A METHOD OF BLOCK ITERATION

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1. Introduction. A method of solving partial difference equations of elliptic type called the *successive overrelaxation* (SOR) *method* was described by Young [1]. He was able to use a Property A possessed by many such systems in order to prove theorems relating the convergence of the simultaneous displacements, Gauss-Seidel and SOR methods. The new method was of importance because a considerable gain in the convergence rate over the Gauss-Seidel method was possible with the use of an optimum "relaxation factor."

The authors have been studying a method of iteration analogous to the SOR method but in which blocks of unknowns are adjusted rather than individual unknowns. This technique finds application in difference systems of elliptic type where the blocks consist of unknowns at grid intersections on a single grid line. This application was first made known to the authors by R. H. Stark of the Knolls Atomic Power Laboratory.

It has been found that the results of [1] can be generalized rather simply to the block methods, using a generalized definition of Property A.

2. Basic definitions and theorems. We consider a system of linear equations

(2.1)
$$\sum_{i=1}^{n} a_{ij} x_{j} = b_{i} \qquad (i = 1, 2, \dots, n),$$

or

$$Ax = b$$

where the unknowns x_i are partitioned into groups numbered $1, 2, \dots, N$. We specify that the unknowns x_i , $i = 1, 2, \dots, n_1$, constitute the first group; the unknowns x_i , $i = (n_1 + 1)$, $(n_1 + 2)$, \dots , n_2 , constitute the second group, in general the unknowns x_i , $i = n_s + 1$, $n_s + 2$, \dots , n_{s+1} , constitute the (s + 1)st group and $n_N = n$.

This partitioning π evidently imposes a partitioning of the matrix $A = (a_{ij})$ into blocks A_{kl} composed of the intersection of the rows whose numbers i satisfy

$$n_{k-1} < i \leq n_k$$

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with the columns whose numbers j satisfy

$$n_{l-1} < j \leq n_e$$
.

Here and in the sequel we indicate blocks by indexed Roman capitals. If $n_1 = 1$, $n_2 = 2$, \cdots , $n_N = n = N$ then the groups are the individual unknowns, and the blocks are the matrix entries.

DEFINITION 2.1. A has Property A^* if there exist two disjoint subsets S and T of W, the set of the first N integers, such that $S \cup T = W$, and if $A_{kl} \neq 0$ then either k = l, or $k \in S$ and $l \in T$, or $k \in T$ and $l \in S$.

This definition is a natural generalization of Young's definition, ([1], p. 92), to the case of block partition and reduces to Young's in the case where $A_{kl} = a_{kl}$. In this latter case we retain the designation "Property A."

DEFINITION 2.2. An ordering N-tuple for A will be an N-tuple $\gamma^{\pi} = (\gamma_1^{\pi}, \gamma_2^{\pi}, \dots, \gamma_N^{\pi})$, where each γ_k^{π} is an integer, such that, if $A_{kl} \neq 0$, and $k \neq l$, then $|\gamma_k^{\pi} - \gamma_l^{\pi}| = 1$.

As with Property A^{π} this definition is a natural generalization of Young's definition of an "ordering vector." The latter, used where $A_{kl} = a_{kl}$, will be designated by γ .

Theorem 2.1. A matrix has Property A^{π} if and only if there exists an ordering N-tuple for A.

The proof is exactly the same as in [1] (Theorem 2.1). If A has Property A^{π} , one takes $\gamma_k^{\pi} = 1$ if $k \in S$ and $\gamma_k^{\pi} = 0$ if $k \in T$. If a γ^{π} exists, one takes S and T to be the sets of integers k such γ_k^{π} is odd and even, respectively.

DEFINITION 2.3. A matrix A will be said to be ordered by γ^{π} if, whenever $A_{kl} \neq 0$ and $\gamma_{k}^{\pi} > \gamma_{l}^{\pi}$, the kth row of blocks follows the lth row, and, whenever $\gamma_{l}^{\pi} > \gamma_{k}^{\pi}$, the lth row follows the kth row. This is a generalization of the definition of a consistent ordering in [1].

Theorem 2.2. If $A=(A_{kl})$ has Property A^{π} and $|A_{kk}| \neq 0$ for all k and if

$$(2.2) B = -C^{-1}A + I,$$

where

$$C = \begin{pmatrix} \ddots & 0 \\ & A_{kk} \\ 0 & \ddots \end{pmatrix},$$

then B has Property A.

