

Harmonic Analysis for Star Graphs and the Spherical Coordinate Trapezoidal Rule

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Abstract

Aspects of continuous and discrete harmonic analysis on the circle are generalized to star graphs, and through spherical coordinates to the two sphere. The resulting function theory is used to analyze trapezoidal rule integration on the two sphere.

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1 Introduction

Differential operators on graphs arise in various settings, including the modeling of carbon nanostructures [11], boundary control of elastic multi-structures [8], and studies of the human circulatory system [13]. Eigenfunctions of the second derivative operator can provide an extension of Fourier analysis to metric graphs [3]. This extension has additional structure, including Fast Fourier transform algorithms, for graphs whose edge lengths are integer multiples of a common value [5]. The present work explores the harmonic analysis of star graphs and their 'doubles', which arise in the construction of spherical coordinate grids for the two sphere S^2 . Here we see three levels of intimately connected harmonic analysis. Orthogonal eigenfunctions for a Laplace operator with nonlocal boundary conditions on a two dimensional cylinder descend by restriction to orthogonal eigenfunctions of the graph Laplacian, and these in turn descend by restriction to orthogonal eigenfunctions of difference operators on spherical coordinate grids.

Discrete and continuous harmonic analysis for the circle are tightly linked to the trapezoidal rule for integration. A similar linkage is present for our star graph harmonic analysis. We consider trapezoidal rule integration for S^2 , a subject of recent interest [2, 14]. With the aid of Sobolev type spaces, rapid convergence of the trapezoidal rule is established in Corollary 3.4 for rather singular functions on the sphere. An alternative approach is also provided to some of the results of [2, 14].

The paper begins with a study of eigenfunctions for differential and difference operators. After a review of the graph Laplace operator, a family of trigonometric functions on $[0, 1] \times [0, 1]$ is introduced. These are shown to be a complete orthogonal basis for a two dimensional Laplace operator satisfying periodic boundary conditions in one variable, and nonlocal conditions in the other variable. The nonlocal conditions are related to the construction of spherical coordinates on S^2 . These functions are then sampled, first in one coordinate, then in both coordinates. The sampled eigenfunctions are shown to give eigenfunctions for graph and difference operators. The discrete Fourier transform algorithms discussed in [5] have a simple direct development in the present context; this fact offers the prospect of extending spectral methods [6, 9, 10] to problems on networks, a topic for future work.

This function theory is then applied to problems of numerical integration on S^2 . By using Sobolev spaces associated to the two dimensional Laplace operator with nonlocal boundary conditions it is possible to recognize cer-

tain function singularities compatible with accurate trapezoidal rule computations. The integration of smooth functions on S^2 , previously treated in [2, 14], is reconsidered with our harmonic analysis tools.

2 Operators and eigenfunctions

2.1 Graph differential operators

Suppose $\mathcal{S}$ is a star graph with M edges of equal length, numbered $0, \dots, M-1$. Pick coordinates which identify each edge with the interval $[0, 1/2]$, so that the interior vertex of $\mathcal{S}$ on each edge is identified with $x = 0$. A function F on $\mathcal{S}$ may then be written as a vector

$$F = [f_0(x), \dots, f_{M-1}(x)], \quad 0 \leq x \leq 1/2,$$

with the natural constraint $f_0(0) = \dots = f_{M-1}(0)$.

Self-adjoint second derivative operators d^2/dx^2 acting on the Hilbert space $\oplus_{m=0}^{M-1} L^2[0, 1/2]$ may be defined using boundary conditions [7, S107-S128]. The boundary conditions at $x = 1/2$ are either the Dirichlet condition $f_m(1/2) = 0$ for all edges $m = 0, \dots, M-1$, or the Neumann condition $f'_m(1/2) = 0$ for $m = 0, \dots, M-1$. Continuity and a standard derivative condition are imposed at the interior vertex,

$$f_m(0) = \dots = f_{M-1}(0), \quad \sum_{m=0}^{M-1} f'_m(0) = 0. \quad (2.1)$$

These are the most common interior vertex conditions [11, 8]. Special features of the eigenvalues and eigenfunctions for these boundary conditions in combination with equal edge lengths will be exploited.

It will be convenient to introduce another graph $\mathcal{G}$, which arises in the definition of a spherical coordinate grid for the two sphere $S^2 = \{(X, Y, Z); X^2 + Y^2 + Z^2 = 1\}$, using the spherical coordinates

$$X = \rho \sin(\pi x) \cos(2\pi y), \quad Y = \rho \sin(\pi x) \sin(2\pi y), \quad Z = \rho \cos(\pi x),$$

with $0 \leq x \leq 1$ and $0 \leq y \leq 1$. Sampling y at M equally spaced points $y_m = m/M$ for $m = 0, \dots, M-1$, but leaving x unsampled, leaves a topological

graph $\mathcal{G}$ with M edges joining the two polar vertices as illustrated in Figure 1. A function F on $\mathcal{G}$ may then be identified with a vector function

$$F = [f_0(x), \dots, f_{M-1}(x)], \quad 0 \leq x \leq 1,$$

subject to the constraints

$$f_0(0) = \dots = f_{M-1}(0), \quad f_0(1) = \dots = f_{M-1}(1). \quad (2.2)$$

With $\mathcal{G}$ in mind, define the self-adjoint operator $\mathcal{L}$ acting on $\oplus_{m=0}^{M-1} L^2[0, 1]$ by d^2/dx^2 , with a domain defined using the boundary conditions (2.1) at both $x = 0$ and $x = 1$. The functions that are even, respectively odd, about $x = 1/2$ are invariant subspaces for $\mathcal{L}$. The restriction of $\mathcal{L}$ to the even, respectively odd, subspace may be identified with the operator defined above using Neumann, respectively Dirichlet, conditions at $x = 1/2$. Our study is thus mainly aimed at the Fourier analysis for $\mathcal{L}$ on $\mathcal{G}$.

