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STABILITY AND ERROR ANALYSIS
OF LINEAR MULTISTEP METHODS

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CHAPTER I: INTRODUCTION

The general linear multistep method may be defined by a difference equation of the form

$$y_n=\sum_{i=1}^{k} a_i y_{n-i}+h\left[b_0 f(x_n,y_n)+\sum_{i=1}^{k} b_i f(x_{n-i},y_{n-i})\right] \tag{1.1}$$

where k is a fixed integer, $k\geq 2$ (If k=1, (1.1) is called a single step method.); a_i i=1, 2, . . ., k and b_i i=0, 1, . . ., k are real constants; $h=x_n-x_{n-1}=x_{n-1}-x_{n-2}=\ldots=x_{n-k-1}-x_{n-k}$ is called the stepsize and is assumed constant throughout. The method is called linear as the values y_{n-i} and $f(x_{n-i},y_{n-i})$ $i=0,1,\ldots,k$ appear in a linear fashion.

The differential equation to be numerically solved by means of (1.1) is

$$y'=f(x,y),\quad y(a)=y_0. \tag{1.2}$$

It is well known from the theory of ordinary differential equations that if

(i) $f(x,y)$ is a continuous function for $a\leq x\leq b$ and $-\infty<y<+\infty$ and

(ii) $f(x,y)$ satisfies a Lipschitz condition with respect to y

then for any real y_0, (1.2) possesses a unique solution $z(x)$ on the interval $[a,b]$.

The linear multistep method given in (1.1) defines a numerical algorithm which determines a sequence $\{y_n\}$ which may be used to approximate the solution function $z(x)$ at points x_n $n=k, k+1, \ldots$ when $y_0, y_1, \ldots, y_{k-1}$ are initially specified. The accuracy of such an approximation will be determined by the size of the discretization error $\epsilon_n \equiv z(x_n) - y_n$. This error will in general be a function of n and h.

The first restriction imposed on (1.1) in order that it be an acceptable method for approximating the solution $z(x)$ of (1.2) is that it be convergent.

Definition: The linear multistep method defined by (1.1) is called convergent if the following statement is true for all functions $f(x,y)$ which satisfy conditions (i) and (ii) above and all values y_0. If $z(x)$ denotes the solution of the initial value problem (1.2) then $\lim\limits_{\substack{h\to 0\\ x_n=x}} y_n = z(x)$ holds for all $x \in [a,b]$ and all solutions $\{y_n\}$ of the difference equation (1.1) having starting values $y_j = y_j(h)$ satisfying $\lim\limits_{h\to 0} y_j(h) = y_0$ $j=0, 1, \ldots, k-1$.

An intuitive interpretation may be helpful. Let x be chosen in $(a,b]$ and divide the interval $[a,x]$ into n equal parts with $n > k-1$. Now choose $h=(x-a)/n$. By solving (1.1) n-k+1 times (as the first k values of y must be initially specified) an approximation y_n of $z(x)$ is obtained. The definition above insures that for a convergent method y_n may be made arbitrarily close to $z(x)$ by choosing the stepsize h sufficiently small, i.e. ϵ_n must approach zero as the stepsize h approaches zero.

In order to investigate the restrictions convergence places on the method (1.1) it is convenient to define an associated linear operator:

$$(1.3)\quad L[z(x_n), h] \equiv z(x_n) - \left(\sum_{i=1}^{k} a_i z(x_{n-i}) + h b_0 z'(x_n) + \sum_{i=1}^{k} b_i z'(x_{n-i}) \right)$$

For a sufficiently differentiable function $z(x)$

$$L[z(x_n),h] = C_0 z(x_n) + C_1 h z'(x_n) + \ldots + C_q h^q z^{(q)}(x_n) + C_{q+1} h^{q+1} z^{(q+1)}(x_n) + \ldots .$$

where

$$C_0 = 1 - \sum_{i=1}^{k} a_i$$

$$C_1 = \sum_{i=1}^{k} i a_i - \sum_{i=1}^{k} b_i$$

(1.4) $\vdots$

$$C_q = \frac{(-1)^{q+1}}{q!} \sum_{i=1}^{k} i^q a_i + \frac{(-1)^q}{(q-1)!} \sum_{i=1}^{k} i^{q-1} b_i, \quad q \geq 2.$$

A linear multistep method is defined to be of order p if for the associated linear operator $C_0 = C_1 = \ldots = C_p = 0$ but $C_{p+1} \neq 0$.

It is shown by Henrici (6) that if (1.1) is of order p, then for a sufficiently differentiable function $z(x)$

$$(1.5)\quad z(x_n) = \sum_{i=1}^{k} a_i z(x_{n-i}) + h\left(b_0 z'(x_n) + \sum_{i=1}^{k} b_i z'(x_{n-i})\right) + T(x_n)$$

where $T(x_n) = c_{p+1} h^{p+1} z^{(p+1)}(x_n) + O(h^{p+2})$. $T(x_n)$ is called the truncation error and is said to be of order p+1. Observe $T(x_n) = 0$ if $z(x)$ is a polynomial of degree q, where $q \leq p$. A truncation error is introduced each time (1.1) is applied to find a value y_n from previously obtained values $y_{n-1}, y_{n-2}, \ldots, y_{n-k}$.

The linear multistep method (1.1) is said to be consistent provided it is of order q for $q \geq 1$.

In the multistep method (1.1) there are 2k+1 constants to be determined so by solving the equations $C_0 = C_1 = \cdots = C_{2k+1} = 0$ a method of order 2k+1 could be obtained. However high order is not by itself sufficient to determine an acceptable method. High order reduces the truncation error but it does not control the propagated error, i.e. the error introduced by using only approximate values in the calculation of new values. The concept of zero stability is introduced to control the propagated error.

Definition: The linear multistep method (1.1) is said to be zero stable if the polynomial

$$a(r) \equiv r^k - \sum_{i=1}^{k} a_i r^{k-i}$$

has no root of absolute value larger than one and that the roots of absolute value one are simple roots.

Observe that the polynomial a(r) is the characteristic equation for the difference equation (1.1) when $h = 0$.

Results relating the concepts of convergence, order, and zero stability have been established by Dahlquist (4) and reported in Henrici (6):

Theorem (1.1): A necessary and sufficient condition for the convergence of the linear multistep method (1.1) is that the method be consistent and zero stable.

Theorem (1.2): The maximum order of a zero stable method is k+1 if k is odd and k+2 if k is even.

It is obvious how convergence requires a condition of order on the multistep method but how the property of zero stability is related is perhaps not so apparent.

To examine this connection subtract (1.1) from (1.5) to obtain

$$(1.6) \quad \epsilon_n = z(x_n) - y_n$$
$$= \sum_{i=1}^{k} a_i \epsilon_{n-i} + h \sum_{i=1}^{k} b_i \Big(f(x_{n-i}, z(x_{n-i})) - f(x_{n-i}, y_{n-i}) \Big)$$
$$+ T(x_n).$$

If $h = 0$ in (1.6) the difference equation becomes

$$(1.7) \qquad \epsilon_n = \sum_{i=1}^{k} a_i \epsilon_{n-i}$$

From the theory of linear difference equations it is known that if $r_1, r_2, \ldots, r_j$ $(j \leq k)$ are the distinct roots of the characteristic equation $a(r) = 0$ and if root r_i has multiplicity m_i, then the general solution of (1.7) is of the form

$$(1.8) \quad \begin{array}{l} A_{11} r_1^n + A_{12} r_1^n n + A_{13} r_1^n n(n-1) + \ldots + \\ \qquad + A_{1m_1} r_1^n n(n-1) \ldots (n-m_1+2) \; + \\ \vdots \\ A_{j1} r_j^n + A_{j2} r_j^n n + A_{j3} r_j^n n(n-1) + \ldots + \\ \qquad + A_{jm_j} r_j^n n(n-1) \ldots (n-m_j+2) \end{array}$$

where A_{ij} are arbitrary constants. Therefore from the form of the general solution it is clear that if $a(r)$ has a root of magnitude greater than one the associated componet of the solution of (1.7) grows exponentially with n and if $a(r)$ has a root of magnitude one which is not a simple root the associated component of the solution of (1.7) grows with n. In either case ϵ_n approaches infinity as n approaches infinity so convergence cannot be achieved.

In practical situations however h may not be made arbitrarily small and therefore the above theory is not necessarily sufficient to describe the linear multistep method (1.1).

To examine what happens to ϵ_n when $h \neq 0$ define

$$(1.9)\quad g_{n-i} = \begin{cases} \dfrac{f(x_{n-i}, z(x_{n-i})) - f(x_{n-i}, y_{n-i})}{\epsilon_{n-i}} & \text{if } \epsilon_{n-i} \neq 0 \\ 0 & \text{if } \epsilon_{n-i} = 0 \end{cases}$$

for $i = 0, 1, \ldots, k$.

Using this definition (1.6) becomes

$$(1.10)\quad \epsilon_n = \sum_{i=1}^{k} a_i \epsilon_{n-i} + h \sum_{i=0}^{k} b_i g_{n-i} \epsilon_{n-i} + T(x_n).$$

Consider now the case where $T(x_n) = T$ a constant and $g_{n-i} = g$ a constant $i=0,1,\ldots,k$ and $s_1(H), \ldots, s_k(H)$ are distinct roots of the characteristic polynomial

$$(1.11)\qquad I(r,H) = a(r) - Hb(r)$$

where

$$a(r) \equiv r^k - \sum_{i=1}^{k} a_i r^{k-i},\quad b(r) \equiv \sum_{i=0}^{k} b_i r^{k-i},\ \text{and } H \equiv hg.$$

In this case the solution of (1.10) is

(1.12) $\epsilon_n = A_1(s_1(H))^n + \ldots + A_k(s_k(H))^n + T/I(1,H)$

where $A_1, \ldots, A_k$ are constants which satisfy the initial conditions

$$E_j = A_1(s_1(H))^j + \ldots + A_k(s_k(H))^j$$

where $E_j = \epsilon_j - T/I(1,H)$ $j=0,1,\ldots,k-1$; i.e. $A_1, \ldots, A_k$ are determined by the error in the initially specified values $y_0, \ldots, y_{k-1}$.

It is intuitively obvious that for small values of H $I(r,H) \approx a(r)$ and therefore the roots $s_1(H), \ldots, s_k(H)$ should be approximately equal to the roots $r_1, r_2, \ldots, r_k$ of $a(r)=0$. By the use of Rouche's theorem it may be shown that for any $\epsilon > 0$ there exists a $\delta > 0$ such that for $0 \leq H < \delta$ the equation $I(r,H)=0$ has exactly as many roots in each of the disks $|t-r_i| < \delta$ $i=1,\ldots,k$ as does the equation $a(r)=0$. Further if r_i is a root of multiplicity m_i it can be shown to be the m_i different values of an analytic function of H^{1/m_i} obtained by assigning to H^{1/m_i} its m_i different values. It follows that if $b(r_i) \neq 0$ then these m_i roots are distinct for H sufficiently small, $H \neq 0$.

Thus letting $s_i(H) = r_i + c_iH + d_iH^2 + O(H^3)$ and substituting this into (1.11) it follows, by the method of undetermined coefficients, that

$$(1.13) \quad s_i(H) = r_i + \left[\frac{b(r_i)}{a'(r_i)}\right] H + \left[\frac{b(r_i)b'(r_i) - \dfrac{a''(r_i)b^2(r_i)}{2a'(r_i)}}{(a'(r_i))^2}\right] H^2$$

$$+ O(H^3).$$

If the linear multistepmethod (1.1) is consistent then $C_0 = C_1 = 0$, but observe $C_0 = 0$ if, and only if, $1 - \sum_{i=1}^{k} a_i = a(1) = 0$, and $C_1 = 0$, if and only if $\sum_{i=1}^{k} ia_i = \sum_{i=0}^{k} b_i$. Next observe $a'(1) = k - \sum_{i=1}^{k-1} (k-i)a_i =$

$$k(1 - \sum_{i=1}^{k-1} a_i) + \sum_{i=1}^{k-1} ia_i = ka_k + \sum_{i=1}^{k-1} ia_i = \sum_{i=1}^{k} ia_i.$$

Thus $C_1 = 0$ if, and only if, $a'(1) = b(1)$.

By these results, if $r_1 = 1$,

$s_1(H) = 1 + \left[\frac{b(1)}{a'(1)}\right] H + O(H^2) = 1 + H + O(H^2)$, the first terms agreeing with the series expansion of e^H. It is shown in Henrici (6) that if method (1.1) is of order q then

$$s_1(H) = e^H + O(H^{q+1}).$$

Thus if $H = hg > 0$ then $|s_1(H)| > 1$ and so the error ϵ_n will grow exponentially with n. Keep in mind however that if

$g > 0$ then the solution itself is increasing with x and relative accuracy may still be maintained if the error does not grow more rapidly than the solution. It is now necessary to define the concept of stability in more general terms.

Let $I(r,H)$ be a polynomial in r of degree k. Assume $I(r,H) = 0$ is the characteristic equation corresponding to the difference equation (1.10) and $s_1(H), \ldots, s_k(H)$ are the roots of $I(r,H) = 0$. The linear multistep method (1.1) is said to be

(i) absolutely stable on an interval $[H_1,H_2]$ if for H in $[H_1,H_2]$, $|s_i(H)| \leq 1$ $i=1,2, \ldots, k$ and the roots of absolute value one are simple roots.

(ii) relatively stable on an interval $[H_1,H_2]$ if for any H in $[H_1,H_2]$ $|s_i(H)| < |s_1(H)|$ $i=2, \ldots, k$

where $s_1(H) = e^H + O(H^{q+1})$. Observe in (i) $H_2 \leq 0$ for if $H_2 > 0$ then the root $s_1(H)$ has an absolute value larger than one.

In the preceding analysis and in what follows it is assumed that g_{n-i} $i=0,1, \ldots, k$ as defined by (1.9) are constant. Observe that if $f(x,y)$ has a derivative with respect to y, then by the mean value theorem $g_{n-i} = \frac{\partial f}{\partial y}(x_{n-i},y^*_{n-i})$ where y^*_{n-i} is between $z(x_{n-i})$ and y_{n-i}. Thus in this case, if we assume g_{n-i} is constant, we are assuming that $\frac{\partial f}{\partial y}$ is constant over the region.

The purpose of making such an assumption is to have a linear difference equation in ϵ_n so that the theory for such may be used to obtain a general solution for ϵ_n. Thus although the theory developed assuming g_{n-i} is constant is not rigorously applicable to the general case, it does provide considerable insight into the stability problems which arise. For instance if $\frac{\partial f(x,y)}{\partial y}$ is approximately constant over a region the true error would be approximated very closely by the above analysis. By choosing h small the size of the region can be restricted enough so that $\frac{\partial f}{\partial y}$ is approximately constant over such a restricted region. Also it is verified by experience that this type of assumption yields pertinent information as regards the stability of the method.

A common application of a linear multistep method involves the use of a pair of difference equations. The first, called the predictor, is of the form

$$(1.14)\quad y_n = \sum_{i=1}^{k} a_i^* y_{n-i} + h\sum_{i=1}^{k} b_i^* f(x_{n-i}, y_{n-i}).$$

The second, called the corrector, is of the form

$$(1.15)\quad y_n = \sum_{i=1}^{k} a_i y_{n-i} + h\left(b_0 f(x_n, y_n) + \sum_{i=1}^{k} b_i f(x_{n-i}, y_{n-i})\right).$$

As commonly implemented a first approximation of $z(x_n)$ is obtained by the use of an open formula (the predictor) followed by an evaluation of the derivative corresponding to this first approximation. This is followed by an application of a closed formula (the corrector) to obtain a new approximation to $z(x_n)$ and then the derivative is evaluated with this new value. This last step may be repeated m times leading to a class of algorithms which are denoted as $PE(CE)^m$ methods.

A variation of the above implementation of the predictor and corrector equations is obtained by eliminating the final derivative evaluation. This slight variation has a pronounced effect on the discretization error ϵ_n. Such a variation is denoted by $P(EC)^m$.

In Chapter II the difference equation for the discretization error of a $PE(CE)^m$ implementation is derived and analyzed. In Chapter III a $P(EC)^m$ is studied.

Next a generalization of the linear multistep method (1.1) is introduced. The generalization is defined by a difference equation of the form

$$(1.16)\quad y_n = \sum_{i=1}^{k} a_i y_{n-i} + h\left(b_{-1} f(x_{n-e}, y_{n-e}) + b_o f(x_n, y_n) + \sum_{i=1}^{k} b_i f(x_{n-i}, y_{n-i})\right),$$

where $0<\theta<1$. Observe the generalization consists merely of adding the extra term $b_{-1}f(x_{n-\theta},y_{n-\theta})$ to the right hand side of (1.1). The purpose of making such a generalization is that the method (1.16) may be convergent, zero stable, and of order p, $p\geq k+3$. This result has been established in a paper by Stetter and Gragg (13). In fact Butcher (2) has displayed methods of the form of (1.16) of order $2k+1$ for $k\leq 7$ which are convergent and zero stable.

The practical use of method (1.16) requires that $y_{n-\theta}$ be estimated so that the extra term $hb_{-1}f(x_{n-\theta},y_{n-\theta})$ may be evaluated. This may be done by the use of a predictor equation of the form

$$(1.17)\quad y_{n-\theta} = \sum_{i=1}^{k} A_i y_{n-i} + h\sum_{i=1}^{k} B_i f(x_{n-i},y_{n-i}).$$

Also (1.16) is, in general, an implicit equation for y_n and so a predictor equation to obtain a first estimate of y_n is also required. Such a predictor may also take advantage of the knowledge of $f(x_{n-\theta},y_{n-\theta})$. It will be of the form

$$(1.18)\quad y_n = \sum_{i=1}^{k} a_i^* y_{n-i} + h\left(b_{-1}^* f(x_{n-\theta},y_{n-\theta}) + \sum_{i=1}^{k} b_i^* f(x_{n-i},y_{n-i})\right).$$

As for the linear multistep method (1.1) two implementations of (1.16) are possible. In each $y_{n-\theta}$ is predicted by (1.17) and $f(x_{n-\theta}, y_{n-\theta})$ is evaluated for use in (1.17) and (1.16). After an approximation y_n^p is obtained by (1.17), $f(x_n, y_n^p)$ is evaluated and then (1.16) is used to obtain a value y_n^c which is an approximation to $z(x_n)$. The two implementations differ in whether or not $f(x_n, y_n^c)$ is evaluated. If $f(x_n, y_n^c)$ is evaluated before moving to the next step such a method will be called a generalized predictor-corrector method and denoted as a GPC method. If $f(x_n, y_n^c)$ is not evaluated the method will be called a simplified generalized predictor-corrector method and will be denoted as a SGPC method. Observe a GPC method requires the evaluation of $f(x,y)$ 3 times for each forward step whereas a SGPC method requires 2 derivative evaluations.

In Chapter IV the difference equation satisfied by the discretization error for a GPC method is derived and analyzed and SGPC methods are discussed in Chapter V.

In Chapter VI various special cases of the above methods are discussed and a comparison is made.

CHAPTER II: $PE(CE)^m$ METHODS

In this chapter the difference equation satisfied by the discretization error $\epsilon_n^{(m)} \equiv z(x_n) - y_n^{(m)}$ for a $PE(CE)^m$ implementation of the predictor and corrector equations will be derived.

It is assumed that the predictor equation given by

$$(2.1)\quad y_n^{(0)} = \sum_{i=1}^{k} a_i^* y_{n-i}^{(m)} + h \sum_{i=1}^{k} b_i^* f(x_{n-i}, y_{n-i}^{(m)})$$

is of order p, $p \geq 1$, and $y_{n-i}^{(m)}$ $i=1,2, \ldots, k$ are previously calculated values and are regarded as approximations to $z(x_{n-i})$, the true solution evaluated at $x = x_{n-i}$. Define now $z_{n-i} = z(x_{n-i})$ $i=1, 2, \ldots, k$. Thus for a sufficiently differentiable function $z(x)$

$$(2.2)\quad z_n = \sum_{i=1}^{k} a_i^* z_{n-i} + \sum_{i=1}^{k} b_i^* f(x_{n-i}, z_{n-i}) + T_p(x_n)$$

where $T_p(x_n) = C_{p+1}^* h^{p+1} z^{(p+1)}(x_n) + O(h^{p+2})$.

