Numerical evaluation of the spheroidal wave functions

November 5, 2021

Spaces of bandlimited functions

A function F has bandlimit γ if it is the Fourier transform of a function supported on the interval $(-\gamma, \gamma)$; that is, if

$$F(z) = \int_{-\gamma}^{\gamma} \exp(izt)\sigma(t)\ dt$$

with $\sigma \in L^2(-\gamma, \gamma)$.

Bandlimited functions have many applications in numerical analysis and signal processing because any function obtained via sampling at finite time steps is necessarily bandlimited.

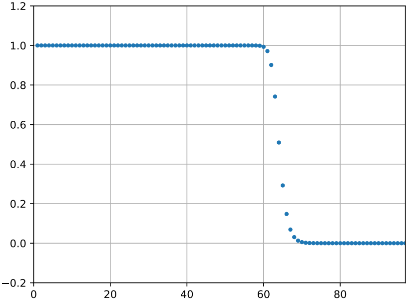
Spaces of bandlimited functions

We can identify the space of functions with bandlimit γ with the image of the restricted Fourier operator $\mathscr{F}_\gamma : L^2(-1,1) \to L^2(-1,1)$, which is defined via

$$\mathscr{F}_\gamma[\sigma](z) = \sqrt{\frac{\gamma}{2\pi}} \int_{-1}^{1} \exp(i\gamma z t)\sigma(t)\, dt.$$

The operator $\mathscr{F}_\gamma$ is normal and it has:

- roughly $\frac{2}{\pi}\gamma$ eigenvalues whose magnitudes are close to 1
- $\mathcal{O}(\log(\gamma))$ eigenvalues whose magnitudes are decaying and non-negligible



$\gamma = 100$

An efficient mechanism for representing bandlimited functions

The restricted Fourier operator $\mathscr{F}_\gamma$ has roughly

$$N_\gamma = \frac{2}{\pi}\gamma + 7.44\log(\gamma),$$

eigenvalues whose magnitudes are greater than machine zero ϵ_0. This implies that the first N_γ eigenfunctions of $\mathscr{F}_\gamma$ suffice to represent functions with bandlimit γ with relative precision ϵ_0 (in the $L^2(-1,1)$ norm).

Approximately γ orthogonal polynomials or trigonometric functions are required to represent functions in this space with comparable accuracy.

Indeed:

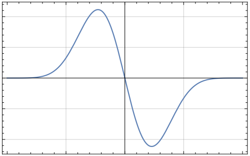
The variational characterization of the eigenvalues of $\mathscr{F}_\gamma^*\mathscr{F}_\gamma$ gives a sense in which the eigenfunctions of $\mathscr{F}_\gamma$ are an optimal mechanism for representing functions with bandlimit γ.

An efficient mechanism for representing bandlimited functions

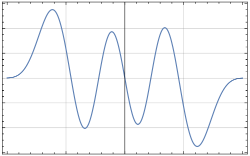
We denote the eigenfunctions of $\mathscr{F}_\gamma$ via

$$Ps_0(z;\gamma),\ Ps_1(z;\gamma),\ Ps_2(z;\gamma),\ldots$$

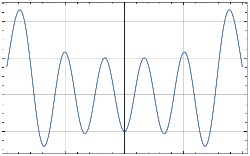
and the eigenvalue corresponding to $Ps_n(z;\gamma)$ by $\lambda_n(\gamma)$.



$Ps_1(z;20)$



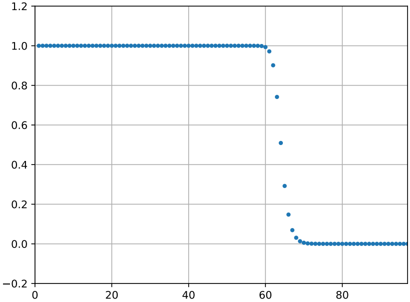
$Ps_5(z;20)$



$Ps_{10}(z;20)$

Numerical difficulties are encountered when discretizing $\mathscr{F}_\gamma$

The behavior of the spectrum of $\mathscr{F}_\gamma$ makes the numerical calculation of $Ps_n(z;\gamma)$ through the discretization of $\mathscr{F}_\gamma$ challenging.



When the gaps between eigenvalues are small, the problem of computing eigenfunctions is ill-conditioned.

