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DATA APPROXIMATION USING POLYHARMONIC RADIAL BASIS FUNCTIONS

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Abstract: The paper is concerned with the approximation and interpolation employing polyharmonic splines in multivariate problems. The properties of approximants and interpolants based on these radial basis functions are shown. The methods of such data fitting are applied in practice to treat the problems of, e.g., geographic information systems, signal processing, etc. A simple 1D computational example is presented.

Keywords: polyharmonic spline, radial basis function, approximation, data fitting, interpolation

MSC: 65D07, 65D12, 65D10, 41A63

1. Introduction

Continuous approximation of functions given by the values sampled at discrete nodes is a problem first solved in numerical analysis several centuries ago. It is of practical importance in many branches of engineering and science. Recently, data fitting is vastly used also with the data obtained by measurements in 2D or 3D for geographic information systems, computer aided geometric design, signal processing, etc.

For approximation, we use polyharmonic splines simply as radial basis functions with an additional property: they solve the corresponding polyharmonic equation. Moreover, we use them as they are the basis functions resulting from minimization of the $\mathcal{L}_2$ norm of the corresponding derivatives of the interpolant or approximant, i.e., they make the resulting curve or surface smooth in some sense. The best known example is the cubic spline in 1D.

Last but not least, we use them since the corresponding approximation formula based on them can be obtained as a solution of a polyharmonic partial differential equation. If the polyharmonic equation is of order m, the resulting formula provides the minimum $\mathcal{L}_2$ norm of the mth derivatives of the approximant or interpolant.

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In the paper, we show some relations among the approaches mentioned as far as both the interpolation and approximation are concerned. The simplest approach is just the plain use of polyharmonic splines (Section 2). Some further notation is introduced in Sections 3 and 4.

The more sophisticated treatment employs the smooth approximation (Sections 5 and 6) with a simple computational example in Sec. 6. Construction of the interpolation formula with the help of solving a boundary value problem is treated in Section 7.

2. Polyharmonic splines

Let us start with some definitions and notation, cf. [6]. Let n be a positive integer, $x, y \in R^n$, $x = (x_1, \dots, x_n)$, $y = (y_1, \dots, y_n)$, and $r(x, y) = \|x - y\|_{\mathrm{E}}$ be the Euclidean norm of $x - y$. The functions

$$r^k,\ k = 1, 3, \dots, \quad \text{and} \quad r^k \ln r,\ k = 2, 4, \dots, \tag{1}$$

are called *polyharmonic splines* of (algebraic) degree k. If k is even, we define the value of the spline for $x = y$ by the limit as $r \to 0$, i.e., by 0. Let $\Delta = \sum_{s=1}^{n} \partial^2/\partial x_s^2$ be the Laplace (harmonic) operator. The equation

$$\Delta^m \vartheta(x_1, \dots, x_n) = 0$$

is then called the *polyharmonic equation of order m*.

Fix the vector $y \in R^n$. The polyharmonic spline r^k ($r^k \ln r$) solves the polyharmonic equation with

$$m = \tfrac{1}{2}(k + n) \tag{2}$$

in $R^n \setminus \{x = y\}$ for n odd. Further, the polyharmonic spline $r^k \ln r$ solves the polyharmonic equation of order (2) in $R^n \setminus \{x = y\}$ for n even, cf. [6].

In other notation,

$$\Delta^m r^k = \delta(x - y) \quad \text{and} \quad \Delta^m r^k \ln r = \delta(x - y) \quad \text{in } R^n \tag{3}$$

for n odd and n even, respectively, where δ is the Dirac generalized function. It is easy to see that if a function solves the equation with the operator Δ^m, it solves the equation with the operator Δ^{m+1}, too.

