ESTIMATING EIGENVALUES[1]

CHANDLER DAVIS

1. **Introduction.** In §2 of this note is pointed out a simple generalization of the ingenious method of Kato [3][2] for locating eigenvalues.

In the remaining sections, a similar idea is used to demonstrate an iterative procedure for finding arbitrarily good upper and lower bounds for any isolated eigenvalue of a bounded self-adjoint operator. It is the only procedure available which will do this; the previously existing method which comes closest is that giving simultaneous convergence to n eigenvalues which are lower (or higher) than any other point of the spectrum (see [4, §14.5, and references there]).

2. **Extension of the method of Kato.** Let A be a self-adjoint operator on a Hilbert space $\mathfrak{H}$ (not necessarily separable; real or complex scalars); let $E(\lambda)$ be the resolution of the identity for A, and $\mathfrak{S}(A)$ its spectrum. Suppose $\mathfrak{S}(A)$ is disjoint from each of the n open intervals[3] $(\alpha_1, \alpha_2), \cdots, (\alpha_{2n-1}, \alpha_{2n})$. If we define

$$P(\lambda) \equiv \prod_{i=1}^{n} P_i(\lambda), \quad \text{with} \quad P_i(\lambda) \equiv (\lambda - \alpha_{2i-1})(\lambda - \alpha_{2i}),$$

then $P(\lambda) \geqq 0$ on $\mathfrak{S}(A)$, since each $P_i(\lambda)$ is. (If $\alpha_1 = -\infty$, omit $(\lambda - \alpha_1)$ from P_1.) Therefore,

$$(1) \qquad (P(A)x, x) = \int_{-\infty}^{\infty} P(\lambda) d(E(\lambda)x, x) \geqq 0$$

for any $x \in \mathfrak{H}$ in the domain of $P(A)$. Notice that $(P(A)x, x)$ is a linear polynomial $Q_x(\alpha_1, \cdots, \alpha_{2n})$ in the α, and that, for any chosen x, the coefficients may be calculated. These are the fundamental ideas of the method.

Now assume we have $n+1$ open intervals $(a_1, b_1), \cdots, (a_{n+1}, b_{n+1})$, all known to be disjoint from $\mathfrak{S}(A)$.[4] Our objective is to gain further information about $\mathfrak{S}(A)$, therefore to replace some a by a lower value

Received by the editors January 17, 1952.

[1] The author thanks C. L. Dolph for providing him, in several lectures and private conversations, with an excellent introduction to approximation problems.

[2] Numbers in brackets refer to the bibliography.

[3] This notation for open intervals is the same as that which will be used for inner products in $\mathfrak{H}$, but it will always be clear from context which is meant.

[4] It is not necessary to exclude the case $a_i = b_i$, that is, (a_i, b_i) void.

or some b by a higher value. Consider, for example, the problem of improving a_k, $k>1$, when we know that the portion of the spectrum between b_{k-1} and a_k consists of *one isolated point* λ_k. We may proceed as follows.

Choose a nonzero $y\in\mathfrak{H}$. By (1), we have

$$Q_y(a_1, b_1, \cdots, a_{k-1}, \beta, a_{k+1}, b_{k+1}, \cdots, a_{n+1}, b_{n+1}) \geqq 0 \quad \text{for } \beta = b_{k-1}.$$

Examine the coefficient of β; if it is non-negative, the method fails and we must try a different choice of y. If it is negative, then increasing β decreases Q_y. We find the solution $\beta=\beta_0$ of $Q_y(\cdots, \beta, \cdots)=0$; then $\beta_0\geqq b_{k-1}$. Also, $\mathfrak{S}(A)\cap[a_{k-1}, \beta_0]$ is not empty. For if it were we could prove $Q_y(\cdots, \beta, \cdots)\geqq 0$ for some $\beta>\beta_0$, by (1) and the fact $\mathfrak{S}(A)$ is closed, contradicting the linearity of Q_y. Therefore $a_{k-1}<\lambda_k\leqq\beta_0$, so that if $\beta_0<a_k$ we have improved our information about the value of λ_k in the direction desired. (If $\beta_0\geqq a_k$, we have learned nothing.)

