Stiffly Stable Linear Multistep Methods of Extended Order

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Abstract

In this paper we discuss some desirable properties of linear multistep methods applied to stiff equations. We then proceed to produce and examine a class of methods with these properties. These schemes are extensions of those discussed by Gear (1968), and are of higher order.

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1. Introduction

For the general initial value problem

$$y' = f(x,y),\ y(o) = y_0\ , \tag{1.1}$$

the general linear k-step method is defined by

$$\sum_{i=o}^{k} \alpha_i y_{j+1} = h \sum_{i=o}^{k} \beta_i f(x_{j+1},\ y_{j+1}),\ j = 0,\ 1,\ 2,\ \ldots\ . \tag{1.2}$$

In this paper we shall be concerned with the behavior of (1.2) on stiff equations; that is, problems (1.1) where $\frac{\partial f}{\partial f} < < 0$ or, for a system of equations $y' = \underline{f}(x,y)$, when the Jacobian matrix $\frac{\partial f_i}{\partial y_j}$ has some eigenvalues with large negative real parts.

Much can be seen from the behavior of (1.2) on the simple linear homogeneous problem

$$y' = \lambda y\ ,\ y(0) = y_0 \tag{1.3}$$

for $Re(\lambda) < 0$. For this problem, the general solution of (1.2) is (assuming no multiple roots)

$$y_j = \sum_{i=1}^{k} c_i(\xi_i(h\lambda))^j \quad ,$$

where $\{\xi_i(h\lambda)\}^k$ are the roots of $\rho(\xi) - h\lambda\sigma(\xi) = 0$

$$\rho(\xi) = \sum_{i=0}^{k} \alpha_i \xi^i \quad , \quad \sigma(\xi) = \sum_{i=0}^{k} \beta_i \xi^i \ .$$

Since the solution of (1.3) decays for $\mathrm{Re}(\lambda) < 0$, we would like the solution of (1.2) to do so as well; however Dahlquist (1963) has shown that this can happen in the whole left half-plane $\mathrm{Re}(\lambda) < 0$ only for methods of order two or less. For other methods then, it is of interest to define the region of the complex plane where the solution of (1.2) applied to (1.3) does decay; this is the <u>region of absolute stability</u>:

$$S = \{w \in \mathbb{C} \mid \text{all roots } \xi_i(w) \text{ or } \rho(\xi) - w\sigma(\xi) = 0 \text{ satisfy } |\xi_i(w)| < 1\}. \qquad (1.4)$$

As is well known, every useful linear multistep method must be strongly stable: i.e., the roots of $\rho(\xi) = 0$ must satisfy $\xi_1 = 1, |\xi_i| < 1,\ 1 < i \le k$. This is equivalent to saying $w = 0$ belongs to S, or more precisely, to the <u>boundary</u> of S, since on the boundary one or more roots $|\xi_i(w)| = 1$, and the other $|\xi_j(w)| < 1$. We shall call such a method <u>stable at 0</u>, and assume this holds throughout the paper. Moreover, applying (1.2) ot a stiff equation (1.3), i.e., $\mathrm{Re}(\lambda) << 0$, h must be chosen so $h\lambda \in S$ in order to get any kind of decay in the approximate solution. This places a substantial restriction on h unless the region S is unbounded, i.e., unless $\infty \in S$. We call such a method stable at ∞; of course this is equivalent to the roots of $\sigma(\xi) = 0$ satisfying $|\xi_i| < 1$.

Another desirable property of (1.2) for stiff equations can be seen as follows: the true solution of (1.3) satisfies

$$\left| \frac{y(x_{j+1})}{y(x_j)} \right| = |e^{h\lambda}| \to 0 \text{ as } h\lambda \to -\infty,$$

that is the solution damps more and more over one step as $h\lambda \to -\infty$. If the same holds for the discrete solution of (1.3), i.e., $\left| \frac{y_{j+1}}{y_j} \right| \to 0$ as $h\lambda \to -\infty$, we say the method is damped at ∞. Also we define the asymptotic decay rate as $D = \lim_{h\lambda \to -\infty} \left| \frac{y_{j+1}(h\lambda)}{y_j(h\lambda)} \right|$; thus for the backwards Euler method $y_{j+1} = y_j + hf(x_{j+1}, y_{j+1})$, $D = 0$ so the method is damped at ∞, and for the trapezoidal method $y_{j+1} = y_j + \frac{h}{2}(f(x_{j+1}, y_j) + f(x_{j+1}, y_{j+1}))$, $D = 1$ (so asymptotically there is no damping).

For further background and discussion of linear multistep methods applied to stiff equations, see Gear (1971) or Lambert(1973). In this paper, we first discuss properties of any k-step method which is stable at ∞. Then we proceed to produce and examine k-step methods which are in addition damped at ∞, and are of higher order than any previously found.

2. Methods which are Stable at ∞

For this analysis, it is more convenient to transform from the ξ-plane to the z-plane via

$$z = \frac{\xi-1}{\xi+1}\,, \quad \xi = \frac{1+z}{1-z}\,. \tag{2.1}$$

This maps the unit circle $|\xi| < 1$ onto the left half-plane $\mathrm{Re}(z) < 0$, so that the region of absolute stability is now described as

$$S = \{w\varepsilon\mathbb{C} \mid \text{all roots } z_i(w) \text{ of } r(z) - ws(z) = 0 \text{ satisfy } \mathrm{Re}(z_i(w)) < 0\}. \tag{2.2}$$

Here $r(z)$ and $s(z)$ are the (polynomial) transforms of $\rho(\xi)$ and $\sigma(\xi)$,

