Notes on Scattered-Data Radial-Function Interpolation

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I. Interpolation

We will be considering two types of interpolation problems. Given a continuous function h: $\mathbf{R}^n \to \mathbf{R}$, a set of vectors $X = \{x_j\}_{j=1}^N$ in $\mathbf{R}^n$ and scalars $\{y_j\}_{j=1}^N$, one version of the scattered data interpolation problem consists in finding a function f such that the system of equations

$$f(x_j) = y_j, \quad j = 1, \ldots, N$$

has a solution of the form

$$f(x) = \sum_{j=1}^N c_j h(x - x_j). \tag{1.1}$$

Equivalently, one wishes to know when the $N \times N$ matrix A with entries $A_{j,k} = h(x_j - x_k)$ is invertible.

In the second version of the scattered data interpolation problem, we require polynomial reproduction. Let $\pi_{m-1}(\mathbf{R}^n)$ be the set of polynomials in n variables having degree $m-1$ or less. In multi-index notation, $p \in \pi_{m-1}(\mathbf{R}^n)$ has the form

$$p(x) = \sum_{|\alpha| \le m-1} p_\alpha x^\alpha,$$

where $\alpha = (\alpha_1, \ldots, \alpha_n)$ is an n-tuple of nonnegative integers and $|\alpha| = \sum_{j=1}^n |\alpha_j|$.

If every polynomial $p \in \pi_{m-1}(\mathbf{R}^n)$ is determined by its values on X, then we will say that the data set X is *unisolvent* (for $\pi_{m-1}(\mathbf{R}^n)$). This condition can also be rephrased in terms of matrices. Order the monomials x^α in some convenient way. Form the matrix P for which the rows are an x^α evaluated at x_j, $j = 1, \ldots, N$; that is, the row corresponding to α is $(\, x_1^\alpha \quad \cdots \quad x_N^\alpha \,)$. For example, if $n = 2$, $m = 2$ – so we are working in $\pi_1(\mathbf{R}^2)$ – and $N = 5$, then P would be

$$P = \begin{pmatrix} 1 & 1 & 1 & 1 & 1 \\ x_1 & x_2 & x_3 & x_4 & x_5 \\ y_1 & y_2 & y_3 & y_4 & y_5 \end{pmatrix}$$

In general, X is unisolvent if and only the rank of the associated matrix P is the dimension of the corresponding space of polynomials, $\pi_{m-1}(\mathbf{R}^n)$.

For a polynomial reproduction, we consider an interpolant having the form

$$f(x) = \sum_{j=1}^N c_j h(x - x_j) + \sum_{|\alpha| \le m-1} b_\alpha x^\alpha, \tag{1.2}$$

The interpolation conditions $y_k = f(x_k)$, $k = 1, \ldots, N$, imply that the c_j's and b_α's satisfy

$$y_k = \sum_{j=1}^{N} c_j h(x_k - x_j) + \sum_{|\alpha| \leq m-1} b_\alpha x_k^\alpha, \ k = 1, \ldots, N,$$

or, in an equivalent matrix form,

$$y_{data} = Ac + P^T b.$$

These give us N equations in the $N + \dim \pi_{m-1}(\mathbf{R}^n)$ unknowns; not enough to determine the unknowns.

The extra equations will come from requiring polynomial reproduction. If the data comes from a polynomial $p \in \pi_{m-1}(\mathbf{R}^n)$ — that is, $y_k = p(x_k)$, $k = 1, \ldots, N$ — then the interpolant must *coincide* with p, so $p(x) \equiv f(x)$. Since the set of functions $\{h(x - x_j\}_{j=1}^N \cup \{x^\alpha\}_{|\alpha| \leq m-1}$ is at the very least linearly independent, the sum $\sum_{j=1}^N c_j h(x - x_j)$ vanishes identically and $p(x) \equiv \sum_{|\alpha| \leq m-1} b_\alpha x^\alpha$. This implies two things. First, the values of p on X are sufficient to determine $p(x)$ for all $x \in \mathbf{R}^n$; X is thus unisolvent. Second, $y_{poly\ data} = P^T \tilde{b} = Ac + P^T b$ has $c = 0$ as its only solution; this condition requires additional equations involving c, as well as conditions on A itself.

We remark that the book by Holger Wendland [18] contains an excellent survey of results concerning scattered data surface fitting and approximation, and a discussion of recent results concerning radial basis functions and and other similar basis functions.

II. Conditionally Positive Definite Functions

The conditions on A can be met when the function h belongs to the following class, which has played an important role in the study of both types of scattered-data interpolation problems [1-15].

