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The Role of Difference Equations in Numerical Analysis

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Abstract—The central role of difference equations and, principally, the role of their stability properties in Numerical Analysis is discussed by analyzing the special problem of approximating the solutions of ordinary differential equations. We show how a deeper knowledge of the stability properties of difference equations may be useful in designing numerical methods.

Keywords—Difference equations, Ordinary differential equations, Initial value problems, Boundary value problems, Stability.

1. INTRODUCTION

According to Threfethen's definition [1], Numerical Analysis is the study of algorithms for the problems of continuous mathematics. At the hearth of algorithms, one often finds difference equations. Moreover, since the solutions of such difference equations must be "near" to the solutions of the continuous problems, the stability properties of the difference equations assume a central role. The fact that one is forced to work with finite arithmetic, instead of the infinite precision arithmetic, adds additional perturbation to the difference equations, making sometime the stability request even more crucial.

The prominence of the role of the stability properties makes the difference among the Numerical Analysis and other branches of mathematics which also use the difference equations as a main tool. For example, in Combinatorics, difference equations are very important, but their stability properties are not, since the problems involved are often unstable and the interesting part concerning the solutions is their asymptotic behavior.

A comprehensive discussion about the role of difference equations (and the related stability properties) in Numerical Analysis, would require much more space than the length of a paper. We shall confine ourselves to discuss three aspect of the same problem, that is the approximation of the solutions of a differential equation. In Section 2, we shall review the problem of approximating the solution of an initial value problem by means of a discrete one. The same continuous problem will be treated in Section 4, but there the discrete problem will become a boundary value one. In Section 3, as an example of boundary value problem, the singular perturbation boundary value problem will be analyzed.

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2. INITIAL VALUE PROBLEMS

Often the problem of approximating the solution of an initial value problem by means of a discrete one is not precisely stated, since part of the needed hypothesis are not explicitly mentioned. This is not a shortcoming of the Numerical Analysts only, but it is an aspect of the more general "dogma of stability" which has characterized for many years the physical models (see, for example, [2]). Consider the approximation of the Initial Value Problem:

$$y' = f(t, y), \qquad y(t_0) = y_0 \tag{1}$$

where $y, f \in \mathbb{R}$. We suppose that the solution is unique in the interval (t_0, T). A discrete problem is usually obtained from (1) by approximating the continuous quantities by discrete ones, obtaining

$$F_h\left(y(t_n), y(t_{n+1}), \ldots, y(t_{n+k}), f(t_n, y(t_n)), f(t_{n+1}, y(t_{n+1})), \ldots, f(t_{n+k}, y(t_{n+k}))\right) = \tau_n. \tag{2}$$

We shall not go into the details on the way of obtaining the previous formula. The interested reader may refer to the excellent books on the subject (see for example [3–6]). For our purpose, $y(t_n)$ are the values of the solution in a discrete set of points, h is the stepsize, and τ_n is the local error which is $O(h^{p+1})$ for some integer $p \geq 1$, said order of the method. Moreover, n may range between 0 and N which will be considered large, and it does not matter because the problem requires h to be small or T to be large. The relation (2) is a difference equation of degree k. Since τ_n is not known, except for the above-mentioned asymptotic behavior with respect to h, the numerical method will disregard it, solving instead of (2) the difference equation:

$$F_h\big(y_n, y_{n+1}, \ldots, y_{n+k}, f(t_n, y_n), f(t_{n+1}, y_{n+1}), \ldots, f(t_{n+k}, y_{n+k})\big) = 0. \tag{3}$$

Actually, because of the necessity of using finite precision arithmetic, instead of (3), a further perturbation of (2) is solved, that is

$$F_h\big(y_n, y_{n+1}, \ldots, y_{n+k}, f(t_n, y_n), f(t_{n+1}, y_{n+1}), \ldots, f(t_{n+k}, y_{n+k})\big) = \varepsilon_n. \tag{4}$$

The quantities ε_n, which take into account the errors due to the finite precision, are small, depending on the machine precision used, but they do not depend on h. The different nature of the two perturbation τ_n and ε_n will have a certain theoretical importance, as stressed below.

