Computing Rational Gauss-Chebyshev Quadrature Formulas with Complex Poles: the Algorithm.

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Abstract

We provide an algorithm to compute arbitrarily many nodes and weights for rational Gauss-Chebyshev quadrature formulas integrating exactly in spaces of rational functions with *complex* poles outside $[-1, 1]$. Contrary to existing rational quadrature formulas, the computational effort is very low, even for extremely high degrees, and under certain conditions on the poles it can be shown that the complexity is of order $O(n)$. This algorithm is based on the derivation of explicit expressions for the Chebyshev (para-)orthogonal rational functions on $[-1, 1]$ with arbitrary *complex* poles outside this interval.

Keywords: quadrature formulas, orthogonal rational functions, complex poles, algorithm, numerical integration, Gauss-Chebyshev.

1 Introduction

Since the fundamental work of Szegő [1], orthogonal polynomials have been an essential tool in the analysis of basic problems in mathematics and engineering. For example, moment problems, numerical quadrature, rational and polynomial approximation and interpolation, linear algebra, and all the direct or indirect applications of these techniques in engineering are all indebted to the basic properties of orthogonal polynomials.

Orthogonal rational functions are a generalization of orthogonal polynomials in such a way that the polynomial case is recovered when all the poles are at infinity. They were first introduced by Djrbashian in the 1960s. Most of his papers appeared in Russian literature, but an accessible survey in English can be found in [2], while details about this section can be found in book [3]. For a survey about the use of orthogonal rational functions in numerical quadrature and system identification, see respectively survey paper [4] and [5], while several results about matrix-valued orthogonal rational functions can be found in [6]–[8].

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In [2]–[8], orthogonality was considered mainly on the unit circle or the whole real line. Of course, many of the classical orthogonal polynomials are not defined with respect to a measure on the unit circle or the whole real line, but they are orthogonal over a finite interval or a half-line. Not much is known about the generalization of these cases to the rational case. It has a lot of potential, because the analysis of orthogonal rational functions on the real line suffered from technical difficulties due to the poles of the function spaces being in the support of the measure. If the support of the measure is only a finite interval or a half-line, the poles can easily be located on the real axis, but outside the support of the measure. New intriguing questions about the location of the zeros, the quadrature formulas and the moment problems arise. For further details on this topic in the case of all *real* poles outside the support of the measure, see e.g. [9]–[13], while some extensions to the case of arbitrarily *complex* poles outside the support of the measure can be found in [14, 15].

A class of Gaussian quadrature formulas on $[-1, 1]$, based on orthogonal rational functions, and their fast and efficient computation, has been dealt with in [16]. These formulas are rational generalisations of the Gauss-Chebyshev formulas and are exact in a maximal space of rational functions with arbitrary but prefixed real poles outside $[-1, 1]$. In contrast to most existing rational quadrature formulas, the computational effort of the algorithm for computing the nodes and weights is very low, and under certain conditions on the poles the complexity can be shown to be of order $O(n)$.

Further, in [17] the expressions of the nodes and weights for the Gauss-Chebyshev quadrature formulas, as well as the theorem on the asymptotic distribution of the nodes, are extended to the case of complex poles, arbitrary but fixed outside $[-1, 1]$. The main purpose of this paper is to extend the algorithm in [16] to this case. In Section 2 we give the necessary theoretical preliminaries. Then, because the nonlinear equation defining the nodes cannot be solved analytically, in Section 3 we perform a thorough analysis of this equation based on the distribution of the poles in the complex plane. Afterwards, in Section 4, we discuss some numerical methods to compute the nodes. Once the nodes are known, the computation of the weights is straightforward, so we will not discuss this in detail. Finally in Section 5 we conclude the paper with some numerical examples.

This paper is an updated and revised version of the conference paper [18]. First, we have included a proof of Lemma 2.2 and Theorem 2.3, because those proofs have never been published before in the case of arbitrary complex poles. Secondly, the method described in Section 4.3 is an improvement of the method proposed in [18, Sec. 4.3] in such a way that it works well on its own for any sequence of poles and that every combination of method can now be considered for determining the initial values for Newton’s method (see also the last paragraph of [18, Sec. 6]). Consequently, we have adapted the numerical examples in accordance with this improvement. Finally, we have performed some timings to illustrate the complexity of the algorithm.

2 Preliminaries

The extended real line will be denoted by $\overline{\mathbb{R}} = \mathbb{R} \cup \{\infty\}$ and the Riemann sphere by $\overline{\mathbb{C}} = \mathbb{C} \cup \{\infty\}$. The unit circle and the open unit disc are denoted respectively by $\mathbb{T} = \{z : |z| = 1\}$ and $\mathbb{D} = \{z : |z| < 1\}$. The complement of the interval $I = [-1, 1]$ with respect to a set X will be given by X^I , e.g. $\overline{\mathbb{C}}^I = \overline{\mathbb{C}} \setminus I$. Furthermore, if $b = \lfloor a \rfloor$ with $a \in \mathbb{R}$, then b is the largest integer so that $b \leq a$.

i	$w_i(x)$	c_i	d_i	p_i	q_i
1	$(1-x^2)^{-1/2}$	1	1	1	-1
2	$\left(\frac{1-x}{1+x}\right)^{1/2}$	3/2	0	1	1
3	$(1-x^2)^{1/2}$	2	0	2	1

Table 1: Definition of the weight function $w_i(x)$ and parameters c_i , d_i , p_i and q_i for $i = 1, 2, 3$.

Suppose a sequence of poles $A = \{\alpha_1, \alpha_2, \dots\} \subset \overline{\mathbb{C}}^I$ is given and define the factors

$$Z_k(x) = \frac{x}{1-x/\alpha_k}, \quad k = 1, 2, \dots$$

and the basis functions

$$b_0(x) \equiv 1, \quad b_k(x) = b_{k-1}(x)Z_k(x), \quad k = 1, 2, \dots$$

Then the space of rational functions with poles in A is defined as $\mathcal{L}_n = \text{span}\{b_0(x), \dots, b_n(x)\}$. Let $\mathcal{P}_n$ denote the space of polynomials of degree less than or equal to n and define $\pi_n(x) = \prod_{k=1}^n (1-x/\alpha_k)$, then we may write equivalently $\mathcal{L}_n = \{p_n/\pi_n, p_n \in \mathcal{P}_n\}$.

Let w be any of the weight functions $w_i(x)$, $i = 1, 2, 3$, as defined in Table 1. Orthonormalising the basis functions $\{b_0(x), \dots, b_n(x)\}$ with respect to the weight function $w_i(x)$, i.e. with respect to the inner product

$$\langle f, g \rangle_w = \int_{-1}^1 f(x) \overline{g(x)} w_i(x) dx,$$

we obtain a basis of Chebyshev orthonormal rational functions (ORFs) $\{\varphi_0(x), \dots, \varphi_n(x)\}$ for the space $\mathcal{L}_n$ on the interval I , so that

$$\langle \varphi_k, \varphi_l \rangle_w = \begin{cases} 0 & , \quad k \neq l \\ 1 & , \quad k = l \end{cases}, \quad 0 \leq k, l \leq n. \quad (1)$$

We define the involution operation or substar conjugate of a function $f(x)$ as

$$f_*(x) = \overline{f(\bar{x})}$$

and the superstar transformation as

$$f^*(x) = \frac{\pi_{n*}(x)}{\pi_n(x)} f_*(x).$$

Note that the factor $\frac{\pi_{n*}(x)}{\pi_n(x)}$ merely replaces the poles $\{\bar{\alpha}_k\}_{k=1}^n$ of $f_*(x)$ by the poles $\{\alpha_k\}_{k=1}^n$ so that $\mathcal{L}_n^* = \mathcal{L}_n$.

