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ON THE ZEROS OF SOME POLYNOMIALS THAT ARISE IN NUMERICAL QUADRATURE AND CONVERGENCE ACCELERATION*

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Abstract. In this work the zeros of a sequence of polynomials that arise in convergence acceleration and some new numerical quadrature formulas are studied. In particular, it is proved that those polynomials that arise in numerical quadrature have all their zeros on [0, 1] and that they are simple, and a characterization theorem for these polynomials is also provided. Furthermore, the zeros are shown to have an interlacing property.

1. Introduction. In a recent work, Sidi (1980a), new numerical quadrature formulas $I_k[f]$ for integrals $I[f]$, where

$$I[f]=\int_0^1 (1-x)^\alpha x^\beta(-\log x)^\nu f(x)\,dx, \qquad \beta>-1, \quad \alpha+\nu>-1, \tag{1.1}$$

and

$$I_k[f]=\sum_{i=1}^{k} A_{k,i}f(x_{k,i}), \qquad k=1,2,\cdots, \tag{1.2}$$

have been introduced. The abscissas $x_{k,i}$ and the weights $A_{k,i}$ in these formulas are the poles and residues of a sequence of rational functions $H_k(z)$; i.e.,

$$H_k(z)=\sum_{i=1}^{k}\frac{A_{k,i}}{z-x_{k,i}}, \tag{1.3}$$

which are approximations to the function

$$H(z)=\int_0^1 \frac{(1-x)^\alpha x^\beta(-\log x)^\nu}{z-x}\,dx, \tag{1.4}$$

in the complex z-plane cut along the real interval [0, 1]. The approximations $H_k(z)$ are obtained by applying a modification of the Levin (1973) T-transformation to the moment series of $H(z)$. For a motivation and details of this approach the reader is referred to Sidi (1980a).

The abscissas $x_{k,i}$ above are the zeros of the polynomial $D_{k,1,k+\alpha+\nu}(x)$, where

$$D_{k,n,m}(x)=\sum_{j=0}^{k}(-1)^j\binom{k}{j}(n+j)^m x^{n+j-1}; \tag{1.5}$$

hence they are independent of β and dependent only on $\alpha+\nu$. In Sidi (1980a) it is shown that when m and n are integers such that $m\geqq 0$ and $n\geqq 1$, the polynomial $D_{k,n,m}(x)$ has all its zeros in [0, 1], $x=0$ and $x=1$ being zeros of multiplicity $n-1$ and $\max(k-m,0)$ respectively, and the rest being simple zeros in (0, 1). It is shown furthermore that when $m\geqq 2$, the simple zeros of $D_{k,n,m}(x)$ and $D_{k-1,n,m-1}(x)$ on (0, 1) interlace. An immediate consequence of these results is that for $\alpha+\nu=0,1,2,\cdots$, the abscissas $x_{k,i}$ in (1.2) are simple and lie in (0, 1), and $\{x_{k,i}\}$ and $\{x_{k-1,i}\}$ interlace.

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The purpose of the present work is to extend these results to the case in which $\alpha+\nu$, and therefore m, are not integers; and we shall also relax the requirement that n be an integer. In the course of development we shall also prove a characterization theorem for $D_{k,n,m}(x)$ when $m>k-1$.

Finally, we note that, for n a positive integer, the polynomials $D_{k,n,k+\varepsilon}(x)$, for all ε, come up as the denominators of the rational approximations obtained by applying a modification of the Levin (1973) T-transformation to the infinite series $\sum_{r=1}^{\infty} a_r/x^r$, with $a_r=r^{-1-\varepsilon}w(r)$, where $w(\rho)$, as a function of the continuous variable ρ, has a Poincaré-type asymptotic expansion of the form

$$w(\rho)\sim\sum_{i=0}^{\infty} w_i/\rho^i \quad \text{as } \rho\to\infty. \tag{1.6}$$

For details see Sidi (1980b).

