A fast (and simple) algorithm for the computation of Legendre coefficients

Arieh Iserles

March 13, 2010

Abstract

We present an $\mathcal{O}(N \log N)$ algorithm for the calculation of the first N coefficients in an expansion of an analytic function in Legendre polynomials. In essence, the algorithm consists of an integration of a suitably weighted function along an ellipse, a task which can be accomplished with Fast Fourier Transform, followed by some post-processing.

The mathematical underpinning of this algorithm is an old formula that expresses expansion coefficients $\hat{f}_m$ as infinite linear combinations of derivatives. We evaluate the latter with the Cauchy theorem, thereby expressing each $\hat{f}_m$ as a scaled integral of $f(z)\varphi_m(z)/z^{m+1}$ along an appropriate contour, where φ_m is a slowly-converging hypergeometric function. Next, we transform φ_m into another hypergeometric function which converges rapidly. Once we replace the latter function by its truncated Taylor expansion and choose an appropriate elliptic contour, we obtain an expression for the $\hat{f}_m$s which is amenable to rapid computation.

1 Introduction

Expansion of functions in fast-converging series is of central importance in approximation theory and is, through the agency of spectral methods, fundamental in designing efficient computational methods for partial differential equations. Particularly effective are Fourier expansions, since their first N terms can be computed in $\mathcal{O}(N \log N)$ terms using the Fast Fourier Transform (FFT). Moreover, because

$$\int_{-1}^{1} f(x)\mathrm{T}_m(x)(1-x^2)^{-\frac{1}{2}}\,\mathrm{d}x = \int_{-\pi}^{\pi} f(\cos\theta)\cos(m\theta)\,\mathrm{d}\theta, \qquad m \in \mathbb{Z}_+,$$

the computation of Chebyshev expansions can be reduced to that of their Fourier counterparts and likewise accomplished in $\mathcal{O}(N \log N)$ operations. However, an $\mathcal{O}(N \log N)$ algorithm for the computation of the *Legendre expansion*

$$f(x) = \sum_{m=0}^{\infty} \hat{f}_m \mathrm{P}_m(x), \tag{1.1}$$

where

$$\hat{f}_m = (m+\tfrac{1}{2}) \int_{-1}^{1} f(x)\mathrm{P}_m(x)\,\mathrm{d}x, \qquad m \in \mathbb{Z}_+, \tag{1.2}$$

is not known. This is not for a want of trying. In particular, the idea of computing Chebyshev coefficients first, subsequently converting them into Legendre coefficients, has been considered in (Alpert & Rokhlin 1991) and (Potts, Steidl & Tasche 1998) and it results in an $\mathcal{O}\big(N(\log N)^2\big)$ algorithm.

The challenge of computing (1.2) directly is compounded by the fact that the integrand oscillates rapidly for large m. The obvious recourse is thus to use a quadrature formula with large number of nodes: essentially, to compute the first N coefficients we need $\mathcal{O}(N)$ quadrature nodes. Although this can be effectively accomplished with Clenshaw–Curtis quadrature (Trefethen 2008), the outcome is an $\mathcal{O}\big(N^2\big)$ algorithm: no joy. An appealing alternative is to use one of the modern methods for the computation of highly oscillatory integrals (Huybrechs & Olver 2009). Such methods produce exceedingly precise approximations using a very small data set of function values and derivatives. Unfortunately, these methods are based upon asymptotic expansion of highly oscillatory integrals and they apply only to algebraically-decaying coefficients, while Legendre coefficients (like their Fourier and Chebyshev brethren) decay exponentially fast (or faster) for an analytic function f. Thus, we cannot expect salvation from this quarter either.

Our approach proposes to abandon (1.2) altogether. Our starting point is an explicit expression for x^m as a linear combination of P_k, $k = 0, 1, \ldots, m$, which was already familiar to Adrien-Marie Legendre (1817). (Cf. also (Whittaker & Watson 1902, p. 310) and (Rainville 1960, p. 181).) This leads to an explicit expression for $\hat{f}_m$ which, albeit well known, is on the face of it without much merit in numerical computation: Given that

$$f(z) = \sum_{n=0}^{\infty} f_n z^n$$

is analytic in an open domain $\Omega \subseteq \mathbb{C}$ such that $[-1, 1] \in \Omega$, it is true that

$$\hat{f}_m = (2m+1) \sum_{n=0}^{\infty} \frac{(m+2n)! f_{m+2n}}{2^{m+2n} n! (\frac{3}{2})_{m+n}}, \qquad m \in \mathbb{Z}_+, \tag{1.3}$$

where the *Pochhammer symbol* $(a)_k$ is defined as $(a)_0 = 1$, $(a)_k = (a)_{k-1}(a+k-1)$, $k \geq 1$ (Rainville 1960, p.182). Although (1.3) has been occasionally applied to direct (and fairly laborious) evaluation of Legendre coefficients in their explicit form for specific (and simple) functions f (Brunner, Iserles & Nørsett 2010), its apparent lack of appeal in computation is obvious: evaluating a sufficient number of derivatives by finite differences to render (1.3) useful is both expensive and exceedingly unstable. Obvious but, fortunately, wrong.

The first critical step is to compute derivatives by means of complex integration, rather than by finite differences (Bornemann 2010). Thus,

$$f_n = \frac{1}{2\pi \mathrm{i}} \int_\gamma \frac{f(z)}{z^{n+1}} \, \mathrm{d}z,$$

where γ is a simple, closed Jordan curve circling the origin in Ω with positive orientation. Therefore, choosing the circle $\gamma = \{r\mathrm{e}^{\mathrm{i}\theta} \,:\, \theta \in [-\pi, \pi]\}$ with $r > 1$ and given sufficiently large $N \in \mathbb{Z}$, the sequence $\{f_n/n!\}_{n=0}^{N-1}$ can be computed with the Discrete Fourier Transform (DFT)

$$f_n \approx \frac{r^{-n}}{N} \sum_{k=0}^{N-1} f(r\omega_N^k)\omega_N^{-kn}, \qquad n = 0, 1, \ldots, N-1,$$

where $\omega_N = \exp\frac{2\pi\mathrm{i}}{N}$: this can be done in $\mathcal{O}(N\log N)$ operations. Unfortunately, even once the derivatives are known, we need $\mathcal{O}\big(N^2\big)$ operations to compute

$$\hat{f}_m \approx (2m+1)\sum_{n=0}^{\lfloor (N-m)/2\rfloor -1} \frac{(m+2n)!f_{m+2n}}{2^{m+2n}n!(\frac{3}{2})_{m+n}}, \qquad m=0,1,\ldots,N-2$$

– another dead end. However, suppose that, instead of computing derivatives with FFT, we apply the Cauchy theorem formally to (1.3). After some algebra, this results in

$$\hat{f}_m = \frac{2^m(m!)^2}{(2m)!}\frac{1}{2\pi\mathrm{i}}\int_\gamma \frac{f(z)}{z^{m+1}}\,{}_2\mathrm{F}_1\left[\begin{matrix}\frac{m+1}{2},\frac{m+2}{2};\\ m+\frac{3}{2};\end{matrix}\ \frac{1}{z^2}\right]\mathrm{d}z, \qquad m\in\mathbb{Z}_+. \tag{1.4}$$

The *hypergeometric function* ${}_2\mathrm{F}_1$ is defined for $a,b,c\in\mathbb{C}$, where c is neither zero nor a negative integer, by

$${}_2\mathrm{F}_1\left[\begin{matrix}a,b;\\ c;\end{matrix}\ z\right] = \sum_{k=0}^{\infty}\frac{(a)_k(b)_k}{k!(c)_k}z^k \tag{1.5}$$

(Rainville 1960, p. 45).

Our hope by this stage is to replace the hypergeometric function in (1.4) by its truncated Taylor expansion, since then, having chosen a suitable contour γ, the expression (1.4) can be approximated by DFT and computed with FFT in $\mathcal{O}(N\log N)$ operations. Unfortunately, even when γ is chosen in the domain of analyticity of the hypergeometric function, the Taylor expansion for large m converges excruciatingly slowly. We would need an enormous number of terms, of vastly different orders of magnitude, and the computation is bound to be both expensive and contaminated by unacceptable roundoff error. Another hope dashed!

Except that the magic of special functions theory allows us to replace the hypergeometric function in (1.4) by a rapidly convergent expression, which can be approximated by truncated Taylor series with a small number of terms. Moreover, we can choose an elliptic trajectory γ so that our new expression is in a form suitable for discretization with DFT and the outcome is a high-accuracy approximation for the Legendre coefficients obtained with a single FFT, hence in $\mathcal{O}(N\log N)$ operations, followed by $\mathcal{O}(N)$ post-processing.

The outcome of this rather convoluted mathematical journey is thus a surprisingly simple numerical algorithm.

In Section 2 we derive the expression (1.4) by two different routes. We commence from the formula (1.3): this has the virtue of simplicity and of reliance on known formulæ. However, we believe that an alternative, direct derivation of (1.4) is of interest, since it explains in a much more profound manner *why* this strange expression makes sense.

Section 3 is devoted to the derivation of our numerical algorithm. Thus, we subject (1.4) to a transformation that converts the hypergeometric function into rapidly-convergent expression, choose a contour γ which is amenable to DFT and conclude with our algorithm for an $\mathcal{O}(N\log N)$ calculation of Legendre coefficients.

