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Generalized Multistep Methods and Applications to Satellite Orbit Trajectory Computation

James Dyer

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by

James Dyer

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Generalized Multistep Methods and Applications to Satellite Orbit Trajectory Computation

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James Dyer

ABSTRACT

Recent ideas in the theory of multistep methods of solving a differential equation of the first order are extended to methods of solving the special second order equation $y'' = f(x,y)$. A slight modification of the usual multistep method permits a significantly higher order approximation of the difference equation to the differential equation without loss of stability.

The method of constructing the generalized difference equations is based on a quasi-Hermite polynomial approximation. An outline of this theory is given along with some related unsolved problems. This method permits the construction of new classes of stable difference equations with high order of accuracy for solving both a first order differential equation and the above special second order equation.

Some of the new methods have been tested in experiments including the computation of an unperturbed satellite orbit trajectory. Machine time used and accuracy obtained are compared with a standard multistep method.

Although further theoretical and experimental work remains to be done towards the analysis of accumulated round-off error and truncation error in the new methods, it is expected that they can eventually be incorporated into efficient algorithms for solving the general equations of motion of an earth satellite.

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1. Introduction

The research reported in this paper was motivated by a desire to construct new predictor-corrector methods for numerically solving the equations of motion of an earth satellite.

Among many others, the Gauss-Jackson method of solving these equations has been in use for many years with comparatively good results. This method is based in part on a difference equation corresponding to a special differential equation of the second order (with first derivative absent). It appears to owe to this characteristic some of its advantages over other more general numerical integration schemes. It is, moreover, in part a result of applying a particular process of summation to the above-mentioned difference equation. A clear advantage can be shown [5] in certain cases for the summed form in the control of the propagation of round-off error. If arithmetic is carried out with "sufficient" precision, the advantage is not clear. Neither is the advantage of the summed form clear if the so-called process of double precision accumulation is used with the orthodox form. This problem has been very briefly considered here. The results of an experiment are given where the summed and unsummed forms of a simple difference equation are used with and without the relatively inexpensive process of double precision accumulation. With this important exception, difference equations used in the present are unsummed. We are primarily concerned with reducing local truncation (discretization) error.

The order of accuracy (Definitions 3.6 and 3.10) of the correcting difference equations of the Gauss-Jackson method (summed or unsummed), if kth differences

are considered, is k+1. In the last decade much work has been accomplished in the analysis of linear multistep methods for solving differential equations. In 1956, G. Dahlquist showed that the order of a stable k-step method could not exceed k+2 and that the order could be k+2 only in a highly restricted number of cases. Henrici proved [5] this result for a stable second order difference equation, i.e., for a difference equation corresponding to the special equation, $y''=f(x,y)$.

If stability is ignored, a k-step linear difference equation corresponding to a first order differential equation can always be constructed, based on the Hermite interpolating polynomial, with an order of accuracy of 2k+1. (This is, of course, as much as one can normally hope for in an operator derived from an osculatory interpolating polynomial, because we impose conditions on the polynomial and its derivative at k+1 points.) Thus it is seen that a considerable gap exists between the maximum possible order of accuracy of a k-step difference equation and the maximum possible order of accuracy of a stable k-step difference equation. Stability is a necessary condition for convergence [5, p. 217] of a linear multistep method. To close the gap it is necessary to abandon the traditional equally-spaced multistep methods.

In 1964, Gragg and Stetter introduced [4] a class of difference operators for a first order equation which they called generalized multistep predictor-corrector methods. The derivative value is used at exactly one "non-step" point. These methods represent a compromise between Runga-Kutta methods and conventional multistep methods. They use information previous to the last point computed, as do the latter; and derivative evaluations are made part

way through a step, as in the former. The authors prove that convergent generalized methods (of solving a first order equation) with an order of accuracy of 2k+1 exist for $k \leq 4$. Actually they are able to choose the non-step point so that an order of 2k+2 is obtainable. Moreover they show that the methods converge like h^{2k+2} uniformly in a given interval of integration. They provide s:ant computational evidence of the value of their schemes.

Butcher [1], still considering first order differential equations only, developed an elegant method of constructing stable methods with order of accuracy 2k+1 for $k < 8$. His method of construction employed the familiar Hermite interpolating polynomial.

In view of the foregoing remarks, it was felt wise to study multistep operators, generalized in the direction noted above, with respect to a second order equation $y''=f(x,y)$. This problem is interesting in itself; and it was felt that if satisfactory results were achieved, a method of this sort could be incorporated, in analogy with the structure of the Gauss-Jackson algorithm, into one which applied to perturbed satellite motion and could retain its effectiveness for certain types of, if not most, trajectories.

Our difference equations are based on an interpolating polynomial $P(x)$ of degree m such that

$$P(x) = g(x) \qquad x \varepsilon \sigma$$

$$P''(x) = g''(x) \qquad x \varepsilon \tau$$

where σ and τ are subsets of S_K, a set of k+1 equally spaced points. The set $\sigma U \tau$ contains m+1 points, and g is a twice differentiable function.

The uniqueneaa of such a polynomial is in question. It does not depend on the values of g and its second derivative. This problem of the uniqueness of the generalized Hermite interpolating polynomial, even in its simplest form where $\sigma=\tau=S_k$, does not appear to be considered in the literature. Although we are practically concerned only with fitting a function and its second derivative at equally spaced points, there are many associated problems of theoretical interest. One may replace the second derivative in the above problem by the nth derivative, impoae conditions on derivatives of mixed orders, or remove the requirement of the equal spacing of the points.

A theory of generalized Hermitian interpolation was needed. Some results pertaining to this study are given in Section 2. Professor T. S. Motzkin of the University of California, Los Angeles, was consulted during the preparation of this section. A subsequent paper by Professor Motzkin and the author will treat this subject more fully.

The study of conditions for the uniqueness of the generalized Hermitian interpolational polynomial leads to the consideration of the question of independence of certain sets of polynomials, to the definition of generalized Vandermonde determinants and to the study of Hankel determinants associated with the sequence of coefficients in the Maclaurin series for $\log^n(1+x)$.

In Section 3 some of the above theory is used to construct stable high-order k-step methods of numerical integration generalized as above. We are concerned with relatively small k, $k < 8$. The difference operators constructed depend on a parameter θ. Graphs are included indicating the ranges of θ where stability occurs, in some successful cases. The constructive process was used

also to produce stable generalized explicit methods of order of accuracy 2k, not known to exist, for a first order differential equation.

A final section reports the results of simple computational experiments comparing machine time required for the new operators with that required for a standard operator to compute a solution with comparable accuracy. The Appendix contains the coefficients in constructed equations.

Theorem 2.17 is due to T. S. Motzkin. The truth of Lemma 2.3 was demonstrated by R. B. Barrar.

2. Generalized Hermite Interpolation

Our method of constructing a high-order generalized k-step difference equation to solve numerically the equation

$$y'' = f(x,y)$$

requires a generalization of the notion of Hermitian interpolation. The usual k + 1 point second-order Hermite interpolational polynomial P(x) is of degree 3k + 2 and for a twice differentiable function g(x) satisfies

$$P^{(\mu)}(x_i) = g^{(\mu)}(x_i) \qquad \mu = 0,1,2 \qquad i = 0,1,\ldots,k$$

$$g^{(0)} = g \qquad P^{(0)} = P .$$

In general, if higher derivatives appear, all derivatives of lower order are considered. See [11]. Here we wish to fit the function and second derivative and not to impose conditions on the first derivative. We consider here only the case of equally spaced points x_i. The symbol X will always denote the set $\{x_0, x_1, \ldots, x_k\}$.

The generalization of the usual osculatory interpolation consists in defining a polynomial P of degree m, if possible, by imposing m + 1 conditions of the type

$$P^{(\mu)}(x_i) = g^{(\mu)}(x_i)$$

with $0 \leqq \mu \leqq n$ and $0 \leq i \leq k$. For any such set of conditions, a unique polynomial is or is not defined. Conditions for the uniqueness are of interest. One may begin with the following determinantal form [9],

$$
(2.1)\quad \left|\begin{array}{ccccccccc}
p(x) & 1 & x & x^2 & \cdots & x^j & x^{j+1} & \cdots\cdots & x^m \\
g(x_0) & 1 & x_0 & x_0^2 & \cdots & x_0^j & x_0^{j+1} & \cdots\cdots & x_0^m \\
g(x_1) & 1 & x_1 & x_1^2 & \cdots & x_1^j & x_1^{j+1} & \cdots\cdots & x_1^m \\
\hline
g(x_k) & 1 & x_k & x_k^2 & \cdots & x_k^j & x_k^{j+1} & \cdots\cdots & x_k^m \\
g'(x_0) & 0 & 1 & 2x_0 & \cdots & jx_0^{j-1} & (j+1)x_0^j & \cdots\cdots & mx_0^{m-1} \\
\hline
g'(x_k) & 0 & 1 & 2x_k & \cdots & jx_k^{j-1} & (j+1)x_k^j & \cdots\cdots & mx_k^{m-1} \\
\hline\hline
g^{(n)}(x_0) & 0 & 0 & 0 & \cdots & j! & (j+1)!x_0 & \cdots\cdots & \frac{m!}{(m-n)!}x_0^{m-n} \\
\hline
g^{(n)}(x_k) & 0 & 0 & 0 & \cdots & j! & (j+1)!x_k & \cdots\cdots & \frac{m!}{(m-n)!}x^{m-n}
\end{array}\right|
$$

defining the usual Hermite interpolating polynomial $P(x)$. Here $m=(n+1)(k+1)-1$. For $m < (n+1)(k+1)-1$, the more general determinantal form is obtained from the above form by eliminating rows corresponding to conditions not imposed and eliminating an equal number of columns on the right. The coefficients of the interpolating polynomial P are uniquely determined if and only if the fundamental

determinant which results from deleting the first row and first column from the general form (2.1) is different from zero. We call this determinant a generalized Vandermonde determinant. Some special cases (Hermite interpolation) have been carefully considered. They satisfy the following condition:

> If a derivative condition is given at a point, then conditions on all lower derivatives are given at that point.

It is well known that uniqueness occurs in these cases.

In this paper we are interested primarily in another special case, that resulting from the imposition of a condition on the polynomial and its nth derivative at all k + 1 points ($n \leq k + 1$). The resulting generalized Vandermonde determinant is

$$(2.2)\quad D(k,n,X) = |M(k,n,X)| = \begin{vmatrix} 1 & x_0 & x_0^2 & \cdots\cdots & x_0^{2k+1} \\ 1 & x_1 & x_1^2 & \cdots\cdots & x_1^{2k+1} \\ \hline 1 & x_k & x_k^2 & \cdots\cdots & x_k^{2k+1} \\ \sigma_0 x_0^n & \sigma_1 x_0^{1-n} & \sigma_2 x_0^{2-n} & \cdots\cdots & \sigma_{2k+1} x_0^{2k+1-n} \\ \sigma_0 x_1^n & \sigma_1 x_1^{1-n} & \sigma_2 x_1^{2-n} & \cdots\cdots & \sigma_{2k+1} x_1^{2k+1-n} \\ \hline \sigma_0 x_k^n & \sigma_1 x_k^{1-n} & \sigma_2 x_k^{1-n} & \cdots\cdots & \sigma_{2k+1} x_k^{2k+1-n} \end{vmatrix}$$

where $\sigma_i = i(i-1)(i-2)\ldots(i-n+1)$. If $M(k,n,X)$ is non-singular, a uniquely defined interpolating polynomial may be associated with it. Denote this polynomial by $P(k,n,x)$. The following lemma is true more generally. For this report only the case $n = 2$ is of interest.

Lemma 2.3. Let $m = 2k + 1$. $M(k,2,X)$ is non-singular if and only if the polynomials $(x + x_0)^m$, $(x + x_1)^m, \ldots, (x + x_k)^m$, $m(m-1)(x + x_0)^{m-2}$, $m(m-1)(x + x_1)^{m-2}$, $\ldots, m(m-1)(x + x_k)^{m-2}$ are linearly independent.

Proof. Denote the polynomials as ordered by $P_1(x), P_2(x), P_3(x), \ldots, P_{m+1}(x)$. Expand $P_i(x)$ in powers of x:

$$P_i(x) = \sum_{j=1}^{j=m+1} a_{ij} x^{m-j+1} \qquad i = 1,2,\ldots,m+1$$

and consider the matrix (a_{ij}). For $\lambda > 1$ entries $a_{1,\lambda+1}, a_{2,\lambda+1}, \ldots$ in the $(\lambda+1)$th column are:

$$\binom{m}{\lambda} x_0^\lambda, \binom{m}{\lambda} x_1^\lambda, \ldots\ldots, \binom{m}{\lambda} x_k^\lambda, m(m-1)\binom{m-2}{\lambda-2} x_0^{\lambda-2},$$

$$m(m-1)\binom{m-2}{\lambda-2} x_1^{\lambda-2}, \ldots\ldots, m(m-1)\binom{m-2}{\lambda-2} x_k^{\lambda-2}.$$

Division now by $\binom{m}{\lambda}$ gives the $(\lambda + 1)$th column of $M(k,2,X)$. For the first two columns the result is obvious.

Define the translation operator T_a on the vector space V_n of nth degree polynomials

(2.4) $\quad T_a P(x) = P(x+a) \qquad P \varepsilon V_n$

Obviously this linear translation is non-singular. (Apply it to the natural basis.) Define for real a:

$$X+a = \{x_0+a,\ x_1+a,\ \ldots,\ x_k+a\} \quad .$$

Corollary. $|M(k,\ 2,\ X)| \neq 0 \iff |M(k,\ 2,\ X+a)| \neq 0$.

Proof. Because T_a is non-singular, the set $P_1,\ P_2,\ \ldots,\ P_{m+1}$ of the lemma is linearly independent if and only if the set $T_aP_1,\ T_aP_2,\ \ldots,\ T_aP_{m+1}$ is linearly independent.

The non-singularity (singularity) of M(k, 2, X) is invariant under translation by a real number. Because of this property, we may sometimes write M(k, n) instead of M(k, n, X). It is understood that there are k+1 equally spaced points and that the rows of M(k,n) are ordered to correspond to conditions on the interpolating polynomial and its nth derivative as in (2.2). The following fact is obvious:

Lemma 2.5. M(k, k+1) is non-singular. M(k, n) is singular if $n > k+1$.

Corollary. There exists a unique polynomial of degree 2k+1 which vanishes along with its (k+1)th derivative at k+1 equally spaced points for all $k \geq 0$.

It is clear that a matrix $A = (a_{ij})$ of the form

$$(2.6)\qquad \begin{pmatrix} a_{11} & 0 & a_{13} & 0 & a_{15} & 0 & - & - \\ 0 & a_{22} & 0 & a_{24} & 0 & a_{26} & - & - \\ a_{31} & 0 & a_{33} & 0 & a_{35} & 0 & - & - \\ 0 & a_{42} & 0 & a_{44} & 0 & a_{40} & - & - \\ - & - & - & - & - & - & - & - \\ - & - & - & - & - & - & - & - \end{pmatrix}$$

can, by elementary row operations, be triangularized in the usual manner giving

$$(2.7)\qquad \begin{pmatrix} b_{11} & 0 & b_{13} & 0 & b_{15} & 0 & - & - \\ 0 & b_{22} & 0 & b_{24} & 0 & b_{26} & - & - \\ 0 & 0 & b_{33} & 0 & b_{35} & 0 & - & - \\ 0 & 0 & 0 & b_{44} & 0 & b_{46} & - & - \\ - & - & - & - & - & - & - & - \\ - & - & - & - & - & - & - & - \end{pmatrix} .$$

<u>Theorem 2.8.</u> $M(k, n)$ is singular if both the following conditions are satisfied:

1) n even, $n > 0$

2) k even, $k \geq 0$.

