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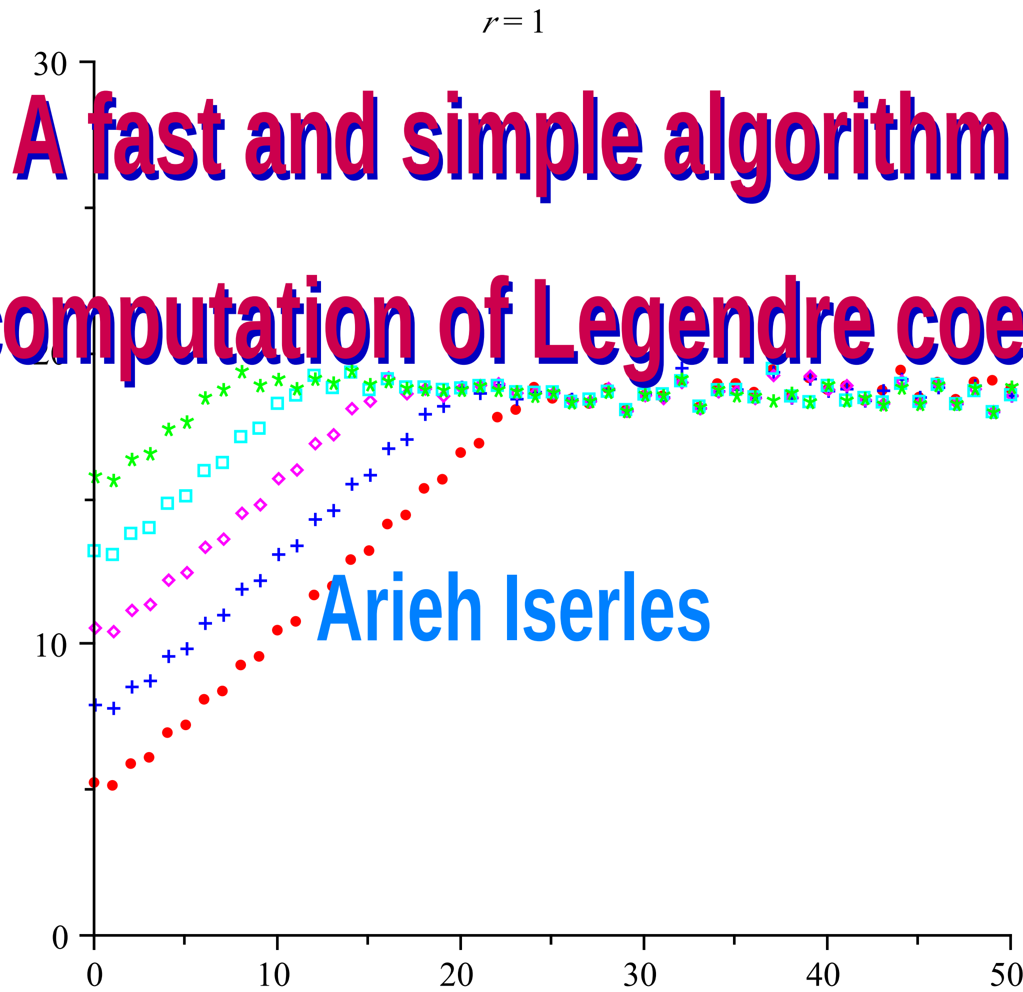
& THEORETICAL PHYSICS

A fast and simple algorithm for the computation of Legendre coefficients



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FAST ORTHOGONAL EXPANSIONS

Let $\mathrm{d}\mu$ be a Borel measure with an infinite number of points of increase, $\mathrm{supp}\ \mathrm{d}\mu = \Omega \subseteq \mathbb{C}$, and let $f \in \mathbb{H}$, the Hilbert space of functions bounded w.r.t. the norm induced by the inner product

$$\langle f, g \rangle = \int_\Omega f(x)\overline{g(x)}\,\mathrm{d}\mu(x).$$

Then

$$f \sim \sum_{m \in \mathcal{M}} \hat{f}_m \varphi_m \qquad \text{where} \qquad \hat{f}_m = \frac{\langle f, \varphi_m \rangle}{\langle \varphi_n, \varphi_n \rangle},$$

where $\{\varphi_m\}_{m \in \mathcal{M}}$ is an orthogonal basis of $\mathbb{H}$.

If $\Omega \subseteq \mathbb{R}$, $\mathrm{d}\mu(x) = w(x)\,\mathrm{d}x$, where $0 < w \in \mathrm{C}^\infty(\Omega)$, while $f \in \mathrm{C}^\infty(\Omega)$, then the convergence is spectral: faster than the reciprocal of any polynomial!

This explains the fundamental role of such expansions in approximation theory, signal processing and numerical analysis of PDEs.

Fourier expansions: $\Omega = \mathbb{T}$, $\mu(x) = x$, $\mathcal{M} = \mathbb{Z}$, $\varphi_m(x) = \mathrm{e}^{\mathrm{i}m\pi x}$.

$$\hat{f}_m \approx \frac{1}{N} \sum_{k=-N/2+1}^{N/2} f(\mathrm{e}^{2k\pi\mathrm{i}/N})\mathrm{e}^{2km\pi\mathrm{i}/N}, \qquad -N/2+1 \le m \le N/2,$$

(the Discrete Fourier Transform) has itself spectral accuracy and can be calculated using the Fast Fourier Transform in $\mathcal{O}(N \log N)$ operations.

