Approximation of Radial Functions by Piecewise Polynomials on Arbitrary Grids

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We study the approximation of radial functions in IR^N, $N \geq 2$, by means of Lagrange finite elements on arbitrary grids. As an application, error estimates are obtained for the finite-element discretization of the radial Schrödinger equation. (AMS subject classification number: 65M60.)

1. INTRODUCTION

For $N \geq 2$, let $\Omega \subset IR^N$ be the open ball of radius R centered at the origin. A function $f(x)$ defined in Ω is said to be radial if it is constant on each set $r = |x| =$ constant. In this note, we are concerned with the approximation of radial functions by piecewise polynomials in r, a topic that arises naturally when analyzing Galerkin discretizations of problems with radial symmetry. We first explain the notation. If Δ is a partition of $[0, R]$

$$\Delta: 0 = r_0 < r_1 < \cdots < r_n = R$$

we denote

$$h = \max_{1 \leq i \leq n}(r_i - r_{i-1})$$

$$\underline{h} = \min_{1 \leq i \leq n}(r_i - r_{i-1})$$

and we consider the space $S_{\Delta,k}$ consisting of all the continuous functions f such that, for $i = 1, \ldots, n$, the restriction $f|_{[r_{i-1}, r_i]}$ is a polynomial of degree $k \geq 1$, k an integer. This definition means that we are using Lagrange finite elements on the interval $[0, R]$. It excludes polynomial splines in the sense of Varga [1], except for the special case of piecewise linear functions. The subspace of $S_{\Delta,k}$ consisting of functions f with $f(R) = 0$ is denoted by $\mathring{S}_{\Delta,k}$. Functions $f(r)$ of a scalar variable defined on $(a, b) \subset (0, R)$ can

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clearly be interpreted as radial functions defined on the hollow open ball with inner radius a and outer radius b. The same symbol f is used for both interpretations. We write $H_r^m(\Omega)$ for the subspace of $H^m(\Omega)$, $m = 0, 1, \ldots$ consisting of radial functions.

The main results of this article are given in Section 2 where, for $f \in H_r^{k+1}(\Omega)$, optimal rates of convergence are shown for the approximation error in the L^2 and H^1 norms. Our analysis applies on arbitrary meshes. It is perhaps worth noting that for N large and fixed $k \geq 1$, functions f in $H_r^{k+1}(\Omega)$ may be very singular near $r = 0$. The approximation properties of $S_{\Delta,k}$ have been investigated by Eriksson and Thomée [2] and Eriksson and Nie [3]. The analysis in [2] is restricted to quasi-uniform grids, i.e., to grids such that

$$\frac{h}{\underline{h}} = O(1), \qquad \text{as } h \to 0$$

while [3] only considers the case where f is suitably smooth at the origin. As an application of the results of Section 2, we analyze in section 3 a Galerkin discretization of the radial Schrödinger equation which has attracted much attention in plasma physics and nonlinear optics [4, 5].

In the remainder, we shall use the letter C to denote a generic constant, not necessarily the same at each occurrence, which does not depend on the mesh size h.

2. THE MAIN RESULT

Our basic approximation result is the following

Theorem 2.1. *For $f \in H_r^{k+1}(\Omega)$, $k \geq 1$, $\Omega \subset IR^N$, there exists a function $v \in S_{\Delta,k}$ such that*

$$\|\nabla(v - f)\|_{L^2(\Omega)} \leq C\, h^k\, \|f\|_{h^{k+1}(\Omega)}$$

where C is a constant depending only on k and N.

Proof. Without loss of generality, we may assume that f is real-valued. For simplicity, we first consider the special case $N = 3$. We determine v through the conditions

$$v(R) = f(R) \tag{2.1}$$

$$\lim_{0<\varepsilon\to 0} v^{(i)}(r_j - \varepsilon) = f^{(i)}(r_j), \qquad 1 \leq j \leq n, 1 \leq i \leq k \tag{2.2}$$

where the superscripts denote derivatives with respect to r. The conditions in (2.2) make sense and determine v uniquely. Indeed, if $0 < \delta < r_1$

$$\int_\delta^R (f^{(k+1)})^2\, dr \leq \frac{1}{\delta^2} \int_0^R (f^{(k+1)})^2\, r^2\, dr$$

$$= \frac{1}{\delta^2}\frac{1}{4\pi} \int_\Omega \left[\left(\sin\phi\, \cos\theta \frac{\partial}{\partial x_1} + \sin\phi\, \sin\theta \frac{\partial}{\partial x_2} + \cos\phi \frac{\partial}{\partial x_3}\right)^{k+1} f\right]^2 dx$$

