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Iterative Methods for Solving Large Systems of Linear Equations

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The paper is concerned with iterative methods for solving large systems of linear algebraic equations with sparse matrices. Such systems frequently arise in the numerical solution by finite difference methods of boundary value problems involving elliptic partial differential equations. In particular, the symmetric successive overrelaxation (SSOR) method and its acceleration by semi-iteration are considered. Estimates of the best relaxation parameter to be used with the SSOR method are given and certain convergence properties are studied. For a large class of elliptic boundary value problems, it is shown that the number of iterations needed to achieve a given convergence level using the accelerated method varies as $h^{-1/2}$, where h is the mesh size.

I. Introduction

In this paper we study certain convergence properties of the symmetric successive overrelaxation method (SSOR method) for solving systems of linear algebraic equations. We shall be primarily concerned with large systems with sparse matrices such as frequently arise in the solution by finite difference methods of certain boundary value problems involving elliptic partial differential equations.

It is shown that if one can determine bounds on three quantities, one can make a good estimate of the best acceleration parameter, ω , to use with the SSOR method, and one can also give an upper bound for the computational effort needed to achieve satisfactory convergence. This information can be used to construct an effective semi-iterative method to accelerate the convergence. The necessary parameters can be determined for a large class of elliptic boundary value problems. For such problems it is shown that the number of iterations needed to achieve a given convergence level using the accelerated method is $0(h^{-1/2})$. This compares favorably with $0(h^{-1})$ iterations needed for the successive overrelaxation method (SOR method). The theoretical results are tested by the actual solution of several numerical problems.

It is hoped that with the availability of explicit procedures for applying the accelerated *SSOR* method in a large class of cases and with the possibility of achieving large savings in computational effort, the method will find increased usage.

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In this brief presentation it is only possible to sketch the high points of the theory. For details the reader is referred to [8].

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2. The SSOR Method

Let us consider the linear system

$$Au = b \tag{2.1}$$

where A is a real, symmetric, positive definite, square matrix of order N. The real $N \times 1$ column matrix b is given, and the $N \times 1$ column matrix u is to be determined.

In order to define the SSOR method it is convenient to rewrite (2.1) in the form

$$u = Bu + c \tag{2.2}$$

where

$$\begin{array}{c} B = I - D^{-1} A - L + U \\ c = D^{-1} b \end{array}$$
 (2.3)

and where D is the diagonal matrix with the same diagonal elements as A. The matrices L and U are strictly lower and strictly upper triangular, respectively. The SSOR method is defined as follows. Let $u^{(0)}$ be an arbitrary initial approximation to the solution of (2.1). We define the sequence $u^{(1/2)}$, $u^{(1)}$, $u^{(3/2)}$, $u^{(2)}$, ... by

$$\begin{array}{c} u^{(n+1/2)} = \omega(Lu^{(n+1/2)} + Uu^{(n)} + c) + (1 - \omega) u^{(n)} \\ u^{(n+1)} = -\omega(Lu^{(n+1/2)} + Uu^{(n+1)} + c) + (1 - \omega) u^{(n+1/2)}. \end{array}$$

$$(2.4)$$

Here the "relaxation factor" ω is a real number such that $0 < \omega < 2$.

It should be noted that even though (2.4) appears to define $u^{(n+1/2)}$ and $u^{(n+1)}$ implicitly, nevertheless, the calculation can be carried out explicitly. Thus, if N = 3 the system (2.1) becomes

$$\begin{pmatrix} a_{1,1} & a_{1,2} & a_{1,3} \\ a_{2,1} & a_{2,2} & a_{2,3} \\ a_{3,1} & a_{3,2} & a_{3,3} \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \\ u_3 \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \\ b_3 \end{pmatrix}.$$
(2.5)

The related system (2.2) becomes

$$\begin{pmatrix} u_1 \\ u_2 \\ u_3 \end{pmatrix} = \begin{pmatrix} 0 & b_{1,2} & b_{1,3} \\ b_{2,1} & 0 & b_{2,3} \\ b_{3,1} & b_{3,2} & 0 \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \\ u_3 \end{pmatrix} + \begin{pmatrix} c_1 \\ c_2 \\ c_3 \end{pmatrix}$$
(2.6)

