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Applications of radial basis functions: Sobolev-orthogonal functions, radial basis functions and spectral methods

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Abstract

In this paper we consider an application of Sobolev-orthogonal functions and radial basis function to the numerical solution of partial differential equations. We develop the fundamentals of a spectral method, present examples via reaction–diffusion partial differential equations and discuss briefly some links with theory of wavelets.

1 Introduction

Radial basis functions are a well-known and useful tool for functional approximation in one or more dimensions. The general form of approximations is always a linear combination (finite or infinite) number of shifts of a single function, the *radial basis function.* In more than one dimension, this function is made rotationally invariant by composing a univariate function, usually called ϕ, with the Euclidean norm. In one dimension such approximation usually simplifies to univariate polynomial splines. For a recent review of radial basis function approximations, see [5].

This note is about applications for radial basis functions and other approximation schemes such as Sobolev-orthogonal polynomials and more general Sobolev-orthogonal functions to the numerical solution of partial differential equations. The basic ideas stem from the theory of Sobolev-orthogonal polynomials ([13]), and in this paper there is a remarkable connection developed between applications of Sobolev-orthogonality with radial basis functions (e.g. [5]), and wavelets are mentioned as well (e.g. [8, 9]). Sobolev-orthogonal polynomials are a device to extend the standard theory of orthogonal polynomials (see, for instance, [12]) by requiring orthogonality with respect to non-selfadjoint inner products of the form

$$(f,g)_\lambda = \int_a^b f(x)g(x)\,\mathrm{d}x + \lambda \int_a^b f'(x)g'(x)\,\mathrm{d}x$$

for a positive parameter λ and a suitable interval (a,b), $a,b \in \mathbb{R} \cup \{\pm\infty\}$. The $\mathrm{d}x$ in the two integrals is often replaced by more general Borel measures, $\mathrm{d}\psi$, say. The scheme which we want to discuss in this short article is one of spectral type: in lieu of e.g. finite element spaces as underlying piecewise polynomial approximation spaces for the solution, we take purpose-build approximations which make the linear systems which we need to solve particularly simple, sometimes even diagonal.

Therefore, in the first instance, we develop a theory of applying Sobolev-orthogonal polynomial basis functions for the numerical solution of partial differential equations via a spectral method. Then we extend this idea to general classes of radial basis function-type methods, where shift-invariant approximation spaces are generated with Sobolev-orthogonal basis functions. Due to the introductory character of this paper, our discussion is restricted to relatively simple cases. Our presentation is illustrated with the one-dimensional reaction–diffusion partial differential equation.

This is the place to note that radial basis functions have found a number of other applications in the discretisation of PDEs. Thus, for example, Driscoll and Fornberg [10] have used fast-converging 'flat' multiquadrics in pseudospectral methods, while Frank and Reich [11] applied radial basis functions with particle methods in order to conserve enstrophy in the solution of certain shallow-water equations. Our application is of an altogether different nature.

1.1 Examples of PDEs and Sobolev-orthogonality

Consider the partial differential equation

$$\frac{\partial u}{\partial t} = \nabla\left(a\nabla u\right) + bu + c, \tag{1.1}$$

where $u = u(\mathbf{x},t)$ is of sufficient smoothness with respect to $\mathbf{x}$ and t, $\mathbf{x}$ is given in a cube $\mathcal{V} \subset \mathbb{R}^d$ (more generally, in a finite domain), $t \geq 0$, $a = a(\mathbf{x}) > 0$, $b = b(\mathbf{x})$ and $c = c(\mathbf{x})$. We impose zero Dirichlet boundary conditions. The stipulation of cube as a domain and zero Dirichlet conditions is unduly restrictive, but it will suffice for the short presentation in this paper and adequately illustrate the main novel concepts in our presentation. In the next section, we shall also introduce a nonlinearity into the underlying PDE.

We wish to approximate the solution $u(\mathbf{x},t)$ as a finite linear combination of the generic form

$$u(\mathbf{x},t) = \sum_{l=1}^{m} \alpha_l(\mathbf{x}) w_l(t),$$

where t is nonnegative and $\mathbf{x}$ resides in the domain. In the sequel we shall also use expansions into infinite series with $l \in \mathbb{Z}$. Thus, a Galerkin ansatz (in the usual L_2 inner product on $\mathbb{R}^d$ which we denote by $(\cdot,\cdot)$ in contrast to the specialised Sobolev-inner product $(\cdot,\cdot)_\lambda$ above) gives

$$\sum_{l=1}^{m}(\alpha_l,\alpha_k)w_l' = \sum_{l=1}^{m}\left(\nabla(a\nabla\alpha_l),\alpha_k\right)w_l + \sum_{l=1}^{m}(b\alpha_l,\alpha_k)w_l + (c,\alpha_k), \qquad k=1,2,\ldots,m.$$

Integration by parts in the second term above and substitution of the requisite zero boundary conditions yield the alternative formulation

$$\sum_{l=1}^{m}(\alpha_l,\alpha_k)w_l' = -\sum_{l=1}^{m}\left(a\nabla\alpha_l,\nabla\alpha_k\right)w_l + \sum_{l=1}^{m}(b\alpha_l,\alpha_k)w_l + (c,\alpha_k), \qquad k=1,2,\ldots,m. \tag{1.2}$$

