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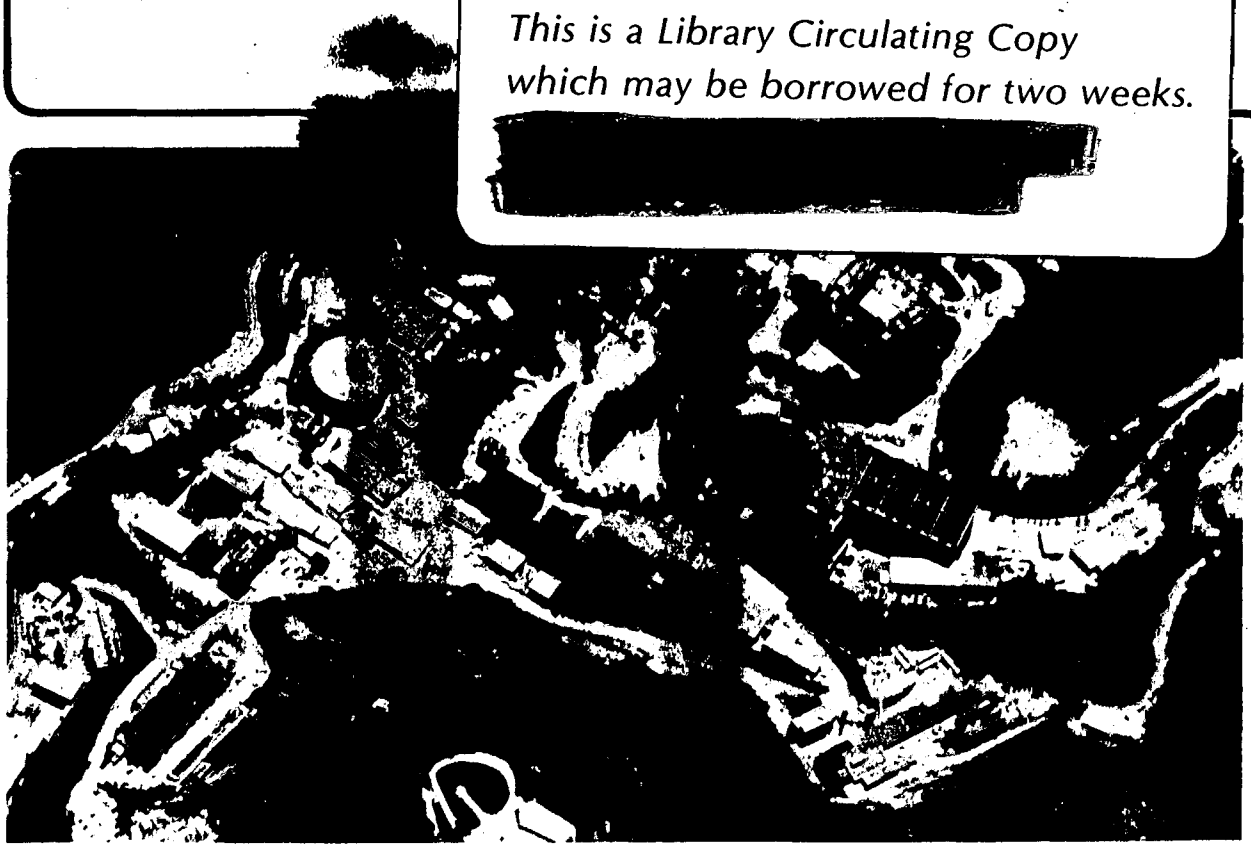

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BLOCK PRECONDITIONING FOR THE CONJUGATE GRADIENT METHOD

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BLOCK PRECONDITIONING FOR THE CONJUGATE GRADIENT METHOD

1. Introduction

In this paper we study some preconditioning techniques for the conjugate gradient method to solve the linear systems of equations that arise from the discretization of partial differential equations. We consider for example elliptic equations such as

$$-\sum_{i=1}^{d} \frac{\partial}{\partial \xi_i}\left(\lambda_i(\xi)\,\frac{\partial u}{\partial \xi_i}\right) + \sigma(\xi)u = f \quad \text{in} \quad \Omega \subset R^d \ , \ \xi = (\xi_1, \xi_2, \ldots, \xi_d) \tag{1}$$

with

$$u(\xi) = g(\xi) \ \text{ or } \ \frac{\partial u}{\partial n} = g(\xi) \qquad \text{on } \partial\Omega \ ,$$

where n is the exterior normal, and $\lambda_i(\xi) > 0$. The techniques that we describe are suitable for standard finite-difference discretizations of equations such as the above that yield certain symmetric positive definite block tridiagonal linear systems of the form

$$Ax = b \ , \tag{2}$$

where

$$A = \begin{pmatrix} D_1 & A_2^T & & & \\ A_2 & D_2 & A_3^T & & \\ & \ddots & \ddots & \ddots & \\ & & A_{n-1} & D_{n-1} & A_n^T \\ & & & A_n & D_n \end{pmatrix} .$$

Such equations can arise also from finite element discretizations with node groupings that form a tree [11].

The prototype model problem in two dimensions is the Dirichlet problem,

$\sigma \equiv 0$, $\lambda_i \equiv 1$, $g \equiv 0$, Ω the unit square,

$$-\Delta u = f$$

$$u = 0 \quad \text{on the boundary},$$

with standard five-point differencing on a uniform mesh of width h. We focus attention on the matrix structure obtained for natural ordering, which yields (after multiplication by h^2)

$$A_i = -I \ , \ D_i = \begin{pmatrix} 4 & -1 & & & \\ -1 & 4 & -1 & & \\ & \cdot & \cdot & \cdot & \\ & & -1 & 4 & -1 \\ & & & -1 & 4 \end{pmatrix} .$$

In three dimensions, standard 7-point differencing with this ordering would yield D_i that have two additional non-zero diagonals. Different orderings or higher order approximations would give rise to different structures, to which our techniques could be applied also.

To solve (2) we use the generalized or preconditioned conjugate gradient method, which may be written as follows [3]. Let x^0 be given, define p^{-1} arbitrarily, and let $r^0 = b - Ax^0$. For $k = 0, 1, \ldots$ perform the steps

$$Mz^k = r^k$$

$$\beta_k = \frac{(z^k, Mz^k)}{(z^{k-1}, Mz^{k-1})} \ , \quad k \geq 1 \ ; \quad \beta_0 = 0$$

$$p^k = z^k + \beta_k p^{k-1}$$

$$\alpha_k = \frac{(z^k, Mz^k)}{(p^k, Ap^k)}$$

$$x^{k+1} = x^k + \alpha_k p^k$$

$$r^{k+1} = r^k - \alpha_k A p^k \ .$$

The matrix M is the preconditioning matrix, which should be in some sense an approximation of A. It is known that the preconditioned conjugate gradient

method converges rapidly if the condition number $\kappa(M^{-1}A)$, which is the ratio of the largest to the smallest eigenvalue of $M^{-1}A$, is small or if the eigenvalues are clustered (cf. [3]).

The goal of this study is to devise good preconditioning matrices M. For this purpose we exploit the structure of A in constructing some block preconditionings, one special case of which is the one introduced by R.R. Underwood [19].

In Section 2 to motivate the use of our block techniques we recall some results on block Cholesky factorization. Section 3 deals with the main problem --finding good approximate inverses for tridiagonal matrices that are diagonally dominant. New block techniques for two-dimensional problems ($d = 2$ in (1)) are introduced in Section 4. Three-dimensional problems will be discussed in detail in a subsequent study.

In Section 5 we present numerical experiments for several test problems. As comparisons are made with point preconditioning techniques, some of them are recalled briefly there. We compare the methods on the basis of number of iterations and the number of floating point operations required. Also, we illustrate graphically the spectral properties of the matrices corresponding to the various preconditionings.

2. Block Cholesky factorization

Let A be the symmetric positive definite block tridiagonal matrix of (2). Let m_i be the order of the i^{th} square diagonal block D_i and $N = \sum_{i=1}^{n} m_i$ the order of A. We denote

$$D = \begin{pmatrix} D_1 & & & \\ & D_2 & & \\ & & \ddots & \\ & & & D_n \end{pmatrix} \qquad L = \begin{pmatrix} 0 & & & \\ A_2 & 0 & & \\ & \ddots & \ddots & \\ & & A_n & 0 \end{pmatrix} .$$

$$A = D + L + L^T ,$$

and we denote by a_{ij} the elements (pointwise) of A.

Since A is positive definite, there holds $a_{ii} > 0$, $i = 1, \ldots, N$. We assume that the following holds also.

Hypothesis (H1). (a). *The off-diagonal elements a_{ij}, $i \neq j$ of A are non-positive.*

(b). *A is (weakly) diagonally dominant; i.e., there holds*

$$a_{ii} \geq \sum_{j \neq i} |a_{ij}| \quad , \quad i = 1, \ldots, N ,$$

and there exists at least one k, $1 \leq k \leq N$, such that

$$a_{kk} > \sum_{j \neq k} |a_{kj}| .$$

(c). *Each column of A_i, $i = 2, \ldots, n$, has at least one non-zero element.*

Hypothesis (H1)(a) implies that A is a Stieltjes matrix, i.e., a positive definite M−matrix.

Let Σ be the symmetric block diagonal matrix with $m_i \times m_i$ blocks Σ_i satisfying

$$\begin{aligned} \Sigma_1 &= D_1 \\ \Sigma_i &= D_i - A_i \Sigma_{i-1}^{-1} A_i^T \quad , \quad 2 \leq i \leq n . \end{aligned} \tag{3}$$

Then the block Cholesky factorization of A can be written as

$$A = (\Sigma + L)\Sigma^{-1}(\Sigma + L^T) .$$

The factor $\Sigma + L$ is block lower bidiagonal. Since A is positive definite symmetric, the factorization can be carried out.

The following results concerning the properties of the Σ_i are well known, but as we did not find them in the literature in a form suitable for our application, we give them here for completeness. These properties provide guidance in our selection of preconditioning matrices for the conjugate gradient method.

Let

$$B = \begin{pmatrix} B_1 & -C^T \\ -C & B_2 \end{pmatrix}$$

be a symmetric positive definite M-matrix with B_1 and B_2 square. This implies (cf. [2]) that the diagonal elements are positive, the off-diagonal elements are non positive, and B is generalized strictly diagonally dominant, i.e., there exists a diagonal positive matrix E such that $E^{-1}BE$ is strictly diagonally dominant.

Lemma 1. *$B'_2 = B_2 - CB_1^{-1}C^T$ is a symmetric positive definite M-matrix.*

B'_2 is called the Schur complement of B_1 in B. For other properties of the Schur complement see [4].

Proof. We can write

$$\begin{pmatrix} B_1 & 0 \\ 0 & B_2 - CB_1^{-1}C^T \end{pmatrix} = \begin{pmatrix} I & 0 \\ CB_1^{-1} & I \end{pmatrix} B \begin{pmatrix} I & B_1^{-1}C^T \\ 0 & I \end{pmatrix}.$$

Since the leading principal minors of B are unchanged by the transformation on the right side of the equality, the matrix on the left side is positive definite, and hence so is B'_2. In particular the diagonal elements of B'_2 are positive and, as $B_1^{-1} > 0$ and $C \geq 0$ hold, it follows that the off diagonal elements are non positive.