More specifically, for the benefit of readers who do not wish to wade through mathematical details, just to acquint themselves with the algorithm, we choose $r\in(0,1]$ so that the ellipse $\frac{1}{2}(r^{-1}\mathrm{e}^{-\mathrm{i}\theta}+r\mathrm{e}^{\mathrm{i}\theta})$, $\theta\in[-\pi,\pi]$, lies in the domain of analyticity of the function f (or, for $r=1$, 'collapses' to $[-1,1]$) and compute the FFT $\{\kappa_{N,k}\}_{k=0}^{N-1}$ of the sequence

$$\{(1-r^2\omega_M^{2k})f(\tfrac{1}{2}(r^{-1}\omega_N^{-k}+r\omega_N^{r}))\ :\ k=0,1,\ldots,N-1\},$$

where $\omega_N = \exp\frac{2\pi\mathrm{i}}{N}$ and N is a suitably large integer. Next, choose $M \in \mathbb{Z}_+$ and, for all $m = 1, 2, \ldots, N-1-2M$ and $m = 1, 2, \ldots, N-1-2M$ calculate

$$\tilde{g}_{0,0} = 1, \qquad \tilde{g}_{m,0} = \frac{mr}{m-\frac{1}{2}}\tilde{g}_{m-1,0}, \qquad \tilde{g}_{m,j} = \frac{(m+j)(j-\frac{1}{2})r^2}{j(m+j+\frac{1}{2})}\tilde{g}_{m,j-1}.$$

Finally, approximate

$$\tilde{f}_m \approx \sum_{j=0}^{M} \tilde{g}_{m,j}\kappa_{N,m+2j}, \qquad m = 0, 1, \ldots, N-1-2M.$$

In Section 4 we present few numerical examples, briefly debate implementation details and discuss future directions.

It is a matter for intense satisfaction that two ideas due to mathematical giants of the early Nineteenth Century – Carl Friedrich Gauss's Fast Fourier Transform (Gauss 1866)[1] and Adrien-Marie Legendre's expression of general powers of x in the basis of 'his' polynomials – combine to address an important computational challenge of the Twenty First Century.

2 An integral expression for Legendre coefficients

2.1 The functions φ_m

Substitution of the Cauchy formula into the expression (1.3) results in

$$\hat{f}_m = (2m+1)\sum_{n=0}^{\infty} \frac{(m+2n)!}{2^{m+2n}n!(\frac{3}{2})_{m+n}} \frac{1}{2\pi\mathrm{i}}\int_\gamma \frac{f(z)}{z^{m+n+1}}\,\mathrm{d}z, \qquad m \in \mathbb{Z}_+.$$

However,

$$(\tfrac{3}{2})_{m+n} = (\tfrac{3}{2})_m(m+\tfrac{3}{2})_n, \qquad (m+2n)! = 2^{2n}m!(\tfrac{m+1}{2})_n(\tfrac{m+2}{2})_n.$$

Therefore

$$\begin{aligned}\hat{f}_m &= \frac{(2m+1)m!}{2^m(\frac{3}{2})_m}\frac{1}{2\pi\mathrm{i}}\int_\gamma \sum_{n=0}^{\infty}\frac{f(z)}{z^{m+1}}\frac{(\frac{m+1}{2})_n(\frac{m+2}{2})_n}{n!(m+\frac{3}{2})_n}\frac{1}{z^{2n}}\,\mathrm{d}z\\ &= \frac{2^m(m!)^2}{(2m)!}\frac{1}{2\pi\mathrm{i}}\int_\gamma \frac{f(z)}{z^{m+1}}\,{}_2\mathrm{F}_1\left[\begin{matrix}\frac{m+1}{2}, \frac{m+2}{2}; & \frac{1}{z^2}\\ m+\frac{3}{2}; & \end{matrix}\right]\mathrm{d}z\\ &= \frac{c_m}{2\pi\mathrm{i}}\int_\gamma \frac{f(z)}{z^{m+1}}\varphi_m(z)\,\mathrm{d}z, \qquad m \in \mathbb{Z}_m,\end{aligned}$$

where

$$c_m = \frac{2^m(m!)^2}{(2m)!}, \quad \varphi_m(z) = {}_2\mathrm{F}_1\left[\begin{matrix}\frac{m+1}{2}, \frac{m+2}{2}; & \frac{1}{z^2}\\ m+\frac{3}{2}; & \end{matrix}\right], \qquad m \in \mathbb{Z}_+.$$

[1] Gauss apparently discovered the FFT in 1805 but never bothered to publish it in his lifetime, a unique exemplar of 'perish and publish'.

This proves (1.4) but note that we have left the exact nature of the contour γ deliberately vague. While *any* closed curve γ surrounding the origin with winding number 1 in Ω will do for the computation of an arbitrary derivative of f by means of the Cauchy theorem, this need not (and is not) the case with (1.4). Indeed, the simplicity of the proof of this formula is deceptive because it rests upon the interchange of infinite summation and integration. This in turn depends on the properties of the integrand and cannot be taken for granted.

Our first observation is that the analyticity of the hypergeometric function (1.5) is assured only for $|z| < 1$. This might indicate that γ must lie in the exterior of the closed unit disc, but this is unnecessarily restrictive.

Proposition 1 *The domain of analyticity of the function φ_m, $m \in \mathbb{Z}_+$, is $\mathbb{C} \setminus [-1, 1]$.*

Proof Although the statement of this proposition would not surprise experts in special functions, we believe that it is valuable to present its proof for the sake of completeness. We commence from the integral representation

$$
{}_2\mathrm{F}_1\left[\begin{matrix} a, b; \\ c; \end{matrix}\; z\right] = \frac{\Gamma(c)}{\Gamma(b)\Gamma(c-b)} \int_0^1 t^{b-1}(1-t)^{c-b-1}(1-zt)^{-a}\,\mathrm{d}t
$$

where b, c and $c - b$ are neither zero nor a negative integer (Rainville 1960, p. 47). Therefore

$$
\varphi_n(z) = \int_0^1 t^{\frac{1}{2}n}(1-t)^{\frac{1}{2}(m-1)}\left(1 - \frac{t}{z^2}\right)^{-\frac{1}{2}(m+1)}\,\mathrm{d}t,
$$

which is integrable (and analytic) for $z \in \mathbb{C} \setminus [-1, 1]$. It remains to show that φ_m cannot be analytic anywhere on $[-1, 1]$. We commence by showing that $z = 1$ (hence, φ_m being even, also $z = -1$) results in divergence. To this end we use the classical formula

$$
{}_2\mathrm{F}_1\left[\begin{matrix} a, b; \\ c; \end{matrix}\; 1\right] = \frac{\Gamma(c)\Gamma(c-a-b)}{\Gamma(c-a)\Gamma(c-b)},
$$

which is valid for all $a, b, c \in \mathbb{C}$ provided that c is neither zero nor a negative integer and that $\mathrm{Re}\,(c-a-b) > 0$ (Rainville 1960, p. 49). Therefore, letting $c = a+b+\varepsilon$, where $0 < \varepsilon \ll 1$, we have

$$
{}_2\mathrm{F}_1\left[\begin{matrix} a, b; \\ a+b+\varepsilon; \end{matrix}\; 1\right] = \frac{\Gamma(a+b)}{\Gamma(a)\Gamma(b)}\Gamma(\varepsilon)[1 + \mathcal{O}(\varepsilon)].
$$

Letting $a = \frac{m+1}{2}$, $b = \frac{m+2}{2}$ and allowing $\varepsilon \to 0$ confirms that $\varphi_m(1) = +\infty$.

It remains to prove that φ_m fails to be analytic for $x \in (-1, 1) \setminus \{0\}$. But in that case

$$
\varphi_m(x) = \sum_{k=0}^{\infty} \frac{(\frac{m+1}{2})_k(\frac{m+2}{2})_k}{k!(m+\frac{3}{2})_k}\frac{1}{x^{2k}} \geq \sum_{k=0}^{\infty} \frac{(\frac{m+1}{2})_k(\frac{m+2}{2})_k}{k!(m+\frac{3}{2})_k} = \varphi_m(1)
$$

and the assertion follows. □

We have just demonstrated that the analyticity of each φ_m fails exactly along the support of the Legendre measure, where φ_m has a branch cut.

But what is φ_m? It is easy to verify that

$$
\varphi_0(z) = \tfrac{1}{2} z \log \frac{z+1}{z-1} \tag{2.1}
$$

but general form of φ_m for all $m \in \mathbb{Z}_+$ is not available. Fortunately, it is possible to establish a relationship between φ_m and φ_0 which identifies contours γ which are allowed in (1.4) and, incidentally, proves the above formula in an alternative manner.

2.2 A direct proof of (1.4)

Let

$$\mathcal{K}_m(z) = \frac{c_m}{2m+1} \frac{\varphi_m(z)}{z^{m+1}}, \qquad m \in \mathbb{Z}_+.$$

Direct computation confirms that

$$\begin{aligned} \mathcal{K}_1(z) &= \mathrm{P}_1(z)\mathcal{K}_0(z) - 1, \\ \mathcal{K}_2(z) &= \mathrm{P}_2(z)\mathcal{K}_0(z) - \tfrac{3}{2}z, \\ \mathcal{K}_3(z) &= \mathrm{P}_3(z)\mathcal{K}_0(z) - \tfrac{5}{2}z^2 + \tfrac{2}{3}, \end{aligned}$$

motivating the next lemma.

Lemma 2 *For every $m \in \mathbb{Z}_+$ is it true that*

$$\mathcal{K}_m(z) = \mathrm{P}_m(z)\mathcal{K}_0(z) + q_m(z), \qquad m \in \mathbb{Z}_+, \tag{2.2}$$

where q_m is a polynomial.

