A Block Lanczos Method for Computing the Singular Values and Corresponding Singular Vectors of a Matrix

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We present a block Lanczos method for computing the greatest singular values and associated vectors of a large and sparse matrix, say A. Our algorithm does not transform A but accesses it through a user-supplied routine that computes the product AX or $A'X$ for a given matrix X.

This paper includes a discussion of the various ways to compute the singular-value decomposition of an upper triangular band matrix, this problem arises as a subproblem to be solved in the block Lanczos procedure.

Key Words and Phrases: block Lanczos method, singular values, singular vectors, large sparse matrix, singular-value decomposition, upper triangular band matrix
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1. INTRODUCTION

In this paper, we construct a block Lanczos method for the following problem.

> Compute the k greatest singular values and associated vectors of a large and sparse $m \times n$ matrix A, where k is much smaller than m or n.

This problem finds applications in factor analysis, regression, and image enhancement (cf. [6]).

We assume without loss of generality that $m \geq n$. For $i = 1, 2, \ldots, n$, let σ_i be a singular value of A, and let $\mathbf{u}_i$ and $\mathbf{v}_i$ be the corresponding left and right singular vectors, respectively. The singular values are ordered so that

$$\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_n. \tag{1.1}$$

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Let us exploit an idea of Lanczos' [10, Chapter 3] and consider the $(m + n) \times (m + n)$ matrix

$$\tilde{A} = \begin{pmatrix} 0 & A \\ A^t & 0 \end{pmatrix}, \tag{1.2}$$

whose eigenvalues are $\pm\sigma_1, \pm\sigma_2, \ldots, \pm\sigma_n$, plus $(m - n)$ zeros. The eigenvectors corresponding to $+\sigma_i$ and $-\sigma_i$ are

$$\begin{pmatrix} \mathbf{u}_i \\ \mathbf{v}_i \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} \mathbf{u}_i \\ -\mathbf{v}_i \end{pmatrix},$$

respectively, for $i = 1, 2, \ldots, n$. The remaining eigenvectors are all of the form $\binom{\mathbf{u}}{0}$, where $\mathbf{u}$ is a vector of order m, which is orthogonal to $\mathbf{u}_1, \mathbf{u}_2, \ldots, \mathbf{u}_n$. We address the equivalent problem:

Compute the k algebraically greatest eigenvalues and corresponding eigenvectors of the large and sparse matrix $\tilde{A}$ of (1.2).

An efficient scheme for this eigenproblem is the block Lanczos method developed by several researchers, in particular, Cullum and Donath ([1] and [2]), Golub and Underwood ([9] and [18]), Lewis [11], and Ruhe [15]. We choose to consider the variant described by Golub and Underwood.

We are going to present a theoretical development of the block Lanczos method and give two theorems on its convergence rate. The practical implementation aspects are then discussed and particular attention is paid to the choice of the block size. Our paper includes a discussion of the various ways for computing the singular-value decomposition of an upper triangular band matrix; this problem arises as a subproblem to be solved in the block Lanczos procedure. We should mention that Cullum and Willoughby have recently published a related point Lanczos algorithm for computing singular values and vectors (see [3]).

An alternative procedure for solving our problem would be to apply a standard Lanczos method to find the greatest eigenvalues and the corresponding eigenvectors of the matrix A^tA or AA^t. This approach is probably adequate for determining the greatest singular value, but the loss of accuracy can become severe for the smaller singular values. This point is discussed and well illustrated in [3].

In this paper, we use the Euclidean vector norm

$$\|\mathbf{x}\| = \|\mathbf{x}\|_2 = (\mathbf{x}^t\mathbf{x})^{1/2},$$

and refer to an $n \times b$ matrix X with $n \geq b$ as an orthonormal matrix if

$$X^tX = I.$$

2. BLOCK BIDIAGONALIZATION ALGORITHM

We first study the generation of a block bidiagonal form with the use of a block Lanczos procedure. This bidiagonalization algorithm was suggested by Golub and Kahan [5] and described in detail by Paige [13] for the single-vector recurrence. Palmer [14] discussed the block recurrence in his doctoral thesis.

Let us develop the block Lanczos method for

$$\tilde{A} = \begin{pmatrix} 0 & A \\ A^t & 0 \end{pmatrix} \tag{1.2}$$

with the initial $(m + n) \times b$ orthonormal matrix

$$X_1 = \begin{pmatrix} 0 \\ Q_1 \end{pmatrix}, \tag{2.1}$$

where Q_1 is an $n \times b$ matrix. It follows that

$$M_1 = X_1^t \tilde{A} X_1 = 0,$$

$$Z_1 = \begin{pmatrix} AQ_1 \\ 0 \end{pmatrix}, \qquad \text{and} \qquad X_2 = \begin{pmatrix} P_1 \\ 0 \end{pmatrix},$$

where P_1 is an $m \times b$ matrix. Thus,

$$M_2 = X_2^t \tilde{A} X_2 = 0.$$

Using the relations defining the block Lanczos method (cf. [18]), we can prove by induction that, for $j = 1, 2, \ldots,$

$$X_{2j-1} = \begin{pmatrix} 0 \\ Q_j \end{pmatrix} \qquad \text{and} \qquad M_{2j-1} = 0, \tag{2.2}$$

where Q_j is an $n \times b$ orthonormal matrix, and

$$X_{2j} = \begin{pmatrix} P_j \\ 0 \end{pmatrix} \qquad \text{and} \qquad M_{2j} = 0, \tag{2.3}$$

where P_j is an $m \times b$ orthonormal matrix. Since the X_j form a sequence of mutually orthonormal matrices, that is,

$$X_i^t X_j = 0 \qquad \text{for} \quad i \neq j,$$

we deduce that the P_j and Q_j form two sequences of mutually orthonormal matrices.