$$\leq \frac{1}{\delta^2} C(k) \|f\|^2_{H^{k+1}(\Omega)}.$$

Here, we have noted by θ and ϕ the polar and azimutal angles. We have also used the notation $dx = dx_1 \cdots dx_N$. This shows that $f \in H^{k+1}(\delta, R) \subset C^k(\delta, R)$ so that the derivatives in (2.2) are meaningful. On the other hand, (2.1) and (2.2) with $j = n$ are satisfied if and only if $v|_{[r_{n-1}, r_n]}$ is the kth-degree Taylor polynomial of f about r_n. Once $v|_{[r_{n-1}, r_n]}$ is determined, (2.2) with $j = n - 1$ together with the continuity of v at r_{n-1} clearly determine the Taylor expansion of $v|_{[r_{n-2}, r_{n-1}]}$ about r_{n-1}. The iteration of this argument shows the existence and uniqueness of $v \in S_{\Delta,k}$ satisfying (2.1)–(2.2).

In order to establish the bound in the theorem, we note that, since $f \in H^{k+1}(\delta, R)$ for each $0 < \delta < R$, the Taylor formula gives, for $r_j < r < r_{j+1}$,

$$f'(r) - v'(r) = \frac{1}{(k-1)!} \int_{r_{j+1}}^{r} (r - s)^{k-1} f^{(k+1)}(s)\, ds$$

which implies

$$\begin{aligned}
\int_{r_j}^{r_{j+1}} (f'(r) - v'(r))^2 r^2\, dr &= \frac{1}{((k-1)!)^2} \int_{r_j}^{r_{j+1}} \left[\int_{r}^{r_{j+1}} (r - s)^{k-1} f^{(k+1)}(s)\, ds \right]^2 r^2\, dr \\
&\le \frac{1}{((k-1)!)^2} \int_{r_j}^{r_{j+1}} \left[\int_{r}^{r_{j+1}} (r - s)^{2(k-1)} (f^{(k+1)}(s))^2 s^2\, ds \right] \\
&\quad \cdot \left[\int_{r}^{r_{j+1}} \frac{ds}{s^2} \right] r^2\, dr \\
&\le \frac{1}{((k-1)!)^2} h^{2(k-1)} \int_{r_j}^{r_{j+1}} (f^{(k+1)}(r))^2 r^2\, dr \\
&\quad \cdot \int_{r_j}^{r_{j+1}} \left(\frac{1}{r} - \frac{1}{r_{j+1}} \right) r^2\, dr.
\end{aligned}$$

Now after some manipulations

$$\int_{r_j}^{r_{j+1}} \left(\frac{1}{r} - \frac{1}{r_{j+1}} \right) r^2\, dr = \frac{3r_{j+1}(r_{j+1} - r_j)^2 - 2(r_{j+1} - r_j)^3}{6r_{j+1}} \le \frac{h^2}{2} \tag{2.3}$$

and the theorem follows.

Only minor adjustments are needed to adapt the proof to the case $N \neq 3$. For $N = 2$, one obtains, in lieu of the integral in (2.3)

$$\begin{aligned}
\int_{r_j}^{r_{j+1}} (\ln r_{j+1} - \ln r) r\, dr &= \frac{1}{2} r_j (r_{j+1} - r_j) + \frac{1}{4} (r_{j+1} - r_j)^2 \\
&\quad - \frac{1}{2} r_j^2 \ln\left(1 + \frac{r_{j+1} - r_j}{r_j} \right).
\end{aligned} \tag{2.4}$$

Note that the last term in the right-hand side vanishes for $r_j = 0$. On using the inequality $\ln(1 + \varepsilon) \ge \varepsilon - \frac{1}{2}\varepsilon^2$, valid for $\varepsilon \ge 0$, it is readily concluded that (2.4) is $O(h^2)$ uniformly in r_j and the proof of the theorem can be continued as in the three-dimensional case. On the other hand, for $N > 3$, (2.3) must be replaced by

$$\frac{1}{N-2}\int_{r_j}^{r_{j+1}}\left(r-\frac{r^{N-1}}{r_{j+1}^{N-2}}\right)dr=\frac{1}{N-2}\left[\frac{1}{2}(r_{j+1}^2-r_j^2)-\frac{r_{j+1}^N-r_j^N}{Nr_{j+1}^{N-2}}\right].$$