We denote the Joukowski Transformation $x = \frac{1}{2}(z + z^{-1})$ by $x = J(z)$, mapping the open unit disc $\mathbb{D}$ onto the cut Riemann sphere $\overline{\mathbb{C}}^I$ and the unit circle $\mathbb{T}$ onto the interval I . The inverse mapping is denoted by $z = J^{inv}(x)$ and is chosen so that $z \in \mathbb{D}$ if $x \in \overline{\mathbb{C}}^I$. With the sequence $A = \{\alpha_1, \alpha_2, \dots\} \subset \overline{\mathbb{C}}^I$ we associate a sequence $B = \{\beta_1, \beta_2, \dots\} \subset \mathbb{D}$ so that $\beta_k = J^{inv}(\alpha_k)$.

Given this sequence of complex numbers $B = \{\beta_1, \beta_2, \dots\} \subset \mathbb{D}$, we define the Blaschke factors

$$\zeta_k(z) = \frac{z - \beta_k}{1 - \overline{\beta_k}z}, \quad k = 1, 2, \dots$$

and the Blaschke products

$$B_0(z) \equiv 1, \quad B_k(z) = B_{k-1}(z)\zeta_k(z), \quad k = 1, 2, \dots$$

Note that the sequence $\{B_0(z), \dots, B_n(z)\}$ forms a basis for the space of rational functions on the unit circle with poles among $\{1/\overline{\beta_1}, \dots, 1/\overline{\beta_n}\}$.

In [17, Lem. 3.1] a relation has been proven between the factors $Z_k(x)$ and the Blaschke factors $\zeta_k(z)$ and $1/\zeta_k(z)$, so that for $k = 0, \dots, n$ it holds that $b_k(x)$ is a linear combination of $1/B_k(z), 1/B_{k-1}(z), \dots, 1/B_0(z) = B_{0*}(z), \dots, B_{k-1*}(z), B_{k*}(z)$. Based on this relation and the property of orthonormality given by (1), the following explicit expressions for the Chebyshev ORFs $\varphi_n(x)$ related to the i^{th} weight in Table 1 have been proven in [17, Thm. 3.2].

Theorem 2.1. *Let $x = J(z) \in \overline{\mathbb{C}}$ and $\alpha_k = J(\beta_k) \in \overline{\mathbb{C}}^I$. Suppose we define the numbers p_i and q_i for $i = 1, 2, 3$ according to Table 1. Then the orthonormal rational functions $\varphi_n(x)$ related to the i^{th} weight in Table 1, with $n \geq 1$, are given by*

$$\varphi_n(x) = \sqrt{\frac{2^i}{\pi}} \sqrt{1 - |\beta_n|^2} \frac{q_i}{2z^{i-1} + q_i - 3} \left(\frac{z^i B_{n-1*}(z)}{1 - \beta_n z} - \frac{q_i}{(z - \beta_n) B_{n-1}(z)} \right)$$

and for $n = 0$ by

$$\varphi_0 = \sqrt{\frac{p_i}{\pi}}.$$

The expressions in this theorem can also be proven by means of Theorem 5 in [15], which gives a relation between ORFs on the interval I and ORFs on the unit circle $\mathbb{T}$, in the case in which explicit expressions are known for the latter one (see [15, Sec. 5 and Sec. 6]). Further, note that when all poles are equal to infinity, $\varphi_n(x)$ becomes the Chebyshev polynomial of the first (respectively second) kind for $i = 1$ (respectively $i = 3$). Furthermore, in this case we have that $\mathcal{L}_n = \mathcal{L}_{n*} = \mathcal{P}_n$.

We define the para-orthogonal rational functions $Q_n(x, \tau)$ with respect to the ORFs $\varphi_n(x)$ as

$$Q_n(x, \tau) = \varphi_n(x) + \tau \varphi_n^*(x), \quad \tau \in \mathbb{T}, \quad n \geq 1.$$

The use of these para-orthogonal rational functions lies in the fact that their zeros are simple and real and can be used as nodes in the quadrature formulas (see also [10, Sec. 3]). A proof will be given in the following lemma.

Lemma 2.2. *The zeros of the para-orthogonal rational function $Q_n(x, \tau) = \frac{q_n(x, \tau)}{\pi_n(x)}$ are simple and real.*

Proof. (The proof is similar to the proof of [3, Thm. 5.2.1]). First, note that $Q_n^*(x, \tau) = \overline{\tau} Q_n(x, \tau)$. Further, we have that $Q_n^*(x, \tau) = \frac{q_{n*}(x, \tau)}{\pi_n(x)}$, so that $q_n(x, \tau) = \tau q_{n*}(x, \tau)$. Or equivalently,

$$r_n(x) \triangleq \gamma q_n(x, \tau) = \overline{\gamma} q_{n*}(x, \tau) \triangleq r_{n*}(x),$$

where $\gamma \in \mathbb{T}$ and $\gamma^2 = \overline{\tau}$. Hence, the coefficients of $r_n(x)$ are real, and so are the zeros of $r_n(x)$.

It remains to prove that these zeros are simple. Suppose there are only $s \leq n - 2$ zeros with an odd multiplicity. Call them $x_1, \dots, x_s$, possibly repeated if they are multiple. The remaining zeros are all of even multiplicity, and hence we can arrange them in doublets (x_j, x_j) for $j = s + 1, \dots, s + r$ with $r = (n - s)/2 \geq 1$. Again, we assume that the doublet (x_j, x_j) is repeated if the multiplicity of x_j is more than 2. Consequently, $q_n(x, \tau)$ is of the form

$$q_n(x, \tau) = c \prod_{j=1}^s (x - x_j) \prod_{j=s+1}^{s+r} (x - x_j)^2$$

for some nonzero constant c . Consider now the function

$$T(x) = \frac{c(1 - x/\bar{\alpha}_n) \prod_{j=1}^s (x - x_j)}{\pi_{n-1}(x)} \in (Z_{n-1}/Z_{n*})\mathcal{L}_{n-2}.$$

It is easy to verify that $Q_n \perp (Z_{n-1}/Z_{n*})\mathcal{L}_{n-2}$, so that $\langle Q_n, T \rangle_w = 0$. In contrast, we have that

$$\langle Q_n, T \rangle_w = |c|^2 \int_{-1}^1 \frac{\prod_{j=1}^{s+r} (x - x_j)^2}{|\pi_{n-1}(x)|^2} w_i(x) dx > 0.$$

This is a contradiction, so that $s \geq n - 1$, which means that all the zeros are simple. $\square$

The quadrature formulas now follow from the next theorem (see also [10, Sec. 3]).