Chebyshev expansions: $\Omega = (-1,1)$, $\mathrm{d}\mu(x) = \frac{\mathrm{d}x}{\sqrt{1-x^2}}$, $\mathcal{M} = \mathbb{Z}_+$, $\varphi_m(x) = \mathrm{T}_m(x)$. Changing variables,

$$\hat{f}_m = \frac{2}{\pi} \int_{-1}^{1} f(x)\mathrm{T}_m(x)\frac{\mathrm{d}x}{\sqrt{1-x^2}} = 2\int_{-1}^{1} f(\cos \pi t)\cos(m\pi t)\,\mathrm{d}t$$

(except that $\hat{f}_0$ should be halved) and this can be computed by FFT. We obtain an $\mathcal{O}(N \log N)$ algorithm again!

Legendre expansions: $\Omega = (-1,1)$, $\mu(x) = x$, $\mathcal{M} = \mathbb{Z}_+$, $\varphi_m(x) = \mathrm{P}_m(x)$. Now

$$\hat{f}_m = (m + \tfrac{1}{2}) \int_{-1}^{1} f(x)\mathrm{P}_m(x)\,\mathrm{d}x.$$

How to calculate this fast?

Previous work (Gallagher, Wise & Allen, Alpert & Rokhlin, Potts, Steidl & Tasche): Calculate first either Fourier or Chebyshev coefficients and then convert them to Legendre coefficients. Alternatively, use the fast multipole method. The algorithms are complicated, difficult to program and at best $\mathcal{O}\left(N(\log N)^2\right)$. They are not in wide use.

Why is this important? For 'straight' approximation Chebyshev polynomials are arguably better (error equi-oscillation, no Gibbs phenomenon!) but often the nature of the problem forces upon us the choice of the weight function.

A COMPLETELY USELESS FORMULA...

Let us suppose that f is analytic in the interior of the Bernstein ellipse

$$\mathfrak{B}_r = \{\tfrac{1}{2}(r^{-1}\mathrm{e}^{-\mathrm{i}\theta} + r\mathrm{e}^{\mathrm{i}\theta}) \;:\; \theta \in [0, 2\pi]\}$$

for some $r \in (0,1)$,

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

(This guarantees convergence of the Legendre expansion!) Then

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

where $(a)_0 = 1$, $(a)_k = (a)_{k-1}(a+k-1)$, $k \geq 1$ (the Pochhammer symbol) (Whittaker & Watson, Rainville).

Except that this formula is useless for numerical calculations! Firstly, an approximation of derivatives is notoriously unstable. Secondly, suppose that by some magic we have calculated the f_ns cheaply and stably – we'll then need $\mathcal{O}\left(N^2\right)$ operations to calculate the first N coefficients $\hat{f}_m$.

But did uselessness ever stop a full-bloodied mathematician?

We subject the formula to the Cauchy integral theorem: Let γ be a simple Jordan curve circling the origin with positive orientation. Since

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

we have

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

where

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

– recall that

$${}_2\mathrm{F}_1\left[\begin{matrix} a, b; \\ c; \end{matrix} \; \zeta\right] = \sum_{n=0}^{\infty} \frac{(a)_n (b)_n}{n! (c)_n} \zeta^n.$$

Of course, not any γ will do: we must integrate in the domain of analyticity of φ_m. It is possible to prove that each φ_m is analytic in $\mathbb{C} \setminus [-1,1]$, with branch points at ± 1 and a branch cut along $(-1,1)$. Therefore γ must encircle the support $[-1,1]$ of the underlying Legendre measure.

But what is φ_m? It is easy to verify that

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

In general, let

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

Direct computation:

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

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

$$\mathcal{K}_m(z) = \mathsf{P}_m(z)\mathcal{K}_0(z) + q_m(z),$$

where q_m *is a polynomial.*

Proof Very long, yet elementary, algebra. $\square$

THEOREM *Let* γ *be a closed Jordan curve in* $\mathfrak{B}_r \setminus [-1, 1]$*, circling the origin with winding number* 1*. Then*

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

Proof We have

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

It is well-known (and trivial to prove) that

$$\frac{1}{2\pi \mathrm{i}}\int_\gamma g(z)\log\frac{z+1}{z-1}\,\mathrm{d}z=\int_{-1}^{1} g(x)\,\mathrm{d}x,\qquad g \text{ analytic in } \mathfrak{B}_r,$$