PROOF

$$C^{-1} = \begin{pmatrix} & \ddots & & 0 & \\ & & A_{kk}^{-1} & & \\ & 0 & & \ddots & \end{pmatrix}$$

so that B plainly exists. If A has Property A^{π} , there exists a γ^{π} for A by Theorem 2.1.

Now

$$B = (B_{kl}) = \begin{cases} -A_{kk}^{-1} A_{kl} & (k \neq l), \\ 0 & (k = l), \end{cases}$$

and we can define a γ for B as follows: If $b_{ij} \neq 0$ and $i \neq j$ then set $\gamma_i = \gamma_k^{\pi}$ and $\gamma_j = {\gamma_l}^{\pi}$, where B_{kl} is the block containing b_{ij} . Now $b_{ij} \neq 0$ and $i \neq j$ implies that $A_{kl} \neq 0$ and $k \neq l$. Therefore $|\gamma_i - \gamma_j| = |\gamma_k^{\pi} - {\gamma_l}^{\pi}| = 1$, which assures that γ is indeed an ordering n-tuple. By Theorem 2.1, B must have Property A. Furthermore, if A is ordered by γ^{π} then B will be ordered by γ .

THEOREM 2.3. If A is symmetric and A_{ii} is positive definite for each i, then B has real eigenvalues.

PROOF. If A_{ii} is positive definite then $A_{ii} = P_i D_i P_i'$ where D_i is a diagonal matrix with positive entries and P_i' is orthogonal. We can define a square root for A_{ii} by

$$A_{ii}^{\frac{1}{2}} = P_i D_i^{\frac{1}{2}} P_i',$$

and for C by

$$C^{\frac{1}{2}} = \left(egin{array}{ccc} \cdot & & & 0 & \\ & A^{\frac{1}{2}}_{ii} & & \\ 0 & & \ddots & \end{array}
ight).$$

It can easily be shown that $C^{-\frac{1}{2}}$ exists and is the inverse of $C^{\frac{1}{2}}$ as well as the square root of C^{-1} . These matrices are all symmetric. Thus

$$B^* = C^{\frac{1}{2}}BC^{-\frac{1}{2}}$$

$$= -C^{\frac{1}{2}}C^{-1}AC^{-\frac{1}{2}} + C^{\frac{1}{2}}IC^{-\frac{1}{2}}$$

$$= -C^{-\frac{1}{2}}AC^{-\frac{1}{2}} + I,$$

and

$$B^{*\prime} = B^*.$$

Since B is similar to the symmetric matrix B^* it has real eigenvalues.

3. Generalization of Young's results. Equations 2.1 can be written in the block form

(3.1)
$$\sum_{l=1}^{N} A_{kl} \mathbf{x}_{l} = \mathbf{b}_{k} \qquad (k = 1, 2, \dots, N),$$

where

$$\mathbf{x}_{l+1} = (x_{n_{l+1}}, x_{n_{l+2}}, \cdots, x_{n_{l+1}})$$

and

$$\mathbf{b}_{k+1} = (b_{n_k+1}, b_{n_k+2}, \cdots, b_{n_{k+1}}).$$

If $|A_{kk}| \neq 0$ for all k, these equations can be written

(3.2)
$$\mathbf{x}_{k} = -\sum_{l \neq k} A_{kk}^{-1} A_{kl} \mathbf{x}_{l} + A_{kk}^{-1} \mathbf{b}_{k}.$$

We can define an iterative sequence of vectors $\mathbf{x}_k^{(t)}$ analogous to the SOR method by

(3.3)
$$\mathbf{x}_{k}^{(t+1)} = \omega \left[-\sum_{l=1}^{k-1} A_{kk}^{-1} A_{kl} \mathbf{x}_{l}^{(t+1)} - \sum_{l=k+1}^{N} A_{kk}^{-1} A_{kl} \mathbf{x}_{l}^{(t)} + A_{kk}^{-1} \mathbf{b}_{k} \right] + (1 - \omega) \mathbf{x}_{k}^{(t)} \quad (k = 1, 2, \dots, N).$$

