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A Finite-Difference Construction of the Spheroidal Wavefunctions

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Abstract

A fast and simple finite-difference algorithm for computing the spheroidal wave functions is described. The resulting eigenvalues and eigenfunctions for real and complex spheroidal bandwidth parameter, $c$, agree with those in the literature from four to more than eleven significant figures. The validity of this algorithm in the extreme parameter regime, up to $c^2 = 10^{14}$, is demonstrated. The prolate spheroidal functions and the spectral concentration problem in relation to band-limited and time-limited signals is discussed. We review the properties of these eigenfunctions in the context of Sturm-Liouville theory and the implications for a finite difference algorithm. A number of new suggestions for data-fitting using prolate spheroidal wave functions with a heuristic for optimally choosing the value of $c$ and the number of basis functions are described.

Keywords: [Spheroidal wave functions, Slepian functions, Prolate spheroidal wave equation, Eigenvalues, Finite Differences, Matlab, Data Fitting]

1. Introduction

A common problem in the physical and engineering sciences is the expansion of experimental data in different functional bases followed by a minimum least-squares condition for selecting appropriate eigenvalues. In the fields of optics and acoustics, the orthogonal basis of trigonometric functions over $\mathbb{R}$ (i.e. Fourier series) are typically used to reconstruct and analyze physical signals. More generally, the eigenfunctions of the Laplacian operator form
a smooth \((C^\infty)\) orthonormal basis over any compact Riemannian manifold with a boundary. The form of the Laplacian is determined by the geometry of the problem which usually determines the choice of coordinates. The spheroidal wave functions are the eigenfunctions of the Laplacian operator in spheroidal coordinates and have many applications in areas such as acoustic scattering [Sammelmann, 2002], spectroscopy and optical scattering from spheroidal particles [Rysakov and Ston, 2001; Asano, 1979] and the polar gap problem in geophysics [Simons and Dahlen, 2006].

The spheroidal wave functions were originally studied for modeling heat conduction in ellipsoids [Niven, 1880]. More recently, the spheroidal wave functions have been applied to chemistry and quantum mechanics for solving the Schrödinger equation for the hydrogen atom in spheroidal coordinates [Sung and Herschbach, 1991]. Unlike the Legendre polynomials and spherical harmonics, the spheroidal wave functions do not have a simple analytic form such as that provided by Rodrigues’ formula [DLMF, 2012]. Instead, the spheroidal wave functions are typically constructed by expanding in an orthonormal basis for \(L^2(\mathbb{R})\), such as the Legendre polynomials, then numerically solving for the expansion coefficients [Flammer, 1957; Li et al., 1998; Boyd, 2005]. A review of these algorithms is presented in section 3.

Existing algorithms for generating spheroidal wave functions vary in their limitations and complexity of their implementation. We have developed a simple and efficient algorithm for generating the spheroidal functions which is presented in section 3.1. A sample second-order numerical accuracy, Matlab code of the algorithm is included in the Appendix. The motivation for constructing these functions originated from a number of applications in space physics where experimental data obtained over irregularly spaced locations are used to estimate related values over a regular spatial grid. Examples include reconstructing ionosphere electric field data from high frequency (HF: 3-30 MHz) over-the-horizon radars and estimating the auroral electric current using magnetic field perturbation data from the Iridium satellite constellation [Anderson et al., 2000; Waters et al., 2001]. Therefore, the algorithm we developed generates the spheroidal functions numerically at discrete grid points which is appropriate for dealing with experimental data.
2. Prolate Spheroidal Wavefunctions

The prolate spheroidal functions originally studied by Slepian and Pollak [1961] and Slepian [1983] are the real-valued functions that solve the Shannon spectral concentration problem for band-limited functions. The task is to find band-limited functions which are simultaneously maximally localised in the time domain. In particular, for any fixed $W \in \mathbb{R}^+$ we have the Paley-Weiner subspace $B_W \subset L^2(\mathbb{R})$ of $W$-bandlimited functions. These functions are characterised by the bandlimit condition

$$f(t) = \frac{1}{2\pi} \int_{-W}^{W} F(\omega) \exp(i\omega t) \, d\omega, \quad (1)$$

$\forall f \in B_W$, where $F$ is the Fourier transform of $f$

$$F(\omega) = 2\pi \int_{-\infty}^{\infty} f(t) \exp(-i\omega t) \, dt. \quad (2)$$

The spectral concentration problem is to find the square-integrable (finite-energy) function $f \in B_W$ that maximises the ratio

$$\alpha^2(T) = \frac{\int_{-T/2}^{T/2} |f(t)|^2 \, dt}{\int_{\mathbb{R}} \|F(\omega)\|^2 \, d\omega}. \quad (3)$$

Since $f(t)$ is bandlimited, from Eqn. (2) the spectral concentration problem reduces to a Fredholm integral equation of the second kind [Gosse, 2010]

$$\int_{-1}^{1} \frac{\sin(c(\omega - \hat{\omega}))}{\pi(\omega - \hat{\omega})} F(\hat{\omega}) \, d\hat{\omega} = \lambda F(\omega) \quad (4)$$

$\forall \omega \in [-1, 1]$ where the 'prolateness' or 'confinement' factor, $c = WT$ is a product of band-limit and time-limit factors. The eigenvalues $\lambda(c)$ are functions of $c$ and are positive-definite. The kernel $K : R^2 \rightarrow R$ of this integral transform is given by

$$K(\omega, \hat{\omega}) = \chi_{[-1,1]} \frac{\sin[c(\omega - \hat{\omega})]}{\pi(\omega - \hat{\omega})} \quad (5)$$

where $\chi_{[-1,1]}$ is the indicator function which takes the value 1 on $[-1, 1]$ and zero elsewhere. The kernel is continuous and symmetric. From Bochner’s theorem, it is also positive definite [Slepian and Pollak, 1961]. Thus it follows
that the integral operator in Eqn. (4) is compact [Gosse, 2010]. Furthermore, to see that the operator is self-adjoint one can apply Fubini’s theorem. Hence, from the spectral theorem it follows that the spectrum \( \{ \lambda_n(c) \} \) of this operator is countable and the corresponding eigenfunctions, known as the Slepian functions, form an orthogonal basis for \( L^2([-1,1]) \).