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where

$$b_{i,j} = -\frac{a_{i,j}}{a_{i,i}}, \quad i, j = 1, 2, 3; \quad i \neq j$$

$$c_i = \frac{b_i}{a_{i,i}}, \quad i = 1, 2, 3.$$
(2.7)

We remark that

$$L = \begin{pmatrix} 0 & 0 & 0 \\ b_{2,1} & 0 & 0 \\ b_{3,1} & b_{3,2} & 0 \end{pmatrix}, \qquad U = \begin{pmatrix} 0 & b_{1,2} & b_{1,3} \\ 0 & 0 & b_{2,3} \\ 0 & 0 & 0 \end{pmatrix}.$$
 (2.8)

To analyze the convergence of the SSOR method we write (2.4) in the form

$$u^{(n+1)} = \mathscr{S}_{\omega} u^{(n)} + k_{\omega}$$
(2.9)

where

$$\mathcal{G}_{\omega} = (I - \omega U)^{-1} (\omega L + (1 - \omega) I) (I - \omega L)^{-1} (\omega U + (1 - \omega) I))$$

$$k_{\omega} = \omega (2 - \omega) (I - \omega U)^{-1} (I - \omega L)^{-1} c.$$

$$(2.10)$$

Evidently (2.9) is a linear stationary method of first degree. For such a method the error $\varepsilon^{(n)} = u^{(n)} - \bar{u}$, where \bar{u} is the exact solution of (2.1), is approximately multiplied by $S(\mathscr{S}_{\omega})$ when one computes $u^{(n+1)}$. Here $S(\mathscr{S}_{\omega})$ denotes the spectral radius of \mathscr{S}_{ω} , i.e., the maximum of the moduli of the eigenvalues of \mathscr{S}_{ω} . Thus, roughly speaking, to reduce $\varepsilon^{(n)}$ to a fraction ζ of $\varepsilon^{(0)}$ we find the smallest integer n such that

$$S(\mathscr{G}_{\omega})^{n} \leq \zeta. \tag{2.11}$$

Thus we have

$$n \doteq \frac{-\log \zeta}{-\log S(\mathscr{G}_{\omega})} . \tag{2.12}$$

We define the quantity

$$RR(\mathscr{G}_{\omega}) = \frac{-1}{\log S(\mathscr{G}_{\omega})}$$
(2.13)

as the *reciprocal rate of convergence* of (2.9). The number of iterations needed for convergence is approximately proportional to $RR(\mathscr{S}_{\omega})$.

Clearly, for convergence, we need $S(\mathscr{G}_{\omega}) < 1$. This condition holds for $0 < \omega < 2$ since A is positive definite (see, for instance [6]). Of greater importance than mere convergence is the *rapidity* of convergence; this is discussed in the next section.

3. Determination of ω

We now show that if we can give bounds on three quantities, we can explicitly compute a "good" value of ω and a bound on the corresponding value of $S(\mathscr{G}_{\omega})$.

Since A is positive definite, it follows that the eigenvalues of B are real and less than unity. We let m and M be lower and upper bounds, respectively, for the eigenvalues of B. (We require⁺ that M < 1.) We let $\overline{\beta}$ be a bound on S(LU). In [8] it is shown that

$$S(\mathscr{S}_{\omega}) \leq \begin{cases} 1 - \omega(2 - \omega) \frac{1 - M}{1 - \omega M + \omega^2 \overline{\beta}} & \text{if } \overline{\beta} \geq \frac{1}{4} \text{ or if } \overline{\beta} < \frac{1}{4} \\ \text{and } \omega \leq \omega^{\star} & (3.1) \\ 1 - \omega(2 - \omega) \frac{1 - m}{1 - \omega m + \omega^2 \overline{\beta}} & \text{if } \overline{\beta} < \frac{1}{4} \text{ and } \omega > \omega^{\star}. \end{cases}$$

