

Estimating Optimum Overrelaxation Parameters

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1. Introduction. In using the successive overrelaxation (S.O.R.) iteration method to solve the matrix equation

$$(1.1) \quad A\mathbf{x} = \mathbf{f},$$

finding the optimum overrelaxation parameter ω_b is an important and often a difficult part of the problem [1, p. 257]. When A is a 2-cyclic, consistently ordered, real symmetric, positive-definite matrix (this will be assumed in the rest of the paper), only the spectral radius $\rho(\mathcal{L}_1)$ of the associated Gauss-Seidel iteration matrix \mathcal{L}_1 is needed to determine the optimum parameter ω_b [2, p. 109]. When $\rho(\mathcal{L}_1)$ is close to unity, small changes in the estimate for $\rho(\mathcal{L}_1)$ can drastically affect the rate of convergence of the S.O.R. iterations and, thus, an accurate estimate of $\rho(\mathcal{L}_1)$ is needed.

In practice, two basic approaches are often used to estimate $\rho(\mathcal{L}_1)$ or equivalently ω_b . One approach is to carry out a number of S.O.R. iterations with some $\omega < \omega_b$ and then on the basis of numerical results obtain a new estimate for ω_b [1], [3], [4], [12]. A second approach is to obtain an estimate for $\rho(\mathcal{L}_1)$, using the power method, prior to carrying out the S.O.R. iterations [1], [2], [5], [6]. The second approach is useful when the iterative process is slowly convergent, when the matrix problem (1.1) is to be solved a number of times for different vectors \mathbf{f} , or when very accurate solutions are required.

In this paper it is shown how to use Chebyshev polynomials to accelerate the convergence of the power method. The description of the procedure includes a method for terminating the iterations in an attempt to minimize the total computer time required to solve the problem. The method has worked well in practice in a number of difficult problems. More details are given in [13].

The numerical procedures given in this paper apply equally well when the cyclic Chebyshev semi-iterative method [2], [7] is used to solve the matrix problem (1.1).

2. The Chebyshev Polynomial Method. By the S.O.R. method for solving (1.1) is meant the iterative process

$$(2.1) \quad D\mathbf{x}^{n+1} = \omega\{L\mathbf{x}^{n+1} + U\mathbf{x}^n + \mathbf{f}\} + (1 - \omega)D\mathbf{x}^n$$

where D is a block diagonal matrix and L and U are respectively strictly lower and upper triangular matrices. With the assumptions of Section 1, (2.1) converges most rapidly when $\omega = \omega_b$, where

$$(2.2) \quad \omega_b = 2 / \{1 + [1 - \rho(\mathcal{L}_1)]^{1/2}\}$$

and $\rho(\mathcal{L}_1)$ is the spectral radius of the Gauss-Seidel matrix $\mathcal{L}_1 = (D - L)^{-1}U$ [2, p. 111]. Also, the eigenvalues λ_i of the $q \times q$ matrix \mathcal{L}_1 lie in the interval $[0, 1)$ and may be ordered as

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$$1 > \lambda_1 = \lambda_2 = \dots = \lambda_{s-1} > \lambda_s = \lambda_{s+1} = \dots = \lambda_{t-1} > \lambda_t \geq \dots \geq \lambda_q \geq 0,$$

where we assume that $t > s$ [2, p. 107]. The ratio $\sigma = \lambda_s/\lambda_1$ is called the dominance ratio. We are concerned with finding $\lambda_1 = \rho(\mathcal{L}_1)$.

In this section we assume that \mathcal{L}_1 has q linearly independent eigenvectors. Starting with a vector

$$(2.3) \quad \mathbf{x}(0) = a_1 \mathbf{u}_1 + a_s \mathbf{u}_s + \sum_{i=t}^q a_i \mathbf{u}_i, \quad a_1 \neq 0,$$

where $\mathcal{L}_1 \mathbf{u}_j = \lambda_j \mathbf{u}_j$, we define

$$(2.4) \quad \begin{aligned} \mathbf{x}(r) &= P_r(\mathcal{L}_1) \mathbf{x}(0) \\ &= P_r(\lambda_1) \left\{ a_1 \mathbf{u}_1 + \frac{P_r(\lambda_s)}{P_r(\lambda_1)} a_s \mathbf{u}_s + \sum_{i=t}^q \frac{P_r(\lambda_i)}{P_r(\lambda_1)} a_i \mathbf{u}_i \right\} \end{aligned}$$

