Numerical Work of Hans F. Weinberger

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In the abstract, I listed the following papers:

Approximation of Eigenvalues

[1] Upper and lower bounds for eigenvalues by finite difference methods. Communications on Pure and Appl. Math. 9 (1956), pp. 613-623.

[2] Lower bounds for higher eigenvalues by finite difference methods. Pacific J. Math. 8 (1958), pp. 339-368.

Approximation Theory Issues

[3] Optimal approximations and error bounds (joint with M. Golomb). In Proc. Symposium on Numerical Approximation, Univ. of Wisconsin Press, 1959, pp. 117-190.

[4] Optimal approximation for functions prescribed at equally spaced points. Nat. Bureau of Standards J. of Research 65B, 2 (1961), pp. 99-104.

[5] On optimal numerical solution of partial differential equations. SIAM J. Numer. Anal. 9 (1972), pp. 182-198.

[6] Optimal numerical approximation of a linear operator. Linear Alg. and its Appl. 52/53 (1983), pp. 717-737.

Error Bounds for Iterative Methods for Matrix Inversion

[7] A posteriori error bounds in iterative matrix inversion. In Numerical Treatment of Partial Differential Equations, Academic Press 1965, pp. 153-163. Proceedings of Symposium on Partial Differential Equations, held at the Univ. of Maryland in 1965 (Edited by J. Bramble).

We will discuss the main results in several of these papers. Let's first consider paper [1]:

[1] Upper and lower bounds for eigenvalues by finite difference methods.Communications on Pure and Appl. Math. 9 (1956), pp. 613-623.

Consider the membrane eigenvalue problem

$$\begin{cases} \Delta u + \lambda u = 0 \text{ in the domain } R \\ u = 0 \text{ on the boundary } \partial R \end{cases}, \tag{1}$$

This problem has eigenvalues

$$0 < \lambda_1 \leq \lambda_2 \leq \cdots \nearrow \infty$$

and corresponding eigenvectors

$$u_1, u_2, u_3, \ldots; \qquad \int\int_R u_i u_j \, dx \, dy = \delta_{i,j}.$$

The minimum principle for the lowest eigenvalue is

$$\lambda = \lambda_1 = \min_{v=0 \text{ on } \partial R} \frac{D(v,v)}{\int\int_R v^2 \, dx \, dy}, \tag{2}$$

where

$$D(v,v) = \int\int_R \left[\left(\frac{\partial v}{\partial x} \right)^2 + \left(\frac{\partial v}{\partial y} \right)^2 \right] dx \, dy$$

is the Dirichlet integral; the quotient in (2) is referred to as the Rayleigh quotient.

Since the eigenvalues can be found explicitly for only very simple domains, it is of interest to be able to have computable lower and upper bounds for them. We will concentrate on the lowest eigenvalue $\lambda = \lambda_1$.

Upper Bounds It follows immediately from the minimum principle that upper bounds for $\lambda = \lambda_1$ can be obtained by substituting in the Rayleigh quotient any function w vanishing on ∂R.

Lower Bounds Lower bounds are more difficult to obtain. In paper [1] Hans obtained a lower bound in terms of the lowest eigenvalue of an appropriate finite difference eigenvalue problem, which for simplicity we describe in one dimension: Let R_h be a grid consisting of the union of squares of side h with their sides adjacent and parallel to the $x-$ and $y-$ axes.

R_h contains not only the region R on which the membrane problem is to be solved, but also all of its left and downward translates of distance at most h:

$$R_h \supset \{(x, y) : (x + \alpha, y + \beta) \in R, \text{ for some } 0 \leq \alpha \leq h, 0 \leq \beta \leq h\}$$

Consider now grid functions $w = w_i$ that vanish on the boundary of R_h and consider the "finite difference" equations

$$\Delta_h w + \underline{\lambda}^{(h)} w = 0, \tag{3}$$

where

$$\Delta_h w = \frac{1}{h^2}[w_{i+1} - 2w_i + w_{i-1}],$$

with eigenvalues

$$\underline{\lambda}_1^{(h)} \leq \underline{\lambda}_2^{(h)} \leq \cdots .$$

In [1], the following is proved:

Theorem

$$\underline{\lambda}_1^{(h)} \leq \lambda_1. \tag{4}$$

As mentioned above, upper bounds can be obtained by substituting in the Rayleigh quotient any function that vanishes on ∂R. These upper bounds can be calculated from the following "finite difference" method:

$$\Delta_h w + \lambda^{(h)} S_h w = 0, \tag{5}$$

where

$$\Delta_h w = \frac{1}{h^2}[w_{i+1} - 2w_i + w_{i-1}], \text{ as above,}$$

and

$$S_h w = \frac{1}{6}[w_{i-1} + 4w_i + w_{i+1}].$$

This problem has eigenvalues and eigenvectors

$$0 < \overline{\lambda}_1^{(h)} \leq \overline{\lambda}_2^{(h)} \leq \ldots,$$

$$w_1^{(h)}, w_2^{(h)}, \ldots.$$

If one substitutes in the minimum principle the broken linear function taking on the values of the finite difference eigenvector at the mesh points one gets $\overline{\lambda}_1^{(h)}$, and one thus has

$$\lambda_1 \leq \overline{\lambda}_1^{(h)}. \tag{6}$$

Eigenvalue problem (3) differs from problem (5) in two ways: the domain is larger and the mass matrix has been lumped.