It will be observed that A_{kk} is a square matrix of order n_k , A_{kl} is a rectangular matrix of dimension n_k by n_l and \mathbf{x}_l is a vector of order n_l , so that all matrix operations are defined. Now, if one defines the error vectors

$$\mathbf{e}_{k}^{(t)} = \mathbf{x}_{k}^{(t)} - \mathbf{x}_{k}, \quad k = 1, 2, \dots, N, \quad \mathbf{e}^{(t)} = \mathbf{x}^{(t)} - \mathbf{x},$$

it is easily shown that

$$(3.4) \quad \mathbf{e}_{k}^{(t+1)} = \omega \left[-\sum_{l=1}^{k-1} A_{kk}^{-1} A_{kl} \mathbf{e}_{l}^{(t+1)} - \sum_{l+k+1}^{N} A_{kk}^{-1} A_{kl} \mathbf{e}_{l}^{(t)} \right] + (1-\omega) \mathbf{e}_{k}^{(t)}.$$

But this is equivalent to the matrix equation

$$(3.5) E\mathbf{e}^{(t+1)} = F\mathbf{e}^{(t)}.$$

where

$$E = (E_{kl}) = \begin{cases} I_{kk} & (k = l), \\ \omega A_{kk}^{-1} A_{kl} & (k > l), \\ 0 & (k < l), \end{cases}$$

and

$$F = (F_{kl}) = \begin{cases} (1 - \omega)I_{kk} & (k = l), \\ 0 & (k > l), \\ -\omega A_{kk}^{-1} A_{kl} & (k < l), \end{cases}$$

and $|E| \neq 0$. Now the eigenvalues of the iterative procedure (3.3) are the values of λ for which

$$(3.6) H_{\omega} \mathbf{e} = E^{-1} F \mathbf{e} = \lambda \mathbf{e} \text{ for } \mathbf{e} \neq 0,$$

and therefore are the solutions of

$$(3.7) |G| = |F - \lambda E| = 0$$

where

(3.8)
$$G = (G_{kl}) = \begin{cases} (1 - \omega - \lambda) I_{kk} & (k = l), \\ -\omega \lambda A_{kk}^{-1} A_{kl} & (k > l), \\ -\omega A_{kk}^{-1} A_{kl} & (k < l). \end{cases}$$

Thus we have

Theorem 3.1. The eigenvalues of the iteration procedure (3.3) are solutions of |G| = 0 where G is given by (3.8).

Now we assume that A has Property A^{π} and is ordered by some γ^{π} . We know from Theorem 2.2 that B has Property A and is ordered by the γ derived from γ^{π} . The same obviously applies to G and an inspection of G shows that it has the form

$$G = (g_{ij}) = \begin{cases} (1 - \omega - \lambda) & (i = j), \\ \omega \lambda b_{ij} & (i > j), \\ \omega b_{ij} & (i < j). \end{cases}$$

We have now displayed matrices B and G which relate respectively, to the iterative methods of simultaneous block displacements (defined by $\mathbf{e}^{(t+1)} = B\mathbf{e}^{(t)}$) and successive block overrelaxation. The matrices B and G have the same properties as do their analogues in [1]. Specifically B and G have Property A when A has Property A^{π} , B has real eigenvalues when A is symmetric and positive definite, and G has the same form with regard to B as in [1]. Finally, it is possible to generalize a theorem of Geiringer's [2] quoted for use in the proof of Corollary 2.2, [1], p 100. One gets

Theorem 3.2. If A is symmetric and A_{kk} is positive definite for each k then the method of successive block displacements (equation (3.3) with $\omega = 1$) converges if, and only if, A is positive definite.

The proof is similar to that in [2], p. 389, except that blocks must be manipulated rather than entries.

It therefore follows that the results of [1] may be applied to the method of successive block overrelaxation. These results will now be briefly outlined in their generalized form.

Property A and an ordering of A (or B) allow one to show that |G| = |G'|, where

$$g'_{ij} = \begin{cases} 1 - \omega - \lambda & (i = j), \\ \lambda^{\frac{1}{2}} \omega b_{ij} & (i \neq j), \end{cases}$$

and that if μ is a k-fold eigenvalue of B, then so also is $-\mu$. These results lead to the theorem ([1], Theorem 2.3).

THEOREM 3.3. Let A be a matrix with Property A^* , ordered by some γ^* . If $\omega \neq 0$, and if λ is a non-zero eigenvalue of H^{ω} , and if μ satisfies

$$(3.9) \qquad (\lambda + \omega - 1)^2 = \omega^2 \mu^2 \lambda,$$

then μ is an eigenvalue of B. If μ is an eigenvalue of B and if λ satisfies (3.9), then λ is an eigenvalue of H_{ω} .