<u>Proof:</u> Consider first the case $k = n = 2$. We have equally spaced points x_0, x_1, x_2. By the corollary to Lemma 2.3 we may take $x_1=0$. We use the notation $M \sim N$ to state the fact that matrices M and N are row-equivalent.

Now it is clear that

$$M(2,2,X) \sim \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & -1 & 1 & -1 \\ 0 & 0 & 2 & 0 & 0 & 0 \\ 0 & 0 & 2 & 6 & 12 & 20 \\ 0 & 0 & 2 & -6 & 12 & -20 \end{pmatrix}$$

and that

$$M(2,2,X) \sim \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 6 & 0 & 20 \\ 0 & 0 & 2 & 0 & 12 & 0 \\ 0 & 0 & 2 & 0 & 0 & 0 \end{pmatrix} . \tag{2.9}$$

Triangularizing the matrix found by deleting the last row and last column from the matrix on the right as in the statement preceding the theorem, we have

$$M(2,2,X) \sim \begin{pmatrix} b_{11} & 0 & b_{13} & 0 & b_{15} & 0 \\ 0 & b_{22} & 0 & b_{24} & 0 & b_{26} \\ 0 & 0 & b_{33} & 0 & b_{35} & 0 \\ 0 & 0 & 0 & b_{44} & 0 & b_{46} \\ 0 & 0 & 0 & 0 & b_{55} & 0 \\ 0 & 0 & 2 & 0 & 0 & 0 \end{pmatrix} .$$

Now it is apparent that M is row-equivalent to a triangular matrix with a zero on the diagonal, i.e., the last row can be annihilated by row operations, using interchanges if necessary. Clearly, for even k, we may take the interpolating set X to include the origin and the remaining members of X to be symmetrically distributed about the origin. If in addition n is even, a form analogous to (2.6) can be achieved, i.e., for elements a_{ij} not in the last row, i+j odd implies $a_{ij}=0$. The entries in the final row can then be systematically reduced to zero.

The above theorem shows that a polynomial of degree 2k+1 is not uniquely determined by its values and the values of its nth derivative at k+1 equally spaced points if k is even and n is even.

M(1,2) is non-singular by Lemma 2.5. It can be verified by hand computation that M(3,2) is also non-singular. Machine computations of $|M(k,2)|$ for k=5,7,9 indicate that the matrices are non-singular in support of the following conjecture:

Conjecture 2.10. There exists a unique polynomial of degree 2k+1 which vanishes along with its second derivative at k+1 equally spaced points if k is odd.

A further condition for the uniqueness.

It has been noted that a generalized Hermitian interpolating polynomial is unique if and only the associated generalized Vandermonde determinant is different from zero. We have also given a condition for the non-singularity of M(k,2) involving the polynomials $\{T^i x^{2k+1}, T^i x^{2k-1}; i=0,1,2,\ldots,k\}$. We now derive a third necessary and sufficient condition for the uniqueness of P(k,2,x).

The linear transformation $T=T_a$ on the space V_p of polynomials of degree p has been previously defined (2.4). Another linear transformation $D=D_p$, the differentiation operator, can also be defined on this space. See [10]. Let $T=T_1$. D is uniquely given as a polynomial in T-I.

$$D(T-I) = (T-I) - 1/2(T-I)^2 + 1/3(T-I)^3 - \ldots + \frac{(-1)^{p-1}}{p}(T-I)^p \quad .$$

<u>Lemma 2.11</u>. If $g(x) \epsilon V_p$ and if $g(T)x^p=0$, then g(x) is the zero polynomial.

<u>Proof</u>. The independence of the polynomials x^p, Tx^p, T^2x^p, ..., T^px^p is a consequence of the fact that the usual Vandermonde determinant is different from zero. The lemma follows.

<u>Corollary</u>. Let $g_i(x)\epsilon V_p$ $i=0,1,2,\ldots,p$. Denote by S this set of polynomials. Denote by S_x the set $g_i(T)x^p$ $i=0,2,\ldots,p$. Then S is independent if and only if S_x is independent.

It is clear that the <u>nth</u> order differentiation operator $D_p^n = D^n = D^n(T-I)$ is given by polynomial multiplication.

$$D^n(T-I) = \sum_{i=0}^{i=p} d_i^{(n)}(T-I)^i \quad .$$

For future reference we note that the sequence $\{d_i^{(2)}: \ i=0,1,2,\ldots\}$ begins $0, 0, 1, -1, \frac{11}{12}, -\frac{5}{6}, \frac{137}{180}, -\frac{7}{10}, \ldots$.

We let $m=2k+1$ and consider the question of the independence of the polynomials

$$\begin{array}{cc} x^m & D^2(T-I)x^m \\ T\,x^m & T\,D^2(T-I)x^m \\ T^2x^m & T^2D^2(T-I)x^m \\ \vdots & \vdots \\ T^kx^m & T^kD^2(T-I)x^m \end{array} \quad .$$

One may write the T^j as polynomials in T-I and equivalently consider the independence of the set

$$\begin{array}{cc} x^m & D^2(T-I)x^m \\ (T-I)x^m & (T-I)D^2(T-I)x^m \\ (T-I)^2x^m & (T-I)^2D^2(T-I)x^m \\ \vdots & \vdots \\ (T-I)^kx^m & (T-I)^kD^2(T-I)x^m \end{array} \quad .$$

Finally using the fact that $(T-I)^j=0$ for $j > m$, and using the corollary to Lemma 2.11, we consider the independence of the polynomials in the operator T-I in the latter set above. Writing $\lambda=T-I$ we write the matrix of coefficients of these polynomials relative to the basis $1, \lambda, \lambda^2, \ldots, \lambda^{2k+1}$. Because the above discussion is not restricted to the second derivative, let $n \leq k+1$ and write

$$(2.12) \qquad D^n(T-I) = d_n^{(n)}(T-I)^n + d_{n+1}^{(n)}(T-I)^{n+1} + \ldots + d_{2k+1}^{(n)}(T-1)^{2k+1} \ .$$

The following matrix is then written for such n, (here $n < k$) and d_j is written for $d_j^{(n)}$ for convenience. The composition of the matrix is clear. The

k+1 x k+1 matrix in the lower left corner is always the identity. That in the lower right is zero. The first non-zero element in the first row appears under λ^{n+k}, in the second row under λ^{n+k-1}, and in the (k+1)th row under λ^{n} .

(2.13)

	1	λ	λ^2	$\dots$	λ^{n-1}	λ^n	λ^{n+1}	$\dots$	λ^{k-3}	λ^{k-2}	λ^{k-1}	λ^k	λ^{k+1}	$\dots$	λ^{n+k-2}	λ^{n+k-1}	λ^{n+k}	λ^{n+k+1}	$\dots$	λ^{2k}	λ^{2k+1}
$\lambda^k D^n(\lambda)$	0	0	0	$\dots$	0	0	0	$\dots$	0	0	0	0	0	$\dots$	0	0	d_n	d_{n+1}	$\dots$	d_k	d_{k+1}
$\lambda^{k-1} D^n(\lambda)$	0	0	0	$\dots$	0	0	0	$\dots$	0	0	0	0	0	$\dots$	0	d_n	d_{n+1}	d_{n+2}	$\dots$	d_{k+1}	d_{k+2}
$\lambda^{k-2} D^n(\lambda)$	0	0	0	$\dots$	0	0	0	$\dots$	0	0	0	0	0	$\dots$	d_n	d_{n+1}	d_{n+2}	d_{n+3}	$\dots$	d_{k+2}	d_{k+3}
$\vdots$																					
$\lambda D^n(\lambda)$	0	0	0	$\dots$	0	0	d_n	$\dots$	d_{k-4}	d_{k-3}	d_{k-2}	d_{k-1}	d_k	$\dots$	d_{n+k-3}	d_{n+k-2}	d_{n+k-1}	d_{n+k}	$\dots$	d_{2k-1}	d_{2k}
$D^n(\lambda)$	0	0	0	$\dots$	0	d_n	d_{n+1}	$\dots$	d_{k-3}	d_{k-2}	d_{k-1}	d_k	d_{k+1}	$\dots$	d_{n+k-2}	d_{n+k-1}	d_{n+k}	d_{n+k+1}	$\dots$	d_{2k}	d_{2k+1}
λ^k	0	0	0	$\dots$	0	0	0	$\dots$	0	0	0	1	0	$\dots$	0	0	0	0	$\dots$	0	0
λ^{k-1}	0	0	0	$\dots$	0	0	0	$\dots$	0	0	1	0	0	$\dots$	0	0	0	0	$\dots$	0	0
λ^{k-2}	0	0	0	$\dots$	0	0	0	$\dots$	0	1	0	0	0	$\dots$	0	0	0	0	$\dots$	0	0
λ^{k-3}	0	0	0	$\dots$	0	0	0	$\dots$	1	0	0	0	0	$\dots$	0	0	0	0	$\dots$	0	0
$\vdots$																					
λ^2	0	0	0	$\dots$	0	0	0	$\dots$	0	0	0	0	0	$\dots$	0	0	0	0	$\dots$	0	0
λ	0	1	0	$\dots$	0	0	0	$\dots$	0	0	0	0	0	$\dots$	0	0	0	0	$\dots$	0	0
1	1	0	0	$\dots$	0	0	0	$\dots$	0	0	0	0	0	$\dots$	0	0	0	0	$\dots$	0	0

Denote this array by $\overline{M}(k,n)$. From the form of the matrix of dimension $2k+1 \times 2k+1$ in the lower left hand quarter of $\overline{M}(k,n)$, it is evident that the latter matrix is non-singular if and only if the matrix $\overline{N}(k,n)$, given by the array below, is non-singular.

$$
\begin{array}{lcccccccccc}
 & \lambda^{k+1} & \lambda^{k+2} & \ldots\lambda^{n+k-2} & \lambda^{n+k-1} & \lambda^{n+k} & \lambda^{n+k+1} & \ldots\lambda^{2k} & \lambda^{2k+1} \\
\lambda^{k}D^{n}(\lambda) & 0 & 0 & \ldots\ 0 & 0 & d_n & d_{n+1} & \ldots\ d_k & d_{k+1} \\
\lambda^{k-1}D^{n}(\lambda) & 0 & 0 & \ldots\ 0 & d_n & d_{n+1} & d_{n+2} & \ldots\ d_{k+1} & d_{k+2} \\
\lambda^{k-2}D^{n}(\lambda) & 0 & d_n & \ldots\ d_n & d_{n+1} & d_{n+2} & d_{n+3} & \ldots\ d_{k+2} & d_{k+3} \\
\hline
\lambda^{n+2}D^{n}(\lambda) & 0 & d_n & \ldots\ d_k & d_{k+1} & d_{k+2} & d_{k+3} & \ldots\ d_{2k-n} & d_{2k-n+1} \\
\lambda^{n-1}D^{n}(\lambda) & d_n & d_{n+1} & \ldots\ d_{k+1} & d_{k+2} & d_{k+3} & d_{k+4} & \ldots\ d_{2k-n+1} & d_{2k-n+2} \\
\hline
\lambda D^{n}(\lambda) & d_k & d_{k+1} & \ldots\ d_{n+k-3} & d_{n+k-1} & d_{n+k-2} & d_{n+k} & \ldots\ d_{2k-1} & d_{2k} \\
D^{n}(\lambda) & d_{k+1} & d_{k+2} & \ldots\ d_{n+k-2} & d_{n+k-1} & d_{n+k} & d_{n+k-1} & \ldots\ d_{2k} & d_{2k+1}
\end{array}
\tag{2.14}
$$

<u>Theorem 2.15</u>. $M(k,n)$ is non-singular if and only if $\overline{N}(k,n)$ is non-singular.

Some special cases are given below concerning the case of current interest, i.e., $n=2$. We take all entries to be positive and call the resulting matrix $N(k,n)$. Clearly $|N(k,2)| = (-1)^{k+1}|\overline{N}(k,2)|$.

$$|N(1,2)| = \begin{vmatrix} 0 & 1 \\ 1 & 1 \end{vmatrix}$$

$$|N(2,2)| = \begin{vmatrix} 0 & 1 & 1 \\ 1 & 1 & 11/12 \\ 1 & 11/12 & 5/6 \end{vmatrix} = 0$$

$$|N(3,2)| = \begin{vmatrix} 0 & 1 & 1 & 11/12 \\ 1 & 1 & 11/12 & 5/6 \\ 1 & 11/12 & 5/6 & 137/180 \\ 11/12 & 5/6 & 137/180 & 7/10 \end{vmatrix} = (1/240)^2$$

The matrix $\overline{N}(k,n)$ can be determined in a slightly different manner. Define the sets

$$\sigma = \{1, \lambda, \lambda^2, \ldots, \lambda^k\}$$
$$\sigma^{(n)} = \{D^n(\lambda), \lambda D^n(\lambda), \lambda^2 D^n(\lambda), \ldots, \lambda^k D^n(\lambda)\}$$

and let S and $S^{(n)}$ be the vector spaces generated over the real numbers by σ and $\sigma^{(n)}$ respectively. The sets σ and $\sigma^{(n)}$ are both independent sets in V_{2k+1}. For the set $\sigma \cup \sigma^{(n)}$ to be independent, the formula

$$\dim(S) + \dim(S^{(n)}) = \dim(S+S^{(n)}) + \dim(S \cap S^{(n)}) ,$$

relating the dimensions of two subspaces to the dimensions of their join and intersection, shows that it is necessary and sufficient that $S \cap S^{(n)} = \phi$.

A necessary and sufficient condition for this is that $(a_0+a_1\lambda+a_2\lambda^2+\ldots+a_k\lambda^k)D^n(\lambda)$ be a kth degree polynomial for no kth degree polynomial $a_0+a_1\lambda+a_2\lambda^2+\ldots+a_k\lambda^k$. Conditions on the coefficients a_i give the necessary and sufficient condition that $\overline{N}(k,n)$ be non-singular.

Associated with any sequence $\{a_i\}$ are the so-called Hankel determinants H_j^i :

$$H_j^i = \begin{vmatrix} a_i & a_{i+1} & \cdots & a_{i+j-1} \\ a_{i+1} & a_{i+2} & \cdots & a_{i+j} \\ \hline \hline a_{i+j-1} & a_{i+j} & \cdots & a_{i+2j-2} \end{vmatrix} .$$

If we write $\log^n(1+x) = \sum_{i=0}^{\infty} a_i x^i$ to define the sequence $\{a_i\}$ then the following is evidently true.

Theorem. 2.16. $M(k,n)$ is non-singular and $P(k,n,x)$ is uniquely determined if and only if H_{k+1}^1 is non-zero.

One can prove a general theorem about Hankel determinants which has an application in the theory of generalized Hermitian interpolation.