We solve the ODE system (1.2) with respect to t, for example with the backward Euler scheme (we use backward Euler for the sake of simplicity, but it should be noted that the same analysis applies to any implicit multistep method, because our use of Sobolev-orthogonality is only linked to the implicitness of the solution method)

$$w_l^{n+1} = w_l^n + \Delta t F_l(\mathbf{w}^{n+1}), \qquad n\in\mathbb{Z}_+, \quad l=1,2,\ldots,m, \tag{1.3}$$

where the function F_l is given implicitly by the equations (1.2) and where $\mathbf{w}^{n+1}$ in the expression above is the vector with components w_l^{n+1}, $l=1,2,\ldots,m$. Let us now multiply expression (1.3) by (α_l,α_k) and sum up for $l=1,2,\ldots,m$. Then, exploiting (1.2), a little algebra yields

$$\sum_{l=1}^{m}\left\{\int_{\mathcal{V}}[1-\Delta t b(\mathbf{x})]\,\alpha_l(\mathbf{x})\alpha_k(\mathbf{x})\mathrm{d}\mathbf{x} + \Delta t\int_{\mathcal{V}}a(\mathbf{x})\nabla^T\alpha_l(\mathbf{x})\nabla\alpha_k(\mathbf{x})\mathrm{d}\mathbf{x}\right\}w_l^{n+1}$$
$$= \sum_{l=1}^{m}\int_{\mathcal{V}}\alpha_l(\mathbf{x})\alpha_k(\mathbf{x})\mathrm{d}\mathbf{x}w_l^n + \int_{\mathcal{V}}c(\mathbf{x})\alpha_k(\mathbf{x})\mathrm{d}\mathbf{x}. \tag{1.4}$$

The connection with Sobolev-inner products is clear. Indeed, let us now choose the set $\mathbf{W}_{m,n} := \{w_1, w_2, \ldots, w_m\}$ as a set of functions that are orthogonal with respect to the homogeneous Sobolev $\overset{\circ}{H}_{d,2}$ inner product (see, e.g., [13])

$$\langle f,g\rangle_{\Delta t} := \int_{\mathcal{V}}[1-\Delta t b(\mathbf{x})]f(\mathbf{x})g(\mathbf{x})\mathrm{d}\mathbf{x} + \Delta t\int_{\mathcal{V}}a(\mathbf{x})\nabla^T f(\mathbf{x})\nabla g(\mathbf{x})\mathrm{d}\mathbf{x} \tag{1.5}$$

(this of course requires that $\Delta t b(\mathbf{x}) \le 1$, hence may restrict in a minor way the choice of the time step Δt). Further below we shall also use infinite sets $\mathbf{W}$ instead of the finite set $\mathbf{W}_{m,n}$. It is important to note that in general the Sobolev inner-product depends upon the step size. Subject to this formulation, the linear system (1.4) diagonalises and its numerical solution becomes trivial. We turn now to a more elaborate example in the next subsection, namely the reaction-diffusion equation.

1.2 Reaction-diffusion as a paradigm for nonlinear PDEs

Let us consider the nonlinear partial differential equation

$$\frac{\partial u}{\partial t} = \nabla(a\nabla u) + f(u), \tag{1.6}$$

where otherwise all the quantities are as in (1.1), including the boundary conditions. Suppose that an approximation u^n to $u(\mathbf{x}, n\Delta t)$ is available at all the spatial grid points. We commence by interpolating u^n to requisite precision by some function v. Thus, v is defined throughout the cube $\mathcal{V}$ and coincides with u^n at the grid points. This allows us to linearise the source function f about u^n, the outcome being

$$\frac{\partial u}{\partial t} = \nabla(a\nabla u) + c + bu + g(u), \tag{1.7}$$

where

$$\begin{aligned} b(\mathbf{x}) &= f'(v(\mathbf{x})), \\ c(\mathbf{x}) &= f(v(\mathbf{x})) - f'(v(\mathbf{x}))v(\mathbf{x}), \\ g(\mathbf{x}, u) &= f(u) - f(v(\mathbf{x})) - f'(v(\mathbf{x}))[u - v(\mathbf{x})]. \end{aligned}$$

Note that

$$g(\mathbf{x}, u) = O(|u - v|^2).$$

We can now solve the nonlinear system (1.7) by functional iteration, i.e. by letting as a start

$$w_l^{n+1,0} = w_l^n, \qquad l = 1, 2, \ldots, m,$$

and recurring, employing the inner product (1.5),

$$\begin{aligned} &\sum_{l=1}^{m} \langle \alpha_l, \alpha_k \rangle_{\Delta t} w_l^{n+1,j+1} \qquad (1.8) \\ = \; &\sum_{l=1}^{m} (\alpha_l, \alpha_k) w_l^n + \left(g\left(\cdot, \sum_{l=1}^{m} \alpha_l w_l^{n+1,j} \right), \alpha_k \right), \quad k = 1, 2, \ldots, m, \end{aligned}$$

for $j \in \mathbb{Z}_+$.

If, as in the previous subsection, we choose $\mathbf{W}_m$ so as to diagonalise the linear system, each step of (1.8) becomes relatively cheap. Hence this approach might offer a realistic means to derive spectral approximation to nonlinear PDEs. Indeed, a special one-dimensional case can be treated straightforwardly and it is presented in the sequel.

