

# On rapid computation of expansions in ultraspherical polynomials

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## Abstract

We present an  $\mathcal{O}(N \log_2 N)$  algorithm for the computation of the first  $N$  coefficients in the expansion of an analytic function in ultraspherical polynomials. We first represent expansion coefficients as an infinite linear combination of derivatives and then as an integral transform with a hypergeometric kernel along the boundary of a Bernstein ellipse. Following a transformation of the kernel, we approximate the coefficients to arbitrary accuracy using Discrete Fourier Transform.

## 1 Introduction

Let  $\{\varphi_n\}_{n \in \mathbb{Z}_+}$  be a set of orthogonal functions with respect to the Borel measure  $d\mu$ , supported by the real interval  $(a, b)$ . Then any  $f \in L_2(a, b)$  can be expanded in the form

$$f(x) \sim \sum_{n=0}^{\infty} \hat{f}_n \varphi_n(x), \quad \text{where} \quad \hat{f}_n = \frac{\langle f, \varphi_n \rangle}{\langle \varphi_n, \varphi_n \rangle}, \quad n \in \mathbb{Z}_+, \quad (1.1)$$

and that the expansion converges in norm. Moreover, if both  $f$  and the  $\varphi_n$ s are all analytic, the convergence is pointwise and *spectral*:  $\left\| f - \sum_{n=0}^N \hat{f}_n \varphi_n \right\|$  decays faster than  $N^{-\alpha}$  for any real  $\alpha > 0$ . A familiar example is the *Fourier expansion*, whereby  $\gamma$  is the complex unit circle,  $\mu(z) = z$ ,  $\varphi_{2n}(z) = e^{\pi i n z}$  and  $\varphi_{2n+1}(z) = e^{-\pi i n z}$ . Another important example is when  $\{\varphi_n\}$  is an orthogonal polynomial basis, i.e. when each  $\varphi_n$  is an  $n$ th degree polynomial.

Expansions (1.1) are of fundamental importance in many branches of computational mathematics. This is true in particular once the coefficients  $\hat{f}_n$  can be computed rapidly. It is elementary that for Fourier expansions the coefficients can be discretized with the Discrete Fourier Transform (DFT), incurring spectrally small error. Moreover, the first  $N$  terms of the DFT can be computed in just  $\mathcal{O}(N \log_2 N)$  operations by means of the Fast Fourier Transform (FFT). Likewise, the computation of expansions in Chebyshev polynomials (thus,  $\gamma = [-1, 1]$ ,  $d\mu(z) = (1 - z^2)^{-1/2} dz$  and  $\varphi_n(z) = T_n(z)$ , the  $n$ th Chebyshev polynomial of the first kind) can be reduced by a simple change of variable to the computation of a Fourier expansion, resulting again in a  $\mathcal{O}(N \log_2 N)$  price tag.

In a recent paper Iserles (2011) presented an  $\mathcal{O}(N \log_2 N)$  algorithm for the computation of an expansion into Legendre polynomials: thus,  $\gamma = [-1, 1]$ ,  $\mu(z) = z$  and  $\varphi_n = P_n$ , the  $n$ th Legendre polynomial. The purpose of the current paper is to explore a generalisation of (Iserles 2011) to more general framework of *ultraspherical polynomials*  $\{P_n^{(\alpha, \alpha)}\}_{n \in \mathbb{Z}_+}$ , orthogonal in  $[-1, 1]$  with respect to the measure  $(1 - x^2)^\alpha d\mu$ ,  $\alpha > -1$  (Rainville 1960).

The approach of (Iserles 2011) rests upon three steps. Firstly, the  $n$ th expansion coefficient is expressed as a linear combination of derivatives,

$$\hat{f}_n = (2n + 1) \sum_{m=0}^{\infty} \frac{(2m + n)! f^{(2m+n)}(0)}{2^{2m+n} m! (\frac{3}{2})_{m+n}}, \quad n \in \mathbb{Z}_+, \quad (1.2)$$

where the *Pochhammer symbol*  $(a)_k$  is defined recursively as  $(a)_0 = 1$ ,  $(a)_k = (a + k - 1)(a)_{k-1}$  for  $k \in \mathbb{N}$ . The expression (1.2) is classical (Rainville 1960) but, on its own, of little practical use in computing the expansion coefficients  $\{\hat{f}_n\}$ .

Secondly, assuming analyticity of  $f$  on and within the *Bernstein ellipse*  $\mathcal{B}_r = \{\frac{1}{2}(re^{i\theta} + r^{-1}e^{-i\theta}) : \theta \in [-\pi, \pi]\}$  for some  $r \in (0, 1)$ , we compute the derivatives in (1.2) using the Cauchy integral formula. Thus, let  $\gamma$  be a simple Jordan curve encircling  $[-1, 1]$  within  $\mathcal{B}_r$  with winding number 1. It has been established in (Iserles 2011) that

$$\hat{f}_n = \frac{2^n (n!)^2}{(2n)!} \frac{1}{2\pi i} \int_{\gamma} \frac{f(z)}{z^{m+1}} {}_2F_1 \left[ \begin{matrix} \frac{n+1}{2}, \frac{n+2}{2} \\ n + \frac{3}{2} \end{matrix}; \frac{1}{z^2} \right] dz, \quad n \in \mathbb{Z}_+, \quad (1.3)$$

where  ${}_2F_1$  is the usual hypergeometric function (Rainville 1960).

Suppose that  $r \leq \sqrt{2} - 1$ . In that case it is possible to fit a circle of radius  $\rho > 1$ , centred at the origin, into  $\mathcal{B}_r$ , truncate the Taylor expansion of the hypergeometric function and discretize (1.3) along this circle by means of DFT. In principle this leads to an algorithm bearing the cost of  $\mathcal{O}(N \log_2 N) + \mathcal{O}(NM)$  for the calculation of the first  $N$  coefficients, where  $M$  is the degree of the Taylor polynomial replacing the hypergeometric function. This approach, however, is doomed, since the Taylor series of the hypergeometric function in question decays *very* slowly indeed: computer experiments indicate that, in general,  $M = \mathcal{O}(N)$  and the algorithm costs  $\mathcal{O}(N^2)$  operations: a dead end. This is precisely the moment we apply our third ingredient: an identity replacing the hypergeometric function in (1.3) by another (scaled)

hypergeometric function, which converges rapidly. Specifically, we use the identity

$${}_2F_1\left[\begin{matrix} a, a + \frac{1}{2}; \\ c; \end{matrix} 2\zeta - \zeta^2\right] = \frac{1}{(1 - \frac{1}{2}\zeta)^{2a}} {}_2F_1\left[\begin{matrix} 2a, 2a - c + 1; \\ c; \end{matrix} \frac{\zeta}{2 - \zeta}\right], \quad (1.4)$$

valid for all  $a, b, c \in \mathbb{C}$ ,  $-c \notin \mathbb{Z}_+$  and  $\operatorname{Re} \zeta < 1$ <sup>1</sup> with  $a = \frac{1}{2}(n + 1)$ ,  $c = n + \frac{3}{2}$ . Once we choose the curve  $\gamma$  as a Bernstein ellipse  $\mathcal{B}_\rho$ ,  $\rho \in (r, 1)$ <sup>2</sup>, the outcome is

$$\hat{f}_n = \frac{c_n \rho^n}{2\pi} \int_{-\pi}^{\pi} (1 - \rho^2 e^{2i\theta}) f\left(\frac{1}{2}(\rho e^{i\theta} + \rho^{-1} e^{-i\theta})\right) {}_2F_1\left[\begin{matrix} n + 1, \frac{1}{2}; \\ n + \frac{3}{2}; \end{matrix} \rho^2 e^{2i\theta}\right] e^{in\theta} d\theta, \quad (1.5)$$

where

$$c_n = \frac{4^n (n!)^2}{(2n)!}, \quad n \in \mathbb{Z}_+.$$

The Taylor expansion of the hypergeometric function in (1.5) converges rapidly. Hence, once we replace it by a Taylor polynomial, we incur small error: it has been proved in (Iserles 2011) that, given any  $\varepsilon > 0$ , there exists  $M = M(\varepsilon)$  such that, once we replace the hypergeometric function in (1.4) by its  $M$ -degree Taylor polynomial, we commit an error less than  $\varepsilon$  in magnitude *uniformly* for all Legendre coefficients  $\hat{f}_n$ . Therefore, allowing for an error of  $\varepsilon$ , once we replace the integral in (1.5) by DFT, we can reduce the evaluation of  $\hat{f}_n$ ,  $n = 0, 1, \dots, N - 1$  to a single FFT over  $N$  values, followed by  $\mathcal{O}(MN)$  additional operations, and the outcome is an  $\mathcal{O}(N \log_2 N)$  algorithm.

Although the mathematical journey leading this algorithm might be long, convoluted and counter-intuitive, the algorithm itself is surprisingly simple, easy to implement and trivially scaleable to higher dimensions.

The purpose of this paper is to explore generalizations of this algorithm. We commence in Section 2 by extending the underlying framework to expansions in *ultraspherical polynomials*  $P_n^{(\alpha, \alpha)}$ ,  $\alpha > -1$ . Expansions of this kind are highly relevant for spectral methods for partial differential equations (Ben-Yu 2001) and Gegenbauer filtering (Gelb & Tanner 2006, Shu & Wong 1995, Tadmor 2007). In Section 3 we introduce two  $\mathcal{O}(N \log_2 N)$  algorithms for the computation of the first  $N$  terms in the expansion (1.1), which extend the methodology of (Iserles 2011) to this setting. Finally, in Section 4 we report few numerical experiments and discuss optimal implementation of our algorithm.

It is fair to mention the existence of competing means to compute expansions in orthogonal polynomials. Thus, Alpert & Rokhlin (1991) have developed an  $\mathcal{O}(N(\log N)^2)$  algorithm for Legendre expansions, based upon the fast multipole method which, however, is considerably more complicated than that in (Iserles 2011), lending itself less easily to multivariate generalization, while Potts, Steidl & Tasche (1998) have presented a general divide-and-conquer  $\mathcal{O}(N(\log N)^2)$  algorithm for OPRL expansions: although it appears to be less effective for ultraspherical expansions, it has the redeeming virtue of generality. Another approach is due to Keiner (2009) – although formulated in the terminology of Gegenbauer polynomials it can be easily translated to an ultraspherical setting for  $\alpha \geq -\frac{1}{2}$ . It converts an expansion in one set of Gegenbauer polynomials (e.g., Chebyshev or Legendre) into another at the cost of a single

<sup>1</sup><http://functions.wolfram.com/HypergeometricFunctions/Hypergeometric2F1/16/01/01/0004/>.

<sup>2</sup>Of course,  $\mathcal{B}_r$  has winding number  $-1$ , but this can be addressed trivially.

FFT. Therefore the operation count is  $\mathcal{O}(N \log N)$ , similarly to our algorithm, except that Keiner's approach requires two FFTs (one to obtain the original expansion, another to convert), while a single FFT suffices for ours. (By the end of Section 3 we describe a situation in which our approach enjoys more substantive advantage over Keiner's.) Note that all these algorithms use function values of  $f$  from the interval  $[-1, 1]$ , while our approach typically uses values on a Bernstein ellipse.

