Numerical evaluation of the prolate spheroidal wave functions of order 0

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Motivation

The spheroidal wave equation

$$(1-t^2)y''(t) - 2ty'(t) + \left(\chi - \frac{\mu^2}{1-t^2} - \gamma^2 t^2\right) y(t) = 0$$

arises, among other ways, from the separation of the Helmholtz equation in spheroidal coordinates.

The solutions are typically indexed via the explicit parameters μ (order) and γ (bandlimit), as well as by an implicit parameter ν (characteristic exponent). The parameter χ usually plays the role of a Sturm-Liouville eigenvalue and is viewed as a function of ν, μ and γ.

When $\gamma^2 > 0$, the solutions are known as prolate spheroidal wave functions and this is the case we are most interested in.

The spheroidal wave functions can be defined for all complex values of ν, μ and γ^2.

The standard reference is:

> J. Meixner and F. Schäfke. *Mathieusche Funktionen und Sphäroidfunktionen*. Springer-Verlag, Berlin, 1954.

Motivation

It was famously observed by Slepian that the eigenfunctions of the restricted Fourier operator

$$T[f](x) = \int_{-1}^{1} \exp(i\gamma xt) f(t) dt$$

are a collection of prolate spheroidal wave functions of order $\mu = 0$ and nonnegative integer characteristic exponents ν.

These functions provide a mechanism for representing bandlimited functions which is optimal in a certain sense.

The standard method for evaluating them is the Xiao-Rokhlin algorithm, which solves a discrete eigenproblem in order to construct a Legendre expansion of one of the prolate functions. Its running time grows with γ and ν.

Motivation

I will describe an $\mathcal{O}(1)$ algorithm for evaluating the eigenfunctions of the restricted Fourier operator on the interval $[0, 1)$.

This algorithm can be easily extended to prolate and oblate spherical wave functions of integer orders and characteristic exponents.

The rapid numerical evaluation of the prolate spheroidal wave functions is interesting in its own right. When combined with butterfly algorithms, an $\mathcal{O}(1)$ algorithm for the evaluation of the prolate functions provides a robust and efficient mechanism for rapidly applying the prolate spheroidal wave function transform and its inverse.

A similar approach was recently used to construct a practical $\mathcal{O}\left(N^2 \log^3(N)\right)$ algorithm for computing spherical harmonic transforms:

> James Bremer, Ze Chen and Haizhao Yang. *Rapid Application of the Spherical Harmonic Transform via Interpolative Decomposition Butterfly Factorization*
> arXiv:2004.11346

The angular spheroidal wave functions

It is the angular spheroidal wave functions of the first kind, which we will denote by $Ps_\nu^\mu(z;\gamma^2)$, which we wish to calculate.

The function $Ps_\nu^\mu(z;\gamma^2)$ admits an expansion of the form

$$\sum_{n=-\infty}^{\infty} a_n P_{\nu+2n}^\mu(x),$$

where P_ν^μ is the associated Legendre function of the first kind of order μ and degree ν. Requiring this form for $Ps_\nu^\mu(z;\gamma^2)$ determines it up to a constant. We normalize it through the condition

$$\begin{cases} Ps_\nu^\mu(0;\gamma^2) = P_\nu^\mu(0) & \text{when} \quad P_\nu^\mu(0) \neq 0 \\ \dfrac{dPs_\nu^\mu}{dx}(0;\gamma^2) = \dfrac{dP_\nu^\mu}{dx}(0) & \text{otherwise.} \end{cases}$$

The radial spheroidal wave function of the third kind

The radial spheroidal wave function of the third kind is defined via the formula

$$S_\nu^{\mu(3)}(z;\gamma^2) = C_\nu^\mu(\gamma^2)(1-z^2)^{\mu/2}\int_1^\infty (1-t^2)^{\mu/2}\exp(i\gamma tz)Ps_\nu^\mu(t;\gamma^2)\ dt.$$

Although the real and imaginary parts of $S_\nu^{\mu(3)}(z;\gamma^2)$ oscillate in many regions, its logarithm is nonoscillatory. The existence of solutions of this type is a general feature of second order differential equations whose coefficients are nonoscillatory.

The nonoscillatory phase function

The real and imaginary parts of the logarithm of $S_\nu^{\mu(3)}(z;\gamma^2)$ are related to each other by a simple formula, at least on the interval $[0,1)$. Indeed, there the logarithm is necessarily of the form

$$i\,\Psi S_\nu^\mu(x;\gamma^2) - \frac{1}{2}\log\left(\frac{d\,\Psi S_\nu^\mu}{dx}(x;\gamma^2)\right)$$

with $\Psi S_\nu^\mu(x;\gamma^2)$ real-valued and increasing.

