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MULTIVARIATE SMOOTH INTERPOLATION THAT EMPLOYS POLYHARMONIC FUNCTIONS

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Abstract: We study the problem of construction of the smooth interpolation formula presented as the minimizer of suitable functionals subject to interpolation constraints. We present a procedure for determining the interpolation formula that in a natural way leads to a linear combination of polyharmonic splines complemented with lower order polynomial terms. In general, such formulae can be very useful e.g. in geographic information systems or computer aided geometric design. A simple computational example is presented.

Keywords: data interpolation, smooth interpolation, polyharmonic spline, radial basis function, Fourier transform

MSC: 65D05, 41A05, 41A63, 31B30, 42A38

1. Introduction

In science and technology, measurements of the values of a continuous function of one or more independent variables are performed. We get a finite number of function values measured at a finite number of nodes but we are interested also in the values corresponding to other points in some domain of interest. This is the general problem of *data approximation*. In particular, the interpolating curve can be defined as the solution of a constrained variational problem.

Smooth approximation with radial basis functions is very useful in solving problems of interpolation or data fitting, in particular in 2D and 3D. Note that the number of linear algebraic equations of the system to be solved in the course of the construction of the interpolant is, in principle, proportional to the number N of measured values. In practice, such interpolants are employed e.g. in geographic information systems or computer aided geometric design.

Polyharmonic splines satisfy the polyharmonic equation. Moreover, polyharmonic splines are radial basis functions. In the paper, we present a particular procedure for construction of the interpolation formula that in a natural way leads to a linear

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combination of polyharmonic splines, possibly complemented with lower order polynomial terms. The 1D cubic spline interpolation is known to be the approximation of this kind where the $\mathcal{L}^2$ norm of the second derivative (curvature) of the interpolating function is minimized.

We generalize the approach of Talmi and Gilat [6], and Mitáš and Mitášová [2], and introduce the problems to be solved and the tools necessary to this aim in Sections 2 and 3. We present the general existence theorem for smooth interpolation in Section 4. A particular basis system $\exp(-\mathrm{i}\rho \cdot x)$ of functions for the space, where the smooth interpolation is performed, is introduced in Section 5. The next section is concerned with the polyharmonic spline interpolation in particular. In Section 7 we show results of the computational experiment employing various versions of the smooth interpolation. We finally sum up the results in Section 8.

2. Data interpolation. Interpolation with radial basis functions

Consider a finite number N of (complex, in general) measured (sampled) values $f_1, \ldots, f_N \in C$ obtained at N given nodes $X_1, \ldots, X_N \in \Omega$ that are mutually distinct and $\Omega \subset R^n$ is a hypercube. To understand the quantity measured, we look for the unknown values corresponding to other points in Ω. Assume that $f_j = f(X_j)$ are measured values of some function f continuous in Ω and z is an approximating function to be constructed.

The *interpolating function* (interpolant) z is constructed to fulfil the interpolation conditions

$$z(X_j) = f_j, \quad j = 1, \ldots, N. \tag{1}$$

Various additional conditions can be considered, e.g. minimization of some functionals applied to z. In this way we come to the *smooth interpolation* treated e.g. in [6] and [5].

We do not treat the general problem of smooth approximation in this paper.

Let $x, y \in R^n$ and

$$r(x,y) = \|x - y\|_E = \sqrt{\sum_{s=1}^{n} (x_s - y_s)^2} \tag{2}$$

be the Euclidean distance of the points x, y. The dimension n of the independent variable can be arbitrary. The function F is called a *radial basis function* if $F(x,y) = \widehat{F}(r(x,y))$. Radial basis functions are often used for interpolation as well as approximation. It is expected that every item f_j of data measured at the node X_j influences the result of interpolation and/or approximation at a point in the vicinity of X_j proportionally to its distance from X_j if this vicinity can be considered "homogeneous".

The vector $\alpha = (\alpha_1, \ldots, \alpha_n)$, where α_s, $s = 1, \ldots, n$, are integers, is called a *multiindex*. Denote the *length of a multiindex* α by

$$|\alpha| = \sum_{s=1}^{n} |\alpha_s|, \tag{3}$$

where $|\alpha_s|$ means the absolute value of the component α_s. We say that α is a *nonnegative multiindex* if $\alpha_s \geq 0$ holds for all $s = 1, \ldots, n$.

