Computing Eigenmodes of Elliptic Operators Using Radial Basis Functions

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Abstract

Radial basis function (RBF) approximations have been successfully used to solve boundary-value problems numerically. We show that RBFs can also be used to compute eigenmodes of elliptic operators. Special attention is given to the Laplacian operator in two dimensions. We include techniques to avoid degradation of the solution near the boundaries and corner singularities. Numerical results compare favorably to basic finite element methods.

Keywords. radial basis functions, eigenvalues, elliptic operators, numerical methods, Laplacian

1 Introduction

Many positive properties of RBF methods have been identified in connection with boundary-value problems (BVPs) [1-4]. They are grid-free numerical schemes very suitable for problems in irregular geometries. They can exploit accurate and smooth representations of the boundary, are very easy to implement, and can be spectrally accurate [5, 6]. It would be expected that the benefits experienced by the use of RBFs in BVPs would carry over for eigenvalue problems. In this article we formulate and apply an RBF-based method to compute eigenmodes of elliptic operators.

Given a linear elliptic second order partial differential operator $L$ and a bounded region $\Omega$ in $\mathbb{R}^n$ with boundary $\partial \Omega$, we seek eigenpairs $(\lambda, u) \in (C, C(\Omega))$ satisfying

\begin{equation}
Lu + \lambda u = 0 \quad \text{in } \Omega \quad \text{and} \\
L_B u = 0 \quad \text{on } \partial \Omega,
\end{equation}

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where $L_B$ is a linear boundary operator of the form

$$L_B u = a u + b (n \cdot \nabla u).$$

Here $a$ and $b$ are given constants and $n$ is the unit outward normal vector defined on the boundary. We assume that $\Omega$ is open and that the eigenvalue problem is well-posed.

We use an interpolating RBF approximation of an eigenfunction of (1) and replace the eigenvalue problem above with a finite-dimensional eigenvalue problem. In order to compute the eigenpairs of the modified system, we approximate the operator $L$ by a matrix that incorporates the boundary conditions and then use standard techniques to find the eigenvalues and eigenvectors of this matrix.

Unfortunately, as pointed out in [2, 7], straightforward RBF approximations are relatively inaccurate near the boundaries, and special attention should be given to this issue. We study the boundary clustering of nodes and the collocation of the PDE on the boundary and verify that they are effective techniques for preventing degradation of the solution near the edges of the domain.

We also consider the effect of corner singularities in 2-D regions, i.e., corners with interior angle $\pi/\varphi$ where $\varphi$ is not integer. It is known that some eigenfunctions are not smooth at such corners, and as a result a typical RBF approximation gives very poor results in this case. In fact, our tests show that the numerical solution does not converge if the method is not modified. In [8] Driscoll exploits the singular behavior of an eigenfunction at the corners and propose an efficient algorithm to compute eigenvalues for polygonal regions. With that as motivation, we append terms to the RBF expansion that approximate the singular behavior of an eigenfunction.

The remainder of this article is organized as follows: In the next section we introduce RBF approximations. In section 3 we formulate the problem in matrix form. In section 4 we present the boundary treatment techniques. In section 5 numerical results are presented. We carry out several experiments in 2-D regions for the Laplacian operator for a disk, an isosceles right triangle, and an L-shaped region, as shown in Fig. 1, and compare to finite elements and spectral methods.
2 Radial basis functions

Let \( \{y_i\}_{i=1}^{N} \) be a finite set of distinct points in \( \mathbb{R}^n \). Given a function \( \phi \) from \( \mathbb{R}^+ \) to \( \mathbb{R} \), we write the standard RBF approximation of a function \( u(x) \):

\[
\tilde{u}(x) = \sum_{i=1}^{N} \alpha_i \phi(||x - y_i||) \ , \quad x \in \mathbb{R}^n.
\]  

The points \( y_i \) are called centers and \( \phi \) the radial basis function [9]. The coefficients \( \alpha_i \) are chosen so that \( \tilde{u} \) satisfies certain interpolation criteria to be discussed later.

Several choices for \( \phi \) have been presented in the literature [7, 9, 10]. Some of the most commonly used RBFs are:

\[
\begin{align*}
\phi(r) &= r^3, & \text{(cubic)}, \\
\phi(r) &= r^2 \log(r), & \text{(thin plate spline)}, \\
\phi(r) &= (1 - r^2)^p p(r), & \text{(Wendland functions [11], where } p \text{ is polynomial)}, \\
\phi(r) &= \exp(-cr^2), & \text{(Gaussian)}, \\
\phi(r) &= \sqrt{c^2 + r^2}, & \text{(multiquadric)},
\end{align*}
\]

where \( r \) is real and non-negative and \( c \) is a positive constant. The multiquadric, in particular, has been successfully used to solve elliptic problems numerically [2, 4]. It was introduced by Hardy [12], and Kansa applied it to solve PDEs in the early 1990s [1].