where P_r is a polynomial of degree r satisfying $P_r(\lambda_1) \neq 0$. If $P_r(y) = y^r$, (2.4) is the power method of iteration. In general $\mathbf{x}(r)$ approaches (in direction) the eigenvector \mathbf{u}_1 at a rate governed by $\max |P_r(\lambda_i)/P_r(\lambda_1)|$, $2 \leq i \leq q$, if this maximum is < 1 . For the Chebyshev method we take $P_r(y) = P_{r,\sigma}(y)$, where

$$(2.5) \quad P_{r,\sigma}(y) = \frac{T_r(2y/\lambda_1\sigma - 1)}{T_r(2/\sigma - 1)}$$

and where $T_r(z)$ is the Chebyshev polynomial of degree r . Among all polynomials P_r of degree r in y and such that $P_r(\lambda_1) = 1$, $P_{r,\sigma}(y)$ is the polynomial having the least maximum modulus over the range $0 \leq y \leq \lambda_s$ [8]. For σ close to unity, the Chebyshev polynomial method is much faster than the power method [9].

For computational purposes the vectors $\mathbf{x}(r)$ of the Chebyshev method can be formed in sequence by the procedure [10]

$$(2.6) \quad \begin{aligned} \mathbf{v}(r) &= \mathcal{L}_1 \mathbf{x}(r-1), \\ \lambda(r) &= \frac{[\mathbf{v}(r), \mathbf{x}(r-1)]}{[\mathbf{x}(r-1), \mathbf{x}(r-1)]}, \\ \mathbf{x}(r) &= \mathbf{x}(r-1) + \alpha_r \left[\frac{\mathbf{v}(r)}{\lambda(r)} - \mathbf{x}(r-1) \right] + \beta_r [\mathbf{x}(r-1) - \mathbf{x}(r-2)], \end{aligned}$$

where $\alpha_1 = 2/(2 - \sigma)$, $\beta_1 = 0$ and for $r \geq 2$

$$\alpha_r = \frac{4}{\sigma} \frac{T_{r-1}((2 - \sigma)/\sigma)}{T_r((2 - \sigma)/\sigma)}, \quad \beta_r = \frac{T_{r-2}((2 - \sigma)/\sigma)}{T_r((2 - \sigma)/\sigma)}.$$

In the formula for $\lambda(r)$ the notation $[\mathbf{v}, \mathbf{w}]$ denotes the inner product of two vectors \mathbf{v} and \mathbf{w} . We note that (2.6) reduces to the power method when $\alpha_r = 1$ and $\beta_r = 0$, $r = 1, 2, \dots$. Also, since the matrix vector product $\mathcal{L}_1 \mathbf{x}(r-1)$ may be obtained using (2.1) by setting $\mathbf{f} = \mathbf{o}$ and $\omega = 1$, the iterative procedure (2.6) takes essentially the same coding as that required by the S.O.R. iterations. However, (2.6) requires one and possibly two more vectors of storage than do the S.O.R. iterations. This could be troublesome in the solution of large problems. This will be discussed further in Section 3.

An accurate estimate for σ is important in the effective use of the Chebyshev polynomial method. This problem is discussed in Section 4.

3. Linear Elementary Divisors for \mathcal{L}_1 . In general, the elementary divisors of the Gauss-Seidel matrix are not all linear. However, if the $q \times q$ positive-definite matrix A of (1.1) is partitioned in the "normal 2-cyclic" form [2, p. 101],

$$(3.1) \quad A = \begin{bmatrix} A_1 & B \\ B^T & A_2 \end{bmatrix}$$

then Tee [11] has shown that the Gauss-Seidel matrix associated with the partitioning (3.1) has only linear elementary divisors. (Another proof of this fact can be found in [13].) Thus, when A is partitioned in the form (3.1), the Chebyshev procedure of (2.6) may be used to obtain an estimate for $\rho(\mathcal{L}_1)$. However, when A is of the form (3.1), one may use a different (and, perhaps, a better) Chebyshev procedure.