As observed in (Potts et al. 1998), once a fast algorithm is available to compute an expansion in orthogonal polynomials, one immediately obtains an equally fast algorithm for fast evaluation of the function  $f$  from its expansion in an appropriate grid – essentially, the two algorithms are transposes of each other. Thus, our algorithms can be used also to this end.

## 2 Expansions in ultraspherical polynomials

### 2.1 $x^n$ as a linear combination of orthogonal polynomials

The *ultraspherical polynomial*  $P_n^{(\alpha, \alpha)}$ , where  $\alpha > -1$ , is orthogonal in the interval  $(-1, 1)$  with respect to the Borel measure  $(1 - x^2)^\alpha dx$  (Rainville 1960, p. 276). Important special cases are  $\alpha = 0$  (Legendre polynomials  $P_n$ ),  $\alpha = -\frac{1}{2}$  (Chebyshev polynomials of the first kind  $T_n = n!P_n^{(-\frac{1}{2}, -\frac{1}{2})}/(\frac{1}{2})_n$ ) and  $\alpha = \frac{1}{2}$  (Chebyshev polynomials of the second kind  $U_n = (n+1)!P_n^{(\frac{1}{2}, \frac{1}{2})}/(\frac{3}{2})_n$ ).

The standard explicit representation of ultraspherical polynomials follows from a hypergeometric form of Jacobi polynomials,

$$P_n^{(\alpha, \alpha)}(x) = \frac{(1 + \alpha)_n}{n!} {}_2F_1 \left[ \begin{matrix} -n, 1 + 2\alpha + n; \\ 1 + \alpha; \end{matrix} \frac{1 - x}{2} \right]$$

(Rainville 1960, p. 254). The polynomials  $P_n^{(\alpha, \alpha)}$ , under different normalisation, are often known as *Gegenbauer polynomials*  $C_n^\nu$ :

$$P_n^{(\alpha, \alpha)}(x) = \frac{(1 + \alpha)_n}{(1 + 2\alpha)_n} C_n^{\alpha+1/2}(x), \quad \alpha \neq -\frac{1}{2}. \quad (2.1)$$

We commence by expanding  $x^n$  as a linear combination of  $P_m^{(\alpha, \alpha)}$  for  $m = 0, \dots, n$ : since the latter span  $n$ -degree polynomials, such a linear combination

$$x^n = \sum_{m=0}^n a_{n,m} P_m^{(\alpha, \alpha)}(x), \quad n \in \mathbb{Z}_+, \quad (2.2)$$

always exists. Note that each  $P_n^{(\alpha, \alpha)}$  has the parity of  $n$ , therefore  $a_{n, n-2m-1} \equiv 0$  and we are seeking just  $a_{n, n-2m}$ ,  $m = 0, 1, \dots, \lfloor n/2 \rfloor$ . Excluding for the time being the case  $\alpha = -\frac{1}{2}$ , we substitute (2.1) in (2.2),

$$x^n = \sum_{m=0}^{\lfloor n/2 \rfloor} \frac{(1 + \alpha)_{n-2m}}{(1 + 2\alpha)_{n-2m}} a_{n, n-2m} C_{n-2m}^{\alpha+1/2}(x).$$

**Proposition 1** *It is true that*

$$a_{n,n-2m} = \frac{n!(2\alpha + 1)_{n-2m}}{2^n(\alpha + \frac{1}{2})_n(\alpha + 1)_{n-2m}} \frac{q_m(n + \alpha + \frac{1}{2})}{m!}, \quad m = 0, 1, \dots, \lfloor n/2 \rfloor, \quad (2.3)$$

where

$$q_m(z) = (-1)^m \frac{(-z)_m (z - 2m)}{z}$$

is an  $m$ th-degree polynomial.

*Proof* Since

$$C_n^\nu = \sum_{k=0}^{\lfloor n/2 \rfloor} \frac{(-1)^k (\nu)_{n-k} (2x)^{n-2k}}{k!(n-2k)!}$$

(Rainville 1960, p. 277), we have

$$\begin{aligned} x^n &= \sum_{m=0}^{\lfloor n/2 \rfloor} \frac{(1 + \alpha)_{n-2m}}{(1 + 2\alpha)_{n-2m}} a_{n,n-2m} \sum_{k=0}^{\lfloor n/2 \rfloor - m} \frac{(-1)^k (\alpha + \frac{1}{2})_{n-2m-k} (2x)^{n-2m-2k}}{k!(n-2m-2k)!} \\ &= \sum_{m=0}^{\lfloor n/2 \rfloor} \frac{(1 + \alpha)_{n-2m}}{(1 + 2\alpha)_{n-2m}} a_{n,n-2m} \sum_{k=m}^{\lfloor n/2 \rfloor} \frac{(-1)^{m+k} (\alpha + \frac{1}{2})_{n-m-k} (2x)^{n-2k}}{(k-m)!(n-2k)!} \\ &= \sum_{k=0}^{\lfloor n/2 \rfloor} \frac{(-1)^k (2x)^{n-2k}}{(n-2k)!} \left[ \sum_{m=0}^k (-1)^m \frac{(1 + \alpha)_{n-2m} (\alpha + \frac{1}{2})_{n-m-k}}{(1 + 2\alpha)_{n-2m} (k-m)!} a_{n,n-2m} \right]. \end{aligned}$$

From  $k = 0$  we obtain

$$a_{n,n} = \frac{n!(2\alpha + 1)_n}{2^n(\alpha + \frac{1}{2})_n(\alpha + 1)_n},$$

which is consistent with (2.3). Moreover,

$$\sum_{m=0}^k (-1)^m \frac{(1 + \alpha)_{n-2m} (\alpha + \frac{1}{2})_{n-m-k}}{(1 + 2\alpha)_{n-2m} (k-m)!} a_{n,n-2m} = 0, \quad k = 1, 2, \dots, \lfloor n/2 \rfloor.$$

Therefore we need to prove, substituting the postulated form of the  $a_{n,n-2m}$ s and discarding nonzero common factors, that

$$\sum_{m=0}^k (-1)^m \frac{(\alpha + \frac{1}{2})_{n-m-k}}{m!(k-m)!} q_m(n + \alpha + \frac{1}{2}) = 0, \quad k = 1, 2, \dots, \lfloor n/2 \rfloor. \quad (2.4)$$

Since

$$(\nu)_{n-m-k} (-\nu - n)_m = (-1)^m \frac{(\nu)_{n+1} (-\nu - n)_m}{(-\nu - n)_k (-\nu - n + k + 1)_m},$$

a substitution of the  $q_m$ s and letting  $\nu = \alpha + \frac{1}{2}$  yield

$$\begin{aligned}
& \sum_{m=0}^k (-1)^m \frac{(\alpha + \frac{1}{2})_{n-m-k}}{m!(k-m)!} q_m(n + \alpha + \frac{1}{2}) \\
&= \sum_{m=0}^k \frac{(n - 2m + \alpha + \frac{1}{2})(\alpha + \frac{1}{2})_{n-m-k}(-\alpha - n - \frac{1}{2})_m}{m!(k-m)!(\alpha + n + \frac{1}{2})} \\
&= \frac{(\alpha + \frac{1}{2})_n}{(-\alpha - n - \frac{1}{2})_k} \sum_{m=0}^k (-1)^m \frac{(n - 2m + \alpha + \frac{1}{2})(-\alpha - n - \frac{1}{2})_m}{m!(k-m)!(-\alpha - n + k + \frac{1}{2})_m}.
\end{aligned}$$

Letting  $y = n + \alpha + \frac{1}{2}$ , it follows from

$$\sum_{m=0}^k \frac{(-1)^m (y - 2m)(-y)_m}{m!(k-m)!(-y + k + 1)_m} = 0$$

that (2.4), hence also (2.3), is true. But

$$\begin{aligned}
& \sum_{m=0}^k \frac{(-1)^m (y - 2m)(-y)_m}{m!(k-m)!(-y + k + 1)_m} \\
&= \frac{y}{k!} \sum_{m=0}^k \binom{k}{m} \frac{(-1)^m (-y)_m}{(-y + k + 1)_m} - \frac{2}{(k-1)!} \sum_{m=1}^k (-1)^m \binom{k-1}{m-1} \frac{(-y)_m}{(-y + k + 1)_m} \\
&= \frac{y}{k!} {}_2F_1 \left[ \begin{matrix} -k, -y; \\ -y + k + 1; \end{matrix} 1 \right] + \frac{2}{(k-1)!} \frac{y}{y - k - 1} {}_2F_1 \left[ \begin{matrix} -k + 1, -y + 1; \\ -y + k + 2; \end{matrix} 1 \right] \\
&= \frac{y}{k!} \frac{\Gamma(-y + k + 1)(2k)!}{\Gamma(-y + 2k + 1)k!} + \frac{2y}{(k-1)!(y - k - 1)} \frac{\Gamma(-y + k + 2)(2k - 1)!}{\Gamma(-y + 2k + 1)k!} \\
&= 0,
\end{aligned}$$

since  $\Gamma(z + 1) = z\Gamma(z)$ . Note that we have used the standard formula from (Rainville 1960, p. 49) to sum up hypergeometric functions with unit argument.

This completes the proof of the proposition.  $\square$

We now deduce from (2.3) that

$$\begin{aligned}
\frac{x^n}{n!} &= \sum_{m=0}^{\lfloor n/2 \rfloor} \frac{(-1)^m (\alpha + n - 2m + \frac{1}{2})(-\alpha - n - \frac{1}{2})_m (2\alpha + 1)_{n-2m}}{2^n (\alpha + \frac{1}{2})_{n+1} m! (\alpha + 1)_{n-2m}} P_{n-2m}^{(\alpha, \alpha)}(x) \\
&= \frac{1}{2^n} \sum_{m=0}^{\lfloor n/2 \rfloor} \frac{\alpha + n - 2m + \frac{1}{2}}{m! (\alpha + \frac{1}{2})_{n-m+1}} \cdot \frac{(2\alpha + 1)_{n-2m}}{(\alpha + 1)_{n-2m}} P_{n-2m}^{(\alpha, \alpha)}(x). \tag{2.5}
\end{aligned}$$

Note that for  $\alpha = 0$  we obtain the familiar formula

$$\frac{x^n}{n!} = \frac{1}{2^n} \sum_{m=0}^{\lfloor n/2 \rfloor} \frac{2n + 1 - 4m}{m! (\frac{3}{2})_{n-m}} P_{n-2m}(x)$$

(Rainville 1960, p. 181), which has already featured in the original Legendre (1817) paper. For  $\alpha = \frac{1}{2}$  we have

$$\begin{aligned} \frac{x^n}{n!} &= \frac{1}{2^n} \sum_{m=0}^{\lfloor n/2 \rfloor} \frac{n-2m+1}{m!(n-m+1)!} \frac{(n-2m+1)!}{\left(\frac{3}{2}\right)_{n-2m}} P_{n-2m}^{(\frac{1}{2}, \frac{1}{2})}(x) \\ &= \sum_{m=0}^{\lfloor n/2 \rfloor} \frac{n-2m+1}{m!(n-m+1)!} U_{n-2m}(x). \end{aligned}$$