Similarly it is assumed that the corrector equation

$$(2.3)\quad y_n^{(j)} = \sum_{i=1}^{k} a_i y_{n-i}^{(m)} + h\left(b_0 f(x_n, y_n^{(j-1)}) + \sum_{i=1}^{k} b_i f(x_{n-i}, y_{n-i}^{(m)})\right)$$

for $j = 1, 2, \ldots, m$ is of order q, $q \geq 1$, so that for a sufficiently differentiable function $z(x)$

$$(2.4)\quad z_n = \sum_{i=1}^{k} a_i z_{n-i} + h\left(b_0 f(x_n, z_n) + \sum_{i=1}^{k} b_i f(x_{n-i}, z_{n-i})\right)$$
$$+ T_c(x_n)$$

where $T_c(x_n) = C_{q+1} h^{q+1} z^{(q+1)}(x_n) + O(h^{q+2})$.

Subtracting (2.1) from (2.2) one obtains

$$(2.5)\quad \epsilon_n^{(0)} \equiv z_n - y_n^{(0)}$$
$$= \sum_{i=1}^{k} a_i^*(z_{n-i} - y_{n-i}^{(m)})$$
$$+ h\sum_{i=1}^{k} b_i^*\left(f(x_{n-i}, z_{n-i}) - f(x_{n-i}, y_{n-i}^{(m)})\right) + T_p(x_n).$$

Subtracting (2.3) from (2.4) one obtains

$$(2.6)\quad \epsilon_n^{(j)} \equiv z_n - y_n^{(j)}$$
$$= \sum_{i=1}^{k} a_i(z_{n-i} - y_{n-i}^{(m)}) + h\left(b_0\left(f(x_n, z_n) - f(x_n, y_n^{(j-1)})\right)\right.$$
$$\left. + \sum_{i=1}^{k} b_i\left(f(x_{n-i}, z_{n-i}) - f(x_{n-i}, y_{n-i}^{(m)})\right)\right) + T_c(x_n)$$

for $j = 1, 2, \ldots, m$.

To study these equations further it is convenient to define

$$g_{n-i}^{(j)} = \begin{cases} \dfrac{f(x_{n-i}, z_{n-i}) - f(x_{n-i}, y_{n-i}^{(j)})}{\epsilon_{n-i}^{(j)}} & \text{if } \epsilon_{n-i}^{(j)} \neq 0 \\ 0 & \text{if } \epsilon_{n-i}^{(j)} = 0 \end{cases}$$

for $j = 1, \ldots, m$ $i = 0, 1, \ldots, k$ and then to assume that $g_{n-i}^{(j)} = g$, a constant for $j = 1, \ldots, m$ and $i = 0, 1, \ldots, k$. Thus (2.5) and (2.6) may be written

$$(2.7)\quad \epsilon_n^{(0)} = \sum_{i=1}^{k} a_i^* \epsilon_{n-i}^{(m)} + h \sum_{i=1}^{k} b_i^* g \epsilon_{n-i}^{(m)} + T_p(x_n)$$

and

$$(2.8)\quad \epsilon_n^{(j)} = \sum_{i=1}^{k} a_i \epsilon_{n-i}^{(m)} + h\left(b_0 g \epsilon_n^{(j-1)} + \sum_{i=1}^{k} b_i g \epsilon_{n-i}^{(m)} \right) + T_c(x_n), \quad j = 1, \ldots, m.$$

In order to obtain the difference equation for $\epsilon_n^{(m)}$ it is necessary to eliminate $\epsilon_n^{(j-1)}$ from (2.8) for $j = 1, \ldots, m$. Doing this one obtains the result

$$(2.9)\quad \epsilon_n^{(m)} = \sum_{i=1}^{k} a_i \epsilon_{n-i}^{(m)} + \left(\sum_{j=1}^{m-1} (hb_0 g)^j \sum_{i=1}^{k} (a_i + hgb_i) \epsilon_{n-i}^{(m)} + (hb_0 g)^m \sum_{i=1}^{k} (a_i^* + hgb_i^*) \epsilon_{n-i}^{(m)} \right) + h \sum_{i=1}^{k} b_i g \epsilon_{n-i}^{(m)} + T_c^{(m)}(x_n)$$

where

$$(2.10)\quad T_c^{(m)}(x_n) = T_c(x_n) \sum_{j=0}^{m-1} (hb_0 g)^j + (hb_0 g)^m T_p(x_n).$$

Observe from the form of (2.10) that in order for the truncation error of the $PE(CE)^m$ implementation to be of the same order as the truncation error for the corrector alone it is necessary that $p \geq (q - m)$.

Next, assuming $T_c^{(m)}(x_n) = T$, a constant and defining $H = hg$ and $\theta = Hb_0$, (2.9) may be written

$$(2.11)\ \epsilon_n^{(m)} = \sum_{j=0}^{m-1} \theta^j \sum_{i=1}^{k} (a_i + Hb_i)\epsilon_{n-i}^{(m)} + \theta^m \sum_{i=1}^{k} (a_i^* + Hb_i^*)\epsilon_{n-i}^{(m)} + T.$$

The characteristic equation for the difference equation in (2.11) is

$$(2.12)\ \rho^m(r,H) \equiv r^k - \left(\sum_{j=0}^{m-1} \theta^j\right) \sum_{i=1}^{k} (a_i + Hb_i)r^{k-i} - \theta^m \sum_{i=1}^{k} (a_i^* + Hb_i^*)r^{k-i}$$

If $s_1(H), \ldots, s_k(H)$ are distinct roots of $\rho^m(r,H) = 0$, from the theory of linear difference equations, the general solution of (2.11) is

$$(2.13)\ \epsilon_n^{(m)} = A_1(s_1(H))^n + \ldots + A_k(s_k(H))^n + T/\rho^m(1,H)$$

where $A_1, \ldots, A_k$ are constants which satisfy the initial conditions

$$E_j = A_1(s_1(H))^j + \ldots + A_k(s_k(H))^j$$

for $j = 0, \ldots, k-1$ where $E_j = \epsilon_j - T/\rho^m(1,H)$, i.e. the constants $A_1, \ldots, A_k$ are determined by the error in the initially specified values $y_0, y_1, \ldots, y_{k-1}$. If $s_1(H), \ldots, s_k(H)$ are not distinct, the form of the solution of (2.11) as given in (2.13) must be modified to be in agreement with the general form of (1.8).

Now observing $\dfrac{1-\theta^m}{1-\theta} = \sum_{j=0}^{m-1} \theta^j$ the characteristic equation (2.12) may be written:

$$(2.14)\quad (1-\theta)\rho^m(r,H) = (1-\theta)r^k + (\theta^m-1)\sum_{i=1}^{k}(a_i+Hb_i)r^{k-i}$$
$$-(1-\theta)\theta^m\sum_{i=1}^{k}(a_i^*+Hb_i^*)r^{k-i}.$$

The right hand side of (2.14) is the characteristic equation for the difference equation as given by Hull and Creemer (7).

In order to further study the discretization error $\epsilon_n^{(m)}$ it is apparent from (2.13) that the roots $s_1(H), \ldots, s_k(H)$ of $\rho^m(r,H)$ need to be examined. To do this it is convenient to make the following definitions:

$$(2.15)\quad \begin{aligned} &\text{(i)}\ a(r) = r^k - \sum_{i=1}^{k} a_i r^{k-i} \\ &\text{(ii)}\ b(r) = \sum_{i=0}^{k} b_i r^{k-i} \\ &\text{(iii)}\ a^*(r) = r^k - \sum_{i=1}^{k} a_i^* r^{k-i} \\ &\text{(iv)}\ b^*(r) = \sum_{i=1}^{k} b_i^* r^{k-i} \end{aligned}$$

Using these definitions and adding in zero in the form $\Theta^{m+1}r^k - \Theta^{m+1}r^k$ equation (2.14) may be written

$$(2.16)\quad (1-\Theta)\rho^m(r,H) = (1-\Theta^m)\left[a(r) - Hb(r)\right] + \Theta^m(1-\Theta)\left[a^*(r) - Hb^*(r)\right].$$

Observe from (2.16) that, assuming $|\Theta| = |Hb_0| < 1$,

$$(2.17)\quad \lim_{m\to\infty} (1-\Theta)\rho^m(r,H) = a(r) - Hb(r) \equiv I(r,H).$$

The reader will recall from Chapter I that the right hand side of (2.17) is the characteristic equation (1.11) for the linear multistep method (1.1) when $h \neq 0$. Thus the error analysis of the $PE(CE)^\infty$ method is the same as that for the linear multistep method (1.1). The reason for such is that assuming the corrector has converged, i.e. $y_n^{(m)} = y_n^{(m-1)}$, the corrector equation (2.3) and the linear multistep method (1.1) are identical. Under the assumption that the corrector is iterated to convergence the predictor serves merely to furnish a starting value for the iterations. Thus $I(r,H)=0$ will be referred to as the characteristic equation of the iterated corrector. From (2.17) it follows that the roots of $\rho^m(r,H)=0$ will approach the roots of $I(r,H)=0$ as m approaches infinity.

To examine the relationship between these two sets of roots observe from (2.16) and (2.17) that

$$(2.18) \quad \lim_{H\to 0} (1-\theta)\rho^m(r,H) = a(r) = \lim_{H\to 0} I(r,H).$$

Let (i) $r_1, r_2, \ldots, r_k$ be the k distinct roots of $a(r) = 0$; (ii) $s_1(H), s_2(H), \ldots, s_k(H)$ be the k roots of $I(r,H) = 0$; and (iii) $t_1^{(m)}, t_2^{(m)}, \ldots, t_k^{(m)}$ be the k roots of $\rho^m(r,H) = 0$. From (2.18) it follows that for H sufficiently small

$$(2.19) \quad \begin{aligned} &\text{(i)} \quad s_i(H) = r_i + c_{i1}H + c_{i2}H^2 + \ldots \\ &\text{(ii)} \quad t_i^{(m)}(H) = r_i + d_{i1}H + d_{i2}H^2 + \ldots \end{aligned}$$

for $i = 1, 2, \ldots, k$. Thus

$$(2.20) \quad t_i^{(m)}(H) = s_1(H) + e_{i1}H + e_{i2}H^2 + \ldots$$

where $e_{ij} = d_{ij}-c_{ij}$ $i=1,2,\ldots,k$ $j=1,2,3,\ldots$.

In order to solve for e_{ij} in terms of the predictor and corrector coefficients let the root $t_i^{(m)}(H)=s_i(H)+e_j'H^j + O(H^{j+1})$ where $j\geq 1$. Substituting this into the characteristic equation $\rho^m(r,H) = 0$ and grouping terms in powers of H one obtains the equation

$$\rho^m(t_i^{(m)},H)=0=\left[a'(s_i(H))e_j'\right]H^j + \left[a^*(s_i(H))-Hb^*(s_i(H))\right]H^m b_0^m + O(H^{j+1}).$$

Equating coefficients of like powers of H results in

$$(2.21)\qquad e_j' = \begin{cases} 0 & \text{if } j<m \\ \dfrac{-b_0^m a^*(s_i(H))}{a'(s_i(H))} & \text{if } j=m. \end{cases}$$

By the use of (2.19i) and Taylor series

$$\frac{a^*(s_i(H))}{a'(s_i(H))} = \frac{a^*(r_i)}{a'(r_i)} + O(H).$$

Thus from (2.21) and (2.20) one obtains the result

$$(2.22)\quad t_i^{(m)}(H) = s_i(H) + \left[\frac{-b_0^m a^*(r_i)}{a'(r_i)}\right]H^m + O(H^{m+1})$$

for $i = 1, 2, \ldots, k$.

The two most widely used $PE(CE)^m$ implementations are with $m = \infty$ and $m = 1$. The analysis above with $m = \infty$ coincides with the assumption that the iterated corrector has converged, i.e. $y_n^{(m)} = y_n^{(m-1)}$. In practice the corrector is assumed to have converged provided that $\left|y_n^{(m)} - y_n^{(m-1)}\right| < \delta$, where δ is some predetermined tolerance. Observe from (2.17) and from (2.22) that if $m = \infty$ the error is determined by the corrector equation. However since the evaluation of the derivative function $f(x,y)$ is commonly the dominating factor in computation time for computer applications of predictor-corrector techniques, it may not be feasible to iterate the corrector to convergence. Under this assumption the case $m = 1$ is most commonly used. From (2.22) it is apparent that for $m = 1$ the predictor as well as the corrector influences the discretization error $\epsilon_n^{(m)}$.

If $m = 1$, using the expansion of $s_i(H)$ as given by (1.13) in equation (2.22), one obtains

$$(2.23)\quad t_i^{(1)}(H) = r_i + \left[\frac{d(r_i)}{a'(r_i)}\right]H + \left[\frac{\dfrac{-d^2(r_i)a''(r_i)}{2a'(r_i)} + d(r_i)d'(r_i) + b_0 a'(r_i)b^*(r_i)}{(a'(r_i))^2}\right]H^2 + O(H^3)$$

where $d(r_i) = b(r_i) - b_0 a^*(r_i)$, $i = 1, \ldots, k$.

In determining whether $\epsilon_n^{(m)}$ will grow or decay as n approaches ∞ it is the absolute values of the roots $t_i^{(m)}(H)$ that are important. Letting $r_j = \rho_j e^{iw}$ in (2.23) it follows that for H sufficiently small

$$(2.24)\quad \left|t_j^{(1)}(H)\right| = \rho_j + A_j H + B_j H^2 + O(H^3)$$

where

$$A_j = \mathrm{Re}\left[\frac{e^{-iw}d(\rho_j e^{iw})}{a'(\rho_j e^{iw})}\right]$$

$$B_j = \mathrm{Re}\left[e^{-iw}\Psi_2(\rho_j e^{iw})\right] + \frac{\mathrm{Img}\left[\dfrac{e^{-iw}d(\rho_j e^{iw})}{a'(\rho_j e^{iw})}\right]}{2\rho_j}$$

with $\Psi_2(\rho_j e^{iw})$ being the coefficient of H^2 in (2.23).

A convenient device for studying the stability properties of a predictor-corrector method or for comparing various methods is a root-locus plot for the method. In a root-locus plot the absolute values of the roots $t_i^{(m)}(H)$ of $\rho^m(r,H) = 0$ $i = 1, \ldots, k$ are plotted as functions of H. From such a graph the intervals of absolute and relative stability are easily seen.

In Appendix A root-locus plots are made for several commonly used $PE(CE)^m$ implementations with various values of m to illustrate the effect of iterating the corrector.

CHAPTER III: $P(EC)^m$ METHODS

In this chapter the difference equation satisfied by the discretization error $\epsilon_n^{(m)} \equiv z_n - y_n^{(m)}$ for a $P(EC)^m$ implementation of the predictor and corrector equations is derived and analyzed.

It is assumed that the predictor equation given by

$$(3.1)\quad y_n^{(0)} = \sum_{i=1}^{k} a_i^* y_{n-i}^{(m)} + h \sum_{i=1}^{k} b_i^* f(x_{n-i}, y_{n-i}^{(m-1)})$$

is of order p and $y_{n-i}^{(m)}$ and $y_{n-i}^{(m-1)}$ $i = 1, 2, \ldots, 2k$ are previously calculated values and are regarded as approximations to $z_{n-i} \equiv z(x_{n-i})$ $i = 0, 1, \ldots, 2k$ so that for a sufficiently differentiable function $z(x)$

$$(3.2)\quad z_n = \sum_{i=1}^{k} a_i^* z_{n-i} + h \sum_{i=1}^{k} b_i^* f(x_{n-i}, z_{n-i}) + T_p(x_n)$$

where $T_p(x_n) = C_{p+1}^* h^{p+1} z^{(p+1)}(x_n) + O(h^{p+2})$.

Similarly it is assumed that the corrector equation

$$(3.3)\quad y_n^{(j)} = \sum_{i=1}^{k} a_i y_{n-i}^{(m)} + h \left[b_0 f(x_n, y_n^{(j-1)}) + \sum_{i=1}^{k} b_i f(x_{n-i}, y_{n-i}^{(m-1)}) \right], \quad j = 1, \ldots, m$$

is of order q so that for a sufficiently differentiable function $z(x)$

$$(3.4)\quad z_n = \sum_{i=1}^{k} a_i z_{n-i} + h\left[b_0 f(x_n, z_n) + \sum_{i=1}^{k} b_i f(x_{n-i}, z_{n-i})\right]$$
$$+ T_c(x_n)$$

where $T_c(x_n) = C_{q+1} h^{q+1} z^{(q+1)}(x_n) + O(h^{q+2})$.

Now define $\epsilon_{n-i}^{(j)} = z_{n-i} - y_{n-i}^{(j)} = z(x_{n-i}) - y_{n-i}^{(j)}$ for $j = 0,\ldots,m$ $i = 0,1,\ldots,2k$ so that subtracting (3.1) from (3.2) and (3.3) from (3.4) one obtains

$$(3.5)\quad \epsilon_n^{(0)} = \sum_{i=1}^{k} a_i^* \epsilon_{n-i}^{(m)} + h\sum_{i=1}^{k} b_i^*\left[f(x_{n-i}, z_{n-i}) - f(x_{n-i}, y_{n-i}^{(m-1)})\right]$$
$$+ T_p(x_n)$$

and

$$(3.6)\quad \epsilon_n^{(j)} = \sum_{i=1}^{k} a_i \epsilon_{n-i}^{(m)} + h\left[b_0\left[f(x_n, z_n) - f(x_n, y_n^{(j-1)})\right]\right.$$
$$\left. + \sum_{i=1}^{k} b_i\left[f(x_{n-i}, z_{n-i}) - f(x_{n-i}, y_{n-i}^{(m-1)})\right]\right] + T_c(x_n),$$

for $j = 1, 2, \ldots, m$.

Now define

$$g_{n-i}^{(j)} = \begin{cases} \dfrac{f(x_{n-i}, z_{n-i}) - f(x_{n-i}, y_{n-i}^{(j)})}{\epsilon_{n-i}^{(j)}} & \text{if } \epsilon_{n-i}^{(j)} \neq 0 \\ 0 & \text{if } \epsilon_{n-i}^{(j)} = 0 \end{cases}$$

and then assume that $g_{n-i}^{(j)} = g$, a constant, for $i = 0,\ldots,2k$ and $j = 1,\ldots,m$. With this (3.5)and (3.6) may be written as

$$(3.7)\ \epsilon_n^{(0)} = \sum_{i=1}^{k} a_i^* \epsilon_{n-i}^{(m)} + hg \sum_{i=1}^{k} b_i^* \epsilon_{n-i}^{(m-1)} + T_p(x_n)$$

and

$$(3.8)\ \epsilon_n^{(j)} = \sum_{i=1}^{k} a_i \epsilon_{n-i}^{(m)} + hg\left[b_0 \epsilon_n^{(j-1)} + \sum_{i=1}^{k} b_i \epsilon_{n-i}^{(m-1)}\right] + T_c(x_n)$$

for $j = 1,\ldots,m$.

Next, defining $H = hg$ and $\theta = Hb_0 = hgb_0$, by eliminating $\epsilon_n^{(j-1)}$ from (3.8) one obtains

$$(3.9)\ \epsilon_n^{(j)} = \sum_{i=1}^{k}\left[\sum_{s=0}^{j-1} \theta^s\, a_i + \theta^j a_i^*\right]\epsilon_{n-i}^{(m)}$$

$$+ H \sum_{i=1}^{k}\left[\sum_{s=0}^{j-1} \theta^s\, b_i + \theta^j b_i^*\right]\epsilon_{n-i}^{(m-1)} + T^{(j)}(x_n) .$$

where

$$(3.10)\ T^{(j)}(x_n) = T_c(x_n)\sum_{s=0}^{j-1} \theta^s + \theta^j T_p(x_n),\ j \le m.$$

In order to obtain a difference equation for $\epsilon_n^{(m)}$ it is now necessary to eliminate the term $\epsilon_{n-i}^{(m-1)}$ for $i = 1,2,\ldots,k$ from equation (3.9) when $j = m$.

