On the Stability of Nonlinear Differential Sequences Generated Numerically

R. Leonard Brown

Dept. of Applied Mathematics and Computer Science
Thornton Hall, University of Virginia
Charlottesville, VA 22903 USA

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1. Introduction

The numerical solution of the initial value problem for a system of ordinary differential equations

$$y'(t) = f(y(t),t) \tag{1a}$$

$$y(t_o) = y_o \tag{1b}$$

can be considered locally as the computation of a sequence of approximations $Y_n = \{y_{n-k+1},\ldots,y_{n-1},y_n\}$ with each y_n being a numerical approximation to $y(t_n)$ for $t_n = t_o + \sum_{i=1}^{n} h_i$. While many sophisticated packages [1,2,3,4] exist which change the stepsize h_i in order to achieve stability and specified accuracy, the stepsize usually remains constant for a number of steps, and the the change of stepsize is usually accompanied by an interpolatory change in the solution sequence Y_n, although not always [5]. For these reasons the local analysis, limited to k steps, given in the sequel will assume constant stepsize h. The actual numerical solution element y_n is usually computed from elements of the sequence Y_{n-1} and $f(y,t)$ using one of several formulas, each of which has a local discretization error term $\phi_n Ch^{r+1}$ where ϕ depends on f and t_n, C is a constant dependent on the formula, and r is called the order of the method. This work is concerned with how errors are propagated when numerical methods are applied to a differential function $f(y,t)$ which is nonlinear in y, with emphasis on stable propagation of the errors.

The most typical formulas in use are Runge-Kutta multistage formulas [6] and Adams type multistep methods. An s-stage Runge-Kutta formula is

$$K_o = hf(y_n,t_n) \tag{2a}$$

$$K_q = hf(y_n + \sum_{j=0}^{q-1} \beta_{qj}K_j,\ t_n + \sum_{j=0}^{q-1} h\beta_{qj}),\ q = 1,2,\ldots,s-1 \tag{2b}$$

$$y_{n+1} = y_n + \sum_{q=0}^{s-1} \gamma_q K_q. \tag{2c}$$

Families of explicit formulas exist for orders one through four, with the order equal to the number of stages. Fifth order formulas require at least six stages, and more accurate implicit formulas formed by replacing (2b) by

$$K_q = hf(y_n + \sum_{j=0}^{q} \beta^*_{qj} K_j,\ t_n + \sum_{j=0}^{q} h\beta^*_{qj}),$$ and requiring solution of systems of nonlinear equations, also exist [7]. The Adams-Bashforth and Adams-Moulton formulas are of the form

$$y_n = y_{n-1} + h\sum_{i=1}^{k} b_i f(y_{n-i}, t_{n-i}), \tag{3}$$

$$y_n = y_{n-1} + h\sum_{i=0}^{k} b_i^* f(y_{n-i}, t_{n-i}) \tag{4}$$

respectively. A k-step Adams Bashforth formula is of order k, and a k-step Adams-Moulton of order k+1. Since the latter may require iterative solution of a system of nonlinear equations, the initial solution guess may be predicted by an Adams-Bashforth formulas of the same or one lower order, and the difference may be used to approximate the discretization error [6]. Many methods iterate (4) a set number of times, often one, rather than to convergence.

The concept of multistep methods is useful since order of accuracy as high as k+1 [8] can be achieved by a stable formula with only a few evaluations of $f(y,t)$, whereas a correspondingly accurate Runge-Kutta formula requires at least one evaluation of $f(y,t)$ for each additional order of accuracy. Newer methods have been developed to handle special circumstances. The backward differentiation implicit formulas

$$y_n = \sum_{i=1}^{k} a_i y_{n-1} + h\, b_o f(y_n, t_n) \tag{5}$$

are useful in solving stiff systems of equations [1]. For systems with known complex time constants λ, such as are often encountered in simulation of physical systems such as aircraft, formulas dependent on $h\lambda$ for constant h are known. Such formulas have the general form

$$y_n = \sum_{i=1}^{k} a_i(h\lambda)\, y_{n-i} + h\sum_{i=0}^{k} b_i(h\lambda) f(y_{n-i}, t_{n-i}). \tag{6}$$

The coefficients a_i, b_i are chosen to fit exactly the case $\hat{y}(t) = C_1 e^{\mu t}\cos\gamma t + C_2 e^{\mu t}\sin\gamma t$ where $\lambda = \mu \pm i\gamma$ and h is constant. The order of these methods is generally two lower than would be expected since two degrees of freedom are lost in forcing the solution to follow $\hat{y}(t)$.

