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Error Bounds in the Rayleigh-Ritz Approximation of Eigenvectors

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The difference between any eigenvector u_p of a linear operator A and its Rayleigh-Ritz approximation w_p is bounded in terms of the differences between the eigenvalues λ_i of A and their Rayleigh-Ritz upper bounds κ_i. The bound for the difference between u_p and w_p approaches zero with $\kappa_p-\lambda_p$.

1. Introduction

The most common method of approximating the eigenvalues $\lambda_1\leq\lambda_2\leq \ldots$ of a symmetric linear operator A is the Rayleigh-Ritz method [1,5,19].[1] This reduces an eigenvalue problem on a space of a large or even infinite number of dimensions to an eigenvalue problem on a space of relatively few dimensions.

If the desired eigenvalues λ_i are characterized as minima, the Rayleigh-Ritz approximations κ_i give upper bounds for them.

Along with the upper bounds κ_i for the eigenvalues the Rayleigh-Ritz method yields associated vectors w_i. It is to be expected that these vectors approximate the eigenvectors of A in some sense. Furthermore, it is to be expected that the better the eigenvalue λ_i is approximated by κ_i, the better will be the approximation of w_i to the corresponding eigenvector.

Indeed, this is easily seen in the case of the first eigenvector. If the unit vector w_1 is expanded in terms of the normalized eigenvectors u_i of A, we have

$$w_1=\sum a_i u_i, \tag{1.1}$$

$$\sum a_i^2=1, \tag{1.2}$$

and

$$\sum \lambda_i a_i^2=\kappa_1. \tag{1.3}$$

Subtracting λ_1 times (1.2) from (1.3) and noting that $\lambda_2\leq\lambda_3\leq \ldots$ we find that

$$a_1^2\geq\frac{\lambda_2-\kappa_1}{\lambda_2-\lambda_1} \tag{1.4}$$

or equivalently

$$\left[1-\frac{1}{2}(w_1-u_1,w_1-u_1)\right]^2\geq 1-\frac{\kappa_1-\lambda_1}{\lambda_2-\lambda_1}. \tag{1.5}$$

In general the λ_i are unknown, and we must express our results in terms of the κ_i and any lower bounds $\bar{\lambda}_i$ for the λ_i that may be available. Such bounds can be obtained by various methods (see for example [1,2,3,4,5,6,10,11,12,13,14,19,20,21,22,23,24,25,26]).

If $\lambda_i\geq\bar{\lambda}_i$, the inequality (1.5) leads to

$$\left[1-\frac{1}{2}(w_1-u_1,w_1-u_1)\right]^2\geq 1-\frac{\kappa_1-\bar{\lambda}_1}{\bar{\lambda}_2-\bar{\lambda}_1}. \tag{1.6}$$

This inequality shows that if the maximum error $\kappa_1-\bar{\lambda}_1$ is small compared with the interval $\bar{\lambda}_2-\bar{\lambda}_1$, the difference w_1-u_1 is small in norm. The bound (1.6) is sharp in the sense that equality is attained when $\lambda_i=\bar{\lambda}_i$ and $a_i=0$ for $i>2$. The inequality (1.6) is trivial for $\kappa_1\geq\bar{\lambda}_2$.

In this paper we generalize the bound (1.6). We give a bound for the norm of w_p-u_p in terms of the given bounds κ_i and $\bar{\lambda}_i$. This bound is again sharp in the sense that equality may be attained. The bound for (w_p-u_p,w_p-u_p) is small if the maximum error $\kappa_p-\bar{\lambda}_p$ is small relative to both $\bar{\lambda}_{p+1}-\kappa_p$ and $\bar{\lambda}_p-\kappa_{p-1}$. It becomes trivial if $\kappa_p\geq\bar{\lambda}_{p+1}$ or $\kappa_{p-1}\geq\bar{\lambda}_p$. The case $p=1$ gives an improved but more complicated version of (1.6).

If λ_p is multiple eigenvalue, we can only expect w_p to approximate one of the associated eigenvectors. Hence if λ_p lies near to several other eigenvalues we must expect w_p to approximate not u_p but a linear combination of the eigenvectors corresponding to the nearby eigenvalues. This approximation is established in section 3.

It is possible to find a bound for (w_p-u_p,w_p-u_p) by determining to what extent w_p satisfies the eigenvalue equation. Such bounds, which involve $(Aw_p-\kappa_p w_p,Aw_p-\kappa_p w_p)$ have been found by several authors [12, 20, 23]. Our bound, however, involves only the κ_i and the lower bounds $\bar{\lambda}_i$. It should be particularly useful in the case of differential operators where the Rayleigh-Ritz trial functions may not be sufficiently differentiable to give a finite value of (Aw_p,Aw_p). Our bounds are established by algebraic means for the case when A is an $N\times N$ matrix. They are independent of N. Consequent-

[1] Figures in brackets indicate the literature references at the end of this paper.

ly, the bounds also hold for infinite-dimensional operators A whose first p eigenvalues and eigenvectors are approximated uniformly by those of a sequence A_N of $N \times N$ matrices. This is certainly the case if A is completely continuous. It also holds under the weaker condition that A have p discrete eigenvalues defined by a minimum maximum principle. These must lie below any continuous spectrum. Thus A may be a Schroedinger operator corresponding to both bound and unbound states.

The fact that the eigenvalues λ_i are stationary values of the Rayleigh quotient tends to make the approximation of the eigenvectors worse than that of the eigenvalues. In fact, the bound (2.41) shows that the square of the norm of the error $w_p - u_p$ is of the order $\kappa_p - \bar{\lambda}_p$.

The error bounds in sections 2 and 3 are in the sense of the norm. If A is a differential operator, its eigenvectors u_i are functions. It is often of interest to approximate the value of the function at a particular point. An adaptation of the method of Diaz and Greenberg [7, 9] which leads to such a pointwise approximation is presented in section 4.

2. Separated Eigenvalues

Let A be an hermitian $N \times N$ matrix. It is a linear operator on Euclidean N-space. Let the usual scalar product between two vectors u and v on this space be denoted by (u,v).