Let $e = (1,1,\ldots,1)^T$. The condition that B is generalized strictly diagonally dominant corresponds to the existence of a diagonal matrix $E > 0$

$$E = \begin{pmatrix} E_1 & 0 \\ 0 & E_2 \end{pmatrix}$$

such that $E^{-1}BE$ is strictly diagonally dominant, i.e.,

$$E^{-1}BEe > 0 .$$

But we have

$$E^{-1}BE = \begin{pmatrix} E_1^{-1}B_1E_1 & -E_1^{-1}C^TE_2 \\ -E_2^{-1}CE_1 & E_2^{-1}B_2E_2 \end{pmatrix}$$

and

$$E_1^{-1}B_1E_1e > E_1^{-1}C^TE_2e$$

$$E_2^{-1}B_2E_2e > E_2^{-1}CE_1e ,$$

where, with a looseness of notation, we denote by e vectors of different length with all elements equal to 1.

As $CB_1^{-1}E_1$ is a positive matrix, the first inequality implies

$$CE_1e \geq CB_1^{-1}C^TE_2e$$

and

$$E_2^{-1}CE_1e \geq E_2^{-1}CB_1^{-1}C^TE_2e .$$

Thus there holds

$$E_2^{-1}B_2E_2e > E_2^{-1}CB_1^{-1}C^TE_2e ,$$

from which one obtains

$$E_2^{-1}(B_2 - CB_1^{-1}C^T)E_2e = E_2^{-1}B'_2E_2e > 0 .$$

Hence B'_2 is an M-matrix.

Using the same techniques we can show also that if B satisfies Hypothesis (H1)(a),(b) then B'_2 does also.

Now we apply these results to A with $B_1 = D_1$, $-C^T = (A_2^T\ 0\ \cdots\ 0)$, and

$$B_2 = \begin{pmatrix} D_2 & A_3^T & & & \\ A_3 & D_3 & A_4^T & & \\ & \ddots & \ddots & \ddots & \\ & & A_{n-1} & D_{n-1} & A_n^T \\ & & & A_n & D_n \end{pmatrix}.$$

We have

$$B'_2 = \begin{pmatrix} D_2 - A_2 D_1^{-1} A_2^T & A_3^T & & & \\ A_3 & D_3 & A_4^T & & \\ & \ddots & \ddots & \ddots & \\ & & A_{n-1} & D_{n-1} & A_n^T \\ & & & A_n & D_n \end{pmatrix}.$$

There follows

Theorem 1. *Under Hypothesis (H1) all the Σ_i are symmetric strictly diagonally dominant M-matrices.*

It is of interest to note, that in the particular case of the model problem, the block Cholesky factorization can be shown to reduce to a Fast Poisson Solver [18].

3. Incomplete Block Cholesky Factorization

Because of the work and storage that may be required in large problems for computing the Σ_i, carrying out the complete block Cholesky factorization is not of interest to us here as a general means for solving (2). For example, for the two-dimensional model problem, although $\Sigma_1 = D_1$ is tridiagonal, Σ_1^{-1} and hence Σ_i, $i \geq 2$, are dense.

In this paper our interest focuses on approximate block Cholesky factorizations obtained by using in (3) instead of Σ_{i-1}^{-1} a sparse approximation Λ_{i-1}. One thereby obtains instead of Σ the block diagonal matrix Δ with $m_i \times m_i$ blocks Δ_i satisfying

$$\Delta_1 = D_1 \tag{4a}$$

$$\Delta_i = D_i - A_i \Lambda_{i-1} A_i^T \quad , \quad 2 \le i \le n \ , \tag{4b}$$

where for each i in (4b), Λ_{i-1} is the sparse approximation to Δ_{i-1}^{-1}. The incomplete block Cholesky preconditioning matrix for use with the conjugate gradient algorithm is then

$$M = (\Delta + L)\Delta^{-1}(\Delta + L^T) \ . \tag{5}$$

One has

$$M = A + \Delta - D + L\Delta^{-1}L^T = A + R \ ,$$

where R is a block diagonal matrix

$$R = \begin{pmatrix} R_1 & & & & \\ & R_2 & & & \\ & & \cdot & & \\ & & & R_{n-1} & \\ & & & & R_n \end{pmatrix}$$

with

$$R_1 = \Delta_1 - D_1 = 0$$

$$R_i = \Delta_i - D_i + A_i \Delta_{i-1}^{-1} A_i^T \quad , \quad 2 \le i \le n \ .$$

The factor $\Delta + L$ in (5) is lower block bidiagonal. Using the Cholesky factors L_i of Δ_i,

$$\Delta_i = L_i L_i^T \ ,$$

one can express M in terms of (point) lower and upper triangular factors

$$M = \begin{bmatrix} L_1 & & & \\ W_2 & L_2 & & 0 \\ & \cdot & \cdot & \\ & & W_{n-1} & L_{n-1} \\ & & & W_n \quad L_n \end{bmatrix} \begin{bmatrix} L_1^T & W_2^T & & \\ & L_2^T & W_3^T & \\ & & \cdot & \cdot \\ 0 & & L_{n-1}^T & W_n^T \\ & & & L_n^T \end{bmatrix}, \tag{6}$$

where

$$W_i = A_i L_{i-1}^{-T} \quad , \quad i = 2,\ldots,n \ .$$

This form is generally more efficient computationally than is (5). For specific Λ_i of interest, we show in subsequent sections that all the Δ_i are positive definite, which implies that the above factorization can be carried out.

Note that in the conjugate gradient algorithm M is not required explicitly, only the linear system $Mz^k = r^k$ need be solved for z^k. Since this can be done with block backward and forward substitution, the block off-diagonal elements W_i need not be computed explicitly. The requisite products with vectors can be obtained by solving linear systems with triangular coefficient matrices L_i and L_i^T. Generally, for preconditionings of interest, the Δ_i, and correspondingly the L_i, will be sparse. These features were first used in this context by R.R. Underwood in [20], where block incomplete Cholesky preconditioning for the conjugate gradient algorithm was introduced.

For the standard five point discretization of (1) in two dimensions, D_i is tridiagonal, and A_i is diagonal. This is the case on which this paper focuses: of central interest is the choice that the Λ_{i-1} be tridiagonal, so that all the Δ_i in (4b) are tridiagonal. Correspondingly, in this section we discuss techniques for approximating the inverse of a tridiagonal, diagonally-dominant matrix.

Let

$$T = \begin{pmatrix} a_1 & -b_1 & & & \\ -b_1 & a_2 & -b_2 & & \\ & \cdot & \cdot & \cdot & \\ & & -b_{m-2} & a_{m-1} & -b_{m-1} \\ & & & -b_{m-1} & a_m \end{pmatrix} \tag{7}$$

be a non singular tridiagonal matrix. We assume that the following holds.

Hypothesis (H2). *The elements a_i and b_i of T satisfy*

$$\begin{aligned} a_i &> 0 \quad , \quad 1 \le i \le m \\ b_i &> 0 \quad , \quad 1 \le i \le m-1 \, , \end{aligned}$$

and T is strictly diagonally dominant, i.e.

$$\begin{aligned} a_1 &> b_1 \\ a_i &> b_{i-1} + b_i \quad , \quad 2 \le i \le m-1 \\ a_m &> b_{m-1} \, . \end{aligned}$$

3.1 Diagonal approximation

The simplest approximation $\widetilde{T}_1$ of T^{-1} we consider is the diagonal matrix whose elements are

$$(\widetilde{T}_1)_{ii} = \frac{1}{(T)_{ii}} . \tag{8}$$

3.2 Banded approximation from the exact inverse

One can do much better than the diagonal approximation $\widetilde{T}_1$ by using the following powerful result, which characterizes the inverses of symmetric tridiagonal matrices, (cf. [1],[10]).

Theorem 2. *There exist two vectors u and $v \in R^m$ such that*

$$(T^{-1})_{ij} = u_i v_j \qquad for \quad i \le j \ .$$

Since the inverse of T is

$$T^{-1} = \begin{pmatrix} u_1v_1 & u_1v_2 & \cdots & u_1v_m \\ u_1v_2 & u_2v_2 & \cdots & u_2v_m \\ \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot \\ u_1v_m & u_2v_m & \cdots & u_mv_m \end{pmatrix},$$

one can compute recursively the components of u and v. Under Hypothesis (H2) T is positive definite, so that T^{-1} is also, which implies that $u_i \neq 0$, $v_i \neq 0$, for all i. We remark that all of Hypothesis (H2), which will be used later, is not required for Theorem 2. It is necessary only that T in (7) be nonsingular and irreducible (all of the b_i non-zero).

Lemma 2. *The components of u and v can be computed as follows:*

$$u_1 = 1 \ , \ u_2 = \frac{a_1}{b_1}$$

$$u_i = \frac{a_{i-1}u_{i-1} - b_{i-2}u_{i-2}}{b_{i-1}} \ , \quad 3 \le i \le m$$

$$v_m = \frac{1}{-b_{m-1}u_{m-1} + a_m u_m} \tag{9}$$

$$v_i = \frac{1 + b_i u_i v_{i+1}}{a_i u_i - b_{i-1}u_{i-1}} \ , \quad 2 \le i \le m-1$$

$$v_1 = \frac{1 + b_1 u_1 v_2}{a_1 u_1} \ .$$

Proof. By substitution.

Alternative recurrences for generating u and v can be obtained by several means, such as by computing the first and last columns of T^{-1} from the Cholesky factors of T. For numerical computation scaling may be required in (9) to prevent underflow or overflow or it may be desirable to work with the ratios u_{i+1}/u_i and v_{i+1}/v_i considered below.

Several papers have characterized the elements of inverses of diagonally dominant matrices. D. Kershaw [15] proved results for tridiagonal matrices and S. Demko [5] extended them to banded matrices. It is known that the elements of $(T^{-1})_{ij}$ are bounded in an exponentially decaying manner along each row or column. Specifically, there exist $\rho < 1$ and a constant C_0 such that

$$(T^{-1})_{ij} \leq C_0 \rho^{|i-j|}.$$

This result does not prove that the elements actually decay along each row; it merely provides a bound. With Hypothesis (H2), however, one can prove the following:

Lemma 3. *Under Hypothesis (H2) the sequence $\{u_i\}_{i=1}^m$ is strictly increasing and the sequence $\{v_i\}_{i=1}^m$ is strictly decreasing.*

Proof. It is clear that $u_2 = \dfrac{a_1}{b_1} > 1 = u_1$. The proof continues by induction using formulas of Lemma 2. Since $u_{i-1} > u_{i-2}$, one has from (9) that

$$u_i > u_{i-1}\left(\frac{a_{i-1} - b_{i-2}}{b_{i-1}}\right) > u_{i-1},$$

because $a_{i-1} - b_{i-1} - b_{i-2} > 0$. To prove that the v_i are decreasing we need to modify the formulas of Lemma 2 slightly, using the ones for u to simplify those for v. Note that

$$a_i u_i - b_{i-1} u_{i-1} - b_i u_{i+1} = 0$$

and

$$(a_{i+1} u_{i+1} - b_i u_i) v_{i+1} = 1 + b_{i+1} u_{i+1} v_{i+2} .$$

Thus

$$v_i = \frac{a_{i+1} u_{i+1} v_{i+1} - b_{i+1} u_{i+1} v_{i+2}}{b_i u_{i+1}} = \frac{a_{i+1}}{b_i} v_{i+1} - \frac{b_{i+1}}{b_i} v_{i+2} \quad , \text{ for } i \leq m-2 ,$$

and

$$v_{m-1} = \frac{a_m}{b_{m-1}} v_m .$$

Clearly $v_{m-1} > v_m$, and by induction $v_i > v_{i+1} \left(\frac{a_{i+1} - b_{i+1}}{b_i} \right) > v_i$.