Proof The assertion of the theorem will be proved separately for even and odd values of m, commencing from an explicit representation of Legendre polynomials,

$$\begin{aligned} \mathrm{P}_{2m}(z) &= \sum_{k=0}^{m} \frac{(-1)^{m-k}(\frac{1}{2})_{m+k}}{(m-k)!(2k)!} X^{-2k}, \\ \mathrm{P}_{2m+1}(z) &= \sum_{k=0}^{m} \frac{(-1)^{m-k}(\frac{1}{2})_{m+k+1}}{(m-k)!(2k+1)!} X^{-2k-1}, \end{aligned}$$

where $X = (2z)^{-1}$ (Rainville 1960, p. 157). Thus,

$$\begin{aligned} \mathcal{K}_{2m}(z) - \mathrm{P}_{2m}(z)\mathcal{K}_0(z) &= \frac{2^{4m+1}(2m)!(\frac{3}{2})_{2m}}{(4m+1)!} \sum_{k=0}^{\infty} \frac{(2m+2k)!}{k!(\frac{3}{2})_{2m+k}} X^{2k+2m+1} \\ &\quad - 2\sum_{j=0}^{m} \frac{(-1)^{m-j}(\frac{1}{2})_{m+j}}{(m-j)!(2j)!} \sum_{k=0}^{\infty} \frac{(2k)!}{k!(\frac{3}{2})_k} X^{2k-2j+1} \\ &= 2^{4m+1}\frac{(2m)!(\frac{3}{2})_{2m}}{(4m+1)!} \sum_{k=m}^{\infty} \frac{(2k)!}{(k-m)!(\frac{3}{2})_{m+k}} X^{2k+1} \\ &\quad - 2\sum_{j=0}^{m} \sum_{k=-j}^{\infty} \frac{(-1)^{m-j}(\frac{1}{2})_{m+j}}{(m-j)!(2j)!} \frac{(2k+2j)!}{(k+j)!(\frac{3}{2})_{k+j}} X^{2k+1}. \end{aligned}$$

Since

$$\frac{2^{4m}(2m)!(\frac{3}{2})_{2m}}{(4m+1)!} = 1,$$

we thus deduce that

$$\mathcal{K}_{2m}(z) - \mathrm{P}_{2m}(z)\mathcal{K}_0(z) = 2\sum_{k=m}^{\infty} \frac{(2k)!}{(k-m)!(\frac{3}{2})_{m+k}} X^{2k+1} \tag{2.3}$$

$$- 2\sum_{k=-m}^{\infty}\left[\sum_{j=\max\{0,-k\}}^{\infty} \frac{(-1)^{m-j}(\frac{1}{2})_{m+j}(2k+2j)!}{(n-j)!(2j)!(k+j)!(\frac{3}{2})_{k+j}}\right] X^{2k+1}.$$

Let $k \geq 0$. Then the coefficient of X^{2k+1} in the second sum is

$$\alpha_k = 2\sum_{j=0}^{m} \frac{(-1)^{m-j}(\frac{1}{2})_{m+j}(2k+2j)!}{(m-j)!(2j)!(k+j)!(\frac{3}{2})_{k+j}}.$$

Moreover, for every $0 \leq j \leq m$, $k \geq 0$

$$(\tfrac{1}{2})_{m+j} = (\tfrac{1}{2})_m(m+\tfrac{1}{2})_j, \qquad (2k+2j)! = (2k)!2^{2j}(k+\tfrac{1}{2})_j(k+1)_j,$$
$$\frac{1}{(m-j)!} = \frac{(-1)^j(-m)_j}{m!}, \qquad \frac{1}{(2j)!} = \frac{1}{2^{2j}(\frac{1}{2})_j j!}, \qquad \frac{1}{(\frac{3}{2})_{k+j}} = \frac{1}{(\frac{3}{2})_k(k+\frac{3}{2})_j}$$

and therefore

$$\alpha_k = 2(-1)^m \frac{(2k)!(\frac{1}{2})_m}{m!k!(\frac{3}{2})_k}\, {}_3\mathrm{F}_2\left[\begin{matrix} -m, m+\frac{1}{2}, k+\frac{1}{2}; \\ \frac{1}{2}, k+\frac{3}{2}; \end{matrix}\ 1\right], \qquad k \geq 0.$$

(We refer to (Rainville 1960) to the definition of generalized hypergeoemtric functions.) However, according to (Rainville 1960, p. 87) and provided that neither c nor $1+a+b-c-m$ are zero or a negative integer, it is true that

$${}_3\mathrm{F}_2\left[\begin{matrix} -m, a, b; \\ c, 1+a+b-c-m; \end{matrix}\ 1\right] = \frac{(c-a)_m(c-b)_m}{(c)_m(c-a-b)_m}.$$

In our case $a = m+\frac{1}{2}$, $b = k+\frac{1}{2}$, $c = \frac{1}{2}$ and, since

$$(-m)_m = (-1)^m m!, \qquad (-k)_m = \frac{(-1)^m k!}{(k-n)!}, \qquad \frac{1}{(-m-k-\frac{1}{2})_m} = \frac{(-1)^m}{(k+\frac{3}{2})_m},$$

we deduce that

$$\alpha_k = \frac{2(2k)!}{(k-n)!(\frac{3}{2})_{k+m}}, \qquad k \geq 0.$$

This is a perfect match for the first sum in (2.3), we deduce that

$$\mathcal{K}_{2m} = \mathrm{P}_{2m}(z)\mathcal{K}_0(z) - \sum_{k=1}^{n-1}\left[\sum_{j=k}^{m-1} \frac{(-1)^{m-j}(\frac{1}{2})_{m+j}(2j-2k)!}{(m-j)!(2j)!(j-k)!(\frac{3}{2})_{j-k}}\right] z^{2(k-1)}$$

and obtain the polynomial q_{2n} explicitly.

Likewise (and with fewer details)

$$\begin{aligned}
&\mathcal{K}_{2m+1} - \mathrm{P}_{2m+1}(z)\mathcal{K}_0(z)\\
&= \frac{2^{4m+3}(2m+1)!(\frac{3}{2})_{2m+1}}{(4m+3)!}\sum_{k=0}^{\infty}\frac{(2m+2k+1)!}{k!(\frac{3}{2})_{2m+k+1}}X^{2(k+m+1)}\\
&\quad - 2\sum_{j=0}^{m}\frac{(-1)^{m-j}(\frac{1}{2})_{m+j+1}}{(m-j)!(2j+1)!}\sum_{k=0}^{\infty}\frac{(2k)!}{k!(\frac{3}{2})_k}X^{2(k-j)}\\
&= 2\sum_{k=m+1}^{\infty}\frac{(2k-1)!}{(k-m-1)!(\frac{3}{2})_{m+k}}X^{2k}\\
&\quad - 2\sum_{k=-m}^{\infty}\left[\sum_{j=\max\{0,-k\}}^{m}\frac{(-1)^{m-j}(\frac{1}{2})_{m+j+1}(2k+2j)!}{(m-j)!(2j+1)!(k+j)!(\frac{3}{2})_{k+j}}\right]X^{2k}.
\end{aligned}$$

For $k \geq 0$ the coefficient of X^{2k} in the first sum is

$$\begin{aligned}
&2\sum_{j=0}^{m}\frac{(-1)^{m-j}(\frac{1}{2})_{m+j+1}(2k+2j)!}{(m-j)!(2j+1)!(k+j)!(\frac{3}{2})_{k+j}}\\
&= 2\frac{(-1)^m(\frac{1}{2})_{m+1}(2k)!}{m!k!(\frac{3}{2})_k}\sum_{j=0}^{m}\frac{(-m)_j(m+\frac{3}{2})_j(k+\frac{1}{2})_j}{j!(\frac{3}{2})_j(k+\frac{3}{2})_j}\\
&= 2\frac{(-1)^m(\frac{1}{2})_{m+1}(2k)!}{m!k!(\frac{3}{2})_k}\,{}_3\mathrm{F}_2\left[\begin{matrix}-m, m+\frac{3}{2}, k+\frac{1}{2};\\ \frac{3}{2}, k+\frac{3}{2};\end{matrix}\,1\right]\\
&= 2\frac{(-1)^m(\frac{1}{2})_{m+1}(2k)!}{m!k!(\frac{3}{2})_k}\times\frac{(-m)_m(-k+1)_m}{(\frac{3}{2})_m(-m-k-\frac{1}{2})_m} = \frac{2(2k-1)!}{(k-m-1)!(\frac{3}{2})_{k+m}},
\end{aligned}$$

perfectly matching the coefficient of X^{2k+1} in the second sum. We deduce that also $\mathcal{K}_{2m+1} - \mathrm{P}_{2m+1}(z)\mathcal{K}_0(z)$ is a polynomial. The proof of (2.2) is thus complete. □

Theorem 3 *Let γ be an arbitrary closed curve in $\Omega \setminus [-1,1]$, circling the origin with winding number 1. Then*

$$\hat{f}_m = \frac{c_m}{2\pi\mathrm{i}}\int_\gamma \frac{f(z)}{z^{m+1}}\varphi_m(z)\,\mathrm{d}z, \qquad m \in \mathbb{Z}_+. \tag{2.4}$$

Proof Because of (2.2), substituting the explicit form of $\mathcal{K}_0$ (cf. (2.1)) into the integral, we have

$$\begin{aligned}
\frac{c_m}{2\pi\mathrm{i}}\int_\gamma \frac{f(z)}{z^{m+1}}\varphi_m(z)\,\mathrm{d}z &= -\frac{2m+1}{2\pi\mathrm{i}}\int_\gamma f(z)\mathcal{K}_m(z)\,\mathrm{d}z\\
&= -\frac{2m+1}{2\pi\mathrm{i}}\int_\gamma f(z)[\mathrm{P}_m(z)\mathcal{K}_0(z)+q_n(z)]\,\mathrm{d}z\\
&= \frac{m+\frac{1}{2}}{2\pi\mathrm{i}}\int_\gamma f(z)\mathrm{P}_m(x)\log\frac{z+1}{z-1}\,\mathrm{d}z,
\end{aligned}$$

because $\int_\gamma f(z)q_n(z)\,\mathrm{d}z = 0$ for analytic f and polynomial q_n. However, for any function g analytic in Ω

$$\frac{1}{2\pi\mathrm{i}}\int_\gamma g(z)\log\frac{z+1}{z-1}\,\mathrm{d}z = \int_{-1}^{1} g(x)\,\mathrm{d}x$$

(Trefethen 2008), thus we deduce that

$$\frac{c_m}{2\pi\mathrm{i}}\int_\gamma \frac{f(z)}{z^{m+1}}\varphi_m(z)\,\mathrm{d}z = (m+\tfrac{1}{2})\int_{-1}^{1} f(x)\mathrm{P}_m(x)\,\mathrm{d}x = \hat{f}_m,$$

as asserted in (2.4). □

The method of proof of the theorem indicates that $\mathcal{K}_m$ is, up to rescaling, nothing else but $\mathrm{P}_m \log\frac{z+1}{z-1}$, plus a polynomial which makes no difference to the integral. This might lead us to consider the computation of

$$\hat{f}_m = \frac{m+\frac{1}{2}}{2\pi\mathrm{i}}\int_\gamma f(z)\mathrm{P}_m(z)\log\frac{z+1}{z-1}\,\mathrm{d}z, \qquad m\in\mathbb{Z}_+, \tag{2.5}$$

in place of (2.4). An added attraction of (2.5) is that, replacing $(m+\frac{1}{2})\mathrm{P}_m$ therein by other orthogonal polynomials, this approach might lead to a more general methodology, applicable to other orthogonal polynomial systems. Unfortunately, this idea does not lead anywhere.

