Computational Ordinary Differential Equations

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Stability Criteria in the Numerical Solution of Initial Value Problems

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1 Introduction

1.1. Consider the system of ordinary differential equations

$$U'(t) = f(t, U(t)) \tag{1.1}$$

with an initial condition $U(0) = u_0$. Here u_0 is a given vector in the s-dimensional real vector space $\mathbb{R}^s$ while $U(t) \in \mathbb{R}^s$ is unknown for $t > 0$. In all of the following $f(t, \xi)$ is assumed to be a given, continuous function from $\mathbb{R} \times \mathbb{R}^s$ to $\mathbb{R}^s$ with $s \geq 1$.

We will be concerned with numerical processes which yield approximations $u_n \in \mathbb{R}^s$ to the true solution $U(t_n)$ at the *grid points* $t_n = nh$. Here $h > 0$ denotes the *step size* of the process. We assume u_n to be computed from u_{n-1}, without using the former approximations u_{n-2}, $u_{n-3}, \cdots$.

We will deal with the *stability* analysis of the numerical process. Here the term stability is used to indicate that *any numerical errors introduced at some stage of the calculations are propagated in a mild fashion* in the subsequent steps of the process.

1.2. Much of the stability analysis in the numerical solution of equation (1.1) consists of studying the numerical method when applied to a very simple, linear, scalar *test equation*. In justification of focussing on such a simple test equation one can appeal to *two principles*.

The *first principle* underlies the replacement of (1.1) by the linear system

$$U'(t) = AU(t). \tag{1.2}$$

Here f is assumed to be differentiable, and A stands for the Jacobian matrix of f "frozen" at any point t^* belonging to the time-interval under consideration, i.e.

$$A = \frac{\partial}{\partial \xi} f(t^*, U(t^*)).$$

The first principle asserts that stability in the numerical solution of all linear equations (1.2) under consideration guarantees a stable behaviour of the original numerical process for (1.1).

The *second principle* is applied when one replaces (1.2) by the still simpler equation

$$U'(t) = \lambda U(t). \tag{1.3}$$

Here λ stands for any eigenvalue belonging to the spectrum $\sigma[A]$ of A. The second principle asserts that stability of the method in the solution of all relevant equations (1.3) guarantees stability in the solution of (1.2).

Clearly, a combination of these two principles provides a justification for basing the stability analysis of numerical methods for (1.1) on the test equation (1.3). See e.g. [1], [7], [8].

In this paper we will review some situations where the above principles break down, and other principles have to be used.

1.3. Suppose that the numerical calculations for approximating the solution to (1.1) are performed using a slightly perturbed starting vector $\widetilde{u}_0$ say, instead of u_0. We then would obtain new approximations, denoted by $\widetilde{u}_n$.

In a stability analysis of the numerical process for (1.1) the crucial question is whether the difference $\widetilde{u}_n - u_n$ can be bounded suitably in terms of the perturbation $\widetilde{u}_0 - u_0$. Therefore, one is looking for estimates of the type

$$\begin{array}{l} |\widetilde{u}_n - u_n| \le \gamma n^q |\widetilde{u}_0 - u_0| \qquad \text{(whenever } n \ge 1, \text{ and} \\ \{u_n\}, \{\widetilde{u}_n\} \text{ are generated by the same numerical process).} \end{array} \tag{1.4}$$

Here $|\cdot|$ is a given norm in $\mathbb{R}^s$ and $\gamma \ge 0$, $q \ge 0$ are independent of n, $\{u_n\}$, $\{\widetilde{u}_n\}$. Clearly, the estimate (1.4) amounts to *stability* if both γ and q are of moderate size. Property (1.4) with $q = 0$, $\gamma = 1$ is called *contractivity*.

2 Failing of the first principle: Runge–Kutta methods

2.1. As an illustration consider the method

$$u_n = u_{n-1} + \frac{h}{2}[f(t_{n-1}, u_{n-1}) + f(t_n, u_n)], \quad n = 1, 2, 3, \cdots$$

in the numerical solution of the problem

$$U'(t) = -1 + \exp[10^5(1 - 3U(t))], \quad U(0) = 1/3.$$

The true solution is $U(t) \equiv 1/3$.

We apply the method wi
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where $x_j \in \mathbb{R}^s$ are comput

$$x_i = hf(t_{n-1} + c_i h, u$$
for $i = 1, 2, \cdots, m$.

The coefficients a_{ij}, b_i are
$a_{i1} + a_{i2} + \cdots + a_{im}$.