For notational purposes define

$$(3.11)\quad \begin{aligned} \bar{a}_i &= \sum_{s=0}^{m-2} \theta^s a_i + \theta^{m-1} a_i^* \\ \bar{b}_i &= \sum_{s=0}^{m-2} \theta^s a_i + \theta^{m-1} b_i^* \end{aligned}$$

where $\sum_{s=0}^{m-2}\theta^{s} = 0$ if $m = 1$; $i = 1,\ldots,k$. Now observe that

$$(3.12)\quad \theta\bar{b}_i + b_i = \sum_{s=0}^{m-1}\theta^{s}b_i + \theta^{m}b_i^{*},$$

the coefficient of $\epsilon_{n-i}^{(m-1)}$ in equation (3.9) when $j = m$. Using the definitions from (3.11) in (3.9) with $j = m-1$ one has

$$(3.13)\quad \epsilon_n^{(m-1)} = \sum_{i=1}^{k}\bar{a}_i\epsilon_{n-i}^{(m)} + H\sum_{i=1}^{k}\bar{b}_i\epsilon_{n-i}^{(m-1)} + T^{(m-1)}(x_n).$$

Next observe that equation (3.8) with $j = m$ may be written as

$$(3.14)\quad \theta\epsilon_n^{(m-1)} = \epsilon_n^{(m)} - \sum_{i=1}^{k}a_i\epsilon_{n-i}^{(m)} - H\sum_{i=1}^{k}b_i\epsilon_{n-i}^{(m-1)} - T_c(x_n).$$

Replacing n by n-j in (3.13) and (3.14) it follows that

$$(3.15)\quad \sum_{j=1}^{k}(\theta\bar{b}_j + b_j)\epsilon_{n-j}^{(m-1)} = \Bigg\{\sum_{j=1}^{k}\bar{b}_j\epsilon_{n-j}^{(m)} + \sum_{j=1}^{k}\sum_{i=1}^{k}(b_j\bar{a}_i - \bar{b}_j a_i)\epsilon_{n-j-i}^{(m)} + H\sum_{j=1}^{k}\sum_{i=1}^{k}(b_j\bar{b}_i - \bar{b}_j b_i)\epsilon_{n-j-i}^{(m-1)} + \sum_{j=1}^{k}\left[b_j T^{(m-1)}(x_{n-j}) - \bar{b}_j T_c(x_{n-j})\right]\Bigg\}.$$

Next using (3.12) and $\sum_{j=1}^{k}\sum_{i=1}^{k}(b_j\bar{b}_i-\bar{b}_j b_i)\epsilon_{n-j-i}^{(m-1)} = 0$

(3.15) may be written

$$(3.16)\quad \sum_{j=1}^{k}\left(\sum_{s=0}^{m-1}\theta^s\, b_j + \theta^m b_j^*\right)\epsilon_{n-j}^{(m-1)} = \Bigg\{ \sum_{j=1}^{k}\bar{b}_j\epsilon_{n-j}^{(m)} + \sum_{j=1}^{k}\sum_{i=1}^{k}(b_j\bar{a}_i-\bar{b}_j a_i)\epsilon_{n-j-i}^{(m)} + \sum_{j=1}^{k}\left(b_j T^{(m-1)}(x_{n-j}) - \bar{b}_j T_c(x_{n-j})\right)\Bigg\}.$$

Using (3.16) in (3.9) with $j = m$ one has the difference equation

$$(3.17)\quad \epsilon_n^{(m)} = \sum_{i=1}^{k}\left[\sum_{s=0}^{m-1}\theta^s\, a_i + \theta^m a_i^*\right]\epsilon_{n-i}^{(m)} + H\sum_{i=1}^{k}\bar{b}_i\epsilon_{n-i}^{(m)} + H\sum_{i=1}^{k}\sum_{j=1}^{k}(b_i\bar{a}_j-\bar{b}_i a_j)\epsilon_{n-j-i}^{(m)} + H\sum_{i=1}^{k}\left[b_i T^{(m-1)}(x_{n-i}) - \bar{b}_i T_c(x_{n-i})\right] + T^{(m)}(x_n).$$

Now using the definitions of $\bar{a}_i$ and $\bar{b}_i$ as given in (3.11) one obtains the difference equation for the discretization error $\epsilon_n^{(m)}$ for the $P(EC)^m$ implementation:

$$(3.18)\ \epsilon_n^{(m)} = \left(\sum_{s=0}^{m-2}\theta^s\right)\sum_{i=1}^{k}(a_i + Hb_i)\epsilon_{n-i}^{(m)}$$

$$+ \theta^{m-1}\left\{\sum_{i=1}^{k}(a_i + \theta a_i^* + Hb_i^*)\epsilon_{n-i}^{(m)}\right.$$

$$\left. + H\sum_{i=1}^{k}\sum_{j=1}^{k}(b_i a_j^* - a_j b_i^*)\epsilon_{n-i-j}^{(m)}\right\} + T_n$$

where

$$(3.19)\ T_n = H\theta^{m-1}\sum_{j=1}^{k}\left[b_j T_p(x_{n-j}) - b_j^* T_c(x_{n-j})\right]$$

$$+ T_c(x_n)\sum_{s=0}^{m-1}\theta^s + \theta^m T_p(x_n)$$

with $\sum_{s=0}^{m-2}\theta^s = 0$ if $m = 1$.

Observe from (3.19) that in order for T_n, the truncation error for the $P(EC)^m$ implementation, to be of the same order as the truncation error for the corrector alone, $T_c(x_n)$, it is necessary that the order of the predictor, p, satisfy the inequality $p \geq q-m$, where q is the order of the corrector and m is the number of times the corrector equation is used.

The characteristic equation for the difference equation in (3.18) is

$$(3.20)\quad P^m(r,H) = r^{2k} - \sum_{s=0}^{m-1}\Theta^s\sum_{i=1}^{k}(a_i + Hb_i)r^{2k-i}$$
$$- \Theta^{m-1}\left(\sum_{i=1}^{k}(a_i + \Theta a_i^* + Hb_i^*)r^{2k-i}\right.$$
$$\left. + H\sum_{i=1}^{k}\sum_{j=1}^{k}(b_i a_j^* - a_j b_i^*)r^{2k-i-j}\right).$$

Consider now the case where $T_n = T$, a constant, and $u_1(H), \ldots, u_{2k}(H)$ are distinct roots of $P^m(r,H) = 0$. From the theory of linear difference equations the solution $\epsilon_n^{(m)}$ of (3.18) may be written

$$(3.21)\quad \epsilon_n^{(m)} = A_1(u_1(H))^n + \ldots + A_{2k}(u_{2k}(H))^n + T/P^m(1,H)$$

where $A_1, \ldots, A_{2k}$ are constants which satisfy the initial conditions $E_j = A_1(u_1(H))^j + \ldots + A_{2k}(u_{2k}(H))^j$ where $E_j = \epsilon_j - T/P^m(1,H)$ for $j = 0,1,\ldots,2k-1$. If the roots $u_1(H), \ldots, u_{2k}(H)$ are not distinct the form of (3.21) must be modified to be in agreement with the general form of (1.8).

In order to examine the roots of $P^m(r,H) = 0$ define

$$(3.22)\quad \begin{aligned} &\text{(i) } a(r) = r^k - \sum_{i=1}^{k} a_i r^{k-i}, \quad \text{(ii) } b(r) = \sum_{i=0}^{k} b_i r^{k-i}, \\ &\text{(iii) } a^*(r) = r^k - \sum_{i=1}^{k} a_i^* r^{k-i}, \quad \text{(iv) } b^*(r) = \sum_{i=1}^{k} b_i^* r^{k-i}. \end{aligned}$$

By the use of these definitions and considerable algebraic manipulation the characteristic equation (3.20) may be written in the form

$$(3.23)\quad (1-\theta)P^m(r,H) = (1-\theta^m)r^k\left[a(r) - Hb(r)\right] - \theta^{m-1}(1-\theta)H\left[a(r)b^*(r) - a^*(r)b(r)\right].$$

Observe from (3.23) that, assuming $|\theta| = |Hb_0| < 1$,

$$(3.24)\quad \lim_{m\to\infty}(1-\theta)P^m(r,H) = r^k\left[a(r) - Hb(r)\right] = r^k I(r,H)$$

where $I(r,H)$ is the characteristic equation for the iterated corrector. From this it follows that as $m\to\infty$, k roots of $P^m(r,H) = 0$ approach zero and k roots approach the roots of $I(r,H) = 0$. Since for H sufficiently small the roots which are approaching zero will have small absolute values, it follows that the error $\epsilon_n^{(m)}$ will be essentially determined by those roots of $P^m(r,H) = 0$ which are approaching the non-zero roots of the iterated corrector.

Consider now the case where $r_1, \ldots, r_j$ $(j \leq k)$ are the simple non-zero roots of $a(r) = 0$; $s_1(H), \ldots, s_j(H)$ are the corresponding roots of $I(r,H) = 0$; and $u_1^{(m)}(H)$, $u_2^{(m)}(H), \ldots, u_j^{(m)}(H)$ are the corresponding roots of $P^m(r,H) = 0$. In order to examine the manner in which these roots are related observe from (3.23) and (3.24) that

$$(3.25)\quad \lim_{H\to 0}(1-\theta)P^m(r,H) = r^k a(r) = \lim_{H\to 0} r^k I(r,H).$$

From this it follows that for H sufficiently small, assuming a suitable ordering,

$$
\text{(3.26)} \qquad
\begin{aligned}
s_i(H) &= r_i + c_{i1}H + c_{i2}H^2 + \ldots \\
u_i^{(m)}(H) &= r_i + d_{i1}H + d_{i2}H^2 + \ldots, \qquad i \leq j
\end{aligned}
$$

so that

$$
\text{(3.27)} \qquad u_i^{(m)}(H) = s_i(H) + e_{i1}H + e_{i2}H^2 + \ldots
$$

where $e_{is} = d_{is} - c_{is} \qquad i \leq j, \; s = 1,2,\ldots$

In order to solve for e_{is} in terms of the coefficients of the predictor and corrector equations it is convenient to let $u_i^{(m)}(H) = s_i(H) + \bar{e}_{is}H^s + O(H^{s+1}) \quad i \leq j, \; s \geq 1$. By the method of undetermined coefficients it is determined that

$$
\bar{e}_{is} = \begin{cases} 0 & s < m, \\ \dfrac{-b_0^{m-1} b(s_i(H))\; a^*(s_i(H))}{(s_i(H))^k a'(s_i(H))} & s = m, \; i \leq j. \end{cases}
$$

By the use of (3.25i) and Taylor series it follows that

$$
\bar{e}_{im} = \frac{-b_0{}^{m-1} b(r_i) a^*(r_i)}{(r_i)^k a'(r_i)} + O(H), \; i \leq j.
$$

Using this information in (3.27) one obtains the result

$$
\text{(3.28)} \quad u_i^{(m)}(H) = s_i(H) + \left[\frac{-b_0^{m-1} b(r_i) a^*(r_i)}{(r_i)^k a'(r_i)} \right] H^m + O(H^{m+1})
$$

for $i \leq j$.

If $m = 1$, using the expansion of $s_i(H)$ as given in (1.13) it follows from (3.28) that

$$(3.29)\quad u_i^{(1)}(H) = r_i + \left[\frac{f(r_i)}{r_i^k a'(r_i)}\right] H$$

$$+H^2\left[\frac{-f^2(r_i)\left[\frac{a''(r_i)}{2a'(r_i)} + \frac{k}{r_i}\right] + f(r_i)\left[a'(r_i)b^*(r_i) + f'(r_i)\right]}{(r_i^k\, a'(r_i))^2}\right] -$$

$$+\ O(H^3) \qquad i = 1,2,\dots,j$$

where $f(r) = b(r)\left[r^k - a^*(r)\right]$.

In determining the effect of the root $u_i^{(1)}(H)$ on the error $\epsilon_n^{(1)}$ it is the absolute value of the root which is of interest. Letting $r_s = \rho_s e^{iw}$ in equation (3.29) it follows that

$$(3.30)\quad u_s^{(1)}(H) = \rho_s + A_s H + B_s H^2 + O(H^3)$$

where

$$A_s = \mathrm{Re}\left\{\frac{e^{-i(k+1)w}\ f(\rho_s e^{iw})}{(\rho_s)^k\ a'(\rho_s e^{iw})}\right\}$$

and

$$B_s = \frac{\mathrm{Img}\left\{\frac{e^{-i(k+1)w}\ f(\rho_s e^{iw})}{(\rho_s)^k\ a'(\rho_s e^{iw})}\right\}}{2\rho_s} + \mathrm{Re}\left\{e^{-iw} C_2(\rho_s e^{iw})\right\}$$

where $C_2(r_i)$ is the coefficient of H^2 in equation (3.29).

In Appendix A root-locus plots are made for several commonly used predictor-corrector methods with a $P(EC)^m$ implementation using various values of m to illustrate the effect of iterating the corrector.

CHAPTER IV: GPC METHODS

In this chapter the difference equation satisfied by the discretization error for a generalized predictor-corrector method is derived.

However before starting such a derivation the concept of order for a generalized method will be examined.

A difference equation of the form

$$(4.1)\quad y_{n-\theta} = \sum_{i=1}^{k} A_i y_{n-i}^{(c)} + h \sum_{i=1}^{k} B_i f(x_{n-i}, y_{n-i}^{(c)})$$

is said to be of order s provided that the associated difference operator

$$L\left[z(x_{n-\theta}),h\right] \equiv z(x_{n-\theta}) - \left(\sum_{i=1}^{k} A_i z(x_{n-i}) + h \sum_{i=1}^{k} B_i z'(x_{n-i})\right)$$

$$= C_0^\theta z(x_n) + C_1^\theta h z'(x_n) + C_2^\theta h^2 z''(x_n) + \dots + C_q^\theta h^{q+1} z^{(q+1)}(x_n) + \dots$$

is such that $C_0^\theta = C_1^\theta = \dots = C_s^\theta = 0$ but $C_{s+1}^\theta \neq 0$. Using Taylor series to expand $L\left[z(x_{n-\theta}),h\right]$ it follows that

$$C_0^\theta = 1 - \sum_{i=1}^{k} A_i$$

$$(4.2)\quad C_1^\theta = -\theta + \sum_{i=1}^{k} i A_i - \sum_{i=1}^{k} B_i$$

$$C_q^{\theta} = (-1)^q \left\{ \frac{\theta^q - \sum_{i=1}^{k} i^q A_i}{q!} + \frac{\sum_{i=1}^{k} i^{q-1} B_i}{(q-1)!} \right\}, \quad q \geq 2.$$

Observe from (4.2) that as $\theta \neq 0$ C_i^{θ}, $i \geq 1$, is different from the corresponding coefficient for the difference operator associated with the linear multistep method (1.1).

Thus if (4.1) is of order s it follows that for a sufficiently differentiable function $z(x)$, with $z(x_n - th)$ defined to be z_{n-t}, $0 \leq t \leq k$, that

$$(4.3) \quad z_{n-\theta} = \sum_{i=1}^{k} A_i z_{n-i} + h \sum_{i=1}^{k} B_i z'_{n-i} + T_{\theta}(x_n)$$

where

$$(4.4) \quad T_{\theta}(x_n) = C_{s+1}^{\theta} h^{s+1} z^{(s+1)}(x_n) + O(h^{s+2}).$$

Similarly a difference equation of the form

$$(4.5) \quad y_n = \sum_{i=1}^{k} a_i y_{n-i}^{(c)} + h \Big[b_{-1} f(x_{n-\theta}, y_{n-\theta}) + b_0 f(x_n, y_n^{(p)}) + \sum_{i=1}^{k} b_i f(x_{n-i}, y_{n-i}^{(c)}) \Big]$$

is said to be of order q provided that the associated difference operator

$$L\left[z(x_n), h\right] \equiv z_n - \left(\sum_{i=1}^{k} a_i z_{n-i} + h \left[b_{-1} z'_{n-\theta} + b_0 z'_n + \sum_{i=1}^{k} b_i z'_{n-i} \right] \right)$$

$$L\left[z(x_n),h\right] = C_0 z(x_n) + \ldots + C_p h^p z^{(p)}(x_n) + \ldots$$

is such that $C_0 = C_1 = \ldots = C_q = 0$ but $C_{q+1} \neq 0$. Using Taylor series to expand $L\ z(x_n),h$ it follows that

$$C_0 = 1 - \sum_{i=1}^{k} a_i$$

$$C_1 = \sum_{i=1}^{k} i a_i - b_{-1} - b_0 - \sum_{i=1}^{k} b_i$$

(4.6)

$$\vdots$$

$$C_q = (-1)^q \left\{ \frac{-\sum_{i=1}^{k} i^q a_i}{q!} + \frac{b_{-1}\theta^{q-1} + \sum_{i=1}^{k} i^{q-1} b_i}{(q-1)!} \right\},\ q \geq 2.$$

Thus if (4.5) is of order q it follows that for a sufficiently differentiable function $z(x)$

$$(4.7)\quad z_n = \sum_{i=1}^{k} a_i z_{n-i} + h\left[b_{-1} z'_{n-\theta} + b_0 z'_n + \sum_{i=1}^{k} b_i z'_{n-i}\right] + T_c(x_n)$$

where

$$(4.8)\quad T_c(x_n) = C_{q+1} h^{q+1} z^{(q+1)}(x_n) + O(h^{q+2}).$$

For the GPC method to be analyzed let $y_{n-\theta}$ be predicted by equation (4.1) and let $y_n^{(p)}$ be obtained by the equation

$$(4.9)\quad y_n^{(p)} = \sum_{i=1}^{k} a_i^* y_{n-i}^{(c)} + h\left[b_{-1}^* f(x_{n-\theta}, y_{n-\theta}) + \sum_{i=1}^{k} b_i^* f(x_{n-i}, y_{n-i}^{(c)})\right]$$

which is of the form of equation (4.5). If (4.9) is of order p then for a sufficiently differentiable function $z(x)$

$$(4.10)\quad z_n = \sum_{i=1}^{k} a_i^* z_{n-i} + h\left[b_{-1}^* z'_{n-\theta} + \sum_{i=1}^{k} b_i^* z'_{n-i}\right] + T_p(x_n)$$

where

$$(4.11)\quad T_p(x_n) = C_{p+1}^* h^{p+1} z^{(p+1)}(x_n) + O(h^{p+2}).$$

Defining $\epsilon_{n-\theta} = z(x_{n-\theta}) - y_{n-\theta}$, $\epsilon_n^{(p)} = z(x_n) - y_n^{(p)}$, and $\epsilon_{n-i}^{(c)} = z(x_{n-i}) - y_{n-i}^{(c)}$ $i = 0,1,\ldots,k$ it follows by subtracting (4.1) from (4.3), (4.9) from (4.10), and (4.5) from (4.6) that

$$(4.12)\quad \epsilon_{n-\theta} = \sum_{i=1}^{k} A_i \epsilon_{n-i}^{(c)} + h\sum_{i=1}^{k} B_i \left[f(x_{n-i}, z_{n-i}) - f(x_{n-i}, y_{n-i}^{(c)})\right] + T_\theta(x_n),$$

$$(4.13)\quad \epsilon_n^{(p)} = \sum_{i=1}^{k} a_i^* \epsilon_{n-i}^{(c)} + h\Bigg[b_{-1}^* \left[f(x_{n-\theta}, z_{n-\theta}) - f(x_{n-\theta}, y_{n-\theta})\right] + \sum_{i=1}^{k} b_i^* \left[f(x_{n-i}, z_{n-i}) - f(x_{n-i}, y_{n-i}^{(c)})\right]\Bigg] + T_p(x_n),$$

and

$$(4.14)\quad \epsilon_n^{(c)} = \sum_{i=1}^{k} a_i \epsilon_{n-i}^{(c)} + h\Bigg[b_{-1}\left[f(x_{n-\theta}, z_{n-\theta}) - f(x_{n-\theta}, y_{n-\theta})\right] \; b_0\left[f(x_n, z_n) - f(x_n, y_n^{(p)})\right] + \sum_{i=1}^{k} b_i \left[f(x_{n-i}, z_{n-i}) - f(x_{n-i}, y_{n-i}^{(c)})\right]\Bigg] + T_c(x_n).$$