2. Theory. In what follows we assume that $D_{k,n,m}(x)$ is as given in (1.5) and that m and n are real numbers satisfying $m>-1$ and $n>0$. Write $m=\gamma+p$, where $-1<\gamma\leqq 0$, and $p\geqq 0$ is an integer. Obviously γ and p are uniquely determined by these conditions.

LEMMA 2.1.

$$D_{k,n,m}(x)=\frac{d}{dx}[xD_{k,n,m-1}(x)]. \tag{2.1}$$

Proof. Follows easily from (1.5). □

LEMMA 2.2. *When m is not an integer or when m is an integer $\geqq k$,*

$$\operatorname{sgn} D_{k,n,m}(1)=(-1)^{\min(p,k)}; \tag{2.2}$$

otherwise $D_{k,n,m}(1)=0$.

Proof. We start by expressing $D_{k,n,m}(x)$ as

$$D_{k,n,m}(x)=(-1)^k\Delta^k(n^m x^{n-1}), \tag{2.3}$$

where Δ is the forward difference operator operating on n. Setting $x=1$ in (2.3), and using the fact that

$$\Delta^k u(n)=\frac{d^k}{d\sigma^k}u(\sigma)\bigg|_{\sigma=\bar\sigma} \quad \text{for some } \bar\sigma\in(n, n+k), \tag{2.4}$$

whenever $u(\sigma)$ is k times differentiable on $(n, n+k)$, we obtain

$$D_{k,n,m}(1)=(-1)^k\left[\prod_{i=0}^{k-1}(m-i)\right]\bar\sigma^{m-k} \quad \text{for some } \bar\sigma\in(n, n+k). \tag{2.5}$$

The result now follows easily. □

THEOREM 2.1. *Define*

$$r(t)=\int_0^1(-\log x)^t D_{k,n,m}(x)\,dx, \tag{2.6}$$

and, for $p\geqq 1$, define

$$t_i=\gamma+i+\max(0, p-k), \qquad i=0,1,\cdots,s, \quad s=\min(p-1, k-1). \tag{2.7}$$

Then

$$r(t_i)=0, \qquad i=0,1,\cdots,s. \tag{2.8}$$

Proof. Substituting (1.5) in (2.6), and using the result

$$\int_0^1 (-\log x)^t x^{a-1}\,dx = \frac{t!}{a^{t+1}}, \qquad t>-1, \quad a>0, \tag{2.9}$$

we obtain

$$r(t) = t! \sum_{j=0}^{k} (-1)^j \binom{k}{j} (n+j)^{m-t-1} = (-1)^k t!\,\Delta^k (n^{m-t-1}), \tag{2.10}$$

where Δ is the forward difference operator operating on n. From (2.7) and the fact that $\gamma > -1$, it is clear that $t_i > -1$ for all $i \geqq 0$. Furthermore, $m - t_i - 1 = s - i$, $i = 0, 1, \cdots, s$, so that $r(t_i) = (-1)^k t_i!\,\Delta^k(n^{s-i})$, $i = 0, 1, \cdots, s$. This, together with $s \leqq k-1$ and

$$\Delta^k(n^b) = 0, \qquad b = 0, 1, \cdots, k-1, \tag{2.11}$$

results in (2.8). □

THEOREM 2.2. *The polynomial* $\tilde{D}_p(x) = x^{1-n} D_{k,n,m}(x)$ *has exactly* $\min(p, k)$ *zeros on* $(0, 1)$ *and they are all simple. Furthermore, the zeros of* $\tilde{D}_{p-1}(x)$ *on* $(0, 1)$ *interlace those of* $\tilde{D}_p(x)$ *there, such that the smallest positive zero of* $\tilde{D}_p(x)$ *is less than the smallest positive zero of* $\tilde{D}_{p-1}(x)$.

