Interpolation by Basis Functions of Different Scales and Shapes

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Abstract

Under very mild additional assumptions, translates of conditionally positive definite radial basis functions allow unique interpolation to scattered multivariate data, because the interpolation matrices have a symmetric and positive definite dominant part. In many applications, the data density varies locally, and then the translates should get different scalings that match the local data density. Furthermore, if there is a local anisotropy in the data, the radial basis functions should be distorted into functions with ellipsoids as level sets. In such cases, the symmetry and the definiteness of the matrices are lost. However, this paper provides sufficient conditions for the unique solvability of such interpolation processes. The basic technique is a matrix perturbation argument combined with the Ball–Narcowich–Ward stability results.

Keywords: Conditionally positive definite radial basis functions, shape parameters, scaling, solvability.

Classification: 41A05, 41A15, 41A17, 41A27, 41A30, 41A40, 41A63, 65D10

[1]) Supported by a research stay sponsored by ??? in the University of Milan–Bicocca

1 Introduction

Let $\Omega \subset I\!R^d$ be a compact set, and let us denote the space of d-variate polynomials of order not exceeding m by $I\!P_m^d$. We shall study multivariate interpolation by conditionally positive definite radial functions

$$\phi \;:\; I\!R_{\geq 0} \to I\!R$$

of order $m \geq 0$. This means that for all possible choices of sets

$$X = \{x_1, \ldots, x_N\} \subset \Omega$$

of N distinct points the quadratic form induced by the $N \times N$ matrix

$$A = (\phi(\|x_j - x_k\|_2))_{1 \leq j,k \leq N} \tag{1}$$

is positive definite on the subspace

$$V := \left\{ \alpha \in I\!R^N \;:\; \sum_{j=1}^{N} \alpha_j p(x_j) = 0 \text{ for all } p \in I\!P_m^d \right\}.$$

Note that $m = 0$ implies $V = I\!R^d$ because of $I\!P_m^d = \{0\}$, and then the matrix A in (1) is positive definite. The most prominent examples of conditional positive definite radial basis functions of order m on $I\!R^d$ are

$$\begin{array}{lcll}
\phi(r) & = & (-1)^{\lceil \beta/2 \rceil} r^\beta, \beta > 0, \beta \notin 2I\!N_0 & m \geq \lceil \beta/2 \rceil \\
\phi(r) & = & (-1)^{k+1} r^{2k} \log(r), \quad k \in I\!N & m \geq k+1 \\
\phi(r) & = & (c^2 + r^2)^{\beta/2}, \quad \beta < 0 & m \geq 0 \\
\phi(r) & = & (-1)^{\lceil \beta/2 \rceil} (c^2 + r^2)^{\beta/2}, \quad \beta > 0, \beta \notin 2I\!N_0 & m \geq \lceil \beta/2 \rceil \\
\phi(r) & = & e^{-\alpha r^2}, \quad \alpha > 0 & m \geq 0 \\
\phi(r) & = & (1-r)_+^4 (1+4r) & m \geq 0, d \leq 3.
\end{array}$$

See e.g. [17] for a comprehensive derivation of the properties of these functions.

It is customary to scale a radial basis function ϕ by going over to $\phi(\cdot/\delta)$ with a positive value δ that is roughly proportional to the distance between "neighbouring" data locations. In particular, for the Wendland function $\phi(r) = (1-r)_+^4(1+4r)$ the scaled function has support $[0, \delta]$. From now on, we use

$$A = (\phi(\|x_j - x_k\|_2/\delta))_{1 \leq j,k \leq N}$$

instead of (1).

Interpolation of real values $f_1, \ldots, f_N$ on a set $X = \{x_1, \ldots, x_N\}$ of N distinct scattered points of Ω by such a scaled function $\phi(\cdot/\delta)$ is done by solving the $(N+Q) \times (N+Q)$ system

$$\begin{array}{rcrcl}
A\alpha & + & P\beta & = & f \\
P^T\alpha & + & 0 & = & 0
\end{array} \tag{2}$$

where $Q = \dim I\!P_m^d$ and

$$P = (p_i(x_j))_{1\le j\le N, 1\le i\le Q}$$

for a basis $p_1, \dots, p_Q$ of $I\!P_m^d$. In fact, if the additional assumption

$$\text{rank } (P) = Q \le N \tag{3}$$

holds, then the system (2) is uniquely solvable. The resulting interpolant has the form

$$s(x) = \sum_{j=1}^{N} \alpha_j \phi(\|x_j - x\|_2/\delta) + \sum_{i=1}^{Q} \beta_i p_i(x) \tag{4}$$

with the additional condition $\alpha \in V$.