In order to determine the coefficients \( \alpha_i \), a set of \( N \) distinct interpolation points in \( \Omega \) is needed. Usually, the same set of points is used for centers and interpolation. Taking centers outside the domain appropriately, however, has been shown to be an effective way of improving accuracy near the boundary — see, e.g., Fedoseyev et al. [2] and Fornberg et al. [7]. If \( u(x_j) \), \( j = 1, 2, \ldots, N \), were known, finding the \( \alpha_i \) would require solution of an \( N \times N \) linear system \( A\alpha = u \), \( A \equiv [\phi(||x_i - y_j||)]_{N \times N} \), \( \alpha \equiv [\alpha_1, \alpha_2, \ldots, \alpha_N]^T \) and \( u \equiv [u(x_1), u(x_2), \ldots, u(x_N)]^T \). \( A \) is called the RBF interpolation matrix and, for some RBFs, is positive definite [9].

3 Algorithm

There are different ways to use (3) to derive a finite-dimensional eigenvalue problem. We shall start with the method we find the most efficient. The idea behind this scheme is to approximate the operator \( L \) by a matrix \( L_\phi \) that also incorporates the boundary conditions.

For \( N_I \) nodes in the interior of the domain and \( N_B \) nodes on the boundary, \( N = N_I + N_B \), we denote the interpolation points by \( \{x_i\}_{i=1}^{N_I} \in \Omega \) and \( \{x_i\}_{i=N_I+1}^{N} \in \partial \Omega \). In order to obtain \( L_\phi \), we enforce the boundary condition at every point \( x_i \) on the boundary, and evaluate the RBF approximation (3) at
the interior interpolation points to obtain
\[ \sum_{i=0}^{N} \alpha_i \phi(\|x_j - y_i\|_2) = \tilde{u}(x_j), \quad j = 1, 2, ..., N, \]
\[ \sum_{i=0}^{N} \alpha_i L_B \phi(\|x_j - y_i\|_2) = 0, \quad j = N_I + 1, N_I + 2, ..., N. \]

In the notation \( L_B \phi(\|x_j - y_i\|_2) \) it is understood that \( L_B \) is applied to the first variable, then evaluated. This can be written in matrix form as
\[ \alpha = A^{-1} \begin{bmatrix} \tilde{u}^T \\ 0_{N_p \times 1} \end{bmatrix}, \quad (4) \]
where \( \tilde{u}^T \equiv [\tilde{u}(x_1), \tilde{u}(x_2), ..., \tilde{u}(x_{N_I})]^T, 0_{p \times q} \) is the \( p \times q \) zero matrix,
\[ A \equiv \begin{bmatrix} A^T \\ B \end{bmatrix}, \quad A^T \equiv [\phi(\|x_i - y_j\|_2)]_{N_I \times N_I}, \quad \text{and} \quad B \equiv [L_B \phi(\|x_{N_I+i} - y_j\|_2)]_{N_p \times N_I}. \]

For the Dirichlet boundary condition, the matrix \( A \) becomes the usual RBF interpolation matrix.

For the interior points, we also have that
\[ \sum_{i=1}^{N} \alpha_i L \phi(\|x_j - y_i\|_2) = \lambda \tilde{u}(x_j) \quad j = 1, 2, ..., N_I, \]
which can be expressed as
\[ L^I \alpha = \lambda \tilde{u}^I, \quad (5) \]
where
\[ L^I \equiv [L \phi(\|x_i - y_j\|_2)]_{N_I \times N_I}. \]
Combining (4) and (5) we obtain
\[ L_0 \tilde{u}^I = \lambda \tilde{u}^I. \quad (6) \]
\( L_\phi \) is the \( N_I \times N_I \) matrix given by
\[ L_\phi \equiv L^I A^{-1} \begin{bmatrix} I_{N_I \times N_I} \\ 0_{N_p \times N_I} \end{bmatrix}. \]
Here \( I_{p \times p} \) is the identity matrix of order \( p \).