Fig. 2.1 displays the functions $\mathrm{P}_{20}(z)\log\frac{z+1}{z-1}$ and $\varphi_{20}(z)$ on the circle $|z|=2$. The first function oscillates rapidly – this is not surprising since the Argument Principle implies that P_m winds m times along the circle $|z|=r>1$. This indicates that the calculation of the integral for large values of m is likely to be problematic. The second function, however, does not appear to be oscillatory at all, and this makes it much more amenable for quadrature.

Most importantly, while it is not clear at all how to compute $\int_\gamma f(z)\mathrm{P}_m(z)\log\frac{z+1}{z-1}\,\mathrm{d}z$ rapidly with the FFT, we demonstrate in the next section that, subject to further work, this can be accomplished for (2.4).

2.3 An interpretation in terms of Legendre functions of the second kind

Both formula (2.4) and the representation (2.2) can be interpreted in terms of *Legendre functions of the second kind* Q_ν (Abramowitz & Stegun 1964, p. 332). Such functions are solutions of Legendre's equations valid in the plane cut along the real axis from $+1$ to $-\infty$ (Whittaker & Watson 1902, p. 316). In particular, for integer parameters the *Neumann representation* holds,

$$\mathrm{Q}_m(z) = \tfrac{1}{2}\int_{-1}^{1}\frac{\mathrm{P}_m(x)}{z-x}\,\mathrm{d}x, \qquad m\in\mathbb{Z}_+$$

(Whittaker & Watson 1902, p. 320). Legendre coefficients can be expressed explicitly in terms of integrals with Legendre functions of the second kind,

$$\hat{f}_m = \frac{2m+1}{2\pi\mathrm{i}}\int_\gamma f(z)\mathrm{Q}_m(z)\,\mathrm{d}z, \qquad m\in\mathbb{Z}_+ \tag{2.6}$$

(Whittaker & Watson 1902, p. 322). Since both (2.4) and (2.6) are valid for all analytic f, it follows that

$$\mathrm{Q}_m(z) = \frac{c_m}{2m+1}\frac{\varphi_m(z)}{z^{m+1}}, \qquad m\in\mathbb{Z}_+ \tag{2.7}$$

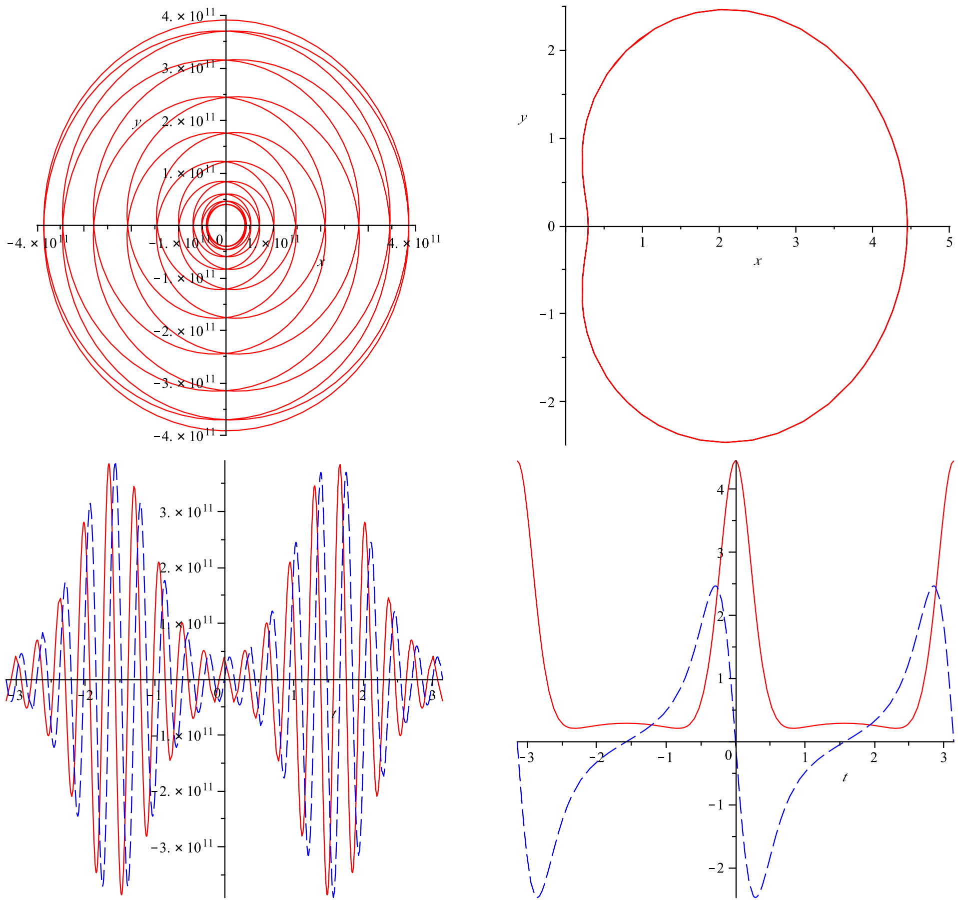

Figure 2.1: The plots of $\mathrm{P}_{20}(2\mathrm{e}^{\mathrm{i}\theta})\log\frac{2\mathrm{e}^{\mathrm{i}\theta}+1}{2\mathrm{e}^{\mathrm{i}\theta}-1}$ (on the left) and $\varphi_{20}(2\mathrm{e}^{\mathrm{i}\theta})$, $\theta\in[-\pi,\pi]$ in the complex plane (upper row) and their real (solid line) and imaginary (dashed line) parts.

is nothing else but our function $\mathcal{K}_m$! Note that this expression of Legendre functions of the second kind in hypergeometric form appears to be new. [2] Moreover,

$$\mathrm{Q}_m(z)=\tfrac{1}{2}\mathrm{P}_m(z)\log\frac{1+z}{1-z}+\sum_{k=0}^{\lfloor (m-1)/2\rfloor}\frac{2k-4k-1}{(2k+1)(m-k)}\mathrm{P}_{m-2k-1}(z)$$

(Abramowitz & Stegun 1964, p. 334), which confirms (2.2).

[2] Cf. the page `/HypergeometricFunctions/LegendreQGeneral/26/01/01/` on the `http://functions.wolfram.com` website for seven assorted – yet different – expressions of Q_ν in hypergeometric form, all lacking relevance for our purpose.

3 A hypergeometric transformation and a numerical algorithm

3.1 The integral formula and FFT

The formula (2.4) can *in principle* be approximated by DFT, lending itself to calculation with FFT. Thus, let

$$\varphi_m(z) = \sum_{j=0}^{\infty} \frac{h_{m,j}}{z^{2j}}, \qquad \text{where} \qquad h_{m,j} = \frac{(\frac{m+1}{2})_j(\frac{m+2}{2})_j}{j!(m+\frac{3}{2})_j}, \qquad j,m \in \mathbb{Z}_+.$$

By virtue of the analyticity of f and φ_m, (2.4) is equivalent to

$$\hat{f}_m = \frac{c_m}{2\pi\mathrm{i}} \sum_{j=0}^{\infty} h_{m,j} \int_\gamma \frac{f(z)}{z^{m+2j+1}}\,\mathrm{d}z, \qquad m \in \mathbb{Z}_+,$$

and this can be approximated by truncating the infinite series,

$$\hat{f}_m = \frac{c_m}{2\pi\mathrm{i}} \sum_{j=0}^{M} h_{m,j} \int_\gamma \frac{f(z)}{z^{m+2j+1}}\,\mathrm{d}z, \qquad m \in \mathbb{Z}_+,$$

for sufficiently large $M \in \mathbb{N}$. (Note that this procedure is nothing else but truncating the expansion (1.3) and evaluating derivatives by Cauchy integrals.) This can be approximated by DFT, considering a circular countour $|z| = r^{-1}$, where $r \in (0,1)$. The outcome is

$$\hat{f}_m \approx c_m r^m \sum_{j=0}^{M} h_{m,j} r^{2j} \frac{1}{N} \sum_{k=0}^{N-1} f(r^{-1}\omega_N^k)\omega_N^{k(m+2j)}, \tag{3.1}$$

where $\omega_N = \exp\frac{2\pi\mathrm{i}}{N}$ and $N \in \mathbb{N}$ is a sufficiently large composite integer. Let

$$\sigma_{N,m} = \frac{1}{N} \sum_{k=0}^{N-1} f(r^{-1}\omega_N^k)\omega_N^{km}, \qquad m = 0,1,\ldots,N-1.$$

Then (3.1) yields

$$\hat{f}_m \approx c_m r^m \sum_{j=0}^{M} h_{m,j} r^{2j} \sigma_{N,m+2j}, \qquad m = 0,1,\ldots,N-1-2M.$$

The overall cost of this procedure is $\mathcal{O}(N\log) + \mathcal{O}(MN)$ and everything hinges upon our choice of M. As long as the Taylor expansion of φ_m decays rapidly, we may choose small M – ideally either $M = \mathcal{O}(1)$ or, at most, $M = \mathcal{O}(\log N)$. This, unfortunately, is not the case.

Fig. 3.1 displays the order of magnitude (in decimal digits) of $r^{-2j}h_{m,j}$ for three different values of m. Thus, for $m = 10$, to attain accuracy of 20 decimal digits, we require $M = 61$. This increases to $M = 120$ for $m = 100$ and to $M = 295$ for $m = 400$. Worse, since the $r^{-2j}h_{m,j}$ tend first to increase, before asymptotic decrease sets in, we need about 43 decimal digits to calculate $\hat{f}_{400}$ to 20 significant digits. This is a clear nonstarter!

