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# ACCURATE BOUNDS FOR THE EIGENVALUES OF THE LAPLACIAN AND APPLICATIONS TO RHOMBICAL DOMAINS*

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1. Introduction. By an eigenvalue and eigenfunction of Laplace's operator on a bounded two-dimensional domain $G$ we mean a positive number $\lambda$ and a non-zero function $u(x,y)$ which satisfy

$$\Delta u(x,y) + \lambda u(x,y) = 0 \ , \ (x,y) \in G \tag{1}$$

and

$$u(x,y) = 0 \ , \ (x,y) \in \Gamma \tag{2}$$

where $\Gamma$ is the boundary of $G$ and $\Delta = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}$. We enumerate the eigenvalues so that $0 < \lambda_1 < \lambda_2 \leq \lambda_3 < \ldots$ .

In [1] and [2] a method is described for finding accurate approximations to these eigenvalues and eigenfunctions together with rigorous bounds on the error in the approximations. The method makes use of known particular solutions of the differential equation (1) and involves two main steps. First, a linear combination of the particular solutions is determined which approximately satisfies the boundary condition (2). Second, the error on the boundary is measured and used to compute upper and lower bounds for a true solution. The pertinent portions of [1] and [2] are summarized in Section 2.

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This paper is primarily concerned with the first step of this process. A generalization of the interpolation technique of [1] for determining a good linear combination is described in Section 3. The basic tool is a Householder-QR algorithm [5]-[6] for computing the singular values of rectangular matrices.

In Section 4 the revised method is illustrated by taking the domain G to be a rhombus. Such domains are difficult to handle with the original method. The Weinstein method of intermediate problems has also been applied to rhombical domains by Stadter [3]. We conclude by comparing Stadter's results with our own.

2. Summary of [1] and [2]. Introducing polar coordinates $(r,\theta)$ and scaled Bessel functions $s_\nu J_\nu(\xi)$ we note that for any $\nu$ the functions

$$p_\nu(r,\theta;\lambda) = s_\nu J_\nu(\sqrt{\lambda}\, r)\cos \nu\theta\ , \quad \nu = 0,1,2,\ldots \text{ and}$$

(3)

$$p_{-\nu}(r,\theta;\lambda) = s_\nu J_\nu(\sqrt{\lambda}\, r)\sin \nu\theta\ , \quad \nu = 1,2,3,\ldots$$

are solutions of the differential equation (1). Consequently, finite linear combinations of these functions may approximate the desired eigenfunctions. These "particular" solutions are chosen because results of S. Bergman and I.Vekua imply that linear combinations of them can approximate any eigenf'unction arbitrarily closely and because similar particular solutions can, in prinicple, be generated for more general differential equations.

Any symmetries in the domain $G$ can be used to eliminate terms from the linear combination. For example, if $G$ is symmetric with respect to both the $x$ and $y$ axes, then the first eigenfunction (corresponding to $\lambda_1$) can be approximated with n terms by

$$u_*(r,\theta) = \sum_{j=1}^{n} c_j p_{2j-2}(r,\theta;\lambda_*) \quad . \tag{4}$$

The parameter $\lambda_*$ and coefficients $c_j$ are to be determined so that $u_*$ is close to zero on $\Gamma$.

The method used in [1] involves choosing n points $(r_i,\theta_i)$ on $\Gamma$ and requiring that $u_*$ interpolate zero at these points, that is

$$u_*(r_i,\theta_i) = 0 \ , \ i = 1,\ldots,n \ .$$

This determines the coefficients to be the solution of $A(\lambda)c = 0$ where $c = (c_1,\ldots,c_n)^T$ and $A(\lambda)$ is the n-by-n matrix whose i,j-th element is $a_{i,j}(\lambda) = p_{2j\ 2}(r_i,\theta_i;\lambda)$ , $i,j = 1,\ldots,n$ . Non-zero coefficients are obtained if and only if $A(\lambda)$ is singular, consequently $\lambda_*$ is taken to be a zero of determinant $(A(\lambda))$.

