NUMERICAL COMPUTATION OF THE LAPLACE-BELTRAMI OPERATOR ON THE SPHERE

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Abstract. We propose a method for computation of the Laplace-Beltrami operator of a spherical function. It is proved that differentiation may be replaced by integration with a kernel derived from the Poisson kernel, followed by a limit computation. Theoretical results show uniform convergence, but in practice, limiting process is difficult to be performed and it turns out that the error is too big. Numerical experiments show that under assumption that the test function is bandlimited, computation of its Laplace-Beltrami operator can be performed via integration with a proper polynomial kernel.

1. Introduction

Laplace-Beltrami operator on a manifold is used for shape analysis and segmentation [13]. It can be applied for instance to characterize the topology of human body shapes. Numerical methods developed for computation of the Laplace-Beltrami operator on manifolds are based on its discretization [13, 11] and lead to a solution of the eigenvalue and eigenvector problem [8, 18, 19, 11, 13]. Another are concerned with partial differential equations, see, e.g., [7, 5]. In [2, 1] Álvarez *et al.* present a methos that uses radial basis functions. Algorithms based on integration are described in [4, 3, 12]. The method we use resembles the one presented in [12], however, the difference lies in the way tthe integral is computed: by direct application of integration schemes in the present paper or by solving an optimization problem in [12].
Numerical differentiation based on differences is quite difficult and unstable [9]. If a function can be extended to the complex domain, a method to reduce the computational error is use of Taylor formula [16]; however, this method can hardly be applied to computation of higher order derivatives. Another possibility is to use Cauchy formula [10] that replaces differentiation by integration. Similarly, the formula we derive in the present paper allows to replace differentiation by integration, and therefore it can be regarded as a kind of spherical counterpart of the latter method.

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2. Preliminaries

A square integrable function f over the n-dimensional unit sphere $\mathbb{S}^n \subseteq \mathbb{R}^{n+1}$, $n \geq 2$, with the rotation-invariant measure $d\sigma$ normalized such that

$$\Sigma_n = \int_{\mathbb{S}^n} d\sigma(x) = \frac{2\pi^{(n+1)/2}}{\Gamma((n+1)/2)},$$

can be represented as a Fourier series in terms of the hyperspherical harmonics,

$$f = \sum_{l=0}^{\infty} \sum_{k\in \mathcal{M}_{n-1}(l)} a_l^k(f)\, Y_l^k, \tag{1}$$

where $\mathcal{M}_{n-1}(l)$ denotes the set of sequences $k = (k_0, k_1, \dots, k_{n-1})$ in $\mathbb{N}_0^{n-1} \times \mathbb{Z}$ such that $l \geq k_0 \geq k_1 \geq \dots \geq |k_{n-1}|$ and $a_l^k(f)$ are the Fourier coefficients of f. The hyperspherical harmonics of degree l and order k are given by

$$Y_l^k(x) = A_l^k \prod_{\tau=1}^{n-1} C_{k_{\tau-1}-k_\tau}^{\frac{n-\tau}{2}+k_\tau}(\cos\theta_\tau)\sin^{k_\tau}\theta_\tau \cdot e^{\pm i k_{n-1}\phi} \tag{2}$$

for some constants A_l^k. Here, $(\theta_1, \dots, \theta_{n-1}, \phi)$ are the hyperspherical coordinates of $x \in \mathbb{S}^n$,

$$\begin{aligned}
x_1 &= \cos\theta_1,\\
x_2 &= \sin\theta_1\cos\theta_2,\\
&\dots\\
x_n &= \sin\theta_1 \dots \sin\theta_{n-2}\sin\theta_{n-1}\cos\phi,\\
x_{n+1} &= \sin\theta_1 \dots \sin\theta_{n-2}\sin\theta_{n-1}\sin\phi,
\end{aligned}$$

and C_κ^K are the Gegenbauer polynomials of degree κ and order K. The set of degree l hyperspherical harmonics is denoted by $\mathcal{H}_l$.