The Gauss-Seidel matrix \mathcal{L}_1 associated with (3.1) may be written as

$$(3.2) \quad \mathcal{L}_1 = \begin{bmatrix} A_1 & 0 \\ B^T & A_2 \end{bmatrix}^{-1} \begin{bmatrix} 0 & -B \\ 0 & 0 \end{bmatrix} = \begin{bmatrix} 0 & -A_1^{-1}B \\ 0 & A_2^{-1}B^T A_1^{-1}B \end{bmatrix}.$$

Thus, the nonzero eigenvalues of \mathcal{L}_1 are the same as those of $A_2^{-1}B^T A_1^{-1}B$ and $\rho(\mathcal{L}_1) = \rho(A_2^{-1}B^T A_1^{-1}B)$. Also, the elementary divisors of $A_2^{-1}B^T A_1^{-1}B$ are linear, since the matrix $A_2^{-1}B^T A_1^{-1}B$ is similar to the symmetric matrix $A_2^{-1/2}B^T A_1^{-1}B A_2^{-1/2}$. Hence, the Chebyshev polynomial method may be applied to the matrix $A_2^{-1}B^T A_1^{-1}B$ and can be carried out by the procedure

$$(3.3) \quad \begin{aligned} \hat{\mathbf{v}}(r) &= A_2^{-1}B^T A_1^{-1}B \hat{\mathbf{x}}(r-1), \\ \lambda(r) &= \frac{[\hat{\mathbf{v}}(r), \hat{\mathbf{x}}(r-1)]}{[\hat{\mathbf{x}}(r-1), \hat{\mathbf{x}}(r-1)]}, \\ \hat{\mathbf{x}}(r) &= \hat{\mathbf{x}}(r-1) + \alpha_r \left[\frac{\hat{\mathbf{v}}(r)}{\lambda(r)} - \hat{\mathbf{x}}(r-1) \right] + \beta_r [\hat{\mathbf{x}}(r-1) - \hat{\mathbf{x}}(r-2)], \end{aligned}$$

where α_r and β_r are as defined in (2.6).

It is not necessary to form the matrix $A_2^{-1}B^T A_1^{-1}B$ explicitly in order to carry out (3.3). The vector $\hat{\mathbf{v}}(r)$ may be obtained implicitly by

$$(3.4) \quad \begin{aligned} \hat{\mathbf{y}}(r) &= A_1^{-1}B \hat{\mathbf{x}}(r-1), \\ \hat{\mathbf{v}}(r) &= A_2^{-1}B^T \hat{\mathbf{y}}(r). \end{aligned}$$

Thus, to obtain $\hat{\mathbf{v}}(r)$ requires the same work as does the $\mathbf{v}(r)$ of (2.6). However, the eigenvalue and extrapolation calculations in (3.3) use vectors with fewer components than those used in (2.6). For example, if A_1 and A_2 are matrices of the same order, then the vectors $\mathbf{x}(r)$ of (2.6) contain twice as many components as do the $\hat{\mathbf{x}}(r)$ of (3.3). Thus, the arithmetic computations and the vector storage requirements of (3.3) are less than those of (2.6).

4. Computational Strategy and Numerical Results. In this section it is assumed that A is partitioned in the normal 2-cyclic form (3.1). Thus, the Chebyshev iterative procedure (2.6) or (3.3) may be used to estimate $\rho(\mathcal{L}_1)$. To complete the description of the Chebyshev algorithm, we shall (a) specify a means of estimating σ , (b) discuss the strategy of the algorithm, and (c) give a criterion for terminating the

iterative procedure (2.6) or (3.3). Finally, we discuss some numerical results.

a. *Estimating* σ . Numerical estimates for σ are obtained by observing the decay rate of the residual vector $\mathbf{y}(r) \equiv \mathbf{v}(r)/\lambda(r) - \mathbf{x}(r)$, where $\mathbf{v}(r)$, $\lambda(r)$, and $\mathbf{x}(r)$ are defined by (2.6). We define the residual vector quotient as

$$(4.1) \quad Q(r) = \|\mathbf{y}(r)\|/\|\mathbf{y}(r - 1)\| ,$$

where $\|\cdot\|$ denotes some suitable vector norm. Since for the power method, $Q(r) \rightarrow \sigma$ [13], an initial estimate for σ may be obtained by doing a few power iterations and computing $Q(r)$ before starting the use of Chebyshev polynomials.

