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Modern convergence theory for stiff initial-value problems

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Abstract

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In this paper we give a brief review of available theoretical results about convergence and error structures for discretizations of stiff initial-value problems. We point out limitations of the various approaches and discuss some recent developments.

Keywords: Stiff differential equations; stability; convergence.

1. An overview on existing convergence concepts

More or less efficient codes have been used more or less successfully for the numerical solution of stiff ODEs; at present, backward differentiation schemes (BDFs) are without doubt among the most widely used methods. However, as it is often the case in numerical mathematics and its applications, the theoretical foundations are still incomplete. Many problems which arise in practice — and which are solved numerically — are of such a complexity that the available theory (e.g., concerning convergence properties or error structures of the methods used) is not applicable. Algorithms and control mechanisms used within the respective codes are often based on model concepts or heuristic principles only. This is obviously reasonable from a practical point of view; but a convergence theory as universal as possible is of course desirable.

In this paper we give a brief review on existing theoretical approaches and results about convergence and error structures for discretizations of stiff initial-value problems

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

$$y(0) = y_0. \tag{1.1b}$$

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We point out some limitations of the various approaches and discuss some recent developments.

Historically, the first theoretical concept especially suited for the assessment of numerical methods for stiff problems was A-stability (cf. [12]), respectively $A(\alpha)$-stability (cf. [35]). Based on this model concept, rigorous conclusions can only be drawn for linear constant-coefficient problems $y' = Jy$. Nevertheless it has been used, with doubtful reliability, as a guideline to select methods for the solution of more difficult problems. First serious attempts to develop a rigorous, comprehensive convergence theory for *nonlinear* stiff problems go back to the early seventies. The respective ideas are based on the observation that the so-called *logarithmic norm* (with respect to the underlying domain $\mathscr{G}$)

$$\mu(f) := \sup_{\substack{(t,y_1),(t,y_2)\in\mathscr{G} \\ y_1\neq y_2}} \lim_{\tau\to 0+} \frac{\| y_1 - y_2 + \tau(f(t, y_1) - f(t, y_2))\| - \| y_1 - y_2 \|}{\tau \| y_1 - y_2 \|} \tag{1.2}$$

is a canonical parameter in the assessment of the condition behavior of an initial-value problem (1.1) (see [11,15] and Section 2 below). Namely, it enables estimates for the effect of perturbations (of the initial value or of the direction field) which are, in a certain sense, sharp (cf. the discussion in Section 2). Consequently, these estimates have been considered as a natural improvement over the well-known "classical" estimates based on a Lipschitz constant L for f, the improvement being dramatic for such stiff problems where the optimal (smallest possible) Lipschitz constant $L(f)$ is significantly larger than $\mu(f)$. (Recall that, inevitably, $L(f) \gg 0$ for stiff problems in spite of their good condition; thus, the typical condition number $e^{tL(f)}$ dramatically increases with t — in contrast to $e^{t\mu(f)}$ if $\mu(f)$ is moderate.) In the analysis of discretization methods, it is equally natural to strive for stability estimates also based on the problem-characterizing parameter $\mu(f)$ to overcome the obvious fact that classical stability inequalities based on $L(f) \gg 0$ are of no use in stiff situations. In the concept of G-stability (introduced by Dahlquist in 1975, see [13]) this idea was realized for multistep methods. For one-step methods (in particular implicit Runge–Kutta methods), Butcher [9] introduced an analogous stability concept called B-stability.

Norms induced by a scalar product $\langle \cdot, \cdot \rangle$ turned out to be particularly convenient. In this case the logarithmic norm $\mu(f)$ can be expressed as the *optimal one-sided Lipschitz constant* $m(f)$ for f, i.e., the smallest real number m for which

$$\langle f(t, y_1) - f(t, y_2), y_1 - y_2 \rangle \leqslant m \| y_1 - y_2 \|^2 \tag{1.3}$$