The spheroidal wave functions of interest are also solutions of a Sturm-Liouville problem

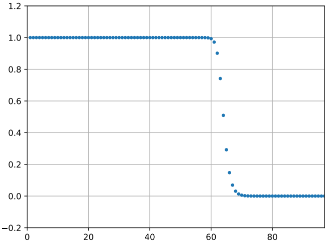
The functions

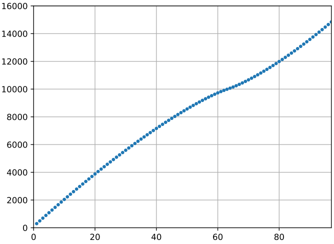
$$Ps_0(z;\gamma),\ Ps_1(z;\gamma),\ Ps_2(z;\gamma),\ \ldots$$

are also the solutions of the singular self-adjoint Sturm-Liouville problem

$$\begin{cases} (1-z^2)y''(z) - 2zy'(z) - \gamma^2 z^2 y(z) = -\chi\ y(z), \quad -1 < z < 1, \\ \lim\limits_{z\to\pm 1} y'(z)(1-z^2) = 0. \end{cases}$$

We denote the Sturm-Liouville eigenvalue corresponding to $Ps_n(z;\gamma)$ by $\chi_n(\gamma)$.





The Osipov-Xiao-Rokhlin algorithm

The standard approach to the numerical solution of

$$\begin{cases} (1-z^2)y''(z) - 2zy'(z) - \gamma^2 z^2 y(z) = -\chi\ y(z), \quad -1 < z < 1, \\ \lim\limits_{z \to \pm 1} y'(z)(1-z^2) = 0. \end{cases}$$

calls for representing its solutions via Legendre expansions. In the case when n is even:

$$Ps_n(z;\gamma) = \sum_{k=0}^{\infty} \beta_k P_{2k}(z)$$

In the case when n is odd:

$$Ps_n(z;\gamma) = \sum_{k=0}^{\infty} \beta_k P_{1+2k}(z)$$

Why Legendre functions?

The Legendre functions

$$P_0(z),\ P_1(z),\ P_2(z),\ \ldots$$

are a set solutions of

$$\begin{cases} (1-z^2)y''(z) - 2zy'(z) = -\chi\ y(z), & -1 < z < 1, \\ \qquad \lim\limits_{z\to\pm 1} y'(z)(1-z^2) = 0 \end{cases}$$

which comprise an orthonormal basis in $L^2(-1,1)$

Any f in $L^2(-1,1)$ can be represented as

$$f(z) = \sum_{k=-\infty}^{\infty} \beta_k P_k(z).$$

In general, the coefficients β_k need only decay fast enough to ensure convergence in $L^2(-1,1)$. If, however, f is smooth and satisfies the boundary conditions, then they decay "faster than any polynomial."

The Osipov-Xiao-Rokhlin algorithm

When one of these expansions is inserted into the reduced spheroidal wave equation

$$(1 - z^2)y''(z) - 2zy'(z) + (\chi - \gamma^2 z^2)y(z) = 0$$

a set of three term recurrence relations for its coefficients emerges. These relations can be written as:

$$\begin{pmatrix} A_0(\gamma) & B_1(\gamma) & & & & \\ B_1(\gamma) & A_1(\gamma) & B_2(\gamma) & & & \\ & B_2(\gamma) & A_2(\gamma) & B_3(\gamma) & & \\ & & B_3(\gamma) & A_3(\gamma) & B_4(\gamma) & \\ & & & \ddots & \ddots & \ddots \end{pmatrix} \begin{pmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \\ \vdots \end{pmatrix} = \chi \begin{pmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \\ \vdots \end{pmatrix}$$

This matrix is truncated and an eigenproblem for it is solved. This gives both the eigenvalue $\chi_n(\gamma)$ and an expansion representing $Ps_n(z;\gamma)$.

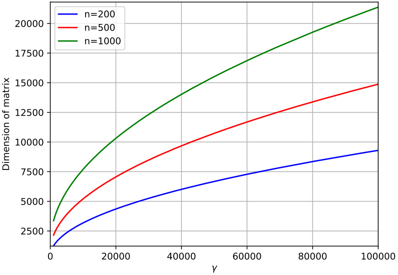
Only solutions satisfying the boundary conditions arise because only their coefficients decay rapidly enough to satisfy the truncated problem.