The RBF approximation of the eigenpairs of (1) is now obtained by computing the eigenvalues and eigenvectors of the matrix \( L_\phi \).

In some instances it is necessary or useful to add functions to the RBF approximation (3),
\[ \tilde{u}(x) \equiv \sum_{i=1}^{N} \alpha_i \phi(\|x - y_i\|_2) + \sum_{i=1}^{M} \beta_i g_i(x), \quad x \in \mathbb{R}^n. \quad (7) \]

To make this system uniquely solvable, it is usually required that
\[ \sum_{i=1}^{N} \alpha_i g_j(x) = 0, \quad j = 1, 2, ..., M. \]
For multiquadrics, the choice $M = 1$, $g \equiv 1$ leads to a positive definite RBF interpolation matrix [13]. For the Neumann problem, augmentation by a constant is especially appropriate due to the trivial zero mode.

Repeating the procedure above for (7), one obtains the following expression for the operator of the finite-dimensional system:

$$L_\phi \equiv L_2^I A_2^{-1} \begin{bmatrix} I_{N_I \times N_I} \\ 0_{(N_B + M) \times N_I} \end{bmatrix},$$

where

$$L_2^I \equiv \begin{bmatrix} A^I & Lg_j(x_i) \end{bmatrix}_{N_I \times M},$$

$$A_2 \equiv \begin{bmatrix} A^I & Lg_j(x_i) \\ B & [L_Bg_j(x_{N_I+i})]_{N_B \times M} \end{bmatrix}_{M \times N}.$$

A few remarks should be made about the method:

- The matrix $A$ (or $A_2$) usually becomes ill-conditioned as the number of nodes increases. This is a common problem when RBFs of global support are used [14].

- The eigenvalue system is of size $N_I$, the number of interior nodes, although as an intermediate step one must invert a matrix of size $N$, the total number of nodes.

- One could rewrite the matrix eigenvalue system using the “inverse RBF operator”. In this case one would seek the eigenpairs $(\nu, \tilde{u}^I)$ of the matrix $H_\phi$,

$$H_\phi \equiv A^I \begin{bmatrix} L^I \\ B \end{bmatrix}^{-1} \begin{bmatrix} I_{N_I \times N_I} \\ 0_{N_B \times N_I} \end{bmatrix}.$$

The approximate eigenvalues and eigenvectors of (1) would then be $1/\nu$ and $\tilde{u}^I$, respectively.

Another approach is to write the finite-dimensional problem as a generalized eigenvalue problem. The idea is to substitute the RBF approximation (3) into the eigenvalue problem (1), leading to the following system:

$$\begin{bmatrix} L^I \\ B \end{bmatrix} \alpha = \lambda \begin{bmatrix} A^I \\ 0_{N_B \times N} \end{bmatrix} \alpha.$$

In this case, one would seek the generalized eigenvalues and eigenvectors of these matrices. This system is of size $N$, not $N_I$, but unlike $L_\phi$, does not require a matrix inversion. Notice that in principle the accuracy of the approximation does not depend on how the eigenpairs of the finite-dimensional problem are computed, but on the RBF and the set of nodes used. The generalized eigenvalue problem also suffers from ill-conditioning.
4 Boundary treatment

RBF approximations are, in general, inaccurate near the boundary [15, 16]. In this section we consider several techniques for improving accuracy near boundaries.

4.1 Boundary clustering of nodes

Clustering of nodes near the boundary was found to be very successful in [7]. Clustering in a 1-D interval is essential for a high-degree polynomial interpolation to be successful. Chebyshev points, given by $\cos(j\pi/N)$, $j = 0, 1, ..., N$ on [-1,1], are commonly used to avoid large errors near the boundary for spectral methods based on polynomials. This motivates clustering the nodes more densely at boundaries for RBFs. In [7] numerical experiments were run based on nodes in [-1,1] with density proportional to $(1-x^2)^{-\gamma}$. The case $\gamma = 0$ gives equispaced nodes, $\gamma > 0$ clusters nodes toward the endpoints, and $\gamma = 0.5$ gives the Chebyshev points; see [17] for more detail.

Figure 2 shows node distributions obtained with $\gamma = 0.4$. On top, the nodes on an 1-D interval are shown. Using these points, it is possible to generate nodes in 2-D regions as presented for the disk, triangle, and L-shaped region.

4.2 Collocation of the PDE on the boundary

The idea of adding equations obtained via collocation of the PDE on the boundary was introduced for boundary-value problems in [2]. We shall explore this approach in connection with the eigenvalue problem.