Let us carry out $2s$ steps of the block Lanczos scheme. We obtain the matrix equation

$$\tilde{A} \bar{X}_{2s} = \bar{X}_{2s} T_{2s} + \bar{Z}_{2s}, \tag{2.4}$$

where

$$T_{2s} = \begin{pmatrix} 0 & R_2^t & & & 0 \\ R_2 & 0 & R_3^t & & \\ & \ddots & \ddots & \ddots & \\ & & R_{2s-1} & 0 & R_{2s}^t \\ 0 & & & R_{2s} & 0 \end{pmatrix}, \tag{2.5}$$

$$\bar{X}_{2s} = (X_1, X_2, \ldots, X_{2s}), \qquad \bar{Z}_{2s} = (0, \ldots, 0, Z_{2s+1}),$$

and

$$Z_{2s+1} = \begin{pmatrix} 0 \\ A^t P_s - Q_s R_{2s}^t \end{pmatrix}. \tag{2.6}$$

Let

$$\bar{P}_s = (P_1, P_2, \ldots, P_s) \tag{2.7}$$

and

$$\bar{Q}_s = (Q_1, Q_2, \ldots, Q_s). \tag{2.8}$$

We can rewrite eq. (2.4) as

$$\begin{pmatrix} 0 & A \\ A^t & 0 \end{pmatrix}\begin{pmatrix} \bar{P}_s & 0 \\ 0 & \bar{Q}_s \end{pmatrix} = \begin{pmatrix} \bar{P}_s & 0 \\ 0 & \bar{Q}_s \end{pmatrix}\begin{pmatrix} 0 & J_s \\ J_s^t & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ \hat{Z}_{2s+1} & 0 \end{pmatrix}, \tag{2.9}$$

where

$$J_s = \begin{pmatrix} R_2 & R_3^t & & & 0 \\ & R_4 & R_5^t & & \\ & & \ddots & \ddots & \\ & 0 & & R_{2s-2} & R_{2s-1}^t \\ & & & & R_{2s} \end{pmatrix} \tag{2.10}$$

and

$$\hat{Z}_{2s+1} = (0, \ldots, 0, Z_{2s+1}). \tag{2.11}$$

Furthermore, the matrix eq. (2.9) is reducible into two lower order matrix equations,

$$A\bar{Q}_s = \bar{P}_s J_s \tag{2.12}$$

and

$$A^t\bar{P}_s = \bar{Q}_s J_s^t + \hat{Z}_{2s+1}. \tag{2.13}$$

The block Lanczos method therefore generates a block bidiagonal matrix J_s of order bs. As the R_i are upper triangular matrices, the matrix J_s is also a band upper triangular matrix with b superdiagonals. Therefore we have constructed a scheme that produces a block bidiagonal matrix J_s from a given rectangular matrix A while preserving the singular values. In Section 4 we discuss how to compute the singular-value decomposition of J_s.

ALGORITHM 2.1 (Block Bidiagonalization Method)

1. Let Q_1 be a given $n \times b$ orthonormal matrix.
   Compute

$$W_1 := AQ_1,$$

   and factorize W_1 so that

$$W_1 = P_1 R_2,$$

   where P_1 is orthonormal and R_2 is upper triangular.
2. For $i = 2, 3, \ldots, s$, do
   (a) Compute

$$Z_i := A^t P_{i-1} - Q_{i-1} R_{2i-2}^t,$$

   and factorize Z_i so that

$$Z_i = Q_i R_{2i-1},$$

   where Q_i is orthonormal and R_{2i-1} is upper triangular.

(b) Compute

$$W_i := AQ_i - P_{i-1}R_{2i-1}^t,$$

and factorize W_i so that

$$W_i = P_iR_{2i},$$

where P_i is orthonormal and R_{2i} is upper triangular.

In Algorithm 2.1, if the matrix Z_i were rank deficient, we would choose the columns of Q_i so that they are orthogonal to those of all previous Q_j. The remedy is similar for a rank-deficient matrix W_i. We may use the Householder transformations for this construction.

Suppose that μ_i is a singular value of J_s with corresponding left and right singular vectors $\mathbf{w}_i$ and $\mathbf{z}_i$, respectively. Let

$$\mathbf{p}_i = \bar{P}_s\mathbf{w}_i \quad \text{and} \quad \mathbf{q}_i = \bar{Q}_s\mathbf{z}_i.$$

From (2.12) and (2.13) we get

$$A\mathbf{q}_i = \mu_i\mathbf{p}_i \tag{2.14}$$

and

$$A^t\mathbf{p}_i = \mu_i\mathbf{q}_i + \hat{Z}_{2s+1}\mathbf{w}_i,$$

or equivalently,

$$A^t\mathbf{p}_i = \mu_i\mathbf{q}_i + Z_{2s+1}\mathbf{h}_i, \tag{2.15}$$

where the vector $\mathbf{h}_i$ is a vector of order b consisting of the last b components of $\mathbf{w}_i$. Accordingly, if we had that $Z_{2i+1}\mathbf{h}_i = \mathbf{0}$, then the value μ_i would be a singular value of matrix A with corresponding left and right singular vectors $\mathbf{p}_i$ and $\mathbf{q}_i$, respectively. In the next section we give error bounds that indicate that the greatest singular values of J_s are usually accurate approximations to those of A.

3. ERROR BOUNDS FOR THE SINGULAR-VALUE APPROXIMATIONS

Let us consider the matrix

$$\tilde{A} = \begin{pmatrix} 0 & A \\ A^t & 0 \end{pmatrix}. \tag{1.2}$$

Its $(b + 1)$ algebraically greatest eigenvalues are $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_{b+1}$, and its algebraically smallest eigenvalue is $-\sigma_1$. For $i = 1, 2, \ldots, b$, the normalized eigenvector of $\tilde{A}$ corresponding to the eigenvalue σ_i is

$$\mathbf{g}_i = \frac{1}{\sqrt{2}}\begin{pmatrix} \mathbf{u}_i \\ \mathbf{v}_i \end{pmatrix}.$$

Now, the eigenvalues of the block tridiagonal matrix T_{2s} of (2.5) are $\mu_1 \geq \mu_2 \geq \cdots \mu_{bs} \geq -\mu_{bs} \geq \cdots \geq -\mu_2 \geq -\mu_1$. But the matrix T_{2s} is generated by $2s$ steps of the block Lanczos method applied to $\tilde{A}$ with initial matrix

$$X_1 = \begin{pmatrix} 0 \\ Q_1 \end{pmatrix}.$$

If we let

$$G_1 = (\mathbf{g}_1, \mathbf{g}_2, \ldots, \mathbf{g}_b) \quad \text{and} \quad V_1 = (\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_b),$$

then

$$G_1^t X_1 = \frac{1}{\sqrt{2}} V_1^t Q_1.$$

The following theorem is a direct consequence of a theorem due to Underwood [18, pp. 37–38].