Estimates for σ are obtained at every Chebyshev iteration by comparing the convergence rate actually being obtained with the theoretical convergence rate one would obtain if the σ being used were correct. If a Chebyshev polynomial using σ_0 as the estimate for σ is started on iteration $k + 1$ and if

$$(4.2) \quad \begin{aligned} & \text{(i) } \lambda(k + r + 1) \text{ is sufficiently close to } \lambda_1 \text{ for all } r \geq 0, \text{ and} \\ & \text{(ii) } \sum_{i=t}^q P_{r,\sigma_0}(\lambda_i) a_i \mathbf{u}_i \text{ is small relative to } \|P_{r,\sigma_0}(\lambda_s) a_s \mathbf{u}_s\| , \end{aligned}$$

then from (2.4) and since $P_{r,\sigma_0}(\lambda_1) = 1$, we may approximate $\mathbf{x}(k + r)$ by $a_1 \mathbf{u}_1 + P_{r,\sigma_0}(\lambda_s) a_s \mathbf{u}_s$. Hence, the residual vector $\mathbf{y}(k + r + 1)$ may be approximated by $\mathbf{y}(k + r + 1) \approx (\sigma - 1) P_{r,\sigma_0}(\lambda_s) a_s \mathbf{u}_s$ and the residual vector quotient by

$$(4.3) \quad Q(k + r + 1) \approx |P_{r,\sigma_0}(\lambda_s)/P_{r-1,\sigma_0}(\lambda_s)| ,$$

where $P_{0,\sigma_0}(y) = 1.0$. With $Q_{r+1} \equiv \prod_{l=2}^{r+1} Q(k + l)$, it follows from (4.3) that

$$(4.4) \quad Q_{r+1} \approx |P_{r,\sigma_0}(\lambda_s)| .$$

Solving for the largest positive solution λ_s of (4.4) and dividing by λ_1 , one obtains the estimate*

$$(4.5) \quad \sigma \approx \frac{\sigma_0}{2} \left\{ \cosh \left[\frac{\cosh^{-1} \{ Q_{r+1} T_r(2/\sigma_0 - 1) \}}{r} \right] + 1.0 \right\} .$$

Thus, if the assumptions given in (4.2) are valid, expression (4.5) will give a good estimate for σ . Obviously, these assumptions do not always hold. However, they may be reasonable under certain conditions. The Chebyshev strategy given below is designed toward this end.

b. *Chebyshev Strategy*. Let the k th iterate in the Chebyshev procedure be expressed in the form

$$(4.6) \quad \mathbf{x}(k) = P_{r_n,\sigma_n}(\mathcal{E}_1) \cdots P_{r_1,\sigma_1}(\mathcal{E}_1) P_{r_0,\sigma_0}(\mathcal{E}_1) \mathcal{E}_1^4 \mathbf{x}(0) ,$$

where $P_{r,d}(\mathcal{E}_1)$ is the Chebyshev polynomial of degree r in which d is used as the estimate for σ and where $k = 4 + r_0 + \cdots + r_n$. Using the notation of (4.6), the Chebyshev strategy is first to do four iterations of the power type to obtain an initial estimate, σ_0 , for σ and a reasonable estimate for λ_1 . In addition, these power iterates tend to eliminate from the eigenvector guess $\mathbf{x}(0)$ those eigenvector modes corresponding to small eigenvalues. Starting with iteration 5, low-degree Chebyshev polynomials are repeatedly applied, with the estimates for the dominance ratio being con-

* If $\{Q_{r+1} T_r(2/\sigma_0 - 1)\} < 1$, then \cos and \cos^{-1} should be used in (4.5) instead of \cosh and \cosh^{-1} .

tinuously updated. Upper limits of the form $\sigma_0 \leq .9$, $\sigma_1 \leq .95$, $\sigma_2 \leq .985$ are imposed on the first few estimates for σ in an attempt to insure that these initial estimates be less than σ . Those polynomials for which σ is underestimated will greatly reduce all the eigenvector modes in the estimated vector $\mathbf{x}(0)$ except those with the larger eigenvalues.* This results in assumption (ii) of (4.2) being more nearly satisfied which, in turn, enables the estimates for σ to converge to the correct value. As σ_n approaches σ , high-degree polynomials are applied.

The strategy for terminating a Chebyshev polynomial and starting the generation of a new polynomial using an improved estimate for σ is made by comparing the convergence rate being obtained with the theoretical convergence rate one would obtain if the estimate for σ were correct. If a Chebyshev polynomial using σ_0 as the estimate for σ is started on iteration $k + 1$, then from Eq. (4.3) the convergence rate actually being obtained on iteration $k + r$ is $-\ln[Q(k + r + 1)]$. Now if $\sigma_0 = \sigma$, the Chebyshev theory of Section 2 implies that the theoretical convergence rate of iteration $k + r$ should be $-\ln[T_{r-1}(2/\sigma_0 - 1)/T_r(2/\sigma_0 - 1)]$. Thus, the criterion

$$(4.7) \quad R(k + r + 1) = \frac{\ln [Q(k + r + 1)]}{\ln [T_{r-1}(2/\sigma_0 - 1)/T_r(2/\sigma_0 - 1)]} < .6$$

for starting the generation of a new polynomial automatically causes the degrees r_n to become larger as σ_n tends to σ . It is often helpful to require all polynomials generated to be at least of degree r^* , where r^* is 3 or 4.

