# Computing orthogonal rational functions with poles near the boundary

*J. Van Deun, A. Bultheel, and P. González Vera*

*Report TW 450, February 2006*




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**Abstract**

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**Keywords :** Orthogonal rational functions

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## 1 Introduction

Orthogonal rational functions with prescribed poles outside the support of a given measure generating orthogonality represent a nice extension of the well known theory of orthogonal polynomials (all the poles located at infinity) and have become a tool widely used in system theoretical applications, see e.g. [4, 5, 6, 9, 14, 15, 16, 17]. It may therefore come as a surprise that very little attention has gone to the accurate and efficient numerical computation of these functions. A possible explanation could be that most applications so far have used explicitly known orthogonal systems, see e.g. [16, 17] (this is the same explanation Gautschi [3] gives for the lack of interest in computational aspects of orthogonal polynomials), or that in many cases the orthogonality measure is discrete with finite support, so that the computation of the rational functions is rather straightforward. For more general measures we proposed a method of computing the coefficients in the three term recurrence relation satisfied by orthogonal rational functions in [12]. This is basically just a rational generalization of what Gautschi calls the *discretized Stieltjes procedure*. As is shown in that paper, this procedure works very well for orthogonal rational functions that have poles not too close to the boundary of the support of the orthogonality measure. The computation of orthogonal rational functions with poles very close to the boundary is a complicated matter. In the present paper it is our aim to analyze the problem and indicate some possible solutions. Some examples serve as illustration. As in [12], we will limit our attention to the case of a finite interval.

## 2 Preliminaries

Let the real line be denoted by $\mathbb{R}$ and the extended real line by $\overline{\mathbb{R}} = \mathbb{R} \cup \{\infty\}$. For the interval $[-1, 1]$ and its complement with respect to the real line we use $I = [-1, 1]$ and $\overline{\mathbb{R}}^I = \overline{\mathbb{R}} \setminus I$. Given a positive bounded Borel measure $\mu$ on $I$ whose support $\text{supp}(\mu) \subset I$ is an infinite set, we can define an inner product on $L^2(\mu)$ as

$$\langle f\,, g\rangle = \int_{-1}^{1} f(x)g(x)d\mu(x)$$

(since we will only be dealing with real functions, there is no need for a complex conjugate bar in the definition of the inner product). Furthermore, we assume that the measure is normalized such that $\mu(I) = 1$.

Now let us introduce the spaces of rational functions. For the sake of simplicity and contrary to the approach in [12], we assume that all poles are equal to each other, so that there is only one pole of high multiplicity. It is reasonable to assume (and confirmed by numerical experiments) that the computational effort for the case of one multiple pole close to the boundary is comparable to the case of a cluster of poles all close to the boundary, and the analysis is much easier for the former case. So assuming there is a pole $\alpha > 1$ (this is not an essential restriction; the case $\alpha < -1$ is completely similar), we define the basis functions

$$b_n(z) = \left(\frac{x}{1 - x/\alpha}\right)^n, \quad n = 0, 1, 2, \ldots$$

The space of rational functions with a multiple pole $\alpha$ is defined as

$$\mathcal{L}_n = \text{span}\{b_0, b_1, \ldots, b_n\}.$$

Note that if $\alpha = \infty$, then we are in the polynomial case and $\mathcal{L}_n = \mathcal{P}_n$, the space of polynomials of degree $n$. Orthonormalizing the canonical basis we obtain the orthogonal rational functions $\{\phi_0, \phi_1, \ldots, \phi_n\}$ which satisfy the following three term recurrence relation,

$$\phi_n(x) = \left(E_n \frac{x}{1 - x/\alpha} + F_n\right) \phi_{n-1}(x) - \frac{E_n}{E_{n-1}} \phi_{n-2}(x) \tag{1}$$

for $n = 3, 4, \ldots$, where we take the coefficient $E_n$ positive (the cases $n = 1$ and $n = 2$ are a little different, but this is not relevant for our discussion). For more information we refer to [12]. As in the polynomial case [3] we take the position that the recurrence coefficients $E_n$ and $F_n$ are the fundamental quantities in constructing orthogonal rational functions. In [12] we derive explicit expressions for these quantities, which in the case of one multiple pole take the following form,

$$\begin{aligned} F_n &= -E_n G_n \quad \text{with} \\ G_n &= \left\langle \frac{x}{1 - x/\alpha} \phi_{n-1}(x)\,, \phi_{n-1}(x) \right\rangle \quad \text{and} \\ E_n &= \frac{1}{\|\hat{\phi}_n\|}, \end{aligned}$$

where

$$\hat{\phi}_n(x) = \left(\frac{x}{1 - x/\alpha} - G_n\right) \phi_{n-1}(x) - \frac{1}{E_{n-1}} \phi_{n-2}(x).$$

