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SPHERICAL BASIS FUNCTION APPROXIMATION WITH PARTICULAR TREND FUNCTIONS

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Abstract: The paper is concerned with the measurement of scalar physical quantities at nodes on the $(d-1)$-dimensional unit sphere surface in the d-dimensional Euclidean space and the spherical RBF interpolation of the data obtained. In particular, we consider $d = 3$. We employ an inverse multiquadric as the radial basis function and the corresponding trend is a polynomial of degree 2 defined in Cartesian coordinates. We prove the existence of the interpolation formula of the type considered. The formula can be useful in the interpretation of many physical measurements. We show an example concerned with the measurement of anisotropy of magnetic susceptibility having extensive applications in geosciences and present numerical difficulties connected with the high condition number of the matrix of the system defining the interpolation.

Keywords: spherical interpolation, spherical radial basis function, trend, inverse multiquadric, magnetic susceptibility

MSC: 65D12, 65D05, 65Z05

1. Introduction

The aim of this paper is to present some ways of approximating and mapping measured physical quantities exhibiting anisotropy that can be expressed by means of a second-order tensor. A typical example is the measurement of magnetic susceptibility of rock having extensive applications in geosciences [11].

In the paper, we develop the data interpolation and approximation with the help of spherical radial basis functions in such a case, cf. [6]. The functions appearing in the formula are the basis functions chosen as radial functions and the trends, cf. [1].

In the laboratory determination of raw data, cf. [5], [8], [11], the rock sample rotates in magnetic field in a set of selected directions and the data items s_i measured are of the form

$$s_i = z_i^{\mathrm{T}} K z_i + e_i, \tag{1}$$

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where z_i are the unit vectors in the ith direction of measurement in Cartesian coordinates, K is a tensor and e_i are deviations from the theoretical tensor model.

An appropriate rotation of the coordinate system can make the tensor K diagonal,

$$K = \begin{bmatrix} K_1 & 0 & 0 \\ 0 & K_2 & 0 \\ 0 & 0 & K_3 \end{bmatrix},$$

where K_1, K_2, K_3 are *principal susceptibilities*. These Cartesian coordinates are basically used for the description of the problem in what follows. We call the graphical representation of the directional susceptibilities (1) the *lemniscate surface,* see Fig. 1. The function s corresponding to (1) is taken for the trend in our considerations that follow.

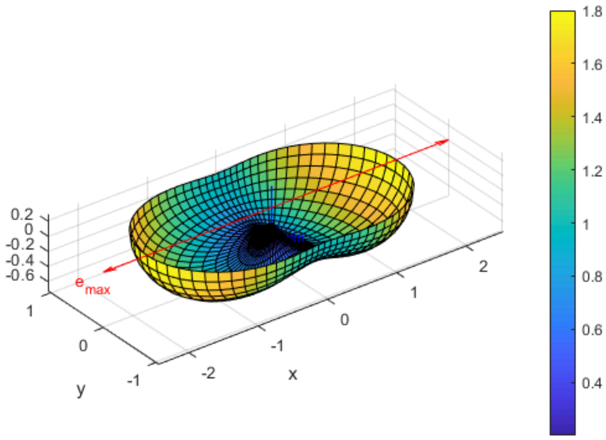

Figure 1: Lower half of the lemniscate surface with $K_1 = 1.8, K_2 = 1.0, K_3 = 0.2$. The magnitude of directional susceptibility in the ith direction z_i is given by the distance between the origin and the surface measured along the vector z_i. The red arrows indicate the direction of the first eigenvector of the susceptibility tensor.

2. Exact and smooth approximation of spherical data

Let d be the dimension of a real Euclidean space $\mathbb{R}^d$. Put

$$S^{d-1} = \{x = (x_1, \ldots, x_d) \in \mathbb{R}^d \mid \sum_{i=1}^{d} x_i^2 = 1\}.$$

Then S^{d-1} is the $(d-1)$-*dimensional surface of unit sphere* in the d-dimensional Euclidean space.