1.3 The one-dimensional case using polynomial splines

Let (1.1) be given in one space dimension and without source terms, whence it becomes the familiar diffusion equation with variable diffusion coefficient,

$$\frac{\partial u}{\partial t} = \frac{\partial}{\partial x}\left(a \frac{\partial u}{\partial x} \right).$$

Thus, provided that $0 \le x \le 1$ and t nonnegative, we require the 'usual' Sobolev orthogonality [13] with respect to the inner product

$$\langle f, g \rangle_{\Delta t} = (f, g)_1 = \int_0^1 f(x)g(x)\mathrm{d}\varphi(x) + \int_0^1 f'(x)g'(x)\mathrm{d}\psi(x),$$

where

$$\frac{\mathrm{d}\varphi(x)}{\mathrm{d}x} = 1 - \Delta t b, \qquad \frac{\mathrm{d}\psi(x)}{\mathrm{d}x} = \Delta t a.$$

We emphasise again the dependence of the Sobolev-inner product on the step size. Taking the approach of the previous subsection as our point of departure, an obvious option is to use Sobolev-orthogonal polynomials. An alternative approach which can be worked out explicitly and which we wish to demonstrate in this subsection, is to use univariate polynomial spline approximations. It has the advantage of being more amenable to a generalisation to several space dimensions.

We suppose that the unit-interval $[0,1]$ is divided into N intervals of length $h := \frac{1}{N}$ and consider a piecewise-quadratic basis of continuous functions $s_1, s_2, \ldots, s_N$ such that

$$s_l(x) := \begin{cases} \frac{1}{h}[x-(l-1)h] + \alpha_l(x-lh)[x-(l-1)h], & (l-1)h \le x \le lh, \\ \frac{1}{h}[(l+1)h - x] + \beta_l(x-lh)[x-(l+1)h], & lh \le x \le (l+1)h, \\ 0, & |x-lh| \ge h. \end{cases}$$

Clearly, s_l is a continuous, $C[0,1]$ cardinal function of Lagrange interpolation at the knots (hence, a quadratic spline with double knots, cf., Powell [16], the added degree of freedom taken up by the requirement of Sobolev-orthogonality). Next, we need just to impose Sobolev orthogonality, and solve for the coefficients α_l and β_l. This is equivalent to the requirement that

$$\langle s_l, s_{l+1}\rangle_{\Delta t} = 0, \qquad l = 1, 2, \ldots, N-1.$$

In the special case $a(x) \equiv 1$, $b(x), c(x) \equiv 0$, we have $\varphi(x) = x$, $\psi(x) = \Delta t x$ and

$$\begin{aligned} \langle s_l, s_{l+1}\rangle_{\Delta t} &= \int_0^h \left[\frac{x}{h} + \alpha_{l+1}(x-h)x\right]\cdot\left[\frac{h-x}{h} + \beta_l x(x-h)\right]\mathrm{d}x \\ &\quad + \Delta t \int_0^h \left(\frac{1}{h} + 2\alpha_{l+1}x - \alpha_{l+1}h\right)\left(-\frac{1}{h} + 2\beta_l x - \beta_l h\right)\mathrm{d}x \\ &= h\int_0^1 \left[\xi + \alpha_{l+1}h^2(\xi-1)\xi\right]\cdot\left[1-\xi-\beta_l h^2\xi(1-\xi)\right]\mathrm{d}\xi \\ &\quad - \frac{\Delta t}{h}\int_0^1 (1+2\alpha_{l+1}\xi - \alpha_{l+1})(1+\beta_l - 2\beta_l\xi)\mathrm{d}\xi \\ &= h\left[\left(\frac{1}{6} - \frac{h^2}{12}(\alpha_{l+1}+\beta_l) + \frac{h^4}{30}\alpha_{l+1}\beta_l\right) + \frac{\Delta t}{h^2}\left(-1 + \frac{1}{3}\alpha_{l+1}\beta_l\right)\right]. \end{aligned}$$

Let $\mu = \Delta t/h^2$ be the Courant number. Since we have two degrees of freedom for each l and because each equation is otherweise independent of l, we may fix $\alpha \equiv \alpha_l \equiv \beta_l$. Then, letting $\hat{\alpha} := h^2\alpha$, requiring $\langle s_l, s_{l+1}\rangle_{\Delta t} = 0$ is equivalent to

$$5 - 5\hat{\alpha} + \hat{\alpha}^2 + 10\mu\alpha^2 - 30\mu = 0 \tag{1.9}$$

or

$$(10\mu + h^4)\alpha^2 - 5h^2\alpha + 5 - 30\mu = 0.$$

We wish to solve this quadratic equation for α for a suitable range of Courant numbers. Indeed, the equation (1.9) has two real solutions α for every $\mu > \frac{1}{6}$ if h is small enough, since its discriminant is