Definition 2.1. *Let h: $\mathbf{R}^n \to \mathbf{C}$ be continuous. We say that h is* conditionally positive definite (CPD) of order m *(denoted $\mathcal{P}_m^n$) if for every finite set $\{x_j\}_1^N$ of distinct points in $\mathbf{R}^n$ and for every set of complex scalars $\{c_j\}_1^N$ satisfying*

$$\sum_{j=1}^{N} c_j q(x_j) = 0, \qquad \forall q \in \pi_{m-1}(\mathbf{R}^n), \ \textit{equivalently, } Pc = 0$$

we have $c^H Ac = \sum_{j,k=1}^N \bar{c}_j c_k h(x_k - x_j) \geq 0$. If in addition $c^H Ac = 0$ implies that $c = 0$, we say that h is strictly *CPD of order m.*

Going back to our discussion of interpolation with polynomial reproduction, observe that if h is strictly CPD of order m and if c satisfies $Pc = 0$, then taking adjoints we also have $c^H P^T = 0$. (P is real, so $P^T = P^H$.) Consequently, multiplying the polynomial interpolation equations, $P^T \tilde{b} = Ac + P^T b$, on the left by c^H yields $0 = c^H Ac + 0$, or $c^H Ac = 0$. Since h is strictly CPD of order m, we have that $c = 0$. This gives us the result below.

Proposition 2.2. *Let h be strictly CPD order m. The function f defined in equation (1.2) is the unique solution to the problem of interpolation with polynomial reproduction, provided that c is required to satisfy $Pc = 0$.*

If $h(x) = F(|x|)$, then h is called *radial*. It is easy to show that if h is radial and CPD of order m in $\mathbf{R^n}$, then it is still an order m CPD function on $\mathbf{R^{n-1}}$. The converse is false, however. For example, the function $F(r) = \max(1-r, 0)$ is strictly positive definite in $\mathbf{R}$, but not in higher dimensions.

Are there any radial functions that are order m CPD in all dimensions? Let's start with order 0. The answer is, "yes." Obviously, Gaussians are, because their Fourier transforms are still Gaussians, no matter what the dimension n is. By Bochner's Theorem, they are positive definite, and so are sums and positive (constant) multiples of them. One can also add limits of such functions to this list, provided one is careful about how one takes limits. Is there anything else? Surprisingly, no. This is what I. J. Schoenberg proved some sixty years ago. We will now describe his result.

We begin with the following definition. A function $f : (0, \infty) \to \mathbf{R}$ is said to be *completely monotonic on* $(0, \infty)$ if $f \in C^\infty(0, \infty)$ and if its derivatives satisfy $(-1)^k f^{(k)}(\sigma) \geq 0$ for all $0 < \sigma < \infty$ and all $k = 0, 1, \ldots$. We will call this class of functions $CM(0, \infty)$. If, in addition, f is continuous at $\sigma = 0$, we will say that f is completely monotonic on $[0, \infty)$. We denote the class of such functions by $CM[0, \infty)$.

Here are a few examples. The function $\frac{1}{\sigma}$ is in $CM(0, \infty)$ and $e^{-\sigma}$ is in $CM[0, \infty)$. In general, completely monotonic functions are characterized by this result.

Theorem 2.3 (Bernstein-Widder [19])**.** *A function f belongs to $CM(0, \infty)$ if and only if there is a nonnegative Borel measure $d\eta$ defined on $[0, \infty)$ such that*

$$f(\sigma) = \int_0^\infty e^{-\sigma t} d\eta(t)$$

is convergent for $0 < \sigma < \infty$. Moreover, f is in $CM[0, \infty)$ if and only if the the integral converges for $\sigma = 0$.

Schoenberg found that every radial function that is positive definite in all dimensions is a monotonic function in r^2. The precise statement is this.

Theorem 2.4 (Schoenberg [16])**.** *A radial function $F(r)$ is positive definite on $\mathbf{R^n}$ for all n if and only if $f(\sigma) := F(\sqrt{\sigma})$ is in $CM[0, \infty)$; that is, f is completely monotonic and continuous at $\sigma = 0$.*

Let's look at the Hardy multiquadric, $-\sqrt{1 + r^2}$. Recall that the Laplace transform $\mathcal{L}[t^{-1/2}](s) = \sqrt{\pi} s^{-1/2}$. Integrating this from $s = s_1$ to $s = s_2$ gives us

$$2\sqrt{\pi}(s_2^{1/2} - s_1^{1/2}) = \int_{s_1}^{s_2} \left(\int_0^\infty t^{-1/2} e^{-st} dt \right) ds$$

As long as s_1 as s_2 are positive, Fubini's theorem applies and we get

$$\begin{aligned} s_2^{1/2} - s_1^{1/2} &= (2\sqrt{\pi})^{-1} \int_0^\infty t^{-1/2} \int_{s_1}^{s_2} e^{-st} ds dt \\ &= (2\sqrt{\pi})^{-1} \int_0^\infty t^{-3/2} \left(e^{-s_1 t} - e^{-s_2 t} \right) dt \end{aligned}$$