Choose a nonnegative integer L and consider the interpolant

$$z(x) = \sum_{j=1}^{N} \lambda_j F(x, X_j) + \sum_{|\alpha| \leq L-1} a_\alpha \varphi_\alpha(x), \tag{4}$$

where α is a nonnegative multiindex, $F(x, y)$ a radial basis function (e.g. a proper polyharmonic spline), φ_α are all the monomials of the form

$$\varphi_\alpha(x) = x_1^{\alpha_1} \ldots x_n^{\alpha_n} \tag{5}$$

of degree at most $L - 1$ called *trend functions*, and λ_j, $j = 1, \ldots, N$, and a_α, $|\alpha| \leq L - 1$, are coefficients to be found; the second sum in the formula (4) is empty if $L = 0$. The term trend function has nothing in common with trends in statistics and was first introduced in [2].

3. Polyharmonic splines

Let $r(x, y)$ be given by (2). The functions

$$r^k, \quad k = 1, 3, \ldots, \tag{6}$$

$$r^k \ln r, \quad k = 2, 4, \ldots, \tag{7}$$

are called *polyharmonic splines*. The equation $\Delta^m\, u(x_1, \ldots, x_n) = 0$, where $\Delta = \partial^2/\partial x_1^2 + \cdots + \partial^2/\partial x_n^2$ is the Laplace operator, is called the *polyharmonic equation of order* m.

Fix the vector $y \in R^n$. Then it is easy to show that the polyharmonic spline r^k (or $r^k \ln r$) solves the polyharmonic equation with $m = \frac{1}{2}(k+n)$ in $R^n \setminus \{x = y\}$ for n odd (or for n even). Note that the term *spline* is used here also for a nonpolynomial function.

Apparently, $r(x, y)$ is a real radial basis function. All polyharmonic splines possess the same property, too. For practical use, the polyharmonic splines are combined with lower order polynomial terms to form an interpolation or approximation formula.

4. Smooth interpolation

We are going to show briefly the role of polyharmonic splines in interpolation using the *smooth interpolation* or *variational spline theory.*

We follow [6], and formulate and solve the problem of smooth interpolation. We generalize the problem for $n > 1$ as compared with [5]. Choose a set $\{B_\alpha\}$ of nonnegative numbers, where α is a nonnegative multiindex. Let L be the smallest nonnegative integer such that $B_\alpha > 0$ for at least one α, $|\alpha| = L$, while $B_\alpha = 0$ for all α, $|\alpha| < L$.

Recall that the nodes $X_1, \ldots, X_N \in \Omega$ are supposed to be mutually distinct. Let W_L be a linear vector space of complex valued functions g continuous together with all their partial derivatives of all orders in Ω. For $g, h \in W_L$ we put

$$(g, h)_L = \sum_{L \le |\alpha|} B_\alpha \int_\Omega \frac{\partial^{|\alpha|} g(x)}{\partial x_1^{\alpha_1} \ldots \partial x_n^{\alpha_n}} \left(\frac{\partial^{|\alpha|} h(x)}{\partial x_1^{\alpha_1} \ldots \partial x_n^{\alpha_n}} \right)^* \mathrm{d}x, \tag{8}$$

where * denotes the complex conjugate, for the inner product and similarly for the norm if the values of $\|g\|_L$ and $\|h\|_L$ exist and are finite.

If $L > 0$ we first have to construct the quotient space W_L/P_{L-1} with the zero class P_{L-1} whose basis $\{\varphi_\alpha\}$, $|\alpha| \le L-1$, consists of all the trend functions (5) of degree at most $L-1$. Denote the number of these functions by T.

W_L is the normed space where we minimize functionals and measure the smoothness of the interpolation as prescribed by the choice of $\{B_\alpha\}$. We complete the space W_L in the norm $\|\cdot\|_L$ (cf. e.g. [7]) and denote the completed space again W_L. For an arbitrary $L \ge 0$, choose a *basis system* of functions $\{g_\varkappa\} \subset W_L$, $\varkappa$ being a nonnegative multiindex, that is complete and orthogonal. Then, moreover, all the trend functions $\{\varphi_\alpha\}$ are orthogonal and also the basis and trend functions are mutually orthogonal. The set $\{\varphi_\alpha\}$ of trend functions is empty for $L = 0$. For details, see [2] and [5].

We will also employ the usual Lebesgue space $\mathcal{L}^2(\Omega)$ of generalized functions with the norm $\|g\|_{\mathcal{L}^2}$.