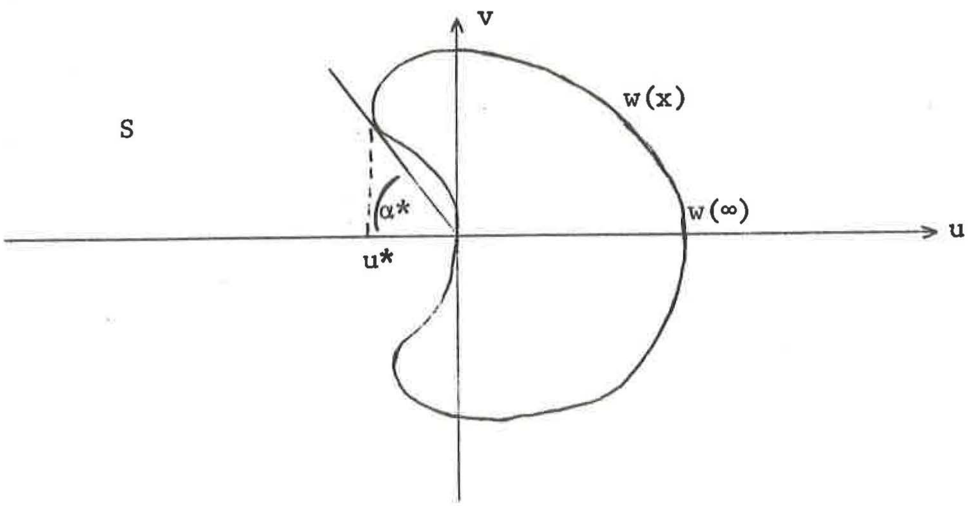
$$r(z) = \left(\frac{1-z}{2}\right)^k \rho\left(\frac{1+z}{1-z}\right) \equiv \sum_{j=0}^{k} a_j z^j\,, \quad s(z) = \left(\frac{1-z}{2}\right)^k \sigma\left(\frac{1+z}{1-z}\right) \equiv \sum_{j=0}^{k} b_j z^j. \tag{2.3}$$

The final definition we need is that of order of accuracy: as is well known, for given $r(z)$, $s(z)$, the method is of order m if

$$\frac{r(z)}{s(z)} = \log\left(\frac{1+z}{1-z}\right) + 0(z^{m+1}). \tag{2.4}$$

Notice that for S to include as much of the left half-plane as possible, we want the function $w(z) = \frac{r(z)}{s(z)}$ to map the left half-plane onto itself as mach as possible. Since $w = \log(\frac{1+z}{1-z})$ does this, we see from (2.4) that a method of order m maps correctly for $|z|$ small. For the trapezoidal rule, $\frac{r(z)}{s(z)} = 2z$, which maps perfectly for all z; unfortunately higher order stable methods cannot map as well for $|z|$ away from 0.

In the z-plane, any strongly stable method has $r(z)$ with one root $z_1 = 0$ and $\mathrm{Re}\, z_i < 0$ for $i > 1$. Hence $w = 0$ is on the boundary of S; and we can plot the locus of the boundary by the curve $w(x) = \frac{r(ix)}{s(ix)}$, $-\infty < x < \infty$. If the method is also stable at ∞, $s(z) = 0$ has all roots with $\mathrm{Re}\, z_i < 0$ and the complement of S will be a bounded region, typically with the following form:



(2.5)

Clearly, $w(o) = 0$, $w(\infty) = {}^{a_k}/_{b_k}$ $w(-x) = \overline{w(x)}$, and for small $|x|$, the curve follows the imaginary axis. In fact, from (2.4) we have

$$w(x) = \frac{r(ix)}{s(ix)} = \log\left(\frac{1+ix}{1-ix}\right) + 0(x^{m+1})$$

$$= 2\left(ix + \frac{(ix)^3}{3} + \frac{(ix)^5}{5} + \ldots\right) + 0(x^{m+1}).$$

Thus

$$\mathrm{Re}\, w(x) \sim x^{m+1}, \quad \mathrm{Im}\, w(x) \sim x$$

for $|x|$ small, so the real part stays very close to zero for $|x|$ small, and increases sharply as $|x| \to 1$; this accounts for the sudden bend in these curves for $|x| \cong 1$ (see for example Gear (1971), page 215).

Since we want $w(z)$ to map the left half-plane onto itself as much as possible, we can measure this by, for example, the angle α^* subtended by the boundary S at 0 (as in Widlund (1967), where this property is referred to as $A(\alpha^*)$ stability) and by $u^* = \min_x \mathrm{Re}(w(x))$. We shall use these later when discussing particular methods.

It is tempting to speculate that if the method is stable at 0 and ∞, $w(x)$ always looks like (2.5); i.e., it crosses the x-axis only at $x = 0$ and $x = \infty$. This would mean in particular that the stability region would include the negative real axis ($A(o)$ - stability). However in general this is false: take the method of third order with $r(z) = 2(4z + z^2 + \frac{19}{3} z^3)$, $s(z) = 4 + z + 5z^2 + z^3$. This is stable at 0 and ∞, but $w(ix)$ crosses the negative real axis at $-^8/_3$ and -6.

Of course the number and position of such crossings can be readily determined: they are the real λ such that

$$\begin{aligned} o = r(ix) - \lambda s(ix) &= (\Sigma(-1)^j a_{2j} x^{2j} - \lambda\Sigma(-1)^j b_{2j} x^{2j}) \\ &\quad + ix(\Sigma(-1)^j a_{2j+1} x^{2j} - \lambda\Sigma(-1)^j b_{2j+1} x^{2j}). \end{aligned}$$

Eliminating λ, $x^2 = y$ must be a real root of the polynomial

$$P(y) = (\Sigma(-1)^j b_{2j} y^j)(\Sigma(-1)^j a_{2j+1} y^j) - (\Sigma(-1)^j a_{2j} y^j)(\Sigma(-1)^j b_{2j+1} y^j). \tag{2.6}$$

Thus is $P(y)$ has no real positive roots, $w(x)$ has no extra crossings of the real axis. In particular, since the constant term in (2.6) is $2b_o{}^2 > 0$, we have

Theorem 2.1: A linear k-step method which is stable at 0 and ∞ is in fact $A(\alpha)$-stable for some α if the coefficients of the polynomial $P(y)$ in (2.6) are all positive.