Zonal (rotation-invariant) functions are those depending only on the first hyperspherical coordinate $\theta = \theta_1$. Unless it leads to misunderstandings, we identify them with functions of θ or $t = \cos\theta$. A zonal $\mathcal{L}^1$-function f has the following Gegenbauer expansion

$$f(t) = \sum_{l=0}^{\infty} \hat{f}(l)\, C_l^\lambda(t), \qquad t = \cos\theta, \tag{3}$$

where $\hat{f}(l)$ are the Gegenbauer coefficients of f and λ is related to the space dimension by

$$\lambda = \frac{n-1}{2}.$$

Consequently, for a zonal $\mathcal{L}^2$-function f one has

$$\hat{f}(l) = A_l^0 \cdot a_l^0(f),$$

compare (1), (2), and (3). Further, Funk-Hecke theorem states that for a zonal L^1-function f and $Y_l \in \mathcal{H}_l(S^n)$, $l \in \mathbb{N}_0$,

$$\int_{S^n} Y_l(y)\, f(x \cdot y)\, d\sigma(y) = Y_l(x) \cdot \frac{(4\pi)^\lambda\, l!\, \Gamma(\lambda)}{(2\lambda + l - 1)!} \int_{-1}^{1} f(t)\, C_l^\lambda(t) \left(1 - t^2\right)^{\lambda - 1/2} dt. \tag{4}$$

For $f, g \in L^1(S^n)$, g zonal, their convolution $f * g$ is defined by

$$(f * g)(y) = \frac{1}{\Sigma_n} \int_{S^n} f(x)\, \tau_y g(x)\, d\sigma(x), \qquad \tau_y g(x) = g(x \cdot y), \tag{5}$$

and for $f \in L^2(S^n)$ it is equal to

$$f * g = \sum_{l=0}^{\infty} \sum_{k \in M_{n-1}(l)} \frac{\lambda}{\lambda + l}\, a_l^k(f)\, \hat{g}(l)\, Y_l^k.$$

If f is a zonal function, then

$$\widehat{f * g}(l) = \frac{\lambda}{\lambda + l} \hat{f}(l)\, \hat{g}(l). \tag{6}$$

With this notation we have

$$Y_l(f; x) = \frac{\lambda + l}{\lambda} \left(f * C_l^\lambda\right)(x),$$

hence, the function $\frac{\lambda+l}{\lambda} C_l^\lambda$ is the reproducing kernel for $\mathcal{H}_l(S^n)$, and Funk–Hecke formula can be written as

$$Y_l * f = \frac{\lambda}{\lambda + l} \hat{f}(l)\, Y_l.$$

The Laplace-Beltrami operator Δ^* on the sphere is defined by

$$\begin{aligned} \Delta^* f(\theta_1, \dots, \theta_{n-1}, \phi) &= \sum_{k=1}^{n-1} \left(\prod_{j=1}^{k-1} \sin\theta_j\right)^{-2} (\sin\theta_k)^{k+2-n} \frac{\partial}{\partial\theta_k} \left(\sin^{n-k}\theta_k \frac{\partial f(\theta_1, \dots, \theta_{n-1}, \phi)}{\partial\theta_k}\right) \\ &\quad + \left(\prod_{j=1}^{k} \sin\theta_j\right)^{-2} \frac{\partial^2 f(\theta_1, \dots, \theta_{n-1}, \phi)}{\partial\phi^2}. \end{aligned}$$

It is known that the hyperspherical harmonics are the eigenfunctions of Δ^*, i.e.,

$$\Delta^* Y_l^k = -l(n + l - 1) Y_l^k, \tag{7}$$

see [15, Chapter II, Theorem 4.1]. The relation of Δ^* and the Laplace operator Δ is given by

$$\Delta f = R^{-n} \frac{\partial}{\partial R} \left(R^n \frac{\partial f}{\partial R}\right) + \frac{1}{R^2} \Delta^* f, \tag{8}$$

where $R \geq 0$ is the radial distance of $\mathbf{x} \in \mathbb{R}^{n+1}$ in the hyperspherical coordinates, see [15, Chapter II, Proposition 3.3].