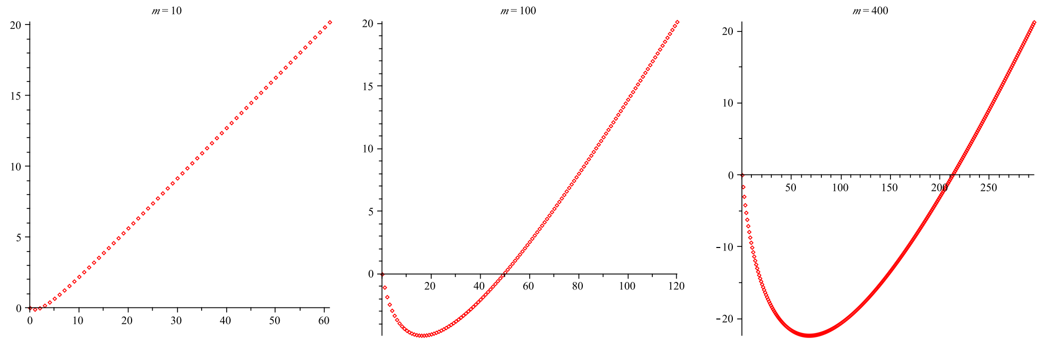

Figure 3.1: $-\log_{10}(r^{-2j}h_{m,j})$ for $r=\frac{3}{2}$ and different values of m.

3.2 A hypergeometric transformation

With many mathematical constructs the underlying problem is scarcity of information. Insofar as hypergeometric functions are concerned, the problem is arguably of an information glut. The Wolfram Research website `http://functions.wolfram.com` has 111951 different formulæ for the ${}_2\mathrm{F}_1$ functions: 111950 of those are not very helpful to the task in hand. Fortunately, the one designated

`HypergeometricFunctions/Hypergeometric2F1/16/01/01/0004/`

therein, can be used to transform the integrand into considerably more tractable form.

Thus, let $a,b,c\in\mathbb{C}$ be given, where c is neither zero nor negative integer, and suppose that $\zeta\in\mathbb{C}$, $\mathrm{Re}\,\zeta<1$. Then

$$ {}_2\mathrm{F}_1\left[\begin{array}{l} a, a+\frac{1}{2};\\ c;\end{array} 2\zeta-\zeta^2\right]=(1-\tfrac{1}{2}\zeta)^{-2a}{}_2\mathrm{F}_1\left[\begin{array}{l} 2a, 2a-c+1;\\ c;\end{array} \frac{\zeta}{2-\zeta}\right]. \tag{3.2}$$

We set $a=\frac{m+1}{2}$, $c=m+\frac{3}{2}$, whereby (3.2) yields

$$ {}_2\mathrm{F}_1\left[\begin{array}{l} \frac{m+1}{2},\frac{m+2}{2};\\ m+\frac{3}{2};\end{array} 2\zeta-\zeta^2\right]=\frac{1}{(1-\frac{1}{2}\zeta)^{n+1}}{}_2\mathrm{F}_1\left[\begin{array}{l} m+1,\frac{1}{2};\\ m+\frac{3}{2};\end{array} \frac{\zeta}{2-\zeta}\right].$$

Note that

$$ {}_2\mathrm{F}_1\left[\begin{array}{l} m+1,\frac{1}{2};\\ m+\frac{3}{2};\end{array} z\right]=\sum_{j=0}^{\infty} g_{m,j}z^j, \qquad \text{where} \qquad g_{m,j}=\frac{(m+1)_j(\frac{1}{2})_j}{j!(m+\frac{3}{2})_j}\in(0,1).$$

Therefore the hypergeometric function on the right converges rapidly for small $|\zeta/(2-\zeta)|$.

Let $r\in(0,1)$. We choose a negatively-oriented *Bernstein ellipse*, namely the contour

$$\{z=\tfrac{1}{2}(r^{-1}\mathrm{e}^{-\mathrm{i}\theta}+r\mathrm{e}^{\mathrm{i}\theta})\,:\,\theta\in[-\pi,\pi]\}.$$

Requiring $2\zeta-\zeta^2=z^{-2}$ results in

$$\zeta=\frac{2r\mathrm{e}^{\mathrm{i}\theta}}{r^{-1}\mathrm{e}^{-\mathrm{i}\theta}+r\mathrm{e}^{\mathrm{i}\theta}}, \qquad \frac{\zeta}{2-\zeta}=r^2\mathrm{e}^{2\mathrm{i}\theta}, \qquad \frac{1}{1-\frac{1}{2}\zeta}=r\mathrm{e}^{\mathrm{i}\theta}(r^{-1}\mathrm{e}^{-\mathrm{i}\theta}+r\mathrm{e}^{\mathrm{i}\theta}),$$

therefore, by serendipitous cancellation,

$$\frac{1}{z^{m+1}}\varphi_m(z) = 2^{m+1}r^{m+1}\mathrm{e}^{\mathrm{i}(m+1)\theta}{}_2\mathrm{F}_1\left[\begin{array}{c} m+1, \frac{1}{2}; \\ m+\frac{3}{2}; \end{array} r^2\mathrm{e}^{2\mathrm{i}\theta}\right].$$

Since

$$\mathrm{d}z = -\tfrac{1}{2}\mathrm{i}r^{-1}\mathrm{e}^{-\mathrm{i}\theta}(1-r^2\mathrm{e}^{2\mathrm{i}\theta})\,\mathrm{d}\theta,$$

we deduce from (2.4) that

$$\hat{f}_m = \frac{\tilde{c}_m r^m}{2\pi}\int_{-\pi}^{\pi}(1-r^2\mathrm{e}^{2\mathrm{i}\theta})f(\tfrac{1}{2}(r^{-1}\mathrm{e}^{-\mathrm{i}\theta}+r\mathrm{e}^{\mathrm{i}\theta}))_2\mathrm{F}_1\left[\begin{array}{c} m+1, \frac{1}{2}; \\ m+\frac{3}{2}; \end{array} r^2\mathrm{e}^{2\mathrm{i}\theta}\right]\mathrm{e}^{\mathrm{i}m\theta}\,\mathrm{d}\theta, \quad (3.3)$$

where

$$\tilde{c}_m = 2^m c_m = \frac{2^{2m}(m!)^2}{(2m)!}, \qquad m \in \mathbb{Z}_+.$$

3.3 A Fast Legendre Transform

We proceed as in Subsection 3.1, truncating the Taylor expansion of an ${}_2\mathrm{F}_1$ function, except that our starting point is the formula (3.3). Thus, let N be a suitably large composite integer and

$$\kappa_{N,m} = \frac{1}{N}\sum_{k=0}^{N-1}(1-r^2\omega_N^{2k})f(\tfrac{1}{2}(r^{-1}\omega_N^{-k}+r\omega_N^k))\omega_N^{mk}, \qquad m=0,1,\ldots,N-1 \quad (3.4)$$

be the DFT of the sequence

$$\{(1-r^2\omega_N^{2k})f(\tfrac{1}{2}(r^{-1}\omega_N^{-k}+r\omega_N^k)) \,:\, k=0,\ldots,N-1\}.$$

We approximate (3.3), replacing the hypergeometric function by its truncated Taylor expansion and the integral by DFT, whence

$$\begin{aligned}\hat{f}_m &\approx \frac{\tilde{c}_m}{2\pi}\sum_{j=0}^{M} g_{m,j}r^{m+2j}\frac{1}{2\pi}\int_{-\pi}^{\pi}(1-r^2\mathrm{e}^{2\mathrm{i}\theta})f(\tfrac{1}{2}(r^{-1}\mathrm{e}^{-\mathrm{i}\theta}+r\mathrm{e}^{\mathrm{i}\theta}))\mathrm{e}^{\mathrm{i}(m+2j)\theta}\,\mathrm{d}\theta \\ &\approx \tilde{c}_m\sum_{j=0}^{M} g_{m,j}r^{m+2j}\frac{1}{N}\sum_{k=0}^{N-1}(1-r^2\omega_N^{2k})f(\tfrac{1}{2}(r^{-1}\omega_N^{-k}+r\omega_N^k))\omega_N^{(m+2j)k} \\ &= \sum_{j=0}^{M}\tilde{g}_{m,j}(r)\kappa_{N,m+2j}, \qquad m=0,1,\ldots,N-1-2M, \end{aligned} \quad (3.5)$$

where

$$\tilde{g}_{m,j}(r) = \tilde{c}_m g_{m,j}r^{m+2j} = \frac{2^{2m}(m!)^2(m+1)_j(\frac{1}{2})_j}{(2m)!j!(m+\frac{3}{2})_j}r^{m+2j}, \qquad m\in\mathbb{Z}_+, \quad j=0,\ldots,M.$$

Note that the $\tilde{g}_{m,j}$s can be obtained by recursion in $\mathcal{O}(MN)$ operations,

$$\left.\begin{aligned}&\tilde{g}_{0,0}=1, \qquad \tilde{g}_{m,0}=\frac{mr}{m-\frac{1}{2}}\tilde{g}_{m-1,0},\\ &\tilde{g}_{m,j}=\frac{(m+j)(j-\frac{1}{2})r^2}{j(m+j+\frac{1}{2})}\tilde{g}_{m,j-1}, \quad j=1,2,\ldots,M,\end{aligned}\right\} \qquad m=1,2,\ldots,N-1-2M.$$

Since (3.4) can be accomplished with FFT in $\mathcal{O}(N\log N)$ operations, while both (3.5) and the computation of the $\tilde{g}_{g,j}$s bear the price tag of $\mathcal{O}(MN)$ flops, the basic requirement is that M is small – ideally, $M=\mathcal{O}(1)$, but even with $M=\mathcal{O}(\log N)$ we still have an $\mathcal{O}(N\log N)$ algorithm.