Now we wish to investigate limits on the order of a method which is stable at 0 and stable at ∞. First of all, a necessary condition for a polynomial to have all its roots in the left half-plane is that all its coefficients be non-negative; thus we can assume that the coefficients $\{a_j\}$ of $r(z)$ and $\{b_j\}$ of $s(z)$ are non-negative. Also $a_0 = 0$ and $a_1 > 0$ since 0 is a simple root of $r(z)$. From (2.4) we have

$$r(z) - s(z) \log \left(\frac{1+z}{1-z}\right) = O(z^{m+1})$$

or,

$$\sum_{o}^{k} a_j z^j - 2\left(\sum_{o}^{k} b_j z^j\right)\left(z + \frac{z^3}{3} + \frac{z^5}{5} + \ldots\right) = O(z^{m+1}) \tag{2.7}$$

for a method of order m. Thus we have

$$\left.\begin{array}{l} \dfrac{a_1}{2} = b_o\,, \quad \dfrac{a_2}{2} = b_1 \\[2ex] \dfrac{a_3}{2} = b_2 + \dfrac{b_o}{3}\,, \quad \dfrac{a_4}{2} = b_3 + \dfrac{b_1}{3}\,, \\[2ex] \quad \cdot \; \cdot \; \cdot \; \cdot \\[1ex] \dfrac{a_j}{2} = b_{j-1} + \frac{1}{3}b_{j-3} + \frac{1}{5}b_{j-5} + \ldots + \begin{cases} \frac{1}{j}b_o\,, & \text{if } j \text{ odd} \\[1ex] \frac{1}{j-1}b_1\,, & \text{if } j \text{ even} \end{cases} \end{array}\right\} \tag{2.8}$$

for $j \le \min(m,k)$. If $m \ge k$, this defines the $\{a_j\}_1^k$ uniquely in terms of the $\{b_j\}$. If $m < k$, it defines $a_1, \ldots, a_m$.

Limits on the order of a method which is stable at 0 were obtained long ago by Dahlquist (1956):

Theorem 2.2: A linear k-step method is stable at 0 only for $m \le k + 1$ (for k odd) and $m \le k + 2$ (for k even). Those with $m = k + 2$ are only weakly stable.

For a proof see Gear (1971), page 197. The proof involves the positivity of the coefficients in the expansion of $z/\log\left(\frac{1+z}{1-z}\right)$.

In a very similar way we can show

Theorem 2.3: A linear k-step method is stable at ∞ only for $m \le k$ (for k even) and $m \le k + 1$ (for k odd). Those with $m = k + 1$ are only weakly stable.

Proof: We need only look at the coefficient of z^{k+1} in (2.7).

For k even, this coefficient is

$$-2\left(b_k + \frac{b_{k-2}}{3} + \dots + \frac{b_o}{k+1}\right)$$

which is strictly negative since all $b_j \ge 0$ and $b_o = a_1/2 > 0$.

Hence $m \le k$.

For k odd, this coefficient is

$$-2\left(b_k + \frac{b_{k-2}}{3} + \dots + \frac{b_1}{k+1}\right)$$

which is certainly less than or equal to zero, and equals zero only if $b_1 = b_3 = \dots = b_k = 0$. But this in turn implies $a_2 = a_4 = \dots = a_{k+1} = 0$, which means that at best both r(z) and s(z) have roots on the imaginary axis, giving a weakly stable method. And of course even for this method, the next coefficient (of z^{k+2}) is strictly negative so the order $m \le k + 1$.

QED.

This theorem says essentially that the best order we can achieve with a useful k-step method is m = k (except for the trapezoidal scheme which has k = 1, m = 2). Note that in this case the method is completely specified by the coefficients $\{b_j\}$; the $\{a_j\}$ are given by (2.8). An example of such a class of methods is the backward differentiation formulas, recently popularized by Gear (1968) where $s(z) = (z+1)^k$ or $\sigma(\xi) = \xi^k$. These are obviously stable at ∞, and have the further property of being damped at ∞; for the problem $y' = \lambda y$, as $\mathrm{Re}(h\lambda) \to -\infty$, $|y_{n+1}/y_n| \to 0$, so the damping effect is always greater for larger decay rates. In fact these are the only linear k-step methods of order k with this property, because with any other $\sigma(\xi)$, $|y_{n+1}/y_n| \to |\xi_1(\sigma)|$, the biggest root of $\sigma(\xi)$. Unfortunately these methods are stable at 0 only for $k \le 6$.

Various other k-step methods of order k have been derived, with the aim of extending the order of those stable at 0 and ∞. Instead of $s(z) = (z+1)^k$ as in Gear, Cryer (1973) tried $s(z) = (z+d)^k$; for d close to 1, these may still be useful for stiff problems. Cryer showed such schemes could be made stable along the negative real axis for any k, by taking d small enough. More recently, Jeltsch (1974) has shown these methods are actually $A(\alpha)$-stable for certain α.

In fact, this is not difficult to see: since $s(z) = (z+d)^k$,

$$\frac{r(z)}{2} = z[(z+d)^k - z^k](1 + O(d^2)) \equiv c(z)(1 + O(d^2)).$$

Thus for d small, the roots of $r(z)$ are close to the roots $\{z_j\}$ of $c(z)$, which are

$$z_j = \frac{-d}{1 - e^{2\pi ij/k}}, \ j = 1, \ldots, k - 1, \text{ and } z_k = 0.$$

So the method is stable at 0 for d small enough, and one need only show that the roots $\{z_j(\lambda)\}$ of $[r(z) + \lambda s(z)]$ stay in the left half-plane for $0 < \lambda < \infty$ to ensure $A(\alpha)$-stability for some α.

Cryer and Jeltsch require $d \sim 2^{-k}$ for stability. This is easily seen to be unrealistic when the methods are computed: for $k = 10$ the method is stable for $d < 0.2$; for $k = 20$, stable for $d < 0.1$. Even so however, these methods are not of practical use: the asymptotic decay rate $|y_{n+1}/y_n|$ for the model problem $y' = \lambda y$ as $\mathrm{Re}(h\lambda) \to -\infty$, is $c = \frac{1-d}{1+d}$ which is $\geq 1/3$ for $d < 0.5$, and approaches 1 as $d \to 0$. Thus although the region of absolute stability looks like (2.5), the decay rate in the whole left half-plane is close to 1 if d is close to zero.

3. k-step Methods of Order m

Because of the apparent impossibility of obtaining k-step methods of order k which are useful for stiff problems and are of order higher than 6, it is natural to try methods of degree k and order $m < k$. More specifically, let us assume the polynomial $s(z) = \sum_o^k b_j z^j$ is given, and try to determine coefficients $\{a_j\}_1^k$ so that

$r(z) = \sum_1^k a_j z^j$ is stable (i.e., all roots in left half-plane) and the k-step method thus formed has order m. From (2.8), we see that the order requirement determines exactly $a_1, \ldots, a_m$, and we are free to choose the rest. To ensure stability, we must choose these coefficients carefully, and it is not at all clear how to do this. Let us examine this problem more closely.

