which the added terms with  $j = 1, 2, \dots, n$  are again written in the form of (1a), we arrive at

$$\begin{aligned} \mathbf{W}_{n+2} &= (-\alpha_1 - \theta) \mathbf{W}_{n+1} + \beta_1 \Delta t \mathbf{F}_{n+1} \\ &\quad + \sum_{j=0}^{n-1} \theta^j \left[ (-\alpha_0 - \theta \alpha_1 - \theta^2) \mathbf{W}_{n-j} + (\beta_0 + \theta \beta_1) \Delta t \mathbf{F}_{n-j} \right] \\ &\quad + \theta^{n-1} \left[ \theta^2 \mathbf{W}_1 - \theta \alpha_0 \mathbf{W}_0 + \theta \beta_0 \Delta t \mathbf{F}_0 \right], \quad n \geq 0, \end{aligned} \quad (6)$$

where  $\mathbf{F}_j$  denotes  $\mathbf{F}(t_j, \mathbf{W}_j)$ . Since  $\mathbf{W}_1$  was calculated by the forward Euler method and  $\alpha_1 = -1 - \alpha_0$  (see (1b)), this relation can be written as

$$\begin{aligned} \mathbf{W}_{n+2} &= (-\alpha_1 - \theta) \mathbf{W}_{n+1} + \beta_1 \Delta t \mathbf{F}_{n+1} \\ &\quad + \sum_{j=0}^{n-1} \theta^j \left[ (1 - \theta)(\theta - \alpha_0) \mathbf{W}_{n-j} + (\beta_0 + \theta \beta_1) \Delta t \mathbf{F}_{n-j} \right] \\ &\quad + \theta^n \left[ (\theta - \alpha_0) \mathbf{W}_0 + (\theta + \beta_0) \Delta t \mathbf{F}_0 \right], \quad n \geq 0. \end{aligned}$$

Considering this step as a linear combination of scaled forward Euler steps, we see that  $\mathbf{W}_{n+2} \geq 0$  if all coefficients are non-negative, i.e.

$$-\alpha_1 - \theta \geq 0, \quad \beta_1 \geq 0, \quad (1 - \theta)(\theta - \alpha_0) \geq 0, \quad \beta_0 + \theta \beta_1 \geq 0, \quad \theta - \alpha_0 \geq 0, \quad \theta + \beta_0 \geq 0. \quad (7)$$

These conditions imply the step size restriction  $\Delta t \leq \gamma(\theta) \Delta t_{FE}$ , where

$$\gamma(\theta) = \min \left( \frac{-\alpha_1 - \theta}{\beta_1}, \frac{(1 - \theta)(\theta - \alpha_0)}{\beta_0 + \theta \beta_1}, \frac{\theta - \alpha_0}{\theta + \beta_0} \right) =: \min(A(\theta), B(\theta), C(\theta)). \quad (8)$$

Obviously, the larger  $\gamma(\theta)$ , the better are the positivity properties of the scheme.

The conditions (7) define an eligible  $\theta$ -interval, viz.  $\theta \in [\theta_{min}, \theta_{max}]$ , where

$$\begin{aligned} \theta_{min} &= \max(\alpha_0, -\frac{\beta_0}{\beta_1}, -\beta_0) = -\beta_0, \\ \theta_{max} &= \min(-\alpha_1, 1). \end{aligned}$$

Observe that  $A(\theta)$ ,  $B(\theta)$  and  $C(\theta)$  are monotonic decreasing functions of  $\theta$  (recall the condition  $0 < \xi \leq 2$ ). Therefore, we obtain the maximal  $\gamma(\theta)$ -value

$$\gamma_{max} = \min(A(\theta_{min}), B(\theta_{min}), C(\theta_{min})) = \begin{cases} B(\theta_{min}) = \frac{\xi}{2-\xi} & \text{if } 0 < \xi \leq \frac{2}{3}, \\ A(\theta_{min}) = \frac{2-\xi}{2+\xi} & \text{if } \frac{2}{3} \leq \xi \leq 2. \end{cases} \quad (9)$$

