

THE USE OF STABILITY CHARTS IN THE SYNTHESIS OF NUMERICAL QUADRATURE FORMULAE*

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Abstract. A classification of quadrature formulae is made according to their stability chart characteristics. Methods are described for synthesizing formulae with such characteristics, emphasis being placed upon those methods used for formulae which are applicable in real-time simulation problems. The relations between the stability chart characteristics and computed results are also discussed.

1. Introduction. The notion of the stability chart was first introduced by Gray [1] in connection with the problem of digital real-time simulation. He described the original use of these charts as a check upon the feasibility of using a particular given numerical integration method in solving a system of linear, constant-coefficient differential equations. In this paper we are going to describe another use of these charts, the development of new quadrature formulae, i.e. formulae to be used in solving differential equations.

2. The concept of the stability chart. The quadrature methods which we consider fall in three categories:

1) The open formula

$$x_n = \sum_{i=1}^M a_{i0} x_{n-i} + h \sum_{i=1}^N b_{i0} x'_{n-i},$$

where x_i means $x(ih)$ and $x'_i = dx/dt_{i-h}$. Such a formula is denoted as an O_{MN} formula; (or an open formula of type O_{MN}).

2) The closed or repeated closure formula

$$x_n = \sum_{i=1}^P a_{ic} x_{n-i} + h \sum_{i=0}^{Q-1} b_{ic} x'_{n-i},$$

where this is an iterative procedure with the value of x'_0 at any step being obtained from x_0 of the previous step (at the first step we use an educated guess—some open method). This is denoted by rC_{PQ} .

3) The mixed formula $O_{MN}C_{PQ}$ is the open method O_{MN} followed by one application of the closed method where all ordinates (x_i) in both the open and closed formulae use the values computed from the closed and all derivatives (x'_i) are computed using the value computed from the open formula (see Gray [1]).

In all of the above formulae the a 's and b 's are real.

Suppose now we are concerned with the problem of integrating an equation of the type

$$x' = \lambda x, \tag{1}$$

where λ is complex. Assume we have decided upon a fixed quadrature formula of one of the types mentioned above. Let h be the interval of integration and assume that we are given a set of initial conditions for a function $x(t)$ satisfying an equation of type (1).

Let $z = \lambda h$. Then it is known that there exists a positive integer s , constants c_i

*Received April 13, 1954. The work described here was performed in connection with Contract Nonr-551(02) with Special Devices Center, O.N.R.

($i = 1, \dots, s$) dependent on the initial conditions and complex valued functions $r_i(z)$ ($i = 1, \dots, s$) such that the computed solution of (1) is

$$x(nh) = \sum_{i=1}^s c_i [r_i(z)]^n \quad \text{for } n \geq 0. \tag{2}$$

For $i = 1, \dots, s$, let $w_i(z)$ be the principal value of $\log [r_i(z)]$. Then the given quadrature formula yields polynomials P and Q such that

$$z = \frac{P\{\exp [-w_i(z)]\}}{Q\{\exp [-w_i(z)]\}} \quad \text{for } i = 1, \dots, s,$$

where $P(0) = 1$ and $Q(0) = 0$ for an open or mixed formula, and $P(0) = 1$ and $Q(0) = b_{0c} \neq 0$ for a closed formula [1].

Let $\phi(w) = [P(e^{-w})]/[Q(e^{-w})]$ for all complex numbers w . Then the roots of

$$\phi(w) - z = 0 \tag{3}$$

are exactly the values $w_i(z)$, $i = 1, \dots, s$. We call ϕ the characteristic function of the given quadrature formula.

Let $w_d(z) = w_i(z)$, where $R[w_i(z)] \geq R[w_j(z)]$ $j = 1, \dots, s$. Thus in general w_d is a many-valued function of z . The stability chart for a given quadrature formula is simply a picture of the mapping $z \rightarrow w_d(z)$ in a neighborhood of the origin.

For the moment let us only consider domains where w_d is a single valued function of z . In this case we call $w_d(z)$, the dominant root of Eq. (3).

In the problem of real-time simulation our foremost aim is stability, i.e.

$$\frac{\text{computed solution}}{\text{true solution}} \rightarrow 1 \quad \text{as } t \rightarrow \infty.$$

Because of this and since by (2) $x(nh) = c \exp [nw_d(z)]$ for large n , we certainly would like to have the relation $w_d(z) = \phi[w_d(z)] = z$ for each z in the domain under consideration. In particular we want $w_d(0) = 0$, i.e. we certainly want stability for the equation $x' = 0$. Thus we would like $w_d(z) = z$ in a neighborhood of the origin. Looking at this from the opposite point of view we would want $\phi(w) = w$ in a neighborhood of the origin in the w -plane in which $w = w_d[\phi(w)]$.