The main approximation step consists of replacing infinite series with its truncated Taylor series. Let $\|f\|_\infty$ be the maximum of $|f|$ on the ellipse. The discarded tail can be bounded with ease,

$$\begin{aligned}T_{M,m} &:= \left|\tilde{c}_m \sum_{j=M+1}^{\infty} g_{m,j} r^{m+2j}\frac{1}{2\pi}\int_{-\pi}^{\pi}(1-r^2\mathrm{e}^{2\mathrm{i}\theta})f(\tfrac{1}{2}(r^{-1}\mathrm{e}^{-2\mathrm{i}\theta}+r\mathrm{e}^{\mathrm{i}\theta}))\mathrm{e}^{\mathrm{i}(m+2j)\theta}\,\mathrm{d}\theta\right|\\ &\le \tilde{c}_m(1+r^2)\|f\|_\infty\sum_{j=M+1}^{\infty}|g|_{m,j}r^{m+2j} \le \tilde{c}_m\frac{1+r^2}{1-r^2}\|f\|_\infty r^{m+2M+2},\end{aligned}$$

because $|g_{m,j}|\le 1$. It is trivial to prove with the Stirling formula (Abramowitz & Stegun 1964, p. 257) that

$$(\pi m)^{\frac{1}{2}} \le \tilde{c}_m \le 2m^{\frac{1}{2}}, \qquad m=1,2,\ldots.$$

Therefore

$$|T_{M,m}| \le \max\{1,2m^{\frac{1}{2}}\}\frac{1+r^2}{1-r^2}\|f\|_\infty r^{m+2M+2}, \qquad m=0,1,\ldots,N-2M-1.$$

The function $x^{\frac{1}{2}}r^x$ reaches its maximum for $x>0$ at $x_{\max}=(-2\log r)^{-1}$, where it equals $\mathrm{e}^{-\frac{1}{2}}(-2\log r)^{-\frac{1}{2}}$. Therefore we obtain the uniform bound

$$|T_{M,m}| \le \max\left\{1,\mathrm{e}^{-\frac{1}{2}}\left(-\frac{2}{\log r}\right)^{\frac{1}{2}}\right\}\frac{1+r^2}{1-r^2}\|f\|_\infty r^{2M+2}.$$

It follows that, in order to restrict the magnitude of the tail uniformly below given tolerance $\delta>0$, it is enough to choose

$$M \ge \frac{1}{2}\frac{\log\max\left\{1,\mathrm{e}^{-\frac{1}{2}}\left(-\frac{2}{\log r}\right)^{\frac{1}{2}}\right\}+\log\frac{1+r^2}{1-r^2}+\log\|f\|_\infty-\log\delta}{-\log r}-1. \tag{3.6}$$

The bound (3.6) depends just on the tolerance $\delta>0$, the size of $|f|$ on the ellipse and the parameter $r\in(0,1)$: clearly, our lower bound on M becomes large the nearer r is to 1. It is however independent of N and we deduce that $M=\mathcal{O}(1)$: our algorithm is truly $\mathcal{O}(N\log N)$.

It is important to emphasize (a point which we reiterate in the next section) that the bound (3.6) typically vastly overestimates the least value of M required to produce the coefficients to given accuracy. Its sole role is in establishing the cost of the algorithm and it should not be used as a practical means for choosing M.

3.4 Betwixt Legendre and Chebyshev

An obvious question is what happens once we allow $r=1$ in (3.3). The outcome,

$$\hat{f}_m = \frac{\tilde{c}_m}{2\pi}\int_{-\pi}^{\pi}(1-\mathrm{e}^{2\mathrm{i}\theta})f(\cos\theta){}_2\mathrm{F}_1\left[\begin{matrix} m+1,\frac12;\\ m+\frac32;\end{matrix}\,\mathrm{e}^{2\mathrm{i}\theta}\right]\mathrm{e}^{\mathrm{i}m\theta}\,\mathrm{d}\theta \tag{3.7}$$

$$= \frac{\tilde{c}_m}{2\pi}\int_{-\pi}^{\pi}(1-\mathrm{e}^{2\mathrm{i}\theta})f(\cos\theta)\psi_m(\mathrm{e}^{2\mathrm{i}\theta})\mathrm{e}^{\mathrm{i}m\theta}\,\mathrm{d}\theta, \quad \text{where} \quad \psi_m(z) = {}_2\mathrm{F}_1\left[\begin{matrix} m+1,\frac12;\\ m+\frac32;\end{matrix}\,z\right],$$

can be used to design an alternative to algorithm (3.5), but first we need to consider the convergence of the integral in (3.7). It follows from (2.1) that

$$\psi_0(z) = \tfrac12 z^{-1}\log\frac{1+z}{1-z}.$$

Moreover, $\varphi_m(z) = \mathrm{e}^{\mathrm{i}m\theta}\psi_m(\mathrm{e}^{2\mathrm{i}\theta})$. But $\psi_m(z) = (2m+1)c_m^{-1}z^{m+1}\mathcal{K}_m(z)$ and we deduce from (2.2) that the integrand of (3.7) has logarithmic singularity at $\theta=\pm\pi$. Such singularity is too weak to disrupt existence and boundedness of the integral (3.7) for analytic f and all $m\in\mathbb{Z}_+$.

We next replace ψ_m by its Taylor expansion and interchange integration and summation, whence

$$\hat{f}_m = \frac{\tilde{c}_m}{2\pi}\sum_{j=0}^{\infty} g_{m,j}\int_{-\pi}^{\pi} f(\cos\theta)(1-\mathrm{e}^{2\mathrm{i}\theta})\mathrm{e}^{\mathrm{i}(m+2j)\theta}\,\mathrm{d}\theta$$

$$= \tfrac12\tilde{c}_m\sum_{j=0}^{\infty} g_{m,j}(\check{f}_{m+2j}-\check{f}_{m+2j+2}), \qquad m\in\mathbb{Z}_+,$$

where

$$\check{f}_m = \frac{1}{\pi}\int_{-\pi}^{\pi} f(\cos\theta)\mathrm{e}^{\mathrm{i}m\theta}\,\mathrm{d}\theta, \qquad m\in\mathbb{Z}_+.$$

Note however that $f(\cos\theta)$ is an even function, therefore $\int_{-\pi}^{\pi} f(\cos\theta)\sin m\theta\,\mathrm{d}\theta = 0$ and

$$\check{f}_m = \frac{1}{\pi}\int_{-\pi}^{\pi} f(\cos\theta)\cos m\theta\,\mathrm{d}\theta, \qquad m\in\mathbb{Z}_+,$$

is the mth *Chebyshev coefficient* of f,

$$f(x) = \tfrac12\check{f}_0\mathrm{T}_0(x) + \sum_{m=1}^{\infty}\check{f}_m\mathrm{T}_m(x).$$

Let

$$\sigma_{N,m} = \frac{2}{N}\sum_{k=0}^{N-1} f(\cos\tfrac{2\pi k}{N})\cos\tfrac{2\pi km}{N}, \qquad m=0,\ldots,N-1,$$

be the Discrete Cosine Transform discretization of $\{\check{f}_m\}_{m=0}^{N-1}$. Analogously to (3.5), we deduce the approximation

$$\hat{f}_m \approx \tfrac12\tilde{c}_m\sum_{j=0}^{M}\tilde{g}_{m,j}(1)(\sigma_{N,m+2j}-\sigma_{N,m+2j+2}), \qquad j=0,1,\ldots,N-2M-3, \tag{3.8}$$

where the functions $\tilde{g}_{m,j}$ have been already defined in Subsection 3.3.

The algorithm (3.8), being restricted to $[-1,1]$, enjoys an important advantage over (3.5) when the function f has singularities near the interval.

The calculation of (3.8) requires $\mathcal{O}(N\log N)+\mathcal{O}(MN)$ operations. However, the analysis of Subsection 3.3 which led to the $\mathcal{O}(N\log N)$ cost of the algorithm (3.5) is no longer valid in the present setting. Instead, recalling that

$$\psi_m(z)=\sum_{j=0}^{\infty} g_{m,j}z^j, \qquad \text{where} \qquad |g_{m,j}|\le 1,$$

and, like in Subsection 3.3, denoting the tail by $T_{M,m}$, we observe that

$$\begin{aligned}
T_{M,m} &= \frac{\tilde{c}_m}{2\pi}\int_{-\pi}^{\pi} f(\cos\theta)(1-\mathrm{e}^{2\mathrm{i}\theta})\mathrm{e}^{\mathrm{i}m\theta}\sum_{j=M+1}^{\infty} g_{m,j}\mathrm{e}^{2\mathrm{i}j\theta}\,\mathrm{d}\theta\\
&= \frac{\tilde{c}_m}{2\pi}\sum_{j=M+1}^{\infty} g_{m,j}\int_{-\pi}^{\pi} f(\cos\theta)[\cos((m+2j)\theta)-\cos((m+2j+2)\theta)]\\
&= \tfrac{1}{2}\tilde{c}_m\sum_{j=M+1}^{\infty} g_{m,j}[\check{g}_{m+2j}-\check{f}_{m+2j+2}],
\end{aligned}$$

where we have used the parity of $f(\cos\theta)$. Therefore

$$|T_{M,m}|\le \tfrac{1}{2}\tilde{c}_m\sum_{j=M+1}^{\infty}(|\check{f}_{m+2j}|+|\check{f}_{m+2j+2}|). \tag{3.9}$$

Recall that f is analytic in an open set Ω such that $[-1,1]\subset\Omega$. Therefore there exist $d>0$ and $\alpha>0$ (whose size depends solely on the eccentircity of the largest Bernstein ellipse that can be fitted into Ω) such that $|\check{f}_k|\le d\mathrm{e}^{-\alpha k}$, $k\in\mathbb{Z}_+$. We thus deduce from (3.9) that

$$|T_{M,m}|\le \tfrac{1}{2}\tilde{c}_m d\frac{1+\mathrm{e}^{2\alpha}}{1-\mathrm{e}^{2\alpha}}\mathrm{e}^{-\alpha(m+2M+2)}, \qquad m,M\in\mathbb{Z}_+.$$

Recall from Subsection 3.3 that $(\pi m)^{\frac{1}{2}}\tilde{c}_m\le 2m^{\frac{1}{2}}$, $m\in\mathbb{Z}$. Therefore

$$\tilde{c}_m\mathrm{e}^{-\alpha m}\le \max\{1,2m^{\frac{1}{2}}\mathrm{e}^{-\alpha m}\}\le \max\left\{1,\frac{1}{(2\alpha\mathrm{e})^{\frac{1}{2}}}\right\}, \qquad m\in\mathbb{Z}_+,$$

where we have used the fact that $1/(2\alpha)>0$ is the global maximum of $x^{\frac{1}{2}}\mathrm{e}^{-\alpha x}$. We thus deduce that for every $M,m\in\mathbb{Z}_+$ the magnitude of the tail can be uniformly bounded by $\tilde{d}\mathrm{e}^{-2\alpha M}$, where $\tilde{d}\ge 0$ depends only upon the function f. We thus can, given tolerance $\delta>0$, choose $M\in\mathbb{Z}_+$ so that all the computed coefficients carry at most error δ, thereby deducing that the cost of the method is indeed $\mathcal{O}(N\log N)$.