hence

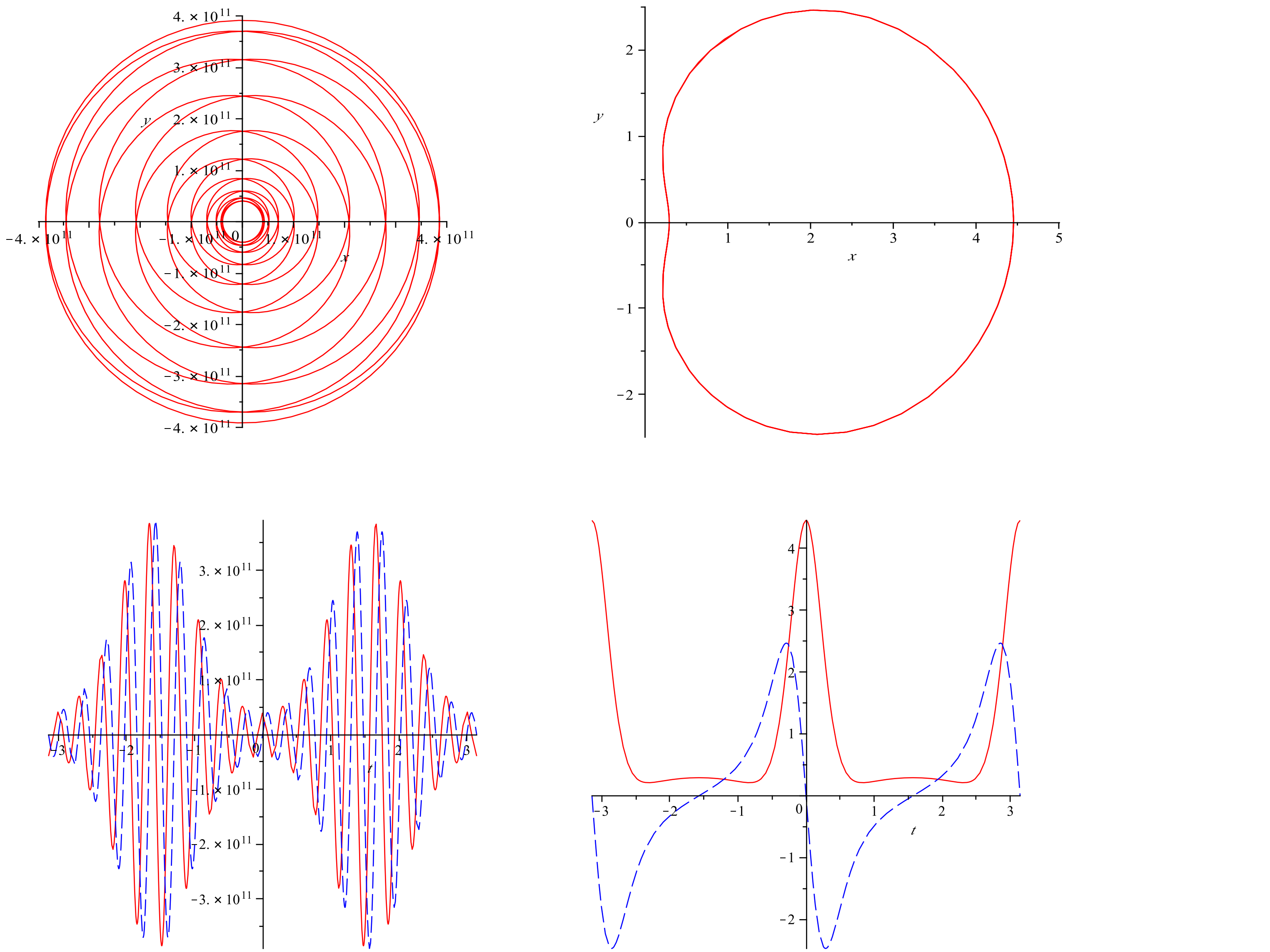
$$\frac{c_m}{2\pi \mathrm{i}}\int_\gamma \frac{f(z)}{z^{m+1}}\varphi_m(z)\,\mathrm{d}z=(m+\tfrac{1}{2})\int_{-1}^{1} f(x)\mathrm{P}_m(x)\,\mathrm{d}x=\hat{f}_m,$$

as asserted. □

There might be a natural temptation to throw away the meaningless polynomial q_m and compute directly

$$\hat{f}_m=\frac{m+\frac{1}{2}}{2\pi \mathrm{i}}\int_\gamma f(z)\mathrm{P}_m(z)\log\frac{z+1}{z-1}\,\mathrm{d}z.$$

This will be a disaster! Intuitively speaking, the difference is that $\mathrm{P}_m(z)\log\frac{z+1}{z-1}$ oscillates very rapidly, thereby making the computation of the integral difficult, while φ_m is nonoscillatory.



The plots of $P_{20}(2e^{i\theta}) \log \frac{2e^{i\theta}+1}{2e^{i\theta}-1}$ (on the left) and $\varphi_{20}(2e^{i\theta})$, $\theta \in [-\pi, \pi]$.

A HYPERGEOMETRIC TRANSFORMATION

The integral formula and FFT In principle, we can approximate

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

by FFT. Thus,

$$\varphi_m(z) = \sum_{j=0}^{\infty} \frac{h_{m,j}}{z^{2j}}, \qquad h_{m,j} = \frac{(\frac{m+1}{2})_j (\frac{m+2}{2})_j}{j!(m+\frac{3}{2})_j},$$

and, truncating,

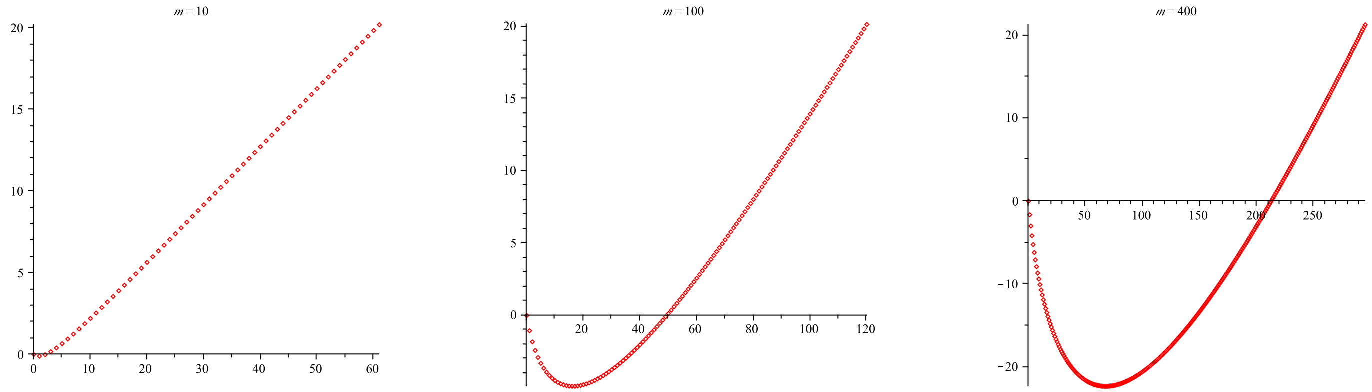
$$\hat{f}_m \approx \frac{c_m}{2\pi \mathrm{i}} \sum_{j=0}^{M} h_{m,j} \int_\gamma \frac{f(z)}{z^{m+2j+1}} \, \mathrm{d}z, \qquad m \in \mathbb{Z}_+,$$

for a suitable $M \in \mathbb{N}$. Suppose we can fit a circular countour $|z| = \rho^{-1} > 1$ into $\mathfrak{B}_r$, then we can approximate with DFT,

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

where $\omega_N = \exp \frac{2\pi \mathrm{i}}{N}$. This can be computed with FFT.