The above indicates some of the wide variety of problems which can be handled by multistep formulas. However, a better understanding of the stability problems inherent in using them would be helpful.

2. Stability of Solution Sequences

The standard linear stability analysis is formula specific and describes the behavior of a numerical formula applied to the complex test equation $y' = \lambda y$, $y(t_o) \neq 0$. Let $E_n = \{e(t_{n-k+1}), \ldots, e(t_{n-1}), e(t_n)\}$ be the difference sequence for $y(t_n) - Z(t_n)$ where each solves the test equation for a different initial value y_0, z_o. Then $e(t_n) = (y_0 - z_0)e^{\lambda t}$ is nonincreasing in norm for $\mathrm{Re}(\lambda) \leq 0$. Such a condition is called stability. It is desirable for the numerical solution y_n to be stable if the true solution is stable, so for a given stepsize h, one finds all complex λ such that any numerical sequence $\hat{E}_n = \{e_{n-k+1}, \ldots, e_{n-1}, e_n\}$ has the property $|e_{i+1}| \leq |e_i|$ for all i, where $e_i = y_i - z_i$, the difference between the numerical solution sequences with initial values y_0, z_0.

For Euler's formula, $y_n = (1+h\lambda)y_{n-1}$, hence the numerical solution is stable for $|1+h\lambda| \leq 1$. For multistep formulas, linear stability is characterized by the generating polynomials

$$\rho(\xi) = \sum_{i=0}^{k} a_i\, \xi^{k-i}, \tag{7a}$$

$$\sigma(\xi) = \sum_{i=0}^{k} b_i\, \xi^{k-i} \tag{7b}$$

where ρ and σ have no common divisors. The region of linear stability is all $h\lambda$ such that $\rho(\xi) + h\lambda\, \sigma(\xi)$ has all roots inside the unit circle, or on the unit circle and simple [6]. For Euler's formula, $\rho(\xi) + h\lambda\, \sigma(\xi)$ is $(-\xi+1) + h\lambda$. Since this analysis is formula specific, tc investigate the formula's effect on an actual $f(y,t)$ one considers all the eigenvalues λ_i of the Jacobian matrix $\partial f(y,t)/\partial y$; if all $h\lambda_i$ are inside the stability region for all y_n, t_n of interest, then the numerical solution will be stable. Insuring that such a condition holds is usually not desirable and often is impossible.

To develop a stability analysis for nonlinear $f(y,t)$, let $f(y,t)$ have the property

$$\mathrm{Re} \langle y-z,\ f(y,\ t) - f(z,t)\rangle \leq \mu \|\ y-z\|^2 \tag{8}$$

for all t, y, and z of interest. Here $\langle u,v\rangle = U^{*}Qv$ for some positive definite Hermitian matrix Q, and $\|\ u\ \|^2 = \langle u,u\rangle$. Then for any two solutions

$y(t)$, $z(t) = y(t)-e(t)$, $e(t)$ satisfies

$$\frac{de(t)}{dt} = f(y(t),t) - f(z(t),t)$$

and (8) implies that

$$\frac{d}{dt} \|e(t)\|^2 = 2\ \mathrm{Re}\langle e(t),\ \frac{de(t)}{dt}\rangle \leq 2\mu\|e(t)\|^2$$

and thus

$$\|e(t)\| \leq e^{\mu t}\|e(t_o)\|,$$

which is non-increasing for $\mu \leq 0$.