Theorem. 2.17. Let H_j^i be the Hankel determinants associated with a sequence $a_0, a_1, a_2, \ldots$. Let k be an integer greater than 2 and assume $H_{k-1}^0 = 0$ and $H_{k-2}^1 \neq 0$. Then

$$H_k^0 = \frac{H_{k-2}^0}{(H_{k-2}^1)^2} (H_{k-1}^1)^2 .$$

Proof. Denote by A_j^i the array associated with the Hankel determinant H_j^i. Let ${}_\ell C_j^i$ be the ℓth column of A_j^i and let ${}_\ell A_j^i$ be the matrix formed by replacing the ℓth column of A_j^i by ${}_1C_j^{i-1}$. Let ${}_\ell H_j^i$ be used to denote $|{}_\ell A_j^i|$.

The columns ${}_\ell C_{k-1}^0$ of A_{k-1}^0 are linearly dependent by hypothesis. Thus the equation

$$(2.18) \qquad \sum_{\ell=1}^{\ell=k-1} \alpha_\ell \, {}_\ell C_{k-1}^0 = \phi$$

may be solved non-trivially. Because $H_{k-2}^1 \neq 0$ a solution to (2.18) is clearly

$$(2.19) \qquad \alpha_1 = -H_{k-2}^1 \qquad \alpha_\ell = {}_{\ell-1}H_{k-2}^1 \qquad \ell=2,3,\ldots,k-1 .$$

Replacing the first column of A_k^0 by this combination of its first k-1 columns and computing H_k^0 in terms of the entries of the last row of the resulting matrix and their cofactors, we have

$$H_k^0 = -\frac{1}{\alpha_1} H \, H_{k-1}^1$$

where $H = \sum_{i=1}^{i=k-1} \alpha_i a_{k-2+i} = \sum_{i=1}^{i=k-1} a_{k-2+i} \, {}_iH_{k-2}^1$. Consider the k+1 x k+1 matrix

$$\tilde{A} = \begin{pmatrix} a_0 & a_1 & \cdots & a_{k-3} & a_{k-1} \\ a_1 & a_2 & \cdots & a_{k-2} & a_k \\ a_2 & a_3 & \cdots & a_{k-1} & a_{k+1} \\ - & - & - & - & - \\ - & - & - & - & - \\ a_{k-2} & a_{k-1} & \cdots & a_{2k-5} & a_{2k-3} \end{pmatrix} .$$

It is clear that

$$H = (-1)^{k+1} |\tilde{A}| \ .$$

Let the columns of A be called ${}_iC$ $i=1,2,\ldots,k-1$ and list the columns of $\tilde{A}$, A^1_{k-1}, A^0_{k-1} for convenience.

Columns of $\tilde{A}$: ${}_1C$, ${}_2C$, ${}_3C$, ... ${}_{k-3}C$, ${}_{k-2}C$, ${}_{k-1}C$

Columns of A^1_{k-1}: ${}_2C$, ${}_3C$, ${}_4C$, ... ${}_{k-2}C$, ${}_{k-1}C^0_{k-1}$, ${}_{k-1}C$

Columns of A^0_{k-1}: ${}_1C$, ${}_2C$, ${}_3C$, ... ${}_{k-3}C$, ${}_{k-2}C$, ${}_{k-1}C^0_{k-1}$

It follows from these sequences of columns and from the equations (2.18), (2.19) expressing the linear dependence of the columns of A^0_{k-1}, that

$$|\tilde{A}| = (-1)^k \frac{\alpha_{k-1}}{\alpha_1} H^1_{k-1}$$

or

$$|\tilde{A}| = (-1)^{k-1} \frac{H^0_{k-2}}{H^1_{k-2}} H^1_{k-1}$$

and hence that

$$H^0_k = \frac{H^0_{k-2}}{(H^1_{k-2})^2} (H^1_{k-1})^2 \ .$$

The proof is complete.

It is clear, of course, that under the obvious hypotheses we have proved

$$(2.20) \qquad H_k^n = \frac{H_{k-2}^n}{(H_{k-2}^{n+1})^2} (H_{k-1}^{n+1})^2 ,$$

which is really no more general.

Let the sequence a_0, a_1, a_2, ... be defined by

$$\log(1+x) = \sum_{\ell=0}^{\infty} \alpha_\ell x^\ell .$$

From the uniqueness of the usual Hermite interpolating polynomial one knows that M(k, 1, X) is non-singular for all k. If the H_j^i are associated with the above sequence, it follows from Theorem 2.16 that $H_j^1 \neq 0$ for j=1,2,3,... .

If the sequence a_0, a_1, a_2, ... is defined by

$$\log^2(1+x) = \sum_{\ell=0}^{\infty} \alpha_\ell x^\ell$$

and the H_j^i are associated with this sequence, then we know from Theorem 2.8 and Theorem 2.15 that $H_j^1=0$ for j=3,5,7, ... We wish knowledge of H_j^1 for even j. $H_j^1 \neq 0$ for j=2,4. These determinants appear as $|N(1,2)|$ and $|N(3,2)|$ on page 21. As a corollary to the last theorem we have:

<u>Corollary</u>. With the last definition of the H_j^i, if $H_k^2 \neq 0$ for $k \geq 4$ then $H_k^1 \neq 0$ for k=2,4,6,... and for such k,M(k-1,2) is non-singular and P(k-1,2,x) is uniquely defined.

3. Existence and Construction of Operators

Consider a differentiable function $y(x)$ and the differential equation

$$y' = g(x,y). \tag{3.1}$$

Most k-step methods of solving (3.1) are specializations of the formula

$$\alpha_k y_{\nu-k} + \ldots + \alpha_1 y_{\nu-1} + \alpha_0 y_\nu = h(\beta_k g_{\nu-k} + \ldots + \beta_1 g_{\nu-1} + \beta_0 g_\nu) \tag{3.2}$$

where $y_j = y(x_j)$ and $g_j = g(x_j, y_j)$. One may associate with (3.2) the difference operator

$$\begin{aligned} L_h[y(x)] = {} & \alpha_k y(x-kh) + \alpha_{k-1} y(x-(k-1)h) + \ldots + \alpha_1 y(x-h) + \alpha_0 y(x) \\ & - h\{\beta_k y'(x-kh) + \beta_{k-1} y(x-(k-1)h) + \ldots + \beta_1 y'(x-h) + \beta_0 y'(x)\}. \end{aligned} \tag{3.3}$$

L_h operates on any differentiable function. Assume that $y(x)$ possesses an indefinite number of derivatives. Each term in the right member of (3.3) can then be expanded by Taylor's formula to give:

$$L_h[y(x)] = C_0 y(x) + C_1 h y^1(x) + \ldots + C_q h^q y^{(q)}(x) + \ldots \tag{3.4}$$

The coefficients are given by

$$\begin{aligned} C_0 &= \alpha_0 + \alpha_1 + \ldots + \alpha_k \\ C_1 &= -[\alpha_1 + \alpha\alpha_2 + \ldots + k\alpha_k - (\beta_0 + \beta_1 + \ldots + \beta_k)] \\ &- \\ C_q &= (-1)^q[1/q!(\alpha_1 + 2^q\alpha_2 + \ldots + k^q\alpha_k) - \frac{1}{(q-1)!}(\beta_1 + 2^{q-1}\beta_2 + \ldots + k^{q-1}\beta_k)] \end{aligned} \tag{3.5}$$

for $q=2,3,\ldots$.

Definition 3.6. The difference operator (3.3) is of order of accuracy p if $C_0=C_1=\ldots=C_p=0$ and $C_{p+1} \neq 0$.

The order of a difference operator is the first crude measure of its accuracy. Among methods of the same accuracy p, the coefficient C_{p+1}, which of course is independent of the choice of function y(x), may be considered as a finer measure of the accuracy. The coefficient must be suitably normalized because it can be made as small as one wishes by multiplying (3.2) by a suitably small constant.

It is clear from the definition of C_i that the order of an operator is p if and only if $L_h[y(x)] = 0$ whenever y is a polynomial of degree not exceeding p, but is non-zero for some polynomial of degree p+1.

There is a theory [5] similar to the above if one begins with a special second order differential equation of the form

$$y'' = g(x,y). \tag{3.7}$$

We give here only the difference equation

$$\alpha_k y_{\nu-k} + \ldots + \alpha_1 y_{\nu-1} + \alpha_0 y_\nu = h^2(\beta_k g_{\nu-k} + \ldots + \beta_1 g_{\nu-1} + \beta_0 g_\nu), \tag{3.8}$$

the difference operator

$$\begin{aligned} L_{h^2}[y(x)] = {} & \alpha_k y(x-kh) + \alpha_{k-1} y(x-(k-1)h) + \ldots + \alpha_1 y(x-h) + \alpha_0 y(x) \\ & - h^2\{\beta_k y''(x-kh) + \beta_{k-1} y''(x-(k-1)h) + \ldots + \beta_1 y''(x-h) + \beta_0 y''(x)\}, \end{aligned} \tag{3.9}$$

and the corresponding definition of the order of accuracy, after expanding, as above.

Definition 3.10. The difference operator L_{h^2} is said to be of order of accuracy p if $C_0 = C_1 = \ldots = C_{p+1} = 0$ and $C_{p+2} \neq 0$.

It is again true that the order can determined from a knowledge of polynomials annihilated by L_{h^2} and also that C_{p+2} suitably normalized here can be used as a finer gauge of accuracy among operators of order p.

Method of Construction.

Associate with the left side of equation (3.2) the polynomial

$$\rho(\xi) = \alpha_{k+1} + \alpha_k \xi + \alpha_{k-1}\xi^2 + \ldots + \alpha_0 \xi^{k+1} \quad . \tag{3.11}$$

Definition 3.12. A multistep method defined by (3.2) is said to be stable if and only if all roots of $\rho(\xi)=0$ lie within or on the unit circle and a root of modulus 1 has multiplicity at most 1.

This definition applies to (3.8) also. Here the multiplicity of a root of modulus 1 must not exceed 2. A definition of stability in general is clear.

Definition 3.13. A multistep method is said to be consistent if it has order at least 1.

Stability and consistency together are necessary and sufficient conditions for methods defined by (3.2) and (3.8) to converge. The concepts of stability and consistency extend themselves to the slightly modified multistep methods considered here. We are concerned now with the construction of methods with order of accuracy approaching 2k and stable in the above sense.

In 1956 G. Dahlquist proved (see [1], [4], [5] for appropriate reference) that the order of a stable k-step method as defined by (3.12) cannot exceed k+2 and can be equal to k+2 in only fairly unusual circumstances. Henrici extended this result [5] to apply to methods for second order equations. Thus a method of order greater than k+2 is divergent. Gragg and Stetter [4] and Butcher [1] apparently independently showed that by including a term $\beta g_{\nu-\theta}$ where $x_{\nu-\theta}=x_\nu-\theta h$ in equation (3.2) it is possible, for an appropriate value of θ in the interval $0 < \theta < 1$ and for small k, to determine the coefficients so that the resulting method is stable and has order of accuracy 2k+1 (sometimes 2k+2). This theory was applied only to a method for first order equations. Gragg and Stetter proved the assertion for $k \leq 4$, and exhibited some implicit and explicit methods for such k. They also proved that, under reasonable hypotheses on the accuracy of the starting values and the differentiability of the solution function, the pth order methods produced true pth order convergence uniformly on a fixed interval of integration. Butcher used the usual Hermite interpolation theory to construct high-order generalized implicit methods for first order equations and for $k < 8$.

The present author has used as a point of departure the work described above. To extend the theory to apply to multistep methods of solving a special second order equation $y''=g(x,y)$ in a constructive way, the Hermite interpolational theory needed to be generalized in a direction apparently not before considered. Thus was partially accomplished in Section 1. This extended theory enables us to define for $k < 8$ high-order implicit and explicit stable generalized k-step methods of solving the second order equation mentioned above as well as explicit methods for $3 < k < 8$ for first order equations.

Consider again a set S_k of k+1 equally spaced points $x_{\nu-k}, x_{\nu-k+1}, \ldots, x_\nu$ on the line and a sufficiently often differentiable function f(x). Under certain conditions we have already shown the existence of a unique generalized Hermitian interpolating polynomial P(x) = P(k,n,x) such that

$$(3.13) \qquad \left.\begin{aligned} P(x) &= f(x) \\ P^{(n)} &= f^{(n)}(x) \end{aligned}\right\} \quad x \in S_k \quad .$$

It is possible to generalize still further. Let m be an integer such that $0 \leq m < 2k+1$. Let σ, and τ be subsets of S_k with the set $\sigma \cup \tau$ containing m+1 points. A unique polynomial $P(x) = P(\sigma, \tau, k, n, x)$ of degree m again exists such that

$$(3.14) \qquad \begin{aligned} P(x) &= f(x) & x \in \sigma \\ P^{(n)}(x) &= f^{(n)}(x) & x \in \tau \end{aligned}$$

if and only if the fundamental determinant is different from zero. Although we have not extended theoretical results to this more general setting, computation of the determinant by machine shows that this uniqueness "often" occurs.

Recall the general determinantal form derived from (2.1) by eliminating rows corresponding to conditions not imposed and by eliminating a corresponding number of columns on the right, reducing the degree of the polynomial. The determinant is an m<u>th</u> degree polynomial, Q(x). If the fundamental determinant, Δ, is not zero, $Q(x) \equiv 0$, and we can compute it in terms of the entries in the first column and their cofactors. Dividing by Δ, we have

$$(3.15) \qquad P(x) \equiv \sum_{x_i \varepsilon \sigma} h_i(x) f(x_i) + \sum_{x_i \varepsilon \tau} \bar{h}_i(x) f^{(n)}(x_i) \ .$$

The functions h_i, $\bar{h}_i$ are polynomials of degree m and depend on σ, τ, k, and n. They generalize the usual Hermitian interpolational functions of the first and second kind respectively. For n=1 and $\sigma=\tau=S_k$ it is well known that they have a simple analytical form. (This is true, of course, also when all derivatives less than or equal to the nth appear in a form analogous to (3.15)). In general, however, no simple form was found for the functions $h_i(\sigma, \tau, k, n, x)$ and $\bar{h}_i(\sigma, \tau, k, n, x)$. For this study they were computed from the determinantal form.

Most familiar methods of numerical integration are obtained as a result of polynomial approximation. We note without proof that by proper choice of n, σ, τ, x one may obtain from (3.15) all Adams type difference equations among a variety of other methods. For example, by specializing

$$x = x_\nu$$
$$n = 1$$
$$\sigma = \{x_{\nu-1}\}$$
$$\tau = \{x_{\nu-1}, x_{\nu-2}, \ldots, x_{\nu-k}\}$$

we have the first order explicit Adams formula--the k-step Adams-Bashforth equation which is usually derived by integrating both sides of (3.1) between proper limits.

Definition: The method defined by (3.2) or (3.8) is called explicit if $\beta_0=0$ and is called implicit if $\beta_0 \neq 0$.

This notation will also be applied to methods involving a "non-step" point about to be described.

