A PROOF OF THE DANIEL-MOORE CONJECTURES FOR A-STABLE MULTISTEP TWO-DERIVATIVE INTEGRATION FORMULAS

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Abstract

A simple proof is given of the following particular case of the Daniel-Moore conjectures, recently proved in full generality by Wanner, Hairer and Nørsett. The maximum error order achievable by an A-stable $k$-step two-derivative formula equals four and the optimum value of the corresponding error constant is achieved by the second Obrechkoff method. The arguments presented in this paper reveal some new properties of two-variable Hurwitz polynomials of degree $(k,2)$ which, when applied to the canonical polynomial associated with the integration formula, directly yield a proof of the Daniel-Moore conjectures in the case considered herein.

1. Introduction

The problem of the maximum error order compatible with A-stability for multistep multiderivative integration formulas has been recently tackled in an important paper by Wanner, Hairer and Nørsett 1). In their contribution, in addition to several other results, these authors present a proof of the Daniel-Moore conjectures 2) saying that the maximum error order achievable by an $n$-derivative formula equals $2n$ and that the minimum absolute value of the corresponding error constant is

$$(n!)^2/(2n)! (2n+1)!.$$ 

The aim of the present paper is to offer an alternative proof of the Daniel-Moore conjectures for the case $n = 2$, which reveals some interesting properties of two-variable Hurwitz polynomials and of positive algebraic functions of degree 2. These properties have the remarkable feature of being expressible in terms of positive reality of certain one-variable rational functions. In that respect, it is worth mentioning that the power of the approach to stability problems via positive functions is nowadays well recognized, not only in numerical analysis as shown by Dahlquist 3) but also in various other fields of applied mathematics 4-9).

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The twofold aspect of the paper is reflected in its organization. In the first part (secs 2 and 3), the Daniel-Moore conjectures are discussed with the help of the canonical polynomial introduced in ref. 10 and a proof of the conjectures is worked out, which relies upon some properties exhibited by positive algebraic functions of degree 2. The properties in question are then proved in the second part (sec. 4) independently of the Daniel-Moore environment and thus are, it is hoped, capable of applications in other areas.

The general properties of $A$-stable $k$-step $n$-derivative formulas as described in ref. 10 are briefly recalled in sec. 2. Two technical modifications with respect to ref. 10 are introduced. The first one pertains to the very definition of the error order, oddly defined in ref. 10 and corrected here to comply with standard practice in the field as suggested by Gear, Jeltsch and Wanner et al. The second modification affects the question of the exact properties of the even and odd parts of the canonical polynomial that are implied by the assumption of asymptotic convergence.

The main part of the paper is concerned with the particular case $n = 2$. Sec. 3 contains the preliminary steps of the proof of the Daniel-Moore conjectures. Even and odd canonical polynomials associated with $k$-step 2-derivative formulas of error order 4 are expressed into a well-defined parametric form. Then the problem reduces to discovering the properties of the one-variable parameter polynomials that result from the stability condition.

This problem is solved in sec. 4, in its most natural framework. The main result, which directly yields a proof of the Daniel-Moore conjectures for $n = 2$, asserts that a certain one-variable rational function derived from a two-variable Hurwitz polynomial of degree $(k, 2)$ has to be a positive real function. An interesting interpretation of this result in terms of transformations of Hurwitz polynomials is emphasized.

### 2. Definitions and preliminaries

In the present paper we are mainly interested in $A$-stable strongly convergent integration methods, but we also consider certain weakly convergent methods in the process of argumentation. Let us recall the algebraic characterization of these properties in terms of the so-called canonical polynomial. Let

$$
\sum_{t=0}^{n} \sum_{j=0}^{k} (-1)^{t} a_{t,j} h^{t} D^{j} x_{t-j} = 0, \quad t = k, k + 1, \ldots
$$

be any $k$-step $n$-derivative integration formula, and let

$$
H(p, q) = a_0(p) + q a_1(p) + \ldots + q^n a_n(p)
$$

be its associated canonical polynomial$^{10}$, where
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\[
a_k(p) = (p - 1)^k \sum_{j=0}^{k} a_{k,j} \left( \frac{p + 1}{p - 1} \right)^{k-j}.
\]  \hspace{1cm} (3)