Equation (3.9) leads to an explicit formula for the optimal relaxation factor ω_b in terms of $\bar{\mu}$ (the spectral norm of B) when the matrix A is symmetric and positive definite. The value of ω_b is optimal in the sense that the spectral norm $\bar{\lambda}$ is minimal and so the convergence rate is greatest. The relations are

(3.10)
$$\omega_b = \frac{2}{1 + (1 - \bar{\mu}^2)^{\frac{1}{2}}},$$

$$\bar{\lambda}(\omega_b) = \omega_b - 1.$$

Under these circumstances one can obtain an asymptotic relation (as $\bar{\mu} \to 1$) between the rate of convergence $R(H_1)$ of the successive block displacements method and the rate $R(H_{\omega b})$ of the optimal successive block overrelaxation method. As in [1], p. 96, we define the rates by

$$R(H_{\omega}) = -\log \bar{\lambda}(\omega).$$

The relation mentioned is

(3.13)
$$R(H\omega_b) \sim 2[R(H_1)]^{\frac{1}{2}}$$

([1], Theorem 3.3).

4. Application of the SBOR method to the equation $\nabla^2 \varphi - A\varphi = B$, rectangular region. Consider the problem of finding a function φ which satisfies the elliptic partial differential equation,

(4.1)
$$\nabla^2 \varphi - A \varphi = B \quad (A \ge 0 \text{ and constant}, B = B(x, y))$$

in the interior of the rectangle x = 0, x = a, y = 0, y = b and has prescribed values on the boundary. An approximate solution can be obtained by covering the region with the grid whose lines are

$$x = nh$$
 $(n = 0, 1, 2, \dots, N = a/h),$
 $y = mh$ $(m = 0, 1, 2, \dots, M = b/h),$

and replacing the differential equation by a difference equation for the function $\phi(n, m)$ defined at the grid intersections. We replace the derivatives in (4.1) by their usual five point difference approximations and get the equations

$$\frac{1}{h^2} [\phi(n+1,m) + \phi(n-1,m) + \phi(n,m-1) + \phi(n,m+1) - 4\phi(n,m)] - A\phi(n,m) = B(n,m)$$

$$(n = 1, 2, \dots, N-1, m = 1, 2, \dots, M-1),$$

 $\phi(0, m)$, $\phi(N, m)$, $\phi(n, 0)$, $\phi(n, M)$ prescribed. The iterative method of successive line displacements is defined by the equations

(4.4)
$$\phi^{(t+1)}(n,m) = \frac{1}{4 + Ah^2} [\phi^{(t+1)}(n+1,m) + \phi^{(t+1)}(n-1,m) + \phi^{(t+1)}(n,m-1) + \phi^{(t)}(n,m+1) - h^2 B(n,m)],$$

$$\phi^{(t)}(0,m) = \phi(0,m), \text{ etc.},$$

and $\phi^{(0)}(n, m)$ arbitrary for $n \neq 0, N, m \neq 0, M$. The quantities $\phi^{(t)}(n, m)$ are the t'th trial values of $\phi(n, m)$. The descriptive term "successive line displacements" refers to the fact that for each m, in increasing order, a solution of the system of simultaneous linear equations in the variables $\phi^{(t+1)}(0, m), \phi^{(t+1)}(1, m), \cdots, \phi^{(t+1)}(N, m)$ is obtained. As can be seen from the equivalent form

$$(4.5) - \phi^{(t+1)}(n-1, m) + (4 + Ah^2) \phi^{(t+1)}(n, m) - \phi^{(t+1)}(n+1, m)$$
$$= \phi^{(t+1)}(n, m-1) + \phi^{(t)}(n, m+1) - h^2B(n, m),$$

each subsystem has a coefficient matrix of the form

(4.6)
$$\begin{bmatrix} 4 + Ah^2 & -1 & & 0 \\ -1 & 4 + Ah^2 & \ddots & & \\ & \ddots & \ddots & -1 \\ 0 & & -1 & 4 + Ah^2 \end{bmatrix}.$$

This is a matrix of Jacobi type and can easily be inverted by a simple elimination algorithm (see, for example, Peaceman and Rachford [3], p. 34). The unknowns ϕ (n, m) for fixed m are evidently the groups of unknowns numbered $1, 2, \dots, m, \dots, M-1$ of Section (3), and the matrices (4.6) are the blocks A_{kk} . This determines the partitioning π . A γ^{π} for the matrix A, whose coefficients can be determined from (4.3), is defined by $\gamma_m^{\pi} = m$.