c. *Terminating the Iterative Procedure.* Let I_{opt} be the number of iterations required by the successive overrelaxation method using optimum ω , and let $I_{\omega(k)}$ be the number of iterations required when

$$\omega(k) = 2/\{1 + (1 - \lambda(k))^{1/2}\}$$

is determined from the k th approximation, $\lambda(k)$, of the λ iterations. We wish to terminate the λ iterations when $\lambda(k)$ is so close to $\rho(\mathcal{L}_1)$ that

$$(4.8) \quad I_{\omega(k)}/I_{\text{opt}} - 1 < \delta,$$

where δ is a number at our disposal. The quantity δ represents the relative number of additional S.O.R. iterations required because $\omega(k)$ rather than ω_b is used in (2.1).

In order to use (4.8) to terminate the λ iterations, we must find some way to estimate $I_{\omega(k)}$ and I_{opt} . Assuming that $\rho(\mathcal{L}_1) \approx 1$ and $\lambda(k) \approx \rho(\mathcal{L}_1)$ it is shown in [13] that (4.8) may be approximated by

$$(4.9) \quad \frac{|\lambda(k) - \lambda(k-1)|}{2[1 - \lambda(k)][1 - Q(k)]} < \delta, \quad \lambda(k) > \rho(\mathcal{L}_1),$$

$$(4.10) \quad \left\{ \frac{|\lambda(k) - \lambda(k-1)|}{[1 - \lambda(k)][1 - Q(k)]} \right\}^{1/2} < \delta, \quad \lambda(k) < \rho(\mathcal{L}_1).$$

Since in practice it usually happens that $\lambda(k) < \rho(\mathcal{L}_1)$, we terminate the iterations when (4.10) is satisfied.

The convergence quantity δ of (4.8) determines the total number of iterations required to solve the problem. To minimize computer time, it is desired to find the

* For example, if $\sigma = .889$ and if a 5th-degree Chebyshev polynomial is generated with $\sigma_0 = .8$, then all eigenvector modes u_i with $(\lambda_i/\lambda_1) \leq .8$ are multiplied by a factor smaller than .017, while the u_n eigenvector mode is multiplied by a factor of .211.

value of δ which minimizes this total number of iterations. In what follows we attempt to determine this optimum value experimentally.

d. *Numerical Results.* We now give two numerical examples which illustrate the effectiveness of the Chebyshev polynomial method. In each example A is partitioned in the form (3.1). We take $\mathbf{f} = \mathbf{0}$ so that the solution of (1.1) is $\mathbf{x} = \mathbf{0}$. All components of the initial guess vector are taken to be 1.0 and the S.O.R. iterations are continued until the maximum vector component is less than 10^{-6} . The λ iterations performed prior to the S.O.R. iterations are carried out using the procedure given by (3.3) and the Chebyshev strategy is that as described in parts a and b of this section. For comparison purposes, the λ iterations were also carried out using the power method.

TABLE 1. PROBLEM A
Chebyshev Acceleration

k	$\lambda(k)$	$\omega(k)$	$\sigma(k)$	$\delta(k)$	$I_{\omega(k)}$	$I_{T(k)}$
5	.997684	1.90816	.89864	.79	> 5,000	> 5,000
33	.999782	1.97091	.99798	.9	1,522	1,555
49	.999797	1.97189	.99978	1.15	1,442	1,489
70	.999813	1.97302	.99982	.87	1,354	1,424
82	.999834	1.97453	.99980	.69	1,228	1,310
103	.999865	1.97706	.99976	.45	987	1,090
115	.999876	1.97798	.99974	.31	870	985
130	.999884	1.97869	.99972	.13	739	869
132	.999885	1.97874	.99972	.11	722	854

Power Iterations

k	$\lambda(k)$	$\omega(k)$	$\sigma(k)$	$\delta(k)$	$I_{\omega(k)}$	$I_{T(k)}$
5	.997684	1.90816	.89864	.75	> 5,000	> 5,000
38	.999190	1.94499	.97795	1.00	3,322	3,360
103	.999674	1.96451	.98529	.76		
200	.999782	1.97092	.99802	.88	1,522	1,722
250	.999793	1.97163	.99934	.98	1,465	1,715
300	.999797	1.97193	.99970	1.02	1,441	1,741

In Tables 1 and 2, k is the iteration index for the λ iterations, $I_{\omega(k)}$ is the number of iterations required to solve (1.1) to the required degree of accuracy using $\omega(k)$ as the overrelaxation parameter, $I_{T(k)} = k + I_{\omega(k)}$, and $\delta(k)$ is the left-hand side of

(4.10). A graph of k vs $I_{T(k)}$ for problem B is given in Fig. 1. Table 3 clearly shows the advantage of the Chebyshev polynomial method over the power method.