The Laplace operator is commutative with $SO(n+1)$-rotations Y,

$$\Delta\,[f(\mathrm{YX})] = (\Delta f)(\mathrm{YX}), \tag{9}$$

see [20, Chapter IX, Par. 2, Subsec. 4]. Consequently, it follows from (8) that the same holds for the Laplace-Beltrami operator, see also [15, Chapter II, formula (3.15)],

$$\Delta_{S^2}\,[f(\mathrm{YX})] = (\Delta_{S^2} f)(\mathrm{YX}). \tag{10}$$

Since S^n is a manifold without boundary, the Green second surface identity implies that for f, g of class C^2 the following holds:

$$\int_{S^n} \Delta^* f(\mathrm{X}) \cdot g(\mathrm{X})\, d\sigma(\mathrm{X}) = \int_{S^n} f(\mathrm{X}) \cdot \Delta^* g(\mathrm{X})\, d\sigma(\mathrm{X}). \tag{11}$$

The scalar product in $L^2(S^n)$ is antilinear in the first variable,

$$\langle f, g\rangle = \frac{1}{\Sigma_n} \int_{S^n} \overline{f(\mathrm{X})}\, g(\mathrm{X})\, d\sigma(\mathrm{X}).$$

With this notation we have

$$(f * g)(\mathrm{Y}) = \langle \overline{f}, \tau_{\mathrm{Y}} g \rangle .$$

Since Δ^* is a linear operator, one has

$$\overline{\Delta^* f} = \Delta^* \overline{f}$$

and (11) can be also written as

$$\langle \Delta^* f, g\rangle = \langle f, \Delta^* g\rangle . \tag{12}$$

Denote by D^n the interior of the sphere, $D^n = \{\mathbf{x} \in \mathbb{R}^{n+1} : |\mathbf{x}| < 1\}$. Let $\xi \in D^n$ with $r = |\xi|$ and $\mathrm{X} \in S^n$. The Poisson kernel for the sphere is given by

$$p(\xi, \mathrm{X}) = \frac{1}{\Sigma_n} \cdot \frac{1 - |\xi|^2}{|\xi - \mathrm{X}|^n} = \frac{1}{\Sigma_n} \cdot \frac{1 - r^2}{(1 - 2r\cos\theta + r^2)^{(n+1)/2}} \tag{13}$$

where θ denotes the angle between the vectors ξ and X. It is given as a series

$$p(\xi, \mathrm{X}) = \frac{1}{\Sigma_n} \cdot \sum_{l=0}^{\infty} r^l \cdot \frac{\lambda + l}{\lambda}\, C_l^{\lambda}(\cos\theta) \tag{14}$$

and it is a harmonic function of the variable ξ,

$$\Delta_{\xi}\, p(\xi, \mathrm{X}) = 0.$$

Since the Gegenbauer polynomials C_l^{λ} over the interval $[-1, 1]$ are bounded by

$$\left| C_l^{\lambda}(\cos\theta) \right| \le (n + l - 2)^{n-2}$$

uniformly in θ (compare [17, Theorem 7.33.1]), the series in (14) is uniformly (in θ) convergent for each $r \in [0, 1)$.

The following statement is the content of [14, Chap. II, Theorem 1.10]

Theorem 2.1. *Suppose f is a continuous function on $\mathbb{S}^n$, then the function defined by*

$$u(\xi) = \int_{\mathbb{S}^n} f(x)\, p(\xi, x)\, d\sigma(x) \tag{15}$$

when $|\xi| < 1$, and $u(\xi) = f(\xi)$ when $|\xi| = 1$ is harmonic for $|\xi| < 1$ and continuous for $|\xi| \leq 1$.