Since in this paper we wish to study the quadrature error of computing these coefficients, we are only interested in orders of magnitude. Therefore we can limit our attention to the study of the quantity $G_n$ defined above. The other inner products (those needed in taking the norm of $\hat{\phi}_n$) will be of the same order of magnitude (especially for large $n$; for a justification of this remark see [12]). So in the rest of this paper we will study the computation of the integral

$$G_n = \int_{-1}^{1} \frac{x}{1 - x/\alpha} \phi_{n-1}^2(x) d\mu(x).$$

The computed approximation to $G_n$ will be denoted by $\tilde{G}_n$.

# 3 Quadrature error

In [12] we discuss Gauss-type quadrature formulas which integrate exactly in certain maximal spaces of rational functions. More precisely we have

$$\int_{-1}^{1} f(x)d\mu(x) = \sum_{k=1}^{N} \lambda_k f(\xi_k), \quad f \in \mathcal{L}_N \cdot \mathcal{L}_{N-1} \tag{2}$$

where $\xi_k$ are the zeros of $\phi_N$ and both weights and zeros can be easily computed from the recurrence coefficients using linear algebra techniques. In this section we study the quadrature error $\Delta_{n,N} = |G_n - \tilde{G}_n|$ if $\tilde{G}_n$ is computed using a quadrature formula like (2) based on rational functions $\{\tilde{\phi}_N\}$ with a multiple pole in $\tilde{\alpha}$ (if $\tilde{\alpha} = \infty$ then this is the classical Gauss quadrature formula). We assume that the orthogonality measure $\mu$ is the same for $\phi_n$ and $\tilde{\phi}_N$. Recall that $n$ is the degree of the coefficient we wish to compute (for the function $\phi_n$), and $N$ is the number of nodes in the quadrature formula (based on functions $\tilde{\phi}_N$).

The quadrature error $\Delta_{n,N}$ can be approximated for large $n$ and $N$ using asymptotic results for orthogonal rational functions. As a special case of the more general theorem in [12] we have $\Delta_{n,N} \approx |\Delta(n, N, \beta, \tilde{\beta})|$, where

$$\Delta(n, N, \beta, \tilde{\beta}) = \frac{1}{2}(1-\beta^4)\frac{1}{2\pi \mathbf{i}} \oint_{\Gamma} \frac{(1+z^2)(z-\tilde{\beta})^{(2N-1)}(1-\beta z)^{(2n-5)}}{(1-\tilde{\beta}z)^{(2N-1)}(z-\beta)^{(2n-1)}} dz, \tag{3}$$

the numbers $\beta$ and $\tilde{\beta}$ are given by the relations

$$\alpha = \frac{1}{2}\left(\beta + \frac{1}{\beta}\right), \quad |\beta| < 1,$$
$$\tilde{\alpha} = \frac{1}{2}\left(\tilde{\beta} + \frac{1}{\tilde{\beta}}\right), \quad |\tilde{\beta}| < 1$$

and $\Gamma$ is a Jordan curve inside the unit disc, surrounding the pole $\beta$. Convergence of $|\Delta(n, N, \beta, \tilde{\beta})|$ to $\Delta_{n,N}$ will be slower if $\beta$ and $\tilde{\beta}$ are very close to 1, so $n$ and $N$ will have to be larger to obtain a good approximation. Since the integrand is a rational function and the only pole surrounded by the integration curve is $\beta$, we can use the residue theorem to get an explicit representation for this integral.

