Jiří Fiala

Zeroes of orthogonal polynomials by QD-algorithm

Aplikace matematiky, Vol. 14 (1969), No. 3, 210–219

Persistent URL: http://dml.cz/dmlcz/103226

ZEROES OF ORTHOGONAL POLYNOMIALS BY QD-ALGORITHM

Jiří Fiala

(Received January 22, 1968)

1. INTRODUCTION

When using quadrature formulas of the highest algebraic order (see e.g. [1]) we need to know the abscissas of those formulas, which are the zeroes of some orthogonal polynomials of high degree. If we use standard methods, two difficulties arise: fist of all we need to have sufficient approximations for the roots. Secondly the coefficients of some polynomials are too large to be handled by up-to-date computers. On the other hand, the roots are normally small numbers. E.g., for Laguerre polynomial of the n-th order $L_n^{(0)}$ (the coefficient at x^n being equal to 1) the absolute coefficient is equal to $(-1)^n \cdot n!$, but the largest root satisfies the inequality

$$x_n < 2n + 1 + \{(2n + 1)^2 + \tfrac{1}{4}\}^{1/2} \cong 4n$$

([2] § 6.31, theorem 6.31.2). Thus, for $n = 101$ this root is equal to 378.892 ...

In this note we propose a method for computing roots of polynomials defined by some recurrence relations and for which the explicit knowledge of coefficients is not necessary. The class of polynomials considered below contains all orthogonal polynomials. The method is based on a direct computation of the top row of the QD-scheme from the recurrence relations.

2. QD-ALGORITHM

If we want to calculate the poles of a rational function, say

$$N_1(x)/N_0^*(x)\,,$$
$$N_1(x) = x^{n-1} + \ldots$$
$$N_0^*(x) = x^n + \ldots$$

we should get the values

$$q_1^{(0)}, q_2^{(1)}, \dots, q_n^{(0)}$$
$$e_1^{(0)}, e_2^{(0)}, \dots, e_n^{(0)}$$

from the recurrence relations

$$N_k^*(x) = \frac{x\,N_k(x) - N_{k-1}^*(x)}{q_k^{(0)}}, \quad k = 1, 2, \dots, n\,;$$

$$N_{k+1}(x) = \frac{N_k^*(x) - N_k(x)}{e_k^{(0)}}, \quad k = 1, 2, \dots, n-1\,.$$

These values are determined uniquely by equating to 1 the highest coefficients of the polynomials $N_k^*(x)$, $N_{k+1}(x)$. In this way the computed numbers form the top row of the QD-scheme:

$$\begin{array}{cccccccccc}
 & q_1^{(0)} & & & & & & & & \\
0 & & e_1^{(0)} & & & & & & & \\
 & q_1^{(1)} & & q_2^{(0)} & & & & & & \\
0 & & e_1^{(1)} & & e_2^{(0)} & & & & & \\
 & q_1^{(2)} & & q_2^{(1)} & & \cdot & & & & \\
0 & & e_1^{(2)} & & e_2^{(1)} & & \cdot & & & \\
 & q_1^{(3)} & & q_2^{(2)} & & \cdot & & \cdot & & \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & e_{n-1}^{(0)} & & \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & q_n^{(0)} & \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & e_{n-1}^{(1)} & & 0 \\
 & & & & & & & & q_n^{(1)} & \dots
\end{array}$$

in which we get the following rows by using the rules:

$$q_\sigma^{(\nu+1)} = q_\sigma^{(\nu)} + e_\sigma^{(\nu)} - e_{\sigma-1}^{(\nu+1)}, \quad e_\sigma^{(\nu+1)} = \frac{e_\sigma^{(\nu)} q_{\sigma+1}^{(\nu)}}{q_\sigma^{(\nu+1)}}, \quad e_0^{(\nu+1)} = 0\,.$$

Supposing the poles of our function to be real and distinct in magnitude, the q-columns converge to their values. Moreover we can easily write the continued fraction expansion of the type S (for continued fractions see e.g. [9]) for our function:

$$\frac{N_1(x)}{N_0^*(x)} = \frac{1|}{|x} - \frac{q_1^{(0)}|}{|1} - \frac{e_1^{(0)}|}{|x} - \frac{q_2^{(0)}|}{|1} - \frac{e_2^{(0)}|}{|x} - \dots - \frac{q_n^{(0)}|}{|1}\,.$$

Concluding the paragraph we refer to the basic Rutishauser's paper [3] and subsequent papers, in which the QD-algorithm is modified to give a better convergence. (See e.g. [4].)