Note that we can prove the same result if we suppose only that T is diagonally dominant with $a_1 > b_1$ and $a_m > b_{m-1}$.

One can characterize the decay of the element along a row away from the diagonal. Let $\bar{\alpha}_i$ and $\bar{\beta}_i$ be such that $u_i = \bar{\alpha}_{i-1} u_{i-1}$, $v_i = \left(\frac{1}{\bar{\beta}_{i-1}} \right) v_{i-1}$, $i \geq 2$. We have

$$\bar{\alpha}_i = \frac{a_i}{b_i} - \frac{b_{i-1}}{b_i} \frac{1}{\bar{\alpha}_{i-1}} \quad , \quad \bar{\alpha}_1 = \frac{a_1}{b_1}$$

$$\bar{\beta}_i = \frac{a_{i+1}}{b_i} - \frac{b_{i+1}}{b_i} \frac{1}{\bar{\beta}_{i+1}} \quad , \quad \bar{\beta}_{m-1} = \frac{a_m}{b_{m-1}} .$$

In the general case we do not know the solution of the recurrences (which are simply the recurrences for computing the elements of T^{-1}), but the previous discussion gives us the bounds

$$\bar{\alpha}_i > \frac{a_i - b_{i-1}}{b_i} > 1 ,$$

$$\bar{\beta}_i > \frac{a_{i+1} - b_{i+1}}{b_i} > 1 .$$

In particular, we have, for $i > j$,

$$(T^{-1})_{ij} = \frac{1}{\bar{\alpha}_{i-1} \cdots \bar{\alpha}_j} (T^{-1})_{ii} \leq \frac{(T^{-1})_{ii}}{\prod_{k=j}^{i-1} \left(\frac{a_k - b_{k-1}}{b_k} \right)} .$$

If $\frac{1}{\rho} = \min_{k \geq 2} \left(\frac{a_k - b_{k-1}}{b_k} \right)$ we find, for $i > j$,

$$(T^{-1})_{ij} \leq (T^{-1})_{ii} \rho^{i-j} \quad , \quad \rho < 1 .$$

This latter bound is not very sharp. For example, for the matrix T with $a_i = 4$, $i = 1, \ldots, m$ and $b_i = 1$, $i = 1, \ldots, m-1$, which will be of interest later, we get $\rho = 1/3$. But for this case

$$\bar{\alpha}_1 = 4 , \quad \bar{\alpha}_i = 4 - \frac{1}{\bar{\alpha}_{i-1}} \quad , \quad i \geq 2 .$$

The $\bar{\alpha}_i$ form a decreasing sequence that converges very quickly towards $2 + \sqrt{3} \approx 3.732$, which corresponds to a reduction factor of $1/(2+\sqrt{3}) \approx 0.2679$, which is considerably less than $1/3$. Of course if the a_i's and b_i's are constant, we could construct the inverse in another way from the eigenvalues and eigenvectors of T, which are known in this case.

It is of importance to observe that if T is strictly diagonally dominant the elements of the inverse decrease strictly away from the diagonal -- the stronger the diagonal dominance the faster the decay. This suggests the following means for approximating the inverse of T with a matrix of small bandwidth.

If A is any matrix, denote by $\mathbf{B}(A,q)$ the band matrix consisting of the $2q+1$ main diagonals of A. For a banded approximation $\tilde{T}_2$ to the inverse of T we consider

$$\tilde{T}_2 = \mathbf{B}(T^{-1},q) \tag{10}$$

with q small, say 1 or 2.

3.3 Approximation from Cholesky factors

Another way of approximating T^{-1} is to use the Cholesky factorization of T,

$$T = U^T U ,$$

with

$$U^T = \begin{pmatrix} \gamma_1 & & & \\ -\delta_1 & \gamma_2 & & 0 \\ & \ddots & \ddots & \\ & & -\delta_{m-2} & \gamma_{m-1} \\ & & & -\delta_{m-1} \quad \gamma_m \end{pmatrix}$$

a lower bidiagonal matrix. We have

$$\gamma_1^2 = a_1 \quad , \ \gamma_1 \delta_1 = b_1 \ ,$$
$$\delta_{i-1}^2 + \gamma_i^2 = a_i \ , \ \gamma_i \delta_i = b_i \ , \ i \geq 2 \ .$$

The δ_i's are positive and the diagonal dominance of T implies

$$\delta_i < \gamma_i \quad , \quad 1 \leq i \leq m-1 \ .$$

The matrix U^{-T} is lower triangular and dense. We denote

$$U^{-T} = \begin{pmatrix} \frac{1}{\gamma_1} & & & \\ \zeta_1 & \frac{1}{\gamma_2} & & 0 \\ \eta_1 & \zeta_2 & \frac{1}{\gamma_3} & \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \eta_{m-2} \quad \zeta_{m-1} & \frac{1}{\gamma_m} \end{pmatrix} .$$

It is easy to see that the elements of U^{-T} can be computed diagonal by diagonal, since

$$\zeta_i = \frac{\delta_i}{\gamma_i \gamma_{i+1}} \qquad 1 \le i \le m-1$$
$$\eta_i = \frac{\delta_i \zeta_{i+1}}{\gamma_i} \qquad 1 \le i \le m-2 ,$$

and so on. We note also that U^{-T} can be generated diagonal by diagonal by taking successive terms of its Neumann series in U^T.

We have the following result similar to the one for the inverse of T.

Lemma 4. *For each row, the elements of U^{-T} decrease away from the diagonal.*

Proof. Since $\frac{\delta_i}{\gamma_i} < 1$ we have $\eta_{i-1} < \zeta_i < \frac{1}{\gamma_{i+1}}$; the proof is the same for the other elements.

As an approximation for U^{-T} we can, therefore, take $\mathbf{B}(U^{-T},k)$ with k small. As an approximation for T^{-1} we can use correspondingly

$$\tilde{T}_3 = \mathbf{B}(U^{-1},k)\mathbf{B}(U^{-T},k) . \tag{11}$$

Note that $\tilde{T}_3$ is positive definite. If $k=1$, $\tilde{T}_3$ is tridiagonal, with

$$\tilde{T}_3 = \begin{pmatrix} \frac{1}{\gamma_1^2} + \zeta_1^2 & \frac{\zeta_1}{\gamma_2} & & \\ \frac{\zeta_1}{\gamma_2} & \frac{1}{\gamma_2^2} + \zeta_2^2 & \frac{\zeta_2}{\gamma_3} & \\ & \cdot & \cdot & \cdot \end{pmatrix} .$$

Unless the Cholesky decomposition is needed explicitly, it is necessary to compute only the square of the γ_i's to obtain $\tilde{T}_3$, because

$$\frac{\zeta_i}{\gamma_{i+1}} = \frac{b_i}{\gamma_i^2 \gamma_{i+1}^2} \quad , \quad \zeta_i^2 = \frac{a_{i+1} - \gamma_{i+1}^2}{\gamma_i^2 \gamma_{i+1}^2} .$$

Thus one obtains $\tilde{T}_3$ directly from a_i, b_i, and γ_i^2.

Note that $T\tilde{T}_3$ is the five diagonal matrix

$$T\tilde{T}_3 = \begin{pmatrix} 1 & -b_2u_1v_3 & b_2u_1v_2 & & \\ -b_2u_1v_3 & 1 & -b_3u_2v_4 & b_3u_2v_3 & \\ b_2u_1v_2 & -b_3u_2v_4 & 1 & -b_4u_3v_3 & b_4u_3v_4 \\ & & \cdot & \cdot & \cdot \end{pmatrix} .$$

Since the u_iv_j are expected to be small, $\tilde{T}_3$ can be expected to be a good approximation to T^{-1}.

3.4 Polynomial approximation

A classical way to obtain an approximation of T^{-1} is to use a polynomial expansion in powers of T. For convenience let D_T be the diagonal of T and denote

$$\bar{T} = T - D_T .$$

Then

$$T^{-1} = (I + D_T^{-1}\bar{T})^{-1}D_T^{-1} .$$

Since T is strictly diagonally dominant, the corresponding Jacobi iteration is convergent, which implies that the eigenvalues of $D_T^{-1}\bar{T}$ (which are real) are contained in (-1,+1) (see for example [12],[21]). Thus one can write

$$(I + D_T^{-1}\bar{T})^{-1} = \sum_{k=0}^{\infty}(-1)^k(D_T^{-1}\bar{T})^k ,$$

the series being convergent.

Of course, the powers of $D_T^{-1}\bar{T}$ contain more and more nonzero diagonals as k increases. As an approximate inverse we can take simply the first few terms (which are the sparsest ones)

$$\tilde{T}_{4,1} = D_T^{-1} - D_T^{-1}\bar{T}D_T^{-1}$$

or

$$\tilde{T}_{4,2} = D_{\bar{T}}^{-1} - D_{\bar{T}}^{-1}\bar{T}D_{\bar{T}}^{-1} + D_{\bar{T}}^{-1}\bar{T}D_{\bar{T}}^{-1}\bar{T}D_{\bar{T}}^{-1} .$$

It is well known, however, that if the eigenvalues of $D_{\bar{T}}^{-1}\bar{T}$ are not close enough to zero, the series could be a poor approximation. Better polynomial approximations can be found (cf. [14]).

Let $S = D_{\bar{T}}^{-1}\bar{T}$, and suppose we want to find a polynomial P of degree less than or equal to ν that minimizes $\|(I+S)^{-1} - P(S)\|_2$. Since S is similar to a symmetric matrix there exists a unitary matrix Q such that

$$S = Q\Theta Q^T ,$$

where Θ is a diagonal matrix whose elements are the eigenvalues of S.

We have

$$P(S) = QP(\Theta)Q^T ,$$

so that

$$\|(I+S)^{-1} - P(S)\|_2 = \|(I+\Theta)^{-1} - P(\Theta)\|_2 \le C_1 \max_i \| \frac{1}{1+\vartheta_i} - P(\vartheta_i) \| ,$$

where C_1 is constant and ϑ_i, $1 \le i \le m$, are the eigenvalues of S. To minimize the right-hand side (the minimum, of course, need not minimize also the left-hand side) we must find the polynomial approximation of $1/(1+x)$ on the set of eigenvalues ϑ_i of S. Instead we could solve the simpler problem of finding

$$\min \max_{\vartheta \in [\vartheta_1, \vartheta_m]} \| \frac{1}{1+\vartheta} - P(\vartheta) \| ,$$

where ϑ_1 (resp. ϑ_m) is the smallest (resp. largest) eigenvalue of S. The solution to this problem is given by the Chebyshev polynomials.

