# Radial Basis Functions
# Viewed From Cubic Splines

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**Abstract.** In the context of radial basis function interpolation, the construction of native spaces and the techniques for proving error bounds deserve some further clarification and improvement. This can be described by applying the general theory to the special case of cubic splines. It shows the prevailing gaps in the general theory and yields a simple approach to local error bounds for cubic spline interpolation.

## 1. Optimal Recovery

The theoretical starting point for both cubic splines and radial basis functions is provided by optimal recovery of functions $f$ from scattered data in a set $X = \{x_1, x_2, \ldots, x_M\}$ of *centers* or *knots*. The functions must be in some space $\mathcal{F}$ of real–valued functions on some domain $\Omega \subset \mathbb{R}^d$ containing $X = \{x_1, x_2, \ldots, x_M\}$. The space carries a semi–inner product $(.,.)_\mathcal{F}$ that has a finite–dimensional nullspace $\mathcal{P} \subset \mathcal{F}$ such that $\mathcal{F}/\mathcal{P}$ is a Hilbert space. Once the space $\mathcal{F}$ and its semi–inner product $(.,.)_\mathcal{F}$ are fixed, the recovery problem consists in finding a function $s \in \mathcal{F}$ that minimizes $|s|^2_\mathcal{F} = (s,s)_\mathcal{F}$ under the constraints $s(x_j) = f(x_j)$, $1 \le j \le M$.

For cubic splines, the space $\mathcal{F}$ is known beforehand as Sobolev space

$$\mathcal{F} = W_2^2[a,b] = \left\{ f \;:\; f^{''} \in L_2[a,b] \right\}, \quad (f,g)_\mathcal{F} = (f'', g'')_{L_2[a,b]} \tag{1}$$

while the case of radial basis functions usually requires a fairly abstract construction of the space $\mathcal{F}$ from some given radial basis function $\Phi$ (see e.g.: [5,6,9] for details). We shall mainly consider the special function $\Phi(x) = |x|^3$ on $\mathbb{R}^1$ here and show how this construction works to recover the theory of natural cubic splines. We note in passing that it is possible (see [8] for a simple presentation) to go the other way round, i.e.: to construct $\Phi$ from $\mathcal{F}$, but this is not the standard procedure.

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## 2. Native Spaces

The radial basis function setting starts out with the space $\mathbb{P}_m^d$ of $d$-variate $m$-th order polynomials, a subset $\Omega$ of $\mathbb{R}^d$, and defines the linear space $(\mathbb{P}_m^d)_\Omega^\perp$ of all linear functionals

$$f \mapsto \lambda_{X,M,\alpha}(f) := \sum_{j=1}^{M} \alpha_j f(x_j)$$

that vanish on $\mathbb{P}_m^d$ and are finitely supported in $\Omega \subseteq \mathbb{R}^d$. The functionals $\lambda_{X,M,\alpha}$ depend each on a finite support set $X = \{x_1, x_2, \ldots, x_M\} \subseteq \Omega$ and a vector $\alpha \in \mathbb{R}^M$, where $M$ is unrestricted, but where $\alpha$ and $X$ are subject to the condition $\lambda_{X,M,\alpha}(\mathbb{P}_m^d) = \{0\}$. We shall write $\lambda^x f(x)$ to indicate the action of a functional $\lambda$ with respect to the variable $x$ on a function $f$.

**Definition 1.** *An even continuous function $\Phi$ on $\mathbb{R}^d$ is conditionally positive definite of order $m$ on $\Omega \subseteq \mathbb{R}^d$, iff the symmetric bilinear form*

$$(\lambda, \mu)_\Phi := \lambda^x \mu^y \Phi(x - y) \tag{2}$$

*is positive definite on $(\mathbb{P}_m^d)_\Omega^\perp$.*

**Definition 2.** *With*

$$s_\lambda := \lambda^y \Phi(\cdot - y) \tag{3}$$

*the native space associated to the conditionally positive definite function $\Phi$ of order $m$ on $\mathbb{R}^d$ is*

$$\mathcal{F} := \mathbb{P}_m^d + \operatorname{clos}_{(\cdot,\cdot)_\Phi} \left\{ s_\lambda : \lambda \in (\mathbb{P}_m^d)_\Omega^\perp \right\} \tag{4}$$

The above definition of the native space involves an abstract closure with respect to a somewhat unusual inner product. At this point it is not even clear that it consists of well–defined functions on $\Omega$ or $\mathbb{R}^d$ (see [9] for a discussion). Altogether, it is a major problem to characterize the native space as a space of functions with one of the usual differentiability properties. This seems to be the major obstacle for understanding the theory of radial basis functions.