The formulas

$$\alpha_k y_{\nu-k}+\alpha_{k-1}y_{\nu-k+1}+\ldots+\alpha_0 y_\nu = h^n(\beta_k g_{\nu-k}+\beta_{k-1}g_{\nu-k+1}+\ldots+\beta_\theta g_{\nu-\theta}+\beta_0 g_\nu)$$

(3.16)

$$g_j = g(x_j,y_j) \qquad x_{\nu-\theta} = x_\nu-\theta h \qquad 0 < \theta < 1$$

for numerically solving the equation $y^{(n)}=g(x,y)$ are similar to the usual formulas with the exception of the term $h^n\beta_\theta g_{\nu-\theta}$ on the right. We wish to determine the coefficients α_i, β_i, β_θ so that (3.16) is stable and has order of accuracy approaching 2k for $k < 8$. If (3.16) is rewritten

$$(3.17) \qquad h^n\beta g_{\nu-\theta} = \sum \alpha_i y_{\nu-i} - h^n \sum \beta_i g_{\nu-i} ,$$

one sees that if $\alpha_0= 1$, the remaining coefficients can be determined from the nth derivatives of the Hermitian interpolational functions $h(\sigma, \tau, k, n, x)$, $\bar{h}(\sigma, \tau, k, n, x)$. Before considering the question of stability, note that by setting $\tau=S_k-x_\nu$ one eliminates the condition

$$P(x_\nu) = y^{(n)}(x_\nu) .$$

The term involving the derivative at x_ν is absent from (3.16). Thus we may choose $\beta_0=0$ and an explicit method is constructed. The order of accuracy of the method is reduced by 1.

It remains to examine the question of stability of the method. Writing θ as independent variable instead of x, consider the equation

$$(3.18) \qquad \sum_{i=0}^{i=k} \alpha_i(\theta)\xi^i = 0 \qquad 0 < \theta < 1 \ .$$

Let $\xi_1(\theta)$, $\xi_2(\theta)$, ..., $\xi_k(\theta)$ be the roots of (3.18) and let n=2 in (3.16). Consistency of the method implies that (3.18) always has a double root $\xi_1=\xi_2=1$. Define the function

$$N(\theta) = \max_{2<i} |\xi_i(\theta)| \ .$$

Of interest are the θ such that $N(\theta) < 1$. Motivated by the concept of strong stability [5] only such θ are admitted. The process as described above will fail if the generalized Hermite interpolating polynomial P resulting from a definition of subsets σ and τ is not unique. As seen, this always happens if k is even and $\sigma=\tau=S_k$. If a unique polynomial is not defined, we may redefine σ and τ and try again, although we wish to maximize the number of conditions in order to maximize the order of the resulting operator.

The process also fails if

$$N(\theta) = N_{\sigma,\tau}(\theta) \geq 1 \qquad 0 \leq \theta \leq 1 \ .$$

In this case we may again redefine τ and try again.

Figures 1 through 5 show the function $N(\theta)$ in some successful cases where stable high-order operators were found. For $n=1,2$ (applying to a first or special second order equation respectively) the curves are labelled by the step number k and the set $\bar{\tau}=S_k-\tau$ which is the set of interpolation points at which the derivative condition is omitted. For example, $k=4$, $\bar{\tau}=\{x_\nu\}$ labels the function $N(\theta)$ associated with the highest order explicit θ-family of operators of the type considered. Labels omitting $\bar{\tau}$ are meant to imply $\bar{\tau}=\emptyset$. Again it is remarked that in most cases considered we have relied on an approximate machine computation as a criterion for the uniqueness of P. In all cases $\sigma=S_k$.

Although usually of a lower order of accuracy, we have included explicit methods in the investigation because they require only one prediction, $y_{\nu-\theta}$, whereas implicit methods require two, y_ν and $y_{\nu-\theta}$. It was felt that they could be of some practical value. We are concerned primarily with solving a special second order differential equation; however, we have given some explicit methods for solving a first order equation because they have not been included in the literature.

The error constant $C(\theta)$ associated with the θ-family of integration methods is a smooth function of θ. If $N(\theta) < 1$ in some interval $\theta_0 \leq \theta \leq \theta_1$, it is reasonable to attempt to find a value of θ in the above interval which minimizes $|C|$. That problem has not been considered here because the resulting reduction in error would usually be of a lower order than the one we are principally investigating. Results of computation, however, show that the error constants $C(\theta)$ associated with the maximal order 4-step explicit θ-family of operators for

a special second order differential equation (curve $k=4$; Fig. 4) can be made to vanish in the range of stability by an appropriate choice of θ. Thus another complete order of accuracy can be attained in this case (see Table 1 below). We have not determined that particular value of θ.

A tabulation of the maximal order of accuracy observed for stable k-step operators constructed in the investigation is given below for $k < 8$. Although column two is well known [1], it is included here for completeness.

TABLE 1

Orders of Accuracy

	for $y'=f(x,y)$		for $y''=g(x,y)$	
k	explicit	implicit	explicit	implicit
1	2k	2k+1	2k-1	2k
2	2k	2k+1	2k-1	2k-1
3	2k	2k+1	2k-1	2k
4	2k	2k+1	2k-1*	2k-1
5	2k	2k+1	2k-2	2k
6	2k-1	2k+1	2k-3	
7		2k+1	2k-2	

* 2k can probably be attained here.

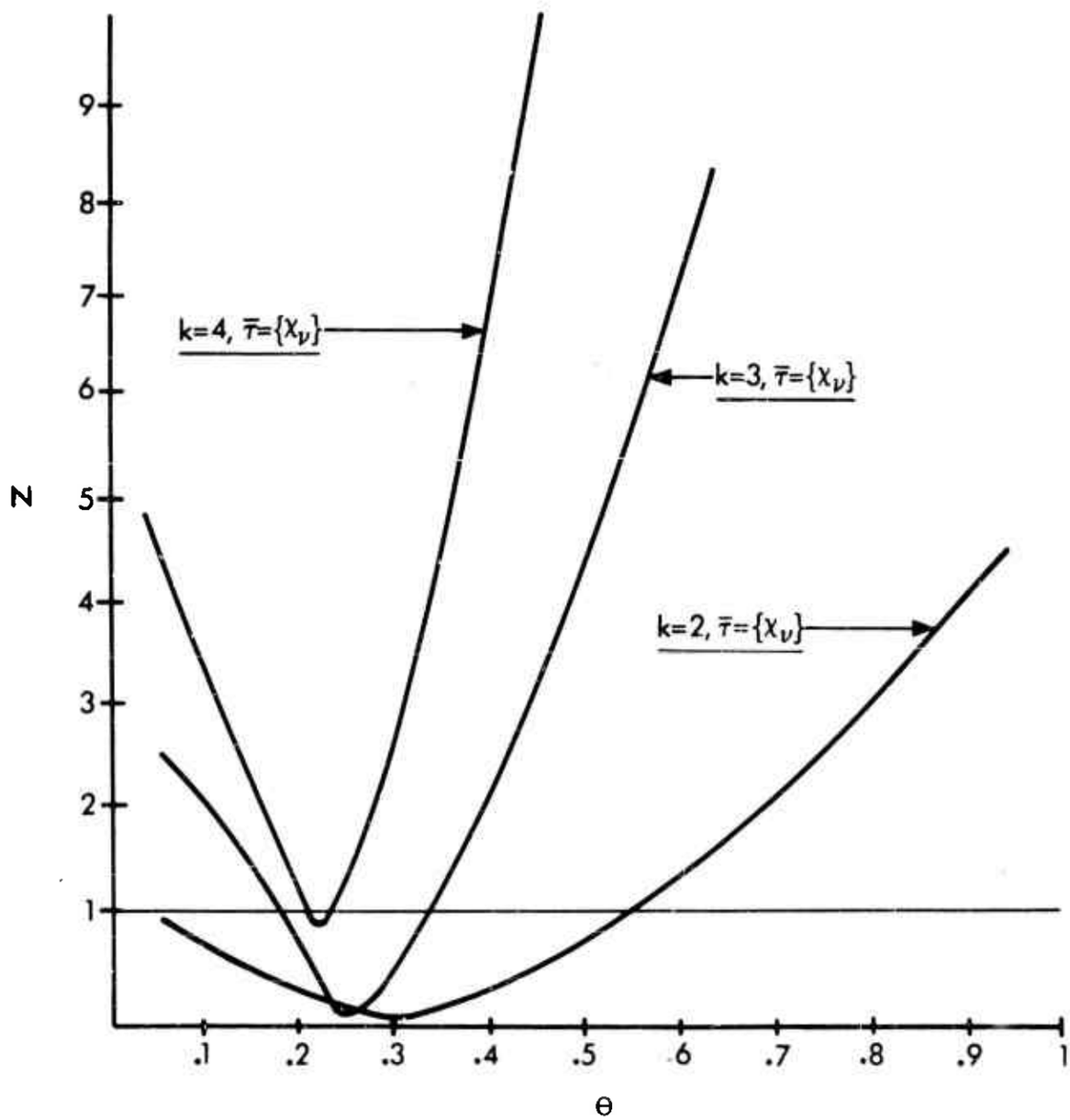

FIGURE 1. N(θ) FOR n=1 AND INDICATED k, $\bar{\tau}$.

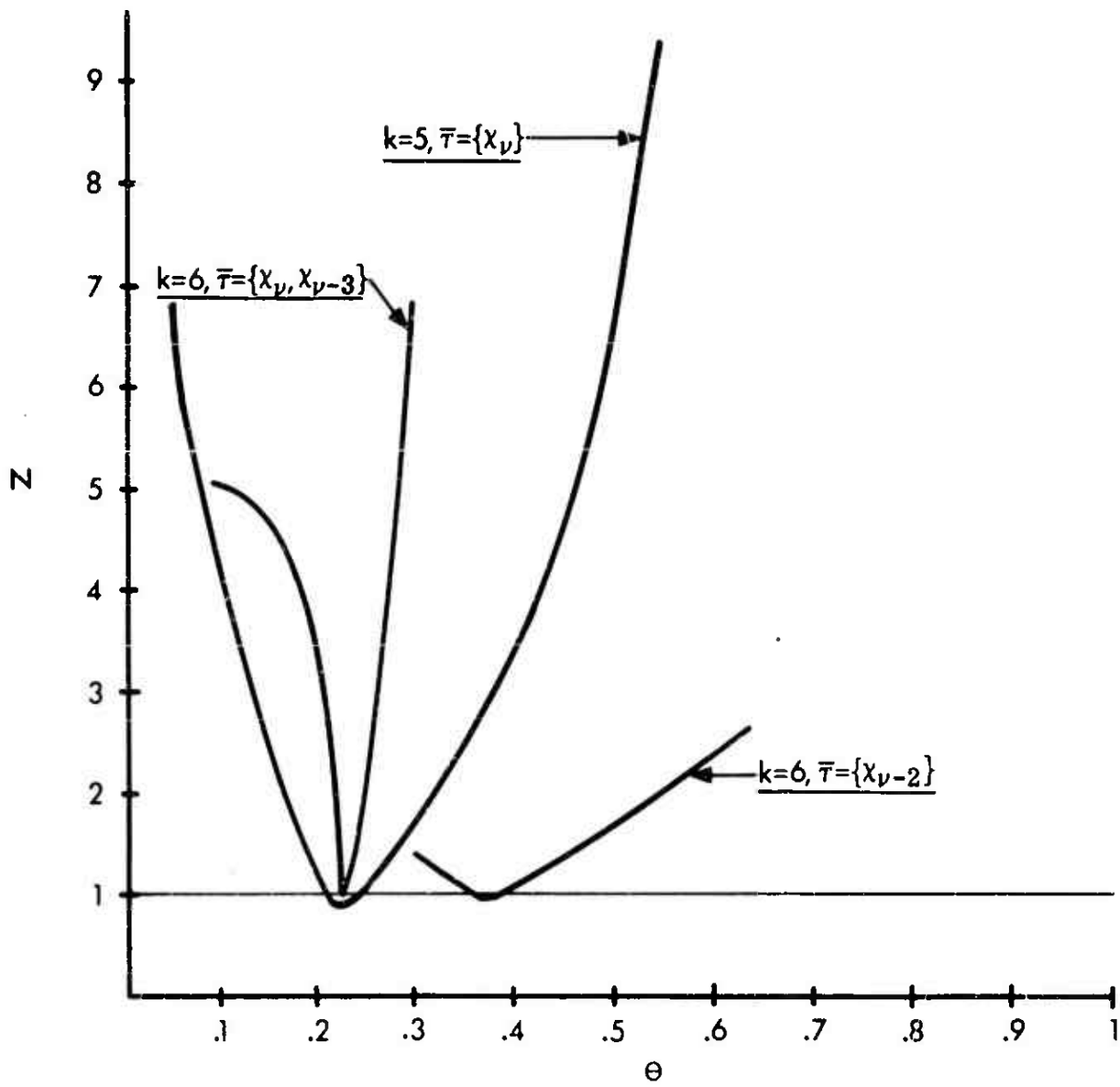

FIGURE 2. N(Θ) FOR n=1 AND INDICATED k, $\bar{\tau}$.

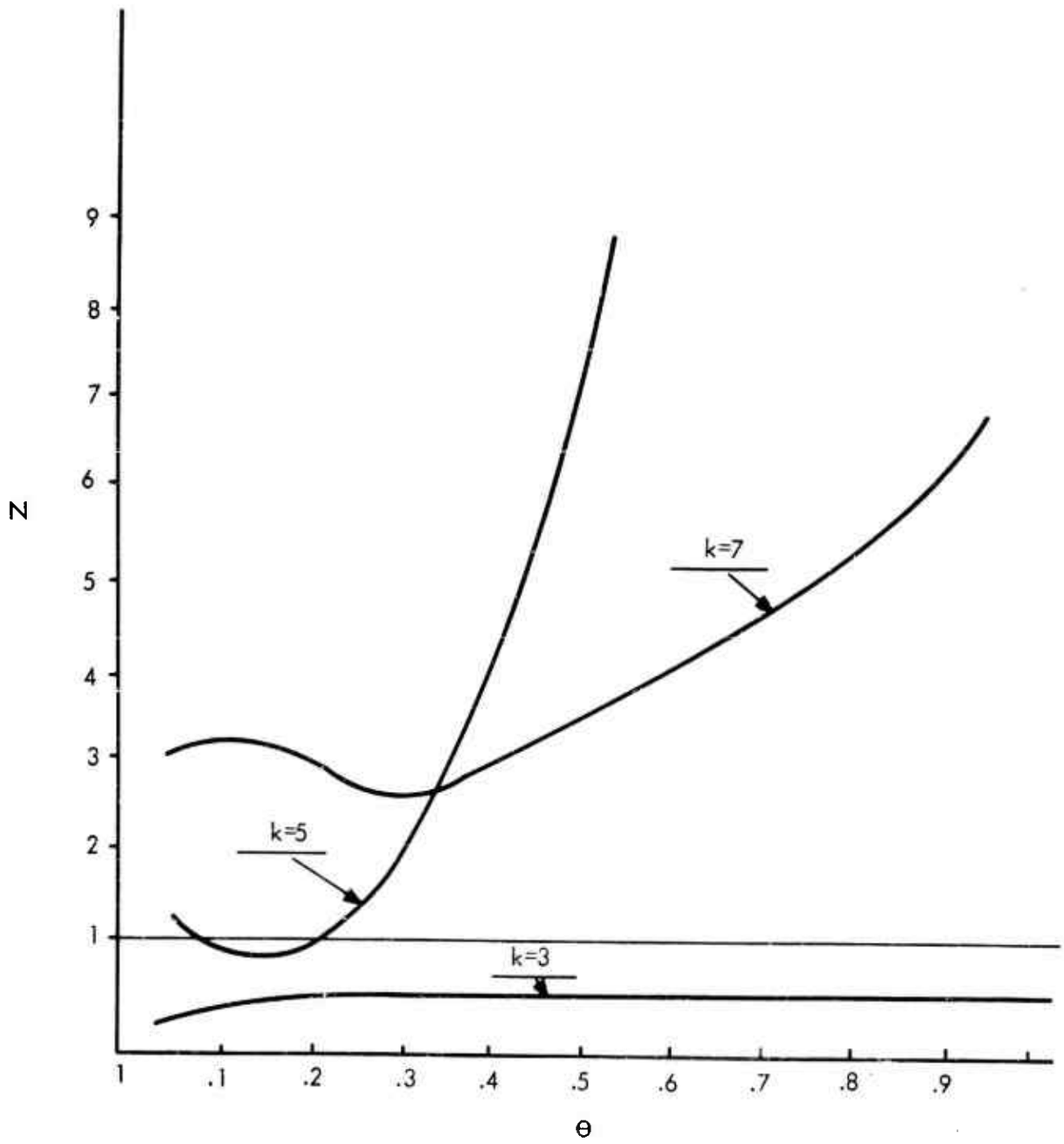

FIGURE 3. N(Θ) FOR n=2 AND INDICATED k.