(for all (t, y_1), (t, y_2) in the domain $\mathscr{G}$ under consideration). Let us now, for example, recall the precise definition of B-stability. Assume that m is a one-sided Lipschitz constant for f, and consider two "parallel" steps $(t_{\nu-1}, \eta_{\nu-1}) \to (t_\nu, \eta_\nu)$ and $(t_{\nu-1}, \tilde{\eta}_{\nu-1}) \to (t_\nu, \tilde{\eta}_\nu)$ of a one-step method applied to (1.1). The method is called *B-stable* if there exists a smooth function Φ with $\Phi(0) = 1$ such that

$$\| \eta_\nu - \tilde{\eta}_\nu \| \leqslant \Phi(hm) \| \eta_{\nu-1} - \tilde{\eta}_{\nu-1} \|, \tag{1.4}$$

where $h = t_\nu - t_{\nu-1}$ is the steplength. Note that (1.4) is an immediate discrete analogue to the condition inequality

$$\| y(t+h) - \tilde{y}(t+h) \| \leqslant e^{hm} \| y(t) - \tilde{y}(t) \|, \tag{1.5}$$

where y, $\tilde{y}$ denote a pair of solutions to (1.1a) (see, e.g., [16]).

B-stability turned out to be a very successful concept; in particular, several classes of implicit Runge–Kutta methods have been shown to be B-stable. The essential technical tool for the derivation of stability results are certain algebraic conditions on the Runge–Kutta coefficients like *algebraic stability* and *diagonal stability* (cf., for instance, [8,10,18]). For multistep methods it turns out that, unfortunately, G-stability is a rather restrictive requirement in the following sense. A-stability is of course a necessary condition and therefore, due to well-known order barriers, a G-stable multistep method cannot have an order of consistency higher than 2.

For higher-stage one-step methods it is important to notice that — apart from stability questions — also the local error analysis is by no means trivial. For implicit Runge–Kutta methods the local error (i.e., the error induced by a single integration step) is a complicated expression involving various derivatives of the right-hand side f, the norm of which is inevitably affected by large problem parameters like $L(f)$, and therefore the actual magnitude of the local error is not a priori obvious. This difficulty had almost consistently been ignored in the earlier literature (see, however, [29]). Frank et al. were the first to give a systematical local error analysis (see [17,19]). The essential aspect is that, from a reasonable *quantitative* point of view, an assertion like "the order of the local error is $O(h^p)$" makes only sense if the O-constant is not influenced by prohibitively large problem parameters — but only by the local smoothness of the ODE solution (the latter dependence is quite natural). It turns out that, in this quantitative order concept, the local error of an implicit Runge–Kutta method usually suffers from an *order reduction* (compared to the classical, nonstiff order). In general, the order actually observed reduces to the so-called stage order, i.e., the minimal order of the truncation errors occurring in the individual Runge–Kutta stages. But even that the stage order can be achieved is by no means simple to prove and requires a careful "internal" stability analysis (concept of BS-stability). The concepts of B-stability and BS-stability led to a quantitative convergence theory (B-convergence) for stiff problems satisfying a one-sided Lipschitz condition (1.3) (see [17,19]). A typical B-convergence result reads

$$\| \eta_\nu - y(t_\nu) \| \leqslant \mathscr{C}(m, M_l) h^p, \tag{1.6}$$

where the quantitity $\mathscr{C}(m, M_l)$ depends only on the one-sided Lipschitz constant m and on bounds M_l for the derivatives of $y(t)$ entering the expression for the local error. In recent years, a large number of results concerning B-stability (and rélated stability concepts) and B-convergence have been derived for various types of implicit Runge–Kutta methods (for an overview see, for example, [15,20]).

An alternative approach towards a convergence analysis for stiff problems is based on the concepts of *singular perturbations*. A standard problem considered in singular perturbation theory is

$$u' = \phi(t, u, v), \tag{1.7a}$$

$$v' = \frac{1}{\epsilon} \psi(t, u, v), \tag{1.7b}$$

with

$$\mu\left(\frac{\partial \psi}{\partial v} \right) \leqslant -\kappa < 0. \tag{1.8}$$

Here, $\epsilon > 0$ is a small parameter characterizing the stiffness. A problem of this form has a quite particular structure. All stiff eigenvalues are of the same magnitude $-O(1/\epsilon)$; furthermore, the dependence of the right-hand side on the stiffness parameter ϵ is rather special. The behavior of solutions to (1.7) is well understood; it can be analyzed by asymptotic methods and the necessary condition estimates can, e.g., be derived using contraction arguments, without relying on a one-sided Lipschitz condition for the right-hand side (cf., e.g., [28]). In recent years, convergence results have been derived for implicit Runge–Kutta methods and, recently, also for BDF methods applied to (1.7) (see [22,26]). These results constitute a nontrivial extension of the convergence theory, since — as will turn out in Section 2 — problem class (1.7) is *not* satisfactorily covered by the concept of B-convergence.