It is convenient to normalize $u_*$ so that

$$\int_0^{2\pi}\int_0^{\delta} u_*^2(r,\theta) r \ dr \ d\theta = 1 \tag{5}$$

where $\delta$ is the rauius of the largest circle centered at the origin and contained in $G$ . This can be achieved without numerical integration because the particular solutions (3) are orthogonal over this circle and become orthonormal if $s_\nu$ is defined by

$$
\begin{aligned}
&\cdot\ 2\pi \int_0^{\delta} J_0^2(\sqrt{\lambda}\, r)\, r\, dr = 1 \ , \\
(6)\qquad &\\
&s_\nu^2 \cdot \pi \int_0^{\delta} J_\nu^2(\sqrt{\lambda}\, r)\, r\, dr = 1 \ , \quad \nu = 1,2,\ldots \ .
\end{aligned}
$$

The desired normalization (5) of $u_*$ can then be achieved by requiring

$$
(7)\qquad \sum_{j=1}^{n} c_j^2 = 1 \ .
$$

Note that the normalization depends upon $\delta$ and $\lambda$ .

The approximate eigenf'unction $u_*(r,\theta)$ determined in this way is a solution of the differential equation which is zero at n selected boundary points and hopefully small on the rest of the boundary. To obtain error bounds, we compute

$$
(8)\qquad \epsilon = \max_{(r,\theta)\in\Gamma} |u_*(r,\theta)| \cdot \sqrt{\text{area of } G} \ .
$$

The first theorem of [2] then implies that there is an eigenvalue $\lambda_k$ in the interval

$$
(9)\qquad \frac{\lambda_*}{1+\epsilon} \le \lambda_k \le \frac{\lambda_*}{1-\epsilon} \ .
$$

The other theorems in [2] bound the error in $u_*$ . Thus it is possible to obtain upper and lower bounds for both the eigenvalues and eigenfunctions.

3. New methods for determining the coefficients. The interpolation technique described above is a special case of the following general method for determining the $c_j$'s, $\lambda_*$ and hence $u_*$ and $\epsilon$ . Let m

points $(r_i,\theta_i)$ , $i = 1,\ldots,m$ , be chosen on the boundary, let n be the number of terms to be used and assume $m \geq n$ . (In practice, we will take n to be 10 or 20 and m two or three times n .) Let A(h) be the rectangular matrix with elements

$$a_{i,j}(\lambda) = p_{\nu_j}(r_i,\theta_i;\lambda), \quad i = 1,\ldots,m, \quad j = 1,\ldots,n \tag{10}$$

where the $\nu_j$ are determined by any symmetries in the domain. Let $c = (c_1,\ldots,c_n)^T$ and let $\|\cdot\|_m$ and $\|\cdot\|_n$ be norms on m -vectors and n -vectors respectively. Compute .

$$\min_{\lambda} \min_{c} \frac{\|A(\lambda)\underline{c}\|_m}{\|\underline{c}\|_n} \tag{11}$$

by an algorithm which also computes the minimizing $\lambda$ and c . Let the minimizing $\lambda$ be the approximate eigenvalue $\lambda_*$ and the minimizing c be the coefficients in the approximate eigenfunction .

$$u_*(r,\theta) = \sum_{j=1}^{n} c_j\, p_{\nu_j}(r,\theta;\lambda) .$$

The actual value of the minimum is not used. In principle, infinitely many $\lambda_*$ 's could be found, each giving a local minima and each approximating an eigenvalue of the original problem. In practice, a rough estimate of an eigenvalue is known from other considerations and the minimizing search is carried'out near the estimate.

The quotient in (11) should not be confused with the Rayleigh quotient occurring in variational methods. The value of our quotient is hopefully very small and is a measure of the error in satisfying the

boundary condition. In most variational methods the base functions in the linear combination already satisfy the boundary condition, but not the differential equation, and the value of the Rayleigh quotient approximates the eigenvalue itself.