Though quite abstractly defined, the native space carries a useful Hilbert space structure that is induced via continuity arguments by

$$(s_\lambda, s_\mu)_\Phi := (\lambda, \mu)_\Phi = \lambda(s_\mu) = \mu(s_\lambda),$$

which is an inner product on the second summand of $\mathcal{F}$. There are several ways to define an inner product on all of $\mathcal{F}$, but for most purposes it suffices to extend the above bilinear form to $\mathcal{F}$ by setting it to zero on $\mathbb{P}_m^d$, and to work in the Hilbert space $\mathcal{F}/\mathbb{P}_m^d$ instead of $\mathcal{F}$. The Hilbert space structure is the major tool for analysis of the native space.

These things will be somewhat more transparent if we specialize to the cubic spline case. Here we have $d = 1$, $\Phi(x) = |x|^3$ and we will see soon that $\Phi$ is conditionally positive definite of order 2 on $\mathbb{R}$, which is not immediately clear. We first connect the two bilinear forms in

**Theorem 3.** *For $\Phi(x) = |x|^3$, $d = 1$, $\Omega = [a, b] \subset \mathbb{R}$, and $m = 2$ we have*

$$(\lambda, \mu)_\Phi = (s_\lambda, s_\mu)_\Phi = \frac{1}{12}(s_\lambda^{''}, s_\mu^{''})_{L_2[a,b]}$$

*for all $\lambda, \mu \in (\mathbb{P}_m^d)_\Omega^\perp$.*

**Proof:** We can assume $X = \{x_1, x_2, \ldots, x_M\} \subset \Omega = [a, b] \subset \mathbb{R}$ to be ordered as $a \le x_1 < x_2 < \ldots < x_M \le b$. For any $\lambda_{X,M,\alpha} \in (\mathbb{P}_m^d)_\Omega^\perp$ we have

$$s_{\lambda_{X,M,\alpha}}(x) = \sum_{j=1}^{M} \alpha_j |x - x_j|^3$$

due to (3), and with $|x|^3 = 2x_+^3 - x^3$ we find

$$s_{\lambda_{X,M,\alpha}}(x) = 2\sum_{j=1}^{M} \alpha_j (x - x_j)_+^3 + \sum_{j=1}^{M} \alpha_j (x_j^3 - 3xx_j^2) + 0$$

because $\lambda_{X,M,\alpha}$ annihilates linear polynomials. Then

$$s''_{\lambda_{X,M,\alpha}}(x) = 12 \sum_{j=1}^{M} \alpha_j (x - x_j)_+^1 \tag{5}$$

is a piecewise linear function. Its support lies in $[x_1, x_M]$, again because $\lambda_{X,M,\alpha}$ annihilates linear polynomials. If two functionals

$$\lambda_{X,M,\alpha}(f) = \sum_{j=1}^{M} \alpha_j f(x_j), \quad \lambda_{Y,N,\beta}(f) = \sum_{k=1}^{N} \beta_k f(y_k)$$

from $(\mathbb{P}_m^d)_\Omega^\perp$ are given, then

$$(\lambda_{X,M,\alpha}, \lambda_{Y,N,\beta})_\Phi = \sum_{j=1}^{M} \sum_{k=1}^{N} \alpha_j \beta_k |x_j - y_k|^3 \tag{6}$$

by (2), and we want to compare this to

$$\begin{aligned}
&(s''_{\lambda_{X,M,\alpha}}(x), s''_{\lambda_{Y,N,\beta}}(x))_{L_2(\mathbb{R})} \\
&:= \int_{-\infty}^{\infty} s''_{\lambda_{X,M,\alpha}}(x) s''_{\lambda_{Y,N,\beta}}(x) dx. \\
&= \int_a^b s''_{\lambda_{X,M,\alpha}}(x) s''_{\lambda_{Y,N,\beta}}(x) dx.
\end{aligned}$$