Defining

$$g_{n-\theta} = \begin{cases} \dfrac{f(x_{n-\theta}, z_{n-\theta}) - f(x_{n-\theta}, y_{n-\theta})}{\epsilon_{n-\theta}} & \text{if } \epsilon_{n-\theta} \neq 0 \\ 0 & \text{if } \epsilon_{n-\theta} = 0 \end{cases}$$

$$g_n^{(p)} = \begin{cases} \dfrac{f(x_n, z_n) - f(x_n, y_n^{(p)})}{\epsilon_n^{(p)}} & \text{if } \epsilon_n^{(p)} \neq 0 \\ 0 & \text{if } \epsilon_n^{(p)} = 0 \end{cases}$$

$$g_{n-i}^{(c)} = \begin{cases} \dfrac{f(x_{n-i}, z_{n-i}) - f(x_{n-i}, y_{n-i}^{(c)})}{\epsilon_{n-i}^{(c)}} & \text{if } \epsilon_{n-i}^{(c)} \neq 0 \\ 0 & \text{if } \epsilon_{n-i}^{(c)} = 0 \end{cases}$$

one may write equations (4.12), (4.13) and (4.14) as

$$(4.15)\quad \epsilon_{n-\theta} = \sum_{i=1}^{k} A_i \epsilon_{n-i}^{(c)} + h \sum_{i=1}^{k} B_i g_{n-i}^{(c)} \epsilon_{n-i}^{(c)} + T_\theta(x_n),$$

$$(4.16)\quad \epsilon_n^{(p)} = \sum_{i=1}^{k} a_i^* \epsilon_{n-i}^{(c)} + h \left[b_{-1}^* g_{n-\theta} \epsilon_{n-\theta} + \sum_{i=1}^{k} b_i^* g_{n-i}^{(c)} \epsilon_{n-i}^{(c)} \right] + T_p(x_n),$$

and

$$(4.17)\quad \epsilon_n^{(c)} = \sum_{i=1}^{k} a_i \epsilon_{n-i}^{(c)} + h \left[b_{-1} g_{n-\theta} \epsilon_{n-\theta} + b_0 g_n^{(p)} \epsilon_n^{(p)} + \sum_{i=1}^{k} b_i g_{n-i}^{(c)} \epsilon_{n-i}^{(c)} \right] + T_c(x_n).$$

Eliminating $\epsilon_{n-\theta}$ and $\epsilon_n^{(p)}$ from (4.17) by the use of (4.15) and (4.16) one obtains the difference equation for the discretization error for a generalized predictor-corrector method:

$$(4.18)\quad \epsilon_n^{(c)} = \sum_{i=1}^{k} \Big\{ a_i + h\left[b_i g_{n-i}^{(c)} + b_{-1}A_i g_{n-\theta} + b_0 a_i^* g_n^{(p)}\right] + h^2\left[b_{-1}B_i g_{n-\theta} g_{n-i}^{(c)} + b_0 b_{-1}^* A_i g_{n-\theta} g_n^{(p)} + b_0 b_i^* g_n^{(p)} g_{n-i}^{(c)}\right] + h^3\left[b_0 b_{-1}^* B_i g_n^{(p)} g_{n-\theta} g_{n-i}^{(c)}\right] \Big\} \epsilon_{n-i}^{(c)} + T_n(x_n)$$

where

$$(4.19)\quad T_n(x_n) = T_c(x_n) + h\left[b_{-1} g_{n-\theta} T_\theta(x_n) + b_0 g_n^{(p)} T_p(x_n)\right] + h^2\left[b_0 b_{-1}^* g_n^{(p)} g_{n-\theta} T_\theta(x_n)\right].$$

Observe from (4.19) that in order to have the truncation error $T_n(x_n)$ for the GPC method to be of the same order as the truncation error $T_c(x_n)$ for the generalized corrector alone it is necessary that $T_\theta(x_n)$ and $T_p(x_n)$ each be at least of order t, $t \geq q-1$.

Consider now the case where $g_{n-\theta} = g_n^{(p)} = g_{n-i}^{(c)} = g$, a constant, for $i = 0,1,\ldots,k$ and $T_n(x_n) = T$, a constant. Defining $H = hg$, (4.18) may be written

$$(4.20)\quad \epsilon_n^{(c)} = \sum_{i=1}^{k} \Big\{ a_i + H\left[b_i + b_{-1}A_i + b_0 a_i^*\right] + H^2\left[b_{-1}B_i + b_0 b_{-1}^* A_i + b_0 b_i^*\right] + H^3\left[b_0 b_{-1}^* B_i\right] \Big\} \epsilon_{n-i}^{(c)} + T.$$

The characteristic equation corresponding to this difference equation is

$$(4.21)\quad G(r,H) \equiv r^k - \sum_{i=1}^{k}\Big(a_i + H\big[b_i + b_{-1}A_i + b_0 a_i^*\big] + H^2\big[b_{-1}B_i + b_0 b_{-1}^* A_i + b_0 b_i^*\big] + H^3\big[b_0 b_{-1}^* B_i\big]\Big) r^{k-i}.$$

If $s_1(H), \ldots, s_k(H)$ are distinct roots of $G(r,H) = 0$, from the theory of linear difference equations, the solution of (4.20) may be written

$$(4.22)\quad \epsilon_n^{(c)} = A_1(s_1(H))^n + \ldots + A_k(s_k(H))^n + T/G(1,H)$$

where $A_1, \ldots, A_k$ are constants which satisfy the initial conditions

$$E_j = A_1(s_1(H))^j + \ldots + A_k(s_k(H))^j$$

where $E_j = \epsilon_j - T/G(1,H)$ for $j = 0,1,\ldots,k-1$. If $s_1(H), \ldots, s_k(H)$ are not distinct the form of (4.22) must be modified to be in agreement with the general form of (1.8).

In order to examine the behavior of the roots $s_1(H)$, $s_2(H), \ldots, s_k(H)$ of $G(r,H) = 0$ define

$$(4.23)\quad \begin{aligned} &(i)\ a(r) = r^k - \sum_{i=1}^{k} a_i r^{k-i} \\ &(ii)\ C_1(r) = \sum_{i=1}^{k} (b_i + b_{-1}A_i + b_0 a_i^*) r^{k-i} \end{aligned}$$

$$\text{(iii)}\quad C_2(r) = \sum_{i=1}^{k} (b_{-1}B_i + b_0 b^*_{-1}A_i + b_0 b^*_i) r^{k-i}$$

$$\text{(iv)}\quad C_3(r) = \sum_{i=1}^{k} b_0 b^*_{-1} B_i r^{k-i}$$

so that (4.21) becomes

$$(4.24)\quad G(r,H) = a(r) - HC_1(r) - H^2 C_2(r) - H^3 C_3(r).$$

Observe from this that $\lim_{H\to 0} G(r,H) = a(r)$, so that if $r_1, \ldots, r_k$ are the roots of $a(r) = 0$, assuming a suitable ordering and H sufficiently small,

$$(4.25)\quad s_i(H) = r_i + d_{i1}H + d_{i2}H^2 + d_{i3}H^3 + \ldots \quad i = 1,\ldots;k.$$

If $r_1, \ldots, r_v$ $v \leq k$ are the simple roots of $a(r) = 0$ it follows by the method of undetermined coefficients that

$$(4.26)\quad \begin{aligned} d_{j1} &= \frac{C_1(r_j)}{a'(r_j)} \\ d_{j2} &= \frac{\left(C_2(r_j) + d_{j1}C_1'(r_j) - \dfrac{d_{j1}^2 a''(r_j)}{2}\right)}{a'(r_j)} \\ d_{j3} &= \Bigg(C_3(r_j) + d_{j1}C_2'(r_j) + \frac{d_{j1}^2 C_1''(r_j)}{2} + d_{j2}C_1'(r_j) \\ &\qquad - \frac{d_{j1}^3 a^{(3)}(r_j)}{6} - d_{j1}d_{j2}a''(r_j)\Bigg) \Big/ a'(r_j) \end{aligned}$$

when $j \leq v$.

It follows from the work by Stetter and Gragg (13) that for H sufficiently small the root $s_1(H)$ approaching $r_1 \equiv 1$ is of the form

$$s_1(H) = e^H + O(H^q).$$

The GPC method is zero stable, relatively stable or absolutely stable provided that $G(r,H)$ satisfies the definitions of such as given in the introduction.

In Appendix B root-locus plots are made for some GPC methods.

CHAPTER V: SGPC METHODS

In this chapter the difference equation satisfied by the discretization error for a simplified generalized predictor-corrector (SGPC) method is derived.

Assume that a value of $y_{n-\theta}$ is predicted by the formula

$$(5.1)\quad y_{n-\theta} = \sum_{i=1}^{k} A_i y_{n-i}^{(c)} + h\sum_{i=1}^{k} B_i f(x_{n-i}, y_{n-i}^{(p)})$$

which is of order s, so that for a sufficiently differentiable function z(x)

$$(5.2)\quad z_{n-\theta} = \sum_{i=1}^{k} A_i z_{n-i} + h\sum_{i=1}^{k} B_i z'_{n-i} + T_\theta(x_n)$$

where

$$(5.3)\quad T_\theta(x_n) = C_{s+1}^{\theta} h^{s+1} z^{(s+1)}(x_n) + O(h^{s+2}).$$

Note that (5.1) is the same as (4.1) except that the function f(x,y) on the right side is evaluated at the point $(x_{n-i}, y_{n-i}^{(p)})$.

Next assume that a first approximation to z_n is obtained by the use of the difference equation

$$(5.4)\quad y_n^{(p)} = \sum_{i=1}^{k} a_i^* y_{n-i}^{(c)} + h\Big[b_{-1}^* f(x_{n-\theta}, y_{n-\theta}) + \sum_{i=1}^{k} b_i^* f(x_{n-i}, y_{n-i}^{(p)})\Big]$$

which is of order p, so that for a sufficiently differentiable function z(x)

$$(5.5)\quad z_n = \sum_{i=1}^{k} a_i^* z_{n-i} + h\left[b_{-1}^* z'_{n-e} + \sum_{i=1}^{k} b_i^* z'_{n-i}\right] + T_p(x_n)$$

where

$$(5.6)\quad T_p(x_n) = C_{p+1}^* h^{p+1} z^{(p+1)}(x_n) + O(h^{p+2}).$$

Now assume that the final approximation to z_n is obtained by the use of the generalized corrector

$$(5.7)\quad y_n^{(c)} = \sum_{i=1}^{k} a_i y_{n-i}^{(c)} + h\Big[b_{-1} f(x_{n-e}, y_{n-e}) + b_0 f(x_n, y_n^{(p)})$$
$$+ \sum_{i=1}^{k} b_i f(x_{n-i}, y_{n-i}^{(p)})\Big]$$

which is of order q, so that for a sufficiently differentiable function z(x)

$$(5.8)\quad z_n = \sum_{i=1}^{k} a_i z_{n-i} + h\left[b_{-1} z'_{n-e} + b_0 z'_n + \sum_{i=1}^{k} b_i z'_{n-i}\right] + T_c(x_n)$$

where

$$(5.9)\quad T_c(x_n) = C_{q+1} h^{q+1} z^{(q+1)}(x_n) + O(h^{q+2}).$$

Defining $\epsilon_{n-e} = z_{n-e} - y_{n-e}$; $\epsilon_{n-i}^{(p)} = z_{n-i} - y_{n-i}^{(p)}$ and $\epsilon_{n-i}^{(c)} = z_{n-i} - y_{n-i}^{(c)}$ for $i = 0,1,\ldots,2k$ it follows by subtracting (5.1) from (5.2), (5.4) from (5.5), and (5.7) from (5.8) that

$$(5.10)\quad \epsilon_{n-\theta} = \sum_{i=1}^{k} A_i \epsilon_{n-i}^{(c)} + h \sum_{i=1}^{k} B_i \left[f(x_{n-i}, z_{n-i}) - f(x_{n-i}, y_{n-i}^{(p)}) \right]$$

$$+ T_\theta(x_n),$$

$$(5.11)\quad \epsilon_n^{(p)} = \sum_{i=1}^{k} a_i^* \epsilon_{n-i}^{(c)} + h \left[b_{-1}^* \left[f(x_{n-\theta}, z_{n-\theta}) - f(x_{n-\theta}, y_{n-\theta}) \right] \right.$$

$$\left. + \sum_{i=1}^{k} b_i^* \left[f(x_{n-i}, z_{n-i}) - f(x_{n-i}, y_{n-i}^{(p)}) \right] \right]$$

$$+ T_p(x_n),$$

and

$$(5.12)\quad \epsilon_n^{(c)} = \sum_{i=1}^{k} a_i \epsilon_{n-i}^{(c)} + h \left[b_{-1} \left[f(x_{n-\theta}, z_{n-\theta}) - f(x_{n-\theta}, y_{n-\theta}) \right] \right.$$

$$\left. + \sum_{i=0}^{k} b_i \left[f(x_{n-i}, z_{n-i}) - f(x_{n-i}, y_{n-i}^{(p)}) \right] \right]$$

$$+ T_c(x_n).$$

Now defining

$$g_{n-\theta} = \begin{cases} \dfrac{f(x_{n-\theta}, z_{n-\theta}) - f(x_{n-\theta}, y_{n-\theta})}{\epsilon_{n-\theta}} & \text{if } \epsilon_{n-\theta} \neq 0 \\ 0 & \text{if } \epsilon_{n-\theta} = 0 \end{cases}$$

$$g_{n-i}^{(p)} = \begin{cases} \dfrac{f(x_{n-i}, z_{n-i}) - f(x_{n-i}, y_{n-i}^{(p)})}{\epsilon_{n-i}^{(p)}} & \text{if } \epsilon_{n-i}^{(p)} \neq 0 \\ 0 & \text{if } \epsilon_{n-i}^{(p)} = 0 \end{cases}$$

for $i = 0,1,\ldots,2k$ equations (5.10), (5.11), and (5.12) may be written as

$$(5.13)\quad \epsilon_{n-\theta} = \sum_{i=1}^{k} A_i \epsilon_{n-i}^{(c)} + h\sum_{i=1}^{k} B_i g_{n-i}^{(p)} \epsilon_{n-i}^{(p)} + T_\theta(x_n),$$

$$(5.14)\quad \epsilon_n^{(p)} = \sum_{i=1}^{k} a_i^* \epsilon_{n-i}^{(c)} + h\left[b_{-1}^* g_{n-\theta}\epsilon_{n-\theta} + \sum_{i=1}^{k} b_i^* g_{n-i}^{(p)} \epsilon_{n-i}^{(p)}\right] + T_p(x_n),$$

and

$$(5.15)\quad \epsilon_n^{(c)} = \sum_{i=1}^{k} a_i \epsilon_{n-i}^{(c)} + h\left[b_{-1} g_{n-\theta}\epsilon_{n-\theta} + \sum_{i=0}^{k} b_i g_{n-i}^{(p)} \epsilon_{n-i}^{(p)}\right] + T_c(x_n).$$

By eliminating $\epsilon_{n-\theta}$ from (5.14) by the use of (5.13) it follows that

$$(5.16)\quad \epsilon_n^{(p)} = \sum_{i=1}^{k} (a_i^* + hg_{n-\theta} b_{-1}^* A_i)\epsilon_{n-i}^{(c)} + \sum_{i=1}^{k} (hg_{n-i}^{(p)} b_i^* + h^2 g_{n-\theta} g_{n-i}^{(p)} b_{-1}^* B_i)\epsilon_{n-i}^{(p)} + T_n^p$$

where

$$(5.17)\quad T_n^p = T_p(x_n) + hg_{n-\theta} b_{-1}^* T_\theta(x_n).$$

By eliminating $\epsilon_{n-\theta}$ and $\epsilon_n^{(p)}$ from (5.15) by the use of (5.13) and (5.16) it follows that

$$(5.18)\quad \epsilon_n^{(c)} = \sum_{i=1}^{k}\Big\{\Big[a_i\Big] + h\Big[g_{n-\theta}b_{-1}A_i + g_n^{(p)}b_0a_i^*\Big] + h^2\Big[g_n^{(p)}g_{n-\theta}b_0b_{-1}^*A_i\Big]\Big\}\epsilon_{n-i}^{(c)}$$
$$+\sum_{i=1}^{k}\Big\{h\Big[g_{n-i}^{(p)}b_i\Big] + h^2\Big[g_{n-\theta}g_{n-i}^{(p)}b_{-1}B_i + g_n^{(p)}g_{n-i}^{(p)}b_0b_i^*\Big] + h^3\Big[g_n^{(p)}g_{n-\theta}g_{n-i}^{(p)}b_0b_{-1}^*B_i\Big]\Big\}\epsilon_{n-i}^{(p)} + T_n^c$$

where

$$(5.19)\quad T_n^c = T_c(x_n) + h\Big[g_{n-\theta}b_{-1}T_\theta(x_n) + g_n^{(p)}b_0T_p(x_n)\Big] + h^2\Big[g_n^{(p)}g_{n-\theta}b_0b_{-1}^*T_\theta(x_n)\Big].$$

In order to obtain the difference equation for the discretization error $\epsilon_n^{(c)}$ for a SGPC method it is now necessary to eliminate the terms $\epsilon_{n-i}^{(p)}$ $i = 1,\ldots,k$ from equation (5.18).

Consider now the case where $g_{n-\theta} = g_{n-i}^{(p)} = g$, a constant, for $i = 0,1,\ldots,2k$. For notational purposes define

$$(5.20)\quad \begin{aligned} &\text{(i)}\ H = hg\\ &\text{(ii)}\ C_i = a_i^* + Hb_{-1}^*A_i\\ &\text{(iii)}\ D_i = Hb_i^* + H^2b_{-1}^*B_i\\ &\text{(iv)}\ E_i = a_i + H\Big[b_{-1}A_i + b_0a_i^*\Big] + H^2b_0b_{-1}^*A_i\\ &\text{(v)}\ F_i = Hb_i + H^2\Big[b_{-1}B_i + b_0b_i^*\Big] + H^3b_0b_{-1}^*B_i \end{aligned}$$

for $i = 1,2,\ldots,k$. With these definitions (5.16) and (5.18) may be written as

$$(5.21)\quad \epsilon_n^{(p)} = \sum_{i=1}^{k} C_i \epsilon_{n-i}^{(c)} + \sum_{i=1}^{k} D_i \epsilon_{n-i}^{(p)} + T_n^p$$

and

$$(5.22)\quad \epsilon_n^{(c)} = \sum_{i=1}^{k} E_i \epsilon_{n-i}^{(c)} + \sum_{i=1}^{k} F_i \epsilon_{n-i}^{(p)} + T_n^c.$$

If one now uses equation (5.21) with n replaced by n-i in equation (5.22) it follows that

$$(5.23)\quad \epsilon_n^{(c)} = \sum_{i=1}^{k} E_i \epsilon_{n-i}^{(c)} + \sum_{i=1}^{k} \sum_{j=1}^{k} F_i C_j \epsilon_{n-i-j}^{(c)}$$

$$+ \sum_{j=1}^{k} D_j \sum_{i=1}^{k} F_i \epsilon_{n-j-i}^{(p)} + \sum_{i=1}^{k} F_i T_{n-i}^p + T_n^c.$$

Next observe from equation (5.22) with n replaced by n-j that

$$\sum_{i=1}^{k} F_i \epsilon_{n-j-i}^{(p)} = \epsilon_{n-j}^{(c)} - \sum_{i=1}^{k} E_i \epsilon_{n-j-i}^{(c)} - T_{n-j}^c.$$

Using this in equation (5.23) it follows that

$$(5.24)\quad \epsilon_n^{(c)} = \sum_{i=1}^{k} (E_i + D_i) \epsilon_{n-i}^{(c)} + \sum_{i=1}^{k} \sum_{j=1}^{k} (F_i C_j - D_j E_i) \epsilon_{n-j-i}^{(c)}$$

$$+ \sum_{i=1}^{k} (F_i T_{n-i}^p - D_i T_{n-i}^c) + T_n^c.$$

Observe that the terms $\epsilon_{n-i}^{(p)}$ do not appear in (5.24).