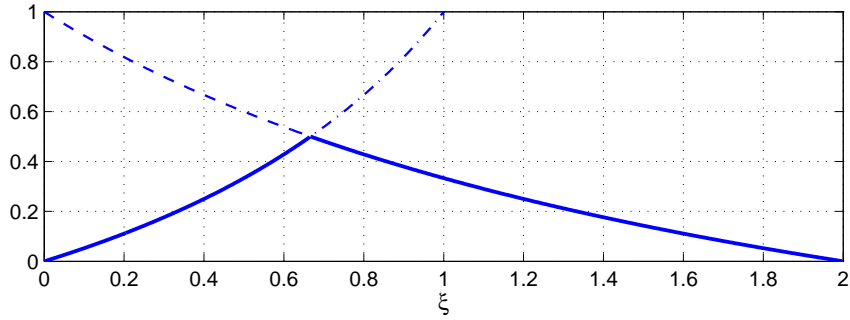


Figure 1:  $\gamma_{max}$  (solid),  $A(\theta_{min})$  (dashed), and  $B(\theta_{min})$  (dash-dotted) as functions of  $\xi$ .

The result is plotted in Figure 1. The ascending part of the  $\gamma_{max}$ -curve (i.e. for  $0 < \xi < \frac{2}{3}$ ) is an extension to the work in [4]. We note that in that paper only the minimum of  $A(\theta)$  and  $B(\theta)$  was considered in (8), leading to a different value of  $\theta_{min}$ . The forward Euler starting procedure (5) was introduced afterwards, but this does not lead to a positivity result for  $0 < \xi < \frac{2}{3}$ .

From Figure 1 we see that, within the class of explicit second-order two-step method, the optimal method with respect to positivity is the  $\xi = \frac{2}{3}$  method (known as the extrapolated BDF2 method [5]). The resulting value for  $\gamma_{max}$  is  $\frac{1}{2}$ .

**Remark.** In (6), the sequence of subtracting and adding  $\theta^j \mathbf{W}_{n+2-j}$  was performed until  $j = n + 1$ . In [4] these terms were subtracted and added up to  $j = n$ . It has been proved [6] that the latter choice has no advantages compared with the choice made in (6), i.e., does not lead to a more relaxed condition on  $\Delta t$ . The proof is rather lengthy and technical and therefore is not included in this paper.

### 3 Positivity for one-leg methods

One-leg schemes were introduced by Dahlquist [1] to facilitate the analysis of linear multistep methods. Therefore, it is of interest to study the positivity properties of methods when formulated in the one-leg form. Similar to the preceding section, we will consider explicit methods. We will see that the results are slightly better than those derived for the linear multistep formulation.

A natural scaling for one-leg methods is to require  $\beta_0 + \beta_1 = 1$ . Starting from the linear multistep formulation (1) we multiply the coefficients by a factor  $\frac{1}{\xi}$  to obtain

$$\alpha_2 \mathbf{W}_{n+2} = \sum_{j=0}^1 \left[ -\alpha_j \mathbf{W}_{n+j} + \beta_j \Delta t \mathbf{F}(t_{n+j}, \mathbf{W}_{n+j}) \right], \quad (10a)$$

where

$$\alpha_0 = \frac{1}{\xi} - 1, \quad \alpha_1 = 1 - \frac{2}{\xi}, \quad \alpha_2 = \frac{1}{\xi}, \quad \beta_0 = \frac{1}{2} - \frac{1}{\xi}, \quad \beta_1 = \frac{1}{2} + \frac{1}{\xi}. \quad (10b)$$



Since  $\xi > 0$  we have

$$0 < \alpha_2 = -(\alpha_1 + \alpha_0). \quad (11)$$

The one-leg form of (10a) reads

$$\begin{aligned} \alpha_2 \mathbf{W}_{n+2} &= -\alpha_1 \mathbf{W}_{n+1} - \alpha_0 \mathbf{W}_n + \Delta t \mathbf{F}(\bar{t}, \bar{\mathbf{W}}_{n+2}), \\ \bar{\mathbf{W}}_{n+2} &= \beta_1 \mathbf{W}_{n+1} + \beta_0 \mathbf{W}_n, \end{aligned} \quad (12)$$

where  $\bar{t} = \beta_1 t_{n+1} + \beta_0 t_n = t_n + \beta_1 \Delta t$ . This one-leg formulation is second-order accurate if the coefficients satisfy (10b).