Using the methods of Frankel [4] one can find the eigenvalues of (4.4). If $\phi^{(t)}(n, m) - \phi(n, m) = e^{(t)}(n, m)$, and λ is an eigenvalue of the matrix operation H defined by $e^{(t+1)} = He^{(t)}$, then the eigenvalues will be solutions of

(4.7)
$$\lambda e(n,m) = \frac{1}{4 + Ah^2} [\lambda e(n+1,m) + \lambda e(n-1,m) + \lambda e(n,m-1) + e(n,m+1)],$$

e(0, m) = e(N, m) = e(n, 0) = e(n, M) = 0, $e(n, m) \not\equiv 0$). It can be verified that

(4.8)
$$e_{p,q}(n,m) = \lambda^{m/2} \sin \frac{p\pi n}{N} \sin \frac{q\pi m}{M}$$

$$(p = 1, 2, \dots, N-1, q = 1, 2, \dots, M-1),$$

contain all the eigenvectors corresponding to non-zero eigenvalues and that the eigenvalues satisfy the equation

$$(4.9) (4 + Ah^2)\lambda = 2\lambda \cos \frac{p\pi}{N} + 2\lambda^{\frac{1}{2}} \cos \frac{q\pi}{M}.$$

The non-zero eigenvalues are, therefore,

$$\lambda_{p,q} = \left[\frac{\cos \frac{q\pi}{M}}{2 + Ah^2/2 - \cos p\pi/N} \right]^2$$

Now consider the iteration scheme defined by

$$(4.10) \quad \psi^{(t+1)}(n,m) = \frac{1}{4 + Ah^2} \left[\psi^{(t+1)}(n+1,m) + \psi^{(t+1)}(n-1,m) + \varphi^{(t+1)}(n,m-1) + \varphi^{(t)}(n,m+1) - h^2 B(n,m) \right]$$

$$\phi^{(t+1)}(n,m) = \omega \psi^{(t+1)}(n,m) + (1-\omega)\phi^{(t)}(n,m)$$

with prescribed boundary values, and $\phi^{(0)}$ arbitrary. These equations describe the successive line (block) overrelaxation method and are of the type defined by (3.3). They reduce to (4.4) when $\omega = 1$.

It can be shown that the matrix A defined by (4.3) is symmetric and positive definite. Substituting $\omega = 1$ into (3.9) we get the relation between the eigenvalues of the simultaneous displacements and successive displacements methods.

$$\lambda = \mu^2.$$

Thus

$$\mu_{p,q} = \frac{\cos\frac{q\pi}{M}}{2 + \frac{Ah^2}{2} - \cos\frac{p\pi}{N}}.$$

Evidently $\bar{\mu}$ is that value of μ for which p = q = 1. For large values of M and N, equations (3.10) and (3.11) give the approximate results

(4.12)
$$\omega_b \cong 2 - 2h\sqrt{C}, \\ \bar{\lambda}(\omega_b) \cong 1 - 2h\sqrt{C},$$

where

$$C = A + \pi^2 \left(\frac{1}{a^2} + \frac{1}{\overline{b^2}} \right).$$

These results may also be obtained directly using the same arguments as are found in [4]. The spectral norm given in (4.12) compares favorably with that for the same problem using the SOR method ($\tilde{\lambda} \cong 1 - h\sqrt{2C}$).

Using an extension of the methods of [5], it can be shown that an advantage is always obtained by using successive block overrelaxation (rather than SOR) when the (sufficient) conditions

(i)
$$|A| \neq 0$$
,
(ii) $\sum_{\substack{j=1\\j\neq 1}}^{n} |a_{ij}| \leq a_{ii}$,
(ii) $a_{ij} \leq 0$ $(i \neq j)$.

are satisfied. Counter examples have been constructed, however, to show that this is not true in general, even for positive definite matrices.

In [6], Sheldon has demonstrated that reversing the order of iteration in the SOR method produces an iteration operator with real non-negative eigenvalues, when A is symmetric, positive definite, and has Property A. A similar demonstration will give the same result for the SBOR method under the hypothesis that A has Property A^{\dagger} , symmetry, and positive definiteness.

An advantage of the block methods is that there is less restriction on the difference equations in order to preserve Property A^{π} . For example, a nine point difference approximation is permissible using line relaxation but not using point relaxation. Also, individual points may be deleted using block iteration although termination of lines (accompanying changes in grid size, for example) causes trouble. This can most easily be seen from the obser-

vation that with respect to line iteration, Property A^{τ} means that the lines (blocks) may be divided into two groups, and that unknowns on a given line in one group are expressed as linear combinations of unknowns on the *same* line or on lines of the *other* group only.

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