

Floating-point versus Symbolic Computations in the QD-algorithm

ANNIE CUYT

Research Director NFWO, Department of Mathematics and Computer Science, University of Antwerp, UIA, Universiteitsplein 1, B-2610 Wilrijk, Belgium

The convergence of columns in the univariate qd-algorithm to reciprocals of polar singularities of meromorphic functions has often proved to be very useful. Any q-column corresponding to a "simple pole of isolated modulus" converges to the reciprocal of the corresponding pole. By performing an equivalence transformation of the underlying corresponding continued fraction and programming the new qd-like scheme so as to compute algebraic expressions, the difference in convergence behaviour between the "simple pole" case and the "equal modulus" pole case of the floating-point algorithm is eliminated. (© 1997 Academic Press Limited

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1. The Floating-point QD-algorithm

Let the function f(z) be known by its formal series expansion

$$f(z) = \sum_{i=0}^{\infty} c_i z^i.$$
 (1)

The series expansion is taken around the origin only to simplify the notation. We set $c_i = 0$ for i < 0. For arbitrary integers n and for integers $m \ge 0$ we define determinants

	c_n	c_{n+1}	• • •	c_{n+m-1}
$H_m^{(n)} =$	c_{n+1}	c_{n+2}		c_{n+m}
	÷	÷	·	÷
	c_{n+m-1}	c_{n+m}		c_{n+2m-2}

with $H_0^{(n)} = 1$. The series (1) is termed k-normal if $H_m^{(n)} \neq 0$ for m = 0, 1, ..., k and $n \geq 0$. It is ultimately called k-normal if for every $0 \leq m \leq k$ there exists an n(m) such that $H_m^{(n)} \neq 0$ for n > n(m). With (1) as input we can also define the *qd*-scheme (Henrici, 1974, p. 609):

(a) the start columns are given by

$$e_0^{(n)} = 0$$
 $n = 1, 2, \dots$

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$$q_1^{(n)} = \frac{c_{n+1}}{c_n}$$
 $n = 1, 2, \dots$

(b) and the rhombus rules for continuation of the scheme by

$$e_m^{(n)} = q_m^{(n+1)} - q_m^{(n)} + e_{m-1}^{(n+1)} \qquad m = 1, 2... \qquad n = 1, 2, ...$$
$$q_{m+1}^{(n)} = \frac{e_m^{(n+1)}}{e_m^{(n)}} q_m^{(n+1)} \qquad m = 1, 2... \qquad n = 1, 2, ...$$

Usually the values $q_m^{(n)}$ and $e_m^{(n)}$ are arranged in a table where subscripts indicate columns and superscripts downward sloping diagonals and the continuation rules link elements in a rhombus:



THEOREM 1.1. Let (1) be the Taylor series at z = 0 of a function f meromorphic in the disk $B(0, R) = \{z : |z| < R\}$ and let the poles z_i of f in B(0, R) be numbered such that

$$z_0 = 0 < |z_1| \le |z_2| \le \dots < R$$

each pole occurring as many times in the sequence $\{z_i\}_{i\in\mathbb{N}}$ as indicated by its order. If f is ultimately k-normal for some integer k > 0, then the qd-scheme associated with f has the following properties (put $z_{k+1} = \infty$ if f has only k poles):

(a) For each
$$m$$
 with $0 < m \le k$ and $|z_{m-1}| < |z_m| < |z_{m+1}|$,

$$\lim_{n \to \infty} q_m^{(n)} = z_m^{-1}$$
(2)

(b) For each m with $0 < m \le k$ and $|z_m| < |z_{m+1}|$,

$$\lim_{n \to \infty} e_m^{(n)} = 0. \tag{3}$$

PROOF. The proof can be found in Henrici (1974, pp. 612–613). \Box

Any index m such that the strict inequality

$$|z_m| < |z_{m+1}|$$

holds is called a critical index. It is clear that the critical indices of a function do not depend on the order in which the poles of equal modulus are numbered. The theorem above states that if m is a critical index and f is ultimately m-normal, then

$$\lim_{n \to \infty} e_m^{(n)} = 0$$

Thus the qd-table of a meromorphic function is divided into subtables by those e-columns tending to zero. Any q-column corresponding to a simple pole of isolated modulus is flanked by such e-columns and converges to the reciprocal of the corresponding pole. If a subtable contains j > 1 columns of q-values, the presence of j poles of equal modulus is indicated. In Henrici (1974, p. 642) it is also explained how to determine these poles if j > 1.