The \((k, n)\) method based on (1) is weakly stable provided the polynomial \(a_0(p) = H(p, 0)\) has exact degree \(k - 1\), does not vanish in the open right-half plane \(\text{Re} p > 0\) and has at most simple zeros on the imaginary axis \(\text{Re} p = 0\). In case \(a_0(p)\) does not vanish on \(\text{Re} p = 0\), such a method is strongly stable. A weakly (strongly) stable method is weakly (strongly) convergent provided it is consistent, which means that \(a_1(p)\) has exact degree \(k\) and satisfies \(2a_1(p) = pa_0(p) + o(p^{k-1})\). In the sequel, \(a_1(p)\) is then assumed to be monic, which is a simple matter of normalization.

A weakly stable \((k, n)\) integration formula is said to have the error order \(\nu\) and the corresponding error constant \(K_{\nu+1}\) if its associated canonical polynomial satisfies

\[
\frac{1}{p^k} H\left( p, -\log \frac{p + 1}{p - 1} \right) \sim K_{\nu+1} \left( \frac{2}{p} \right)^{\nu+1}, \quad \text{for } p \to \infty.
\]  \hspace{1cm} (4)

Note that the assumption of consistency implies (4) with \(\nu = 1\). It is clear that (4) remains satisfied if the possible one-variable divisors of \(H(p, q)\) are factored out. Henceforth we assume, without loss of generality, that \(H(p, q)\) has no factors of the form \(u(p)\) or \(v(q)\). In this case, the integration formula (1) is known to be A-stable if and only if (2) is a Hurwitz polynomial in the narrow sense \(^{4,10}\), which means that \(H(p, q)\) does not vanish in both regions \(\text{Re} p \geq 0, \text{Re} q > 0\), and \(\text{Re} p > 0, \text{Re} q \geq 0\).

Decomposing the canonical polynomial into its even and odd parts, and using well-known properties of two-variable Hurwitz polynomials, one obtains the following result, which provides a significant simplification in the theory of the maximal order achievable by A-stable integration formulas \(^{10,12}\).

**THEOREM 1.** Let there exist an A-stable strongly convergent \((k, n)\) formula of error order \(\nu\) and error constant \(K_{\nu+1}\). Then there exists an A-stable weakly convergent \((k', n')\) formula, with \(k' \leq k\) and \(n' \leq n\), of same error order \(\nu\) and error constant \(K_{\nu+1}\), admitting an even or odd canonical polynomial.

The statement of theorem 1 differs from the corresponding statement given by Jeltsch \(^{12}\), in regard to the distinction between strong and weak stability. However, the argument used by Jeltsch precisely leads to the conclusion of theorem 1.
3. A-stable \((k, 2)\) integration formulas

From now on, we restrict our attention to the case \(n = 2\). We shall establish the following version of the Daniel–Moore conjectures ². (In fact, the present section contains only the preliminary steps of the proof; the crux of the proof is in section 4.)

**THEOREM 2.** The maximum error order reachable by an \(A\)-stable strongly convergent \((k, 2)\) formula is \(v = 4\), and the minimum value of the corresponding error constant is \(K_6 = 1/720\). (This optimum is achieved by the second Obrechkoff method, the canonical polynomial of which is \(H(p, q) = 2 + pq + \frac{1}{2} q^2\).)

The first step of the argument consists in using theorem 1. Thus we shall consider the class of even or odd polynomials (2) characterizing \(A\)-stable weakly convergent \((k, 2)\) formulas. In fact, we shall treat in full detail the even case only; it turns out that the odd case can be treated by a mere duplication of the method used in the even case.

Let then \(k = 2m + 1\) and let

\[
H(p, q) = a(p) + pq b(p) + q^2 c(p)
\]  

be an even polynomial associated with a \((2m + 1)\)-step 2-derivative formula. By definition, \(a(p)\), \(b(p)\) and \(c(p)\) are even polynomials of formal degree \(2m\).