Remark 2.2. *Denote by n the north pole of the sphere,*

$$\mathrm{n} = (1, 0, \ldots, 0)$$

and set

$$\eta = r \cdot \mathrm{n}.$$

Let

$$p_r(x) = p_r(\cos\theta) = p(\eta, x)$$

for $x \in \mathbb{S}^n$. Then, (15) *can be expressed in terms of convolution or scalar product (over $\mathbb{S}^n$),*

$$u(\xi) = (f * p_r)(y) = \langle \bar{f}, \tau_y p_r \rangle,$$

where

$$y = \frac{\xi}{r} \in \mathbb{S}^n.$$

3. The Laplace-Beltrami operator

Numerical computation of derivatives is quite difficult and unstable, whereas algorithms for numerical integration are more robust. In the case of a function over $\mathbb{R}$, a way to replace differentiation by integration is use of Cauchy integral [10] which proves to be quite effective. In the present paper, we show how to compute $\Delta^j_{\mathbb{S}^2} f$ of a $2j$-times differentiable function as a convolution with an integral kernel. In this way, differentiation is replaced by a numerically more stable integration.

Theorem 3.1. *Suppose $f \in \mathcal{C}^{2j}(\mathbb{S}^n)$ for $j \in \mathbb{N}$. Then,*

$$(\Delta_{\mathbb{S}^2})^j f(y) = \lim_{r\to 1} (f * \mathcal{K}_r^{(j)})(y) \tag{16}$$

pointwise, where $\mathcal{K}_r^{(j)}$ is given by

$$\mathcal{K}_r^{(j)}(x) = (\Delta_{\mathbb{S}^2})^j p_r(x). \tag{17}$$

Proof. Since $f \in \mathcal{C}^{2j}(\mathbb{S}^n)$, $(\Delta_{\mathbb{S}^2})^j f$ is continuous and Theorem 2.1 applies. The function

$$v_r(y) = \langle (\Delta_{\mathbb{S}^2})^j \bar{f}, \tau_y p_r \rangle, \qquad y \in \mathbb{S}^n,\ r \in [0, 1)$$

yields $(\Delta_{\mathbb{S}^2})^j f$ in limit $r \to 1$. Now, by (12) and (10),

$$v_r(y) = \langle (\Delta_{\mathbb{S}^2})^{j-1} \bar{f}, \Delta_{\mathbb{S}^2}(\tau_y p_r) \rangle = \langle (\Delta_{\mathbb{S}^2})^{j-1} \bar{f}, \tau_y (\Delta_{\mathbb{S}^2} p_r) \rangle. \tag{18}$$

The Laplace-Beltrami operator in expression $\Delta_{\mathbb{S}^2}(\tau_y p_r)$ is taken with respect to the variable x. Repeat the operation described in (18) j times to obtain

$$v_r(y) = \langle \bar{f}, \tau_y \left((\Delta_{\mathbb{S}^2})^j p_r \right) \rangle. \tag{19}$$

TABLE 1. Relative error of computation of $\Delta_{S^2} f$ for homogeneous harmonic polynomials of distinct degrees – convolution with kernel K_r

Degree of polynomial	Convolution with $K^{(1)}_{0.99}$	Convolution with $K^{(1)}_{0.995}$	Convolution with $K^{(1)}_{0.999}$
4	3.9%	2%	0.4%
5	4.9%	2.5%	0.5%
6	5.8%	3%	0.6%
7	6.8%	3.4%	0.7%
8	7.7%	3.9%	0.8%
9	8.6%	4.4%	0.9%

Expressed as a convolution and with notation (17), this yields (16) 2

The following lemma gives a recipe how to compute kernels $K_r^{(j)}$.