Theorem 2.3. *Assume that the para-orthogonal rational function $Q_n(x, \tau) = \frac{q_n(x, \tau)}{\pi_n(x)}$ is regular, i.e. none of the zeros $x_{nk}(\tau)$ of $q_n(x, \tau)$ coincide with any of the poles. Define*

$$\lambda_{nk}(\tau) = \left[\sum_{j=0}^{n-1} |\varphi_j(x_{nk}(\tau))|^2 \right]^{-1}.$$

Then the quadrature formula

$$\int_{-1}^1 f(x) w_i(x) dx \approx \sum_{k=1}^n \lambda_{nk}(\tau) f(x_{nk}(\tau))$$

is exact for $f \in \mathcal{L}_{n-1} \cdot \mathcal{L}_{n-1}$. In the special case in which α_n is real, this quadrature formula is exact for $f \in \mathcal{L}_n \cdot \mathcal{L}_{n-1*}$.*

Proof. (The proof is almost the same as the proof of [3, Thm. 11.6.1]). In the remainder of this proof, we will omit the parameter τ to simplify our notation. Define the fundamental interpolating functions as

$$L_{nk}(x) = \frac{(1 - x/\alpha_n)}{(1 - x_{nk}/\alpha_n)} \frac{Q_n(x)}{(x - x_{nk})Q'_n(x_{nk})} \in \mathcal{L}_{n-1},$$

where the prime denotes the derivative, and let the weights λ_{nk} be given by

$$\lambda_{nk} = \langle L_{nk}, 1 \rangle_w.$$

Now consider the auxiliary function

$$h(x) = f(x) - \sum_{k=1}^n f(x_{nk}) L_{nk}(x).$$

For $f \in \mathcal{L}_{n-1} \cdot \mathcal{L}_{n-1*}$, this can be written as

$$h(x) = \frac{p_{2n-2}(x)}{\pi_{n-1}(x)\pi_{n-1*}(x)} = \frac{(1 - x/\alpha_n)p_{2n-2}(x)}{\pi_n(x)\pi_{n-1*}(x)}, \quad p_{2n-2} \in \mathcal{P}_{2n-2}.$$

Since $h(x_{nk}) = 0$ for $k = 1, \dots, n$ (interpolation property), and since the numerator of $Q_n(x)$ is a nonzero constant times the nodal polynomial $(x - x_{n1}) \cdots (x - x_{nn})$, we can write

$$h(x) = Q_n(x)g(x), \quad g(x) = \frac{(1 - x/\alpha_n)q_{n-2}(x)}{\pi_{n-1*}(x)}, \quad q_{n-2} \in \mathcal{P}_{n-2}.$$

By its form, $g \in (Z_{n-1*}/Z_n)\mathcal{L}_{n-2*}$, and hence, $g_* \in (Z_{n-1}/Z_{n*})\mathcal{L}_{n-2}$. Consequently,

$$\langle h, 1 \rangle_w = \langle Q_n, g_* \rangle_w = 0.$$

Thus the quadrature is exact for all $f \in \mathcal{L}_{n-1} \cdot \mathcal{L}_{n-1*}$.

For $f \in \mathcal{L}_n \cdot \mathcal{L}_{n-1*}$ we have that

$$\begin{aligned} h(x) &= \frac{p_{2n-1}(x)}{\pi_n(x)\pi_{n-1*}(x)}, \quad p_{2n-1} \in \mathcal{P}_{2n-1} \\ &= Q_n(x)g(x), \quad g \in \mathcal{L}_{n-1*}. \end{aligned}$$

If α_n is real, it follows from [10, Lem. 3.1]¹ that there exists a nonzero constant c_n so that $Q_n(x) = c_n\varphi_n(x) \perp \mathcal{L}_{n-1}$. Consequently, we then have that

$$\langle h, 1 \rangle_w = \langle Q_n, g_* \rangle_w = 0$$

as well, so that in the special case in which α_n is real, the quadrature is exact for all $f \in \mathcal{L}_n \cdot \mathcal{L}_{n-1*}$.

Finally, define the reproducing kernel by

$$k_n(x, y) = \sum_{j=0}^n \varphi_j(x)\varphi_{j*}(y).$$

This has the property that $\langle f(\cdot), k_n(\cdot, y) \rangle_w = f(y)$ for every $f \in \mathcal{L}_n$ and y in the domain of f . Consequently, it holds that

$$\langle L_{nk}(\cdot), k_n(\cdot, x_{nk}) \rangle_w = 1.$$

At the same time we have that

$$\langle L_{nk}(\cdot), k_n(\cdot, x_{nk}) \rangle_w = \sum_{j=0}^n \varphi_j(x_{nk}) \langle L_{nk}, \varphi_j \rangle_w = \lambda_{nk} \sum_{j=0}^{n-1} \varphi_j(x_{nk}) \varphi_{j*}(x_{nk}).$$

This concludes the proof of the theorem. $\square$

Expressions for the computation of the nodes and weights in the quadrature formula, related to the i^{th} weight in Table 1, are given in the next theorem. For the proof we refer to [17, Thm. 4.1 and Thm. 4.6].

¹The statement in [10, Lem. 3.1] has been proven in the case of complex poles in the lower half-plane in [3, Cor. 3.2.2], but this proof remains valid for arbitrary complex poles.

Theorem 2.4. Let $x = J(z) \in \overline{\mathbb{C}}$ and $\alpha_k = J(\beta_k) \in \overline{\mathbb{C}}^I$. Suppose we define the numbers c_i and d_i for $i = 1, 2, 3$ according to Table 1. The nodes $x_{nk}(\tau) = \cos \theta_{nk}(\tau) \in [-1, 1]$ of the rational Gauss-Chebyshev quadrature formula are the zeros of the para-orthogonal rational function $Q_n(x, \tau)$. They satisfy

$$F_n(\theta_{nk}(\tau)) = \pi k - d_i \frac{\pi}{2}, \quad k = 1, 2, \dots, n, \quad (2)$$

where

$$\begin{aligned} F_n(\theta) &= \sum_{j=1}^{n-1} f_{\beta_j}(\theta) + \frac{1}{2} f_{\beta_{n,\tau}}(\theta) - (n - c_i) \theta, \\ f_{\beta}(\theta) &= \arctan \frac{\sin \theta - \Im(\beta)}{\cos \theta - \Re(\beta)} + \arctan \frac{\sin \theta + \Im(\beta)}{\cos \theta - \Re(\beta)} \end{aligned} \quad (3)$$

and

$$\beta_{n,\tau} = \frac{\beta_n + \tau \bar{\beta}_n}{1 + \tau}$$

supposing $\tau \in \mathbb{T} \setminus \{-1\}$ is chosen so that $\beta_{n,\tau} \in]-1, 1[$.