Let the eigenvalues of A be $\lambda_1 \leq \lambda_2 \leq \ldots \leq \lambda_N$. The corresponding eigenvectors are denoted by $u_1, \ldots, u_N$ so that the equations

$$Au_i = \lambda_i u_i \qquad i=1, \ldots, N \tag{2.1}$$

are satisfied. The u_i are normalized so that

$$(u_i, u_j) = \delta_{ij} \qquad i,j=1, \ldots, N. \tag{2.2}$$

Then (2.1) implies

$$(Au_i, u_j) = \lambda_i \delta_{ij} \qquad i,j=1, \ldots, N. \tag{2.3}$$

We suppose that the Rayleigh-Ritz method [1, 5, 19] is applied to find upper bounds

$$\kappa_\alpha \geq \lambda_\alpha \qquad \alpha=1, \ldots, M \tag{2.4}$$

for the first $M < N$ eigenvalues of A. This is done by choosing M linearly independent vectors $v_1, \ldots, v_M$ and finding the roots $\kappa_1 \leq \kappa_2 \leq \ldots \leq \kappa_M$ of the secular equation

$$\det [(Av_\alpha, v_\beta) - \kappa (v_\alpha, v_\beta)] = 0 \qquad \alpha,\beta=1, \ldots, M. \tag{2.5}$$

Associated with each of the κ_α is a linear combination

$$w_\alpha = \sum_{\beta=1}^{M} C_\alpha^\beta v_\beta \tag{2.6}$$

of unit length such that the M linear equations

$$(Aw_\alpha, v_\beta) = \kappa_\alpha (w_\alpha, v_\beta) \qquad \beta=1, \ldots, M. \tag{2.7}$$

are satisfied. Then

$$(w_\alpha, w_\beta) = \delta_{\alpha\beta} \tag{2.8}$$

and

$$(Aw_\alpha, w_\beta) = \kappa_\alpha \delta_{\alpha\beta} \qquad \alpha,\beta=1, \ldots, M. \tag{2.9}$$

We assume that in addition to the upper bounds κ_α we have determined some lower bounds $\bar{\lambda}_i$ such that

$$\lambda_i \geq \bar{\lambda}_i \qquad i=1, \ldots, N. \tag{2.10}$$

This means that we have at least some idea of the degree of approximation of the κ_α to the eigenvalues λ_α

We seek to determine from this degree of approximation of the κ_α to the eigenvalues the degree of approximation of a particular Rayleigh-Ritz eigenvector w_p to the eigenvector u_p of A.

We assume that $\lambda_{p-1} < \lambda_p < \lambda_{p+1}$ and that the bounds κ_{p-1}, κ_p, $\bar{\lambda}_p$, and $\bar{\lambda}_{p+1}$ are sufficiently good that

$$\kappa_p < \bar{\lambda}_{p+1} \tag{2.11}$$

and

$$\kappa_{p-1} < \bar{\lambda}_p. \tag{2.12}$$

Our problem is the following: Given the M vectors $w_1, \ldots, w_M$ satisfying (2.8), find the largest value of the deviation $(w_p - u_p, w_p - u_p)$ of w_p from the pth normalized eigenvector of any matrix A satisfying the eq (2.9) and having eigenvalues λ_i satisfying (2.10).

If the eigenvalues λ_i of A are given, A is completely specified by prescribing its normalized eigenvectors. These eigenvectors $u_1, \ldots, u_N$ form a basis, so that the w_α can be written as linear combinations of them. Let

$$w_\alpha = \sum_{i=1}^{N} a_\alpha^i u_i \qquad \alpha=1, \ldots, M. \tag{2.13}$$

Since the u_i satisfy (2.2) and (2.3), the eqs (2.8) and (2.9) become

$$\sum_{i=1}^{N} a_\alpha^i a_\beta^i = \delta_{\alpha\beta} \tag{2.14}$$

and

$$\sum_{i=1}^{N} \lambda_i a_\alpha^i a_\beta^i = \kappa_\alpha \delta_{\alpha\beta} \qquad \alpha,\beta=1, \ldots, M. \tag{2.15}$$

On the other hand,

$$(w_p - u_p, w_p - u_p) = 2(1 - a_p^p). \tag{2.16}$$

If u_p satisfies (2.2) and (2.3), so does $-u_p$. We choose the sign to make a_p^p non-negative. Thus, our problem of maximizing $(w_p - u_p, w_p - u_p)$ is reduced to that of minimizing $(a_p^p)^2$ under the constraints (2.14), (2.15), and (2.10).

We first keep the eigenvalues λ_i fixed and unequal. If a_α^i is the minimizing set of coefficients, we find by direct differentiation that the equations

$$a_p^p\delta_{ip}\delta_{\alpha p}+\sum_{\beta=1}^{M}(r_{\alpha\beta}+\lambda_i s_{\alpha\beta})a_\beta^i=0 \qquad i=1,\ldots,N \quad \alpha=1,\ldots,M \tag{2.17}$$

must be satisfied. The $r_{\alpha\beta}$ and $s_{\alpha\beta}$ are Lagrange multipliers, and are symmetric:

$$r_{\alpha\beta}=r_{\beta\alpha}, \qquad s_{\alpha\beta}=s_{\beta\alpha}. \tag{2.18}$$

To solve the eq (2.17), we multiply by a_γ^i and sum with respect to i. Using (2.14) and (2.15) we find that

$$a_p^pa_\gamma^p\delta_{\alpha p}+r_{\alpha\gamma}+\kappa_\gamma s_{\alpha\gamma}=0. \tag{2.19}$$

Interchanging α and γ and using (2.18), we find

$$r_{\alpha\gamma}=-(\kappa_\alpha-\kappa_\gamma)^{-1}\kappa_pa_p^p[a_\gamma^p\delta_{\alpha p}-a_\alpha^p\delta_{\gamma p}],$$

$$s_{\alpha\gamma}=(\kappa_\alpha-\kappa_\gamma)^{-1}a_p^p[a_\gamma^p\delta_{\alpha p}-a_\alpha^p\delta_{\gamma p}] \qquad \alpha\neq\gamma. \tag{2.20}$$

In particular, $r_{\alpha\gamma}$ and $s_{\alpha\gamma}$ vanish unless $\alpha=\gamma$ or either α or γ is p.

Letting $\alpha=\gamma$ in (2.19), we find

$$r_{\alpha\alpha}+\kappa_\alpha s_{\alpha\alpha}=-(a_p^p)^2\delta_{\alpha p}. \tag{2.21}$$

We substitute (2.20) and (2.21) in (2.17) to obtain

$$(\kappa_p-\kappa_\alpha)(\lambda_i-\kappa_\alpha)s_{\alpha\alpha}a_\alpha^i+(\lambda_i-\kappa_p)a_p^pa_\alpha^pa_p^i=0 \qquad \alpha\neq p \tag{2.22}$$

and

$$a_p^p\delta_{ip}+[(\lambda_i-\kappa_p)s_{pp}-(a_p^p)^2]a_p^i-\sum_{\beta\neq p}\frac{\lambda_i-\kappa_p}{\kappa_\beta-\kappa_p}a_p^pa_\beta^pa_\beta^i=0, \qquad i=1,\ldots,N. \tag{2.23}$$