The following definitio
Crouzeix [4]: Method (2.1)

$$\begin{cases} \text{all } b_i \ge 0, \text{ an} \\ Q_{ij} = b_i a_{ij} + \end{cases}$$

Similarly to [3], [4], we rest
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$$|\xi| = |$$

and to differential equation

$$\begin{cases} |\widetilde{U}(t) - \\ \text{whenev} \end{cases}$$

We apply the method with $h = 0.1$. Starting with $u_0 = 1/3$ the method yields $u_1 = 1/3$. But, starting from $\widetilde{u}_0 = 0.333$ the method yields

$$\widetilde{u}_1 \simeq 10^{42}.$$

Clearly, (1.4) does not hold here with any γ of moderate size.

The derivative with respect to ξ of the function

$$f(t,\xi) = -1 + \exp[10^5(1 - 3\xi)]$$

satisfies

$$\frac{\partial}{\partial \xi} f(t,\xi) \leq 0.$$

Further, the method under consideration is A–stable, which implies contractivity in the solution of (1.2) and (1.3) with $A = \lambda \leq 0$. Therefore, the first principle of section 1.2 is misleading for the situation at hand. A related example was given by Wanner [20].

2.2. The above example shows that there is some need for a reliable stability theory relevant to nonlinear differential equations. We now review such a theory for general *Runge-Kutta methods* of the following type.

$$u_n = u_{n-1} + b_1 x_1 + b_2 x_2 + \cdots + b_m x_m \tag{2.1a}$$

where $x_j \in \mathbb{R}^s$ are computed from u_{n-1} in such a way that

$$\begin{aligned} &x_i = hf(t_{n-1} + c_i h,\ u_{n-1} + a_{i1}x_1 + a_{i2}x_2 + \cdots + a_{im}x_m) \\ &\text{for } i = 1, 2, \cdots, m. \end{aligned} \tag{2.1b}$$

The coefficients a_{ij}, b_i are real parameters defining the method, and $c_i = a_{i1} + a_{i2} + \cdots + a_{im}$.

The following definition originated with Butcher, Burrage [3] and Crouzeix [4]: Method (2.1) is called *algebraically stable* if

$$\begin{cases} \text{all } b_i \geq 0, \text{ and the } m \times m \text{ matrix } Q = (Q_{ij}) \text{ with} \\ Q_{ij} = b_i a_{ij} + b_j a_{ji} - b_i b_j \text{ is positive semi-definite.} \end{cases}$$

Similarly to [3], [4], we restrict ourselves in the sequel, up to section 3, to the Euclidean norm

$$|\xi| = |\xi|_2 = \sqrt{\xi^{\mathrm{T}}\xi} \qquad \text{for } \xi \in \mathbb{R}^s, \tag{2.2a}$$

and to differential equations (1.1) such that

$$\begin{cases} |\widetilde{U}(t) - U(t)| \leq |\widetilde{U}(t-h) - U(t-h)| \\ \text{whenever } h > 0 \text{ and } \widetilde{U},\ U \text{ satisfy (1.1).} \end{cases} \tag{2.2b}$$

Consider the property

> There is contractivity whenever the method is applied with *any* $h > 0$ to *any* equation (1.1) satisfying (2.2). (2.3)

Theorem 1. Algebraic stability is a necessary and sufficient condition on the method to guarantee property (2.3).

This theorem is valid provided method (2.1) is irreducible (cf. [1], [9], [17]).

2.3. Clearly, algebraic stability is a favourable property. However, within the class of Runge–Kutta methods that fail to be algebraically stable, there are methods with other favourable properties, e.g. requiring only little computational labour for computing u_n from u_{n-1}. Therefore, it seems worth looking closer at the methods which are A-stable without being algebraically stable. In particular, consider the following *question*: Are there methods failing to be algebraically stable and still stable [(1.4), with moderately sized γ, q] for all $h > 0$ and for all equations (1.1) satisfying (2.2)?

The method in the example of Section 2.1 corresponds to a Runge–Kutta method with $m = 2$, $a_{11} = a_{12} = 0$, $a_{21} = a_{22} = b_1 = b_2 = 1/2$. This method fails to be algebraically stable. The differential equation in Section 2.1 belongs to the class of equations under consideration, defined by requirement (2.2). Therefore, the disastrous error propagation in Section 2.1 suggests that the answer to the above question is negative.