Stiffness also frequently occurs in problems connected with partial differential equations (e.g., for parabolic initial/boundary value problems); often a stiff ODE system arises after a PDE has been discretized in space. The one-sided Lipschitz constant m frequently appears in a natural way (often it has a direct physical meaning, e.g., $m \leqslant 0$ may indicate dissipation of energy). Therefore the concepts and results of the B-theory are often useful here; for an overview of results, cf., for instance, [31]. Also certain modifications of the one-sided Lipschitz condition are of relevance; in the analysis of non-self-adjoint parabolic equations, for instance, a strengthened one-sided Lipschitz condition (a so-called "sectorial condition") plays an important role (cf., for instance, [2,24,26] for its significance in the analysis of numerical methods). To put these concepts in perspective, however, it should be emphasized that they are of minor relevance for PDEs involving significant nonlinearities.

Concerning the *structure* of discretization errors (i.e., asymptotic error expansions in powers of the stepsize), useful results have been derived only recently for special classes of stiff problems (e.g., for class (1.7) and simple one-step methods (see [1–4,7,21,34]). It turned out that the usual arguments (following the lines of the general procedure described in [33]) are of little use in the stiff case. Already for very simple schemes as, e.g., implicit Euler or implicit midpoint rule, the global error cannot be described by smooth functions, but strongly varying (decaying or oscillating) components may play a dominant role. The particular error structure strongly depends on the type of problem under consideration, on various problem parameters like, for instance, the magnitude of the stiff eigenvalues, and on the method and stepsize actually used.

These results about error structures form the basis for the analysis of extrapolation or defect correction methods and for a sound justification of stepsize control mechanisms; but the theory is far from complete. For multistep schemes, results about error structures in the stiff case do not seem to exist.

2. Norms, logarithmic norms and one-sided Lipschitz constants: a critical discussion

The overview given in Section 1 shows that one-sided Lipschitz constants are an essential tool in the analysis of stiff problems; a large number of results are based on this concept. As already mentioned, the use of one-sided Lipschitz constants is, in a sense, natural, because typical stability estimates like (1.4) are obvious discrete analogues of condition estimates of the form (1.5) for the solutions of the given ODE. Note that the estimate (1.5) is even *optimal in a local sense*, i.e., for arbitrary $y(t)$ there exists a perturbed $\tilde{y}(t)$ such that the estimate (1.5) (with the best possible choice $m = m(f)$ is asymptotically sharp for $h \to 0$ (cf. [15,16]).

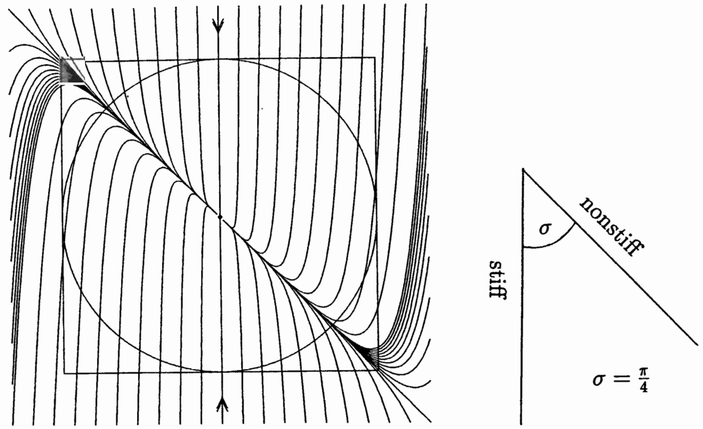

Fig. 1. Phase portrait for example (2.1) (J nonsymmetric).