THEOREM 1.2. Let m and m+j with j > 1 be two consecutive critical indices and let f be (m+j)-normal. Let the polynomials $p_k^{(n)}$ be defined by

$$p_0^{(n)}(z) = 1$$

$$p_{k+1}^{(n)}(z) = z p_k^{(n+1)}(z) - q_{m+k+1}^{(n)} p_k^{(n)}(z) \qquad n \ge 0 \quad k = 0, 1, \dots, j-1.$$

Then there exists a subsequence $\{n(\ell)\}_{\ell \in \mathbb{N}}$ such that

$$\lim_{\ell \to \infty} p_j^{(n(\ell))}(z) = (z - z_{m+1}^{-1}) \dots (z - z_{m+j}^{-1})$$

From the above theorem the qd-scheme seems to be an ingenious tool for determining, under certain conditions, the poles of a meromorphic function f directly from its Taylor series at the origin. If f is rational, the last e-column is even theoretically equal to zero, as can be seen from the following theorem. The proof hereof is based on the next lemma (Henrici, 1974, pp. 610–613).

LEMMA 1.1. Let f be given by its formal Taylor series expansion (1). If there exists a positive integer k such that f is k-normal then the values $q_m^{(n)}$ and $e_m^{(n)}$ exist for $m = 1, \ldots, k$ and $n \ge 0$ and they are given by

$$q_m^{(n)} = \frac{H_m^{(n+1)}H_{m-1}^{(n)}}{H_m^{(n)}H_{m-1}^{(n+1)}}$$
$$e_m^{(n)} = \frac{H_{m+1}^{(n)}H_{m-1}^{(n+1)}}{H_m^{(n+1)}H_m^{(n)}}.$$

THEOREM 1.3. Let (1) be the Taylor series at z = 0 of a rational function of degree n in the numerator and $m \leq n$ in the denominator. Then if the series f is m-normal,

$$e_m^{(n-m+h)} = 0 \qquad h > 0.$$

In order to compare the output of the floating-point qd-algorithm with the results of the next section, we now display the results of a run for

$$f(z) = \frac{e^z}{(z-1)(z-2)(z+2)}.$$

INPUT :

floating-point representation of $(c_0, c_1, \ldots, c_{18})$

OUTPUT :

$$q_1^{(17)} = 0.100\,0004\text{E}+01$$

 $e_1^{(16)} = -0.367\,4957\text{E}-05$

$$\begin{array}{l} q_2^{(15)} = 0.447\,9084\mathrm{E}{+}00\\ e_2^{(14)} = -0.110\,2231\mathrm{E}{+}00\\ q_3^{(13)} = -0.558\,1391\mathrm{E}{+}00\\ e_3^{(12)} = -0.300\,3665\mathrm{E}{-}07 \end{array}$$