Now we are in the position to prove a theorem enabling us to compute directly the top row of the QD-scheme for some recurrently defined polynomials.

Theorem 1. *Let $a_1, \ldots, a_n, b_1, \ldots, b_{n-1}, b_n = 0$ be real numbers,*

$$a_0 = b_0 = 0\,, \quad p_0(x) = 1\,,$$
$$p_{i+1}(x) = (x - a_{i+1})\, p_i(x) - b_i p_{i-1}(x)\,, \quad i = 0, 1, 2, \ldots, n-1\,.$$

Then, if all the following values are defined, we can get the top row of the QD-scheme for computing the zeroes of the polynomial $p_n(x)$ either from

(I)

$$q_1^{(0)} = a_n \qquad e_1^{(0)} = \frac{b_{n-1}}{q_1^{(0)}}$$

$$q_2^{(0)} = a_{n-1} - e_1^{(0)} \qquad e_2^{(0)} = \frac{b_{n-2}}{q_2^{(0)}}$$

$$\cdots\cdots\cdots\cdots\cdots\cdots$$

$$q_n^{(0)} = a_1 - e_{n-1}^{(0)} \qquad e_n^{(0)} = 0$$

or from

(II)

$$q_1^{(0)} = a_1 \qquad e_1^{(0)} = \frac{b_1}{q_1^{(0)}}$$

$$q_2^{(0)} = a_2 - e_1^{(0)} \qquad e_2^{(0)} = \frac{b_2}{q_2^{(0)}}$$

$$\cdots\cdots\cdots\cdots\cdots\cdots$$

$$q_n^{(0)} = a_n - e_{n-1}^{(0)} \qquad e_n^{(0)} = 0$$

Proof. Let us put $N_o^*(x) = p_n(x)$ and $N_1(x) = p_{n-1}(x)$. We can get the values q and e as stated above:

$$q_1^{(0)} N_1^* = x p_{n-1} - x p_{n-1} + a_n p_{n-1} + b_{n-1} p_{n-2}$$

$$q_1^{(0)} = a_n\,, \quad N_1^* = p_{n-1} + \frac{b_{n-1}}{a_n}\, p_{n-2}$$

$$e_1^{(0)} N_2 = N_1^* - N_1 = \frac{b_{n-1}}{a_n}\, p_{n-2}$$

$$e_1^{(0)} = \frac{b_{n-1}}{a_n}\,, \quad N_2 = p_{n-2}$$

$$q_2^{(0)} N_2^* = x p_{n-2} - p_{n-1} - e_1^{(0)} p_{n-2} = \left(a_{n-1} - e_1^{(0)}\right) p_{n-2} + b_{n-2} p_{n-3}$$

$$q_2^{(0)} = a_{n-1} - e_1^{(0)}\,, \quad N_2^* = p_{n-2} + \frac{b_{n-2}}{q_2^{(0)}} \ \ldots \text{ and so on.}$$

The second expression for the top row may be obtained simply by applying the following

Lemma. *If we define the numbers* $\tilde{a}_i$, $\tilde{b}_i$ *by the relations*

$$\tilde{a}_i = a_{n+1-i}, \quad \tilde{b}_i = b_{n-i}$$

and polynomials $\tilde{p}_i(x)$ *by*

$$\tilde{p}_0 = 1, \quad \tilde{p}_{i+1} = (x - \tilde{a}_{i+1})\,\tilde{p}_i - \tilde{b}_i\tilde{p}_{i-1},$$

then the equality $p_n(x) = \tilde{p}_n(x)$ *holds.*

We obtain the proof from expressing $p_n(x)$ as a determinant:

$$p_n(x) = \begin{vmatrix} x - a_1 & 1 & 0 & \dots & 0 & 0 \\ b_1 & x - a_2 & 1 & \dots & 0 & 0 \\ 0 & b_2 & x - a_3 & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & & \vdots & \vdots \\ 0 & 0 & 0 & & b_{n-1} & x - a_n \end{vmatrix}$$

4. ZEROES OF ORTHOGONAL POLYNOMIALS

Now we are going to apply successively Theorem 1 to some classical orthogonal polynomials. The notation is the same as e.g. in [2].