THEOREM 3.1. *Assume that* $\sigma_b > \sigma_{b+1}$. *Let* $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_{bs}$ *be the singular values of the* $bs \times bs$ *matrix* J_s *generated by the block bidiagonalization method with an initial* $n \times b$ *orthonormal matrix* Q_1. *Suppose that the* $b \times b$ *matrix*

$$W = \frac{1}{\sqrt{2}} V_1^t Q_1,$$

where

$$V_1 = (\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_b),$$

is nonsingular so that its smallest singular value τ *is positive. Note that* $\tau \leq 1/\sqrt{2}$. *Then, for* $i = 1, 2, \ldots, b$, *we have that*

$$\sigma_i \geq \mu_i \geq \sigma_i - \epsilon_i^2,$$

where

$$\epsilon_i^2 = \frac{(\sigma_i + \sigma_1)\tan^2\theta}{T_{2s-1}^2\left(\dfrac{1+\gamma_i}{1-\gamma_i}\right)},$$

$$\theta = \cos^{-1}\tau,$$

$$\gamma_i = \frac{\sigma_i - \sigma_{b+1}}{\sigma_i + \sigma_1},$$

and T_{2s-1} *is the* $(2s-1)$*st Chebyshev polynomial of the first kind.*

Example 3.1. Suppose that A is an $m \times n$ matrix with singular values $\sigma_1 = 1.0$, $\sigma_2 = 0.9$, $\sigma_3 = 0.5$, ... Let us apply the block bidiagonalization algorithm with $b = 2$ and $s = 5$. Then

$$\gamma_1 = \frac{1.0 - 0.5}{1.0 + 1.0} = 0.25,$$

$$\gamma_2 = \frac{0.9 - 0.5}{0.9 + 1.0} \doteq 0.21,$$

$$T_9\left(\frac{1+\gamma_1}{1-\gamma_1}\right) \doteq T_9(1.67) \doteq 1.0 \times 10^4,$$

and

$$T_9\left(\frac{1+\gamma_2}{1-\gamma_2}\right) \doteq T_9(1.53) \doteq 3.7 \times 10^3.$$

Let

$$\tau = \frac{1}{\sqrt{2}} \times 0.04,$$

so that

$$\tan^2 \theta \doteq 1249.$$

Thus,

$$\epsilon_1^2 \doteq \frac{2.0 \times 1249}{1.0 \times 10^8} \doteq 2.5 \times 10^{-5},$$

and

$$\epsilon_2^2 \doteq \frac{1.9 \times 1249}{1.37 \times 10^7} \doteq 1.7 \times 10^{-4}.$$

The two greatest singular values μ_1 and μ_2 of J_s therefore satisfy the inequalities

$$\sigma_1 \geq \mu_1 \geq \sigma_1 - 2.5 \times 10^{-5}$$

and

$$\sigma_2 \geq \mu_2 \geq \sigma_2 - 1.7 \times 10^{-4}.$$

However, we suspect that the bounds of Theorem 3.1 may be gross overestimates. Suppose that

$$Q_1 = V_1.$$

Then we have

$$\tau = \frac{1}{\sqrt{2}}$$

and

$$\tan \theta = 1.$$

The last value is quite unsatisfactory for an initial matrix consisting of the correct singular vectors.

We seek to construct tighter bounds. From the matrix equations

$$A\bar{Q}_s = \bar{P}_s J_s \tag{2.12}$$

and

$$A^t \bar{P}_s = \bar{Q}_s J_s^t + \hat{Z}_{2s+1}, \tag{2.13}$$

we get

$$\begin{aligned} A^t A \bar{Q}_s &= A^t \bar{P}_s J_s \\ &= \bar{Q}_s J_s^t J_s + \hat{Z}_{2s+1} J_s. \end{aligned}$$

Thus,

$$A^t A \bar{Q}_s = \bar{Q}_s J_s^t J_s + (0, \ldots, 0, Z_{2s+1} R_{2s}). \tag{3.1}$$

We observe that the matrix $\bar{Q}_s$ is orthonormal and that the matrix $J_s^t J_s$ is block tridiagonal. It can be proved (cf. [18, Chapter 2]) that the matrix equation (3.1) characterizes an application of the block Lanczos method to the matrix $A^t A$ with

the initial matrix Q_1. Since the matrix A^tA has eigenvalues $\sigma_1^2 \geq \sigma_2^2 \geq \cdots \geq \sigma_n^2$ and corresponding normalized eigenvectors $\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_n$, we obtain the next result from Underwood's theorem [18, pp. 37–38].

THEOREM 3.2. *Assume that $\sigma_b > \sigma_{b+1}$. Let $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_{bs}$ be the singular values of the $bs \times bs$ matrix J_s generated by the block bidiagonalization method with an initial $n \times b$ orthonormal matrix Q_1. Suppose that the $b \times b$ matrix*

$$W = V_1^t Q_1,$$

where

$$V_1 = (\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_b),$$

is nonsingular so that its smallest singular value τ is positive. Note that $\tau \leq 1$. Then, for $i = 1, 2, \ldots, b$, we have that

$$\sigma_i \geq \mu_i \geq (\sigma_i^2 - \epsilon_i^2)^{1/2},$$

or

$$\sigma_i \geq \mu_i \geq \sigma_i - \frac{1}{\sigma_i}\epsilon_i^2 \qquad \text{for} \quad \frac{\epsilon_i^2}{\sigma_i^2} < 1,$$

where

$$\epsilon_i^2 = \frac{(\sigma_i^2 - \sigma_n^2)\ tan^2\ \theta}{T_{s-1}^2\left(\dfrac{1+\gamma_i}{1-\gamma_i}\right)},$$

$$\theta = cos^{-1}\ \tau,$$

$$\gamma_i = \frac{\sigma_i^2 - \sigma_{b+1}^2}{\sigma_i^2 - \sigma_n^2},$$

and T_{s-1} is the $(s-1)$st Chebyshev polynomial of the first kind.