In many applications it is desirable not to use the same scale δ in all terms of (4). In fact, if x_j lies in some local cluster of points, one would rather use $\phi(\|x_j - x\|_2/\delta_j)$ for a small positive δ_j that is adapted to the local data density near x_j. This approach was suggested by various authors, see e.g. [11, 5, 7, 9]. In particular, Buhmann and Micchelli [4] considered monotonic scalings for multiquadrics and claimed that they improve the interpolation. Fasshauer [6] observed that varying scales of multiquadrics worked well in accelerating the convergence of his multilevel method. Carlson and Foley [5] studied the variation of a constant multiquadric scaling for the interpolation of various test functions. They concluded that test functions with large curvature such as the surface of a sphere require large scales, while those with considerable variation require smaller scales. Based upon their results, Hon and Kansa [10] conjectured that the scaling of multiquadrics should be proportional to the local radius of curvature. Galperin and Zheng [8] suggested to optimize local scaling factors along with the data points. There is some need for data–dependent strategies for optimal choice of data locations and scales. Most of the above papers use multiquadrics of different scales for solving partial differential equations. For interpolation, recent numerical methods can be found in [3].

So far, there are no known conditions for solvability of interpolation problems at different scales, but this paper will be a first step. Numerical evidence suggests that singular systems can occur [7].

If we introduce the nonsymmetric matrix

$$\tilde{A} = (\phi(\|x_j - x_k\|_2/\delta_j))_{1\le j,k\le N},$$

the system (2) is perturbed into

$$\begin{array}{rcrcl} \tilde{A}\tilde{\alpha} & + & P\tilde{\beta} & = & f \\ P^T\tilde{\alpha} & + & 0 & = & 0. \end{array} \tag{5}$$

This paper will provide sufficient conditions for nonsingularity of (5). Sections 6 and 7 will treat the perturbation of shape instead of scale.

2 Basic Argument

We shall modify a classical perturbation argument from Numerical Analysis. Let $T : V \times I\!R^Q \to V \times I\!R^Q$ be the linear mapping defined via

$$T := \begin{pmatrix} A & P \\ P^T & 0 \end{pmatrix}^{-1} \begin{pmatrix} \tilde{A} & P \\ P^T & 0 \end{pmatrix}, \begin{pmatrix} \tilde{\alpha} \\ \tilde{\beta} \end{pmatrix} \mapsto \begin{pmatrix} \alpha \\ \beta \end{pmatrix}, \tilde{\alpha} \in V. \tag{6}$$

The final goal is to derive sufficient conditions for the invertibility of T, which proves solvability of (5). Note that T is just a perturbation of the identity. A crucial tool will consist of inequalities of the form

$$\gamma^T A \gamma \geq \lambda \|\gamma\|_2^2 \tag{7}$$

for all $\gamma \in V$ and fixed positive numbers λ that will still depend on properties of ϕ and X. Our source for such inequalities will be [16], which in turn is based on the fundamental work started by Ball, Narcowich, and Ward [1, 2, 12, 13, 14].