Equation (4) is a perturbation of equation (2), which, if the initial condition are exactly stated, gives the values of the continuous solution at the grid points. The sources of perturbation are:

1. the local errors τ_n
2. the precision errors ε_n
3. the k initial points: only one of them, y_0, may be exactly known.

When will all the previous perturbation not affect "too much" the solution? This is a problem of structural (or total) stability, very similar to the structural stability typical of physical models. Here the hidden hypothesis comes in:

(a) the differential equation (1) has an equilibrium point $\overline{y}$ and one is interested to approximate the solution in a neighborhood of this point;
(b) the function $f(t, y)$ has a Taylor expansion with nonzero linear part around $\overline{y}$ and, for the linearized problem, $\overline{y}$ is uniformely asymptotically stable.

Under such hypothesis, one obtains the needed structural stability, and the first approximation stability theorem can be used. This permits us to linearize the discrete problem and, consequently, justifies the use of the popular linear test equation $y' = \lambda y$, $\mathrm{Re}(\lambda) < 0$, to study the numerical methods. It is true that seldom one studies the methods for $\mathrm{Re}(\lambda) > 0$ but still there is the hidden hypothesis that one is integrating in a neighborhood of an (unstable) equilibrium point.

Numerical methods applied to problems far from the equilibrium points, for example in chaotic regime, have, so far, not been extensively studied. To be more clear, let us analyze the case of linear multistep formulas. In this case, (2) and (4) become

$$\sum_{j=0}^{k} \alpha_j y(t_{n+j}) - h \sum_{j=0}^{k} \beta_j f\big(t_{n+j}, y(t_{n+j})\big) = \tau_n, \tag{5}$$

$$\sum_{j=0}^{k} \alpha_j y_{n+j} - h \sum_{j=0}^{k} \beta_j f_{n+j} = \varepsilon_n. \tag{6}$$

By subtracting and posing $e_n = y(t_n) - y_n$, one obtains the error equation:

$$\sum_{j=0}^{k} \alpha_j e_{n+j} - h \sum_{j=0}^{k} \beta_j \big(f(t_{n+j}, y_{n+j} + e_{n+j}) - f_{n+j}\big) = \tau_n - \varepsilon_n. \tag{7}$$

The unperturbed equation has $e_n = 0$ as a constant solution. Of course the numerical solution is meaningful if this constant solution is at least stable. Here the different nature of τ_n and ε_n plays a role (essentially of theoretical nature). In fact, if ε_n is not considered, provided that h tends to zero as n tends to infinite, one may show that the stability of the constant solution of $\sum_{j=0}^{k} \alpha_j e_{n+j} = 0$, which is only part of (7), implies the convergence of the perturbed equation. This is called 0-stability and it is only of theoretical interest. In fact, the condition $h \to 0$ is very heavy, and moreover, $\varepsilon_n = 0$ is not realistic. It is remarkable that for $\varepsilon_n \neq 0$, no convergence results can be provided. Much more realistic is to ask for the asymptotic stability of the unperturbed equation derived from (7). This was established first by Dahlquist [7]. Supposing that (1) satisfies the hypotheses (a) and (b), one may linearize and study the linear error equation:

$$\sum_{j=0}^{k} (\alpha_j - h\lambda\beta_j)\, e_{n+j} = \tau_n - \varepsilon_n, \tag{8}$$

whose stability properties are dictated by the polynomial ($q = h\lambda$):

$$\prod(z, q) = \sum_{j=0}^{k} (\alpha_j - q\beta_j)\, z^j \tag{9}$$

The asymptotic stability of the zero solution of the unperturbed equation is obtained for the values of q for which the polynomial $\prod(z, q)$ is a Schur polynomial, that is when the roots are all inside the unit disk in the complex plane. Let $\mathcal{D}$ be the set of values of q for which $\prod(z, q)$ is a Schur polynomial. It is called region of absolute stability. It represents the values of $h\lambda$ ($\lambda \in \mathbb{C}^-$) for which the continuous problem and the discrete one have similar qualitative behavior. Depending on the choice of the parameters α_j and β_j (and then on the methods), it may happen that

$$\mathcal{D} \begin{matrix} \subset \\ \equiv \\ \supset \end{matrix} \mathbb{C}^-.$$

