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# A Note on Monotonicity of a Rosenbrock Method

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For a dissipative differential equation with stationary solution  $u^*$ , the difference between any solution  $U(t)$  and  $u^*$  is nonincreasing with  $t$ . In this note we present necessary and sufficient conditions in order for a similar monotonicity property to hold for numerical approximations computed from a Rosenbrock method. Our results also provide global convergence results for some modifications of Newton's method.

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## 1. INTRODUCTION

Consider an initial value problem in  $\mathbb{R}^m$

$$U'(t) = f(U(t)) \quad (t \geq 0), \quad (1.1a)$$

$$U(0) = u_0 \quad (1.1b)$$

whose solution  $U(t)$  tends to a stationary solution  $u^* \in \mathbb{R}^m$ . For the numerical solution of (1.1) we consider the Rosenbrock method

$$u_{n+1} = u_n + (I - h\theta f'(u_n))^{-1} h f(u_n) \quad (1.2)$$

where  $\theta$  is a positive parameter,  $h > 0$  is the stepsize and the vectors  $u_n \in \mathbb{R}^m$  approximate  $U(t_n)$ ,  $t_n = nh$  ( $n = 0, 1, 2, \dots$ ).

Assume the function  $f$  is dissipative with respect to an inner product  $\langle \cdot, \cdot \rangle$  on  $\mathbb{R}^m$  ( $\langle f(\tilde{u}) - f(u), \tilde{u} - u \rangle \leq 0$  for all  $\tilde{u}, u \in \mathbb{R}^m$ ) and let  $\|x\| = \langle x, x \rangle^{1/2}$  (for  $x \in \mathbb{R}^m$ ). This assumption implies that the difference  $\|\tilde{U}(t) - U(t)\|$  of any two solutions of the differential equation (1.1a) is nonincreasing with  $t$ . The corresponding property for the numerical approximations,  $\|\tilde{u}_{n+1} - u_{n+1}\| \leq \|\tilde{u}_n - u_n\|$ , only holds under additional, rather restrictive conditions on  $f$  (see e.g. [3]). In this note we look at the less exacting monotonicity property

$$\|u_{n+1} - u^*\| \leq \|u_n - u^*\|, \quad (1.3)$$

and we shall present conditions on  $f$  which are necessary and sufficient for (1.3) to hold with arbitrary stepsize  $h$ . Under somewhat stronger conditions on  $f$  the convergence of  $u_n$  to  $u^*$  can be guaranteed. These results are relevant to stiff ordinary differential equations and to partial differential equations (via the method of lines) since neither the Lipschitz constant of  $f$  nor the dimension  $m$  are involved.

The monotonicity property (1.3) is of particular interest if scheme (1.2) is regarded as a time-marching procedure for finding stationary solutions. The scheme has been used for this purpose in [4] with  $\theta = 1$  (and with an approximation to the Jacobian matrix  $f'(u_n)$ ; cf.(2.1)). We note that in such a situation (1.2) can be considered as a modified Newton procedure for solving  $f(u) = 0$ . By introducing  $\omega = 1/\theta$  and  $\lambda = 1/h\theta$  we can rewrite (1.2) as

$$u_{n+1} = u_n - \omega(f'(u_n) - \lambda I)^{-1} f(u_n),$$

in which  $\omega > 0$  can be viewed as a relaxation parameter and  $\lambda > 0$  ensures that  $f'(u_n) - \lambda I$  is

nonsingular whenever  $f$  is dissipative (see [5; sect.5.4,7.1]).

## 2. MONOTONICITY FOR NUMERICAL APPROXIMATIONS

Besides the Rosenbrock method (1.2) we also consider the more general linearly implicit scheme

$$u_{n+1} = u_n + (I - h\theta J(u_n))^{-1} h f(u_n) \quad (2.1)$$

where  $J(u_n)$  is an  $m \times m$  matrix. Further we shall use the following notation. By  $L(\mathbb{R}^m)$  we denote the space of linear operators on  $\mathbb{R}^m$ . If  $\|\cdot\|$  is a norm on  $\mathbb{R}^m$ , the corresponding operator norm on  $L(\mathbb{R}^m)$  is also denoted by  $\|\cdot\|$ , and  $\mu[\cdot]$  will stand for the logarithmic norm (cf.[2]).