If $m = n$, we technically have the original interpolation method because a minimum equal to zero occurs when $\lambda$ and $c$ are such that $A(\lambda)$ is singular and $A(\lambda)\underline{c} = \underline{0}$. If $m > n$, the minimum will not be zero except in special circumstances and $u_*$ will not be exactly zero at the chosen boundary points.

In the experiments to be described in the next section, we have taken both $\|\cdot\|_m$ and $\|\cdot\|_n$ to be Euclidean length, thus obtaining a discrete least squares fit to the boundary condition. It is known that any m-by-n matrix A, and in particular our $A(\lambda)$, can be factored into a singular value decomposition $U \Sigma V^T$ where U is m-by-m orthogonal, $V^T$ is n-by-n orthogonal and $\Sigma$ is m-by-n with the form

$$\Sigma = \begin{pmatrix} \sigma_1 & & & 0 \\ & \sigma_2 & & \\ & & \ddots & \\ 0 & & & \sigma_n \\ & & 0 & \end{pmatrix}$$

where $\sigma_1 \geq \sigma_2 > \ldots \geq \sigma_n > 0$. The singular values $\sigma_i$ are the square roots of the eigenvalues of $A^TA$ and in our case are functions of $\lambda$. It is immediate that

$$\min_{c} \frac{\|Ac\|}{\|c\|} = \sigma_n = \frac{\|Av_n\|}{\|v_n\|} \tag{12}$$

where $\underline{v}_n$ is the last row of $V^T$ .

Several algorithms for computing the singular value decomposition without the loss of accuracy resulting from the use of $A^TA$ are proposed by Golub and Kahan in [4] and by Golub in [5]. The algorithm in [5] uses Householder transformations to reduce A to a bidiagonal matrix J and then a variant of the QR algorithm to compute the singular values of J . An **Algol** procedure for the algorithm is given by Businger [6]. The matrix $V^T$ and hence our coefficient vector c is a **biproduct** of the algorithm. The $\underline{c}$ automatically satisfies (7). To complete the process we carry out a one-dimensional minimizing search to find local minima of $\sigma_n(\lambda)$ . The minimizing $\lambda$ are our approximate eigenvalues.

This method is often superior to the original interpolation approach. The boundary points must still be chosen, but their effect on the final approximation and bounds is less pronounced. Furthermore, the Householder-m algorithm provides a stable, accurate method for computing the coefficients, the most critical portion of the process.

It might appear even more desirable to use a Chebyshev criterion at the boundary by taking $\|\cdot\|_m$ in (11) to be the maximum norm. But now we see no natural choice for $\|\cdot\|_n$ . If the maximum norm is also used for $\|\cdot\|_n$ we do not know of an algorithm for computing the minimizing c . If we take $\|\underline{c}\|_n = |c_1|$ , the inner minimization in (11) in effect becomes

$$\min_{c_2,\ldots,c_n} \max_i \left|a_{i,1} - \sum_{j=2}^{n} c_j a_{i,j}\right| \tag{13}$$

The resulting coefficients must be renormalized to satisfy (7). We have not had much experience with this approach. Some preliminary experiments encountered difficulties possibly related to the fact that $\lambda$ is chosen so that the particular solutions $p_\nu(r,\theta;\lambda)$ do not form a Chebyshev system on the boundary. Further investigation is planned.

4. Experiments with a rhombus. The least squares method described above was tested by taking G to be a rhombus with sides of length $\pi$ and obtuse interior angle $\beta$ for various values of $\beta$. This region was chosen for several reasons. First, the corners in the region have a direct effect on the accuracy of the method. Second, the rhombus has been used by Stadter to illustrate the method of intermediate problems and we wish to compare the two methods. Third, we wish to extend Stadter's tabulations to include eigenvalues of all symmetry classes.

Since we are not interested in just the rhombus itself, we have avoided using any of its special properties. It is possible to use our computer program to bound the eigenvalues and eigenf'unctions of any other star-shaped symmetric domain by "just changing one card".

