Finite Precision Behavior of Stationary Iteration for Solving Singular Systems

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ABSTRACT

A stationary iterative method for solving a singular system $Ax = b$ converges for any starting vector if $\lim_{i\to\infty} G^i$ exists, where G is the iteration matrix, and the solution to which it converges depends on the starting vector. We examine the behavior of stationary iteration in finite precision arithmetic. A perturbation bound for singular systems is derived and used to define forward stability of a numerical method. A rounding error analysis enables us to deduce conditions under which a stationary iterative method is forward stable or backward stable. The component of the forward error in the null space of A can grow linearly with the number of iterations, but it is innocuous as long as the iteration converges reasonably quickly. As special cases, we show that when A is symmetric positive semidefinite the Richardson iteration with optimal parameter is forward stable, and if A also has unit diagonal and property A, then the Gauss-Seidel method is both forward and backward stable. Two numerical examples are given to illustrate the analysis.

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1. INTRODUCTION

Singular linear systems occur in various applications, such as the computation of the stationary distribution vector in a Markov chain [1, 8] and the solution of a Neumann boundary value problem by finite difference methods [11]. Because of the structure and the possibly large dimension of the coefficient matrices in these applications, iterative methods are frequently used to solve the systems. A potential danger is that the rather delicate convergence properties of the iterative methods will be destroyed by rounding errors. Keller [9] discusses this possibility for stationary iteration, and gives a short argument from which he concludes that "the spurious contributions in null(A) grow at worst linearly and if the rounding errors are small the scheme can be quite effective." In this work we extend our analysis in [6] to provide a quantitative error analysis of stationary iteration for singular systems.

In Section 2 we set up our notation and review the behavior of stationary iteration in exact arithmetic. In Section 3 we define normwise and componentwise forward and backward stability of a numerical method for solving singular systems. Backward stability can be defined as in the nonsingular case; forward stability cannot, so we derive a new perturbation result to help us formulate an appropriate definition.

A forward error analysis is presented in Section 4. We split the error into its components in null(A) and its complement. The error bounds enable us to identify conditions under which stationary iteration is normwise or componentwise forward stable. A bound for the residual, and hence for the normwise backward error, is derived in Section 5. In Sections 6 and 7 we give examples of how unconditional stability can be deduced in special cases: we show that (1) the Richardson iteration with optimal parameter is normwise forward stable if A is symmetric positive semidefinite and (2) the Gauss-Seidel method is both normwise forward stable and normwise backward stable if A is symmetric positive semidefinite with unit diagonal and has property A. Finally, two numerical experiments with the Gauss-Seidel method are described in Section 8. One shows how the analysis correctly predicts forward and backward stability for a Neumann problem, and the other displays instability of the Gauss-Seidel method, with linear growth of the component of the error in null(A), which again is in accord with the analysis.

A useful tool in analyzing the behavior of stationary iteration for a singular system is the Drazin inverse. This can be defined, for $A \in \mathbb{R}^{n\times n}$, as the unique matrix A^D such that

$$A^DAA^D = A^D, \qquad AA^D = A^DA, \quad \text{and} \quad A^{k+1}A^D = A^k,$$

where $k = \text{index}(A)$. The index of A is the smallest nonnegative integer k such that $\text{rank}(A^k) = \text{rank}(A^{k+1})$; it is characterized as the dimension of the largest Jordan block of A with eigenvalue zero. If index(A) $= 1$, then A^D is also known as the group inverse of A, and is denoted by $A^{\#}$. The Drazin inverse is an "equation-solving inverse" precisely when index(A) ≤ 1, for then $AA^DA = A$, and so if $Ax = b$ is a consistent system then A^Db is a solution. As we will see, however, the Drazin inverse of the coefficient matrix A itself plays no role in the analysis. The Drazin inverse can be represented explicitly as follows. If

$$A = P\begin{bmatrix} B & 0 \\ 0 & N \end{bmatrix}P^{-1},$$

where P and B are nonsingular and N has only zero eigenvalues, then

$$A^D = P\begin{bmatrix} B^{-1} & 0 \\ 0 & 0 \end{bmatrix}P^{-1}.$$

Further details of the Drazin inverse can be found in the excellent reference [2, Chapter 7].

2. THEORETICAL BACKGROUND

Let $A \in \mathbb{R}^{n\times n}$ be a singular matrix. We consider solving $Ax = b$ by stationary iteration, using a splitting $A = M - N$, where M is nonsingular. The iteration takes the form

$$Mx_{k+1} = Nx_k + b.$$

First, we examine the convergence of the iteration in exact arithmetic. Since any limit point x of the sequence $\{x_k\}$ must satisfy $Mx = Nx + b$, or $Ax = b$, we restrict our attention to consistent linear systems. (For a thorough analysis of stationary iteration for inconsistent systems see [4].) Writing the iteration as $x_{k+1} = Gx_k + M^{-1}b$, where $G = M^{-1}N$, and solving this recurrence, we obtain

$$x_{m+1} = G^{m+1}x_0 + \sum_{i=0}^{m} G^iM^{-1}b. \tag{2.1}$$

Since A is singular, G has an eigenvalue 1, so G^m does not tend to zero as $m \to \infty$, that is, G is not convergent. If the iteration is to converge for all x_0 then $\lim_{m\to\infty} G^m$ must exist. Following [10], we call a matrix B for which $\lim_{m\to\infty} B^m$ exists semiconvergent.

We assume from this point on that G is semiconvergent. It is easy to see [1, Lemma 6.9] that G must have the form

$$G = P\begin{bmatrix} I & 0 \\ 0 & \Gamma \end{bmatrix}P^{-1}, \tag{2.2}$$

where P is nonsingular and $\rho(\Gamma) < 1$. Hence

$$\lim_{m\to\infty} G^m = P\begin{bmatrix} I & 0 \\ 0 & 0 \end{bmatrix}P^{-1}.$$

To rewrite this limit in terms of G, we note that

$$I - G = P\begin{bmatrix} 0 & 0 \\ 0 & I-\Gamma \end{bmatrix}P^{-1}, \tag{2.3}$$

and, since $I - \Gamma$ is nonsingular,

$$(I-G)^D = P\begin{bmatrix} 0 & 0 \\ 0 & (I-\Gamma)^{-1} \end{bmatrix}P^{-1}. \tag{2.4}$$

Hence

$$\lim_{m\to\infty} G^m = I - (I-G)^D(I-G). \tag{2.5}$$

To evaluate the limit of the second term in (2.1) we note that, since the system is consistent, $M^{-1}b = M^{-1}Ax = (I-G)x$, and so

$$\begin{aligned}\sum_{i=0}^{m} G^iM^{-1}b &= \sum_{i=0}^{m} G^i(I-G)x \\ &= (I - G^{m+1})x \\ &\to (I-G)^D(I-G)x = (I-G)^DM^{-1}b,\end{aligned}$$

using (2.5). We note in passing that the condition that G is semiconvergent is equivalent to $I - G$ having index 1, in view of (2.3), but that this condition does not imply that $A = M(I-G)$ has index 1.