Notice that if $\mathfrak{S}(A)\cap[b_{k-1}, a_k]$ were not known to consist of a single point, β_0 would give merely an upper bound on the value of the left-hand end point of that set.

Of course in the above we might use a trial function y containing parameters, which then could be adjusted to minimize β_0.

Lower bounds are treated in a similar way.

The classical Rayleigh-Ritz method is a special case of the above, for $n=1$, $a_1=-\infty$, $b_1=0$, $P(\lambda)=\lambda-\beta$.

The general case for $n=1$ is given by Kato [3].

The extension given here, which consists in increasing n, is believed to have serious limitations in computational work, at least when A is unbounded. For if the trial function has components in the subspaces $(I-E(\lambda))\mathfrak{H}$ for large λ, these will give an inordinately large contribution to the integral in (1) when high powers of λ are present. It is easy to find an A and a y such that Kato's method, even though it is unable to use all the information one has to begin with about $\mathfrak{S}(A)$, still gives better estimates than the extended method.

3. Convergence to an arbitrary eigenvalue. Let A, $E(\lambda)$, $\mathfrak{S}(A)$ be as before. Suppose for definiteness that $E(\lambda)=E(\lambda^-)$. Again we use the spectral representation of a polynomial in A, but it suffices here to consider (for real b)

$$B \equiv (A-b)^2 = \int_{-\infty}^{\infty} (\lambda-b)^2 dE(\lambda). \tag{2}$$

We make the following observation:

If $\mathfrak{S}(A)\cap(b-k,\ b+k)$ *consists of a finite number of eigenvalues* $\lambda_i, \cdots, \lambda_{i'}$, *then* $\mathfrak{S}(B)\cap[0,\ k^2)$ *consists of the corresponding eigenvalues* $(\lambda_i-b)^2, \cdots, (\lambda_{i'}-b)^2$; *the eigenfunctions belonging to a* λ_j *here belong also to the corresponding* $(\lambda_j-b)^2$. (Also, the rest of the spectrum of A transforms in the same way.)

The proof is easy. Rewriting (2) and making the necessary changes of variable, we get

$$B = \int_{-\infty}^{b} (\lambda - b)^2 dE(\lambda) + \int_{b}^{\infty} (\lambda - b)^2 dE(\lambda)$$

$$= -\int_{0}^{\infty} \nu dE(-\nu^{1/2} + b) + \int_{0}^{\infty} \nu dE(\nu^{1/2} + b).$$

Thus, if we write the spectral resolution of B as $\int_{-\infty}^{\infty}\nu dF(\nu)$, with $F(0)=0$ and $F(\nu)=F(\nu^-)$, we have $F(\nu)=E(\nu^{1/2}+b)-E'(-\nu^{1/2}+b)$, where E' is simply E renormalized: $E'(\lambda)\equiv E(\lambda^+)=E'(\lambda^+)$.

The italicized observation above follows.

Henceforth assume A (therefore also B) *bounded.* Define $\nu_1\equiv\inf\mathfrak{S}(B)$, and assume it is an isolated point of $\mathfrak{S}(B)$.

Iterative methods are available which provide a sequence of numbers μ_i converging to ν_1 from above, and a sequence of elements $y_i\in\mathfrak{H}$ converging strongly to an eigenfunction x_1 of B belonging to ν_1; see, for example, [2].

The assumption that ν_1 is an isolated point of $\mathfrak{S}(B)$ is equivalent to the assumption that the nearest point λ' of $\mathfrak{S}(A)$ to b is an isolated point. (This can of course be guaranteed in advance in many of the most important problems.) Suppose for a moment that it is also known in advance that $\lambda'\geqq b$. Then the sequence of numbers $\mu_i^{1/2}+b$ converges to λ' from above, and the x_1 above is an eigenfunction of A belonging to λ'.

A similar situation exists if $\lambda'<b$.