The calculation of Chebyshev coefficients forms a central role in two existing algorithms for the computation of Legendre coefficients (Alpert & Rokhlin 1991, Potts et al. 1998). Yet, both the mathematical premise of these methods and their practice are different from (3.8).

4 Numerical examples and conclusions

4.1 Numerical examples

In Fig. 4.1 we display the number of significant decimal digits, once Legendre coefficients of the entire function $f(x) = \mathrm{e}^x$ are computed with the algorithm from Subsection 3.3. We have used $N = 512$ in all computations and the calculations have been carried out to 20 significant decimal digits.[3] Further numerical evidence for this function is exhibited in Table 1.

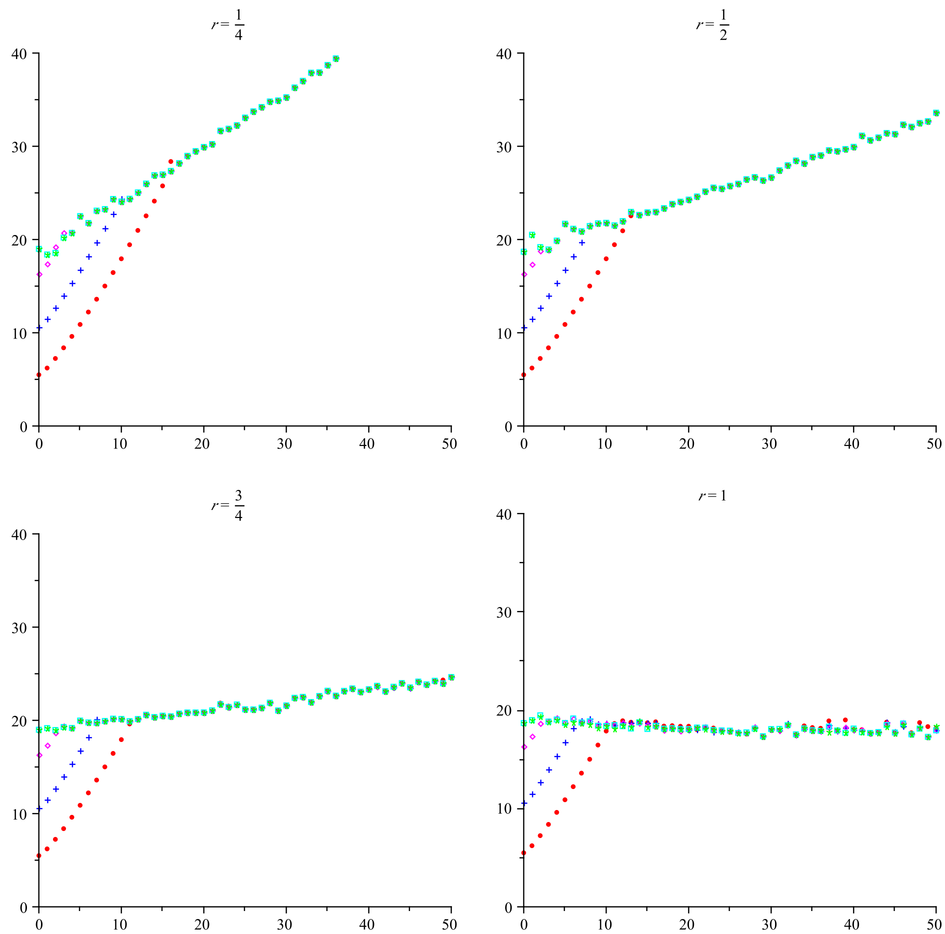

Figure 4.1: The number of significant digits recovered in computing $\hat{f}_m$, $m = 0, \ldots, 50$, for $f(x) = \mathrm{e}^x$ with $N = 512$ and different values of $r \in (0, 1)$: here • corresponds to $M = 2$, $+$ to $M = 4$, $\diamondsuit$ to $M = 6$, $\square$ to $M = 8$ and $*$ to $M = 10$.

[3]Except that, in order to calculate sufficiently reliable reference values of $\hat{f}_m$ by ordinary quadrature in MAPLE, we have been forced to use up to 200 significant digits.

Table 1: Absolute errors in computing $\hat{f}_m$ for $f(x) = \mathrm{e}^x$ and $m = 0, 10$.

$m = 0$	$M = 2$	$M = 4$	$M = 6$	$M = 8$	$M = 10$	$M = 12$
$r = \frac{1}{4}$	3.21_{-06}	2.50_{-11}	4.73_{-17}	1.00_{-19}	1.00_{-19}	1.00_{-19}
$r = \frac{1}{2}$	3.21_{-06}	2.50_{-11}	4.72_{-17}	2.00_{-19}	2.00_{-16}	2.00_{-19}
$r = \frac{3}{4}$	3.21_{-06}	2.50_{-11}	4.74_{-17}	1.70_{-19}	1.70_{-19}	1.70_{-19}
$r = 1$	3.21_{-06}	2.50_{-11}	4.74_{-17}	1.39_{-20}	1.20_{-20}	1.19_{-20}
$r = \frac{3}{4}$ (30 digits)	3.21_{-06}	2.50_{-11}	4.74_{-17}	1.76_{-20}	1.76_{-20}	1.76_{-20}
$r = \frac{3}{4}$ ($N = 256$)	3.21_{-06}	2.50_{-11}	4.70_{-17}	4.00_{-19}	4.00_{-19}	4.00_{-19}
$m = 10$	$M = 2$	$M = 4$	$M = 6$	$M = 8$	$M = 10$	$M = 12$
$r = \frac{1}{4}$	1.16_{-18}	3.68_{-25}	8.23_{-25}	8.23_{-25}	8.23_{-25}	8.23_{-25}
$r = \frac{1}{2}$	1.16_{-18}	1.28_{-22}	1.28_{-22}	1.28_{-22}	1.28_{-22}	1.28_{-22}
$r = \frac{3}{4}$	1.16_{-18}	8.62_{-21}	8.77_{-21}	8.80_{-21}	8.79_{-21}	8.79_{-21}
$r = 1$	1.33_{-18}	2.05_{-19}	2.27_{-19}	4.01_{-19}	4.18_{-19}	3.89_{-19}
$r = \frac{3}{4}$ (30 digits)	1.16_{-18}	4.58_{-25}	2.83_{-29}	2.84_{-25}	2.84_{-29}	2.84_{-29}
$r = \frac{3}{4}$ ($N = 256$)	1.16_{-18}	1.17_{-20}	1.20_{-20}	1.19_{-20}	1.19_{-20}	1.19_{-20}

Several observations are evident from both Fig 4.1 and Table 1.

1. For small values of m we need relatively large value of M in (3.5) to ensure that the error is suitably small.[4] Moreover, larger values of $r \in (0, 1]$ appear to produce better performance in this regime.

2. The picture changes completely for large m, when very good results can be obtained with small values of M – in fact, increasing M brings no benefit. Moreover, for $r \in (0, 1)$ accuracy goes on increasing geometrically with m, faster for *small* r. In all likelihood, this is caused by the term $\tilde{g}_{m,j}(r)$ in (3.5), which scales like r^{m+2j}.

3. The choice $r = 1$, whereby the Bernstein ellipse 'collapses' to $[-1, 1]$, seems to produce small uniform error and is competitive with $r \in (0, 1)$.

4. There are three possible sources of error in our algorithm: (a) replacing integrals by DFT, (b) truncating the ${}_2\mathrm{F}_1$ function, and (c) finite accuracy of floating-point arithmetic. The first source of error is quantified by N, the second by M and the last by the number of significant digits (or the "machine epsilon"). In Table 1 we have displayed the error for $r = \frac{3}{4}$ also when 30 decimal digits have been used. A comparison with the third row (which corresponds to the same r with just 20 significant digits) is instructive. For $m = 0$ the outcome is fairly similar: increasing computer accuracy does not improve

[4]Yet, these values are *much* smaller than those in inequality (3.6)!

the algorithm while increasing M definitely does! However, the picture changes for $m = 10$. For $M = 2$ the results are identical, but taking $M \geq 4$ increased computer accuracy definitely improves performance for $m = 10$. On the other hand, once we replace $N = 512$ with $N = 256$, another result reported in the table, the errors do not change significantly.

The conclusion we draw is that the number of points N used in DFT need not to be unduly large unless the function f itself changes rapidly. What matters is the size of M for small m, while for large m we are restricted by computer accuracy. Moreover, although small $r \in (0,1)$ produces superior error for large m, uniform error is smaller for large $r \in (0,1]$.

An obvious tweak to the algorithm (3.5) is to allow M to depend upon m. Thus, for small m we use larger M but allow M to be smaller for large m. Specifically, revisiting the error analysis in Subsection 3.3 while keeping $\tilde{c}_m$ intact results in an m-dependent choice of M, namely

$$M_m \geq \frac{1}{2}\frac{\log\tilde{c}_m + \log\frac{1+r^2}{1-r^2} + \log\|f\|_\infty - \log\delta}{-\log r} - 1 - \frac{1}{2}m, \qquad m \in \mathbb{Z}_+. \tag{4.1}$$

However, checking again the performance of the algorithm, we conclude that the upper bound (4.1) is so pessimistic as to be practically useless. Thus, in our case, letting $\delta = 10^{-19}$ and $r = \frac{3}{4}$ results in $M_0 = 79$ and $M_{10} = 77$, while an error consistent with tolerance δ is obtained in actual computation already with $M = 7$ for $m = 0$ and $M = 3$ for $m = 10$. (Note that the purpose of the bound (3.6) was to argue that the algorithm (3.5) is $\mathcal{O}(N\log N)$, rather than to offer a realistic choice of M.)