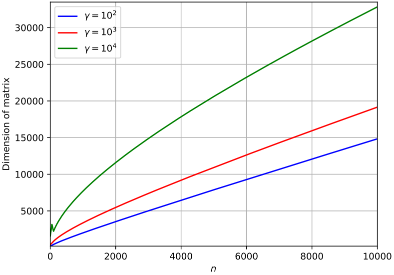
The Osipov-Xiao-Rokhlin algorithm

The dimension of the matrix dictates the running time of the algorithm. From numerical experiments, it is believed to behave as

$$\mathcal{O}\left(n + \sqrt{\gamma n}\right)$$

for large values of the parameters.

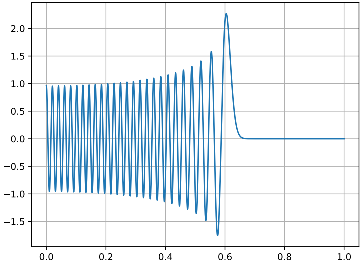


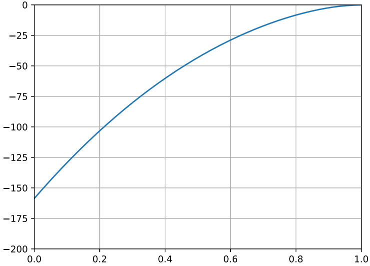


We can do better ...

Like many second order linear ordinary differential equations, the reduced spheroidal wave equation admits solutions whose logarithms can be represented much more efficiently than the solutions themselves.

This is the observation which underlies WKB methods. However, rather than use it to construct asymptotic approximations of $Ps_n(z;\gamma)$, we will simply solve a differential equation to construct the logarithm directly.





$\gamma = 500$ and $n = 100$

Riccati's equation and its variants

If $y(z) = \exp(r(z))$ satisfies

$$y''(z) + q(z)y(z) = 0$$

then r solves the Riccati equation

$$r''(z) + (r'(z))^2 + q(z) = 0.$$

When q is real-valued, r must be of the form

$$r(z) = i\psi(z) - \frac{1}{2}\log\left(\psi'(z)\right)$$

so that

$$u(z) = \frac{\sin\left(\psi(z)\right)}{\sqrt{\psi'(z)}} \quad \text{and} \quad v(z) = \frac{\cos\left(\psi(z)\right)}{\sqrt{\psi'(z)}}$$

are a basis of solutions of the original ordinary differential equation.

We call ψ a phase function for the differential equation.

Riccati's equation and its variants

We refer to

$$m(z) = \frac{1}{\psi'(z)} = \left(u(z)\right)^2 + \left(v(z)\right)^2$$

as a modulus function for the ordinary differential equation since

$$u(z) = \sqrt{m(z)}\sin(\psi(z)) \;\text{ and }\; v(z) = \sqrt{m(z)}\cos(\psi(z))$$

are solutions.

It can be easily verified that m satisfies Appell's equation

$$m'''(z) + 4q(z)m'(z) + 2q'(z)m(z) = 0.$$

Because of the close relationship between the logarithms of solutions, phase functions and modulus functions we can demonstrate the existence of a "well-behaved" logarithm by establishing properties of the corresponding modulus function.

The phase function generated by a pair of solutions

If u, v is a pair of real-valued solutions of

$$y''(z) + q(z)y(z) = 0$$

on the interval I whose Wronskian is 1 then

$$m(z) = (u(z))^2 + (v(z))^2$$

does not vanish on I and any antiderivative of

$$\psi'(z) = \frac{1}{m(z)}$$

is a phase function. Requiring that

$$u(z) = \frac{\sin(\psi(z))}{\sqrt{\psi'(z)}} \quad \text{and} \quad v(z) = \frac{\cos(\psi(z))}{\sqrt{\psi'(z)}}$$

determines ψ up to an additive constant which is an integral multiple of 2π.

The radial spheroidal wave function of the third kind

We define a new solution of the reduced spheroidal wave equation via

$$S_n^{(3)}(z;\gamma) = \frac{\sqrt{\gamma}}{Ps_n(1)} \int_1^\infty \exp(iz\gamma t) Ps_n(t;\gamma)\, dt.$$

It is immediately clear that

$$S_n^{(3)}(z;\gamma) = \frac{\exp(i\gamma z)}{\sqrt{\gamma} z} + \mathcal{O}\left(\frac{1}{z^2}\right) \quad \text{as} \quad z \to \infty,$$

This asymptotic formula suggests that $M_n(z;\gamma) = \left| S_n^{(3)}(z;\gamma) \right|^2$ is well-behaved.