It would be desirable to have $\mathcal{D} \equiv \mathbb{C}^-$ but it turns out that this is possible only when (Dahlquist barriers) $\beta_k \neq 0$ and $p \leq 2$ (p is the order of the method). Even when this happens, as for the trapezoidal method,

$$y_{n+1} - y_n = \frac{h}{2}(f_n + f_{n+1}),$$

one must say that, even if the two solutions (the continuous and the discrete ones) share the property of decaying, for relatively large values of q the discrete solution shows up an oscillating

behavior which is absent in the continuous solution. This means that only approximatively the qualitative behavior can be considered similar. Let us, for example, assume that $\lambda = -60$, $h = 0.1$, $t_0 = 0$. One has $y(t_n) = (e^{-6})^n y_0$ and $y_n = (-\frac{1}{2})^n y_0$ from which it is evident that the two solutions only share the generic property that they tend to zero. If the hypothesis (b) is not satisfied, the discrete solution may even not exist for q not very small. Consider for example the problem $y' = -y^2, y(0) = y_0$. The continous solution is $y = y_0/(1 + y_0 t)$. By applying the trapezoidal rule one has

$$y_{n+1}^2 + \frac{2}{h} y_{n+1} - \frac{2}{h} y_n + y_n^2 = 0.$$

This is a second degree equation in y_{n+1}. It is evident that if $hy_n > 1 + \sqrt{2}$ it has not real solutions and the numerical method is not defined. For smaller values of h one may recover the numerical method, but in this case, the region of absolute stability loses its importance. It is interesting to note that if one uses, as usual, the Newton method to solve the nonlinear equations at each step, it converges for $hy_n < \eta < 1 + \sqrt{2}$. By a little analysis, one may show that the condition $hy_n < 2$ is sufficient for the convergence. This condition is the same which guarantees the root $z_1 = \frac{1+q/2}{1-q/2}$ of the characteristic polynomial associated to a linearization of the equation around an approximate solution $\hat{y}_n$, to be positive (for $q \in \mathbb{R}^-$). This is not surprising considering that z_1 has to approximate e^q.

The case $\mathcal{D} \supset \mathbb{C}^-$ presents similar limitations and moreover if $\lambda \in \mathbb{C}^+$, the qualitative behavior of the two solutions may be completely different.

The case $\mathcal{D} \subset \mathbb{C}^-$ can be easily realized but it is not sufficient for a large class of problems (stiff problems).

Without going into more details, we shall say that this approach, which is the most widely used, is not the only possible, as shown is Section 4.

3. BOUNDARY VALUE PROBLEMS

When it is well conditioned, a Boundary Value Problem is characterized by having the solution made up of components which are both decreasing and increasing for $t \to \infty$. The numerical methods need to generate discrete problems which show similar characteristics. If one tries to use numerical methods which do not fulfill this request, as in the popular shooting method, the discrete problem presents very serious instability. A deeper analysis of this question may be found in [8,9].

In order to show how the knowledge of the stability properties of a difference equation are essential in designing efficient numerical methods, let us discuss in details the second order singular perturbation problem:

$$\begin{aligned} &\epsilon y'' + s(t)y' + c(t)y = f(t), \qquad && t \in [t_{\min}, t_{\max}], \\ &y(t_{\min}) = a, \quad y(t_{\max}) = b, \end{aligned}$$

where ϵ is positive (it could be very small), $c(t)$ and $f(t)$ are continuous functions on the integration interval $[t_{\min}, t_{\max}]$ and $s(t)$ is differentiable.