The case  $\alpha = -\frac{1}{2}$  is more complicated, because the sum has removable singularities and care need be taken distinguishing between even and odd  $n$ s: the outcome of the calculation is

$$\begin{aligned} \frac{x^{2n}}{(2n)!} &= \frac{1}{2^{2n-1}(2n)!} \sum_{m=0}^{n-1} \binom{2n}{m} T_{2n-2m}(x) + \frac{1}{2^{2n}(n!)^2} T_0(x), \\ \frac{x^{2n+1}}{(2n+1)!} &= \frac{1}{2^{2n}(2n+1)!} \sum_{m=0}^n \binom{2n+1}{m} T_{2n+1-2m}(x). \end{aligned}$$

## 2.2 Expressing $\hat{f}_n$ using derivatives

**Theorem 2** *Let the function  $f$  be analytic in the interior of the Bernstein ellipse  $\mathcal{B}_r = \{\frac{1}{2}(re^{i\theta} + r^{-1}e^{-i\theta}) : \theta \in [-\pi, \pi]\}$  for some  $r \in (0, 1)$ . Letting  $f_n = f^{(n)}(0)$ ,  $n \in \mathbb{Z}_+$ , it is true that*

$$f(x) = \sum_{n=0}^{\infty} \hat{f}_n P_n^{(\alpha, \alpha)}(x),$$

where

$$\hat{f}_n = (\alpha + n + \frac{1}{2}) \frac{(2\alpha + 1)_n}{(\alpha + 1)_n} \sum_{m=0}^{\infty} \frac{f_{n+2m}}{2^{n+2m} m! (\alpha + \frac{1}{2})_{n+m+1}}, \quad n \in \mathbb{Z}_+. \quad (2.6)$$

*Proof* Substituting (2.5) into the Taylor expansion,

$$\begin{aligned} f(x) &= \sum_{n=0}^{\infty} \frac{f_n}{2^n} \sum_{m=0}^{\lfloor n/2 \rfloor} \frac{\alpha + n - 2m + \frac{1}{2}}{m!(\alpha + \frac{1}{2})_{n-m+1}} \cdot \frac{(2\alpha + 1)_{n-2m}}{(\alpha + 1)_{n-2m}} P_{n-2m}^{(\alpha, \alpha)}(x) \\ &= \sum_{n=0}^{\infty} \frac{f_{2n}}{2^{2n}} \sum_{m=0}^n \frac{\alpha + 2n - 2m + \frac{1}{2}}{m!(\alpha + \frac{1}{2})_{2n-m+1}} \cdot \frac{(2\alpha + 1)_{2n-2m}}{(\alpha + 1)_{2n-2m}} P_{2n-2m}^{(\alpha, \alpha)}(x) \\ &\quad + \sum_{n=0}^{\infty} \frac{f_{2n+1}}{2^{2n+1}} \sum_{m=0}^n \frac{\alpha + 2n - 2m + \frac{3}{2}}{m!(\alpha + \frac{1}{2})_{2n-m+2}} \cdot \frac{(2\alpha + 1)_{2n-2m+1}}{(\alpha + 1)_{2n-2m+1}} P_{2n-2m+1}^{(\alpha, \alpha)}(x) \end{aligned}$$

and, interchanging sums,

$$\begin{aligned}
f(x) &= \sum_{m=0}^{\infty} \frac{1}{m!} \sum_{n=m}^{\infty} \frac{(\alpha + 2n - 2m + \frac{1}{2})(2\alpha + 1)_{2n-2m}}{(\alpha + \frac{1}{2})_{2n-m+1}(\alpha + 1)_{2n-2m}} \cdot \frac{f_{2n}}{2^{2n}} \mathbf{P}_{2n-2m}^{(\alpha, \alpha)}(x) \\
&\quad + \sum_{m=0}^{\infty} \frac{1}{m!} \sum_{n=m}^{\infty} \frac{(\alpha + 2n - 2m + \frac{3}{2})(2\alpha + 1)_{2n-2m+1}}{(\alpha + \frac{1}{2})_{2n-m+2}(\alpha + 1)_{2n-2m+1}} \cdot \frac{f_{2n+1}}{2^{2n+1}} \mathbf{P}_{2n-2m+1}^{(\alpha, \alpha)}(x) \\
&= \sum_{m=0}^{\infty} \frac{1}{m!} \sum_{n=0}^{\infty} \frac{(\alpha + 2n + \frac{1}{2})(2\alpha + 1)_{2n}}{(\alpha + \frac{1}{2})_{2n+m+1}(\alpha + 1)_{2n}} \cdot \frac{f_{2n+2m}}{2^{2n+2m}} \mathbf{P}_{2n}^{(\alpha, \alpha)}(x) \\
&\quad + \sum_{m=0}^{\infty} \frac{1}{m!} \sum_{n=0}^{\infty} \frac{(\alpha + 2n + \frac{3}{2})(2\alpha + 1)_{2n+1}}{(\alpha + \frac{1}{2})_{2n+m+2}(\alpha + 1)_{2n+1}} \cdot \frac{f_{2n+2m+1}}{2^{2n+2m+1}} \mathbf{P}_{2n+1}^{(\alpha, \alpha)}(x) \\
&= \sum_{n=0}^{\infty} (\alpha + 2n + \frac{1}{2}) \frac{(2\alpha + 1)_{2n}}{(\alpha + 1)_{2n}} \sum_{m=0}^{\infty} \frac{f_{2n+2m}}{2^{2n+2m} m! (\alpha + \frac{1}{2})_{2n+m+1}} \mathbf{P}_{2n}^{(\alpha, \alpha)}(x) \\
&\quad + \sum_{n=0}^{\infty} (\alpha + 2n + \frac{3}{2}) \frac{(2\alpha + 1)_{2n+1}}{(\alpha + 1)_{2n+1}} \sum_{m=0}^{\infty} \frac{f_{2n+2m+1}}{2^{2n+2m+1} m! (\alpha + \frac{1}{2})_{2n+m+2}} \mathbf{P}_{2n+1}^{(\alpha, \alpha)}(x).
\end{aligned}$$

The explicit formula (2.6) follows.  $\square$

Note that for  $\alpha = 0$  we recover (1.2), while for  $\alpha = \frac{1}{2}$  and  $\alpha = -\frac{1}{2}$  we have

$$\hat{f}_n = (n+1) \frac{(n+1)!}{(\frac{3}{2})_n} \sum_{m=0}^{\infty} \frac{f_{n+2m}}{2^{n+2m} m! (n+m+1)!}, \quad n \in \mathbb{Z}_+$$

and

$$\hat{f}_n = \begin{cases} \sum_{m=0}^{\infty} \frac{f_{2m}}{2^{2m} (m!)^2}, & n = 0, \\ \frac{2n!}{(\frac{1}{2})_n} \sum_{m=0}^{\infty} \frac{f_{n+2m}}{2^{n+2m} m! (n+m)!}, & n \in \mathbb{N} \end{cases}$$

respectively.

### 2.3 Hypergeometric representation

Let  $\gamma$  be a simple, closed and positively-oriented Jordan curve in the interior of  $\mathcal{B}_r$  which does not intersect  $[-1, 1]$ . It follows from (2.6) by the Cauchy Integral Theorem that

$$\begin{aligned}
\hat{f}_n &= (\alpha + n + \frac{1}{2}) \frac{(2\alpha + 1)_n}{(\alpha + 1)_n} \sum_{m=0}^{\infty} \frac{f^{(n+2m)}(0)}{2^{n+2m} m! (\alpha + \frac{1}{2})_{n+m+1}} \\
&= (\alpha + n + \frac{1}{2}) \frac{(2\alpha + 1)_n}{(\alpha + 1)_n} \sum_{m=0}^{\infty} \frac{(n+2m)!}{2^{n+2m} m! (\alpha + \frac{1}{2})_{n+m+1}} \frac{1}{2\pi i} \int_{\gamma} \frac{f(z)}{z^{n+2m+1}} dz \\
&= (\alpha + n + \frac{1}{2}) \frac{(2\alpha + 1)_n}{2^n (\alpha + 1)_n} \frac{1}{2\pi i} \int_{\gamma} \frac{f(z)}{z^{n+1}} \sum_{m=0}^{\infty} \frac{(n+2m)!}{m! (\alpha + \frac{1}{2})_{n+m+1} (2z)^{2m}} dz,
\end{aligned}$$



where interchanging summation and integration is justified by analyticity. Since  $(n+2m)! = n!2^{2m}(\frac{n+1}{2})_m(\frac{n+2}{2})_m$  and  $(\alpha+\frac{1}{2})_{n+m+1} = (\alpha+\frac{1}{2})_{n+1}(\alpha+n+\frac{3}{2})_m$ , we conclude that

$$\begin{aligned}\hat{f}_n &= \frac{(2\alpha+1)_n n!}{2^n(\alpha+1)_n(\alpha+\frac{1}{2})_n} \frac{1}{2\pi i} \int_\gamma \frac{f(z)}{z^{n+1}} \sum_{m=0}^{\infty} \frac{(\frac{n+1}{2})_m(\frac{n+2}{2})_m}{m!(\alpha+n+\frac{3}{2})_m} \frac{1}{z^{2m}} dz \\ &= \frac{c_n}{2\pi i} \int_\gamma \frac{f(z)}{z^{n+1}} \varphi_n(z) dz,\end{aligned}\quad (2.7)$$

where

$$c_n = \frac{(2\alpha+1)_n n!}{2^n(\alpha+1)_n(\alpha+\frac{1}{2})_n}, \quad \varphi_n(z) = {}_2F_1\left[\begin{matrix} \frac{n+1}{2}, \frac{n+2}{2} \\ \alpha+n+\frac{3}{2} \end{matrix}; z^{-2}\right], \quad n \in \mathbb{Z}_+. \quad (2.8)$$

Note that for  $\alpha = 0$  we recover (1.3), for  $\alpha = \frac{1}{2}$  we obtain  $c_n = (n+1)!/[2^n(\frac{3}{2})_n]$ , while for  $\alpha = -\frac{1}{2}$  simple computation confirms that  $c_0 = 1$  and  $c_n = n!/[2^{n-1}(\frac{1}{2})_n]$  for  $n \in \mathbb{N}$ .