Here for $\overline{\beta} < \frac{1}{4}$ we let

$$\omega^{\star} = \frac{2}{1 + \sqrt{1 - 4\overline{\beta}}} . \tag{3.2}$$

A "good" choice of ω in the sense of minimizing the bound given by (3.1) is

$$\omega_{1} = \begin{cases} \frac{2}{1 + \sqrt{1 - 2M + 4\bar{\beta}}} & \text{if } M \leq 4\bar{\beta} \\ \frac{2}{1 + \sqrt{1 - 4\bar{\beta}}} & \text{if } M > 4\bar{\beta}. \end{cases}$$
(3.3)

Moreover, with this choice we have

$$S(\mathscr{G}_{\omega_{1}}) \leq \begin{cases} \left[1 - \frac{1 - M}{\sqrt{1 - 2M + 4\overline{\beta}}}\right] \left[1 + \frac{1 - M}{\sqrt{1 - 2M + 4\overline{\beta}}}\right]^{-1}, & \text{if } M \leq 4\overline{\beta} \\ \frac{1 - \sqrt{1 - 4\overline{\beta}}}{1 + \sqrt{1 - 4\overline{\beta}}} = \omega^{\star} - 1, & \text{if } M > 4\overline{\beta}. \end{cases}$$

$$(3.4)$$

As an example, let us consider the following model problem. Given a function g(x, y) defined on the boundary S of the unit square $0 \le x \le 1$, $0 \le y \le 1$, find a function u(x, y) continuous in the closed region and of class $C^{(2)}$ in the interior R such that u(x, y) = g(x, y) on S and such that u satisfies in R the Laplace differential equation

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = 0.$$
 (3.5)

We consider the use of the five-point difference equation

$$\frac{u(x+h,y)+u(x-h,y)+u(x,y+h)+u(x,y-h)-4u(x,y)}{h^2}=0.$$
 (3.6)

+ It is easy to show that $m \le 0 \le M$ and that $S(B) \le 2\sqrt{S(LU)}$. Therefore if $-m > 2\sqrt{\overline{\beta}}$ we replace m by $-2\sqrt{\overline{\beta}}$. Similarly, if $M > 2\sqrt{\overline{\beta}}$ we replace M by $2\sqrt{\overline{\beta}}$.

Here we choose a positive integer \mathcal{J} and let \mathcal{J}^{-1} be the mesh size, h. The equation (3.6) is to be satisfied at all mesh points (ph, qh), where p, q are integers, in R. It is easy to verify that if one multiplies (3.6) by $-h^2$ and brings the known boundary values to the right-hand side, one obtains a system of the form (2.1) where A is symmetric and positive definite.

In this case it can be shown that

$$S(B) = \cos \pi h$$

$$S(LU) = \frac{1}{4} \cos^2 \frac{\pi h}{2(1-h)} \le \frac{1}{4} \cos^2 \frac{\pi h}{2}$$
(3.7)

(see, for instance, [8]). Hence we can let

$$\frac{M = -m = \cos \pi h}{\overline{\beta}} = \frac{1}{4} \cos^2 \frac{\pi h}{2}.$$
(3.8)

From (3.3) we have

$$\omega_1 = \frac{2}{1 + \sqrt[3]{3} \sin \frac{\pi h}{2}}$$
(3.9)

and by (3.4)

$$S(\mathscr{S}_{\omega_{1}}) \leq \frac{1 - \frac{2}{\sqrt{3}} \sin \frac{\pi h}{2}}{1 + \frac{2}{\sqrt{3}} \sin \frac{\pi h}{2}} \sim 1 - \frac{2\pi h}{\sqrt{3}}$$
(3.10)

for small h. Therefore,

$$RR\left(\mathscr{G}_{\omega_{1}}\right) \stackrel{\leq}{\sim} \frac{\sqrt[]{3}}{2\pi} h^{-1}.$$
(3.11)

Thus the reciprocal rate of convergence of the SSOR method varies as h^{-1} . This is the same order of magnitude (but with a slightly larger constant) as that of the SOR method.