If the value $a_p^p=0$ is compatible with the constraints (2.14) and (2.15), the minimum value of $(a_p^p)^2$ is clearly zero. We suppose for the moment that this is not the case, so that

$$a_p^p\neq 0. \tag{2.24}$$

Then we can solve (2.23) with $i=p$ for s_{pp} in terms of the a_β^p. We can also eliminate $s_{\alpha\alpha}$ between (2.22) with $i=p$ and any other value of i to obtain

$$a_p^pa_\beta^pa_\beta^i=\frac{(\lambda_i-\kappa_p)(\lambda_p-\kappa_\beta)}{(\lambda_p-\kappa_p)(\lambda_i-\kappa_\beta)}a_p^i(a_\beta^p)^2. \tag{2.25}$$

Substituting this and the value of s_{pp} in (2.23) we obtain

$$a_p^i\left\{\frac{\lambda_i-\kappa_p}{\lambda_p-\kappa_p}\left[1-\sum_{\beta=1}^{M}(a_\beta^p)^2+\sum_{\beta=1}^{M}\frac{\lambda_p-\kappa_\beta}{\lambda_i-\kappa_\beta}(a_\beta^p)^2\right]\right\}=0, \qquad i\neq p. \tag{2.26}$$

Suppose now that exactly L of the coefficients a_β^p are nonzero:

$$a_\beta^p\neq 0 \quad \text{for} \quad \beta=\beta_1,\beta_2,\ldots,\beta_L \qquad \beta_1<\beta_2<\ldots<\beta_L. \tag{2.27}$$

By (2.24) one of the $\beta_\nu=p$. The term in braces in (2.26) times the product of the $(\lambda_i-\kappa_{\beta_\nu})$ with $\beta_\nu\neq p$ is a polynomial of degree L in λ_i. Hence it vanishes for at most L values of i. Consequently, $a_p^i\neq 0$ for $\bar{L}\leq L$ values of $i\neq p$.

From (2.22) it follows that $a_p^i=0$ implies $s_{\alpha\alpha}a_\alpha^i=0$ for all α. But $s_{\alpha\alpha}=0$ implies $a_\alpha^p=0$. Hence $a_p^i=0$ implies $a_{\beta_\nu}^i=0$. Thus our vectors w_α split into two subsets: The subset S_1 consists of L orthonormal vectors $w_{\beta_1},\ldots,w_{\beta_L}$ (including w_p) having only components in the $\bar{L}+1$ directions $u_{i_1},\ldots,u_{i_{\bar{L}+1}}$. The subset S_2 consists of $M-\bar{L}-1$ vectors orthogonal to u_p.

It follows that $\bar{L}$ must be either L or $L-1$. In the latter case, the L vectors w_{β_ν} in the first set will be the eigenvectors $u_{i_1},\ldots,u_{i_L}$ themselves. In particular, w_p is u_p so that the corresponding maximum of (w_p-u_p,w_p-u_p) is zero. This occurs if and only if $\kappa_p=\lambda_p$. The more interesting case is that in which

$$\bar{L}=L. \tag{2.28}$$

The term in the braces in (2.26) vanishes for $i=i_1,i_2,\ldots,i_{L+1}(i_1<i_2<\ldots<i_{L+1})$ except when $i_\nu=p$. This represents a set of L linear equations in the L unknowns $(a_{\beta_1}^p)^2\ldots,(a_{\beta_L}^p)^2$. It can be solved explicitly to yield

$$(a_{\beta_\mu}^p)^2=\prod_{\substack{\nu=1\\ \nu\neq\mu}}^{L}\frac{\lambda_p-\kappa_{\beta_\nu}}{\kappa_{\beta_\mu}-\kappa_{\beta_\nu}}\prod_{\substack{\tau=1\\ i_\tau\neq p}}^{L+1}\frac{\kappa_{\beta_\mu}-\lambda_{i_\tau}}{\lambda_p-\lambda_{i_\tau}} \tag{2.29}$$

(This result can be checked by the Lagrange interpolation formula [17]. A similar solution of a closely related equation was given by K. Loewner, Math. Z. *38*, 180–181 (1934).)

We now let $\beta=\beta_\mu$ in (2.25), multiply by a_p^i, and sum. By (2.14) we have

$$\sum_{i_\tau\neq p}\frac{\lambda_{i_\tau}-\kappa_p}{\lambda_{i_\tau}-\kappa_{\beta_\mu}}(a_p^{i_\tau})^2+\frac{\lambda_p-\kappa_p}{\lambda_p-\kappa_{\beta_\mu}}(a_p^p)^2=\delta_{p\beta_\mu} \qquad \mu=1,\ldots,L. \tag{2.30}$$

Again, we can solve explicitly for the L unknowns $(a_p^{i_\tau})^2, i_\tau\neq p$. Using (2.25) and (2.29), we find that

$$(a_{\beta_\mu}^{i_\tau})^2=\prod_{\substack{\nu=1\\ \nu\neq\mu}}^{L}\frac{\lambda_{i_\sigma}-\kappa_{\beta_\nu}}{\kappa_{\beta_\mu}-\kappa_{\beta_\nu}}\prod_{\substack{\tau=1\\ \tau\neq\sigma}}^{L+1}\frac{\kappa_{\beta_\mu}-\lambda_{i_\tau}}{\lambda_{i_\sigma}-\lambda_{i_\tau}} \tag{2.31}$$

The solution (2.31) formally satisfies the conditions (2.14), (2.15), and (2.17). (The square roots must be chosen so that $a\,\beta_{\beta_\mu}^{i_\sigma}$ is $(\lambda_{i_\sigma}-\kappa_{\beta_\mu})^{-1}$ times a function of i_σ only times a function of β_ν only.) In order to be admissible, the coefficients must be real. It is easily seen that this is the case if and only if

$$\lambda_{i_1}<\kappa_{\beta_1}<\lambda_{i_2}< \ . \ . \ . \ <\kappa_{\beta_L}<\lambda_{i_{L+1}}. \tag{2.32}$$

The vectors w_β in the subset S_2 are orthogonal to $w_{\beta_1}, \ldots, w_{\beta_L}$ and u_p. It follows from (2.31) that they are orthogonal to $u_{i_1}, \ldots, u_{i_{L+1}}$. This is possible if and only if to each i with $i\neq i_1, \ldots, i_{L+1}$ there corresponds a separate κ_β with $\beta\neq\beta_1, \ldots, \beta_L$ such that $\kappa_\beta\geq\lambda_i$.