It is well known that the imaginary part of $S_\nu^{\mu(3)}(x;\gamma^2)$ is equal to $Ps_\nu^\mu(x;\gamma^2)$ on the interval $[0,1)$, so that

$$Ps_\nu^\mu(x;\gamma^2) = \frac{\sin\left(\Psi S_\nu^\mu(x;\gamma^2)\right)}{\sqrt{\frac{d\,\Psi S_\nu^\mu}{dx}(x;\gamma^2)}}.$$

We refer to $\Psi S_\nu^\mu(x;\gamma^2)$ as the nonoscillatory phase function for the spheroidal wave equation.

The nonoscillatory phase function

We note that at this stage $\Psi S_\nu^\mu(1;\gamma^2)$ is only defined up to a constant modulo 2π. We fix it by requiring that

$$0 \le \lim_{x\to 1^-} \Psi S_\nu^\mu(x;\gamma^2) < 2\pi.$$

It is well known that

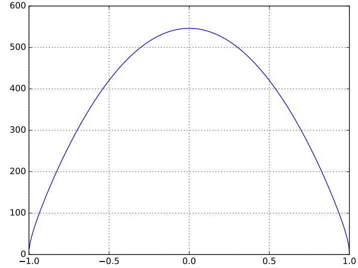
$$Ps_\nu^\mu(x;\gamma^2) = C_\nu^\mu(\gamma^2)(1-x^2)^{\mu/2}\left(1+\mathcal{O}\left(1-x\right)\right) \quad \text{as} \quad x \to 1^-,$$

and that there is a second independent solution of the spheroidal wave equation which has a logarithmic singularity at 1. Together with

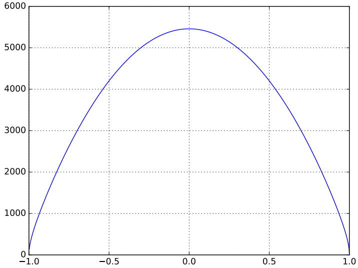
$$Ps_\nu^\mu(x;\gamma^2) = \frac{\sin\left(\Psi S_\nu^\mu(x;\gamma^2)\right)}{\sqrt{\frac{d\,\Psi S_\nu^\mu}{dx}(x;\gamma^2)}},$$

this implies that

$$\lim_{x\to 1^-} \Psi S_\nu^\mu(x;\gamma^2) = 0.$$



The derivative of $\Psi S_{\nu}^{\mu}(x;\gamma^2)$ when $\gamma = 500$ and $\nu = 400$.



The derivative of $\Psi S_{\nu}^{\mu}(x;\gamma^2)$ when $\gamma = 5000$ and $\nu = 4000$.

The nonoscillatory phase function

There is an interesting observation which we will exploit later.

When $\nu = n$ and $\mu = m$ are integers, $Ps_n^m(x;\gamma^2)$ has $n-m$ zeros on $(-1,1)$.

When $n-m$ is odd, $Ps_n^m(x;\gamma^2)$ is odd. And when $n-m$ is even, $Ps_n^m(x;\gamma^2)$ is even.

From this, the formula

$$Ps_\nu^\mu(x;\gamma^2) = \frac{\sin\left(\Psi S_\nu^\mu(x;\gamma^2)\right)}{\sqrt{\frac{d\Psi S_\nu^\mu}{dx}(x;\gamma^2)}},$$

and the fact that the phase function increases to 0 as $x \to 1^-$, we deduce that

$$\Psi S_n^m(0;\gamma^2) = -\frac{\pi}{2}(n-m+1).$$

In particular, for integer values of the parameters ν and μ the value of the phase function at 0 is known to us.

The Riccati equation

The logarithmic derivative of $S_\nu^{\mu(3)}(z;\gamma^2)$ satisfies a Riccati equation of the form

$$r'(t) + (r(t))^2 + q(t) = 0$$

and the well-known formula

$$S_\nu^{\mu(3)}(z;\gamma^2) = \frac{\exp\left(i\gamma z - \frac{i\pi}{2}\nu\right)}{\gamma z}\left(1 + \mathcal{O}\left(\frac{1}{z}\right)\right).$$

tells us its behavior at infinity. This, together with the fact that

$$\Psi S_n^m(0;\gamma^2) = -\frac{\pi}{2}(n - m + 1),$$

gives us everything we need to calculate $\Psi S_n^m(x;\gamma^2)$ on $[0,1)$.

Outline of the algorithm for constructing $\mathit{\Psi S}_\nu^\mu(z;\gamma^2)$

We take as inputs the values of the parameters μ, γ and χ BUT NOT ν.