Consider the following set of assumptions (2.2)-(2.6), with  $\delta > 0$  and  $\epsilon \geq 0$ , which will be denoted by  $(A_1)$ .

$$m \in \mathbb{N} \text{ and } \|\cdot\| \text{ is a norm on } \mathbb{R}^m \text{ generated by an inner product } \langle \cdot, \cdot \rangle; \quad (2.2)$$

$$f: \mathbb{R}^m \rightarrow \mathbb{R}^m, u^* \in \mathbb{R}^m \text{ is a zero of } f, \text{ and } J: \mathbb{R}^m \rightarrow L(\mathbb{R}^m); \quad (2.3)$$

$$\left\{ \begin{array}{l} D = \{u: u \in \mathbb{R}^m, \|u - u^*\| < \delta\}, f \text{ is continuously differentiable on } D \\ \text{and } J \text{ is continuous on } D; \end{array} \right. \quad (2.4)$$

$$\left\{ \begin{array}{l} \text{for any } u \in D \text{ we have } \mu[f'(u)] \leq 0 \\ \text{and } J(u) \text{ does not have positive real eigenvalues;} \end{array} \right. \quad (2.5)$$

$$\left\{ \begin{array}{l} \text{for all } u, v \in D \text{ there is a } E(u, v) \in L(\mathbb{R}^m) \text{ such that} \\ f'(v) = J(u)(I + E(u, v)), \|E(u, v)\| \leq \epsilon. \end{array} \right. \quad (2.6)$$

Further  $(A_2)$  will stand for these assumptions (2.2)-(2.6) together with

$$J(u) = f'(u) \text{ (for all } u \in D). \quad (2.7)$$

In (2.4) continuously differentiable means that that the matrix of partial derivatives  $f'(u) = (\partial f_i(u) / \partial u_j)$  exists and depends continuously on  $u$ . The condition  $\mu[f'(u)] \leq 0$  on  $D$  is equivalent to requiring that  $f$  is dissipative on  $D$  (see e.g.[5, sect.5.4]). The condition in (2.6) states that the relative difference between  $f'(v)$  and  $J(u)$  is bounded by  $\epsilon$ ; in case  $J(u)$  is regular it reads  $\|J(u)^{-1}(f'(v) - J(u))\| \leq \epsilon$ . Thus, in a relative sense, the variation of  $f'$  on  $D$  may not be too large and  $J(u)$  has to approximate  $f'(u)$  accurately enough.

In order to formulate our main results we define the real functions  $\psi_k(k = 1, 2)$  on the interval  $[1/2, \infty)$  by

$$\psi_1(\theta) = \min\{2\theta - 1, 1\}, \quad (2.8)$$

$$\psi_2(\theta) = \min\{2\theta - 1, \sqrt{(2\theta - 1)/\theta}\}. \quad (2.9)$$

**THEOREM 2.1.** *Let  $h$  and  $\delta$  be positive, and  $k$  equal to 1 or 2. We have  $\|u_{n+1} - u^*\| \leq \|u_n - u^*\|$  (whenever  $u_n \in D$  and  $(A_k)$  is valid) iff  $\theta \geq 1/2$  and  $\epsilon \leq \psi_k(\theta)$ .*

This theorem is an extension of a result by M.N. SPIJKER and the present author, see [7; sect. 4]. The proof will be given in the next section. The restriction  $\theta \geq 1/2$  in this theorem is not surprising since the methods with  $\theta < 1/2$  are not  $A$ -stable. For  $\theta = 1/2$  we see that the monotonicity property only holds for linear problems ( $\epsilon=0$ ).

Under slightly stronger conditions on  $f$  it can be shown that  $\|u_{n+1} - u^*\| < \|u_n - u^*\|$  (for  $u_n \in D, u_n \neq u^*$ ). This leads to the following result which will also be proved in section 3.