Using $x_+^1 = (-x)_+^1 + x$ we rewrite $s''_{\lambda_{X,M,\alpha}}$ as

$$\begin{aligned} s''_{\lambda_{X,M,\alpha}}(x) &= 12 \sum_{j=1}^{M} \alpha_j (x_j - x)_+^1 + 12 \sum_{j=1}^{M} \alpha_j (x - x_j) \\ &= 12 \sum_{j=1}^{M} \alpha_j (x_j - x)_+^1. \end{aligned}$$

with a remarkable swap of $x$ with $x_j$ when compared to (5). We now use Taylor's formula

$$f(x) = f(a) + (x-a)f'(a) + \int_a^b f''(u)(x-u)_+^1 du$$

for functions $f \in C^2[a,b]$ and $a \le x \le b$. Fixing $y \in [a,b]$, we insert $f_y(x) := (y-x)_+^3/3!$ and get

$$\begin{aligned} \frac{(y-x)_+^3}{3!} = \frac{(y-a)^3}{3!} - (x-a)\frac{(y-a)^2}{2!} + \int_a^b (y-u)_+^1 (x-u)_+^1 du \\ = \frac{1}{2 \cdot 3!}(|y-x|^3 + (y-x)^3). \end{aligned}$$

To the two right–hand sides of this identity we now apply functionals $\lambda_{X,M,\alpha}$ and $\lambda_{Y,N,\beta}$. This yields

$$\begin{aligned} & \sum_{j=1}^{M}\sum_{k=1}^{N} \alpha_j \beta_k |x_j - y_k|^3 && + \sum_{j=1}^{M}\sum_{k=1}^{N} \alpha_j \beta_k (y_k - x_j)^3 \\ = & \sum_{j=1}^{M}\sum_{k=1}^{N} \alpha_j \beta_k |x_j - y_k|^3 && + 0 \\ = & \ 2\sum_{j=1}^{M}\sum_{k=1}^{N} \alpha_j \beta_k (y_k - a)^3 && - 6\sum_{j=1}^{M}\sum_{k=1}^{N} \alpha_j \beta_k (x_j - a)(y_k - a)^2 \\ & && + 12\sum_{j=1}^{M}\sum_{k=1}^{N} \alpha_j \beta_k \int_a^b (y_k - u)_+^1 (x_j - u)_+^1 du \\ = & \ 0 - 0 && + 12 \int_a^b \sum_{j=1}^{M} \alpha_j (x_j - u)_+^1 \sum_{k=1}^{N} \beta_k (y_k - u)_+^1 du \\ = & && \frac{1}{12}\left(s''_{\lambda_{X,M,\alpha}}, s''_{\lambda_{Y,N,\beta}}\right)_{L_2(\mathbb{R})}, \end{aligned}$$

where the functions $s''_{\lambda_{X,M,\alpha}}$ and $s''_{\lambda_{Y,N,\beta}}$ are supported in $[x_1, x_M]$ and $[y_1, y_M]$, respectively, such that the $L_2$ integral can be restricted to $[a,b]$. ■

**Corollary 4.** *The function $\Phi(x) := |x|^3$ is conditionally positive definite of order 2 on $\mathbb{R}$.*

**Proof:** Theorem 3 yields that the quadratic form (2) is positive semidefinite for $\Phi(x) = |x|^3$. If $\|\lambda_{X,M,\alpha}\|_\Phi$ vanishes, then $s''_{\lambda_{X,M,\alpha}} = 0$ holds, and the representation (5) as a piecewise linear function implies that all coefficients $\alpha_j$ must vanish. ■

**Theorem 5.** *The spaces $\mathcal{F}$ of (1) and (4) coincide for $\Phi(x) = |x|^3$.*

**Proof:** By standard arguments, taking the $L_2$ closure of the space of piecewise linear continuous functions. ■

We have cut the above proof short because we want to illustrate the use of the abstract space

$$\mathcal{G}_\Omega = \{f \ : \ \Omega \to \mathbb{R} \ : \ |\lambda(f)| \le C_f \|\lambda\|_\Phi \text{ for all } \lambda \in (\mathbb{P}_m^d)_\Omega^\perp\} \tag{7}$$

that occurs in the fundamental papers of Madych and Nelson [5,6] and provides another possibility to define a native space for $\Phi$.