We first solve a Riccati equation going down the imaginary axis from $i\infty$ to 0 in order to find the value of the logarithmic derivative of $S_\nu^{\mu(3)}(z;\gamma^2)$ at 0. The correct initial value is determined from the well-known asymptotic approximation for $S_\nu^{\mu(3)}(z;\gamma^2)$ mentioned earlier.

We then solve the Riccati equation across the interval $(0,1)$ in order to calculate the logarithmic derivative of $S_\nu^{\mu(3)}(z;\gamma^2)$ there.

We integrate the imaginary part of the logarithmic derivative going backward from 1 to 0 in order to construct $\mathit{\Psi S}_\nu^\mu(x;\gamma^2)$. We use the fact that

$$\lim_{x\to 1^-} \mathit{\Psi S}_\nu^\mu(x;\gamma^2) = 0$$

to set the constant.

Details, details, details ...

I am being somewhat glib as there are a number of important details that must be dealt with if one wants a robust and accurate numerical method.

First, we do not actually solve the Riccati equation over $(0, 1)$. There are several forms of the Riccati equation. If y is a complex-valued solution of

$$y''(t) + q(t)y(t) = 0$$

then $w(t) = |y(t)|^2$ satisfies Appell's equation

$$w'''(t) + 4q(t)w'(t) + 2q'(t)w(t) = 0.$$

We actually solve Appell's equation rather than the Riccati equation to compute $\mathit{\Psi S}_\nu^\mu(x;\gamma^2)$ on $(0, 1)$.

Appell's equation has the advantage that its solution is real-valued and increasing on $[0, 1)$.

Moreover, we do so under the change of variables $x = 1 - \exp(-u)$ because for small values of the parameters, $\mathit{\Psi S}_\nu^\mu(x;\gamma^2)$ goes to 0 very slowly as $x \to 1^-$.

Problems, problems, problems ...

The algorithm just described allows us to compute $\mathit{\Psi S}_\nu^\mu(x;\gamma^2)$, and hence $Ps_\nu^\mu(x;\gamma^2)$, given the parameters χ, ν and μ.

But the computation of χ given ν, μ and γ is not easy. Indeed, the standard algorithm requires solving an eigenproblem and its running time grows with the parameters.

An obvious solution is to build a precomputed expansion of χ as a function of the other parameters.

The trouble is that the relationship between χ and the characteristic exponent ν is complicated.

Problems, problems, problems ...

If the spheroidal wave equation has a solution which admits a Laurent expansion of the form

$$z^{\nu} \sum_{n=-\infty}^{\infty} a_n z^{2n}$$

around $z = \infty$ then we say ν is a characteristic exponent. Obviously if ν is a characteristic exponent then so are

$$\nu + 2k \quad \text{and} \quad 1 - \nu + 2k$$

for all integers k.

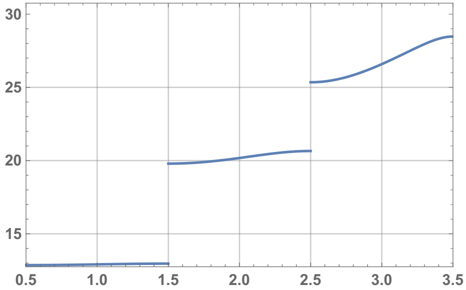
We uniquely determine ν as a function of the other parameters by requiring that

$$\lim_{\gamma \to 0^+} \chi_{\nu}^{\mu}(\gamma^2) = \nu(\nu + 1).$$

This makes it consistent with the associated Legendre differential equation.

Problems, problems, problems ...

The trouble is that $\chi_\nu^\mu(\gamma^2)$, when viewed as a function of ν, has a branch point at each half integer.



A plot of $\chi_\nu^0(\gamma^2)$ as a function of ν when $\gamma = 5$.

A solution

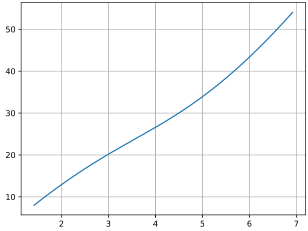
Rather than index the spheroidal wave functions via ν, μ and γ^2, we introduce a new variable

$$\xi_\nu^\mu(\gamma^2) = -\frac{2}{\pi}\Psi S_\nu^\mu(0;\gamma^2)$$

and construct expansions of χ as a function of ξ, μ and γ.

From our earlier discussion, we know that ξ is a real-valued generalization of the number of roots of $Ps_\nu^\mu(x;\gamma^2)$ on the interval $(-1,1)$ whose value is known when ν and μ are integers.

And, of course, χ is smooth as a function of these variables:



A plot of $\chi_\nu^0(\gamma^2)$ as a function of ξ when $\gamma = 5$.

A solution

Since I am primarily interested in spheroidal wave functions of order 0, in the first instance I have taken $\mu = 0$ and only computed expansions of χ as a function of ξ and γ. This is the only aspect of the algorithm I describe today which is restricted to spheroidal wave functions of order 0.