The eigenvalues, \( \lambda_n(c) \) are non-degenerate for all real-valued \( c \neq 0 \) so each eigenfunction of Eqn. (4) corresponds to a unique eigenvalue [Slepian and Pollak, 1961]. Furthermore, it turns out that the zeroth order prolate spheroidal function of the first degree, \( S^1_0(t; c) \) corresponds to the largest eigenvalue \( \lambda(c) \) and hence solves the Shannon problem for the maximum energy concentration. The W-bandlimited function orthogonal to \( S^1_0(t; c) \) that gives the next maximal concentration is then the spheroidal function of degree 2, and so forth.

The spectral concentration result was generalized by Rhodes [1970]. For any order \( m > -1 \), the first \( L + 1 \) spheroidal wavefunctions \( S^l_m(\eta; c) \) are the \( L + 1 \) linearly independent functions which are maximally concentrated on the interval \([-1,1]\). This characteristic is important for more general applications of the general order spheroidal wavefunctions. For example, in spheroidal harmonic fitting where the spectral concentration and localisation properties may be desirable.

The terminology, ‘order’ and ‘degree’ are inherited from the Legendre polynomials \( P^l_m(t; c = 0) \) of degree \( l \) and order \( m \). However, for \( c = 0 \) and \( m \neq 0 \), the spheroidal functions reduce to associated Legendre functions of the first kind which are not polynomials [DLMF, 2012]. Likewise, for \( m = 0 \) and \( c \neq 0 \), the spheroidal functions are not polynomials. Therefore, we use the term ‘degree’ loosely when referring to the index, \( l \) of the eigenfunction \( S^l_m(t; c) \).

In addition to being eigenfunctions of an integral operator, the Slepian functions are also the ‘latitudinal’ angular component of the eigenfunctions of the Laplacian in prolate spheroidal coordinates. In particular, the differential equation that they satisfy is a perturbation to Legendre’s differential equation

\[
\left[ \partial_\eta (1 - \eta^2) \partial_\eta + (\lambda_{ml}(c) - c^2 \eta^2 - \frac{m^2}{1 - \eta^2}) \right] S_{ml} = 0
\]  

(6)
where the bandlimit-timelimit product, $c$, has a geometrical interpretation as the 'prolateness' (or ellipticity) of the prolate spheroid surfaces in a prolate spheroidal coordinate system. Geometrically, when $c = 0$ the foci of the spheroids collapse into a single point which is the center of a sphere. Algebraically, it can be seen that for $c = 0$, the prolate spheroidal wave equation reduces to the associated Legendre equation which arises in the construction of the spherical harmonics [DLMF, 2012].

The fact that the Slepian functions are eigenfunctions of both the Sturm-Liouville differential operator in Eqn. (6) and the Shannon integral operator in Eqn. (4) when $m = 0$ is the ‘lucky accident’ that the operators commute if and only if $m = 0$, as discussed by Slepian [1983]. Historically, this has led to the computation of the Slepian functions by expressing them as a linear combination of Legendre polynomials. Therefore, the problem of calculating the Slepian functions and their eigenvalues has typically resulted in recursion-based methods and asymptotic approximations.

Methods that use the property that the Slepian functions are eigenfunctions of the integral operator are complicated by the fact that for large values of the parameter, $c$ the first few eigenvalues are close to unity making the associated eigenfunctions difficult to resolve. Similarly, for all values of $c$, the Slepian functions of order $m \gg c$ are close to zero and the corresponding eigenfunctions are difficult to resolve.

Utilising the Sturm-Liouville form and the speed of modern eigensolver routines, we have developed a simple approach for generating the prolate spheroidal functions over a finite interval. In particular, we discretise the differential equation and solve using the method of finite differences. From our review of the literature, this approach seems to be unique. Furthermore, using this method we generalise the idea of spherical cap harmonics to spheroidal cap harmonics, for which there are presently no constructive algorithms.

2.1. Prolate Spheroidal Coordinates

The prolate spheroidal coordinates are generated by intersecting three mutually orthogonal families of surfaces: prolate spheroids, hyperboloids of revolution and half-planes. The convention used follows that of Sammelmann
The transformation from spheroidal \((\xi, \eta, \phi)\) to Cartesian coordinates \((x, y, z)\) is

\[
x = f \sqrt{(\xi^2 - 1)(1 - \eta^2)} \cos(\phi)
\]
\[
y = f \sqrt{(\xi^2 - 1)(1 - \eta^2)} \sin(\phi)
\]
\[
z = f \xi \eta
\]

(7)

These are related to the elliptic coordinate \((\mu, \nu, \phi)\) definition of the prolate spheroidal coordinates by \(\xi = \cosh(\mu)\) and \(\eta = \cos(\nu)\). Hence \(\xi \geq 1, -1 \leq \eta \leq 1, \phi \in [0, 2\pi]\). The isosurfaces of the radial coordinate \(\xi\) form prolate spheroids centered at the origin with major axis along the z-axis and distance \(2f\) between focii. Similarly, surfaces of constant angular coordinate form hyperboloids of revolution and surfaces of constant azimuthal angle, \(\phi\) form half-planes. A detailed description of the prolate spheroidal coordinate system was given by Sammelmann [2002].