In general, however, even the extremal eigenvalues ϑ_1 and ϑ_m are not known; all one knows is that $-1 < \vartheta_1 \le \vartheta_m < 1$ holds. Since $1/(1+x)$ is discontinuous at $x = -1$, we could simply compute P to yield

$$\min_{P} \max_{\vartheta \in [0,1]} \| \frac{1}{1+\vartheta} - P(\vartheta) \| .$$

This should give a good result for the eigenvalues between 0 and 1, but a poor one for the smaller eigenvalues. For a first degree polynomial we obtain

$$P(\Theta) \approx 0.9412 - 0.4706\,\Theta .$$

As shall be seen later, one can often obtain a better approximation if additional information about the eigenvalues is available. In general, we shall be considering tridiagonal polynomial approximations $\tilde{T}$ to T^{-1} of the form

$$\tilde{T}_4 = \alpha D_T^{-1} + \beta D_T^{-1} \bar{T} D_T^{-1} , \tag{12}$$

where α and β are real numbers.

3.5 Comparison of approximations for the model problem

We now compare the above approximations for the model problem, for which in (7) $a_i = 4$, $i = 1, \ldots, m$, and $b_i = 1$, $i = 1, \ldots, m-1$. The case $m = 10$ is considered. The upper triangular part of the inverse T^{-1} as computed in double precision FORTRAN on an IBM 3081 by MATLAB [19] to four places is

$$\begin{bmatrix}
0.2679 & 0.0718 & 0.0192 & 0.0052 & 0.0014 & 0.0004 & \ldots \\
 & 0.2872 & 0.0770 & 0.0206 & 0.0055 & 0.0015 & \ldots \\
 & & 0.2886 & 0.0773 & 0.0207 & 0.0056 & \ldots \\
 & & & 0.2887 & 0.0773 & 0.0207 & \ldots \\
 & & & & 0.2887 & 0.0773 & \ldots \\
 & & & & & 0.2887 & \ldots \\
 & & & & & \ldots & \ldots
\end{bmatrix} .$$

For the different approximations $\tilde{T}_i$ to T^{-1} we get the following results (using MATLAB):

(i) Diagonal approximation (Sec. 3.1). $\tilde{T}_1$ is diagonal with $(\tilde{T}_1)_{ii} = \frac{1}{T_{ii}}$. For this case

$$\| \tilde{T}_1 - T^{-1} \|_2 \approx 0.2305 .$$

The eigenvalues of $\tilde{T}_1 T$ are approximately

0.5203, 0.5794, 0.6726, 0.7923, 0.9288, 1.0712, 1.2077, 1.3274, 1.4206, 1.4797.

(ii) Banded approximation from the exact inverse (Sec. 3.2). For the tridiagonal case $\tilde{T}_2 = \mathbf{B}(T^{-1},1)$ one has

$$\| \tilde{T}_2 - T^{-1} \|_2 \approx 0.0456 .$$

The eigenvalues of $\tilde{T}_2 T$ are approximately

0.8295, 0.8939, 0.9073, 0.9482, 0.9874, 1.0129, 1.0716, 1.0810, 1.1332, 1.1351.

For the five-diagonal case $\tilde{T}_2' = \mathbf{B}(T^{-1},2)$ one has

$$\| \tilde{T}_2' - T^{-1} \|_2 \approx 0.0104 .$$

The eigenvalues of $\tilde{T}_2' T$ are approximately

0.9633, 0.9665, 0.9781, 0.9871, 0.9993, 1.0007, 1.0129, 1.0257, 1.0271, 1.0393.

(iii) Approximation from Cholesky factors (Sec. 3.3). $\tilde{T}_3 = \mathbf{B}(U^{-1},1)\mathbf{B}(U^{-T},1)$, $T = U^T U$. For this case

$$\| \tilde{T}_3 - T^{-1} \|_2 \approx 0.0569 .$$

The eigenvalues of $\tilde{T}_3 T$ are approximately

0.8804, 0.8811, 0.9321, 0.9333, 1.0033, 1.0034, 1.0742, 1.0756, 1.1283, 1.1290.

The norms are a little greater than for (ii), but the eigenvalues are more clustered around 1. If we take $\tilde{T}_3' = \mathbf{B}(U^{-1},2)\mathbf{B}(U^{-T},2)$ we have

$$\| \tilde{T}_3' - T^{-1} \|_2 \approx 0.0134 ,$$

and the eigenvalues of $\tilde{T}_3' T$ are approximately

0.9695, 0.9731, 0.9731, 0.9887, 1.0002, 1.0002, 1.0118, 1.0274, 1.0275, 1.0311.

(iv) Polynomial approximations (Sec. 3.4). $\tilde{T}_4 = D_T^{-1} - D_T^{-1}\bar{T}D_T^{-1}$. For this case

$$\| \tilde{T}_4 - T^{-1} \|_2 \approx 0.1106 .$$

The eigenvalues of $\tilde{T}_4 T$ are approximately

0.7698, 0.7698, 0.8231, 0.8231, 0.8928, 0.8928, 0.9569, 0.9569, 0.9949, 0.9949.

Note that all the eigenvalues are less than 1 and occur doubly in pairs. That this should be the case is seen from the relationship

$$\tilde{T}_4 T = I - D_T^{-1}\bar{T}D_T^{-1}\bar{T} .$$

The eigenvalues of $\tilde{T}_4 T$ are $1-\mu_i^2$, where μ_i is an eigenvalue of $D_T^{-1}\bar{T}$, which is the Jacobi iteration matrix. For the T in (7), $D_T^{-1}\bar{T}$ has eigenvalues $\pm\mu_i$. If we take $\tilde{T}_4' = 0.9412\, D_T^{-1} - 0.4706\, D_T^{-1}\bar{T}D_T^{-1}$, then

$$\| \tilde{T}_4' - T^{-1} \|_2 \approx 0.1888 .$$

The eigenvalues of $\tilde{T}_4' T$ are approximately

0.6071, 0.6600, 0.7367, 0.8232, 0.9053, 0.9723, 1.0186, 1.0448, 1.0559, 1.0587.

A good result is obtained for the model problem by a Chebyshev approximation over [-0.5,0.5], which gives

$$\tilde{T}_4'' = 1.1429\, D_T^{-1} - 1.1429\, D_T^{-1}\bar{T}D_T^{-1}$$

$$\| \tilde{T}_4'' - T^{-1} \|_2 \approx 0.0577 .$$

The eigenvalues of $\tilde{T}_4'' T$ are approximately

0.8799, 0.8799, 0.9407, 0.9407, 1.0204, 1.0204, 1.0936, 1.0936, 1.1371, 1.1371.

The eigenvalues for all the above cases are tabulated in Fig. 1 in a format that permits a rough comparison of their distributions. The eigenvalues are

rounded to two decimal places, and the least significant digit is entered in the column corresponding to the first digit(s).

It is evident that for this model problem the banded approximations from the exact inverse (ii) and the approximations from Cholesky factors (iii) give better approximations to T^{-1} than the polynomial expansions (iv). It would be of interest to know if the same results would hold for matrices T of larger bandwidth.

	.5	.6	.7	.8	.9	1.0	1.1	1.2	1.3	1.4
$\mathcal{T}_1 T$	2,8	7	9		3	7		1	3	2,8
$\mathcal{T}_2 T$				3,9	1,5,9	1,7,8	3,4			
$\mathcal{T}'_2 T$					6,7,8,9	0,0,1,3,3,4				
$\mathcal{T}_3 T$				6,6	3,3	0,0,7,8	3,3			
$\mathcal{T}'_3 T$					7,7,7,9	0,0,1,3,3,3				
$\mathcal{T}_4 T$			7,7	2,2,9,9	6,6,9,9					
$\mathcal{T}'_4 T$		1,6	4	2	1,7	2,4,6,6				
$\mathcal{T}''_4 T$				6,6	4,4	2,2,9,9	4,4			

Fig. 1. *Tabular display of eigenvalue distributions.*

4. Block preconditionings for the two-dimensional case

Using the preceding results we now are able to define some block preconditioning techniques for the two-dimensional problem. For this case the D_i are tridiagonal, and our goal is to keep the Δ_i, $i \geq 2$, in (4b) tridiagonal, or possibly of slightly greater bandwidth. For the preconditionings discussed below, only the Cholesky factors L_i of the Δ_i are actually stored for computational purposes, corresponding to (6).

4.1 The block preconditionings

4.1.1 BDIA

The diagonal approximation (8) is used; Λ_{i-1} is diagonal with

$$(\Lambda_{i-1})_{jj} = \frac{1}{(\Delta_{i-1})_{jj}}.$$

The Δ_i's are tridiagonal matrices at each stage differing from D_i only in their diagonal elements.

4.1.2 INV(1)

The banded approximation (10) from the exact inverse is used,

$$\Lambda_{i-1} = B(\Delta_{i-1}^{-1}, 1) .$$

Each of the Δ_i's are tridiagonal. At each stage we compute two vectors u and v and use them to obtain the three main diagonals of Δ_{i-1}^{-1}. We then compute and store the Cholesky factors of Δ_i. $2N$ words of storage are needed for M, as in BDIA. We do not consider here keeping more diagonals in the approximation to Δ_{i-1}^{-1} for this case, as the particularly simple expression in Theorem 2 becomes

more complex if the Δ_i's have more than 3 diagonals.

4.1.3 CHOL(q)

We use (11),

$$\Lambda_{i-1} = \mathbf{B}(U_{i-1}^{-1}, q)\mathbf{B}(U_{i-1}^{-T}, q) ,$$

where $\Delta_{i-1} = U_{i-1}^T U_{i-1}$, with U_{i-1} an upper triangular matrix. At each stage we compute U_{i-1}, which is (except possibly for $i=2$) a matrix with $q+1$ nonzero main diagonals. The first $q+1$ diagonals of U_{i-1}^{-1} can be computed diagonalwise starting from the main diagonal. Since Λ_{i-1} is a symmetric matrix of bandwidth $2q+1$, approximately $(q+1)\sum_{i=2}^{n} m_i + 2m_1$ words of storage are needed for Δ_i. CHOL(q) is a special case of the following method proposed by Underwood [20] in a slightly different setting.

4.1.4 UND(p,q)

For this case

$$\Lambda_{i-1} = \mathbf{B}(\mathbf{B}(U_{i-1}^{-1}, q-1)\mathbf{B}(U_{i-1}^{-T}, q-1), 2p-1) ,$$

with $q \geq p$. One computes the q main diagonals of U_{i-1}^{-T}, but then stores only the $2p-1$ main diagonals of the product to form Λ_{i-1}. More information about U_{i-1}^{-T} is used here than in CHOL(q). The storage needed is $p\sum_{i=2}^{n} m_i + 2m_1$. Note that UND($q,q$) $\equiv$ CHOL($q-1$).