An obvious option to reduce the computation of the  $\hat{f}_n$ s to a single FFT, based upon (2.7), is as follows. Suppose that  $r < \sqrt{2} - 1$ . In that case we can choose  $\gamma$  as a circle  $\Gamma_\rho$  of radius  $\rho > 1$  (specifically, for radius  $\rho > 1$  we need  $r \in (0, \sqrt{1+\rho^2} - \rho)$ ). Suppose that  $\varphi_n$  is replaced by its Taylor section,

$$\varphi_n(z) \approx \varphi_n^{[M]}(z) = \sum_{m=0}^M \varphi_{n,m} z^{-2m}, \quad \text{where} \quad \varphi_{n,m} = \frac{(\frac{n+1}{2})_m(\frac{n+2}{2})_m}{m!(\alpha+n+\frac{3}{2})_m}$$

(cf. (2.8)). Because of the analyticity of  $\varphi_n$  on  $\Gamma_\rho$ , we can choose  $M$  large enough so that the error in the above approximation is arbitrarily small for  $|z| = \rho$ . Replacing the integral in (2.7) by a DFT we have

$$\begin{aligned}\hat{f}_n &\approx \frac{c_n}{2\pi i} \sum_{j=0}^{N-1} f(\rho\omega_N^j) \omega_N^{-(n+1)j} \sum_{m=0}^M \varphi_{n,m} \omega_N^{-2mj} \rho^{-2m} \\ &= \frac{c_n}{2\pi i} \sum_{m=0}^M \varphi_{n,m} \rho^{-2m} \sum_{j=0}^{N-1} f(\rho\omega_N^j) \omega_N^{-(n+2m+1)j},\end{aligned}$$

where  $\omega_N = \exp \frac{2\pi i}{N}$  is the  $N$ th primitive root of unity. Let

$$\sigma_r = \sum_{j=0}^{N-1} f(\rho\omega_N^j) \omega_N^{-rj}, \quad r = 0, 1, \dots, N-1$$

be the DFT of the sequence  $\{f(\rho\omega_N^j)\}_{j=0}^{N-1}$ . It now follows that

$$\hat{f}_n \approx \frac{c_n}{2\pi i} \sum_{m=0}^M \varphi_{n,m} \sigma_{n+2m+1} \rho^{-2m}, \quad n = 0, 1, \dots, N-2M-2. \quad (2.9)$$

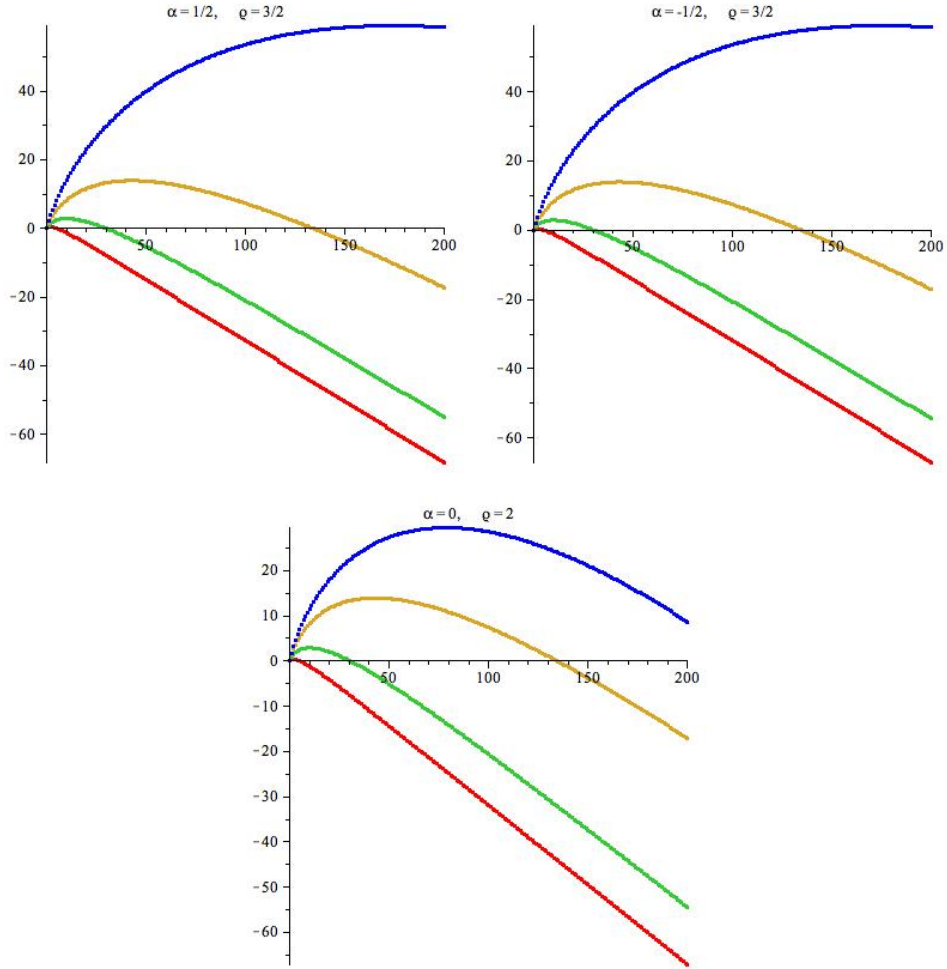


Figure 2.1: Plots of  $\log_{10}(|\varphi_{n,m}|\rho^{-2m})$  for  $m = 0, 1, \dots, 200$  and different values of  $\alpha$  and  $\rho > 1$ . In each plot the bottom curve corresponds to  $n = 16$ , the next to  $n = 64$ , then  $n = 256$  and finally  $n = 1024$ .

The cost of computing (2.9) is  $\mathcal{O}(N \log_2 N) + \mathcal{O}(MN)$ . Therefore, were it possible to choose  $M = \mathcal{O}(1)$  (or even  $M = \mathcal{O}(\log_2 N)$ ) for large  $N$ , while incurring small error, we would have had an  $\mathcal{O}(N \log_2 N)$  algorithm. Unfortunately, this is impossible.

Figure 2.1 displays the order of magnitude (in decimal digits) of the expansion terms  $|\varphi_{n,m}|\rho^{-2m}$  for increasing  $m$ . While for small  $n$  the terms decay exponentially, this is not true even for moderate values of  $n$ : the terms first increase substantially and only then commence the asymptotic decay at an exponential rate. This information is further fleshed out in Table 1, where (for  $\alpha = \frac{1}{2}$ ,  $\rho = \frac{3}{2}$  and different values on  $n$ )

we have displayed the quantities

$$M_n^* = \min\{m \in \mathbb{Z}_+ : |\varphi_{n,k}| \rho^{-2k} < \varepsilon \forall k \geq m\}, \quad d_n^* = \log_{10} \frac{|\varphi_{n,M_n^*}| \rho^{-2M_n^*}}{\varepsilon}$$

for  $\varepsilon = 10^{-12}$ . Thus,  $M_n^*$  is the number of terms required in (2.9) to reach accuracy  $\varepsilon$  (in the truncation of  $\varphi_n$  – we are disregarding here the error committed in replacing integrals by DFT), while  $d_n^*$  is the number of significant digits needed in the calculation, considering that we need to sum up terms of widely different magnitudes.

Table 1: The number of terms  $M_n^*$  and of significant digits  $d_n^*$  required to compute  $\varphi_n$  up to accuracy  $10^{-12}$  for  $\alpha = \frac{1}{2}$  and  $\rho = \frac{3}{2}$ .

$n$	16	32	64	128	256	512	1024	2048	4096
$M_n^*$	42	53	73	110	181	332	603	1165	2287
$d_n^*$	12	13	15	18	26	41	71	131	252

A clear conclusion from both Figure 2.1 and Table 1 is that  $M = \mathcal{O}(N)$ . Therefore the cost of (2.9) is  $\mathcal{O}(N^2)$  and by no stretch of imagination can it be considered a “fast” algorithm. The idea of integrating along a circle of radius  $\rho > 1$  (which, anyway, has a number of other obvious drawbacks) leads nowhere. Instead, like in (Iserles 2011), we use the transformation

$${}_2F_1 \left[ \begin{matrix} a, a + \frac{1}{2}; \\ c; \end{matrix} 2\zeta - \zeta^2 \right] = \frac{1}{(1 - \frac{1}{2}\zeta)^{2a}} {}_2F_1 \left[ \begin{matrix} 2a, 2a - c + 1; \\ c; \end{matrix} \frac{\zeta}{2 - \zeta} \right], \quad (2.10)$$

valid for all  $a, c \in \mathbb{C}$ , where  $c$  is neither zero nor a negative integer, and  $\zeta \in \mathbb{C}$ ,  $\operatorname{Re} \zeta < 1$ . Letting  $a = \frac{n+1}{2}$  and  $c = \alpha + n + \frac{3}{2}$ , the outcome is

$$\varphi_n((2\zeta - \zeta^2)^{-1/2}) = \frac{1}{(1 - \frac{1}{2}\zeta)^{n+1}} {}_2F_1 \left[ \begin{matrix} n + 1, \frac{1}{2} - \alpha; \\ n + \alpha + \frac{3}{2}; \end{matrix} \frac{\zeta}{2 - \zeta} \right].$$

Let  $\rho \in (r, 1)$ , in which case  $\mathcal{B}_\rho$  lies inside the analyticity boundary  $\mathcal{B}_r$ . We choose  $\zeta$  so that  $|\zeta/(2 - \zeta)| = \rho^2$ : this gives us a point on  $\mathcal{B}_\rho$ . Specifically,

$$z = \frac{1}{2}(\rho e^{i\theta} + \rho^{-1} e^{-i\theta}), \quad \zeta = \frac{2\rho^2 e^{2i\theta}}{1 + \rho^2 e^{2i\theta}},$$

hence

$$\frac{\zeta}{2 - \zeta} = \rho^2 e^{2i\theta}, \quad 2\zeta - \zeta^2 = \frac{1}{z^2}, \quad \frac{1}{1 - \frac{1}{2}\zeta} = 1 + \rho^2 e^{2i\theta}.$$

Since  $dz = -\frac{1}{2}i\rho^{-1}e^{-i\theta}(1 - \rho^2 e^{2i\theta})d\theta$  (the minus sign is a consequence of the negative orientation of the Bernstein ellipse), it follows from (2.7) that

$$\hat{f}_n = \frac{c_n(2\rho)^n}{2\pi} \int_{-\pi}^{\pi} (1 - \rho^2 e^{2i\theta}) f\left(\frac{1}{2}(\rho e^{i\theta} + \rho^{-1} e^{-i\theta})\right) e^{in\theta} \chi_n(\rho^2 e^{2i\theta}) d\theta, \quad (2.11)$$

where

$$\chi_n(z) = {}_2F_1 \left[ \begin{matrix} n+1, \frac{1}{2} - \alpha; \\ n + \alpha + \frac{3}{2}; \end{matrix} z \right], \quad n \in \mathbb{Z}_+.$$

Note that  $\chi_n$  reduces to a constant when  $\alpha = \frac{1}{2}$  (Chebyshev polynomials of the second kind), while  $\chi_n(z) = (1-z)^{-1}$  for  $\alpha = -\frac{1}{2}$  (Chebyshev polynomials of the first kind).  $\chi_n$  makes sense even when  $\alpha \downarrow -1$ , in which case some fairly messy algebra yields

$$\chi_n(z) = \frac{\pi^{1/2} (\frac{1}{2})_n}{z^{(2n-1)/4} (1-z)^{3/2}} P_{\frac{1}{2}}^{\frac{1}{2}-n} \left( \frac{1+z}{1-z} \right), \quad 0 < |z| < 1,$$

where  $P_\nu^\mu$  is a *Legendre function* (Abramowitz & Stegun 1964, p. 332).

