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Factorization and Normalized Iterative Methods

§1. Introduction

In studying the literature on iterative methods for solving elliptic difference equations, one finds that these iterative methods can be phrased so that they all depend upon the ability to directly solve appropriate matrix equations in few unknowns. In some cases, such as the Young-Frankel successive overrelaxation iterative method [38, 10] and the Richardson iterative method [24,39], the matrix equations to be directly solved involve only one linear equation in one unknown. In the other cases, such as the Peaceman-Rachford iterative method [21], and the Douglas-Rachford iterative method [8], tridiagonal matrix equations are directly solved. While the idea of group relaxation [19, 13, 4], the direct solution of matrix equations in few unknowns, has for some time been recognized to be advantageous, it appears that only the systematic direct solution of tridiagonal matrix equations has gained popularity in practical machine codes for solving elliptic difference equations.

The main purpose of this article is to introduce a class of iterative methods which depend upon the direct solution of matrix equations involving matrices more general than tridiagonal matrices. We shall show how these appropriate matrix equations can be directly and efficiently solved, and we shall show in addition how standard methods for accelerating convergence can be applied.

§2. Regular Splittings

We seek to solve the matrix equation

$$A\underline{x} = \underline{k} \ , \tag{2.1}$$

where $A = (a_{i,j})$ is a given $n \times n$ non-singular matrix, and $\underline{k}$ is a given column vector with n components. As in [17], we split the matrix A into

$$A = B - C \ , \tag{2.2}$$

where B and C are $n \times n$ matrices. If, for an arbitrary $n \times n$

matrix M , M has nonnegative entries, we write $M \geq 0$. If M has only positive entries, we write $M > 0$. Similarly, if the matrix $M_1 - M_2$ has nonnegative entries, we write $M_1 \geq M_2$.

Definition 1. $A = B - C$ is a regular splitting of A if and only if $B^{-1} \geq 0$ and $C \geq 0$.

In what is to follow, we assume that matrix equations of the form

$$(2.3) \qquad B\underline{x} = \underline{g} ,$$

where $\underline{g}$ is a given column vector, can be directly solved for the vector $\underline{x}$. If (2.2) represents a regular splitting of A , then the iterative method

$$(2.4) \qquad B\underline{x}^{(m+1)} = C\underline{x}^{(m)} + \underline{k} , \quad m = 0, 1, 2, \ldots ,$$

where $\underline{x}^{(0)}$ is an arbitrary vector, can be carried out. Equivalently, we write (2.4) in the form

$$(2.4') \qquad \underline{x}^{(m+1)} = B^{-1} C\underline{x}^{(m)} + B^{-1} \underline{k} , \quad m = 0, 1, 2, \ldots .$$

The matrix $D \equiv B^{-1}C$ has non-negative entries if (2.2) represents a regular splitting of A . Using (2.2), we express the matrix D as

$$(2.5) \qquad D = (A + C)^{-1} C = (I + A^{-1}C)^{-1} A^{-1} C .$$

If $E \equiv A^{-1}C$, then

$$(2.5') \qquad D = (I + E)^{-1}E .$$

If $A^{-1} > 0$, and $A = B - C$ is a regular splitting of A , then the matrix E has only non-negative entries. If, for an arbitrary square matrix M , $\bar{\mu}[M]$ denotes the spectral radius of M ,i.e. $\bar{\mu}[M] = \max_k |\lambda_k|$, where λ_k is an eigenvalue of M , then we say M is convergent if and only if $\bar{\mu}[M] < 1$.

Lemma 1. If $A = B - C$ is a regular splitting of A and $A^{-1} > 0$, then

$$(2.6) \qquad \bar{\mu}[D] = \frac{\bar{\mu}[E]}{1 + \bar{\mu}[E]} ,$$

and the matrix D is convergent.

Proof. It is clear from (2.5') that eigenvectors of E are also eigenvectors of D . Thus, if $E\underline{a}_j = \lambda_j \underline{a}_j$, then $D\underline{a}_j = \frac{\lambda_j}{1 + \lambda_j} \underline{a}_j$.

Since both D and E are non-negative matrices, the result of (2.6) is an immediate consequence of the Perron-Frobenius theory of non-negative matrices [22, 12, 7]. From (2.6) it follows that $\bar{\mu}[D] < 1$ and thus D is convergent.

As a consequence of this lemma, the iterative method of (2.4) is necessarily convergent.

We now assume that $A = B_1 - C_1 = B_2 - C_2$ are two regular splittings of A. With $D_i \equiv B_i^{-1} C_i$, we now compare the spectral radii of the matrices D_1 and D_2.

<u>Theorem 1.</u> Let $A = B_1 - C_1 = B_2 - C_2$ be two regular splittings of A, where $A^{-1} > 0$. If $C_2 \geq C_1 \geq 0$, equality excluded*, then

$$1 > \bar{\mu}[D_2] > \bar{\mu}[D_1] > 0 . \tag{2.7}$$

<u>Proof.</u> From (2.6), $\bar{\mu}[D]$ is monotone with respect to $\bar{\mu}[E]$, and it thus suffices to prove that $\bar{\mu}[E_2] > \bar{\mu}[E_1] > 0$. Since $C_2 \geq C_1 \geq 0$, equality excluded. and $A^{-1} > 0$, it follows that $E_2 \geq E_1 \geq 0$, equality excluded. We first assume that the matrix E_1 is irreducible, i.e. there exists no $n \times n$ permutation matrix Λ such that

$$\Lambda E_1 \Lambda^{-1} = \begin{bmatrix} E^{(1)}_{1,1} & E^{(1)}_{1,2} \\ 0 & E^{(1)}_{2,2} \end{bmatrix}, \tag{2.8}$$

where $E^{(1)}_{1,1}$ and $E^{(1)}_{2,2}$ are square submatrices. With E_1 irreducible, and $E_2 \geq E_1 \geq 0$, equality excluded, it follows [7, p. 598] that $\bar{\mu}[E_2] > \bar{\mu}[E_1] > 0$. If E_1 is reducible, let Λ be $n \times n$ permutation matrix for which (2.8) is valid. With