The snag: The convergence of the functions φ_m for large m is very slow:



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

To attain accuracy of 20 decimal digits, we need $M = 61$ for $m = 10$, $M = 120$ for $m = 100$ and $M = 295$ for $m = 400$. Worse: we need 43 decimal digits to calculate $\widehat{f}_{400}$ to 20 digits.

Clearly, this is a non-starter!

A hypergeometric transformation The `http://functions.wolfram.com` website has 111951 different formulæ for ${}_2F_1$ functions. Of these 111950 are not helpful, fortunately one is! Thus, let $a, b, c \in \mathbb{C}$, $\zeta \in \mathbb{C}$, $\operatorname{Re} \zeta < 1$. Then

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

Set $a = \frac{m+1}{2}$, $c = m + \frac{3}{2}$, whereby

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

Note that

$$ {}_2F_1\left[\begin{matrix} m+1, \frac{1}{2}; \\ m+\frac{3}{2}; \end{matrix}\; z\right] = \sum_{j=0}^{\infty} g_{m,j} z^j, \quad \text{where} \quad g_{m,j} = \frac{(m+1)_j (\frac{1}{2})_j}{j!\,(m+\frac{3}{2})_j} > 0 $$

decay! Hence we can expect rapid convergence once we truncate this ${}_2F_1$ function.

Choosing the contour: Ultimately, we wish to reduce everything to DFT, and this means that we need to choose γ so that $|\zeta/(2-\zeta)|$ is constant. We choose the Bernstein ellipse

$$\mathfrak{B}_r = \{\tfrac{1}{2}(r^{-1}\mathrm{e}^{-\mathrm{i}\theta} + r\mathrm{e}^{\mathrm{i}\theta}) \,:\, \theta \in [-\pi, \pi]\}, \qquad r \in (0,1).$$

Strictly speaking, $\mathfrak{B}_r$ has negative orientation. OK, all it takes is to flip the sign... We have

$$2\zeta - \zeta^2 = \frac{1}{z^2} \quad \Rightarrow \quad \zeta = \frac{r\mathrm{e}^{\mathrm{i}\theta}}{z}, \quad \frac{\zeta}{2-\zeta} = r^2\mathrm{e}^{2\mathrm{i}\theta}, \quad \frac{1}{1-\frac{1}{2}\zeta} = 2r\mathrm{e}^{\mathrm{i}\theta}z$$

and, by wonderfully serendipitous cancellation,

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

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

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

where $\tilde{c}_m = 2^m c_m = 2^{2m}(m!)^2/(2m)!$.

A FAST LEGENDRE TRANSFORM

Let N be a large composite integer and

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

be the DFT of

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

Replacing the integral with DFT and truncating the hypergeometric series,

$$\hat{f}_m \approx \tilde{c}_m \sum_{j=0}^{M} g_{m,j} r^{m+2j} \frac{1}{N}\sum_{k=0}^{N-1}(1-r^2\omega_N^{2k})f(\tfrac{1}{2}(r^{-1}\omega_N^{-k}+r\omega_N^k))\omega_N^{(m+2j)k}$$

$$= \sum_{j=0}^{M} \tilde{g}_{m,j}(r)\kappa_{N,m+2j}, \qquad m = 0, \ldots, N-1-2M,$$

where

$$\tilde{g}_{m,j}(r) = \tilde{c}_m g_{m,j} r^{m+2j} = \frac{2^{2m}(m!)^2(m+1)_j(\frac{1}{2})_j}{(2k)!j!(m+\frac{3}{2})_j} r^{m+2j}.$$

Since

$$\tilde{g}_{0,0} = 1, \qquad \tilde{g}_{m,0} = \frac{mr}{m-\frac{1}{2}}\tilde{g}_{m-1,0},$$

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

can be computed in MN operation and, provided that $M = \mathcal{O}(1)$, we have an $\mathcal{O}(N \log N)$ algorithm: the cost is dominated by a single FFT!

How large is the error? The error in replacing integral with DFT is exponentially small but we need to show that our truncation of the Taylor series doesn't lead to large error: essentially, given tolerance $\varepsilon > 0$, we need to show that M may depend on ε, but not on N. The discarded tail is

$$T_{M,m} := \left| \sum_{j=M+1}^{\infty} \frac{\tilde{g}_{m,j}(r)}{2\pi} \int_{-\pi}^{\pi} (1-r^2 e^{2i\theta}) f(\tfrac{1}{2}(r^{-1}e^{-i\theta}+re^{i\theta}))e^{i(m+2j)\theta}d\theta \right|$$

$$\leq \tilde{c}_m(1+r^2)\|f\|_\infty \sum_{j=M+1}^{\infty} |g|_{m,j} r^{m+2j} \leq \tilde{c}_m \frac{1+r^2}{1-r^2}\|f\|_\infty r^{m+2M+2}.$$

Since

$$\tilde{c}_m \le 2m^{\frac{1}{2}}, \qquad x^{\frac{1}{2}} r^x \le \mathrm{e}^{-\frac{1}{2}} (-2 \log r)^{-\frac{1}{2}},$$

we have

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

and we can choose M, independent of N, s.t. the error is smaller than ε,

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

Health warnining: This is a *terrible* means of choosing a good M, since it overestimates it by orders of magnitude!