Solutions in Hardy spaces have well-behaved modulus functions

We know that $Ps_n(z;\gamma)$ is regular at 1 and

$$Ps_n(z;\gamma) = C_1 \frac{\sin(\gamma z)}{z} + C_2 \frac{\cos(\gamma z)}{z} + \mathcal{O}\left(\frac{1}{z^2}\right) \quad \text{as} \quad z \to \infty.$$

It follows that $Ps_n(z;\gamma)$ is an element of $L^2(1,\infty)$ and

$$S_n^{(3)}(z;\gamma) = \frac{\sqrt{\gamma}}{Ps_n(1)} \int_1^\infty \exp(iz\gamma t) Ps_n(t;\gamma)\, dt$$

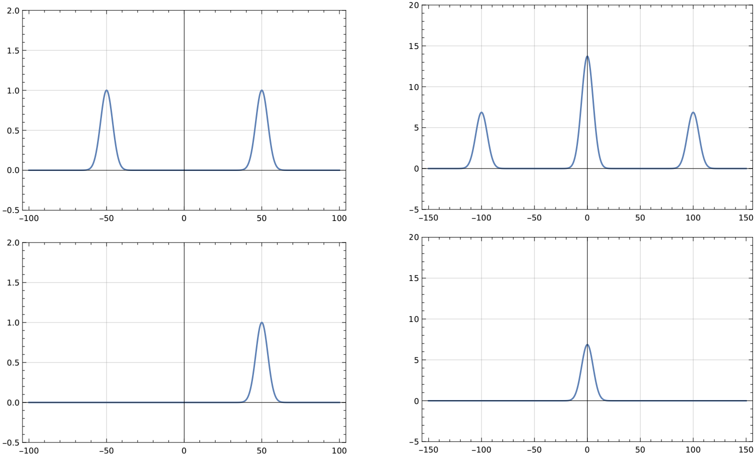
is an element of the Hardy space of functions analytic in the upper half of the complex plane whose boundary values are square integrable.

Solutions of second order differential equations in Hardy spaces generally have nonoscillatory modulus functions.

Solutions in Hardy spaces have well-behaved modulus functions

$$G''(z) + k^2 q(z) G(z) = 0$$

If $G(z) = \int_{-\infty}^{\infty} \exp(izt) f(t)\, dt$ then $|G(z)|^2 = \int_{-\infty}^{\infty} \exp(izt) \left(\int_{-\infty}^{\infty} f(t+s) f(s)\, ds \right) dt$



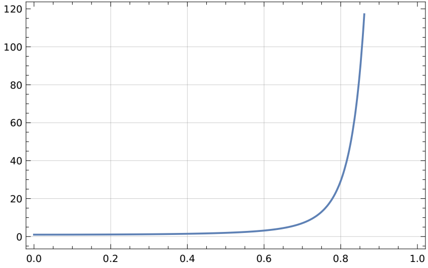
Monotonicity properties of $M_n(z;\gamma)$ and $S_n^{(3)}(z;\gamma)$

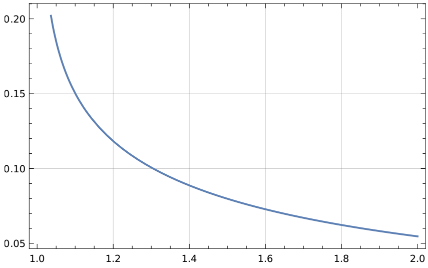
Conjecture

For fixed $\gamma > 0$ and $n \geq 0$, when viewed as a function of z, $M_n(z;\gamma)$ is absolutely monotone on the interval $(0,1)$ and completely monotone on the interval $(1,\infty)$

Conjecture

For fixed $\gamma > 0$ and $n \geq 0$, when viewed as a function of z, $S_n^{(3)}(iz;\gamma)$ is $(n+2)$-times monotone on the interval $(0,\infty)$.





The modulus and phase functions associated with $S_n^{(3)}(Z;\gamma)$

The normal form of the reduced spheroidal wave equation is

$$w''(z) + \left(\frac{1}{(1-z^2)^2} + \frac{\chi_n(\gamma) - \gamma^2 z^2}{1-z^2}\right) w(z) = 0.$$

Its solutions are of the form $y(z)\sqrt{1-z^2}$, where y solves the reduced spheroidal wave equation.