In order to add equations, an extra set of centers is needed. We add centers outside the domain and adjacent to the boundary. In Figure 3, we show uniformly distributed nodes for the circle, the dots represent collocation nodes and the open circles represent centers.
Figure 3: Example of distribution of centers (circles) and collocation nodes (dots) in a disk for collocation of the PDE on the boundary.

The implementation of this scheme is straightforward. For \( b \neq 0 \) in (2), one just needs to consider the boundary collocation nodes as both boundary points and interior points (in the sense that both equations in (1) should be satisfied). The resulting \( L_\phi \) matrix has the same structure presented previously.

For the Dirichlet boundary condition this simple procedure breaks down since \( Lu = \lambda u \) implies that the matrix \( A \) (or \( A_2 \)) would be singular. A non-singular system can be obtained by rewriting the matrix

\[
L_\phi \equiv L_\lambda A_3^{-1} \left[ I_{N_B \times N_B} \right], \quad A_3 \equiv \left[ A_1^{I} \right]_{N_B \times N_B}
\]

### 4.3 Corner singularities

We now turn our attention to the eigenvalue problem in 2-D regions with corners and assume that \( L \) is the Laplacian operator. In a corner with interior angle \( \pi / \varphi \) an eigenfunction has a particular singular behavior if \( \varphi \) is not integer. For the L-shaped region, for instance, the singularity occurs at the reentrant corner. Generic numerical procedures are inefficient because of the loss of smoothness at such corners. In particular, a typical RBF approximation gives a very poor approximation of an eigenfunction near a singularity. Clustering of points at the reentrant corner and collocation of the PDE on the boundary did not prevent poor convergence rates in our numerical experiments.

In order to improve our numerical scheme, we exploit the local behavior of the eigenfunction at a corner of the boundary. Let \( (r, \theta) \) be polar coordinates originating from a corner. An eigenfunction \( u \) of (1) with Dirichlet boundary condition can be represented as

\[
u(r, \theta) = \sum_{n=1}^{\infty} c_n J_{\nu}(\sqrt{\lambda} r) \sin(n \varphi \theta),
\]

where \( J_{\nu} \) is a Bessel function of first kind. Using the ascending series

\[
J_{\nu}(z) = \left( \frac{1}{2} \right)^{\nu} \sum_{k=0}^{\infty} \frac{(-\frac{1}{4} z^2)^k}{k! \Gamma(\nu + k + 1)}
\]
we have that
\[ u(r, \theta) = \sum_{n=1}^{\infty} \sum_{k=0}^{\infty} b_{nk} r^{n\varphi + 2k} \sin(n\varphi \theta) , \]
where the coefficients \( b_{nk} \) are independent of \( r \) and \( \theta \).

Motivated by the last expansion, we add terms of the form \( r^{n\varphi + 2k} \sin(n\varphi \theta) \) to the RBF approximation, i.e., in (7) we let \( g_i = r^{n\varphi + 2k} \sin(n\varphi \theta) \), where \( n \) and \( k \) are chosen appropriately so that the smallest powers of \( r \) are used. We believe that these extra terms help to capture the singular behavior of an eigenfunction at a corner. For the Neumann problem, we have that
\[ u(r, \theta) = \sum_{n=0}^{\infty} \sum_{k=0}^{\infty} d_{nk} r^{n\varphi + 2k} \cos(n\varphi \theta) , \]
which suggests a similar modification.

5 Numerical results

Numerical experiments were run for the Laplacian operator in 2D regions. The regions chosen are the circle of radius \( \pi \), the triangle of vertices \((0,0), (\pi,0) \) and \((\pi,\pi)\), and the L-shaped region of vertices \((0,\frac{\pi}{2}), (\frac{\pi}{2},\pi), (\pi,0), (0,0), (\pi,\pi) \) and \((0,\pi)\), as pictured in Fig. 1.

We used multiquadric RBFs \((\phi(r) = \sqrt{c^2 + r^2})\) to generate the results and considered the expansion (7) with \( M = 1 \) and \( g_1 \equiv 1 \). We used \( c = 4 \) for the disk, \( c = 1 \) for the triangle and \( c = 0.85 \) for the L-shaped region. These choices are not proved to be optimal but appear to be sufficiently close. More information on selecting the parameter \( c \) can be found in [10, 18].