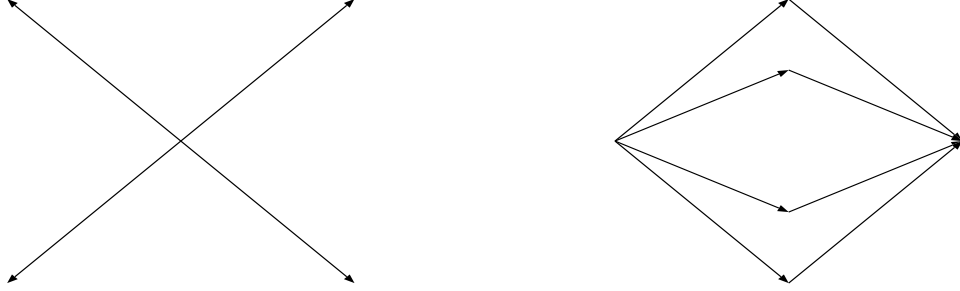


Figure 1: A star graph $\mathcal{S}$ and the graph $\mathcal{G}$

2.2 A partial differential operator

The construction of $\mathcal{G}$ from the partially discretized spherical coordinate grid on S^2 suggests that the eigenfunctions for $\mathcal{L}$ might be related to eigenfunctions for a partial differential operator. For $(x, y) \in [0, 1] \times [0, 1]$, define the families of functions

$$\Phi(k, x, y) = \cos(\pi k x), \quad k = 0, 1, 2, \dots, \quad (2.3)$$

$$\Psi(j, k, x, y) = \sin(\pi k x) \exp(2\pi i j y), \quad k = 1, 2, 3, \dots, \quad j = \pm 1, \pm 2, \pm 3, \dots$$

Each of these functions $f(x, y)$ has y -period 1,

$$f(x, y + 1) = f(x, y), \quad (2.4)$$

and satisfies the boundary conditions

$$f(0, y_1) = f(0, y_2), \quad f(1, y_1) = f(1, y_2), \quad 0 \leq y_1, y_2 \leq 1, \quad (2.5)$$

so they extend continuously to functions on S^2 . They also satisfy

$$\int_0^1 \partial_x f(0, y) \, dy = \int_0^1 \partial_x f(1, y) \, dy = 0. \quad (2.6)$$

Let Δ_p denote the partial differential operator

$$\Delta_p = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}, \quad (2.7)$$

initially defined on the smooth (that is, infinitely differentiable) functions of $(x, y) \in [0, 1] \times [0, 1]$ which extend to smooth 1-periodic functions of y , and which satisfying the boundary conditions (2.5) and (2.6).

Theorem 2.1. *The operator Δ_p is symmetric and essentially self adjoint on $L^2([0, 1] \times [0, 1])$. The functions $\Phi(k, x, y)$ and $\Psi(j, k, x, y)$ form a complete orthogonal basis of eigenfunctions for Δ_p .*

Proof. The symmetry of Δ_p is verified by a simple computation. Let $I^2 = [0, 1] \times [0, 1]$. For f, g in the domain of Δ_p , iterated integration and integration by parts gives

$$\begin{aligned} \int_{I^2} (\Delta_p f) \bar{g} - f \overline{\Delta_p g} &= \int_0^1 \int_0^1 f_{xx} \bar{g} - f \overline{g_{xx}} \, dx \, dy = \int_0^1 f_x \bar{g} - f \overline{g_x} \Big|_0^1 \, dy \\ &= \overline{g(1, y)} \int_0^1 f_x(1, y) \, dy - \overline{g(0, y)} \int_0^1 f_x(0, y) \, dy \\ &\quad - f(1, y) \int_0^1 \overline{g_x(1, y)} \, dy + f(0, y) \int_0^1 \overline{g_x(0, y)} \, dy = 0. \end{aligned}$$

We already observed that the functions $\Phi(k, x, y)$ and $\Psi(j, k, x, y)$ lie in the domain of Δ_p . These functions satisfy

$$\Delta_p \Phi(k, x, y) = -k^2 \pi^2 \Phi(k, x, y),$$

and

$$\Delta_p \Psi(j, k, x, y) = -(k^2 + 4j^2) \pi^2 \Psi(j, k, x, y)$$

The orthogonality of the eigenfunctions is easily checked, as are the norming calculations

$$\int_{I^2} |\Phi(k, x, y)|^2 = \int_0^1 \cos(k\pi x)^2 dx = \begin{cases} 1/2, & k = 1, 2, 3, \dots, \\ 1, & k = 0, \end{cases} \quad (2.8)$$

$$\int_{I^2} |\Psi(j, k, x, y)|^2 = \int_0^1 \sin(k\pi x)^2 dt = 1/2.$$

To establish the completeness of the eigenfunctions, consider the related set $\sigma(j, k, x, y)$ obtained by augmenting the set of functions $\Psi(j, k, x, y)$ with the functions $\sin(k\pi x)$,

$$\sigma(j, k, x, y) = \sin(k\pi x) \exp(2\pi i j y), \quad k = 1, 2, 3, \dots, \quad j = 0, \pm 1, \pm 2, \dots$$

These are separable eigenfunctions for

$$\Delta_1 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2},$$

where d^2/dx^2 has a domain defined by the Dirichlet conditions $f(0) = 0 = f(1)$, and d^2/dy^2 has a domain defined by the periodicity of (2.4).