$$(120\mu + 5)h^4 + 1200\mu^2 - 200\mu.$$

In the case $\mu = \frac{1}{6}$ each s_l reduces, upon the choice of $\hat{\alpha} = 0$, to a *chapeau* function. Otherwise we obtain $\alpha = O(1)$. We may give up a small support, characteristic of spline functions (which, anyway, is of marginal importance, since we do not solve linear systems!). This is a case discussed in the next section. Another obvious alternative is to construct an orthogonal basis from *chapeau* functions. This, however, is easily seen to be identical to the LU factorization of the standard FEM matrix

$$\begin{bmatrix} \frac{2}{3} & \frac{1}{6} & 0 & 0 & 0 & \cdots & 0 \\ \frac{1}{6} & \frac{2}{3} & \frac{1}{6} & 0 & 0 & \cdots & 0 \\ 0 & \frac{1}{6} & \frac{2}{3} & \frac{1}{6} & 0 & \cdots & 0 \\ \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \vdots \\ 0 & \cdots & 0 & \frac{1}{6} & \frac{2}{3} & \frac{1}{6} & 0 \\ 0 & \cdots & 0 & 0 & \frac{1}{6} & \frac{2}{3} & \frac{1}{6} \\ 0 & \cdots & 0 & 0 & 0 & \frac{1}{6} & \frac{2}{3} \end{bmatrix}.$$

2 Applications of radial basis functions and wavelets

2.1 Sobolev-orthogonal translates of a radial basis function

In this section, we wish to develop a more general approach employing the concepts of wavelets and radial basis functions and employ shift-invariant spaces of approximations for our spectral methods. We begin by giving up the compactness of the domain $\mathcal{V}$ and work on the entire real line instead. For this, we shall demonstrate the use of Sobolev-inner products and shift-invariant spaces and concentrate solely on this part of the analysis in the present article. So, in particular, the set $\mathbf{W}$ above is of the form $\{\phi(\cdot - nh) \mid n \in \mathbb{Z}\}$. In the sequel we shall add several remarks about how to find compactly-supported ϕ that allow the treatment of partial differential equations on compact domains. We remark that n is no longer used for the time-steps in the differential equation solver but for the shifts of the radial functions.

To start with, we wish to find a function $\phi \in \mathbf{H}^2(\mathbb{R})$, where $\mathbf{H}^2(\mathbb{R})$ is a non-homogeneous Sobolev space, such that for a positive constant λ and positive spacing h it is true that

$$\int_{-\infty}^{\infty} \phi(x)\phi(x-hn)\,\mathrm{d}x + \lambda \int_{-\infty}^{\infty} \phi'(x)\phi'(x-hn)\,\mathrm{d}x = \delta_{0n}, \qquad n \in \mathbb{Z}. \tag{2.1}$$

We multiply both left- and right-hand-side of the general pattern (2.1) by $\exp(\mathrm{i}\theta n)$ and sum over $n \in \mathbb{Z}$,

$$\sum_{n=-\infty}^{\infty} \exp(\mathrm{i}\theta n) \left\{ \int_{-\infty}^{\infty} \phi(x)\phi(x-hn)\,\mathrm{d}x + \lambda \int_{-\infty}^{\infty} \phi'(x)\phi'(x-hn)\,\mathrm{d}x \right\} = 1, \;\; \theta \in [-\pi, \pi]. \tag{2.2}$$

In order to be able to exchange summation and integration and apply the Poisson summation formula (Stein and Weiss [17], p. 252) we make a number of assumptions. The version of the Poisson summation formula that we wish to use states that for a univariate function f with

$$|f(x)| = O\Big((1+|x|)^{-1-\epsilon}\Big)$$

and

$$|\hat{f}(x)| = O\Big((1+|x|)^{-1-\epsilon}\Big)$$

and positive ϵ, the following equality holds (note that the first bound in the above implies existence and continuity of the one-dimensional Fourier transform)

$$\sum_{j=-\infty}^{\infty} \hat{f}(\theta + 2\pi j) = \sum_{j=-\infty}^{\infty} \exp(\mathrm{i}\theta j) f(j).$$

Specifically, we assume that the following three decay estimates hold:

$$|\phi(x)| \le c(1+|x|)^{-1-\varepsilon},$$
$$|\phi'(x)| \le c(1+|x|)^{-1-\varepsilon},$$

and

$$|\hat{\phi}(\xi)| \le c(1+|\xi|)^{-3-\varepsilon},$$

where c is a generic positive constant, $\varepsilon > 0$, $\hat{\phi}$ denotes the Fourier transform and we demand the faster rate of decay in the last display because we shall later require summability of translates of the Fourier transform multiplied by the square of its argument. Note in particular that the first decay condition renders the Fourier transform $\hat{\phi}$ continuous and well defined.

An example for a function ϕ that satisfies the three decay conditions above is the second divided difference of the multiquadric radial basis function [4] $\sqrt{r^2+C^2}$ that is

$$\phi(x) = \frac{1}{2}\sqrt{(x-1)^2+C^2} - \sqrt{x^2+C^2} + \frac{1}{2}\sqrt{(x+1)^2+C^2}.$$

Here, C is a positive constant parameter. The above function decays cubically [4] and its Fourier transform even decays exponentially due to the exponential decay of the modified Bessel function K_1 [1] that features in the generalised Fourier transform of the multiquadric, here stated only in the one-dimensional case,

$$-2C\frac{K_1(C|\xi|)}{|\xi|}$$

(cf. Jones [14]).