On the other hand, it is easy to write down examples which show an uncritical error sensitivity in the sense that the global effect of perturbations remains moderately bounded, even though m may be large and positive. Consider, for instance, the simple constant-coefficient problem

$$y' = Jy, \quad \text{with } J = \begin{pmatrix} -1 & 0 \\ \dfrac{1}{\epsilon} - 1 & -\dfrac{1}{\epsilon} \end{pmatrix}, \tag{2.1}$$

where ϵ is a small positive parameter. This is a linear problem of the type (1.7). The logarithmic norm $\mu_2(J)$ with respect to the Euclidean norm $\|\cdot\|_2$ (i.e., the best possible one-sided Lipschitz constant $m(f)$ for $f(t, y) = Jy$) can be expressed as the spectral abscissa of $\frac{1}{2}(J + J^{\mathrm{T}})$ (cf., e.g., [15]), and we easily obtain

$$\mu_2(J) = \tfrac{1}{2}(\sqrt{2} - 1) \cdot \frac{1}{\epsilon} - \tfrac{1}{2}(\sqrt{2} + 1) = O\left(+\frac{1}{\epsilon}\right). \tag{2.2}$$

Consequently, (2.1) is *locally ill-conditioned* with respect to the Euclidean norm. The worst propagation of a perturbation δ of the initial value y_0, measured in $\|\cdot\|_2$, qualitatively behaves like $e^{+t/\epsilon}\|\delta\|_2$ for small t, despite the fact that the eigenvalues of J are -1 and $-1/\epsilon$. On the other hand, the *global* effect of such a perturbation is easily seen to be uniformly bounded by $\sqrt{2}\,\|\delta\|_2$ for arbitrary $t > 0$. That is, a rapid growth of perturbations can only occur during a very short transient phase.

To illustrate this situation we study the behavior of solutions to (2.1) by means of its phase portrait [1] (cf. Fig. 1). Without limitation of generality we consider all y with $\|y\|_2 = 1$. For

[1] By linearity, it is not necessary here to distinguish between solutions and perturbations.

certain y on the unit circle, the direction field is outwardly directed; hence for a solution trajectory $y(t)$ passing through such a point, the norm $\| y(t)\|_2$ increases. Moreover, the local growth of $\| y(t)\|_2$ is enormous due to the large size of the stiff eigenvalue. However, after a very short time interval the rapid variation vanishes and the solution trajectory smoothly follows the direction corresponding to the nonstiff eigenvalue.

This situation, namely that there is a dramatic discrepancy between local and global condition, is not exceptional, but, in a sense, *typical*. It has been shown in [5] that for two-dimensional stiff problems

$$y' = Jy = SAS^{-1}y, \quad \text{with } A = \begin{pmatrix} c_1 & 0 \\ 0 & -\dfrac{c_2}{\epsilon} \end{pmatrix}, \; c_2 > 0, \tag{2.3}$$

the logarithmic norm $\mu_2(J)$ is moderate-sized (i.e., not affected by a factor $+1/\epsilon$) if and only if J is "nearly symmetric" in the sense that the angle σ between the eigendirections of J must satisfy $\sigma = \frac{1}{2}\pi + O(\epsilon^{1/2})$. This can also directly be seen from Fig. 1. Only if the eigendirections would be orthogonal (symmetric case) or at least "nearly orthogonal", a locally strong increase of perturbations could not occur. (In example (2.1) we have $c_1 = -1$, $c_2 = 1$ and $\sigma = \frac{1}{4}\pi$.) Thus, in the nonsymmetric case we inevitably must have $\mu_2(J) \gg 0$ due to the potentially strong local increase; but the good global condition — i.e., the fact that such a strong increase can only occur on a very short time interval — is not reflected by this local concept. (Only in the symmetric case there is no such difficulty.) Numerical experience indicates that a similar discrepancy is also typical for higher-dimensional stiff systems; however, to derive rigorous characterizations as for the two-dimensional case would be a highly nontrivial task. In the PDE field (initial/boundary value problems, method of lines context) examples are known where a strongly positive logarithmic norm is caused by certain types of boundary conditions (cf., e.g., [15, Section 10.6]). A comprehensive *general* characterization of cases where the logarithmic norm concept is reasonably applicable or not does not exist; but in view of the results of [5] we must expect that $m(f) \gg 0$ is often the case, i.e., that a strong discrepancy between local and global condition is often present. Naturally, B-convergence bounds based on $m(f)$ are of no use in all these situations.

This restricted applicability of the B-theory is not too surprising in the light of a result given in [8]. There it was shown for nonconfluent Runge–Kutta methods that B-stability for problems with $m \leqslant 0$ is equivalent to AN-stability (the generalization of A-stability for scalar problems $y' = \lambda(t)y$). Thus a stability property for nonlinear problems is directly related to a stability property for scalar linear problems. A similar equivalence also holds in the context of multistep methods. A-stability is not only necessary, but even sufficient for G-stability (cf. [14]). With this background in mind, one may say (and some people indeed do so) that B-stability and G-stability are scalar concepts which do not take account of time-dependent or nonlinear coupling.