The conclusion is that if G is semiconvergent, stationary iteration converges to a solution of $Ax = b$ that depends on x_0:

$$\lim_{m\to\infty} x_m = [I - (I-G)^D(I-G)]x_0 + (I-G)^DM^{-1}b. \tag{2.6}$$

The first term in this limit is in null$(I-G)$, and the second term is in range$(I-G)$. To obtain the unique solution in range$(I - G)$ we should take for x_0 any vector in range$(I - G)$ ($x_0 = 0$, say). In Section 4 we modify the above analysis to incorporate the effects of rounding errors. To guide the error analysis we need to know what we are aiming to prove. Therefore in the next section we examine forward and backward stability for singular systems.

3. STABILITY FOR SINGULAR SYSTEMS

The notion of numerical stability is well understood for nonsingular systems $Ax = b$. A method is said to be normwise backward stable in floating point arithmetic if it produces a computed solution $\widehat{x}$ that satisfies

$$\|b - A\widehat{x}\| \leq c_n u(\|A\| \, \|\widehat{x}\| + \|b\|) \tag{3.1}$$

for some constant c_n, where u is the unit roundoff. As is well known, this condition is equivalent to the condition that $\widehat{x}$ solves a slightly perturbed system (see [6], for example). The definition of componentwise backward stability is obtained by replacing the norms with absolute values in (3.1). These definitions are applicable also to consistent singular systems, but in this case the size of the residual $b - Ay$ cannot be used to bound the error $x - y$ for a particular solution x; indeed, the error can be arbitrarily large even when $b - Ay = 0$.

However, it is possible to bound the distance from y to the nearest solution vector,

$$\delta_2(y) = \min\{\|y - x\|_2 \ : \ Ax = b\}. \tag{3.2}$$

The constrained least squares problem defining $\delta_2(y)$ is easily solved by noting that if $Ax = b$, then $z = y - x$ satisfies $Az = Ay - b = r$. The required z is the solution of minimum 2-norm to the consistent system $Az = r$, and so $\delta_2(y) = \|A^+ r\|_2$, where A^+ is the Moore-Penrose pseudoinverse. Hence, like the error in the nonsingular case, $\delta_2(y)$ can be bounded in terms of the residual, but with $\|A^+\|_2$ replacing $\|A^{-1}\|_2$. We do not need δ_2 for our stability definitions, but we will make use of it in Section 4.

A method for solving nonsingular systems is normwise forward stable if

$$\|x - \widehat{x}\| \leq c_n' u \kappa(A) \|x\|, \tag{3.3}$$

where $\kappa(A) = \|A\| \, \|A^{-1}\|$, and componentwise forward stable if

$$\|x - \widehat{x}\| \leq c_n' u \big\| |A^{-1}| \, |A| \, |x| \big\|. \tag{3.4}$$

Here, and throughout, the norm is assumed to be monotonic (that is, $|x| \leq |y| \Rightarrow \|x\| \leq \|y\|$ [7, p. 285]). These definitions are clearly unsuitable for a singular system, since they involve A^{-1}. Moreover, since the solution to which stationary iteration converges depends on the method [as shown by (2.6)], a useful definition of forward stability must be method-dependent. We use the following perturbation result as the basis for our definition of forward stability. The result projects the perturbations into range$(I - G)$ and so can be thought of as gauging the effect of perturbations to the "nonsingular part of the system."

THEOREM 3.1. *Let x be a particular solution of the consistent and singular linear system $(I - G)x = M^{-1}b$, where $G, M \in \mathbb{R}^{n\times n}$ and G is semiconvergent. Consider the perturbed system*

$$E[I - (G + \Delta G)](x + \Delta x) = E(M + \Delta M)^{-1}(b + \Delta b), \tag{3.5}$$

where E is the projector $(I - G)^D(I - G)$, the underlying perturbations are ΔM, ΔN and Δb, and

$$\begin{aligned} G &= M^{-1}N, \quad G + \Delta G = (M + \Delta M)^{-1}(N + \Delta N), \\ A &= M - N, \quad A + \Delta A = (M + \Delta M) - (N + \Delta N). \end{aligned}$$

Suppose that $\|\Delta M\| = O(\epsilon)$, $\|\Delta N\| = O(\epsilon)$, and $\|\Delta b\| = O(\epsilon)$. If $\rho((I - G)^D \Delta G) < 1$, then there exists a vector Δx satisfying (3.5) such that

$$\Delta x = (I - G)^D M^{-1}(\Delta b - \Delta A x) + O(\epsilon^2).$$

Proof. We define f to be the vector satisfying

$$(M + \Delta M)^{-1}(b + \Delta b) = M^{-1}b + f.$$

Expanding (3.5) and simplifying, we have

$$(I - G)\big[I - (I - G)^D \Delta G\big]\Delta x = E(f + \Delta G x),$$

which has a particular solution

$$\big[I - (I - G)^D \Delta G\big]\Delta x = (I - G)^D(f + \Delta G x). \tag{3.6}$$

Since $\rho((I - G)^D \Delta G) < 1$, the matrix $I - (I - G)^D \Delta G$ is nonsingular, and so (3.6) has the unique solution

$$\begin{aligned} \Delta x &= \big[I - (I - G)^D \Delta G\big]^{-1}(I - G)^D(f + \Delta G x) \\ &= (I - G)^D(f + \Delta G x) + O(\epsilon^2). \end{aligned} \tag{3.7}$$

It is simple to show that

$$\begin{aligned} f &= M^{-1}(\Delta b + \Delta M G x - \Delta M x) + O(\epsilon^2), \\ \Delta G &= M^{-1}(\Delta N - \Delta M G) + O(\epsilon^2), \end{aligned}$$

and substituting these formula into (3.7) completes the proof. ∎

Our definition of componentwise forward stability is motivated by assuming that $|\Delta A| \leq \epsilon |A|$ and $|\Delta b| \leq \epsilon |b|$, where $\epsilon = c_n u$, and using the theorem to obtain the first order bound, for any absolute norm, $\|\Delta x\| \leq c_n u \| \, |(I - G)^D M^{-1}| (|A| \, |x| + |b|) \, \|$. Thus we define a stationary iterative method to be componentwise forward stable if the computed solution $\widehat{x}$ satisfies

$$\|x - \widehat{x}\| \leq c_n u \left\| \, |(I - G)^D M^{-1}| \, |A| \, |x| \, \right\|, \tag{3.8}$$

where x is the solution that would be computed by the method in exact arithmetic. Note that we have omitted b from the right-hand side, but since $|b| \leq |A||x|$ this merely changes the constant c_n.