We use (2) and (5) to get

$$\begin{array}{rcl} A\alpha + P\beta & = & \tilde{A}\tilde{\alpha} + P\tilde{\beta} \\ \tilde{\alpha}^T A\alpha & = & \tilde{\alpha}^T \tilde{A}\tilde{\alpha} \\ & = & \tilde{\alpha}^T(\tilde{A} - A)\tilde{\alpha} + \tilde{\alpha}^T A\tilde{\alpha} \\ & \geq & (\lambda - \|\tilde{A} - A\|_2)\|\tilde{\alpha}\|_2^2 \end{array}$$

with λ from (7). If we can make sure that

$$\|\tilde{A} - A\|_2 < \lambda \tag{8}$$

holds, we get

$$\|\tilde{\alpha}\|_2 \leq \frac{\|A\|_2\|\alpha\|_2}{\lambda - \|\tilde{A} - A\|_2}.$$

Furthermore, if we look at

$$P\tilde{\beta} = A\alpha + P\beta - \tilde{A}\tilde{\alpha}$$

and use the property (3), we see that we can bound $\|(\tilde{\alpha}, \tilde{\beta})\|$ above in terms of $\|(\alpha, \beta)\|$. But this means that the mapping T of (6) is invertible under the assumption (8), and thus we have proven

Theorem 2.1 *The system* (5) *for perturbed interpolation is solvable, if the perturbation $\tilde{A}$ of the standard matrix A is bounded by* (8)*, where the constant λ comes from* (7)*.*

Sections 3 to 6 of the paper will center around evaluation of (8) and (7) in various situations.

3 Matrix Perturbations by Scaling

We first concentrate on the left–hand side of (8), and for convenience we use

$$\|B\|_2 \le n \max_{1\le j,k\le n} |b_{jk}|$$

for any $n \times n$ matrix B. To avoid complications, we restrict the variable scalings to

$$\delta_j \ge \kappa\delta$$

with a small positive constant $\kappa < 1$. Then the absolute values of the entries of $\tilde{A} - A$ have the bounds

$$|\phi(\|x_j - x_k\|_2/\delta_j) - \phi(\|x_j - x_k\|_2/\delta)| \quad \le \quad |\phi'(\xi)| \|x_j - x_k\|_2 \left| \frac{1}{\delta} - \frac{1}{\delta_j} \right|$$

with

$$0 \le \xi \le \frac{\max_{1\le k\le N} \|x_j - x_k\|_2}{\kappa\delta} \le \frac{|X|_2}{\kappa\delta},$$

if ϕ is continuously differentiable. Here, we have used the shorthand notation $|X|_2 :=$ diam$_2(X)$ for the L_2 diameter of X. With

$$C(\delta) := |X|_2 \max_{\xi\in[0,|X|_2/\kappa\delta]} |\phi'(\xi)| \tag{9}$$

we have

$$\|\tilde{A} - A\|_2 \le C(\delta) N \max_{1\le j\le N} \left| \frac{1}{\delta} - \frac{1}{\delta_j} \right|$$

and (8) takes the form

$$\max_{1\le j\le N} \left| \frac{1}{\delta} - \frac{1}{\delta_j} \right| < \frac{\lambda}{C(\delta)N}, \tag{10}$$

which leaves us to work on λ.

4 Lower Bounds on Eigenvalues

Clearly, the value λ of (7) is a lower bound on the eigenvalues of the quadratic form induced by the matrix A when restricted to V. If the function ϕ were not scaled, the value λ would take the form $G(q_X)$ with the separation distance

$$q := q_X := \frac{1}{2} \min_{1\le j<k\le N} \|x_j - x_k\|_2$$

in practically every situation [16]. The function G still depends on ϕ, Ω and the space dimension d, but not on any other property of the data set X, in particular not on the cardinality of X.

We now need a scaled version of this approach. The basic trick is to replace x_j by $y_j := x_j/\delta$ to define a data set Y. Then the new q_Y is q_X/δ, and we can take $\lambda = G(q_X/\delta)$, because the scaled matrix A defined for the data X coincides with the unscaled matrix defined for Y. Altogether we get

Theorem 4.1 *If ϕ is a continuously differentiable radial basis function, and if the scalings δ_j are perturbations of δ that satisfy*

$$\max_{1\leq j\leq N}\left|\frac{1}{\delta}-\frac{1}{\delta_j}\right| < \frac{G(q_X/\delta)}{C(\delta)N}, \tag{11}$$

with C from (9) *and G from [16], then the general system* (5) *is uniquely solvable.*

5 Examples for Scalings

It does not make any sense to scale the powers $\phi(r) = (-1)^{\lceil \beta/2\rceil} r^\beta$. Similarly, the thin–plate splines $\phi(r) = (-1)^{k+1}r^{2k}\log(r)$ need not be scaled, because their orders of conditional positive definiteness allow to absorb the additional polynomials.