Finally, the weights $\lambda_{nk}(\tau)$ of the rational Gauss-Chebyshev quadrature formula are given by

$$\lambda_{nk}(\tau) = 2\pi \frac{1 - (1 - d_i)[x_{nk}(\tau)]^{i-1}}{i + g_n(x_{nk}(\tau))}, \quad k = 1, 2, \dots, n,$$

where

$$\begin{aligned} g_n(x) &= \sum_{j=1}^{n-1} \{P(z, \beta_j) + P(z, \bar{\beta}_j)\} + P(z, \beta_{n,\tau}), \\ P(z, \beta) &= \frac{1 - |\beta|^2}{|z - \beta|^2} \quad \text{and} \quad x = J(z). \end{aligned}$$

The distribution of the points $x_{nk}(\tau)$ as $n \rightarrow \infty$ depends on the asymptotic distribution of the poles, as formulated in the next theorem. For a proof, see [17, Thm. 4.3].

Theorem 2.5. Assume that the sequence of poles $A = \{\alpha_1, \alpha_2, \dots\}$ is bounded away from I and that the asymptotic distribution of the poles is given by a measure ν on (a subset of) $\overline{\mathbb{C}}^I$, i.e. for any continuous function f with compact support,

$$\lim_{n \rightarrow \infty} \frac{1}{n} \sum_{k=1}^n f(\alpha_k) = \int f(z) d\nu(z).$$

If $\nu = p\delta_\infty + (1 - p)\nu_0$ with $0 \leq p \leq 1$ (where δ_z is the unit measure whose support is the point z) and

$$\int \log |t| d\nu_0(t) < \infty,$$

then the asymptotic distribution of the zeros of $Q_n(x, \tau)$ is given by an absolutely continuous measure λ with weight function

$$\lambda'(x) = \frac{1}{\pi} \frac{1}{\sqrt{1 - x^2}} \int \Re \left\{ \frac{\sqrt{t^2 - 1}}{t - x} \right\} d\nu(t)$$

where the square root is positive for $t > 1$ and the branch cut is $[-1, 1]$.

In general, Equation (2) cannot be solved analytically. Assume for the remainder of this section that $A = \{\alpha_1, \alpha_2, \dots\} \subset \overline{\mathbb{R}}^I$ (and thus $B = \{\beta_1, \beta_2, \dots\} \subset I$, and the nodes and weights independent of τ). Then it is possible to numerically calculate the nodes in the quadrature formulas using Newton's method. In this respect, the following properties are particularly interesting (see [16, p. 316]).

Lemma 2.6. *Suppose $A = \{\alpha_1, \alpha_2, \dots\} \subset \overline{\mathbb{R}}^I$. Then the functions $F_n(\theta)$ from Theorem 2.4, with c_i given by Table 1, are strictly increasing for $0 \leq \theta \leq \pi$. If all poles have equal sign, these functions are concave (positive poles) or convex (negative poles) on $]0, \pi[$. In general there can only be one interior inflection point.*

Newton's method for finding zeros works particularly well for monotonic functions, especially if the initial values are not too far from the exact solutions. We discuss two different methods for determining these initial values (see also [16, p. 316–318]).

The first method is based on linear extrapolation (LE). Let $\{\theta_{nk}\}_{k=1}^n$ denote the n exact zeros, then the initial values can be determined using one of the following equations

$$\theta_{n,k+1}^{(0)} = \theta_{n,k} + (\theta_{n,k} - \theta_{n,k-1}), \quad \theta_{n,1}^{(0)} = \theta_{n,0} = 0 \quad (4)$$

or

$$\theta_{n,n-k}^{(0)} = \theta_{n,n-k+1} + (\theta_{n,n-k+1} - \theta_{n,n-k+2}), \quad \theta_{n,n}^{(0)} = \theta_{n,n+1} = \pi \quad (5)$$

for $k = 1, 2, \dots, n-1$.

The advantage of LE is that it can be used for any sequence of arbitrary poles $\{\alpha_k\}_{k=1}^n \subset \overline{\mathbb{R}}^I$. The disadvantage, however, is that the initial values cannot be determined all at the same time.

The second method for determining the initial values is based on the asymptotic zero distribution (AZD). First we assume that the poles tend to a fixed limit with increasing n , i.e. $\lim_{n \rightarrow \infty} \alpha_n = \alpha$, so that the zero distribution is given by a measure λ whose derivative is equal to

$$\lambda'(x) = \frac{1}{\pi} \frac{1}{\sqrt{1-x^2}} \frac{\sqrt{1-1/\alpha^2}}{1-x/\alpha}.$$

The zero density on the interval $[-1, x]$ equals

$$t(x) = \int_{-1}^x \lambda'(u) du = \frac{1}{\pi} \arcsin \frac{\alpha x - 1}{\alpha - x} + \frac{1}{2}.$$

Solving for x gives

$$x = \frac{1 - \alpha \cos(\pi t)}{\alpha - \cos(\pi t)}, \quad t \in [0, 1], \quad (6)$$

so if we evaluate this in n equidistant points

$$t_{nk} = \frac{2k-1}{2n} \in [0, 1], \quad k = 1, 2, \dots, n, \quad (7)$$

then we get an estimation for the zeros x_{nk} .

For a more general case of a finite number of arbitrary poles $\{\alpha_k\}_{k=1}^n \subset \overline{\mathbb{R}}^I$ for which the distribution is not known, we can use the cubic interpolating spline $s(t)$ through the points $(t_n(\xi_k), \arccos \xi_k)$, with

$$t_n(x) = \frac{1}{n\pi} \sum_{j=1}^n \arcsin \frac{\alpha_j x - 1}{\alpha_j - x} + \frac{1}{2} \quad (8)$$

and

$$\xi_k = \cos\left(\pi \frac{2k-1}{2m}\right), \quad k = 1, 2, \dots, m, \quad (9)$$

which are the zeros of the Chebyshev polynomial $T_m(x)$ for a suitable value of m . Note that the spline is an approximation for the inverse of (8) and that (8) converges pointwise to $t(x)$ for $n \rightarrow \infty$. The initial values for the zeros θ_{nk} are then given by

$$\theta_{nk}^{(0)} = s(t_{nk}) \quad (10)$$

with t_{nk} the points from Equation (7).

The advantage of AZD is that all the initial values can be computed at the same time using vector or matrix operations (depending on whether the sequence contains all equal poles). Of course the estimates will be better for larger n because the method is based on the asymptotic behaviour of the poles.

Finally, we mention the following theorem, which has been proven in [16, Thm. 4.4] in the case of arbitrary *real* poles outside $[-1, 1]$, but which will still hold in the case of arbitrary *complex* poles outside this interval.

Theorem 2.7. *Let there be m different poles among the first n . Then it will take $O(mn)$ operations to compute the nodes and weights in the quadrature formulas. In particular, if all poles are different, the complexity is of order $O(n^2)$, while if there is only a finite number of different poles (m does not depend on n for large n), then the complexity is of order $O(n)$.*

3 Analysis of $F_n(\theta)$ in the case of complex poles

As mentioned in Section 2, Equation (2) cannot be solved analytically, so the nodes have to be computed numerically using an iterative method. An analysis of the equation for the nodes has been done in the case of all real poles in Lemma 2.6. The equation had certain properties that justified the use of Newton's method in computing the nodes. In the case of arbitrary complex poles, not all these properties hold in general. Instead, we have the following lemma.