**THEOREM 2.2.** *Let  $h$  and  $\delta$  be positive, and  $k$  equal to 1 or 2. Assume  $u_0 \in D, \theta \geq 1/2, \epsilon \leq \psi_k(\theta)$  and*

( $A_k$ ). Assume in addition that either  $\epsilon < \psi_k(\theta)$  and  $J(u)$  is regular (for all  $u \in D$ ) or  $\mu[f'(u)] < 0$  (for all  $u \in D$ ). Then  $u^*$  is the unique zero of  $f$  in  $D$  and  $\lim_{n \rightarrow \infty} u_n = u^*$ .

### 3. PROOF OF THE MONOTONICITY RESULTS

#### 3.1. Preliminaries

In order to prove the theorems of section 2 we first derive some technical results. Consider arbitrary  $A, B \in L(\mathbb{R}^m)$  with  $m \in \mathbb{N}$ , and suppose  $\|\cdot\|$  is a norm on  $\mathbb{R}^m$  generated by an inner product  $\langle \cdot, \cdot \rangle$ . For any  $C \in L(\mathbb{R}^m)$  we denote by  $C^*$  its adjoint with respect to this inner product ( $\langle Cx, y \rangle = \langle x, C^*y \rangle$  for all  $x, y \in \mathbb{R}^m$ ).

The relation  $\|Bx\| \leq \gamma \|Ax\|$  (for all  $x \in \mathbb{R}^m$ ), with  $\gamma > 0$  given, implies the existence of a  $C \in L(\mathbb{R}^m)$  such that  $B = CA$ ,  $\|C\| \leq \gamma$ ; if  $A$  is regular we can take  $C = BA^{-1}$  and for singular  $A$  the inverse  $A^{-1}$  can be replaced by the generalized inverse of  $A$  (see e.g. [1; ch.8]). Since  $\|C^*\| = \|C\|$  for any  $C \in L(\mathbb{R}^m)$  one easily arrives at the following result.

**LEMMA 3.1.** *Let  $\gamma > 0$ . We have  $\|B^*x\| \leq \gamma \|A^*x\|$  (for all  $x \in \mathbb{R}^m$ ) iff  $B = AC$  for some  $C \in L(\mathbb{R}^m)$  with  $\|C\| \leq \gamma$ .*

Consider the following statements, with  $\theta \geq \frac{1}{2}$  and  $\epsilon \geq 0$ ,

$$B = A(I + E_1) \text{ for some } E_1 \in L(\mathbb{R}^m) \text{ with } \|E_1\| \leq \epsilon, \quad (3.1a)$$

$$A = B(I + E_2) \text{ for some } E_2 \in L(\mathbb{R}^m) \text{ with } \|E_2\| \leq \epsilon, \quad (3.1b)$$

and

$$B = \theta A(I + F) \text{ for some } F \in L(\mathbb{R}^m) \text{ with } \|F\| \leq 1. \quad (3.2)$$

**LEMMA 3.2.** *(3.1a) implies (3.2) iff  $\epsilon \leq \psi_1(\theta)$ .*

**PROOF.** Assuming (3.1a) and  $\epsilon \leq \psi_1(\theta)$  we set  $F = \theta^{-1}[E_1 + (1-\theta)I]$ , in which case  $B = \theta A(I + F)$  and

$$\|F\| \leq \theta^{-1}(\epsilon + |1-\theta|) \leq \theta^{-1}(\psi_1(\theta) + |1-\theta|) = 1.$$

To construct a counterexample in case  $\epsilon > \psi_1(\theta)$  we first consider the simple scalar (complex) example  $A = a$ ,  $B = b$  with  $a, b \in \mathbb{C}$ . The condition in (3.1a) corresponds to

$$|b - a| \leq \epsilon |a| \quad (3.3)$$

and (3.2) corresponds to

$$|b - \theta a| \leq \theta |a|. \quad (3.4)$$

By simple geometrical arguments it follows that for  $\epsilon > \psi_1(\theta)$  there exist  $a, b \in \mathbb{C}$  satisfying (3.3) but violating (3.4).