The *problem of smooth interpolation* [6] consists in finding the coefficients $A_\varkappa$ and a_α of the *smooth interpolant*

$$z(x) = \sum_\varkappa A_\varkappa g_\varkappa(x) + \sum_{|\alpha| \le L-1} a_\alpha \varphi_\alpha(x) \tag{9}$$

such that

$$z(X_j) = f_j, \quad j = 1, \ldots, N, \tag{10}$$

and

$$\text{the quantity } \ \|z\|_L^2 \ \text{ attains its minimum on } W_L. \tag{11}$$

The second sum in the interpolant is empty for $L = 0$. Apparently the quantity $\|z\|_L^2$ is the weighted sum of the squares of $\mathcal{L}^2$ norms of the derivatives of z of all orders $|\alpha|$ with weights B_α. Putting $B_\alpha > 0$ for some set of multiindices α, we can specify the partial derivatives of z whose $\mathcal{L}^2$ norms are to be minimized, i.e. the behavior of the smooth interpolant z.

Moreover,

$$\|z\|_L^2 = \sum_\varkappa A_\varkappa A_\varkappa^* \|g_\varkappa\|_L^2$$

due to the mutual orthogonality of the basis $\{g_\varkappa\}$ and trend functions $\{\varphi_\alpha\}$, and (9).

The infinite sum in (9) is inconvenient for practical computation. Therefore, we introduce the generating function [6]. If the series

$$R(x,y) = \sum_\varkappa \frac{g_\varkappa(x) g_\varkappa^*(y)}{\|g_\varkappa\|_L^2} \tag{12}$$

converges for all $x, y \in \Omega$ and is continuous in Ω we call the fuction $R(x,y)$ the *generating function.*

If $L > 0$, introduce an $N \times T$ matrix Φ with entries $\Phi_{j\alpha} = \varphi_\alpha(X_j)$, $j = 1, \dots, N$, $|\alpha| \le L-1$. The matrix Φ is, in general, rectangular.

We state in following Theorem 1 that a finite linear combination of the values of the generating function $R(x,y)$ at nodes is used for the practical interpolation instead of the infinite linear combination of the values of the basis functions in (9).

Theorem 1. *Let $X_i \neq X_j$ for all $i \neq j$. Assume that the series (12) converges for all $x, y \in \Omega$ and the generating function $R(x,y)$ is continuous in Ω. Moreover, let* rank $\Phi = T$, *i.e. Φ has full rank T. Then the problem (9), (10), and (11) of smooth interpolation has the unique solution*

$$z(x) = \sum_{j=1}^N \lambda_j R(x, X_j) + \sum_{|\alpha| \le L-1} a_\alpha \varphi_\alpha(x), \tag{13}$$

where the coefficients λ_j, $j = 1, \dots, N$, and a_α, $|\alpha| \le L-1$, are the unique solution of a nonsingular system of $N+T$ linear algebraic equations.

Proof. The proof including the linear algebraic system to be solved is for $n = 1$ and arbitrary $L \ge 0$ presented in [3]. The proof of Theorem 1 in the general case of $n \ge 1$ and $L \ge 0$ differs from this proof only in details. □

The smooth interpolant z given by (9) can now be, for a radial basis function $R(x,y)$, rewritten in the form (13), i.e. (4).

5. A particular choice of basis function system

Let the function $f(x) = f(x_1, \dots, x_n)$ to be interpolated be 2π-periodic in each independent variable x_s, $s = 1, \dots, n$. Periodic functions with other periods in the individual variables can be formally transformed to the period 2π. Let us consider f

in the hypercube $\widetilde{\Omega} = [0, 2\pi]^n$. We choose exponential functions of pure imaginary argument for the periodic basis system $\{g_\rho\}$ in W_L, where $g_\rho(x) = \exp(-\mathrm{i}\rho \cdot x)$. We have to change the notation properly with respect to the fact that the integer components of the multiindex ρ are also negative. The definition (3) of the length $|\rho|$ of the multiindex ρ remains without change. The following theorem shows important properties of the system $\{g_\rho\}$.

Theorem 2. *Let there be an integer U, $U \geq L$, such that $B_\alpha = 0$ for all $|\alpha| > U$ in W_L. The system of periodic exponential functions of pure imaginary argument*

$$g_\rho(x) = \exp(-\mathrm{i}\rho \cdot x), \ \ x \in \widetilde{\Omega}, \tag{14}$$

ρ being a multiindex with integer components $\rho_s = 0, \pm 1, \pm 2, \ldots,\ s = 1, \ldots, n$, is complete and orthogonal in W_L.