Choose a positive integer N and a nonnegative integer M, $N \geq M$. Given a set $X = \{X_j\}_{j=1}^N$ of mutually distinct nodes $X_j = (X_{j1}, X_{j2}, \dots, X_{jd})$ on S^{d-1}, then a general formula for the *exact spherical approximant* (interpolant) v has for $x \in S^{d-1}$ the form

$$v(x) = \sum_{j=1}^{N} a_j \psi(g(x, X_j)) + \sum_{k=1}^{M} b_k p_k(x), \tag{2}$$

where a_j, $j = 1, \dots, N$, and b_k, $k = 1, \dots, M$, are real coefficients to be found. If $M = 0$, the second sum in (2) is empty.

Further, $\psi \colon [0, \pi] \to \mathbb{R}$ is a continuous real function called the *spherical basis function* (SBF) or *spherical radial basis function* (SRBF). A function $\sigma(x, y)$, $x, y \in \mathbb{R}^d$, is called *radial* if there exists a function $\tau(r)$, $r \geq 0$, such that $\sigma(x, y) = \tau(r)$, where $r = \|x - y\| \in \mathbb{R}$ is the Euclidean norm. The nonnegative function g is the *geodesic metric*, usually $g \colon S^{d-1} \times S^{d-1} \to [0, \pi]$, cf. [6], Section 2.3.

Finally, let $\Pi_t(\mathbb{R}^d)$ be the set of all polynomials $p \colon \mathbb{R}^d \to \mathbb{R}$ with real coefficients and of total degree less then or equal to some nonnegative integer t (called *trends*). Let us formulate the exact approximation (interpolation) problem to be solved, cf. [6], [7]. The smoothing problem will be mentioned in the end of this section.

Given a continuous real target function $f \colon S^{d-1} \to \mathbb{R}$, find the spherical interpolant (2), i.e., a continuous function $v \colon S^{d-1} \to \mathbb{R}$ that satisfies the *interpolation conditions*

$$v(X_i) = f(X_i), \quad i = 1, \dots, N, \tag{3}$$

where $f(X_i)$ are the values measued at X_i. We use the SBF interpolation formula (2) with a proper geodesic metric g, spherical radial basis function ψ, and trends $p_k \in \Pi_t(\mathbb{R}^d)$, $k = 1, \dots, M$. We confine ourselves only to real-valued functions and real data in this paper to make the exposition clearer.

Let us employ the matrix notation. We substitute X_i, $i = 1, \dots, N$, for x in the formula (2) to get

$$v(X_i) = \sum_{j=1}^{N} a_j \psi(g(X_i, X_j)) + \sum_{k=1}^{M} b_k p_k(X_i), \quad i = 1, \dots, N, \tag{4}$$

and replace the left hand parts $v(X_i)$ of the interpolation conditions (3) with the expressions (4).

Introduce an $N \times N$ symmetric matrix Ψ with the entries

$$\psi_{ij} = \psi(g(X_i, X_j)), \quad i, j = 1, \dots, N, \tag{5}$$

and an $N \times M$ matrix P with the entries

$$p_{jk} = p_k(X_j), \quad j = 1, \dots, N, \ k = 1, \dots, M.$$

Moreover, we denote by $a \in \mathbb{R}^N$, $b \in \mathbb{R}^M$, and $f \in \mathbb{R}^N$ the vectors of the unknowns and the vector of the right hand parts $f(x_i)$ of the interpolation conditions (3).

Note that if $M > 0$ then we have only N interpolation conditions (3) for $N+M$ interpolation coefficients a_j and b_k in the formula (2). Thus, we can impose M additional linear constraints for the individual trends p_k,

$$\sum_{j=1}^{N} a_j p_k(X_j) = \sum_{j=1}^{N} a_j p_{jk} = 0, \quad k = 1, \ldots, M. \tag{6}$$

Now the system of linear algebraic equations to be solved for the unknown vectors a and b consists of (3) and (6), i.e.

$$\Psi a + Pb = f,$$
$$P^{\mathrm{T}} a = 0$$

or

$$\begin{bmatrix} \Psi & P \\ P^{\mathrm{T}} & 0 \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} f \\ 0 \end{bmatrix}. \tag{7}$$

We put

$$Q = \begin{bmatrix} \Psi & P \\ P^{\mathrm{T}} & 0 \end{bmatrix}, \tag{8}$$

which is a symmetric $(N+M) \times (N+M)$ matrix of the system (7).

We have formulated the general spherical interpolation problem. Apparently, the problem possesses the unique solution if and only if the matrix Q of the system (7) is nonsingular. We employ some conditions guaranteeing that Q is nonsingular. To prove them we need two statements.