The question arises how to circumvent this drawback. For constant-coefficient problems like (2.3) this is simple. Instead of the Euclidean norm one chooses another scalar product norm, the so-called "elliptic norm" $\| y\|_S := \| S^{-1}y\|_2$. This corresponds to a complete decoupling and, obviously, the corresponding logarithmic norm is simply $\mu_S(J) = \mu_2(A)$, the spectral abscissa of J. However, already for two-dimensional linear systems $y' = J(t)y$ with time-dependent coefficients there is no such simple remedy because it turns out that, even for smoothly

varying eigendirections, there is *no fixed elliptic norm* for which the corresponding logarithmic norm remains moderate-sized on a time interval of length O(1) (cf. [5]). In other words, the logarithmic norm $\mu_S(J)$ is extremely sensitive with respect to rotations of the eigendirections of J; unless the norm $\|\cdot\|_S$ (or, equivalently, the unit ellipse $\{y: \| y\|_S = 1\}$) is chosen precisely adapted to these eigendirections, there always exist points y on that unit ellipse where, for a solution trajectory $y(t)$ passing through this point, $\| y(t)\|_S$ is subject locally to rapid increases.

This latter observation causes surprising complications in the analysis of discretization methods. In the following section we briefly review recent work concerning the convergence of implicit Runge–Kutta methods applied to a class of weakly nonlinear stiff problems for which the B-theory is not applicable.

3. An extension of B-convergence

As explained in Section 2, the applicability of results from the B-theory is more restricted than usually believed. In particular, not even simple linear stiff systems $y' = J(t)y$ with time-dependent coefficients are satisfactorily covered. For any scalar product norm, the supremum of $\mu(J(t))$ on some time interval of length O(1) must be expected to be strongly positive (affected by the moduli of the stiff eigenvalues) except in special cases ($J(t)$ normal). But a theoretical concept like B-stability relies heavily on a suitable scalar product norm; therefore an immediate application of the concepts of the B-theory to such problems cannot lead to reasonable convergence results. (Also the arguments from singular perturbation theory are only applicable in special cases.) In the following we briefly discuss this point further and review a recent result, given in [6], concerning the convergence of implicit Runge–Kutta methods.

Problems of the form $y' = J(t)y$ can be studied by means of a suitable time-dependent change of coordinates. Assume, for instance, that $J(t)$ is diagonalizable: $J(t) = S(t)A(t)S^{-1}(t)$, with a well-conditioned, smoothly varying eigensystem $S(t)$. Then the time-dependent transformation $\bar{y} := S^{-1}(t)y$ leads to the transformed ODE

$$\bar{y}' = \bar{J}(t)\bar{y}, \quad \text{with } \bar{J}(t) := A(t) - S^{-1}(t)S'(t) \tag{3.1}$$

(the eigenvalues of $\bar{J}(t)$ are sometimes called the *kinematic eigenvalues* of $J(t)$). This time-dependent change of coordinates may also be viewed as a time-dependent adaption of the norm (generalization of the concept of elliptic norms). Under appropriate smoothness assumptions with respect to $S(t)$, the logarithmic norm $\mu_2(\bar{J}(t))$ (i.e., the largest kinematic eigenvalue of $J(t)$) is obviously of the magnitude of the spectral abscissa of $J(t)$; it is not affected by prohibitively large problem parameters like the moduli of the stiff eigenvalues.

Let us now consider implicit Runge–Kutta methods applied to (3.1). One could think that for a study of stability one would simply have to apply an analogous time-dependent transformation to the discrete scheme (including the internal Runge–Kutta stages) and to apply the B-theory to this transformed scheme. Unfortunately, such a procedure does not lead to a useful result, because the Runge–Kutta scheme transformed in that way cannot be interpreted as a Runge–Kutta scheme applied to the transformed ODE (3.1). Still one could believe that a straightforward modification of the arguments from the B-theory would lead to a successful stability analysis of the transformed scheme; but this is also not the case. Actually, the derivation of satisfactory quantitative stability and convergence results requires a careful use of perturbation arguments; the respective technical details can be found in [6].