Since $t^{-3/2}\left(e^{-s_1 t} - e^{-s_2 t}\right) \le t^{-3/2}\left(1 - e^{-s_2 t}\right)$, which is integrable, we may apply the Lebesgue Dominated Convergence theorem to obtain

$$s^{1/2} = (2\sqrt{\pi})^{-1} \int_0^\infty t^{-3/2}\left(1 - e^{-st}\right) dt$$

This gives us the following representation representation [6,11] for the Hardy multiquadric

$$-\sqrt{1+r^2} = (2\sqrt{\pi})^{-1} \int_0^\infty \frac{e^{-(1+r^2)t} - 1}{t^{3/2}} dt$$

If we replace r^2 by σ and differentiate with respect to σ, we recover

$$\frac{-1}{2\sqrt{1+\sigma}} = -(2\sqrt{\pi})^{-1} \int_0^\infty \frac{e^{-(1+\sigma)t}}{t^{1/2}} dt$$

This the negative of a completely monotonic function. In [11], Micchelli showed that a continuous radial function $F(r)$ was an order 1 CPD function if and only if $-\frac{d}{d\sigma}F(\sqrt{\sigma})$ is completely monotonic on $(0,\infty)$. This generalizes Schoenberg's theorem to the $m = 1$ case.

What about $m > 1$? Is there an analogue then? Yes. K. Guo, S. Hu and X. Sun [6,17] proved the following result.

Theorem 2.5. *A continuous radial function $F(r)$ is order m conditionally positive definite on $\mathbf{R^n}$ for all n if and only $(-1)^m \frac{d^m}{d\sigma^m} F(\sqrt{\sigma})$ is completely monotonic on $(0,\infty)$.*

Consider Duchon's thin-plate spline [2], $F(r) = r^2 \ln r^2$. To use the theorem, we note that $F(\sqrt{\sigma}) = \sigma \ln \sigma$. It is easy to check that $(-1)^2 \frac{d^2}{d\sigma^2}(\sigma \ln \sigma) = 1/\sigma$, which – as we mentioned above – is in $CM(0,\infty)$. Thus, the thin plate spline is an order 2 CPD radial function.

III. Order m Radial Basis Functions

Continuous radial functions that are order m *strictly* conditionally positive definite in all $\mathbf{R^n}$ are called *radial basis functions* (RBFs) of order m. The simplest and probably most important example of an order 0 radial basis function is the Gaussian, $G(x) = e^{-t|x|^2}$, where $t > 0$ is a parameter. The Fourier transform convention

$$\widehat{G}(\xi) = \int_{\mathbf{R^n}} G(x) e^{-i\xi\cdot x} d^n x = (\pi/t)^{n/2} e^{-|\xi|^2/(4t)}$$

The quadratic form associated with the Gaussian is

$$Q_t := \sum_{j,k=1}^{N} c_j \bar{c}_k e^{-|x_k - x_j|^2 t}. \tag{3.1}$$

If we write the Gaussian using the Fourier inversion theorem for $\mathbf{R^n}$, interchange the finite sums and the integral, and do an algebraic manipulation, this quadratic form becomes

$$Q_t = (\pi/t)^{n/2} \int_{\mathbf{R^n}} e^{-|\xi|^2/(4t)} \left| \sum_j c_j e^{-ix_j \cdot \xi} \right|^2 d^n\xi.$$

If $Q_t = 0$, then since the integrand is nonnegative and continuous, we have that the integrand vanishes identically; hence, we have that

$$\sum_j c_j e^{-ix_j \cdot \xi} \equiv 0.$$

The complex exponentials are linearly independent, so all c_j's are 0. Thus the Gaussian is strictly positive definite in all dimensions.

We can use this to establish that the Hardy multiquadric is an order 1 RBF. From the integral representation for $-\sqrt{1+r^2}$, we see that the quadratic form associated with the multiquadric is

$$c^H Ac = (2\sqrt{\pi})^{-1} \int_0^\infty \frac{e^{-t}Q_t - |\sum c_j|^2}{t^{3/2}} dt$$

To establish that the multiquadric is SCPD of order 1, we assume that $\sum_j c_j = 0$ and set $c^H Ac = 0$. From the previous equation, we obtain

$$\int_0^\infty \frac{e^{-t}Q_t}{t^{3/2}} dt = 0.$$

The integrand is nonnegative and continuous, even at $t = 0$. Consequently, it must vanish. We then have for all $t > 0$, $Q_t = 0$. By the result above, we again have that $c = 0$. Thus the multiquadric is an order 1 RBF. Similar considerations can be used to show that $F(r)$ is an order m RBF if $(-1)^m \frac{d^m}{d\sigma^m} F(\sqrt{\sigma})$ is a non-constant, completely monotonic function on $(0, \infty)$. The thin-plate spline is thus an order 2 RBF.

We close by remarking that the results described here concerning RBFs can be used to discuss how well interpolants approximate a function belonging to certain classes of smooth functions [9,10] – band-limited ones, for example – and to discuss the numerical stability of interpolation matrices associated with RBFs, in terms of both norms of inverses and condition numbers [1,12-14].

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