TABLE 2. PROBLEM B
Chebyshev Acceleration

k	$\lambda(k)$	$\omega(k)$	$\sigma(k)$	$\delta(k)$	$I_{\omega(k)}$	$I_{T(k)}$
5	.995636	1.87607	.88427	.77	1,372	1,377
13	.998096	1.91639	.97447	.93	864	877
24	.998798	1.93298	.99392	.74	640	664
40	.998920	1.93638	.99957	1.19	590	630
64	.999278	1.94768	.99931	.44	394	458
78	.999353	1.95041	.99914	.13	311	389
80	.999358	1.95058	.99912	.09	299	379
120	.999361	1.95068		.03	289	409

Power Iterations

k	$\lambda(k)$	$\omega(k)$	$\sigma(k)$	$\delta(k)$	$I_{\omega(k)}$	$I_{T(k)}$
5	.995636	1.87607	.88427	.77	1,372	1,377
35	.998140	1.91732	.97724	.81	854	889
99	.998789	1.93278	.99559	.77	642	741
150	.998882	1.93529	.99899	.97	608	758
200	.998922	1.93642	.99954	1.12	588	788
250	.998950	1.93722	.99961	1.12	576	826
300	.998974	1.93794	.99958	1.06	565	865

TABLE 3

<i>Problem</i>	<i>Minimum $I_{T(k)}$</i>	
	<i>Chebyshev Method</i>	<i>Power Method</i>
A	854	1,715
B	379	741

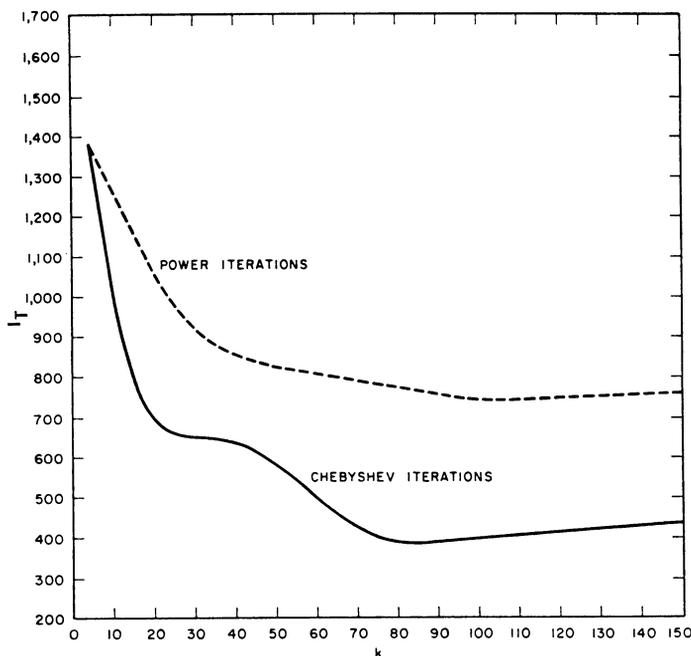


FIGURE 1
PROBLEM B GRAPH OF k VS I_T

For the two problems considered here, $I_{T(k)}$ is minimized for the Chebyshev iterations when δ is about .1. Obviously, a different value for δ would minimize $I_{T(k)}$ for other problems. It has been found, however, that a convergence criterion for the λ iterations of $\delta(k) \leq .2$ works well for most problems.

Other numerical examples are given in [13].

e. *Nonnormal Partitionings of A*. It is sometimes more convenient from a programming point of view to use a 2-cyclic partitioning of A which is not normal. For this case, however, the Chebyshev algorithm (2.6) usually requires many more iterations to estimate $\rho(\mathcal{L}_1)$ accurately than would comparable problems with the normal partitioning (3.1). This is because \mathcal{L}_1 may have nonlinear elementary divisors corresponding to the eigenvalue 0. In [13] there is presented a modification of the Chebyshev polynomial method which helps to overcome this difficulty.

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