First of all, a well-known necessary and sufficient stability condition for $r(z) = \sum_1^k a_j z^k$ with <u>all</u> coefficients prescribed, is that the Hurwitz determinants be positive (see e.g. Marden [1966, pg. 181]). That is, we form the matrix

$$\begin{pmatrix} a_2 & a_4 & a_6 & a_8 \cdots & \\ a_1 & a_3 & a_5 & a_7 \cdots & \\ 0 & a_2 & a_4 & a_6 & a_8 \cdots \\ 0 & a_1 & a_3 & a_5 & a_7 \cdots \\ & \cdots\cdots & & \ddots & \\ & & & & a_k \end{pmatrix}, \tag{3.1}$$

where each $a_j = 0$ for $j > k$, and take the determinants of the leading principal minors; these must all be positive. (Notice that since $a_0 = 0$, all our coefficients have subscripts advanced by 1 from the normal discussion of stable polynomials.) To put this criterion in a more tractable form for computation, we can reduce the matrix to upper triangular form by a judicious choice of row eliminations. Since this will not change the determinants, the criterion will be equivalent to the diagonal elements of the triangular matrix being positive.

We perform this triangular reduction by first eliminating all coefficients a_1 from below the diagonal, then all a_2's, etc. Because of the repetitive form of the rows, if we eliminate a by subtracting a multiple of row 1 from row 2, then the same multiple of row 3 from row 4, etc., we keep the repetitive pattern of the rows, and the even rows become

$$a_3^{(1)},\ a_5^{(1)},\ a_7^{(1)},\ \ldots.$$

via

$$a_{2j+1}^{(1)} = a_{2j+1} - \frac{a_1}{a_2}\, a_{2j+2},\ j = 1, \ldots, [\tfrac{k-2}{2}].$$

In particular, $a_3^{(1)}$ is the second diagonal element of the triangular form. Now we eliminate all a_2's by subtracting the proper multiple of row 2 from row 3, row 4 from row 5, etc., forming the new odd row

$$a_4^{(1)},\ a_6^{(1)},\ a_8^{(1)},\ \ldots$$

via

$$a_{2j+2}^{(1)} = a_{2j+2} - \frac{a_2}{a_3^{(1)}}\, a_{2j+3}\ ,\ j = 1, \ldots, [\tfrac{k-3}{2}].$$

Again, the first element so formed, $a_4^{(1)}$, is the third diagonal element of the reduced triangular form. We continue in this way, eliminating in turn all a_3's, a_4's, ..., a_{k-2}'s from below the diagonal. The entire reduction can be expressed as follows:

$$
\begin{aligned}
a^{(1)}_{2j+1} &= a_{2j+1} - \frac{a_1}{a_2} a_{2j+2}\ , \quad j = 1, \ldots, [\tfrac{k-2}{2}] \\
a^{(1)}_{2j+2} &= a_{2j+2} - \frac{a_2}{a_3^{(1)}} a_{2j+3}, \quad j = 1, \ldots, [\tfrac{k-3}{2}] \\
a^{(2)}_{2j+3} &= a^{(1)}_{2j+3} - \frac{a_3^{(1)}}{a_4^{(1)}} a^{(1)}_{2j+4}\ , \quad j = 1, \ldots, [\tfrac{k-4}{2}] \\
a^{(2)}_{2j+4} &= a^{(1)}_{2j+4} - \frac{a_4^{(1)}}{a_5^{(2)}} a^{(2)}_{2j+5}\ , \quad j = 1, \ldots, [\tfrac{k-5}{2}] \\
&\cdots
\end{aligned}
\tag{3.2}
$$

This set of recurrence relations provides an $O(k^2)$ process for deciding the stability of a given polynomial. We shall refer to the diagonal elements thus obtained $(a_3^{(1)}, a_4^{(1)}, a_5^{(2)}, a_6^{(2)}, \ldots) \equiv (c_3, c_4, \ldots, c_{k-1})$ as the Hurwitz factors of $r(z)$. Computationally this reduction can be carried out using only one array, with the Hurwitz factors as the final values obtained by the array. Schematically, the reduction can be expressed in a tableau

$$
\begin{array}{ccccccccccc}
a_1 & & a_3 & & a_5 & & a_7 & \cdots & & & \\
& a_2 & & a_4 & & a_6 & & a_8 \cdots & & & \\
& & a_3^{(1)} & & a_5^{(1)} & & a_7^{(1)} \cdots & & & & \\
& & & a_4^{(1)} & & a_6^{(1)} & & a_8^{(1)} \cdots & & & \\
& & & & a_5^{(2)} & & a_7^{(2)} \cdots & & & & \\
& & & & & a_6^{(2)} & & a_8^{(2)} \cdots & & & \\
& & & & & & a_7^{(3)} \vdots & & & & \\
& & & & & & & \ddots & & &
\end{array}
\tag{3.3}
$$

Now let us return to the problem posed at the beginning of this section: given $r_m(z) = a_1 z + \ldots + a_m z^m$, when and how can we extend this to a polynomial of degree k which is stable?

Theorem 3.1: A sufficient condition for the existence of a stable extension of degree k is that the given polynomial $r_m(z)$ be stable.

Proof: We need only show that we can extend $r_m(z)$ to a stable polynomial $r_m(z) + a_{m+1} z^{m+1}$ of degree m+1; for then we can repeat the process up to degree k. But this is surely possible for a_{m+1} small enough; the Hurwitz determinants (see (3.1)) of the new polynomial are continuous functions of this last coefficient a_{m+1}, and are all positive for $a_{m+1} = 0$, so they must remain positive for a_{m+1} slightly positive as well. QED.

This seems like a simple straightforward criterion to use; however it turns out to be too strong for the polynomials we are interested in, so we must seek weaker conditions. To see that this criterion is not necessary for a stable extension, consider the example with m = 5, k = 6:

$$r_5(z) = z + z^2 + \tfrac{4}{3}z^3 + z^4 + \tfrac{1}{2}z^5$$

is unstable; however $r_6(z) = r_5(z) + \frac{1}{3}z^6$ is stable.