2.2. Prolate Spheroidal Wave Equation

The prolate spheroidal coordinate system is one of eleven coordinate systems in \(\mathbb{R}^3\) where the Laplace and Helmholtz equations are separable. Eigenfunctions of the Laplacian are equivalently in the kernel of the Helmholtz wave operator. Therefore, constructing the prolate spheroidal functions amounts to solving the Helmholtz equation in spheroidal coordinates. Using the expression for the Laplacian in spheroidal coordinates yields

\[
(\nabla^2 + k^2)\psi = \frac{1}{f^2(\xi^2 - \eta^2)} \left[ \partial_\xi (\xi^2 - 1) \partial_\xi \psi + \partial_\eta (1 - \eta^2) \partial_\eta \psi \right]
\]
\[
+ \frac{(\xi^2 - \eta^2)}{(\xi^2 - 1)(1 - \eta^2)} \partial_\eta^2 \psi + c^2(\xi^2 - \eta^2)\psi \right] = 0.
\]

(8)

The parameter, \(c\) is a geometric constant related to the bandwidth of the resulting angular functions. In particular, \(c = fk\) where \(k\) is the wavenumber and \(f\) is the semi-focal length defined in Eqn. (7). Using separation of variables, \(\psi = R(\xi)S(\eta)\Phi(\phi)\) and applying partial fractions

\[
\left[ \partial_\xi (\xi^2 - 1) \partial_\xi - (\lambda_{ml}(c) - c^2 \xi^2 + \frac{m^2}{\xi^2 - 1}) \right] R_{ml} = 0
\]

(9)

\[
\left[ \partial_\eta (1 - \eta^2) \partial_\eta + (\lambda_{ml}(c) - c^2 \eta^2 - \frac{m^2}{1 - \eta^2}) \right] S_m = 0
\]

(10)

\[
\left[ \partial_\phi^2 + m^2 \right] \Phi_m = 0.
\]

(11)
The spherical harmonic complex exponential (sinusoidal) solutions are obtained for the azimuthal component giving the usual Fourier basis for $L^2(S^1)$. The periodicity requirement, $\Phi_m(0) = \Phi_m(2\pi)$ forces the condition $m \in \mathbb{Z}$. The solutions $S_{lm}$ to the angular component in Eqn. (10) are referred to as the ‘prolate spheroidal wavefunctions’.

The differential equations (9), (10) and (11) are in Sturm-Liouville form. However, the radial component of Eqn. (9) is singular since its domain $[1, \infty)$ is unbounded. The domains $[-1, 1]$ and $[0, 2\pi]$ for the angular and azimuthal eigenfunctions are bounded. It follows from Sturm-Liouville theory that the eigenfunctions $S_{lm}$ and $\Phi_m$ form an orthogonal basis for the $L^2$ Hilbert spaces over their domains. Therefore, the product of the angular functions, the spheroidal harmonics, $S_{lm}\Phi_m$, form an orthogonal basis over the product domain, i.e. the prolate spheroid $S^1 \otimes E$, where $E$ is the ellipse described by $\eta \in [-1, 1]$.

Eqn. (10) is a perturbation to the Associated Legendre equation with the extra term $c^2\eta^2$. Setting $c = 0$ corresponds to setting the focal length of the spheroids to zero, which collapses them back into spheres. Hence, the quantity $f\xi$ becomes the radial quantity $r$ as $c \to 0$ and the resulting differential equations (9), (10) and (11) become those for spherical Bessel functions and the spherical harmonics, respectively. In particular, setting $c = 0$ returns Eqn. (10) to the associated Legendre equation with eigenvalues given by $\lambda_{lm}^l = l(l + 1)$. Both $l$ and $m$ are integers for solutions over the full sphere while $l$ is non-integer for solutions over a spherical cap or spherical ring. For the Legendre equation, the eigenvalues are ordered starting from $l = 0$ with increasing $l$ and for full sphere solutions, the integer parameter $m$ is restricted by $l$ such that $-l \leq m \leq 1$.

When $c \neq 0$, the eigenfunctions and eigenvalues of Eqn. (10) can still be indexed by $l$ since Sturm-Liouville theory guarantees that the eigenvalues are real and form a positive, increasing sequence. Furthermore, for small values of the prolateness factor, $c$ the prolate spheroidal eigenfunctions are very similar to the corresponding associated Legendre functions. This suggests that using $l$ to label the eigenvalues $\lambda_{lm}(c)$ of Eqn. (10) in order of increasing size creates a sensible indexing of the prolate spheroidal functions $S_{lm}(\eta; c)$.

When $m = 0$, the differential operator for the prolate spheroidal wave
equation of Eqn. (10) commutes with the integral operator [Slepian, 1983]. Thus, the bandlimited Slepian functions are a special case of the prolate spheroidal functions. In particular, for \( m = 0 \) the spheroidal functions possess a remarkable double orthogonality property [Slepian and Pollak, 1961]. In fact, the double orthogonality also holds for positive integer orders \( m = 1, 2, 3... \) as shown by Rhodes [1970]. They form orthogonal bases for both \( L^2([-1,1]) \) and band limited functions \( B_W \) for some band limit, \( W \) [Zayed, 2007]. For prolate spheroids with a geometric factor \( c \), we have \( W = c/T \) where \( T \) is the time limit of the functions.

The prolate spheroidal functions are somewhat unique in the sense of their double orthogonality. However, the periodic Mathieu functions possess double orthogonality [Rhodes, 1970]. More recently a method for generating other systems of orthogonal functions with the double orthogonality property was developed that showed the oblate spheroidal eigenfunctions are orthogonal on \((-1,1)\) and along the imaginary axis \(i\mathbb{R} \) [Zayed, 2007]. This result may be related to the fact that the prolate and oblate spheroidal differential equations are equivalent under the isomorphism \( c \to ic \), which replaces \( c^2 \) by \(-c^2\).