Once summation and integration are interchanged, (2.2) becomes

$$\int_{-\infty}^{\infty} \phi(x) \sum_{n=-\infty}^{\infty} \exp(\mathrm{i}\theta n)\phi(x-hn)\,\mathrm{d}x$$

$$+\lambda\int_{-\infty}^{\infty}\phi'(x)\sum_{n=-\infty}^{\infty}\exp(i\theta n)\phi'(x-hn)\,dx=1,\qquad \theta\in[-\pi,\pi], \tag{2.3}$$

or, applying the Poisson Summation Formula (Stein and Weiss, [17], p. 252)

$$\int_{-\infty}^{\infty}\phi(x)\sum_{n=-\infty}^{\infty}\exp\Big(ih^{-1}x(\theta+2\pi n)\Big)\hat{\phi}\Big(h^{-1}(\theta+2\pi n)\Big)\,dx+i\lambda h^{-1} \tag{2.4}$$
$$\times\int_{-\infty}^{\infty}\phi'(x)\sum_{n=-\infty}^{\infty}\exp\Big(ih^{-1}x(\theta+2\pi n)\Big)(\theta+2\pi n)\hat{\phi}\Big(h^{-1}(\theta+2\pi n)\Big)\,dx=h,$$

where $\theta\in[-\pi,\pi]$. Because ϕ vanishes at infinity, integration by parts of the second term of (2.4) gives

$$\int_{-\infty}^{\infty}\phi(x)\sum_{n=-\infty}^{\infty}\exp\Big(ih^{-1}x(\theta+2\pi n)\Big)\hat{\phi}\Big(h^{-1}(\theta+2\pi n)\Big)\,dx$$
$$+\frac{\lambda}{h^2}\int_{-\infty}^{\infty}\phi(x)\sum_{n=-\infty}^{\infty}\exp(ih^{-1}x(\theta+2\pi n))(\theta+2\pi n)^2\hat{\phi}(h^{-1}(\theta+2\pi n))dx$$
$$=\sum_{n=-\infty}^{\infty}\hat{\phi}(h^{-1}(\theta+2\pi n))\hat{\phi}\Big(-h^{-1}(\theta+2\pi n)\Big)\Big[1+\lambda h^{-2}(\theta+2\pi n)^2\Big]=h.$$

Since ϕ is real, $\hat{\phi}(-\xi)=\overline{\hat{\phi}}(\xi)$, and this implies

$$\sum_{n=-\infty}^{\infty}|\hat{\phi}(h^{-1}(\theta+2\pi n))|^2(1+\lambda h^{-2}(\theta+2\pi n)^2)=h,\qquad \theta\in[-\pi,\pi]. \tag{2.5}$$

This is our condition that leads to the required Sobolev-orthogonality. In summary, we have established the following theorem.

Theorem 2.1 *If the decay conditions on ϕ, as stated above, hold in tandem with the expression* (2.5), *then the required orthogonality condition* (2.1) *is satisfied.*

We note that, if we are given a ψ such that

$$\sum_{n=-\infty}^{\infty}\left|\hat{\psi}\Big(h^{-1}(\theta+2\pi n)\Big)\right|^2=h,\qquad \theta\in[-\pi,\pi], \tag{2.6}$$

then

$$\hat{\phi}(\xi):=\frac{\hat{\psi}(\xi)}{\sqrt{1+\lambda\xi^2}} \tag{2.7}$$

satisfies (2.5). This expression can be used to derive an explicit transformation which takes a ψ that satisfies (2.6), into a ϕ satisfying (2.5), although its practical computation may be nontrivial. Indeed, by the Parseval–Plancherel theorem [17], we get the useful identity

$$\phi(x)=\frac{1}{\pi\sqrt{\lambda}}\int_{-\infty}^{\infty}\psi(x-y)K_0\left(\frac{|y|}{\sqrt{\lambda}}\right)\,dy, \tag{2.8}$$

which is a convolution and whose Fourier transform is therefore (2.7) (cf., for instance, Jones [14]). In (2.8), K_0 is the 0th modified Bessel function (Abramowitz and Stegun [1]) which is positive on positive reals and satisfies $K_0(t) \sim -\log t$ near zero and $K_0(t) \sim \sqrt{\pi/(2t)}e^{-t}$ for large t, similar to the asymptotics we have used before for the K_1 modified Bessel function. Hence, by a lemma in [7], see also (Light and Cheney [15]) ϕ decays algebraically of a certain order if ψ does. Moreover, because $1/\sqrt{1+\lambda x^2}$ is positive, integer translates of ϕ are dense in L^2, say, provided that this is the case with integer translates of ψ [18].

In some trivial cases we may evaluate the integral (2.8) explicitly, for instance for $\psi(x) = \cos x$, where the integral is again a constant multiple of the cosine function (Abramowitz and Stegun [1]). Otherwise, the smoothness and fast exponential decay of the modified Bessel function can be used together with a quadrature formula.

We may now use the translates of such Sobolev-orthogonal functions in the spectral approximation of a PDE as above, letting $\mathbf{W} := \{\phi(\cdot - nh) \mid n \in \mathbb{Z}\}$.