Let us write

\[
a(p) = \sum_{i=0}^{m} a_i p^{2(m-i)},
\]

and similarly for \(b(p)\) and \(c(p)\). In view of (4), assuming the formula to have the error order \(v = 4\) imposes the constraints

\[
a_0 = 2b_0 = 2, \quad a_1 = \frac{7}{3} b_0 + 2b_1 - 4c_0,
\]

and yields the following value for the error constant

\[
K_6 = \frac{1}{32} (a_2 - \frac{7}{3} b_0 - \frac{8}{3} b_1 - 2b_2 + 4c_0 + \frac{8}{3} c_1).
\]

It will prove quite useful to parametrize \(H(p, q)\) in terms of the polynomials \(a(p), x(p), y(p)\), where \(x(p)\) and \(y(p)\) are defined as

\[
x(p) = b(p) - \frac{1}{2} a(p), \quad y(p) = c(p) - \frac{1}{15} a(p) - \frac{1}{2} p^2 x(p).
\]

With the help of (9) one can rewrite (5) as

\[
H(p, q) = (1 + \frac{1}{3} pq + \frac{1}{15} q^2) a(p) + pq (1 + \frac{1}{3} pq) x(p) + q^2 y(p).
\]
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It is easily seen that the constraints (7) are equivalent to $x_0 = y_0 = 0$ (and $a_0 = 2$). As a result, substituting for $a(p)$, $x(p)$ and $y(p)$ in (10) even polynomials of respective formal degrees $2m$ (with $a_0 = 2$), $2m - 2$ and $2m - 2$ yields the general form of even canonical polynomials associated with $(2m + 1, 2)$ integration formulas exhibiting order $v \geq 4$. In addition, (8) becomes

$$K_5 = \frac{[1 + 15(x_1 + 6y_1)]}{720}. \quad (11)$$

In the present situation, the first Daniel–Moore conjecture amounts to saying that the properties of $A$-stability and weak convergence force $K_5 > 0$ and hence $v \leq 4$; their second conjecture is stronger, saying that $K_5$ is bounded from below by 1/720 and achieves this value only in the degenerate case $m = 0$. In view of (11), the latter conjecture reduces to $x_1 + 5y_1 \geq 0$, with equality if and only if $x(0) = y(0) = 0$ and $a(p) = 2$. The truth of this conjecture is established in sec. 4, in a framework where the basic ideas underlying the theory appear more clearly than in the present context. To obtain the result mentioned above, if suffices to specialize theorem 3 of sec. 4 to the case $\lambda = 1/2$, $\mu = 1/12$.

To have a complete proof of theorem 1, one should also treat the case of an odd polynomial $H(p, q)$. The simplest way to do so consists in duplicating the methods of the present and next sections for the even polynomial $H'(p, q) = pH(p, q)$. The only difference lies in the presence of a double zero of $H'(p, 0)$ at the origin, but this gives rise to no real difficulty. The details are omitted.

4. Even Hurwitz polynomials of degree $(2m + 1, 2)$

Let $H(p, q)$ be an even two-variable polynomial, with real coefficients, of degree $2m + 1$ in $p$ and degree 2 in $q$. Then $H(p, q)$ can be written in the form $a(p) + pq b(p) + q^2 c(p)$, as in (5), with

$$a(p) = \sum_{i=0}^{m} a_i p^{2(m-i)}$$

and similarly for $b(p)$ and $c(p)$. We shall now analyse the properties of such polynomials $H(p, q)$ which are Hurwitzian in the narrow sense, with the additional requirements that $a_0$ and $b_0$ are strictly positive and that $a(p)$ has only simple zeros (necessarily on the imaginary axis). Thus we shall treat a slightly generalized version of the problem raised in sec. 3.

A first consequence of Hurwitzity is that both rational functions $pb(p)/a(p)$ and $pb(p)/c(p)$ are positive real \(^4\). Hence one can write \(^6\)
with \( \lambda = b_0/a_0 > 0 \), where the \( \alpha_s \) and \( \beta_s \) are positive real numbers satisfying 
\[ 0 < \alpha_1 < \alpha_2 < \ldots < \alpha_m \] (since \( a(p) \) is assumed to have simple zeros) and 
\[ \beta_s \leq \alpha_s \leq \beta_s \] for \( s = 1, 2, \ldots, m \). Because \( H(p, q) \) is even, it is clear, as a further consequence of Hurwitzity, 
that the zeros of the trinomial \( H(i\omega, q) \) must lie on the imaginary axis 
\( \text{Re} q = 0 \), for any given real number \( \omega \). In other words, the corresponding 
discriminant of (5) must be nonpositive, i.e.