3. Constructing Prolate Spheroidal Wavefunctions

Spheroidal harmonics \( Y_{lm}(\eta,\phi;c) \) (similar to spherical harmonics) can be generated by multiplying the angular solutions \( S_{lm}(\eta;c) \) by the azimuthal functions \( \Phi_m(\phi) = \Phi_m(0)e^{im\phi} \). Although the radial functions \( R_{lm}(\xi;c) \) are not of interest here, the radial and angular differential equations (9) and (10) are isomorphic under the interchange \( \xi \leftrightarrow \eta \). Therefore, the radial functions can be seen as an analytic continuation of the angular functions to the domain \( \eta \in (1,\infty) \). Using this observation, the radial functions can be constructed either by expanding them in terms of the angular functions or expanding them as spherical Bessel functions [Sammelmann, 2002; Falloon, 2001].

The usual approach for generating the spheroidal wavefunctions is to expand them in an orthogonal basis for the Hilbert space \( L^2(-1,1) \) and solve for the expansion coefficients. The most common choice of basis involves expansion in terms of an infinite series of associated Legendre polynomials [Flammer, 1957; Boyd, 2005; Hogan and Lakey, 2012]. The coefficients for expansion are then found by recursion. However, solving for the spheroidal
eigenfunctions in this manner requires the solution of a transcendental equation. A more numerically robust method, presented by Abbott [1997] is to solve for the expansion coefficients by finding the eigenvectors and eigenvalues of a symmetric tri-diagonal matrix. This method has the advantage of being readily generalized to a complex-valued prolateness factor, c [Sammelmann, 2002].

Another class of methods used for solving the spheroidal wave equation is the ‘shooting-method’ schemes based on Newton-interpolation. A typical example is the ‘sfroid’ algorithm presented in Chapter 17.4 of Press et al. [1992]. The resulting eigenfunctions and eigenvalues agree to within a few digits in comparison with the results of Flammer [1957] and Li et al. [1998].

Traditional approaches to generating the spheroidal wavefunctions have some important limitations. For large |c|, the recursion or Newton-interpolation methods tend to fail. Newton’s method, claimed to be capable of producing spheroidal eigenvalues to an accuracy of ‘100 significant digits or more’ [Li et al., 1998] becomes inaccurate and impractical for $c^2 > 1000$. Barrowes et al. [2004] used an asymptotic expansion to generate spheroidal wave functions for $|c|^2 \leq 8 \times 10^4$. The algorithm we present here can handle $|c|^2$ as large as $10^{14}$.

4. Finite Difference Solution Method

The finite difference strategy for constructing the spheroidal wavefunctions arises quite naturally given the Sturm-Liouville formulation of the problem. The eigenvalue problem from the prolate spheroidal wave equation is

$$\left[ \partial_\eta (1 - \eta^2) \partial_\eta + \left( -c^2 \eta^2 - \frac{m^2}{1 - \eta^2} \right) \right] S_m^l = \lambda_{ml}(c) S_m^l, \quad (12)$$

Discretise Eqn. (12) to any desired order. We use the method of finite differences. In order to facilitate this process for high order schemes which require multiple formulae for discretisation about successive points near the boundaries, we developed a matrix algorithm to compute the finite difference formulae for arbitrary order using any number of grid points.

For a discrete grid of $N + 1$ points, Eqn. (12) is satisfied on the $N - 1$ interior points. At the boundary we apply Sturm-Liouville boundary conditions.
The Dirchlet; $S^d_{m}(0; c) = S^d_{m}(N+1; c)$, Neumann; $S^d_{m}(0; c) = S^d_{m}(N+1; c)$ or mixed boundary conditions may be used according to the application. Given a domain, the boundary conditions and specific values for $m$ and $c$, the first $N-1$ eigenfunctions of Eqn. (12) and their corresponding eigenvalues, $\lambda^d_{m}(c)$ may be generated, ordered in magnitude by the degree\(^1\).

Appendix A contains Matlab source code for a second order finite difference algorithm for solving the spheroidal wave equation. Higher order finite difference schemes, such as the 8th-order scheme used to generate the results in this paper are easily extended from this code. The algorithm gives the option of Dirichlet or Neumann boundary conditions and the ability to specify an arbitrary domain, giving the option of generating spherical and spheroidal cap harmonics. The parameters, $c$ and $m$ are adjusted by the user and the code can solve for complex-valued $m$ and $c$. The eigenvalue problem is converted to a matrix eigenvalue problem which calls the eigensolver routines available in modern programs such as Matlab or Interactive Data Language (IDL).

Although the algorithm solves for the first $N − 1$ eigenfunctions, only the first $\frac{N-1}{2}$ eigenfunctions are usable for a mesh with $N + 1$ points. In practice, due to numerical rounding error typically only the first $\frac{1}{5}(N − 1)$ eigenfunctions are acceptably accurate. The discretisation error in the finite difference formula for a $k$th order scheme with a grid spacing $h$ is proportional to $h^k$. Increasing the number of grid points, $N$ increases both the accuracy of the results and the number of usable eigenfunctions.

One important feature of the algorithm is that the eigenfunctions which are returned by the numerical solver do not have any particular normalisation. One may simply use a numerical integration method such as the trapezoidal rule, or Boole’s 5th order rule [Press et al., 1992] to divide the eigenfunctions by their $L^2$ norm. The resulting eigenfunctions will then be orthonormal with respect to the standard $L^2$ norm over their domain. Our algorithm allows the user to select values of the order $m$ and spheroidal $c$ pa-

---

\(^1\)The indexing begins at $l = 1$. However, in comparison to the Legendre polynomials, the first eigenfunction is technically degree 2 since it has two zeros over its domain. Nonetheless, we have conformed here to the convention employed in the literature.
rameters. The algorithm will also solve the differential equation for complex $m$.

5. Results

The results were obtained using an 8th-order version of the Matlab code listed in Appendix A with 20,001 grid points.

5.1. Eigenvalues for real-valued spheroidal parameter, $c$

Table 1 shows the computed eigenvalues of the spheroidal wave functions for real valued parameter, $c$. Most of our eigenvalues agree with results in the literature to an accuracy of between five and eleven or more significant figures. A grid size of 20,001 points is not necessary to obtain this level of accuracy. There was no difference in the number of accurate significant figures when $N$ was reduced to 8001 points. Furthermore, if we run our algorithm with 1001 grid points using Matlab 2011b, the computation reproduces the eigenvalue corresponding to $l = 2, m = 2, c^2 = 0.1$ with an accuracy of more than ten significant figures compared with the results of Li et al. [1998].