**Theorem 6.** *The spaces $\mathcal{F}$ of (1) and (4) coincide with $\mathcal{G}_{[a,b]}$ of (7) for $\Phi(x) = |x|^3$.*

**Proof:** We shall be somewhat more explicit this time, and start with

**Lemma 7.** *We have the inclusion $W_2^2[a,b] \subseteq \mathcal{G}_{[a,b]}$.*

**Proof:** Generalizing Taylor's formula for $f \in W_2^2[a,b]$, we find the identity

$$\begin{aligned}
\lambda_{X,M,\alpha}(f) &= \sum_{j=1}^M \alpha_j f(x_j) = 0 + \int_a^b f''(u) \sum_{j=1}^M \alpha_j (x_j - u)_+^1 du \\
&= \frac{1}{12}(f'', s''_{\lambda_{X,M,\alpha}})_{L_2[a,b]} \\
&\le \frac{1}{12}\|f''\|_{L_2[a,b]} \cdot \|s''_{\lambda_{X,M,\alpha}}\|_{L_2[a,b]} \\
&\le \frac{1}{\sqrt{12}}\|f''\|_{L_2[a,b]} \cdot \|\lambda_{X,M,\alpha}\|_\Phi.
\end{aligned}$$

for all $\lambda_{X,M,\alpha} \in (\mathbb{P}_m^d)_\Omega^\perp$. ■

**Lemma 8.** *The other inclusion is $\mathcal{G}_{[a,b]} \subseteq W_2^2[a,b]$.*

**Proof:** Define the subspace $\mathcal{F}_0 := \{s''_\lambda : \lambda \in (\mathbb{P}_m^d)_\Omega^\perp\}$ of $L_2[a,b]$. It carries an inner product $(s''_\lambda, s''_\mu)_{L_2[a,b]} = 12(\lambda,\mu)_\Phi$ constructed from the inner product $(\cdot,\cdot)_\Phi$, and we define $\mathcal{F} := \overline{\mathcal{F}_0}$ to be the $L_2$ closure of $\mathcal{F}_0$ with respect to $(\cdot,\cdot)_{L_2[a,b]}$. Any $g \in \mathcal{G}_{[a,b]}$ defines a linear functional on $\mathcal{F}_0$ by

$$s''_\lambda \mapsto \lambda(g), \qquad \lambda \in (\mathbb{P}_m^d)_\Omega^\perp.$$

Here, we used that the map $\lambda \mapsto s''_\lambda$ is one–to–one. The above functional is continuous on $\mathcal{F}_0$ by definition of $\mathcal{G}_{[a,b]}$. Thus there is some $h_g \in \mathcal{F}_{[a,b]} = \overline{\mathcal{F}_0} \subseteq L_2[a,b]$ such that $\lambda(g) = (h''_g, s''_\lambda)_{L_2[a,b]}$ for all $\lambda \in (\mathbb{P}^d_m)^\perp_\Omega$, and we can assume $h_g \in W_2^2[a,b]$ because we can start with $h''_g = f_g \in L_2[a,b]$ and do integration. Now Taylor's formula for $h_g$ yields

$$\lambda(h_g) = 0 + \frac{1}{12}(h''_g, s''_\lambda)_{L_2[a,b]} = \lambda(g)$$

for all $\lambda \in (\mathbb{P}^d_m)^\perp_\Omega$. By considering a fixed $\mathbb{P}^d_m$–unisolvent set $X = \{x_1, x_2, \ldots, x_M\}$ and functionals supported on $\{x, x_1, \ldots, x_M\}$ defined by interpolation in Lagrange form

$$\lambda(p) := p(x) - \sum_{j=1}^M u_j(x)p(x_j) = 0 \text{ for all } p \in \mathbb{P}^d_m,$$

we can form the interpolating polynomial

$$p_g(x) := \sum_{j=1}^M u_j(x)(g - h_g)(x_j)$$

to $g - h_g$ and use $\lambda(g - h_g) = 0$ to see that $g = h_g + p_g$ holds. ■

Thus we have proven $\mathcal{G}_{[a,b]} = W_2^2[a,b]$ in detail. A full proof of Theorem 5 can be given by similar techniques. Furthermore, the abstractly defined spaces $\mathcal{G}_{[a,b]}$ and $\mathcal{F}$ can be proven to coincide using abstract Hilbert space arguments. ■

This finishes the proof of Theorem 6, and we can reconstruct functions from $\mathcal{G}_{[a,b]} = W_2^2[a,b]$ from data at locations $a \leq x_1 < x_2 < \ldots < x_M \leq b$ uniquely by cubic splines of the form

$$s(x) = \sum_{j=1}^M \alpha_j |x - x_j|^3 + \sum_{k=0}^1 \beta_k x^k \tag{8}$$

under the two additional conditions

$$\sum_{j=1}^M \alpha_j x_j^k = 0, \; k = 0, 1. \tag{9}$$

The representation (5) shows that these conditions imply linearity of $s$ outside of $[x_1, x_M]$. Thus the solution is a *natural cubic spline*, defined on all of $\mathbb{R}$.