Similarly, a stationary iterative method is normwise forward stable if the computed solution $\widehat{x}$ satisfies

$$\|x - \widehat{x}\| \leq c_n u \|(I - G)^D M^{-1}\| \, \|A\| \, \|x\|. \tag{3.9}$$

That these are appropriate definitions of forward stability is supported by the properties that they are method-dependent when A is singular, and that when A is nonsingular they reduce to (3.3) and (3.4), since then $(I - G)^D M^{-1} = A^{-1}$.

4. FORWARD ERROR ANALYSIS

We use the same assumptions and model of floating point arithmetic as in [6]. Thus we assume that x_{k+1} is computed by forming $Nx_k + b$ and then solving $Mx_{k+1} = Nx_k + b$, and we use the standard model of floating point arithmetic (in its weaker form that is valid for machines without a guard digit). The computed vectors $\widehat{x}_k$ satisfy an equality of the form

$$(M + \Delta M_{k+1})\widehat{x}_{k+1} = N\widehat{x}_k + b + f_k,$$

or

$$M\widehat{x}_{k+1} = N\widehat{x}_k + b - \xi_k, \tag{4.1}$$

where

$$\xi_k = \Delta M_{k+1} \widehat{x}_{k+1} - f_k.$$

For the Jacobi, Gauss-Seidel, SOR, and Richardson iterations it is easy to show [6] that

$$|\xi_k| \leq c_n u (|M| \, |\widehat{x}_{k+1}| + |N| \, |\widehat{x}_k| + |b|), \tag{4.2}$$

where c_n is a constant of order n; for the rest of the analysis we will assume that (4.2) is satisfied.

Solving the recurrence (4.1), we obtain [cf. (2.1)]

$$\widehat{x}_{m+1} = G^{m+1}x_0 + \sum_{i=0}^{m} G^i M^{-1}(b - \xi_{m-i}). \tag{4.3}$$

We wish to bound $e_{m+1} = x - \widehat{x}_{m+1}$, where x is the limit in (2.6) corresponding to the given starting vector x_0. Since the iteration is stationary at the solution x, we have, from (2.1),

$$x = G^{m+1}x + \sum_{i=0}^{m} G^i M^{-1}b. \tag{4.4}$$

Subtracting (4.3) from (4.4), we obtain

$$e_{m+1} = G^{m+1}e_0 + \sum_{i=0}^{m} G^i M^{-1}\xi_{m-i}.$$

The first term, $G^{m+1}e_0$, is negligible for large m, because it is the error after $m+1$ stages of the exact iteration and this error tends to zero. To obtain a useful bound for the second term, we cannot simply take norms or absolute values, because $\sum_{i=0}^{m} G^i$ grows unboundedly with m (recall that G has an eigenvalue 1). Our approach is to split the vectors ξ_i according to $\xi_i = \xi_i^{(1)} + \xi_i^{(2)}$, where $M^{-1}\xi_i^{(1)} \in \mathrm{range}(I-G)$ and $M^{-1}\xi_i^{(2)} \in \mathrm{null}(I-G)$; this is a well-defined splitting because range$(I - G)$ and null$(I - G)$ are complementary subspaces [since index$(I - G) = 1$, or equivalently, G is semiconvergent]. Using the properties of the splitting, the error can be written as

$$\begin{aligned} e_{m+1} &= G^{m+1}e_0 + \sum_{i=0}^{m} G^i M^{-1}\xi_{m-i}^{(1)} + \sum_{i=0}^{m} G^i M^{-1}\xi_{m-i}^{(2)} \\ &= G^{m+1}e_0 + \sum_{i=0}^{m} G^i M^{-1}\xi_{m-i}^{(1)} + M^{-1}\sum_{i=0}^{m} \xi_{m-i}^{(2)}. \end{aligned}$$

We achieve the required splitting for ξ_i via the formulae

$$\xi_i^{(1)} = MEM^{-1}\xi_i, \quad \xi_i^{(2)} = M(I - E)M^{-1}\xi_i,$$

where

$$E = (I - G)^D(I - G).$$

Hence the error can be written as

$$e_{m+1} = G^{m+1}e_0 + \sum_{i=0}^{m} G^i EM^{-1}\xi_{m-i} + (I - E)M^{-1}\sum_{i=0}^{m} \xi_{m-i}. \tag{4.5}$$

Clearly, as $m \to \infty$ the final term in this expression can become unbounded, but since it grows only linearly in the number of iterations, it is unlikely to have a significant effect in applications where stationary iteration converges quickly enough to be of practical use. This point is also addressed in [9] (see the quotation in Section 1), but without the benefit of an explicit expression for the error.