We now consider the possible minima of $(a_p^p)^2$. Choosing a particular set of β_ν and i_σ, we find from (2.31) that

$$(a_p^p)^2=\prod_{\beta_\nu\neq p}\frac{\lambda_p-\kappa_{\beta_\nu}}{\kappa_p-\kappa_{\beta_\nu}}\prod_{i_\tau\neq p}\frac{\kappa_p-\lambda_{i_\tau}}{\lambda_p-\lambda_{i_\tau}} \tag{2.33}$$

Because of (2.32)

$$\frac{(\lambda_p-\kappa_{\beta_\nu})(\kappa_p-\lambda_{i_\nu})}{(\kappa_p-\kappa_{\beta_\nu})(\lambda_p-\lambda_{i_\nu})}=1-\frac{(\kappa_p-\lambda_p)(\kappa_{\beta_\nu}-\lambda_{i_\nu})}{(\kappa_p-\kappa_{\beta_\nu})(\lambda_p-\lambda_{i_\nu})}<1 \tag{2.34}$$

for $i_\nu>p$ or $\beta_\nu<p$.

Thus, the right-hand side of (2.33) is increased by dropping any pair λ_{i_ν}, κ_{β_ν}. This means that its minimum will be attained when the sets $i_1, \ldots, i_{L+1}, \beta_1, \ldots, \beta_L$ are maximal with respect to the properties required of them. We further note that the right-hand side of (2.33) is an increasing function of λ_{i_τ} for $i_\tau\neq p$ and a decreasing function of κ_{β_ν} for $\beta_\nu\neq p$.

Keeping these facts in mind, we construct the sets $i_1, \ldots, i_{L+1}, \beta_1, \ldots, \beta_L$ which minimize $(a_p^p)^2$ for fixed unequal λ_i as follows.

Let

$$i_1=1. \tag{2.35}$$

Let

$$i_2=\min\{i|\exists\beta\ni\lambda_1<\kappa_\beta<\lambda_i\}. \tag{2.36}$$

Let

$$\beta_1=\max\{\beta|\kappa_\beta<\lambda_{i_2}\}. \tag{2.37}$$

Then inductively, let

$$i_{\nu+1}=\min\{i|\exists\kappa_\beta\ni\lambda_{i_\nu}<\kappa_\beta<\lambda_i\}, \tag{2.38}$$

$$\beta_\nu=\max\{\beta|\kappa_\beta<\lambda_{i_{\nu+1}}\}.$$

Because of (2.11) the set of β_ν includes p. If p is not included in the i_σ, we can easily construct a solution of the eqs (2.14) and (2.15) with $a_p^p=0$. To do this we define the $(a_{\beta_\mu}^{i_\sigma})^2$ by (2.31). Then $a_p^p=(w_p,u_p)=0$.

Conversely, if (2.24) is violated so that the minimum of $(a_p^p)^2$ is zero, we can consider the problem of minimizing a coefficient $(a_p^q)^2$ with $q<p$ under the constraints (2.14), (2.15), and $a_p^i=0$ for some set of $i<p$ including p. Since $\kappa_p<\lambda_{p+1}$, not all the a_p^q can vanish. Therefore this minimum problem will have a non-zero solution for some q and some set of $i\leq p$. The minimizing conditions again lead to the determination of sets i_σ and β_ν by (2.35), (2.36), (2.37), and (2.38). The integer p is included in the β_ν but not in the i_σ.

Thus, $a_p^p\neq0$ if and only if p is one of the i_σ. It follows from the construction of the i_σ that this will be the case if and only if there is a κ_β such that $\lambda_{p-1}<\kappa_\beta<\lambda_p$. This is assured by (2.12) for any λ_i satisfying (2.10). Condition (2.12) is therefore necessary and sufficient for $(a_p^p)^2$ to have a nonzero minimum.

The minimum value of $(a_p^p)_2$ is now given by (2.33). It is a continuous nondecreasing function of the eigenvalues λ_i. Hence its minimum with respect to the λ_i satisfying (2.10) will occur for $\lambda_i=\bar{\lambda}_i$. We may remove the assumption that the λ_i are unequal by a limiting process. This will alter the inequalities in (2.37) and (2.38) slightly.

As we pointed out in the introduction, we can replace the matrix A by a symmetric operator on a Hilbert space. We need only assume that A has at least p discrete eigenvalues defined by a minimum maximum principle [1,5,19]. For then the first N eigenvalues of A and their corresponding eigenvectors are uniformly approximated by those of an $N'\times N'$ matrix $A_{N'}$ for N' sufficiently large. If $\bar{\lambda}_i$ $i=1, \ldots, N$ are lower bounds for the first N eigenvalues of A, there is an $\epsilon_{N'}$ which goes to zero as $N'\to\infty$ such that $\bar{\lambda}_i-\epsilon_{N'}$ are lower bounds for the first N eigenvalues of $A_{N'}$. Also, $\bar{\lambda}_N-\epsilon_{N'}$ is a lower bound for the higher eigenvalues of $A_{N'}$. We let $N'\to\infty$ for fixed M and N. Using (2.33) and (2.34), we obtain the following theorem.

THEOREM 1. *Let $\kappa_1\leq\kappa_2\leq \ldots \leq\kappa_M$ be the Rayleigh-Ritz upper bounds for the first* M *of the eigenvalues $\lambda_1\leq\lambda_2\leq \ldots$ of a symmetric linear operator A. Let $\bar{\lambda}_1\leq \ldots \leq\bar{\lambda}_N$ be lower bounds for the first N eigenvalues of A, $N\geq M$.*

Let

$$\kappa_{p-1}<\bar{\lambda}_p<\kappa_p<\bar{\lambda}_{p+1}. \tag{2.39}$$

Define the numbers
$i_1<i_2< \ldots <i_{L+1}$, $\beta_1<\beta_2< \ldots <\beta_L$ by

$$i_1=1$$

$$i_2=\min\{i|\bar{\lambda}_i>\kappa_1\}$$

$$\beta_1=\max\{\beta|\kappa_\beta\leq\bar{\lambda}_{i_2}\}$$

$$i_{\nu+1}=\min\{i|\exists\beta\ni\bar{\lambda}_{i_\nu}<\kappa_\beta<\bar{\lambda}_i\}$$

$$\beta_\nu=\max\{\beta|\kappa_\beta\leq\bar{\lambda}_{i_{\nu+1}}\} \tag{2.40}$$

Then if w_p is the normalized Rayleigh-Ritz eigenvector corresponding to the bound κ_p and u_p is the normalized eigenvector of A corresponding to the eigenvalue λ_p,

$$\left[1-\frac{1}{2}(w_p-u_p, w_p-u_p)\right]^2 \geq\left\{1-\frac{\kappa_p-\bar{\lambda}_p}{\bar{\lambda}_{i_{L+1}}-\bar{\lambda}_p}\right\}\prod_{\substack{\nu=1\\ \beta_\nu\neq p}}^{L}\left\{1-\frac{(\kappa_p-\bar{\lambda}_p)(\kappa_{\beta_\nu}-\bar{\lambda}_{i_\nu})}{(\kappa_p-\kappa_{\beta_\nu})(\bar{\lambda}_p-\bar{\lambda}_{i_\nu})}\right\} \tag{2.41}$$

The right-hand side of this inequality approaches zero if either κ_p approaches $\bar{\lambda}_{p+1}$ or κ_{p-1} approaches $\bar{\lambda}_p$. It is near one if the error $\kappa_p-\bar{\lambda}_p$ is small relative to the approximate spacing $\bar{\lambda}_{i_{L+1}}-\bar{\lambda}_p$ and if the products of errors $(\kappa_p-\bar{\lambda}_p)(\kappa_{\beta_\nu}-\bar{\lambda}_{i_\nu})$ are small relative to the products of approximate spacings $(\kappa_p-\kappa_{\beta_\nu})(\bar{\lambda}_p-\bar{\lambda}_{i_\nu})$.

