TECHNICAL NOTES AND SHORT PAPERS

Estimation of the Successive Over-Relaxation Factor

By A. K. Rigler

1. Introduction. Successive over-relaxation and its several variants are well-known methods for solving finite difference equations of elliptic type. To obtain the greatest rate of convergence one must know the spectral radius ρ of the basic simultaneous displacement iteration matrix. It is also well known (see Varga [5], for example) that using a value slightly larger than ρ is less serious than using an estimate too small by the same amount.

In obtaining an estimate of ρ, one is willing to expend some small fraction of the total computing time required to solve a set of difference equations. If too little attention is given to the estimate of ρ, the convergence rate suffers; if too much effort is spent on estimating ρ, it will not be recovered in the improved convergence rate in the main calculation.

It is the purpose of this paper to show how the Kohn-Kato formula for an upper bound of an eigenvalue (see Crandall [1]) is especially well suited for use in the estimation of ρ for successive over-relaxation.

2. The Kohn-Kato Formula. The following discussion assumes that the matrix Q is symmetric with non-negative eigenvalues. The Kohn-Kato theorem is presented here in the particular context of estimating the spectral radius of Q, although it is much more general.

Let the eigenvalues of Q be

$$0 \leqq \lambda_n \leqq \lambda_{n-1} \leqq \cdots \leqq \lambda_2 < \lambda_1 = \rho,$$

and $\mathbf{x}$ be any vector. Let $(\mathbf{x}, \mathbf{y})$ denote the inner product of the vectors $\mathbf{x}$ and $\mathbf{y}$. Define

$$\gamma = \frac{(\mathbf{x}, Q\mathbf{x})}{(\mathbf{x}, \mathbf{x})}, \qquad \sigma = \frac{(Q\mathbf{x}, Q\mathbf{x})}{(\mathbf{x}, Q\mathbf{x})}, \qquad \epsilon^2 = \frac{(Q\mathbf{x} - \gamma\mathbf{x}, Q\mathbf{x} - \gamma\mathbf{x})}{(\mathbf{x}, \mathbf{x})},$$

and

$$\mu(\alpha) = \gamma + \frac{\epsilon^2}{\gamma - \alpha}, \tag{1}$$

where α is an arbitrary number greater than λ_2. Then the Kohn-Kato theorem states that $\mu \geqq \rho$ whenever $\gamma > \alpha$.

Now suppose that $\mathbf{x}$ is an approximation to the dominant eigenvector of Q. Then σ is probably the most commonly used quantity as an estimate for ρ. Unfortunately, the extremal property of ρ assures that $\sigma \leqq \rho$; that is, σ lies on the more sensitive

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side of ρ. If, instead, $\mu(\alpha)$ is used with $\lambda_2 < \alpha < \gamma$, then the Kohn-Kato theorem asserts that $\mu(\alpha) \geqq \rho$.

It might appear that the use of Eq. (1) to estimate ρ simply shifts the problem to that of estimating λ_2, a much more difficult task to carry out accurately. However, only a crude estimate of λ_2 will do. Moreover, any positive $\alpha < \lambda_2$ will make μ larger than σ. This follows from the observation that $\mu(0) = \sigma$ and $\mu(\alpha)$ is monotone increasing in $0 < \alpha < \gamma$.

Thus, given an approximation to the dominant eigenvector $\mathbf{x}$ and an estimate α of λ_2, then one of the three following cases holds:

(a) $\mathbf{x}$ is exactly the dominant eigenvector and $\mu = \sigma = \gamma = \rho$.

(b) $\mu \geqq \rho$. The error is on the less sensitive side of ρ.

(c) $\sigma \leqq \mu \leqq \rho$. The error is on the more sensitive side of ρ but an improvement over the more conventional modified Rayleigh quotient σ.

It is interesting to note that if $\mathbf{x}$ were a linear combination of only two eigenvectors, those corresponding to ρ and λ_2, and if $\alpha = \lambda_2$, then $\mu = \rho$.

It is possible, of course, that a poor choice of α will cause $\mu(\alpha)$ to be much larger than ρ. However, when $\mathbf{x}$ is a reasonably accurate approximation to the dominant eigenvector and α is the best current estimate of λ_2, then $\mu(\alpha)$ will be quite close to ρ.

When the power method or a polynomial acceleration of the power method is used to construct the approximate eigenvector, $\mu(\alpha)$ requires no appreciable increase of computing time over σ. The current values of $(Q\mathbf{x}, Q\mathbf{x})$ and $(\mathbf{x}, Q\mathbf{x})$ are needed for both, and $(\mathbf{x}, \mathbf{x})$ has already been calculated for the previous iterate.