The boundary conditions for both d^2/dx^2 and d^2/dy^2 determine self adjoint ordinary differential operators on $L^2[0, 1]$ with complete sets of eigenfunctions

$$\begin{aligned} \exp(2\pi i j y), \quad j = 0, \pm 1, \pm 2, \dots, \\ \sin(k\pi x), \quad k = 1, 2, 3, \dots, \end{aligned}$$

respectively. Thus [12, pp. 51–52] the set $\sigma(j, k, x, y)$ gives a complete orthogonal basis for $L^2(I^2)$. To finish the proof of completeness for the functions $\Phi(k, x, y)$ and $\Psi(j, k, x, y)$ in $L^2(I^2)$, notice that the closed span of $\sin(k\pi x)$ for $k = 1, 2, 3, \dots$ is the same as the closed span of $\cos(k\pi x)$ for $k = 0, 1, 2, \dots$, this last set being a complete set of eigenfunctions for the self adjoint operator d^2/dx^2 on $L^2[0, 1]$ with domain defined by the Neumann conditions $f'(0) = 0 = f'(1)$.

Finally, since Δ_p is symmetric, and has a complete orthonormal set of eigenfunctions, it is essentially self adjoint.

□

Henceforth, Δ_p will refer to the self adjoint closure of the symmetric operator defined above. The eigenfunctions for the graph operator $\mathcal{L}$ may be obtained by sampling some of the functions $\Phi(k, x, y)$ and $\Psi(j, k, x, y)$.

Theorem 2.2. For a positive integer M and for $m = 0, \dots, M-1$, let $y_m = m/M$. If

$$\Phi(k, x, y_m) = \cos(\pi k x), \quad \Psi(j, k, x, y_m) = \sin(\pi k x) \exp(2\pi i \frac{jm}{M}),$$

then the M -vector functions

$$\phi(k, x) = [\Phi(k, x, y_0), \dots, \Phi(k, x, y_{M-1})],$$

for $k = 0, 1, 2, \dots$, together with

$$\psi(j, k, x) = [\Psi(j, k, x, y_0), \dots, \Psi(j, k, x, y_{M-1})],$$

for $j = -\lfloor (M-1)/2 \rfloor, \dots, -1, 1, \dots, \lfloor (M-1)/2 \rfloor$, and $k = 1, 2, \dots$, form a complete orthogonal basis of eigenfunctions for $\mathcal{L}$ on $\oplus_{m=0}^{M-1} L^2[0, 1]$.

Proof. The proof is similar to that of the previous theorem. The equations $\phi''(k, x) = -k^2 \pi^2 \phi(k, x)$ and $\psi''(j, k, x) = -k^2 \pi^2 \psi(j, k, x)$ are satisfied, as well as the continuity conditions of (2.1) at $x = 0$ and $x = 1$. The derivative portion of (2.1) is satisfied for $\phi(k, x)$ since $\phi'(k, 0) = 0 = \phi'(k, 1)$. For $\psi(j, k, x)$ and any $x \in [0, 1]$ we have

$$\sum_{m=0}^{M-1} \psi'(j, k, x) = \pi k \cos(\pi k x) \sum_{m=0}^{M-1} \exp(2\pi i \frac{jm}{M}) = 0,$$

since the last sum is geometric,

$$\sum_{m=0}^{M-1} \exp(2\pi i jm/M) = \frac{1 - \exp(2\pi i j)}{1 - \exp(2\pi i j/M)} = 0,$$

for

$$j = -\lfloor (M-1)/2 \rfloor, \dots, -1, 1, \dots, \lfloor (M-1)/2 \rfloor.$$

The orthogonality is easily verified, as are the norming calculations

$$\int_0^1 |\phi(k, x)|^2 dx = M \int_0^1 \cos(k\pi x)^2 dx = M/2, \quad (2.9)$$

$$\int_0^1 |\psi(j, k, x)|^2 dx = M \int_0^1 \sin(k\pi x)^2 dx = M/2.$$

If the functions $\phi(k, x)$ are replaced by $\sin(\pi kx)$, the resulting set

$$\sigma(j, k, x, y_m) = \sin(k\pi x) \exp(2\pi i \frac{jm}{M}), \quad k = 1, 2, 3, \dots,$$

for

$$j = -\lfloor (M-1)/2 \rfloor, \dots, -1, 1, \dots, \lfloor (M-1)/2 \rfloor.$$

is complete. The functions $\sin(k\pi x)$ form a basis of eigenfunctions for d^2/dx^2 with $f(0) = 0 = f(1)$, as before. The exponential factors are eigenvectors for, say, the averaging operator

$$A_y[f_0, \dots, f_{M-1}] = \frac{1}{2}[f_{M-1} + f_1, f_0 + f_2, \dots, f_{M-2} + f_0]$$

acting on functions on the set $\{y_m\}$, allowing the use of the abstract result cited above, or they can be handled by direct computation. Then one notes as before that the closed span of $\sin(k\pi x)$ for $k = 1, 2, 3, \dots$ is the same as the closed span of $\cos(k\pi x)$ for $k = 0, 1, 2, \dots$

□

Since $\exp(2\pi i(j+M)m/M) = \exp(2\pi ijm/M)$, the j -index for $\psi(j, k, x)$ admits alternative choices, such as $j = 1, \dots, M-1$.