Let us start with unscaled multiquadrics

$$\phi(r) = (-1)^{\lceil \beta/2\rceil}(1+r^2)^{\beta/2}, \quad \beta > 0, \beta \notin 2I\!N_0,\ m \geq \lceil \beta/2\rceil.$$

From [16] we take $G(q_X) = c(\beta,d)q_X^\beta \exp(-12.76d/q_X)$ and get the sufficient condition

$$\max_{1\leq j\leq N}\left|\frac{1}{\delta}-\frac{1}{\delta_j}\right| < c(\beta,d)\frac{q_X^\beta \exp(-12.76d\delta/q_X)}{\delta^\beta C(\delta)N}$$

for the scaled system (5) to be solvable. In the standard case $\beta = 1$ we have $|\phi_c'| \leq 1$ and can take $C(\delta) = |X|_2$. Note that one can keep δ/q_X small by proper choice of the basic scaling. This is necessary anyway, because the stability estimates, which are quite realistic due to [15], blow up like $\exp(12.76d\delta/q_X)$. The constant $c(\beta,d)$ is explicitly given in [16], and the method of that paper will also give the corresponding constants for all the other examples to follow. We refrain from repeating those constants here.

The above general scaling is not the standard one for multiquadrics. In fact, most applications will use $\phi_c(r) = (-1)^{\lceil \beta/2\rceil}(c^2+r^2)^{\beta/2}$ and perturb this function into ϕ_{c_j} for positive values $c_j \approx c$. Due to $\phi_c(r) = c^\beta\phi(r/c)$ we have additional factors that spoil the argument of section 3. Clearly, the appropriate value of λ is

$$c^\beta G(q_X/c) = c(\beta,d)q_X^\beta \exp(-12.76dc/q_X),$$

and the differences in the matrix entries are bounded by

$$\begin{aligned} |(c_j^2+r^2)^{\beta/2}-(c^2+r^2)^{\beta/2}| &= \beta(\tilde c^2+r^2)^{-1+(\beta+1)/2}\frac{\tilde c}{\sqrt{\tilde c^2+r^2}}|c_j-c| \\ &\leq \beta(\tilde c^2+r^2)^{(\beta-1)/2}|c_j-c| \end{aligned}$$

for some $\tilde c$ between c and c_j. In the most interesting case $\beta = 1$ we thus get the sufficient condition

$$\max_{1\leq j\leq N}|c-c_j| \leq \frac{q_X}{N}c(\beta,d)\exp(-12.76dc/q_X)$$

for solvability of the scaled system.

For cases where $\phi'(r)$ attains its maximum on $[0,\infty)$, e.g. for the Gaussian, the Wendland functions or the inverse multiquadrics, we can bound the derivative of the scaled function via

$$\|\phi'(r/\delta)\|_\infty \le \delta^{-1}\|\phi'(r)\|_\infty$$

and just have to find the maximum absolute value of the derivative of the unscaled function. For the Gaussian e^{-t^2} this is $\sqrt{2/e}$, and from [16] we get the criterion

$$\max_{1\le j\le N}\left|\frac{1}{\delta}-\frac{1}{\delta_j}\right| < c\frac{\sqrt{2}\delta^{d+1}\exp(-40.71d^2\delta^2/q_X^2)}{\sqrt{e}Nq_X^d|X|_2}.$$

In the case of inverse multiquadrics $\phi(r)=(1+r^2)^{\beta/2},\quad \beta<0$ the absolute value of the unscaled derivative can be bounded by

$$\frac{|\beta|}{\sqrt{1-\beta}}\left(\frac{2-\beta}{1-\beta}\right)^{\beta/2-1}.$$

Then we get

$$\max_{1\le j\le N}\left|\frac{1}{\delta}-\frac{1}{\delta_j}\right| < c(\beta,d)\frac{\sqrt{1-\beta}}{|\beta|}\left(\frac{1-\beta}{2-\beta}\right)^{\beta/2-1}\frac{q_X^\beta\exp(-12.76dq_X/\delta)}{\delta^{\beta-1}N|X|_2}.$$