However, the following counterexample, due to Kraaijevanger [11], shows that the answer is positive. Let $m = 2$, and consider method (2.1) with

$$\begin{array}{llll} a_{11} & = 1/2, & a_{12} & = 0 \\ a_{21} & = -1/2, & a_{22} & = 2 \\ b_1 & = -1/2, & b_2 & = 3/2. \end{array}$$

Since $b_1 < 0$, this method is *not algebraically stable.* Still,

> (1.4) holds with $\gamma = 2$, $q = 0$ whenever this method is applied with *any* $h > 0$ to *any* equation (1.1) satisfying (2.2).

This example thus suggests that algebraic stability is an unnecessarily strong demand upon a method if one is not looking for contractivity but only for stability in the sense (1.4) with moderate γ, q.

2.4. Up to now we have been dealing with a constant stepsize $h > 0$. In actual calculations one will often use *variable stepsizes* $h_n > 0$ and non-equidistant gridpoints $t_n = t_{n-1} + h_n$. In this situation it is natural to consider the following stability property of a Runge–Kutta method:

> There are fixed γ, q such that (1.4) holds whenever the method is applied with *any* variable $h_n \in (0, 1]$ to *any* equation (1.1) satisfying (2.2). (2.4)

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Theorem 2. Algebraic stability is a necessary and sufficient condition on the method to guarantee that (2.4) holds.

Thus, after all, algebraic stability turns out to be the appropriate demand upon a Runge–Kutta method — if one is looking for the variable stepsize stability property (2.4). For the proof of Theorem 2 we refer to [11].

2.5. The stability estimates in (2.3), (2.4), present under the assumption of algebraic stability, are quite satisfactory in that they are still valid for highly nonlinear differential equations, for which the first principle of Section 1 may break down. However, the condition of algebraic stability is rather strong and not satisfied by various methods of practical interest (cf. e.g. [1]). Therefore it is important to note that rigorous stability estimates exist as well for some methods which fail to be algebraically stable. Such estimates were derived e.g. by Hundsdorfer [8] and Schmitt [16] for mildly nonlinear differential equations, where the first principle of Section 1 applies. The estimates in [8] cover some A-stable methods applied to equations (1.1) satisfying (2.2). The estimates in [16] are relevant to some $A(\theta)$-stable methods ($0 < \theta < \pi/2$) applied to differential equations where the (classical) numerical range of the Jacobian matrix lies within an appropriate wedge in the complex plane. Since these results lie outside the actual scope of the present paper we refer to [16] for more details.

3 Failure of the second principle: general methods

3.1. In the above we dealt with highly nonlinear equations (1.1) and variable h_n. From now on we consider the numerical solution of the linear problem (1.2) with a constant stepsize $h > 0$. An application of the Runge–Kutta method (2.1) to equation (1.2) yields a numerical process of the type

$$u_n = \varphi(hA)u_{n-1}, \qquad n = 1, 2, 3, \cdots. \tag{3.1}$$

Here $\varphi(\zeta) = \frac{P(\zeta)}{Q(\zeta)}$ is a rational function with $\varphi(0) = \varphi'(0) = 1$, and we use the notation

$$\varphi(hA) = P(hA)[Q(hA)]^{-1}.$$

Note that Rosenbrock methods and higher derivative methods, when applied to (1.2), also reduce to numerical processes of type (3.1).

The second principle of Section 2.1 asserts that the condition

$$|\varphi(h\lambda)| < 1, \quad \text{for all } \lambda \in \sigma[A]$$

is sufficient to guarantee a stable behaviour of process (3.1). Defining the *stability region*

$$S = \{\zeta : \zeta \in \mathbb{C} \text{ with } |\varphi(\zeta)| < 1\}$$

the above condition can be cast into the form

$$h\sigma[A] \subset S. \tag{3.2}$$

This condition can be reliable. E.g. if A is a normal matrix, then (3.2) guarantees estimate (1.4) for the process (3.1) with $|\cdot| = |\cdot|_2$, $\gamma = 1$, $q = 0$.

From now on, A is an arbitrary $s \times s$ matrix, and we confine ourselves to the important maximum norm,

$$|\xi| = |\xi|_\infty = \max_{1 \le j \le s} |\xi_j| \quad \text{for } \xi = (\xi_1, \xi_2, \ldots, \xi_s)^{\mathrm{T}} \in \mathbb{R}^s.$$

In this general setting condition (3.2) is very unreliable. This was pointed out e.g. in [6], [10], [14], [18], [19]. Although (3.2) guarantees (1.4), even with $q = 0$, the corresponding γ can be excessively large. The fact is that γ depends not only on the set $h\sigma[A]$ occurring in (3.2) but also on the condition number of the (generalized) eigenvectors of A. Therefore, under condition (3.2) the size of γ is not under control. This is particularly important in solving partial differential equations by semi-discretization, since Lax stability requires uniform boundedness of the condition number of eigenvectors as $\Delta x \to 0+$.