Replacing C_i, D_i, E_i, and F_i $i = 1,\ldots,k$ by their definitions as given in (5.20) and performing considerable algebraic manipulation of terms, it follows that the difference equation for the discretization error in a SGPC method is

$$(5.25)\quad \epsilon_n^{(c)} = \sum_{i=1}^{k}\left\{a_i + H(b_{-1}A_i + b_0 a_i^* + b_i^*) + H^2(b_{-1}^* b_0 A_i + b_{-1}^* B_i)\right\}\epsilon_{n-i}^{(c)}$$
$$+ \sum_{i=1}^{k}\sum_{j=1}^{k}\left\{H(a_j^* b_i - a_i b_j^*) + H^2\left[b_{-1}(a_j^* B_i - b_j^* A_i) + b_{-1}^*(b_i A_j - a_i B_j)\right]\right\}\epsilon_{n-i-j}^{(c)} + T_n$$

where

$$(5.26)\quad T_n = T_c(x_n) + T_\theta(x_n)\left[Hb_{-1} + H^2 b_0 b_{-1}^*\right] + T_p(x_n)\left[Hb_0\right]$$
$$+ \sum_{i=1}^{k}\left\{T_c(x_{n-i})\left[-Hb_i^* - H^2 b_{-1}^* B_i\right] + T_\theta(x_{n-i})H^2\left[b_{-1}^* b_i - b_{-1} b_i^*\right] + T_p(x_{n-i})\left[Hb_i + H^2 b_{-1} B_i\right]\right\}.$$

Observe from (5.26) that in order for the truncation error T_n of the SGPC method to be of the same order as the truncation error $T_c(x_n)$ for the generalized corrector it is necessary that each of $T_\theta(x_n)$ and $T_p(x_n)$ be of order t, $t \geq q-1$.

The characteristic equation for the difference equation (5.25) is

$$(5.27)\quad SG(r,H) \equiv r^{2k} - \sum_{i=1}^{k}\Big[a_i + H\big[b_{-1}A_i + b_0a_i^* + b_i^*\big] + H^2\big[b_{-1}^*b_0A_i - b_{-1}^*B_i\big]\Big]r^{2k-i}$$
$$-\sum_{i=1}^{k}\sum_{j=1}^{k}\Big[H\big[a_j^*b_i - a_ib_j^*\big] + H^2\big[b_{-1}(a_j^*B_i - b_j^*A_i) + b_{-1}^*(b_iA_j - a_iB_j)\big]\Big]r^{2k-i-j}.$$

If $s_1(H), \ldots, s_k(H)$ are distinct roots of $SG(r,H) = 0$ then by the theory of linear difference equations the solution of (5.25), assuming $T_n = T$, a constant, may be written

$$(5.28)\quad \epsilon_n^{(c)} = A_1(s_1(H))^n + \ldots + A_{2k}(s_{2k}(H))^n + T/SG(1,H)$$

where $A_1, \ldots, A_{2k}$ are constants which satisfy the initial conditions

$$E_j = A_1(s_1(H))^j + \ldots + A_{2k}(s_{2k}(H))^j$$

where $E_j = \epsilon_j - T/SG(1,H)$ for $j = 0,1,\ldots,2k-1$. If the roots of $SG(r,H) = 0$ are not distinct the form of (5.28) must be modified slightly in order to be in agreement with the general form of (1.8).

In order to study the behavior of the roots of $SG(r,H) = 0$ it is convenient to define the polynomials

$$\text{(i)}\quad a(r) = r^k - \sum_{i=1}^{k} a_i r^{k-i}$$

$$\text{(ii)}\quad C_1(r) = \sum_{i=1}^{k} (b_{-1}A_i + b_0 a_i^* + b_i^*) r^{2k-i}$$

$$(5.29)\qquad + \sum_{i=1}^{k} \sum_{j=1}^{k} (a_j^* b_i - a_i b_j^*) r^{2k-i-j}$$

$$\text{(iii)}\quad C_2(r) = \sum_{i=1}^{k} (b_{-1}^* b_0 A_i + b_{-1}^* B_i) r^{2k-i}$$

$$+ \sum_{i=1}^{k} \sum_{j=1}^{k} \Big(b_{-1}(a_j^* B_i - b_j^* A_i) + b_{-1}^*(b_i A_j - a_i B_j) \Big) r^{2k-i-j}$$

so that the characteristic equation (5.27) may be written

$$(5.30)\quad SG(r,H) = r^k a(r) - HC_1(r) - H^2 C_2(r).$$

Observe from (5.30) that $\lim_{H\to 0} SG(r,H) = r^k a(r)$. From this it follows that as H approaches zero k roots of $SG(r,H) = 0$ approach zero and k roots approach the k roots $r_1, \ldots, r_k$ of $a(r) = 0$. Thus for H sufficiently small the error $\epsilon_n^{(c)}$ for the SGPC method will be essentially determined by those roots of SG(r,H) which are approaching the non-zero roots of $a(r) = 0$.

If $r_1, \ldots, r_t$ $(t \leq k)$ are the simple non-zero roots of $a(r) = 0$ and $s_1(H), \ldots, s_t(H)$ are the corresponding roots of $SG(r,H) = 0$ it follows from the above and the method of undetermined coefficients that

$$(5.31) \quad s_i(H) = r_i + d_{i1}H + d_{i2}H^2 + O(H^3)$$

where

$$d_{i1} = \frac{C_1(r_i)}{a'(r_i)}$$

$$d_{i2} = \frac{d_{i1}C_1'(r_i) - \dfrac{d_{i1}^2 a''(r_i)}{2} + C_2(r_i)}{a'(r_i)}$$

for $i \leq t$.

It follows from the work by Stetter and Gragg (13) that for H sufficiently small the root $s_1(H)$ approaching $r_1 \equiv 1$ is of the form

$$s_1(H) = e^H + O(H^q).$$

The SGPC method is zero stable, absolutely stable, or relatively stable provided $SG(r,H)$ satisfies the definitions for such as given in the introduction.

In Appendix B root-locus plots are made for some SGPC methods.

CHAPTER VI: COMPARISONS AND CONCLUSIONS

The first point to be considered in this chapter is that neither a $PE(CE)^m$ or a $P(EC)^m$ implementation is necessarily more stable (in the sense of possessing a larger region of stability) than the other. To show this consider now methods which use the predictor formula

$$(6.1)\quad y_n^{(p)} = (1 - a_2^* - a_3^*)y_{n-1} + a_2^* y_{n-2} + a_3^* y_{n-3} + h\left[\left(\frac{4a_3^* + 5a_2^* + 23}{12}\right)f(x_{n-1},y_{n-1}) + \left(\frac{16a_3^* + 8a_2^* - 16}{12}\right)f(x_{n-2},y_{n-2}) + \left(\frac{4a_3^* - a_2^* + 5}{12}\right)f(x_{n-3},y_{n-3})\right]$$

which is of order 3 for arbitrary a_2^* and a_3^*, and the corrector formula

$$(6.2)\quad y_n^{(c)} = y_{n-1} - y_{n-2} + y_{n-3} + \frac{h}{12}\left[5f(x_n,y_n^{(p)}) + 7f(x_{n-1},y_{n-1}) + 7f(x_{n-2},y_{n-2}) + 5f(x_{n-3},y_{n-3})\right]$$

which is of order 4.

The roots of $a(r) = 0$, for this method $a(r) = r^3 - r^2 + r - 1$, are $1, +i, -i$. The stability of either implementation will be determined by the manner in which the roots of the characteristic equation for the respective difference equations approach these roots of $a(r) = 0$ as as H approaches zero. Let (i) $s_1(H)$ be the root approaching 1 as H approaches zero, (ii) $s_2(H)$ be the root approaching $+i$, and (iii) $s_3(H)$ be the root approaching $-i$. As shown by Henrici (6), for H sufficiently small, $s_1(H) = e^H + O(H^5)$ for either implementation. By the use of equation (2.24) it follows that for a PE(CE) implementation, assuming H is sufficiently small,

$$(6.3) \quad \left|s_i(H)\right| = 1 + \left(\frac{-7 + 5a_3^*}{24}\right)H + O(H^2) \qquad i = 2, 3.$$

By the use of equation (3.30) it follows that for a P(EC) implementation, assuming H is sufficiently small,

$$(6.4) \quad \left|s_i(H)\right| = 1 + \left(\frac{a_2^*}{12}\right)H + O(H^2) \qquad i = 2, 3.$$

Choosing $a_2^* = +12$ and $a_3^* = -5$ it follows that the PE(CE) implementation has no region of absolute stability whereas the P(EC) implementation does possess a region of absolute stability. For a root-locus plot of the PE(CE) implementation see Figure 1 and for the root-locus plot for a P(EC) implementation see Figure 2. In these and all following figures magnitudes only are plotted. A circle will indicate a positive root, a square a negative root, and a triangle indicates a complex pair.

On the other hand if one chooses $a_2^* = -12$ and $a_3^* = +5$ it follows that the P(EC) implementation has no region of absolute stability whereas a PE(CE) implementation does.

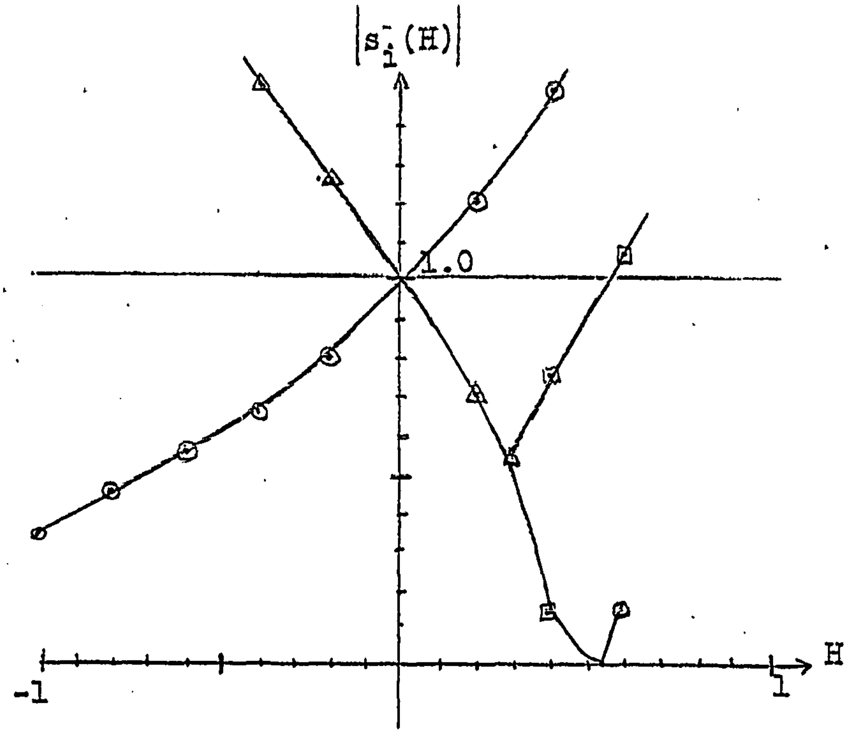

Figure 1. PE(CE)

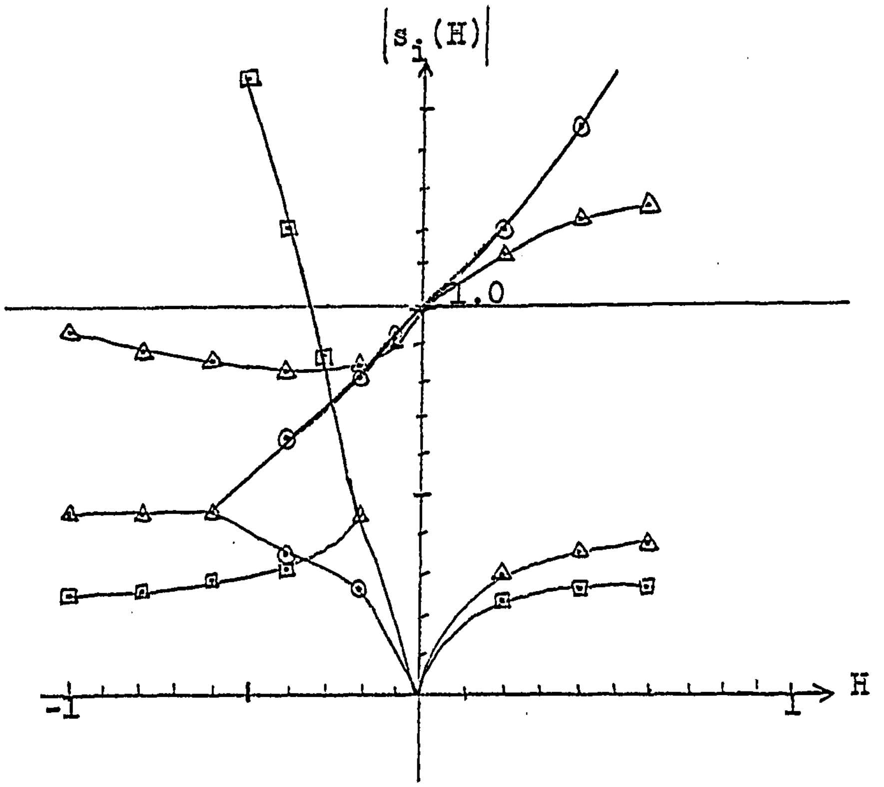

Figure 2. P(EC)

For a root-locus plot of the PE(CE) implementation see Figure 3 and for the P(EC) implementation see Figure 4.

In a recent paper F. T. Krogh (11) states "The author has additional evidence that $P(EC)^{m+1}$ algorithms are less stable than $PE(CE)^m$ ones. It is planned to discuss this matter further in a later paper . . . ." To show that this statement is not in general true recall from the analysis in Chapter II and Chapter III that the simple non-zero roots of the characteristic equation for either a $P(EC)^m$ or a $PE(CE)^m$ implementation agree with the roots of the iterated corrector to $O(H^m)$ (see equation (2.22) and equation (3.28)). Thus from this if the iterated corrector is convergent and the non-zero roots are controlling the error a $P(EC)^{m+1}$ implementation should be expected to be more stable than a $PE(CE)^m$ implementation as the roots of its characteristic equation will be closer to the roots of the iterated corrector.

One example of a predictor-corrector method which is more stable in a $P(EC)^2$ implementation than in a PE(CE) implementation is a method using the predictor

$$(6.5)\quad y_n^{(p)} = 7y_{n-1} - 6y_{n-2} + \frac{h}{2}\left[-3f(x_{n-1},y_{n-1}) - 7f(x_{n-2},y_{n-2})\right]$$

and the corrector

$$(6.6)\quad y_n^{(c)} = \frac{1}{4}(y_{n-1} + 3y_{n-2}) + \frac{h}{48}\Big[17f(x_n,y_n^{(p)}) + 56f(x_{n-1},y_{n-1}) - 33f(x_{n-2},y_{n-2})\Big].$$

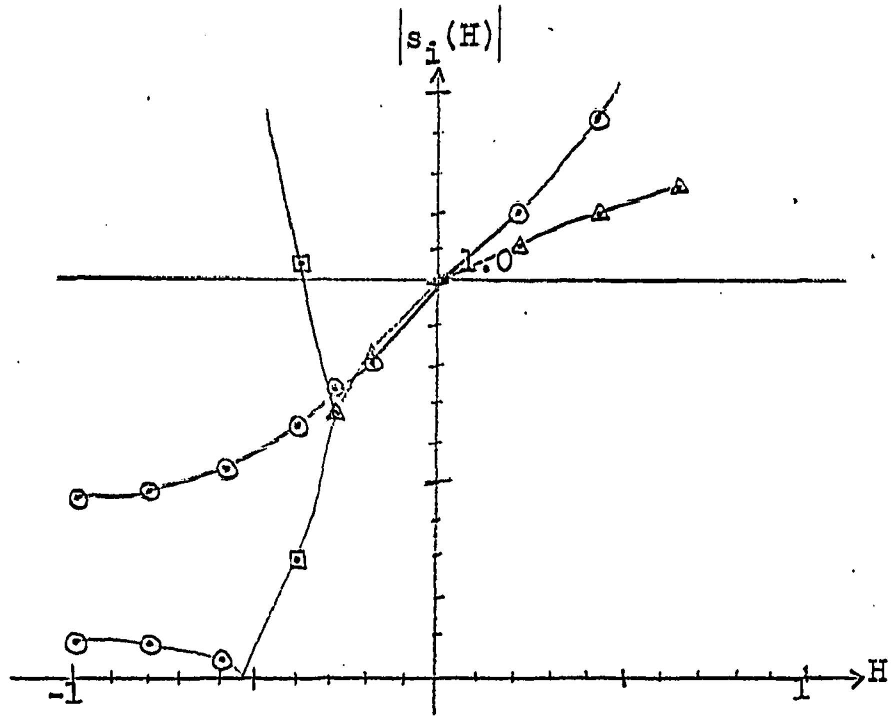

Figure 3. PE(CE)

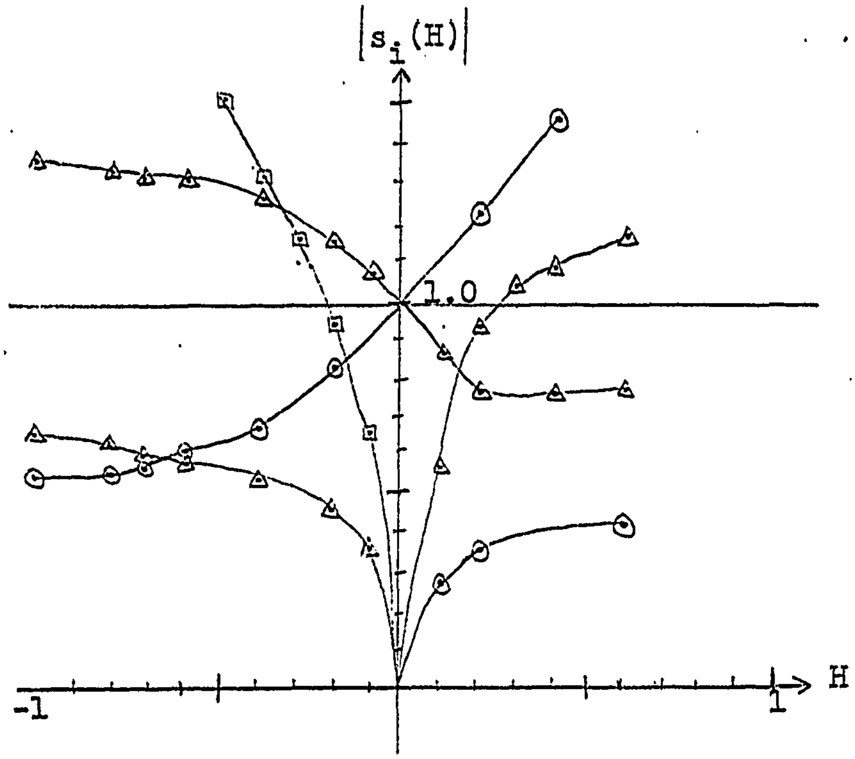

Figure 4. P(EC)

By the use of equation (1.13) and equation (3.28) it follows that for a $P(EC)^2$ implementation, assuming H is sufficiently small,

$$s_2(H) = -\frac{3}{4} + \left(\frac{349}{448}\right)H + O(H^2).$$

For the PE(CE) implementation, using equation (2.24) and assuming that H is sufficiently small,

$$s_2(H) = -\frac{3}{4} + \left(\frac{1265}{768}\right)H + O(H^2).$$

The root-locus plot for the PE(CE) implementation is given in Figure 5, for the $P(EC)^2$ method see Figure 6, and a root-locus plot for the iterated corrector is given in Figure 7.