There appears to be an error in the eigenvalue recorded by Li et al. [1998] for $l = 11, m = 4, c^2 = -1$ in the form of an additional zero in the third decimal place. Without this zero, our results agree to at least eleven decimal places. Increasing the grid size has no effect on the first nine significant figures which appear to be stable and accurate.

<table>
<thead>
<tr>
<th>$l$</th>
<th>$m$</th>
<th>$c^2$</th>
<th>Flammer $\lambda_{m}^l(c)$</th>
<th>Numerical Recipes $\lambda_{m}^l(c)$</th>
<th>Li et al $\lambda_{m}^l(c)$</th>
<th>$0(h^2)$ FD scheme $\lambda_{m}^l(c)$</th>
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<tr>
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<td>4</td>
<td>-1</td>
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<td>2</td>
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<td>37.0135</td>
<td>36.996 267 50</td>
<td>36.996 267 483 327 900</td>
</tr>
</tbody>
</table>

Table 1: Comparison of spheroidal eigenvalues for real-valued parameter, $c$. 


<table>
<thead>
<tr>
<th>l</th>
<th>m</th>
<th>c</th>
<th>Barrowes et al $\lambda^c_m(c)$</th>
<th>$0(h^8)$ FD scheme $\lambda^c_m(c)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0</td>
<td>(1+i)20</td>
<td>19.2453281 + 20.049941i</td>
<td>19.245328130215245 + 20.064994147104926i</td>
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<tr>
<td>3</td>
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<td>58.2267144e + 60.0256155i</td>
<td>58.226714355451151 + 60.025615481889362i</td>
</tr>
<tr>
<td>3</td>
<td>1</td>
<td>20√2 e^{67.5°}</td>
<td>11.0776528 + 26.1296172i</td>
<td>11.07765281339274 + 26.129617504573941i</td>
</tr>
<tr>
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<td>4.23515050e+02 + 7.34845178e+02i</td>
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</tr>
<tr>
<td>5</td>
<td>3</td>
<td>200√2 e^{30°}</td>
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Table 2: Comparison of spheroidal eigenvalues for complex valued parameter, $c$.

### 5.2. Eigenvalues and eigenfunctions for complex $c$

Table 2 shows the solutions for various values of complex $c$. In all cases, our eigenvalues are at least as accurate (9 significant figures) as the eigenvalues obtained by the asymptotic methods of Barrowes et al. [2004]. In order to further test the accuracy of the spheroidal eigenvalues produced by our algorithm, we ran a 2nd order grid with 1001 points and an 8th order grid with 20,001 points for comparison. The branching of the eigenvalues in the complex plane is easily handled by the finite difference algorithm.

Figure 1 shows a selected set of eigenfunctions for complex valued $c$. The real part of the spheroidal wavefunctions with $m = 0$ and $c = 20(1 + i)$ follow a similar shape to the prolate wavefunctions with a real-valued prolate factor $c = 20$. The difference is that for the complex case, the real part of the spheroidal wavefunctions gain an additional pair of side-lobes, which are smaller in size compared with the usual turning points in the real $c$ case. The real part of the $l = 1$ eigenfunction has $1 + 2$ turning points. For $l = 2$ we have $2 + 2$ turning points and so forth. Plotting the subsequent functions, one finds that this trend continues past $l = 4$. These complex eigenfunctions may differ by up to a complex phase factor compared to those generated by other programs or routines. Therefore, the figures and qualitative descriptions for the complex eigenfunctions we have given are specific to the eigensolver routine used in Matlab 2011b.
Figure 1: Spheroidal Wavefunctions for complex size parameter, $c = 20(1 + i)$, generated with an $O(h^8)$ finite difference scheme with 4001 grid points.

<table>
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<th>$\eta$</th>
<th>$\lambda_{lm}(c)$</th>
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<td>0.05</td>
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</tr>
</tbody>
</table>

Table 3: Eigenvalues for large $|c|$. 

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5.3. Eigenvalues and eigenfunctions for $|c| \geq 1000$

Table 3 shows the eigenvalues computed by our algorithm for large, real valued $c$. The results agree with those obtained by Falloon [2001] with an accuracy of eight to eleven decimal places for an 8th-order differencing scheme with $N=1,001$ points. Therefore, our results also agree with Slepian and Sonnenblick [1965]. With the smaller grid, the computation time on a 2.8 GHz personal computer was of the order of 10 seconds. However, unlike Falloon’s method, this amounts to the computation of the first 499 eigenfunctions of the prolate spheroidal wave equation.

Table 3 shows that our algorithm can handle values of $|c|$ as large as $10^7$, which to our knowledge is the largest magnitude of $|c|$ for which the prolate spheroidal wavefunctions have been computed. This corresponds to a $c^2$ value of $10^{14}$. In this particular example, we have computed the eigenvalues for $m = 0$ which are the Slepian functions. For such large values of $|c|$, comparisons with published values are not possible. However, we are confident the values in Table 3 are valid for a number of reasons.

Our results for $c = 1000$ agree with those of Falloon [2001]. Starting from $c = 100$ the same pattern occurs in the results of both Falloon and ours. In particular, up to the fourth or more decimal place, increasing $c$ by a factor of 10 corresponds to increasing the eigenvalues by a factor in
10, i.e. the eigenvalues in the asymptotic range of large \( c \) increase linearly with \( c \). This observation corresponds to the analytic result that as \( c \to \infty \), the \( l \)th prolate function \( S_{lm}(c) \) approximates a scaled version of a Hermite polynomial. Furthermore, the \( l \)th eigenvalue of the associated differential operator is asymptotically [Boyd, 2004]

\[
\lambda_l(c) = (2l + 1)c - (l^2 + l + 3/2)/2 + O(1/c).
\] (13)

Hence, for a fixed order, \( l \) the eigenvalues \( \lambda_l(c) \) increase linearly with \( c \) for large \( c \). Numerically we see that this occurs at around \( c = 100 \). We see this trend in our results up to \( c = 10^7 \).

