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ON MONOTONICITY AND SIGN-CONSTANCY OF SOME RATIONAL EXPLICIT METHODS FOR NONLINEAR SYSTEMS OF ORDINARY DIFFERENTIAL EQUATIONS

ПРО МОНОТОННІСТЬ І ЗНАКОСТАЛІСТЬ ДЕЯКИХ ДРОБОВО-РАЦІОНАЛЬНИХ ЯВНИХ МЕТОДІВ ДЛЯ НЕЛІНІЙНИХ СИСТЕМ ЗВИЧАЙНИХ ДИФЕРЕНЦІАЛЬНИХ РІВНЯНЬ

One particular type of explicit rational numerical methods for nonlinear systems of ordinary differential equations is studied. A property called sign-constancy of an integration method is considered. This means that the product of approximate solutions at two consecutive grid points is positive for the corresponding differential equation. Unconditional (i.e., for all step sizes) monotonicity and sign-constancy of rational methods are proved.

Вивчається один тип числових дробово-раціональних явних методів для розв'язування нелінійних систем звичайних диференціальних рівнянь. Розглядається властивість знакосталості методу інтегрування. Знакосталість означає, що скалярний добуток наближених розв'язків, взятих у двох сусідніх точках сітки, є додатним для відповідного диференціального рівняння. Доведено безумовну (для всіх значень кроку) монотонність і знакосталість дробово-раціональних методів.

1. Introduction. Let $(\cdot,\cdot)$ be an inner product on $\mathbb{C}^m$ and let $\|\cdot\|$ be the corresponding inner product norm.

We consider the Cauchy problem for the class $\mathcal{F}_1$ of *monotone nonlinear autonomous systems* of ordinary differential equations, i.e.,

$$y'(t) = f(y(t)), \quad \operatorname{Re}\Big(f(y(t)), y(t)\Big) < 0, \tag{1}$$
$$y(0) = y_0, \quad t \in [0; T],$$

where $f\colon \mathbb{C}^m \to \mathbb{C}^m$ is a sufficiently smooth function.

For the inner product norm and (1), it is easy to verify that, for all $h > 0$, any solution $y(t)$ satisfies

$$\|y(t+h)\| \le \|y(t)\|.$$

According to [1], we call an integration method *monotone* for (1) if the corresponding inequality holds also with respect to this norm for two consecutive approximations with step size $h \in (0; h_0)$. In the present note, we call the method *unconditionally monotone* if it is monotone for all $h > 0$.

We consider the following standard explicit one-step integration methods of the first and second order applied to (1):

$$\bar{u} = u + hf(u), \tag{2}$$

$$\hat{u} = u + 0{,}5\, h\left[f(u) + f(\overline{u})\right], \tag{3}$$

where u is an approximate solution at a certain grid point t, $\overline{u}$ and $\hat{u}$ are approximate solutions at the grid point $t+h$ obtained by methods (2) and (3), respectively.

Methods (2) and (3) are monotone with corresponding values of h_0 which depend on the given equation (1) and, therefore, they are not unconditionally monotone.

Let $\mathcal{F}_2 \subset \mathcal{F}_1$ denote a class of *sign-constant systems* (on the interval $[a;b]$) of ordinary differential equations, which means that, for the corresponding exact solutions, the inequality

$$\operatorname{Re}(y(t_1), y(t_2)) > 0$$

holds for all $t_1, t_2 \in [a;b] \subseteq [0;T]$.

Now we introduce a property of the numerical method called the *sign-constancy*, which is useful for the theoretical study of integration methods applied to $\mathcal{F}_2$.

Definition 1. *The integration method is called unconditionally sign-constant if, for a system from the class $\mathcal{F}_2$ and for all $h>0$, the following inequality holds:*

$$\operatorname{Re}(u, \overline{u}) > 0.$$

In [2], it was shown that, for a particular rational first-order method, we have

unconditional sign-constancy $\Rightarrow$ unconditional monotonicity.

Explicit methods (2) and (3) are not unconditionally monotone and (2) is not unconditionally sign-constant. One can prove the unconditional sign-constancy of (3) for the linear system $y' = Ay$ with a self-adjoint matrix A only. It is easy to see that implicit mid-point, trapezoidal, and some other methods are not unconditionally sign-constant even for the scalar equations $y' = ay$ with $a<0$. However, the implicit Euler method possesses this property.

Some classes of rational explicit Runge–Kutta formulas were investigated also in [3–6]. In this note, some new rational methods are introduced and their unconditional monotonicity and sign-constancy are proved.