Unless $\beta$ is a submultiple of $180^\circ$, some high order derivatives of the eigenf'unctions will be unbounded near the corners of this domain. However, the particular solutions and hence our approximating eigenfunctions have bounded derivatives of all orders. Consequently, we can expect slow convergence of the approximations and will have to take many terms in the linear combinations to get reasonable accuracy.

In [1] an L -shaped domain with one reentrant corner was studied using particular solutions of fractional order to match the boundary condition and derivative singularities at the corner. Upper and lower bounds which agreed to better than eight significant figures were obtained rather easily. We avoided such an approach with the rhombus because it becomes too special when more than one "bad" corner is involved and because we were interested in the effect of the singularities on convergence.

Upper and lower bounds for the first five eigenvalues of six different rhombuses are given in Table 1. (The approximation $\lambda_*$ may be easily recomputed from the table using $\lambda_* = a - d^2/a$ where a and d are respectively the average and half the difference of the given upper and lower bounds.) The first five eigenvalues of the corresponding square, that is $\beta = 90^\circ$ , are 2, 5, 5, 8 and 10 .

If the rhombus is oriented as in Figure 1, then the first five eigenfunctions have the following qualitative properties. With respect to the x -axis, $u_1$ , $u_2$ , and $u_4$ are symmetric, $u_3$ and $u_5$ are antisymmetric. With respect to the y -axis, $u_1$ , $u_3$ , and $u_4$ are symmetric, $u_2$ and $u_5$ are antisymmetric. Only $u_4$ has curved nodal lines; they are sketched in the figure and they approach the lines $y = \pm x$ as $\beta$ approaches $90^\circ$ . The nodal lines of $u_2$ , $u_3$ and $u_5$ are the y -axis, the x -axis and both axes, respectively, Because of the symmetries, the particular solutions used from (3) were those involving only even cosines for $u_1$ and $u_4$ , odd cosines for $u_2$ , odd sines for $u_3$ and even sines for $u_5$ .

For all the values tabulated, 40 boundary points and 20 terms in the series were used. The number of boundary points and their distribution did not have a marked effect on the accuracy, although it was found helpful to space the points more closely together near the corners.

As $\beta$ varies, the effect of the corners upon accuracy can be seen immediately from the values of $\epsilon$ given in Table 2. In general, as the angle at a corner increases, the severity of the singularity also increases (see [7]) and consequently the accuracy for a fixed number of terms will decrease. This is observed for $k = 1$, 3 and 4 where $\epsilon$ increases as $\beta$ increases. In these three cases, the second derivatives of $u_k$ are unbounded near the obtuse corner.

For $k = 2$, the nodal line bisects the obtuse angle and hence all the angles are effectively acute. The second derivatives are now bounded but the third derivatives are unbounded. The largest angle is $180^\circ-\beta$, which decreases as $\beta$ increases. The net effect is significantly greater accuracy for $k = 2$ than for $k = 1$, 3 or 4 and decreasing $\epsilon$ with increasing $\beta$.

For $k = 5$, the nodal lines bisect both angles and all angles are effectively less than $60^\circ$. The third derivatives are bounded while the fourth derivatives are not. The accuracy is greater than even $k = 2$, but its dependence upon $\beta$ is complicated, apparently by the presence of two comparable angles.

A special situation occurs with $\beta = 120^\circ$ and $k = 2$ or 5. The eigenfunctions $u_2$ and $u_5$ are then also eigenfunctions of equilateral and $30\text{-}60\text{-}90^\circ$ triangles respectively. It can be shown that such eigenfunctions are analytic. We can actually obtain several decimal places of accuracy with only a few terms.

The canputations were done on an IBM 360/67 using long form arithmetic (roughly 16 significant decimal digits). Each 40-by-20 case took about 20 seconds. Some 20-by-10 cases were also tried; they each took 2 or 3 seconds. A Fortran version of the Algol procedure in [6] was used for the singular value decompositions. The one-dimensional minimizations were done using repeated quadratic interpolation.