The function $M_n(z;\gamma)(1-z^2)$, where

$$M_n(z;\gamma) = \left|S_n^{(3)}(z;\gamma)\right|^2,$$

is a modulus function for the normal form of the reduced spheroidal wave equation.

The modulus and phase functions associated with $S_n^{(3)}(Z;\gamma)$

We define a phase function $\Psi S_n(z;\gamma)$ via

$$w''(z) + \left(\frac{1}{(1-z^2)^2} + \frac{\chi_n(\gamma) - \gamma^2 z^2}{1-z^2} \right) w(z) = 0$$

via the formula

$$\Psi S_n(z;\gamma) = \int_1^z \frac{1}{M_n(u;\gamma)(1-u^2)}\, du.$$

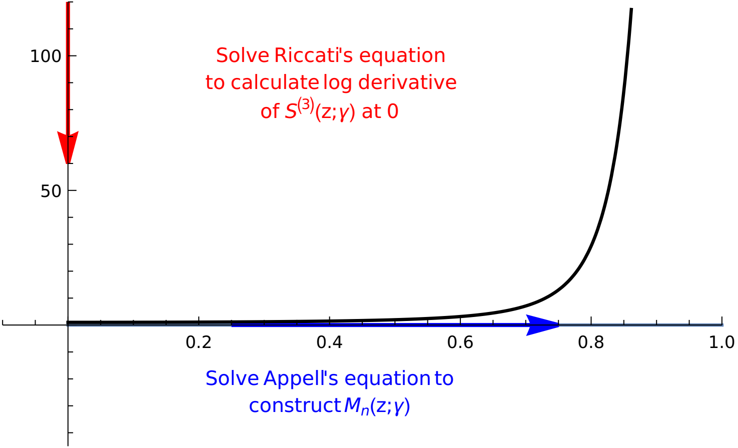
The constant of integration is chosen so that

$$\frac{\sin\left(\Psi S_n(z;\gamma)\right)}{\sqrt{\frac{d\Psi S_n}{dz}(z;\gamma)}}$$

is regular at 1. Since $Ps_n(z;\gamma)$ is also regular at 1, we have

$$Ps_n(z;\gamma)\sqrt{1-z^2} = C_n(\gamma)\frac{\sin\left(\Psi S_n(z;\gamma)\right)}{\sqrt{\frac{d\Psi S_n}{dz}(z;\gamma)}}.$$

Algorithm for constructing $\Psi S_n(z;\gamma)$

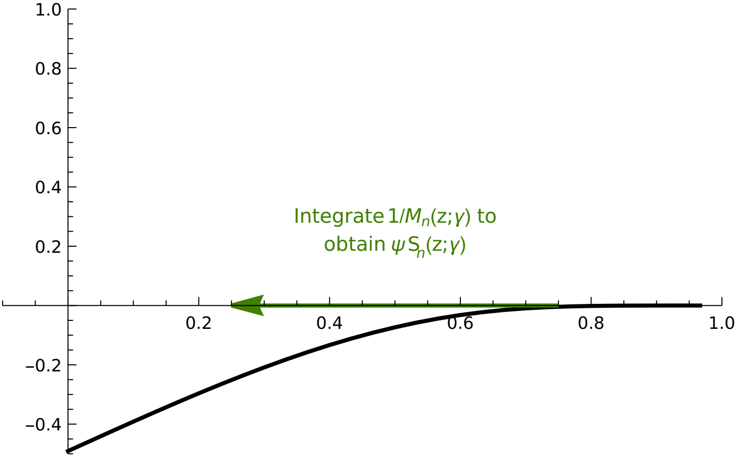


$$\frac{d}{dz}\log\left(S_n^{(3)}(z;\gamma)\right) = i\gamma + \mathcal{O}\left(\frac{1}{z}\right)$$

Functions are represented as piecewise Chebyshev expansions

An adaptive solver suitable for stiff problems is used

Algorithm for constructing $\Psi S_n(z;\gamma)$



$$\frac{d}{dz}\log\left(S_n^{(3)}(z;\gamma)\right) = i\gamma + \mathcal{O}\left(\frac{1}{z}\right)$$