## 3. Working Equations

Note that the standard approach of radial basis functions cannot use the piecewise polynomial structure of the underlying basis function. Thus it has to start with the linear system

$$\begin{pmatrix} 0 & |x_1-x_2|^3 & \dots & |x_1-x_M|^3 & 1 & x_1 \\ |x_2-x_1|^3 & 0 & \dots & |x_2-x_M|^3 & 1 & x_2 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ |x_M-x_1|^3 & |x_M-x_2|^3 & \dots & 0 & 1 & x_M \\ 1 & 1 & \dots & 1 & 0 & 0 \\ x_1 & x_2 & \dots & x_M & 0 & 0 \end{pmatrix} \begin{pmatrix} \alpha_1 \\ \alpha_2 \\ \vdots \\ \alpha_M \\ \beta_0 \\ \beta_1 \end{pmatrix} = \begin{pmatrix} f(x_1) \\ f(x_2) \\ \vdots \\ f(x_M) \\ 0 \\ 0 \end{pmatrix}$$

when interpolating a function $f$ in $X = \{x_1, x_2, \dots, x_M\}$ by a function represented as in (8) with the conditions (9). This is a non-sparse system with entries increasing when moving away from the diagonal. The usual systems for cubic splines, however, are tridiagonal and diagonally dominant, allowing a solution at $\mathcal{O}(M)$ computational cost. By going over to a new basis of second divided differences of $|\,.\,|^3$, and by taking second divided differences of the above equations, one can bring them down to tridiagonal form. This was already pointed out in the early paper [7]. In modern terminology this is a preconditioning process, and it was thoroughly investigated for general radial basis functions by Jetter and Stöckler [3].

## 4. Power Functions

We now want to explain the technique of error analysis for radial basis functions in terms of cubic splines; the results will yield explicit local error bounds that seem to be new.

**Definition 9.** *For any general quasi–interpolant of the form*

$$s_{u,f}(x) := \sum_{j=1}^{M} u_j(x) f(x_j) \tag{10}$$

*reproducing* $\mathbb{P}_m^d$ *the power function*

$$P_u(x) := \sup_{|f|_\Phi \neq 0} \frac{|f(x) - s_{u,f}(x)|}{|f|_\Phi}.$$

*is the pointwise norm of the error functional in* $(\mathbb{P}_m^d)_\Omega^\perp$.

Introducing the Lagrange formulation

$$s_{u^*,f}(x) := \sum_{j=1}^{M} u_j^*(x) f(x_j)$$

of the radial basis function interpolant on $X = \{x_1, x_2, \dots, x_M\}$ to some function $f$, we have $u_j^*(x_k) = \delta_{jk},\ 1 \le j,k \le M$ by interpolation, but the functions $u_j$ in (10) need not satisfy these conditions. The crucial fact for error analysis is the optimality principle

**Theorem 10.** *[5,11] For all $x$, the power function for radial basis function interpolation minimizes*

$$P_{u^*}(x) = \inf_u P_u(x),$$

*where all quasi–interpolants (10) are admitted, provided that they reproduce $\mathbb{P}_m^d$.*

This allows to insert piecewise polynomial quasi–interpolation processes in order to get explicit error bounds. It is a major problem to do this for scattered multivariate data. If we consider the univariate cubic spline case, things are much easier. We have to assume reproduction of linear polynomials and can apply Taylor's formula to the error:

$$\begin{aligned} f(x) - s_{u,f}(x) &= f(x) - \sum_{j=1}^M u_j(x) f(x_j) \\ &= \int_a^b f''(t) \left( (x-t)_+^1 - \sum_{j=1}^M u_j(x)(x_j - t)_+^1 \right) dt \\ &\le \|f''\|_{L_2[a,b]} \|(x - \cdot)_+^1 - \sum_{j=1}^M u_j(x)(x_j - \cdot)_+^1\|_{L_2[a,b]}. \end{aligned}$$

Since the Cauchy–Schwarz inequality is sharp, we have

$$\begin{aligned} P_u(x)^2 &= \|(x-\cdot)_+^1 - \sum_{j=1}^M u_j(x)(x_j - \cdot)_+^1\|_{L_2[a,b]}^2 \\ &= \int_a^b \left( (x-t)_+^1 - \sum_{j=1}^M u_j(x)(x_j - t)_+^1 \right)^2 dt \end{aligned}$$

as an explicit representation of any upper bound of the power function. We now fix an index $k$ such that $x \in [x_{k-1}, x_k]$ and use the piecewise linear interpolant defined by

$$\begin{aligned} u_{k-1}(x) &= \frac{x_k - x}{x_k - x_{k-1}} \\ u_k(x) &= \frac{x - x_{k-1}}{x_k - x_{k-1}} \\ u_j(x) &= 0, \quad j \ne k, \quad j \ne k-1. \end{aligned}$$