3. Computational Technique. This method of estimating ρ is easily adapted for use with the cyclic Chebyshev variant of successive over-relaxation presented by Golub and Varga [2]. A brief description follows:

The symmetric algebraic equations to be solved are written in the partitioned matrix form

$$\begin{bmatrix} D_1 & -B \\ -B^t & D_2 \end{bmatrix} \begin{bmatrix} \varphi_1 \\ \varphi_2 \end{bmatrix} = \begin{bmatrix} \mathbf{k}_1 \\ \mathbf{k}_2 \end{bmatrix}.$$

The cyclic Chebyshev iteration is

$$\text{(2a)} \qquad \begin{aligned} D_1 \hat{\varphi}_1^{(2m+1)} &= \mathbf{k}_1 + B\varphi_2^{(2m)}, \\ \varphi_1^{(2m+1)} &= \varphi_1^{(2m-1)} + \omega_{2m+1}[\hat{\varphi}_1^{(2m+1)} - \varphi_1^{(2m-1)}], \end{aligned}$$

$$\text{(2b)} \qquad \begin{aligned} D_2 \hat{\varphi}_2^{(2m+2)} &= \mathbf{k}_2 + B^t \varphi_1^{(2m+1)}, \\ \varphi_2^{(2m+2)} &= \varphi_2^{(2m)} + \omega_{2m+2}[\hat{\varphi}_2^{(2m+2)} - \varphi_2^{(2m)}], \qquad m \geqq 0. \end{aligned}$$

The extrapolation factors ω_j are elements of the sequence

$$\text{(3)} \qquad \begin{aligned} \omega_1 &= 1, \\ \omega_2 &= \frac{2}{2 - q^2}, \\ \omega_{j+1} &= \frac{1}{1 - \frac{q^2}{4}\omega_j}, \qquad j \geqq 2, \end{aligned}$$

where q, $0 < q < 1$, is an estimate of the spectral radius ρ of the matrix

$$\begin{bmatrix} 0 & D_1^{-1}B \\ D_2^{-1}B^t & 0 \end{bmatrix}.$$

From the form of this matrix it follows that ρ^2 is the spectral radius of $H = D_2^{-1}B^tD_1^{-1}B$, a matrix similar to a symmetric matrix and of smaller dimension than the original.

To calculate the spectral radius of H by the "power method," one can set $q = 0$, $\mathbf{k}_1 = \mathbf{0}$, and $\mathbf{k}_2 = \mathbf{0}$ in the iteration (2a, 2b) and (3). The initial vector $\varphi_2^{(0)}$ is an arbitrary nonzero vector. The result is a sequence of vectors $\varphi_2^{(2m)}$ converging to the dominant eigenvector of H. The quantities γ and ϵ^2 were defined in terms of a symmetric matrix $Q = D_2^{1/2}HD_2^{-1/2}$. Application of this transformation and some algebraic manipulation produces sequences γ_{2m} and ϵ_{2m}^2 defined in terms of inner products of vectors already available in the iteration (2b). These redefined quantities are

$$\gamma_{2m} = \frac{(\varphi_2^{(2m)}, B^t\varphi_1^{(2m+1)})}{(\varphi_2^{(2m)}, B^t\varphi_1^{(2m-1)})} \tag{4}$$

and

$$\epsilon_{2m}^2 = \frac{(\varphi_2^{(2m+2)}, B^t\varphi_1^{(2m)})}{(\varphi_2^{(2m)}, B^t\varphi_1^{(2m-2)})} - \gamma_{2m}^2. \tag{5}$$

A rough estimate of λ_2 to be used as the parameter α may be computed from Eq. (5) in a manner proposed by Varga [4],

$$\lambda_2^2 \approx \frac{(\varphi_2^{(2m)}, B^t\varphi_1^{(2m-1)})\epsilon_{2m}^2}{(\varphi_2^{(2m-2)}, B^t\varphi_1^{(2m-3)})\epsilon_{2m-2}^2}. \tag{6}$$

4. Two Examples. The first example is taken from a realistic problem; that of solving the biharmonic problem on a square with boundary values prescribed for the solution and its normal derivative. A uniform mesh of 900 unknown points was used and the difference equations were solved by the two line cyclic Chebyshev method, see Griffin and Varga [3].