Let us define

$$\mathbf{V}_n = \mathbf{W}_n - \theta \mathbf{W}_{n-1}, \quad \theta \in [0, 1), \quad n \geq 1. \quad (13)$$

Furthermore, we introduce the coefficients

$$\begin{aligned} \alpha_1^* &= -\alpha_1 - \alpha_2 \theta, & \alpha_2^* &= -\alpha_0 - \alpha_1 \theta - \alpha_2 \theta^2 = (1 - \theta)(\alpha_2 \theta - \alpha_0), \\ \beta_1^* &= \beta_1, & \beta_2^* &= \beta_0 + \beta_1 \theta. \end{aligned} \quad (14)$$

The parameter  $\theta$  in (13) and (14) will be chosen such that the coefficients in (14) satisfy

$$\alpha_j^* \geq 0, \quad \beta_j^* \geq 0, \quad j = 1, 2. \quad (15)$$

Assuming positive starting values

$$\mathbf{V}_1 \geq 0 \text{ and } \mathbf{W}_1 \geq 0, \quad (16)$$

we have the following theorem.

**Theorem 1.** *Suppose that  $\Delta t \leq \mathcal{C} \Delta t_{FE}$ , with  $\mathcal{C} = \min\left(\frac{\alpha_1^*}{\beta_1^*}, \frac{\alpha_2^*}{\beta_2^*}\right)$ , and  $\theta$  is such that the conditions (15) and (16) are satisfied. Then  $\mathbf{V}_n \geq 0$  and  $\mathbf{W}_n \geq 0$  for all  $n \geq 1$ .*

*Proof.* The formulae (12)–(13) give

$$\alpha_2 \mathbf{V}_{n+2} = \alpha_1^* \mathbf{V}_{n+1} + \alpha_2^* \mathbf{W}_n + \Delta t \mathbf{F}(\bar{t}, \bar{\mathbf{W}}_{n+2}), \quad (17)$$

$$\bar{\mathbf{W}}_{n+2} = \beta_1^* \mathbf{V}_{n+1} + \beta_2^* \mathbf{W}_n. \quad (18)$$

Adding  $\mathcal{C} \bar{\mathbf{W}}_{n+2}$  to both sides in equation (17) we obtain

$$\alpha_2 \mathbf{V}_{n+2} = (\alpha_1^* - \mathcal{C} \beta_1^*) \mathbf{V}_{n+1} + (\alpha_2^* - \mathcal{C} \beta_2^*) \mathbf{W}_n + \mathcal{C} \bar{\mathbf{W}}_{n+2} + \Delta t \mathbf{F}(\bar{t}, \bar{\mathbf{W}}_{n+2}).$$

The coefficients in this relation are non-negative, due to the definition of  $\mathcal{C}$  and (11). Therefore,  $\mathbf{V}_{n+2} \geq 0$  if

$$\mathbf{V}_{n+1} \geq 0, \quad \mathbf{W}_n \geq 0, \quad \mathcal{C} \bar{\mathbf{W}}_{n+2} + \Delta t \mathbf{F}(\bar{t}, \bar{\mathbf{W}}_{n+2}) \geq 0. \quad (19)$$

The term  $\mathcal{C} \bar{\mathbf{W}}_{n+2} + \Delta t \mathbf{F}(\bar{t}, \bar{\mathbf{W}}_{n+2})$  can be seen as a scaled forward Euler step. Thus, it is non-negative if  $\bar{\mathbf{W}}_{n+2} \geq 0$  and  $\Delta t \leq \mathcal{C} \Delta t_{FE}$ . From (18) and (15) we see that  $\bar{\mathbf{W}}_{n+2} \geq 0$  if

$$\mathbf{V}_{n+1} \geq 0 \quad \text{and} \quad \mathbf{W}_n \geq 0. \quad (20)$$

Combining (19) and (20) we have

$$\mathbf{V}_{n+2} \geq 0 \text{ if } \mathbf{V}_{n+1} \geq 0 \text{ and } \mathbf{W}_n \geq 0. \quad (21)$$

By assumption, we know that  $\mathbf{V}_1 \geq 0$ ,  $\mathbf{W}_1 \geq 0$  (see (16)) and  $\mathbf{W}_0 \geq 0$ . Thus, (21) yields  $\mathbf{V}_2 \geq 0$ . As a result, relation (13) gives  $\mathbf{W}_2 = \mathbf{V}_2 + \theta\mathbf{W}_1 \geq 0$ . Having  $\mathbf{V}_2 \geq 0$  and  $\mathbf{W}_1 \geq 0$ , we obtain  $\mathbf{V}_3 \geq 0$  (again by (21)) which results in  $\mathbf{W}_3 = \mathbf{V}_3 + \theta\mathbf{W}_2 \geq 0$ , etc. for all  $n \geq 4$ .  $\square$