Consider the Wendland functions $\phi_{\ell,k}(r)$, $k=1,2,3$ with $\ell=\lfloor\frac{d}{2}\rfloor+k+1$ defined as in [6]:

$$\begin{aligned}
\phi_{\ell,1}(r) &= (1-r)_+^{\ell+1}[1+r(\ell+1)]\\
\phi_{\ell,2}(r) &= (1-r)_+^{\ell+2}[3+r(3\ell+6)+r^2(\ell^2+4\ell+3)]\\
\phi_{\ell,3}(r) &= (1-r)_+^{\ell+3}[15+r(15\ell+45)\\
&\quad +r^2(6\ell^2+36\ell+45)+r^3(\ell^3+9\ell^2+23\ell+15)].
\end{aligned}$$

We can easily compute the derivatives of the unscaled version and bound them by calculating their maximum absolute value. In particular,

$$|\phi'_{\ell,1}(r)| = (\ell+1)(\ell+2)r(1-r)_+^{\ell} \le (\ell+1)(\ell+2).$$

The next case is

$$|\phi'_{\ell,2}(r)| = (\ell+3)(\ell+4)r(1-r)_+^{\ell+1}((\ell+1)r+1).$$

Now, since $(\ell+1)r+1\le(1+r)^{\ell+1}$, we get

$$|\phi'_{\ell,2}(r)| \le (\ell+3)(\ell+4)r(1-r^2)_+^{\ell+1} \le (\ell+3)(\ell+4).$$

Finally

$$|\phi'_{\ell,3}(r)| = 3(\ell+5)(\ell+6)r(1-r)_+^{\ell+2}((\ell^2/3+4\ell/3+1)r^2+(\ell+2)\ell+1).$$

It is easy to see that $(\ell^2/3 + 4\ell/3 + 1)r^2 + (\ell + 2)\ell + 1 \le (1 + r)^{\ell+2}$, then

$$|\phi'_{\ell,3}(r)| \le 3(\ell + 5)(\ell + 6)r(1 - r^2)_+^{\ell+2} \le 3(\ell + 5)(\ell + 6).$$

If we write these bounds as

$$\|\phi'_{\ell,k}(r)\|_\infty \le \epsilon_{\ell k},$$

we get

$$\max_{1\le j\le N}\left|\frac{1}{\delta} - \frac{1}{\delta_j}\right| < \frac{c(\ell, k)}{\epsilon_{\ell k} N|X|_2}\left(\frac{q_X}{\delta}\right)^{2k+1},$$

where $c(\ell, k)$ is available from [18].

6 Matrix Perturbations by Shape

We now want to replace $\phi(\|x - x_j\|_2)$ by a function with elliptic contours. To this end, we define $\psi(t) := \phi(\sqrt{t})$ and introduce for each j a d–variate positive definite quadratic form via a positive definite $d \times d$–matrix Q_j. Its eigenvalues will be denoted by $\lambda_{j\ell}$, $1 \le \ell \le d$, $1 \le j \le N$, and we replace $\phi(\|x - x_j\|_2)$ by $\psi((x - x_j)^T Q_j (x - x_j))$. This coincides with $\phi(\|x - x_j\|_2)$ if Q_j is the identity matrix.

The basic perturbation argument will be the same as for the scaling case, but we now have to use a different technique to bound the perturbations of the matrix entries. In fact,

$$\begin{array}{ll} & |\psi((x - x_j)^T Q_j (x - x_j)) - \psi((x - x_j)^T I (x - x_j))| \\ \le & |\psi'(\tau_j)||(x - x_j)^T (Q_j - I)(x - x_j)| \end{array}$$

with some value τ_j between $(x-x_j)^T Q_j (x-x_j)$ and $(x-x_j)^T I(x-x_j)$. To get a handle on these, we restrict ourselves to matrices Q_j with eigenvalues satisfying