If lower bounds $\bar{\lambda}_i$ are not given for all the eigenvalues λ_i, we can always use a lower bound for any particular eigenvalue as a lower bound for a higher eigenvalue. In particular, we can let $\bar{\lambda}_i=\bar{\lambda}_{p+1}$ for $i>p$ and $\bar{\lambda}_i=\bar{\lambda}_1$ for $i<p$. If $p>1$, (2.39) requires that $\kappa_{p-1}<\bar{\lambda}_p$. Then $L=2$, $i_1=1$, $\beta_1=p-1$, $i_2=\beta_2=p$, $i_3=p+1$. This leads to the simpler bound

$$\left[1-\frac{1}{2}(w_p-u_p, w_p-u_p)\right]^2 \geq\left\{1-\frac{\kappa_p-\bar{\lambda}_p}{\bar{\lambda}_{p+1}-\bar{\lambda}_p}\right\}\left\{1-\frac{(\kappa_p-\bar{\lambda}_p)(\kappa_{p-1}-\bar{\lambda}_1)}{(\kappa_p-\kappa_{p-1})(\bar{\lambda}_p-\bar{\lambda}_1)}\right\} \tag{2.42}$$

Even though this bound has fewer factors than (2.41), it is, in general, smaller.

For $p=1$ we can take $\bar{\lambda}_i=\bar{\lambda}_2$ for $i\geq2$. Then $L=1$, $i_1=\beta_1=1$, $i_2=2$, and (2.41) reduces to (1.6).

Example. We apply the Rayleigh-Ritz method to the matrix

$$A=\begin{pmatrix}1 & 1 & 0\\ 1 & 3 & 1\\ 0 & 1 & 23\end{pmatrix} \tag{2.43}$$

using trial vectors with vanishing third component. This amounts to finding the eigenvalues and eigenvectors of the 2×2 matrix obtained by striking out the third row and column of A. We obtain

$$\kappa_1=2-\sqrt{2},\ \kappa_2=2+\sqrt{2} \tag{2.44}$$

with the corresponding vectors

$$w_1\sim\left(\frac{1}{2}(2+\sqrt{2})^{1/2},\frac{1}{2}(2-\sqrt{2})^{1/2},0\right)$$

$$w_2\sim\left(\frac{1}{2}(2-\sqrt{2})^{1/2},\frac{1}{2}(2+\sqrt{2})^{1/2},0\right) \tag{2.45}$$

If the first two coordinate directions are replaced by the w_1 and w_2 directions, the matrix A becomes

$$A^*=\begin{pmatrix}\kappa_1 & 0 & -\frac{1}{2}\kappa_1^{1/2}\\ 0 & \kappa_2 & -\frac{1}{2}\kappa_2^{1/2}\\ -\frac{1}{2}\kappa_1^{1/2} & -\frac{1}{2}\kappa_2^{1/2} & 23\end{pmatrix} \tag{2.46}$$

We now obtain lower bounds for the eigenvalues by means of Hadamard's theorem on determinants [16].

$$\bar{\lambda}_1=\kappa_1-\frac{1}{2}\kappa_1^{1/2},$$

$$\bar{\lambda}_2=\kappa_2-\frac{1}{2}\kappa_2^{1/2}. \tag{2.47}$$

For $\bar{\lambda}_3$ we use the fact that the largest eigenvalue must exceed the largest diagonal element. Then

$$\bar{\lambda}_3=23. \tag{2.48}$$

Substituting these values in (2.41) we find that

$$(w_1-u_1, w_1-u_1)\leq0.08025,$$
$$(w_2-u_2, w_2-u_2)\leq0.09980. \tag{2.49}$$

In this problem one can, of course, determine the eigenvalues and the corresponding eigenvectors explicitly. We find that

$$(w_1-u_1, w_1-u_1)=0.000328,$$
$$(w_2-u_2, w_2-u_2)=0.002238. \tag{2.50}$$

Thus, the error bounds (2.49) are a good deal larger than the errors themselves.

Our error bounds depend upon the lower bounds $\bar{\lambda}_i$. These were chosen rather crudely and could be improved in various ways (see, for example [5]). In order to determine the effect of such an improvement, we replace the $\bar{\lambda}_i$ by the eigenvalues λ_i in (2.41). We then obtain the bounds

$$(w_1-u_1, w_1-u_1)\leq0.000330,$$
$$(w_2-u_2, w_2-u_2)\leq0.002243. \tag{2.51}$$

These are very close to the actual values (2.50).

The simpler bound (1.6) gives

$$(w_1-u_1, w_1-u_1)\leq 0.195136 \tag{2.52}$$

if the values (2.47) of $\bar{\lambda}_i$ are used, and

$$(w_1-u_1, w_1-u_1)\leq 0.002364 \tag{2.53}$$

if they are replaced by the λ_i themselves. In both cases we see that the bound (2.41) is significantly better than the simplified bound (1.6).

3. Neighboring Eigenvalues

The condition (2.39) implies that the eigenvalue λ_p is simple. If this is not the case, the corresponding eigenvector u_p is not uniquely defined. In fact, if λ_p has multiplicity m, u_p may be any element of an m-space. If $m>1$, there will always be such a u_p orthogonal to w_p, so that the minimum of (w_p,u_p) is zero.

We must reformulate our problem. We seek the minimum value of $(w_p,u_p)^2$ when u_p is taken to be that element of the m-space which best approximates w_p. This u_p is the projection of w_p into the m-space of eigenvectors corresponding to λ_p.

The condition (2.39) implies not only that λ_p is simple, but that our bounds κ_{p-1}, κ_p, $\bar{\lambda}_p$, and $\bar{\lambda}_{p+1}$ are good enough to reveal its simplicity. That is, the error in our bounds is smaller than the separations between λ_{p-1}, λ_p, and λ_{p+1}. If this is not the case, we cannot distinguish between a simple and a multiple eigenvalue.