CONCLUSION:

$$z_1 \approx \frac{1}{q_1^{(17)}} = 0.999\,9960\text{E} + 00$$

$$z_i^{-2} - (q_2^{(14)} + q_3^{(13)})z_i^{-1} + q_2^{(13)}q_3^{(13)} \approx 0 \qquad i = 2, 3$$

$$z_2 \approx 0.200\,0095\text{E} + 01$$

$$z_3 \approx -0.200\,0032\text{E} + 01$$

These convergence results are closely linked to the well-known theorem of de Montessus de Ballore on the uniform convergence of Padé approximants for meromorphic functions (Baker and Graves-Morris, 1981, pp. 246–254). The reason is that the q- and e-values appear in the partial numerators and denominators of the corresponding continued fraction

$$f(z) = c_0 + \sum_{i=1}^{\infty} \left(\frac{-q_i^{(n-m+1)}z}{1} + \frac{-e_i^{(n-m+1)}z}{1} \right)$$
(4)

of which the (2m)th convergent is the Padé approximant to f of degree n in the numerator and m in the denominator. The theorem of de Montessus de Ballore states that if fis meromorphic with m poles in a disk B(0,R) with radius R centered at the origin (or the point around which f is developed into a Taylor series), then the sequence of Padé approximants with fixed denominator degree m and increasing numerator degree n, converges to f uniformly on compact subsets of B(0, R) excluding the poles. This makes sense because the Padé approximants considered in the sequence are rational functions with denominator degree m and the only singularities of f inside the disk are its m poles. The problem that arises from poles of equal modulus is now easy to understand. Since convergence is proved on compact subsets of a disk of meromorphy, poles equidistant from the origin (or the point around which f is developed into a Taylor series) cannot be treated separately. Increasing the radius of the disk (in *qd*-terminology moving to the next critical index) includes all the next poles of equal modulus simultaneously. If $|z_i| = |z_{i+1}|$ then we cannot define a disk centered at the origin that contains only one of the points but not both of them. The jumps in the modulus of the poles z_i are, moreover, indicated by the critical indices in the qd-algorithm.

2. Towards a Symbolic *QD*-like Algorithm

By performing an equivalence transformation (Perron, 1977, pp. 3–5) from (4) to

$$f(z) = c_0 + \sum_{i=1}^{\infty} \left(\frac{-Q_i^{(1)}(z)}{1 + Q_i^{(1)}(z)} + \frac{-E_i^{(1)}(z)}{1 + E_i^{(1)}(z)} \right)$$
(5)

we obtain new computation rules for the $Q_m^{(n)}(z)$ and $E_m^{(n)}(z)$ which are now rational functions of z (Cuyt, 1988):

(a) help entries $g_{0,m}^{(n)}$ are given by

$$g_{0,m}^{(n)} = -c_{n-m+1}z^{n-m+1} \tag{6a}$$

$$g_{r,m}^{(n)} = \frac{g_{r-1,m}^{(n)} g_{r-1,r}^{(n+1)} - g_{r-1,m}^{(n+1)} g_{r-1,r}^{(n)}}{g_{r-1,r}^{(n+1)} - g_{r-1,r}^{(n)}} \qquad r = 1, \dots, m-1$$
(6b)

where the values $g_{r,m}^{(n)}$ are stored as below

(b) and the symbolic qd-like algorithm is defined by

$$Q_1^{(n)}(z) = \frac{c_{n+1}}{c_n} z \frac{g_{0,1}^{(n)}}{g_{0,1}^{(n)} - g_{0,1}^{(n+1)}} \qquad n \ge 1$$
(7a)

$$E_m^{(n)}(z) + 1 = \frac{g_{m-1,m}^{(n+m-1)} - g_{m-1,m}^{(n+m)}}{g_{m-1,m}^{(n+m-1)}} (Q_m^{(n+1)}(z) + 1) \qquad m \ge 1 \quad n \ge 1$$
(7b)

$$Q_m^{(n)}(z) = \frac{E_{m-1}^{(n+1)}(z)Q_{m-1}^{(n+1)}(z)}{E_{m-1}^{(n)}(z)} \frac{g_{m-2,m-1}^{(n+m-2)} - g_{m-2,m-1}^{(n+m-1)}}{g_{m-2,m-1}^{(n+m-2)}} \frac{g_{m-1,m}^{(n+m-1)}}{g_{m-1,m}^{(n+m-1)} - g_{m-1,m}^{(n+m)}}$$
(7c)
$$m \ge 2 \quad n \ge 1.$$