Note. For $\gamma = 0$ this theorem has been proved in Sidi (1980a). Therefore, in the proof below, we shall take $\gamma \neq 0$. This is necessary especially at those places in the proof where we make use of Lemma 2.2.

Proof. We start by proving that $\tilde{D}_p(x)$ has at least $\min(p, k)$ sign changes in (0, 1). Since this is trivially so for $p = 0$, we take $p \geqq 1$. Making the change of integration variable $x = e^{-y}$ in (2.6), (2.8) can be expressed as

$$\int_0^\infty y^{\delta+i} e^{-y} D_{k,n,m}(e^{-y})\,dy = 0, \qquad i = 0, 1, \cdots, s, \tag{2.12}$$

where $\delta = \gamma + \max(0, p-k) > -1$. Taking appropriate linear combinations of the equalities in (2.12), we have

$$\int_0^\infty y^{\delta} e^{-y} L_i^{(\delta)}(y) D_{k,n,m}(e^{-y})\,dy = 0, \qquad i = 0, 1, \cdots, s. \tag{2.13}$$

where $L_i^{(\delta)}(y)$ are the generalized Laguerre polynomials that form an orthogonal set of polynomials with respect to the weight function $y^\delta e^{-y}$ on $[0, \infty)$. Therefore, $D_{k,n,m}(e^{-y})$ has at least $s+1$ sign changes on $(0, \infty)$; see Cheney (1966, p. 110). This implies that $\tilde{D}_p(x)$ has at least $s + 1 = \min(p, k)$ sign changes on (0, 1).

Now for $p \geqq k$, the number of sign changes of $\tilde{D}_p(x)$ on (0, 1) is at least k. But $\tilde{D}_p(x)$ is a polynomial of degree exactly k. Therefore, it follows that when $p \geqq k$, $\tilde{D}_p(x)$ has exactly k zeros on (0, 1) which are all simple.

For $p < k$, we next show that $\tilde{D}_p(x)$ has exactly p sign changes on (0, 1). For this we shall make use of Lemmas 2.1 and 2.2. Suppose that $\tilde{D}_p(x)$ changes its sign at exactly $p+q$ points on (0, 1) with $q \geqq 1$, and denote these points by x_i, $i = 1, 2, \cdots, p+q$, such that $0 < x_1 < x_2 \cdots < x_{p+q} < 1$. Now from (1.5) and the fact that $n > 0$, it follows that $xD_{k,n,m}(x) = 0$ at $x = 0$. Again from (1.5) we have that, for $x > 0$ but sufficiently close to zero, $D_{k,n,m}(x) > 0$. Consequently, for $x_i < x < x_{i+1}$, we have $(-1)^i D_{k,n,m}(x) \geqq 0$, $i = 0, 1, \cdots, p+q$, where we have also set $x_0 \equiv 0$. But for $x_{p+q} \leqq x \leqq 1$ we should have $(-1)^p D_{k,n,m}(x) \geqq 0$, according to Lemma 2.2. This implies that q is an even integer, hence $q \geqq 2$. By applying Rolle's theorem to $(d/dx)[xD_{k,n,m}(x)]$, and using Lemma 2.1, we have that $D_{k,n,m+1}(x)$ has an odd number of sign changes in each of the subintervals (x_i, x_{i+1}), $i = 0, 1, \cdots, p+q-1$, which implies that $D_{k,n,m+1}(x)$ has at least $p+q \geqq p+2$ sign changes on $(0, 1)$. But from above we know that $D_{k,n,m+1}(x)$ has at least $p+1$ sign changes on $(0, 1)$, and if it has more, they should be $p+1+q'$ in number, where $q' \geqq 2$ is an even integer. Consequently, $D_{k,n,m+1}(x)$ must have at least $p+3$ sign changes on $(0, 1)$. If $p+1 = k$, this leads to a contradiction, as we have already shown that $D_{k,n,\gamma+k}(x)$ has exactly k simple zeros on $(0, 1)$; hence $D_{k,n,\gamma+k-1}(x)$ has exactly $k-1$ sign changes on $(0, 1)$. If $p+1 = k-1$, then this implies that $D_{k,n,\gamma+k-1}(x)$ has at least $k+1$ sign changes on $(0, 1)$, and this is a contradiction, since we have already shown that $D_{k,n,\gamma+k-1}(x)$ has exactly $k-1$ sign changes on $(0, 1)$. The proof can now be completed by letting $p = k-3, \cdots, 1, 0$, in this order.