Now we bound the term

$$S_m = \sum_{i=0}^{m} G^i E M^{-1} \xi_{m-i}. \tag{4.6}$$

The inequality (4.2) gives us a bound on the size of the error vectors ξ_k that depends on the iterates $\widehat{x}_k$. As in [6], we define the ratios

$$\theta_x = \sup_k \max_{1\le i\le n} \left(\frac{|\widehat{x}_k|_i}{|x_i|} \right), \qquad \gamma_x = \sup_k \frac{\|\widehat{x}_k\|}{\|x\|}, \tag{4.7}$$

in terms of which $|\widehat{x}_k| \le \theta_x |x|$ and $\|\widehat{x}_k\| \le \gamma_x \|x\|$ for all k. Here, x is the vector given in (2.6). We have the componentwise and normwise bounds

$$\begin{aligned} |\xi_k| &\le c_n u(1+\theta_x)(|M| + |N|)|x| \equiv \xi_C, \\ \|\xi_k\| &\le c_n' u(1+\gamma_x)(\|M\| + \|N\|)\|x\| \equiv \xi_N, \end{aligned}$$

where $c_n' = c_n$ for the ∞-norm and $c_n' = \sqrt{n}\, c_n$ for the 2-norm. Returning to (4.6), we obtain the bound

$$\begin{aligned} |S_m| &= \left| \sum_{i=0}^{m} G^i E M^{-1} \xi_{m-i} \right| \\ &\le \sum_{i=0}^{m} |G^i E M^{-1}| \xi_C \\ &\le \sum_{i=0}^{\infty} |G^i E M^{-1}| \xi_C, \end{aligned} \tag{4.8}$$

and also the normwise bound

$$\|S_k\| \le \sum_{i=0}^{\infty} \|G^i E M^{-1}\| \xi_N.$$

The convergence of the two infinite sums is assured by Lemma 2.1 in [6], since by (2.2), (2.3), and (2.4),

$$\begin{aligned} G^iE &= G^i(I-G)^D(I-G) \\ &= P\begin{bmatrix} I & 0 \\ 0 & \Gamma^i \end{bmatrix} P^{-1} \cdot P \begin{bmatrix} 0 & 0 \\ 0 & (I-\Gamma)^{-1} \end{bmatrix} P^{-1} \cdot P \begin{bmatrix} 0 & 0 \\ 0 & (I-\Gamma) \end{bmatrix} P^{-1} \\ &= P\begin{bmatrix} 0 & 0 \\ 0 & \Gamma^i \end{bmatrix} P^{-1} = (GE)^i \quad (i \geq 1), \end{aligned} \tag{4.9}$$

where $\rho(\Gamma) < 1$.

We conclude that we have the normwise error bound

$$\begin{aligned} \|e_{m+1}\| &\leq \|G^{m+1}e_0\| + c_n' u(1+\gamma_x)(\|M\| + \|N\|)\|x\| \\ &\quad \times \left\{ \sum_{i=0}^{\infty} \|G^iEM^{-1}\| + (m+1)\|(I-E)M^{-1}\| \right\}. \end{aligned} \tag{4.10}$$

On setting $E = I$ we obtain the result for the nonsingular case given in [6]. If we assume that Γ is diagonal, so that P in (4.9) is a matrix of eigenvectors of G, then for any absolute norm,

$$\sum_{i=0}^{\infty} \|G^iEM^{-1}\| \leq \kappa(P)\|M^{-1}\| \frac{1}{1-\rho(\Gamma)}.$$

This bound shows that a small forward error is guaranteed if $\kappa(P)\|M^{-1}\| = O(1)$ and the second largest eigenvalue of G is not too close to 1. (It is this subdominant eigenvalue that determines the asymptotic rate of convergence of the iteration.)

Turning to the componentwise case, we see from (2.4) and (4.9) that

$$\sum_{i=0}^{\infty} G^iE = (I-G)^D.$$

Because of the form of the bound (4.8), this prompts us to define the scalar $c(A) \geq 1$ by

$$c(A) = \min \left\{ \epsilon : \sum_{i=0}^{\infty} |G^iEM^{-1}| \leq \epsilon |(I-G)^D M^{-1}| \right\},$$

in terms of which we have the componentwise error bound

$$\begin{aligned} |e_{m+1}| &\leq |G^{m+1}e_0| + c_n u(1+\theta_x)\big\{c(A)|(I-G)^DM^{-1}| \\ &\quad + (m+1)|(I-E)M^{-1}|\big\}(|M| + |N|)|x|. \end{aligned} \tag{4.11}$$

Again, as a special case we have the result for nonsingular A given in [6].

As in the nonsingular case, the bound (4.11) has desirable scaling properties. If the elements of M and N are linear combinations of those of A, then $c(A)$ is independent of scalings $A \to D_1AD_2$ (D_i diagonal and nonsingular) and in most respects (4.11) is invariant under such scalings—the exception is the term θ_x, which can be expected to depend only mildly on the scaling.

From (4.11) and (3.8), we deduce conditions on a stationary iterative method that ensure it is componentwise forward stable: the constants θ_x and $c(A)$ should be bounded by d_n, a slowly growing function of n; the inequality $|M|+|N| \le d_n'|A|$ should hold, as it does for the Jacobi method, and for the SOR method when $\omega \in [\beta, 2]$, where β is positive and not too close to zero; and the "exact error" $G^{m+1}e_0$ must decay quickly enough to ensure that the term $(m+1)|(I-E)M^{-1}|$ does not grow too large before the iteration is terminated.

Unlike for the case of nonsingular A, it does not seem possible to identify important classes of matrices and methods for which componentwise forward stability is guaranteed. As an indication of the difficulty, whereas $c(A) = 1$ for the Jacobi and Gauss-Seidel methods if A is a nonsingular M-matrix [6], when A is a singular M-matrix $c(A)$ can be infinite. An example for the Gauss-Seidel method is the $n \times n$ matrix with $a_{ii} \equiv n-1$ and $a_{ij} = -1$ for $i \ne j$, for which, for certain n, $(I-G)^DM^{-1}$ has zero elements that are nonzero in the terms G^iEM^{-1}. There is, however, a theoretically interesting class of iterations and matrices for which $c(A)$ is likely to be small. This is the class for which $A = M - N$ is a regular splitting, that is, for which $M^{-1} \ge 0$, $I - G$ has index 0 or 1, and $NE \ge 0$; this definition, from [10], generalizes the classical definition of Varga [14] to singular matrices. For a regular splitting, for $i \ge 1$ we have

$$G^iEM^{-1} = (GE)^iM^{-1} = (M^{-1}NE)^iM^{-1} \ge 0,$$

and so if also $EM^{-1} \ge 0$ then $c(A) = 1$. Of more practical interest is the fact that normwise stability results can be obtained for some standard methods, as we show in Sections 6 and 7.