This problem is considered a difficult one since, because of the small parameter ε, the solution may present very different behaviors in different subintervals of (a, b). In a recent paper [10], Kreiss *et al.* have discussed the necessity, in order to avoid very small values of steplengths on large intervals, to use different methods (characterized as forward, backwards and symmetric) on different subintervals. They should be chosen according to the signs and the magnitude of the eigenvalues of a suitable matrix. Our approach, based on the stability properties of a second order difference equation, will lead to similar conclusions, but, in our case the choice among backward, symmetric or forward methods is automatic since the nature of the method is imbedded in a unique difference equation.

By using a three point scheme to approximate the derivatives of the problem, we obtain, as discrete problem, the second order difference equation:

$$\begin{aligned} &\sigma_{i-1}y_{i-1} + y_i + \tau_i y_{i+1} = f_i, \\ &y_0 = a, \quad y_{n+1} = b, \end{aligned} \tag{10}$$

where

$$\sigma_i = \frac{-h_{i+1}(2\epsilon - s(t_{i+1})h_{i+1})}{(h_{i+1}+h_i)(2\epsilon + s(t_{i+1})(h_i - h_{i+1}) - c(t_{i+1})h_i h_{i+1})}, \tag{11}$$

$$\tau_i = \frac{-h_{i-1}(2\epsilon + s(t_i)h_{i-1})}{(h_{i-1}+h_i)(2\epsilon + s(t_i)(h_{i-1} - h_i) - c(t_i)h_i h_{i-1})}, \tag{12}$$

hence, the coefficients depend on the stepsizes. Note that if $\tau_i = 0$, the method behaves as a forward one, while, if $\sigma_i = 0$, the method behaves as a backward one. Of course, if $\sigma_i = \tau_i$, the method is a symmetric one. Since each σ_i and τ_i, as functions of the stepsizes, are able to assume all the values, it is evident the flexibility of the method to adapt itself to the different situations in the subintervals.

In [11], it was shown that it is possible to find values of the stepsize in order to have

$$\max|y_n| \leq k\,(|y_0|, |y_{n+1}|, \max|f_n|),$$

which is equivalent to the definition of stability. The study of the stability of difference equations with variable coefficients was done by studying the equivalent problem in matrix form,

$$T\mathbf{y} = \mathbf{f},$$

where $\mathbf{y} = (y_1, \ldots, y_n)^\top$, $\mathbf{f} = (\mathbf{f}(t_1) - \sigma_0 y_0, \mathbf{f}(t_2), \ldots, \mathbf{f}(t_n) - \tau_n y_{n+1})^\top$ and

$$T = \begin{pmatrix} 1 & \tau_1 & & \\ \sigma_1 & \ddots & \ddots & \\ & \ddots & \ddots & \tau_{n-1} \\ & & \sigma_{n-1} & 1 \end{pmatrix}_{n\times n}.$$

To obtain a stable difference equation, it is sufficient to choose σ_i and τ_i so that T^{-1} exists and $\|T^{-1}\|$ is either independent from n (well conditioned), or it grows as n or n^2 (weakly well conditioned). In this way, the global error can be controlled.

Let $\mathbf{x} = (y(t_1), \ldots, y(t_n))^\top$ be the vector of the exact solution at the gridpoints; the global error $\mathbf{e} = \mathbf{y} - \mathbf{x}$ satisfies

$$T\mathbf{e} = \zeta,$$

where $\zeta = (\zeta_1, \ldots, \zeta_n)^\top$ is the vector of the local truncation errors. One has then

$$\|\mathbf{e}\| \leq \|T^{-1}\|\,\|\zeta\|,$$

and, if $\|T^{-1}\|$ depends at most on n^2, we may conclude that

$$\|\mathbf{e}\| \leq kO(h^q), \qquad q \geq 1, \quad h = \max(h_i), \quad k \text{ a constant.}$$