This simplifies the integral to

$$P_u(x)^2 = \int_{x_{k-1}}^{x_k} \left( (x-t)_+^1 - \frac{(x_k - x)(x_{k-1} - t)_+^1 + (x - x_{k-1})(x_k - t)_+^1}{x_k - x_{k-1}} \right)^2 dt,$$

because the integrand vanishes outside $[x_{k-1}, x_k]$. Furthermore, the bracketed function is a piecewise linear B–spline with knots $x_{k-1}$, $x$, $x_k$ and absolute value $(x - x_{k-1})(x_k - x)/(x_k - x_{k-1})$ at $t = x$. This suffices to evaluate the integral as

$$\begin{aligned} P_u^2(x) &= \frac{1}{3}(x_k - x)^3 \left(\frac{x - x_{k-1}}{x_k - x_{k-1}}\right)^2 + \frac{1}{3}(x - x_{k-1})^3 \left(\frac{x_k - x}{x_k - x_{k-1}}\right)^2, \\ P_u(x) &= \frac{1}{\sqrt{3}} \frac{(x_k - x)(x - x_{k-1})}{\sqrt{x_k - x_{k-1}}} \end{aligned}$$

to get

**Theorem 11.** *The natural cubic spline $s_f$ interpolating a function $f$ with $f'' \in L_2$ has the local error bound*

$$|f(x) - s_f(x)| \le \frac{1}{\sqrt{3}} \frac{(x_k - x)(x - x_{k-1})}{\sqrt{x_k - x_{k-1}}} \|f''\|_{L_2[x_{k-1}, x_k]} \tag{11}$$

*for all $x$ between two adjacent knots $x_{k-1} < x_k$.*

If we define the local meshwidth $h_k := x_k - x_{k-1}$, we thus get local convergence of order $3/2$ by

$$|f(x) - s_f(x)| \le \frac{h_k^{3/2}}{4\sqrt{3}} \|f''\|_{L_2[x_{k-1}, x_k]},$$

and $3/2$ is known to be the optimal approximation order for functions with smoothness at most of the type $f'' \in L_2$. Taking the Chebyshev norm of $f''$ instead of the $L_2$ norm we similarly get

$$|f(x) - s_f(x)| \le \frac{1}{2}(x_k - x)(x - x_{k-1}) \|f''\|_{L_\infty[x_{k-1}, x_k]}$$

proving that natural cubic splines satisfy the standard error bound for piecewise linear interpolation.

Note that these bounds have the advantage to be local and of optimal order, but the disadvantage to be no better than those for piecewise linear interpolation. This is due to their derivation via local linear interpolation. To improve the bounds one must add more regularity to the function $f$, and this is the topic of the next section. Piecewise linear interpolation is optimal in its native space of functions $f$ with $f' \in L_2$ and has optimal order $1/2$ there, but at the same time it is used to provide bounds of the optimal order $3/2$ for cubic spline interpolation of functions with $f'' \in L_2[a, b]$, forming the native space of cubic splines.

## 5. Improved Error Bounds

For interpolation of sufficiently smooth functions by cubic splines, the following facts about improved approximation orders in the $L_\infty$ norm are well–known [1]:

a) The approximation order can reach four, but

b) order four is a saturation order in the sense that any higher order can only occur for the trivial case of $f \in \mathbb{P}_4^1$.

c) For orders greater than 2 on all of $[a,b]$ one needs additional boundary conditions. These can be imposed in several ways:

   c1) Conditions that force $f$ to be linear outside of $[a,b]$ while keeping splines natural (i.e.: with linearity outside of $[a,b]$), or

   c2) additional interpolation conditions for derivatives at the boundary, or

   c3) periodicity requirements for both $f$ and the interpolant.

d) General Hilbert space techniques including boundary conditions lead to orders up to 7/2 for functions with $f^{(4)} \in L_2$, but

e) techniques for order four (as known so far) require additional stability arguments (diagonal dominance of the interpolation matrix or bounds on elements of the inverse matrix providing exponential off-diagonal decay) and need $f \in C^4[a,b]$.