However, (8) is again a condition that cannot be easily verified, so a concept relating the true solution sequence $Y_n^t = \{y(t_{n-k+1}),\ \ldots,$

$y(t_{n-1}), y(t_n)\}$ to the computed sequence $Y_n^C = \{y_{n-k+1}, \ldots y_{n-1}, y_n\}$ is presented in the sequel. The following definitions and theorem are helpful. They occur in Dahlquist [9] and the theorem proof is presented in Brown [10].

Definition: a <u>linear</u> <u>k-step</u> <u>formula</u> satisfies

$$0 = \sum_{j=0}^{k} [a_j \hat{y}_{n-j} + h\, b_j f(\hat{y}_{n-j}, t_{n-j})] \tag{9}$$

Definition: a <u>one-leg</u> <u>k-step</u> <u>formula</u> corresponding to (9) satisfies

$$0 = \sum_{j=0}^{k} a_j y_{n-j} + hsf\left(\frac{1}{s}\sum_{j=0}^{k} b_j y_{n-j}, \frac{1}{s}\sum_{j=0}^{k} b_j t_{n-j}\right) \tag{10}$$

where $s = \sigma(1)$. Without loss of generality, set $s=1$.

<u>Theorem</u> <u>1</u> [9] Let Y_n be a sequence which satisfies (10), and let $\hat{Y}_n = \{\hat{y}_n\}$ be such that

$$\hat{y}_n = \sum_{j=0}^{k} b_j y_{n-j} = \sigma(E)\ y_n, \tag{11}$$

where E denotes the back shifting operator. Then $\hat{Y}_n$ satisfies (9). Conversely, if $\hat{Y}_n$ satisfies (9) then there exists a sequence Y_n such that $\hat{y}_n = \sigma(E) y_n$, and y_n satisfies (10).

This shows that Y_n given by the one-leg k-step formula will have similar stability properties to its corresponding linear k-step sequence $\hat{Y}$. Dahlquist [9] has described a discrete Liapunov function $V_{G,\ell,h}$ which, applied to a sequence Y_n , characterizes the stability of that sequence generated by a non-linear system (1). Let

$$V_{G,\ell,h}(Y_n) = \sum_{i=1}^{\ell} \sum_{j=1}^{\ell} g_{ij} \langle y_{n-i+1}, y_{n-j+1} \rangle$$ where G is a

positive definite, $\ell \times \ell$ matrix. The structure of G assures that $V_{G,\ell,h}$ is positive for $Y_n \neq \{0\}$.

Definition: The (G,ℓ,h)-domain of attraction of (the numerical solution to) the system (1) is all z_0 such that $\Delta V_{G,\ell,h}(Z_0) = V_{G,\ell,h}(Z_1) - V_{G,\ell,h}(Z_0) \leq 0$, where $Z_0 = \{z((1-\ell)h),\ldots,z(-h),z_0\}$, $Z_1 = \{z((2-\ell)h),\ldots,z_0, z_1\}$ for the numerical solution and $Z_1 = \{z((2-\ell)h), \ldots, z_0, z(h)\}$ for the exact solution.

Definition: The (G, ℓ, h)-stability region of (the numerical solution to) the non-linear system (1) is all z_0 such that

$$V_{G,\ell,h}(Z_0) \leq \inf_{z_0 \in \partial D} \{V_{G,\ell,h}(Z_0)\}$$ where ∂D is the boundary of the

(G,ℓ,h)-domain of attraction.

This has the following application. Rather than requiring that $\text{Re}\langle y-z, f(t,y)-f(t,z) \rangle \leq 0$, a connected subset of initial values y_0 is found such that $y(h)$ will be in that subset if y_0 was; this is the stability region. This insures that the difference $y(h)-z(h)$ is bounded since both $y(h)$ and $z(h)$ are in the stability region if y_0 and z_0 were. If $f(y,t)$ is autonomous, $y(t_n)$ will remain in the region as $n\to\infty$. For most well behaved functions $f(y,t)$, the boundary of the region around a stable point can be approximated computationally. Once the analytic stability region is known, the numerical stability region can be calculated using the one-leg k-step method for the same sequence $\{y(1-k)h), \ldots, y(-h), y_0\}$ to get y_1. The two regions can then be compared.