The stability chart shows how good an approximation of $w_d(z) = z$ is obtained for a given quadrature formula. Thus it gives an indication of the stability of the numerical solution of a linear differential equation using the given formula.

3. Synthesis of new formulae. In the synthesis of new formulae our aim has been to make $w_d(z) \approx z$ in as large a region around the origin as possible. Thus we want w_d to be single valued there. We have found, however, that it is much more feasible to work with the inverse relations. Thus the main criteria considered in the development of new quadrature formulae have been:

- 1) $w_d(0) = 0$
- 2) $\phi(w) \approx w$ in as large a neighborhood of the origin as possible where $w_d[\phi(w)] = w$.

We first consider 2).

If $\phi(w) = w$ were to hold exactly in some neighborhood of the origin, then we would have

$$\left. \begin{aligned} \phi(0) &= 0, \\ \phi'(0) &= 1, \\ \phi^{(n)}(0) &= 0 \quad \text{for } n > 1. \end{aligned} \right\} \tag{4}$$

However, since there are only a finite number of quadrature coefficients which determine the coefficients of the polynomial P and Q , we see that the infinite set of conditions (4) cannot be fulfilled.

For an open or closed formula, the Eqs. (4) are linear in the quadrature coefficients. If we consider these coefficients as unknown and if there are n of them, then the first n linear equations above are independent. Thus they can be solved simultaneously. The coefficients so obtained are called "classical" and the corresponding formula, the "classical quadrature formula" of the particular type in question. The reason for the name is that the formulae so obtained are just those which can be obtained by Taylor series matching. For an open or closed formula we call the first k conditions of (4) the first k "classical conditions". When a mixed formula is such that the open and closed formulae forming it are classical then we also call the mixed formula "classical".

Now consider the characteristic function ϕ for a mixed formula. Suppose the formula uses n^* quadrature coefficients. The coefficients of the polynomials P and Q are functions of these n^* quadrature coefficients. Let the polynomial coefficients be p_i, q_i , where $i = 0, 1, \dots, r$ and $j = 0, 1, \dots, s$ and r and s are the respective degrees of P and Q . Let R be the range of all possible $(r + s + 2)$ -tuples $(p_0, p_1, \dots, p_r, q_0, q_1, \dots, q_s)$ when the quadrature coefficients take on all real values. Suppose it is possible to find $k < n^*$, such that all points in R can be obtained with k of the quadrature coefficients held constant. Then really only $N = n^* - k$ quadrature coefficients are necessary to determine ϕ .

Consider the first N of the Eqs. (4) for a mixed formula of a given type with undetermined coefficients. In general all the equations will not be linear; some will be quadratic. However, if we can solve them simultaneously and we set the k non-essential quadrature coefficients noted above equal to 1, then we get a set of quadrature coefficients which we call "completely classical". The corresponding formula is a "completely classical" mixed formula and indeed the various conditions given by (4) are the "completely classical" conditions.

It must be stressed that the completely classical conditions and not the combination of open and closed classical conditions must be satisfied by the mixed formula coefficients in order that $\phi(w) \approx w$. The classical coefficients for a mixed formula will always satisfy some completely classical conditions but usually not all (indeed no such case has been found). Thus in order to investigate the validity of $\phi(w) \approx w$ near the origin without actually inspecting the stability chart itself one should see if the completely classical conditions are satisfied (or almost satisfied).

Another important point is that a completely classical mixed formula may not exist for every method $O_{MN}C_{RS}$. And indeed when one does exist there may appear to be more than one such formula (since our simultaneous equations are quadratic). It is necessary that for each formula found, classical, completely classical or otherwise, the original condition be satisfied, i.e. the condition that $w_2(0) = 0$. Although necessary and sufficient conditions that this be satisfied have not been found, several necessary conditions have been found and may be used as a quick check on the possibility of a stability chart corresponding to a useful quadrature formula. We might list a few of the simpler ones:

If

$$r^N P\left(\frac{1}{r}\right) = R(r) = r^N - \sum_{i=1}^N a_i r^{N-i}$$

then the following must hold:

- I. $|a_N| < 1$ unless $R(r) = (r - 1)^N$,
- II. $\left. \frac{dR(r)}{dr} \right|_{r=1} = N - \sum_{i=1}^N (N - j)a_i \geq 0$,
- III. $\left. \frac{dR(r)}{dr} \right|_{r=-1} = N(-1)^{M-1} - \sum_{i=1}^N (N - j)a_i(-1)^{N-i} \left. \begin{array}{l} > 0 \quad N \text{ odd} \\ < 0 \quad N \text{ even} \end{array} \right\}$

Other similar conditions can also be found.