First we will look at the simpler situation where $\tilde{\beta} = 0$ (this corresponds to ordinary Gauss quadrature). Using the residue theorem and Leibniz' formula for the high order derivative of a product of two functions, we can obtain an explicit expression for the function $\Delta$. Some computations yield

$$\Delta(n, N, \beta, 0) = \frac{1}{2}(1-\beta^4)\beta^{2N-2n+1} \sum_{k=0}^{2n-5} \frac{(-1)^k}{k!(2n-2-k)!} \cdots$$
$$\cdots \left[(2N+1)_{2n-2-k}\beta^2 + (2N-1)_{2n-2-k}\right] \cdots$$
$$\cdots \beta^{2k}(2n-5)_k(1-\beta^2)^{2n-5-k}$$

where we have used the symbol $(a)_n = a(a-1)(a-2)\ldots(a-n+1)$. This formula clearly shows that for fixed $n$ and $\beta$ and for large enough $N$, the function $\Delta$ will be decreasing with increasing $N$, which corresponds to saying that the quadrature error decreases when the number of nodes increases. More interesting, however, is the fact that for large $N$ the function $\Delta$ will be increasing if $\beta$ increases from 0 to 1, since for large $N$ the behaviour of $\Delta$ is dominated by the exponential term in front of the summation.

For the general situation $\tilde{\beta} \neq 0$ it is also possible to give an explicit representation of $\Delta(n, N, \beta, \tilde{\beta})$, using Leibniz' rule twice. The formula, however, is quite

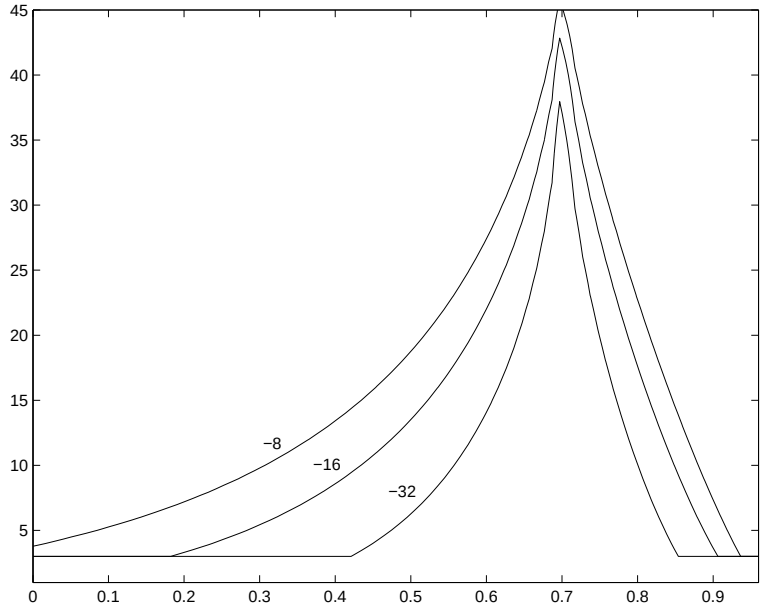



Figure 1: Contour plot of $\log_{10}|\Delta(n, 50, \beta, 0.7)|$

complicated and it is difficult to deduce the behaviour of $\Delta$ by simple inspection of the expression. But it is an explicit expression which allows a direct computation. We give it only for the sake of completeness:

$$\Delta(n, N, \beta, \tilde{\beta}) = \frac{1}{2}(1-\beta^4)\frac{1}{(2n-2)!}\Big[F^{(2n-2)}(\beta)(1+\beta^2)$$

$$+4(n-1)\beta F^{(2n-3)}(\beta) + 2(n-1)(2n-3)F^{(2n-4)}(\beta)\Big]$$

where the $k$-th derivative of the function $F(z)$ is given by

$$F^{(k)}(z) = \sum_{i=0}^{k}\binom{k}{i}\sum_{j=0}^{k-i}\binom{k-i}{j}(2N-1)_{k-i-j}(2N-1)^{(j)}\tilde{\beta}^j$$

$$\frac{(z-\tilde{\beta})^{2N-1-k+i+j}}{(1-\tilde{\beta}z)^{2N-1+j}}(2n-5)_i(1-\beta z)^{2n-5-i}(-\beta)^i$$

and we have used the symbol $(a)^{(n)} = a(a+1)(a+2)\ldots(a+n-1)$. One conclusion we can draw from this formula, is that the quadrature error will be small if $\beta$ is close to $\tilde{\beta}$ (which is of course not very surprising).