Lemma 1. ([3], Theorem 1.23) *Let*

$$A = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix}$$

be a square matrix, A_{11} its nonsingular submatrix. Then

$$\det[A/A_{11}] = \det A / \det A_{11},$$

where

$$[A/A_{11}] = A_{22} - A_{21} A_{11}^{-1} A_{12}$$

is the Schur complement of the submatrix A_{11} in A.

Lemma 2. ([4], Theorem 4.2.1) *Let the $N \times N$ matrix A be symmetric positive definite and the $N \times M$ matrix Y have rank M, $N \geq M > 0$. Then the $M \times M$ matrix $Y^{\mathrm{T}} AY$ is also symmetric positive definite.*

Theorem 1. *Let the $N \times N$ principal submatrix Ψ of the $(N+M) \times (N+M)$ matrix Q introduced in (8) be symmetric positive definite and let* rank $P = M$*. Then the matrix Q is nonsingular.*

Proof. (Cf. the proof of Theorem 1 in [9].) Let $[Q/\Psi] = -P^{\mathrm{T}}\Psi^{-1}P$ be the Schur complement of the submatrix Ψ in Q. Then

$$\det Q = \det[Q/\Psi] \det \Psi$$

according to Lemma 1. Further,

$$\det[Q/\Psi] = \det(-P^{\mathrm{T}}\Psi^{-1}P) \neq 0$$

follows for the positive definite matrix Ψ from Lemma 2 as we have assumed rank $P = M$. Finally, we get $\det Q \neq 0$, the matrix Q is nonsingular, and the system (7) has the unique solution. □

Theorem 1 holds only for Ψ positive definite. On the other hand, different assumptions can be imposed on the matrix Q of the system (7), e.g., positive definiteness or conditional positive definiteness of the function ψ, see [7].

Definition 1. ([6]) A continuous function $\psi\colon [0,\pi] \to \mathbb{R}$ is said to be *positive definite on S^{d-1}* (i.e., $\psi \in \mathrm{PD}(S^{d-1})$) if the quadratic form

$$c^{\mathrm{T}}\Psi c = \sum_{i=1}^{N}\sum_{j=1}^{N} c_i c_j \psi(g(Y_i, Y_j)) \tag{9}$$

is positive on $\mathbb{R}^N \setminus \{0\}$ for any finite set $Y = \{Y_k\}_{k=1}^{N}$ of distinct points on S^{d-1}.

Definition 2. ([7]) Let the span of the trends p_k, $k = 1, \ldots, M$, be the space $\pi_t(\mathbb{R}^d)$ of polynomials in d variables of total degree t, where t is a nonnegative integer. A continuous function $\psi\colon [0,\pi] \to \mathbb{R}$ is said to be *conditionally positive definite of order t on S^{d-1}* (i.e., $\psi \in \mathrm{CPD}_t(S^{d-1})$) if the quadratic form (9) is positive for any finite set $Y = \{Y_k\}_{k=1}^{N}$ of distinct points on S^{d-1} and scalars $c_1, c_2, \ldots, c_N$ such that

$$\sum_{j=1}^{N} c_j p(Y_j) = 0$$

for all $p \in \pi_t(\mathbb{R}^d)$.

Remark 1. In Theorem 1, we use the hypothesis that the matrix Ψ is positive definite and rank $P = M$. Moreover, any function $\psi \in \mathrm{PD}(S^{d-1})$ can be used to provide a unique interpolant of the form

$$v(x) = \sum_{j=1}^{N} a_j \psi(g(x, X_j)).$$

However, most books and papers (see, e.g., [1], [6], [7]) employ the condition that the spherical basis function ψ is positive definite or conditionally positive definite to prove that the matrix Q is nonsingular (cf., e.g., [6]).

Remark 2. The simplest spherical interpolant v can be considered if we omit the second sum in (2), i.e., we set $M = 0$ and employ no trends. If Ψ is symmetric positive definite, there is no matrix P in the formulation, $Q = \Psi$ and, instead of (7), we get the $N \times N$ symmetric positive definite system

$$\Psi a = f. \tag{10}$$

Apparently, the system (10) possesses the unique solution a.