Finally, we suggest another approach to dealing with the potentially dangerous term $(I-E)M^{-1}\sum \xi_i$ in (4.5). Premultiplying a vector by $I-E$ moves it into the null space of $I-G$, which is also the null space of A. If we measure error by the distance $\delta_2(\widehat{x}_k)$ from the iterate $\widehat{x}_k$ to the nearest solution vector [see (3.2)], then we can ignore $(I-E)M^{-1}\sum \xi_i$, as this term moves us parallel to the solution space. Hence, in the normwise case, by a slight modification of the above analysis,

$$\begin{aligned}\delta_2(\widehat{x}_{m+1}) \le\ & \|G^{m+1}e_0\|_2 \\ & + c_n' u\gamma_m\big[(\|M\|_2 + \|N\|_2)\|x_{m+1}^*\|_2 + \|b\|_2\big] \\ & \times \sum_{i=0}^{\infty} \|G^iEM^{-1}\|_2,\end{aligned}$$

where x_{m+1}^* is the nearest solution vector to $\widehat{x}_{m+1}$ and

$$\gamma_m = \max_{0 \le k \le m} \frac{\|\widehat{x}_k\|}{\|x_{m+1}^*\|}.$$

A possible drawback of this approach is that x_{m+1}^* can be large normed, which may make it an unacceptable solution.

5. THE RESIDUAL

Now we investigate the size of the residual, $r_{m+1} = b - A\widehat{x}_{m+1}$, in order to bound the backward error. From (4.3) and (4.4) we find that

$$r_{m+1} = AG^{m+1}(x - x_0) + \sum_{i=0}^{m} AG^i M^{-1} \xi_{m-i}.$$

It is easy to show that $AG^i = H^i A$, where $H = NM^{-1}$ (recall that $G = M^{-1}N$). Therefore

$$r_{m+1} = H^{m+1} r_0 + \sum_{i=0}^{m} H^i (I - H) \xi_{m-i}. \tag{5.1}$$

Since the right-hand side of (3.1) contains $\widehat{x}$ rather than x, we modify the definitions of θ_x and γ_x in (4.7):

$$\theta_m = \max_{0 \le k \le m} \max_{1 \le i \le n} \frac{|\widehat{x}_k|_i}{|\widehat{x}_{m+1}|_i}, \qquad \gamma_m = \max_{0 \le k \le m} \frac{\|\widehat{x}_k\|}{\|\widehat{x}_{m+1}\|}.$$

With these definitions, $|\widehat{x}_k| \le \theta_m |\widehat{x}_{m+1}|$ and $\|\widehat{x}_k\| \le \gamma_m \|\widehat{x}_{m+1}\|$ for $0 \le k \le m$, and so, using (4.2),

$$\begin{aligned} |\xi_k| &\le c_n u\big[\theta_m(|M| + |N|)|\widehat{x}_{m+1}| + |b|\big], \\ \|\xi_k\| &\le c_n' u\big[\gamma_m(\|M\| + \|N\|)\|\widehat{x}_{m+1}\| + \|b\|\big]. \end{aligned}$$

From (5.1) we obtain the componentwise bound

$$|r_{m+1}| \le |H^{m+1} r_0| + c_n u S\big[\theta_m(|M| + |N|)|\widehat{x}_{m+1}| + |b|\big], \tag{5.2}$$

where

$$S = \sum_{i=0}^{\infty} |H^i (I - H)|.$$

The first term, $H^{m+1}r_0$, is the residual of the exact iteration after $m+1$ stages, so it tends to zero. Since G is semiconvergent and $H = MGM^{-1}$, H is also semiconvergent. Therefore H has the form

$$H = Q\begin{bmatrix} I & 0 \\ 0 & \Gamma \end{bmatrix} Q^{-1},$$

where $\rho(\Gamma) < 1$, and

$$H^i(I-H) = Q\begin{bmatrix} 0 & 0 \\ 0 & \Gamma^i(I-\Gamma) \end{bmatrix} Q^{-1}.$$

It follows from Lemma 2.1 in [6] that the sum defining S exists.

The bound (5.2) is essentially the same as the one that holds in the case of nonsingular A [6]. As in that case, we are not aware of any classes of matrix or iteration for which (5.2) implies componentwise backward stability. The normwise analogue of (5.2) is

$$\|r_{m+1}\| \le \|H^{m+1}r_0\| + c_n' u\sigma\big[\gamma_m(\|M\| + \|N\|)\|\widehat{x}_{m+1}\| + \|b\|\big], \tag{5.3}$$

where

$$\sigma = \sum_{i=0}^{\infty} \|H^i(I-H)\|.$$

As is shown in [6], if $H = XDX^{-1}$, with $D = \mathrm{diag}(\lambda_i)$, then for any p-norm

$$\sigma \le \kappa(X) \max_{\lambda_i \ne 1} \frac{|1-\lambda_i|}{1-|\lambda_i|}. \tag{5.4}$$

Thus σ is guaranteed to be small if H is diagonalizable with a well conditioned matrix of eigenvectors and if H has no eigenvalues of modulus close to 1 other than the eigenvalue 1.

For large m the normwise backward error satisfies

$$\frac{\|r_m\|}{\|A\|\,\|\widehat{x}_{m+1}\| + \|b\|} \le c_n'' u \gamma_m \sigma\left(\frac{\|M\| + \|N\|}{\|A\|}\right),$$

and for the ∞-norm the factor $(\|M\| + \|N\|)/\|A\|$ is bounded by 2 for the Jacobi method and for the SOR method with $1 \le \omega \le 2$. As we show in the next two sections, normwise backward stability can be deduced in certain cases.

6. RICHARDSON ITERATION

In this section we specialize our normwise forward and backward error bounds to the stationary Richardson iteration, for which $M = \alpha I$ and $N = \alpha I - A$, where α is a parameter. We will assume that A is symmetric positive semidefinite, with eigendecomposition $A = Q\Lambda Q^T$, where Q is orthogonal and

$$\Lambda = \operatorname{diag}(\lambda_i), \quad \lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_r > \lambda_{r+1} = \cdots = 0.$$