Theorem 3.2: The following are necessary conditions for the existence of a stable extension of degree k:

1. the Hurwitz factors $c_3, \ldots, c_{[\frac{m+2}{2}]}$ of $r_m(z)$ must be positive.

2. the polynomial $d_m(z) = a_1 z + [\frac{(k-2)\ \ldots\ (m-1)}{(k-1)\ \ldots\ m}] a_2 z^2 + \ldots + [\frac{(k-m)\ \ldots\ 1}{(k-1)\ \ldots\ m}] a_m z^m$ must be stable.

Proof: From the tableau (3.3), the Hurwitz factors of (1) are precisely those which depend only on the given coefficients $a_1, \ldots, a_m$; since they are unaffected by the choice of $a_{m+1}, \ldots, a_k$, they must be positive to begin with.

And, if $r(z)$ is to be stable, all derivatives of $r(z)$ must also be stable, since the roots of a derivative lie in the convex hull of the roots of the original polynomial (see for example Marden (1966; pg 22)). Similarly the reciprocal polynomial $z^k r(\frac{1}{z})$ must also be stable. Thus

$$(z^k r(\tfrac{1}{z}))^{(k-m)} = [(k-1) \ldots m]a_1 z^{m-1} + [(k-2) \ldots (m-1)]a_2 z^{m-2} + \ldots + [(k-m) \ldots 1]a_m$$

must be stable. But $d_m(z)$ is merely a constant multiple of the reciprocal of this polynomial, so must also be stable. QED.

The following examples show that neither of these conditions implies the other, and thus neither condition is sufficient for a stable extension to exist.

(a) $m = 5$, $k = 6$; $r_5(z) = z + \frac{5}{4}z^2 + \frac{20}{9}z^3 + \frac{5}{2}z^4 + \frac{5}{2}z^5$

$$d_5(z) = z + z^2 + \tfrac{4}{3}z^3 + z^4 + \tfrac{1}{2}z^5$$

Here (1) holds ($c_3 > 0$) but (2) doesn't.

(b) $m = 4$, $k = 5$; $r_4(z) = z + \frac{4}{3}z^2 + \frac{8}{3}z^3 + 4z^4$

$$d_4(z) = z + z^2 + \tfrac{4}{3}z^3 + z^4$$

Here (2) holds but (1) doesn't ($c_3 < 0$).

4. Higher Order Methods Damped at ∞

As we mentioned earlier, a particularly useful set of multistep methods for stiff equations are those with $\sigma(\xi) = \xi^k$. Gear (1968) shows the k-step methods of order k generated this way are stable for $k \leq 6$. By reducing the stability requirement to $m < k$, we can find stable methods of higher order.

Proceding as in Section 3, we prescribe k and $s(z) = (z+1)^k$. Then we determine coefficients $a_1, \ldots, a_m$ of $r(z) = \sum_o^k a_j z^j$ by the accuracy requirements (2.8). This gives

$$\left.\begin{aligned}
&\frac{a_1}{2} = 1,\ \frac{a_2}{2} = k,\ \frac{a_3}{2} = \binom{k}{2} + \frac{1}{3},\ \frac{a_4}{2} = \binom{k}{3} + \frac{k}{3},\\
&\frac{a_5}{2} = \binom{k}{4} + \frac{1}{3}\binom{k}{2} + \frac{1}{5}\binom{k}{0},\ \frac{a_6}{2} = \binom{k}{5} + \frac{1}{3}\binom{k}{3} + \frac{1}{5}\binom{k}{1},\\
&\ldots\ldots\\
&\frac{a_m}{2} = \begin{cases} \binom{k}{m-1} + \frac{1}{3}\binom{k}{m-3} + \ldots + \frac{1}{m}\binom{k}{0}, & \text{if m odd} \\ \binom{k}{m-1} + \frac{1}{3}\binom{k}{m-3} + \ldots + \frac{1}{m-1}\binom{k}{1}, & \text{if m even.} \end{cases}
\end{aligned}\right\} \quad (4.1)$$

Now we check to see if the polynomial $r_m(z)$ defined by these coefficients has a stable extension to degree k, and then try to find suitable coefficients $a_{m+1}, \ldots, a_k$.

First, we merely checked the sufficient condition (Theorem 3.1) for a stable extension, namely that the polynomial $r_m(z)$ itself be stable; this we did by constructing the Hurwitz factors using (3.2). However, this showed a stable extension only for m = 7 and k = 8, 9, 10.... So we switched to the less stringent necessary conditions (Theorem 3.2).

In fact, the first of the necessary condition is automatically satisfied for these polynomials: going back to the Hurwitz determinants (3.1), the Hurwitz factors $c_3, \ldots, c_{[\frac{m+2}{2}]}$ are determined by the top $[\frac{m}{2}] \times [\frac{m}{2}]$ block; for m = 8 this is

$$\begin{pmatrix} a_2 & a_4 & a_6 & a_8 \\ a_1 & a_3 & a_5 & a_7 \\ 0 & a_2 & a_4 & a_6 \\ 0 & a_1 & a_3 & a_5 \end{pmatrix}.$$

Now express these coefficients in terms of the coefficients $\{b_j\}$ of s(z) using (4.1) or, more generally, (2.8). By subtracting column multiples, it is easy to see that these first $[\frac{m}{2}]$ Hurwitz determinants are the same as those using the coefficients $\{b_j\}_o^{m-1}$; for m = 8 we mean the subdeterminants of

$$\begin{pmatrix} b_1 & b_3 & b_5 & b_7 \\ b_0 & b_2 & b_4 & b_6 \\ 0 & b_1 & b_3 & b_5 \\ 0 & b_0 & b_2 & b_4 \end{pmatrix}.$$

And these, of course, are all positive since s(z) is stable. This can be stated more formally as

<u>Lemma 4.1</u>: Given the stable polynomial s(z) of degree k, if we demand that the corresponding polynomial r(z) be such that the corresponding linear multistep method have order m < k, then

the Hurwitz factors $c_3, \ldots, c_{[\frac{m+2}{2}]}$ are positive.