Remark 3. Let us formulate the least squares smoothing problem. Keep the notation introduced. Further, let w_j, $j = 1, \ldots, N$, be positive weights chosen and put $W = \mathrm{diag}(w_1, w_2, \ldots, w_N)$. In solving the data smoothing problem we employ the least squares functional minimization. The approximant is assumed in the form

$$\widehat{v}(x) = \sum_{j=1}^{N} (\widehat{f}_j - \widehat{a}_j) w_j \psi(g(x, X_j)) + \sum_{k=1}^{M} \widehat{b}_k p_k(x), \tag{11}$$

where $\widehat{a}_j$, $j = 1, \ldots, N$, and $\widehat{b}_k$, $k = 1, \ldots, M$, are real coefficients to be found, and, moreover, we have

$$\widehat{v}(X_j) = \widehat{a}_j, \quad j = 1, \ldots, N.$$

If $M = 0$, the second sum in (11) is empty.

Now the system of linear algebraic equations to be solved for the unknown vectors $\widehat{a}$ and $\widehat{b}$ is

$$\begin{bmatrix} \Psi W + I & -P \\ P^{\mathrm{T}} W & 0 \end{bmatrix} \begin{bmatrix} \widehat{a} \\ \widehat{b} \end{bmatrix} = \begin{bmatrix} \Psi W f \\ P^{\mathrm{T}} W f \end{bmatrix}. \tag{12}$$

No interpolation conditions are imposed. An analog of Theorem 1 concerned with the system (12) is proved e.g. in [10], Theorem 2.

3. Magnetic susceptibility measurement

As we have mentioned in the introduction, the particular physical quantity whose measured values are approximated by the means presented in this paper is magnetic susceptibility. Put $d = 3$, then S^2 is the usual two-dimensional unit sphere in the three-dimensional space. Choose a fixed positive integer N and put $M = 1$. Consider the interpolation formula (2) in the form

$$v(x) = \sum_{j=1}^{N} a_j \psi(g(x, X_j)) + b s(x), \tag{13}$$

where $x, X_j \in S^2$, i.e., in (7), P is a single column N-vector and b and 0 are scalars.

The interpolation conditions (4) now read

$$v(X_i) = \sum_{j=1}^{N} a_j \psi(g(X_i, X_j)) + bs(X_i), \quad i = 1, \dots, N. \tag{14}$$

Moreover, we add a single constraint

$$\sum_{j=1}^{N} a_j s(X_j) = 0 \tag{15}$$

corresponding to (6).

To define a SBF formula (13) uniquely, we have to choose a proper spherical basis function ψ, geodesic metric g, and trend s. For $x, y \in S^2$ (both x and y are unit vectors), one usually puts

$$g(x,y) = \sqrt{1 - (x^{\mathrm{T}} y)^2},$$

where the angle α, $0 \le \alpha \le \pi$, between the vectors x and y is given by

$$\cos\alpha = x^{\mathrm{T}} y. \tag{16}$$

For our purposes, we consider the angle between vectors of parallel directions to be zero regardless of their orientation. At the same time, we take into account always the acute angle α of the vectors x, y, i.e., the range of α is $[0, \frac{1}{2}\pi]$. We now change the formula (16) for

$$\cos\alpha = |x^{\mathrm{T}} y|, \quad \text{i.e. } \alpha = \cos^{-1}(|x^{\mathrm{T}} y|),$$

and use the geodesic metric

$$g(x,y) = \sqrt{1 - \cos^2\alpha} = \sin\alpha = \sin(\cos^{-1}(|x^{\mathrm{T}} y|)) \tag{17}$$

with α acute. Thus, this geodesic metric is the function $g\colon S^2 \times S^2 \to [0, \frac{1}{2}\pi]$.

The metric (17) does not distinguish the vectors x and $-x$. Therefore, in what follows, we assume that the elements X_j of the set X are mutually distinct and, moreover, that it is $X_i \ne -X_j$ for every $i, j = 1, \dots, N$.

We have chosen the *inverse multiquadric*

$$\psi(r) = \frac{1}{\sqrt{(r^2 + c^2)}} \tag{18}$$

for the spherical radial basis function, where $r \in [0, \frac{1}{2}\pi]$ (the range of the function g) and c is a positive shape parameter that controls tension of the interpolation surface.