5. Comparison with the method of intermediate problems. The method of intermediate problems, introduced by A. Weinstein and extended by N. Aronszajn, is the basis for several techniques for computing bounds for the eigenvalues of certain semibounded, self-adjoint operators on Hilbert space. As the survey articles [8] and [9] indicate, the method has both a rich theoretical background and important applications to many problems in physics and engineering. One of the techniques, the so-called B*B method of N. Bazley and D. Fox, has been used by Stadter [3] to bound the eigenvalues of Laplace's operator on a rhombus.

Stadter chooses to consider only eigenfunctions which are symmetric with respect to both axes, although he could easily handle others. Consequently, his $\lambda_1$, $\lambda_2$, $\lambda_3$, ... $\lambda_1$, $\lambda_4$, $\lambda_6$, . . . . He tabulates results corresponding to our $\beta = 105^\circ, 120^\circ, \ldots, 165^\circ$. Hence our tables overlap in the following four places:

| | Our bounds | | Difference | Stadter's bounds | | Difference |
|---|---|---|---|---|---|---|
| $\lambda_1(105^\circ)$ | 2.1138 | 2.1150 | .0012 | 2.1137 | 2.1163 | .0016 |
| $\lambda_1(120^\circ)$ | 2.5192 | 2.5261 | .0069 | 2.5210 | 2.5307 | .0097 |
| $\lambda_4(105^\circ)$ | 8.0043 | 8.0133 | .0090 | 7.9960 | 8.0286 | .0326 |
| $\lambda_4(120^\circ)$ | 8.4751 | 8.5100 | .0349 | 8.4807 | 8.5365 | .0558 |

We see that the accuracies of the two methods are comparable for this particular problem. Our bounds are somewhat tighter, but Stadter's parameter which roughly corresponds to our n was only 15, versus our 20. With our n also set to 15 , we obtain accuracies very similar to Stadter's.

It is also interesting to note that the center of Stadter's intervals are close to the upper ends of our intervals. This, combined with the fact that our $\lambda_*$ 's are probably much more accurate approximations than the bounds indicate, leads us to suspect that Stadter's lower bounds may be much closer to the actual eigenvalues than his upper bounds.

Our method also produces approximate eigenfunctions and bounds on their accuracy. The method of intermediate problems does not do this.

In a sense, this domain leads to a very easy test of the method of intermediate problems because a rhombus can be mapped onto a square by a simple affine coordinate transformation. The resulting eigenvalue problem on the square provides a very natural application of the method. However, with other domains for which the transformation is more complicated, or unknown, the application becomes more difficult or impossible. For example, we do not see how to apply the method to the L-shaped domain in [1]. On the other hand, our method has the advantage that it can be applied directly to any other domain.Apparently the accuracy of both methods -is affected by singularities at the corners.

It should be pointed out that, although the theoretical basis of our method is quite general [2], it has so far been applied only to the

"fixed, homogeneous vibrating membrane" problem (1)-(2). The method of intermediate problems has been successfully applied to a number of other differential equation eigenvalue problems.

In summary, for the specific problem of Laplace's operator on a rhombus the two methods give comparable results. For Laplace's operator on other domains, especially if eigenf'unctions are also desired, our method is to be preferred because it can be applied with no change. For certain other types of eigenvalue problems involving other operators, the method of intermediate problems may be applicable where ours is not.

6. Acknowledgements. Part of this work was done during a visit to the Computer Science Department of Stanford University at the invitation of Professor George Forsythe and under a grant from the Office of Naval Research. Professor Gene Golub kindly supplied Dr. Peter Businger's Fortran version of his Algol singular values procedure [6]. Drs. R. J. Hanson and C. L. Lawson also supplied a Fortran version of [6] which produced essentially the same results, although it used a different shift strategy in the Q,R algorithm. Lyle Smith carried out the preliminary experiments-with (13).