The solvability of the discrete problem is related to the solvability of the continous one. It turns out that the conditions of existence of the solution for the problem (10) are very similar to the conditions of existence for the continuous problem. Consider, for example, the following widely used condition [12]:

$$c(t) \leq \frac{s^2(t)}{4\epsilon} + \frac{s'(t)}{2} + \left(\frac{\pi}{t_{\max} - t_{\min}}\right)^2 \epsilon, \tag{13}$$

which is sufficient for the continous problem to have solution; a similar result holds for the discrete problem. In fact, one has:

THEOREM 1. *Suppose a constant stepsize is used. A sufficient condition for the matrix T to be invertible is the following:*

$$c(\zeta) \leq \frac{s(t_{i+1})s(t_i)}{4\epsilon} + \frac{s'(\eta)}{2}, \qquad c(t_{i+1})\, c(t_i) > 0. \tag{14}$$

with $\zeta, \eta \in [t_i, t_{i+1}]$.

PROOF. A sufficient condition for T to be invertible is (see [13])

$$\sigma_i \tau_i \leq 1/4, \qquad \text{for all } i.$$

By substituting the values of σ_i and τ_i in (11) and (12), it results that this inequality is satisfied if:

$$-2\epsilon s'(\eta) - s(t_{i+1})s(t_i) \leq -4\epsilon c(\zeta) + c(t_{i+1})c(t_i)h^2,$$

with $\zeta, \eta \in [t_i, t_{i+1}]$. The previous inequality is certainly satisfied if (14) holds true. ∎

The conditions on τ_i and σ_i which ensure the well conditioning of the matrix T are known [13]. By applying these conditions it is possible to choose, by using (11) and (12), the optimal stepsizes. From this point of view one could say that an inverse problem is solved in order to obtain an optimal sequence of stepsizes.

In particular, the next result gives the possibility to choose a constant stepsize.

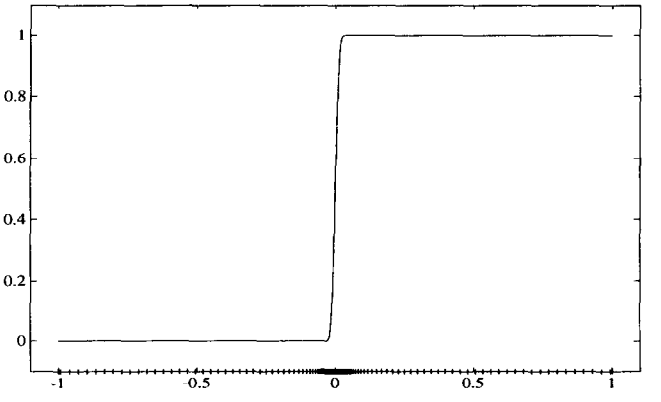

Figure 1. $\epsilon = 10^{-4}$.

THEOREM 2. *Suppose that, for $t \in [t_{\min}, t_{\max}]$, $k \geq 0$,*

(i) $c(t) \leq -k$

(ii) $s'(t) \geq -k$

(iii) *h is constant and,*

if $s'(t) > k$, $h \leq \left(2\epsilon/(\max|s'_t| - k)\right)^{1/2}$

if $s(t_{\min}) > 0, h \leq -2\epsilon/s(t_{\min})$

if $s(t_{\max}) < 0$, $h \leq -2\epsilon/s(t_{\max})$,

then T is invertible and well conditioned or weakly well conditioned.

If the continous problem is ill conditioned or one wish to use fewer grid points, it is necessary to use a variable stepsize. This can be efficiently done but we skip here the details (see [11]).

As an example consider the solution of the following BVP [11]:

$$\epsilon y'' + ty' = 0, \qquad -1 < t < 1,$$
$$y(-1) = 0, \qquad y(1) = 1,$$

which has a turning point at $t = 0$.

This problem was solved by choosing the stepsize according to what was said above. In Figure 1 we report the solution for $\epsilon = 10^{-4}$, and the stepsize variation.