Laguerre polynomilas satisfy the following recurrence formula

$$(\nu + 1)\,L_{\nu+1}^{(\alpha)}(x) = (2\nu + \alpha + 1 - x)\,L_\nu^{(\alpha)}(x) - (\nu + \alpha)\,L_{\nu-1}^{(\alpha)}(x).$$

Here we put $p_\nu(x) = (-1)^\nu\,\nu!\,L_\nu^{(\alpha)}(x)$. After simple calculations we shall get the sought recurrence relation

$$p_{\nu+1}(x) = [x - (2\nu + \alpha + 1)]\,p_\nu(x) - \nu(\nu + \alpha)\,p_{\nu-1}(x).$$

From this we have immediately:

Theorem 2. *The zeroes of Laguerre polynomial* $L_n^{(\alpha)}$ *can be computed by using QD-algorithm in which we take as the first row the values calculated from* (I) *or* (II) *with*

$$a_\nu = 2\nu - 1 + \alpha, \quad b_\nu = \nu(\nu + \alpha).$$

In the second case we have the explicit equalities for q and e:

$$q_i^{(0)} = i + \alpha \quad (i = 1, 2, 3, \dots, n)$$
$$e_i^{(0)} = i \qquad (i = 1, 2, 3, \dots, n - 1)$$

Example. The beginning of the scheme for $L_3^{(0)}(x)$ reads according to (II):

0						
	1					
0		1				
	2		2			
0		1		2		
	3		3		3	
0		1		2		0
	4		4		1	
0		1		0·5		0
	5·7		3·5		0·5	
0		0·35263		0·071428		0
	6·05263		2·52946		0·42857	
.	.	0·14737		0·001761		0
.	.	.	2·38385		0·416149	
.	.	.	.	0·000307		0
.	.	.	.	.	0·415841	
.	.	.	.	.	.	.
.			.	.	.	.
				.	.	.

The exact values are: 6·28994 ..., 2·29428 ..., 0·41577 ... We can get easily also the following continued fraction expansion:

$$-\frac{1}{n}\frac{L_{n-1}^{(\alpha)}(x)}{L_n^{(\alpha)}(x)} = \frac{1|}{|x} - \frac{1+\alpha|}{|1} - \frac{1|}{|x} - \frac{2+\alpha|}{|1} - \frac{2|}{|x} - \dots - \frac{n+\alpha|}{|1}.$$

Hermite polynomials. The zeroes of Hermite polynomials can be calculated as square roots of the zeroes of the polynomials $L_n^{(-1/2)}$ for n even or $L_n^{(1/2)}$ for n odd. Actually, we have these well known formulas

$$H_{2n}(x) = (-1)^n 2^{2n} n!\, L_n^{(-1/2)}(x^2),$$
$$H_{2n+1}(x) = (-1)^n 2^{2n+1} n!\, x\, L_n^{(1/2)}(x^2).$$

Thus, we can take as the top row in the case (II) the following numbers

$$0{\cdot}5 \quad 1 \quad 1{\cdot}5 \quad 2 \quad 2{\cdot}5 \quad 3 \quad \dots \quad n-\tfrac{1}{2} \quad 0 \quad (n \text{ even})$$

and

$$1{\cdot}5 \quad 1 \quad 2{\cdot}5 \quad 2 \quad 3{\cdot}5 \quad 3 \quad \dots \quad n+\tfrac{1}{2} \quad 0 \quad (n \text{ odd}).$$

In both cases the q-columns converge to the squares of the corresponding zeroes.