Example 3.2. We use the same given data as in Example 3.1, with the additional assumption that $\sigma_n = 0.0$. Thus,

$$\sigma_1^2 = 1.00,\ \sigma_2^2 = 0.81,\ \sigma_3^2 = 0.25, \ldots, \sigma_n^2 = 0.00,$$

so that

$$\gamma_1 = \frac{1.00 - 0.25}{1.00 - 0.00} = 0.75,$$

$$\gamma_2 = \frac{0.81 - 0.25}{0.81 - 0.00} \doteq 0.69,$$

$$T_4\left(\frac{1+\gamma_1}{1-\gamma_1}\right) = T_4(7) \doteq 1.88 \times 10^4,$$

and

$$T_4\left(\frac{1+\gamma_2}{1-\gamma_2}\right) \doteq T_4(5.45) \doteq 6.82 \times 10^3.$$

Also,

$$\tan^2 \theta = 624.$$

Consequently,

$$\epsilon_1^2 \doteq \frac{1.00 \times 624}{3.55 \times 10^8} \doteq 1.7 \times 10^{-6}$$

and

$$\epsilon_2^2 \doteq \frac{0.81 \times 624}{4.65 \times 10^7} \doteq 1.1 \times 10^{-5}.$$

As

$$\frac{1}{\sigma_1} \epsilon_1^2 \doteq 1.7 \times 10^{-6}$$

and

$$\frac{1}{\sigma_2} \epsilon_2^2 \doteq 1.2 \times 10^{-5},$$

the two greatest singular values μ_1 and μ_2 of J_s therefore satisfy the inequalities

$$\sigma_1 \geq \mu_1 \geq \sigma_1 - 1.7 \times 10^{-6}$$

and

$$\sigma_2 \geq \mu_2 \geq \sigma_2 - 1.2 \times 10^{-5}.$$

We observe that the bounds given by Theorem 3.2 are much smaller than those given by Theorem 3.1.

4. COMPUTATION OF SINGULAR VALUES AND VECTORS OF J

We wish to compute the singular values and vectors of the $bs \times bs$ block bidiagonal matrix J_s. In the rest of this section we omit the subscript s from J_s and denote its order by $t = bs$. Since the $b \times b$ blocks that form the block diagonal of J are upper triangular and the $b \times b$ blocks that form the block superdiagonal are lower triangular, we see that the blocks all fit together to form an upper triangular band matrix, dense within the band and with bandwidth (number of superdiagonals) equal to b. The rest of this section treats the problem of computing the singular values and vectors of an upper triangular band matrix J. The case where the vectors are not required is also considered, since this section may be useful outside the block Lanczos context.

The method consists of two phases. The first phase reduces J to bidiagonal form by a finite sequence of orthogonal transformations. The problem of doing this efficiently is the main subject of this section. The singular values of J are preserved under the transformations. The second phase reduces the bidiagonal form to diagonal form by a modified version of the QR algorithm. This process is described in detail in Golub and Reinsch [8] and is not discussed any further here. The singular values of J are the final diagonal elements, and the matrices of left and right singular vectors are the products of all the left and right transformations (respectively) used in the two phases of the reduction.

We are left with the first phase, reducing J to bidiagonal form. The methods of Givens and Householder for reducing a full symmetric matrix to tridiagonal form

preserving eigenvalues are well known and are described, for example, in Wilkinson [20]. In order to preserve eigenvalues, the same elementary transformations (either Givens or Householder) are applied to both the left and right sides of the matrix.

A similar method for reducing a nonsymmetric matrix to bidiagonal form preserving singular values (but not, of course, eigenvalues) is described in Golub and Reinsch [8]. Singular values are preserved when different elementary transformations are applied to the left and right sides of the matrix. Golub and Reinsch use Householder transformations, but Givens transformations could easily be used instead. For the reduction of a full matrix to bidiagonal or tridiagonal form, the method of Householder is about twice as fast as the method of Givens. However, in 1973 Gentleman [4] showed how "fast Givens" transformations can be implemented. These are also described in Van Loan [19], and it appears that there is now little difference in the speed or effectiveness of the two methods.

Reducing a symmetric band matrix to tridiagonal form in a straightforward manner immediately fills in the zeros off the band. Rutishauser [16] shows how this may be avoided and the reduction completed while preserving the band structure, using either Givens or Householder transformations. Here we describe how to generalize this to the reduction of an upper triangular band matrix to bidiagonal form. In general, a similar process would apply to any nonsymmetric band matrix.

Recall that a Givens transformation matrix $P^{(i,j)}$ is given by

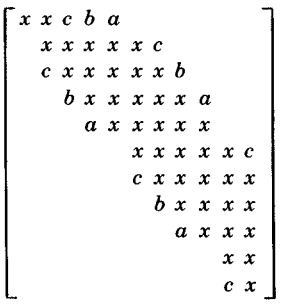
$$P^{(i,j)} = \begin{array}{c} \\ 1 \\ \\ \\ i \\ \\ \\ j \\ \\ \end{array} \begin{array}{c} \begin{array}{ccccccc} & & i & & j & & \end{array} \\ \begin{bmatrix} 1 & & & & & & \\ & \ddots & & & & & \\ & & 1 & & & & \\ & & & c & & d & \\ & & & & 1 & & \\ & & & & & \ddots & \\ & & & & & & 1 \\ & & & -d & & c & \\ & & & & & & & 1 \\ & & & & & & & & \ddots \\ & & & & & & & & & 1 \end{bmatrix} \end{array}$$

where $c^2 + d^2 = 1$ and has the property that if it is applied to J on the left, then the resulting matrix $J' = P^{(i,j)}J$ has elements different from J only in rows i and j, with zeros in both rows in those columns where there were zeros in both before, and, if c and d are chosen appropriately, with its (j, i) element equal to zero. Let us write $J = (\gamma_{ij})$, $J' = (\gamma'_{ij})$. Then, in particular, we have

$$\gamma'_{ik} = c\gamma_{ik} + d\gamma_{jk}, \qquad \gamma'_{jk} = -d\gamma_{ik} + c\gamma_{jk}, \qquad 1 \le k \le t,$$

so $\gamma'_{ji} = 0$, if

$$c = \gamma_{ii}/(\gamma_{ii}^2 + \gamma_{ji}^2)^{1/2},$$
$$d = \gamma_{ji}/(\gamma_{ii}^2 + \gamma_{ji}^2)^{1/2}.$$



STEP 1:
(i) Zero γ_{15} and chase it $a\ a\ a\ a$ off the matrix:
Rotate column 5 against column 4 to zero γ_{15} and introduce γ'_{54}.
Rotate row 5 against row 4 to zero γ'_{54} and introduce γ'_{49}
Rotate column 9 against column 8 to zero γ'_{49} and introduce γ'_{98}.
Rotate row 9 against row 8 to zero γ'_{98}
—chased off
(ii) Zero γ_{14} and chase it $b\ b\ b\ b$ off the matrix similarly.
(iii) Zero γ_{13} and chase it $c\ c\ c\ c\ c\ c$ also
STEP 2: Repeat for the second row, etc

Fig. 1. Bidiagonalizing a pentadiagonal upper triangular matrix of order 11 using Givens rotations by the method band Givens I.

The price paid for the annihilation is that a new nonzero element appears in one row wherever there was one already in the other. We say that row j is rotated against row i by the transformation. Similarly, if $P^{(i,j)}$ is applied on the right, only columns i and j of J are changed with $\gamma'_{ij} = 0$, if c and d are chosen correctly.