4. Acceleration of Convergence

Given a linear stationary iterative method of the form

$$u^{(n+1)} = Gu^{(n)} + k \tag{4.1}$$

where the eigenvalues of the iteration matrix G are real and less than unity, one can accelerate the convergence by an order of magnitude by means of semi-iteration. (See VARGA [5] and GOLUB and VARGA [2].) In the case of the SSOR method, the eigenvalues λ of \mathscr{S}_{ω} are real and nonnegative. Thus we have

$$0 \leq \lambda \leq S(\mathscr{G}_{\omega}) < 1 . \tag{4.2}$$

The optimum semi-iterative method based on the SSOR method is defined by

$$u^{(n+1)} = \varrho_{n+1} \{ \bar{\varrho}(\mathscr{S}_{\omega} u^{(n)} + k_{\omega}) + (1 - \bar{\varrho}) u^{(n)} \} + (1 - \varrho_{n+1}) u^{(n-1)} .$$
(4.3)

Here we let

$$\bar{\varrho} = \frac{2}{2 - S(\mathscr{S}_{\omega})} \tag{4.4}$$

and

$$\varrho_{1} = 1
\varrho_{2} = \left(1 - \frac{\sigma^{2}}{2}\right)^{-1}
\varrho_{n+1} = \left(1 - \frac{\sigma^{2}}{4} \varrho_{n}\right)^{-1}, \quad n = 2, 3, \dots$$
(4.5)

where

$$\sigma = \frac{S(\mathscr{G}_{\omega})}{2 - S(\mathscr{G}_{\omega})} . \tag{4.6}$$

The approximate error reduction after n iterations is approximately

.

$$S_n = \frac{2r^{n/2}}{1+r^n}$$
(4.7)

where

$$r = \left(\frac{\sqrt{S(\mathscr{G}_{\omega})}}{1 + \sqrt{1 - S(\mathscr{G}_{\omega})}}\right)^{4}.$$
(4.8)

The reciprocal asymptotic average rate of convergence is given by

$$RR_{\infty} = \lim_{n \to \infty} \left[-\frac{1}{\frac{1}{n} \log S_n} \right] = -\frac{1}{\frac{1}{2} \log r} \doteq \frac{1}{2} \left(\sqrt[n]{1 - S(\mathscr{G}_{\omega})} \right)^{-1} \quad (4.9)$$
$$\doteq \frac{1}{2} \sqrt[n]{RR(\mathscr{G}_{\omega})}$$

if $S(\mathscr{G}_{\omega})$ is close to unity.

For the model problem we have, by (3.11) and (4.9)

$$RR_{\infty} \doteq \frac{3^{1/4}}{2^{3/2}\sqrt{\pi}} h^{-1/2}$$
 (4.10)

Thus the number of iterations needed to achieve a given level of convergence is $0(h^{-1/2})$ for the model problem. In the next section we show that this result holds for a more general class of problems.

5. More General Elliptic Equations

Let R be a bounded plane region with boundary S consisting of horizontal and vertical line segments. Assume that for some $h_0 > 0$ and for some (x_0, y_0) the set Ω_{h_0} of all points $(x_0 + ih_0, y_0 + jh_0)$ has the following property. If any point of Ω_{h_0} lies in R, then the four adjacent points lie in R or on S. We also assume that this property holds for all positive h such that h_0/h is an integer.

We consider the generalized Dirichlet problem involving the differential equation

$$L[u] = \frac{\partial}{\partial x} \left(A \frac{\partial u}{\partial x} \right) + \frac{\partial}{\partial y} \left(C \frac{\partial u}{\partial y} \right) + Fu = G$$
(5.1)

where A(x, y) > 0, C(x, y) > 0, and $F(x, y) \le 0$ in R + S. Given a continuous function g(x, y) defined on S, the problem is to find a function u(x, y) of class $C^{(2)}$ in R and continuous in R + S such that L[u] = G in R and such that u(x, y) = g(x, y) on S.