Gegenbauer polynomials. Gegenbauer polynomials satisfy the following recurrence relation

$$(n + 1)\, C_{n+1}^{\lambda}(t) = 2(\lambda + n)\, t\, C_n^{\lambda}(t) - (2\lambda + n - 1)\, C_{n-1}^{\lambda}(t)$$

and the highest coefficient is equal to

$$\frac{\Gamma(n + 2\lambda)\,\Gamma(\lambda + \frac{1}{2})}{\Gamma(2\lambda)\,\Gamma(n + \lambda + \frac{1}{2})}\,\frac{1}{2^n}\binom{2n + 2\lambda - 1}{n}.$$

A) even order: we have successively

$$2(n + 1)\, C_{2n+2}^{\lambda}(\sqrt{x}) = 2(\lambda + 2n + 1)\sqrt{(x)}\, C_{2n+1}^{\lambda}(\sqrt{x}) -$$

$$- 2(\lambda + n)\, C_{2n}^{\lambda}(\sqrt{x}) = \frac{4(\lambda + 2n + 1)(\lambda + 2n)}{2n + 1}\, x C_{2n}^{\lambda}(\sqrt{x}) -$$

$$- \frac{2(2\lambda + 2n - 1)(\lambda + 2n + 1)}{2n + 1}\sqrt{(x)}\, C_{2n-1}^{\lambda}(\sqrt{x}) - 2(\lambda + n)\, C_{2n}^{\lambda} =$$

$$= \frac{4(\lambda + 2n + 1)(\lambda + 2n)}{2n + 1}\, x\, C_{2n}^{\lambda}(\sqrt{x}) - 2(\lambda + n)\, C_{2n}^{\lambda}(\sqrt{x}) -$$

$$- \frac{2(2\lambda + 2n - 1)(\lambda + 2n + 1)\, n}{(2n + 1)(\lambda + 2n - 1)}\, C_{2n}^{\lambda}(\sqrt{x}) -$$

$$- \frac{2(\lambda + 2n + 1)(2\lambda + 2n - 1)(\lambda + n - 1)}{(2n + 1)(\lambda + 2n - 1)}\, C_{2n-2}^{\lambda}(\sqrt{x}).$$

Let us denote

$$p_n(x) = \frac{\Gamma(2\lambda)\,\Gamma(2n + \lambda + \frac{1}{2})}{\Gamma(2n + 2\lambda)\,\Gamma(\lambda + \frac{1}{2})}\, 2^{2n}\binom{4n + 2\lambda - 1}{2n}^{-1} C_{2n}^{\lambda}(\sqrt{x}).$$

After some calculations we get the recurrence relation

$$p_{\nu+1}(x) = (x - a_{\nu+1})\, p_\nu(x) - b_\nu\, p_{\nu-1}(x)$$

where

$$(*) \qquad a_{\nu+1} = \frac{8\nu^3 + 12\nu\lambda + \lambda^2 - \lambda}{2(\lambda + 2\nu)(\lambda + 2\nu - 1)(\lambda + 2\nu + 1)}$$

$$b_\nu = \frac{\nu(2\nu - 1)(2\lambda + 2\nu - 1)(\lambda + \nu - 1)}{4(2\nu + \lambda - 2)(2\nu + \lambda)(\lambda + 2\nu - 1)^2}$$

B) odd order: the calculations are similar.

As a result we get the following

Theorem 3. *If we construct QD-scheme using* (I) *or* (II) *and values* (∗), *then the q-columns will converge to the squares of zeroes of Gegenbauer polynomial* C_{2n}^{λ}. *If we take*

$$a_{\nu+1} = \frac{8\nu^3 + 12(\lambda + 1)\,\nu^2 + (4\lambda^2 + 14\lambda + 4)\,\nu + 3\lambda^2 + 3\lambda}{2(2\nu + \lambda)(2\nu + \lambda + 1)(2\nu + \lambda + 2)},$$

$$b_\nu = \frac{\nu(2\nu + 1)(\nu + \lambda)(2\lambda + 2\nu - 1)}{4(2\nu + \lambda - 1)(2\nu + \lambda)^2(2\nu + \lambda - 1)}$$

as initial values, then the q-columns will converge to the squares of zeroes of the polynomial C_{2n+1}^{λ}.