\[ f(\omega) = \omega^2 b^2(i\omega) + 4a(i\omega)c(i\omega) \geq 0, \] (13)

for all real \( \omega \). This readily implies that all inequalities \( \alpha_s \leq \beta_s \leq \alpha_{s+1} \) are 
strictly satisfied, so that \( a(p) \) and \( b(p) \) have no common factor. Indeed, in 
case \( \alpha_s = \beta_i = \omega_0^2 \), i.e., \( a(i\omega_0) = b(i\omega_0) = 0 \) for some \( \omega_0 \), the condition (13) 
forces \( \omega_0 \) to be a double zero of \( f(\omega) \), which in turn forces \( c(i\omega_0) \) to vanish; 
hence \( H(i\omega_0, q) \) should be identically zero, which contradicts the assumption 
of Hurwitzity (in the narrow sense). As a conclusion

\[ 0 < \alpha_1 < \beta_1 < \alpha_2 < \beta_2 < \ldots < \alpha_m < \beta_m. \] (14)

Since (12) is a positive real function, its pole at infinity can be extracted to 
produce a new positive real function \( ^5 \), namely

\[ px(p)/a(p) = \rho[b(p) - \lambda a(p)]/a(p), \] (15)

where \( \lambda = b_0/a_0 > 0 \) and where

\[ x(p) = b(p) - \lambda a(p) = \sum_{i=1}^{m} x_i p^{2(m-i)} \]
is an even Hurwitz polynomial of exact degree \( 2m - 2 \), with \( x_1 > 0 \). With the 
help of \( x(p) \) one can rewrite \( f(\omega) \) in the form

\[ f(\omega) = \omega^2 [\lambda a(i\omega) - x(i\omega)]^2 + 4a(i\omega) [c(i\omega) + \lambda \omega^2 x(i\omega)]. \] (16)

To study this expression, let us first consider

\[ v(p) = \lambda a(p) - x(p) = 2\lambda a(p) - b(p), \] (17)

which is an even polynomial of exact degree \( 2m \). In view of (14), the sign of 
\( v(ia_1^s) \) is known to be \((-1)^s\) for \( s = 1, 2, \ldots, m \). Hence \( v(p) \) can be factorized as

\[ v(p) = \lambda a_0(p^2 + \gamma_1) \prod_{s=2}^{m} (p^2 + \delta_s), \] (18)
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where $\gamma_1$, $\delta_2$, ..., $\delta_m$ are real numbers alternating with the $\alpha_s$ in the following way: $\gamma_1 < \alpha_1 < \delta_2 < \alpha_2 < ... < \delta_m < \alpha_m$. Noting that $\gamma_1$ may be negative, define $\delta_1 = \max(0, \gamma_1)$. For $s = 1, 2, \ldots, m$ one must have

$$a(i \delta_s) [c(i \delta_s) + \lambda \delta_s x(i \delta_s)] \geq 0,$$

(19)
in order to comply with (13) at the point $\omega = \delta_s$.

To progress further in the discussion of (16), we make an important additional assumption, namely

$$\mu = (c_0 - \lambda x_1)/a_0 > 0,$$

(20)
meaning that the polynomial $a(i\omega)[c(i\omega) + \lambda \omega^2 x(i\omega)]$ has exact degree $m$ in $\omega^2$ and is positive for $\omega \to \infty$. As a consequence it appears, in view of (19) and the alternation property $\delta_s < \alpha_s < \delta_{s+1}$, that the polynomial $c(i\omega) + \lambda \omega^2 x(i\omega)$ must vanish at least once for $\omega^2$ in each closed interval $[\delta_s, \delta_{s+1}]$, $[\delta_{s+1}, \delta_{s+2}], \ldots, [\delta_{m-1}, \delta_m]$ and $[\delta_m, \infty]$. Since this polynomial has degree $m$ in $\omega^2$ we are left with the only possibility

$$c(p) - \lambda p^2 x(p) = \mu a_0 \prod_{s=1}^{m} (p^2 + \varepsilon_s),$$

(21)
where $\mu$ is given by (20) and the $\varepsilon_s$ are distinct positive real numbers satisfying $\delta_1 \leq \varepsilon_1 \leq \delta_2 \leq \varepsilon_2 \leq \cdots \leq \delta_m \leq \varepsilon_m$.