We finally show that, for $p < k$, $\tilde{D}_p(x)$ has exactly p zeros on $(0, 1)$, and they are all simple. As above, also here we shall make use of Lemma 2.1 and Rolle's theorem. So far we have shown that $D_p(x)$ has at least p zeros on $(0, 1)$, with exactly p of them, say $x_1 < x_2 < \cdots < x_p$, having odd multiplicities. Assume now that the total multiplicity of the zeros of $\tilde{D}_p(x)$ on $(0, 1)$ is greater than p. Then there are two possibilities:

1) At least one of the x_i, say x_q, has multiplicity $\geqq 3$. Using Lemma 2.1, we see that $\tilde{D}_{p+1}(x)$ has a zero of even multiplicity $\geqq 2$ at x_q, in addition to the $p+1$ points at which it changes sign. Now Lemma 2.1 and Rolle's theorem imply that $\tilde{D}_{p+2}(x)$ should have $p+3$ points of sign changes on $(0, 1)$, one of these points being x_q. But this contradicts the fact that $\tilde{D}_{p+2}(x)$ has exactly $\min(p+2, k)$ sign changes on $(0, 1)$.

2) $\tilde{D}_p(x)$ has at least one zero of even multiplicity $\geqq 2$, say z. As above, this implies that $\tilde{D}_{p+1}(x)$ should have at least $p+2$ sign changes on $(0, 1)$, one of them being at z, and this is a contradiction, since $\tilde{D}_{p+1}(x)$ has exactly $p+1$ sign changes on $(0, 1)$.

The last part of the theorem, on the interlacing property of the zeros of $\tilde{D}_p(x)$ and $\tilde{D}_{p-1}(x)$, is a consequence of Lemma 2.1 and Rolle's theorem. This completes the proof of the theorem. □

THEOREM 2.3. *Let us denote the zeros of $D_{k,n,m}(x)$ on $(0, 1)$ by $x_i^{k,m}$, such that $x_1^{k,m} < k_2^{k,m} < \cdots$. Then for $m \geqq 2$*

$$x_1^{k,m} < x_1^{k-1,m-1} < x_2^{k,m} < x_2^{k-1,m-1} < \cdots. \tag{2.14}$$

Proof. Making use of Theorem 3.2 in Sidi (1982), we have

$$D_{k,n,m}(x) = (n+k)D_{k,n,m-1}(x) - kD_{k-1,n,m-1}(x). \tag{2.15}$$

The rest of the proof now is exactly the same as that of Theorem 4.3 in Sidi (1980a). □

An immediate consequence of this is that for any $\alpha + \nu > -1$, $x_{k,i}$ in (1.2) are simple and lie in $(0, 1)$ and $\{x_{k,i}\}$ and $\{x_{k-1,i}\}$ interlace.

LEMMA 2.3. *Let $m = k + \varepsilon$, such that ε is fixed. Let $x_i^{k,k+\varepsilon}$, $i = 1, 2, \cdots, k$, denote all the zeros (real or otherwise) of $x^{1-n}D_{k,n,k+\varepsilon}(x)$. Then*

$$\lim_{k\to\infty} \frac{\sum_{i=1}^{k} x_i^{k,k+\varepsilon}}{k} = e^{-1}. \tag{2.16}$$

Proof. (2.16) follows easily from the fact that

$$\sum_{i=1}^{k} x_i^{k,k+\varepsilon} = k\left(\frac{n+k-1}{n+k}\right)^{k+\varepsilon}, \tag{2.17}$$

which follows from (1.5). □

From this result and the fact that $e^{-1} < \frac{1}{2}$, we can see that the k real zeros of $D_{k,n,k+\varepsilon}(x)$ for $\varepsilon > -1$ are not symmetrical with respect to $x = \frac{1}{2}$, and it can be argued that they tend to cluster in $(0, \frac{1}{2})$. This statement is made more rigorous in the following theorem.