Proof. For $n = 1$, the proof is given in [4]. For $n \geq 1$, the orthogonality is proven by direct computation. The proof of completeness can be performed for $n > 1$ in a way similar to that in [4]. □

The range of ρ implies a minor change in the notation introduced above. For the basis system (14), the generating function (12) is rewritten as

$$R(x, y) = \sum_\rho \frac{g_\rho(x) g_\rho^*(y)}{\|g_\rho\|_L^2} = \sum_\rho \frac{\exp(-\mathrm{i}\rho \cdot (x - y))}{\|g_\rho\|_L^2}, \tag{15}$$

i.e. the n-dimensional Fourier series in $\mathcal{L}^2(\widetilde{\Omega})$ with the coefficients $\|g_\rho\|_L^{-2}$, where

$$\|g_\rho\|_L^2 = (2\pi)^n \sum_{|\alpha|=L}^{U} B_\alpha \rho_1^{2\alpha_1} \ldots \rho_n^{2\alpha_n}$$

according to (8).

Let now the function f to be interpolated be nonperiodic in R^n. Redefine the generating function

$$R(x, y) = \int_{R^n} \frac{\exp(-\mathrm{i}\rho \cdot (x - y))}{\|g_\rho\|_L^2} \, \mathrm{d}\rho = \mathcal{F}\left(\frac{1}{\|g_\rho\|_L^2} \right) \tag{16}$$

as the n-dimensional Fourier transform $\mathcal{F}$ of the function $\|g_\rho\|_L^{-2}$ of n continuous variables $\rho_1, \rho_2, \ldots, \rho_n$ if the integral exists. Employing the transition from the Fourier series (15) with the coefficients $\|g_\rho\|_L^{-2}$ to the Fourier transform (16) of the function $\|g_\rho\|_L^{-2}$ of continuous variable $\rho \in R^n$ (cf., e.g., [4]), we have transformed the basis functions, enriched their spectrum, and released the requirement of periodicity of f. Moreover, if the integral (16) does not exist in the usual sense, in many instances we can calculate $R(x, y)$ as the Fourier transform $\mathcal{F}$ of the generalized function $\|g_\rho\|_L^{-2}$ of ρ.

The values of the generating function $R(x, y)$ given by (16) depend on x and y only through $x - y$.

6. Polyharmonic spline interpolation

We continue in deriving the polyharmonic spline interpolation. Put

$$K(\alpha) = \frac{|\alpha|!}{\alpha_1! \ \ldots \ \alpha_n!} \tag{17}$$

for a nonnegative multiindex α. Recall that n is the dimension of the problem, fix $L > 0$ and put $B_\alpha = 0$ for all α, $|\alpha| \neq L$, and $B_\alpha = K(\alpha)$ for $|\alpha| = L$. Then

$$\|g_\rho\|_L^2 = (2\pi)^n \left(\sum_{s=1}^{n} \rho_s^2 \right)^L$$

according to the multinomial theorem.

In tables (e.g. [1]), we find easily

$$R(x,y) = \mathcal{F}\left(\left(\sum_{s=1}^{n} \rho_s^2 \right)^{-L} \right) = C_1 r^{2L-n} \text{ for } n \text{ odd,} \tag{18}$$

$$= C_{21} r^{2L-n} \ln r + C_{22} r^{2L-n} \text{ for } n \text{ even,} \tag{19}$$

where $r = r(x,y)$ is given by (2) and C_1, C_{21}, and C_{22} are quantities depending only on n and L. For $2L-n > 0$ the generating function $R(x,y)$ is a radial basis function.

Note that the function (18) has just the form of the polyharmonic function (6) if the dimension n is odd while the function (19) is the sum of the polyharmonic function (7) and $C_{22} r^{2L-n}$ if n is even. We can remove the term $C_{22} r^{2L-n}$ from the formula (19) for the generating function in case of n even and $2L-n > 0$ in the way based on that used in [2].

We now can modify the generating function $R(x,y)$ in (18) and (19) and obtain

$$R(x,y) = r^{2L-n} \text{ for } n \text{ odd,}$$
$$= r^{2L-n} \ln r \text{ for } n \text{ even.}$$

For $2L-n > 0$, the generating function $R(x,y)$ is the polyharmonic function (6), (7), i.e. a radial basis function.

Example 1. Let us minimize the sum of $\mathcal{L}^2$ norms of all the 2nd derivatives of the interpolant. We choose $L = 2$, $B_\alpha = K(\alpha)$ according to (17) for $|\alpha| = 2$, $B_\alpha = 0$ otherwise. In 1D, the 2nd derivative has a simple meaning. It characterizes the curvature of the interpolant. We obtain the generating function $R(x,y)$ in the form

$$\begin{aligned} r^{2L-1} &= r^3 && \text{for } n = 1 \text{ (cubic spline),} \\ r^{2L-2} \ln r &= r^2 \ln r && \text{for } n = 2 \text{ (thin plate spline),} \\ r^{2L-3} &= r && \text{for } n = 3. \end{aligned}$$

The trend functions are monomials of degree at most $L-1 = 1$ in any R^n, i.e. $\{1, x_1\}$ in R^1, $\{1, x_1, x_2\}$ in R^2, and $\{1, x_1, x_2, x_3\}$ in R^3. If $n > 3$, the minimization of $\mathcal{L}^2$ norms of the 2nd derivatives of the interpolant in this way fails.