By the results of [6], stiff initial-value problems of the form

$$y' = J(t)y + g(t, y), \tag{3.2a}$$

$$y(0) = y_0 \tag{3.2b}$$

are covered, with an arbitrary distribution of stiff eigenvalues and with a smooth, Lipschitz-continuous nonlinearity $g(t, y)$ (this excludes highly nonlinear problems). It is assumed that a (not necessarily diagonalizing) time-dependent transformation $S(t)$ exists such that the right-hand side of the correspondingly transformed problem has a logarithmic norm which reflects the well-conditioned behavior of (3.2) in a realistic way. For implicit Runge–Kutta methods applied to such problems, stability and error bounds are derived in [6]. The essence of these results is:

A B-stable respectively B-convergent Runge–Kutta method is also stable respectively convergent when applied to a problem (3.2).

This constitutes a relevant extension of the "conventional" B-theory.

4. Further remarks on problem condition and stability

The above discussions show that, in a convergence theory for stiff problems, the *choice of the norm* is crucial. For the class (3.2), for instance, even a time-dependent adaption of the norm is necessary (cf. Section 3). Also the use of *scalar product norms* is essential in the B-theory and its extension because a technical concept like algebraic stability heavily relies on the underlying scalar product.

On the other hand, a look at examples suggests that *nonscalar product norms* may, in a certain sense, be better suitable for the characterization of the global condition of stiff problems. For an illustration of this point, let us consider singularly perturbed equations of the form (1.7) [2] where the Jacobian of the right-hand side is of the form

$$J = J(t, u, v) = \begin{pmatrix} \dfrac{\partial \phi}{\partial u} & \dfrac{\partial \phi}{\partial v} \\ \dfrac{1}{\epsilon}\dfrac{\partial \psi}{\partial u} & \dfrac{1}{\epsilon}\dfrac{\partial \psi}{\partial v} \end{pmatrix} \tag{4.1}$$

(in general, J is nonsymmetric). For simplicity of presentation we assume that the problem is two-dimensional, i.e., ϕ and ψ in (1.7) are scalar functions. If we assume $|\partial\psi/\partial u| \leqslant \kappa$ in some domain, where $\partial\psi/\partial v \leqslant -\kappa < 0$ (cf. condition (1.8)), then, in contrast to $\mu_2(J)$, the logarithmic norm [3] $\mu_\infty(J)$ is moderately sized, i.e., not affected by a factor $+1/\epsilon$. (Note that $\mu_\infty(A) = \max_i(a_{ii} + \Sigma_{j\neq i}|a_{ij}|)$, cf. [15].) Also the case when $|\partial\psi/\partial u|$ becomes larger than κ would cause no difficulty. It is easy to find an appropriately scaled maximum norm $\|y\|_{\infty,D} := \|Dy\|_\infty$, $D > 0$ diagonal, such that the corresponding logarithmic norm $\mu_{\infty,D}(J)$ is moderately sized (note that for $A = (a_{ij})$ and $D = \mathrm{Diag}(d_i)$, $\mu_{\infty,D}(A) = \mu_\infty(DAD^{-1}) = \max_i(a_{ii} + \Sigma_{j\neq i}|a_{ij}d_i/d_j|)$). The minimal amount of scaling necessary depends on the actual size of $|\partial\psi/\partial u|$ and is related to the global condition of the problem.

[2] This problem class is of course well understood in singular perturbation theory and there is, so to speak, nothing to show. Nevertheless we reconsider problems (1.7) here: they simply serve as illustrative examples for our present discussion concerning the choice of norms.

[3] Note that the logarithmic norm $\mu(f)$ can be expressed as the supremum of $\mu(J)$ with respect to the domain under consideration (here J denotes the Jacobian of f, and $\mu(J)$ denotes the logarithmic norm of the respective locally linearized problem $y' = Jy$).

Geometrically, this can be interpreted as follows. Consider, e.g., the simple linear example (2.1). Obviously, $\mu_\infty(J) = -1$, and therefore the problem is contractive in the maximum norm (i.e., the $\|\cdot\|_\infty$ norm of perturbations never grows). In Fig. 1 this property is reflected by the fact that at each point on the boundary of the unit square $\|y\|_\infty \leqslant 1$, the direction field is inwardly directed. A rescaling of the norm would be necessary if we would alter the nonstiff eigendirection in this example such that the angle σ between the eigenvectors of J would be smaller than $\frac{1}{4}\pi$; i.e., the direction field is inwardly directed for each rectangle sufficiently stretched in the vertical direction. In other words, the norm has to be chosen in such a way that a strong but only local increase of a solution component remains "invisible".