Legendre polynomials. Zeroes of Legendre polynomials can be computed as a particular case of the previous theorem. Actually we have the relation

$$P_n(x) = C_n^{1/2}(x)\,.$$

After an easy arrangement we shall get the

Theorem 4. *If we start with the values*

$$a_{\nu+1} = \frac{8\nu^2 + 4\nu - 1}{(4\nu - 1)(4\nu + 3)},$$

$$b_\nu = \frac{4\nu^2(2\nu - 1)^2}{(4\nu + 1)(4\nu - 1)^2(4\nu - 3)}$$

then the q-columns of the QD-scheme according to (I) *or* (II) *will converge to the squares of the zeroes of Legendre polynomial* P_{2n} *and similarly starting with*

$$a_{\nu+1} = \frac{8\nu^2 + 12\nu + 3}{(4\nu + 1)(4\nu + 5)},$$

$$b_\nu = \frac{4\nu^2(2\nu + 1)^2}{(4\nu - 1)(4\nu + 1)^2(4\nu + 3)}$$

the same algorithm gives the squares of the zeroes of Legendre polynomial P_{2n+1}.

Jacobi polynomials. Zeroes of $P_n^{(\alpha,\beta)}$ for $\alpha = \beta$ can be computed as a particular case of the algorithm for Gegenbauer polynomials, because we have the following equality:

$$P_n^{(\alpha,\beta)}(x) = \frac{\Gamma(2\alpha + 1)\,\Gamma(n + \alpha + 1)}{\Gamma(2\alpha + n + 1)\,\Gamma(\alpha + 1)}\, C_n^{(\alpha+1/2)}(x)\,.$$

Case $\alpha \neq \beta$: The following relation holds:

$$2(n+1)(n+\alpha+\beta+1)(2n+\alpha+\beta)\,P_{n+1}^{(\alpha,\beta)}(x) =$$
$$= (2n+\alpha+\beta)\left[(2n+\alpha+\beta)(2n+\alpha+\beta+2)\,x+\alpha^2-\beta^2\right]P_n^{(\alpha,\beta)}(x) -$$
$$- 2(n+\alpha)(n+\beta)(2n+\alpha+\beta+2)\,P_{n-1}^{(\alpha,\beta)}(x)\,.$$

The coefficient at the highest power of x is

$$\frac{1}{2^n}\binom{2n+\alpha+\beta}{n}.$$

Dividing our recurrence relation by this value and denoting

$$p_\nu(x) = 2^\nu \binom{2\nu+\alpha+\beta}{\nu}^{-1} P_\nu^{(\alpha,\beta)}(x)$$

we shall get after some calculations the relation

$$p_{\nu+1}(x)\,.\,(2\nu+\alpha+\beta)(2\nu+\alpha+\beta+1)(2\nu+\alpha+\beta+2) =$$
$$= \left[(2\nu+\alpha+\beta)(2\nu+\alpha+\beta+1)(2\nu+\alpha+\beta+2)\,x -\right.$$
$$\left.-(2\nu+\alpha+\beta+1)(\beta^2-\alpha^2)\right]p_\nu(x) - \frac{2(\nu+\alpha)(\nu+\beta)(\nu+\alpha+\beta)}{(2\nu+\alpha+\beta)(2\nu+\alpha+\beta-1)}\,p_{\nu-1}(x)\,.$$

Theorem 5. *The zeroes of Jacobi polynomial $P_n^{(\alpha,\beta)}$ for $\alpha \neq \beta$ can be computed by using QD-algorithm with the values q and e given by* (I) *or* (II) *where*

$$a_{\nu+1} = \frac{\beta^2-\alpha^2}{(2\nu+\alpha+\beta)(2\nu+\alpha+\beta+2)},$$
$$b_\nu = \frac{4\nu(\nu+\alpha)(\nu+\beta)(\nu+\alpha+\beta)}{(2\nu+\alpha+\beta-1)(2\nu+\alpha+\beta)^2(2\nu+\alpha+\beta+1)}.$$

The general case. Using Christoffel-Darboux formula we can easily get the general QD-scheme for computing zeroes of orthogonal polynomials. The method is the same as in the preceding particular cases.