A practical application of the function $\Delta(n, N, \beta, \tilde{\beta})$ is explained below. Assume we have at our disposition a quadrature formula (i.e. $N$ different nodes and weights) based on a set of orthogonal rational functions (with respect to $\mu$) with a multiple pole in $\tilde{\beta}$, and we wish to use this quadrature formula to compute the recurrence coefficients for rational functions orthogonal with respect to the same measure, but with a multiple pole in $\beta$. A contourplot of the function $\Delta$ with $N$ and $\tilde{\beta}$ fixed will tell us how many ($n$) coefficients we can compute, as a function of $\beta$ and given a certain precision level (contour) $\epsilon$. Figure 1 shows a contourplot of $\log_{10}|\Delta(n, 50, \beta, 0.7)|$. The contours shown correspond to the machine precision when working in single, double and quadruple precision. For example, if $\beta = 0.58$

($\alpha = 1.15$) and when working in double precision, we can compute more or less 20 coefficients up to machine precision ($\epsilon \approx 10^{-16}$).

The obvious weakness in the previous approach is that we need to know a set of orthogonal rational functions with poles close to the boundary to compute a similar set of functions. In the ideal situation, we want to be able to compute rational functions orthogonal with respect to an arbitrary measure, using a quadrature formula which is easily generated. The solution to this problem is still under investigation, but we have been able to solve it for a certain class of weight functions, using a connection with orthogonal Laurent polynomials. In [7] a quadrature formula is presented to approximate integrals of the form

$$I(g, \lambda, r) = \int_{-1}^{1} \frac{g(u)}{(u+\lambda)^r} \frac{1}{\sqrt{1-u^2}} du,$$

where $g$ is a continuous function in $[-1, 1]$, $\lambda$ is any real number such that $|\lambda| > 1$, and $r$ is an integer. The nodes and weights in this quadrature formula can be computed explicitly from the nodes and weights for Gauss-Chebyshev quadrature. In [1] this type of formulas has been extended to more general weight functions and the following theorem is an immediate consequence of that article.

**Theorem 3.1.** *Let $\mu$ be absolutely continuous with weight*

$$\mu'(x) = (1-x^2)^{c-1/2}, \quad c > -1/2$$

*and let $t_{Nk}$ and $A_{Nk}$ denote respectively the nodes and weights for the (polynomial) Gauss quadrature formula associated with $\mu$. For $\alpha > 1$ define*

$$\xi_{Nk} = \alpha - x_{Nk}, \quad \Lambda_{Nk} = \lambda_{Nk}\sqrt{x_{Nk}}$$

*where*

$$x_{Nk} = \left( \frac{\delta t_{Nk} + \sqrt{(\delta t_{Nk})^2 + 4\gamma}}{2} \right)^2$$

$$\lambda_{Nk} = \frac{2\delta}{1 + \gamma/x_{Nk}} A_{Nk}$$

*with*

$$\delta = \sqrt{\alpha+1} - \sqrt{\alpha-1}, \quad \gamma = \sqrt{\alpha^2-1}.$$

*Then the formula*

$$\int_{-1}^{1} f(x) d\mu(x) \approx \frac{1}{\delta} \left( \frac{4}{\delta^2 + 4\gamma} \right)^c \sum_{k=1}^{N} \Lambda_{Nk} f(\xi_{Nk}) \tag{4}$$

*is exact for every $f$ of the form*

$$f(x) = \frac{p_{2N-1}(x)}{(x-\alpha)^N} \frac{1}{(\alpha - x)^c}, \quad p_{2N-1} \in \mathcal{P}_{2N-1}.$$

It is clear that for integer $c$ these formulas become extremely interesting, integrating exactly rational functions with a multiple pole in $\alpha$. Furthermore, for the case where $c = 0$ or $c = 1$, the orthogonal rational functions are known explicitly and treated in [13]. It may seem that if $c$ is not an integer, then these quadrature formulas are not very useful, because of the factor $(\alpha - x)^c$ in the denominator of the integrand. It will turn out that this is not really a problem, because the high degree of the numerator can compensate for the irrational term in the denominator (in a sense we explain below). First let us look at an example.

| $n$ | rel. err. $E_n$ | rel. err. $F_n$ |
|---|---|---|
| 74 | $5.9868e-15$ | $1.5699e-14$ |
| 75 | $3.9636e-13$ | $4.0155e-13$ |
| 76 | $2.8428e-09$ | $2.8096e-09$ |
| 77 | $1.2139e-06$ | $1.1353e-06$ |
| 78 | $9.8147e-05$ | $8.5249e-05$ |
| 79 | $2.6482e-03$ | $2.0655e-03$ |
| 80 | $2.8900e-02$ | $1.8914e-02$ |
| 81 | $1.4754e-01$ | $7.1077e-02$ |

Table 1: Example 3.2. Relative error for $E_n$ and $F_n$.