To describe the reduction process, let us suppose that J is an upper triangular band matrix with order $t = 11$ and $b = 4$ superdiagonals. Then the first thing the algorithm does is to zero γ_{15} by multiplying J on the right by $P^{(4,5)}$ with c and d chosen correctly, or, in other words, by rotating column 5 against column 4. This introduces one new nonzero element γ'_{54}. This new element is annihilated by multiplying J' on the left by $P^{(4,5)}$, that is, by rotating row 5 against row 4. This in turn introduces a new nonzero element γ'_{49}. Two more transformations, one from the left and one from the right, are now required to completely "chase the element off the matrix." At this point the resulting matrix has the same zero pattern as the original matrix J, except that γ_{15} has been annihilated. Now the process is repeated for γ_{14} and then for γ_{13}, and then the first row has the desired bidiagonal form. Finally, the entire process is repeated for every row until the matrix becomes bidiagonal. The method is illustrated in Figure 1. Let us call this method band Givens I.

Reducing the matrix to bidiagonal form in this way requires approximately $4bt^2$ multiplications using ordinary Givens transformations, or $2bt^2$ using "fast Givens," assuming $1 \ll b \ll t$. This compares with a count of approximately $4t^3/3$ multiplications required to do the reduction by the standard Golub-Reinsch algorithm using Householder transformations and ignoring the band structure, filling in the zeros off the band. This is, of course, a big savings if $b \ll t$;

Table I. Summary of Approximate Multiplication Counts for the Different Algorithms to Reduce a Band Matrix with Order t and Bandwidth b to Bidiagonal Form, Using Ordinary Givens Transformations, Except as Noted in the Last Column[a]

Method	Reduction without vectors	Accumulating the vectors	Total when vectors desired	Total using fast Givens
Golub–Reinsch	$\sum_{i=1}^{t-2} 2(2)(t-i)^2 \sim \frac{4t^3}{3}$	$\sum_{i=1}^{t-2} 2(2)(t-i)^2 \sim \frac{4t^3}{3}$	$\frac{8t^3}{3}$	—
Band Givens I	$\sum_{i=1}^{t-2} \sum_{k=2}^{b} \frac{t-(i+k)+1}{b}(2)(4)(b+1) \sim 4bt^2$	$\sum_{i=1}^{t-2} (b)\frac{t-i}{b}(8)t \sim 4t^3$	$4t^3$	$2t^3$
Band Givens II	$\sum_{k=2}^{b} \sum_{i=1}^{t-2} \frac{t-(i+k)+1}{k}(8)(k+1) \sim 4bt^2$	$\sum_{k=2}^{b} \sum_{i=1}^{t-2} \frac{t-i}{k}(8)t$ $\sim 4t^3 \sum_{k=2}^{b} \frac{1}{k} \sim 4\left(\ln b - \frac{1}{2}\right) t^3$	$4\left(\ln b - \frac{1}{2}\right) t^3$	$2\left(\ln b - \frac{1}{2}\right) t^3$
Band Householder	$\sum_{i=1}^{t-2} \frac{t-i}{b}(2) \sum_{k=1}^{b-1} 2(k)(k+b) \sim \frac{5}{3} b^2 t^2$	$\sum_{i=1}^{t-2} \frac{t-i}{b}(2) \sum_{k=1}^{b} 2(k)t \sim bt^3$	bt^3	—
Triangle Givens	$\sum_{i=1}^{t-2} 4(t-i)^2 \sim \frac{4t^3}{3}$	$\sum_{i=1}^{t-2} (t-i)8t \sim 4t^3$	$\frac{16t^3}{3}$	$\frac{8t^3}{3}$
Band Givens III	$4bt^2$	$\sum_{i=1}^{t-2} (b)\frac{t-i}{b}(8)(t-i) \sim \frac{8t^3}{3}$	$\frac{8t^3}{3}$	$\frac{4t^3}{3}$

[a] It is assumed that $1 \ll b \ll t$, but even for small b the same conclusions regarding the relative efficiency of the methods result except that there is then little difference between band Givens I and II.

furthermore, only $(b + 1)t$ storage locations are required to store the band matrix, while t^2 storage locations are required for the standard Golub–Reinsch reduction. If left and right singular vectors are required, however, the rotations used in band Givens I must be accumulated as the computation proceeds. This requires $4t^3$ multiplications using ordinary Givens transformations or $2t^3$ using "fast Givens," as opposed to $8t^3/3$ multiplications for the Golub–Reinsch reduction. Therefore, if the vectors are required, band Givens I still requires fewer multiplications than Golub–Reinsch if the "fast Givens" transformations are used. Both methods require approximately $2t^2$ storage locations.

There are several other possible methods to reduce J to bidiagonal form. The method we shall call band Givens II applies a sequence of rotations to J as before, but instead of reducing each row in turn to two elements, it systematically reduces the bandwidth by zeroing each superdiagonal in turn. In other words, in the example presented in Figure 1, after zeroing γ_{15} and chasing it off the matrix, it next turns to γ_{26} instead of γ_{14}. This method requires more rotations, since the decreasing bandwidth causes more nonzero elements to be introduced before a certain element is chased off the matrix; but for the same reason each rotation is less work if the vectors are not required. The two considerations cancel each other out, so band Givens I and II require about the same number of multiplications if vectors are not required; but the latter is slower by a factor of about $\ln b$ if vectors are required.

A third method called band Householder zeros all $b - 1$ elements in a row with a single Householder transformation, introducing a triangle of fill-in on the other side of the band at every step. Another method called triangle Givens does not attempt to preserve the band structure, but only the triangle structure. These methods are less efficient than band Givens I. Finally, a complicated version of band Givens I called band Givens III, which requires fewer multiplications when vectors are required, has been devised. The details of these methods appear in [7]. They are omitted here since in the block Lanczos context t may not be large; so there may be little payoff in using a special method. Furthermore, reducing the bidiagonal form to diagonal form to obtain the singular values in the second phase typically takes $8t^3$ multiplications using ordinary Givens or $4t^3$ using fast Givens, so this may dominate any slight savings in the reduction phase. Nonetheless the operation counts for the various methods are summarized in Table I, since they may be useful in other contexts.

5. ITERATING TO IMPROVE ACCURACY

Let us restate our computational procedure. We use the block bidiagonalization method to generate a block bidiagonal matrix J_s of small order and then apply some technique to compute the singular-value decomposition of J_s. Our convergence test depends on the next two lemmas.