Estimates of ρ were formed as described in §3. The results are shown graphically in Figure 1.* To illustrate the effect of α on the estimate, several values were arbitrarily chosen instead of a single value such as from Eq. (6). Of course, any acceleration of the eigenvector calculation will produce a corresponding improvement in each of the curves of Figure 1.

To illustrate the sensitivity of the convergence rate to an accurate value of ρ and the effectiveness of this method in obtaining an adequate approximation, the biharmonic problem described above was solved four times. After 25 iterates of the power method (see Figure 1), μ was computed for three values of α and used as the acceleration parameter. The optimum value ρ was found by experiment. The results appear in Table 1.

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* From a doctoral thesis submitted to the University of Pittsburgh.

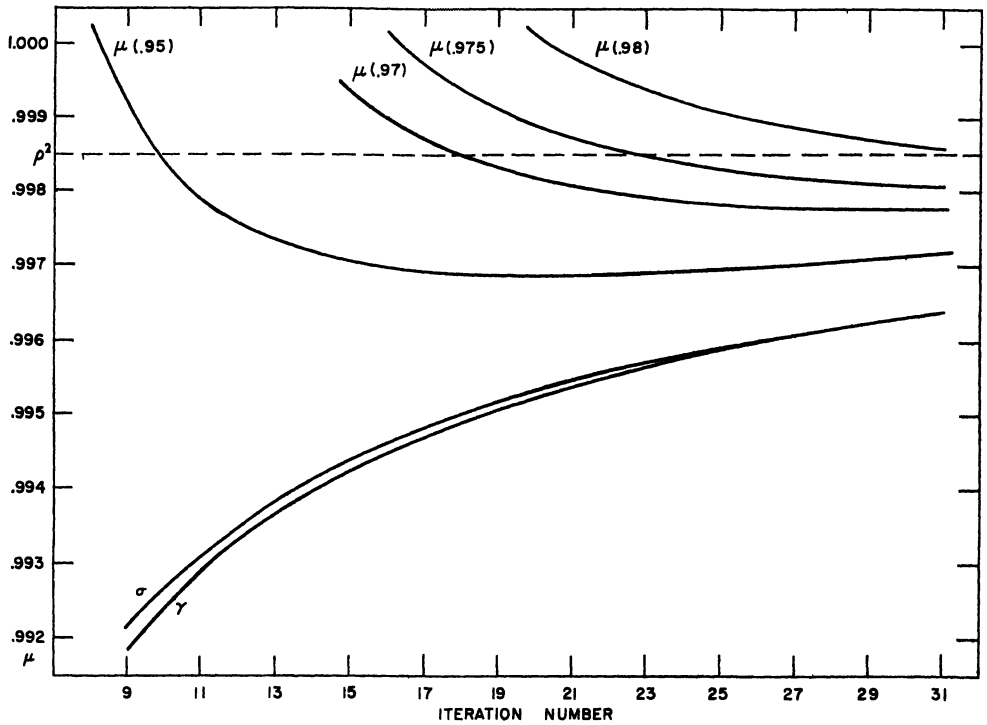

FIGURE 1

TABLE 1

	Acceleration Parameter	Number of Iterations
$\mu(0) = \sigma$	.9960	334
$\mu(.97)$	.9978	263
ρ^2	.9985	117
$\mu(.98)$	.9992	193

The second example is derived from the finite difference approximation of the Dirichlet problem in a square with a uniform mesh of 16 points. The method of solution is the pointwise cyclic Chebyshev method. The purpose of the second example is for comparison between the Kohn-Kato formula, Eq. (1), and another enclosure theorem sometimes used for the same purpose.

This enclosure theorem, due to Collatz [1], states that an eigenvalue λ_j lies in the interval

$$\min_i \frac{(Q\mathbf{x})_i}{(\mathbf{x})_i} \leqq \lambda_j \leqq \max_i \frac{(Q\mathbf{x})_i}{(\mathbf{x})_i}, \qquad j = 1, 2, \cdots, n, \tag{7}$$

where $(\mathbf{x})_i$ denotes the ith component of the vector $\mathbf{x}$. Furthermore, the theory of non-negative matrices [5] gives the more rigorous result that if $\mathbf{x}$ has positive components and Q has non-negative elements than the interval (7) contains the spectral radius ρ. The matrix of example 1 does not have this property. As Crandall [1]

TABLE 2

x_0	x_1	x_2
1	9	93
1	6	58
1	9	93
1	14	150
1	14	150
1	9	93
1	6	58
1	9	93

points out, the Rayleigh quotient, and the formula, Eq. (1), for μ are of second-order accuracy when the eigenvector approximation is of only first-order accuracy. This property is well illustrated in the example.