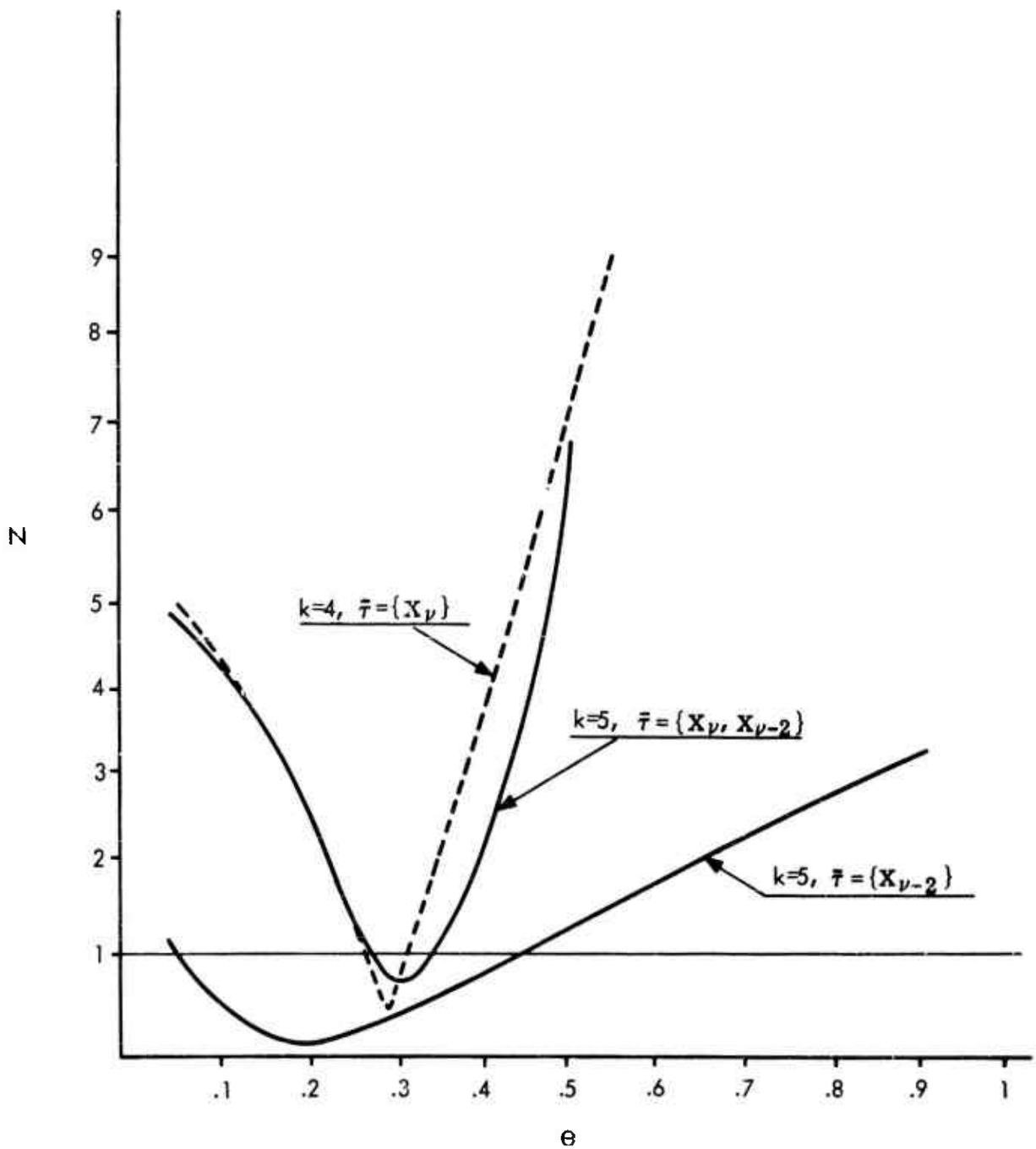

FIGURE 4. N(θ) FOR n=2 AND INDICATED k, $\bar{\tau}$.

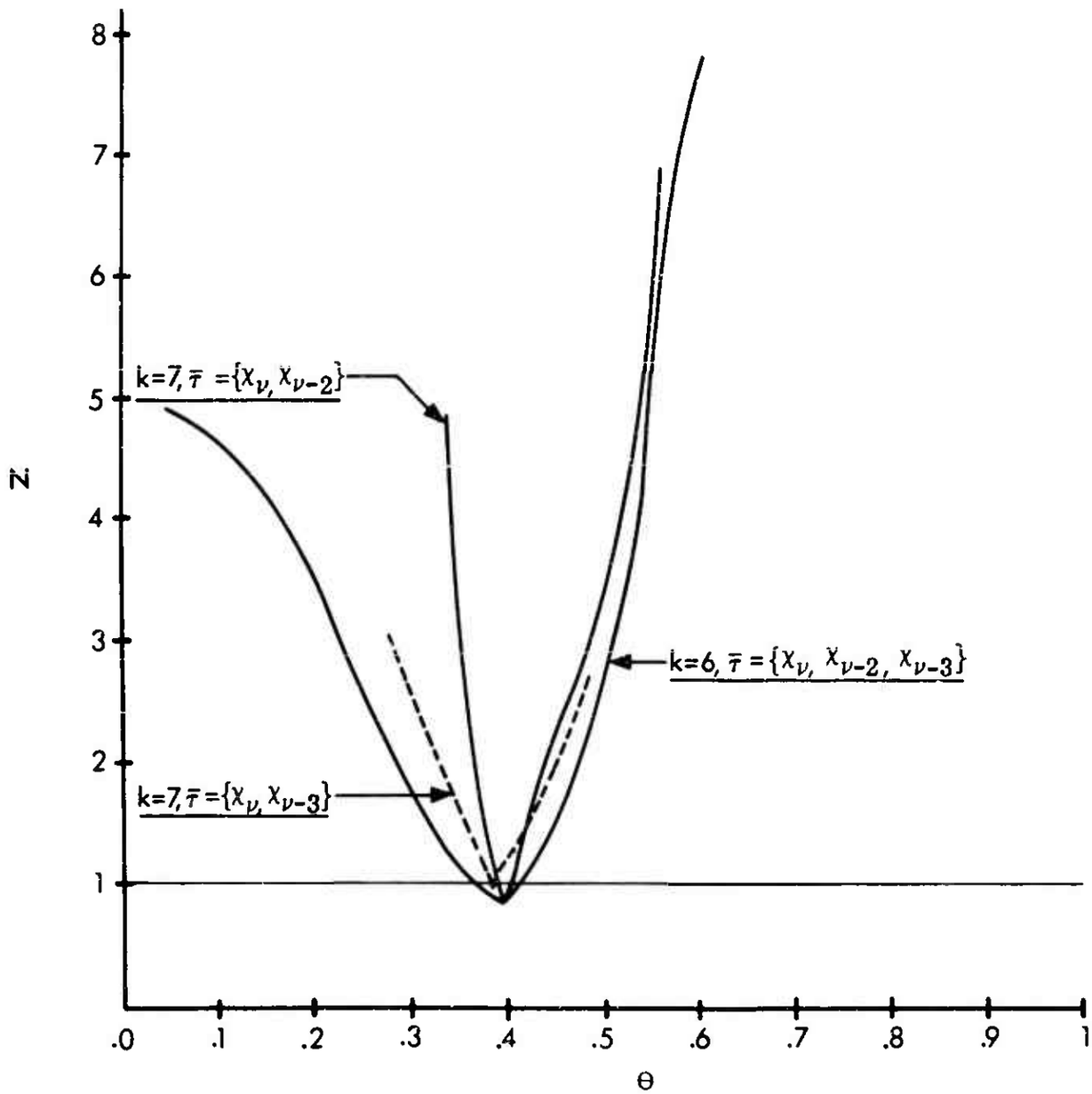

FIGURE 5. N(θ) FOR n=2 AND INDICATED k, $\bar{\tau}$.

This method of constructing stable operators was suggested by the work of Butcher [1] relative to the case described earlier, which we can obtain by specializing $n=1$, $\sigma=\tau=S_k$. Although the coefficients in this case are calculated directly (without determinants) from well known formulas, it is not clear how the roots of (3.18) are determined. In any event, in our work they are calculated (approximately) on computing machinery; and although great care has been taken to insure that adequate significance has been retained, without the inclusion of an error analysis of our results, we have not given a formal proof of stability.

The theory of multistep methods for a special equation of the second order parallels that for a first order equation. It is certain that in the former case, also, a theorem can be proved giving the uniform pth order convergence in a fixed interval of integration for our generalized methods and can be patterned after the analogous theorem for the traditional method (cf. convergence theorem in [4]). The order of accuracy of a method is meaningful only asymptotically as step size, h, approaches zero. Because of this, and because we have already on two occasions of necessity replaced formal proof by a computational argument, we elect to test on available computing machinery in a fairly realistic context some of the methods constructed and to demonstrate convergence and order of convergence in this way.

4. Computational Experiments.

Some of the methods given in the appendix for step number $k=4$ were coded in FORTRAN, and computations were performed on the IBM 7094 in order to give a feeling for their behavior. As a standard of comparison, the computations were also done using what Henrici [5] calls the "Cowell" method of numerical integration. (This is still another use of the term.) A single standard trajectory was selected for computation.

The orbit used is characterized by the initial elements $a=1.5$, $e=.2$, $i=45^{\circ}$, $\Omega=M=\omega=0$, and initial values as given in [2, p.42]. No perturbations have as yet been considered. The period of the orbit is between 155 and 156 minutes.

The well-known Cowell method was selected as a standard of comparison because it is a near-maximal order multistep method and because it is the unsummed form of the Gauss-Jackson method. If no round-off error is present, the summed and unsummed difference equations will yield identical results. The truncation errors are the same.

As noted earlier of our generalized methods, "prediction" and "correction" normally occur at different time points. In the context of the generalization it seems more apt to speak of the process as consisting of one or two "initial" methods and a "terminal" method. Our terminal method may be explicit (open). Such combinations have been selected from methods appearing in the appendix and will be described. The order of the combination we have called the minimum of the orders of the components. The step number of the combination we have called the maximum of the step numbers of the members. Although the advantage

of the generalized methods over the usual multistep methods increases with the step number, we have chosen for the experiments a relatively small step number k=4 for simplicity. The orders of the methods tested vary from 4 to 6.

An error term could be derived analytically for the new methods; however, this would be cumbersome and perhaps practically meaningless. Round-off error effects would not be included. Accumulated error is analytically complex as are instabilities induced by a bad fitting of initial and terminal equations. For these reasons the results of experiments are presented to suggest the efficiency of the new methods.

In addition to the orbit described above, we have tested two methods by numerically solving the equation $y''= -y$, with $y(0) = 0, y'(0)=1$.

The methods used will be described. Initial or predicting methods based on the theory of generalized Hermitian interpolations of Section 2 are here and in the Appendix called quasi-Hermitian methods. They are not necessarily stable. The following five combinations are identified as Programs A, B, C, D and E.

Program A: The maximal order Stormer method (order 4) as predictor; the Cowell method (order 5) as corrector.

Program B: The quasi-Hermitian method I (order 6) as the predicting method; the Cowell method (order 5) as corrector.

Program C: The quasi-Hermitian method II (order 6) as the initial method; the generalized multistep explicit method I (k=3, order 5) as terminal.

Program D: Two initial methods required: The quasi-Hermitian methods I and III (both of order 6) as initial methods; the generalized multistep implicit method I (k=3, order 6) as terminal.

Program E. The quasi-Hermitian method III (order 6) as the initial method; the generalized multistep explicit method II (order 7) as terminal.

Table 2 gives the error in the solution to $y''=-y$ with above initial conditions for indicated integration interval h at three different values of x. Error is experimental value less true value.

TABLE 2

Comparisons of Error in Sin x

Error X 10^{11} at x=3 radians

h	Program A	Program E
.01	0	-1
.05	-46	0
.10	-1971	1
.20	-88389	90

Error X 10^{8} at x=100 radians

h	Program A	Program E
.10	142	0
.20	5374	-8

Error X 10^{7} at x=200 radians

h	Program A	Program E
.10	40	0
.20	1351	-2

Figures 6 through 9 compare errors in one coordinate of the described orbit trajectory as computed by the indicated programs at the stated times for three given values of h. Instead of the error, we plot $-\log_{10} |\text{error}|$ so that the ordinate shows the number of decimal digits of accuracy in the solution.

The truncation error in any of the methods is strongly oscillatory with the period of the orbit and grows with time. In Figure 10 we attempt to eliminate the periodicity and to get a notion of the asymptotic behavior of the propagated truncation error in programs E and A. We have integrated to a point P on the trajectory (represented by the zero abscissa on the graph). As the integration proceeded, the error at P was plotted after every revolution up to nine revolutions.

Figure 11 compares the error in cos x in an experiment using the summed and unsummed form of the difference equation. Stormer's method (k=2) [5] was used. The solution was coded in single-precision FORTRAN and was run on the IBM 7094. The two methods have identical truncation errors. The difference is due to differences in round-off error and error propagation. Henrici outlines [6] a statistical theory of round-off error which shows the summed form to be clearly superior. The theory is verified by computation. Figure 12 shows the results of the same experiment as illustrated by Figure 11 except that the process of "double precision accumulation" [2, p. 21] is used. This process is very inexpensive because the evaluation of the derivatives, normally by far the greater part of the work, is accomplished in single precision. Figure 12 shows that the orthodox form of the difference equation combined with double precision accumulation is superior to the summed form in a simple experiment.