### 3 A fast ultraspherical expansion algorithm

#### 3.1 Algorithm I

Unlike  $\varphi_n$ , the function  $\chi_n$  has rapidly convergent Taylor expansion:

$$\chi_n(z) = \sum_{m=0}^{\infty} \chi_{n,m} z^m, \quad \text{where} \quad \chi_{n,m} = \frac{(n+1)_m}{(n+\alpha+\frac{3}{2})_m} \frac{(\frac{1}{2}-\alpha)_m}{m!}.$$

Using the Stirling formula (Abramowitz & Stegun 1964, p. 257) to approximate Pochhammer symbols for large  $m$ , it is easy to calculate that

$$\chi_{n,m} \sim \frac{\Gamma(n+\alpha+\frac{3}{2})}{n! \Gamma(\frac{1}{2}-\alpha)} \cdot \frac{1}{m^{2\alpha+1}}, \quad m \gg 1, \quad (3.1)$$

hence  $\chi_{n,m}$  decays for large  $m$  for  $\alpha > -\frac{1}{2}$  and increases fairly gently for  $\alpha \in (-1, -\frac{1}{2}]$ , an increase easily counteracted by the rapidly decaying factor  $\rho^{2m}$  in (2.11).

Figure 3.1 illustrates the rapid decay of the scaled Taylor coefficients of  $\chi_n$  for increasing  $n$ , consistent with (3.1). The comparison with Figure 2.1 (where  $\rho^{-1}$  plays the same role as  $\rho$  in the current figure) is striking. Note further for future reference that in the third figure, pre-empting Subsection 3.2, we have allowed  $\rho \uparrow 1$ : the decay for large  $n$  is perceptibly slower but nonetheless acceptable.

Truncating  $\chi_n$  in (2.11), we have

$$\begin{aligned} \hat{f}_n &\approx \frac{c_n (2\rho)^n}{2\pi} \int_{-\pi}^{\pi} (1 - \rho^2 e^{2i\theta}) f(\tfrac{1}{2}(\rho e^{i\theta} + \rho^{-1} e^{-i\theta})) e^{in\theta} \sum_{m=0}^M \chi_{n,m} \rho^{2m} e^{2im\theta} d\theta \\ &= \frac{c_n (2\rho)^n}{2\pi} \sum_{m=0}^M \chi_{n,m} \rho^{2m} \int_{-\pi}^{\pi} (1 - \rho^2 e^{2i\theta}) f(\tfrac{1}{2}(\rho e^{i\theta} + \rho^{-1} e^{-i\theta})) e^{i(n+2m)\theta} d\theta \\ &= c_n (2\rho)^n \sum_{m=0}^M \chi_{n,m} \rho^{2m} \hat{v}_{n+2m}, \end{aligned} \quad (3.2)$$

where

$$\hat{v}_n = \frac{1}{2\pi} \int_{-\pi}^{\pi} (1 - \rho^2 e^{2i\theta}) f(\tfrac{1}{2}(\rho e^{i\theta} + \rho^{-1} e^{-i\theta})) e^{in\theta} d\theta, \quad n \in \mathbb{Z}_+,$$

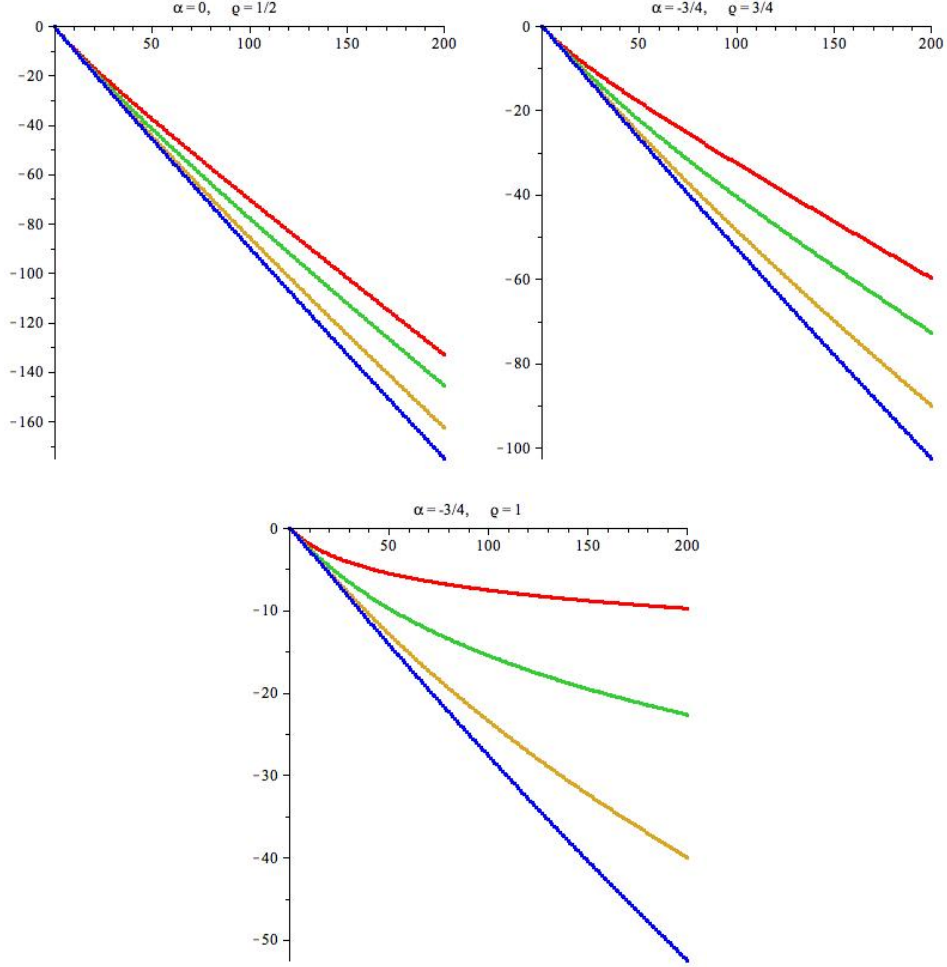


Figure 3.1: The plots of  $\log_{10}(|\chi_{n,m}|\rho^{2m})$  for  $m = 0, 1, \dots, 200$  and different values of  $\alpha$  and  $\rho \in (0, 1)$ . In each plot the bottom curve corresponds to  $n = 16$ , the next to  $n = 64$ , then  $n = 256$  and finally  $n = 1024$ .

is the Fourier transform of  $f$  along the Bernstein ellipse  $\mathcal{B}_\rho$ , modulated by the weight function  $1 - \rho^2 e^{2i\theta}$ . Since the  $\hat{v}_n$ s can be computed for  $n = 0, 1, \dots, N - 1$  in  $\mathcal{O}(N \log_2 N)$  operations using FFT, we deduce that the cost of evaluating (3.2) is  $\mathcal{O}(N \log_2 N) + \mathcal{O}(MN)$ .

Our next task is to compute the difference  $|\hat{f}_n - \hat{f}_n^{[M]}|$ , where

$$\hat{f}_n^{[M]} = c_n (2\rho)^n \sum_{m=0}^M \chi_{n,m} \rho^{2m} \hat{v}_{n+2m}, \quad n, M \in \mathbb{Z}_+.$$

Since we are within the domain of analyticity of  $\chi_n$ , it is true that

$$|\hat{f}_n - \hat{f}_n^{[M]}| = c_n(2\rho)^n \left| \sum_{m=M+1}^{\infty} \chi_{n,m} \rho^{2m} \hat{v}_{n+2m} \right| \leq c_n(2\rho)^n \max_{n \in \mathbb{Z}_+} |\hat{v}_n| \sum_{m=M+1}^{\infty} |\chi_{n,m}| \rho^{2m}.$$

Denoting by  $\|f\|_{\infty} < \infty$  the maximum of  $|f|$  on the Bernstein ellipse  $\mathcal{B}_{\rho}$ , it follows at once that

$$|\hat{v}_n| \leq \frac{\|f\|_{\infty}}{2\pi} \int_{-\pi}^{\pi} |1 - \rho^2 e^{2i\theta}| d\theta := d.$$

The integral on the right can be written explicitly as a complete exponential integral of second kind (Abramowitz & Stegun 1964, p. 589), but this adds little to our understanding: all that matter is that  $\max_{n \in \mathbb{Z}_+} |\hat{v}_n| \leq d$ . Provided that  $\alpha \geq -\frac{1}{2}$ , we have

$$\frac{\chi_{n,m}}{\chi_{n,m-1}} = \frac{n+m}{n+m+\alpha+\frac{1}{2}} \cdot \frac{m-\frac{1}{2}-\alpha}{m} \in (0, 1),$$

therefore  $\chi_{n,m} \in (0, 1)$  for all  $n, m \in \mathbb{Z}_+$  and we deduce that

$$|\hat{f}_n - \hat{f}_n^{[M]}| \leq c_n d (2\rho)^n \sum_{m=M+1}^{\infty} \rho^{2m} = \frac{c_n 2^n d}{1 - \rho^2} \rho^{n+2M+2}. \quad (3.3)$$

Finally, we estimate  $c_n$ , applying the *Stirling formula*  $\Gamma(z) \sim \sqrt{2\pi/z} (e^{-1}z)^z [1 + \mathcal{O}(z^{-1})]$ ,  $|z| \gg 1$  (Abramowitz & Stegun 1964, p. 257) to Pochhammer symbols  $(a)_n = \Gamma(a+n)/\Gamma(a)$ . Straightforward calculation confirms that

$$c_n = \frac{(2\alpha+1)_n n!}{2^n (\alpha+1)_n (\alpha+\frac{1}{2})_n} \sim \tilde{c}_{\alpha} \frac{n^{1/2}}{2^n}, \quad \text{where} \quad \tilde{c}_{\alpha} = \frac{\Gamma(\alpha+1)\Gamma(\alpha+\frac{1}{2})}{\Gamma(2\alpha+1)}. \quad (3.4)$$

Note that this is valid for all  $\alpha > -1$  except that for  $\alpha = -\frac{1}{2}$  we need to use a limiting process for  $n \in \mathbb{N}$ ,

$$c_n = \frac{(2\alpha+2)_{n-1} n!}{2^{n-1} (\alpha+1)_n (\alpha+\frac{3}{2})_{n-1}} \xrightarrow{\alpha \rightarrow -\frac{1}{2}} \frac{n!}{2^{n-1} (\frac{1}{2})_n} \sim \tilde{c}_{-\frac{1}{2}} \frac{n^{1/2}}{2^n},$$

where  $\tilde{c}_{-\frac{1}{2}} = 2\Gamma(\frac{1}{2}) = 2\sqrt{\pi}$ . All this is consistent with (3.4).

In Figure 2.3 we have sketched the values of  $2^n c_n / (\tilde{c}_{\alpha} n^{1/2})$  for three instances of  $\alpha > -1$ . According to (3.4), these values should tend to 1 for  $n \gg 1$  and this is confirmed in the figure.