2.3 Sampling in x

There is still another variation on the theme of sampling eigenfunctions to obtain orthogonal bases on a new space. Given a sequence $a_0, \dots, a_N$, introduce the trapezoidal rule sum

$$\sum_{n=0}^N{}'' a_n = \frac{a_0 + a_N}{2} + \sum_{n=1}^{N-1} a_n.$$

Given positive integers M and N , let $x_n = n/N$ for $n = 0, \dots, N$, and let $\mathbb{V}$ denote the $(N-1)M + 2$ dimensional subspace of complex M -vector valued functions defined on $\{x_n\}$,

$$F(x_n) = [f_0(x_n), \dots, f_{M-1}(x_n)], \quad x_n = n/N, \quad n = 0, \dots, N,$$

subject to the constraints (2.2). Equip $\mathbb{V}$ with the (trapezoidal rule) inner product

$$\langle F, G \rangle = \frac{1}{MN} \sum_{m=0}^{M-1} \sum_{n=0}^N{}'' f_m(x_n) \overline{g_m(x_n)} = \frac{1}{MN} \sum_{n=0}^N{}'' F(x_n) \cdot G(x_n),$$

where $W \cdot Z$ is the usual dot product for vectors $W, Z \in \mathbb{C}^M$,

$$W \cdot Z = \sum_{m=0}^{M-1} w_m \overline{z_m}.$$

The following elementary identities [4, p. 139] are helpful for inner product calculations in $\mathbb{V}$.

Lemma 2.3. *For integers $j, k = 0, \dots, N$,*

$$\sum_{n=0}^N \cos(\pi \frac{jn}{N}) \cos(\pi \frac{kn}{N}) = \begin{cases} 0, & j \neq k, \\ N/2, & j = k, \quad k = 1, \dots, N-1, \\ N, & j = k = 0, \quad \text{or } j = k = N. \end{cases}$$

and for integers $j, k = 1, \dots, N-1$,

$$\sum_{n=1}^{N-1} \sin(\pi \frac{jn}{N}) \sin(\pi \frac{kn}{N}) = \begin{cases} 0, & j \neq k, \\ N/2, & j = k. \end{cases}$$

Theorem 2.4. *Given positive integers M, N , let $y_m = m/M$ for $m = 0, \dots, M-1$, and $x_n = n/N$ for $n = 0, \dots, N$. If*

$$\Phi(k, x_n, y_m) = \cos(\pi k x_n), \quad \Psi(j, k, x_n, y_m) = \sin(\pi k x_n) \exp(2\pi i \frac{jm}{M}),$$

then the M -vector functions defined on $\{x_n\}$,

$$\phi(k, x_n) = [\Phi(k, x_n, y_0), \dots, \Phi(k, x_n, y_{M-1})],$$

for $k = 0, 1, 2, \dots, N$ together with

$$\psi(j, k, x_n) = [\Psi(j, k, x_n, y_0), \dots, \Psi(j, k, x_n, y_{M-1})],$$

for $j = -\lfloor (M-1)/2 \rfloor, \dots, -1, 1, \dots, \lfloor (M-1)/2 \rfloor$ and $k = 1, 2, \dots, N-1$, form a complete orthogonal basis for $\mathbb{V}$.

Proof. One checks easily that the functions $\phi(k, x_n)$ and $\psi(j, k, x_n)$ are in $\mathbb{V}$. Since $\mathbb{V}$ is finite dimensional, it suffices to use Lemma 2.3 to establish the inner product formulas

$$\langle \phi(k_1, x_n), \phi(k_2, x_n) \rangle = \begin{cases} 0, & k_1 \neq k_2, \\ 1, & k_1 = k_2 = 0 \text{ or } k_1 = k_2 = N, \\ 1/2, & k_1 = k_2 = 1, \dots, N-1 \end{cases} \quad (2.10)$$

$$\begin{aligned}\langle \phi(k_1, x_n), \psi(j, k_2, x_n) \rangle &= 0, \\ \langle \psi(j_1, k_1, x_n), \psi(j_2, k_2, x_n) \rangle &= \begin{cases} 1/2, & j_1 = j_2, k_1 = k_2, \\ 0, & \text{otherwise.} \end{cases}\end{aligned}$$

□

With $F(x_n) = [f_0(x_n), \dots, f_{M-1}(x_n)]$, define the adjacency operators $A_x : \mathbb{V} \rightarrow \mathbb{V}$ and $A_y : \mathbb{V} \rightarrow \mathbb{V}$ by

$$A_x F(x_n) = \begin{cases} \frac{F(x_{n-1}) + F(x_{n+1})}{2}, & n = 1, \dots, N-1, \\ \frac{1}{M} \sum_{m=0}^{M-1} f_m(x_1)[1, \dots, 1], & n = 0, \\ \frac{1}{M} \sum_{m=0}^{M-1} f_m(x_{N-1})[1, \dots, 1], & n = N, \end{cases}$$

$$A_y F(x_n) = \frac{1}{2}[f_{M-1}(x_n) + f_1(x_n), f_0(x_n) + f_2(x_n), \dots, f_{M-2}(x_n) + f_0(x_n)].$$

The next result is easily verified.