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| | β 95° | 100° | 105° | 110° | 115° | 120° |
|---|---|---|---|---|---|---|
| k | 2.01218 | 2.04947 | 2.11389 | 2.20923 | 2.34135 | 2.51921 |
| l | 2.01248 | 2.04992 | 2.11494 | 2.21134 | 2.34527 | 2.52606 |
| 2 | 4.90375 | 4.86522 | 4.88407 | 4.96317 | 5.10907 | 5.33333 |
| | 4.90403 | 4.86550 | 4.88424 | 4.96325 | 5.10916 | 5.33334 |
| 3 | 5.15659 | 5.38023 | 5.68125 | 6.07504 | 6.58418 | 7.24150 |
| | 5.15750 | 5.38324 | 5.68840 | 6.08970 | 6.61170 | 7.29028 |
| 4 | 7.99206 | 7.98392 | 8.00439 | 8.07944 | 8.23001 | 8.47510 |
| | 7 . | 7.98866 | 8.01321 | 8.09402 | 8.25296 | 8.50997 |
| 5 | 10.0574 | 10.2334 | 10.5372 | 10. 9864 | 11.6080 | 12.4444 |
| | 10.0578 | 10.2337 | 10.5375 | 10. 9866 | 11.6086 | 12.4445 |

Table 1

Bounds for eigenvalues of rhombus

| | β 95° | 100° | 105° | 110° | 115° | 120° |
|---|---|---|---|---|---|---|
| k | | | | | | |
| l | .071 | .107 | .246 | ● 475 | .834 | 1.36 |
| 2 | .028 | .027 | .017 | ● ♦ | [illegible] | <.001 |
| 3 | .088 | .279 | .627 | 1.21 | 2.09 | 3.36 |
| 4 | .117 | .296 | ● 550 | .900 | [illegible] | 2.05 |
| 5 | .018 | .009 | .006 | .008 | .021 | <.001 |

Table 2

Values of $\epsilon \cdot 10^3$

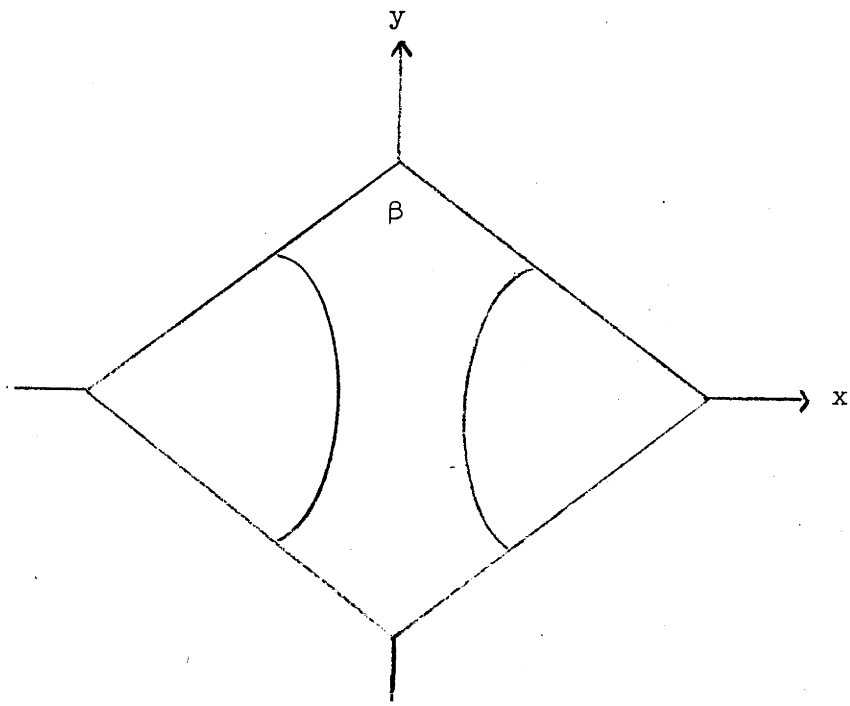


Figure 1

Nodal lines of $u_4$ , $\beta = 105^{\circ}$