If we arrange the values $Q_m^{(n)}(z)$ and $E_m^{(n)}(z)$ in a table where again subscripts indicate columns and superscripts downward sloping diagonals, then (7b) links the elements in the rhombus

$$\begin{array}{ccc}
 E_{m-1}^{(n)}(z) \\
 Q_{m-1}^{(n+1)}(z) & Q_m^{(n)}(z) \\
 & E_{m-1}^{(n+1)}(z)
\end{array}$$

and (7c) links two elements on an upward sloping diagonal

$$E_m^{(n)}(z)$$
$$Q_m^{(n+1)}(z)$$

The continued fraction (5) is especially interesting because it has the same form as the one underlying the general order multivariate Padé approximation theory. The results presented here were discovered when exploring the convergence behaviour of the multivariate version of this qd- like algorithm. Symbolic investigation was necessary because the $Q_m^{(n)}$ and $E_m^{(n)}$ in (5) are no longer merely coefficients. However, successive convergents of the continued fraction (5) again equal the Padé approximants to f. Let us now first generalize Lemma 1.1 and give explicit determinant representations for the rational expressions $Q_m^{(n)}(z)$ and $E_m^{(n)}(z)$. In addition to $H_m^{(n)}$ we define the determinants

$$H_{1,m}^{(n-m+1)}(z) = \begin{vmatrix} z^m & \dots & 1 \\ c_{n-m+1} & \dots & c_{n+1} \\ \vdots & \vdots \\ c_n & \dots & c_{n+m} \end{vmatrix} \qquad H_{1,-1}^{(n)} = 0$$
$$H_{2,m}^{(n-m+1)}(z) = \begin{vmatrix} z^m & \dots & 1 \\ z^m \sum_{k=0}^{n-m} c_k z^k & \dots & \sum_{k=0}^{n} c_k z^k \\ c_{n-m+1} & \dots & c_{n+1} \\ \vdots & & \vdots \\ c_{n-1} & \dots & c_{n+m-1} \end{vmatrix} \qquad H_{2,-1}^{(n)} = 0$$

By means of recurrence relations for these determinants we can prove the following lemma (Cuyt, 1988).

LEMMA 2.1. For well-defined $Q_m^{(n)}(z)$ and $E_m^{(n)}(z)$ the following determinant formulas hold:

$$Q_m^{(n)}(z) = -\frac{H_m^{(n+1)}H_{1,m-1}^{(n)}(z)H_{2,m}^{(n)}(z)}{H_m^{(n)}H_{1,m}^{(n)}(z)H_{2,m-1}^{(n+1)}(z)}$$
$$E_m^{(n)}(z) = -\frac{H_{m+1}^{(n)}H_{1,m-1}^{(n+1)}(z)H_{2,m}^{(n+1)}(z)}{H_m^{(n+1)}H_{1,m}^{(n+1)}(z)H_{2,m}^{(n)}(z)}.$$

We now take a look at how Theorems 1.1 and 1.2 generalize into one powerful theorem for the new qd-like algorithm (7). To this end we introduce

$$\hat{E}_{m}^{(n)}(z) = \frac{H_{m+1}^{(n)}(z)H_{2,m}^{(n+1)}(z)}{H_{m}^{(n+1)}(z)H_{2,m}^{(n)}(z)}$$

which contains only some of the factors appearing in $E_m^{(n)}(z)$.