3. Data interpolation and approximation

Let $f_j = f(X_j)$, $j = 1, \dots, N$, be N values of a complex function f of n real variables (continuous in Ω) measured (sampled) at N mutually distinct given nodes $X_1, \dots, X_N \in \Omega$, where Ω is either a bounded n-cube in R^n or $\Omega = R^n$. The continuous *interpolant* z is constructed in Ω to fulfill the *interpolation conditions*

$$z(X_j) = f_j,\ j = 1, \dots, N. \tag{4}$$

Various additional conditions can be considered, e.g. minimization of some functionals applied to z or a priori fulfillment of some condition (e.g. the polyharmonic equation). The problem does not have a unique solution.

The solution of the problem of *data approximation (data fitting)* is a continuous *approximant* $\widehat{z}$. No interpolation conditions (4) are prescribed. Instead of fulfilling them we minimize the least squares functional

$$\sum_{j=1}^{N} w_j(\widehat{z}(X_j) - f_j)(\widehat{z}(X_j) - f_j)^*, \tag{5}$$

where $w_j,\ j = 1, \ldots, N$, are positive weights and * denotes the complex conjugate. Possible additional conditions for the approximant $\widehat{z}$ can be the same as for the interpolant. If we speak about the approximation, we usually take into account the interpolation, too.

4. Basis function interpolation

Denote by $\alpha = (\alpha_1, \ldots, \alpha_n)$ a *multiindex* in Z^n. The multiindex is called *nonnegative* if $\alpha_s \geq 0$ for all $s = 1, \ldots, n$. For a nonnegative multiindex α we introduce its *length* as $|\alpha| = \sum_{s=1}^{n} \alpha_s$.

We first show the basic notions used for interpolation. These terms are employed for approximation, too. We can assume the interpolant in the form of a finite linear combination

$$z(x) = \sum_{j=1}^{M} Q_j \psi_j(x)$$

with a positive integer M. The continuous complex-valued functions $\psi_j(x)$ of $x \in \Omega$ are called the *basis functions*. The sum, in general, can be infinite. The dependence of the coefficients Q_j on the measured values f_j is usually implicit, realized by a linear algebraic system.

Consider a continuous complex-valued Hermitian function $R(x, y) = R^*(y, x)$ of $x, y \in \Omega$ that is called the *generating function*. We can then put $\psi_j(x) = R(x, X_j),\ j = 1, \ldots, N$, and obtain the interpolant in the form

$$z(x) = \sum_{j=1}^{N} \lambda_j R(x, X_j).$$

Moreover, choose a nonnegative integer L. We put

$$\varphi_\alpha(x) = x_1^{\alpha_1} \cdots x_n^{\alpha_n},$$

where α is a nonnegative multiindex, $|\alpha| < L$. These monomials are of degree $|\alpha|$ and they are called the *trend functions*. Let $T = T(n, L)$ be the actual number of them, see [6].

We add a linear combination of the trend functions to the interpolant and consider it in the form

$$z(x) = \sum_{j=1}^{N} \lambda_j R(x, X_j) + \sum_{|\alpha|<L} a_\alpha \varphi_\alpha(x). \tag{6}$$

In the formula, $\lambda_j,\ j = 1, \ldots, N$, and $a_\alpha,\ |\alpha| < L$, are the coefficients to be found in order that z satisfies the interpolation conditions; the second sum in the formula is empty for $L = 0$.

Theorem 1. *Putting $R(x, y) = r^k(x, y)$ and $R(x, y) = r^k(x, y) \ln r(x, y)$ for k odd and k even, respectively, and choosing $L = m$ according to (2), we obtain*

$$\Delta^L z(x) = \sum_{j=1}^{N} \lambda_j \delta(x - X_j) \quad \textit{in } R^n$$

for the interpolant (6).

Proof. The statement follows from (3) and from the maximum algebraic degree of the trends $\varphi_\alpha(x)$. □

An analogical statement holds for the approximant.

Let the basis function $R(x, y)$ introduced in this section can be written as

$$R(x, y) = \widetilde{R}(\|x - y\|_{\mathrm{E}}) \text{ for all } x, y \in R^n,$$

i.e., it depends only on the Euclidean norm of the difference $x - y$. Then $R(x, y)$ is called a *radial basis function (RBF)*.