We compare the the boundary treatment techniques presented in the previous section. The following abbreviations were adopted: BC for boundary clustering of nodes; PDECB for collocation of the PDE on the boundary; and CST for adding singular terms as discussed in section 4.3. For the CST we used 10 extra terms at the reentrant corner of the L. Clustering of nodes was obtained using \( \gamma = 0.4 \).

We count repeated eigenvalues and denote the exact \( j \)th eigenvalue by \( \lambda^{(j)} \), \( 0 \leq \lambda^{(1)} \leq \lambda^{(2)} \leq \ldots \). For the disk and triangle, the modes are known analytically. For the L, they were estimated using the very accurate algorithm of Driscoll [8]. For an RBF-computed eigenvalue we write \( \lambda^{(j)}_N \).

5.1 Dirichlet boundary conditions

We start with numerical tests for the Dirichlet problem.

Figure 4 shows the relative error, \( |\lambda^{(j)} - \lambda^{(j)}_N|/\lambda^{(j)} \), in selected eigenvalues for the disk as function of \( N \), the total number of centers. The 3rd, 5th, 8th and 12th are repeated eigenvalues and the errors in these are not shown. The graphs show that the lower eigenvalues are usually resolved more accurately than higher ones; however, we note that in most cases the 9th eigenvalue was least accurate among the first 12.
Figure 4: Relative error in selected eigenvalues for the disk (Dirichlet boundary condition).
In order to compare the performance of the boundary treatment schemes we plotted the maximum relative error over the 12 first eigenvalues, $\max_{1 \leq j \leq 12} |\lambda^{(j)}_N - \lambda^{(j)}|/\lambda^{(j)}$, for several values of $N$. The results are shown in Figure 5. For all regions we observed significant gain in accuracy when an edge enhancement technique was used. For the circle and triangle, both BC and PDECB improved the solution, BC giving the most accurate results of the two schemes. Combining the two techniques did not improve the solution over BC alone.

The results for the L-shaped region (last graph in Fig. 5) show that making use of the information about the singularity at the reentrant corner is essential for good approximations. We note that the plain RBF expansion (3) does not converge and that clustering nodes near the singularity worsens the approximations. Combining CST and BC is an efficient approach to this problem; for some values of $N$ an order of magnitude was gained over the CST alone.

Figure 6 shows the error in the first eigenmode of the L-shaped region. CST improves the solution in the whole region. Without singular terms, the error is
No Boundary Treatment  CST  CST and BC

Figure 6: Error of the computed first eigenfunction of the L-shaped region with Dirichlet boundary condition, $N = 481$.

Figure 7: Maximum relative error over the first 12 eigenvalues versus CPU time for the disk with Dirichlet boundary condition.

dominated by the effects of the reentrant corner.

In Figure 7 we compare the performance of the RBF method to a spectral method and second-order finite elements. For the spectral scheme we used the algorithm described in [19]. The finite element results were obtained with the PDE Toolbox for MATLAB. We used a 700MHz Linux PC to generate this data and all algorithms were implemented in MATLAB. Although the RBF method did not converge as fast as the spectral method (which is able to exploit the special structure of the disk), its performance was significantly better than the low-order finite element method.

5.2 Neumann boundary conditions

We now consider the Neumann problem. At a corner of the boundary we define the normal vector by the average of the two nearest normal vectors, see Figure 8.
6 Conclusion

An RBF-based method has been presented for the eigenvalue problem for elliptic operators. The continuous problem is replaced with a finite-dimensional eigenvalue problem. Special attention is given for the approximation near the boundaries in order to improve the accuracy of the method. For 2-D regions with corner singularities, terms were added to the RBF approximation. These terms are obtained from an expansion of an eigenfunction at a corner.

Our numerical experiments show that the RBF method can be effectively used for solving eigenvalue problems. The results computed with the boundary treatment techniques showed considerable improvement in accuracy. In most cases, boundary clustering of nodes gave better results than the collocation of the PDE on the boundary. We note, however, that the latter is easier to implement in irregular domains. For the L-shaped region, the inclusion of singular terms was found to be essential for good approximations.

We believe that the techniques presented here can still be improved. For instance, some numerical experiments suggest that adding more centers outside the domain (as suggested in [7]) would improve accuracy and the conditioning.
Figure 9: Maximum relative error over the first 12 eigenvalues of the Neumann problem.

Figure 10: Contour plot of the 20th eigenfunction of the L-shaped region with Neumann boundary condition (20 contour lines).
of the problem. Another open question is how to cluster nodes near boundaries for general irregular domains and what is the “optimal” clustering of nodes.

References