Obviously any one of the classical open or closed or completely classical mixed formulae corresponds to the stability chart which is most nearly the identity map at the origin among the charts for formulae of the same type. However, as mentioned above, the condition $w_d(0) = 0$ is not always satisfied for such formulae, and even when it is, the neighborhood of the origin where $w_d(z) \approx z$ may be quite small. Thus we would want to develop other formulae which would not suffer from these deficiencies.

As noted previously the only way we can be sure that a formula does not have the first deficiency is to check directly, i.e. we must know all the coefficients. For the second problem, however, several methods have been used with a reasonable amount of success. These are the pseudo-classical or pseudo-completely classical methods (from now on we only use the term classical even though the same procedures are also used in completely classical cases) and the shifting technique.

The pseudo-classical method consists of imposing some but not all of the classical conditions and then imposing enough other conditions to get the necessary number of equations in order to obtain all the quadrature coefficients. The classical conditions are used to keep ϕ under control at the origin, the more such conditions taken, of course, the better $\phi(w) \approx w$ close to the origin. The other conditions are used to help control ϕ at points other than the origin. It is these that we must select carefully in order to get a "good" quadrature formula.

There are many tools that may be used in making the choice of the non-classical conditions in these pseudo-classical methods. Recall that the branch contour of a stability chart is the locus of points z_{bc} in the z -plane such that there exist complex numbers $w_1, w_2, w_1 \neq w_2$ such that $\phi(w_1) = \phi(w_2) = z_{bc}$ and $Rw_1 = Rw_2 = Rw_d(z_{bc})$, i.e. points where w_d is not single valued [1]. In order to make the region where $w_d(z) \approx z$ have a reasonable size, it would be advantageous if it could be shown that the branch contour is not too near the origin. This suggests the use of the theory of schlicht functions. Indeed it was found that the wealth of material about regions in which a function is schlicht (e.g. [2]) was quite useful in putting bounds on the coefficients remaining after the classical conditions had been used to eliminate as many as possible. Some bounds have also been found directly by algebraic methods, by determination of the end points of the branch contour.

The criteria used in these pseudo-classical methods may also depend on the particular problem for which the quadrature formulae are being developed. For example, in the original problem for which this method was used (real-time simulation of a certain phenomenon), we were interested only in values of $z = x + iy$ where $x \leq 0$. For some types of quadrature formulae it was found that we could not make $\phi(w) \approx w$ throughout our whole region of interest. Therefore we tried to increase the size of the region where $w = u + iv, u \leq 0$ corresponds to a $z = x + iy, x \leq 0$. Thus we were assured of damping

when there should be some (even if the true and computed rates of damping were quite different). Bounds were found on certain of the non-classical parameters (i.e. those remaining after classical conditions are used). The bounds themselves represented values such that the intersection of the $u = 0$ and $x = 0$ lines was a maximum (in y) or such that $\phi(\pi i)$ (the intersection of the $u = 0$ and $y = 0$ lines) was a minimum (in x)—this was a desirable property in open or mixed type formulae. These were of particular interest in our problem. In other problems, there might be other aims. In general, bounds might be found for which values a particular type of formula might be as nearly classical as possible, when it cannot be strictly so and still satisfy the condition of $w_d(0) = 0$.

It must be emphasized that such bounds must be found separately for each type of quadrature formula. Indeed, each pseudo-classical method must be tried separately for different types of formulae. So far we have not been able to use any one method for a general type of formula.

The only method of synthesis that is not pseudo-classical and has met with success is the shifting technique. It has been observed that in many cases stability charts for various formulae show a good approximation to the identity map for some portion of the z -plane to the right of the imaginary axis (e.g. classical $O_{12}C_{12}$ — Fig. 1). In some cases this "good" first quadrant region shows a better approximation than the "good" second quadrant region in which we were interested in the real time simulation problem. It may also be the same for regions of interest for other problems. Thus we are led to the following type of translation:

Let w_0 be real such that $\phi(w) \approx w$ is very good in a neighborhood of w_0 .

$$\text{Let } w^* = w - w_0, \quad \Theta(w^*) = \phi(w) - \phi(w_0).$$

We want θ to be the characteristic function of a usable quadrature formula. This will be so provided that

- 1) a quadrature formula having θ as characteristic function can be found;
- 2) the dominant root (i.e. w with largest real part) of the equation $\theta(w) = 0$ is $w = 0$.