Lemma 3.1. *The functions $F_n(\theta)$ are strictly increasing for $0 \leq \theta \leq \pi$.*

Secondly, suppose that all the poles satisfy the condition given by

$$|\Im(\beta)| \leq \sqrt{\frac{|\Re(\beta)|}{4 - |\Re(\beta)|}} (1 - |\Re(\beta)|) \quad (11)$$

(see Figure 1). If the real parts of all the poles have equal sign, then the functions $F_n(\theta)$ are concave (positive real part) or convex (negative real part) on $]0, \pi[$.

Thirdly, if all the poles satisfy the condition given by

$$\begin{aligned} & \Im(\beta)^6 - \{14 + 8|\Re(\beta)| - \Re(\beta)^2\} \Im(\beta)^4 + \\ & \{(1 + |\Re(\beta)|)^2 (1 - 10|\Re(\beta)| - \Re(\beta)^2)\} \Im(\beta)^2 - \{\Re(\beta)^2 (1 + |\Re(\beta)|)^4\} \geq 0, \end{aligned} \quad (12)$$

or if they all satisfy the condition given by (11) together with

$$\begin{aligned} & \Im(\beta)^6 - \{14 - 8|\Re(\beta)| - \Re(\beta)^2\} \Im(\beta)^4 + \\ & \{(1 - |\Re(\beta)|)^2 (1 + 10|\Re(\beta)| - \Re(\beta)^2)\} \Im(\beta)^2 - \{\Re(\beta)^2 (1 - |\Re(\beta)|)^4\} \leq 0 \end{aligned} \quad (13)$$

Figure 1: Partition of $\mathbb{D}$ (figure on the left), respectively the complex plane (figure on the right). Condition (11) holds for poles inside the red curve (figure on the left), respectively outside of the red curve (figure on the right). Furthermore, the poles within the areas marked with an 'x' and an 'o' satisfy condition (13), while the poles within the areas marked with a '+' satisfy condition (12).

(see Figure 1), then there can only be one inflection point $\theta_b \in]0, \pi[$. Further, $\frac{dF_n(\theta)}{d\theta}$ reaches a maximum (respectively minimum) for $\theta = \theta_b$ in the case that condition (12) (respectively the conditions (11) and (13)) is (are) satisfied.

Proof. See [18, Lem. 3.1–3.3] as well as [18, Rem. 3.4]. $\square$

Remark 3.2. If the sequence of poles does not satisfy any of the conditions mentioned in Lemma 3.1, then there can be more than one interior inflection point. Based on many tests, the maximum number of interior inflection points found was $2n - 3$ ($n \geq 2$), for a sequence of poles containing $n - 2$ poles among the first $n - 1$ poles in the areas marked with an 'o', all having different real parts, and two real poles with different sign close to one in absolute value. One can indeed expect that the shape of $F_n(\theta)$ becomes worse when the poles are closer to the boundary $[-1, 1]$. In the remainder of the text, we will assume that this kind of distribution of the poles is the worst situation possible.

Based on the previous remark, the following lemma concerns the behaviour of $F_n(\theta)$ if one or more poles in the sequence tend to a value in $[-1, 1]$.

Lemma 3.3. Consider a finite sequence of n poles and suppose that we let one of the poles α_k in the sequence tend to a value $\alpha \in [-1, 1]$. Then $\frac{dF_n(\theta)}{d\theta}$ has a local maximum in $\theta = \theta_{b_k}$ and $\lim_{\alpha_k \rightarrow \alpha} \theta_{b_k} = \arccos(\alpha)$.

Proof. See [18, Lem. 3.6]. $\square$

Two things are of importance here. In the first place, note that the previous lemma explains the amount of $2n - 3$ interior inflection points mentioned in Remark 3.2. If we have $n - 2$ complex poles all tending to a different value in $] -1, 1[$ and two real poles tending to 1 and -1 , then according to the previous lemma this will result in $\frac{dF_n(\theta)}{d\theta}$

having n local maxima. Between two maxima there has to be a minimum, so we get $n + (n - 1) = 2n - 1$ inflection points of which $2n - 3$ are in the interval $]0, \pi[$.

Secondly, with $\Theta(\beta)$ given by

$$\Theta(\beta) = \frac{1 + |\beta|^2}{2|\Re(\beta)|} - \sqrt{\frac{\left(\frac{1+|\beta|^2}{2\Re(\beta)}\right)^2 - 1}{\left(\frac{\Re(\beta)}{\Im(\beta)}\right)^2 + 1}}, \quad (14)$$

we have that $\cos \theta_\alpha \triangleq \text{sign}(\Re(\beta))\Theta(\beta) \rightarrow \Re(\beta)$ for $|\beta| \rightarrow 1$ while $\Re(\beta) \rightarrow \Re(\alpha) \in [-1, 1]$ for $|\beta| \rightarrow 1$. Furthermore, θ_α is a local maximum for $\frac{df_\beta(\theta)}{d\theta}$ with $f_\beta(\theta)$ given by (3) (see [18, Eq. (16)] and [18, Rem. 3.4]), but not necessarily a local maximum for $\frac{dF_n(\theta)}{d\theta}$. However, based on the previous lemma and the limiting behaviour of θ_α , we can conclude that it will approach the exact local maximum when the related pole or all the other poles come closer to the boundary, or when the multiplicity of the related pole increases.

4 Computing the nodes for complex poles

We will now discuss three methods for determining the initial values for Newton's method. Two of them have already been briefly discussed in Section 2 for the case of all real poles, namely LE and AZD.

4.1 Asymptotic zero distribution

First, consider the case of one multiple pole $\alpha \in \overline{\mathbb{R}}^I$. We can determine β as a function of α by

$$\beta = \alpha - \text{sign}(\alpha)\sqrt{\alpha^2 - 1} = \frac{1}{\alpha + \text{sign}(\alpha)\sqrt{\alpha^2 - 1}}, \quad (15)$$

where the second expression is better, from a numerical point of view, because it avoids computing the difference between two almost equal values. For $\alpha = \infty$, (6) gives us

$$x = -\cos(\pi t) = \cos(\pi(1 - t)).$$

From (15) we can deduce that $\beta = 0$ for the given value of α , which means that we can determine the exact solution of (2) for a given multiplicity n of the pole. This gives us

$$\theta_{nk} = \pi t_{nk},$$

where

$$t_{nk} = \frac{k - d_i/2}{n + c_i - 1} \quad (16)$$

and

$$x_{nk} = \cos(\pi t_{nk}).$$

So when we evaluate (6) in the points

$$t = 1 - t_{nk},$$

with t_{nk} given by (16) instead of (7), the initial values will be the exact solution. When using the same points for an arbitrary pole $\alpha \in \mathbb{R}^I$, this results in the following initial values

$$x_{nk}^{(0)} = \frac{1 + \alpha \cos(\pi t_{nk})}{\alpha + \cos(\pi t_{nk})} = \frac{2\beta + (\beta^2 + 1) \cos(\pi t_{nk})}{\beta^2 + 1 + 2\beta \cos(\pi t_{nk})}. \quad (17)$$

As explained in Section 2, the advantage of AZD for one multiple pole is that we can compute all the initial values at the same time using vector operations. This makes it the fastest method of all. A disadvantage, however, is that it can only be used if all poles are equal to each other. Clearly this has to be a real value, because in the case of complex poles the last pole α_n (if not real already) will be replaced by $\alpha_{n,\tau} = (\beta_{n,\tau} + \beta_{n,\tau}^{-1})/2 \in \mathbb{R}^I$ during the computations.