These considerations on  $\mathbb{C}$  lead to a counterexample with  $A = A_1$  and  $B = B_1 \in L(\mathbb{R}^2)$ ,

$$A_1 = \begin{bmatrix} \text{Re}a & -\text{Im}a \\ \text{Im}a & \text{Re}a \end{bmatrix}, B_1 = \begin{bmatrix} \text{Re}b & -\text{Im}b \\ \text{Im}b & \text{Re}b \end{bmatrix},$$

and with  $\|\cdot\|$  the Euclidian norm on  $\mathbb{R}^2$  (and the corresponding spectral norm on  $L(\mathbb{R}^2)$ ).  $\square$

**LEMMA 3.3.** *(3.1a) & (3.1b) implies (3.2) iff  $\epsilon \leq \psi_2(\theta)$ .*

PROOF. Assume (3.1a), (3.1b) and  $\epsilon \leq \psi_2(\theta)$ . To show that (3.2) holds it is, in view of lemma 3.1, sufficient to consider the remaining case  $1 < \epsilon^2 \leq (2\theta - 1)/\theta$ . From lemma 3.1 it follows that for any  $x \in \mathbb{R}^m$

$$\|B^*x\|^2 - 2\langle A^*x, B^*x \rangle + \|A^*x\|^2 \leq \epsilon^2 \|A^*x\|^2,$$

$$\|B^*x\|^2 - 2\langle A^*x, B^*x \rangle + \|A^*x\|^2 \leq \epsilon^2 \|B^*x\|^2.$$

Combining these inequalities we obtain

$$\langle A^*x, B^*x \rangle \geq (1 - \frac{1}{2}\epsilon^2) \|B^*x\|^2.$$

From our assumption on  $\epsilon$  it follows that

$$\|B^*x\|^2 \leq 2\theta \langle A^*x, B^*x \rangle,$$

and hence

$$\|(B^* - \theta A^*)x\| \leq \theta \|A^*x\|.$$

Statement (3.2) now follows by again applying lemma 3.1.

Now assume  $\epsilon > \psi_2(\theta)$  and  $1/2 \leq \theta \leq 1$ . Then we obtain a (scalar real) counterexample by taking  $m = 1, A = -1, B = -1 - \epsilon$ .

Finally assume  $\epsilon > \psi_2(\theta)$  and  $\theta > 1$ . Let  $\xi \in ((2\theta - 1)/\theta, 2)$  such that  $\xi < \epsilon^2$ , and take  $a, b \in \mathbb{C}$  such that  $b/a$  equals  $(1 - \xi/2) + i\sqrt{\xi(1 - \xi/4)}$ . Then  $|b - a| \leq \epsilon|a|$  and  $|b - a| \leq \epsilon|b|$  but  $|b - \theta a| > \theta|a|$ . As in the proof of lemma 3.2 such  $a, b \in \mathbb{C}$  lead to  $A_2, B_2 \in L(\mathbb{R}^2)$  such that for  $A = A_2, B = B_2$  the statements (3.1a), (3.1b) hold whereas (3.2) is violated.  $\square$

We note that in the above counterexamples which prove the necessity of  $\epsilon \leq \psi_k(\theta)$  we can choose the  $a, b \in \mathbb{C}$  such that  $\operatorname{Re} a \leq 0, \operatorname{Re} b \leq 0$ . This leads to  $A_k, B_k \in L(\mathbb{R}^2)$  satisfying  $\mu[A_k] \leq 0, \mu[B_k] \leq 0$  (for  $k = 1, 2$ ).

The following lemma is a slight generalization of results in [6] and [7; lemma 4.3].

LEMMA 3.5. Assume  $I - \lambda\theta A$  is regular for all  $\lambda > 0$ . We have  $\|I + (I - \lambda\theta A)^{-1}\lambda B\| \leq 1$  (for all  $\lambda > 0$ ) iff  $\mu[B] \leq 0$  and (3.2) holds.