The polyharmonic splines (1) are an example of such radial basis functions. The idea of interpolation by radial basis functions is based on the assumption that the data item f_j measured at the node X_j influences the interpolant mostly in the vicinity of X_j, i.e., that the value of the interpolant at a point x close to X_j depends in some way on f_j and on the distance $r(x, X_j)$.

Many RBFs are often used for interpolation and approximation, see, e.g., [2]. Note that the trend functions φ_α are not radial.

5. Smooth interpolation and approximation

Talmi and Gilat [8] introduced the way of data processing called the *smooth interpolation and approximation*. This approach has been further developed e.g. in [4], [5], or [6]. We use the notation introduced in [6] for the inner product spaces of complex-valued functions defined on Ω with the norm given as a linear combination of $\mathcal{L}_2$ norms of the individual derivatives.

Let $\widetilde{\mathcal{W}}$ be a linear vector space of complex-valued functions g continuous together with their derivatives of all orders on Ω. Let α be a nonnegative multiindex and $\{B_\alpha\}_{|\alpha|\geq 0}$ be a set of nonnegative numbers. Denote by L the smallest nonnegative integer such that $B_\alpha > 0$ for at least one α, $|\alpha| = L$, while $B_\alpha = 0$ for all $|\alpha| < L$. For $g, h \in \widetilde{\mathcal{W}}$, we put

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

and $\|g\|_L^2 = (g,g)_L$, assuming that these expressions exist and are finite.

Let $L = 0$, then $(g,h)_0$ has the properties of the *inner product* and $\|g\|_0$ is the *norm* in the *normed space* $W_0 = \widetilde{\mathcal{W}}$.

Let $L > 0$ and P_{L-1} be the space of all trend functions of degree at most $L-1$, then we construct the *quotient normed space* $W_L = \widetilde{\mathcal{W}}/P_{L-1}$, complete it in the norm $\|\cdot\|_L$, and denote it again by W_L.

Let $\{g_\kappa\}$, where κ is a nonnegative multiindex, be the *complete orthogonal basis* of the space W_L, i.e., $(g_\kappa, g_\nu)_L = 0$ for $\kappa \neq \nu$. W_L is the space where we minimize functionals and measure the smoothness of the approximation as prescribed by the choice of $\{B_\alpha\}_{|\alpha|\geq 0}$.

Assume that the series

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

converges for all $x, y \in \Omega$ and the sum is continuous. $R(x,y)$ can be the generating function for the interpolants and approximants.

In case of interpolation we satisfy the interpolation conditions (4) and minimize $\|z\|_L^2$. Putting $B_\alpha > 0$ for some set of multiindices α, we can specify the required smoothness of the corresponding derivatives of the approximant z.

Theorem 2 (Interpolation)**.** *Let $X_i \neq X_j$ and $R = [R(X_i, X_j)]$, $i,j = 1,\ldots,N$, be an $N \times N$ square Hermitian matrix. If $L > 0$ then let $\Phi = [\Phi_{j\alpha}] = [\varphi_\alpha(X_j)]$, $j = 1,\ldots,N$, $|\alpha| < L$, be an $N \times T$ rectangular matrix of the full column rank, i.e.,* rank $\Phi = T \leq N$. *Then the problem of basis function interpolation has the unique solution $z(x)$ given by* (6)*, where the coefficients λ_j, $j = 1,\ldots,N$, and a_α, $|\alpha| < L$, are the unique solution of a system of $N + T$ linear algebraic equations, see* [6]*, equations* (21), (22).