Proposition 2.5. *The functions $\phi(k, x_n)$ and $\psi(j, k, x_n)$ are eigenfunctions for A_x and A_y ,*

$$A_x \phi(k, x_n) = \cos(\pi k/N) \phi(k, x_n), \quad A_x \psi(j, k, x_n) = \cos(\pi k/N) \psi(j, k, x_n),$$

$$A_y \phi(k, x_n) = \phi(k, x_n), \quad A_y \psi(j, k, x_n) = \cos(2\pi \frac{j}{M}) \psi(j, k, x_n).$$

3 The Trapezoidal Rule in spherical coordinates

Integrals over the two sphere $S^2 \subset \mathbb{R}^3$ may be transformed into integrals over the unit square $I^2 \subset \mathbb{R}^2$ by using spherical coordinates. For a real valued function $F(X, Y, Z)$ defined on S^2 , if

$$g(x, y) = F(\cos(2\pi y) \sin(\pi x), \sin(2\pi y) \sin(\pi x), \cos(\pi x)), \quad (3.1)$$

then

$$\int_{S^2} F = \int_{I^2} 2\pi^2 \sin(\pi x) g(x, y) \, dx \, dy.$$

For notational convenience we will associate $f(x, y) = 2\pi^2 \sin(\pi x) g(x, y)$ with the function $F : S^2 \rightarrow \mathbb{R}$.

Numerical integration schemes such as the product trapezoidal rule

$$T(M, N, f) = \frac{1}{MN} \sum_{m=0}^{M-1} \sum_n'' f(x_n, y_m) \simeq \int_{I^2} f(x, y) dx dy. \quad (3.2)$$

may be defined using a grid with $M(N+1)$ points (x_n, y_m) where $x_n = n/N$, $n = 0, \dots, N$ and $y_m = m/M$, $m = 0, \dots, M-1$. The grid points with $x_n = 0$, respectively $x_n = 1$, are identified on S^2 , so samples of functions $f(x, y)$ coming from functions F defined on S^2 will satisfy the constraints (2.2).

The performance of this algorithm for integration on the sphere can vary dramatically. For $f_1(x, y) = \sin(\pi x)$, the standard one variable error estimates [1, p. 285] show that the computational error is of order N^{-2} , which is not impressive. The performance is markedly better for $f_2(x, y) = \sin(\pi x) \cos(2\pi y)$, where the trapezoidal rule has 0 error when $N \geq 2$ and $M \geq 3$. This section uses harmonic analysis to analyze the performance of the product trapezoidal rule for integrations coming from S^2 . Rapid convergence rates are established for classes of functions $F : S^2 \rightarrow \mathbb{R}$ with rather singular derivative behavior at the poles.

In one variable, trapezoidal rule evaluation of integrals with endpoint singularities can be improved by an elementary change of variables [1, pp. 305–307]. Recent work [2, 14] has considered enhancements of the product trapezoidal rule for integration over the sphere by similar changes of the x variable. Harmonic analysis methods are used to provide a novel approach to these coordinate change problems.

3.1 Sobolev spaces for spherical coordinates

Let Δ_p be the self adjoint closure of the essentially self adjoint Laplacian described in Theorem 2.1. A function $f \in L^2(I^2)$ has a Fourier expansion

$$f(x, y) = \sum_{k=0}^{\infty} \alpha(0, k) \Phi(k, x, y) + \sum_{j,k} \alpha(j, k) \Psi(j, k, x, y)$$

in the orthogonal basis $\{\Phi(k, x, y), \Psi(j, k, x, y)\}$. For $s \geq 0$ introduce the Sobolev style Hilbert space H^s as the set of $f \in L^2(I^2)$ satisfying

$$\|f\|_s^2 = \sum_{j,k} \left[1 + ([k^2 + 4j^2]\pi^2)^s \right] |\alpha_{j,k}|^2 < \infty,$$

where $j = 0, \pm 1, \pm 2, \dots$ and $k = 0, 1, 2, \dots$. Here $\alpha(j, k) = 0$ for $k = 0$ if $j \neq 0$. The space H^s is just the domain of $\Delta_p^{s/2}$ with the usual inner product. Although H^s is defined in terms of Fourier series, it is straightforward to give alternative criteria in some cases.

Proposition 3.1. *Suppose $f(x, y)$ has $2r$ continuous derivatives on I^2 , with*

$$\partial_y^i f(x, 0) = \partial_y^i f(x, 1), \quad i = 0, \dots, 2r - 1, \quad 0 \leq x \leq 1.$$

Assume the Taylor expansion for f is

$$f(x, y) \simeq \sum_{i \geq 0} c_i(x_0, y)(x - x_0)^i, \quad x_0 = 0, 1.$$

about points (x_0, y) . Then $f(x, y) \in H^{2r}$ for $r = 1, 2, 3, \dots$ if

$$c_i(x_0, y) = c_i(x_0), \quad i = 0, 2, 4, \dots, 2(r - 1),$$

that is $c_i(x_0, y)$ is independent of y , and

$$\int_0^1 c_{i+1}(x_0, y) dy = 0, \quad i = 0, 2, 4, \dots, 2(r - 1).$$

Proof. Integration by parts first gives

$$\begin{aligned} & (-4j^2 - k^2)^r \pi^{2r} \int_{I^2} f(x, y) \Psi(j, k, x, y) dy dx \\ &= \int_{I^2} f(x, y) \Delta_p^r \Psi(j, k, x, y) dy dx \\ &= \int_{I^2} f_{yy} \Delta_p^{r-1} \Psi(j, k, x, y) dy dx \\ &+ \int_0^1 \left[f(x, y) \Delta_p^{r-1} \Psi_x - f_x(x, y) \Delta_p^{r-1} \Psi \right] \Big|_0^1 dy \\ &+ \int_{I^2} f_{xx} \Delta_p^{r-1} \Psi(j, k, x, y) dy dx. \end{aligned}$$