$$\Lambda A^{-1} \Lambda^{-1} \equiv \begin{bmatrix} M_{1,1} & M_{1,2} \\ M_{2,1} & M_{2,2} \end{bmatrix}; \Lambda C_1 \Lambda^{-1} \equiv \begin{bmatrix} C^{(1)}_{1,1} & C^{(1)}_{1,2} \\ C^{(1)}_{2,1} & C^{(1)}_{2,2} \end{bmatrix}, \tag{2.9}$$

then since $A^{-1} > 0$ and $E_1 = A^{-1} C_1$, it follows from (2.8) that both $C^{(1)}_{1,1}$ and $C^{(1)}_{2,1}$ are null, and thus $E^{(1)}_{1,1}$ is also null. Thus, if E_1 is reducible, we may assume in (2.8) that $E^{(1)}_{1,1}$ is null, and that $E^{(1)}_{2,2}$ is irreducible since $E_1 \geq 0$, equality excluded. The non-zero eigenvalues of the matrix E_1 are just the non-zero eigenvalues of the irreducible nonnegative submatrix $E^{(1)}_{2,2}$, and $\bar{\mu}[E_1] = \bar{\mu}[E^{(1)}_{2,2}] > 0$. Actually, the irreducibility of $E^{(1)}_{2,2}$ and

$A^{-1} > 0$ imply that $E^{(1)}_{2,2} > 0$ and $E^{(1)}_{1,2} > 0$. Since $C_2 \geq C_1$, equality excluded, then either $E^{(2)}_{2,2} \geq E^{(1)}_{2,2}$, equality excluded, or else $E^{(1)}_{2,2} = E^{(2)}_{2,2}$ is a principal minor of a larger irreducible square submatrix of E_2 , and thus [7], $\bar{\mu}[E_2] > \bar{\mu}[E_1]$, which completes the proof.

The result of Theorem 1 is a generalization of recent results of Householder [16, Theorems 4.12 and 4.13], which generalize results of Fiedler and Pták [9]. The basic idea for this result, however, goes back to the work of Stein and Rosenberg [26]. The particular setting of Theorem 1 will be convenient, as we shall see, for applications to the numerical solution of elliptic difference equations.

It is not difficult to find matrices A which admit regular splittings, and have $A^{-1} > 0$. In fact, consider any $n \times n$ matrix $A = (a_{i,j})$ having the following properties:

(2.10) 1. $a_{i,j} \leq 0$ for all $i \neq j$, $1 \leq i$, $j \leq n$.

2. A is irreducible.

3. $\Sigma^{n}_{j=1} a_{i,j} \geq 0$ for all $1 \leq i \leq n$, with strict inequality for some i .

It follows [7] that A^{-1} has positive entries. From the conditions of (2.10), the diagonal entries of A are positive. Thus, if B is the positive diagonal matrix derived from the diagonal entries of A , then $B^{-1} \geq 0$, and defining $C \equiv B - A$, it follows that $C \geq 0$. Thus $A = B - C$ is a regular splitting of A . Generalizing, if B is any matrix derived from the matrix A satisfying (2.10) by setting certain off-diagonal entries of A to zero, then $B^{-1} \geq 0$ [7, 37], and $A = B - C$ represents a regular splitting of A . Of considerable practical interest is the fact that five-point discrete approximations on a rectangular mesh to the self-adjoint elliptic partial differential equation

$$(2.11) \quad -\nabla \cdot (D \nabla u) + \Sigma u = S \, , \; \Sigma(\underline{x}) \geq 0 \, , \; D(\underline{x}) > 0 \, , \; S = S(\underline{x})$$

for general bounded regions in the plane with suitable boundary conditions, can be derived [31] so that the resulting matrix A , determined by the associated system of linear equations, satisfies (2.10). If a matrix A satisfying (2.10) is symmetric, then it is positive definite [29]. Irreducible symmetric and positive definite matrices A with non-positiv off-diagonal entries are called Stieltjes matrices [3] and for these matrices, it is also known that $A^{-1} > 0$. The original idea for this goes back to an early result of Stieltjes [28].

Lemma 2. Let A be a Stieltjes matrix, and let $A = B - C$ be a regular splitting of the matrix A , where C is symmetric. Then

$$\text{(2.12)} \qquad \bar{\mu}[D] \leq \frac{\bar{\mu}[C]\,\bar{\mu}[A^{-1}]}{1+\bar{\mu}[C]\,\bar{\mu}[A^{-1}]} ,$$

with equality if the matrices A and C commute.

Proof. It suffices to show that $\bar{\mu}[A^{-1}C] \leq \bar{\mu}[A^{-1}]\cdot\bar{\mu}[C]$. For symmetric matrices, it is known [16, p. 219] that the value of the spectral norm is that of the spectral radius. Hence, since A^{-1} and C are symmetric, $\bar{\mu}[A^{-1}C] \leq \|A^{-1}C\| \leq \|A^{-1}\|\cdot\|C\| = \bar{\mu}[A^{-1}]\cdot\bar{\mu}[C]$, from which the inequality of (2.12) follows.

If M is an arbitrary convergent matrix, the rate of convergence [38] of the matrix M is defined by the positive quantity

$$\text{(2.13)} \qquad R(M) = -\ell n\, \bar{\mu}[M] .$$

Theorem 2. Let A be a Stieltjes matrix, and let $A = B_1 - C_1 = B_2 - C_2$ be two regular splittings of A , with $0 \leq C_1 \leq C_2$, equality excluded. If C_1 and C_1 are symmetric and $\bar{\mu}[E_1] \to +\infty$, then

$$\text{(2.14)} \qquad \frac{R(D_1)}{R(D_2)} \sim \frac{\bar{\mu}[E_2]}{\bar{\mu}[E_1]} .$$

Moreover, if C_2 commutes with A , then

$$\text{(2.15)} \qquad \frac{\bar{\mu}[E_2]}{\bar{\mu}[E_1]} \geq \frac{\bar{\mu}[C_2]}{\bar{\mu}[C_1]} > 1 .$$

Proof. From the proof of Theorem 1, $\bar{\mu}[E_2] > \bar{\mu}[E_1]$, and from (2.6) we have that

$$R(D_i) = +\ell n\left(1 + \frac{1}{\bar{\mu}[E_i]}\right) = \frac{1}{\bar{\mu}[E_i]} + 0\left(\frac{1}{\bar{\mu}^{-2}[E_i]}\right), \text{ as } \bar{\mu}[E_i] \to +\infty ,$$

and (2.14) follows. If C_2 commutes with A, the inequalities of (2.15) follow respectively from the proof of Theorem 1, Lemma 2, and the assumption that $C_2 \geq C_1 \geq 0$.