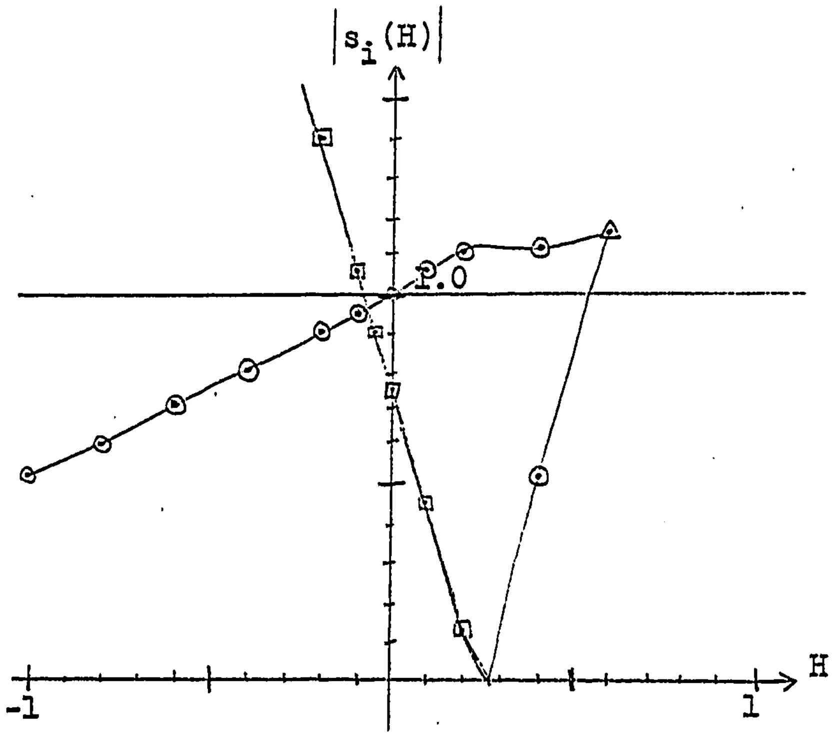

Figure 5. PE(CE)

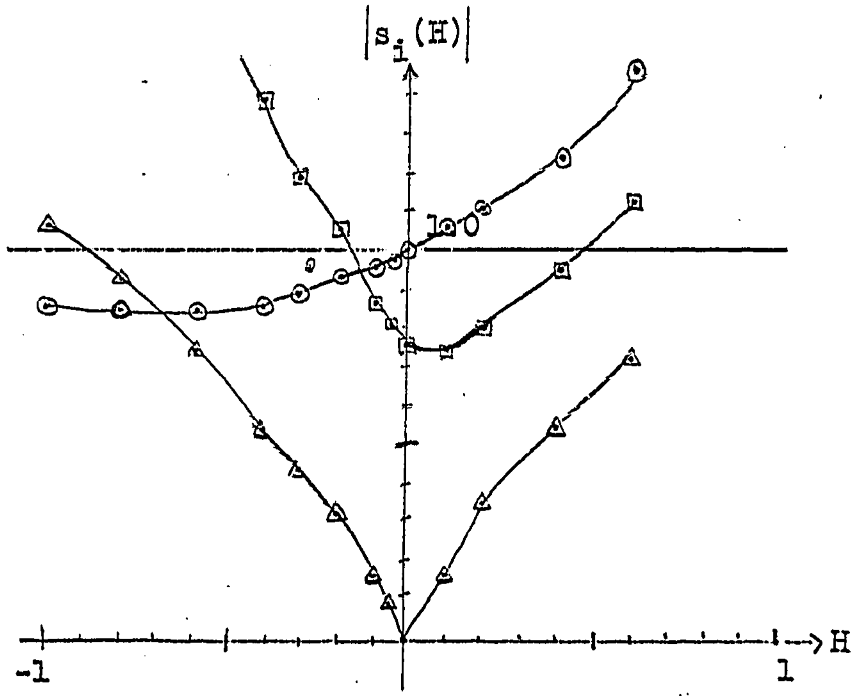

Figure 6. $P(EC)^2$

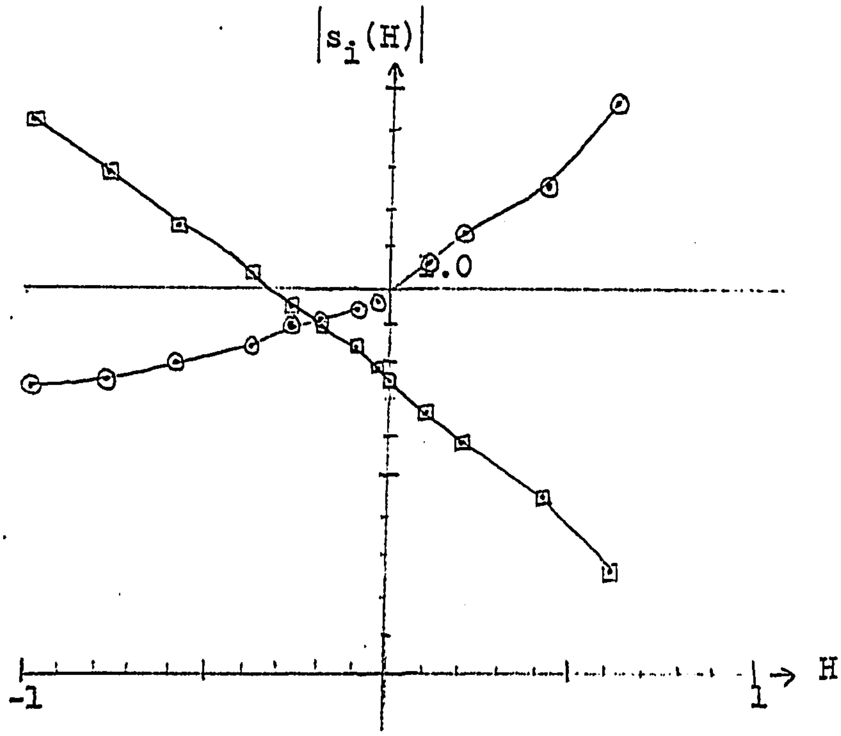

Figure 7. Iterated corrector

The apparent reason for the belief that $P(EC)^m$ methods do not compare favorably with $PE(CE)^m$ methods from the standpoint of stability is a paper by Brown, Riley, and Bennett (1) in which root-locus plots are given for methods using an Adams-Bashforth predictor and an Adams-Moulton corrector for $k = 4$ and various values of m. For such methods a $P(EC)^m$ implementation does not compare favorably with a $PE(CE)^m$ implementation. Observe from the root-locus plots for such methods as given in Appendix A that the stability region is limited by the rapid growth of those roots of the characteristic equation which are approaching zero as H approaches zero. The explanation of this rapid growth is the ill-conditioning of the characteristic equation with respect to the root zero due to the multiplicity of the root. For such methods in a $PE(CE)^m$ implementation zero is a root of multiplicity k-1 and for a $P(EC)^m$ implementation zero is a root of multiplicity 2k-1.

At this point one might ask if there is anything that can be done about the multiplicity of the root at zero for either a $PE(CE)^m$ or a $P(EC)^m$ implementation. In the case of a $PE(CE)^m$ implementation as H approaches zero the characteristic equation approaches $a(r) = 0$ and so one can rid oneself of multiple roots at zero simply by choosing the corrector coefficients so that $a'(0) \neq 0$. In the case of a $P(EC)^m$ implementation as H approaches zero the characteristic equation approaches the equation $r^k a(r) = 0$, so generally zero will be a root of multiplicity p, $p \geq k$. However it is possible to reduce the effect of the multiple root at zero by choosing the predictor and corrector coefficients appropriately in order to change the form of the characteristic equation (3.20). To illustrate this consider the case $k = 3$ using the predictor

$$(6.7) \quad y_n^{(p)} = \sum_{i=1}^{3} a_i^* y_{n-i} + h \sum_{i=1}^{3} b_i^* f(x_{n-i}, y_{n-i})$$

with a_1^*, b_1^*, b_2^*, and b_3^* given as in (6.1) so that (6.7) is of order 3 for arbitrary a_2^* and a_3^*. The corrector to be used is

$$(6.8) \quad y_n^{(c)} = \sum_{i=1}^{3} a_i y_{n-i} + h \left[b_0 f(x_n, y_n^{(p)}) + \sum_{i=1}^{3} b_i f(x_{n-i}, y_{n-i}) \right]$$

with

$$a_1 = 1 - a_2 - a_3 ,$$

$$b_0 = \frac{9 - a_2}{24} ,$$

$$b_1 = \frac{8a_3 + 13a_2 + 19}{24} ,$$

$$b_2 = \frac{32a_3 + 13a_2 - 5}{24} ,$$

and $$b_3 = \frac{8a_3 - a_2 + 1}{24}$$

so that (6.8) is of order 4 for arbitrary a_2 and a_3.

The characteristic equation for a P(EC) method using these is given by (3.20) with $m = 1$ and $k = 3$ and may be written in the form

$$(6.9)\quad P^1(r,H) = r^3\left[r^3 - \sum_{i=1}^{3}(a_i + b_0 H a_i^* + H b_i^*)r^{3-i}\right]$$
$$+ H\Big[(b_1a_1^*-a_1b_1^*)r^4 + (b_2a_1^*-a_1b_2^*+b_1a_2^*-a_2b_1^*)r^3$$
$$+(b_3a_1^*-a_1b_3^*+b_1a_3^*-a_3b_1^*+b_2a_2^*-a_2b_2^*)r^2$$
$$+(b_3a_2^*-a_2b_3^*+b_2a_3^*-a_3b_2^*)r + (b_3a_3^*-a_3b_3^*)\Big].$$

If one now sets the coefficients of the constant and linear terms in (6.9) equal to zero (6.9) is of the form $r^2Q(r,H)$ where $Q(r,H)$ is a polynomial of degree 4 in r. Observe in this form the two zeros at $r = 0$ have no effect on the error $\epsilon_n^{(m)}$ for $H \neq 0$ as may be seen from the form of the solution for $\epsilon_n^{(m)}$ in terms of the roots of the characteristic equation as given by equation (3.21). Thus for $H = 0$, the root zero still has a multiplicity p, $p \geq 3$, but the characteristic equation will no longer be ill-conditioned with respect to this root. The equations necessary to put (6.9) in the form $r^3W(r,H)$ are inconsistent so the best one can do is set the coefficient of r and the constant term equal to zero in (6.9). Solving these equations one obtains the conditions

$$a_2^* = \frac{10a_2 + 18a_3}{a_2 + 2a_3 + 1}\ , \quad a_3^* = \frac{2a_3(8a_3 + 5a_2 - 5)}{(a_2 - 1)(2a_3 + a_2 + 1)}\ .$$

If in addition to this one requires that $a(0) \neq 0$ there is only one root $s_4(H)$ of (6.9) approaching zero as H approaches zero. By the method of undetermined coefficients it follows that for H sufficiently small

$$s_4(H) = 0 + H\left[\frac{9-a_2}{24a_3}\right] - H^2\left[\frac{(9-a_2)^2(4a_3-a_2)}{576a_3^3}\right] + O(H^3).$$

By experimenting it was found that $a_3 = +0.64$ and $a_2 = -3.25a_3$ yields the largest region of absolute stability while maintaining a region of relative stability for $H < 0$. For such a choice of a_3, $P^1(r,0) = 0$ has roots of absolute values 0, +0.8, and 1. The root-locus plot for such an implementation is given in Figure 8.

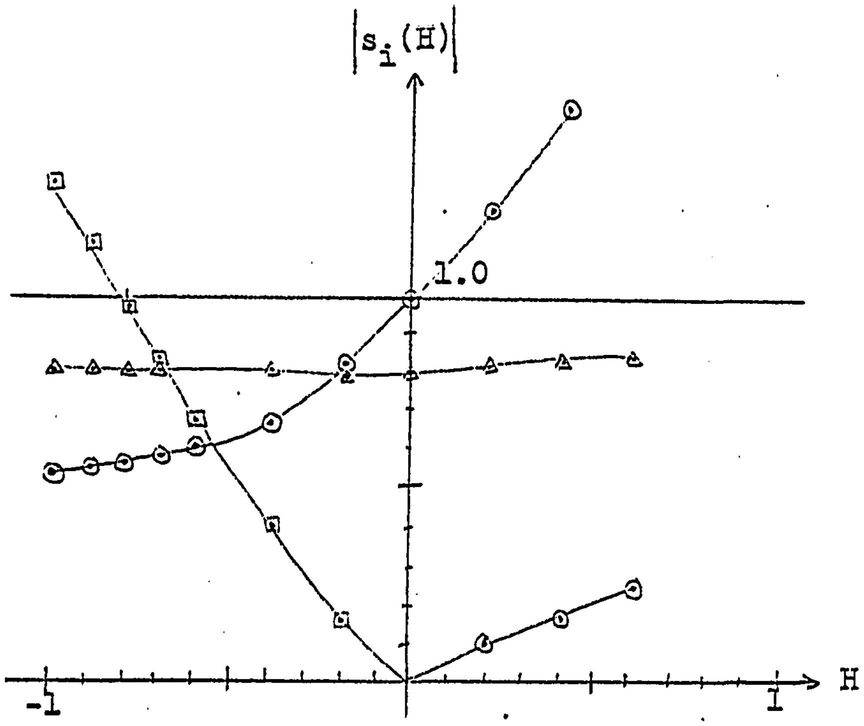

Figure 8.

In recent papers by Klopfenstein and Crane (9) and by Klopfenstein and Millman (10) the question of how does one obtain a predictor-corrector method with the largest possible region of absolute stability for a given implementation has been studied. The method consisted of fixing the corrector to be the Adams-Moulton corrector and then using a gradient technique to select a best possible predictor. The methods obtained and the root-locus plots are given in Appendix A, algorithm 2 and algorithm 3. Observe from a comparison of root-locus plots the method derived above has a larger region of absolute stability than does the method derived by Klopfenstein and Millman (10), algorithm 3 in Appendix A.

An area for future study might be to fix the predictor according to some criterion (such as the one above) and apply a gradient technique to choose the best possible corrector to give the largest possible region of absolute stability.

Another area where more investigation might be fruitful is in a further stability analysis of the generalized predictor-corrector methods. The methods as given in Appendix B have been chosen to be of order 2k+1 and zero stable. One should be able to reduce the order and use the resulting free parameters so as to extend the region of stability.

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APPENDIX A

In this appendix root-locus plots are given for some predictor-corrector algorithms using $PE(CE)^m$ and $P(EC)^m$ implementations with various values of m.

In the figures a circle denotes a positive root, a square denotes a negative root, and a triangle a complex pair.

Algorithm 1 (Adams-Moulton)

$$y_n^{(p)} = y_{n-1} + \frac{h}{24}\left[55y'_{n-1} - 59y'_{n-2} + 37y'_{n-3} - 9y'_{n-4}\right]$$

$$y_n^{(c)} = y_{n-1} + \frac{h}{24}\left[9y_n^{(p)\prime} + 19y'_{n-1} - 5y'_{n-2} + 1y'_{n-3}\right]$$

The root-locus plots for the various implementations are given in Figures 9-13.

Algorithm 2 (Klopfenstein and Crane)

$$y_n^{(p)} = \sum_{i=1}^{4} a_i^* y_{n-i}^{(c)} + h\sum_{i=1}^{4} b_i^* f(x_{n-i}, y_{n-i}^{(c)})$$

$$y_n^{(c)} = y_{n-1}^{(c)} + \frac{h}{24}\Big[9f(x_n, y_n^{(p)}) + 19f(x_{n-1}, y_{n-1}^{(c)}) - 5f(x_{n-2}, y_{n-2}^{(c)}) + 1f(x_{n-3}, y_{n-3}^{(c)})\Big]$$

where

$a_1^* = 1.5476520$ $\quad b_1^* = 2.0022470$

$a_2^* = -1.8675030$ $\quad b_2^* = -2.0316900$

$a_3^* = 2.0172040$ $\quad b_3^* = 1.8186090$

$a_4^* = -0.6973530$ $\quad b_4^* = -0.7143200$

The root-locus plot for this method, designed to have the largest possible region of absolute stability in a PE(CE) implementation, is given in Figure 14.

Algorithm 3 (Klopfenstein and Millman)

$$y_n^{(p)} = \sum_{i=1}^{4} a_i^* y_{n-i}^{(c)} + h \sum_{i=1}^{4} b_i^* f(x_{n-i}, y_{n-i}^{(p)})$$

$$y_n^{(c)} = y_{n-1}^{(c)} + \frac{h}{24}\Big[9f(x_n, y_n^{(p)}) + 19f(x_{n-1}, y_{n-1}^{(p)}) - 5f(x_{n-2}, y_{n-2}^{(p)}) + 1f(x_{n-3}, y_{n-3}^{(p)})\Big]$$

where

$$a_1^* = -0.29 \qquad b_1^* = 2.27$$

$$a_2^* = -15.39 \qquad b_2^* = 6.65$$

$$a_3^* = 12.13 \qquad b_3^* = 13.91$$

$$a_4^* = 4.55 \qquad b_4^* = 0.69$$

The root-locus plot for this method, designed to have the largest possible region of absolute stability in a P(EC) implementation, is given in Figure 15.

Algorithm 4 (Milne)

$$y_n^{(p)} = 1y_{n-4} + \frac{4h}{3}\Big[2y'_{n-1} - 1y'_{n-2} + 2y'_{n-3}\Big]$$

$$y_n^{(c)} = 1y_{n-2} + \frac{h}{3}\Big[y_n^{(p)\prime} + 4y'_{n-1} + 1y'_{n-2}\Big]$$

The root-locus plots for the various implementations are given in Figures 16-20.

Algorithm 5 (Stetter-Milne)

$$y_n^{(p)} = -4y_{n-1}^{(c)} + 5y_{n-2}^{(c)} + 2h\left[2f(x_{n-1},y_{n-1}^{(c)}) + f(x_{n-2},y_{n-2}^{(c)})\right]$$

$$y_n^{(c)} = 1y_{n-2}^{(c)} + \frac{h}{3}\left[f(x_n,y_n^{(p)}) + 4f(x_{n-1},y_{n-1}^{(c)}) + f(x_{n-2},y_{n-2}^{(c)})\right]$$

The root-locus plot for a PE(CE) implementation of this algorithm is given in Figure 21.