Our next example is the rational function $f(x) = (1+x)/(4+x^2)$, with poles at $\pm 2\mathrm{i}$. Thus, we need $r > r_{\min} = \sqrt{5} - 2 \approx 0.2361$ to keep the ellipse within domain of analyticity of f.

The conclusions from Fig 4.2 and Table 2 are fully consistent with the experience that we have already acquired in this section, except for the predictable observation that choosing $r = \frac{1}{4}$, dangerously near $r_{\min}$, leads to significant degradation in performance – in particular, the improvement in accuracy stalls for $M = 8$. This does not represent significant hardship because a conclusion from our both examples is that it is good strategy to take larger values of $r \in (0,1]$.

4.2 Brief conclusions

In this paper we have presented a fast (that is, $\mathcal{O}(N\log N)$) algorithm for the calculation of the coefficients of an expansion in Legendre polynomials. Although the mathematical rationale for the algorithm might appear to be fairly convoluted and perhaps counter-intuitive, the algorithm itself is exceedingly simple, requiring just a single FFT, followed by an $\mathcal{O}(N)$ post-processing.

Preliminary numerical results reported above are not intended to represent comprehensive experimentation with the algorithm, just an initial indication that it works, does so in a stable manner and that there are no hidden perils associated with it. They also allow us to sketch, albeit in a tentative fashion, ideas for the implementation of the algorithm with uniform precision. Thus, we recommend taking large $r \in (0,1]$, perhaps $r = 1$ (a choice which is more robust in the presence of singularities of f near the critical interval $[-1,1]$) and vary the size

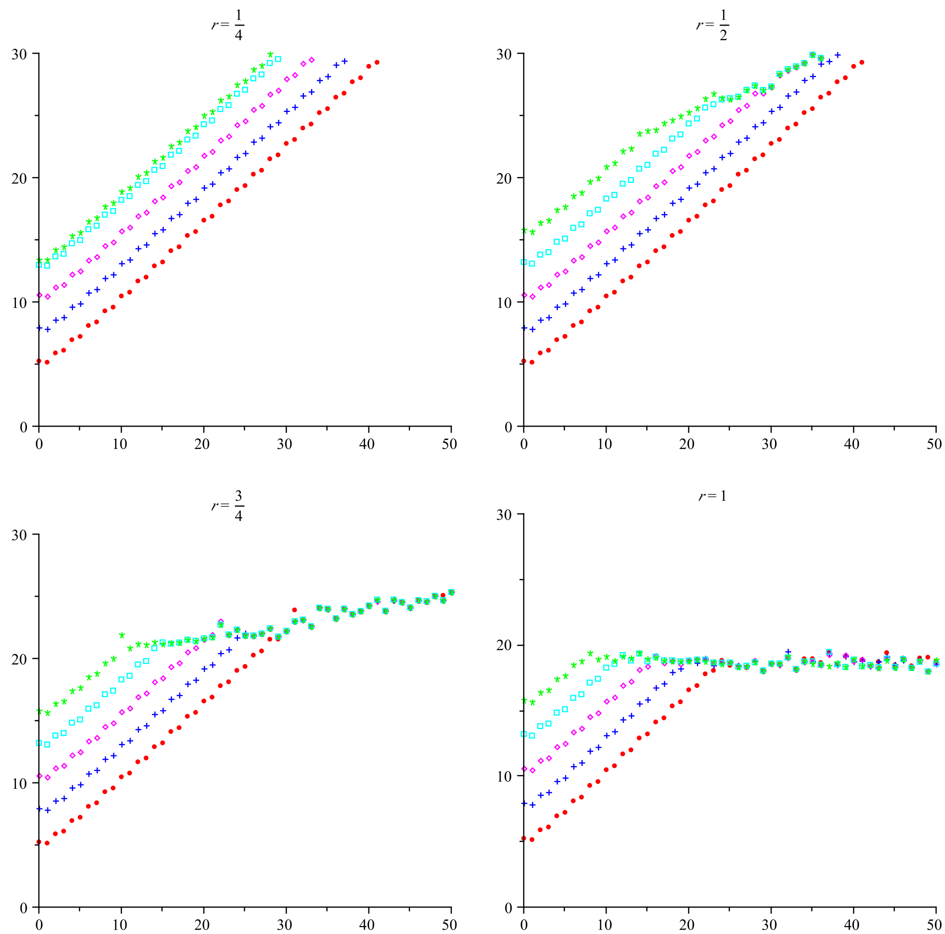

Figure 4.2: The same as Fig. 4.1, except for $f(x) = (1+x)/(4+x^2)$.

of M for different ms: for small m we take larger M but allow the latter to decrease, even down to $M = 0$, for large ms. A good working strategy for the choice of reasonable M for each m is a matter for future research.

A natural question is whether our approach generalises to other orthogonal polynomial systems. This is a subject of ongoing research.

Acknowledgements

I wish to thank a number of colleagues, some for discussions leading toward this paper and others for comments on its draft: Marissa Condon (Dublin), Alfredo Deaño (Madrid), Anders Hansen (Cambridge), Sheehan Olver (Oxford), Jennifer Ryan (Delft) and Nick Trefethen (Ox-

Table 2: Absolute errors in computing $\hat{f}_m$ for $f(x) = (1+x)/(4+x^2)$ and $m = 0, 10$.

$m = 0$	$M = 2$	$M = 4$	$M = 6$	$M = 8$	$M = 10$	$M = 12$
$r = \frac{1}{4}$	5.59_{-06}	1.10_{-08}	2.51_{-11}	1.03_{-13}	4.14_{-14}	4.12_{-14}
$r = \frac{1}{2}$	5.59_{-06}	1.10_{-08}	2.50_{-11}	6.13_{-14}	1.57_{-16}	4.80_{-19}
$r = \frac{3}{4}$	5.59_{-06}	1.10_{-08}	2.50_{-11}	6.13_{-14}	1.57_{-16}	4.70_{-19}
$r = 1$	5.59_{-06}	1.10_{-08}	2.50_{-11}	6.13_{-14}	1.57_{-16}	4.60_{-19}
$r = \frac{3}{4}$ (30 digits)	5.59_{-06}	1.10_{-08}	2.50_{-11}	6.13_{-14}	1.57_{-16}	4.13_{-19}
$r = \frac{3}{4}$ ($N = 256$)	5.59_{-06}	1.10_{-08}	2.50_{-11}	6.31_{-14}	1.57_{-16}	4.10_{-19}

$m = 10$	$M = 2$	$M = 4$	$M = 6$	$M = 8$	$M = 10$	$M = 12$
$r = \frac{1}{4}$	3.29_{-11}	7.50_{-14}	1.87_{-16}	6.10_{-19}	1.26_{-19}	1.25_{-19}
$r = \frac{1}{2}$	3.29_{-11}	7.50_{-14}	1.87_{-16}	4.86_{-19}	1.29_{-21}	9.20_{-24}
$r = \frac{3}{4}$	3.29_{-11}	7.50_{-14}	1.86_{-16}	4.85_{-19}	6.36_{-22}	1.33_{-21}
$r = 1$	3.29_{-11}	7.50_{-14}	1.87_{-16}	5.30_{-19}	6.63_{-20}	6.31_{-20}
$r = \frac{3}{4}$ (30 digits)	3.29_{-11}	7.50_{-14}	1.86_{-16}	4.86_{-19}	1.30_{-21}	3.57_{-24}
$r = \frac{3}{4}$ ($N = 256$)	3.29_{-11}	7.50_{-14}	1.86_{-16}	4.86_{-19}	3.08_{-21}	2.41_{-21}

ford).

References

Abramowitz, M. & Stegun, I. A., eds (1964), *Handbook of Mathematical Functions*, National Bureau of Standards, Washington, DC.

Alpert, B. K. & Rokhlin, V. (1991), 'A fast algorithm for the evaluation of Legendre expansions', *SIAM J. Sci. Statist. Comput.* **12**, 158–179.

Bornemann, F. (2010), Accuracy and stability of computing high-order derivatives of analytic functions by Cauchy integrals, Technical report, Zentrum Mathematik, Technische Universität München.

Brunner, H., Iserles, A. & Nørsett, S. P. (2010), 'The spectral problem for highly oscillatory Fredholm operators', *J. Integral Eqn & Applcs.* (to appear).

Gauss, C. F. (1866), Nachlass, Theoria Interpolationis Methodo Nova Tractata, *in* 'Carl Friedrich Gauss Werke, Band 3', Königlichen Gesellschaft der Wissenschaften, Göttingen, pp. 265–330.

Huybrechs, D. & Olver, S. (2009), Highly oscillatory quadrature, *in* B. Engquist, A. Fokas, E. Hairer & A. Iserles, eds, 'Highly Oscillatory Problems', number 366 *in* 'London Mathematical Society Lecture Note Series', Cambridge University Press, Cambridge, chapter 2, pp. 25–50.

Legendre, A. M. (1817), *Exercices de Calcul Integral. Sur Divers Ordres de Transcendances et sur les Quadratures*, Courcier, Paris.

Potts, D., Steidl, G. & Tasche, M. (1998), 'Fast algorithms for discrete polynomial transforms', *Maths Comp.* **67**, 1577–1590.

Rainville, E. D. (1960), *Special Functions*, Macmillan, New York.

Trefethen, L. N. (2008), 'Is Gauss quadrature better than Clenshaw–Curtis?', *SIAM Review* **50**, 67–87.

Whittaker, E. T. & Watson, G. N. (1902), *A Course of Modern Analysis*, Cambridge University Press, Cambridge.