For simplicity, we drop the factor $1/(N-2)$ so that the above expression becomes

$$r_{j+1}(r_{j+1}-r_j)-\frac{1}{2}(r_{j+1}-r_j)^2-\frac{1}{N}$$
$$\cdot\left\{r_{j+1}^2-\left[r_{j+1}^2-\binom{N}{1}r_{j+1}(r_{j+1}-r_j)+\binom{N}{2}(r_{j+1}-r_j)^2-\binom{N}{3}\right.\right.$$
$$\left.\left.\cdot\frac{(r_{j+1}-r^j)^2}{r_{j+1}}\cdots\right]\right\}=\frac{N-2}{2}(r_{j+1}-r_j)^2+\frac{1}{N}\left[\binom{N}{3}\frac{(r_{j+1}-r_j)^3}{r_{j+1}}-\cdots\right]$$

and the last expression is $O(h^2)$ uniformly in r_{j+1} because $(r_{j+1}-r_j)/r_{j+1}\le 1$.

Remark 2.1. We can replace $\|f\|_{H^{k+1}(\Omega)}$ by $\|(\partial^{k+1}/\partial r^{k+1})f\|_{L^2(\Omega)}$ in the statement of the theorem.

Remark 2.2. Note that, in the above construction, we avoid interpolating f at the origin in view of the possible singularity there. Other techniques to approximate (not necessarily radial) functions lacking in smoothness have been considered in [6] and [7]. In the radial case however, the technique presented here is possibly the most straightforward on arbitrary grids.

Remark 2.3. For $f\in H_r^{k+1}(\Omega)$, an optimal $O(h^{k+1})$ L^2-rate of convergence can be easily obtained by applying Nitsche's trick to the Galerkin solution of the problem

$$-\Delta f=g,\qquad x\in IR^N,\quad g\text{ radial}.$$

with Dirichlet boundary conditions.

The reader interested in L^∞ estimates for functions which are smoother than $H_r^{k+1}(\Omega)$ should consult [3].

3. APPLICATION TO THE RADIAL NONLINEAR SCHRÖDINGER EQUATION

The nonlinear Schrödinger equation in N spatial dimensions

$$i\frac{\partial u}{\partial t}+\Delta u=\mathrm{F}(u)\tag{3.1}$$

where F is a locally Lipschitz function of its argument, has received a great deal of attention in recent years. The case $N=2$ arises in nonlinear optics: u is then the envelope of an electromagnetic beam propagating along the t axis in a three-dimensional optical medium. In the case $N=3$, the equation has been derived in the context of plasma physics: u is then the envelope of a Langmuir wave. It is often assumed in the literature [4, 5] that the solution u of (3.1) is radially symmetric and thus satisfies

$$i\frac{\partial u}{\partial t}(r,t) + \frac{\partial^2 u}{\partial r^2}(r,t) + \frac{N-1}{r}\frac{\partial u}{\partial r}(r,t) = F(u(r,t)). \tag{3.2}$$

Here, we shall consider the case where (3.2) applies for $(r,t) \in]0,R[\times]0,T]$ with initial condition

$$u(r,0) = u_0(r), \qquad r \in [0,R]$$

and a homogeneous Dirichlet boundary condition at $r = R$. The Galerkin approximation u_h: $[0,T] \to \dot{S}_{\Delta,k}$ satisfies

$$i\int_\Omega \frac{du_h}{dt}(t)\bar{\phi}\,dx - \int_\Omega \nabla u_h(t) \cdot \nabla\bar{\phi}\,dx = \int_\Omega F(u_h(t))\bar{\phi}\,dx, \qquad 0 < t \le T \tag{3.3}$$

for all $\phi \in \dot{S}_{\Delta,k}$, and is equipped with an initial condition $u_h(0)$ such that

$$\|u_h(0) - u_0\|_{L^2(\Omega)} = O(h^{k+1}). \tag{3.4}$$

Of course, for practical purposes, the integrals in (3.3) are best written as one-dimensional integrals over the interval $[0,R]$.

In applications, the solution u of (3.2) often focuses at the origin [5] and it is therefore desirable to have a spatial grid that is much finer near the origin than elsewhere. For this reason, we have chosen to avoid the quasi-uniformity requirement on the grid Δ. As we shall see, when the function F is *globally* Lipschitz, the grid may be totally arbitrary. On the other hand, in most cases of interest, F is only *locally* Lipschitz, so that inverse inequalities are needed to prove convergence and consequently, we require some grid structure. More precisely, we shall assume that constants $C > 0$ and $0 < \theta < 1$ exist such that, as the grid is refined,

$$h \le C\underline{h}^\theta. \tag{3.5}$$

Note that (3.5) allows the ratio $h/\underline{h}$ to be arbitrarily large.