4. INITIAL VALUE PROBLEMS SOLVED BY DISCRETE BOUNDARY VALUE METHODS

The possibility of using discrete boundary value problems for the solution of continuous initial value problems is also essentially based on the above mentioned "axiom of stability." In fact the knowledge of the tendency of the solution to a steady state (asymptotic stability to this solution), was the idea which led to this possibility [14–16]. On the other hand, it was noticed that the most difficult initial value problems are those for which the approximation of the subdominant solutions is needed. Subdominant solutions are those which present the smallest growing factor. For example, consider the discrete problem

$$y_{n+2} - 102y_{n+1} + 200y_n = 0.$$

The general solution is $y_n = c_1 2^n + c_2 100^n$. Suppose we have the initial condition $y_0 = \sqrt{3}$, $y_1 = 2\sqrt{3}$, then we need to get the solution $y_n = 2^n\sqrt{3}$. Unfortunately this solution is very unstable because if y_1 is not exactly twice y_0, then an error proportional to 100^n will arise destroying very soon the right solution. Boundary value problems do not have this drawback, as noticed by Miller [17] and Olver [18]. For example, in the previous example one may choose an N large enough and pose $y_N = 0$, $y_{N-1} = 1$ and then solve the problem backward, obtaining, after multiplying the entire sequence by $\sqrt{3}/y_0$, a very good approximation of the solution for $n \ll N$. Many authors, for example Cash [19], Axelsson and Verwer [20], Lopez and Trigiante [21], taking advantage of this fact, have used boundary discrete value methods to approximate the solutions of stiff initial value problems (see also [22,23]). In such problems, in fact, a situation similar to the one in the previous example arises when one uses discrete initial value problems to approximate the continuous solution.

To obtain a discrete boundary value problem one adds extra points to the right of the extreme point T. Let them be $t_N, t_{N+1}, \ldots, t_{N+k-2}$ for some $N > 1$. The initial condition is imposed in t_0, while additional conditions are imposed in the above defined extra points. Usually the extra conditions are imposed not explicitly, by using, at the end, methods which require fewer points (see [21,24,25] for details). The following theorem, wich generalizes previous results, states in more precise form what said before (see [26]).

THEOREM 3. *Suppose that the roots z_i of the characteristic polynomial*

$$p(z) = \sum_{i=0}^{k} p_i z^i$$

are such that

$$|z_1| < |z_2| \leq \cdots \leq |z_k, \tag{15}$$

then there exists k_1 constant and a bounded quantity ξ_{00} such that the solution of the difference equation:

$$\sum_{i=0}^{k} p_i \xi_{n+i} = g_n, \tag{16}$$

with the boundary condition described above, is

$$\xi_n = (\xi_0 + \xi_{00}) z_1^n + k_1 \sum_{j=0}^{n-1} g_j z_1^{n-j-1} + O\left(\left|\frac{z_1}{z_2}\right|^{N-n}\right) + O\left(|z_2|^{-(N-n)}\right) \tag{17}$$

as $N \to \infty$.

To apply the theorem to the problem (2), one must be sure that the problem can be linearized. If this is the case, then the linear problem leads to the characteristic polinomial (9). If the linear

part of the discrete problem has $\mathrm{Re}(\lambda) < 0$, then one needs to have $|z_1| < 1$ in the previous theorem, while all the remaining roots are to stay outside the unit disk of the complex plane. This approach is alternative to the classical approach of Dahlquist. The root conditions are quite different and methods which were considered bad may now be good ones. This is the case, for example, for the so-called Simpson method, which is of order four and has, as boundary value method, a very large region where the conditions of Theorem 3 are satisfied. As matter of fact the root condition is less tight in this approach: There are not barriers such as the Dahlquist barriers. Moreover, convergence results can be done even in the case of constant h and in the case of finite arithmetic. In fact, suppose that h is fixed and $N \to \infty$ and that (16) is the linearized error equation (8), one obtains that $\xi_n \equiv y(t_n) - y_n$ remains bounded (see [24] for details). For $h \to 0$, results similar to the classical ones are obtained.

The pratical use of such methods requires the solution of large systems of linear equations. This can be done on parallel computers, where they become competitive with the classical ones (see [27–29]).

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