Our algorithm for finding stable extensions then proceeded as follows: given k and m, we first formed and checked the stability of the polynomial $d_m(z)$ in Theorem 3.2. If stable, we then integrated $d_m(z)$ (k-m) times, at each step finding one new suitable coefficient (a_{m+1}, then $a_{m+2}, \ldots, a_k$) so the integrated polynomial was still stable (since each of these integrated polynomials is a derivative of the final polynomial r(z), each must be stable). Finally, we locally optimize the choice of coefficients $a_{m+1}, \ldots, a_k$ by using a search routine in these (k-m) dimensions.

First we optimized by minimizing the modulus of the subdominant root $|\xi_2|$ of $\rho(\xi) = 0$, so the method could be "as stable as possible at 0". However the methods so found did not have the largest possible regions of absolute stability, and were not even A(0)-stable necessarily. So we instead optimized by maximizing the angle α^* of (2.5) for the method.

We present here the methods obtained in this way of orders 6, 7, and 8. We give only the coefficients $\{a_j\}_1^k$ of r(z), and these only to at most 5 significant figures. Coefficients $a_1, \ldots, a_m$ can be found as accurately as desired from (4.1) and the accuracy of the remaining coefficients $a_{m+1}, \ldots, a_k$ is not crucial.

m	k	coefficients $a_1, \ldots, a_k$	α^*	u^*	$\lvert\xi_2(0)\rvert$
6	7	2.0, 14.0, 42.667, 74.667, 84.4, 68.133, <u>15.52</u>	29.18°	-3.9	.84
7	9	2.0, 18.0, 72.667, 174.0, 276.4, 311.6, 266.69, <u>113.32</u>, <u>50.25</u>	29.5°	-11.2	.88
8	10	2.0, 20.0, 90.667, 246.67, 450.4, 588.0, 578.28, 458.86 <u>186.79</u>, <u>90.0</u>	-20.8°	-29.0	.99
8	11	2.0, 22.0, 110.67, 337.33 697.06, 1038.4, 1166.3, 1037.1, <u>520.0</u>, <u>270.0</u>, <u>24.5</u>	1.8°	-15.4	.97

In Figures 1-4, we plot the top half of the stability regions for these methods. All were $A(\alpha)$-stable for $\alpha = \alpha^*$ given in the Table, except for the third method ($m = 8$, $k = 10$), where the boundary of S cuts the negative real axis. When we added an extra degree of freedom ($k = 11$), we again found an $A(\alpha)$-stable method. These are not necessarily the best possible for a given m and k, since we could only perform a local search. The method of order 6 is given to show how the stability region can be improved by extending k to 7 from 6 (for the case $k = 6$, $m = 6$, see Gear (1971), page 216).

We shall examine the performance of these methods on some specific stiff problems in a later paper.

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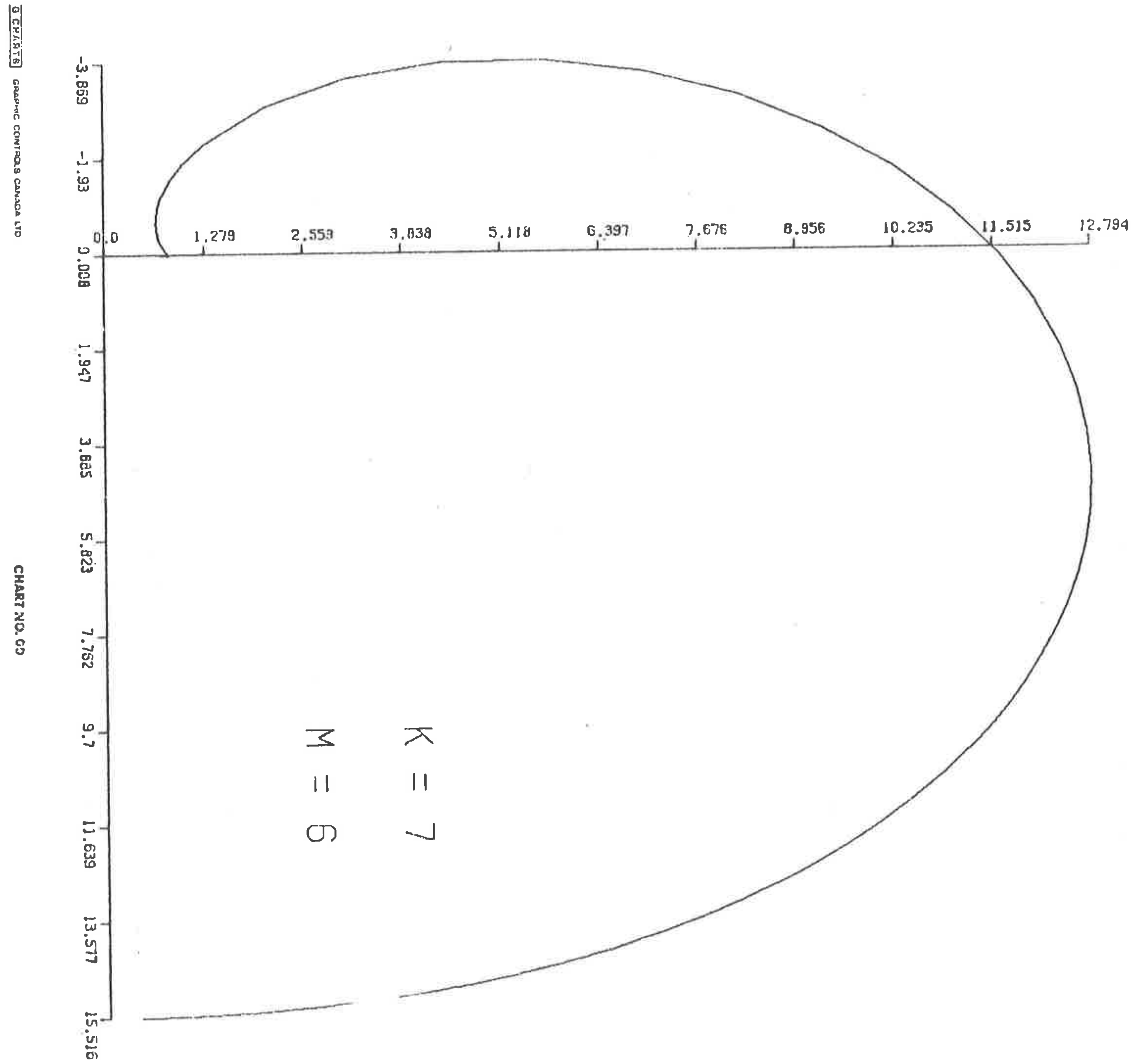