Where $F_n(\theta)$ is strictly increasing concave (respectively convex), Newton's method converges monotonically if $\theta_{nk}^{(0)} \leq \theta_{nk}$ (respectively $\theta_{nk}^{(0)} \geq \theta_{nk}$). The initial values $\theta_{nk}^{(0)} = \arccos(x_{nk}^{(0)})$ with $x_{nk}^{(0)}$ given by (17) satisfy this condition.

Theorem 4.1. *For each $\beta \in]-1, 0]$ (respectively $\beta \in [0, 1[$) we have $\theta_{nk}^{(0)} \geq \theta_{nk}$ (respectively $\theta_{nk}^{(0)} \leq \theta_{nk}$).*

Proof. See [18, Lem. 4.1, Lem. 4.2 and Thm. 4.3]. $\square$

Finally, consider the case of different poles $\{\alpha_k\}_{k=1}^n$ with $\alpha_k \in \overline{\mathbb{C}}^I$. Like before, we can determine the initial values as

$$\theta_{nk}^{(0)} = s(1 - t_{nk}),$$

with t_{nk} given by (16), instead of using (7) and (10), replacing (8) and (9) with

$$t_n(x) = \frac{1}{n\pi} \left\{ \sum_{j=1}^{n-1} \Re \left(\arcsin \frac{\alpha_j x - 1}{\alpha_j - x} \right) + \arcsin \frac{\alpha_{n,\tau} x - 1}{\alpha_{n,\tau} - x} \right\} + \frac{1}{2} \quad (18)$$

and

$$\xi_k = \cos \left(\pi \frac{k - d_i/2}{m + c_i - 1} \right), \quad k = 1, 2, \dots, m.$$

Thus, when all the poles are equal to infinity with multiplicity $n = m$, the initial values will again be the exact solution.

Again, as mentioned in Section 2, the advantage of AZD for different poles is that we can compute all the initial values at the same time using matrix operations. Theoretically, this makes it faster than LE, but slower than AZD for one multiple pole because we first have to form the cubic interpolating spline for the inverse of (18). In practice, however, when the matrices become too large, a bigger but slower memory can become necessary for the computations, which means that LE would become faster. Nevertheless, this can be solved by still determining the initial values using AZD, but computing the nodes in a for-loop using vector operations instead of matrix operations. A disadvantage of AZD for different poles is that the initial values do not necessarily converge monotonically to the exact solution. Another disadvantage of AZD in general is that it does not work well for nodes close to possible peak shaped interior local maxima of $\frac{dF_n(\theta)}{d\theta}$, introduced by poles in the sequence close to the boundary. In this case, however, AZD can still be used to compute those nodes that are not close to these local maxima.

4.2 Linear extrapolation

As we have seen in Section 2, the initial values cannot be determined simultaneously when using LE. Not only is LE slower than AZD because of this, but also convergence while computing the previous node is essential so that it can continue with the computation of the next node. Because of this, LE is more interesting in combination with AZD when some but not all nodes can be computed with the latter, rather than as a method on its own. Nevertheless, LE has an advantage over AZD for sequences of different poles because under certain conditions it converges monotonically to the exact solution.

Theorem 4.2. *If all poles have positive (respectively negative) real parts and satisfy condition (11), Newton's method converges monotonically if the initial values are determined by (4) (respectively (5)).*

Proof. See [18, Thm. 4.4]. □

In the case of poles with positive and negative real parts, we need the extra condition (13) to assure that $F_n(\theta)$ has at most one interior inflection point $\theta_b \in]0, \pi[$, for which $\frac{dF_n(\theta)}{d\theta}$ has a local minimum. In this way, $F_n(\theta)$ will be strictly increasing concave on $]0, \theta_b[$ while the other part will be strictly increasing convex (see Lemma 3.1). So, when applying (4) (respectively (5)) to the interval $[0, \theta_b]$ (respectively $[\theta_b, \pi]$), Newton's method also converges monotonically for these kinds of sequences of poles when using LE.

In practice it is not easy to compute the interior inflection point. Nevertheless, because convergence is not excluded when an initial value lies on the wrong side of the exact solution, computing this is not necessary at all. Instead, we can start with one of both formulas (e.g. (4)) until it does not converge anymore and then continue with the other one (e.g. (5)) if necessary. For other kinds of sequences of poles, convergence with LE cannot be assured but is not necessarily excluded either. However, for sequences containing poles not satisfying condition (11) close to the boundary, it is very unlikely that all the nodes can be computed using LE because of peak shaped interior local maxima of $\frac{dF_n(\theta)}{d\theta}$ introduced by these poles. Compare with AZD, where we had the same problem, but for sequences containing poles close to the boundary (independent of whether they satisfy condition (11)).

4.3 Local maxima of the first derivative

As we have seen before, in the case that the sequence contains poles not satisfying condition (11) close to the boundary, these poles will introduce peak shaped interior local maxima of $\frac{dF_n(\theta)}{d\theta}$. When computing the nodes close to those local maxima, Newton's method can diverge when using AZD as well as when using LE. So the goal is to find another method to determine initial values so that Newton's method will converge (monotonically) to these nodes. To realise this, we can try to estimate all the peak shaped local maxima of $\frac{dF_n(\theta)}{d\theta}$, based on their limiting behaviour (see Lemma 3.3), and then use these estimates as initial values for the nodes close to these local maxima. In the remainder of this text we will refer to this method as the method of the first derivative (MFD).

Let $\alpha = J(\beta)$ be a pole in the sequence of poles different from infinity. Then we have, with $\Theta(\beta)$ defined by (14), that θ_α , satisfying

$$\cos \theta_\alpha = \text{sign}(\Re(\beta)) \min\{1, \Theta(\beta)\}, \quad (19)$$

is a local maximum of $\frac{df_{\beta}(\theta)}{d\theta}$. The closer α is to the boundary, the more this local maximum becomes a peak shaped local maximum of $\frac{df_{\beta}(\theta)}{d\theta}$. And hence, the better it will approximate the local maximum of $\frac{dF_n(\theta)}{d\theta}$ introduced then by α , which will become a peak shaped local maximum as well. When applying (19) to each different pole $\alpha_j \neq \infty$, $j = 1, \dots, m$, in the sequence of poles (note that for the last pole in the sequence, we have to use $\alpha_{n,\tau}$ instead of α_n), we can now define the list $\mathcal{C} = \{\theta_{\alpha_j}\}_{j=1}^m \cup \{0, \pi\}$, so that $\mathcal{C}$ will (also) contain very good estimates of the (possible) peak shaped local maxima of $\frac{dF_n(\theta)}{d\theta}$. With each value in $\mathcal{C}$ we associate the index l_j given by

$$l_j = \frac{F_n(\mathcal{C}[j])}{\pi} - \frac{d}{2}, \quad j = 1, \dots, m+2,$$

where $\mathcal{C}[j]$ represents the j^{th} element of $\mathcal{C}$.