4.1.5 POL(α,β)

We use the polynomial approximations defined in Sec. 3.4,

$$\Delta_{i-1} = D_{T,i-1} + \overline{T}_{i-1}$$

$$\Lambda_{i-1} = \alpha D_{T,i-1}^{-1} + \beta D_{T,i-1}^{-1} \overline{T}_{i-1} D_{T,i-1}^{-1} .$$

Each Δ_i is tridiagonal. Different values of α and β are used. The storage requirements are the same as for BDIA and INV(1).

4.2 Properties of the Δ_i

Now we study the properties of the Δ_i in order to prove that all of the methods described above can be carried out (i.e., we prove that the Δ_i satisfy hypothesis (H2) placed on T).

Theorem 3. *Under Hypothesis (H1) each Δ_i computed by BDIA, INV(1), CHOL(q), UND(p,q), and POL(α,β) with $\beta \leq 0$, $0 < \alpha \leq 1$, $\beta + \alpha \geq 0$ is strictly diagonally dominant with positive diagonal elements and negative off diagonal elements.*

Proof. This can be proved by induction using the same techniques as in Lemma 1. As the proof is essentially the same for all cases, we carry it out only for CHOL(q).

Let

$$B = \begin{bmatrix} B_1 & -C^T \\ -C & B_2 \end{bmatrix}$$

be a positive definite M-matrix with B_1 and B_2 square, and let $B_1 = L_{B_1} L_{B_1}^T$ be the Cholesky decomposition of B_1. Denote

$$L_{B_1}^{-1} = \tilde{L}_{B_1}^{-1} + R_{B_1} ,$$

where $\tilde{L}_{B_1}^{-1}$ contains the $q+1$ diagonals of $L_{B_1}^{-1}$ that are kept for the approximation, and R_{B_1} contains the remaining diagonals. Under hypothesis (H1) both $\tilde{L}_{B_1}^{-1}$ and R_{B_1} are positive. From Lemma 1 we know that $B_2 - CL_{B_1}^{-T}L_{B_1}^{-1}C^T$ is strictly diagonally dominant. We have

$$B_2 - CL_{B_1}^{-T}L_{B_1}^{-1}C^T = B_2 - C\tilde{L}_{B_1}^{-T}\tilde{L}_{B_1}^{-1}C^T - C(\tilde{L}_{B_1}^{-T}R_{B_1} + R_{B_1}^T\tilde{L}_{B_1}^{-1} + R_{B_1}^T R_{B_1})C^T .$$

The last matrix on the right is positive, which implies that $B_2 - C\tilde{L}_{B_1}^{-T}\tilde{L}_{B_1}^{-1}C^T$ is more strongly diagonally dominant than is $B_2 - CL_{B_1}^{-T}L_{B_1}^{-1}C^T$. The desired result for CHOL(q) then follows by induction, taking $B_1 = D_1$, the first diagonal block of A.

4.3 Modified block preconditionings

It is known that the incomplete Cholesky decomposition can be modified to yield a better approximation to A in some cases. The modified incomplete Cholesky decomposition is obtained by computing the remainder R at each stage and subtracting it from the diagonal of M, making the row sums of M equal to the row sums of A. This gives an improvement of the condition number of $M^{-1}A$ for the natural ordering of the unknowns and for A diagonally dominant [7],[13].

As noted previously, the remainder R is a block diagonal matrix whose elements are

$$R_1 = 0$$

$$R_i = \Delta_i - D_i + A_i\Delta_{i-1}^{-1}A_i^T = A_i(\Delta_{i-1}^{-1} - \Lambda_{i-1})A_i^T \quad , \quad 2 \le i \le n .$$

Thus Δ_{i-1}^{-1} must be available if R_i is to be computed.

4.3.1 MINV(1)

For the case of INV(1), Δ_{i-1}^{-1} is readily available, thus it is feasible to define MINV(1), the modified form of INV(1). At each stage, compute the two vectors u and v, from which Δ_{i-1}^{-1} can be obtained. Form the product $R_i = A_i[\Delta_{i-1}^{-1} - \mathbf{B}(\Delta_{i-1}^{-1},1)]A_i^T$, which is a matrix with positive elements except for the 3 main diagonals, which are zero. Then subtract from $D_i - A_i\mathbf{B}(\Delta_{i-1}^{-1},1)A_i^T$ the diagonal matrix made up of the row sums of R_i. Each Δ_i, so modified, gives a remainder with a zero row sum. We note that from Hypothesis (H1) it follows that the remainder matrix is non-positive definite, so that the eigenvalues of $M^{-1}A$ are greater than or equal to 1 for MINV(1).

Theorem 4. *Under Hypothesis (H1) each Δ_i given by MINV(1) is a strictly diagonally dominant matrix with positive diagonal elements and negative off diagonal elements.*

Proof. Consider

$$\begin{pmatrix} B_1 & -C^T \\ -C & B_2 \end{pmatrix}.$$

Let $S_2 = C[B_1^{-1} - \mathbf{B}(B_1^{-1},1)]C^T$ and let R_2 be the diagonal matrix of row sums of S_2. Since $B_1^{-1} \geq 0$, the elements of S_2 and hence of R_2 are positive. Note that $B_2 - C\mathbf{B}(B_1^{-1},1)C^T - R_2$ has the same row sums as $B_2 - C[\mathbf{B}(B_1^{-1},1)]C^T - S_2 = B_2 - CB_1^{-1}C^T$. This, together with the positivity of the elements, shows that $B_2 - C\mathbf{B}(B_1^{-1},1)C^T - R_2$ is diagonally dominant.

4.3.2 MUND(p,q)

For the other block preconditionings there is no simple way to know directly the row sums of R_i without first computing Δ_i^{-1}. However, in UND(p,q) with $q>p$ a part of the remainder is available and can be subtracted from the diagonal. Recall that

$$\Delta_{i-1} = L_{i-1}L_{i-1}^T$$
$$R_i = A_i[\Delta_{i-1}^{-1} - \mathbf{B}(\mathbf{B}(L_{i-1}^{-T},q-1)\mathbf{B}(L_{i-1}^{-1},q-1),2p-1)]\,.$$

Denote by $\tilde{L}_{i-1}^{-1} = \mathbf{B}(L_{i-1}^{-1},q-1)$ the q diagonals of the inverse of L_{i-1} that are computed, and by Q_{i-1} the diagonals that are not computed

$$L_{i-1}^{-1} = \tilde{L}_{i-1}^{-1} + Q_{i-1}\,.$$

Then

$$R_i = A_i[\tilde{L}_{i-1}^{-T}\tilde{L}_{i-1}^{-1} + \tilde{L}_{i-1}^{-T}Q_{i-1} + Q_{i-1}^T\tilde{L}_{i-1}^{-1} + Q_{i-1}^TQ_{i-1} - \mathbf{B}(\tilde{L}_{i-1}^{-T}\tilde{L}_{i-1}^{-1},2p-1)]A_i^T\,.$$

We can obtain $\tilde{L}_{i-1}^{-T}\tilde{L}_{i-1}^{-1} - \mathbf{B}(\tilde{L}_{i-1}^{-T}\tilde{L}_{i-1}^{-1},2p-1)$, since it is made up of the diagonals of the product that are not kept in the algorithm. Thus, instead of discarding these diagonals we could subtract their row sums from the main diagonal. This constitutes the algorithm MUND(p,q): Compute q diagonals of L_i^{-1}. Form the product $\tilde{L}_{i-1}^{-T}\tilde{L}_{i-1}^{-1}$. Use the $2p-1$ main diagonals to form $D_i - A_i\mathbf{B}(\tilde{L}_{i-1}^{-T}\tilde{L}_{i-1}^{-1},2p-1)A_i^T$. Let S_{i-1} be the matrix made up of the $q-p$ outer diagonals of $\tilde{L}_{i-1}^{-T}\tilde{L}_{i-1}^{-1}$. Compute the row sums of $A_iS_{i-1}A_i^T$ and subtract them from the diagonal of $D_i - A_i\mathbf{B}(\tilde{L}_{i-1}^{-T}\tilde{L}_{i-1}^{-1},2p-1)A_i^T$ to obtain Δ_i.

Theorem 5. *Under Hypothesis (H1) each Δ_i given by MUND(p,q) is a strictly diagonally dominant matrix with positive diagonal elements and negative off-diagonal ones.*

Proof. Along the same lines as for Theorem 4.

4.4 Higher dimensions

One can develop block incomplete Cholesky factorizations for three dimensional problems similarly, using, for example, incomplete instead of complete factorizations L_i for the Δ_i. It is planned to investigate these preconditionings in a subsequent study.

5.1 Numerical experiments

In this section we present the results of numerical experiments comparing the preconditionings for two dimensions that were introduced in the previous sections. Comparisons are made also with point preconditionings, which for convenience we recall first.

The first point preconditioning is IC(0), now termed IC(1,1), which was introduced by Meijerink and Van der Vorst [16],[17]. One chooses for preconditioning matrix

$$M = \hat{L}\hat{D}\hat{L}^T$$

where $\hat{D}$ is diagonal and $\hat{L}$ is lower triangular, with the same sparsity pattern as A. According to the notation of [16],[17], $\tilde{a}_i$ are the elements of $\hat{D}$ and

$$\hat{L}^T = \begin{bmatrix} \tilde{a}_1 & \tilde{b}_1 & & \tilde{c}_1 & \\ & \tilde{a}_2 & \tilde{b}_2 & & \tilde{c}_2 \\ & & \ddots & & \ddots \end{bmatrix}.$$

Denote by a_i, b_i, c_i the corresponding elements of A and by m the bandwidth of A. For IC(1,1) one has

$$\tilde{a}_i = \tilde{d}_i^{-1} = a_i - \tilde{b}_{i-1}^2 \tilde{d}_{i-1} - \tilde{c}_{i-m}^2 \tilde{d}_{i-m}$$

$$\tilde{b}_i = b_i$$

$$\tilde{c}_i = c_i \, .$$

This scheme requires the storage of only one N-vector, the $\tilde{d}_i$, in addition to A.

For IC(1,2) Meijerink and Van der Vorst allow one more outer diagonal

$$\hat{L}^T = \begin{bmatrix} \tilde{a}_1 & \tilde{b}_1 & & \tilde{e}_1 & \tilde{c}_1 & \\ & \tilde{a}_2 & \tilde{b}_2 & & \tilde{e}_2 & \tilde{c}_2 \\ & & \ddots & & & \ddots \end{bmatrix},$$

with

$$\tilde{a}_i = \tilde{d}_i^{-1} = a_i - \tilde{b}_{i-1}^2 \tilde{d}_{i-1} - \tilde{e}_{i-m+1}^2 \tilde{d}_{i-m+1} - \tilde{c}_{i-m}^2 \tilde{d}_{i-m}$$

$$\tilde{b}_i = b_i - \tilde{c}_{i-m+1} \tilde{d}_{i-m+1} \tilde{e}_{i-m+1}$$

$$\tilde{e}_i = -\tilde{c}_{i-1} \tilde{d}_{i-1} \tilde{b}_{i-1}$$

$$\tilde{c}_i = c_i \, .$$

Here, 3 N-vectors of storage are required.