We shall later find it convenient to compare the rates of convergence of two iterative methods by means of the (2.14) and (2.15).

§3. Acceleration Methods

We shall henceforth assume that A is a Stieltjes matrix, and (2.2) represents a regular splitting of A , where B is symmetric and positive definite. It follows that C is symmetric and has nonnegative entries. Again we assume that matrix equations of the form (2.3) can be directly solved.

The first acceleration method which we consider is the Young-Frankel successive overrelaxation iterative method [38, 10], and its generalization by Arms, Gates, and Zondek [1]. If the matrix A and the column vectors $\underline{x}$ and $\underline{k}$ are partitioned into the form

(3.1)
$$A = \begin{bmatrix} A_{1,1} & A_{1,2} \cdots A_{1,N} \\ A_{2,1} & A_{2,2} \cdots A_{2,N} \\ \vdots & \vdots \\ A_{N,1} & A_{N,2} \cdots A_{N,N} \end{bmatrix}, \quad \underline{x} = \begin{bmatrix} X_1 \\ X_2 \\ \vdots \\ X_N \end{bmatrix}, \quad \underline{k} = \begin{bmatrix} K_1 \\ K_2 \\ \vdots \\ K_N \end{bmatrix},$$

where the diagonal submatrices $A_{j,j}$ are square, we can write (2.1) equivalently as

$$\text{(3.2)} \qquad \sum_{j=1}^{N} A_{i,j} X_j = K_i \ , \ i = 1, 2, \ldots, N \ .$$

Let B be the diagonal block matrix

(3.3)
$$B = \begin{bmatrix} A_{1,1} & 0 & \cdots 0 \\ 0 & A_{2,2} & \cdots 0 \\ \vdots & & \vdots \\ 0 & 0 & \cdots A_{N,N} \end{bmatrix},$$

and let the matrix C be defined by $A = B - C$. Since A is a Stieltjes matrix, then B and C are both symmetric, and $C \geq 0$. Since B is the direct sum of principal minors of A, then B is positive definite, with non-positive off-diagonal entries. It follows [2] that $B^{-1} \geq 0$, and hence, for this definition of the matrices B and C, we have a regular splitting of A. The successive over-relaxation iterative method, applied to (3.2), is defined by

$$\text{(3.4)} \quad X_i^{(m+1)} = X_i^{(m)} + \omega \left\{ A_{i,i}^{-1} \left(-\sum_{j<i} A_{i,j} X_j^{(m+1)} - \sum_{j>i} A_{i,j} X_j^{(m)} + K_i \right) - X_i^{(m)} \right\},$$

$m = 0, 1, 2, \ldots, i = 1, 2, \ldots, N$, where $\underline{x}^{(0)}$ is an arbitrary vector. The quantity ω is the <u>relaxation factor.</u> In actual computations, the equivalent form of (3.4)

$$\text{(3.5)} \quad A_{i,i} \overset{*}{X}_i^{(m+1)} = -\sum_{j<i} A_{i,j} X_j^{(m+1)} - \sum_{j>i} A_{i,j} X_j^{(m)} + K_i, \ i=1,2,\ldots,N,$$

and

$$(3.5') \quad X_i^{(m+1)} \equiv X_i^{(m)} + \omega \left\{ \overset{*}{X}_i^{(m+1)} - X_i^{(m)} \right\}, \quad i = 1, 2, \ldots, N,$$

may be more useful. We now assume that the matrix A satisfies property A^π, and is (consistently) ordered [1]. We write (3.4) in the form

$$(3.6) \quad \underline{x}^{(m+1)} = \mathscr{L}_\omega \underline{x}^{(m)} + \underline{g}, \quad m = 0, 1, 2, \ldots,$$

where $\mathscr{L}_\omega$ denotes the successive overrelaxation iteration matrix. Since A is by assumption a Stieltjes matrix, and B is, by construction, symmetric and positive definite, we can apply directly the results of Arms, Gates, and Zondek [1], which generalized Young's original results [38], and we obtain

Theorem 3. Let the partitioned Stieltjes matrix A of (3. 1) satisfy property A^π and be (consistently) ordered. Then, the optimum value of ω, ω_b, which minimizes $\overline{\mu}[\mathscr{L}_\omega]$ as a function of the real variable ω, is given by

$$(3.7) \qquad \omega_b = \frac{2}{1+\sqrt{1-\overline{\mu}^2[D]}},$$

and

$$(3.8) \qquad \overline{\mu}[\mathscr{L}_{\omega_b}] = \omega_b - 1.$$

Moreover, as $\overline{\mu}[D] \to 1-$, then

$$(3.9) \qquad R(\mathscr{L}_{\omega_b}) \sim 2\sqrt{2}\,[R(D)]^{\frac{1}{2}}.$$

Since ω_b of (3.7) increases monotonically with $\overline{\mu}[D]$, we obtain from Theorems 2 and 3 the following

Corollary 1. Let $A = B_1 - C_1 = B_2 - C_2$ be two regular splittings of the Stieltjes matrix A, where $0 \leq C_1 \leq C_2$, equality excluded. Let B_1 and B_2 be diagonal block matrices, as in (3. 3), derived from different partitionings of A, where each partitioning of A satisfies property A^π and is consistently ordered. Then,

$$(3.10) \qquad \frac{R(\mathscr{L}_{\omega_b}^{(1)})}{R(\mathscr{L}_{\omega_b}^{(2)})} > 1.$$

Moreover, if both C_1 and C_2 commute with A, and $\overline{\mu}[E_1] \to +\infty$, then

$$(3.11)\qquad \frac{R(\mathscr{L}^{(1)}_{\omega_b})}{R(\mathscr{L}^{(2)}_{\omega_b})} \sim \left(\frac{\bar{\mu}[C_2]}{\bar{\mu}[C_1]}\right)^{1/2}.$$