The boundary conditions for f are also satisfied by Ψ , so the boundary terms vanish and

$$(-4\pi^2 j^2 - \pi^2 k^2)^r \int_{I^2} f(x, y) \Psi(j, k, x, y) dy dx$$

$$= \int_{I^2} (f_{xx} + f_{yy})(x, y) \Delta_p^{r-1} \Psi(j, k, x, y) dy dx.$$

The boundary conditions assumed for f hold for $f_{xx} + f_{yy}$ if r is replaced by $r - 1$. Repeated integration by parts gives the desired result for $\Psi(j, k, x, y)$, and a similar argument works for $\Phi(k, x, y)$. $\square$

The inner product formulas (2.8) and (2.10), applied with one term equal to $\Phi(0, x, y) = 1$, establish the following result on exactness of the trapezoidal rule for the basis functions of (2.3).

Proposition 3.2. *The trapezoidal rule (3.2) is exact on the span of $\Phi(k, x, y)$ for $k = 0, \dots, N$ and $\Psi(j, k, x, y)$ for $j = -\lfloor (M-1)/2 \rfloor, \dots, -1, 1, \dots, \lfloor (M-1)/2 \rfloor$ and $k = 1, \dots, N-1$.*

Suppose $P(M, N, f)$ is the orthogonal projection of f onto the span of the eigenfunctions with indices $j = -\lfloor (M-1)/2 \rfloor, \dots, -1, 1, \dots, \lfloor (M-1)/2 \rfloor$ and $0 \leq k \leq N$. The rate of convergence of $P(M, N, f)$ to f as well as the rate of convergence for the trapezoidal rule (3.2) depends on which Sobolev spaces contain f .

Theorem 3.3. *Suppose $f(x, y)$ is in H^s , and $L = \min(M, N)$. Then for $s > 1$*

$$\|f - P(M, N, f)\| = O(L^{1-s}),$$

and for $s > 2$

$$\sup_{(x,y) \in I^2} |f(x, y) - P(M, N, f)(x, y)| = O(L^{2-s}). \quad (3.3)$$

Proof. We will let C denote various constants. Since $f \in H^s$,

$$|\alpha_{j,k}|^2 \leq C([k^2 + 4j^2]\pi^2)^{-s}.$$

Let B_L denote the set of indices (j, k) with $k \geq 0$ such that $\max(j, k) \leq L$. We have

$$\begin{aligned} \|f - P(M, N, f)\|^2 &\leq \sum_{(j,k) \notin B_L} |\alpha_{j,k}|^2 \leq C \sum_{(j,k) \notin B_L} ([k^2 + 4j^2]\pi^2)^{-s} \\ &\leq C \int_{u^2+v^2 \geq L^2} (u^2 + v^2)^{-s} \leq C \int_{r \geq L} (r^2)^{-s} r dr = C_1 \int_{r \geq L} r^{1-2s} dr \leq CL^{2-2s}. \end{aligned}$$

We also have

$$\begin{aligned} \sum_{(j,k) \notin B_L} |\alpha_{j,k}| &\leq \sum_{(j,k) \notin B_L} C([k^2 + 4j^2]\pi^2)^{-s/2} \\ &\leq C \int_L^\infty (r^2)^{-s/2} r \, dr = C \int_L^\infty r^{1-s} \, dr. \end{aligned}$$

Since the eigenfunctions $\Phi(k, x, y)$ and $\Psi(j, k, x, y)$ are uniformly bounded and continuous on I^2 , the Fourier series converges uniformly to a continuous function if $s > 2$. We also obtain the error estimate

$$\sup_{(x,y) \in I^2} |f(x, y) - P(M, N, f)(x, y)| = O(L^{2-s}).$$

□

Corollary 3.4. *Suppose $f(x, y)$ is in H^s for $s > 2$, and $L = \min(M, N)$. Then*

$$\int_{I^2} f(x, y) \, dx \, dy - T(M, N, f) = O(L^{2-s}).$$

Proof. Approximate f by the orthogonal projection $P(M, N, f)$. By Proposition 3.2,

$$\int_{I^2} P(M, N, f)(x, y) \, dx \, dy - T(M, N, P(M, N, f)) = 0,$$

so

$$\begin{aligned} \int_{I^2} f - T(M, N, f) &= \int_{I^2} [f - P(M, N, f)](x, y) \, dx \, dy \\ &\quad - [T(M, N, f) - T(M, N, P(M, N, f))], \end{aligned}$$

and (3.3) gives the result. □

Corollary 3.4 and Proposition 3.1 show that a function on S^2 may be rather singular while still having its integral approximated well by the trapezoidal rule. For instance, the function

$$F(\cos(2\pi y) \sin(\pi x), \sin(2\pi y) \sin(\pi x), \cos(\pi x)) = \cos(2\pi y), \quad 0 < x < 1,$$

does not extend continuously to the sphere, but the corresponding function

$$f(x, y) = 2\pi^2 \sin(\pi x) \cos(2\pi y)$$

is a linear combination of eigenfunctions for Δ_p , so is in H^s for every $s > 0$.

3.2 Integration of smooth functions

Next we consider the integration of smooth functions over the sphere using the trapezoidal rule. The recent work on this subject in [2, 14] provided motivation and ideas in what follows. This material begins by considering decompositions of polynomials, and then smooth functions.