THEOREM 2.1. Let (1) be the Taylor series at z = 0 of a function f meromorphic in the disk $B(0, R) = \{z : |z| < R\}$ and let the poles z_i of f in B(0, R) be numbered such that

$$z_0 = 0 < |z_1| \le |z_2| \le \dots < R$$

each pole occurring as many times in the sequence $\{z_i\}_{i\in\mathbb{N}}$ as indicated by its order. If f is ultimately k-normal for some integer k > 0, then the symbolic qd-like scheme (7) associated with f has the following properties (put $z_{k+1} = \infty$ if f has only k poles):

(a) For each m with $0 < m \le k$ and $|z_m| < |z_{m+1}|$,

$$\lim_{n \to \infty} H_{1,m}^{(n)}(z) = (z - z_1) \dots (z - z_m)$$

(b) For each m with $0 < m \le k$ and $|z_m| < |z_{m+1}|$,

$$\lim_{n \to \infty} \hat{E}_m^{(n)}(z) = 0$$

PROOF. The proof of both (a) and (b) heavily relies on the theorem of de Montessus de Ballore which states that, under the conditions above with $|z_m| < |z_{m+1}|$, the sequence of Padé approximants $r_{n,m}$ to f with fixed denominator degree m and increasing numerator degree n converges uniformly to f on B(0, R). An elegant proof of this theorem can be found in Baker and Graves-Morris (1981, p. 252).

In order to prove (a) we use the fact that $H_{1,m}^{(n)}(z)$ is the denominator of the Padé approximant $r_{n+m-1,m}(z)$ of degree n+m-1 in the numerator and m in the denominator (Cuyt, 1988, pp. 109–110). If the Padé approximant is normalized such that its denominator is monic, which is possible here because f is ultimately k-normal, then we learn from the proof in Baker and Graves-Morris (1981, p. 252) that

$$\lim_{n \to \infty} H_{1,m}^{(n)}(z) = (z - z_1) \dots (z - z_m).$$

In order to prove (b) we use the fact that both numerator and denominator of $\hat{E}_m^{(n)}(z)$ are remainder series of a Padé approximation procedure. The numerator is $O(z^{n+2m})$ and tends to zero because (Cuyt, 1988, p. 106)

$$E_m^{(n)}(z) = \frac{r_{n+m,m}(z) - r_{n+m-1,m}(z)}{r_{n+m-1,m}(z) - r_{n+m-1,m-1}(z)} = \hat{E}_m^{(n)}(z) \frac{H_{1,m-1}^{(n+1)}(z)}{H_{1,m}^{(n+1)}(z)}$$

and

$$\lim_{n \to \infty} \left(r_{n+m,m}(z) - r_{n+m-1,m}(z) \right) = 0$$

uniformly on B(0, R). The denominator of $\hat{E}_m^{(n)}(z)$ is $O(z^{n+2m-1})$.

We recall from the previous section that any index m such that the strict inequality

$$|z_m| < |z_{m+1}|$$

holds is called a critical index. Note that, in contrast to Theorem 1.1, part (a) of Theorem 2.1 now directly applies to each Q-column with a critical index as column number. The Q-column preceding a vanishing \hat{E} -column contains the factor $H_{1,m}^{(n)}(z)$ in its denominator. Whereas we have to inverse the q-values in the floating-point qd-algorithm, the information on the poles is now contained in the denominator of the Q-values. Moreover, the polynomials containing this information do not have to be composed separately as in Theorem 1.2 and hence the difference between the "simple pole" case and the "equal modulus" pole case is eliminated. The factor $H_{1,m}^{(n)}(z)$ is easily isolated from the other factors in the denominator of $Q_m^{(n)}(z)$ because it is the only one that does not evaluate to zero at z = 0 (or the point around which the Taylor series development was given). The other factors are high order powers of z (which mostly cancel when dealing with a univariate function). In order to know the critical indices, one has to take a look at the \hat{E} -values instead of the *E*-values. These are again obtained by factoring the expression $E_m^{(n)}(z)$, but now retaining the polynomial factors that evaluate to zero. special case of denominator We now display the output of the symbolic *qd*-like algorithm (7), programmed in Mathematica, for the same meromorphic function.