For IC(1,3) one more outer diagonal is kept

$$\hat{L}^T = \begin{bmatrix} \tilde{a}_1 & \tilde{b}_1 & & \tilde{f}_1 & \tilde{e}_1 & \tilde{c}_1 & \\ & \tilde{a}_2 & \tilde{b}_2 & & \tilde{f}_2 & \tilde{e}_2 & \tilde{c}_2 \\ & & \ddots & & & \ddots & \end{bmatrix}$$

with

$$\tilde{a}_i = \tilde{d}_i^{-1} = a_i - \tilde{b}_{i-1}^2\tilde{d}_{i-1} - \tilde{f}_{i-m+2}^2\tilde{d}_{i-m+2} - \tilde{e}_{i-m+1}^2\tilde{d}_{i-m+1} - \tilde{c}_{i-m}^2\tilde{d}_{i-m}$$

$$\tilde{b}_i = b_i - \tilde{c}_{i-m+1}\tilde{d}_{i-m+1}\tilde{e}_{i-m+1} - \tilde{e}_{i-m+2}\tilde{d}_{i-m+2}\tilde{f}_{i-m+2}$$

$$\tilde{f}_i = -\tilde{e}_{i-1}\tilde{d}_{i-1}\tilde{b}_{i-1}$$

$$\tilde{e}_i = -\tilde{c}_{i-1}\tilde{d}_{i-1}\tilde{b}_{i-1}$$

$$\tilde{c}_i = c_i \ .$$

Four N-vectors of storage are required.

The preconditioning IC(2,4) introduce two more diagonals

$$\hat{L}^T = \begin{pmatrix} \tilde{a}_1 & \tilde{b}_1 & \tilde{h}_1 & & \tilde{g}_1 & \tilde{f}_1 & \tilde{e}_1 & \tilde{c}_1 & \\ & \tilde{a}_2 & \tilde{b}_2 & \tilde{h}_2 & & \tilde{g}_2 & \tilde{f}_2 & \tilde{e}_2 & \tilde{c}_2 \\ & & \ddots & \ddots & & \ddots & \ddots & \ddots & \ddots \end{pmatrix},$$

with

$$\tilde{a}_i = \tilde{d}_i^{-1} = a_i - \tilde{b}_{i-1}^2\tilde{d}_{i-1} - \tilde{h}_{i-2}^2\tilde{d}_{i-2} - \tilde{g}_{i-m+3}^2\tilde{d}_{i-m+3} - \tilde{f}_{i-m+2}^2\tilde{d}_{i-m+2} - \\ - \tilde{e}_{i-m+1}^2\tilde{d}_{i-m+1} - \tilde{c}_{i-m}^2\tilde{d}_{i-m}$$

$$\tilde{b}_i = b_i - \tilde{h}_{i-1}\tilde{d}_{i-1}\tilde{b}_{i-1} - \tilde{f}_{i-m+3}\tilde{d}_{i-m+3}\tilde{g}_{i-m+3} - \\ - \tilde{e}_{i-m+2}\tilde{d}_{i-m+2}\tilde{f}_{i-m+2} - \tilde{c}_{i-m+1}\tilde{d}_{i-m+1}\tilde{e}_{i-m+1}$$

$$\tilde{h}_i = -\tilde{e}_{i-m+3}\tilde{d}_{i-m+3}\tilde{g}_{i-m+3} - \tilde{c}_{i-m+2}\tilde{d}_{i-m+2}\tilde{f}_{i-m+2}$$

$$\tilde{g}_i = -\tilde{e}_{i-2}\tilde{d}_{i-2}\tilde{h}_{i-2} - \tilde{f}_{i-1}\tilde{d}_{i-1}\tilde{b}_{i-1}$$

$$\tilde{f}_i = -\tilde{c}_{i-2}\tilde{d}_{i-2}\tilde{h}_{i-2} - \tilde{e}_{i-1}\tilde{d}_{i-1}\tilde{b}_{i-1}$$

$$\tilde{e}_i = -\tilde{c}_{i-1}\tilde{d}_{i-1}\tilde{b}_{i-1}$$

$$\tilde{c}_i = c_i \ .$$

which requires 6 N-vectors of storage.

We consider also the modified versions of the IC preconditionings. The simplest one was introduced by Dupont, Kendall, and Rachford [7], which we denote by DKR. It is equivalent to MIC(1,1). This method allows the use of parameters,

but we choose to use it without parameters, since for practical problems it is almost impossible to know good parameters *a priori*.

DKR is the same as IC(1,1) except that

$$\tilde{d}_i^{-1} = a_i - \tilde{d}_{i-1}\tilde{b}_{i-1}(\tilde{b}_{i-1} + \tilde{c}_{i-1}) - \tilde{d}_{i-m}\tilde{c}_{i-m}(\tilde{c}_{i-m} + \tilde{b}_{i-m}) .$$

MIC(1,2) is the same as IC(1,2) except that

$$\begin{aligned}\tilde{d}_i^{-1} = a_i &- \tilde{b}_{i-1}^2\tilde{d}_{i-1} - \tilde{c}_{i-m}^2\tilde{d}_{i-m} - \tilde{e}_{i-m+1}^2\tilde{d}_{i-m+1} \\ &- \tilde{b}_{i-1}\tilde{e}_{i-1}\tilde{d}_{i-1} - \tilde{b}_{i-m+1}\tilde{e}_{i-m+1}\tilde{d}_{i-m+1} .\end{aligned}$$

MIC(1,3) is the same as IC(1,3) except that

$$\begin{aligned}\tilde{d}_i^{-1} = a_i &- \tilde{b}_{i-1}^2\tilde{d}_{i-1} - \tilde{f}_{i-m+2}^2\tilde{d}_{i-m+2} - \tilde{e}_{i-m+1}^2\tilde{d}_{i-m+1} \\ &- \tilde{c}_{i-m}^2\tilde{d}_{i-m} - \tilde{b}_{i-1}\tilde{f}_{i-1}\tilde{d}_{i-1} - \tilde{b}_{i-m+2}\tilde{f}_{i-m+2}\tilde{d}_{i-m+2} \\ &- \tilde{c}_{i-m+2}\tilde{f}_{i-m+2}\tilde{d}_{i-m+2} - \tilde{c}_{i-m}\tilde{f}_{i-m}\tilde{d}_{i-m} .\end{aligned}$$

Also included in our numerical comparisons is SSOR preconditioning. If $A = \Omega + E + E^T$, where Ω is diagonal and E is the (point) lower triangular part of A, then

$$M = \frac{1}{\omega(2-\omega)}(\Omega + \omega E)\Omega^{-1}(\Omega + \omega E^T) ,$$

where ω is the relaxation parameter. We shall give results also for the block version of SSOR (which in our case is line SSOR). For some cases, results will be given also for a 1-line Jacobi preconditioning (LJAC).

For a five diagonal matrix the work per iteration for each of the methods is given in Table 1. (For simplicity, the technique of [8] for reducing the work requirements of the conjugate gradient method is not incorporated here, since we wish only to compare the relative merits of the different preconditionings.)

Table 1

Work per iteration for the preconditionings

Preconditioning M	Mults.	Adds.	Divs.
I	11N	10N	
DIAG	11N	10N	N
IC(1,1)	15N	14N	
DKR	15N	14N	
SSOR	16N	14N	
IC(1,2),MIC(1,2)	19N	14N	
IC(1,3),MIC(1,3)	21N	18N	
IC(2,4)	25N	22N	
BSSOR,BDIA INV(1), MINV(1) CHOL(1), POL(α,β)	19N	17N	
CHOL(p), UND($p+1,q$) MUND($p+1,q$)			
$p=2$	21N	23N	8N
$p=3$	25N	27N	12N
$p=4$	29N	31N	16N
$p=5$	33N	35N	20N

Table 1 does not include the overhead operations required to construct M. If one carries out many iterations or solves several systems with different right-hand sides, then this overhead can usually be neglected. Specific cases are discussed in Section 5.2..

It should be noted that the quantities in Table 1 depend on the manner in which the program is written. For example, for $INV(1)$ there is no division, because we use Varga's implementation of Gauss elimination for tridiagonal

matrices, which stores the reciprocals of the diagonals [21]. In CHOL(p), factorization routines from LINPACK for banded matrices are used, for which some divisions are required [6]. Thus the entries in Table 1 should be considered as approximate, and as upper bounds in the case of the block methods.

Our implementation of the conjugate gradient algorithm requires 4 N-vectors of storage, plus 4 N-vectors for the matrix A and the right-hand side. If it is not necessary to save the right-hand side, then 1 N-vector of storage could be eliminated. The additional storage required for each of the different preconditionings M is given in Table 2.

Table 2

Storage required by the preconditionings

Preconditioning M	N-vectors of storage
IC(1,1),DKR	1
IC(1,2),MIC(1,2)	3
IC(1,3),MIC(1,3)	4
IC(2,4)	6
SSOR,BSSOR	0
BDIA,INV(1),MINV(1),POL(α,β)	2
CHOL(p),UND($p+1$,q),MUND($p+1$,q)	$p+1$

5.2 First test problem

The first test problem is the model problem

$$-\Delta u = f \qquad \text{in } \Omega \text{ the unit square } (0,1)\times(0,1)$$

with

$$u\big|_{\partial\Omega} = 0 .$$

We use the standard five point stencil on a square mesh with $h = (n+1)^{-1}$, $N = n^2$, and natural ordering to obtain the corresponding linear algebraic system (2). The experimental results are given for different values of h and different stopping criteria. An estimate of the condition number of $M^{-1}A$ is given for each of the preconditionings, as obtained from the conjugate gradient algorithm (cf. [3]), and for small dimension ($n = 10$) the complete spectrum of $M^{-1}A$ is visualized.

The computations were carried out in double precision FORTRAN on an IBM 3081. Unless otherwise noted the solution of the linear system is smooth (the right-hand side b in (2) corresponds to the solution $\xi_i(\xi_i-1)\eta_j(\eta_j-1)\exp(\xi_i\eta_j)$ at a point (ξ_i,η_j)), and the starting vector has random elements in [-1,1]. As the number of additions is roughly the same as the number of multiplications, we indicate only the work required for the multiplications. The divisions that may appear to be needed by some methods are not indicated, since they can be removed with alternative coding. In Table 3 are given the number of iterations and the corresponding total work per point required to achieve the stopping criterion $\|r^k\|_\infty / \|r^0\|_\infty \le 10^{-6}$, for the case $N = 2500$. The value $\omega = 1.7$ for SSOR and BSSOR is the observed optimal for each case to the nearest 0.1.

Table 3

Number of iterations and total work per point for $\|r^k\|_\infty / \|r^0\|_\infty \leq 10^{-6}$. Test problem 1, $N = 2500$.