2. A rational first order method. A two-parameter family of unconditionally monotone and unconditionally sign-constant rational methods of the first order was presented in [2]. In the recent note, we consider the b-parameter first-order family for an arbitrary $b>0$

$$\overline{u} = u + h\,p(r) f, \quad f = f(u), \tag{4}$$

where

$$p(r) = \frac{1}{1+br^2}, \quad r = \frac{h(f,f)}{\operatorname{Re}(f,u)}.$$

The parameter b affects the local error so that we must choose it as small as possible. The following theorems help us to do that:

Theorem 1. *If $b > 1/16$, then method (4) is unconditionally monotone for $\mathcal{F}_1$.*

Proof. Since

$$(\overline{u},\overline{u}) = (u,u) + 2hp\operatorname{Re}(f,u) + h^2p^2(f,f) =$$
$$= (u,u) + h^2p(f,f)\left[p + \frac{2\operatorname{Re}(f,u)}{h(f,f)}\right] =$$
$$= (u,u) + h^2p(f,f)\left[p + \frac{2}{r}\right],$$

for any function $p = p(r)$ such that·

$$0 < p(r) < -\frac{2}{r} \tag{5}$$

and for all $h > 0$, we have

$$\|\bar{u}\| < \|u\|.$$

Choosing

$$p(r) = \frac{1}{1+br^2}, \quad r = \frac{h(f,f)}{\mathrm{Re}(f,u)},$$

it is easy to verify that (5) holds if $b > 1/16$.

Theorem 2. *If* $b > 1/4$, *then method* (4) *is unconditionally sign-constant for* $\mathcal{F}_2$.

Proof. The following relations hold:

$$\mathrm{Re}(\bar{u},u) = (u,u) + hp\,\mathrm{Re}(f,u) = (u,u)\left[1 + hp\frac{\mathrm{Re}(f,u)}{(u,u)}\right] =$$

$$= \frac{(u,u)}{\left(1+br^2\right)}\left[1 + \frac{\mathrm{Re}(f,u)}{(u,u)}h + \frac{b(f,f)^2}{\mathrm{Re}^2(f,u)}h^2\right].$$

This quadratic function of h is positive if

$$\frac{\mathrm{Re}^2(f,u)}{(u,u)^2} - 4b\frac{(f,f)^2}{\mathrm{Re}^2(f,u)} < 0. \tag{6}$$

By using the Cauchy–Schwarz–Bunjakovsky inequality, we establish that inequality (6) will hold for all $u \in \mathbb{C}^m$ if $b > 1/4$, which completes the proof.

Method (4) may be considered as a modification of Euler's scheme (2) (which corresponds to the special choice $b = 0$ in (4)). Here, the function $p(r)$ provides a regularization in the sense that the inequality $\|\bar{u}\| < \|u\|$ holds for all $h > 0$.

3. Rational second-order method. Similar to (4), a rational second-order method can be chosen in the form

$$\begin{aligned} \bar{u} &= u + hp(r)f, \\ \hat{u} &= u + 0{,}5\,h[\,p(r)f + p(\bar{r})\bar{f}\,], \end{aligned} \tag{7}$$

where

$$p(r) = \frac{1}{1+br^2}, \quad r = \frac{h(f,f)}{\mathrm{Re}(f,u)},$$

and

$$\bar{f} = f(\bar{u}) = f(u + hp(r)f), \quad \bar{r} = \frac{h(\bar{f},\bar{f})}{\mathrm{Re}(\bar{u},\bar{f})}.$$

It is easy to verify that method (7) has the second order of accuracy. It may be regarded as a modification of (3). Now we are going to prove unconditional monotonicity and sign-constancy of (7). We need the following lemma:

Lemma 1. *For approximate solutions of problem* (1), *the following inequality holds for all* $h > 0$:

$$\mathrm{Re}(f,u) + 0{,}5\,hp(f,f) < 0. \tag{8}$$

The proof follows from the property of unconditional monotonicity of method (4) because $\|\bar{u}\| < \|u\|$ for $b > 1/16$ and

$$(\bar{u},\bar{u}) = (u,u) + 2hp\operatorname{Re}(f,u) + h^2p^2(f,f) > 0.$$

Theorem 3. *Method* (7) (*with* $b > 1/16$) *is unconditionally monotone for* $\mathcal{F}_1$.

Proof. Let $\bar{p} = p(\bar{r})$. Using inequality (8) three times in the following transformations, we get for all $h > 0$:

$$(\hat{u},\hat{u}) = (u,u) + hp\operatorname{Re}(f,u) + h\bar{p}\operatorname{Re}(\bar{f},u) + 0{,}25h^2\|pf+\bar{p}\bar{f}\|^2 =$$

$$= (u,u) + 0{,}5hp[\operatorname{Re}(f,u) + 0{,}5hp(f,f)] + 0{,}5hp\operatorname{Re}(f,u) +$$

$$+ h\bar{p}\left[\operatorname{Re}(\bar{f},u) + 0{,}5hp\operatorname{Re}(f,\bar{f}) + 0{,}25h\bar{p}(\bar{f},\bar{f})\right] <$$