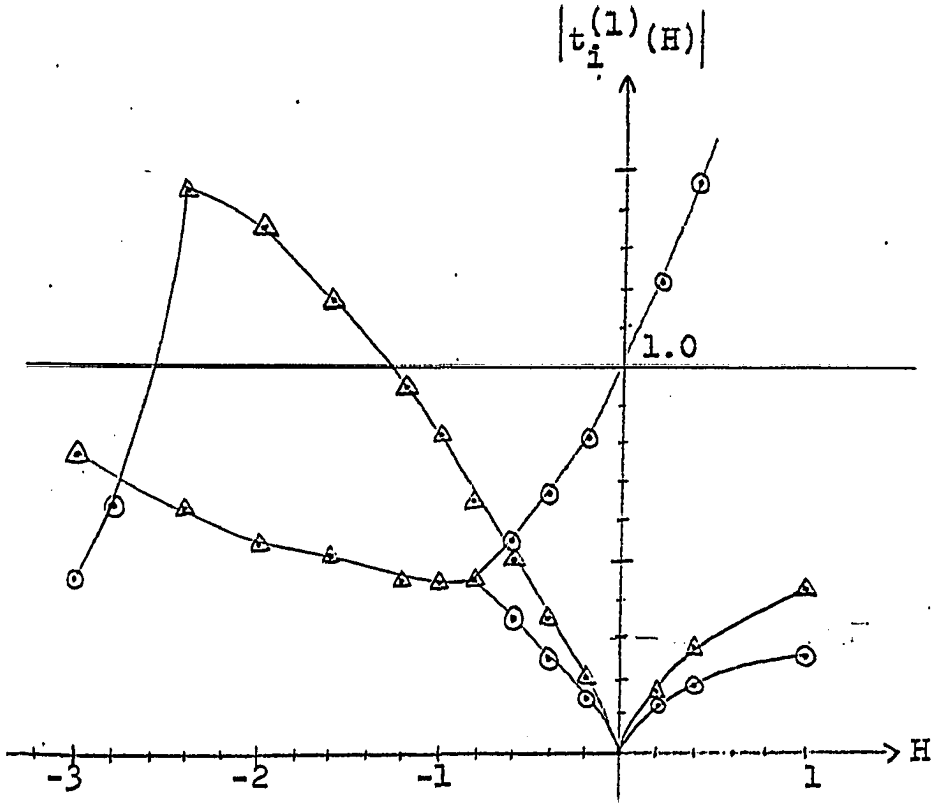

Figure 9. Algorithm 1 PE(CE)

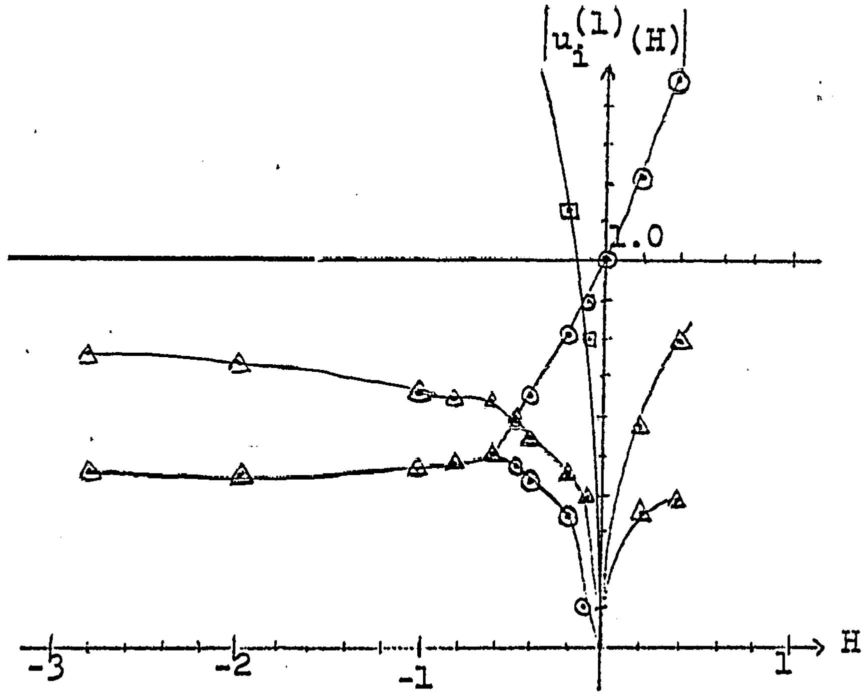

Figure 10. Algorithm 1 P(EC)

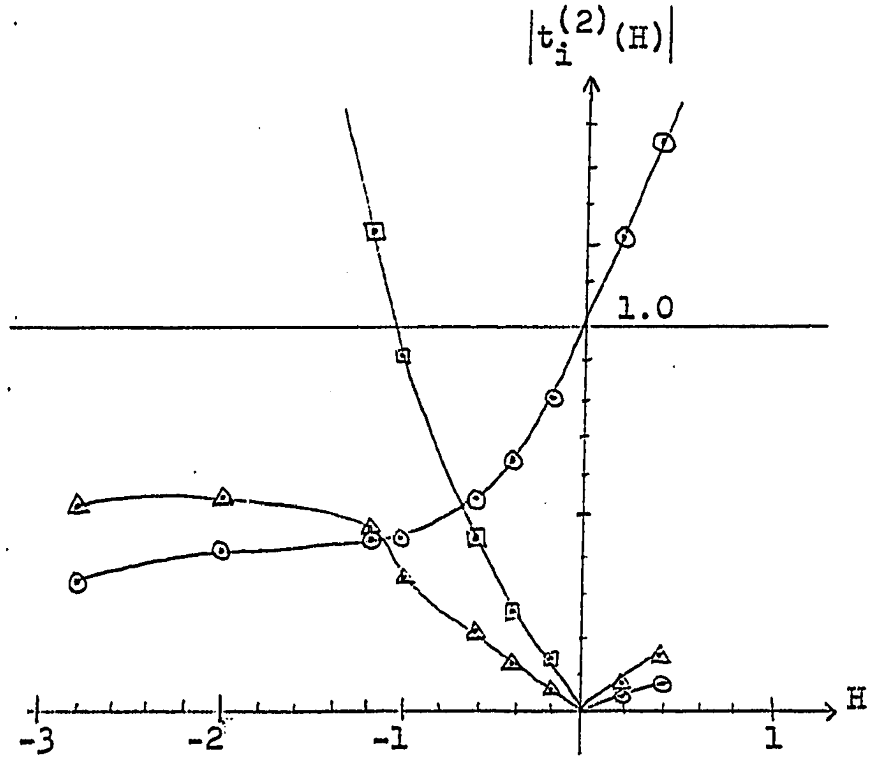

Figure 11. Algorithm 1 $PE(CE)^2$

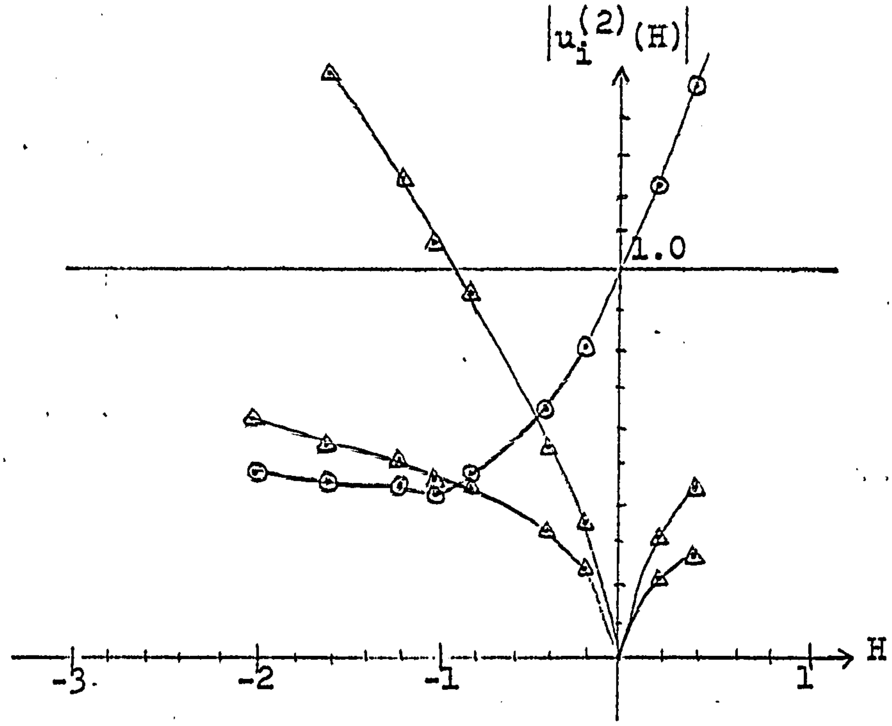

Figure 12. Algorithm 1 $P(EC)^2$

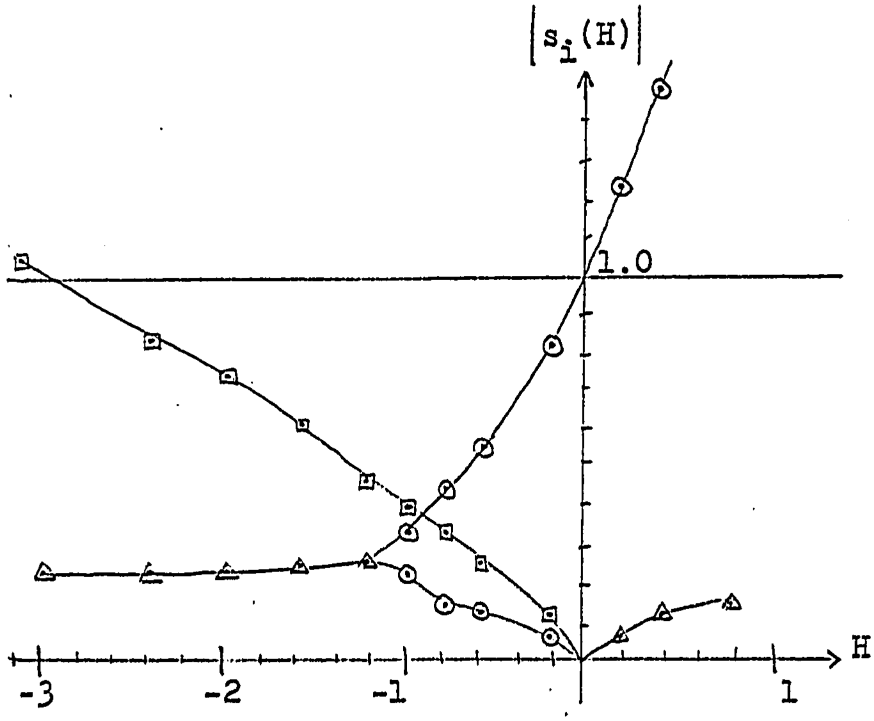

Figure 13. Algorithm 1 Iterated corrector

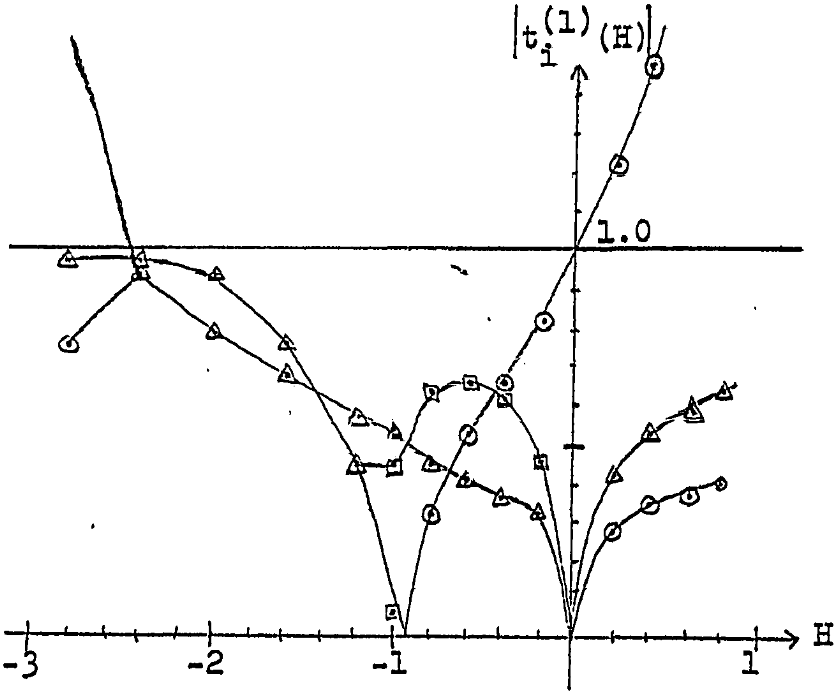

Figure 14. Algorithm 2 PE(CE)

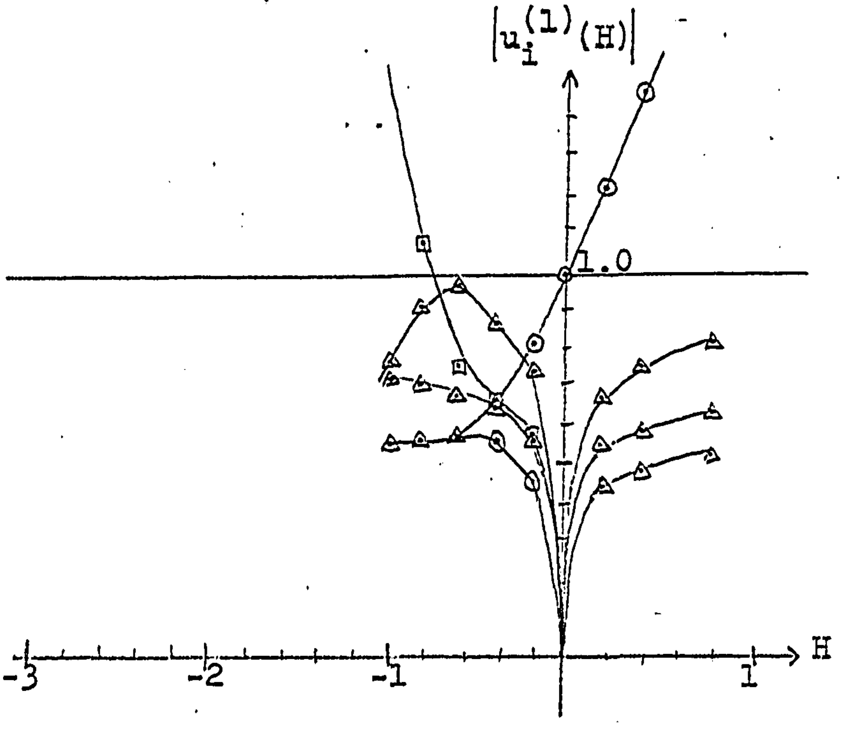

Figure 15. Algorithm 3 P(EC)

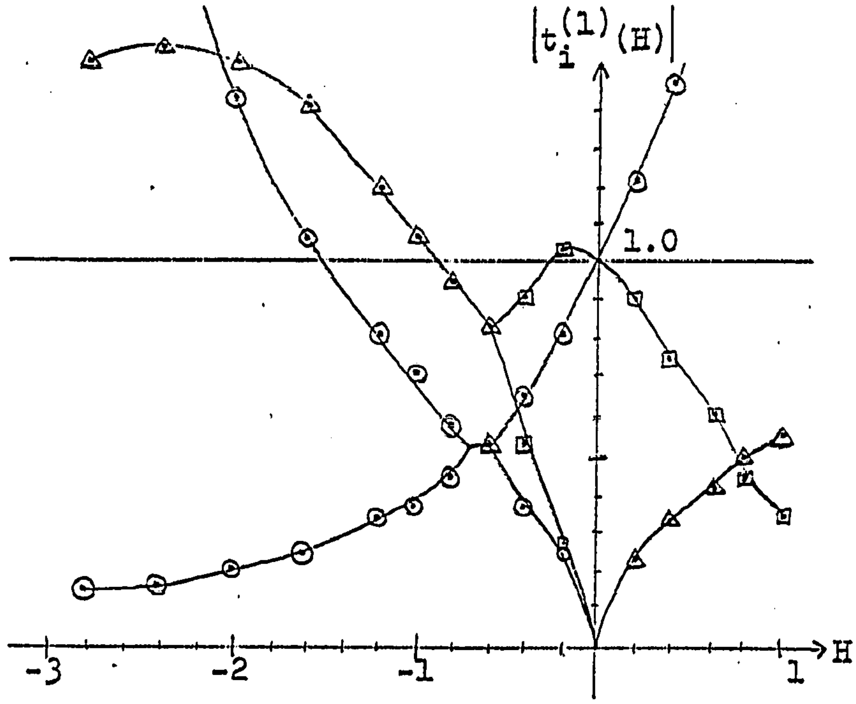

Figure 16. Algorithm 4 PE(CE)

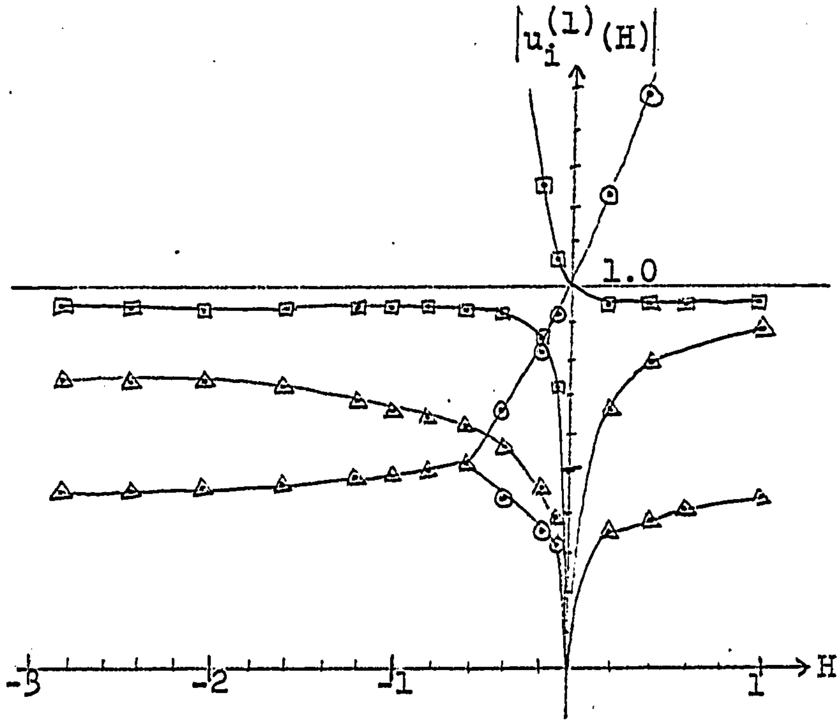

Figure 17. Algorithm 4 P(EC)