The eigenfunctions up to \( c = 10^7 \) retain the same general shape while becoming confined to an increasingly narrow interval, representing localisation of signal energy and narrowing of the bandwidth. Furthermore, the eigenfunctions we obtain retained their Sturm-Liouville properties. The \( l \)th eigenfunction had \( l \) turning points and zeros of successive eigenfunctions retained their alternating property in accord with the Sturm Separation Theorem. This is illustrated in Figure 2 where the general shape of the first few prolate spheroidal wavefunctions of order zero are similar to the first few Legendre polynomials but with Dirichlet boundary conditions \( S_{lm}(\pm 1; c) = 0 \). For this relatively small value of \( c \), the functions are not significantly ‘squashed’ into a narrow interval. Figure 3 shows that for \( c = 10^4 \) the spheroidal functions retain the same shape shown in Figure 2, except that the functions are now confined to the domain \((-0.15, 0.15)\). For much larger \( c \) we have \( c = 10^6 \) \((c^2 = 10^{12})\) in Figure 2 and the spheroidal functions are now confined to the interval \((-0.005, 0.005)\).

Apart from the confinement of the eigenfunctions, the only thing that differs in these graphs is the sign of the eigenfunctions where some sets are reflected about the horizontal axis. This is a consequence of the eigensolver routine, which sometimes returns the negative of a set of eigenfunctions.

### 5.4. Spheroidal Cap Harmonics

A further advantage of our Sturm-Liouville algorithm is the ability to provide a set of basis functions and eigenvalues over a spherical cap or over a latitudinal belt (spherical annulus) often used in geodesy [Haines, 1985] and in space physics [Green et al., 2006; Waters and Sciffer, 2008]. A spherical
Figure 2: Spheroidal wavefunctions generated with an $O(h^8)$ finite difference scheme.
Figure 3: Spheroidal wavefunctions generated with an $O(h^8)$ finite difference scheme and 20,001 grid points.
Figure 4: Spheroidal wavefunctions generated with an $O(h^8)$ finite difference scheme and 20,001 grid points.
cap is obtained by restricting the latitude domain. For experimental data over the Earth surface, the cap does not need to be centred on a geographic pole since spherical coordinate transformations can be applied to shift the basis function ‘pole’. The resulting eigenfunctions have non-integer $l$ degree [Haines, 1985].

A spherical cap domain may also be defined over a spheroid to give spheroidal cap harmonics. Since the caps or latitudinal belt of the spheroid are submanifolds of the spheroid with a boundary it follows that for the set of spheroidal cap harmonics (with fixed parameter, $c$) from the same boundary conditions form an orthonormal basis for the Hilbert space of $l^2$ functions over the spheroidal caps or belts. Eigenfunction sets for different combinations of the boundary conditions are not necessarily orthogonal across these sets. Due to the extra parameter, $c$ that governs the confinement of the spheroidal functions in the spatial and spectral domains, the spheroidal cap harmonics can be tailored to any given set of data over more complex area shapes compared with the spherical cap harmonics, which are designed for data over a sphere.

In the often cited work on spherical cap harmonics for Earth sciences, hypergeometric functions were used to analytically calculate the spherical cap harmonics [Haines, 1985]. However, this method is limited to small order due to precision limitations in computers. Subsequently, a finite difference method was used to obtain higher order spherical cap basis functions over a spherical annulus domain by Waters and Sciffer [2008]. Thus, the computational method presented here is a natural extension of the finite difference scheme employed by Waters and Sciffer [2008] to the case of prolate and oblate spheroids. One simply has to replace the section of code generating the angular component of the spherical cap harmonics with the present algorithm for generating the spheroidal wavefunctions. To our knowledge, an analytic computation of the spheroidal cap harmonics has not yet been explored.

In preliminary tests, we generated the spheroidal cap harmonics numerically and successfully tested conditions such as orthogonality. Furthermore, we performed a least squares, singular value decomposition (SVD) based fit to a 2-dimensional Gaussian function using the spheroidal harmonics for a range of $c$ parameters (including $c = 0$). We found that in this particular
case, using a second order finite difference scheme the spatially confined geometry of the Gaussian was reflected in the improvement of the RMS error from 0.27 for \( c = 0 \) (spherical harmonics) to 0.198 for \( c = 30 \). A more rigorous comparison for random test data and experimental data, perhaps with the suggested fitting criteria described below, is future work.

5.5. An algorithm for choosing the value for \( c \)

Although data fitting comparisons have been made between the spheroidal wavefunctions and the classical families of orthogonal polynomials, there has been little in the way of designing a criterion for choosing the optimal prolate factor, \( c \). Here we outline a procedure for an a-priori criterion for choosing the values for \( c \), given any set of data one wishes to model using the prolate spheroidal functions.

Given a set of data \( X \), the first task is to determine the approximate data bandwidth. One method is to take a Fast Fourier Transform, \( \mathcal{F}(\omega) \), of the data and numerically integrate \( |\mathcal{F}(\omega)|^2 \) over the entire domain. Next, compare the value, \( E_i \), of this integral to the value \( E_i \) of the integral over smaller domains \( D_i = [-W_i, W_i] \)

\[
\int_{-W_i}^{W_i} |F(\omega)|^2 d\omega = E_i \tag{14}
\]

We then set a tolerance parameter, say \( \epsilon = 0.05 \), for which \( \frac{E - E_i}{E} < \epsilon \). The value \( W_i \) corresponding to \( E_i \) is then the approximate bandwidth of the data, \( X \). The process of choosing the intervals \( D_i \) might be aided by focussing on intervals where the amplitudes \( |\mathcal{F}(\omega)|^2 \) are greater than a certain fraction of the maximum amplitude.