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M = 6
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3.838
5.118
6.397
7.676
8.956
10.235
11.515
12.794
-3.869
-1.93
0.008
1.947
3.885
5.823
7.762
9.7
11.639
13.577
15.516
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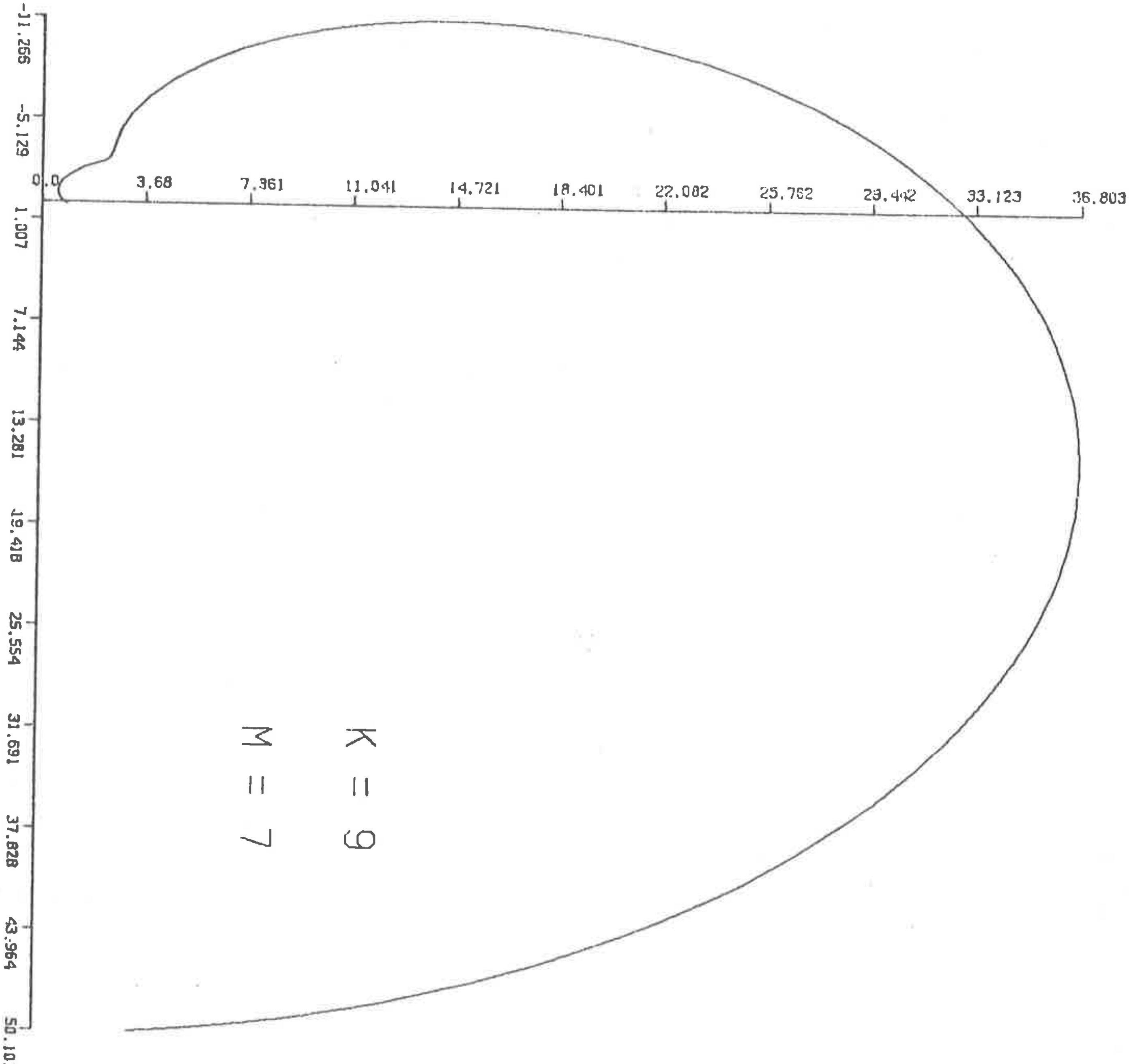
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3.68
7.361
11.041
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33.123
36.803
-11.266
-5.129