In paper [2] lower bounds by means of finite difference methods are obtained for higher eigenvalues.

Hans was on the faculty at the University of Maryland 1950-60, a member of the Institute for Fluid Dynamics and Applied Mathematics (IFDAM). During that period Maryland was a center for eigenvalue studies, with a strong group working in this area: Alexander Weinstein, Larry Payne, and Joe Diaz, in addition to Hans. Much of this work centered on the Method of Intermediate Problems, originated by Weinstein, for providing lower bounds for the eigenvalues of positive, symmetric operators. There were many advances at Maryland during this period, and Hans was in the center of this work. The first result I discussed was one of his contributions. I will now briefly mention another important contribution.

This work is contained in the (unpublished) technical report,

[8] A Theory of lower bounds for eigenvalues, Technical Note BN-183, Institute for Fluid Dynamics and Applied Mathematics, University of Maryland, 1959.

Let A be a symmetric operator on a Hilbert space H, with scalar product $(\cdot,\cdot)$. The domain of A is a linear manifold $V \subset H$. We wish to approximate the eigenvalues $\lambda_1 \leq \lambda_2 \leq \cdots$ of A, which are characterized by the maximum-minimum principle

$$\lambda_k = \sup_{\phi_1,\cdots,\phi_{k-1}\in H} \inf_{\substack{u\in V \\ (u,\phi_\nu)=0,\nu=1,\cdots,k-1}} \frac{(Au,u)}{(u,u)}.$$

We will need some preliminary information on A on the orthogonal complement in V of a finite dimensional subspace of H;

we will assume this information has the form: there are n linearly independent elements $p_1, \cdots, p_n \in H$ and a number ρ_n having the property that

$$u \in V, (v, p_i) = 0, i = 1, \cdots, n \Longrightarrow (Av, v) \geq \rho_n(v, v). \tag{7}$$

Let $q_1, \cdots, q_n$ be linearly independent . Then we define the approximate eigenvalues by

$$\mu_k = \sup_{\phi_1,\cdots,\phi_{k-1}\in H} \inf_{\substack{v\in H \\ (u,\phi_\nu)=0,\nu=1,\cdots,k-1}} Q,$$

where

$$Q = \frac{\sum_{\alpha,\beta=1}^{m}(Aq_\alpha, q_\beta)x_\alpha x_\beta + 2\sum_{\alpha=1}^{m}(Aq_\alpha, v)x_\alpha + \rho_n(v, v)}{\sum_{\alpha,\beta=1}^{m}(q_\alpha, q_\beta)x_\alpha x_\beta + 2\sum_{\alpha=1}^{m}(q_\alpha, v)x_\alpha + (v, v)}.$$

For any $u \in V$, we can write

$$u = \sum_{\alpha=1}^{n} x_\alpha q_\alpha + w,$$

where $(w, q_\alpha) = 0, \alpha = 1, \cdots, n$. Using this relation in (7) see that

$$\frac{(Au, u)}{(u, u)} \geq Q, \quad \forall u \in V,$$

and hence that

$$\mu_k \leq \lambda_k, \quad \mu_k \text{ is a lower bound for } \lambda_k.$$

This is not the full story. More generally, we consider M auxiliary vector $q_1, \cdots, q_m$, where usually $m \geq n$, and modify the definition of μ_k. We again have $\mu_k \leq \lambda_k$. In [8] it is shown that μ is increasing with the number m of the vectors q_α, and conditions are given under which μ_k converges to λ_k as $m \to \infty$ (with n fixed).

We next consider paper

[9] Error bounds in the Rayleigh-Ritz approximation of eigenvectors. Nat. Bureau of Standards J. of Research 64B, 2 (1960), pp. 217-225.