Anticipating some changes of variable, define the class $\mathcal{E}$ of continuous functions $f : I^2 \rightarrow \mathbb{R}$ satisfying

$$(i) \quad f(0, y) = f(1, y) = 0, \quad 0 \leq y \leq 1,$$

and for M sufficiently large, and

$$(ii) \quad \int_0^1 f(x, y) dy = 0 = \sum_{m=0}^{M-1} f(x, m/M), \quad 0 \leq x \leq 1.$$

If $f \in \mathcal{E}$, and M sufficiently large, then the trapezoidal rule is exact, even after a coordinate change $x = \tau(t)$, since

$$\int_{I^2} f(x, y) dx dy = \int_0^1 f(\tau(t), y) dy \tau'(t) dt = 0 = T(M, N, f(\tau(t), y) \tau'(t)).$$

Lemma 3.5. *Suppose $P(X, Y, Z)$ is a polynomial and $\sigma_1 : \mathbb{R} \rightarrow \mathbb{R}$ is a smooth function. If*

$$p(x, y) = 2\pi^2 \sin(\pi x) P(\cos(2\pi y) \sin(\pi x), \sin(2\pi y) \sin(\pi x), \cos(\pi x)),$$

and

$$\sigma(x) = \sigma_1(\cos(\pi x)),$$

then $\sigma(x)p(x, y)$ may be written as a sum

$$\sigma(x)p(x, y) = p_0(x) + p_1(x, y),$$

where $p_0(x)$ is smooth on $[0, 1]$, and p_1 is smooth and in $\mathcal{E}$.

Proof. It suffices to prove the result for the cases $P(X, Y, Z) = X^\alpha Y^\beta Z^\gamma$ with nonnegative integer exponents. Then

$$\sigma(x)p(x, y) = g(x)h(y),$$

where

$$g(x) = 2\pi^2 \sigma(x) \sin^{\alpha+\beta+1}(\pi x) \cos^\gamma(\pi x), \quad h(y) = \cos^\alpha(2\pi y) \sin^\beta(2\pi y).$$

The function $h(y)$ is a trigonometric polynomial

$$h(y) = \sum_{j=-(\alpha+\beta)}^{\alpha+\beta} c_j \exp(2\pi i j y),$$

which is split into constant and nonconstant terms,

$$h(y) = h_0 + h_1(y), \quad h_1(y) = \sum_{j \neq 0} c_j \exp(2\pi i j y).$$

Since

$$\int_0^1 \exp(2\pi i j y) dy = 0 = \sum_{m=0}^{M-1} \exp(2\pi i j m/M)$$

for $j = -\lfloor (M-1)/2 \rfloor, \dots, -1, 1, \dots, \lfloor (M-1)/2 \rfloor$,

$$\int_0^1 h_1(y) dy = 0 = \sum_{m=0}^{M-1} h_1(m/M)$$

for M sufficiently large. The desired functions are

$$p_0(x) = g(x)h_0, \quad p_1(x, y) = g(x)h_1(y).$$

□

Next, consider the decomposition of smooth functions written in spherical coordinates.

Theorem 3.6. *Suppose $F : R^3 \rightarrow \mathbb{R}$ is smooth, and let r be a positive integer. Then the function*

$$f(x, y) = 2\pi^2 \sin(\pi x) F(\cos(2\pi y) \sin(\pi x), \sin(2\pi y) \sin(\pi x), \cos(\pi x))$$

may be written as a sum

$$f(x, y) = f_1(x, y) + f_2(x) + f_3(x, y), \tag{3.4}$$

all summands being smooth, with $f_3 \in \mathcal{E}$,

$$f_2(x) = \int_0^1 f(x, y) dy.$$

and f_1 satisfying

$$\partial_x^i f_1(0, y) = 0 = \partial_x^i f_1(1, y), \quad i = 0, \dots, 2r, \quad 0 \leq y \leq 1, \quad (3.5)$$

and

$$\partial_y^i f_1(x, 0) = \partial_y^i f_1(x, 1), \quad i = 0, 1, 2, \dots, \quad 0 \leq x \leq 1.$$

Thus $f_1 \in H^{2r}$ by Lemma 3.1.

Proof. Let $P(X, Y, Z)$ be the Taylor polynomial of order $2r$ for F at $(0, 0, 1)$, and let $\sigma_1(Z)$ be a smooth function satisfying

$$\sigma_1(Z) = \begin{cases} 1, & Z \geq 1/2, \\ 0, & Z \leq 0. \end{cases}$$

Treat $(0, 0, -1)$ in a similar fashion with Taylor polynomial Q , and a cutoff function

$$\eta_1(Z) = \begin{cases} 1, & Z \leq -1/2, \\ 0, & Z \geq 0. \end{cases}$$

Write F as a sum

$$F = \sigma_1 P + \eta_1 Q + F_1.$$

As in Lemma 3.5, change to spherical coordinates, obtaining

$$\sigma(x)p(x, y) = p_0(x) + p_1(x, y), \quad \eta(x)q(x, y) = q_0(x) + q_1(x, y),$$

with p_0, q_0 smooth and p_1, q_1 smooth and in $\mathcal{E}$. Take $f_3 = p_1 + q_1$, and define $t_2(x) = p_0 + q_0$.