Similar remarks hold if ν_1 is not an isolated point, except that then strong convergence to an eigenfunction can not be guaranteed. For simplicity, *the remainder of this note will not explicitly treat this case.*

There are two limitations to the procedure. The first is that, if one begins the approximation of ν_1 with a trial function orthogonal to the manifold of eigenfunctions belonging to ν_1, one gets convergence, not to ν_1, but to some larger element of the spectrum. This difficulty is familiar and need not be discussed here.

The second difficulty is this: Suppose there is no single closest point of $\mathfrak{S}(A)$ to b, but two, λ_1' and λ_2', $\lambda_1'-b=b-\lambda_2'=\nu_1^{1/2}$. A pro-

cedure such as that of [2] gives a sequence $y_i \in \mathfrak{X}$ converging strongly to an eigenfunction x_1 of B belonging to ν_1; but we have in general

$$x_1 = x_1' + x_2', \quad \text{with} \quad Ax_1' = \lambda_1' x_1', \quad Ax_2' = \lambda_2' x_2',$$

with no assurance that either x_1' or x_2' is null. Call this the "induced degeneracy difficulty" for future reference (§5).

Before stating our result formally and finishing the argument (§5), we give one form of the procedure of this section for which a direct proof of convergence can easily be given without appealing to the literature.

4. **One form of the iteration procedure.** It will readily be seen that the following is equivalent to using the idea of the preceding section together with the Kellogg method [1, III, §10.5].

Let A be as before; let b be a real number such that the *unique* element λ' of $S(A)$ which is closest to b is an isolated point; and let y_0 be of unit norm and not orthogonal to the manifold $\mathfrak{M}(\lambda')$ of eigenfunctions belonging to λ'. Call the projection of y_0 on $\mathfrak{M}(\lambda')$, $a_0' x'$, where $a_0' > 0$, $\|x'\| = 1$.

Define y_i, $i = 1, 2, \cdots$, by $y_{i+1} = Cy_i / \|Cy_i\|$, where $C = -(A-b)^2 + k^2$. The only requirement[5] on k^2 is that

$$2k^2 > \|A - b\|^2 + (\lambda' - b)^2. \tag{3}$$

x' is an eigenfunction of C belonging to the eigenvalue $c' = -(\lambda' - b)^2 + k^2 > 0$.

Each y_i may be written (uniquely) in the form

$$y_i = a_i' x' + a_i'' y_i'', \tag{4}$$

where $a_i' > 0$, $a_i'' > 0$, $y_i'' \perp x'$, $\|y_i''\| = 1$. (Assume no y_i is equal to x', since that case is trivial.) Here $y_i'' \perp \mathfrak{M}(\lambda')$; this is proved by a standard induction on i.

In

$$Cy_i = a_i' c' x' + a_i'' C y_i'',$$

we note that the two orthogonal elements in the right member are respectively equal to $\|Cy_i\| a_{i+1}' x'$ and $\|Cy_i\| a_{i+1}'' y_{i+1}''$. Equating norms of equal elements and eliminating $\|Cy_i\|$ from the two resulting equations gives

$$\frac{a_{i+1}''}{a_{i+1}'} = \frac{\|Cy_i''\|}{c'} \frac{a_i''}{a_i'}.$$

[5] But large k^2 gives slow convergence.

Therefore if we show $\|Cy_i''\|/c'$ is bounded below 1, we shall have shown $a_i''/a_i' \to 0$.

But

$$\|Cy_i''\|^2 = \int_{-\infty}^{\infty} (-(\lambda - b)^2 + k^2)^2 d(E(\lambda)y_i'', y_i'')$$

$$\leqq (-(\lambda'' - b)^2 + k^2)^2 \int_{-\infty}^{\infty} d(E(\lambda)y_i'', y_i'')$$

$$= (-(\lambda'' - b)^2 + k^2)^2 < c'^2.$$

Here λ'' denotes a point which has minimum distance from b of any point of $\mathfrak{S}(A)$ other than λ'; and the inequalities are justified by $y_i'' \perp \mathfrak{M}(\lambda')$ and by (3).