Next, assume AZD was used to compute the nodes, then we get a list $\mathcal{K}$ of indices of nodes that has not been found yet, and hence are close to a peak shaped local maximum of $\frac{dF_n(\theta)}{d\theta}$. Now assume that, with $k \in \mathcal{K}$, the k^{th} node is close to θ_* , where θ_* is a peak shaped local maximum of $\frac{dF_n(\theta)}{d\theta}$. We then have that one element of $\mathcal{C}$ will be a very good estimate of θ_* . At the moment of writing, no method was found to determine which value this is. However, with J_l and J_r given by

$$J_l = \arg \max_j (l_j \leq k) \quad (20)$$

and

$$J_r = \arg \min_j (l_j \geq k), \quad (21)$$

we know for sure that this value has to be $\mathcal{C}[J_l]$ or $\mathcal{C}[J_r]$. So in practice we can start using (20) for each index in $\mathcal{K}$ to determine initial values for the associated nodes, approximating them from the left. And afterwards, continuing with (21) for those nodes for which Newton's method still has not converged, approximating them from the right.

Like in the case of AZD, the advantage of MFD is that we can compute all the initial values at the same time using matrix operations, which theoretically makes it faster than LE too. In Most cases, MFD will also work well if AZD has not been used in advance, even if the sequence contains some or only poles away from the boundary. However, in general Newton's method will converge faster when using AZD for those nodes that can be computed with the initial values determined by AZD.

4.4 Some additional remarks

Remark 4.3. In the case that the sequence only contains poles close to the boundary, it is possible to determine in advance which of both values, $\mathcal{C}[J_l]$ or $\mathcal{C}[J_r]$, is the better one. Suppose we have a sequence of m different poles α_j , each with multiplicity n_j so that $\sum_{j=1}^m n_j = n$. Then the estimates θ_{α_j} of the peak shaped local maxima are given by (19). Further, in the limit case ($\alpha_j \in [-1, 1]$) we have that $\frac{df_{\beta_j}(\theta_{\alpha_j})}{d\theta} = \infty$, while for every other θ we have that $\frac{df_{\beta_j}(\theta)}{d\theta} = 1$. So, with $\delta > 0$ and $\epsilon > 0$ we get that

$$\begin{aligned} f_{\beta_j}(\theta_{\alpha_j} + \delta) - f_{\beta_j}(\theta_{\alpha_j} - \epsilon) &= [f_{\beta_j}(\pi) - (\pi - \theta_{\alpha_j} - \delta)] \\ &\quad - [f_{\beta_j}(0) + (\theta_{\alpha_j} - \epsilon)] = f_{\beta_j}(\pi) - f_{\beta_j}(0) - \pi + \delta + \epsilon = \pi + \delta + \epsilon. \end{aligned}$$

Consequently, $F_n(\theta)$ shows a jump in θ_{α_j} equal to $n_j\pi$ (if $\alpha_j \neq \alpha_{n,\tau}$, otherwise the jump will be equal to $(n_j - 1/2)\pi$), while, if θ_k and θ_{k+1} are two successive exact solutions of (2), then $F_n(\theta_{k+1}) - F_n(\theta_k) = \pi$. Because of this, we can use as a rule that the multiplicity of θ_{α_j} as initial value equals n_j . This rule still works for sequences containing only poles away from the boundary (just because in this case there will be no peak shaped local maxima). But it does not work well if the sequence contains poles away from the boundary as well as poles close to the boundary.

Remark 4.4. At the moment of writing, no example could be found for which not every node could be computed using only MFD. Consider, however, a sequence containing poles away from the boundary for which the distribution of the poles in the sequence is such that one or more nodes are close to a local minimum (respectively a local maximum that is not peak shaped) of $\frac{dF_n(\theta)}{d\theta}$. Further, assume that no value in $\mathcal{C}$ is really close to those nodes. Then it is possible that Newton's method will not converge to these nodes because of intermediate values outside $[0, \pi]$ during the iterations (respectively because of an infinite loop while iterating). When AZD has been used in advance, these nodes would probably already have been computed before continuing with MFD. If not, LE can still be used to compute these nodes, starting from the neighbouring nodes that have been found. In the extreme case that Newton's method does not converge for these nodes with any of the three methods AZD, MFD and LE, some additional computations using the method of bisection can be necessary to compute these nodes. Nevertheless, this additional number of iterations will be negligible compared with the number of iterations needed when only using the method of bisection.

Remark 4.5. For sequences containing poles extremely close to the boundary, the results for the nodes need to be very precise to get accurate results for the weights as well. When using a less severe criterium of accuracy during the iterations, Newton's method will converge when using MFD for the nodes close to the peak shaped local maxima but the results can be very inaccurate. On the other hand, when using a more severe criterium of convergence, rounding errors can cause the desirable accuracy to be unreachable. For this reason, some additional computations using the method of bisection can be necessary to get full precision. This additional number of iterations will now also be negligible compared with the number of iterations needed when only using the method of bisection.

5 Numerical results

We shall now look at three examples of sequences of poles and compare the results for the nodes and weights for the different methods discussed in the previous section with the results for the nodes and weights when only using the method of bisection, assuming the results for the latter are exact. With Δx and $\Delta \lambda$ we denote the maximal difference in absolute value between the resulting nodes and weights. We will also compare the largest number of iterations, denoted by p_{max} , needed for the initial value that converged the slowest, as well as the total number of iterations, denoted by p_{total} , assuming the iterations for each node were done serially like for LE. All the computations in the examples that follow are done with Matlab 6.5 on a Celeron M-processor with a CPU speed of 1.3GHz for the first weight function $i = 1$ (the results for $i = 2, 3$ are similar) and for $\tau = 1$. Further, the Newton iterations are done with an absolute accuracy of $|\theta_k^{(p-1)} - \theta_k^{(p)}| \leq 10^{-10}$, while for the method of bisection the nodes are computed with an absolute accuracy of $|\theta_k^{(p-1)} - \theta_k^{(p)}| \leq 5 \times 10^{-16}$. To check the accu-

racy of the results for each method on its own, the absolute difference $|\pi - \sum_{k=1}^n \lambda_k|$, which theoretically has to be zero, is checked as well.

Example 5.1. Let us first consider the sequence of poles given by

$$A = \{\alpha_{k+6} = 2.005 + 1.905\mathbf{i} + 0.001k(1 + \mathbf{i}), \quad k = -5, \dots, 5\} \cup \{\alpha_{k+17} = -2.000 - 1.900\mathbf{i} - 0.001k(1 + \mathbf{i}), \quad k = -5, \dots, 5\}. \quad (22)$$

Then Figure 2 shows the graph of $F_n(\theta)$, $\frac{dF_n(\theta)}{d\theta}$ and $\frac{d^2F_n(\theta)}{d\theta^2}$. Note that, although the graph of $F_n(\theta)$ looks like a straight line, it is not, as can be deduced from the graph of the first and second derivative. The given sequence does not satisfy any of the conditions given by Lemma 3.1. However, none of the poles are close to the boundary, thus we can expect that Newton's method works well for the given sequence. Table 2 summarises the results for Newton's method and for the method of bisection.