$$f(z) = \frac{e^z}{(z-1)(z-2)(z+2)}$$

INPUT :

$$\sum_{i=0}^{18} c_i z^i \text{ with exact } c_i$$

OUTPUT :

$$\begin{aligned} Q_1^{(17)}(z) &= \frac{-z}{z - 0.999\,9960} \\ E_1^{(16)}(z) &= \frac{3.674\,943\mathrm{E} - 06 * z}{z - 0.999\,9960} \\ Q_2^{(15)}(z) &= \frac{-z * (z - 0.999\,9842)}{(z - 2.232\,566) * (z - 0.999\,9990)} \\ E_2^{(14)}(z) &= \frac{0.246\,0840\mathrm{E} + 00 * z * (z - 0.999\,9842)}{(z - 2.232\,566) * (z - 0.999\,9990)} \\ Q_3^{(13)}(z) &= \frac{-z * (z - 0.999\,9961) * (z - 2.232\,565)}{(z - 1.000\,000) * (z - 2.000\,000) * (z + 2.000\,000)} \\ E_3^{(12)}(z) &= \frac{-5.387\,212\mathrm{E} - 08 * z * (z - 0.999\,9961) * (z - 2.232\,565)}{(z - 1.000\,000) * (z - 2.000\,000) * (z + 2.000\,000)} \end{aligned}$$

CONCLUSION:

$$\begin{aligned} \hat{E}_{1}^{(16)}(z) &= 3.674\,943\mathrm{E}{-}06*z \\ \hat{H}_{1,1}^{(17)}(z) &= z - 0.999\,9960 \\ \hat{E}_{2}^{(14)}(z) &= 0.246\,0840\mathrm{E}{+}00*z \\ \hat{E}_{3}^{(12)}(z) &= -5.387\,212\mathrm{E}{-}08*z \\ \hat{H}_{1,3}^{(13)}(z) &= (z - 1.000\,000)*(z - 2.000\,000)*(z + 2.000\,000) \end{aligned}$$

It is important to emphasize that the entire algorithm should be performed in exact (rational) arithmetic in order to be able to draw the correct conclusions. Only the final display of the results is done in floating-point form. In order to stress the importance of this remark, let us run the same symbolic implementation with floating-point input. Because the symbolic qd-like algorithm (7) cancels a lot of common polynomial factors in its rational expressions $Q_m^{(n)}(z)$ and $E_m^{(n)}(z)$ during the computations, floating-point expressions get into trouble when these common factors are just slightly different due to rounding errors. From the output below it is clear that no conclusions can then be drawn.

INPUT :

$$\sum_{i=0}^{18} c_i z^i \text{ with floating-point } c_i$$

$$\begin{aligned} \text{OUTPUT}: \\ Q_3^{(13)}(z) = \frac{\begin{array}{(} 0.999\ 9912 * z * (z-0.999\ 9990) * (z-2.232\ 566) * \\ (z-0.999\ 9695) * (2.232\ 556 - 3.232\ 561 * z + z^2) * \\ \hline \\ (-3.978\ 324\text{E}-16 - 3.116\ 135 * z + 1.629\ 098\text{E}+10 * z^2 - 4.887\ 340\text{E}+10 * z^3 + \\ \hline \\ 4.887\ 385\text{E}+10 * z^4 - 1.629\ 143\text{E}+10 * z^5 + 7.347\ 068 * z^6 - z^7 \end{array} \right)} \\ \hline \\ (4.000\ 000 - 4.000\ 000 * z - 1.000\ 00 * z^2 + z^3) * \\ (z-0.999\ 9960) * (2.232\ 564 - 3.232\ 565 * z + z^2) * \\ \hline \\ (-2.665\ 543\text{E}-16 + 1.616\ 151 * z - 1.629\ 041\text{E}+10 * z^2 + 4.887\ 210\text{E}+10 * z^3 - \\ \hline \\ 4.887\ 298\text{E}+10 * z^4 + 1.629\ 129\text{E}+10 * z^5 - 7.233\ 991 * z^6 + z^7 \end{array} \right) \end{aligned}$$

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