Functions are represented as piecewise Chebyshev expansions

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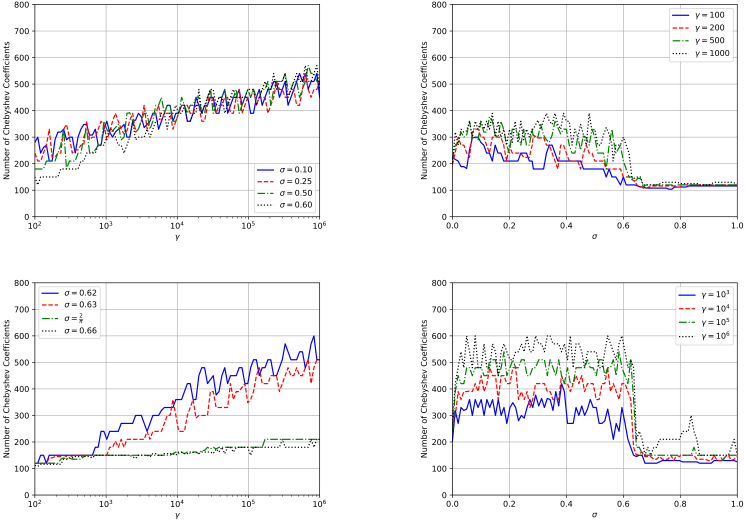
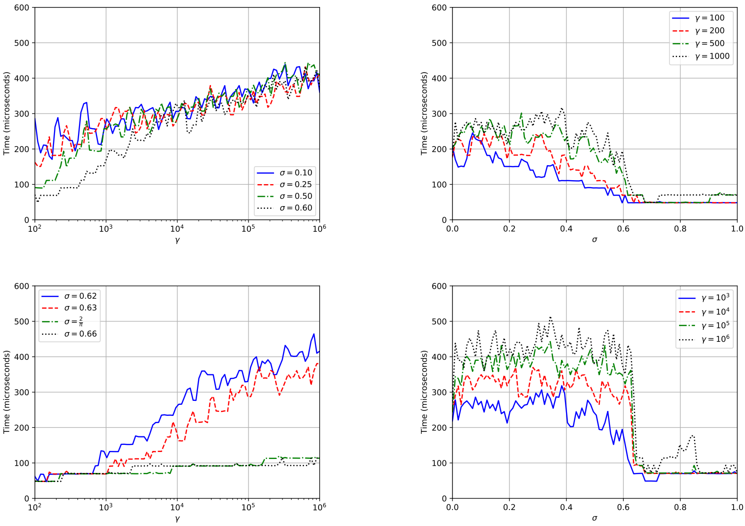
Number of Chebyshev coefficients