As noted before, condition 2) must be checked in any case. Thus condition 1) is all we need worry about. But 1) can always be satisfied since

$$\begin{aligned} \Theta(w^*) &= \phi(w) - \phi(w_0) = \frac{P(e^{-w})}{Q(e^{-w})} - \phi(w_0) \\ &= \frac{P(e^{-w^*} \cdot e^{w_0}) - \phi(w_0)Q(e^{-w^*} \cdot e^{w_0})}{Q(e^{-w^*} \cdot e^{w_0})} = \frac{P^*(e^{-w^*})}{Q^*(e^{-w^*})}, \end{aligned}$$

where P^* , Q^* are polynomials with real coefficients (this was the reason for w_0 being real) of degree N , M respectively, and

$$\begin{aligned} N &= M = \deg Q, & \text{if } \deg P \leq \deg Q, \\ N &= \deg P, & M = \deg Q, & \text{if } \deg P > \deg Q. \end{aligned}$$

Also $P^*(0)$ can be chosen equal to 1 unless $1 - \phi(w_0)Q(0) = 0$; which can be avoided by a slight change in w_0 .

$$Q^*(0) = \begin{cases} b_0 = 0 & \text{if } \phi(w) \text{ corresponds to an open or mixed formula} \\ b_0 \neq 0 & \text{if } \phi(w) \text{ corresponds to a closed formula.} \end{cases}$$

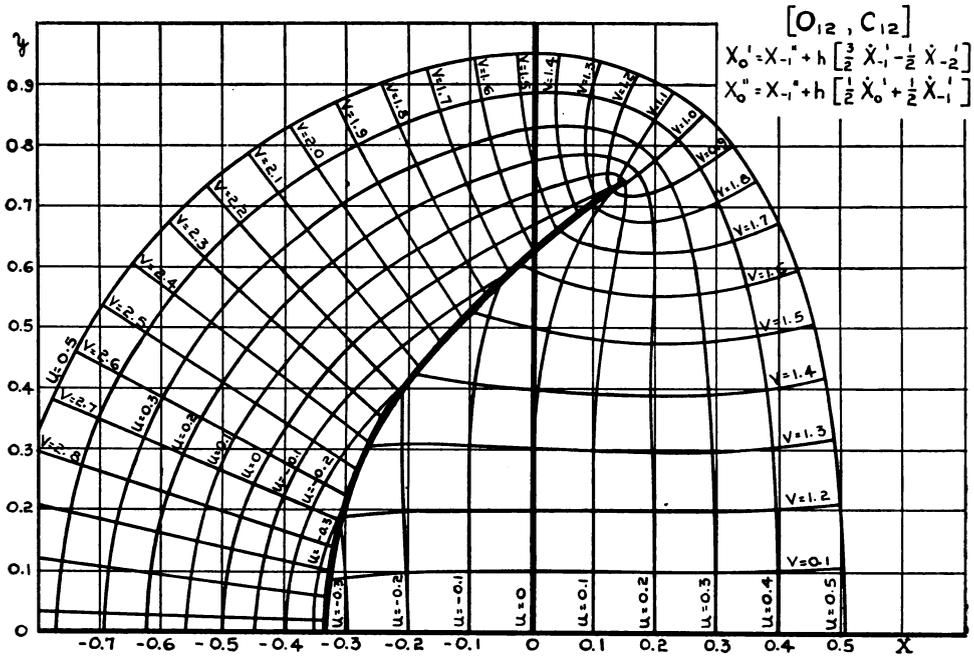


FIG. 1. Stability chart for classical $O_{12}C_{12}$

Thus if

$$P^*(r) = 1 + \sum_{i=1}^N a_i r^i, \quad Q^*(r) = \sum_{i=0}^M b_i r^i,$$

then θ is the characteristic function of

$$x_n = \sum_{i=1}^N (-a_i)x_{n-i} + h \sum_{i=0}^M b_i x'_{n-i},$$

which is really a quadrature formula since the a_i and b_i are real. Such a formula will be useful provided N and M are not too large.

4. Remarks. In conclusion we wish to reiterate that the new formulae were developed for a special purpose—real time simulation—where stability is the essential criterion. However, for any quadrature problem, stability is still very important even if it is not the first criterion to be considered. Thus it seems logical that the methods of synthesis outlined above should be combined with other methods in the development of usable formulae for any such problem.

5. Acknowledgment. The author would like to acknowledge with thanks the help and suggestions of Dr. Morris Rubinoff, Dr. H. J. Gray, and Mr. Paul Slepian, of the Moore School, University of Pennsylvania, as well as the efforts of Mrs. E. L. Fishl in preparing the manuscript for publication.

REFERENCES

- [1] H. J. Gray, Jr., *Numerical methods in digital real-time simulation*, Quart. Appl. Math.
- [2] S. D. Bernardi, *A survey of the development of the theory of schlicht functions*, Duke Math. J. 19, No. 2 (June 1952).