LEMMA 5.1 (Weinstein's Inequality) [12, p. 56]. *Given a symmetric matrix B and a normalized vector $\mathbf{x}$, if there is a scalar μ such that*

$$\|B\mathbf{x} - \mu\mathbf{x}\| \leq \delta,$$

then there is an eigenvalue λ of B within δ of μ.

LEMMA 5.2 [12, pp. 59–60]. *Let B be an $l \times l$ symmetric matrix with eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_l$ and let $\|B\mathbf{x} - \mu\mathbf{x}\| \leq \delta$ for some normalized vector $\mathbf{x}$. Suppose that, for some j,*

$$|\mu - \lambda_i| \geq d > 0 \qquad \text{for} \quad i \neq j.$$

Then B has a normalized eigenvector $\mathbf{y}_j$ corresponding to λ_j such that

$$\|\mathbf{x} - \mathbf{y}_j\| \leq \gamma(1 + \gamma^2)^{1/2},$$

where $\gamma = \delta/d$.

From eqs. (2.14) and (2.15), we obtain

$$\begin{pmatrix} 0 & A \\ A^t & 0 \end{pmatrix} \begin{pmatrix} \mathbf{p}_i \\ \mathbf{q}_i \end{pmatrix} = \mu_i \begin{pmatrix} \mathbf{p}_i \\ \mathbf{q}_i \end{pmatrix} + \begin{pmatrix} \mathbf{0} \\ Z_{2s+1}\mathbf{h}_i \end{pmatrix}. \tag{5.1}$$

Thus, if

$$\|Z_{2s+1}\mathbf{h}_i\| \leq \delta \tag{5.2}$$

for some given tolerance δ, then there is a singular value σ_j of A such that

$$|\mu_i - \sigma_j| \leq \delta.$$

If it is also true that

$$|\mu_i - \sigma_k| \geq d > 0 \qquad \text{for} \quad k \neq j,$$

where $\sigma_1, \sigma_2, \ldots, \sigma_n$ are the singular values of A, then A has normalized left and right singular vectors $\mathbf{u}_j$ and $\mathbf{v}_j$, respectively, corresponding to σ_j such that

$$\|\mathbf{p}_i - \mathbf{u}_j\|^2 + \|\mathbf{q}_i - \mathbf{v}_j\|^2 \leq \gamma^2(1 + \gamma^2),$$

where $\gamma = \delta/d$. For the more complicated case of multiple singular values, we refer the reader to an excellent paper of Stewart [17].

Suppose that our procedure has not computed all the k greatest singular values to the desired accuracy. In Theorem 3.2, the error bounds contain the term $\tan\theta$, where θ is the angle between the two subspaces spanned by the columns of V_1 and Q_1. Let

$$\hat{Q}_1 = (\mathbf{q}_1, \mathbf{q}_2, \ldots, \mathbf{q}_b).$$

The results of the last section indicate that the matrix $\hat{Q}_1$ is a better approximation to the matrix V_1 than the initial matrix Q_1. Thus, we expect to compute more accurate approximations to the greatest singular values of A if we reapply the block bidiagonalization method with the initial matrix $\hat{Q}_1$. This idea leads to the following iterative scheme, where we assume that b equals k.

ALGORITHM 5.1

1. Let b, s, and δ be given parameters and let Q_1 be a given $n \times b$ orthonormal matrix.
2. Repeat until all b greatest singular values have converged:
   (a) Use the block bidiagonalization method with initial matrix Q_1 to generate the matrices J_s, $\bar{P}_s$, and $\bar{Q}_s$.
   (b) Compute the singular value μ_i and corresponding left and right singular vectors $\mathbf{w}_i$ and $\mathbf{z}_i$, respectively, of J_s, for $i = 1, 2, \ldots, bs$.
   (c) Estimate the accuracy of μ_i as an approximation to σ_i for $i = 1, 2, \ldots, b$ (cf. inequality (5.2)).

(d) Let

$$Q_1 := (\mathbf{q}_1, \mathbf{q}_2, \ldots, \mathbf{q}_b),$$

where

$$\mathbf{q}_i = \bar{Q}_s \mathbf{z}_i \qquad \text{for} \quad i = 1, 2, \ldots, b.$$

This iterative algorithm provides a convenient means for estimating the accuracy of the computed singular values. We can show that the ith column of the matrix Z_2 in the block bidiagonalization method computed in each iteration of Algorithm 5.1 after the first is the residual vector for the singular value μ_i computed in the previous iteration. It is thus possible to determine at the start of an iteration the accuracy of the singular values computed at the end of the previous iteration. We also observe that the matrices P_1 and R_2 of the block bidiagonalization method are readily available from the prior iteration.

However, once a few singular values and singular vectors have converged, we need not iterate with them any longer. Since the desired singular values may have different rates of convergence, as indicated by the error bounds of Theorems 3.1 and 3.2, we should modify Algorithm 5.1 so that (1) it does not iterate with those singular values and singular vectors that have converged, and (2) it allows the values of b and s to change from one iteration to the next. We are going to examine these issues in the next two sections.

6. BLOCK BIDIAGONALIZATION METHOD WITH REORTHOGONALIZATION

Suppose that we are given accurate approximations to the k_0 greatest singular values $\sigma_1, \sigma_2, \ldots, \sigma_{k_0}$ and corresponding singular vectors of the matrix A. Let P_0 and Q_0 be the $m \times k_0$ and $n \times k_0$ orthonormal matrices consisting of those given left and right singular vectors, respectively. We want now to compute the next $(k - k_0)$ greatest singular values of A.