The *really* essential point is the following. Recall that for the problem class under consideration, the logarithmic norm with respect to any scalar product norm inevitably gets positive and very large unless the norm is precisely adapted to the actual orientation of the eigendirections of the Jacobian J; this makes scalar product norms unsuitable for nonconstant J. On the other hand, for each problem of the form (1.7) it is easy to find an appropriately scaled maximum norm such that the corresponding logarithmic norm remains moderately sized not only for a single $J(t, u, v)$ but for certain O(1)-domains of arguments (t, u, v); one simply has to choose a sufficiently distorting scaling matrix (i.e., a sufficiently stretched unit rectangle), which is essentially determined by the maximal occurring value of $|\partial\psi/\partial u|$. This has an immediate geometrical interpretation. A simple eigensystem analysis of (4.1) shows that a smooth variation of the occurring partial derivatives corresponds to a smooth (O(1)) rotation of the "nonstiff eigendirection"; the "stiff eigendirection" also rotates but only with a speed $O(\epsilon)$ (the eigenvector of (4.1) corresponding to the stiff eigenvalue is always of the form $(O(\epsilon), 1)^T$). Now the amount of scaling necessary is simply determined by the smallest angle which occurs between these eigendirections, and we finally can express the good problem condition with the help of the logarithmic norm with respect to a certain *fixed*, rescaled maximum norm. In this sense, the (appropriately rescaled) maximum norm is much more "robust" than any scalar product norm.

In view of these considerations it may be hoped that there also exist other interesting nontrivial classes of stiff problems (e.g., certain multi-parameter generalizations of (1.7)) for which a careful choice of (nonscalar product) norm leads to a moderate logarithmic norm; this is a question worth investigating. It is, however, important to notice here that the "inertia" of the stiff eigendirection is essential; the above way of choosing the norm would break down in the case of a O(1)- (and not only $O(\epsilon)$-) rotation of the stiff eigendirection. Thus, this approach appears not to be applicable in the case of such nonlinear problems where, in contrast to (1.7), also the stiff eigendirections vary significantly.

Now, for problem classes where an appropriate norm in the above sense exists, the question is whether it is possible to develop a *convergence theory* for discretization methods based on such a (nonscalar product) norm. Some results in this direction can be found in [23,32]. Unfortunately it turns out that nonscalar product norms are much less convenient to use in a convergence theory than scalar product norms. Furthermore, the results of [23,32] are of a rather negative flavor. It is shown that a one-step method behaving contractively (with respect to $\|\cdot\|_\infty$) for *every* $\|\cdot\|_\infty$-contractive ODE cannot have an order higher than 1.

These results are disappointing; but one should bear in mind that they are formulated in a very general setting and that the requirement of strict contractivity (i.e., step-by-step stability with an amplification factor $\leqslant 1$) is rather strong [4]. A stability and convergence theory, including higher-order convergence results, based on (problem-adapted but otherwise fixed) nonscalar product norms like an appropriate rescaled maximum norm may still be realizable for particular interesting classes of stiff problems, without contradicting the negative results of [23,32]. The following example illustrates this idea.

Example. Assume that the two-stage Radau IA method, characterized by the Runge–Kutta coefficient tableau

$$\begin{array}{c|cc} 0 & \frac{1}{4} & -\frac{1}{4} \\ \frac{2}{3} & \frac{1}{4} & \frac{5}{12} \\ \hline & \frac{1}{4} & \frac{3}{4} \end{array} \tag{4.2}$$

is applied to a linear constant-coefficient singular perturbation problem $y' = Jy$; let us assume that the eigenvalues of J are -1 and $-1/\epsilon$, that the "stiff eigenvector" is $(0, 1)^{\mathrm{T}}$, and that the angle σ between the eigenvectors of J satisfies $\sigma \in [\frac{1}{4}\pi, \frac{1}{2}\pi]$ such that the problem is contractive in the unscaled maximum norm [5]. That is,

$$J = \begin{pmatrix} -1 & 0 \\ \left(\frac{1}{\epsilon} - 1\right) \cot\sigma & -\frac{1}{\epsilon} \end{pmatrix}, \quad \cot\sigma \leqslant 1, \tag{4.3}$$

(example (2.1) is of this type, with $\sigma = \frac{1}{4}\pi$).