Of course, (3.4) is an asymptotic estimate, rather than an upper bound. However, since the tail of the estimate is small, we deduce from (3.4) the existence of a bounded constant  $\tilde{d}$ , independent of  $n$  (but which might depend on  $\rho$ ), such that

$$|\hat{f}_n - \hat{f}_n^{[M]}| \leq \frac{\tilde{d}}{1 - \rho^2} n^{1/2} \rho^{n+2M+2}, \quad n \in \mathbb{Z}_+.$$

Moreover, since the maximum of  $g(x) = x^{1/2} a^x$ ,  $a \in (0, 1)$ , occurs at  $x_{\max} = -1/(2 \log a)$  and  $g(x_{\max}) = [-1/(2e \log a)]^{1/2}$ , we have  $n^{1/2} \rho^n \leq [-1/(2e \log \rho)]^{1/2}$ . Hence

$$|\hat{f}_n - \hat{f}_n^{[M]}| \leq \frac{\tilde{d}_1}{1 - \rho^2} \rho^{2M+2}, \quad n \in \mathbb{Z}_+, \quad \text{where} \quad \tilde{d}_1 = \tilde{d} \sqrt{-\frac{1}{2e \log \rho}}.$$

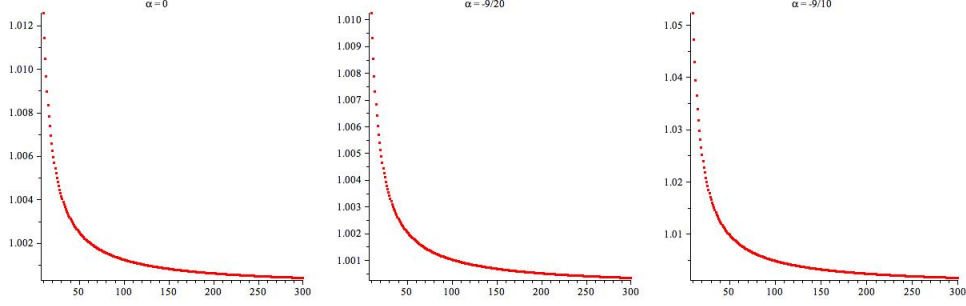


Figure 3.2: The curves  $2^n c_n / (\tilde{c}_\alpha n^{1/2})$  for different values of  $\alpha$  and increasing  $n$ .

Therefore, given  $\varepsilon > 0$ , the choice

$$M > \frac{\log \varepsilon - \log \tilde{d}_1 + \log(1 - \rho^2)}{\log \rho} \quad (3.5)$$

results in  $|\hat{f}_n - \hat{f}_n^{[M]}| < \varepsilon$ , uniformly for all  $n \in \mathbb{Z}_+$ . It is important to remark that (3.5) represents an exceedingly poor and pessimistic practical choice of  $M$  in our algorithm. Its only purpose is to argue that we can choose  $M$ , independent of  $N$  to compute the first  $N$  expansion coefficients. This means that  $M = \mathcal{O}(1)$  and the cost of the algorithm (3.2), where all integrals have been replaced by a single DFT, is  $\mathcal{O}(N \log_2 N)$ .

Extending our analysis to the range  $-1 < \alpha \leq -\frac{1}{2}$  is easy. Since  $\chi_{n,0} = 1$ ,

$$\frac{\chi_{n,m}}{\chi_{n,m-1}} = \frac{(n+m)(m - \alpha - \frac{1}{2})}{(n+m + \alpha + \frac{1}{2})m}, \quad m \in \mathbb{N},$$

and the function  $(n+x)(x - \alpha - \frac{1}{2}) / [(n+x + \alpha + \frac{1}{2})x]$  decreases monotonically for  $x > 0$ . Therefore

$$\left| \frac{\chi_{n,m}}{\chi_{n,m-1}} \right| \leq \frac{(n+1)(\frac{1}{2} - \alpha)}{n + \alpha + \frac{3}{2}}, \quad m \in \mathbb{N},$$

and, by recursion,

$$|\chi_{n,m}| \leq \left(\frac{1}{2} - \alpha\right)^n \left| \frac{\left(1 + \frac{1}{n}\right)^n}{\left(1 + \frac{\alpha + \frac{3}{2}}{n}\right)^n} \right| = \left(\frac{1}{2} - \alpha\right)^n e^{-\alpha - \frac{1}{2}} [1 + \mathcal{O}(n^{-1})], \quad m \in \mathbb{Z}_+.$$

Consequently, we need to replace (3.3) with

$$|\hat{f}_n - \hat{f}_n^{[M]}| \leq \frac{c_n d_1 (\frac{1}{2} - \alpha)^n}{1 - \rho^2} \rho^{n+2M+2}, \quad n \in \mathbb{Z}_+,$$

where we have replaced  $d$  by  $d_1 > d$  to take care of the  $\mathcal{O}(n^{-1})$  term in the above bound. The remainder of the argument that has led to (3.5) is valid also in the current

range of  $\alpha$ , except that we need to replace  $\rho^n$  with  $(\frac{1}{2}-\alpha)^n \rho^n$ : note that  $(\frac{1}{2}-\alpha)\rho/2 < 1$ . Therefore, all we need is to update  $\tilde{d}_1$  and replace  $\log \rho$  by  $\log \rho + \log(\frac{1}{2}-\alpha)$  in the denominator of (3.5). The algorithm is still  $\mathcal{O}(N \log_2 N)$ .

Having determined the cost of the algorithm for all  $\alpha > -1$ , we next present it in a form amenable to practical computation.

**Algorithm I**

**Step 1:** Choose a large composite natural number  $N$ , a (much) smaller natural number  $M$  and a number  $\rho \in (0, 1)$ .

**Step 2:** Compute

$$\check{c}_0 = 1, \quad \check{c}_n = \frac{(2\alpha + n)n\rho}{2(\alpha + n)(\alpha + n - \frac{1}{2})} \check{c}_{n-1}, \quad n = 1, 2, \dots, N-1,$$

$\check{\chi}_{n,0} = 1$  and

$$\check{\chi}_{n,m} = \frac{(n+m)(m-\alpha-\frac{1}{2})}{(n+m+\alpha+\frac{1}{2})m} \rho^2 \check{\chi}_{n,m-1}, \quad m = 1, 2, \dots, M, \quad n = 1, 2, \dots, N-1.$$

**Step 3:** Evaluate the sequence  $v_n = (2\pi)^{-1}(1 - \rho^2 \omega_N^{2n})f(\frac{1}{2}(\rho \omega_N^n + \rho^{-1} \omega_N^{-n}))$ ,  $n = -N/2 + 1, \dots, N/2$ , where  $\omega_N = \exp \frac{2\pi i}{N}$ .

**Step 4:** Compute the DFT  $\{\hat{v}_n\}$  of the sequence  $\{v_n\}$  using FFT.

**Step 5:** Set

$$\hat{f}_n = \check{c}_n \sum_{m=0}^M \check{\chi}_{n,m} \hat{v}_{n+2m}, \quad n = 0, 1, \dots, N-2M-1. \quad (3.6)$$

Note that  $\check{c}_n = c_n \rho^n$  and  $\check{\chi}_{n,m} = \chi_{n,m} \rho^{2m}$ .

The price of the fourth step is  $\mathcal{O}(N \log_2 N)$ , while second and fifth steps bear the price tag of  $\mathcal{O}(MN) = \mathcal{O}(N)$  operations.

A clear implication of numerical experiments in the case  $\alpha = 0$  in (Iserles 2011) which, we have every reason to believe, remains valid for all  $\alpha > -1$ , is that, while computing  $\hat{f}_n$  for small  $n$  requires (relatively) large  $M$ , it suffices to take a small  $M$  for large  $n$  – as a matter of fact, once we wish for uniformly small error, no advantage it to be gained from using large  $M$  for large(ish) values of  $n$ . This indicates that a useful amendment to Algorithm I is to replace (3.6) by

$$\hat{f}_n = \check{c}_n \sum_{m=0}^{M_n} \check{\chi}_{n,m} \hat{v}_{n+2m}, \quad n = 0, 1, \dots, N-1, \quad (3.7)$$

where  $M_n$  is a weakly monotonically decreasing sequence, such that  $M_n = 0$  for  $n = N-2M, \dots, N-1$ . The question, of course, is how to choose well such a sequence, to ensure that the algorithm bears a uniform error not exceeding given tolerance  $\varepsilon$ . Using (3.5) and its modification for  $\alpha \leq -\frac{1}{2}$  is clearly sub-optimal. As things stand,



the authors cannot offer a good means of constructing such a sequence  $\{M_n\}$ , given a function  $f$  and  $\rho \in (r, 1)$ . This is matter for future research but preliminary results and thoughts are reported in Section 4.

An interesting comment on our algorithm, which applies with the same force to the algorithm of the next section, is that Step 3, its  $\mathcal{O}(N \log_2 N)$  part, is independent of the choice of  $\alpha$ . Therefore, in principle, we can compute the first  $N$  expansion coefficients for  $r \geq 1$  different values of  $\alpha$  with a single FFT, in  $\mathcal{O}(N \log_2 N + rMN)$  operations (unlike the algorithm in (Keiner 2009), which would have required  $r + 1$  FFTs). This is useful when testing the algorithm but, more substantively, in the following situation: we wish to construct an approximation to an analytic function  $f$ . This approximation will be used a large number of times, it is important that it contains the least number of terms while attaining given accuracy and this is our main reason to choose  $\alpha > -1$ . In that case we can try different values of  $\alpha$  at the cost of a single FFT.

### 3.2 The case $\rho \uparrow 1$

The nearer  $r$  is to unity in the Bernstein ellipse  $\mathcal{B}_r$ , the weaker analyticity requirements that need be imposed on the function  $f$ . In particular, once  $r \uparrow 1$ , the ellipse ‘collapses’ into the interval  $[-1, 1]$  and we need not be bothered by possible existence of singularities near the interval. This motivates an examination of the case when  $\rho \uparrow 1$ . It has been demonstrated in (Iserles 2011) that in the Legendre case  $\alpha = 0$  Algorithm I survives the limiting process. In this subsection we prove that this remains the case for ultraspherical expansions when  $\alpha > -\frac{1}{2}$ .

Before we go any further, we must check that integrability in (2.11) continues to make sense once  $\rho \rightarrow 1$ . Each function  $\chi_n$  is clearly analytic in  $(-1, 1)$ , thus it is enough to prove that  $\chi_n(\pm 1)$  is bounded. Using the standard formula from Rainville (1960, p. 49) to sum up a hypergeometric function at  $z = 1$ , we have

$$\chi_n(1) = \frac{\Gamma(\alpha + n + \frac{3}{2})\Gamma(2\alpha + 1)}{\Gamma(\alpha + \frac{1}{2})\Gamma(n + 2\alpha + 1)},$$

which is bounded for all  $n \in \mathbb{Z}_+$  and  $\alpha > -\frac{1}{2}$ . Moreover, for  $\alpha > -\frac{1}{2}$  all the Taylor coefficients  $\chi_{n,m}$  are positive, consequently  $|\chi_n(-1)| \leq \chi_n(1)$  and  $\chi_n(-1)$  is also bounded.