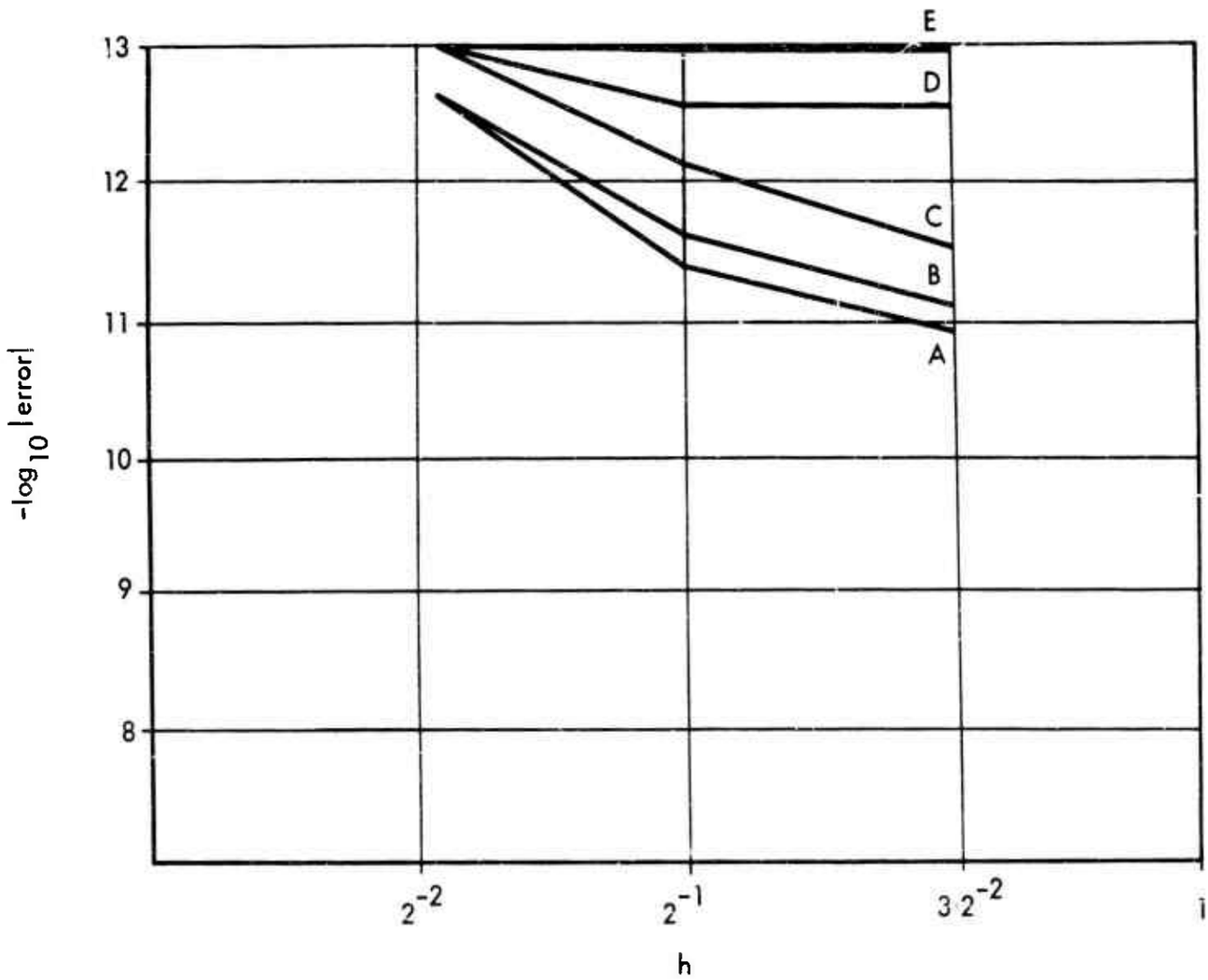

FIGURE 6. PRECISION IN COMPARED METHODS, t = 3min

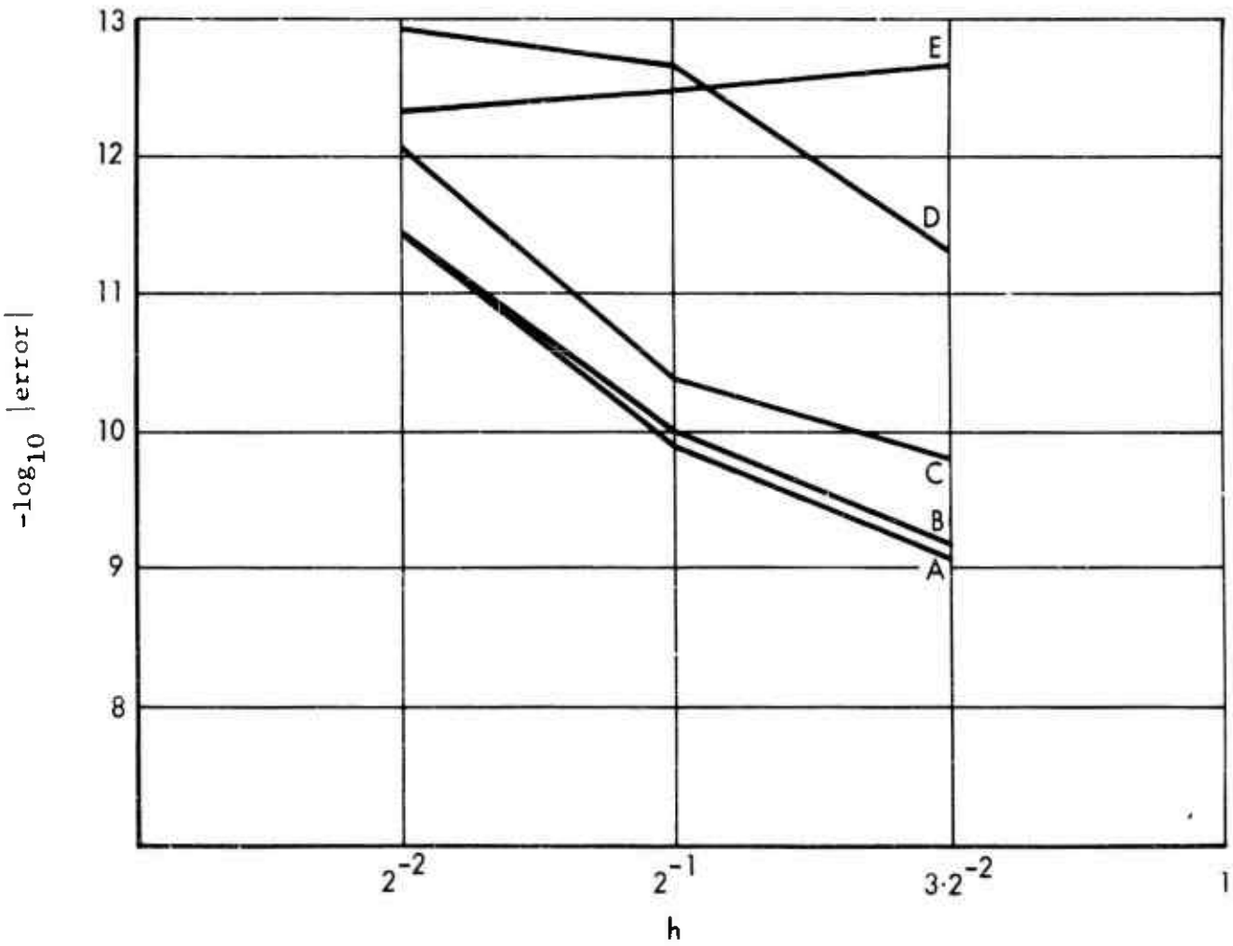

FIGURE 7. PRECISION IN COMPARED METHODS, t=9min

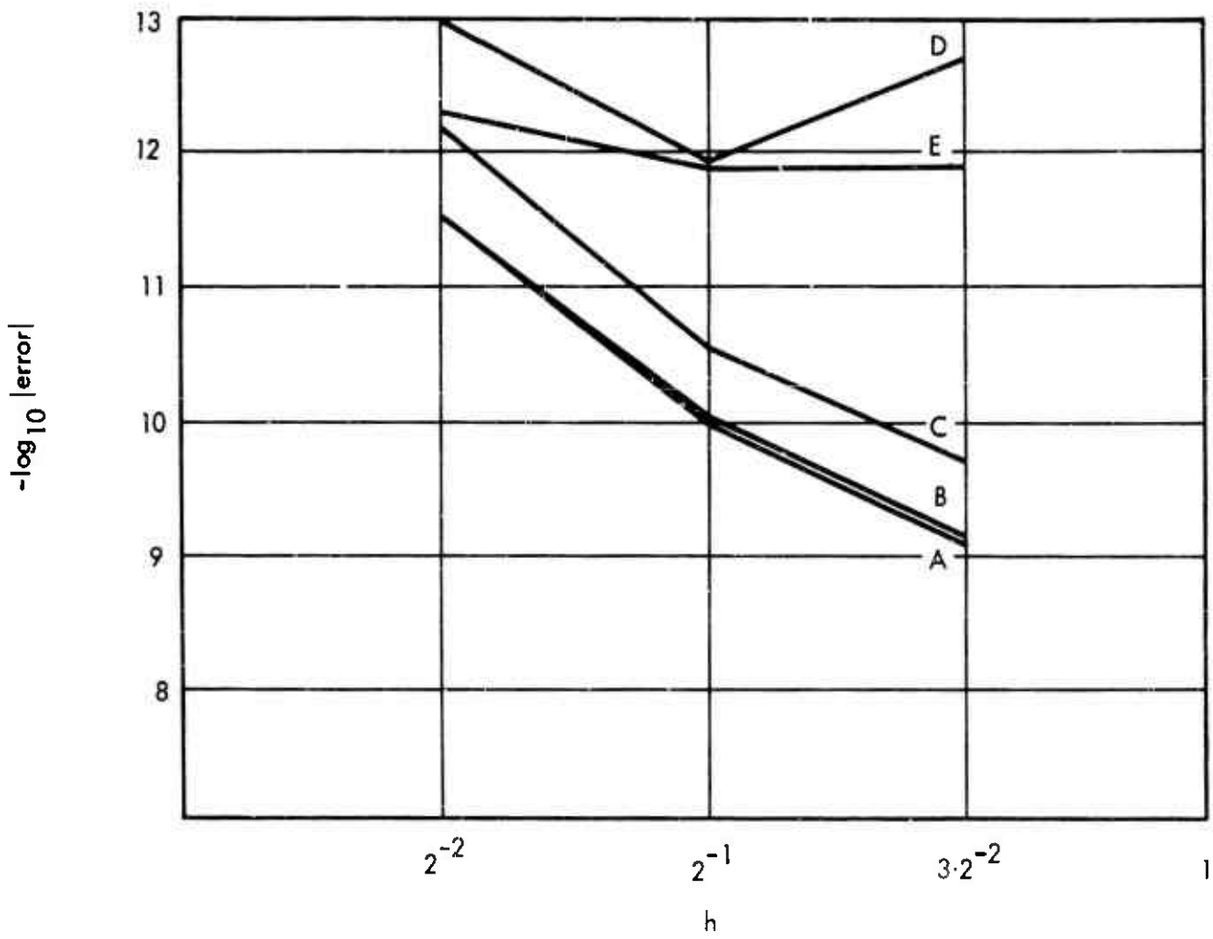

FIGURE 8. PRECISION IN COMPARED METHODS, $t = 30$min.