$$\kappa \le \lambda_{j\ell} \le \frac{1}{\kappa} \tag{12}$$

for some fixed $\kappa \in (0, 1)$. Thus we have

$$\begin{array}{ll} & |\psi((x_j - x_k)^T Q_j (x_j - x_k)) - \psi((x_j - x_k)^T I (x_j - x_k))| \\ \le & D(q_X, \kappa)|X|_2^2 \max_{1\le\ell\le d} |\lambda_{j\ell} - 1| \end{array}$$

with

$$D(q_X) := \max_{t\in[\kappa q_X^2, |X|_2^2/\kappa]} |\psi'(t)|. \tag{13}$$

Note that we have to be careful around the origin, because we are working with ψ instead of ϕ, and in the classical thin–plate case there is no differentiability of $\psi(t) = t \log t$ at zero. But we can safely omit the case $j = k$ from the above discussion. Note that we cannot combine the scale and shape case, because the latter needs bound on the derivative of $\phi(\sqrt{r})$ instead of $\phi(r)$

Applying the results of sections 2 and 4, we get

Theorem 6.1 *If $\psi(t) := \phi(\sqrt{t})$ is a continuously differentiable radial basis function on $[\kappa q_X^2, |X|_2^2/\kappa]$, and if the quadratic forms Q_j at x_j satisfy* (12) *and*

$$\max_{1\leq k\leq d} |\lambda_{jk} - 1| < \frac{G(q_X)}{D(q_X)N|X|_2^2}, \tag{14}$$

with D from (13) *and G from [16], then the general system for the shape perturbation is uniquely solvable.*

7 Examples for Shape Perturbation

The various cases of (14) can be treated by picking the correct G function from [16] as in section 5, but we still have to look at the function $D(q_X)$. The results have to be inserted into (14).

Let us start with multiquadrics $(-1)^{\lceil\beta/2\rceil}(1+r^2)^{\beta/2}$ again. The function ψ is $\psi(t) = (-1)^{\lceil\beta/2\rceil}(1+t)^{\beta/2}$, and for calculating $D(q_X)$ we get

$$\begin{aligned} D(q_X) &= \frac{|\beta|}{2}\left(1+\kappa q_X^2\right)^{\beta/2-1} < \frac{|\beta|}{2} & \beta < 2 \\ D(q_X) &= \frac{|\beta|}{2}\left(1+\frac{1}{\kappa}|X|_2^2\right)^{\beta/2-1} & \beta > 2. \end{aligned}$$

This argument also works for inverse multiquadrics ($\beta < 0$).

Thin–plate splines $\phi(r) = (-1)^{k+1}r^{2k}\log(r)$ with $k \in I\!N$ and $k > 1$ lead to

$$D(q_X) = \frac{1}{2}\kappa^{1-k}|X|_2^{2k-2}\left(1 + |\log(|X|_2^2/\kappa)|\right),$$

while the classical case $k = 1$ yields

$$D(q_X) = \frac{1}{2}\left(1 + \max(|\log(|X|_2^2/\kappa)|, |\log(q_X^2\kappa)|)\right).$$

The monomial case $\phi(r) = (-1)^{\lceil\beta/2\rceil}r^\beta$ has

$$\begin{aligned} D(q_X) &= \frac{\beta}{2}\left(\kappa q_X^2\right)^{\beta/2-1} & \beta < 2 \\ D(q_X) &= \frac{\beta}{2}\left(\frac{|X|^2}{\kappa}\right)^{\beta/2-1} & \beta > 2. \end{aligned}$$

For the Gaussian $\phi(r) = \exp(-\alpha r^2)$ we take

$$D(q_X) = \alpha\exp(-\alpha\kappa q_X^2) < \alpha.$$

Finally, let us look at the Wendland functions. Setting $\psi_{\ell k}(t) = \phi_{\ell k}(\sqrt{t})$ we find

$$D(q_X) \leq c_k \frac{(\ell + 2k)(\ell + 2k - 1)}{2}$$

for $k = 1, 2, 3$ with $c_1 = c_2 = 1,\ c_3 = 3$ by direct differentiation.

Acknowledgement

The authors thank Ed Kansa and H. Wendland for valuable comments on a first draft of the paper.

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