In this area the theory of radial basis functions still lags behind the theory of cubic splines, as far as interpolation of finitely may scattered data on a compact set is concerned (see [2] for better results in case of data on infinite grids). In particular, when specializing to cubic splines,

a) current convergence orders reach only 7/2 at most, and

b) there is no saturation result at all.

c) For orders greater than 2 on all of $[a,b]$ one needs additional boundary conditions which still deserve clarification in the general setting.

d) There is no proper theory for $C^k$ functions.

Let us look at these problems from the classical cubic spline point of view. There, the standard technique [1] uses the orthogonality relation following from the minimum–norm property and applies integration by parts for functions with $f^{(4)} \in L_2[a,b]$. This yields

$$\begin{aligned} \|f'' - s_f''\|_2^2 &= (f'' - s_f'', f'' - s_f'')_2 = (f'' - s_f'', f'')_2 \\ &= (f - s_f, f^{(4)})_2 + f'' \cdot (f' - s_f')|_a^b \end{aligned}$$

and now it is clear that the various possibilities of imposing additional boundary conditions are just boiling down to the condition $f'' \cdot (f' - s_f')|_a^b = 0$ that we assume from now on. Then by Cauchy-Schwarz

$$\|f'' - s_f''\|_2^2 \le \|f - s_f\|_2 \|f^{(4)}\|_2$$

and one has to evaluate the $L_2$ norm of the error. This is done by summing up the bound provided by Theorem 11 in a proper way:

$$\begin{aligned} \|f - s_f\|_2^2 &\le \sum_{k=2}^{M} \frac{\|f''\|^2_{L_2[x_{k-1},x_k]}}{3(x_k - x_{k-1})} \int_{x_{k-1}}^{x_k} (x_k - x)^2 (x - x_{k-1})^2 dx \\ &\le \sum_{k=2}^{M} \frac{\|f''\|^2_{L_2[x_{k-1},x_k]}}{3h_k} \frac{h_k^5}{30} \\ &\le \frac{h^4}{90} \|f''\|^2_{L_2[x_1,x_M]} \end{aligned}$$

with

$$h := \max_{2 \le k \le M} h_k = \max_{2 \le k \le M} (x_k - x_{k-1}).$$

This step used that the right–hand side of (11) has a *localized* norm, and this fact is missing in general radial basis function cases. The technique works for norms that can be localized properly, and this was clearly pointed out in the recent paper [4]. In particular, it works for spaces that are norm–equivalent to Sobolev spaces, and this covers the case of Wendland's compactly supported unconditionally positive definite functions [10].

Using $s_{f-s_f} = 0$, one can replace $\|f''\|_2$ by $\|f'' - s_f''\|_2$ in the right–hand side and combine the above inequalities into

$$\begin{aligned} \|f'' - s_f''\|_2^2 &\le \frac{h^2}{\sqrt{90}} \|f'' - s_f''\|_2 \|f^{(4)}\|_2 \\ \|f'' - s_f''\|_2 &\le \frac{h^2}{\sqrt{90}} \|f^{(4)}\|_2 \\ \|f - s_f\|_2 &\le \frac{h^4}{90} \|f^{(4)}\|_2 \\ \|f - s_f\|_\infty &\le \frac{h^{7/2}}{12\sqrt{30}} \|f^{(4)}\|_2. \end{aligned}$$

This is how far we can get by Hilbert space techniques for cubic splines.

To see the problems occurring for general radial basis functions, we try to repeat the above argument, starting from the necessary and sufficient variational equation

$$(s_f, v)_\Phi = 0 \text{ for all } v \in \mathcal{F},\ v(X) = \{0\} \tag{12}$$

for any minimum–norm interpolant $s_f$ based on data in $X = \{x_1, x_2, \dots, x_M\}$. We want to apply this to $v := f - s_f$ and use integration by parts in some way or other. In view of Theorem 3 it is reasonable to impose the condition

$$(f, g)_\Phi = (Lf, Lg)_2 \text{ for all } f,\ g \in \mathcal{F}$$

with a linear operator $L$ that maps $\mathcal{F}$ into some $L_2$ space, which we would prefer to be $L_2(\Omega)$, not $L_2(\mathbb{R}^d)$. But both the definition of $L$ and the "localization" of the space are by no means trivial, since section 2 made use of very special properties of $\Phi$ that are not available in general. Looking back at cubic splines, we see that the variational equation (12) in its special form

$$(s_f'', v'')_{L_2(\mathbb{R})} = 0 \text{ for all } v'' \in L_2(\mathbb{R}^d),\ v(x_j) = 0$$

contains a lot of information:

1) the function $s_f$ must be a cubic polynomial in all real intervals containing no knot (i.e. also in $(-\infty, x_1)$ and $(x_M, \infty)$), and
2) because of $v'' \in L_2(\mathbb{R}^d)$, the outer cubic pieces must be linear.