One can similarly determine the approximate time limit, \( T \) of time series data, \( X \) by integrating \( |X|^2 \) over its entire domain. Thus, the resulting estimate for the value of \( c \) which optimally fits the spheroidal functions \( S_{l,m}(\eta; c) \) to the data is given by \( c = WT \) with \( W \) and \( T \) estimated by the above procedure. Refinements for the choice of \( c \) may also involve calculating the RMS errors from fitting the data with spheroidal basis functions across a range of \( c \) close to the initial estimate. The value of \( c \) which minimizes the RMS error is then the \emph{a posteriori} refinement for the choice of \( c \).
A process for estimating $N$, the number of spheroidal functions required to fit a set of data is also required. To this effect we employ the heuristic “2 WT theorem” explained by Slepian [1983]. Given a set of data $X$ with the time limit, $T$ and band limit, $W$ determined as above, the $2WT$ theorem states that the Shannon number $2C = 2WT$ is approximately equal to the dimension of the Payley-Weiner subspace of $W$-band limited functions. Therefore, as an initial estimate, one could choose $N = 2C = 2WT$ as the number of spheroidal functions to use for fitting the data.

In practice, one may wish to use more basis functions than given by the estimate $2WT$. Whether this is necessary may be determined by examining the RMS error of the fit, when using extra basis functions. Conversely, since the data can be represented as the coefficients of expansion in the spheroidal function basis, one can compress their data from say, a set of 1000 values to a set of 20 expansion coefficients. Therefore, one may also wish to choose a smaller value of $N$ for applications where data compression is desirable.

Implicit in the estimates of $c$ and $N$ is the assumption that the data is approximately bandlimited. As noted by Slepian [1983], all real world signals are both band limited and time limited due to the origin of the signals and also the discrete nature of measuring instruments. In this manner, the spheroidal wavefunctions and the spheroidal harmonics may provide a more appropriate basis set to fit real-world data compared with the traditional families of orthogonal polynomials [Moore and Cada, 2004; Gosse, 2010].

6. Discussion

The results of our algorithm compare well with results published in the literature for non-zero values for $m$. For the case $m = 0$ and $c \in \mathbb{R}$ Flammer [1957], Li et al. [1998] and Press et al. [1992] do not provide eigenvalues for comparison. This case is of importance since the spheroidal wavefunctions reduce to the Slepian functions for $m = 0$ which gives maximal energy concentration over the unit interval $[-1, 1]$.

Our computed eigenfunctions for fixed Dirichlet boundary conditions agree with those in Figure 6.4 of Falloon [2001] for non-zero $m$. Likewise, our eigenvalues for complex $c$ with $m = 0$ agree with those of Barrowes et al.
[2004] to at least 9 significant figures. However, comparing the work of Gosse [2010] in the case of real $c$ with $m = 0$ we see that the $m = 0, c = 7$ case (Figure 1) eigenfunctions do not seem to satisfy plain Dirichlet or Neumann boundaries. Yet when $c = 27$, Figure 2 of Gosse [2010] shows that the prolate functions essentially satisfy Dirichlet boundary conditions as they decay to zero at $\eta = \pm 1$.

For the case $m = 0$, one can see that the energy or norm-confining property of $c$ acts to force the Slepian functions to decay to zero at the boundaries for sufficiently large $c$, within numerical limits. Therefore, even if one wishes to recover the standard Slepian functions for $m = 0$, the boundary conditions do not seem to be an issue for our algorithm provided that say, $c \geq 27$ using Gosse [2010] as a guide or $c \geq 10$ when comparing with the mathematica code of Falloon [2001]. Nonetheless, the prolate spheroidal wavefunctions still retain their double orthogonality and extremal (energy concentration) properties for non-zero $m$ [Rhodes, 1970].

As solutions to a Sturm-Liouville problem, the functions produced by our algorithm for $m = 0$ still form a complete set over $[-1,1]$. Hence, unless one specifically wants a set of functions in agreement with the standard Slepian functions for small prolate factor $c$, the boundary conditions do not appear to be a major limitation of our algorithm. However, for the specific case of imaginary $c$ with $m = 0$, the standard oblate spheroidal eigenfunctions approach $\pm \infty$ at the boundaries, a behaviour that is not exhibited by our eigenfunctions when using Dirichlet boundaries.

7. Conclusion

The finite-difference algorithm for constructing the spheroidal wavefunctions presented in this paper has several useful features. The eigenfunctions are not normalized and hence they can be numerically normalized by using the preferred scheme of the user. The algorithm was derived from the Sturm-Liouville formalism which allows one to implement an arbitrary mix of Dirichlet and Neumann boundary conditions, a flexibility which can be tailored to the particular problem. One disadvantage is that for $m = 0$ and small real-valued $c$, the boundary conditions implemented in our algorithm do not agree with the standard Slepian functions. However, their important
properties (completeness, double orthogonality and spectral-concentration) are preserved [Rhodes, 1970].

In addition to the normalisation and boundary condition flexibility, our algorithm has been tested for a wide range of parameters including complex order $m$ and complex geometric parameter, $c$. Furthermore, for the case of real and complex valued $c$, with real order $m$, our results are in excellent agreement with those of Barrowes et al. [2004], with an agreement of at least 9 significant figures.

For the extreme parameter regime, with $c^2$ as large as $10^{14}$, we analysed the characteristic properties exhibited by the eigenfunctions, which were found to be in agreement with the behaviour demanded by Sturm-Liouville theory. Furthermore, we identified the linear trend in the eigenvalues for large $c$, found to agree with Falloon [2001] and the asymptotic expression for the eigenvalues of the spheroidal wave equation [Boyd, 2004]. Therefore, our algorithm accurately generates the prolate spheroidal eigenfunctions in the asymptotic regime of $c = 100$ to $c = 10^7$. For even larger values of $c$, one would require a finer mesh (more than 20,000 grid points) to accurately generate the eigenfunctions and eigenvalues of the prolate spheroidal wave equation.