In order to analyze the convergence of (3.3), it is convenient to introduce the Galerkin projection $p_h(t) \in \dot{S}_{\Delta,k}$ of $u(t)$, defined as the solution of the problem

$$\int_\Omega \nabla p_h(t) \cdot \nabla\bar{\phi}\,dx = \int_\Omega \nabla u(t) \cdot \nabla\bar{\phi}\,dx$$

for all $\phi \in \dot{S}_{\Delta,k}$ and $0 \le t \le T$. In view of the approximation results obtained in Section 2, we have

$$\|p_h(t) - u(t)\|_{L^2(\Omega)} + h\|\nabla(p_h(t) - u(t))\|_{L^2(\Omega)} \le Ch^{k+1}\|u(t)\|_{H^{k+1}(\Omega)}. \tag{3.6}$$

Furthermore, if $(\partial u/\partial t)(t)$ belongs to $H_0^1(\Omega)$, then the function p_h: $]0,T[\to H_0^1(\Omega)$ is differentiable at t and it is a simple matter to verify that $(dp_h/dt)(t) \in \dot{S}_{\Delta,k}$ is the Galerkin projection of $(\partial u/\partial t)(t)$. Thus, (3.6) also holds when p_h and u are replaced by their time-derivatives. We begin with

Lemma 3.1. *For $N = 2,3$ and $k \geq 1$, assume that*

$$\theta > \frac{N}{4}.$$

Suppose also that

$$u \in C^1(0,T; H_r^{k+1}(\Omega) \cap H_0^1(\Omega)).$$

Then

$$\lim_{h\to 0} \max_{0\leq t\leq T} \|p_h(t) - u(t)\|_{L^\infty(\Omega)} = 0.$$

Proof. In view of (3.5), we have, for all $\phi \in \dot{S}_{\Delta,k}$,

$$\|\phi\|_{L^\infty(\Omega)} \leq Ch^{-N/2\theta}\|\phi\|_{L^2(\Omega)}.$$

For any $\phi \in \dot{S}_{\Delta,k}$, we may therefore write

$$\begin{aligned}\|u(t) - p_h(t)\|_{L^\infty(\Omega)} &\leq \|u(t) - \phi\|_{L^\infty(\Omega)} + \|p_h(t) - \phi\|_{L^\infty(\Omega)}\\ &\leq \|u(t) - \phi\|_{L^\infty(\Omega)} + Ch^{-N/2\theta}\|p_h(t) - \phi\|_{L^2(\Omega)}\\ &\leq \|u(t) - \phi\|_{L^\infty(\Omega)} + Ch^{-N/2\theta}\|u(t) - \phi\|_{L^2(\Omega)}\\ &\quad + Ch^{-N/2\theta}\|u(t) - p_h(t)\|_{L^2(\Omega)}.\end{aligned}$$

Observe that the last term goes to zero like $O(h^{k+1-N/2\theta})$ and therefore we only need to find $\phi \in \dot{S}_{\Delta,k}$ such that

$$\lim_{h\to 0}\{\|u(t) - \phi\|_{L^\infty(\Omega)} + Ch^{-N/2\theta}\|u(t) - \phi\|_{L^2(\Omega)}\} = 0. \tag{3.7}$$

Now, note that (3.2) can be rewritten as

$$\frac{\partial^2 u}{\partial r^2}(r,t) + \frac{N-1}{r}\frac{\partial u}{\partial r}(r,t) = g(r,t) \equiv -i\frac{\partial u}{\partial t}(r,t) + F(u(r,t)).$$

A first integration with respect to r yields

$$\frac{1}{r}\frac{\partial u}{\partial r}(r,t) = \frac{1}{r^N}\int_0^r g(s,t)s^{N-1}\,ds.$$

Since the integrand on the right-hand side is bounded, this shows that $u \in L^\infty(0,T; H^2(0,R))$. The condition (3.6) can therefore be achieved by choosing ϕ to be the linear interpolant of $u(t)$ with respect to Δ. Indeed, for such a choice, standard one-dimensional approximation theory yields

$$\begin{aligned}&\|\phi - u(t)\|_{L^\infty(\Omega)} + Ch^{-N/2\theta}\|\phi - u(t)\|_{L^2(\Omega)}\\ &\qquad \leq \|\phi - u(t)\|_{L^\infty(0,R)} + Ch^{-N/2\theta}R^{N-1}\|\phi - u(t)\|_{L^2(0,R)}\\ &\qquad \leq C(h + h^{2-N/2\theta})\|u(t)\|_{H^2(0,R)} \to 0.\end{aligned}$$