The parameter $\alpha_{\rm opt}$ that minimizes $\rho(G) = \rho(I - \alpha^{-1}A)$ is easily seen to be $\alpha_{\rm opt} = (\lambda_1 + \lambda_r)/2$. For $\alpha = \alpha_{\rm opt}$, G has eigenvalues $(\lambda_1 + \lambda_r - 2\lambda_i)/(\lambda_1 + \lambda_r)$; since G is symmetric and these eigenvalues are either unity or strictly between -1 and 1, we see that G is semiconvergent and hence the Richardson iteration converges. We assume now that $\alpha = \alpha_{\rm opt}$. To evaluate the bound (4.10) we note that

$$G^iEM^{-1} = \alpha^{-1}(I - \alpha^{-1}A)^iA^DA = \alpha^{-1}Q(I - \alpha^{-1}\Lambda)^i\Lambda^D\Lambda Q^T,$$

from which it follows that

$$\begin{aligned}
\sum_{i=0}^{\infty} \|G^iEM^{-1}\|_2 &= \alpha^{-1}\sum_{i=0}^{\infty} \max_{1\leq j\leq r} |1 - \alpha^{-1}\lambda_j|^i \\
&= \alpha^{-1}\sum_{i=0}^{\infty}\left(\frac{\lambda_1 - \lambda_r}{\lambda_1 + \lambda_r}\right)^i \\
&= \alpha^{-1}\left(\frac{\lambda_1 + \lambda_r}{2\lambda_r}\right) = \lambda_r^{-1} = \|A^D\|_2.
\end{aligned}$$

Since $\|M\|_2 + \|N\|_2 \leq 2\|A\|_2$, the bound (4.10) simplifies to

$$\|e_{m+1}\|_2 \leq \|G^{m+1}e_0\|_2 + c_n''u(1 + \gamma_x)\big[\|A\|_2\|A^D\|_2 + (m+1)\|I - A^DA\|_2\big]\|x\|_2.$$

Therefore, since $A^D = (I - G)^DM^{-1}$, we have normwise forward stability as long as γ_x is not too large and convergence is reasonably quick.

For the residual, since $H = G$, we obtain from (5.4) $\sigma_2 \leq \lambda_1/\lambda_r$. Thus (5.3) yields

$$\|r_{m+1}\|_2 \leq \|H^{m+1}r_0\|_2 + c_n''u\|A\|_2\|A^D\|_2\big(\gamma_m\|A\|_2\|\widehat{x}_{m+1}\|_2 + \|b\|_2\big).$$

This bound is larger by a factor $\|A\|_2\|A^D\|_2$ than what is needed to guarantee normwise backward stability. Of course, stability is assured if A has a small "Drazin condition number" $\kappa_D = \|A\|_2\|A^D\|_2$, and this must be the case if the iteration is to converge at a reasonable rate, since $\rho(G) = (\kappa_D - 1)/(\kappa_D + 1)$.

The results in this section generalize ones in [15] and [16, Theorems 3.3 and 3.4] that apply to the stationary Richardson iteration for symmetric positive definite A. (In [16] the nonstationary cyclic Richardson iteration is also analyzed.)

7. GAUSS-SEIDEL ITERATION

The Gauss-Seidel iteration is the stationary method defined by choosing M to be the lower triangular part of A. It is known to converge in exact arithmetic if A is symmetric positive definite. In [15] Woźniakowski shows that if $A = I - B$ is a symmetric positive definite matrix with property A, and B has zero diagonal elements, then the Gauss-Seidel iteration is normwise forward stable. We now show that this result remains true when we allow A to be positive semidefinite.

Since A has property A, B is of the form

$$B = \begin{bmatrix} 0 & F \\ F^T & 0 \end{bmatrix};$$

hence

$$M = \begin{bmatrix} I & 0 \\ -F^T & I \end{bmatrix}, \qquad G = \begin{bmatrix} 0 & F \\ 0 & F^T F \end{bmatrix}.$$

As $A = I - B$ is positive semidefinite and singular (by assumption), $1 = \rho(B)^2 = \rho(F^T F) = \rho(G)$. It is easy to show that G is semiconvergent, from which it follows that the Gauss-Seidel iteration converges for any starting vector. In fact, the Gauss-Seidel iteration converges for any symmetric positive semidefinite matrix with positive diagonal elements—this follows from general results in [4, Theorem 8; 9, Theorem 2].

Our aim is to bound S_m in (4.6). Therefore we examine closely the term $W_i \equiv G^i E M^{-1}$. Recalling that $E = (I-G)^D(I-G) = (I-G)(I-G)^D$, we have

$$\begin{aligned} W_i &= \begin{bmatrix} 0 & F \\ 0 & F^T F \end{bmatrix}^i \begin{bmatrix} I & -F \\ 0 & I - F^T F \end{bmatrix} \begin{bmatrix} I & -F \\ 0 & I - F^T F \end{bmatrix}^D \begin{bmatrix} I & 0 \\ F^T & I \end{bmatrix} \\ &= \begin{bmatrix} 0 & F(F^T F)^{i-1}(I - F^T F) \\ 0 & (F^T F)^i (I - F^T F) \end{bmatrix} \begin{bmatrix} I & X \\ 0 & (I - F^T F)^D \end{bmatrix} \begin{bmatrix} I & 0 \\ F^T & I \end{bmatrix}, \end{aligned}$$

where $X = F[(I - F^T F)^D + (I - F^T F)^D (I - F^T F) - I]$ (using [2, Theorem 7.7.1]).

Multiplying out, we have

$$W_i = \begin{bmatrix} FY_{i-1}F^T & FY_{i-1} \\ Y_i F^T & Y_i \end{bmatrix},$$

where $Y_i = (F^T F)^i (I - F^T F)(I - F^T F)^D$, which satisfies $Y_i = Y_1^i$. It is straightforward to show that every 1-eigenvector and null vector of B is a null vector of $W_i^T W_i$. (By λ-eigenvector we mean an eigenvector corresponding to the eigenvalue λ.) Now suppose that x is a λ-eigenvector of B and $\lambda \neq 0, 1$. Then

$$Bx = \begin{bmatrix} 0 & F \\ F^T & 0 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} Fx_2 \\ F^T x_1 \end{bmatrix} = \begin{bmatrix} \lambda x_1 \\ \lambda x_2 \end{bmatrix},$$

and if we let $y = [\lambda x_1^T \; x_2^T]^T$, then we see that $W_i^T W_i y = \lambda^{4i-2}(1+\lambda^2)^2 y$. Since B is nondefective, we have found the eigenvalues of $W_i^T W_i$, and so

$$\|W_i\|_2 = \lambda_0^{2i-1}(1+\lambda_0^2), \qquad i \geq 1,$$

where λ_0 is the absolute value of the largest eigenvalue of B that is strictly less than 1 in magnitude.