The function $F_1(X, Y, Z)$ has all derivatives of orders up to $2r$ vanishing at $(0, 0, 1)$ and $(0, 0, -1)$. Let

$$g(x, y) = F_1(\cos(2\pi y) \sin(\pi x), \sin(2\pi y) \sin(\pi x), \cos(\pi x)).$$

Differentiating with respect to x ,

$$\frac{\partial g}{\partial x} = \frac{\partial F_1}{\partial X} \pi \cos(2\pi y) \cos(\pi x) + \frac{\partial F_1}{\partial Y} \pi \sin(2\pi y) \cos(\pi x) - \frac{\partial F_1}{\partial Z} \pi \sin(\pi x).$$

Repeated differentiation shows that if the partial derivatives of F through $2r$ -th order are all zero at $(0, 0, 1)$ and $(0, 0, -1)$, then the derivatives of g through the $2r$ -th with respect to x are also 0 at $x = 0$ and $x = 1$. The same is true for

$$t_1(x, y) = 2\pi^2 \sin(\pi x)g(x, y).$$

So far,

$$f(x, y) = t_1(x, y) + t_2(x) + f_3(x, y). \quad (3.6)$$

Define

$$f_2(x) = \int_0^1 f(x, y) dy, \quad f_1(x, y) = t_1(x, y) + t_2(x) - f_2(x),$$

so

$$f(x, y) = f_1(x, y) + f_2(x) + f_3(x, y).$$

Integration of (3.6) gives

$$\int_0^1 f(x, y) dy = \int_0^1 t_1(x, y) dy + t_2(x),$$

so $t_2(x)$ and $f_2(x)$ have matching derivatives through the $2r$ -th at $x = 0$ and $x = 1$. This implies that f_1 satisfies (3.5). $\square$

Theorem 3.6 can be used as an alternative approach to some ideas of [14]. Denote the one-dimensional trapezoidal rule approximation of $\int_0^1 g$ by

$$T_1(N, g) = \frac{1}{N} \sum_n'' g(x_n), \quad x_n = n/N, \quad n = 0, \dots, N. \quad (3.7)$$

One has the following variant of Theorem 2.2 of [14].

Corollary 3.7. *Suppose $\alpha_0, \alpha_1, \beta$ are positive constants, and*

$$\alpha_0 N^\beta \leq M \leq \alpha_1 N^\beta.$$

Under the assumptions of Theorem 3.6

$$T(M, N, f) = T_1(N, f_2) + O(N^{-s})$$

for s arbitrarily large.

Proof. Picking $s > 0$, let $\gamma = \min(\beta, 1)$ and pick r so that $\gamma(2 - 2r) < -s$. Since

$$\int_0^1 f_3(x, y) dy = 0,$$

Theorem 3.6 gives $f_1 \in H^{2r}$ with

$$\int_0^1 \int_0^1 f_1(x, y) dy dx = 0.$$

By Corollary 3.4,

$$T(M, N, f_1) = O(N^{\gamma(2-2r)}).$$

Thus for M sufficiently large,

$$T(M, N, f) = T_1(N, f_2) + O(N^{\gamma(2-2r)}).$$

□

Trapezoidal rule evaluation of integrals in one variable can often be improved by an elementary change of variables [1, pp. 305–307]. Suppose $\tau : [0, 1] \rightarrow [0, 1]$ is strictly increasing, with $\tau(0) = 0$ and $\tau(1) = 1$. The change of variables $x = \tau(t)$ gives

$$\int_0^1 g(x) dx = \int_0^1 g(\tau(t))\tau'(t)dt. \quad (3.8)$$

High order vanishing of $\tau'(t)$ at 0 and 1 can be used, for instance, to improve the trapezoidal rule convergence rate. The use of this method in conjunction with spherical coordinate integration has been recently considered in [2, 14, 15].

In the context of Theorem 3.6, suppose such a change of variables is applied to (3.4). If

$$g(t, y) = f(\tau(t), y)\tau'(t), \quad g_i(t, y) = f_i(\tau(t), y)\tau'(t), \quad i = 1, 2, 3,$$

then

$$\begin{aligned} \int_{I^2} f(x, y) dx dy &= \int_{I^2} g(\tau(t), y) dt dy \\ &= \int_{I^2} g_1(\tau(t), y) + g_2(\tau(t)) + g_3(\tau(t), y) dt dy. \end{aligned}$$

As mentioned when the class $\mathcal{E}$ was defined, $g_3 \in \mathcal{E}$. Moreover,

$$\partial_y^i g_1(t, 0) = \partial_y^i g_1(t, 1), \quad i = 0, 1, 2, \dots, \quad 0 \leq t \leq 1.$$

Repeated application of the chain rule

$$\partial_t g_1(t, y) = \frac{\partial f_1}{\partial \tau}(\tau')^2 + f_1 \tau''$$

shows that

$$\partial_t^i g_1(0, y) = 0 = \partial_t^i g_1(1, y), \quad i = 0, \dots, 2r, \quad 0 \leq y \leq 1,$$

as long as τ has $2r + 1$ continuous derivatives. Moreover,

$$\int_0^1 g_1(t, y) dy = \int_0^1 f_1(\tau(t), y) dy \quad \tau'(t) = 0,$$

so

$$g_2(t) = \int_0^1 g(t, y) dy.$$

Thus Corollary 3.7 may be applied, yielding the final result.

Corollary 3.8. *Suppose $\tau : [0, 1] \rightarrow [0, 1]$ is smooth and strictly increasing, with $\tau(0) = 0$ and $\tau(1) = 1$. Then Corollary 3.7 holds for $g(t, y)$ in the variables t, y , that is*

$$T(M, N, g) = T_1(N, g_2) + O(N^{-s})$$

for s arbitrarily large.

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