THEOREM 2.4. *Let $m = k + \varepsilon$, $\varepsilon > -1$ fixed. Then for any fixed i*

$$\lim_{k\to\infty} x_i^{k,k+\varepsilon} = 0, \tag{2.18}$$

where $0 < x_1^{k,k+\varepsilon} < x_2^{k,k+\varepsilon} < \cdots < x_k^{k,k+\varepsilon} < 1$.

Proof. Let $z_1, \cdots, z_k$ be the zeros of the polynomial $P(z) = \sum_{j=0}^k \lambda_j z^j$, $\lambda_k = 1$. Then, for $0 \leqq i \leqq k-1$,

$$(-1)^{k-i}\lambda_i = \sum_{1 \leqq j_1 < j_2 < \cdots < j_{k-i} \leqq k} z_{j_1} z_{j_2} \cdots z_{j_{k-i}}, \tag{2.19}$$

with one of the terms in this multiple sum being $z_{i+1}z_{i+2}\cdots z_k$. Since all the zeros of $D_{k,n,k+\varepsilon}(x)$ are positive, we have from (2.19) and (1.5)

$$\prod_{j=i+1}^{k} x_j^{k,k+\varepsilon} < \binom{k}{i}\left(\frac{n+i}{n+k}\right)^{k+\varepsilon}. \tag{2.20}$$

Since $x_j^{k,k+\varepsilon}$ are in ascending order, (2.20) can be replaced by

$$(x_{i+1}^{k,k+\varepsilon})^{k-i} < \binom{k}{i}\left(\frac{n+i}{n+k}\right)^{k+\varepsilon}. \tag{2.21}$$

Therefore,

$$x_{i+1}^{k,k+\varepsilon} < \binom{k}{i}^{1/(k-i)}\left(\frac{n+i}{n+k}\right)^{(k+\varepsilon)/(k-i)}. \tag{2.22}$$

Now $\binom{k}{i}$ is a polynomial in k of degree i. Hence $\binom{k}{i}^{1/(k-i)} = O(1)$ as $k \to \infty$. Consequently,

$$x_{i+1}^{k,k+\varepsilon} = O(k^{-1}) \quad \text{as } k \to \infty. \tag{2.23}$$

This completes the proof of the theorem, providing at the same time an upper bound for the rate at which the $x_i^{k,k+\varepsilon}$ tend to zero as $k \to \infty$. □

THEOREM 2.5. *Let $m = k + \varepsilon$, $\varepsilon > -1$ fixed. Then for σ fixed and $0 < \sigma < \frac{1}{2}$,*

$$\limsup_{k\to\infty} x_{[\sigma k]}^{k,k+\varepsilon} \leqq \frac{\sigma}{1-\sigma}, \tag{2.24}$$

where $[A]$ denotes the greatest integer $\leqq A$.

Proof. We start with (2.20). Since $\sigma k - 1 < [\sigma k] \leqq \sigma k$, we see that for k sufficiently large,

$$\binom{k}{[\sigma k]} \leqq \frac{k!}{(\sigma k - 1)!\,(k - \sigma k)!} \sim \sqrt{\frac{\sigma k}{2\pi(1-\sigma)}}\,\frac{1}{\sigma^{\sigma k}(1-\sigma)^{k(1-\sigma)}}, \tag{2.25}$$

the last part following from Stirling's formula. Similarly, for k sufficiently large,