Figure 2: The graph of $F_n(\theta)$, $\frac{dF_n(\theta)}{d\theta}$ and $\frac{d^2F_n(\theta)}{d\theta^2}$ for the sequence of poles given by (22).

Example 5.2. Next, consider the sequence of poles given by

$$B = \{\alpha_k = 0.75 + 0.01\mathbf{i}, \quad k = 1, \dots, 4\} \cup \{\alpha_k = 2, \quad k = 5, 6\}. \quad (23)$$

Then Figure 3 shows the graph of $F_n(\theta)$, $\frac{dF_n(\theta)}{d\theta}$ and $\frac{d^2F_n(\theta)}{d\theta^2}$. The given sequence contains poles close to the boundary as well as poles away from the boundary. Because of this, not all the nodes can be computed with Newton's method when using only AZD or LE for determining the initial values. But all the nodes can be computed when AZD

method	Δx	$\Delta \lambda$	$ \pi - \sum_{k=1}^n \lambda_k $	p_{max}	p_{total}
bisection	0	0	8.9×10^{-16}	52	1133
AZD	5.6×10^{-16}	2.8×10^{-17}	8.9×10^{-16}	3	66
LE	7.8×10^{-16}	2.8×10^{-17}	8.9×10^{-16}	3	52
MFD	6.7×10^{-16}	2.8×10^{-17}	8.9×10^{-16}	4	85

Table 2: The results for Newton's method and for the method of bisection for the sequence given by (22).

is combined with one of the other two methods or when only MFD is used. Table 3 summarises the results for the two combinations, for MFD alone and for the method of bisection. With n_i we denote the number of initial values that converged for the specific method.

Figure 3: The graph of $F_n(\theta)$, $\frac{dF_n(\theta)}{d\theta}$ and $\frac{d^2F_n(\theta)}{d\theta^2}$ for the sequence of poles given by (23).

Example 5.3. Finally consider the sequence of poles given by

$$C = \{\alpha_k = -\alpha_{k+5} = 0.75 + 0.01i, \quad k = 1, \dots, 4\} \cup \{\alpha_5 = -\alpha_{10} = 2\}. \quad (24)$$

Then Figure 4 shows the graph of $F_n(\theta)$, $\frac{dF_n(\theta)}{d\theta}$ and $\frac{d^2F_n(\theta)}{d\theta^2}$. The given sequence now contains many more poles close to the boundary than poles away from the boundary. In this case not all the nodes can be computed when combining AZD with LE. But they

method	Δx	$\Delta \lambda$	$ \pi - \sum_{k=1}^n \lambda_k $	p_{max}	p_{total}	n_i
bisection	0	0	1.8×10^{-15}	52	309	6
AZD and LE	2.3×10^{-15}	1.3×10^{-15}	1.3×10^{-15}	6 5	26 5	5 1
AZD and MFD	2.3×10^{-15}	1.3×10^{-15}	1.3×10^{-15}	6 5	26 5	5 1
MFD	3.9×10^{-16}	4.4×10^{-16}	8.9×10^{-16}	8	40	6

Table 3: The results for Newton’s method and for the method of bisection for the sequence given by (23).

can be computed when combining AZD with MFD or when only using MFD. Table 4 summarises the results for Newton’s method and for the method of bisection.

Figure 4: The graph of $F_n(\theta)$, $\frac{dF_n(\theta)}{d\theta}$ and $\frac{d^2F_n(\theta)}{d\theta^2}$ for the sequence of poles given by (24).

Example 5.4. To illustrate the complexity of the algorithm, consider a sequence of m different poles among the first n . Then Table 5 summarises the CPU time (seconds) in function of n for $m = 5$. This table clearly shows that for larger n , the CPU time doubles if the total number of poles is doubled, and hence the complexity is of order $O(n)$.

Table 6, on the other hand, summarises the CPU time (seconds) in function of n for $m = n$. This table clearly shows that for larger n , the CPU time almost increases with

method	Δx	$\Delta \lambda$	$ \pi - \sum_{k=1}^n \lambda_k $	p_{max}	p_{total}	n_i
bisection	0	0	5.8×10^{-15}	52	516	10
AZD	2.1×10^{-15}	8.2×10^{-15}	2.2×10^{-15}	5	34	6
and MFD				6	28	4
MFD	1.1×10^{-15}	5.4×10^{-15}	2.7×10^{-15}	9	70	10

Table 4: The results for Newton’s method and for the method of bisection for the sequence given by (24).

n	t	n	t	n	t
8	0.02	256	0.14	8192	3.17
16	0.01	512	0.28	16384	6.35
32	0.02	1024	0.55	32768	12.72
64	0.05	2048	1.08	65536	25.65
128	0.07	4096	2.01	131072	51.26

Table 5: CPU time (seconds) in function of the total number of poles n for a sequence of $m = 5$ different poles among the first n .

a factor 4 if the total number of poles is doubled, and hence the complexity is of order $O(n^2)$.

m	t	m	t	m	t
4	0.08	64	0.05	1024	5.93
8	0.01	128	0.17	2048	22.82
16	0.01	256	0.51	4096	83.54
32	0.02	512	1.70	8192	302.36

Table 6: CPU time (seconds) in function of the total number of poles n for a sequence of $m = n$ different poles among the first n .

6 Conclusion

We have provided a fast algorithm to compute arbitrarily many nodes and weights for rational Gauss-Chebyshev quadrature formulas integrating exactly in spaces of rational functions with arbitrary *complex* poles outside $[-1, 1]$. This algorithm was based on the derivation of explicit expressions for the Chebyshev (para-) orthogonal rational functions.

Once the nodes were known, the computation of the weights was straightforward. These nodes could not be found analytically but had to be solved numerically (using Newton’s method) from the equation $f(x_k) = C_k$, $k = 1, \dots, n$, where C_k is a constant only depending on the node x_k to be computed and f is a smooth, monotonically increasing function that depends on the first n poles. The success of our algorithm depended on obtaining accurate initial values for the exact solutions and on a thorough analysis of the graph of $f(x)$, with $x \in [-1, 1]$, based on the distribution of the poles

in the complex plane.

Some characteristics of this function had already been given for the case of all *real* poles in [16] and two methods had been derived for determining a sequence of initial values for the nodes, assuring convergence of Newton's method. For *complex* poles, however, these characteristics did not hold in general and these two methods were not sufficient to assure convergence to the exact values in every possible case.

We have derived a new method to obtain more accurate initial values for the case of arbitrary complex poles. In all cases under consideration, these values converged to the exact solutions. In some exceptional cases, a few additional iterations using the method of bisection were needed to obtain full precision.

When considering combinations of methods, we have assumed the methods were used one after the other. Thus, the following questions are still open for further investigation:

- Is it possible, when using MFD, to find a method to determine in advance which of both values, $\mathcal{C}[J_l]$ or $\mathcal{C}[J_r]$, is the better one, even when the sequence contains poles away from the boundary?
- Is it possible to predict (based on the distribution of the poles in the sequence) which nodes cannot be computed with AZD so that AZD and MFD can be used simultaneously?
- Or, is it possible to find a single method for determining a set of initial values that is as good as AZD and MFD (and maybe even LE) together?

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