Letting  $\rho \rightarrow 1$  in (2.11) results in

$$\begin{aligned} \hat{f}_n &= \frac{c_n}{2\pi} \int_{-\pi}^{\pi} (1 - e^{2i\theta}) f(\cos \theta) e^{in\theta} \chi_n(e^{2i\theta}) d\theta \\ &= \frac{c_n}{2\pi} \sum_{m=0}^{\infty} \chi_{n,m} \int_{-\pi}^{\pi} f(\cos \theta) [e^{i(n+2m)\theta} - e^{i(n+2m+2)\theta}] d\theta \\ &= \frac{c_n}{2\pi} \sum_{m=0}^{\infty} \chi_{n,m} \int_{-\pi}^{\pi} f(\cos \theta) [\cos((n+2m)\theta) - \cos((n+2m+2)\theta)] d\theta \\ &= c_n \sum_{m=0}^{\infty} \chi_{n,m} [\hat{\tau}_{n+2m} - \hat{\tau}_{n+2m+2}], \end{aligned} \tag{3.8}$$

where

$$\hat{\tau}_n = \frac{1}{2\pi} \int_{-\pi}^{\pi} f(\cos \theta) \cos n\theta \, d\theta, \quad n \in \mathbb{Z}_+,$$

is the  $n$ th *Chebyshev expansion coefficient* of  $f$ .<sup>3</sup> Note that we have used the fact that  $f(\cos \theta)$  is an even function, therefore

$$\int_{-\pi}^{\pi} f(\cos \theta) e^{ik\theta} \, d\theta = \int_{-\pi}^{\pi} f(\cos \theta) [\cos k\theta + i \sin k\theta] \, d\theta = \int_{-\pi}^{\pi} f(\cos \theta) \cos k\theta \, d\theta.$$

The obvious idea, taking a leaf from Algorithm I, is to truncate (3.8). This results in

**Algorithm II**

**Step 1:** Choose a large composite natural number  $N$  and a (much) smaller natural number  $M$ .

**Step 2:** Compute

$$c_0 = 1, \quad c_n = \frac{(2\alpha + n)n}{2(\alpha + n)(\alpha + n - \frac{1}{2})} c_{n-1}, \quad n = 1, 2, \dots, N-1$$

and

$$\chi_{n,0} = 1, \quad \chi_{n,m} = \frac{(n+m)(m-\alpha-\frac{1}{2})}{(n+m+\alpha+\frac{1}{2})m} \chi_{n,m-1}, \quad m = 1, \dots, M, \quad n = 1, \dots, N-1.$$

**Step 3:** Evaluate the sequence  $\tau_n = (2\pi)^{-1} f(\cos \frac{2\pi n}{N})$ ,  $n = 0, 1, \dots, N-1$ .

**Step 4:** Compute the Discrete Cosine Transform  $\{\hat{\tau}_n\}$  of the sequence  $\{\tau_n\}$  using Fast Cosine Transform.

**Step 5:** Set

$$\hat{f}_n^{[M]} = c_n \sum_{m=0}^M \chi_{n,m} (\hat{\tau}_{n+2m} - \hat{\tau}_{n+2m+2}), \quad n = 0, 1, \dots, N-2M-3. \quad (3.9)$$

As a reality check, we consider the case  $\alpha \downarrow -\frac{1}{2}$  in (3.9). As we have already mentioned in Subsection 2.3,  $\chi_n(z)$  reduces to  $(1-z)^{-1}$  in that case, hence  $\chi_{n,m} \equiv 1$  and (3.9) telescopes to

$$\hat{f}_n^{[M]} = c_n \sum_{m=0}^M (\hat{\tau}_{n+2m} - \hat{\tau}_{n+2m+2}) = c_n (\hat{\tau}_n - \hat{\tau}_{n+2M+2}).$$

Since now (cf. Subsection 2.3)  $c_n = n!/[2^{n-1}(\frac{1}{2})_n]$ , while  $P_n^{(-\frac{1}{2}, \frac{1}{2})}(x) = (\frac{1}{2})_n/n! T_n(x)$ , the algorithm yields  $\hat{f}_n^{[M]} = \hat{f}_n - \hat{f}_{n+2M+2}$ . This, incidentally, proves that we have uniform convergence for  $\alpha = -\frac{1}{2}$ . Thus, suppose that  $f$  is analytic within  $\mathcal{B}_r$  for

<sup>3</sup>Strictly speaking, we need to divide  $\hat{\tau}_0$  by two to be the zeroth Chebyshev coefficient.

some  $r \in (0, 1)$ , therefore its Chebyshev expansion converges at a spectral speed. Therefore for every  $\varepsilon$  there exists  $N_\varepsilon$  such that  $|\hat{f}_n| < \varepsilon$  for every  $n \geq N_\varepsilon$ . Choosing  $M \geq N_\varepsilon/2 - 1$ , we thus have  $|\hat{f}_n - \hat{f}_n^{[M]}| = |\hat{f}_{n+2M+2}| < \varepsilon$  for every  $n \in \mathbb{Z}_+$ . Moreover, in this case the optimal choice of  $M_n$ , once we replace (3.9) with

$$\hat{f}_n^{[M]} = c_n \sum_{m=0}^{M_n} \chi_{n,m} (\hat{\tau}_{n+2m} - \hat{\tau}_{n+2m+2})$$

is  $M_n = (\lceil (N_\varepsilon - n)/2 \rceil - 1)_+$ . Of course, there is absolutely no need to use Algorithm II, or for that matter Algorithm I, in the case  $\alpha = -\frac{1}{2}$ , but our observation helps in understanding the case of  $\alpha > -\frac{1}{2}$ .

It remains to demonstrate that, once we wish to approximate (3.8) to uniform accuracy  $\varepsilon$  by truncating the series, we have  $M = \mathcal{O}(1)$ . The bound (3.4) blows up for  $\rho \uparrow 1$  and we need an alternative proof. Fortunately, the relevant proof for the Legendre case  $\alpha = 0$  from (Iserles 2011) works in a more general setting. Thus, recall that  $f$  is analytic in the Bernstein ellipse  $\mathcal{B}_r$ , therefore there exist  $\alpha, d > 0$  such that  $|\hat{\tau}_n| \leq de^{-\alpha n}$ ,  $n \in \mathbb{Z}_+$ . Since  $|\chi_{n,m}| \leq 1$ , we deduce from (3.9) that

$$\begin{aligned} |\hat{f}_n - \hat{f}_n^{[M]}| &= c_n \left| \sum_{m=M+1}^{\infty} \chi_{n,m} (\hat{\tau}_{n+2m} - \hat{\tau}_{n+2m+2}) \right| \\ &\leq c_n \sum_{m=M+1}^{\infty} (|\hat{\tau}_{n+2m}| + |\tau_{n+2m+2}|) \\ &\leq c_n d \sum_{m=M+1}^{\infty} [e^{-\alpha(n+2m)} + e^{-\alpha(n+2m+2)}] = c_n d \frac{1 + e^{-2\alpha}}{1 - e^{-2\alpha}} e^{-\alpha(n+2M+2)}. \end{aligned}$$

It remains to recall the bound on  $c_n$  from the previous subsection,  $c_n \leq c^* n^{1/2}/2^n$  for some  $c^* > 0$ , in order to argue that  $|\hat{f}_n - \hat{f}_n^{[M]}|$  can be made less than  $\varepsilon$  uniformly in  $n$  by choosing sufficiently large  $M$ .

As before, our estimate grossly exaggerates a reasonable choice of  $M$  and should not be used in practical computation. Moreover, exactly like in the case of Algorithm I, it makes good sense to replace (3.9) with a variable- $M$  algorithm,

$$\hat{f}_n^{[M]} = c_n \sum_{m=0}^{M_n} \chi_{n,m} (\hat{\tau}_{n+2m} - \hat{\tau}_{n+2m+2}), \quad n = 0, 1, \dots, N-1, \quad (3.10)$$

where  $M_n$  is a weakly monotonically decreasing sequence such that  $M_n \leq \lfloor (N - n - 3)/2 \rfloor$ . Although practical rules for the choice of a good sequence  $\{M_n\}$  are a matter for future research, useful insight is provided by the numerical experiments of the next section.

## 4 Numerical experiments

Letting  $\rho = \frac{3}{4}$ , we have used Algorithm I to derive the leading coefficients in the expansion into ultraspherical polynomials of the three functions

$$f_a(z) = \sin(z + 1), \quad f_b(z) = e^{-z^2 - z}, \quad f_c(z) = \frac{1}{z^2 + \frac{9}{4}}.$$

Note that, while  $f_a$  and  $f_b$  are entire,  $f_c$  has a polar singularity at  $\pm\frac{3}{2}i$ .

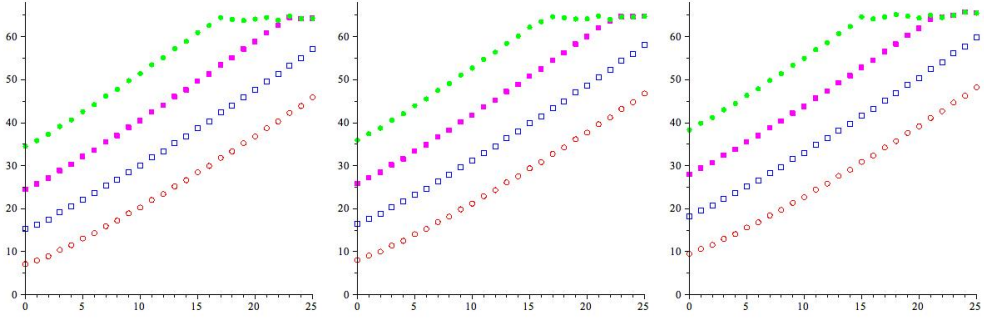


Figure 4.1:  $-\log_{10} |\hat{f}_n^{[M]} - \hat{f}|$  for  $f_a$  and (left to right)  $\alpha = -\frac{1}{2}, 0, 1$ . Circles, boxes, solid boxes and solid circles correspond to  $M = 3, 6, 9, 12$  respectively.

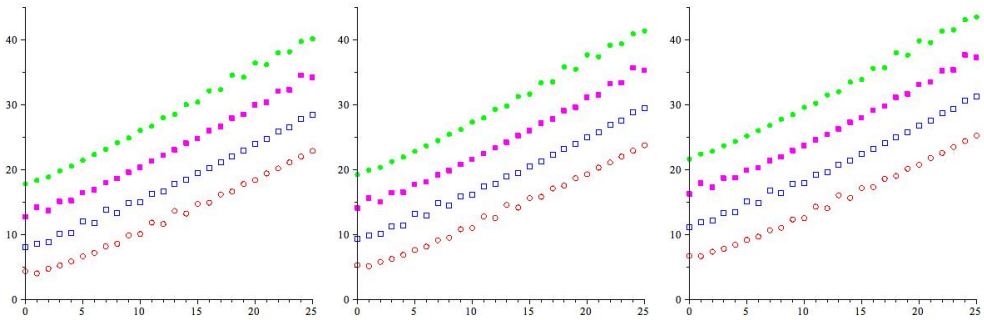


Figure 4.2:  $-\log_{10} |\hat{f}_n^{[M]} - \hat{f}|$  for  $f_b$ .