Finally, let us define the polynomial

$$y(p) = \sum_{i=1}^{m} y_i p^{2(m-i)}$$

to be the remainder in the division of $c(p) - \lambda p^2 x(p)$ by $a(p)$, that is

$$y(p) = c(p) - \lambda p^2 x(p) - \mu a(p).$$

(22)
For $\omega_s^2 = \varepsilon_s$ one has $y(i\omega_s) + \mu a(i\omega_s) = 0$, in view of (21), so that $\mu x(i\omega_s) + \lambda y(i\omega_s)$ equals $-\nu(v(i\omega_s))$, with $\nu(p)$ as in (17). Hence, owing to the alternation of the $\varepsilon_s$ with respect to the $\delta_s$, it appears that $\mu x(i\omega_s) + \lambda y(i\omega_s)$ has sign $(-1)^{s-1}$ or vanishes. Hence there are only two possibilities for the polynomial $\mu x(i\omega) + \lambda y(i\omega)$: either it is identically zero, or it vanishes exactly once for $\omega^2$ in each closed interval $[\varepsilon_s, \varepsilon_{s+1}]$ and is positive at the origin. The first possibility is easily ruled out in the nondegenerate case $m \geq 1$. Indeed, $\mu x + \lambda y \equiv 0$ implies $\mu^2 f = (\nu + \mu a)[\lambda^2 \omega^2 (\nu + \mu a) + 4a]$, so that the condition $f(\omega) \geq 0$ forces the zeros of $y(i\omega) + \mu a(i\omega)$ to coincide with those of $a(i\omega)$, thus implying $y(p) \equiv 0$, hence $x(p) \equiv 0$, in contradiction with $x_1 > 0$.

As a result, in case $m \geq 1$ we can write

$$\mu x(p) + \lambda y(p) = (\mu x_1 + \lambda y_1) \prod_{s=1}^{m-1} (p^2 + \zeta_s),$$

(23)
with $\mu x_1 + \lambda y_1 \neq 0$, where the numbers $\zeta_s$ satisfy

$$\varepsilon_1 \leq \zeta_1 \leq \varepsilon_2 \leq \ldots \leq \zeta_{m-1} \leq \varepsilon_m.$$  

Then, since $\mu x(0) + \lambda y(0)$ is known to be positive, it follows that $\mu x_1 + \lambda y_1$ also is positive. To sum up, we have proved the following theorem, which immediately implies the truth of the Daniel–Moore conjecture.

**Theorem 3.** Let $\lambda$ and $x(p)$ be the quotient and the remainder, respectively, in the division of $b(p)$ by $a(p)$. Let $\mu$ and $y(p)$ be the quotient and the remainder, respectively, in the division of $c(p) - \lambda p^2 x(p)$ by $a(p)$. Then, provided $\mu$ is positive, the requirements on $H(p, q)$ force $\mu x_1 + \lambda y_1$ to be nonnegative and to vanish only in the degenerate case $m = 0$, i.e. in the case $H(p, q) = a_0(1 + \lambda pq + \mu q^2)$.

We shall conclude this paper by explaining the intrinsic significance of the results obtained above in the theory of two-variable Hurwitz polynomials. Let us deduce from $H(p, q)$ a new polynomial, written as $H'(p, z)$, by performing the change of variables

$$q = \frac{-1}{\lambda p - \frac{\mu}{\lambda (p + z)}},$$  

and dropping the common denominator. Note that, by definition of $\lambda$ and $\mu$, the right member of (24) can be viewed as the second order approximation of the continued fraction associated with the algebraic function $q = q(p)$, solution of $H(p, q) = 0$, around the point at infinity. After elementary but tedious computation one obtains

$$H'(p, z) = \mu^2 a(p) + \lambda p^2 [\mu x(p) + \lambda y(p)]$$

$$+ \{\lambda [\mu a(p) + y(p)] + [\mu x(p) + \lambda y(p)]\} pz$$

$$+ [\mu a(p) + y(p)] z^2.$$  

**Theorem 4.** Under the same conditions as above, the polynomial $H'(p, z)$ resulting from $H(p, q)$ by the transformation (24) is a Hurwitz polynomial in the narrow sense.