Since A is symmetric, it has index 1 and

$$A^D = Q^T \begin{bmatrix} 0 & 0 \\ 0 & \Lambda_1^{-1} \end{bmatrix} Q, \tag{7.1}$$

where Q is orthogonal and Λ_1 is the diagonal matrix of nonzero eigenvalues of A. From (7.1) and the definition of B we see that $\lambda_0 = 1 - 1/\|A^D\|_2$. Furthermore, if we evaluate $E^T E$ explicitly in terms of F, we find that the λ-eigenvectors of B ($\lambda \neq 1$) are 1-eigenvectors of $E^T E$, while the 1-eigenvectors of B are 2-eigenvectors of $E^T E$. We deduce that $\|E\|_2 = \sqrt{2}$, and a similar procedure reveals that $\|I-E\|_2 = \sqrt{2}$, too. It is straightforward to show that $\|M^{-1}\|_2 = (1+\sqrt{5})/2$. Hence,

$$\begin{aligned} \|S_m\|_2 &= \|EM^{-1}\xi_m\|_2 + \sum_{i=1}^{m} \|W_i \xi_{m-i}\|_2 \\ &\leq \left(\|EM^{-1}\|_2 + (1+\lambda_0^2) \sum_{i=1}^{m} \lambda_0^{2i-1} \right) \xi_N \\ &\leq \left(3 + \frac{\lambda_0(1+\lambda_0^2)}{1-\lambda_0^2} \right) \xi_N \\ &\leq \left(3 + \frac{1}{1-\lambda_0} \right) \xi_N = (3 + \|A^D\|_2)\xi_N. \end{aligned}$$

Using this bound, together with the inequalities $\|M\|_2 + \|N\|_2 \leq 3\|A\|_2$ and $\|(I-E)M^{-1}\|_2 \leq 3$, we obtain from (4.10) the final bound

$$\|e_{m+1}\|_2 \leq \|G^{m+1}e_0\|_2 + c_n'' u(1+\gamma_x)\|A\|_2[\|A^D\|_2 + (m+1)]\|x\|_2.$$

It can be shown that $\|A^D\|_2 = \|(I-G)^D M^{-1}\|_2$ provided that $F \neq I$. Therefore this bound guarantees normwise forward stability as long as γ_x is not too large and the rate of convergence is not too slow.

Turning to the residual, our task is to bound $\sum_{i=0}^{\infty} \|H^i(I-H)\|_2$. Using a similar approach to the forward error case we find that the eigenvectors of $[H^i(I-H)]^T H^i(I-H)$ are identical to those of W_i, but now with corresponding eigenvalues $\lambda^{4i-2}(1-\lambda^2)^2(1+\lambda^2)$, and these eigenvalues λ of B are real. Hence

$$\|H^i(I-H)\|_2 = \operatorname{sign}(\lambda)\lambda^{2i-1}(1-\lambda^2)(1+\lambda^2)^{1/2}$$

for some eigenvalue λ of B. Through further manipulation we can show that $\|I-H\|_2 < 1.6$ and so, since $\rho(B) = 1$,

$$\begin{aligned}\sum_{i=0}^{\infty} \|H^i(I-H)\|_2 &= \|I-H\|_2 + \sum_{i=1}^{\infty} \operatorname{sign}(\lambda)\lambda^{2i-1}(1-\lambda^2)(1+\lambda^2)^{1/2} \\ &\leq 1.6 + |\lambda|(1+\lambda^2)^{1/2} \\ &\leq 1.6 + \sqrt{2}.\end{aligned}$$

From (5.3) we obtain the final residual bound

$$\|r_{m+1}\|_2 \leq \|H^{m+1} r_0\|_2 + c_n'' u(\gamma_m \|A\|_2 \|\widehat{x}_{m+1}\|_2 + \|b\|_2),$$

which guarantees normwise forward stability for large enough m, provided γ_m is not too large. The derivation of this residual bound is also valid if A is nonsingular. A similar result for the nonsingular case, in which a different infinite sum is considered, can be found in [15].

8. NUMERICAL RESULTS

We illustrate the foregoing analysis with two numerical examples. The computations were done in Matlab, for which the unit roundoff $u = 2^{-53} \approx 1.1 \times 10^{-16}$.

Our first example uses the matrix obtained when a Neumann boundary value problem in two dimensions is discretized with the standard five point operator on a regular mesh, namely, the block tridiagonal matrix [11]

$$A = \begin{bmatrix} D & -2I & & & & & \\ -I & D & -I & & & & \\ & -I & D & \ddots & & & \\ & & \ddots & \ddots & \ddots & & \\ & & & \ddots & D & -I & \\ & & & & -I & D & -I \\ & & & & & -2I & D \end{bmatrix} \in \mathbb{R}^{N^2 \times N^2},$$

where

$$D = \begin{bmatrix} 4 & -2 & & & & & \\ -1 & 4 & -1 & & & & \\ & -1 & 4 & \ddots & & & \\ & & \ddots & \ddots & \ddots & & \\ & & & \ddots & 4 & -1 & \\ & & & & -1 & 4 & -1 \\ & & & & & -2 & 4 \end{bmatrix} \in \mathbb{R}^{N \times N}.$$

The matrix A has a one-dimensional null space spanned by the vector of all ones.

We took $N = 5$ and set $b = Ay$, where $y = (1, 2, \ldots, 25)^T$. We took three different starting vectors x_0: a random vector from the normal (0,1) distribution, the vector of ones, and the vector of zeros. The iterations were terminated when $\widehat{x}_k = \widehat{x}_{k+1}$. We report in Table 1 various numbers of interest, including

$$\eta_\infty(\widehat{x}_k) = \frac{\|b - A\widehat{x}_k\|_\infty}{\|A\|_\infty \|\widehat{x}_k\|_\infty + \|b\|_\infty}, \quad \phi_\infty(\widehat{x}_k) = \frac{\|x - \widehat{x}_k\|_\infty}{\|x\|_\infty}$$

and

$$\mathrm{cond}(A, x) = \frac{\big\| |(I - G)^D M^{-1}| |A| \, |x| \big\|}{\|x\|_\infty}$$

where, in each case, x is the true solution corresponding to x_0. (We computed x from (2.6), evaluating the Drazin inverse by the method in [2, Corollary 7.8.2].) We see from the table that the Gauss-Seidel iteration performs in a componentwise forward-stable and normwise backward-stable way. This is predicted by the error bounds, since $c(A)$, θ_x, σ_∞, and γ_x are all relatively small. The componentwise backward error, which is not shown, is also less than the unit roundoff. Note that, although there are over 100 iterations, the linearly bounded component of the error in null(A) does not appear to influence the forward error.