The expansions I computed work for $0 \leq \gamma \leq 2^{20}$ and $0 \leq \nu \leq 10\gamma$.

The cost of evaluating $\chi_\nu^0(\gamma^2)$

Range of γ	Maximum relative difference	Average time expansion	Average time Xiao-Rokhlin
256 - 512	2.57×10^{-15}	8.23×10^{-07}	4.74×10^{-04}
512 - 1,024	1.91×10^{-15}	7.80×10^{-07}	6.12×10^{-04}
1,024 - 2,048	2.07×10^{-15}	7.76×10^{-07}	1.14×10^{-03}
2,048 - 4,096	1.98×10^{-15}	6.79×10^{-07}	2.19×10^{-03}
4,096 - 8,192	2.09×10^{-15}	6.78×10^{-07}	4.36×10^{-03}
8,192 - 16,384	2.15×10^{-15}	6.94×10^{-07}	8.86×10^{-03}
16,384 - 32,768	1.64×10^{-15}	6.89×10^{-07}	1.79×10^{-02}
32,768 - 65,536	2.06×10^{-15}	6.85×10^{-07}	3.64×10^{-02}
65,536 - 131,072	2.21×10^{-15}	7.19×10^{-07}	7.48×10^{-02}
131,072 - 262,144	2.76×10^{-15}	7.14×10^{-07}	1.66×10^{-01}
262,144 - 524,288	4.93×10^{-15}	7.26×10^{-07}	3.71×10^{-01}
524,288 - 1,048,576	6.40×10^{-15}	7.34×10^{-07}	$1.05\times10^{+00}$

The cost to construct $Ps_\nu^\mu(x;\gamma^2)$

Range of γ	Average precomp time phase algorithm	Average precomp time Xiao-Rokhlin
256 - 512	2.36×10^{-04}	4.38×10^{-04}
512 - 1,024	2.43×10^{-04}	6.91×10^{-04}
1,024 - 2,048	2.73×10^{-04}	1.22×10^{-03}
2,048 - 4,096	2.97×10^{-04}	2.34×10^{-03}
4,096 - 8,192	3.20×10^{-04}	4.53×10^{-03}
8,192 - 16,384	3.36×10^{-04}	9.59×10^{-03}
16,384 - 32,768	3.59×10^{-04}	1.87×10^{-02}
32,768 - 65,536	3.84×10^{-04}	3.71×10^{-02}
65,536 - 131,072	3.96×10^{-04}	7.94×10^{-02}
131,072 - 262,144	4.24×10^{-04}	2.02×10^{-01}
262,144 - 524,288	4.34×10^{-04}	5.00×10^{-01}
524,288 - 1,048,576	4.52×10^{-04}	$1.09\times10^{+00}$

The cost to evaluate $Ps_\nu^\mu(x;\gamma^2)$

Range of γ	Maximum absolute error	Average evaluation time phase algorithm	Average evaluation time Xiao-Rokhlin
256 - 512	9.04×10^{-14}	1.41×10^{-07}	1.29×10^{-05}
512 - 1,024	1.37×10^{-13}	1.40×10^{-07}	2.23×10^{-05}
1,024 - 2,048	2.13×10^{-13}	1.39×10^{-07}	4.07×10^{-05}
2,048 - 4,096	3.02×10^{-13}	1.39×10^{-07}	7.78×10^{-05}
4,096 - 8,192	4.73×10^{-13}	1.39×10^{-07}	1.50×10^{-04}
8,192 - 16,384	6.74×10^{-13}	1.39×10^{-07}	2.99×10^{-04}
16,384 - 32,768	8.71×10^{-13}	1.39×10^{-07}	5.94×10^{-04}
32,768 - 65,536	1.32×10^{-12}	1.44×10^{-07}	1.20×10^{-03}
65,536 - 131,072	1.76×10^{-12}	1.39×10^{-07}	2.51×10^{-03}
131,072 - 262,144	3.62×10^{-12}	1.41×10^{-07}	5.56×10^{-03}
262,144 - 524,288	8.09×10^{-12}	1.39×10^{-07}	1.23×10^{-02}
524,288 - 1,048,576	6.81×10^{-12}	1.39×10^{-07}	2.71×10^{-02}

Future work

This is a preliminary result.

If one really wants to evaluate the prolate spheroidal wave functions of order 0 quickly, they should construct precomputed expansions of $\mathit{\Psi S}_\nu^0(x;\gamma^2)$ as a function of x, ξ and γ.

This should allow for a single evaluation of $Ps_\nu^0(x;\gamma^2)$ to be performed in around 10^{-7} to 10^{-6} seconds on a typical laptop machine.