An example of a function $\hat{\psi}$ that satisfies (2.5) is simply the characteristic function scaled by h of the interval $[-h\pi, h\pi]$. In that case, $|\psi(x)|$ decays like $1/|x|$. In fact, any ψ that satisfies $|\hat{\psi}(\xi)| \le c(1+|\xi|)^{-1/2-\varepsilon}$ for positive ε can be made to satisfy (2.6) by subjecting it to the transformation

$$\hat{\psi}(\xi) \mapsto \hat{\tilde{\psi}}(\xi) := \frac{\sqrt{h}\hat{\psi}(\xi)}{\sqrt{\sum_{n=-\infty}^{\infty} |\hat{\psi}(\xi + h^{-1}2\pi n)|^2}}, \tag{2.9}$$

see for instance (Battle [2]). If ψ is compactly supported then the transformed $\tilde{\psi}$ will not necessarily be compact supported but decay exponentially [6].

In order to find a class of examples of *compactly supported* ψ that satisfy (2.6), see Daubechies [8] for her compactly supported scaling functions ψ which are fundamental for the construction of Daubechies wavelets. For example, the following conditions are sufficient for ψ which shall be defined by its Fourier transform to satisfy (2.6) for $h = 1$ (other h can be used by scaling):

$$\hat{\psi}(\xi) = \prod_{j=1}^{\infty} \tilde{h}\left(\frac{\xi}{2^j}\right),$$

where, for some suitable coefficients $\tilde{h}_k$,

$$\tilde{h}(\xi) = \sum_{k=0}^{2N-1} \tilde{h}_k e^{-ik\xi}$$

has to satisfy $\tilde{h}(0) = 1$, $\tilde{h}(\pi) = 0$, and

$$|\tilde{h}(\xi)|^2 + |\tilde{h}(\xi+\pi)|^2 = 1, \qquad \xi \in [-\pi, \pi].$$

For the construction of such $\tilde{h}$, see [8]. Compactly supported basis functions are important to approximate the numerical solution of a PDE as in the above example defined on a compact $\mathcal{V}$. Moreover, any ψ with the aforementioned decay property can be made to satisfy (2.5) by the transformation

$$\hat{\psi}(\xi) \mapsto \frac{\sqrt{h}\hat{\psi}(\xi)}{\sqrt{\sum_{n=-\infty}^{\infty} |\hat{\psi}(\xi + h^{-1}2\pi n)|^2 (1 + \lambda(\xi + h^{-1}2\pi n)^2}}. \tag{2.10}$$

They can also be found by applying the transformation (2.10) and using the transformation (2.9) as well.

We note finally, that for instance, when ψ is a B-spline then its translates are dense in L^2 if we allow h to become arbitrarily small (see, for instance, Powell [16]) and the last section of this paper).

2.2 Sobolev-orthogonal translates of a function in higher dimensions

Applying the approach of the previous subsection to the Sobolev inner product

$$\int_{\mathbf{R}^d} f(\mathbf{x}) g(\mathbf{x})\, \mathrm{d}\mathbf{x} + \lambda \int_{\mathbf{R}^d} \nabla^T f(\mathbf{x}) \nabla g(\mathbf{x})\, \mathrm{d}\mathbf{x},$$

the outcome is the orthogonality condition

$$\sum_{\mathbf{n}\in\mathbb{Z}^d} |\hat{\phi}(h^{-1}(\theta + 2\pi\mathbf{n}))|^2 (1 + \lambda h^{-2} \|\theta + 2\pi\mathbf{n}\|^2) = h^d, \qquad \theta \in [-\pi, \pi]^d, \tag{2.11}$$

which replaces (2.5). We are now also interested in the more general case of Sobolev-type inner products

$$\int_{\mathbf{R}^d} f(\mathbf{x}) g(\mathbf{x}) \mu(\mathbf{x})\, \mathrm{d}\mathbf{x} + \lambda \int_{\mathbf{R}^d} \nabla^T f(\mathbf{x}) \nabla g(\mathbf{x}) \nu(\mathbf{x})\, \mathrm{d}\mathbf{x},$$

where the weights μ and ν are positive. Here the orthogonality condition becomes more complicated. Specifically, it is

$$\sum_{\mathbf{n}\in\mathbb{Z}^d} \hat{\phi}_\mu\Big(h^{-1}(\theta + 2\pi\mathbf{n})\Big)\overline{\hat{\phi}_\mu}\Big(h^{-1}(\theta + 2\pi\mathbf{n})\Big)$$
$$+ \lambda h^{-2} \hat{\phi}_\nu\Big(h^{-1}(\theta + 2\pi\mathbf{n})\Big)\overline{\hat{\phi}_\nu}\Big(h^{-1}(\theta + 2\pi\mathbf{n})\Big) = h^d, \qquad \theta \in [-\pi, \pi]^d,$$

where

$$\hat{\phi}_\mu \;:=\; \hat{\phi} * \widehat{\sqrt{\mu}},$$
$$\hat{\phi}_\nu \;:=\; (\|\cdot\| \times \hat{\phi}) * \widehat{\sqrt{\nu}},$$

and $*$ denotes continuous convolution, used as in (2.8), where ψ is convolved with a modified Bessel function.