Betwixt Legendre and Chebyshev What happens when $r \uparrow 1$?

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

where

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

But does it make sense?

$\varphi_m(z) = z^m \psi_m(z^2)$ implies $\psi_m(z^2) = (2m+1) c_m^{-1} z^{m+1} \mathcal{K}_m(z)$, therefore we have a logarithmic singularity at $\pm\pi$ and the integral is well defined.

We proceed as before, replacing ψ_m by its truncated Taylor expansion.

We obtain

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

$$= \frac{1}{2} \tilde{c}_m \sum_{j=0}^{\infty} g_{m,j} (\breve{f}_{m+2j} - \breve{f}_{m+2j+2}), \qquad m \in \mathbb{Z}_+,$$

where

$$\breve{f}_m = \frac{1}{\pi} \int_{-\pi}^{\pi} f(\cos\theta) e^{im\theta} \, d\theta = \frac{1}{\pi} \int_{-\pi}^{\pi} f(\cos\theta) \cos m\theta \, d\theta,$$

the mth Chebyshev coefficient! (Since $f(\cos\theta)$ is even, $\int_{-\pi}^{\pi} f(\cos\theta) \sin m\theta \, d\theta = 0$.)

Let

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

be the Discrete Cosine Transform of $\{f(\cos \frac{2\pi k}{N})\}_{k=0}^{N-1}$. Then

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

We again have an $\mathcal{O}(N \log N + MN)$ algorithm – but is there $M = \mathcal{O}(1)$ given tolerance ε? Our previous proof collapses because of the $\frac{1+r^2}{1-r^2}$ factor.

Instead, we note that $|\check{f}_m| \leq d\mathrm{e}^{-\alpha m}$, where $\alpha > 0$ is the eccentricity of the largest Bernstein ellipse within which f is analytic. Hence

$$\begin{aligned} T_{M,m} &\leq \frac{\tilde{c}_m}{2\pi} \sum_{j=M+1}^{\infty} g_{m,j} \left| \int_{-\pi}^{\pi} f(\cos\theta)[\cos((m+2j)\theta) - \cos((m+2j+2)\theta)]\mathrm{d}\theta \right| \\ &\leq \tfrac{1}{2}\tilde{c}_m \sum_{j=M+1}^{\infty} g_{m,j}[|\check{f}_{m+2j}| + |\check{f}_{m+2j+2}|] \\ &\leq \tfrac{1}{2}\tilde{c}_m d(\coth\alpha)\mathrm{e}^{-\alpha(m+2M+2)}, \qquad m, M \in \mathbb{Z}_+. \end{aligned}$$