Let us consider the matrix

$$\tilde{A} = \begin{pmatrix} 0 & A \\ A^t & 0 \end{pmatrix}. \tag{1.2}$$

If we apply the block Lanczos method to compute the eigenvalues $\pm\sigma_{k_0+1}$, $\pm\sigma_{k_0+2}, \ldots, \pm\sigma_k$ of the matrix $\tilde{A}$, then we must maintain the orthogonality of the matrices $X_1, X_2 \ldots, X_s$ with respect to the eigenvectors corresponding to the eigenvalues $\pm\sigma_1, \pm\sigma_2, \ldots, \pm\sigma_{k_0}$ (cf. [18]). But these eigenvectors are accurately approximated by the columns of the matrix (see [10, Chapter 3])

$$\frac{1}{\sqrt{2}} \begin{pmatrix} P_0 & P_0 \\ Q_0 & -Q_0 \end{pmatrix}.$$

We have that

$$I - \frac{1}{\sqrt{2}} \begin{pmatrix} P_0 & P_0 \\ Q_0 & -Q_0 \end{pmatrix} \frac{1}{\sqrt{2}} \begin{pmatrix} P_0 & P_0 \\ Q_0 & -Q_0 \end{pmatrix}^t = \begin{pmatrix} I - P_0 P_0^t & 0 \\ 0 & I - Q_0 Q_0^t \end{pmatrix}.$$

Therefore, if we want to apply the block bidiagonalization method to compute the $(k - k_0)$ next greatest singular values of A, we need to maintain the orthogonality of the matrices $P_1, P_2, \ldots, P_s$ with respect to P_0, and the orthogo-

nality of the matrices $Q_1, Q_2, \ldots, Q_s$ with respect to Q_0. We are thus computing the $(k - k_0)$ greatest singular values of the "deflated" matrix

$$\hat{A} = (I - P_0 P_0^t) A (I - Q_0 Q_0^t). \tag{6.1}$$

Suppose that

$$\|AQ_0 - P_0\Sigma_0\|_F^2 + \|A^t P_0 - Q_0\Sigma_0\|_F^2 \leq \delta^2 \tag{6.2}$$

where $\|\cdot\|_F$ is the Frobenius matrix norm and $\Sigma_0 = \text{diag}(\sigma_1, \sigma_2, \ldots, \sigma_{k_0})$. Note that if both matrices P_0 and Q_0 had been computed by the block Lanczos procedure, then (cf. eq. (2.12))

$$\|AQ_0 - P_0\Sigma_0\| = 0(mk_0\epsilon), \tag{6.3}$$

where ϵ is the machine precision. Using arguments similar to those in Underwood's thesis [18, pp. 62–66], we get from (6.2) that the $(k - k_0)$ greatest singular values of $\hat{A}$ differ from the $(k - k_0)$ next greatest singular values of A by quantities that are less than $|\delta|$ in modulus.

Now, the block bidiagonalization method may be numerically unstable. Although the matrices P_i and Q_i form two sequences of orthonormal matrices in exact arithmetic, they lose orthogonality rapidly in practice owing to the loss of figures in the computation of the matrices Z_i and W_i. To maintain stability in the scheme, we choose to reorthogonalize the matrices P_i and Q_i with respect to all the previous P_j and Q_j, respectively (cf. [18]). We have also implemented the idea of local reorthogonalization due to Lewis [11] (see [7]). But we now feel that complete reorthogonalization is more appropriate for our application of computing a few greatest singular values.

ALGORITHM 6.1 (Block Bidiagonalization Method with Reorthogonalization)

1. Let Q_1 be a given $n \times b$ orthonormal matrix.
   Compute
   $$W_1 := AQ_1.$$
   Orthogonalize W_1 with respect to P_0. Factorize W_1 so that
   $$W_1 = P_1 R_2,$$
   where P_1 is orthonormal and R_2 is upper triangular.
2. For $i = 2, 3, \ldots, s$, do
   (a) Compute
   $$Z_i := A^t P_{i-1} - Q_{i-1} R_{2i-2}^t.$$
   Orthogonalize Z_i with respect to $Q_0, Q_1, \ldots, Q_{i-1}$. Factorize Z_i so that
   $$Z_i = Q_i R_{2i-1},$$
   where Q_i is orthonormal and R_{2i-1} is upper triangular.
   (b) Compute
   $$W_i := AQ_i - P_{i-1} R_{2i-1}^t.$$
   Orthogonalize W_i with respect to $P_0, P_1, \ldots, P_{i-1}$. Factorize W_i so that
   $$W_i = P_i R_{2i},$$
   where P_i is orthonormal and R_{2i} is upper triangular.

In case of rank deficiency of the matrix Z_i or W_i, we apply a remedial procedure similar to that for Algorithm 2.1.

7. ITERATIVE BLOCK LANCZOS METHOD

We should point out that the reorthogonalization process of the last section not only requires a large number of arithmetic operations but also requires that each of the P_j and Q_j be in memory during each step of Algorithm 6.1. Since m and n are large numbers in this application, the available computer memory places an upper bound c on the product bs. It is then necessary to determine optimal values for b and s subject to this upper bound constraint. But the error bounds of Theorem 3.2 indicate that we need accurate knowledge of the singular-value spectrum of the given matrix, which is precisely the same information we are trying to obtain.

A good initial choice of the block size b is the number k of singular values to be computed (see [2] and [18]). This may not be the best choice, as we can see from Example 8.4 of the next section. Our experiments have shown that it seldom pays to have $b > k$ (cf. Example 8.3 of the next section). Underwood [18] made the same observation, but he used a different way to update the block size.

Having chosen b, we compute the number s of blocks by

$$s := \lfloor \frac{c}{b} \rfloor,$$

where $\lfloor \alpha \rfloor$ denotes the integer part of a real number α. If s is less than 2, we compute

$$b := \lfloor \frac{c}{2} \rfloor \qquad \text{and} \qquad s := \lfloor \frac{c}{b} \rfloor.$$

The last computation is necessary so that s would equal 3 if the value of c were 3.

Let us describe how we update the values of c, b, s, and k. Suppose that k_0 singular values and associated singular vectors have converged in an iteration. Then

$$c := c - k_0$$

because those computed singular vectors must reside in the computer memory for the reorthogonalization process. Now, if $b \geq k$, then we decrease the value of b by k_0—that is,

$$b := b - k_0;$$

otherwise we choose the new block size as the smaller value of the old block size and the number of singular values left to be computed—that is,

$$b := \min(b, k - k_0).$$

We update the value of k by

$$k := k - k_0.$$

The new value for s is then computed in the same manner as described in the previous paragraph, with the same modification to the value of b, if necessary.

Our scheme for updating b differs from Underwood's [18] only in the case where $b > k$.