7. A computational example

Example 2. We present results of a simple computational experiment with the polyharmonic spline interpolation for $n = 1$. We consider three cases, i.e. the minimization of the $\mathcal{L}^2$ norm of the 1st, or 2nd, or 3rd derivative of the interpolant. We interpolate the function

$$f(x) = 3(x+1)^2 + \ln(\tfrac{1}{100}x^2 + 10^{-6}) + 1 \tag{20}$$

on $\Omega = [-1, 1]$. Apparently, the function has "almost a singularity" at $x = 0$.

If we put $L = 1$, $B_1 = 1$, and $B_k = 0$ otherwise (k is now a simple index) to minimize the $\mathcal{L}^2$ norm of the 1st derivative of the interpolant then the generating function is $R(x, y) = r^{2L-n} = r$ (piecewise linear function) and the trend function is a constant. If we further put $L = 2$, $B_2 = 1$, and $B_k = 0$ otherwise to minimize the $\mathcal{L}^2$ norm of the 2nd derivative of the interpolant then $R(x, y) = r^{2L-n} = r^3$ (cubic spline), the trend functions are a constant and linear function. If we finally put $L = 3$, $B_3 = 1$, and $B_k = 0$ otherwise to minimize the $\mathcal{L}^2$ norm of the 3rd derivative of the interpolant then $R(x, y) = r^{2L-n} = r^5$ (quintic spline), the trend functions are a constant, linear function, and quadratic function. The graph of the interpolated function (20) and the three smooth interpolants are in Fig. 1.

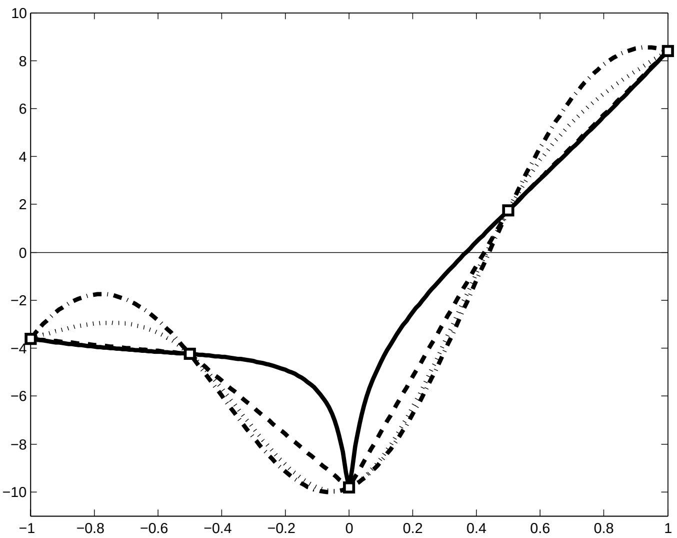

Figure 1: $N = 5$. The horizontal axis: independent variable, the vertical axis: the true function (20) (solid line); the interpolant with $B_1 = 1$ (dashed line, piecewise linear), $B_2 = 1$ (dotted line, cubic spline), and $B_3 = 1$ (dash-dot line, quintic spline).

The results correspond to the general theory. The interpolation conditions (1) are fulfilled. For $n = 1$, the formula (2) gives $r(x, y) = |x - y|$. Minimizing the $\mathcal{L}^2$ norm of the first derivative of the interpolant ($B_1 = 1$) then gives a piecewise linear curve.

Minimizing the same norm of the second derivative of the interpolant ($B_2 = 1$) provides a cubic spline. Putting $B_3 = 1$ we minimize the $\mathcal{L}^2$ norm of the third derivative of the interpolant. As the generating function is r^5 the smooth interpolant is a quintic spline that has four continuous derivatives but tends to oscillate near the ends of the interval Ω.

8. Conclusion

The Fourier transform can be successfully used to determine the generating function also in several other cases including $n = 2$ and $n = 3$. The same means can be used to construct the smooth approximation satisfying no interpolation conditions. The aim of this paper was to show that the construction of a generating function for smooth interpolation can give polyharmonic splines.

We are aware that the example in Fig. 1 is a very simple illustration of smooth interpolation and we can draw no principal conclusions from a single example. 2D or 3D cases are more interesting and can be employed in many practical approximation problems.

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