We illustrate the above point with the tri-diagonal matrix

$$A = \begin{bmatrix} -5 & 2 & & & & \\ 1/2 & -7 & 3 & & & \\ & 1/3 & -9 & 4 & & \\ & & \ddots & \ddots & \ddots & \\ & & & & & s \\ & & & 1/s & -2s-3 & \end{bmatrix}, \text{ with } s = 40.$$

The eigenvalues of this matrix are all different from each other, and satisfy

$$-84 < \lambda < 0.$$

Consider the polynomial, taken from [7],

$$\varphi(\zeta) = 1 + \zeta + \tfrac{1}{8}\zeta^2.$$

Its stability region satisfies

$$(-8, 0) \setminus \{-4\} \subset S.$$

Therefore (3.2) is fulfilled when

$$h \le \tfrac{8}{84} \simeq 0.0952, \quad h \ne \tfrac{-4}{\lambda} \quad \text{for all } \lambda \in \sigma[A].$$

For $h = 0.07$ condition (3.2) is fulfilled, but the smallest γ for which (1.4) holds, with $q = 0$, equals

$$\gamma \simeq 3 \times 10^{10}$$

(cf. [12]).

3.2. The unreliable conditic
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Theorem 3. With the abo
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The latter inclusion is valid

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(cf. [12]).

3.2. The unreliable condition (3.2) can be converted into a reliable one by replacing $\sigma[A]$ by some appropriate larger set $\tau[A] \subset \mathbb{C}$, i.e.

$$h\tau[A] \subset S. \tag{3.2*}$$

Satisfactory stability estimates, with various choices for $\tau[A]$, have been derived in [2], [5], [10], [12], [13], [15], [18], [19].

We now review one of the stability results in [12]. Let the Gerschgorin disk D_j of $A = (\alpha_{jk})$ be defined by

$$D_j = \Big\{\zeta : |\zeta - \alpha_{jj}| \leq \sum_{k \neq j} |\alpha_{jk}|\Big\}.$$

Define $\tau[A]$ to be the convex hull of the union of all Gerschgorin disks, i.e.

$$\tau[A] = \mathrm{conv}(D_1 \cup D_2 \cup \cdots \cup D_s).$$

Theorem 3. With the above $\tau[A]$, condition (3.2*) implies estimate (1.4) with $q = 1$, and γ depending on φ and $h\tau[A]$ only.

Here γ does *not* depend in any transparent manner on the eigenvectors of A. In fact $\gamma = \Gamma(h\tau[A])$ with a fixed function Γ satisfying

$$\Gamma(V_1) \leq \Gamma(V_2) \text{ for } V_1 \subset V_2 \subset S.$$

Moreover, $\max\{\mathcal{R}e\, z : z \in \tau[A]\}$ is precisely the logarithmic norm of A with respect to the maximum norm.

We illustrate the theorem with the same A as above and with h satisfying (3.2*). A straightforward calculation shows that $\tau[A]$ is contained in the union $T_1 \cup T_2$ of the triangle

$$T_1 = \Big\{\zeta : |\pi - \arg\zeta| \leq \frac{\pi}{6} \text{ and } -\frac{3(2s+1)}{4} \leq \mathrm{Re}\,\zeta < 0\Big\}$$

and the disk

$$T_2 = \{\zeta : |\zeta + 2s + 1| \leq s + 1/2\}.$$

Therefore (3.2*) holds when h is so small that

$$h \cdot (T_1 \cup T_2) \subset S.$$

The latter inclusion is valid for all h with

$$h \leq h_0 = \frac{9}{4(2s+1)} \simeq 0.02777.$$

With the choice $h = 0.027$ the theorem thus predicts stability in the sense (1.4) with $q = 1$, and γ only depending on φ and $h \cdot (T_1 + T_2)$.

Straightforward numerical calculations show that, with this h, one actually has

$$|\widetilde{u}_n - u_n| \leq 1.2\, |\widetilde{u}_0 - u_0| \quad (\text{ for all } n \geq 1; u_0, \widetilde{u}_0 \in \mathbb{R}^s).$$

Hence, there is now a very mild error propagation – even better than predicted by theorem 3. We refer to [12] for more details.

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