This follows from standard arguments in the calculus of variations, but it does not easily generalize, because the general form (12) of the variational equation does not admit the same analytic tools as in the cubic case.

If (generalized) direct and inverse Fourier transforms are properly introduced, the radial basis function literature [6,9,11] uses the operator

$$Lf := \left(\frac{f^\wedge}{\sqrt{\Phi^\wedge}}\right)^\vee$$

that (up to a constant factor) is a second derivative operator in the cubic case, as expected. This is due to the fact that $\Phi^\wedge = \|\,.\,\|_2^{-4}$ for $\Phi = \|\,.\,\|_2^3$ in one dimension, and up to a constant factor. Unconditionally positive definite smooth functions $\Phi$ like Gaussians $\Phi(x) = \exp(-\|x\|_2^2)$ or Wendland's function $\Phi(x) = (1 - \|x\|_2)_+^4(1 + 4\|x\|_2)$ have classical Fourier transforms with proper decay at infinity, and then the above operator $L$ is well–defined even without resorting to generalized Fourier transforms. However, it does not represent a classical differential operator, but rather an awkward pseudodifferential operator, making the analysis of the variational equation (12) and the corresponding boundary conditions a hard task. It would be nice to conclude from (12) that a *weak boundary condition* of the form

$$L^*Ls_f = 0 \text{ outside of } \Omega$$

holds, or even a *strong boundary condition*

$$Ls_f = 0 \text{ outside of } \Omega$$

as in the cubic spline case, where $L^*$ is the $L_2$ adjoint of $L$. So far, the proper characterization of necessary boundary conditions following from (12) seems to be an open question whose answer would improve our understanding of the error behavior of radial basis functions considerably.

The paper [9] avoids these problems by simply assuming that the function $f$ satisfies the conditions

$$L^*Lf := \frac{f^\wedge}{\Phi^\wedge} \in L_2(\mathbb{R}^d),\ \ \operatorname{supp} L^*Lf = \operatorname{supp}\left(\frac{f^\wedge}{\Phi^\wedge}\right) \subset \Omega \subset \mathbb{R}^d\,.$$

This allows to mimic part of the cubic spline argument in the form

$$\begin{aligned}|f-s_f|_\Phi^2 &= (f-s_f, f-s_f)_\Phi = (f-s_f, f)_\Phi\\ &= (L(f-s_f), Lf)_{L_2(\mathbb{R}^d)} = (f-s_f, L^*Lf)_{L_2(\mathbb{R}^d)}\\ &= (f-s_f, L^*Lf)_{L_2(\Omega)} \le \|f-s_f\|_{L_2(\Omega)}\|L^*Lf\|_{L_2(\Omega)},\end{aligned}$$

and we are left with the summation argument to form the $L_2$ norm of the error over $\Omega$. But in general we cannot use the localization property of the right–hand side of (11), since we are stuck with

$$|f(x)-s_f(x)| \le P(x)|f-s_f|_\Phi$$

for all $x \in \Omega$. This only yields

$$\|f-s_f\|_{L_2(\Omega)} \le \|P\|_{L_2(\Omega)}|f-s_f|_\Phi$$

and is off by a factor $\sqrt{h}$ if written down in the cubic spline setting, ignoring the additional information. Still, this technique allows to prove error bounds of the form

$$\begin{aligned}|f(x)-s_f(x)| &\le P(x)\|P\|_{L_2(\Omega)}\|L^*Lf\|_{L_2(\Omega)}\\ \|f-s_f\|_{L_2(\Omega)} &\le \|P\|_{L_2(\Omega)}^2\|L^*Lf\|_{L_2(\Omega)}\end{aligned}$$

that roughly double the previously available orders, but still are off from the optimal orders in the cubic case by $1/2$ or $1$, respectively, because $P$, being optimally bounded as in (11), has only $\mathcal{O}(h^{3/2})$ behavior. It it reasonable to conjecture that the above inequalities are off from optimality by orders $d/2$ and $d$ in a $d$-variate setting, respectively. We hope that this presentation helps to clarify the arising problems and to encourage further research in this direction.

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