Of practical importance is the fact that the matrix $D = B^{-1}C \equiv (d_{i,j})$, derived from a regular splitting of A, has nonnegative entries, and thus [7] if $\underline{u}$ is any vector with positive components u_i, then nontrivial upper and lower bounds for the spectral radius of D are given by

$$(3.12)\qquad \min_i \left(\frac{\sum_j d_{i,j} u_j}{u_i}\right) \le \bar{\mu}[D] \le \max_i \left(\frac{\sum_j d_{i,j} u_j}{u_i}\right).$$

If D is, moreover, irreducible, then $\bar{\mu}[D]$ can be expressed [35] as a minimax

$$(3.12')\qquad \max_{\underline{u}\in P}\left\{\min_i \left(\frac{\sum_j d_{i,j} u_j}{u_i}\right)\right\} = \bar{\mu}[D] = \min_{\underline{u}\in P}\left\{\max_i \left(\frac{\sum_j d_{i,j} u_j}{u_i}\right)\right\}$$

where P is the set of all column vectors $\underline{u}$ with positive components. Upper and lower bounds for $\bar{\mu}[D]$ give, respectively, upper and lower bounds[§] for ω_b, defined in (3.7).

Our next acceleration method is what we call the Chebyshev semi-iterative method with respect to the matrix D, and has been widely discussed in various forms in the literature [18, 27, 33, 39].

Here we need only our previous assumptions, A a Stieltjes matrix, B and C defining a regular splitting of A, and B symmetric and positive definite, to enable us to rigorously apply this method. The matrix $D = B^{-1}C$ is nonnegative, and has real eigenvalues, since D is similar to a symmetric matrix. It follows, from the Perron-Frobenius theory of nonnegative matrices and Lemma 1, that the eigenvalues μ of D at least satisfy

$$(3.13)\qquad -\bar{\mu}[D] \le \mu \le \bar{\mu}[D] < 1 .$$

If $C_m(x)$ is the Chebyshev polynomial of degree m, defined by

$$(3.14)\qquad C_m(x) = \cos\left[m \cos^{-1} x\right],\quad |x| \le 1,\quad m = 0, 1, 2, \ldots,$$

then by using the following well known three term recurrence relation for Chebyshev polynomials

$$(3.15)\quad \begin{cases} C_0(x) = 1\ ;\ C_1(x) = x\ , \\ C_{m+1}(x) = 2x\,C_m(x) - C_{m-1}(x)\ ,\ m = 1, 2, \ldots\ , \end{cases}$$

the Chebyshev semi-iterative method with respect to the matrix D, applied to (2.4), is defined[#] by

$$(3.16)\quad \underline{x}^{(m+1)} = a_{m+1}\{D\underline{x}^{(m)} + B^{-1}\underline{k} - \underline{x}^{(m-1)}\} + \underline{x}^{(m-1)},\ m=0, 1, 2, \ldots,$$

where

$$(3.17)\quad a_1 = 1\ ,\ a_{m+1} = \frac{2\,C_m(1/\overline{\mu})}{\overline{\mu}\,C_{m+1}(1/\overline{\mu})}\ ,\ m = 1, 2, \ldots,$$

and $\overline{\mu} \equiv \overline{\mu}[D]$. Again, in actual computations, the equivalent form of (3.16),

$$(3.18)\quad B\underline{x}^{*(m+1)} = C\underline{x}^{(m)} + \underline{k}\ ,$$

and

$$(3.18')\quad \underline{x}^{(m+1)} = a_{m+1}\{\underline{x}^{*(m+1)} - \underline{x}^{(m-1)}\} + \underline{x}^{(m-1)}\ ,$$

may be more useful. If the interval $-\overline{\mu} \le t \le +\overline{\mu}$ is the smallest interval containing all the eigenvalues of D, it is known [33, 39] that the Chebyshev semi-iterative method with respect to the matrix D has the fastest average rate of convergence among all semi-iterative methods, in a certain norm, with respect to the matrix D.

We thus far have considered two acceleration methods applied to the basic iterative method of (2.4). The latter method has the advantage that it requires no further assumptions, such as property A^{π} or a (consistent) ordering to be rigorously applied. The former method on the other hand is, if applicable, faster in rate of convergence [33, 40] and requires in actual computations less vector storage than the Chebyshev semi-iterative method defined in (3.16).

We now consider a new type of splitting of the matrix A, where A is a Stieltjes matrix, B is symmetric and positive definite, but C is now symmetric and non-positive definite. Defining $C \equiv -F$, then F is symmetric and non-negative definite. We furthermore assume that matrix equations of the form

$$(3.19)\quad (B + \rho I)\,\underline{x} = \underline{g}\ ,$$

and

$$(3.19')\quad (F + \rho I)\,\underline{x} = \underline{g}\ ,$$

can be directly solved for the vector $\underline{x}$ for all vectors $\underline{g}$ and all positive scalars ρ. With

$$(3.20) \qquad A = B + F \ ,$$

the Peaceman-Rachford iterative method [21], applied to (2.1), is defined by

$$(3.21) \qquad (B + \rho_m)\, \overset{*}{\underline{x}}^{(m)} = (\rho_m I - F)\, \underline{x}^{(m)} + \underline{k} \ ,$$

and

$$(3.21') \qquad (F + \rho_m I)\, \underline{x}^{(m+1)} = (\rho_m I - B)\, \overset{*}{\underline{x}}^{(m)} + \underline{k} \ ,$$

where the ρ_m are positive scalars. The process can be carried out because of our assumptions concerning (3.19) and (3.19'). Similarly, the Douglas-Rachford iterative method [8], applied to (2.1), is defined by (3.21) and

$$(3.21^*) \qquad (F + \rho_m I)\, \underline{x}^{(m+1)} = F\underline{x}^{(m)} + \rho_m \overset{*}{\underline{x}}^{(m)} \ .$$

Combining (3.21) and (3.21'), we obtain

$$(3.22) \qquad \underline{x}^{(m+1)} = T_{\rho_m} \underline{x}^{(m)} + \underline{g}(\rho_m) \ ,$$

where

$$(3.23) \qquad T_\rho \equiv (F + \rho I)^{-1}(\rho I - B)(B + \rho I)^{-1}(\rho I - F) \ .$$

Similarly, combining (3.21) and (3.21*), we obtain

$$(3.24) \qquad \underline{x}^{(m+1)} = U_{\rho_m} \underline{x}^{(m)} + \underline{h}(\rho_m) \ ,$$

where

$$(3.25) \qquad U_\rho \equiv (F + \rho I)^{-1}(B + \rho I)^{-1} \{\rho^2 I + B \cdot F\} \ .$$

We call the matrices T_ρ and U_ρ respectively the Peaceman-Rachford and Douglas-Rachford iteration matrices. If the matrices B and F commute, then the positive scalars ρ_m can be suitably chosen so as to make these iterative methods rapidly convergent [3, 8, 21, 34]. In the case that B and F do not commute, both of these iterative methods are convergent for fixed $\rho > 0$ [3].