We replace the differential equation by the following symmetric difference equation defined at points (x, y) of $R_h = \Omega_h \cap R$.

$$L_{h}[u] = h^{-2} \left\{ A \left(x + \frac{h}{2}, y \right) \left[u(x+h, y) - u(x, y) \right] - A \left(x - \frac{h}{2}, y \right) \times \left[u(x, y) - u(x-h, y) \right] + C \left(x, y + \frac{h}{2} \right) \left[u(x, y+h) - u(x, y) \right] - C \left(x, y - \frac{h}{2} \right) \left[u(x, y) - u(x, y-h) \right] \right\} + Fu(x, y) = G(x, y) .$$
(5.2)

For this problem we can give the following bounds on M, m, and S(LU).

$$M = -m = \frac{2(\bar{A} + \bar{C})}{2(\bar{A} + \bar{C}) + h^2(-\underline{F})} \cdot$$
(5.3)

$$\cdot \left[1 - \frac{2\underline{A}\sin^2\frac{\pi}{2I} + 2\underline{C}\sin^2\frac{\pi}{2I}}{\frac{1}{2}(\overline{A} + \underline{A}) + \frac{1}{2}(\overline{C} + \underline{C}) + \frac{1}{2}(\overline{A} - \underline{A})\cos\frac{\pi}{I} + \frac{1}{2}(\overline{C} - \underline{C})\cos\frac{\pi}{J}}\right].$$

Here we let

$$\underline{A} \leq A(x, y) \leq \overline{A}, \ \underline{C} \leq C(x, y) \leq \overline{C}, \ (-\underline{F}) \leq -F(x, y)$$
(5.4)

in R + S. It is assumed that the region is included in an $Ih \times \mathcal{J}h$ rectangle. This result is proved in [6, 7]. For the bound on S(LU) we use

$$\overline{\beta} = \max_{(x,y)\in R_h} \{\beta_3(x,y) [\beta_1(x-h,y) + \beta_2(x-h,y)] + \beta_4(x,y) [\beta_1(x,y-h) + \beta_2(x,y-h)]\}.$$
(5.5)

Here we let

$$\beta_{1}(x,y) = \frac{A\left(x + \frac{h}{2}, y\right)}{S(x,y)} \qquad \beta_{2}(x,y) = \frac{C\left(x,y + \frac{h}{2}\right)}{S(x,y)} \\ \beta_{3}(x,y) = \frac{A\left(x - \frac{h}{2}, y\right)}{S(x,y)} \qquad \beta_{4}(x,y) = \frac{C\left(x,y - \frac{h}{2}\right)}{S(x,y)} \\ S(x,y) = A\left(x + \frac{h}{2}, y\right) + A\left(x - \frac{h}{2}, y\right) + C\left(x,y + \frac{h}{2}\right) + \\ + C\left(x,y - \frac{h}{2}\right) - h^{2}F(x,y). \end{cases}$$
(5.6)

Of fundamental importance is the following result, which is proved in [8],

$$S(LU) \le \frac{1}{4} + O(h^2)$$
. (5.7)

It is assumed that A(x, y) and C(x, y) belong to class $C^{(2)}$ in R + S. The significance of this result can be seen by writing (3.4) in the following form $\left(\operatorname{assuming} \overline{\beta} > \frac{1}{4}\right)$.

$$S(\mathscr{G}_{\omega_{1}}) \leq \frac{1-\gamma \left| \frac{\overline{1-M}}{2} \right|}{1+\gamma \left| \frac{1-M}{2} \right|}$$
(5.8)

where

$$\gamma = \left(1 + \frac{2(\overline{\beta} - 1/4)}{1 - M}\right)^{-1/2}.$$
(5.9)