$$< (u,u) + 0{,}5hp[\operatorname{Re}(f,u) + 0{,}5hp(f,f)] - 0{,}25h^2p^2(f,f) +$$

$$+ h\bar{p}\left[\operatorname{Re}(\bar{f},u) + 0{,}5hp\operatorname{Re}(f,\bar{f}) + 0{,}25h\bar{p}(\bar{f},\bar{f})\right] +$$

$$+ 0{,}25h^2p^2\|pf+\bar{p}\bar{f}\|^2 =$$

$$= (u,u) + 0{,}5hp[\operatorname{Re}(f,u) + 0{,}5hp(f,f)] - 0{,}25h^2p^2(f,f) +$$

$$+ h\bar{p}\operatorname{Re}(\bar{f},u) + 0{,}5h\bar{p}p\operatorname{Re}(f,\bar{f}) + 0{,}25h^2\bar{p}^2(\bar{f},\bar{f}) + 0{,}25h^2p^2(f,f) +$$

$$+ 0{,}5h\bar{p}p\operatorname{Re}(f,\bar{f}) + 0{,}25h^2\bar{p}^2(\bar{f},\bar{f}) =$$

$$= (u,u) + 0{,}5hp[\operatorname{Re}(f,u) + 0{,}5hp(f,f)] + h\bar{p}\operatorname{Re}(\bar{f},u) +$$

$$+ hp\bar{p}(f,\bar{f}) + 0{,}5h^2\bar{p}^2(\bar{f},\bar{f}) = (u,u) +$$

$$+ 0{,}5hp[\operatorname{Re}(f,u) + 0{,}5hp(f,f)] + h\bar{p}\left[\operatorname{Re}(\bar{f},u) + 0{,}5h\bar{p}(\bar{f},\bar{f})\right] < (u,u).$$

Theorem 4. *Method* (7) (*with* $b > 1/16$) *is unconditionally sign-constant for* $\mathcal{F}_2$.

Proof. Here, we start again with $(\hat{u},\hat{u})$:

$$(\hat{u},\hat{u}) = \left(u + 0{,}5hpf + 0{,}5h\bar{p}\bar{f},\hat{u}\right) =$$

$$= \operatorname{Re}(u,\hat{u}) + 0{,}5\operatorname{Re}\left(hpf + h\bar{p}\bar{f},\hat{u}\right) =$$

$$= \operatorname{Re}(u,\hat{u}) + 0{,}5h\operatorname{Re}\left(pf+\bar{p}\bar{f},u + 0{,}5h\left(pf+\bar{p}\bar{f}\right)\right) =$$

$$= \operatorname{Re}(u,\hat{u}) + 0{,}5hp\operatorname{Re}(f,u) + 0{,}5h\bar{p}\operatorname{Re}(\bar{f},u) + 0{,}25h^2\|pf+\bar{p}\bar{f}\|^2 =$$

$$= \operatorname{Re}(u,\hat{u}) + 0{,}5hp[\operatorname{Re}(f,u) + 0{,}5hp(f,f)] +$$

$$+ 0{,}5h\bar{p}\left[\operatorname{Re}(\bar{f},u) + hp\operatorname{Re}(f,\bar{f}) + 0{,}5h\bar{p}(\bar{f},\bar{f})\right] =$$

$$= \operatorname{Re}(u,\hat{u}) + 0{,}5hp[\operatorname{Re}(f,u) + 0{,}5hp(f,f)] +$$

$$+ 0{,}5h\bar{p}\left[\operatorname{Re}(\bar{f},\bar{u}) + 0{,}5h\bar{p}(\bar{f},\bar{f})\right] > 0.$$

The expressions in the square brackets are negative due to Lemma 1. Therefore, for all $h > 0$, we have $\operatorname{Re}(u,\hat{u}) > 0$, which was to be proved.

4. Conclusions. For both methods (4) and (7), we set $b = 1/12$, which is sufficient for solving the monotone systems (1). We implemented them as a pair of embeded methods using $\|\hat{u} - \bar{u}\|$ for the step size control.

Our numerical experiments show that we can integrate monotone equations with a step size that is, in average, two or three times larger compared to what methods (2) and (3) allow. We emphasize here that local errors of the rational method are affected by the additional term. Some overhead is needed also for computing inner products; therefore, essential advantages in processing time are possible for equations with a complicated right-hand side.

As a warning, it must be said that the methods discussed above are neither B-stable nor A-stable, [1] though formal applications of the scalar test equation $y' = \lambda y$ give A-acceptability. The reason is not obvious; here, we emphasize only that, for rational methods of this type, the stability for a scalar test equation is not equivalent to the stability for the simple linear system $y' = A y$, as we usually have for nonrational methods. Therefore, these methods cannot be efficiently applied to most stiff systems. But rational methods can be used for the numerical integration of semi-discrete parabolic problems whose solutions are often monotone and sign-constant (see also [1, 3]).

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