$$\left(\frac{n+[\sigma k]}{n+k}\right)^{k+\varepsilon} \leqq \left(\frac{n+\sigma k}{n+k}\right)^{k+\varepsilon} \sim B\sigma^k, \tag{2.26}$$

where B is a constant independent of k. Combining (2.25) and (2.26) in (2.21) with $i = [\sigma k]$, we obtain after some simple manipulations,

$$(x_{[\sigma k]+1}^{k,k+\varepsilon})^{k-\sigma k+1} < C\sqrt{k}\left(\frac{\sigma}{1-\sigma}\right)^{k-\sigma k+1}, \tag{2.27}$$

where C is a constant independent of k. (2.24) now follows easily. □

3. A characterization theorem. Making use of (2.8), we now prove a characterization theorem for $D_{k,n,\gamma+p}(x)$ for $p \geqq k$.

THEOREM 3.1. *Let $\delta > -1$ and $n > 0$. Then there exists a unique (up to a constant multiplicative factor) polynomial $\tilde{D}(x) \not\equiv 0$ from the set of polynomials of degree $\leqq k$, satisfying*

$$\int_0^1 (-\log x)^{\delta+i} x^{n-1} \tilde{D}(x)\, dx = 0, \qquad i = 0, 1, \cdots, k-1, \tag{3.1}$$

and this polynomial is $x^{1-n} D_{k,n,\delta+k}(x)$.

Proof. That $x^{1-n} D_{k,n,\delta+k}(x)$ satisfies (3.1) follows from (2.8), (2.7), and (2.6), together with $\delta = \gamma + p - k$, $-1 < \gamma \leqq 0$, and $p \geqq 0$ an integer, which imply that $p \geqq k$. Let us now prove that there does not exist a polynomial of degree less than k satisfying (3.1). Suppose that $\tilde{D}_1(x)$ were such a polynomial. Then making the change of variable $x = e^{-y}$, and following the steps that lead from (2.8) to (2.13), we would have from (3.1).

$$\int_0^\infty y^\delta e^{-y} L_i^{(\delta)}(y)\, e^{(1-n)y} \tilde{D}_1(e^{-y})\, dy = 0, \qquad i = 0, 1, \cdots, k-1. \tag{3.2}$$

This now implies that $e^{(1-n)y}\tilde{D}_1(e^{-y})$ hence $\tilde{D}_1(e^{-y})$ have k sign changes on $(0, \infty)$ or that $\tilde{D}_1(e^{-y})$ vanishes identically on $[0, \infty)$. Since $\tilde{D}_1(x)$ is a polynomial of degree less than k, this implies that $\tilde{D}_1(x) \equiv 0$ on $[0, 1]$. As for the uniqueness of $\tilde{D}(x)$ we proceed as follows. Let $\tilde{D}(x)$ and $\hat{D}(x)$ be two polynomials of degree exactly k, having equal leading coefficients, and satisfying (3.1). Then $\tilde{D}_1(x) = \tilde{D}(x) - \hat{D}(x)$ is a polynomial of degree less than k, satisfying (3.1). But we proved above that $\tilde{D}_1(x) \equiv 0$ on $[0, 1]$, which implies $\tilde{D}(x) \equiv \hat{D}(x)$. This completes the proof. □

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REFERENCES

E. W. CHENEY (1966), *Introduction to Approximation Theory*, McGraw-Hill, New York.

D. LEVIN (1973), *Development of non-linear transformations for improving convergence of sequences*, Internat. J. Comput. Math., B3, pp. 371–388.

A. SIDI (1980a), *Numerical quadrature and non-linear sequence transformations; unified rules for efficient computation of integrals with algebraic and logarithmic endpoint singularities*, Math. Comp., 35, pp. 851–874.

——— (1980b), *Analysis of convergence of the T-transformation for power series*, Math. Comp., 35, pp. 833–850.

——— (1982), *Numerical quadrature rules for some infinite range integrals*, Math. Comp., 38, pp. 127–142.