PROOF. Let  $C = B - \theta A$ . Then  $I + (I - \lambda\theta A)^{-1}\lambda B = (I - \lambda\theta A)^{-1}(I + \lambda C)$ , and it follows that  $\|I + (I - \lambda\theta A)^{-1}\lambda B\| \leq 1$  iff

$$\|(I + \lambda C^*)x\| \leq \|(I - \lambda\theta A^*)x\| \text{ (for all } x \in \mathbb{R}^m\text{)}.$$

The latter inequality can be written as

$$2\lambda \langle B^*x, x \rangle + \lambda^2 \|C^*x\|^2 \leq \lambda^2 \|\theta A^*x\|^2 \text{ (for all } x \in \mathbb{R}^m\text{)}.$$

Clearly this holds for all  $\lambda > 0$  iff

$$\langle Bx, x \rangle \leq 0 \text{ and } \|C^*x\| \leq \|\theta A^*x\| \text{ (for all } x \in \mathbb{R}^m\text{)}.$$

Application of lemma 3.1 completes the proof.  $\square$

### 3.2. The proof of theorem 2.1

For  $u \in D$  we define

$$\sigma(u) = \int_0^1 \|I + (I - h\theta J(u))^{-1} h f'(u^* + \tau(u - u^*))\| d\tau. \quad (3.5)$$

Since for any  $u_n \in D$

$$\|u_{n+1} - u^*\| = \|u_n - u^* + (I - h\theta J(u_n))^{-1} h(f(u_n) - f(u^*))\|$$

it follows by the mean-value theorem that

$$\|u_{n+1} - u^*\| \leq \sigma(u_n) \|u_n - u^*\|. \quad (3.6)$$

Application of the lemmas 3.2, 3.3 and 3.5 with  $A = hJ(u_n)$  and  $B = hf'(u^* + \tau(u_n - u^*))$  shows the sufficiency of  $\epsilon \leq \psi_k(\theta)$  for having  $\|u_{n+1} - u^*\| \leq \|u_n - u^*\|$  in case  $(A_k)$  holds,  $k = 1, 2$ . The necessity will be proved by some counterexamples.

A counterexample in case  $(A_1)$  holds,  $\epsilon > \psi_1(\theta)$  is given by  $hJ(u) = \lambda A_1$ ,  $hf(u) = \lambda B_1 u$  (for  $u \in \mathbb{R}^2$ ) with  $A_1, B_1$  as in the proof of lemma 3.2,  $\lambda > 0$  and  $\|\cdot\|$  the Euclidean norm on  $\mathbb{R}^2$ . With  $u^* = 0$ ,  $u_n \in \mathbb{R}^2$ , we obtain

$$\begin{aligned} \|u_{n+1} - u^*\| &= \|(I + (I - \lambda\theta A_1)^{-1} \lambda B_1)(u_n - u^*)\| = \\ &= \|I + (I - \lambda\theta A_1)^{-1} \lambda B_1\| \|u_n - u^*\| > \|u_n - u^*\| \end{aligned}$$

provided  $\lambda > 0$  is suitably chosen (see lemma 3.5).

Next we give a scalar (real) example for  $\epsilon > \psi_2(\theta)$ ,  $1/2 \leq \theta \leq 1$  in case  $(A_2)$  is valid. This counterexample is similar to one given by SANDBERG and SHICHMAN [6].

Take, for convenience,  $h = 1, \delta > 1$  and  $u^* = 0, u_0 = 1$ . Let  $\eta \in (2\theta - 1, \epsilon)$  and  $f(u) = \lambda g(u)$  (for  $u \in \mathbb{R}$ ) with  $\lambda > 0$  and  $g: \mathbb{R} \rightarrow \mathbb{R}$  a continuously differentiable function such that

$$\begin{aligned} g(0) &= 0, \quad g'(u) \in [-1 - \epsilon, -1] \text{ (for all } u \in \mathbb{R}), \\ g(u) &= -u + \eta \text{ (for } u \leq 1), \quad g(u) = -u - \eta \text{ (for } u \geq 1). \end{aligned}$$

Such an  $f$  meets the conditions imposed in  $(A_2)$ . Further we have

$$u_1 = (1 + \lambda\theta)^{-1} (1 + \lambda(\theta - 1 - \eta))$$

and thus  $|u_1 - u^*|$  tends to  $\theta^{-1}(\eta + 1 - \theta) > 1 = |u_0 - u^*|$  for  $\lambda \rightarrow \infty$ .