Proof. The theorem is proven for $n = 1$ in [5]. The generalization of the proof for $n > 1$ is straightforward. □

We have denoted the approximant by $\widehat{z}$. In case of approximation we minimize the least squares functional (5) together with $\|\widehat{z}\|_L^2$ added. Put

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

Theorem 3 (Approximation)**.** *Let the assumptions of Theorem 2 hold. Let $W = \operatorname{diag}(w_1, \ldots, w_N)$ be an $N \times N$ diagonal matrix of positive weights w_j. Then the problem of basis function approximation has the unique solution*

$$\widehat{z}(x) = \sum_{j=1}^{N} (\mu_j - f_j) w_j R(x, X_j) + \sum_{|\alpha|<L} \widehat{a}_\alpha \varphi_\alpha(x), \tag{7}$$

where the coefficients μ_j, $j = 1, \ldots, N$, and $\widehat{a}_\alpha$, $|\alpha| < L$, are the unique solution of a system of $N + T$ linear algebraic equations, see [5], equations (23), (24) or [7], equations (19), (20).

Proof. The theorem is proven for $n = 1$ on a bit stronger assumptions in [5]. The generalization of the proof for $n > 1$ is given in [7]. □

Note that the number of operations necessary for the construction of each formula depends primarily on the number N of nodes, not on the dimension n. Only the structure of the set of trend functions and the number of them change with n.

6. Smooth approximation by polyharmonic splines

Put $x \cdot y = \sum_{s=1}^{n} x_s y_s$ for $x, y \in R^n$ and consider the system of periodic exponential functions of pure imaginary argument (ρ is a multiindex)

$$g_\rho(x) = \exp(-\mathrm{i}\rho \cdot x), \; x \in \Omega = [0, 2\pi]^n, \; \rho_s = 0, \pm 1, \pm 2, \ldots, \; s = 1, \ldots, n.$$

Choose an integer U, $U \geq L$, such that $B_\alpha = 0$ for all $|\alpha| > U$ in W_L. The above system $\{g_\rho\}$ is shown to be complete and orthogonal in W_L in [6], Theorem 2. The sum

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

is the *Fourier series* in $x - y$ with the coefficients $\|g_\rho\|_L^{-2}$, where a simple computation gives $\|g_\rho\|_L^2 = (2\pi)^n \sum_{L \leq |\alpha| \leq U} B_\alpha \rho_1^{2\alpha_1} \cdots \rho_n^{2\alpha_n}$. We use the effect of transition from the Fourier series with the coefficients $\|g_\rho\|_L^{-2}$ to the transform

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

i.e., the *Fourier transform* of the function $\|g_\rho\|_L^{-2}$ of n continuous variables $\rho_1, \ldots, \rho_n$, where we put $q = x - y$, $x, y \in R^n$, and eliminate the requirement of periodicity of f.

We are going to show the relation between Sec. 4, where we presented the ways of approximation by polyharmonic splines, and this section. Put $K(\alpha) = |\alpha|!/(\alpha_1! \cdots \alpha_n!)$ for a nonnegative multiindex $\alpha = (\alpha_1, \alpha_2, \ldots, \alpha_n)$. Fix $L > 0$ and put $B_\alpha = 0$ for all α, $|\alpha| \neq L$, $B_\alpha = K(\alpha)$ for $|\alpha| = L$, then

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

In tables, we find easily $\mathcal{F}(\|g_\rho\|_L^{-2})$ and prove that after a simple modification, the transform $\mathcal{F}(\|g_\rho\|_L^{-2})$ is equivalent to the polyharmonic spline of the algebraic degree $2L-n$ as far as the approximation is concerned, i.e., we can use the continuous generating functions

$$R(x,y) = r^{2L-n} \text{ for } n \text{ odd}, \;\; R(x,y) = r^{2L-n}\ln r \text{ for } n \text{ even}, \tag{8}$$

cf. [6]. From the construction of these RBFs we know that they minimize the $\mathcal{L}_2$ norm of the Lth derivatives guaranteeing thus particular smoothness properties of the approximant (as well as interpolant).