2.3 Error estimates

We can offer error estimates for the Sobolev-orthogonal bases, firstly, in the case when ϕ is a univariate spline of fixed degree m, say, with knots on $h\mathbb{Z}$, and, secondly, in the case when ϕ is a linear combination of translates of the radial Gauss kernel

$$e^{-\alpha^2 x^2/2}, \qquad x \in \mathbb{R},$$

along $h\mathbb{Z}$. In the former case it is known that the *uniform* approximation error to a sufficiently smooth function from the linear space spanned by $\phi(\cdot - nh)$, $n \in \mathbb{Z}$, is at most a constant multiple of h^{m+1} ([16]). We have already mentioned that we require $\lambda = O(h^2)$, therefore it can be deduced by twofold integration by parts that the Sobolev error is indeed $O(h^{m+1})$. This can be generalized in a straightforward way to higher dimensions by tensor-product B-splines.

Our $L^2(\mathbb{R})$ error estimates can be carried out as follows: Let f be a band-limited function, that is, one with a compactly-supported Fourier transform, which satisfies such assumptions that imply that the best least-squares approximation using a Sobolev inner product

$$s_h(x) = \sum_{n=-\infty}^{\infty} \langle f, \phi(\cdot - hn)\rangle_{\lambda,h} \phi(x - nh), \qquad x \in \mathbb{R}, \tag{2.12}$$

is well defined. For instance, we may require that $\langle f, f\rangle_{\lambda,h} < \infty$, as well as sufficient decay of the radial basis function ϕ, i.e.

$$\begin{aligned} |\phi(r)| &\leq c(1+|r|)^{-1-\varepsilon}, \\ |\phi'(r)| &\leq c(1+|r|)^{-1-\varepsilon}, \\ |\hat{\phi}(r)| &\leq c(1+|r|)^{-1-\varepsilon} \end{aligned}$$

for a positive ε. Here $\langle\cdot,\cdot\rangle_{\lambda,h}$ is the Sobolev inner product which we study in this note and it is helpful to emphasise its dependence on h in the subscript. We begin with the piecewise polynomial, i.e. spline, case. Hence, let ϕ be from the space of splines of degree m with knots on $h\mathbb{Z}$ such that its translates are Sobolev orthogonal.

Theorem 2.2 *Subject to the assumptions of the last paragraph, we have the error estimate*

$$\|s_h - f\|_2 = O(h^{m+1}), \qquad h \to 0. \tag{2.13}$$

Proof: We shall establish in the course of this proof an error estimate for the first derivative of the error function in (2.13), so that an order of convergence can also be concluded for the norm associated with our Sobolev inner product. Indeed, because the Fourier transform is an $L^2(\mathbb{R})$ isometry, we may prove (2.13) by considering

$$\|\hat{s}_h - \hat{f}\|_2 \tag{2.14}$$

instead of the left-hand side of (2.13). The Fourier transform of (2.12) is

$$\hat{s}_h(\theta) = \sum_{n=-\infty}^{\infty} \langle f, \phi(\cdot - nh)\rangle_{\lambda,h} e^{-i\theta nh} \hat{\phi}(\theta), \qquad \theta \in \mathbb{R}.$$

The absolute convergence of the above is guaranteed by the decay conditions on ϕ. Hence the square of (2.14) is, by the Parseval–Plancherel Formula and periodisation of the integrand with respect to θ,

$$\int_{-\infty}^{\infty}\left|\hat f(\theta)-\sum_{n=-\infty}^{\infty}\langle f,\phi(\cdot-nh)\rangle_{\lambda,h}\mathrm{e}^{-\mathrm{i}\theta hn}\hat\phi(\theta)\right|^2\mathrm{d}\theta$$

$$=\int_{-\infty}^{\infty}\left|\hat f(\theta)-\sum_{n=-\infty}^{\infty}\int_{-\infty}^{\infty}\hat f(\xi)\hat\phi(\xi)\mathrm{e}^{\mathrm{i}\xi hn}(1+\lambda\xi^2)\,\mathrm{d}\xi\mathrm{e}^{-\mathrm{i}\theta hn}\hat\phi(\theta)\right|^2\mathrm{d}\theta$$

$$=\int_{-\pi/h}^{\pi/h}\sum_{k=-\infty}^{\infty}\Bigg|\hat f(\theta+2\pi k/h)-\hat\phi(\theta+2\pi k/h)$$

$$\times\sum_{n=-\infty}^{\infty}\int_{-\infty}^{\infty}\hat f(\xi)\hat\phi(\xi)\mathrm{e}^{\mathrm{i}\xi nh}(1+\lambda\xi^2)\,\mathrm{d}\xi\mathrm{e}^{-\mathrm{i}\theta nh}\Bigg|^2\mathrm{d}\theta. \tag{2.15}$$

The $(1+\lambda\xi^2)$ term in the above comes from the derivative in the Sobolev inner product and Fourier transform. Because f is band-limited, for small enough h (2.15) assumes the form

$$\int_{-\pi/h}^{\pi/h}\sum_{k=-\infty}^{\infty}\left|\hat f(\theta)\delta_{0k}-\hat\phi(\theta+2\pi k/h)\sum_{n=-\infty}^{\infty}\int_{-\infty}^{\infty}\hat f(\xi)\hat\phi(\xi)\mathrm{e}^{\mathrm{i}\xi nh}(1+\lambda\xi^2)\,\mathrm{d}\xi\mathrm{e}^{-\mathrm{i}\theta nh}\right|^2\mathrm{d}\theta. \tag{2.16}$$