Finally we assume  $\epsilon > \psi_2(\theta)$ ,  $\theta > 1$ . For this we construct a complex, scalar counterexample, which can as before be converted to a real one by identifying  $\mathbb{C}$  with  $\mathbb{R}^2$  in the usual way. Suppose  $(2\theta - 1)/\theta < \xi < \min\{2, \epsilon^2\}$  and let  $a, b \in \mathbb{C}$  be such that  $\operatorname{Re} a < 0$ ,  $\operatorname{Re} b < 0$  and  $b/a = (1 - \xi/2) + i\sqrt{\xi(1 - \xi/4)}$  (as in the proof of lemma 3.3). Then  $|b - a| < \epsilon|a|$ ,  $|b - a| < \epsilon|b|$  but  $|b - \theta a| > \theta|a|$ , and thus for  $\lambda > 0$  suitably chosen  $|1 + (1 - \lambda\theta a)^{-1} \lambda b| > 1$  (see lemma 3.5). We put  $\alpha = \lambda a$  and  $\beta = \lambda b$ .

Let  $D$  be the unit disk in  $\mathbb{C}$ ,  $h = 1, u^* = 0$ , and define

$$\begin{aligned} f(u) &= \Phi(0)(\alpha - \beta) + \alpha u + \Phi(u)(\beta - \alpha), \\ \Phi(u) &= -\frac{2k}{k+1} \left(\frac{1}{2} - \frac{1}{2}u\right)^{1+1/k} \end{aligned}$$

for  $u \in \mathbb{C}$ , where  $k \in \mathbb{N}$  is to be specified later. Then  $f(0) = 0$  and

$$\begin{aligned} f'(u) &= \alpha + \phi(u)(\beta - \alpha), \\ \phi(u) &= \left(\frac{1}{2} - \frac{1}{2}u\right)^{1/k}. \end{aligned}$$

The image of  $D$  under  $\phi$  tends to the interval  $(0, 1)$  on the real axis if  $k \rightarrow \infty$ . By using this property it can be shown that, for  $k$  sufficiently large, the conditions on  $f$  in  $(A_2)$  are satisfied. Moreover, since  $f'(1) = \alpha$  and  $f(1)$  tends to  $\beta$  for  $k \rightarrow \infty$ ,

$$|1 + (1 - \theta f'(1))^{-1} f(1)| > 1$$

provided  $k$  is sufficiently large. It follows that, for such  $k$  and  $u_0$  close to 1,

$$|u_1 - u^*| > |u_0 - u^*|.$$

### 3.3. The proof of theorem 2.2

First we show that under the assumptions of theorem 2.2 the function  $\sigma$ , defined by (3.5), satisfies  $\sigma(u) < 1$  (for all  $u \in D$ ). Examination of the proof of lemma 3.5 shows that for  $A, B \in L(\mathbb{R}^m)$  satisfying (3.2) and  $\mu[B] \leq 0$  we have

$$\|I + (I - \lambda\theta A)^{-1}\lambda B\| < 1 \text{ (for all } \lambda > 0\text{)}$$

provided we assume in addition either

$$\mu[B] < 0$$

or

$$A \text{ is regular and } B = \theta A(I + F), \|F\| < 1.$$

Further it is easily seen, by regarding the proofs of lemma 3.2 and lemma 3.3, that if  $A$  is regular and we have (3.1a) with  $\epsilon < \psi_1(\theta)$  or (3.1a), (3.1b) with  $\epsilon < \psi_2(\theta)$  then there is an  $F \in L(\mathbb{R}^m)$  such that  $B = \theta A(I + F), \|F\| < 1$ . By setting  $A = hJ(u), B = hf'(u^* + \tau(u - u^*))$  it follows that the assumptions of theorem 2.2 imply  $\sigma(u) < 1$  on  $D$ .

The function  $\sigma$  is continuous on  $D$ . Therefore we obtain for arbitrary  $u_0 \in D$

$$\|u_n - u^*\| \leq s_0^n \|u_0 - u^*\|$$

with  $s_0 = \max\{\sigma(u) : u \in D, \|u - u^*\| \leq \|u_0 - u^*\|\} < 1$ . From this it is clear that  $u^*$  is the unique zero of  $f$  in  $D$  and that the  $u_n$  converge to  $u^*$  for  $n \rightarrow \infty$ .

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