Example 1. We put $n = 1$ and approximate the function

$$\begin{aligned} f(x) = -(3(x+1)^2 + \ln((x+0.5)^2/100 + 10^{-5}) \\ + \ln((x-0.75)^2/100 + 10^{-5}) + 1) \end{aligned}$$

on $\Omega = [-1,1]$ by the three smooth approximants corresponding to $L = 1,2,3$. To minimize the $\mathcal{L}_2$ norm of the Lth derivative of the approximant, put $B_L = 1$ and $B_k = 0$ otherwise. Then $R(x,y) = r^{2L-1}$ and the trend functions are monomials of degree less than L. The approximant satisfies the polyharmonic equation with $m = L$. The spline of algebraic degree 1 is piecewise linear, that of degree 3 is the minimum curvature cubic spline, and that of degree 5 is the quintic spline. In Fig. 1, $N = 9$ and $w_j = 30$, $j = 1,\ldots,9$.

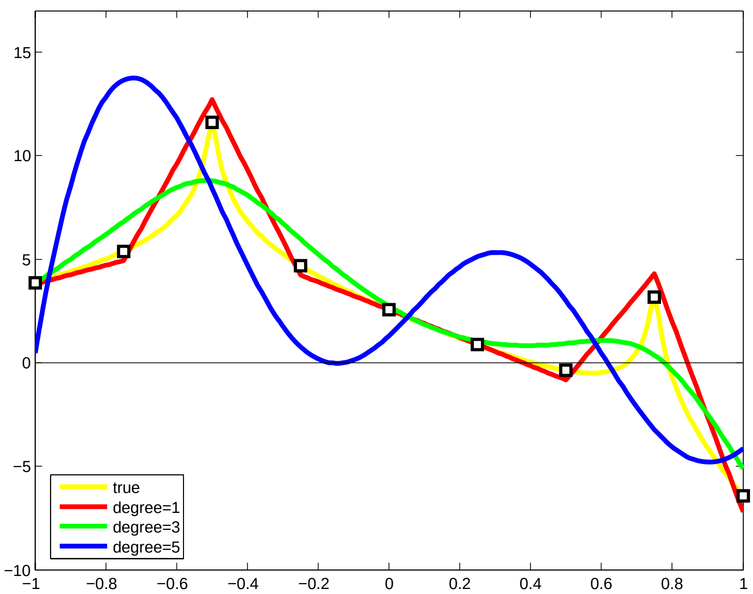

Figure 1: Approximants of Example 1, $2L-1 = 1,3,5$, $N = 9$, $w_j = 30$

7. Interpolant and approximant as a solution of a PDE

If there is a linear differential operator D such that

$$DR(x - X_j) = \delta(x - X_j),\ j = 1, \dots, N,$$
$$D\varphi_\alpha(x) = 0,\ |\alpha| < L,$$

R being the generating RBF, φ_α the trends, and $x \in \Omega$, then

$$Dz(x) = \sum_{j=1}^{N} \lambda_j \delta(x - X_j) \text{ in } \Omega. \tag{9}$$

Conversely, we are now going to find an operator D and to solve the equation (9) to get the interpolant z, see [3].

On the assumptions of Theorem 1, we can put $D = \Delta^m$, where $m = \frac{1}{2}(2L - n + n) = L$ according to (2), as the algebraic degree of the generating functions (8) is $2L - n$. The interpolant is constructed from the solution of the polyharmonic equation with the proper boundary conditions added on the boundary $\partial\Omega$ of a suitable domain Ω. We can add a linear combination of the trend functions φ_α to the interpolant as they are monomials of degree at most $L - 1$ with $D\varphi_\alpha = 0$. The condition we have to fulfill in the next step is to find the coefficients λ_j, $j = 1, \dots, N$, and a_α, $|\alpha| < L$, i.e., to solve the linear algebraic system of Theorem 2.

To set the proper boundary conditions on the continuous boundary of the bounded domain Ω, we can make Ω sufficiently large, in order that the nodes X_j are not close to $\partial\Omega$, and complete the equation (9) with the homogeneous Dirichlet boundary conditions. The partial differential equation can be then solved analytically or numerically.

If we look for an approximant $\widehat{z}$ of the form (7) the procedure is similar, but we solve the linear algebraic system of Theorem 3.