In Fig. 4.1 we display the error committed in approximating  $\hat{f}_n$ ,  $n = 0, \dots, 25$ , for the first function and three different values of  $\alpha$ . Note that  $N = 25$  is sufficient to our purposes because of the very rapid speed of convergence of the expansion – even to obtain the comparisons in Figs 4.1–3 to sufficiently high accuracy we have been compelled to use 60 significant digits. We observe a pattern that will repeat itself again and again and which has been already observed in (Iserles 2011) for  $\alpha = 0$ : the larger  $n$ , the smaller the value of  $M$  required to attain fixed accuracy. Thus, for  $n = 0$

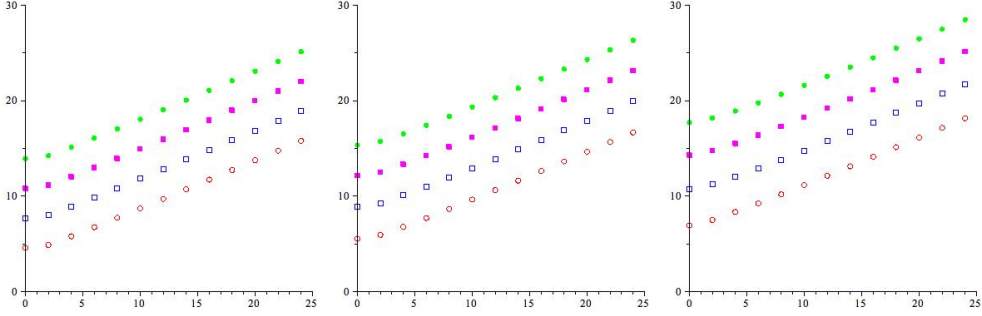


Figure 4.3:  $-\log_{10} |\hat{f}_n^{[M]} - \hat{f}|$  for  $f_c$ .

we obtain with  $M = 3$  roughly 9 significant digits, while with  $M = 6$  the accuracy grows to 15–18 significant digits. For  $n = 25$ , however, the error is less than  $10^{-45}$  (certainly good enough for any realistic calculation) already for  $M = 3$ .

The same pattern repeats itself in Fig. 4.2 and also, for  $f_c$  with finite poles, in Fig. 4.3. The indication is, thus, that a good choice of  $M_n$  in (3.7) (and, as similar computations indicate, (3.10)) is as a monotonically decreasing function.

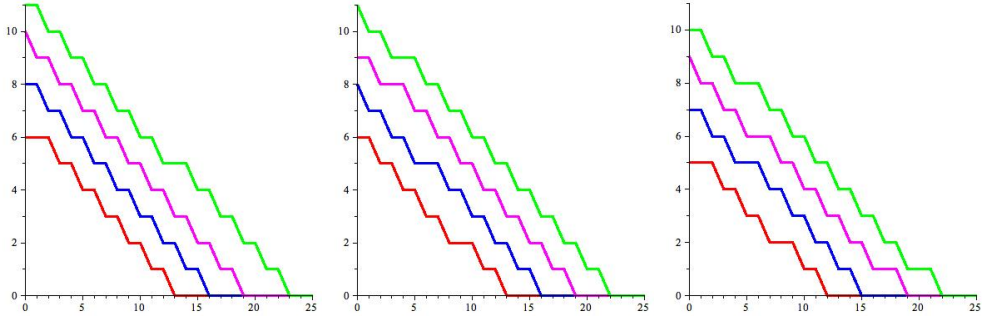


Figure 4.4:  $M_n^{\text{opt}}(\varepsilon)$  for  $f_a$  and (left to right)  $\alpha = -\frac{1}{2}, 0, 1$ . The bottom line corresponds to  $\varepsilon = 10^{-15}$ , then  $10^{-20}$ ,  $10^{-25}$  and, finally,  $10^{-30}$ .

To explore further good choices of  $M_n$ , we define

$$M_n^{\text{opt}}(\varepsilon) = \operatorname{argmin}_{M_n} \left| \tilde{c}_n \sum_{m=0}^{M_n} \tilde{\chi}_{n,m} \hat{v}_{n+2m} - \hat{f}_n \right|, \quad n \in \mathbb{Z}_+, \quad \varepsilon > 0.$$

In Fig. 4.4 we display  $M_n^{\text{opt}}(\varepsilon)$ , the least choice of  $M_n$  consistent with accuracy  $\varepsilon$ , for  $f_a$  and different choices of  $\alpha$ . The picture is consistent: as a function of  $n$ ,  $M_n^{\text{opt}}$  is approximated very well by a function of the form  $\max\{a - bn, 0\}$ . The numbers  $0 < b < a$  clearly depend on  $f$ ,  $\varepsilon$ ,  $\rho$  and  $\alpha$ , yet the dependence on  $\alpha$  appears to be fairly weak, while  $b$  appears to depend just on  $f$ .

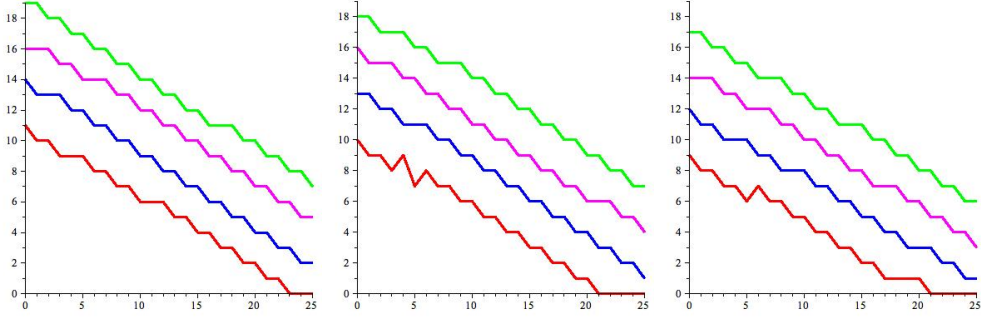


Figure 4.5:  $M_n^{\text{opt}}(\epsilon)$  for  $f_b$  and even  $ns$ .

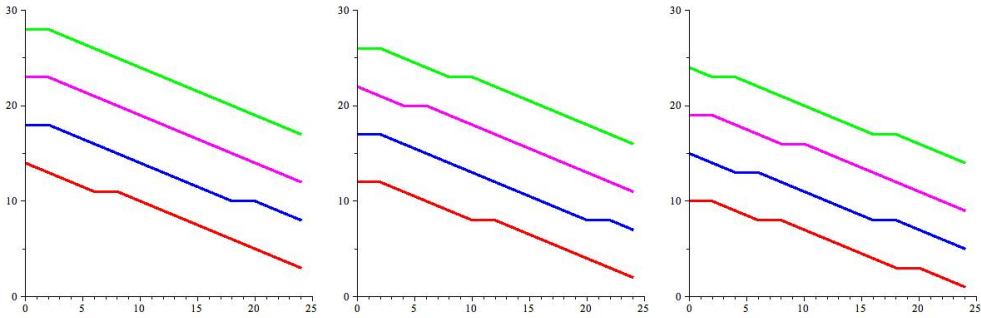


Figure 4.6:  $M_n^{\text{opt}}(\epsilon)$  for  $f_c$ .

Similar behaviour (which was first observed by Edward Mottram in his student project in Cambridge) appears to be universal and this is confirmed by Figs. 4.5–6. (Since  $f_b$  is even,  $\hat{f}_{2n+1}, \hat{f}_{2n+1}^{[M]} \equiv 0, n \in \mathbb{Z}_+$ , hence we display  $M_n^{\text{opt}}$  only for even  $n$  in Fig. 4.6.). Although it is unlikely that optimal parameters  $a$  and  $b$  can be derived explicitly, greater hope resides in determining ‘good’ parameters of this kind: this is a matter for future research. It is clear that the savings in using (3.7), say, in preference to (3.6), are substantial. Provided that our *ansatz* is right and that  $N > a/b$ , the computation of  $\hat{f}_0, \dots, \hat{f}_N$  with (3.7) requires roughly just  $N + a(a-b)/(2b)$  terms  $\hat{v}_m$  altogether.<sup>4</sup>

In all our experiments so far we have assumed  $\rho = \frac{3}{4}$ : this appears to be fairly representative of general behaviour, although singularities of  $f$  near the interval  $[-1, 1]$  require that the Bernstein ellipse  $\mathcal{B}_\rho$  is sufficiently ‘flat’ (Iserles 2011). To demonstrate that the error pattern is fairly insensitive to the choice of  $\rho \in (0, 1]$  for entire functions  $f$ , we have sketched in Fig. 4.7 the number of significant digits once we approximate

<sup>4</sup>All this discussion assumes exact arithmetic and disregards the error in approximating Fourier transforms by FFT.

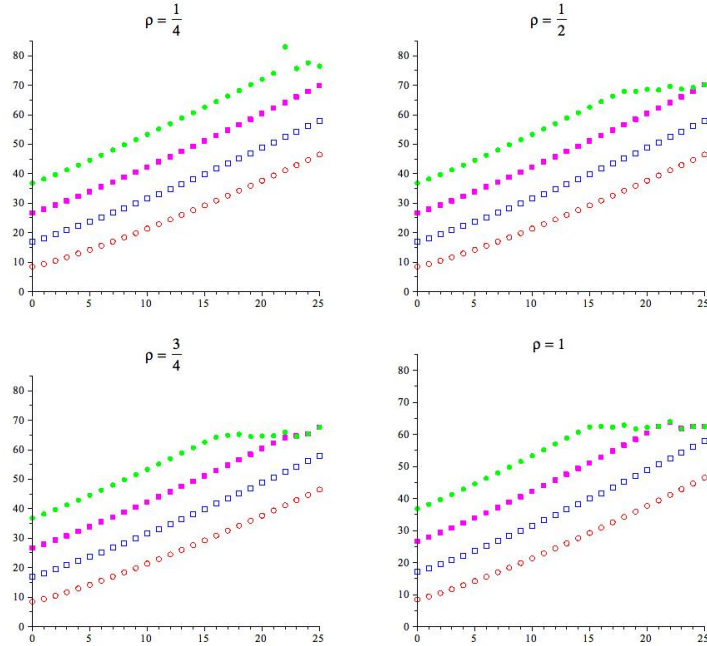


Figure 4.7:  $-\log_{10} |\hat{f}_n^{[M]} - \hat{f}|$  for  $f(z) = ze^z$ ,  $\alpha = 1$  and different values of  $\rho$ .

$\hat{f}_n$  for  $f(z) = ze^z$  with  $\alpha = 1$  and with different values of  $\rho$ . The differences are negligible for small  $n$  but the error decays faster for large  $ns$  for smaller parameter  $\rho$ . Typically, however, our interest is in *uniform* error, in which case the possible gain in seeking ‘good’ values of  $\rho$  does not appear to be of much significance in the case of entire functions .

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