Suppose now that the upper and lower bounds for $\lambda_p, \lambda_{p+1}, \ldots, \lambda_{p+m-1}$ show these eigenvalues to lie close together. Suppose further that

$$\kappa_{p-1}, <<\bar{\lambda}_p, \kappa_{p+m-1}<<\bar{\lambda}_{p+m} \tag{3.1}$$

so that λ_{p-1} and λ_{p+m} are known to lie away from the cluster of eigenvalues about λ_p. Then, to our degree of approximation λ_p behaves like an eigenvalue of multiplicity m. We ask how well w_p can be approximated by a linear combination of unit length of the eigenvectors $u_p, u_{p+1}, \ldots, u_{p+m-1}$.

This problem is equivalent to that of minimizing $\sum_p^{p+m-1} (a_p^i)^2$ under the constraints (2.14), (2.15), and (2.10). By (2.20) we have $r_{\alpha\beta}=s_{\alpha\beta}=0$ unless $\alpha=\beta$ or α or $\beta=p$. Moreover, $r_{\alpha p}+\kappa_p s_{\alpha p}=0$, $r_{\alpha\alpha}+\kappa_\alpha s_{\alpha\alpha}=0$ for $\alpha\neq p$. This means that we would obtain the same minimizing conditions by imposing only the constraints (2.14) with $\alpha=\beta$ or α or $\beta=p$ and the single constraint (2.15) with $\alpha=\beta=p$. The latter may even be replaced by the inequality

$$\sum_{i=1}^{N} \lambda_i (a_p^i)^2\leq \kappa_p. \tag{3.2}$$

The other constraints (2.14) and (2.15) determine which local minima actually occur, but the local minima themselves are determined by (2.14) and (3.2).

The same situation applies in the case under consideration here. Necessary conditions for a maximum of $\sum_p^{p+m-1} (a_p^i)^2$ are determined by the constraints (2.14), (2.10), and (3.2).

Let $\tilde{u}_p$ be the unit vector in the direction of the projection of w_p into the space spanned by $u_p, \ldots, u_{p+m-1}$:

$$\tilde{u}_p=\left\{\sum_{i=p}^{p+m-1} (a_p^i)^2\right\}^{-1/2}\sum_p^{p+m-1} a_p^i u_i. \tag{3.3}$$

Let $\tilde{u}_{p+1}, \ldots, \tilde{u}_{p+m-1}$ be other linear combinations of $u_p, \ldots, u_{p+m-1}$ such that $\tilde{u}_p, \ldots, \tilde{u}_{p+m-1}$ are orthonormal. Let $\tilde{u}_i=u_i$ for $i\neq p, \ldots, p+m-1$ and put

$$\tilde{a}_\alpha^i=(w_\alpha, \tilde{u}_i). \tag{3.4}$$

Then by construction

$$\tilde{a}_p^i=0 \qquad i=p+1, \ldots, p+m-1 \tag{3.5}$$

and

$$(\tilde{a}_p^p)^2=\sum_{i=p}^{p+m-1} (a_p^i)^2. \tag{3.6}$$

Moreover,

$$\sum_{i=1}^{N}\lambda_i(a_p^i)^2\geq\sum_1^{p-1}\lambda_i(\tilde{a}_p^i)^2+\lambda_p(\tilde{a}_p^p)^2+\sum_{p+m}^{N}\lambda_i(\tilde{a}_p^i)^2. \tag{3.7}$$

Thus, if we let

$$\tilde{\lambda}_i=\begin{cases}\lambda_p & i=p, \ldots, p+m-1\\ \lambda_i & \text{otherwise.}\end{cases} \tag{3.8}$$

We have from (3.2) and (3.7) that

$$\sum_1^N\tilde{\lambda}_i(\tilde{a}_p^i)^2\leq\kappa_p. \tag{3.9}$$

Since the $\tilde{u}_i$ are orthonormal, (2.14) becomes

$$\sum\tilde{a}_\alpha^i\tilde{a}_\beta^i=\delta_{\alpha\beta}. \tag{3.10}$$

Our problem is thus reduced to minimizing $(\tilde{a}_p^p)^2$ under the constraints (3.10), (3.9), (2.10), and (3.5). The conditions for local minima are found to be as in section 2. However, the constraints (3.5) together with the fact that $\kappa_{p+m-1}<\bar{\lambda}_{p+m}$ relegate the vectors $w_{p+1}, \ldots, w_{p+m-1}$ to the set S_2 orthogonal to $\tilde{u}_p$. Furthermore, the conditions (3.5) eliminate the values $i=p+1, \ldots, p+m-1$ from the i_σ.

Thus we find the following theorem.

Theorem 2. *Let $\kappa_1\leq\kappa_2\leq \ldots \leq\kappa_M$ be the Rayleigh-Ritz upper bounds for the first M eigenvalues $\lambda_1\leq\lambda_2\leq \ldots$ of an hermitian operator A. Let $\bar{\lambda}_1\leq \ldots \leq\bar{\lambda}_N$ be lower bounds for the first $N\geq M$ eigenvalues. For a certain p and m let*

$$\kappa_{p-1} < \bar{\lambda}_p,$$

$$\kappa_{p+m-1} < \bar{\lambda}_{p+m} \tag{3.11}$$

Define the numbers $i_1, i_2, \ldots, i_{L+1}, \beta_1, \ldots, \beta_L$ *by* (2.40) *with* $\bar{\lambda}_{p+1}, \ldots, \bar{\lambda}_{p+m-1}$ *eliminated from the set of* $\bar{\lambda}_i$, *and* $\kappa_{p+1}, \ldots, \kappa_{p+m-1}$ *eliminated from the set of* κ_α.

Let w_p *be the Rayleigh-Ritz eigenvector that gives the bound* κ_p. *Then there exists a linear combination of unit length* $\tilde{u}_p$ *of the eigenvectors* $u_p, \ldots, u_{p+m-1}$ *of* A *such that*

$$\left[1-\frac{1}{2}(w_p-\tilde{u}_p, w_p-\tilde{u}_p)\right]^2 \geq \left\{1-\frac{\kappa_p-\bar{\lambda}_p}{\bar{\lambda}_{i_{L+1}}-\bar{\lambda}_p}\right\}$$

$$\prod_{\substack{\nu=1\\ \beta_\nu\neq p}}^{L}\left\{1-\frac{(\kappa_p-\bar{\lambda}_p)(\kappa_{\beta_\nu}-\bar{\lambda}_{i_\nu})}{(\kappa_p-\kappa_{\beta_\nu})(\bar{\lambda}_p-\bar{\lambda}_{i_\nu})}\right\} \tag{3.12}$$