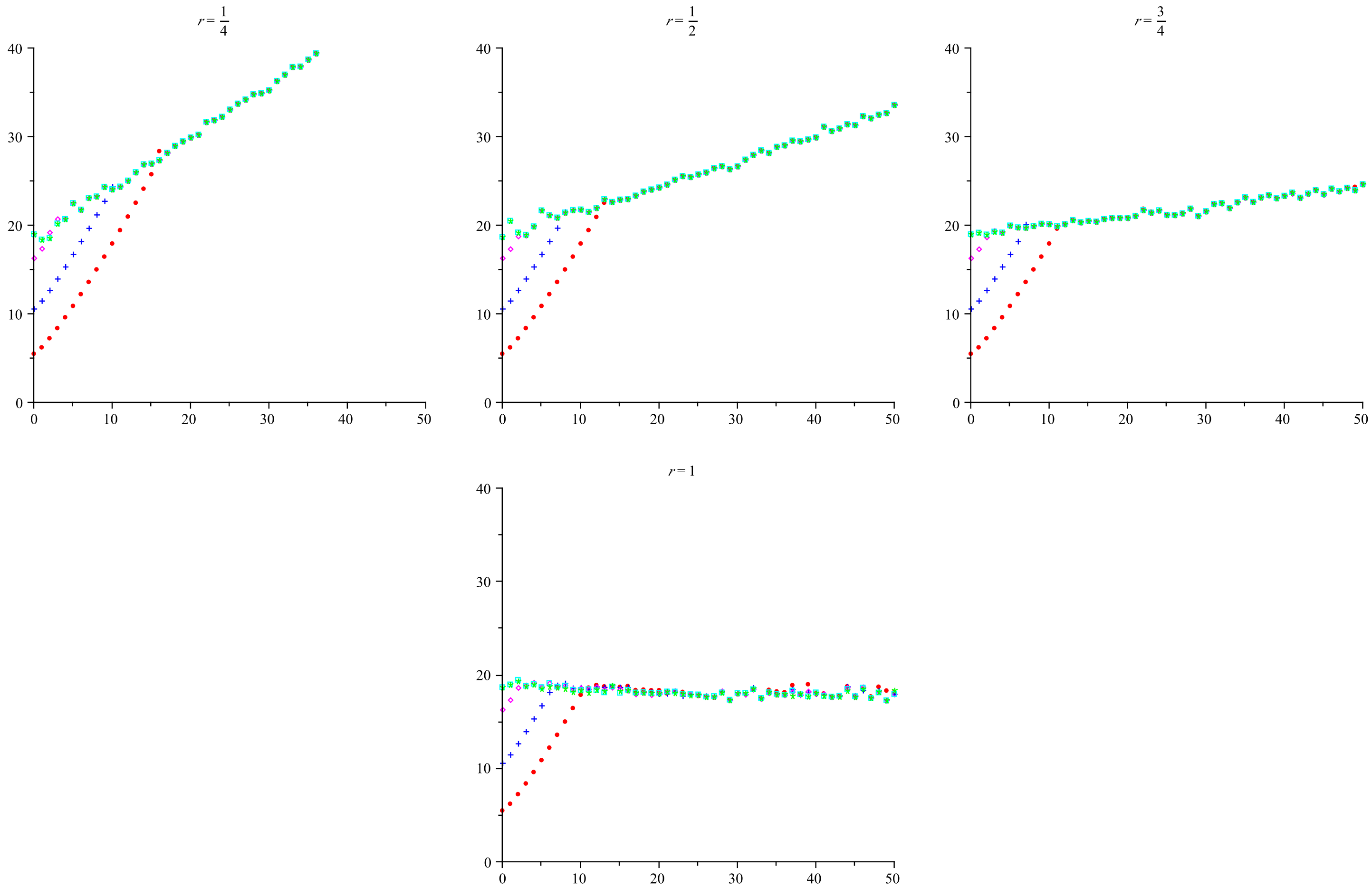
Since

$$\tilde{c}_m \mathrm{e}^{-\alpha m} \leq \max\{1, 2m^{\frac{1}{2}}\mathrm{e}^{-\alpha m}\} \leq \max\{1, (2\alpha\mathrm{e})^{-\frac{1}{2}}\},$$

we again obtain a uniform bound for all $m \in \mathbb{Z}_+$.

NUMERICAL EXAMPLES

We start from $f(x) = \mathrm{e}^x$:



The number of significant digits, computing $\widehat{f}_m$, $m = 0, \ldots, 50$, for $f(x) = \mathrm{e}^x$ with $N = 512$: $M = 2$, $M = 4$, $M = 6$, $M = 8$ and $M = 10$.

Absolute errors in computing $\widehat{f}_m$ for $f(x) = \mathrm{e}^x$

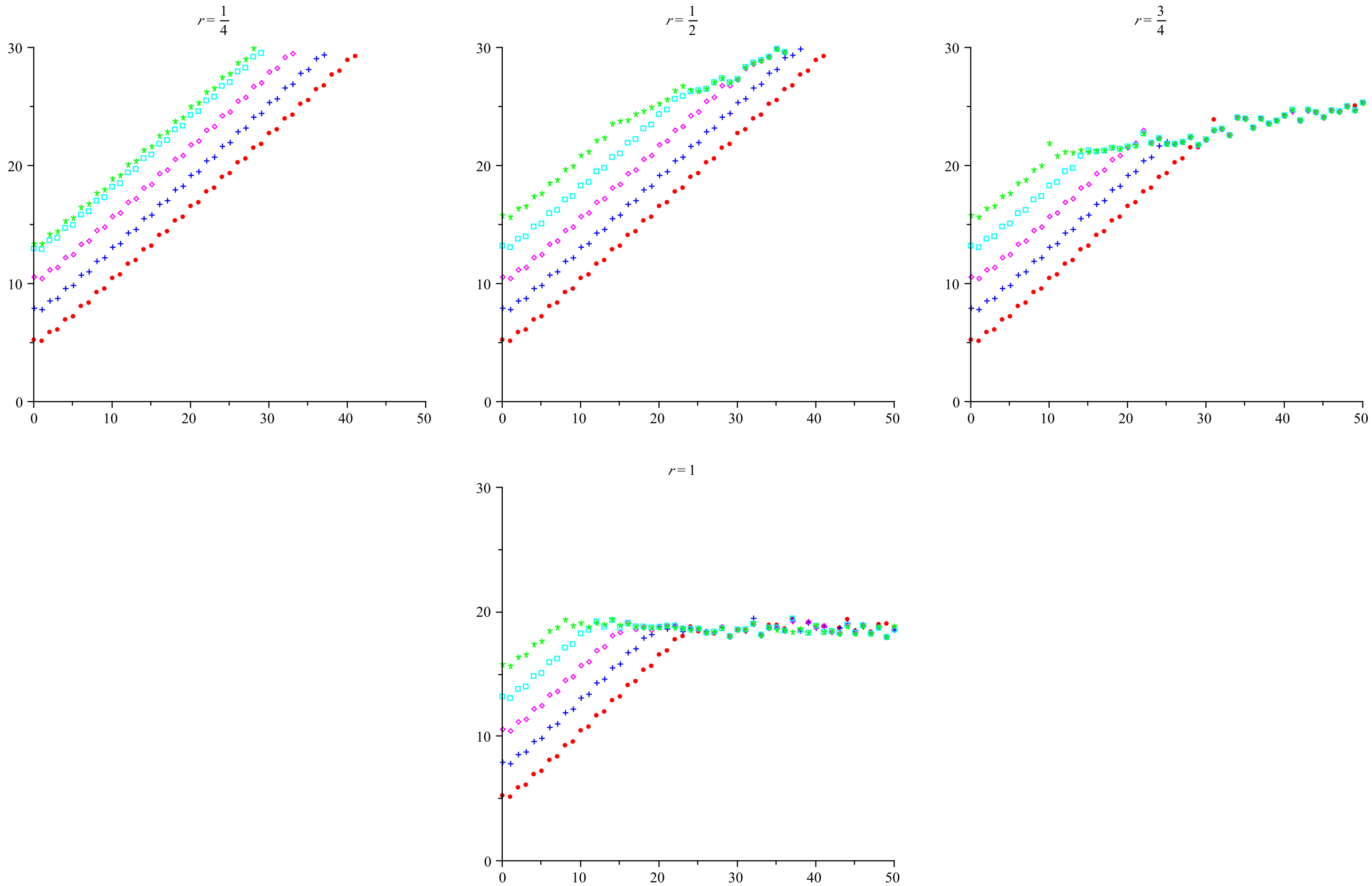
$m = 0$	$M = 2$	$M = 4$	$M = 6$	$M = 8$	$M = 10$	$M = 12$
$r = \frac{1}{4}$	3.21_{-06}	2.50_{-11}	4.73_{-17}	1.00_{-19}	1.00_{-19}	1.00_{-19}
$r = \frac{1}{2}$	3.21_{-06}	2.50_{-11}	4.72_{-17}	2.00_{-19}	2.00_{-16}	2.00_{-19}
$r = \frac{3}{4}$	3.21_{-06}	2.50_{-11}	4.74_{-17}	1.70_{-19}	1.70_{-19}	1.70_{-19}
$r = 1$	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_{-29}	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}