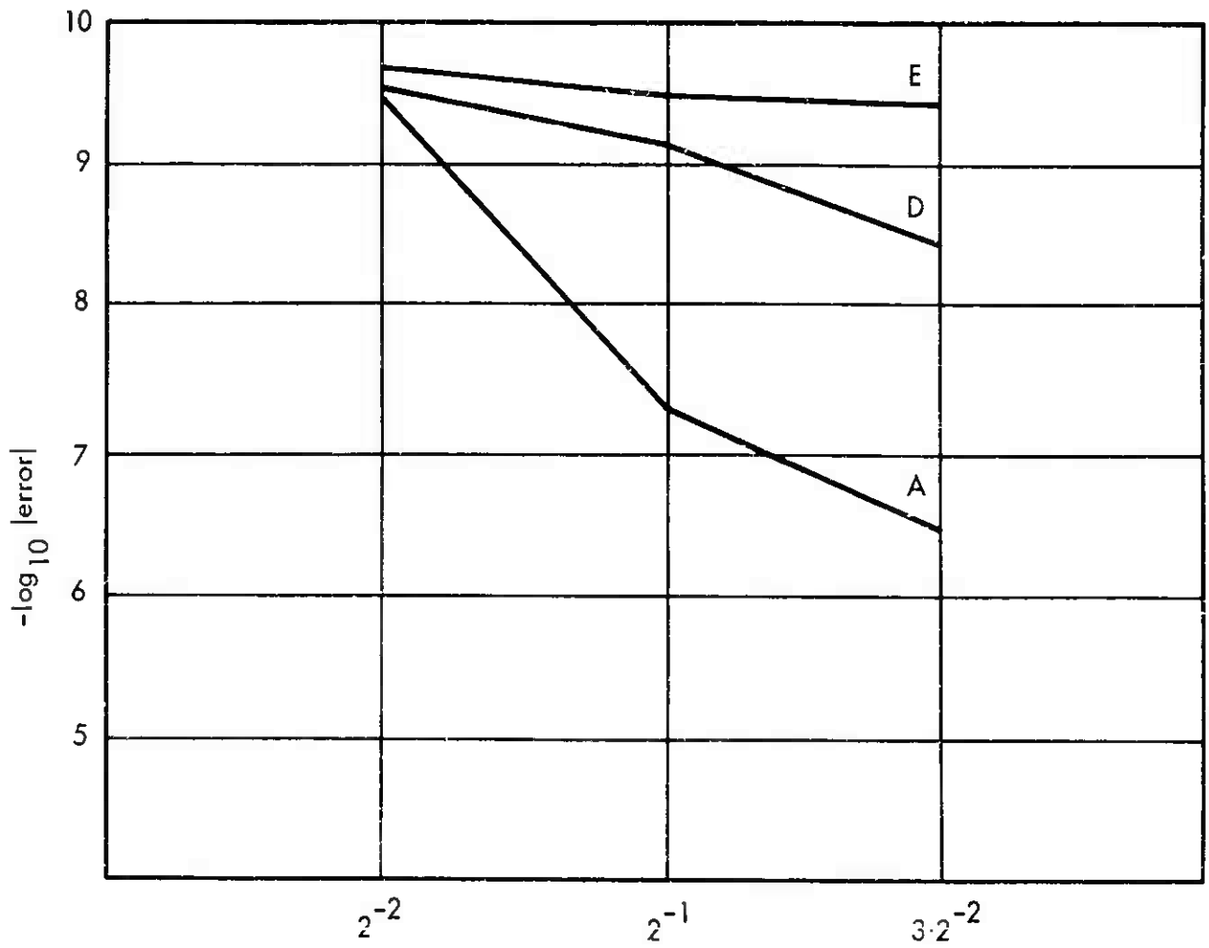

FIGURE 9. PRECISION IN COMPARED METHODS, $t = 498$min

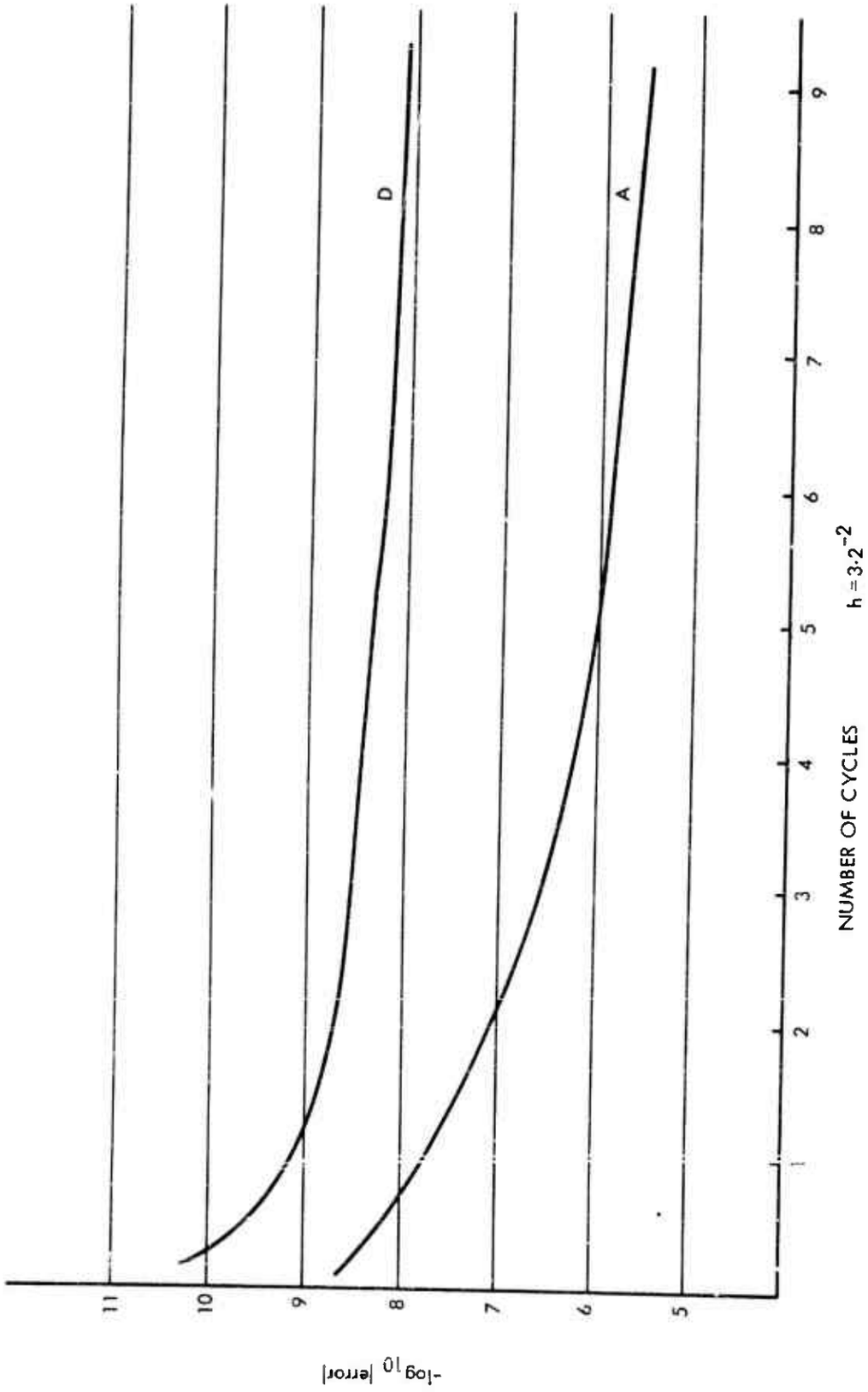

FIGURE 10. PRECISION IN 4-STEP COWELL AND GENERALIZED MULTISTEP

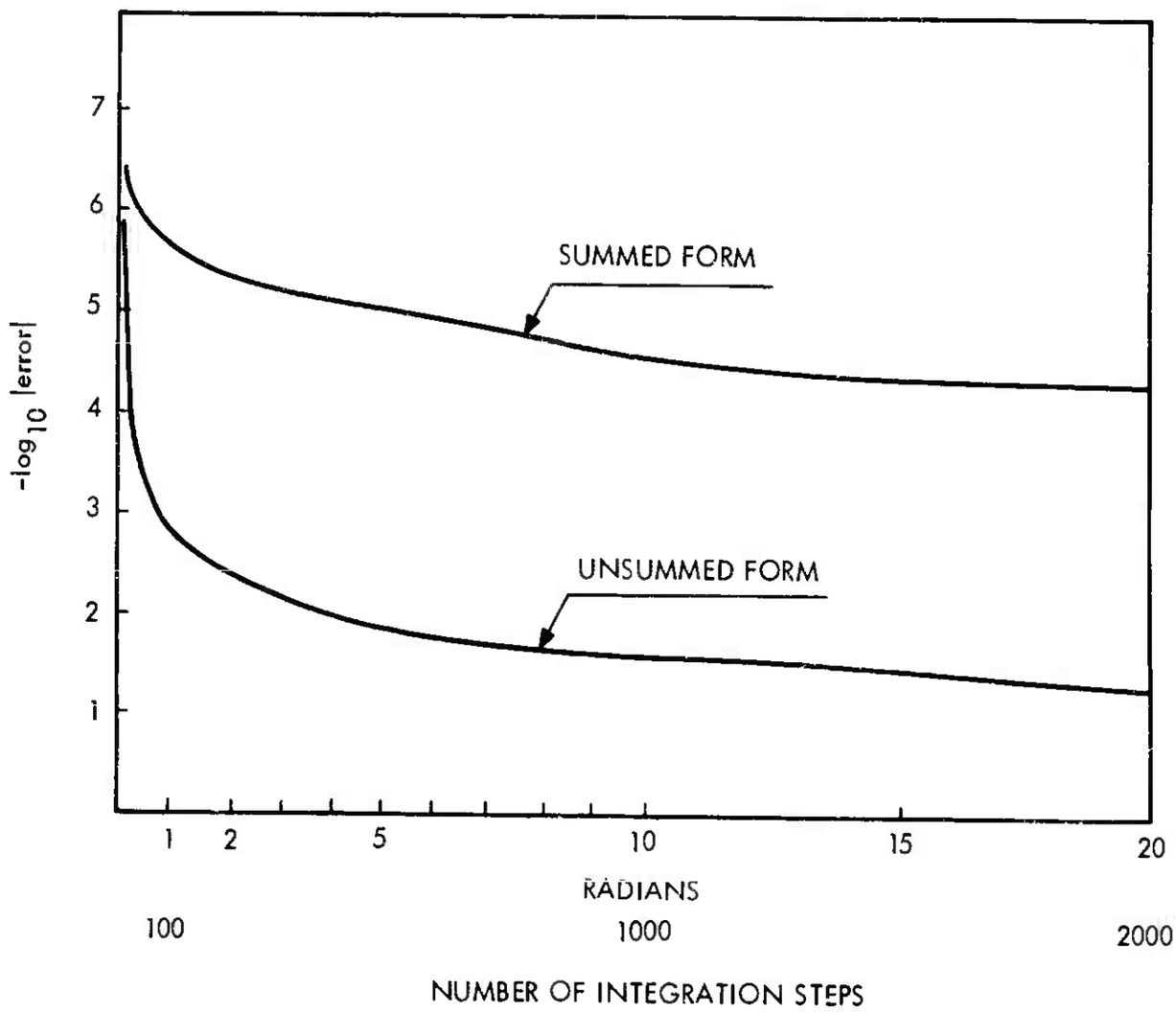

FIGURE 11. ERROR IN SUMMED AND UNSUMMED FORM OF DIFFERENCE EQUATION.

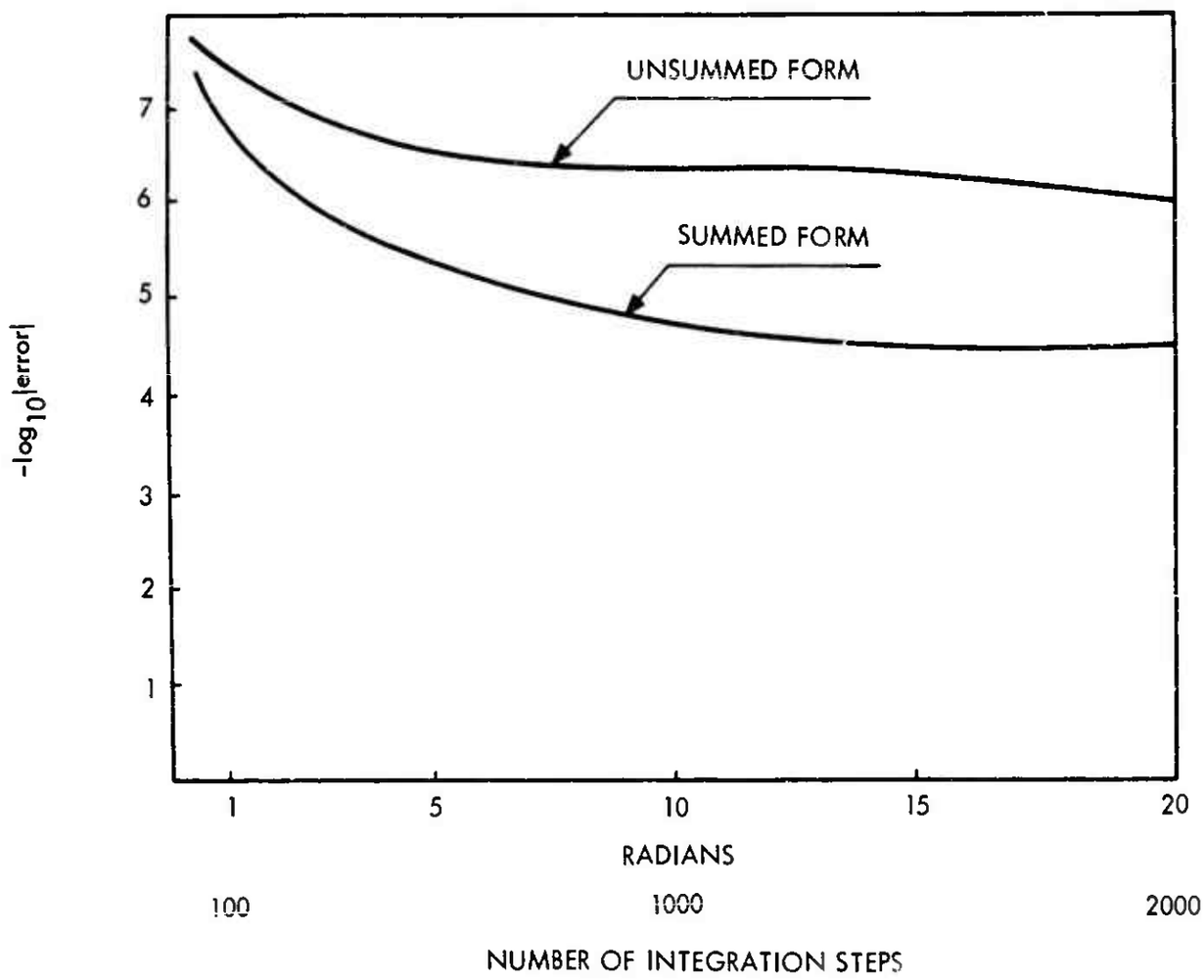

FIGURE 12. ERROR IN SUMMED AND UNSUMMED FORM OF DIFFERENCE EQUATION. DOUBLE PRECISION ACCUMULATION USED.

5. Conclusions.

The purpose of the research, of which this paper reports one phase, is to construct new algorithms for numerically solving the equations of motion of an earth satellite. These algorithms are close to Gauss-Jackson algorithms in structure. Recent developments in the theory of multistep methods have been applied to increase the accuracy of component methods. It is hoped that the final algorithms will increase the ratio of the order of accuracy to the step number (the number of differences used). In this way the starting time for the multistep process may remain unchanged while the interval of integration is increased. If stability characteristics and round-off growth are satisfactory in the new algorithms, the total time consumed in numerical integration may be reduced.

The increase in accuracy of the applied generalized multistep methods for small step number seems sufficiently great to justify the effort of testing higher-order methods that have already been constructed, of fitting these component methods into a final algorithm, and of testing the result in a completely realistic context.

The generalized theory had not before been applied to the equation $y''=f(x,y)$. The pertinent global convergence theorem (cf. [4] Theorem 3.1) is undoubtedly true but is yet to be proved, along with some stability theorems. No work as yet has been done towards deriving a summed form for the new difference equations. This form could be unwieldy. The question, in general, of the need for and effectiveness of a summed form in this work is being seriously considered in various installations. Figures 11 and 12 report a rudimentary experiment relating to this question.

Uniqueness theorems (of which Conjecture 2.10 is an example) are of continuing interest in the theory of quasi-Hermite osculatory polynomial interpolation; also of importance is the question of defining the resulting weighting functions $h_i(x)$, $\bar{h}_i(x)$, etc. by means of simple formulas. For trajectories with significant perturbations, it may be well to base methods on a polynomial of the form

$$P(x) = \sum_{i=0}^{i=k} h_i(x)y(x_{\nu-i}) + \sum_{i=0}^{i=k} \bar{h}_i(x)y'(x_{\nu-i}) + \sum_{i=0}^{i=k} \bar{\bar{h}}_i(x)y''(x_{\nu-i})$$

(cf. the Obrechkoff method) with perhaps nongrid points also appearing. A maximum possible order of accuracy is more than 3k. One can also investigate the feasibility of using least squares polynomials or functions other than polynomials for approximation in orbit trajectory computation.

The author plans also to explore the possible definitions of a reasonable asymptotic average rate ($t \to \infty$) of accumulations of truncation error associated with a multistep method.

6. Bibliography

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Appendix. Coefficients for Generalized Methods

In this Appendix are listed some of the constructed stable generalized methods and some Hermitian predicting equations. A few combinations of these have been tested on computing machinery and the results reported in Section 4.

All methods can be characterized by specifying σ, τ, k, n, θ. And by labelling as Hermitian predicting equation or generalized multistep method, σ and τ have been defined in Section 2. Figures 1 and 2 concern first order equations (n = 1) and show approximate ranges of θ for which stable explicit methods exist. The coefficients of the corresponding difference equations are fairly easily computed and are not included here. In all remaining computational work we have taken n = 2. In the Appendix $\sigma = s_k$ if unspecified. Concerning the generalized multistep methods, for each k, τ pair usually only one stable method is listed (or tested) corresponding to a convenient value of θ. A θ-family of methods always exists.

All predicting (initial) methods are based on the generalized Hermitian (called here "quasi-Hermitian") interpolating polynomial whose unique existence for given k, n, σ, τ was discussed in Section 2.

The form of the quasi-Hermitian predicting equation is

$$y_{\nu-\theta} = \alpha_k y_{\nu-k} + \alpha_{k-1} y_{\nu-k+1} + \cdots + \alpha_1 y_{\nu-1} + h^2(\beta_k f_{\nu-k} + \beta_{k-1} f_{\nu-k+1} + \cdots + \beta_1 f_{\nu-1}).$$

The form of the generalized multistep method is

$$y_\nu = \alpha_k y_{\nu-k} + \alpha_{k-1} y_{\nu-k+1} + \cdots + \alpha_1 y_{\nu-1} + h^2(\beta_k f_{\nu-k} + \beta_{k-1} f_{\nu-k+1} + \cdots + \beta_1 f_{\nu-1} + \beta f_{\nu-\theta} + \beta_0 f_\nu).$$

The coefficients are given with fifteen digits. The error in the coefficients has not yet been completely determined. For k = 3, 4 probably all digits are accurate. For k = 7 probably no more than eight digits should be relied upon. For intermediate k an intermediate number of digits are valid. For convenience, we specify σ and τ in complementary form $\bar{\sigma} = s_k - \sigma$ and $\bar{\tau} = s_k - \tau$.