By (5.3) it follows that $M = 1 - ch^2 + O(h^4)$ for some c > 0. Therefore, (5.7) implies that $\gamma \ge \gamma_0$ as $h \to 0$ for some $\gamma_0 > 0$. By (5.8) it follows that

$$RR(\mathscr{G}_{\omega_1}) = O(h^{-1}), \qquad (5.10)$$

and hence by (4.9) we have

 $RR_{\infty} = O(h^{-1/2}).$ (5.11)

6. Numerical Results

Table 1 gives the number of iterations required for convergence using the accelerated SSOR method for several elliptic boundary value problems. In each case it is assumed that F(x, y) = 0. The function A(x, y) and C(x, y) are as indicated. The values of ω_1 and $S(\mathscr{G}_{\omega_1})$ as estimated using M = -m given by (5.3) and $\overline{\beta}$ given by (5.5) were used. In addition, the experimentally determined optimum ω and the corresponding value of $S(\mathscr{G}_{\omega})$ as determined by the power method were

used. For comparison, the number of iterations required for convergence using the SOR method with the optimum ω is given in each case. It should be noted that each SSOR iteration requires approximately as much work as two SOR iterations. (See, however, NIETHAMMER [4] where it is shown that the computation can be organized so that the number of operations per iteration for each method is approximately the same.)

The numbers of iterations given are those required to satisfy the convergence tolerance

$$\frac{\|u^{(n)} - \bar{u}\|_{A^{1/2}}}{\|\bar{u}\|_{A^{1/2}}} \leq 10^{-6}$$

starting with $u^{(0)} = 0$. Here we define the $A^{1/2}$ norm $||v||_{A^{1/2}}$ of a vector v by

$$\|v\|_{A^{1/2}} = \|A^{1/2}v\| = \sqrt{(v, Av)}$$

From Table 1 it can be seen that the number of iterations \mathcal{N} for the SSOR-SI method varies approximately as $h^{-1/2}$ while for the SOR method \mathcal{N} varies at least as fast as h^{-1} . Even considering the fact that twice as much work per iteration is

Coefficients	h	Accelerated SSOR		
		Estimated Parameters	Optimum Parameters	SOR
A = C = 1	1/20	19	16	44
	1/40	26	23	88
	1/80	37	32	174
$A = C = e^{10(x+y)}$	1/20	10	10	24
	1/40	15	14	48
	1/80	21	20	119
$A = \frac{1}{1 + 2x^2 + x^2}$	1/20	28	17	45
$1 + 2x^2 + y^2$	1/40	40	23	90
$A = \frac{1}{1 + 2x^2 + y^2}$ $C = \frac{1}{1 + x^2 + 2x^2}$	1/80	57	33	177
$A = C = \begin{cases} 1 + x, \ 0 \le x \le \frac{1}{2} \\ 2 - x, \ \frac{1}{2} \le x \le 1 \end{cases}$	1/20	21	17	46
	1/40	32	24	92
	1/80	49	33	180
$A = 1 + 4 x - \frac{1}{2} ^2$	1/20	28	19	43
$(1, 0 \le x < \frac{1}{2})$	1/40	40	25	86
$C = \begin{cases} 1, \ 0 \le x < \frac{1}{2} \\ 9, \ \frac{1}{2} \le x \le 1 \end{cases}$	1/80	56	34	164
$A = 1 + \sin \frac{\pi(x+y)}{2}$	1/20	11	10	24
$A = 1 + \sin \frac{1}{2}$	1/40	15	15	47
$C = e^{10(x+y)}$	1/80	22	21	120

Table 1. Numerical Results

required per iteration and in spite of the additional complication due to the acceleration process, there is a worthwhile saving using the SSOR method as opposed to the SOR method for problems involving small mesh sizes. In some cases, there is an appreciable additional saving achieved in using the optimum ω and the exact $S(\mathcal{D}_{\omega})$ instead of the estimated values. This suggests the desirability of using adaptive, or dynamic, procedures for parameter determination along the lines of Evans and FORRINGTON [1]. The procedure of Evans and Forrington is based on formulas developed by HABETLER and WACHSPRESS [3]. Research on adaptive parameter determination in now underway at The University of Texas at Austin.

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