Analytically, it is possible to form a particular G, based on the coefficients of a one-leg k-step method, such that all numerical sequences based on $f(t,y)$ that satisfy (8) will have a stable solution. Liniger and Odeh [11] have shown how to pick G for second order two-step formulas, second order three-step formulas, and third order, three-step formulas.

It is shown below that even an arbitrary choice of the positive definite hermitian matrix G will generate some usable results, and theorem 2 demonstrates that using some G for a one-leg k-step solution y_n will generate the same stability region for the related solution $\hat{y}_n$ of the linear k-step formula for a modified $\hat{G}$. The proof appears in Brown [10].

<u>Theorem 2</u> If $V_{G,\ell,h}(Y_n) = c$ for the symmetric positive definite matrix G, then there exists a symmetric, positive definite matrix $\hat{G}$, dependent only on G and $\sigma(x)$, such that $V_{\hat{G},\ell,h}(\hat{Y}_n) = c$, where $\hat{Y}_n = \sigma(E)\, Y_n$ are the elements of $\hat{Y}_n$ and Y_n.

3. Existence of Stability Regions

Sufficient conditions can be developed for the existnece of the (G,ℓ,h)-stability regions based on known techniques such as Liapunov's direct method [12] and property (8). An important concept in the development is the equilibrium $\hat{y}(t)$ of the differential function $f(y,t)$. While some references define it for an initial value $\hat{y}(t_0) = 0$ in the space of the dependent variables, this is accomplished by an unnecessary change of variables that could be confusing. The important point is that $\hat{y}(t)$ satisfies $f(\hat{y}(t_0), t_0) = 0$, so that, if f is autonomous, then y(t) is a constant, and otherwise, the Taylor series about t_0 is given by $\hat{y}(t_0) + (t-t_0)^2 f'(z)/2$ and is thus slowly varying and nearly constant for t near t_0.

Definition: The solution $\hat{y}(t)$ of $\hat{y}' = f(\hat{y},t)$ for $\hat{y}(t_0) = \hat{y}_0$, such that $f(\hat{y}_0,t_0) = 0$, is called the <u>equilibrium of f(y,t)</u>.

Definition: The equilibrium of f(y,t) is said to be <u>asymptotically stable</u> if there exists a $\tau_1 \in (t_0,\infty)$ such that for every $\varepsilon>0$ there exists $\delta_1 = \delta_1(\varepsilon,\tau_1)>0$ such that if $||y_0-\hat{y}_0||<\delta_1$, then $||y(t)-\hat{y}(t)||<\varepsilon$ in $[\tau_1, \infty)$, and there exists a $\tau_2 \varepsilon (t_0,\infty)$ and $\delta_2(\tau_2)$ such that if $||y_0-\hat{y}_0||<\delta_2(\tau_2)$ then $\lim_{t\to\infty} ||y(t)-\hat{y}(t)|| = 0$, where y(t) satisfies y'(t) $= f(y,t)$, $y(t_0) = y_0$.

Theorem 3 (Liapunov [12]) The equilibrium of f(y,t) is asymptotically stable if there exists a function v(y,t) which is positive definite in some region D about $\hat{y}(t_0)$ and $\lim v(y,t) = 0$ uniformly in t as $||y-\hat{y}||\to 0$ there, and whose total derivative is negative definite on D.

With this background, it can be shown that a well behaved f(y,t) which has a not necessarily unique Liapunov function v(y,t) with region D implies the existence of a (I,ℓ,h)-domain of attraction and stability region of both the exact solution and of a one-let k-step solution based on a stable multi-step formula. Similar proofs can be developed fro positive definite matrices $G \neq I$.