5. SOME NUMERICAL RESULTS

Large scale computations were made only for Laguerre polynomials and were carried out on the computer Ural-2. We have used a general program for solving algebraic equations by the QD-algorithm (see [5]); however, the top row of the

QD-scheme was computed by using Theorem 2. The tables of zeroes of Laguerre polynomials were made for $n = 3\ (1)\ 50$ and for $n = 101$. (Eight decimal places.) The efficiency of the method was verified for Laguerre polynomial of the 500th order. As the computations in this case were very time-consuming, we got only 80 smallest roots with the precission of 8 decimal places. The following table contains 50 smallest zeroes of the polynomial $L_{500}^{(0)}$. The results can be compared with known asymptotic estimates (see [2], § 6.31, Thm. 6.31.3).

mantissa	exponent	mantissa	exponent	mantissa	exponent
0·28887051	−2	0·56988716	0	0·21234935	+1
0·15220446	−1	0·68083238	0	0·23331686	+1
0·37406324	−1	0·80164407	0	0·25527265	+1
0·69451483	−1	0·93232340	0	0·27821694	+1
0·11136684	0	0·10728716	+1	0·30214994	+1
0·16312296	0	0·12232902	+1	0·32707191	+1
0·22475039	0	0·13835806	+1	0·35298308	+1
0·29623977	0	0·15537444	+1	0·37988371	+1
0·37759180	0	0·17337833	+1	0·40777407	+1
0·46880730	0	0·19236990	+1	0·43665443	+1

mantissa	exponent	mantissa	exponent
0·46652508	+1	0·81976768	+1
0·49738632	+1	0·86055328	+1
0·52923845	+1	0·90233338	+1
0·56208179	+1	0·94510841	+1
0·59591667	+1	0·98887878	+1
0·63074342	+1	0·10336449	+2
0·66656238	+1	0·10794073	+2
0·70337391	+1	0·11261664	+2
0·74117839	+1	0·11739227	+2
0·77997618	+1	0·12226766	+2

The results for small n were successfully compared with the tables computed by other methods. (See e.g. [6], [7], [8].)

References

[1] *Крылов В. И.:* Приближенное вычисление интегралов, Москва 1959.

[2] *G. Szegö:* Orthogonal polynomials, AMS, N.Y. 1959.

[3] *H. Rutishauser:* Der Quotienten-Differenzen-Algorithmus, Birkhäuser Verlag Basel/Stuttgart 1957.

[4] *H. Rutishauser:* On a modification of the QD-algorithm with Graeffe-type convergence. Information Processing 1962, North-Holland, Amsterdam 1963, pp. 93—96.

[5] *J. Fiala:* Řešení algebraických rovnic QD-algoritmem. Zpráva a program 7-07-04, VLD Praha, 1964.

[6] *Айзенштад В. С., Крылов В. И., Метельский А. С.:* Таблицы для численного преобразования Лапласа и вычисления интегралов вида $\int_0^{+\infty} x^s e^{-x} f(x)\,dx$. АН БССР Минск 1962.
[7] *P. Rabinowitz* and *G. Weiss:* Tables of Abscissas and weights for numerical evaluation of integrals of the form $\int_0^{+\infty} e^{-x} x^n f(x)\,dx$ Math. Tables and Other Aids to Comp. *13* (1959) 285—293.
[8] *Head* and *Wilson:* Laguerre functions: Tables and properties. Proc. I.E.E., Part C, 103 (1956) 428.
[9] *H. Wall:* Analytic theory of continued fractions. N.Y. 1948.

Souhrn

NULY ORTHOGONÁLNÍCH POLYNOMŮ QD-ALGORITMEM

JIŘÍ FIALA

V článku se překládá metoda pro výpočet kořenů orthogonálních polynomů. Věta 1. dává algoritmus pro přímý výpočet horního řádku QD-schématu pro třídu polynomů, které jsou definovány rekurentními vztahy tvaru

$$a_0 = b_0 = 0\,, \quad p_0(x) = 1\,,$$
$$p_{i+1}(x) = (x - a_{i+1})\, p_i(x) - b_i\, p_{i-1}(x)\,, \quad i = 0, 1, 2, \ldots, n-1\,.$$

Algoritmus je dán formulemi (I) a (II). Ve zbývající části článku se tato věta aplikuje na klasické orthogonální polynomy. Na konci článku jsou uvedeny numerické výsledky pro Laguerrovy polynomy.

Author's address: Dr *Jiří Fiala,* Výpočetní laboratoř dopravy, Olšanská 7, Praha 3.