Coefficients for generalized multistep (implicit) methods.

I. $k=3$ $\bar{\tau}=\phi$ $\theta=.3$

$\alpha_1 = .164864864864865 \cdot 10$

$\alpha_2 = -.297297297297297$

$\alpha_3 = -.351351351351351$

$\beta_0 = .825825825825825 \cdot 10^{-2}$

$\beta = .140196218627591$

$\beta_1 = .766087516187516$

$\beta_2 = .415871754107048$

$\beta_3 = .209376042709376 \cdot 10^{-1}$

II. $k=4$ $\bar{\tau}=\{x_{\nu-3}\}$ $\theta=.2$

$\alpha_1 = .1564622416043223 \cdot 10$

$\alpha_2 = -.9464169569758374 \cdot 10^{-1}$

$\alpha_3 = -.5045838547345016$

$\alpha_4 = .3460313538886233 \cdot 10^{-1}$

$\beta_0 = -.3027438680537280 \cdot 10^{-1}$

$\beta = .1688144735844922$

$\beta_1 = .7851898795361902$

$\beta_2 = .4800924707582710$

$\beta_3 = 0$

$\beta_4 = .4235373677581134$

III. $k=5$ $\bar{\tau}=\phi$ $\theta=.15$

$\alpha_1 = .167638725140126 \cdot 10$

$\alpha_2 = .278400595805990$

$\alpha_3 = -.150337671295784 \cdot 10$

$\alpha_4 = .466002632892664$

$\alpha_5 = .825862328579257 \cdot 10^{-1}$

$\beta_0 = -.670912228649990 \cdot 10^{-1}$

$\beta = .201329045334982$

$\beta_1 = .784007930456861$

$\beta_2 = .324155404103746$

$\beta_3 = -.494775767295745$

$\beta_4 = -.134034339375600$

$\beta_5 = -.373963322694766 \cdot 10^{-2}$

Coefficients for generalized multistep (explicit) methods.

I. $k=3$ $\bar{\tau}=\{x_\nu\}$ $\theta=.2$

$\alpha_1 = .2 \cdot 10$

$\alpha_2 = -.1 \cdot 10$

$\alpha_3 = 0$

$\beta_0 = 0$

$\beta = .124007936507937$

$\beta_1 = .770833333333333$

$\beta_2 = .111111111111111$

$\beta_3 = -.595238095238095 \cdot 10^{-2}$

II. $k=4$ $\bar{\tau}=\{x_\nu\}$ $\theta=.3$

$\alpha_1 = .205804969722280 \cdot 10$

$\alpha_2 = -.963457924410107$

$\alpha_3 = -.247233242848194$

$\alpha_4 = .152641470035498$

$\beta_0 = 0$

$\beta = .161595975532325$

$\beta_1 = .704431783153855$

$\beta_2 = .872587915934802 \cdot 10^{-1}$

$\beta_3 = -.154458906599228$

$\beta_4 = -.951881093873159 \cdot 10^{-2}$

III. $k=5$ $\bar{\tau}=\{x_\nu, x_{\nu-2}\}$ $\theta=.35$

$\alpha_1 = .307716392780799 \cdot 10$

$\alpha_2 = -.334316264723224 \cdot 10$

$\alpha_3 = .130022320315476 \cdot 10$

$\alpha_4 = .120385824155265$

$\alpha_5 = -.154610307885770$

$\beta_0 = 0$

$\beta = .199342712868876$

$\beta_1 = .542723814092476$

$\beta_2 = 0$

$\beta_3 = -.656160625268288$

$\beta_4 = .171431112289051$

$\beta_5 = .894415771194486 \cdot 10^{-2}$

IV. $k=7$ $\bar{\tau}=\{x_\nu, x_{\nu-2}\}$ $\theta=.36$

$\alpha_1 = .300166612993176 \cdot 10$

$\alpha_2 = -.313714901027128 \cdot 10$

$\alpha_3 = .683807311516383$

$\alpha_4 = .134723867946272 \cdot 10$

$\alpha_5 = -.116171903379676 \cdot 10$

$\alpha_6 = .222241054902451$

$\alpha_7 = .439148682531614 \cdot 10^{-1}$

$\beta_0 = 0$

$\beta = .205438536632750$

$\beta_1 = .539144517864215$

$\beta_2 = 0$

$\beta_3 = -.592537575632003$

$\beta_4 = .484847995513130$

$\beta_5 = -.200181366173655$

$\beta_6 = -.711155078646860 \cdot 10^{-1}$

$\beta_7 = -.193932029482787 \cdot 10^{-2}$

Coefficients for quasi-Hermitian predicting equations .

I. $k=4$ $\bar{\sigma}=\bar{\tau}=\{x_\nu\}$ $\theta=0$

$\alpha_1 = -.160000000000000 \cdot 10^2$ $\beta_1 = .266666666666667 \cdot 10$

$\alpha_2 = .340000000000000 \cdot 10^2$ $\beta_2 = .146666666666667 \cdot 10^2$

$\alpha_3 = -.160000000000000 \cdot 10^2$ $\beta_3 = .266666666666667 \cdot 10$

$\alpha_4 = -.100000000000000 \cdot 10^2$ $\beta_4 = 0$

II. $k=4$ $\bar{\sigma}=\bar{\tau}=\{x_\nu\}$ $\theta=.2$

$\alpha_1 = -.500286720000000 \cdot 10$ $\beta_1 = .129576960000000 \cdot 10$

$\alpha_2 = .124635136000000 \cdot 10^2$ $\beta_2 = .560138240000000 \cdot 10$

$\alpha_3 = -.611842560000000 \cdot 10$ $\beta_3 = .969881600000000$

$\alpha_4 = -.342220800000000$ $\beta_4 = -.194560000000000 \cdot 10^{-2}$

III. $k=4$ $\bar{\sigma}=\bar{\tau}=\{x_\nu\}$ $\theta=.3$

$\alpha_1 = -.193209930000000 \cdot 10$ $\beta_1 = .862500525000000$

$\alpha_2 = .647195490000000 \cdot 10$ $\beta_2 = .303038047500000 \cdot 10$

$\alpha_3 = -.344761190000000 \cdot 10$ $\beta_3 = .433679775000000$

$\alpha_4 = -.922437000000000 \cdot 10^{-1}$ $\beta_4 = -.721777500000000 \cdot 10^{-2}$

IV. $k=5$ $\bar{\sigma}=\{x_\nu\}$ $\bar{\tau}=\{x_\nu, x_{\nu-4}\}$ $\theta=0$

$\alpha_1 = -.168023255813954 \cdot 10^2$ $\beta_1 = .275581395348837 \cdot 10$

$\alpha_2 = .425581395348837 \cdot 10^2$ $\beta_2 = .146666666666667 \cdot 10^2$

$\alpha_3 = -.315116279069767 \cdot 10^2$ $\beta_3 = -.286046511627907 \cdot 10$

$\alpha_4 = -.200996777408638 \cdot 10$ $\beta_4 = 0$

$\alpha_5 = -.802325581395349$ $\beta_5 = -.662494520579550 \cdot 10$

V. $k=5$ $\bar{\sigma}=\{x_\nu\}$ $\bar{\tau}=\{x_\nu, x_{\nu-4}\}$ $\theta=.3$

$\alpha_1 = -.210714719098474 \cdot 10$ $\beta_1 = .881649550039971$

$\alpha_2 = .826695465383721 \cdot 10$ $\beta_2 = .303759825000000 \cdot 10$

$\alpha_3 = -.668751562570494 \cdot 10$ $\beta_3 = -.713862014978198$

$\alpha_4 = -.729126387971761 \cdot 10$ $\beta_4 = 0$

$\alpha_5 = -.175047890984738$ $\beta_5 = -.483931917058517 \cdot 10$

VI. $k=5$ $\bar{\sigma}=\{x_\nu\}$ $\bar{\tau}=\{x_\nu, x_{\nu-4}\}$ $\theta=.5$

$\alpha_1 = .106292724609375 \cdot 10$ $\beta_1 = .341125488281250$

$\alpha_2 = .102539062500000 \cdot 10$ $\beta_2 = .386718750000000$

$\alpha_3 = -.180944824218750 \cdot 10$ $\beta_3 = -.504272460937500$

$\alpha_4 = -.782023005506312 \cdot 10$ $\beta_4 = 0$

$\alpha_5 = -.698852539062500 \cdot 10^{-1}$ $\beta_5 = -.385435703822545 \cdot 10$

VII. $k=5$ $\bar{\sigma}=\{x_\nu\}$ $\bar{\tau}=\{x_\nu, x_{\nu-1}\}$ $\theta=.3$

$\alpha_1 = .157175067554755 \cdot 10^2$ $\beta_1 = 0$

$\alpha_2 = .818655257876087 \cdot 10^2$ $\beta_2 = -.233352230729348 \cdot 10^2$

$\alpha_3 = -.189533965786168 \cdot 10^3$ $\beta_3 = -.911021071886413 \cdot 10^2$

$\alpha_4 = .753013271876087 \cdot 10^2$ $\beta_4 = -.263728213229348 \cdot 10^2$

$\alpha_5 = .176496060554755 \cdot 10^2$ $\beta_5 = -.862500525000000$

VIII. $k=6$ $\bar{\sigma}=\bar{\tau}=\{x_\nu\}$ $\theta=.15$

$\alpha_1 = -.267354410875809 \cdot 10^2$ $\beta_1 = .258741730223803 \cdot 10$

$\alpha_2 = -.542303743902377 \cdot 10^2$ $\beta_2 = .353107545202970 \cdot 10^2$

$\alpha_3 = .163415437280526 \cdot 10^3$ $\beta_3 = .935523697444449 \cdot 10^2$

$\alpha_4 = -.529860381340549 \cdot 10^2$ $\beta_4 = .356880342431044 \cdot 10^2$

$\alpha_5 = -.278255325746131 \cdot 10^2$ $\beta_5 = .251550985402339 \cdot 10$

$\alpha_6 = -.638051094039407$ $\beta_6 = .854784560392494 \cdot 10^{-2}$

IX. k=6 $\bar{\sigma}=\bar{\tau}=\{x_\nu\}$ $\theta=.3$

$\alpha_1 = -.100919643422326 \cdot 10^2$ $\beta_1 = .128647106629316 \cdot 10$

$\alpha_2 = -.227114950680780 \cdot 10^2$ $\beta_2 = .146235774698821 \cdot 10^2$

$\alpha_3 = .665492820631938 \cdot 10^2$ $\beta_3 = .386584562983006 \cdot 10^2$

$\alpha_4 = -.202747607559376 \cdot 10^2$ $\beta_4 = .154121622333216 \cdot 10^2$

$\alpha_5 = -.120925226942311 \cdot 10^2$ $\beta_5 = .122101145605511 \cdot 10$

$\alpha_6 = -.378539202714476$ $\beta_6 = .884987329763802 \cdot 10^{-2}$

X. k=6 $\bar{\sigma}=\bar{\tau}=\{x_\nu\}$ $\theta=.35$

$\alpha_1 = -.677953505973247 \cdot 10$ $\beta_1 = .100266487549777 \cdot 10$

$\alpha_2 = -.168428545345370 \cdot 10^2$ $\beta_2 = .105330757175910 \cdot 10^2$

$\alpha_3 = .480321543101358 \cdot 10^2$ $\beta_3 = .280367261702224 \cdot 10^2$

$\alpha_4 = -.140846861658563 \cdot 10^2$ $\beta_4 = .114420776177617 \cdot 10^2$

$\alpha_5 = -.900799716188439 \cdot 10$ $\beta_5 = .954041971289129$

$\alpha_6 = -.317081388125608$ $\beta_6 = .836468763365225 \cdot 10^{-2}$

XI. k=7 $\bar{\sigma}=\{x_\nu\}$ $\bar{\tau}=\{x_\nu, x_{\nu-1}\}$ $\theta=.15$

$\alpha_1 = .426248672016901 \cdot 10^2$ $\beta_1 = 0$

$\alpha_2 = .106521856117869 \cdot 10^4$ $\beta_2 = -.120432808602138 \cdot 10^3$

$\alpha_3 = .131573055131036 \cdot 10^4$ $\beta_3 = -.131699354325931 \cdot 10^4$

$\alpha_4 = -.473523475391012 \cdot 10^4$ $\beta_4 = -.308091180980903 \cdot 10^4$

$\alpha_5 = .112448958145522 \cdot 10^4$ $\beta_5 = -.140803040314973 \cdot 10^4$

$\alpha_6 = .111881088447489 \cdot 10^4$ $\beta_6 = -.155735015276831 \cdot 10^3$

$\alpha_7 = .693603082892709 \cdot 10^2$ $\beta_7 = -.258741730223803 \cdot 10$

XII. $k=7$ $\bar{\sigma}=\{x_\nu\}$ $\bar{\tau}=\{x_\nu, x_{\nu-4}\}$ $\theta=.36$

$\alpha_1 = -.631355595928052 \cdot 10$ $\beta_1 = .959963291682580$

$\alpha_2 = -.133597097252952 \cdot 10^2$ $\beta_2 = .980492460305444 \cdot 10$

$\alpha_3 = .532090581314935 \cdot 10^2$ $\beta_3 = .229394560344614 \cdot 10^2$

$\alpha_4 = -.344398239116463 \cdot 10^2$ $\beta_4 = 0$

$\alpha_5 = -.197321764953814$ $\beta_5 = -.239793128470220 \cdot 10$

$\alpha_6 = .219776712103132 \cdot 10$ $\beta_6 = -.258511564830275 \cdot 10^{-1}$

$\alpha_7 = -.964138913490856 \cdot 10^{-1}$ $\beta_7 = .711986507800205 \cdot 10^{-2}$

XIII. $k=8$ $\bar{\sigma}=\bar{\tau}=\{x_\nu\}$ $\theta=.15$

$\alpha_1 = -.561616705786098 \cdot 10^2$ $\beta_1 = .372288312743760 \cdot 10$

$\alpha_2 = -.486198844276056 \cdot 10^3$ $\beta_2 = .987049040638957 \cdot 10^2$

$\alpha_3 = -.246075559120176 \cdot 10^3$ $\beta_3 = .637864549912463$

$\alpha_4 = .158204669038749 \cdot 10^4$ $\beta_4 = .123026245967712 \cdot 10^4$

$\alpha_5 = -.251506615194785 \cdot 10^3$ $\beta_5 = .635237310870639 \cdot 10^3$

$\alpha_6 = -.484551151396271 \cdot 10^3$ $\beta_6 = .975616454903224 \cdot 10^2$

$\alpha_7 = -.560120578494670 \cdot 10^2$ $\beta_7 = .345201215578264 \cdot 10$

$\alpha_8 = -.540791966999407$ $\beta_8 = .467686974850554 \cdot 10^{-2}$

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14. KEY WORDS	LINK A ROLE	LINK A WT	LINK B ROLE	LINK B WT	LINK C ROLE	LINK C WT
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