**Example 3.2.** Assume we wish to compute orthogonal rational functions on $I$ with a multiple pole in $\alpha = 1.01$ and with respect to the Lebesgue measure. Now we use the quadrature formula from theorem 3.1 to compute the recurrence coefficients. To get the Lebesgue measure, we have to take $c = 1/2$ in this theorem and then the constant factor in front of the summation in (4) will be equal to 1. The nodes and weights are computed from the nodes and weights for the Gauss-Legendre quadrature, which we assume known. We used $N = 150$ nodes, the relative error for the coefficients $E_n$ and $F_n$ for $n = 74, \ldots, 81$ is as shown in table 1. For $n < 74$ the error was of the order of machine precision. Note that we can compute approximately $n = N/2$ coefficients 'exactly', while for $n > N/2$ the error increases rapidly. In spite of the factor $\sqrt{\alpha - x}$ in the denominator of the function for which the quadrature rule is exact, this quadrature formula seems to work very well and the computational effort is minimal. Of course, one might argue that computing the Gauss-Legendre nodes and weights requires a considerable effort, since they are not explicitly known. However, recent techniques allow the fast and stable computation of these values (especially for large $N$), based on Fourier-Newton methods and not solving the tridiagonal eigenvalue problem. For more information we refer to [8].

As the example already indicated, the quadrature formulas from theorem 3.1 seem to work very well as long as $n \leq N/2$ (or equivalently, as long as the degree of the rational functions we are integrating does not exceed the number of nodes; remember that to compute $E_n$ we have to integrate a function of degree $2n - 1$). In the following theorem we try to explain why this is so.

**Theorem 3.3.** *Let $e_N(f)$ denote the quadrature error for a function $f$ in the formula of theorem 3.1. Then with the notation of that theorem we have*

$$|e_N(f_n)| \leq \epsilon_{N-1} \|f_n\|_I \frac{2\sqrt{\pi}\,\Gamma(c+1/2)\,\delta^{2c}}{\Gamma(c+1)}$$

*for $f_n \in \mathcal{L}_n$ and $n \leq N$, where*

$$\epsilon_{N-1} = \min_{p_{N-1} \in \mathcal{P}_{N-1}} \|(\alpha - x)^c - p_{N-1}(x)\|_I\,, \tag{5}$$

*$\Gamma$ is the Gamma function and $\|\cdot\|_I$ denotes the supremum norm on $I$.*

**Proof.** Let $p_{N-1}$ denote the polynomial which minimizes (5) and define $r_{N-1}(x)$ as

$$r_{N-1}(x) = (\alpha - x)^c - p_{N-1}(x)$$

(it follows that $\epsilon_{N-1} = \|r_{N-1}(x)\|_I$). Then write

$$f_n(x) = f_n(x) \frac{r_{N-1}(x) + p_{N-1}(x)}{(\alpha - x)^c}$$

and note that $e_N(f_n(x)p_{N-1}(x)/(\alpha - x)^c) = 0$ because of theorem 3.1. We then have

$$\begin{aligned}
|e_N(f_n)| &= \left| e_N\left( f_n(x)\frac{r_{N-1}(x)}{(\alpha-x)^c}\right)\right| \\
&= \left| I_\mu\left( f_n(x)\frac{r_{N-1}(x)}{(\alpha-x)^c}\right) - I_N\left( f_n(x)\frac{r_{N-1}(x)}{(\alpha-x)^c}\right)\right| \\
&\leq \epsilon_{N-1}\,\|f_n\|_I\left[I_\mu((\alpha-x)^{-c}) + I_N((\alpha-x)^{-c})\right]
\end{aligned}$$