**Proof:** The result will be established by showing that the three Ansell tests are satisfied, namely

$$H'(i\omega, z) \text{ does not vanish in } Re z > 0,$$

$$H'(p, z) \text{ has no factor } z - iy \text{ with real } y,$$

$$H'(p, 1) \text{ is strictly Hurwitzian.}$$
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Let us abbreviate (25) as $H'(p, z) = a'(p) + pb'(p)z + c'(p)z^2$. The first property, (26), is immediate because the discriminant of $H'(i\omega, z)$ is non-positive, for any real $\omega$. Indeed, with the help of (25) and (13) one obtains $\omega^2 b'^2(i\omega) + 4a'(i\omega)c'(i\omega) = \mu^2 f(\omega) \geq 0$. The second test, (27), is also passed in a straightforward manner, since neither $a'(p)$ nor $b'(p)$ vanishes identically.

Verification of (28) is more difficult. Consider the rational function

$$h(p) = p[\mu x(p) + \lambda y(p)] / [\mu a(p) + y(p)].$$

In view of the alternation property $\varepsilon_s \leq \zeta_s \leq \varepsilon_{s+1}$ obtained above, it immediately follows that $h(p)$ is positive real; this is the fundamental meaning of theorem 3. Now, by definition, $pb'(p)/c'(p)$ equals $\lambda p + h(p)$, hence is a positive real function. Next, let us show that $a'(p)/pb'(p)$ also is positive real. The denominator of this function actually has simple zeros. Let us indeed assume $pb'(p)$ to have a double zero in $p = i\omega_0$. This implies $c'(i\omega_0) = 0$ since $pb'(p)/c'(p)$ is positive real. Hence $a'(i\omega_0)$ cannot vanish, for otherwise $H(p, q)$ would be divisible by $p - i\omega_0$. Then from $\omega^2 b'^2(i\omega) + 4a'(i\omega)c'(i\omega) \geq 0$ it follows that $i\omega_0$ is a double zero of $c'(p)$, hence of $p[b'(p) - \lambda c'(p)] = p[\mu x(p) + \lambda y(p)]$, which is impossible since all zeros of the last polynomial have been shown to be simple. Let now $i\omega_0$ be a zero of $b'(p)$ such that $c'(i\omega_0) \neq 0$. From the condition $f(\omega) \geq 0$ one deduces $a'(i\omega_0) c'(i\omega_0) \geq 0$, which shows that the residue of $a'(p)/pb'(p)$ in $p = i\omega_0$ has the same sign as that of $c'(p)/pb'(p)$ and so is nonnegative. In case $c'(i\omega_0) = b'(i\omega_0) = 0$, the argument above fails to apply. But, in this situation, $i\omega_0$ must be a double zero of $c'(p)$ in order to keep $f(i\omega_0) \geq 0$ and must satisfy $\omega_0^2 = \delta_t$ for a certain $t$ (cf. (18)). Consider the factorization $v(p) = (p^2 + \delta_t) u(p)$. Then the residue of $a'(p)/pb'(p)$ in $p = \pm i\omega_0$ is readily found to be $\mu a(i\omega_0)/2\omega_0^2 u(i\omega_0)$, which clearly is positive in view of the alternation $\alpha_{s-1} < \delta_s < \alpha_s$. To sum up, both functions $a'(p)/pb'(p)$ and $c'(p)/pb'(p)$ are positive real. Hence so is the function

$$\frac{H(p, 1)}{pb'(p)} = 1 + \frac{a'(p)}{pb'(p)} + \frac{c'(p)}{pb'(p)},$$

which immediately proves that $H(p, 1)$ is strictly Hurwitzian, owing to the fact that $a'(p)$, $b'(p)$ and $c'(p)$ have no common factor. This completes the proof.

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