Let us now return to assumption (16) on the starting values. If  $\mathbf{W}_1$  is calculated by the forward Euler method then we have  $\mathbf{W}_1 \geq 0$  for all  $\Delta t \leq \Delta t_{FE}$ . Moreover,  $\mathbf{V}_1 = \mathbf{W}_1 - \theta\mathbf{W}_0 = (1 - \theta)\mathbf{W}_0 + \Delta t\mathbf{F}_0 \geq 0$  under the additional step size restriction  $\Delta t \leq (1 - \theta)\Delta t_{FE}$ .

Using the above considerations we can formulate the following theorem on the positivity condition for the one-leg method.

**Theorem 2.** *If  $\mathbf{W}_1$  is obtained by the forward Euler method (5) and  $\theta$  is such that condition (15) is satisfied, then the one-leg method (12) is positive under the step size restriction  $\Delta t \leq \gamma^{OL}(\theta)\Delta t_{FE}$  where*

$$\gamma^{OL}(\theta) = \min(\mathcal{C}, 1 - \theta) = \min\left(\frac{-\alpha_1 - \alpha_2\theta}{\beta_1}, \frac{(1 - \theta)(\alpha_2\theta - \alpha_0)}{\beta_0 + \beta_1\theta}, 1 - \theta\right). \quad (22)$$

It is illustrative to compare this  $\gamma^{OL}(\theta)$  with the  $\gamma(\theta)$  derived in (8): Condition (15) gives  $\theta \in [\theta_{min}, \theta_{max}]$ , where

$$\begin{aligned} \theta_{min} &= \max\left(\frac{\alpha_0}{\alpha_2}, -\frac{\beta_0}{\beta_1}\right) = -\frac{\beta_0}{\beta_1}, \\ \theta_{max} &= \min\left(-\frac{\alpha_1}{\alpha_2}, 1\right). \end{aligned}$$

Observe that the terms in the minimum function in (22) are monotonic decreasing functions of  $\theta$ . Therefore, the optimal  $\gamma^{OL}(\theta)$ -value is obtained at  $\theta = \theta_{min} = \frac{2-\xi}{2+\xi}$  and is given by

$$\gamma_{max}^{OL} = \min\left(\frac{2(1 + \xi)(2 - \xi)}{(2 + \xi)^2}, \frac{2\xi}{2 + \xi}\right). \quad (23)$$

The result is plotted in Figure 2. From this figure we see that the best method with respect to positivity is no longer the method with  $\xi = \frac{2}{3}$ . The optimal method with respect to positivity is now the method with  $\xi = \frac{1}{4}(\sqrt{17} - 1) \approx 0.78$ . The corresponding  $\gamma_{max}^{OL}$  is then  $\frac{1}{2}(\sqrt{17} - 3) \approx 0.56$ . Comparing (9) and (23) we see that the one-leg method allows a slightly larger time step than the linear two-step method.

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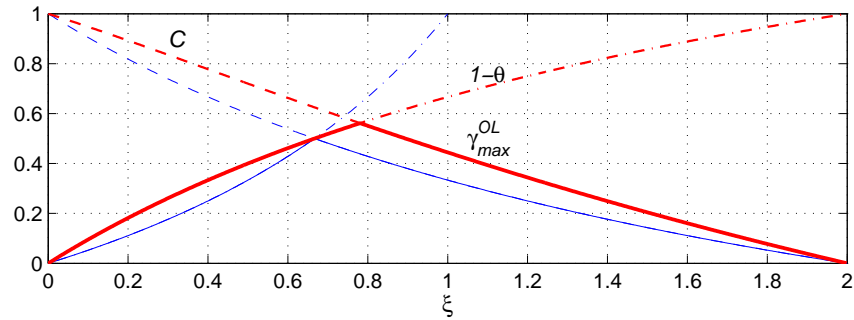


Figure 2: Step size restriction for positivity of the one-leg methods (thick lines) and of the linear two-step methods (thin lines, obtained from Figure 1).

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