where $I_\mu(f) = \int f d\mu$ and $I_N(f)$ denotes the quadrature sum of theorem 3.1. Since the quadrature formula is exact for $(\alpha - x)^{-c}$, this last expression gives

$$|e_N(f_n)| \leq \epsilon_{N-1}\,\|f_n\|_I\, 2I_\mu((\alpha-x)^{-c}).$$

Some computations show that

$$\int_{-1}^{1} \frac{(1-x^2)^{c-1/2}}{(\alpha-x)^c}dx = \frac{\sqrt{\pi}\,\Gamma(c+1/2)\,\delta^{2c}}{\Gamma(c+1)}$$

proving the theorem. □

**Remark.** This theorem shows that for integer $c < N$ the quadrature formula is exact when integrating $f_n \in \mathcal{L}_n$ and $n \leq N$, which also follows immediately from theorem 3.1. For other values of $c$ the quadrature error will depend on how well $(\alpha - x)^c$ can be approximated by a polynomial. To compute $\epsilon_{N-1}$ we could use Remez' algorithm to find the minimax polynomial, but a good estimate is usually given by the coefficient of the first neglected term in a Chebyshev approximation, which is much simpler to compute. Using this estimate in example 3.2 we find

$$\epsilon_{N-1} \approx 8.6311\ 10^{-14}$$

for $N = 150$. The function $f_n$ would in this case be equal to $Z_n\phi_{n-1}^2$ (if we want to estimate the accuracy of $E_n$). For $n = 74$ this gives

$$\left\|Z_n\phi_{n-1}^2\right\|_I = 2.9465\ 10^6.$$

Combining these numbers gives an estimate of $10^{-7}$ which is quite pessimistic compared to the actual error. This is probably due to taking the function $f_n$ outside the integral in the proof of theorem 3.3. For poles close to the boundary, $\|f_n\|_I$ will be large, while the quadrature error remains small. It is not clear, however, how we could get a more accurate estimate.

# 4 Alternative methods

Like in the polynomial case, there are other methods of computing the recurrence coefficients for orthogonal rational functions than the one we discussed (the so-called *discretized Stieltjes procedure*). These other methods, however, do not provide useful alternatives, because they rely on the knowledge of moments as we explain below.

The first method uses the explicit expressions for the recurrence coefficients given in section 2, but instead of approximating the inner products using some kind of quadrature rule, it computes a partial fraction expansion of the integrand and then integrates each fraction separately. This procedure requires the knowledge of the *moments*

$$\mu_k = \int_{-1}^{1} b_k(x)d\mu(x), \quad k = 0, 1, \ldots \tag{6}$$

A second and seemingly very different method is based on certain interpolation properties of the Stieltjes transform of the measure $\mu$. For a detailed description of this method we refer to [10]. The fundamental data for this method, however, are again the moments (6).

The previous methods both fail when working in ordinary (double) precision, for the same reason the moment-based methods for computing orthogonal polynomials fail: the map from the moments to the recurrence coefficients is severely ill-conditioned, as explained in [2] for the polynomial case and in [11] for the rational case.

To overcome this problem, Gautschi introduced the concept of *modified* moments for the case of orthogonal polynomials, see [2]. The algorithm described in that paper can be generalized to the rational case [11] only when all poles are equal to each other (because of the simpler form of the recurrence relation in that case). A more fundamental problem, however, is that the computation of these modified moments for the rational case is more or less of the same complexity as computing the recurrence coefficients, so this only shifts the problem and does not solve it.

# 5 Conclusion

The computation of orthogonal rational functions with poles close to the boundary is a difficult problem. As shown in [12], it becomes unfeasible to use quadrature rules based on polynomials, because of the enormous number of nodes we would need. In this paper we present two different solutions. In the case where we already have a rational Gaussian quadrature formula with poles close to the poles in the target functions, we can easily predict how many coefficients can be computed up to a certain precision level. Rational Gaussian rules are in some sense 'optimal' and tend to converge much faster than simpler quadrature rules. However, if no such quadrature formula is available, a recent development, based on orthogonal Laurent polynomials has given a partial solution to this problem, providing a way to compute the orthogonal rational functions with poles close to the boundary for a number of special weight functions, under the assumption that all poles are equal to each other. For more general measures, the problem is still under investigation.

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