Theorem 4: If the equilibrium $\hat{y}(t)$ of f(y,t) has a Liapunov function of the form $v(y,t) = y^*Qy$ for a positive definite matrix Q, y^* the transpose of y, and $f(y,t)$ is continuously differentiable on a convex domain D whose boundary ∂D is defined by $v'(y_0,t_0) = 0$, and if $f(y,t)$ has the property on D that $(y_1-y_2)^*Q(f(y_1,t)-f(y_2,t)) \leq \mu ||y_1-y_2||_Q^2$ where $\mu \leq 0$ and $x^*Qx = ||x||_Q^2$, then for any point $\tilde{y}_\ell = \tilde{y}(t_\ell)$ in the interior of D, an (I,ℓ,h)-stability region can be constructed using rays for $\tilde{y}_\ell$, provided $h \leq h_0(\ell,f)$.

<u>Proof</u> Note that the solution from t_0 to $t_0 + h$ is spiraling in from ∂D toward the equilibrium, which is inside a circle $||y(t)-y_0||_2 \leq \frac{(h\ell)^2}{2} M$ where $M = \max_{z \in D} f'(z)$, since the hypotheses and (8) gives $||y(t_\ell) - \hat{y}(t_\ell)|| \leq \exp(\mu\ell h)||y(t_0)-\hat{y}(t_0)||$. By definition, $\Delta V_{I,\ell,h}(y_\ell) = ||y(t_\ell)||_Q^2 - ||y(t_0)||_Q^2$, which occurs when $0 = v(y_\ell, t_\ell) - y(y_0,t_0) = (y_\ell - y_0)v'(z)$ by the mean value theorem. Since $v'(z) = 0$ on the boundary ∂D, along any ray from $\tilde{y}_\ell$ one can find $y(t_\ell)$ generated by a y_0 on ∂D, provided $h\ell < h_0\ell$ is small enough that the trajectory from $\tilde{y}_0$ to $\tilde{y}_\ell$ is entirely in D.

The boundary of (I,ℓ,h)-domain of attraction D' can be constructed of all such rays. The (I,ℓ,h)-stability region D" has a boundary of all points such that $V_{I,\ell,h} = v^* = \min_{\partial D'} V_{I,\ell,h}$, which can also be constructed.

Theorem 5: If the hypotheses of theorem 4 are met and $\frac{\partial}{\partial y} \frac{d^p f(z)}{dt^p}$ is continuous in D, then for any $\tilde{y}_\ell$ in the interior of D, an (I,ℓ,h)-stability region can be constructed for a p-th order one-leg k-step method, for $h \leq h_0(\ell,f)$.

<u>Proof</u> $\Delta V = ||y_\ell||_Q^2 - ||y(t_\ell - \ell h)||_Q^2$ where

$$y_\ell = \sum_{j=1}^{k} a_j y(t_{\ell-j}) + hf\left(\sum_{j=0}^{k} b_j y(t_{\ell-j}), \sum_{j=0}^{k} b_j t_{\ell-j}\right)$$

and $y(t_\ell) = y_\ell + K_p h^{p+1} f^{(p)}(z)$, the truncation error formula. If the truncation error varies continuously as $y(t_0)$ varies along ∂D, then two solutions y_ℓ and z_ℓ generated by y_0, z_0 on ∂D have the property that $y_\ell \rightarrow z_\ell$ uniformly as $y_0 \rightarrow z_0$, and a smooth curve $\partial D'$ exists on the boundary of the $(I.\ell,h,)$-domain of attraction. Similar arguments show the existence of the (I,ℓ,h)-stability region.

4. Example

The system [12]

$$x' = -x - 2y + x^2 \sin(t) \tag{12}$$

$$y' = 5x - y + y/(t+4)$$

has a Liapunov function for $Q = q_{ij}$, $q_{11} = 37/44$, $q_{22} = 4/11$, $q_{12} = q_{21} = 3/44$. Figure 1 shows D, as well as D', the (I,2,0.1)-domain and D", the (I,2,0.1)-stability region. The solution was generated by assuming a power series expansion $x(t) = \sum_{j=0}^{\infty} a_j t^j$, $y(t) = \sum_{j=0}^{\infty} b_j t^j$ for which $a_0 = x_0$, $b_0 = y_0$, and a_i and b_i can be generated recursively. The series converges for $|t| < 1$. Figure 2 shows D' and D" for the numerical method based on the Adams-Bashforth 2-step formula