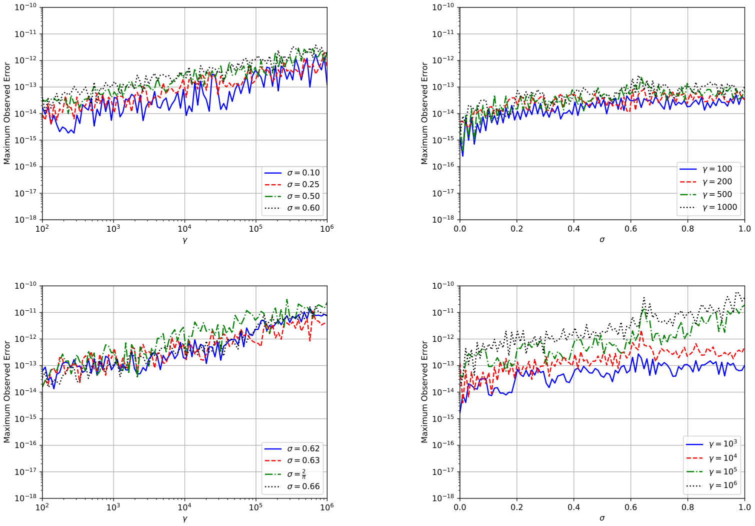
$$n = \gamma\sigma$$

Time in microseconds



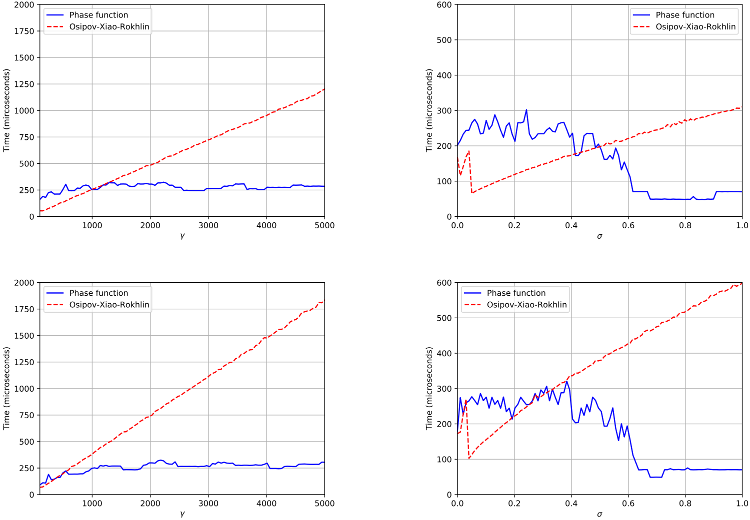
$$n = \gamma\sigma$$

Maximum errors



$$n = \gamma\sigma$$

Comparison with Osipov-Xiao-Rokhlin



Upper left: $\sigma = 0.25$, Lower left $\sigma = 0.50$, Upper right $\gamma = 500$, Lower right $\gamma = 1,000$.

Not so fast ...

The algorithm just described requires knowledge of $\chi_n(\gamma)$.

The standard algorithm for computing $\chi_n(\gamma)$ is the Osipov-Xiao-Rokhlin method, but using it would defeat the purpose of our algorithm.

There are asymptotic estimates for $\chi_n(\gamma)$, but they aren't very accurate.

An obvious brute-force solution: We will precompute a bivariate piecewise polynomial expansion of an analytic continuation $\chi_\tau(\gamma)$ of $\chi_n(\gamma)$.

How do we usually index special functions?

Legendre's differential equation

$$(1 - z^2)y''(z) - 2zy'(z) + \chi y(z) = 0$$

has a regular singularity at $z = \infty$. In particular, there is a solution of the form

$$z^\nu \sum_{k=0}^{\infty} \frac{a_k}{z^{2k}},$$

where $a_0 \neq 0$ and the series converges uniformly in the region $|z| > 1$.

Inserting this expansion into Legendre's differential equation gives us a simple relationship between ν and χ:

$$\chi = \nu(\nu + 1).$$

The standard method for analytically continuing $\chi_n(\gamma)$ is unsuitable

The reduced spheroidal wave equation

$$(1 - z^2)y''(z) - 2zy'(z) + (\chi - \gamma^2 z^2)y(z) = 0$$

has an irregular singularity at ∞. Accordingly, there is a solution of the form

$$z^\nu \sum_{k=-\infty}^{\infty} a_k z^{2k}$$

with the Laurent expansion convergent in $1 < |z| < \infty$.

Inserting this expansion into the differential equation gives a transcendental equation connecting χ and ν. However, there are a countable number of ν associated with each value of χ and a countable number of χ associated with each ν.

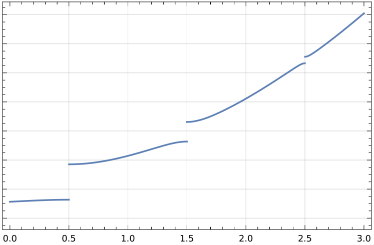
To uniquely associate a value of χ with each ν it is customary to require

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

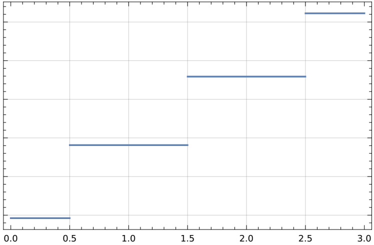
The parameter ν is called the characteristic exponent.

The standard method for analytically continuing $\chi_n(\gamma)$ is unsuitable

Unfortunately, the analytic continuation $\chi_\nu(\gamma)$ obtained in this fashion has branch points at each half-integer value of ν.



$\gamma = 2$



$\gamma = 10$

Phase functions provide a more suitable method

From the formula

$$Ps_n(z;\gamma)\sqrt{1-z^2} = C_n(\gamma)\frac{\sin\left(\Psi S_n(z;\gamma)\right)}{\sqrt{\frac{d\,\Psi S_n}{dz}(z;\gamma)}}.$$

we see that the zeros of $Ps_n(z;\gamma)$ occur at points where the phase function is an integral multiple of π.

It is well known that $Ps_n(z;\gamma)$ has n zeros in $[0,1)$, that $z=0$ is a zero when n is odd, and that $z=0$ is a root of its derivative when n is even.