Example 2. Let us present a very simple example of the construction of an interpolant by solving differential equations. Let $n = 1$, $N = 3$, and let us be given the three nodes and three sampled values, $X_1 = -1$, $X_2 = 0$, $X_3 = 1$, and $f_1 = 1$, $f_2 = 2$, $f_3 = 3$. We are going to construct the interpolant with $L = 1$. The standard solution of the interpolation problem is, according to Theorem 1, the interpolant (6) with $R(x, y) = t(x, y)$, where $m = 1$ according to (2). We look for a piecewise linear function t solving, for a fixed y, the ordinary differential equations

$$\Delta t(x, X_j) = t''(x, X_j) = \delta(x - X_j) \text{ in } \Omega \text{ for } j = 1, 2, 3,$$

where we choose $\Omega = [-2, 2]$. Let us impose the boundary conditions $t(-2, X_j) = 0$, $\mathrm{t}(2, X_j) = 0$ for all j. By the linear finite element method we obtain the exact solutions, i.e., piecewise linear functions $t(x, X_j)$ satisfying the boundary conditions. Moreover, the first derivative of $t(x, X_j)$ is the Haeviside unit step function with the step located at X_j and the second (generalized) derivative of $t(x, X_j)$ is the Dirac function $\delta(x - X_j)$, cf., e.g., [1].

We now have the three individual piecewise linear basis functions $t(x, X_j)$, see the bottom of Fig. 2. We consider a single trend function φ of degree less than $L = 1$, i.e., a constant a. We assemble the system of four linear algebraic equations for four unknowns $\lambda_1, \lambda_2, \lambda_3$, and a according to Theorem 2. Solving this positive definite system we get the coefficients defining the interpolant (6) sought. The interpolant for $x \in [-1, 1]$ is drawn in the top part of the figure. In fact, the computation has been done on $[-2, 2]$ but the interpolant is defined only on $[-1, 1]$.

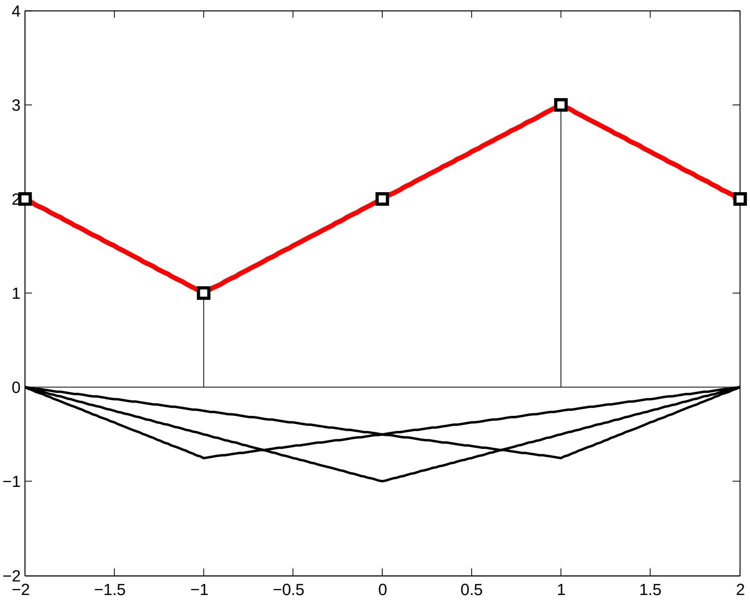

Figure 2: Piecewise linear interpolant of Example 2

8. Conclusion

We have met polyharmonic splines three times in this contribution.

They are radial functions to be used for interpolation/approximation. We have shown that the interpolant/approximant that employs them solves the corresponding polyharmonic equation.

We have proven that they can be used for smooth interpolation/approximation in the sense of [8] as they minimize the $\mathcal{L}_2$ norm of the chosen derivatives of the interpolant/approximant and thus make the resulting curve or surface smooth in a definite sense.

We have also shown that the interpolant/approximant can be obtained by the (exact or numerical) solution of a boundary value problem for a partial differential equation, e.g., the polyharmonic equation.

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