Hence $a_i''/a_i' \to 0$, and, because of $a_i'^2 + a_i''^2 = 1$, $a_i'' \to 0$. Referring to (4), we see that $y_i \to x'$ strongly.

5. **Conclusion.** The main result, accordingly, is this:

Given a bounded self-adjoint operator A on an arbitrary Hilbert space $\mathfrak{H}$; given a real number b such that there is a single point λ' for which $\min \{|b-\lambda|; \lambda \in \mathfrak{S}(A)\}$ *is attained, and λ' is an isolated point of $\mathfrak{S}(A)$; and given an element of $\mathfrak{H}$ not orthogonal to the manifold $\mathfrak{M}(\lambda')$ of eigenfunctions of A belonging to λ'; then we can construct a sequence of elements of $\mathfrak{H}$ converging strongly to an element (of norm 1) of $\mathfrak{M}(\lambda')$, and a sequence of numbers converging to λ'.*

The proof of the last statement is not yet complete. We showed in §3 that we can find a sequence μ_i converging to $(\lambda' - b)^2$; but we did not show how to determine the sign of $\lambda' - b$.

Define for this purpose $\eta_i \equiv (Ay_i, y_i)$, $\epsilon_i^2 \equiv ((A - \eta_i)^2 y_i, y_i)$, where y_i is one member of our approximating sequence of functions of norm 1. Represent y_i again in the form (4). Then

$$\eta_i = a_i'^2 \lambda' + a_i''^2 (Ay_i'', y_i'')$$

$$= \lambda' + a_i''^2 ((A - \lambda')y_i'', y_i''),$$

since $a_i'^2 + a_i''^2 = 1$; hence

$$|\eta_i - \lambda'| \leqq a_i''^2 \|A - \lambda'\| \to 0,$$

and the η_i will serve as the sequence of numbers in the theorem. The proof is therefore finished. We note also the usefulness in this connection of the trivial relation $\epsilon_i^2 \geqq (\lambda_i^0 - \eta_i)^2$, where λ_i^0 is a closest point of $\mathfrak{S}(A)$ to η_i (ultimately $\lambda_i^0 = \lambda'$). This estimate of the error of approximation to λ' is ultimately a good one, since it can be shown that

$\epsilon_i^2 \to 0$ as $a_i'^2/a_i^2$; hence it may be useful in determining the sign of $\lambda' - b$.

The "induced degeneracy difficulty" remains unresolved. It is more serious than it might appear, because if the nearest points of $S(A)$ to b are, say, λ'' below and λ' above, with $b - \lambda''$ very slightly larger than $\lambda' - b$, then even though the procedure succeeds it clearly may require very many steps to give an η_i numerically close to λ'. Of course one can try a new value for b at any stage, but the author has not developed any standardized scheme for deciding when to do so.

However, this observation seems pertinent: Applying the Rayleigh-Ritz approximation to the operator B of §3 is solving an equation of the form $(\{(A-b)^2-\alpha\}y, y)=0$ for α, b being fixed; applying Kato's approximation to A is solving an equation of the form $(\{(A-\alpha)(A-\beta)\}y, y)=0$ for one of α and β, the other being fixed. The latter procedure is much like the first, so that presumably a convergent approximation scheme could be based on it also; and it has the advantage that, essentially, the b above is varied as one goes along, so that the "induced degeneracy" should not arise. The same applies, of course, to the extension given in §2.

The author hopes to develop this idea in a future note, as well as possible extensions to unbounded operators.

Bibliography

1. R. Courant and D. Hilbert, *Methoden der mathematischen Physik*, vol. I, Berlin, 1931.

2. W. Karush, *Determination of the extreme values of the spectrum of a bounded self-adjoint operator*, Proceedings of the American Mathematical Society vol. 2 (1951) pp. 980–989.

3. T. Kato, *On the upper and lower bounds of eigenvalues*, J. Phys. Soc. Japan vol. 4 (1949) pp. 334–339.

4. L. Collatz, *Eigenwertprobleme und ihre numerische Behandlung*, New York, 1951.

University of Michigan