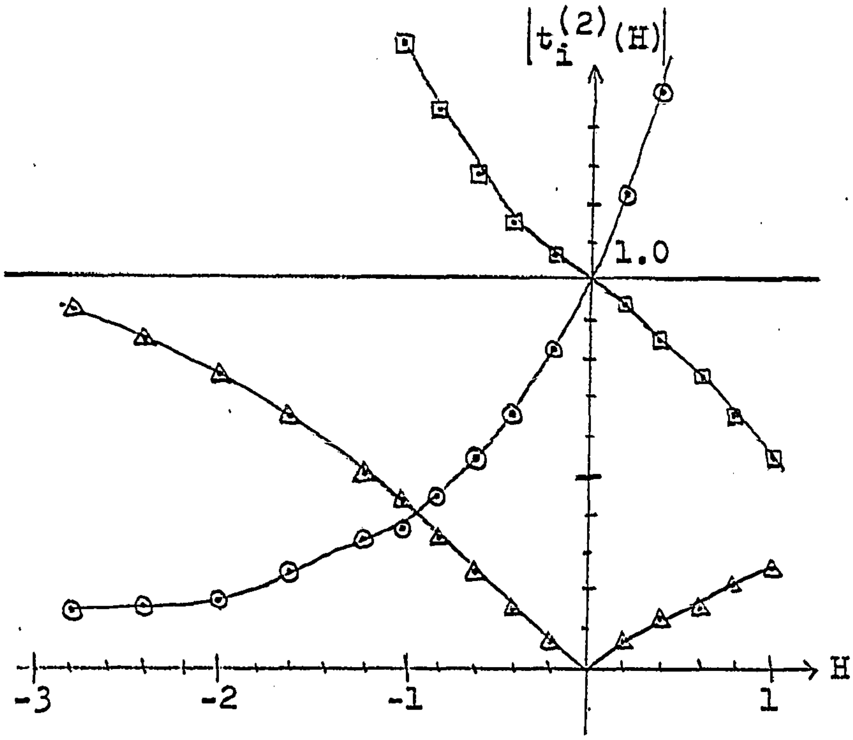

Figure 18. Algorithm 4 $PE(CE)^2$

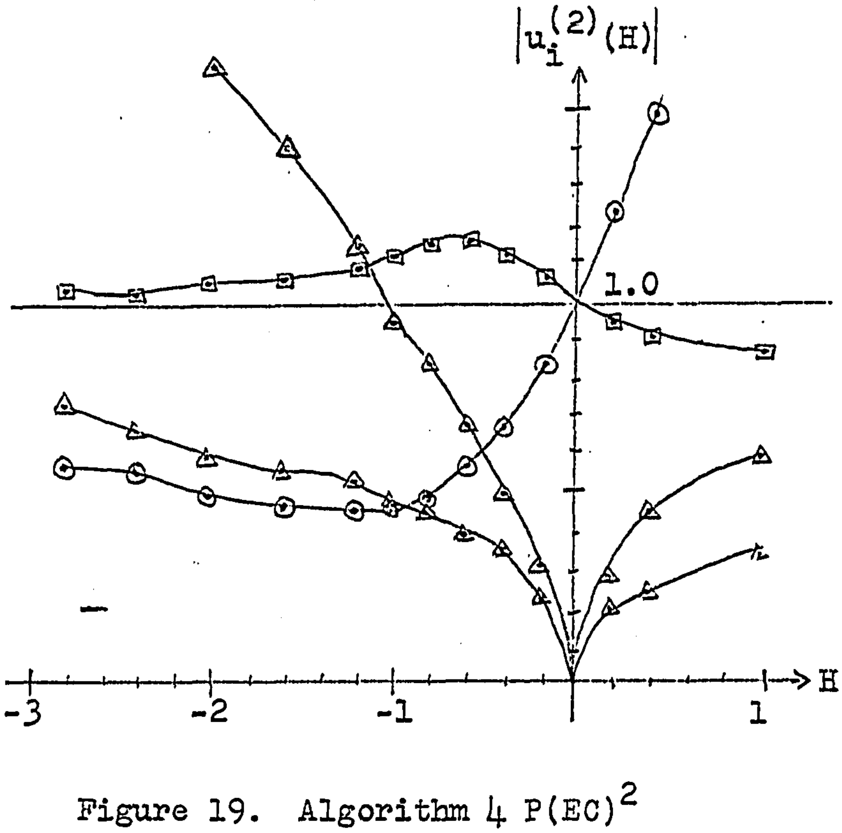

Figure 19. Algorithm 4 $P(EC)^2$

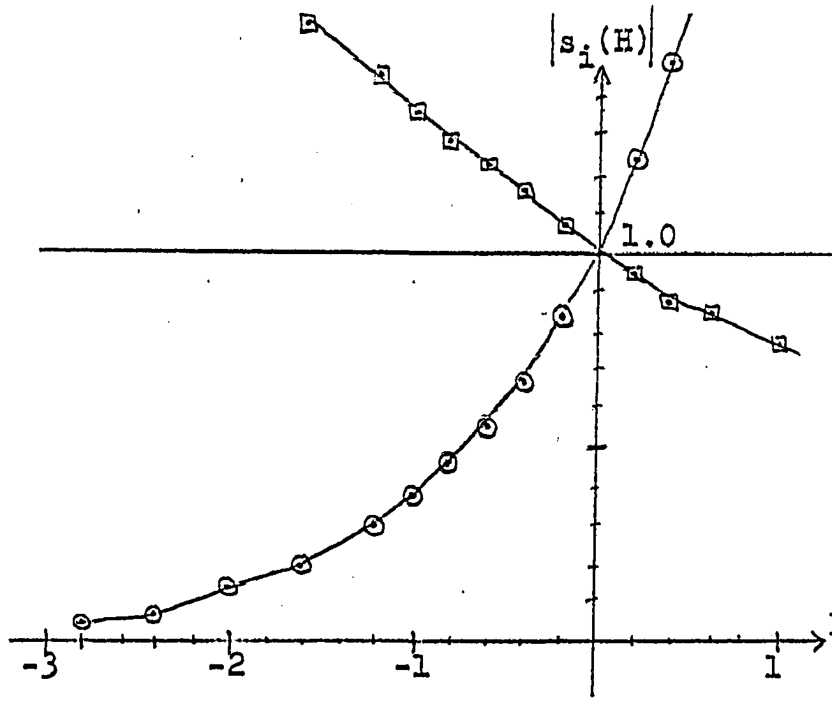

Figure 20. Algorithm 4 Iterated corrector

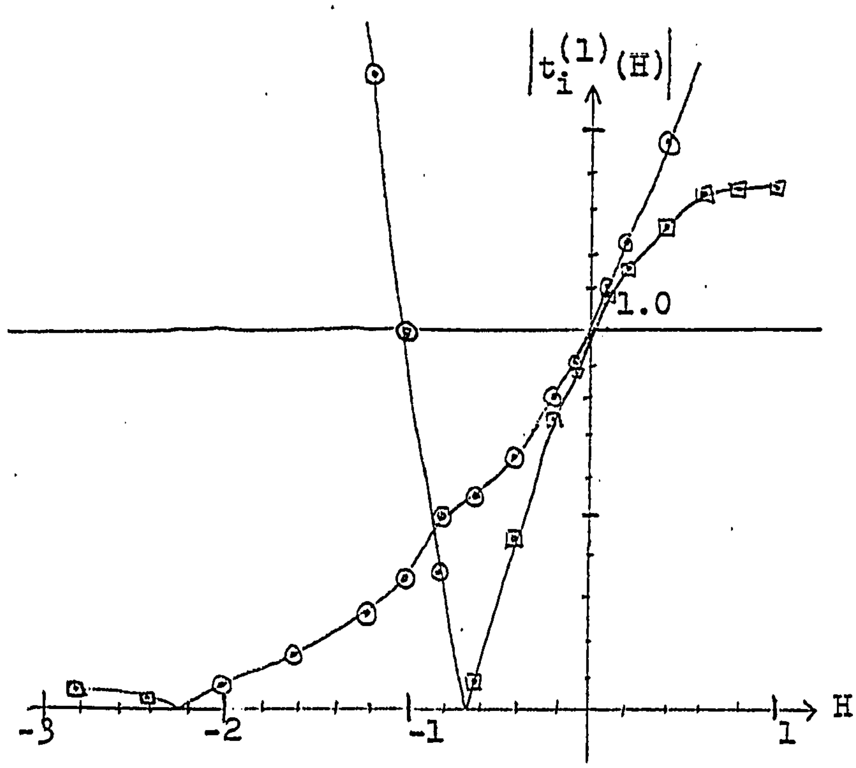

Figure 21. Algorithm 5 PE(CE)

APPENDIX B

In this appendix root-locus plots are given for some generalized predictor-corrector algorithms for both a GPC and a SGPC implementation.

In the figures a circle denotes a positive root, a square denotes a negative root, and a triangle denotes a complex pair of roots.

Algorithm 1

$$y_{n-\frac{1}{2}} = y_{n-1} + \frac{h}{2}\left[f(x_{n-1}, y_{n-1})\right]$$

$$y_n^{(p)} = y_{n-1} + h\left[2f(x_{n-\frac{1}{2}}, y_{n-\frac{1}{2}}) - f(x_{n-1}, y_{n-1})\right]$$

$$y_n^{(c)} = y_{n-1} + \frac{h}{6}\left[4f(x_{n-\frac{1}{2}}, y_{n-\frac{1}{2}}) + f(x_n, y_n^{(p)}) + f(x_{n-1}, y_{n-1})\right]$$

The root-locus plot for a GPC implementation is in Figure 22 and for a SGPC implementation in Figure 23.

Algorithm 2

$$y_{n-\frac{1}{2}} = y_{n-2} + \frac{h}{8}\left[9f(x_{n-1}, y_{n-1}) + 3f(x_{n-2}, y_{n-2})\right]$$

$$y_n^{(p)} = \frac{1}{5}(28y_{n-1} - 23y_{n-2}) + \frac{h}{15}\left[32f(x_{n-\frac{1}{2}}, y_{n-\frac{1}{2}}) - 60f(x_{n-1}, y_{n-1}) - 26f(x_{n-2}, y_{n-2})\right]$$

$$y_n^{(c)} = \frac{1}{31}(32y_{n-1} - y_{n-2}) + \frac{h}{93}\left[64f(x_{n-\frac{1}{2}}, y_{n-\frac{1}{2}}) + 15f(x_n, y_n^{(p)}) + 12f(x_{n-1}, y_{n-1}) - f(x_{n-2}, y_{n-2})\right]$$

The root locus plot for a GPC implementation is given in Figure 24 and for a SGPC in Figure 25.

Algorithm 3

$$y_{n-\frac{1}{2}} = \frac{1}{128}\left(-225y_{n-1} + 200y_{n-2} + 153y_{n-3}\right) + \frac{h}{128}\Big[225f(x_{n-1},y_{n-1}) + 300f(x_{n-2},y_{n-2}) + 45f(x_{n-3},y_{n-3})\Big]$$

$$y_n^{(p)} = \frac{1}{31}(540y_{n-1} - 297y_{n-2} - 212y_{n-3}) + \frac{h}{155}\Big[384f(x_{n-\frac{1}{2}},y_{n-\frac{1}{2}}) - 1395f(x_{n-1},y_{n-1}) - 2130f(x_{n-2},y_{n-2}) - 309f(x_{n-3},y_{n-3})\Big]$$

$$y_n^{(c)} = \frac{1}{617}(783y_{n-1} - 135y_{n-2} - 31y_{n-3}) + \frac{h}{3085}\Big[2304f(x_{n-\frac{1}{2}},y_{n-\frac{1}{2}}) + 465f(x_n,y_n^{(p)}) - 135f(x_{n-1},y_{n-1}) - 495f(x_{n-2},y_{n-2}) - 39f(x_{n-3},y_{n-3})\Big]$$

The root-locus plot for a GPC implementation is in Figure 26 and the root-locus plot for a SGPC implementation is in Figure 27.

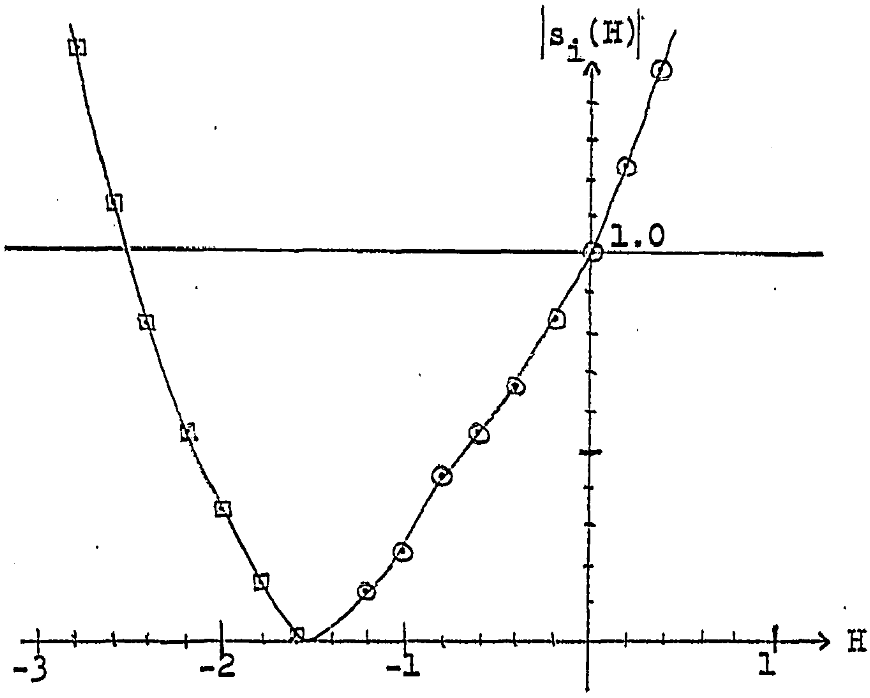

Figure 22. Algorithm 1 GPC

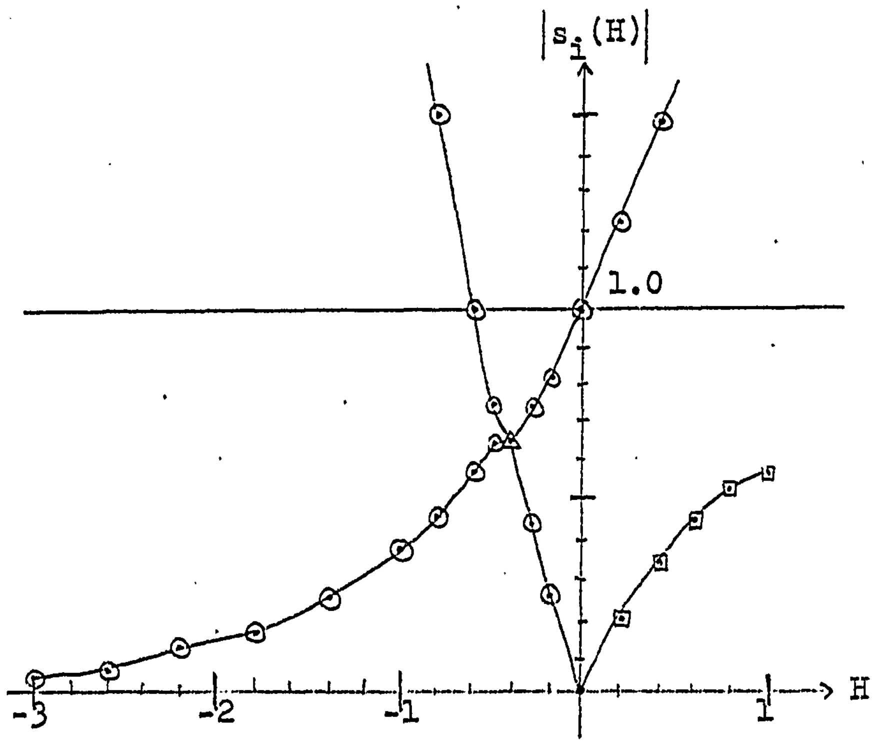

Figure 23. Algorithm 1 SGPC

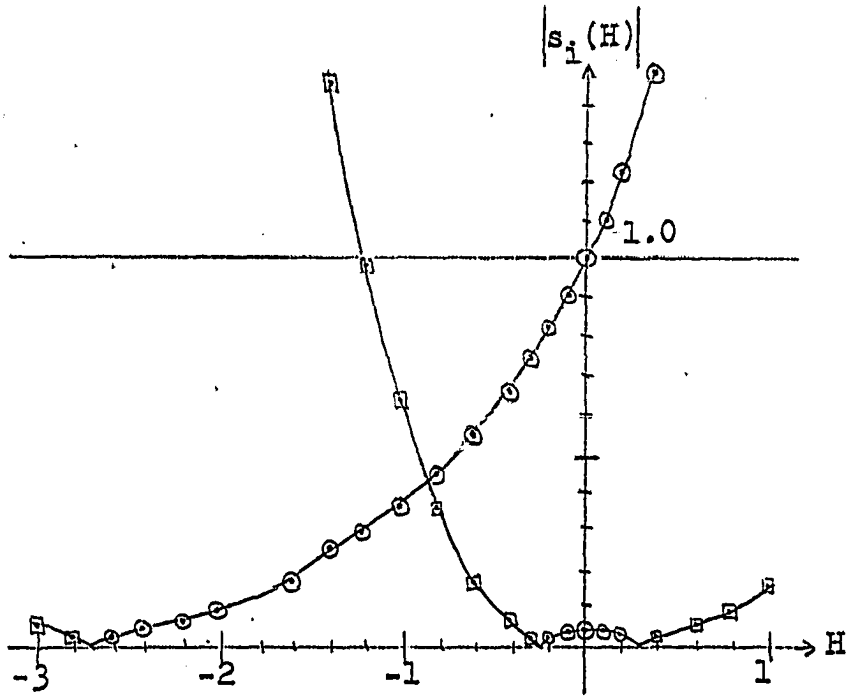

Figure 24. Algorithm 2 GPC

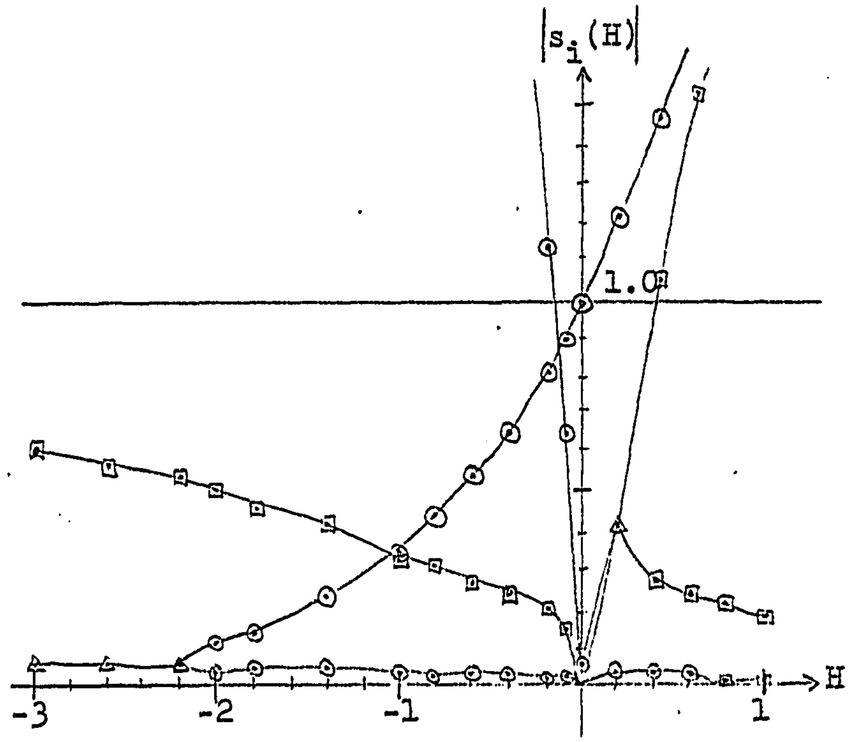

Figure 25. Algorithm 2 SGPC

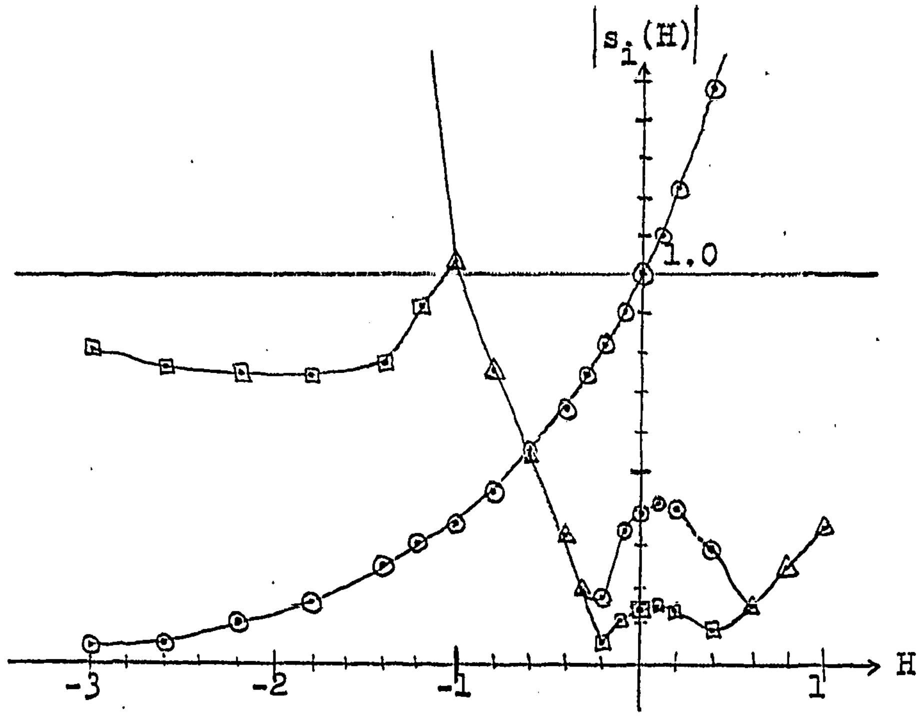

Figure 26. Algorithm 3 GPC

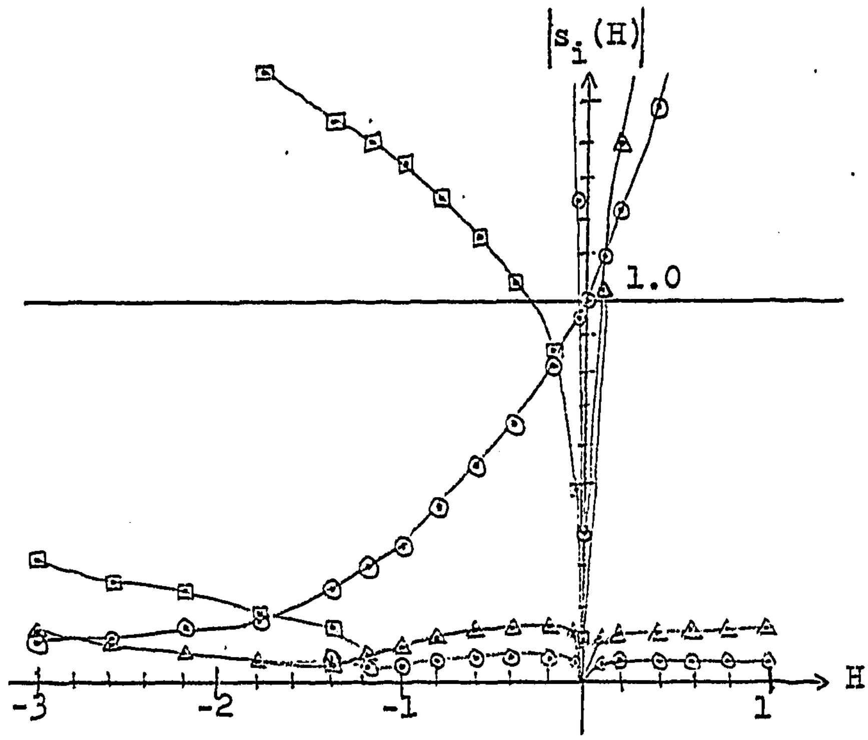

Figure 27. Algorithm 3 SGPC