Lemma 3.2. $K^{(j)}{}_r$ *given by* (17) *can be computed recursively via*

$$K_r^{(0)} = p_r.$$

$$K_r^{(j+1)}(x) = -\frac{\partial}{\partial r}\;\frac{1}{r^{n-2}}\cdot\frac{\partial}{\partial r}\;r^{n-1}\cdot K_r^{(j)}(x)\quad .$$

Proof. Follows from the absolute convergence of the series (14) representing the Poisson kernel, relation (7) and

$$l(n+l-1)r^L = \frac{d}{dr}\;\frac{1}{r^{n-2}}\cdot\frac{d}{dr}\;r^{n-1}\cdot r^L\quad .$$

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4. NUMERICAL EXPERIMENTS

Numerical experiments we performed are to show whether the derived formula is applicable. In order to avoid limit computation, we chose several values of r close to 1 and computed

$$f_1(y) := f * K_r^{(1)}\;(y) \tag{20}$$

for points y belonging to the 38-element Lebedev grid. Convolution is performed via iterated (with respect to the variables θ and ϕ) Gauss-Kronrod integration. The test functions f are homogeneous harmonic polynomials of distinct degrees such that the computed values could be compared to those obtained by direct computation with (7).

Table 1 gives the relative error of the procedure, equal to the quotient of integrated (with Lebedev quadrature) absolute value of the difference between f_1 (defined by (20)) and $\Delta_{S^2} f$ and integrated (with Lebedev quadrature) absolute value of $\Delta_{S^2} f$.

There are two sources of the computational error. One of them is the numerical procedure itself, and the other one is the choice of r. Suppose, P_L is a homogeneous harmonic polynomial of degree l. Then,

$$P_L * K_r^{(1)} = -l(n+l-1)r^L P_L = r^L \Delta_{S^2} P_L.$$

TABLE 2. Relative error of computation of $\Delta_{S^2} f$ for homogeneous harmonic polynomials of distinct degrees – convolution with polynomial kernel

Degree of polynomial	Kernel K^4	Kernel K^5	Kernel K^6	Kernel K^7	Kernel K^8	Kernel K^9
4	$2.2 \cdot 10^{-16}$	$3.1 \cdot 10^{-16}$	$1.5 \cdot 10^{-16}$	$3.9 \cdot 10^{-16}$	$2.7 \cdot 10^{-16}$	$5 \cdot 10^{-16}$
5		$2.4 \cdot 10^{-16}$	$1.3 \cdot 10^{-16}$	$2.9 \cdot 10^{-16}$	$2.6 \cdot 10^{-16}$	$5 \cdot 10^{-16}$
6			$7.3 \cdot 10^{-16}$	$1 \cdot 10^{-15}$	$1 \cdot 10^{-15}$	$1.2 \cdot 10^{-15}$
7				$7.9 \cdot 10^{-16}$	$3.6 \cdot 10^{-16}$	$6.3 \cdot 10^{-16}$
8					$3.8 \cdot 10^{-16}$	$4.6 \cdot 10^{-16}$
9						$6.9 \cdot 10^{-16}$

For $r = 1 - \epsilon$ this is approximately equal to $(1 - l \cdot \epsilon)\Delta_{S^2} P_L$ (see Table 1 to note that the experiment confirms this statement), which turns out to be problematic for big values of l.

However, physical devices transmit spherical harmonics of arbitrary high frequencies with some attenuation and the amplitude spectra of the responses (observations) to functions (signals) of finite energy are negligibly small beyond some finite frequency [6, Section 4.11], i.e., the test function can be assumed to be a polynomial of a certain degree less than or equal to L. In this case, the convolution kernel can be chosen to be equal to

$$K^L = -\frac{1}{\Sigma_n} \sum_{L=0} l(n + l - 1) \cdot \frac{\lambda + l}{\lambda} C_L^{\lambda}.$$

(Factor r^L with $r \in [0, 1)$ in the series (14) is necessary for its convergence, and can be abandoned if the series turns to a finite sum). And indeed, we obtained much better results with those kernels. They are presented in Table 2.

5. CONCLUSIONS

The method presented here can be effectively applied to numerical computation of Laplace-Beltrami operator of band-limited functions over the sphere. It is an alternative to the methods developed so far that are based on computation of differences. Replacement of discrete differentiation by integration yields a method that is stable under perturbations. However, it is a question for further research which integration algorithms should be used in order to optimize the computations.

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Conflict of interest

On behalf of all authors, the corresponding author states that there is no conflict of interest.

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