As in section 2 we obtain a simpler but a weaker inequality by putting $\bar{\lambda}_i=\bar{\lambda}_{p+m}$ for $i>p+m$ and $\bar{\lambda}_i=\bar{\lambda}_1$ for $i<p$ when $p>1$.
This leads to

$$\left[1-\frac{1}{2}(w_p-\tilde{u}_p, w_p-\tilde{u}_p)\right]^2 \geq \left\{1-\frac{\kappa_p-\bar{\lambda}_p}{\bar{\lambda}_{p+m}-\bar{\lambda}_p}\right\}$$

$$\left\{1-\frac{(\kappa_p-\bar{\lambda}_p)(\kappa_{p-1}-\bar{\lambda}_1)}{(\kappa_p-\kappa_{p-1})(\bar{\lambda}_p-\bar{\lambda}_1)}\right\}. \tag{3.13}$$

For $p=1$ we only have to put $\bar{\lambda}_i=\bar{\lambda}_{p+m}$ for $i>p+m$ to obtain

$$\left[1-\frac{1}{2}(w_1-\tilde{u}_1, w_1-\tilde{u}_1)\right]^2 \geq 1-\frac{\kappa_1-\bar{\lambda}_1}{\bar{\lambda}_{m+1}-\bar{\lambda}_1}. \tag{3.14}$$

By the same reasoning we can show that there is a linear combination $\tilde{u}_{p+q}$ of $u_p, \ldots, u_{p+m-1}$ that approximates w_{p+q} with $0<q<m$. We eliminate $\kappa_p, \ldots, \kappa_{p+m-1}$ except for κ_{p+q} from the κ_α and $\bar{\lambda}_{p+1}, \ldots, \bar{\lambda}_{p+m-1}$ from the $\bar{\lambda}_i$ in forming the sets β_v and i_σ. Then we obtain the inequalities (3.12) and (3.13) with w_p replaced by w_{p+q}, $\tilde{u}_p$ by $\tilde{u}_{p+q}$, and κ_p by κ_{p+q}.

Example. We consider the vibrations of a uniform beam which is free at its ends and which lies on an elastic foundation with small linearly varying elastic constant. It satisfies the differential equation

$$u^{\mathrm{IV}}+\epsilon xu=\lambda u \qquad 0<x<1 \tag{3.15}$$

with the end conditions

$$u''(0)=u'''(0)=u''(1)=u'''(1)=0 \tag{3.16}$$

The constant ϵ is positive and small. We introduce the scalar product

$$(u, v)=\int_0^1 uvdx \tag{3.17}$$

and define the symmetric operator A by the bilinear form

$$(Au, v)=\int_0^1 [u''v''+\epsilon uv]dx \tag{3.18}$$

If the eigenvalues $\lambda_1\leq\lambda_2\leq \ldots$ of A are defined as the successive minima of the Rayleigh quotient $(Av, v)/(v, v)$, they coincide with those of the problem (3.15), (3.16).

We are concerned with the two lowest eigenvalues. For $\epsilon=0$ they both vanish. Corresponding eigenfunctions are 1 and $6^{-1/2}(1-2x)$. We use these as trial functions in the Rayleigh-Ritz method. We obtain

$$\kappa_1=\frac{1}{2}(1-6^{-1/2})\epsilon,$$

$$\kappa_2=\frac{1}{2}(1+6^{-1/2})\epsilon, \tag{3.19}$$

with the corresponding vectors

$$w_1=2^{-1/2}[1-6^{-1/2}(1-2x)]$$

$$w_2=2^{-1/2}[1+6^{-1/2}(1-2x)] \tag{3.20}$$

To obtain lower bounds $\bar{\lambda}_i$ we note that (Av, v) is greater for $\epsilon>0$ than for $\epsilon=0$. Thus, the λ_i are bounded below by the eigenvalues λ_i of the problem (3.15), (3.16) with $\epsilon=0$. These can be found explicitly. We find

$$\bar{\lambda}_1=\bar{\lambda}_2=0$$

$$\bar{\lambda}_3=500.462. \tag{3.21}$$

Condition (2.39) is violated so that we cannot say how well w_1 approximates u_1 without improving our bounds. However, we can use theorem 2 to state that there are linear combinations $\tilde{u}_1$ and $\tilde{u}_2$ of u_1 and u_2 such that

$$\int_0^1 (w_1-\tilde{u}_1)^2dx\leq 2[1-\{1-0.0005912\epsilon\}^{1/2}],$$

$$\int_0^1 (w_2-\tilde{u}_2)^2dx\leq 2[1-\{1-0.0014070\epsilon\}^{1/2}]. \tag{3.22}$$

Thus we have shown that w_1 and w_2 approximate linear combinations of u_1 and u_2 in the mean square sense.

When, as in this example, A is unbounded, it is often more desirable to have a bound for the deviation $(A(w_p-\tilde{u}_p), w_p-\tilde{u}_p)$ rather than $(w_p-\tilde{u}_p, w_p-\tilde{u}_p)$ In order to obtain such a bound we note that the quadratic form $(Av,v)+c(v,v)$ is positive definite for $c>-\bar{\lambda}_1$.

Hence we can define a new scalar product

$$[u,v]=(Au,v)+c(u,v). \tag{3.23}$$

We now define the operator $\hat{A}$ by

$$[\hat{A}u,v]=-(u,v). \tag{3.24}$$

Then the eigenvectors of $\hat{A}$ are multiples of those of A, and its eigenvalues are $-(\lambda_i+c)^{-1}$. Applying theorems 1 and 2 to A and expressing the results in terms of $\hat{A}$, we find the following.

THEOREM 3. *Under the hypotheses of theorem 2 there exists for any constant $c>-\bar{\lambda}_1$ a linear combination $\tilde{\tilde{u}}$ of $u_p, \ldots, u_{p+m-1}$ such that*

$$(A\tilde{\tilde{u}},\tilde{\tilde{u}})+c(\tilde{\tilde{u}},\tilde{\tilde{u}})=\kappa_p+c \tag{3.25}$$

and

$$\left[\kappa_p+c+\frac{1}{2}\{(Aw_p-A\tilde{\tilde{u}},w_p-\tilde{\tilde{u}})+c(w_p-\tilde{\tilde{u}},w_p-\tilde{\tilde{u}})\}\right]^2 \geq (\kappa_p+c)(\bar{\lambda}_p+c)\left\{1-\frac{\kappa_p-\bar{\lambda}_p}{\bar{\lambda}_{i_{L+1}}-\bar{\lambda}_p}\right\}\prod_{\substack{\nu=1\\ \beta_\nu\neq p}}^{L}\left\{1-\frac{(\kappa_p-\bar{\lambda}_p)(\kappa_{\beta_\nu}-\bar{\lambda}_{i_\nu})}{(\kappa_p-\kappa_{\beta_\nu})(\bar{\lambda}_p-\bar{\lambda}_{i_\nu})}\right\} \tag{3.26}$$

When the multiplicity $m=1$, $\tilde{\tilde{u}}$ is a multiple of u_p and we have the analog of theorem 1.