Having considered several iterative methods for solving the matrix equation of (2.1), we turn now to the practical question of how these ideas can be actually utilized.

§4. Factorization and Normalized Iterative Techniques

We again assume that A is a Stieltjes matrix, that (2.2) represents a regular splitting of A, and that B is symmetric and positive-definite. It is well known [20] that there exists a real unique upper triangular matrix T with positive diagonal entries such that B can be factored into

(4.1) $$B \equiv T' T \ .$$

If the matrix T is known, then the matrix equation (2.3) can be directly solved by the writing (2.3) in the form

(4.2) $$T' \underline{s} = \underline{g} \ ,$$

where

(4.2') $$T \underline{x} = \underline{s} \ .$$

Both matrix equations of (4.2) and (4.2') can be directly solved by backward substitution.

Now let

(4.3) $$T \equiv \widetilde{T} R \ ,$$

where $\widetilde{T}$ is an upper triangular matrix with unit diagonal entries, and R is a positive diagonal matrix, so that the matrices T , $\widetilde{T}$, and R are all uniquely determined from B . If $R\underline{x} \equiv \underline{y}$, then (2.1) can be written equivalently as

(4.4) $$\widetilde{T}'\widetilde{T}\underline{y} = \widetilde{C}\underline{y} + R^{-1}\underline{k} \ ,$$

where

(4.5) $$\widetilde{C} \equiv R^{-1} C R^{-1} \ .$$

In analogy to the iterative method of (2.4), we consider the iterative method

(4.6) $$\widetilde{T}'\widetilde{T}\underline{y}^{(m+1)} = \widetilde{C}\underline{y}^{(m)} + R^{-1}\underline{k} \ , \quad m = 0, 1, 2, \ldots \ ,$$

where $\underline{y}^{(0)}$ is an arbitrary vector. From the definition of the matrices $\widetilde{T}$, $\widetilde{R}$, and $\widetilde{C}$, it follows that $R^{-1}A R^{-1} = \widetilde{T}'\widetilde{T} - \widetilde{C}$ is a regular splitting of $R^{-1}A R^{-1}$. In the case where the matrix $\widetilde{B}$ is symmetric and positive definite and $\widetilde{C}$ is symmetric, we say that $\widetilde{A} = \widetilde{B} - \widetilde{C}$ is a <u>normalized</u> regular splitting of A if $\widetilde{A} = \widetilde{B} - \widetilde{C}$ is a regular splitting of $\widetilde{A}$ and $\widetilde{B} = \widetilde{T}'\widetilde{T}$, where $\widetilde{T}$ is upper triangular with unit diagonal entries. In analogy to §2, if we define

(4.7) $$\widetilde{D} = (\widetilde{T}'\widetilde{T})^{-1} \widetilde{C} \ ,$$

then

(4.8) $$\widetilde{D} = R D R^{-1} \ .$$

Thus, the matrices D and $\widetilde{D}$ are similar, and evidently have the same spectral radius, proving that the normalization of the basic iterative method of (2.4) does not affect the rate of convergence of the basic iterative method.

The reason for normalizing[±] is purely one of increased efficiency on a digital computing machine, since solving $T'T\underline{x} = \underline{q}$ for the vector $\underline{x}$ requires in general two more multiplications per component than does solving $\widetilde{T}'\widetilde{T}\underline{y} = \underline{h}$ for the vector $\underline{y}$. Thus, if many iterations of (2.4) or (4.6) are anticipated, iterating by means of (4.6) is preferable, since passing finally from the vector $\underline{y}$ to the vector $\underline{x}$ requires but one multiplication per component.

§5. Cyclic Methods

We now consider several practical iterative methods, which can be accelerated by means of the Young-Frankel successive overrelaxation method. We call these methods cyclic iterative methods (as opposed to the primitive methods of §6) since if the partitioned matrix A of (3.1) satisfies property A^{π}, it can be shown [32] that the matrix $D = B^{-1}C$ is cyclic of index 2 in the sense of Romanovsky [25], i.e. there exists a $n \times n$ permutation matrix Λ such that

$$\Lambda D \Lambda^{-1} = \begin{bmatrix} 0 & D_{1,2} \\ D_{2,1} & 0 \end{bmatrix}, \tag{5.1}$$

where the diagonal submatrices are square.

We now consider three iterative techniques simultaneously. Let A be a Stieltjes matrix arising from a five-point approximation on a rectangular mesh in the plane to the self-adjoint elliptic partial differential equation of (2.11), with Dirichlet type boundary conditions. First, let B_3 be the positive diagonal matrix composed of the diagonal entries of A, i.e. B_3 is the matrix of (3.3), corresponding to the partitioning of the matrix A in which the diagonal blocks $A_{j,j}$ of A in (3.1) are all 1×1 matrices. Next, for our rectangular mesh, we number our mesh points along successive horizontal mesh lines, as in Figure 1.

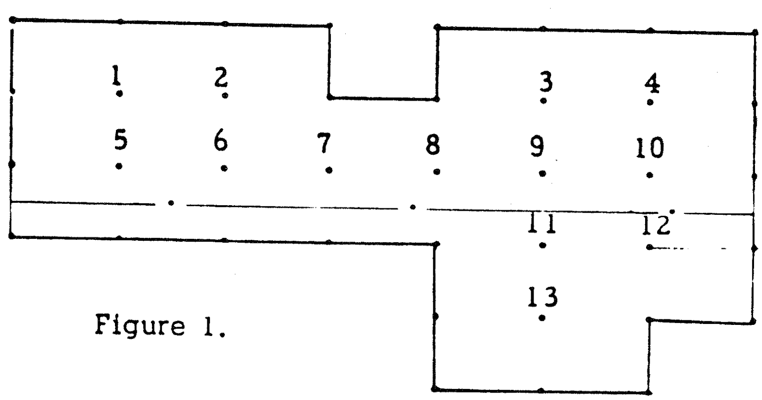

Figure 1.