Using the finite difference, discretised algorithm, one can generate larger and more accurate sets of eigenvalues and eigenfunctions by using larger grids, at the expense of computation time. Using higher order schemes, one may also achieve an improvement in accuracy. In general, the trade-off may be negligible. For a true $n$th order finite difference scheme, one would require at least $n^2 + n + 1$ lines of code to construct the finite-difference coefficient matrix with Dirichlet boundary conditions. For Neumann boundary conditions, one would require $(n+1)^2 + (n+1)$ equations, $(n+1)^2$ for the boundary terms, and $n + 1$ for the central differences.

Since our algorithm relies on the discretisation of the spheroidal Laplacian it is well suited to any physical or mathematical application that requires a discrete set of data to be fitted using a spheroidal function basis. In particular, the discrete eigenfunctions can be interpolated to match the grid on which the data is defined and the accuracy can be tailored by adjusting grid size and using interpolation routines.
In this paper we have introduced the idea of spheroidal cap harmonics as a generalisation of spherical cap harmonics, with their application to data fitting. Since our algorithm can solve over arbitrary finite domains it can be used to construct a complete set of eigenfunctions over a spheroidal annulus (belt) or the caps of a spheroid. Furthermore, because of the extra $c$ parameter which governs the confinement of the prolate spheroidal functions, the spheroidal harmonics and spheroidal cap/belt harmonics can be tailored to a given experimental data set compared with the spherical harmonics. As an example, we found that using a Hilbert-space basis of prolate spheroid functions with $c = 30$, resulted in a more accurate reconstruction of a 2-D Gaussian than the usual spherical harmonics.

Finally, as an extension to the idea of data fitting using spheroidal cap/belt harmonics, we provided a heuristic criterion for optimally selecting the $c$ parameter to fit any given set of data. These criteria were derived from the mathematical properties and estimates such as the 2WT theorem, originally proved by Slepian [1983]. Overall, our algorithm provides a versatile, robust and simple method for numerically constructing the spheroidal wavefunctions.
Appendix A. Second Order Finite Difference Algorithm

The code presented here is a second order finite difference approximation to the eigenvalue problem

\[
(\partial_\eta (1 - \eta^2) \partial_\eta + (-c^2 \eta^2 - \frac{m^2}{1 - \eta^2})) S_{ml} = \lambda_{ml}(c) S_{ml}
\]  

(A.1)

from Eqn. (10). The numerical package in Matlab called by the "eig" function utilises a QR algorithm to solve the eigenproblem in the complex plane. After generating the eigenfunctions, they must be normalized numerically using the preferred normalization scheme of the user. The constant eigenfunction corresponding to \( l = 0 \) must be inserted manually.

Depending on the required accuracy, this second order code along with the 8th order code, have been tested for grids as large as 24,000 points without any errors. This code can handle complex inputs of the geometric factor \( c \), and the order \( m \). Furthermore, it has been tested to work for restricted domains such as subintervals of \([-1, 1]\). To generate the eigenfunctions on a non-uniform grid without interpolation, one may derive the finite-difference formula for a spatially-varying grid step size.

A second order code may have an advantage over higher order algorithms. Due to the tri-diagonal structure of the 2nd order finite difference matrix, one may be able to take advantage of sparse matrix solvers for computations with large grids.

MATLAB Code

BC=0; %Boundary conditions
c=1000; %Spheroidal prolate/oblate parameter
m=0;
MinEta =-1; %Domain for PSWFs [-1,1]
MaxEta = 1;
Npts = 20001; %Number of points to use for grid
h = (MaxEta-MinEta)/(Npts-1); %Grid step size (delta Eta)
eta = -1+h:h:1-h; %TRUNCATED eta grid (boundaries chopped off)
A=double(zeros(Npts-2,Npts-2));
LA=length(A);
for ii=2:LA-1;
A(ii,ii+1)=(1-eta(ii)^2) /(h^2) - eta(ii)/h;
end
A(ii,ii) = 2*(-1+eta(ii)^2) / (h^2) - (c^2)*eta(ii)^2 - (m^2) / (1-eta(ii)^2);
A(ii,ii-1) = (1-eta(ii)^2) / (h^2) + eta(ii) / h;
end

%----Fixed Boundaries (Dirichlet S=0 for now)
A(1,2) = (1-eta(1)^2) / (h^2) - eta(1) / h;
A(1,1) = 2*(-1+eta(1)^2) / (h^2) - (c^2)*eta(1)^2 - (m^2) / (1-eta(1)^2);
A(LA,LA) = 2*(-1+eta(LA)^2) / (h^2) - (c^2)*eta(LA)^2 - (m^2) / (1-eta(LA)^2);
A(LA,LA-1) = (1-eta(LA)^2) / (h^2) + eta(LA) / h;

%----Derivative Zero Boundaries (Neumann: S'=0)
elseif BC==1
LB = (1-eta(1)^2) / (h^2) + eta(1) / h;
A(1,3) = LB*(2/11);
A(1,2) = 2*(-1+eta(1)^2) / (h^2) - (c^2)*eta(1)^2 - (m^2) / (1-eta(1)^2) + LB*(-9/11);
A(LA,LA+0) = 2*(-1+eta(LA)^2) / (h^2) - (c^2)*eta(LA)^2 - (m^2) / (1-eta(LA)^2) + RB*(18/11);
A(LA,LA-1) = (1-eta(LA)^2) / (h^2) + eta(LA) / h - RB*(9/11);
A(LA,LA-2) = RB*(2/11);
end
[V,D] = eig(A);
[lambda,ID] = sort(diag(-D)); % Sort eigenvalues in ascending order
V=V(:,ID); % Sort Eigenfunctions according to eigenvalue magnitude
References


References