Suppose A is a symmetric operator, with eigenvalues $\lambda_1 \leq \lambda_2 \leq \cdots$ and corresponding normalized eigenvectors $u_1, u_2, \ldots$. Let κ_i be the Raleigh-Ritz approximation to $\lambda_i; \kappa_i$ will be an upper bound for λ_i. Along with κ_i, the Rayleigh-Ritz method yields associated vectors w_i. This paper addresses the eigenvector approximation, $u_i \approx w_i$. It is expected that the better the eigenvalue λ_i is approximated by κ_i, the better will be the approximation of u_i by w_i. For the first eigenvector u_1, this is seen to be the case from the estimate

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

which shows that if κ_1 is close to λ_1, then w_1 is close to u_1. If $\overline{\lambda}_1$ and $\overline{\lambda}_2$ are lower bounds for λ_1 and λ_2, respectively, then we have the estimate

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

In [9], Hans generalized this estimate for higher eigenvectors. Here is the bound (under some simplifying assumptions):

$$\begin{aligned}\left[1 - \frac{1}{2}(w_p - u_p, w_p - u_p)\right]^2 \;\geq\; & \left\{1 - \frac{\kappa_p - \overline{\lambda}_p}{\overline{\lambda}_{p+1} - \overline{\lambda}_p}\right\} \\ & \times \left\{1 - \frac{(\kappa_p - \overline{\lambda}_p)(\kappa_{p-1} - \overline{\lambda}_1)}{(\kappa_p - \kappa_{p-1})(\overline{\lambda}_p - \overline{\lambda}_1)}\right\}.\end{aligned}$$

We next turn to paper [5], which is closely related to paper [3]:

[5] On optimal numerical solution of partial differential equations. SIAM J. Numer. Anal. 9 (1972), pp. 182-198.

Suppose

- $$B = \text{ Banach space}$$

- $$\Sigma = \text{ Banach space, with norm or seminorm } \|\cdot\|_\Sigma.$$

- $$N : B \to E_n \text{ (Euclidean n-space), a discretization operator}$$

- $$M : E_m \to \Sigma \text{ an interpolation operator}$$

- $$S : B \to \Sigma, \text{ the solution operator for the problem under consideratio}$$

For input data $\phi, S\phi$ is the solution. Given these spaces and operators, we seek Q (a computational matrix):$E_n \to E_m$ so that MQN approximates S in the sense that

$$\|S\phi - MQN\phi\|_{\Sigma} \text{ is small.}$$

We will be interested in the size of this quantity for ϕ satisfying $\|\phi\|_B \le c$, where c is a given number. Since

$$\sup_{\|\phi\|_B \le c} \|S\phi - MQN\phi\|_\Sigma = c \sup_\phi \frac{\|S\phi - MQN\phi\|_\Sigma}{\|\phi\|_B},$$

we see that it is sufficient to minimize the supremum on the right, which is the operator norm $\|S - MQN\|$. We assume our problem is well-posed in the sense that

$$\frac{\|S\phi\|_\Sigma}{\|\phi\|_B}$$

is bounded for all $\phi \in B$.

We seek the optimum value

$$\mu = \inf_Q \sup_\phi \frac{\|S\phi - MQN\phi\|_\Sigma}{\|\phi\|_B}.$$

If ϕ belongs to the null space of N, then the numerator is independent of Q, so if we define

$$\kappa = \sup_{N\phi=0} \frac{\|S\phi\|_{\Sigma}}{\|\phi\|_B},$$

then $\mu \geq \kappa$. Moreover, we note that the adjoint operator $S^* - N^*Q^*M^*$ has the same norm as $S - MQN$. Therefore, if we define

$$\kappa^* = \sup_{M^*\psi=0} \frac{\|S^*\psi\|_{B^*}}{\|\psi\|_{\Sigma^*}},$$

we see that $\mu \geq \kappa^*$. Thus

$$\mu \geq \max(\kappa, \kappa^*).$$

<u>Theorem</u> There exists an optimal operator $\overline{Q}$ such that

$$\|S - M\overline{Q}N\| = \mu.$$

Theorem If B and Σ are Hilbert spaces, then $\mu = \max(\kappa, \kappa^*)$.

The optimal Q is usually difficult to find, so it is important to know that a computable, nearly optimal Q, is available.

Theorem Let

$$Q_1 = (M^*M)^{-1}M^*S(N^*N^*)^{-1}.$$

Then

$$\|S - MQ_1N\| \le (\kappa^2 + \kappa^{*2})^{1/2} \le \sqrt{2}\mu.$$

One is usually not able to find an explicit optimal computational matrix Q, but one can learn the limit of what can be achieved with a certain discretization of a particular problem. Such a limitation gives a useful basis for the comparison of error estimates for a particular numerical scheme. In one example treated, it is shown that κ is of the order n^{-1} (n is the discretization parameter). Thus the error will be of order n^{-1} for any computational matrix Q.

We next turn to paper [7]:

[7] A posteriori error bounds in iterative matrix inversion. In Numerical Treatment of Partial Differential Equations, Academic Press 1965, pp. 153-163. Proceedings of Symposium on Partial Differential Equations, held at the Univ. of Maryland in 1965 (Edited by J. Bramble).