$$y_{n+1} = y_n + h(1.5*f(y_n,t_n) - .5*f(y_{n-1},t_{n-1})). \tag{13}$$

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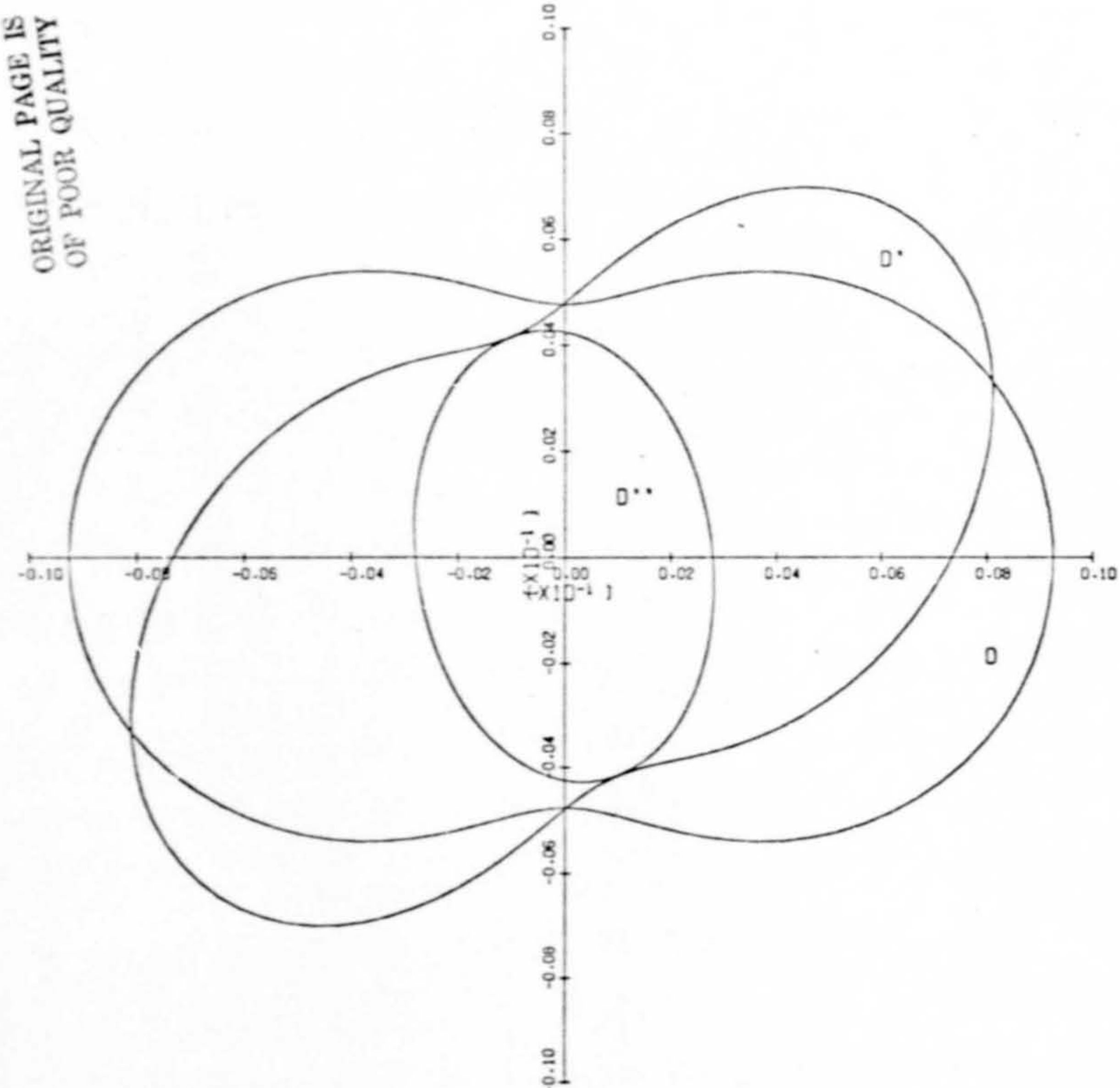