Since each mesh point is coupled only to its four adjacent mesh points, then let B_2 be the diagonal block matrix of (3.3), corresponding to the partitioning of A into successive blocks consisting of mesh points on a single horizontal mesh line. Finally, let B_1 be the diagonal block matrix corresponding to the partitioning of the matrix A into blocks consisting of mesh points on successive pairs of horizontal mesh lines. Specifically, referring to Figure 1, the matrix B_1 can be expressed as

$$B_1 = \begin{bmatrix} A^{(1)}_{1,1} & 0 \\ 0 & A^{(1)}_{2,2} \end{bmatrix}, \tag{5.2}$$

where $A^{(1)}_{1,1}$ is the 10×10 submatrix coupling the unknowns $x_1, \ldots, x_{10}$, and $A^{(1)}_{2,2}$ is the 3×3 submatrix coupling the unknowns x_{11}, x_{12}, and x_{13}. Defining the matrices C_i by

$$A = B_i - C_i \ , \ i = 1, 2, 3, \tag{5.3}$$

it follows that all three different partitionings of the matrix A correspond to regular splittings of A, and in each case the partitioned matrix A satisfies property A^{π}, and can be (consistently) ordered. Moreover,

$$0 \leq C_1 \leq C_2 \leq C_3 \ , \tag{5.4}$$

equality excluded if, as in Figure 1, there are three or more horizontal mesh lines. By means of Corollary 1, it follows that the successive overrelaxation iterative method, with optimum ω, applied to the regular splitting $A = B_1 - C_1$ is faster in rate of convergence than the successive overrelaxation iterative method, with optimum ω's, applied to the remaining cases. The application of the successive overrelaxation iterative method to the regular splitting $A = B_3 - C_3$, which we denote by SOR, is due originally to Young [38] and Frankel [10]. While the theory of [1] applies to both the regular splittings $A = B_1 - C_1 = B_2 - C_2$, only in the latter case has the successive overrelaxation iterative method, denoted by SLOR, been actually considered in solving two-dimensional elliptic difference equations [1, 6, 11, 17]. Since the matrix B_1 couples together adjacent lines of mesh points, we denote the successive overrelaxation iterative method applied to the regular splitting $A = B_1 - C_1$ by S2LOR.

We now show how the iterative method S2LOR can be carried out numerically. Because the matrix A is derived from a five-point formula, the matrix B_1, after a suitable permutation of indices of the mesh points, is a symmetric, positive definite, and five-diagonal matrix. Thus, $B_1 = T'_1 T_1$, where T_1 is an upper tridiagonal matrix with positive diagonal entries. To illustrate this, we have relabled the mesh points of $A^{(1)}_{1,1}$ of (5.2) in Figure 2, which shows that the corresponding matrix coupling the unknowns $x_1, x_2, \ldots, x_{10}$

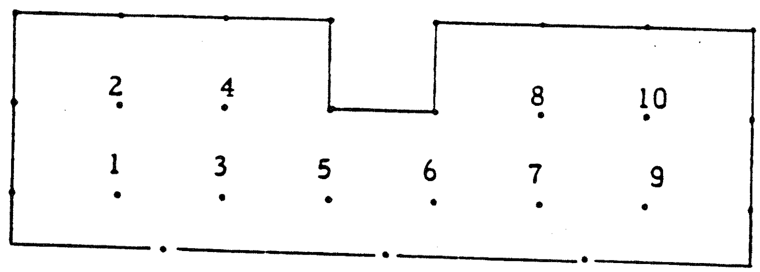

Figure 2.

is a five-diagonal matrix. While matrix equations of the form (2.3), where B is a five-diagonal matrix, can be directly solved by the Gauss elimination method, it is more efficient if one has the upper tridiagonal matrix T_1, where $B = T_1' T_1$, to solve equation (2.3) in the manner of (4.2) - (4.2'). Given the five-diagonal positive definite symmetric matrix B, we can generate the entries of the upper tridiagonal matrix T_1 as follows. Let

(5.5)
$$B = \begin{bmatrix} b_{1,1} & b_{1,2} & b_{1,3} & 0 & 0 & \ldots & 0 \\ b_{1,2} & b_{2,2} & b_{2,3} & b_{2,4} & 0 & \ldots & 0 \\ b_{1,3} & b_{2,3} & b_{3,3} & b_{3,4} & b_{3,5} & \ldots & 0 \\ \vdots & & & & & & \vdots \\ 0 & 0 & 0 & 0 & 0 & \ldots & b_{n,n} \end{bmatrix},$$

(5.5')
$$T = \begin{bmatrix} t_{1,1} & t_{1,2} & t_{1,3} & 0 & 0 & \ldots & 0 \\ 0 & t_{2,2} & t_{2,3} & t_{2,4} & 0 & \ldots & 0 \\ 0 & 0 & t_{3,3} & t_{3,4} & t_{3,5} & \ldots & 0 \\ \vdots & & & & & & \vdots \\ 0 & 0 & 0 & 0 & 0 & \ldots & t_{n,n} \end{bmatrix}$$

If $t_{-1,m} = t_{0,m} \equiv 0$ for $m = 1, 2$, then

$$(5.6)\quad \begin{cases} t^2_{j-2,j} + t^2_{j-1,j} + t^2_{j,j} = b_{j,j} & , j = 1, 2, \ldots, n , \\ t_{j-1,j}\, t_{j-1,j+1} + t_{j,j}\, t_{j,j+1} = b_{j,j+1} & , j = 1, 2, \ldots, n-1 , \\ t_{j,j}\, t_{j,j+2} = b_{j,j+2} & , j = 1, 2, \ldots, n-2 , \end{cases}$$

With (5.6), it is clear how a normalized $\tilde{T}_1$, with unit diagonal entries, can be similarly generated.