Applying theorem 3 to the example (3.15), (3.16), we obtain the inequality

$$\int_0^{\prime} \tilde{u}''^2+(c+\epsilon x)(w_1-\tilde{\tilde{u}})^2]dx\leq 2[c+1.704\epsilon-c^{1/2}\{c+1.704\epsilon\}^{1/2}\{1-0.0005912\epsilon\}^{1/2}] \tag{3.27}$$

for any $c\geq 0$. (The function $\tilde{\tilde{u}}$ depends upon c, however.)

4. Pointwise Bounds for Eigenfunctions

When A is a differential operator, theorems 1 and 3 give bounds for the mean square deviation of the approximate eigenfunction w_p from the exact eigenfunction u_p. It is often of interest to determine the value of u_p at a particular point.

In certain cases a pointwise bound for the deviation $|w_p-\tilde{\tilde{u}}|$ at a point comes directly from the bound (3.26) of theorem 3. For example, we show that for any $0\leq\zeta\leq 1$

$$|w_1(\xi)-\tilde{\tilde{u}}(\xi)|^2\leq G(\xi,\xi)\int_0^1 [(w_1-\tilde{\tilde{u}})''^2+c(w_1-\tilde{\tilde{u}})^2]dx, \tag{4.1}$$

where

$$G(\xi,\xi)=\frac{1}{8}b^{-3}[\sinh^2 b-\sin^2 b]^{-1}$$
$$\times[\sinh b\cosh b-\sin b\cos b+2\sinh b\cosh b(1-2\xi)-2\sin b\cos b\,(1-2\xi)+(\sinh b\cos b+\sin b\cosh b)\sin b\,(1-2\xi)\sinh b(1-2\xi)+(\sinh b\cos b-\sin b\cosh b)\cos b(1-2\xi)\cosh b(1-2\xi)]$$

$$b=\left(\frac{1}{4}c\right)^{1/4} \tag{4.2}$$

(See, for example, [8]). Thus, (3.27) gives a bound for $|w_1(\xi)-\tilde{\tilde{u}}(\xi)|$.

In the case of partial differential operators such a bound may or may not exist. If it exists, it is difficult to find.

However, one can use the following adaptation of the method of Diaz and Greenberg [7,9])cf. [15,18]). For the sake of simplicity we present it only for the case of a special second order operator in two dimensions.

Consider the eigenvalue problem

$$-\Delta u+r(x,y)u=\lambda q(x,y)u \tag{4.3}$$

on a two-dimensional domain D with smooth boundary C. Here Δ is the usual Laplace operator. The function q is positive and r is non-negative, and both are continuous in the closure of D. The boundary C consist of two parts C_1 and C_2, and we have boundary conditions

$$u=0 \quad \text{on} \quad C_1$$

$$\frac{\partial u}{\partial n}+k(x,y)u=0 \quad \text{on} \quad C_2, \qquad k\geq 0. \tag{4.4}$$

We define the scalar product

$$(u,\,v)=\iint_D quvdxdy \tag{4.5}$$

on the linear vector space of functions which are piecewise continuously differentiable in D and vanish on C_1.

Let u_p be the normalized eigenfunction corresponding to the eigenvalue λ_p, and let w_p be the function corresponding to a Rayleigh-Ritz upper bound κ_p for λ_p. Theorem 1 gives a bound for the deviation in norm $(w_p-u_p,\,w_p-u_p)$.

We wish to approximate the value of u_p at an interior point of D, which we choose as the origin of our coordinate system. We use the fact that u_p satisfies the differential equation (4.3) with $\lambda=\lambda_p$ and the boundary conditions (4.4). Let $\Gamma(x,\,y)$ be a parametrix for the differential equation (4.3) satisfying (4.4). That is,

$$\Gamma(x,\,y)=-(4\pi)^{-1}\log\,(x^2+y^2)+\phi(x,\,y), \tag{4.6}$$

where ϕ is any twice continuously differentiable function such that

$$\Gamma=0 \qquad \text{on} \quad C_1$$

$$\frac{\partial\Gamma}{\partial n}+k\Gamma=0 \qquad \text{on} \quad C_2 \tag{4.7}$$

Multiplying (4.3) by Γ and integrating by parts, we find that

$$u_p(0,\ 0)=\iint_D u_p[-\Delta\phi+(r-\lambda_p q)\Gamma]dxdy. \tag{4.8}$$

Replacing u_p by w_p and λ_p by κ_p on the right, we obtain the value

$$w_p^*(0,\ 0)=\iint_D w_p[-\Delta\phi+(r-\kappa_p q)\Gamma]dxdy \tag{4.9}$$

which can be computed by quadratures. Using Schwarz's inequality, the normalization of u_p, and the triangle inequality, we find

$$|w_p^*(0,\ 0)-u_p(0,\ 0)|\leq(\kappa_p-\lambda_p)(\Gamma,\ \Gamma)^{1/2}$$
$$+(w_p-u_p,\ w_p-u_p)^{1/2}$$
$$\left\{\iint_D q^{-1}[-\Delta\phi+(r-\kappa_p q)\Gamma]^2dxdy\right\}^{1/2}\cdot \tag{4.10}$$

Thus, the bound (2.41) for $(w_p-u_p,\ w_p-u_p)$ together with the bound $\kappa_p-\overline{\lambda}_p$ for $\kappa_p-\lambda_p$ provides explicit upper and lower bounds for $u_p(0,\ 0)$. These bounds lie close together if the error bounds (2.41) and $\kappa_p-\overline{\lambda}_p$ are small.

The same method applies to the function $\tilde{u}_p$ of theorem 2. If

$$\tilde{u}_p=\sum_p^{p+m-1} a^i u_i, \tag{4.11}$$

we find from (4.8) that

$$\tilde{u}_p(0,\ 0)=\sum a^i\iint_D u_i[-\Delta\phi+(r-\lambda_i q)\Gamma]dxdy. \tag{4.12}$$

Hence if we again define the approximate value w_p^* by (4.9), we obtain

$$|w_p^*(0,\ 0)-\tilde{u}_p(0,\ 0)|\leq \max\{\kappa_p-\overline{\lambda}_p,\ \kappa_{p+m-1}-\kappa_p\}$$
$$(\Gamma,\ \Gamma)^{1/2}+(w_p-\tilde{u}_p,\ w_p-\tilde{u}_p)^{1/2}$$
$$\left\{\iint_D q^{-1}[-\Delta\phi+(r-\kappa_p q)\Gamma]^2dxdy\right\}^{1/2}\cdot \tag{4.13}$$

This inequality together with theorem 2 gives upper and lower bounds for $\tilde{u}_p(0,\ 0)$.

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