Table 1: Neumann problem

$$\|A^D\|_\infty = 2.82, \quad \|(I-G)^D M^{-1}\|_\infty = 3.55,$$
$$\max\{|\lambda| : \det(G-\lambda I) = 0,\ \lambda \neq 1\} = 0.729,$$
$$c(A) = 23.9, \quad \sigma_\infty = 5.98,$$
$$\theta_x \leq 1.93, \quad \gamma_x \leq 1.00,$$
$$\sum_{i=0}^{\infty} \|G^i E M^{-1}\|_\infty = 4.32, \quad \|(I-E)M^{-1}\|_\infty = 0.5.$$

x_0	Iters.	$\|x\|_\infty$	cond(A,x)	$\min_k \eta_\infty(\widehat{x}_k)$	$\min_k \phi_\infty(\widehat{x}_k)$
Random	119	13.4	13.7	4.46E−17	1.19E−15
Ones	116	12.5	14.6	4.76E−17	1.56E−15
Zeros	119	13.5	13.7	2.96E−17	1.18E−15

For our second example we take a nonsymmetric matrix of the form illustrated by

$$A_4 = \begin{bmatrix} \alpha & \alpha & -1 & 1 \\ \alpha & \alpha & 1 & -1 \\ \alpha & \alpha & \alpha & 1 \\ \alpha & \alpha & \alpha & \alpha \end{bmatrix},$$

that is, $a_{ij} \equiv \alpha$ for $i \geq j$ and $a_{ij} = (-1)^{j-i+1}$ for $j > i$, except that $a_{12} = \alpha$. This is a modified version of a nonsingular matrix used in [5] to illustrate instability of the Gauss-Seidel method. By evaluating G, it is easy to show that the Gauss-Seidel method converges for this matrix (that is, $G = M^{-1}N$ is semiconvergent) whenever $|\alpha| > 1$. We applied the Gauss-Seidel method to the system $A_n x = b$, with $n = 30$ and $\alpha = 4$, where $b = fl(A_n x)$ with the x_i equally spaced on $[-1, 1]$ ($-1 = x_1 < x_2 < \cdots < x_n = 1$). We took for the starting vector the "exact solution" x. The results are displayed in Figure 1, and the relevant statistics are as follows:

$$\|A^D\|_\infty = 1.16\text{E}7, \quad \|(I-G)^D M^{-1}\|_\infty = 1.26\text{E}7,$$
$$\max\{|\lambda| : \det(G-\lambda I) = 0,\ \lambda \neq 1\} = \tfrac{1}{|\alpha|} = 0.25, \quad \text{cond}(A,x) = 7.16\text{E}8,$$
$$c(A) = 4.32\text{E}2, \quad \sigma_\infty = 3.26\text{E}6,$$
$$\theta_x = 1.00, \quad \gamma_x = 1.00,$$
$$\sum_{i=0}^{\infty} \|G^i E M^{-1}\|_\infty = 1.26\text{E}7, \quad \|(I-E)M^{-1}\|_\infty = 8.14\text{E}5,$$
$$\|\widehat{x}_{400}\|_\infty = 1.00, \quad \delta_2(\widehat{x}_{400}) = 2.16\text{E}{-11}.$$

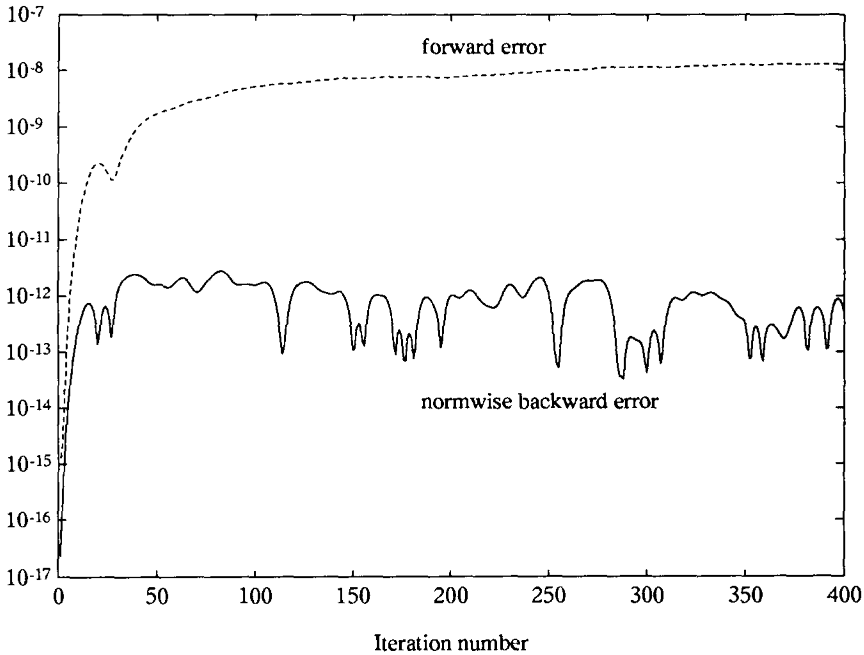

Figure 1: Gauss-Seidel iteration

We see from Figure 1 that the forward and backward errors grow rapidly initially. After about 40 iterations the forward error reaches the level

$$u \sum_{i=0}^{\infty} \|G^i E M^{-1}\|_\infty,$$

which is the order of magnitude of the bound (4.10) for $m = 40$. Thereafter the forward error grows approximately linearly (and continues to do beyond the 400th iteration); this is entirely in accord with (4.10), because the linearly growing term in (4.10) exceeds the infinite sum for $m \geq 15$. The backward error remains bounded for $m \geq 40$, since the growing component of the error lies in null(A). We do not fully understand the scalloping of the backward error curve, but similar behavior with the Richardson iteration has been observed by Trefethen [12] and Chatelin [3], and one way to investigate this phenomenon is via pseudospectra [13]. This failure of the iteration to converge is not restricted to ill-conditioned problems. If we change α to -4, then $\|A^D\|_\infty = 0.65$ and $\|(I-G)^D M^{-1}\|_\infty = 0.64$, and the forward and backward errors both grow rapidly at first and then exhibit scalloping behavior, with the forward error oscillating at around approximately 10^{-11}.

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