Using again the band limitedness of f, together with the Poisson Summation Formula, (2.16) can be brought into the form

$$\int_{-\pi/h}^{\pi/h}\sum_{k=-\infty}^{\infty}\Bigg|\hat f(\theta)\delta_{0k}-\hat\phi(\theta+2\pi k/h)$$

$$\times\frac{1}{h}\sum_{n=-\infty}^{\infty}\hat f(\theta+2\pi n/h)\hat\phi(\theta+2\pi n/h)\Big(1+\lambda(\theta+2\pi n/h)^2\Big)\Bigg|^2\mathrm{d}\theta$$

$$=\int_{-\pi/h}^{\pi/h}\sum_{k=-\infty}^{\infty}\left|\hat f(\theta)\delta_{0k}-h^{-1}\hat\phi(\theta+2\pi k/h)\hat f(\theta)\hat\phi(\theta)(1+\lambda\theta^2)\right|^2\mathrm{d}\theta. \tag{2.17}$$

In the case when ϕ is in the aforementioned spline space, it can be expressed as the inverse Fourier transform of

$$\hat\phi(\xi)=\frac{\sqrt{h}\hat r(\xi)}{\sqrt{\sum_{n=-\infty}^{\infty}|\hat r(\xi+h^{-1}2\pi n)|^2\big(1+\lambda(\xi+h^{-1}2\pi n)^2\big)}},\qquad \xi\in\mathbb{R}, \tag{2.18}$$

where $\hat r(\xi)=\xi^{-m-1}$. This follows from (2.5) and from the fact that all splines from our space are linear combinations of integer translates of $r(x):=|x|^m$, whose generalised Fourier transform is a multiple of ξ^{-m-1} [14]. Since any constant factors in front of the function ξ^{-m-1} in $\hat r$ cancel in the expression for $\hat\phi$ above, we have ignored them straightaway. Substituting (2.18) into (2.17), we get the integral over $[-\pi/h, \pi/h]$ of

$$\sum_{k=-\infty}^{\infty} \left| \hat{f}(\theta)\delta_{0k} - \frac{\hat{r}(\theta + h^{-1}2\pi k)\hat{r}(\theta)}{\sum_{n=-\infty}^{\infty} |\hat{r}(\theta + h^{-1}2\pi n)|^2(1 + \lambda(\theta + h^{-1}2\pi n)^2)} \hat{f}(\theta)(1 + \lambda\theta^2) \right|^2 . \quad (2.19)$$

Considering (2.19) for each m separately, it follows from (2.19) and from $\hat{r}(\xi) = \xi^{-m-1}$ that our claim is true. Indeed for the sum over all terms with $k \neq 0$, it is evident that we obtain a factor of h^{2m+2} from the numerator, because the denominator is periodic, containing one term independent of h, and the nonvanishing expression $h^{-1}2\pi k$ in the argument of $\hat{r}(\theta + h^{-1}2\pi k)$ guarantees $\hat{r}(\theta + h^{-1}2\pi k) \sim h^{m+1}$ due to $\hat{r}(\xi) = \xi^{-m-1}$. Of course, the squares then taken provide the h^{2m+2} instead of h^{m+1}.

On the other hand, for $k = 0$, we have for small enough h

$$\left| \hat{f}(\theta) - \frac{|\hat{r}(\theta)|^2(1 + \lambda\theta^2)\hat{f}(\theta)}{\sum_{n=-\infty}^{\infty} |\hat{r}(\theta + h^{-1}2\pi n)|^2(1 + \lambda(\theta + h^{-1}2\pi n)^2)} \right|^2$$
$$= |\hat{f}(\theta)|^2 \left| \frac{\sum_{n\neq 0} |\hat{r}(\theta + h^{-1}2\pi n)|^2(1 + \lambda(\theta + h^{-1}2\pi n)^2)}{1 + \sum_{n\neq 0} |\hat{r}(\theta + h^{-1}2\pi n)|^2(1 + \lambda(\theta + h^{-1}2\pi n)^2)} \right|^2$$

which is also $O(h^{2m+2})$, as required, because the numerator provides an $O(h^{2m})$, according to the rate of the decay of $\hat{r}$ and the power of h in its argument. This is then squared to provide $O(h^{4m}) = O(h^{2m+2})$.

As for the derivatives, one only has to multiply the Fourier transform of the error function in (2.14) with θ, and we get the same error estimate by multiplying the integrands in all the following integrals with $|\theta|^2$. □

The same analysis remains valid when considering integer translates of the Gauss kernel $e^{-\gamma^2 x^2/2}$ in order to form ϕ. In this case we make use of the fact that the Gauss kernel has a Fourier transform which is a multiple of $e^{-x^2/(2\gamma^2)}$. We put this instead of $\hat{r}$ into (2.19), and we then get arbitrarily-high orders of convergence from (2.14) as long as we take $\gamma = O(h)$, see also [3]. For this choice ϕ is exponentially decaying, whereas for splines of degree m we merely get algebraic decay at infinity of order $-m-1$.

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