It is convenient now to consider the P-condition numbers of the matrices B_i, $i = 1, 2, 3$. Following Todd [30], we define the P-condition number $P(M)$ of an arbitrary non-singular matrix M as

$$(5.7)\qquad P(M) = \frac{\max_k |\lambda_k|}{\min_k |\lambda_k|} ,$$

where the λ_k are eigenvalues of M. Since the matrices B_i are all symmetric and positive definite, the eigenvalues $\lambda_k(i)$ of the matrices B_i are positive real numbers, and thus

$$(5.7')\qquad P(B_i) = \frac{\max_k \lambda_k(i)}{\min_k \lambda_k(i)} , \qquad i = 1, 2, 3 .$$

The following table** gives information about the application of the normalized iterative methods SOR, SLOR, and S2LOR, to the numerical solution of matrix problems arising from a five-point approximation, on a rectangular mesh in the plane, to the partial differential equation of (2.11), with Dirichlet-type boundary conditions. For the second

Method	Operations per Mesh Point		Estimate of $\bar{\mu}[C]$	P(B)
SOR	5m	6a	4	1
SLOR	5m	6a	2	3
S2LOR	6m	7a	1	7

TABLE I. Five-Point Formula in Two Dimensions

and third columns, only Laplace's equation on a uniform mesh is considered. The second column gives upper bounds, by Gerschgorin's lemma [14], for the spectral radii of the corresponding matrices C_i. The third column gives upper bounds for the P-condition numbers of the unnormalized matrices B_i.

It is interesting to note that the numbers in Table I are independent of the actual numbers of mesh points considered. From Table I, we can conclude that, for the matrices B_1, directly solving matrix equations of the form (2.3) does not give rise to serious round-off error difficulties. To illustrate the usefulness of the second column of numbers, we consider the numerical solution of the Dirichlet problem in a unit square on a uniform mesh of side h. For this specific problem, it is known [1, 17] that the matrices C_2, C_3, and A commute, and that

$$\lim_{h \to 0} \frac{R(\mathscr{L}^{(2)}_{\omega_b})}{R(\mathscr{L}^{(3)}_{\omega_b})} = \sqrt{2}\ . \tag{5.8}$$

However, since $\bar{\mu}[C_3] \to 4$, $\bar{\mu}[C_2] \to 2$; $\bar{\mu}[C_1] \to 1$, and $\bar{\mu}[A^{-1}] \to +\infty$ as $h \to 0$, we can obtain the above result as a consequence of Theorem 2 and Corollary 1, as well as the fact that

$$\lim_{h \to 0} \frac{R(\mathscr{L}^{(1)}_{\omega_b})}{R(\mathscr{L}^{(2)}_{\omega_b})} \geq \sqrt{2}\ . \tag{5.8'}$$

Thus, the rate of convergence of the iterative method S2LOR with optimum ω, is, for small mesh spacings h, considerably greater than the rates of convergence of the iterative methods SLOR and SOR, with optimum ω's.

As pointed out in [1], the iterative method SLOR can be rigorously applied to the iterative solution of matrix problems arising from a nine-point approximation to (2.11) in two dimensions. While it is easy to see that the iterative method S2LOR can also be applied to this problem, the surprising result, as indicated in Table II, is that the normalized iterative method S2LOR requires in general the <u>same</u> number of operations per mesh point as does either the normalized iterative method SLOR or the normalized iterative method SOR. As in Table I, the information in Table II concerns the normalized iterative methods SOR, SLOR,

Method	Operations per Mesh Point		Estimate of $\bar{\mu}[C]$	P(B)
SOR	9m	10a	20	1
SLOR	9m	10a	12	7/3
S2LOR	9m	10a	6	17/3

TABLE II. Nine-Point Formula in Two Dimensions

S2LOR, and the last two columns refer to the numerical solution of Laplace's equation on a uniform mesh in the plane. The arguments extend to three dimensions, and we include, for completeness, the seven point approximation in three dimensions to the partial differential equation of (2.11), with given Dirichlet-type boundary conditions.

Method	Operations per Mesh Point		Estimate of $\overline{\mu}[C]$	P(B)
SOR	7m	8a	6	1
SLOR	7m	8a	4	2
S2LOR	8m	9a	3	3

TABLE III. Seven-Point Formula in Three Dimensions

The range of application of iterative method S2LOR is not restricted to rectangular meshes in two and three dimensions. As another application, we consider solving Laplace's equation on a uniform triangular mesh in the plane, and we couple together mesh points on successive pairs of horizontal mesh lines. If we use a seven-point approximation to Laplace's equation in the plane, then, as illustrated in Figure 3, the matrix coupling the unknowns $x_1, \ldots, x_9$ is again a five-diagonal symmetric and positive definite matrix, which can be factored into $T'T$, where T is upper tridiagonal. It is easy to verify that the Stieltjes matrix A, so partitioned, is a tridiagonal block matrix, and therefore [1] satisfies property A^{π} is and (consistently) ordered. Thus, the successive overrelaxation iterative method can be rigorously applied in this case, and the rate of convergence of the iterative method S2LOR is again faster than the rates of convergence of the iterative methods SLOR and SOR.

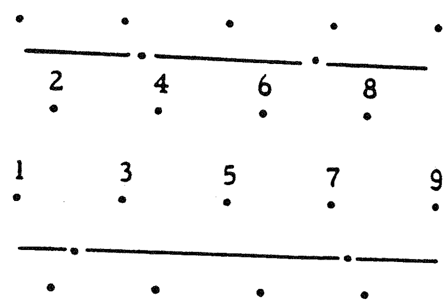

Figure 3.

A far more interesting application of the iterative method S2LOR is to the numerical solution of the biharmonic equation in the plane, over a thirteen-point mesh [5, p. 506]. As pointed out by Heller [15], coupling the mesh points along two neighboring horizontal mesh lines partitions matrix A into a tridiagonal block matrix, which satisfies property A^{π}, and is (consistently) ordered. With suitable boundary conditions, the matrix A can be derived in such a way so that A is symmetric and positive definite, and the diagonal blocks of the partitioned matrix A, corresponding

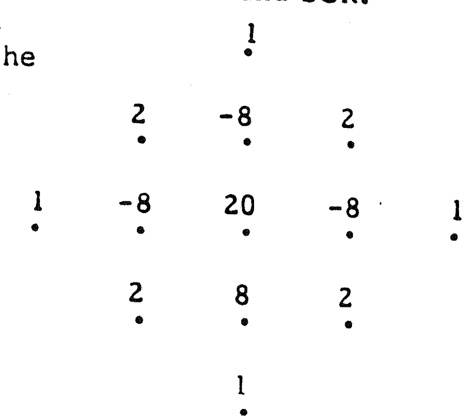

Fig. 4. Thirteen-Point Star

to the coupling of mesh points on two adjacent horizontal mesh lines, are also symmetric and positive definite. Thus, based on a generalization of Reich's Theorem [23], the iterative method S2LOR with $\omega = 1$ (Gauss-Seidel or single step method) is convergent. Since the matrix A satisfies property A^{π} and is (consistently) ordered, it follows [1] that the Richardson iterative method (total step method) is also convergent. The same is not always true for the iterative method SLOR [15, 36]. It is significant, however, that by means of normalization, both the normalized iterative method S2LOR and the normalized iterative method SLOR require 13 multiplications and 14 additions per mesh point. For this application, the matrix B of (3.3) is the direct sum of eight-diagonal symmetric and positive definite matrices, each of which factors into T' T where T is an upper five-diagonal matrix.