Finally, we take the second degree polynomial (1),

$$s(z) = K_1 z_1^2 + K_2 z_2^2 + K_3 z_3^2, \quad z = (z_1, z_2, z_3) \in S^2, \tag{19}$$

where K_1, K_2, K_3 are proper positive constants for the trend.

Notice that the argument of the SBF function ψ is from the interval $[0, \frac{1}{2}\pi]$ since $g\colon S^2 \times S^2 \to [0, \frac{1}{2}\pi]$ is a geodesic metric, while the argument of the trend s is from S^2, similarly to [7].

The advantage of the formula proposed is apparent in cases when we know that the physical field measured does not principally differ from the ideal field whose values can be computed from some explicit formula. This description of an ideal field is then fitted by the trend part of the formula and the contributions obtained from the first, spherical part of the formula are only small.

Let us verify the existence of the formula (13). Since we use the inverse multiquadric (18) for the spherical radial basis function, we shall employ some results of [7] and [6]. Now we can prove that the matrix Ψ corresponding to (18) is symmetric positive definite.

Lemma 3. ([7], p. 19) *The $N \times N$ symmetric matrix Ψ with entries*

$$\psi_{ij} = (r_{ij}^2 + c^2)^{-\alpha},$$

where $r_{ij} = g(X_i, X_j)$, $c > 0$, and $\alpha > 0$, is symmetric positive definite.

Consider the interpolation formula (13) with the functions g, ψ, and s given by the formulae (17), (18), and (19), respectively. Choose positive constants c, K_1, K_2, K_3. For the interpolation formula (13), set up the system (14) corresponding to the interpolation conditions (3) and the equation (15) corresponding to the constraints (6).

Theorem 2. *Let the system (7) correspond to the formula (13). Let the block P in the block matrix Q given by (8) have rank 1. Then the interpolation problem (14), (15) has the unique solution, where the coefficients a_j, $j = 1, \ldots, N$, and b solve uniquely the linear algebraic system (7).*

Proof. According to Lemma 3, the principal submatrix Ψ of the block matrix Q of the system (7) is positive definite. On the assumption that rank $P = 1$, the matrix Q is nonsingular by Theorem 1 and the system (7) has the unique solution a_j, $j = 1, \ldots, N$, and b. ☐

Remark 4. P is a single column N-vector, $P^{\mathrm{T}} = (s(X_1), \ldots, s(X_N))$. The assumption of Theorem 2 that rank $P = 1$ is apparently fulfilled if at least one of the entries $s(X_k)$ is nonzero.

4. Numerical experiments. Conclusions

We present some numerical experience with the interpolation problem described in Section 3. According to Lemma 3, the matrix Ψ with entries (5) is symmetric positive definite and the matrix Q introduced in (8) is nonsingular when the matrix P has rank $P = 1$. But the use of the lemniscate s given by (19) does not prevent a very difficult solving the linear algebraic system (7).

We have chosen the interpolation nodes x_j on the south (lower) "hemisphere" roughly equally. The system (7) can be easily solved for $N = 15$ (i.e., 15 nodes, 16 equations), but for $N = 30$ and higher its solution computed in double precision is useless.

The condition number cond Q of the matrix Q of a linear algebraic system characterizes in some way the accuracy one can reach when solving the system: the higher the condition number, the more ill-conditioned system and the worse (less accurate) the solution. For a symmetric matrix Q, the condition number cond Q can be defined as the quotient of the largest and smallest singular value of Q, i.e. the quotient of the largest in magnitude and smallest in magnitude eigenvalue of the matrix Q, cf. [4].

In our computation with $c \in [0.125, 2.000]$, cond Q reaches about 10^3 in case of $N = 15$, but about 10^8 in case of $N = 60$, which thus provides no acceptable solution. Decreasing c, we can reach a lower condition number.

We have shown sufficient conditions for the existence of SRBF interpolant and approximant. We have considered a particular SRBF interpolation formula employing an inverse multiquadric and using a trend being a second degree polynomial (19) in Section 3.

We have carried out numerical tests with this interpolation formula. The formula performs efficiently only for a small number N of interpolation nodes X_j and the results exhibit week dependency on the parameter c. Further research shall provide a comparison of results obtained using various other SRBFs, e.g. direct multiquadrics [6], thin plate splines [2], etc.

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