Lemma 3.2. *Under the same assumption as in Lemma 3.1, we have*

$$\begin{aligned}i\int_\Omega \frac{dp_h}{dt}(t)\bar{\phi}\,dx - \int_\Omega \nabla p_h(t)\cdot\nabla\bar{\phi}\,dx = \int_\Omega F(p_h(t))\bar{\phi}\,dx\\ + \int_\Omega \delta_h(t)\bar{\phi}\,dx\end{aligned} \tag{3.8}$$

where

$$\|\delta_h(t)\|_{L^2(\Omega)} \leq Ch^{k+1}. \tag{3.9}$$

Proof. Clearly, we have

$$\delta_h(t) = i\left(\frac{dp_h}{dt}(t) - \frac{\partial u}{\partial t}(t)\right) + (F(p_h(t)) - F(u(t))).$$

It suffices to note that $p_h(t)$ and $u(t)$ are bounded. The fact that F is Lipschitz on bounded sets yields the result.

Theorem 3.1. *We make the same assumptions as in Lemma 3.1. Then, the solution u_h of (3.3) with initial condition $u_h(0)$ satisfying (3.4) exists and we have*

$$\|u_h(t) - u(t)\|_{L^2(\Omega)} \leq Ch^{k+1}$$

for $0 \leq t \leq T$.

Proof. Let

$$M = \|u\|_{L^\infty(0,T;\,L^\infty(\Omega))} + 1$$

and introduce the set

$$\Lambda_h = \{\tau \in [0,T]: \quad \text{for all } 0 \leq t \leq \tau, u_h(t) \quad \text{exists and } \|u_h(t)\|_{L^\infty(\Omega)} < M\}.$$

It follows from standard ODE theory that Λ_h is non-empty and we may pose

$$t_h = \sup \Lambda_h.$$

Clearly, u_h exists at t_h and we have either

$$\|u_h(t_h)\|_{L^\infty(\Omega)} = M \tag{3.10}$$

or else

$$t_h = T. \tag{3.11}$$

For $0 \leq i \leq t_h$, we define $e_h(t) = p_h(t) - u_h(t)$. Subtracting (3.3) from (3.7), we obtain

$$i\int_\Omega \dot{e}_h(t)\bar{\phi}\,dx - \int_\Omega \nabla e_h(t)\cdot\nabla\bar{\phi}\,dx = \int_\Omega (F(p_h(t) - F(u_h(t)))\bar{\phi}\,dx + \int_\Omega \delta_h(t)\bar{\phi}\,dx.$$

Now, choose $\phi = e_h(t)$ and take the real part in the above equality. Since both $p_h(t)$ and $u_h(t)$ are bounded for $0 \leq t \leq t_h$, we may use the fact that F is locally Lipschitz to obtain, via Gronwall's lemma,

$$\|e_h(t)\|_{L^2(\Omega)} \leq C\{\|\delta_h\|_{L^\infty(0,T;\,L^2(\Omega)} + \|e_h(0)\|_{L^2(\Omega)}\}.$$

Thus, using the hypothesis, we have, for $0 \leq t \leq t_h$,

$$\|e_h(t)\|_{L^2(\Omega)} \leq Ch^{k+1}. \tag{3.12}$$

Now

$$\begin{aligned}\|u_h(t_h)\|_{L^\infty(\Omega} &\leq \|p_h(t_h)\|_{L^\infty(\Omega)} + \|e_h(t_h)\|_{L^\infty(\Omega)} \\ &\leq \|p_h(t_h)\|_{L^\infty(\Omega)} + Ch^{-N/2\theta}\|e_h(t_h)\|_{L^2(\Omega)} \\ &\leq \|p_h(t_h)\|_{L^\infty(\Omega)} + Ch^{k+1-N/2\theta} < M.\end{aligned}$$

for h sufficiently small. This shows that (3.10) is false if h is small enough and thus (3.12) is valid up to $t = T$.

Convergence proofs for time-discrete Galerkin approximations to (3.1) may be found in [8], along with further material on Schrödinger equations and their numerical solution.

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