M	# its.	work/N
I	109	1199
DIAG	109	1199
IC(1,1)	33	495
IC(1,2)	21	399
IC(1,3)	17	357
IC(2,4)	12	300
DKR	23	345
MIC(1,2)	17	323
MIC(1,3)	14	294
SSOR $\omega = 1$	40	640
SSOR $\omega = 1.7$	21	336
LJAC	80	1120
BSSOR $\omega = 1$	28	532
BSSOR $\omega = 1.7$	16	304
BDIA	22	418
POL(1,-1)	18	342
POL(0.9412,-0.4706)	21	399
POL(1.143,-1.143)	17	323
INV(1)	15	285
MINV(1)	11	209
CHOL(1)	16	304
CHOL(2)	12	252
CHOL(3)	9	225
CHOL(4)	8	232
CHOL(5)	7	231
UND(2,3)	15	255
UND(2,4)	15	255
UND(3,4)	11	231
UND(3,5)	11	231
UND(4,5)	9	225
UND(4,6)	9	225
UND(5,6)	7	203
MUND(2,3)	12	204
MUND(2,4)	10	170
MUND(2,5)	9	153
MUND(3,4)	10	210
MUND(3,5)	8	168
MUND(3,6)	8	168
MUND(4,5)	8	200
MUND(4,6)	7	175
MUND(5,6)	7	203

From Table 3, the following observations can be made.

(i) For the patterns chosen, the larger the number of diagonals in the incomplete Cholesky decomposition, the fewer the number of iterations required for convergence, as observed in [17] for the point preconditionings.

(ii) The modified versions of the preconditionings give better results (for this problem and ordering of the mesh points).

(iii) In general, there is a trade off between storage and execution speed, but if a low storage point-preconditioning is desired, DKR seems a good choice. SSOR can give good results, but an optimal parameter has to be found.

(iv) For methods of comparable storage the block methods give better results than point methods, both in terms of number of iterations and work requirements.

(v) For CHOL(p) it is not effective to go to values of p larger than $p=3$, and, as observed also in [2], to values of q beyond $q=p+1$ for UND(p,q). It is better to use the additional information given by UND(p,q) for larger q to obtain a modified version of the factorization for $q=p+1$.

(vi) The best polynomial, as expected, is POL(1.1429,-1.1429).

(vii) For this problem the best all-around preconditioning appears to be MINV(1), because it has very low storage requirements and gives almost the best work count -- approximately half of IC(1,2) and two thirds of MIC(1,2), which require more storage.

It is of interest to compare the methods for solving the test problem to only moderate accuracy, comparable to truncation error. Comparisons for the more interesting methods are given in Table 4, for which the stopping criterion has been reduced to $\|r^k\|_\infty / \|r^0\|_\infty \leq 10^{-4}$.

Table 4

Number of iterations and total work per point for $\|r^k\|_\infty / \|r^0\|_\infty \leq 10^{-4}$.
Test problem 1, $N = 2500$.

M	# its.	work/N
I	63	693
IC(1,1)	20	300
IC(2,4)	7	175
DKR	16	240
SSOR $\omega = 1.7$	13	208
BSSOR $\omega = 1.7$	10	190
INV(1)	9	171
MINV(1)	7	133
CHOL(1)	9	171
CHOL(5)	4	132

The conclusions drawn from Table 3 for the smaller residuals are in general unaffected.

In Table 5 are given the values of the smallest and largest eigenvalues of $M^{-1}A$ as estimated by the conjugate gradient algorithm, as well as the corresponding condition numbers.

Table 5

Extremal eigenvalues and condition number of $M^{-1}A$.
Test problem 1, $N = 2500$.

M	$\lambda_{min}(M^{-1}A)$	$\lambda_{max}(M^{-1}A)$	$\kappa(M^{-1}A)$
I	0.0076	7.992	1053
IC(1,1)	0.0128	1.206	94.0
IC(1,2)	0.033	1.179	35.6
IC(1,3)	0.049	1.131	23.2
IC(2,4)	0.091	1.138	12.5
DKR	1.003	15.36	15.3
MIC(1,2)	1.003	8.83	8.3
MIC(1,3)	1.006	6.19	6.15
SSOR $\omega = 1.$	0.0075	1.	132.5
SSOR $\omega = 1.7$	0.040	1.	25.1
LJAC	0.0038	1.99	527.
BSSOR $\omega = 1.$	0.0150	1.	66.8
BSSOR $\omega = 1.7$	0.074	1.	13.5
BDIA	0.024	1.023	42.6
POL(1,-1)	0.035	1.	28.7
POL(0.9412,-0.4706)	0.027	1.002	37.2
POL(1.143,-1.143)	0.043	1.023	23.8
INV(1)	0.059	1.073	18.2
MINV(1)	1.006	4.261	4.24
CHOL(1)	0.050	1.050	20.8
CHOL(2)	0.090	1.065	11.8
CHOL(3)	0.142	1.076	7.56
CHOL(4)	0.204	1.078	5.29
CHOL(5)	0.272	1.078	3.97
UND(2,3)	0.058	1.07	18.5
UND(2,4)	0.059	1.073	18.2
UND(2,5)	0.059	1.073	18.2
UND(3,4)	0.104	1.086	10.5
UND(3,5)	0.106	1.089	10.2
UND(4,5)	0.162	1.091	6.75
UND(4,6)	0.166	1.096	6.59
UND(5,6)	0.228	1.088	4.78
MUND(2,3)	0.102	1.242	12.2
MUND(2,4)	0.202	1.564	7.74
MUND(2,5)	0.380	2.024	5.33
MUND(3,4)	0.164	1.242	7.58
MUND(3,5)	0.291	1.518	5.22
MUND(3,6)	0.483	1.887	3.91
MUND(4,5)	0.234	1.221	5.21
MUND(4,6)	0.375	1.449	3.87
MUND(5,6)	0.309	1.197	3.88

It is seen that a considerable reduction in the condition number can be achieved using MINV(1) or, say, MUND(2,5), with only a low cost in storage.

In Table 6 are given the estimated condition numbers $\kappa(M^{-1}A)$ for different values of $n = \frac{1}{h} - 1$.

Table 6

Estimated condition number for different mesh sizes and exponent α of asymptotic dependence on $h = 1/(n+1)$. Test problem 1.

M	$\kappa(M^{-1}A)$				α
	$n=10$	$n=20$	$n=25$	$n=50$	
I	48.37	178.1	273.3	1053	2.00
IC(1,1)	5.10	16.59	25.	94	1.97
IC(1,2)	2.38	6.67	9.8	35.6	1.91
IC(1,3)	1.80	4.56	6.6	23.2	1.87
IC(2,4)	1.32	2.75	3.8	12.5	1.77
DKR	3.04	5.93	7.4	15.3	1.08
MIC(1,2)	1.84	3.36	4.2	8.3	1.01
MIC(1,3)	1.49	2.56	3.15	6.1	0.98
SSOR $\omega = 1.$	6.88	23.12	35.	132	1.97
LJAC	24.68	89.5	137.	527	2.00
BSSOR $\omega = 1.$	3.93	12.04	18.	66.7	1.94
BDIA	2.76	7.9	11.7	42.5	1.91
POL(1,-1)	2.09	5.52	8.	28.6	1.89
POL(0.9412,-0.4706)	2.5	7.	10.3	37.1	1.90
POL(1.143,-1.143)	1.86	4.7	6.7	23.8	1.88
INV(1)	1.61	3.74	5.3	18.2	1.83
MINV(1)	1.3	1.94	2.31	4.23	0.90
CHOL(1)	1.73	4.18	6.	20.8	1.85
CHOL(2)	1.32	2.65	3.65	11.85	1.75
CHOL(3)	1.14	1.93	2.53	7.54	1.62
CHOL(4)	1.06	1.55	1.95	5.28	1.48
CHOL(5)	1.026	1.34	1.61	3.98	1.34
UND(2,3)	1.63	3.8	5.4	18.52	1.83
UND(2,4)	1.62	3.75	5.33	18.24	1.83
UND(3,4)	1.26	2.42	3.3	10.47	1.71
UND(3,5)	1.25	2.39	3.24	10.24	1.71
UND(4,5)	1.12	1.8	2.33	6.73	1.57
UND(4,6)	1.11	1.77	2.28	6.54	1.56
UND(5,6)	1.05	1.47	1.82	4.8	1.44
MUND(2,3)	1.39	2.76	3.79	12.95	1.82
MUND(2,4)	1.29	2.1	2.72	7.74	1.55
MUND(2,5)	1.28	1.89	2.26	5.33	1.27
MUND(3,4)	1.18	1.97	2.58	7.55	1.59
MUND(3,5)	1.15	1.67	2.04	5.22	1.39
MUND(3,6)	1.14	1.6	1.85	3.9	1.11
MUND(4,5)	1.09	1.57	1.96	5.22	1.45
MUND(4,6)	1.07	1.43	1.68	3.8	1.21
MUND(5,6)	1.04	1.35	1.62	3.9	1.30

The quantity α is the estimated value, from the $n = 25$ and $n = 50$ data, of the exponent corresponding to the assumed asymptotic relationship $\kappa(M^{-1}A) \sim Ch^{-\alpha}$.

where C is a constant. It is known theoretically that for $M = I$ and $M = \mathrm{IC}(1,1)$ there holds $\kappa(M^{-1}A) = O(h^{-2})$ and that for $M = \mathrm{DKR}$, $\kappa(M^{-1}A) = O(h^{-1})$. These relationships can be observed as being indicated by the numerical experiments. We see that all the incomplete decompositions $\mathrm{IC}(p,q)$ seem to be $0(h^{-2})$, although the more diagonals that are taken the slower is the convergence to this asymptotic behavior. The MIC methods are $0(h^{-1})$.

For the block methods INV and CHOL the limiting value of α seems to be two, and for MINV one. The observed values of α for the range of h considered are smaller for the block methods than for the point methods with the same storage. It is difficult to assess from the results the order of the MUND methods; we believe that they are somewhere between 1 and 2, closer to 1 if more diagonals are used to form M. Finally, Table 6 shows that even for smaller values of n block methods give better reduction of the condition number than point methods.

It is well known that the rate of convergence of the conjugate gradient method depends not only on the condition number but on the distribution of the interior eigenvalues as well. It is therefore of interest to compare the eigenvalue spectra for the different methods. These are compared for $n = 10$ in Figs. 2-7. Each eigenvalue is designated by a vertical bar drawn at the appropriate abscissa value. This representation depicts in an easily observable manner the separation and clustering of the eigenvalues.