Observations:

- For small m the outcome is insensitive to $r \in (0,1]$ but we need large M.
- For large m we can obtain excellent results with small M, even with $M = 0$. The smaller $r > 0$, the better the accuracy.
- The choice $r = 1$ seems to produce small uniform (in m) error.
- There are three sources of error: (a) replacing integrals with DFT (quantified by N); (b) truncating an ${}_2F_1$ function (quantified by M); and (c) computer arithmetic (quantified by the machine epsilon). The bottom line of the table indicates that (a) is tiny. For small m also (c) is small, everything is dominated by (b), while for large m the error is determined by (c).

Next, $f(x) = (1 + x)/(4 + x^2)$:



The number of significant digits, computing $\widehat{f}_m$, $m = 0, \ldots, 50$, for $f(x) = (1 + x)/(4 + x^2)$ with $N = 512$: $M = 2$, $M = 4$, $M = 6$, $M = 8$ and $M = 10$.

Absolute errors in computing $\widehat{f}_m$ for $f(x) = (1 + x)/(4 + x^2)$

$m = 0$	$M = 2$	$M = 4$	$M = 6$	$M = 8$	$M = 10$	$M = 12$
$r = \frac{1}{4}$	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}

BEYOND LEGENDRE...

A fast (and easy to program) Legendre transform has been sought for at least thirty years. What else remains to be done?

Variable M: We have seen that for smaller m we need larger M but for $m = \mathcal{O}(N)$ we can take even $M = 0$. This suggests an algorithm of the form

$$\hat{f}_m \approx \sum_{j=0}^{M_m} \tilde{g}_{m,j}(r)\kappa_{N,m+2j}, \qquad m = 0, \ldots, N-1,$$

where $M_m \in \mathbb{Z}_+$ decreases monotonically, $M_{N-1} = 0$.

The optimal choice of M_m, however, is f-dependent! (It also depends on the desired accuracy.) We need a good algorithm, at the very least a good heuristic rule of a thumb: initial results due to Ed Mottram.

Multivariate transform: Absolutely straightforward, already implemented in MATLAB and works beautifully.

More general OPSs: What about (more) general Borel measures $\mathrm{d}\mu$?

The work of this paper has been already generalized to ultraspherical (a.k.a. Gegenbauer) polynomials, orthogonal w.r.t.

$$\mathrm{d}\mu(x) = (1-x^2)^\alpha \, \mathrm{d}x, \qquad x \in (-1,1), \quad \alpha > -1.$$

Thus, $\alpha = -\frac{1}{2} \Rightarrow$ Chebyshev, $\alpha = 0 \Rightarrow$ Legendre, $\alpha = \frac{1}{2} \Rightarrow$ Chebyshev of second kind.

What about more general OPSs? Our approach depends on three steps:

1. Express $\widehat{f}_m$ as an infinite linear combination of derivatives;
2. Using the Cauchy Integral Theorem, express $\widehat{f}_m$ as an integral transform over a closed curve in $\mathbb{C}$;
3. Accelerate the convergence of the integral transform by a clever transformation.

Step 1: Turns out that we can express $\widehat{f}_m$ in this form for some familiar OPSs:

Hermite:

$$\mathrm{d}\mu(x) = \mathrm{e}^{-x^2}\,\mathrm{d}x, \quad x \in \mathbb{R}, \qquad \widehat{f}_m = \frac{1}{2^m m!}\sum_{k=0}^{\infty} \frac{f_{m+2k}}{2^{2k}k!};$$

Laguerre:

$$\mathrm{d}\mu(x) = x^\alpha \mathrm{e}^{-x}\,\mathrm{d}x, \quad x \in \mathbb{R}_+, \qquad \widehat{f}_m = (-1)^m \sum_{k=0}^{\infty} \frac{(m+\alpha)_k f_{m+k}}{k!}.$$

Step 2: Unfortunately, it is impossible to encircle an infinite interval by a bounded curve. An impasse.

Conclusion: Let us concentrate on finitely-supported measures.

Variations on the theme of general theory

Let $\{\varphi_m\}_{n\in\mathbb{Z}_+}$ be the monic OPS w.r.t. $\mathrm{d}\mu$, supported by (a,b). Hence

$$\int_a^b \varphi_m(x)\varphi_n(x)\,\mathrm{d}\mu(x) = \begin{cases} \kappa_n > 0, & m=n, \\ 0, & m\neq n \end{cases}$$

and

$$\varphi_{n+1}(x) = (x-a_n)\varphi_n(x) - b_n\varphi_{n-1}(x), \qquad n\in\mathbb{Z}_+,$$

where $\varphi_{-1}\equiv 0$, $b_n>0$.