ALGORITHM 7.1 (Iterative Block Lanczos Method)

1. Let c, b, s, and δ be given parameters and let Q_1 be a given $n \times b$ orthonormal matrix. The matrices P_0 and Q_0 are null.
2. Repeat until all k singular values have converged:
   (a) Use Algorithm 6.1 with initial matrix Q_1 to generate the matrices J_s, $\bar{P}_s$, and $\bar{Q}_s$.
   (b) Compute the singular value μ_i and corresponding left and right singular vectors $\mathbf{w}_i$ and $\mathbf{z}_i$, respectively, of J_s, for $i = 1, 2, \ldots, bs$.
   (c) Estimate the accuracy of μ_i as an approximate singular value, for $i = 1, 2, \ldots, bs$. Assume that k_0 singular values have converged.
   (d) Update the values of c, b, and s.
   (e) For $i = 1, 2, \ldots, k_0 + b$, compute

$$\mathbf{p}_i := \bar{P}_s \mathbf{w}_i$$

   and

$$\mathbf{q}_i := \bar{Q}_s \mathbf{z}_i.$$

   (f) Let

$$P_0 := (P_0 | \mathbf{p}_1, \ldots, \mathbf{p}_{k_0})$$

   and

$$Q_0 := (Q_0 | \mathbf{q}_1, \ldots, \mathbf{q}_{k_0}).$$

   (g) Let

$$Q_1 := (\mathbf{q}_{k_0+1}, \mathbf{q}_{k_0+2}, \ldots, \mathbf{q}_{k_0+b}).$$

8. TEST EXAMPLES

Rectangular diagonal matrices are chosen for all our examples. Such matrices are sufficiently general for the Lanczos method, which does not transform the given matrix. We can thus specify the singular-value spectrum and study the behavior of the algorithm as a function of b and s. The initial matrix is randomly generated.

A set of FORTRAN routines has been written to implement Algorithm 7.1 (see [7]). We ran our tests on an IBM 370/168 computer at the Stanford Linear Accelerator Center.

The computed singular value μ_i and associated singular vectors $\mathbf{p}_i$ and $\mathbf{q}_i$ are accepted if they satisfy the inequality

$$(\|A\mathbf{q}_i - \mu_i \mathbf{p}_i\|^2 + \|A^t \mathbf{p}_i - \mu_i \mathbf{q}_i\|^2)^{1/2} \leq 10^{-3}.$$

In Sections 5 and 6, we have described a way to test for convergence with very little additional work. We have chosen the upper bound c for the product bs to be 12.

The following notation is used in the examples:

$\sigma_1, \sigma_2, \sigma_3, \ldots$ = the computed singular values in the order of convergence.

Iter = total number of iterations.

Time = machine execution time in seconds.

$m' - n = m \times 10^{-n}$.

Example 8.1. A is a 905 × 904 matrix with diagonal elements −1.00, −0.99, -0.98, and 0.000, 0.001, . . . , 0.900.

$k = 3$	$b = 3$
σ_1	1.00 − 4′ − 7
σ_2	0.99 − 9′ − 9
σ_3	0.98 − 3′ − 6
Iter	5
Time	11 36

We note that the computed singular values, as Rayleigh quotients, are accurate to twice the number of digits of the error tolerance.

Example 8.2. A is a 905 × 904 matrix with diagonal elements −1.000, −0.999, -0.998, and 0.9000, 0.9001, . . . , 0.9900. This example is essentially the same as the previous one, except that the gaps between the singular values have been reduced by a factor of 10.

$k = 3$	$b = 3$
σ_1	1.000 − 9′ − 7
σ_2	0.999 − 4′ − 8
σ_3	0 998 − 2′ − 8
Iter	6
Time	13.83

The first two examples illustrate the fact that the convergence rate of the Lanczos algorithm depends on the *relative* spread of the singular values (cf. Theorems 3.1 and 3.2).

Example 8.3. A is an 806 × 805 matrix with diagonal elements 1.0, −1.0, 0.9, -0.9, and 0.000, 0.001, . . . , 0.800.

$k = 1$	$b = 1$	$b = 2$
σ_1	1.0 − 3′ − 10	1.0 − 1′ − 12
Iter	1	3
Time	2.35	6.52

$k = 2$	$b = 1$	$b = 2$
σ_1	1.0 − 3′ − 10	1.0 − 1′ − 12
σ_2	0.9 − 3′ − 16	1.0 − 1′ − 11
Iter	2	3
Time	4.27	6.52

$k = 3$	$b = 1$	$b = 2$	$b = 3$	$b = 4$
σ_1	1.0 − 3′ − 10	1.0 − 1′ − 12	1.0 − 3′ − 8	1.0 − 1′ − 7
σ_2	0.9 + 3′ − 16	1 0 − 1′ − 11	1.0 − 4′ − 9	1.0 − 8′ − 7
σ_3	1.0 + 0′ − 16	0.9 − 1′ − 9	0.9 − 3′ − 9	0.9 − 6′ − 9
Iter	5	4	4	5
Time	9.60	8.28	8 23	10.53

$k = 4$	$b = 1$	$b = 2$	$b = 3$	$b = 4$
σ_1	1.0 − 3′ − 10	1.0 − 1′ − 12	1.0 − 3′ − 8	1.0 − 1′ − 7
σ_2	0.9 + 3′ − 16	1.0 − 1′ − 11	1.0 − 6′ − 8	1.0 − 8′ − 7
σ_3	1.0 + 0′ − 16	0.9 − 3′ − 8	0.9 − 2′ − 7	0.9 − 6′ − 9
σ_4	0.9 + 6′ − 14	0.9 − 7′ − 8	0.9 + 8′ − 10	0.9 − 2′ − 7
Iter	7	5	5	5
Time	12.70	10.00	9.59	10.38

These tests illustrate a couple of important points. First, the Lanczos method does not always compute the greatest singular values (cf. the case where $k = 2$ and $b = 1$). Second, the supposition of Theorems 3.1 and 3.2 that $\sigma_b > \sigma_{b+1}$ is not necessary for the convergence of the Lanczos method.

Example 8.4. A is a 902 × 901 matrix with diagonal elements 0.000, 0.001, . . . , 0.900.

$k = 3$	$b = 1$	$b = 2$	$b = 3$
σ_1	0.900 − 5′ − 6	0.900 − 1′ − 5	0.900 − 9′ − 6
σ_2	0.899 + 3′ − 6	0.899 − 2′ − 6	0.899 − 9′ − 6
σ_3	0.898 − 2′ − 5	0.898 − 4′ − 7	0.898 − 7′ − 5
Iter	13	27	23
Time	28.73	61.85	52.53

This example of a dense singular-value spectrum is one in which the point algorithm ($b = 1$) works better than the block algorithm ($b \geq 2$).

Our iterative block Lanczos method is therefore a good procedure for computing a few greatest singular values of a matrix. A block method with an appropriate block size can (1) have a fast convergence rate, and (2) handle well the case of multiple singular values (see Example 8.3). For problems where the given matrix has to be read from secondary storage, economics may dictate that we multiply the matrix into a block of vectors and thus choose a block method.

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