§6. Primitive Iterative Methods

In the previous section, the basic idea presented involved partitioning the matrix A into a form for which matrix equations, involving only the diagonal blocks of the partitioned matrix A, could be directly solved. It is natural to consider the problem of factoring the entire Stieltjes matrix A into

$$A = T'T \,, \tag{6.1}$$

where T is an upper triangular matrix with positive diagonal entries. §§ Unfortunately, for large practical problems the resulting matrix T is seldom sparse, and the growth of round-off errors is now more serious. The same is true of directly applying the Gauss elimination method to (2.1). Instead, we now attempt to approximately factor the matrix A into the form of (6.1), where the matrix T is sparse. Allowing for an error matrix C, we write

$$A = T'T - C \,. \tag{6.2}$$

In particular, if A is a Stieltjes matrix arising from a five-point approximation to (2.11) on a rectangular mesh in a plane region with given Dirichlet-type boundary conditions, let the directed graph of the upper triangular matrix T be as in Figure 5, where arrows connecting mesh points are interpreted as non-zero coefficients in the matrix T. Specifically, if in Figure 5 the mesh points (k, m), (k+1, m), and (k, m+1) are called the i-th, i+1-st, and j-th mesh points respectively, then the only entries in the i-th row of the matrix $T = (t_{i,j})$ permitted to be non-zero are $t_{i,i}$, $t_{i,i+1}$, and $t_{i,j}$.

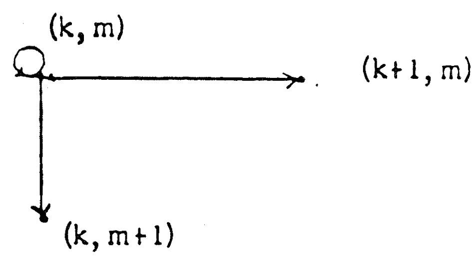

Figure 5. Five-Point Star

While the matrix T so generated is evidently upper triangular and sparse, the matrix C of (6.2) is not in general null. In fact, if $C = (c_{i,j})$, then C is symmetric, and

$$c_{i+1,j} = t_{i,i+1}\, t_{i,j} \tag{6.3}$$

can be different from zero. The matrix T can be derived so that the only non-zero entries of the error matrix C are of the form (6.3). Moreover, with A a Stieltjes matrix, it can be verified that $A = T'T - C$ is a regular splitting of A, so that $(T'T)^{-1} \geq 0$. We include, for completeness, the following

Theorem 4. The matrix $(T'T)^{-1}$ is nonnegative and primitive. If the finite mesh region is convex, then $(T'T)^{-1} > 0$.

Proof. By a classic theorem of Frobenius [12], a primitive matrix is a matrix M such that $M \geq 0$, and such that $M^m > 0$ for some positive integer m. Since (6.2) represents a regular splitting of A, then $(T'T)^{-1} \geq 0$. Moreover, it can be verified that the diagonal entries of $(T'T)^{-1}$ are positive, and, since A is irreducible, the matrix $(T'T)^{-1}$ is also irreducible. Thus [35], $(T'T)^{-1}$ is primitive. If the finite mesh region is convex, then it can be verified that the upper triangular matrix T^{-1} has every entry on or above the main diagonal positive. Thus, $(T'T)^{-1} > 0$.

As consequences of this theorem, we observe, for convex mesh regions, that the matrix $B = T'T$ of (6.2) and the Stieltjes matrix A which B approximates have the common feature that their inverses have only positive entries. Opposed to this, we find that for cyclic iterative methods, the matrix B of (3.3) is such that $B^{-1} \geq 0$, but B^{-1} does not have only positive entries unless C is the null matrix. Next, it follows, for convex mesh regions, that if the matrix C of (6.2) is not null, then the matrix $D \equiv (T'T)^{-1}C$ is not cyclic of index 2. While the successive overrelaxation iterative method cannot directly be used to accelerate the convergence of the basic iterative method of (2.3), the Chebyshev semi-iterative method nevertheless can be applied.##

The use of primitive iterative methods is obviously not restricted to five-point approximations of (2.11). If nine-point approximations of (2.11) in the plane are considered, then the analogous directed graph of the upper triangular matrix T is given in Figure 6. Other extensions are easily obtained.

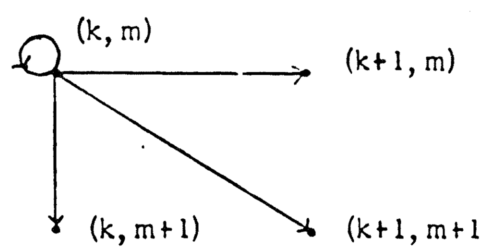

Figure 6. Nine-Point Star

NOTES

*By this, we mean that neither C_1 or $C_2 - C_1$ is the null matrix.

§For special applications of this result, see [6, 31].

#This particular application of Chebyshev polynomials can be derived from (17) of [27], upon making proper identifications.

± An example of a normalized iterative technique is given in [6].

**The quantities m and a refer respectively to multiplications and additions.

§§A similar approach has been considered by T. A. Oliphant in "A direct implicit scheme for solving two dimensional steady-state diffusion problems", The Rice Institute (1958).

##At the present time, Mr. William R. Cadwell, a graduate student at the University of Pittsburgh, is experimenting with this iterative method as well as the iterative method S2LOR on the IBM-704. The numerical results are to be included in his M.A. Thesis.

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