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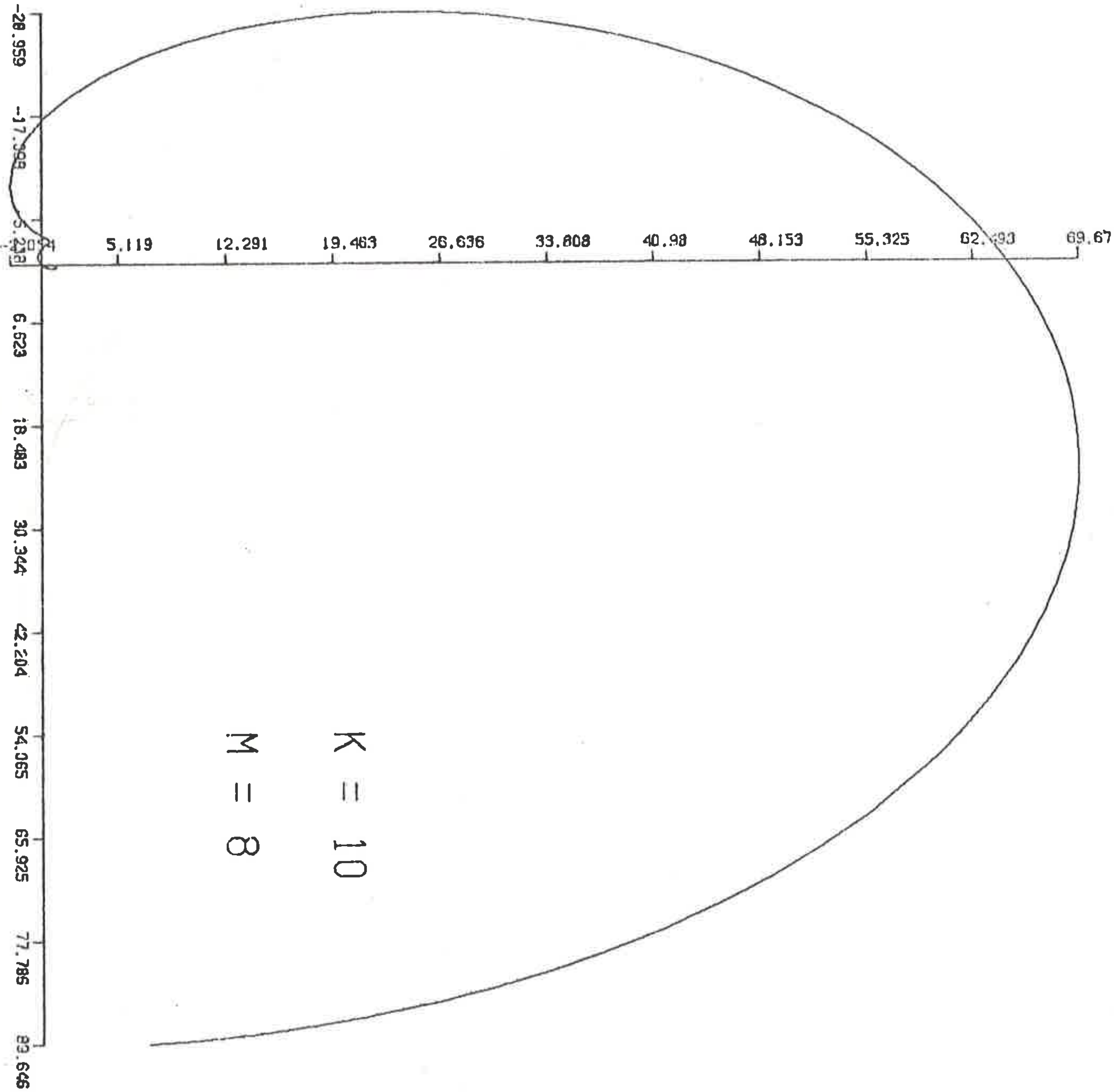
M = 7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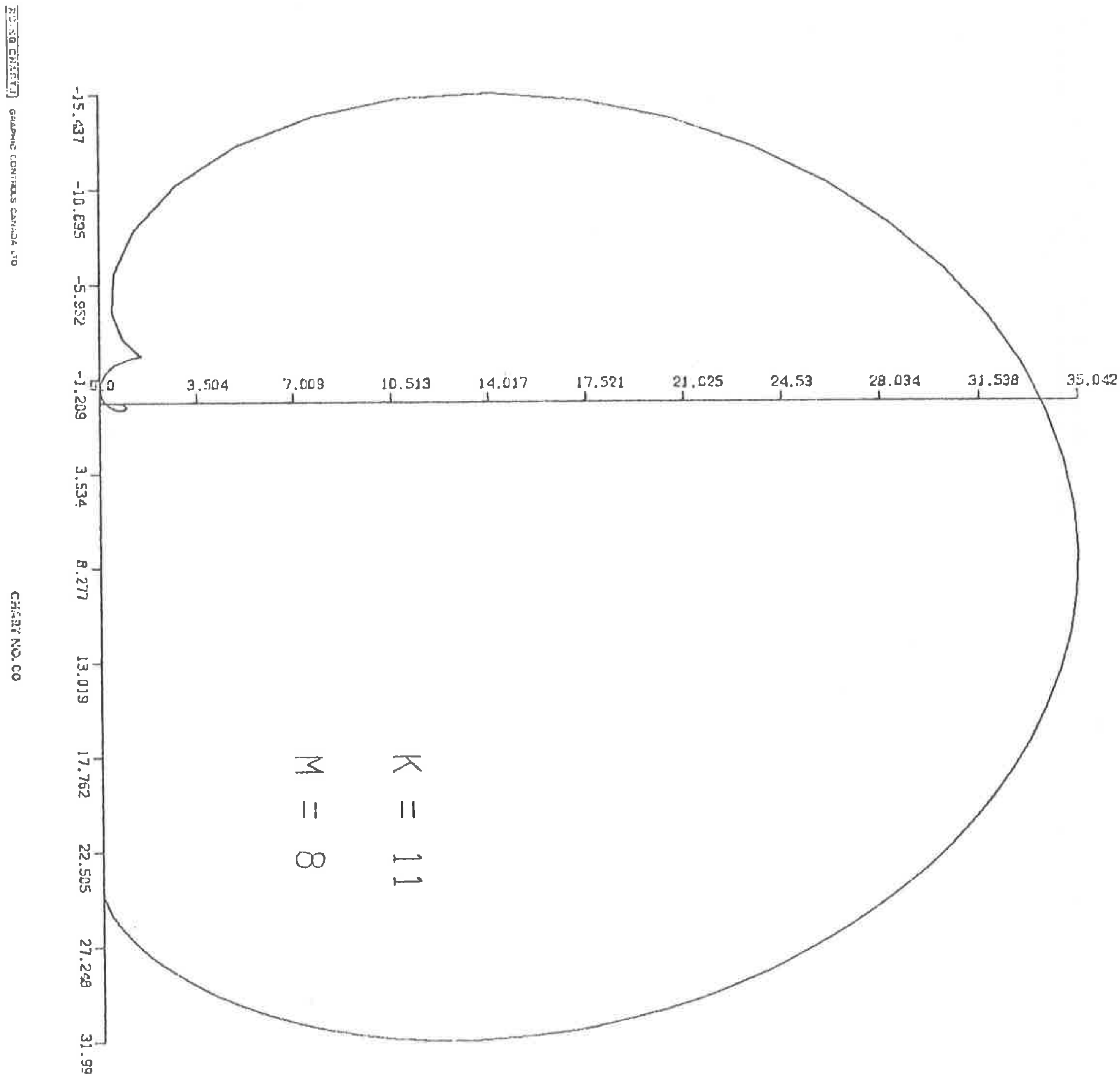
65.925
77.786
89.646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21.025
24.53
28.034
31.538
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-10.695
-5.952
-1.209
3.534
8.277
13.019
17.762
22.505
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31.99
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