FIG. 1 - D. D'. AND D'' FOR EXACT SOLUTION

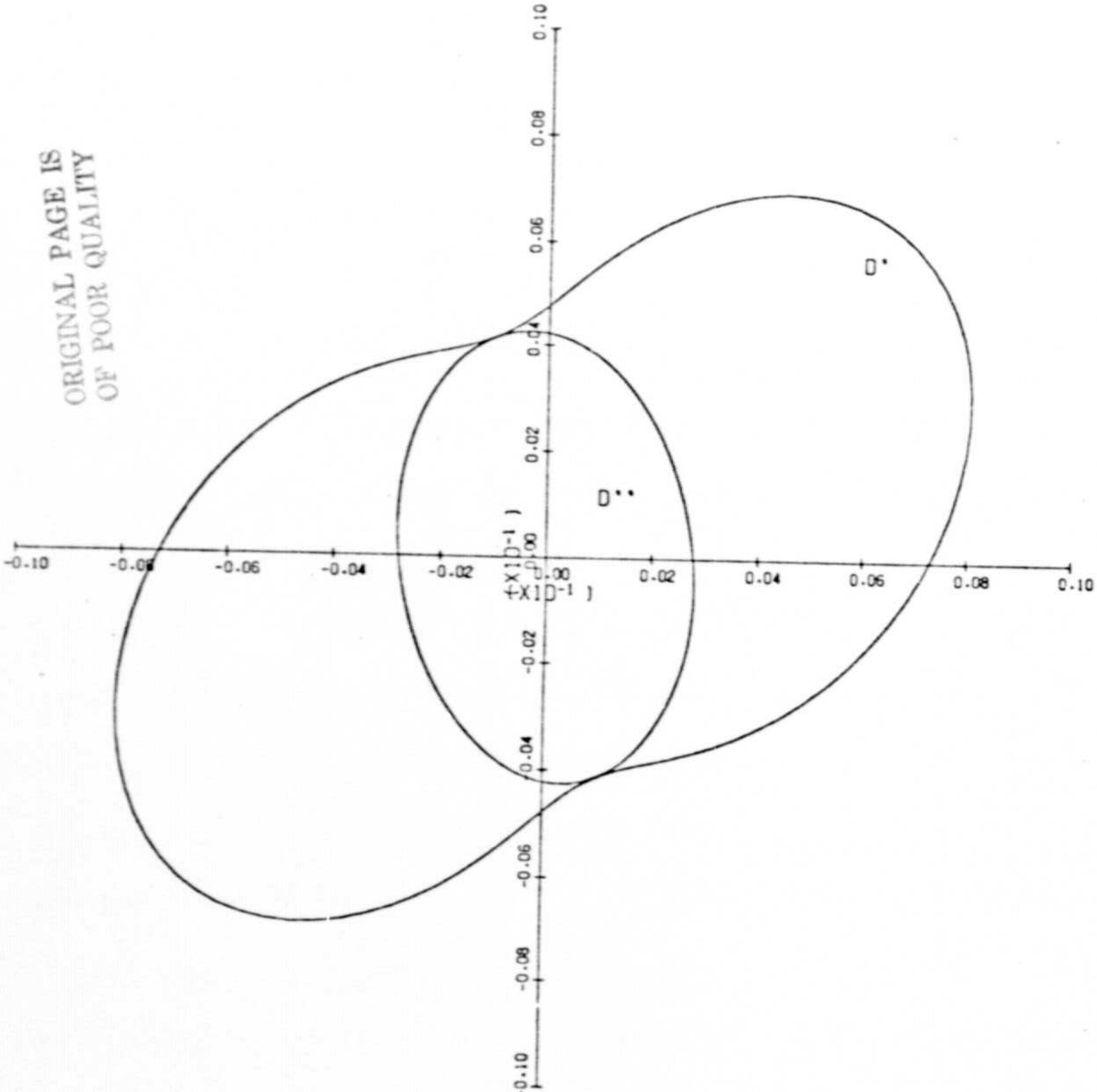

FIG. 2 - D' AND D'' FOR COMPUTED SOLUTION