This paper considers the solution of

$$A\mathbf{x} = \mathbf{b}, \tag{8}$$

where A is an $m \times m$ matrix and $\mathbf{x}$ and $\mathbf{k}$ are m-vectors, by an iterative method. If $M = I - A$ and $\mathbf{k} = \mathbf{b}$, then (8) can be written

$$\mathbf{x} = M\mathbf{x} + \mathbf{k}, \tag{9}$$

so a natural iterative method is

$$\mathbf{x}_{n+1} = M\mathbf{x}_n + \mathbf{k}, \quad n = 0, 1, 2, \ldots. \tag{10}$$

There are other choices for M and $\mathbf{k}$ leading to suitable iterative methods (10); these are the Jacobi methods.

Letting $\mathbf{e}_n = \mathbf{x} - \mathbf{x}_n$ and $\delta_n = \mathbf{x}_n - \mathbf{x}_{n-1}$, the paper addresses the validity of the relation

$$\|\mathbf{e}_n\| \approx \|\delta_n\|,$$

as a stopping criterion. After observing that this relation cannot be valid, the following modified problem is addressed:

Bound $\|\mathbf{e}_n\|$ in terms of $\|\delta_{n-1}\|, \|\delta_n\|, (\delta_{n-1}, \delta_n)$, and a bound $1-\epsilon$ on the spectral radius of M, where $(\cdot,\cdot)$ and $\|\cdot\|$ denote the Euclidean scalar product and norm.

Suppose M is symmetric, with eigenvalues $\lambda_1 \geq \lambda_2 \leq \cdots \lambda_m$, with $|\lambda_i| \leq 1-\epsilon$, and the corresponding normalized eigenvectors $\mathbf{u}_1, \mathbf{u}_2, \ldots, \mathbf{u}_m$. Then, expanding δ_{n-1} in these eigenvectors, we have

$$\delta_{n-1} = \sum_1^m \alpha_i \mathbf{u}_i$$

$$\delta_n = \sum_1^m \alpha_i \lambda_i \mathbf{u}_i$$

$$\mathbf{e}_n = \sum_1^m \frac{\alpha_i \lambda_i^2}{1-\lambda_i} \mathbf{u}_i,$$

so, our problem becomes:

Given the three numbers

$$\sum_1^m \alpha_i^2 = \|\delta_{n-1}\|^2 = A,$$

$$\sum_1^m \alpha_i \lambda_i = (\delta_{n-1}, \delta_n) = B,$$

$$\sum_1^m \alpha_i^2 \lambda_i^2 = \|\delta_n\|^2 = C,$$

find the maximum and minimum possible values of

$$\sum_1^m \frac{\alpha_i^2 \lambda_i^4}{(1-\lambda_i)^2} = \|M(I-M)^{-1}\delta_n\|^2 = \|\mathbf{e}_n\|^2.$$

Using Lagrange multipliers we see that the α_i must satisfy the equations

$$\alpha_i \left[\frac{\lambda_i^4}{(1-\lambda_i)^2} + \mu + \nu\lambda_i + \tau\lambda_i^2 \right] = 0, \quad i = 1, 2, \ldots, m.$$

Thus all the α_i must vanish, except those for which the quantity in the bracket vanishes. Now, μ, ν, and ν can be chosen so that the bracket vanishes for three distinct λ_i, but not for four: call these eigenvalues $\kappa_1 > \kappa_2 > \kappa_3$, and call the corresponding coefficients α_i, β_1, β_2, and β_3. The constraint on the spectral radius of M can now be stated as:

$$-(1-\epsilon) \leq \kappa_1 \leq \kappa_2 \leq \kappa_1 \leq 1 - \epsilon.$$

Define the function

$$R(\kappa_1) = \frac{\frac{(AC-B^2)\kappa_1^4}{1-\kappa_1} + \frac{(B\kappa_1-C)^4}{[(A-B)\kappa_1-(B-C)]^2}}{A\kappa_1^2 - 2B\kappa_2 + C} \tag{11}$$

on the interval

$$\frac{(1-\epsilon)B + C}{(1-\epsilon)A + B} \le \kappa_1 \le 1 - \epsilon \tag{12}$$

(this is the constraint on the spectral radius of M). We now have the following result

<u>Theorem</u> The range of possible values of $\|\mathbf{e}_n\|^2$ when $\|\delta_{n-1}\|^2 = A, (\delta_{n-1}, \delta_n) = B, \delta_n = C$, and M is a symmetric matrix whose spectral radius is at most $1 - \epsilon$ is equal to the range of the function $R(\kappa_1)$ defined by (11) on the interval (12).