Application of the method (4.2) with stepsize h leads to the recursion $\eta_\nu = R(hJ)\eta_{\nu-1}$, with

$$R(hJ) = \begin{pmatrix} R(-h) & 0 \\ \left(R(-h) - R\left(-\frac{h}{\epsilon}\right)\right)\cot\sigma & R\left(-\frac{h}{\epsilon}\right) \end{pmatrix}, \tag{4.4}$$

where $R(z) = (2z+6)/(z^2 - 4z + 6)$ is the stability function of the two-stage Radau IA scheme. This method is A-stable, i.e., $|R(z)| \leqslant 1$ for all Re $z \leqslant 0$. Note that $R(x) < 0$ for real $x < -3$; its minimal value on the negative real axis is attained at $\bar{x} = -3(1+\sqrt{3}) \approx -8.2$, with $R(\bar{x}) \approx -0.098$.

The recursion $\eta_\nu = R(hJ)\eta_{\nu-1}$ does not always behave contractively with respect to $\|\cdot\|_\infty$. For $\sigma \approx \frac{1}{4}\pi$ and $h \approx \epsilon|\bar{x}|$ we have

$$\|R(hJ)\|_\infty \approx \max\left\{1, \left|R(-h) - R\left(-\frac{h}{\epsilon}\right)\right| \cot\sigma + \left|R\left(-\frac{h}{\epsilon}\right)\right|\right\} \approx 1.2, \tag{4.5}$$

because $R(-h/\epsilon) \approx R(\bar{x}) \approx -0.1 < 0$. (A similar "overshooting effect" occurs for any method where $R(x) < 0$ on some section of the negative real axis.) Formula (4.5) also shows that not even a weaker form of step-by-step stability, i.e., $\|R(hJ)\|_\infty \leqslant 1 + Ch$ with a moderate-sized quantity C is satisfied, and therefore no satisfactory convergence result can be based on (4.5).

On the other hand, it is easy to verify that the above recursion behaves contractively, for arbitrary $\sigma \in [\frac{1}{4}\pi, \frac{1}{2}\pi]$, with respect to an appropriately rescaled norm. The choice $\|y\|_{\infty,D} := \|Dy\|_\infty$, $D = \mathrm{Diag}(1, d)$ with $d \approx 0.82$, immediately leads to $\|R(hJ)\|_{\infty,D} \leqslant 1$. Together with an appropriate consistency analysis, this contractivity property could now serve as a basis for estimating the global error norm $\|\eta_\nu - y(t_\nu)\|_{\infty,D}$; eventually, such an argument will also yield an $O(h^2)$-bound for $\|\eta_\nu - y(t_\nu)\|_\infty$.

The "geometry" of the situation described in this example suggests that similar effects will occur for certain Runge–Kutta schemes applied to singularly perturbed problems (linear as well as nonlinear); it may well be possible to base a general convergence argument on related ideas.

Summarizing all this, we see that the choice of norm is crucial in the analysis of stiff problems. One may hope that a careful choice of norms will lead to interesting stability and convergence results for some particular classes of stiff problems (e.g., multi-parameter singular perturbation problems) and particular discretization schemes.

On the other hand, the concept of step-by-step stability will presumably be too weak for sufficiently "difficult" problem classes, i.e., *global* stability approaches will have to be used in general. Note that even for certain classes of *linear* problems (e.g., in strongly nonnormal situations) global stability approaches are suitable (cf., for instance, [30]). In linear situations the global stability analysis leads to the question of power-boundedness of certain linear operators, and results like the Kreiss Matrix Theorem (cf., e.g., [25]) providing characterizations of power-boundedness via resolvent inequalities are of major importance (cf., e.g., [27,30]).

Still, we are far from understanding all phenomena in strongly nonlinear stiff situations. It is an interesting question whether global stability concepts based on characterizations of power-boundedness can be generalized in order to cover relevant classes of highly nonlinear problems.

[4] A step-by-step stability inequality with an amplification factor $1 + Ch$ (C moderate-sized), relaxing the requirement of contractivity, is usually sufficient in a convergence argument.

[5] None of these assumptions is essential, they are only made to simplify the presentation.

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