There necessarily exist $d_{n,m}$, $0\le m\le n$, s.t.

$$x^n = \sum_{m=0}^{n} d_{n,m}\varphi_m(x), \qquad n\in\mathbb{Z}_+.$$

Clearly,

$$d_{n,m} = \frac{1}{\kappa_m}\int_a^b x^n\varphi_m(x)\,\mathrm{d}\mu(x), \qquad m=0,\ldots,n.$$

Using the recurrence relation inside the integral,

$$d_{n+1,m} = \frac{1}{\kappa_m}(\kappa_{m-1} b_m d_{n,m-1} + \kappa_m a_m d_{n,m} + \kappa_{m+1} d_{n,m+1}).$$

Letting $\tilde{d}_{n,m} = \kappa_m d_{n,m}/\kappa_0$, this simplifies to

$$\tilde{d}_{n+1,m} = b_m \tilde{d}_{n,m-1} + a_m \tilde{d}_{n,m} + \tilde{d}_{n,m+1}.$$

Let $d_{n,m} = 0$ for $m \geq n+1$ and

$$\boldsymbol{d}_n = \begin{bmatrix} \tilde{d}_{n,0} \\ \tilde{d}_{n,1} \\ \tilde{d}_{n,2} \\ \vdots \end{bmatrix}, \qquad \mathcal{H} = \begin{bmatrix} a_0 & 1 & 0 & \cdots & \cdots & 0 \\ b_1 & a_1 & 1 & \ddots & & \vdots \\ 0 & b_2 & a_2 & 1 & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & & \end{bmatrix}.$$

Then $\boldsymbol{d}_0 = \boldsymbol{e}_0$ and $\boldsymbol{d}_{n+1} = \mathcal{H}\boldsymbol{d}_n$, therefore

$$\boldsymbol{d}_n = \mathcal{H}^n \boldsymbol{e}_0, \qquad n \in \mathbb{Z}_+.$$

Note that $\mathcal{H}$ is similar to the Jacobi matrix $\mathcal{J}$,

$$\Sigma\mathcal{H}\Sigma^{-1} = \begin{bmatrix} a_0 & b_1^{\frac{1}{2}} & 0 & \cdots & \cdots & 0 \\ b_1^{\frac{1}{2}} & a_1 & b_2^{\frac{1}{2}} & \ddots & & \vdots \\ 0 & b_2^{\frac{1}{2}} & a_2 & b_3^{\frac{1}{2}} & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & \end{bmatrix},$$

where $\Sigma = \mathrm{diag}\,\boldsymbol{\sigma}$ with $\sigma_0 = 1$ and $\sigma_m = (b_{m-1}/b_m)^{\frac{1}{2}}$, $m \in \mathbb{N}$ (with $b_0 = 1$). Therefore $\sigma(\mathcal{H}) = \sigma(\mathcal{J})$ and $\sigma(\mathcal{H})$ coincides with $[a, b]$, the support of the measure.

Supposing $0 \in [a, b]$, let $f(x) = \sum_{n=0}^{\infty} f_n x^n$ be analytic. Then

$$f(x) = \kappa_0 \sum_{n=0}^{\infty} f_n \sum_{m=0}^{n} \frac{\tilde{d}_{n,m}}{\kappa_m} \varphi_m(x) = \kappa_0 \sum_{m=0}^{\infty} \frac{1}{\kappa_m} \left(\sum_{n=m}^{\infty} \tilde{d}_{n,m} f_n \right) \varphi_m(x)$$

and we deduce that

$$\hat{f}_m = \frac{\kappa_0}{\kappa_m} \sum_{n=m}^{\infty} \tilde{d}_{n,m} f_n, \qquad m \in \mathbb{Z}_+.$$

Let the support of $\mathrm{d}\mu$ be compact and γ be a simple Jordan curve surrounding it with winding number one. Then

$$\hat{f}_m = \frac{\kappa_0}{\kappa_m} \frac{1}{2\pi \mathrm{i}} \int_\gamma f(z) \sum_{n=m}^{\infty} \frac{\tilde{d}_{n,m}}{z^{n+1}} \, \mathrm{d}z.$$

But $\tilde{d}_{n,m} = \boldsymbol{e}_m^\top \mathcal{H}^n \boldsymbol{e}_0$, therefore

$$\sum_{n=m}^{\infty} \frac{\tilde{d}_{n,m}}{z^{n+1}} = \frac{1}{z} \boldsymbol{e}_m^\top \left(\sum_{n=m}^{\infty} \mathcal{H}^n z^{-n} \right) \boldsymbol{e}_0 = \frac{1}{z^{m+1}} \boldsymbol{e}_m^\top \mathcal{H}^m (I - z^{-1} \mathcal{H})^{-1} \boldsymbol{e}_0$$

and we deduce that

$$\hat{f}_m = \frac{\kappa_0}{\kappa_m} \frac{1}{2\pi \mathrm{i}} \int_\gamma \frac{f(z)}{z^{m+1}} \boldsymbol{e}_m^\top \mathcal{H}^m (I - z^{-1} \mathcal{H})^{-1} \boldsymbol{e}_0 \, \mathrm{d}z, \qquad m \in \mathbb{Z}_+.$$

Note that (subject to very generous conditions) the essential spectrum of $\mathcal{H}$ is $[a, b]$, inside the contour.

All this has been recently extended (with María-José Cantero) to orthogonal polynomials on the complex unit circle.

And this is the state of the art as of this moment in time…