The matrix of interest is

$$\begin{bmatrix} 3 & 1 & 2 & 2 & 1 & & & \\ 1 & 2 & & 2 & & 1 & & \\ 2 & & 3 & 1 & 2 & & 1 & \\ 2 & 2 & 1 & 4 & 2 & 2 & & 1 \\ 1 & & 2 & 2 & 4 & 1 & 2 & 2 \\ & 1 & & 2 & 1 & 3 & & 2 \\ & & 1 & & 2 & & 2 & 1 \\ & & & 1 & 2 & 2 & 1 & 3 \end{bmatrix}.$$

An initial guess for the dominant eigenvector and two successive power iterates appears in Table 2.

The following quantities are calculated from Table 2.

$$\gamma_1 = 10.4619289,$$

$$\sigma_1 = 10.4711305,$$

$$\epsilon_1^2 = .09626686,$$

$$\lambda_2 \approx 1.07,$$

$$\mu(1.07) = 10.47221,$$

$$\min_i \frac{(x_2)_i}{(x_1)_i} = 9.666666,$$

$$\max_i \frac{(x_2)_i}{(x_1)_i} = 10.71428.$$

If several more iterates are computed one finds that the correct value of the spectral radius is

$$\rho = 10.47214.$$

5. Summary. The proposed method for estimating the spectral radius ρ of a real symmetric matrix is particularly useful when, first, an eigenvector of mediocre

accuracy is available (perhaps from a few iterates of the power method); second, when an over-estimate is preferred to an under-estimate; and third, when no further improvement of the eigenvector is contemplated. These conditions are found in the problem of computing the optimum successive over-relaxation parameter.

No cases have been found for which σ gives a faster convergence rate than $\mu(\alpha)$ for any reasonable value of α. Dangers of many kinds exist for slowly convergent problems but this particular one has not been observed. Furthermore, any increase in convergence rate gained by use of this method reduces the likelihood that the sequence (2a, 2b) and (3) will be terminated by a false convergence indication.

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1. S. H. CRANDALL, *Engineering Analysis, A Survey of Numerical Procedures*, McGraw-Hill, New York, 1956. MR **18**, 674.
2. G. H. GOLUB & R. S. VARGA, "Chebyshev semi-iterative methods, successive over-relaxation methods, and second order Richardson iterative methods. I, II," *Numer. Math.*, v. 3, 1961, pp. 147–168. MR **26** #3207.
3. D. S. GRIFFIN & R. S. VARGA, "Numerical solution of plane elasticity problems," *J. Soc. Indust. Appl. Math.*, v. 11, 1963, pp. 1046–1062. MR **28** #3544.
4. R. S. VARGA, *On Estimating Rates of Convergence in Multigroup Diffusion Problems*, WAPD-TM-41, OTS, U. S. Dept. of Commerce, Washington, D. C., 1957.
5. R. S. VARGA, *Matrix Iterative Analysis*, Prentice-Hall, Englewood Cliffs, N. J., 1962. MR **28** #1725.

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A Practical Application of Block Diagonally Dominant Matrices

By H. S. Price

Introduction. In this note the concept of block diagonally dominant matrices (see references [3], [4], [5]) is applied to a problem from electromagnetic theory. The actual problem considered here is to find the vector potential $P(r, z)$, induced in a piecewise homogeneous, axially symmetric, infinite region Ω, by a current loop of radius r_t located at $z = 0$. Using Maxwell's first two equations (see references [6], [7]), it can be shown that $P(r, z)$ satisfies the following differential equation:

$$(1) \quad \frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial P(r,z)}{\partial r}\right) + \frac{\partial^2 P(r,z)}{\partial z^2} + \left(k^2(r,z) - \frac{1}{r^2}\right)P(r,z) = 0, \qquad (r,z)\in\Omega.$$

The complex-valued function $k^2(r, z)$ is given by

$$(2) \qquad k^2 = \epsilon(r,z)\mu(r,z)\omega^2 - i\mu(r,z)\sigma(r,z)\omega = \alpha(r,z) - i\beta(r,z),$$

where μ is the permeability, σ the conductivity, ϵ the inductive capacity, and ω is the angular frequency. At the source, for a current loop of radius r_t whose plane is normal to the z-axis and whose center is located at the origin, we have

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