All of this implies that

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

Phase functions provide a more suitable method

The formula $\Psi S_n(0;\gamma) = -\frac{\pi}{2}(n+1)$ suggests that we define a new parameter

$$\tau_\chi(\gamma) = -\frac{2}{\pi}\Psi S_\chi(0;\gamma) - 1$$

and use it to index the spheroidal wave functions of order zero. This is a noninteger generalization of the concept of the "number of zeros of $Ps_n(z;\gamma)$."

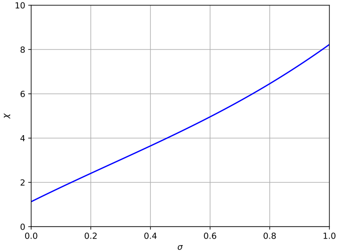
Conjecture

For fixed $\gamma > 0$ and $-1 < z < 1$, when viewed as a function of χ, $\Psi S_\chi(z;\gamma)$ is strictly decreasing on the interval $(0,\infty)$.

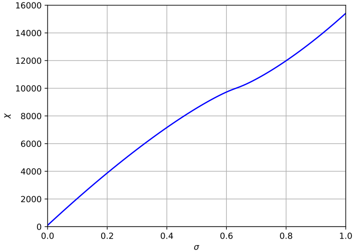
In fact, for reasons which will be clear very shortly, we find it preferable to use the parameter:

$$\sigma_\chi(\gamma) = \frac{\tau_\chi(\gamma)}{\gamma}.$$

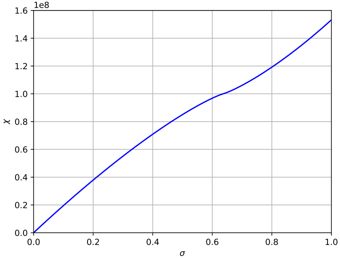
χ as a function of σ



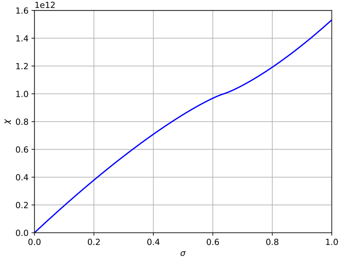
$\gamma = 2$



$\gamma = 100$



$\gamma = 10,000$



$\gamma = 10^6$

The expansion of $\chi_\sigma(\gamma)$

Around 0.75MB of memory are required for an expansion of $\chi_\sigma(z;\gamma)$ which holds for

$$2^6 \leq \gamma \leq 2^{20} \quad \text{and} \quad 0 \leq \sigma \leq 1.1.$$

The range $0 \leq \sigma \leq 1.1$ was chosen because

$$\lambda_m(\gamma) < \epsilon_0 \approx 2.22 \times 10^{-16}$$

for all $\gamma \geq 2^6$ and

$$m = \lfloor 1.1\gamma \rfloor.$$

The time to evaluate this expansion for any pair of the parameters is less than 10^{-7} seconds on a standard desktop computer.

Further work

There is a better strategy which will give an $\mathcal{O}(1)$ algorithm:

- Phase functions should be used to represent solutions in oscillatory regions
- Near turning points the solutions themselves should be constructed
- In the nonoscillatory regime, logarithms of solutions should be used

Rather than precomputing an expansion for $\chi_\xi(\gamma)$ and using it to construct $\mathit{\Psi S}_n(z;\gamma)$ on-the-fly, we should precompute an expansion of $\mathit{\Psi S}_\xi(z;\gamma)$.

The conjectures should be proved and generalized (e.g., similar results hold for any equation which admits a solution which is an element of a Hardy space).

Results regarding monotonicity are nice, but it would be better to have bounds on the number of coefficients needed to represent various functions.

Further work

Many quantities related to special funcitons are defined only on the integers. There is a large body of work on smooth extensions of discrete functions, including classical results (Ramanujan's master theorem, Whitney) and more recent methods (Fefferman, Luli).

The prolate transform

$$T\left[f\right](n) = \int_{-1}^{1} Ps_n(z;\gamma) f(z)\ dz$$

is related to the Fourier integral operator

$$\hat{T}\left[f\right](\tau) = \int_{-1}^{1} \exp\left(i\Psi S_\tau(z;\gamma) - \frac{1}{2}\log\left(\Psi S'_\tau(z;\gamma)\right)\right) f(z)\ dz.$$

Because ΨS_τ is smooth and nonoscillatory, butterfly transforms can be used to rapidly apply $\hat{T}$. The ability to evaluate $\Psi S_\tau(z;\gamma)$ rapidly is essential.