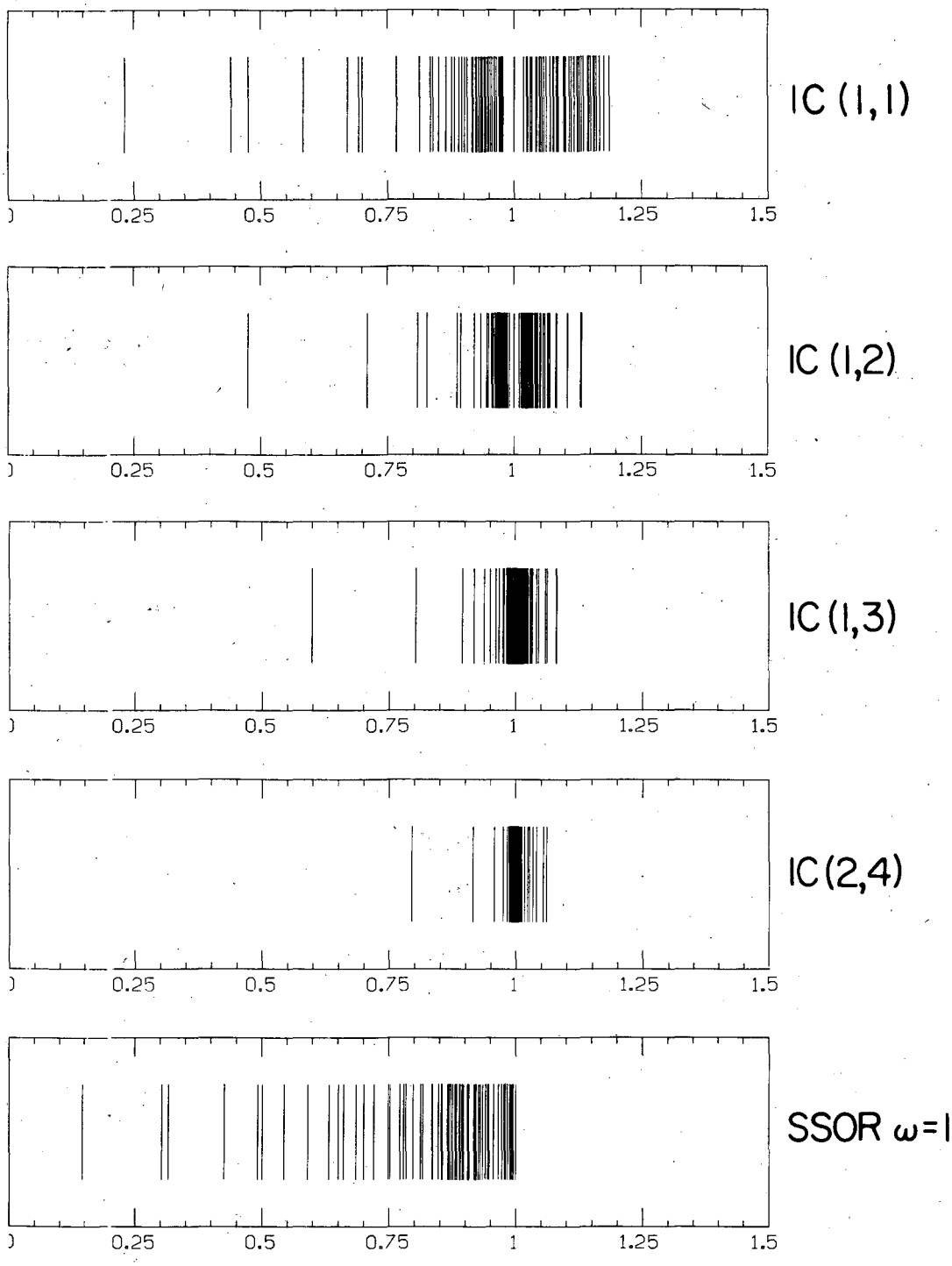


Fig. 2. *Spectra of $M^{-1}A$ for different preconditionings M. Test problem 1. $N = 100$.*

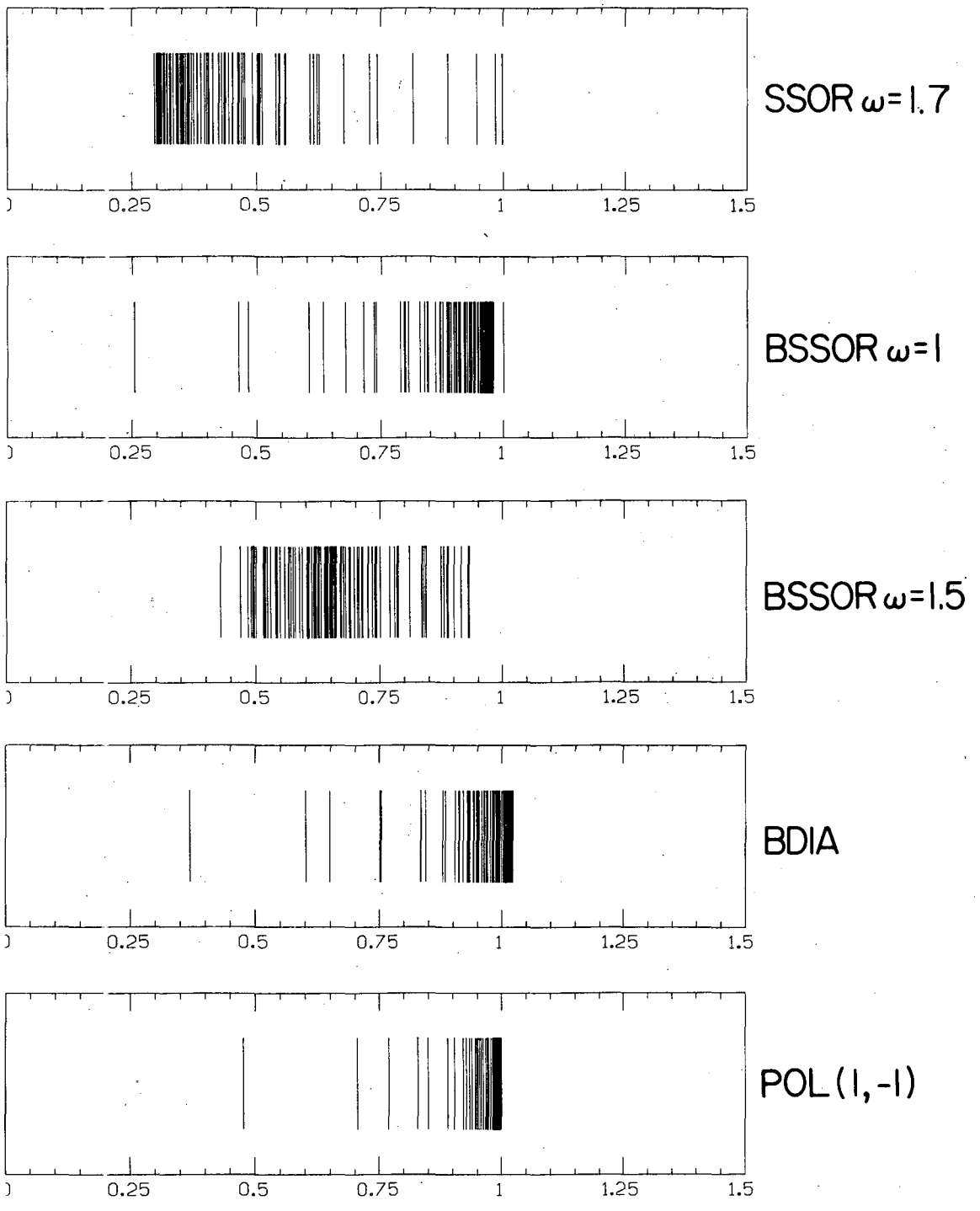

SSOR ω=1.7
BSSOR ω=1
BSSOR ω=1.5
BDIA
POL(1,-1)
0.25
0.5
0.75
1
1.25
1.5
XBL 832-8294

Fig. 2. *(cont.)*

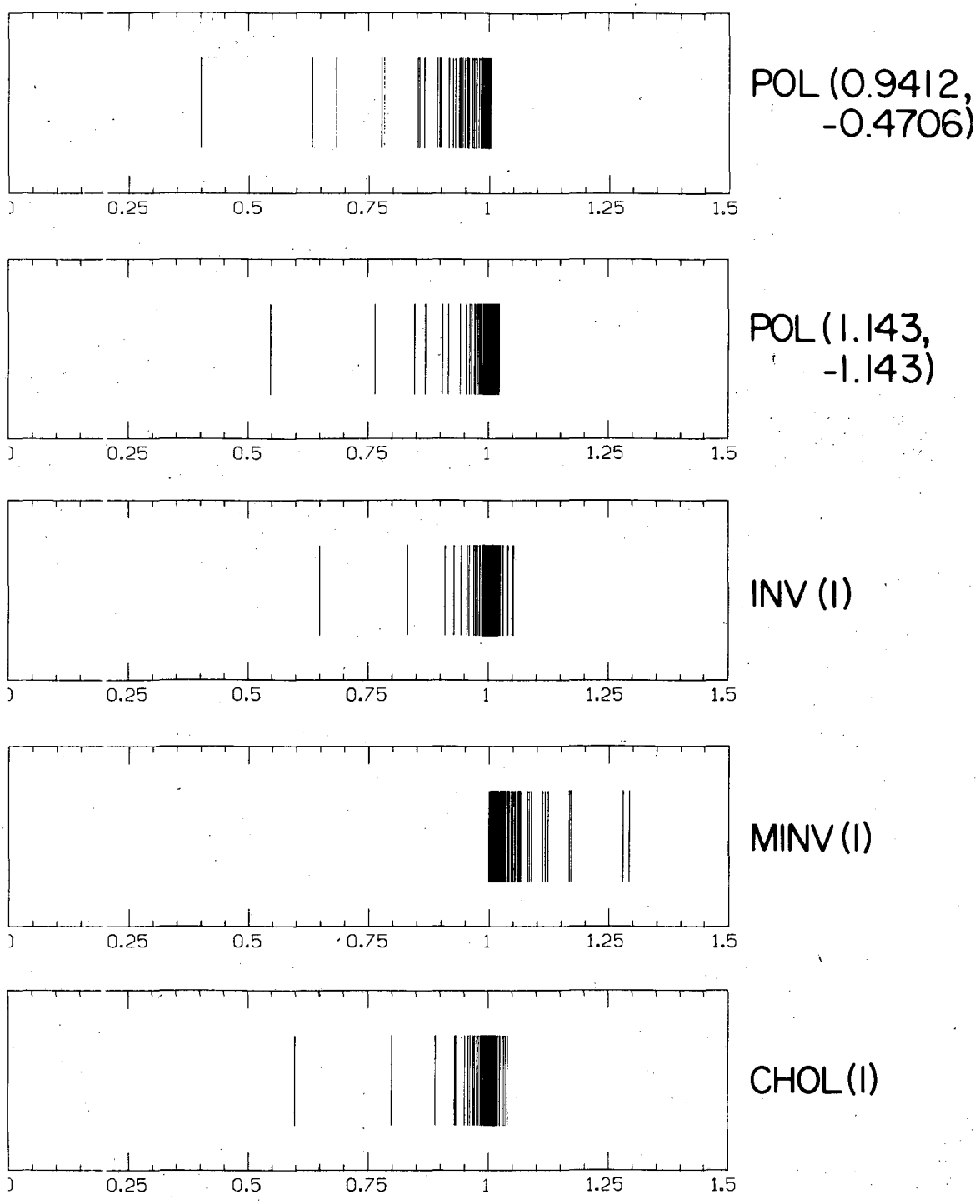

POL (0.9412, -0.4706)
POL (1.143, -1.143)
INV (1)
MINV (1)
CHOL (1)
0.25
0.5
0.75
1
1.25
1.5
XBL 832-8295

Fig. 2. *(cont.)*

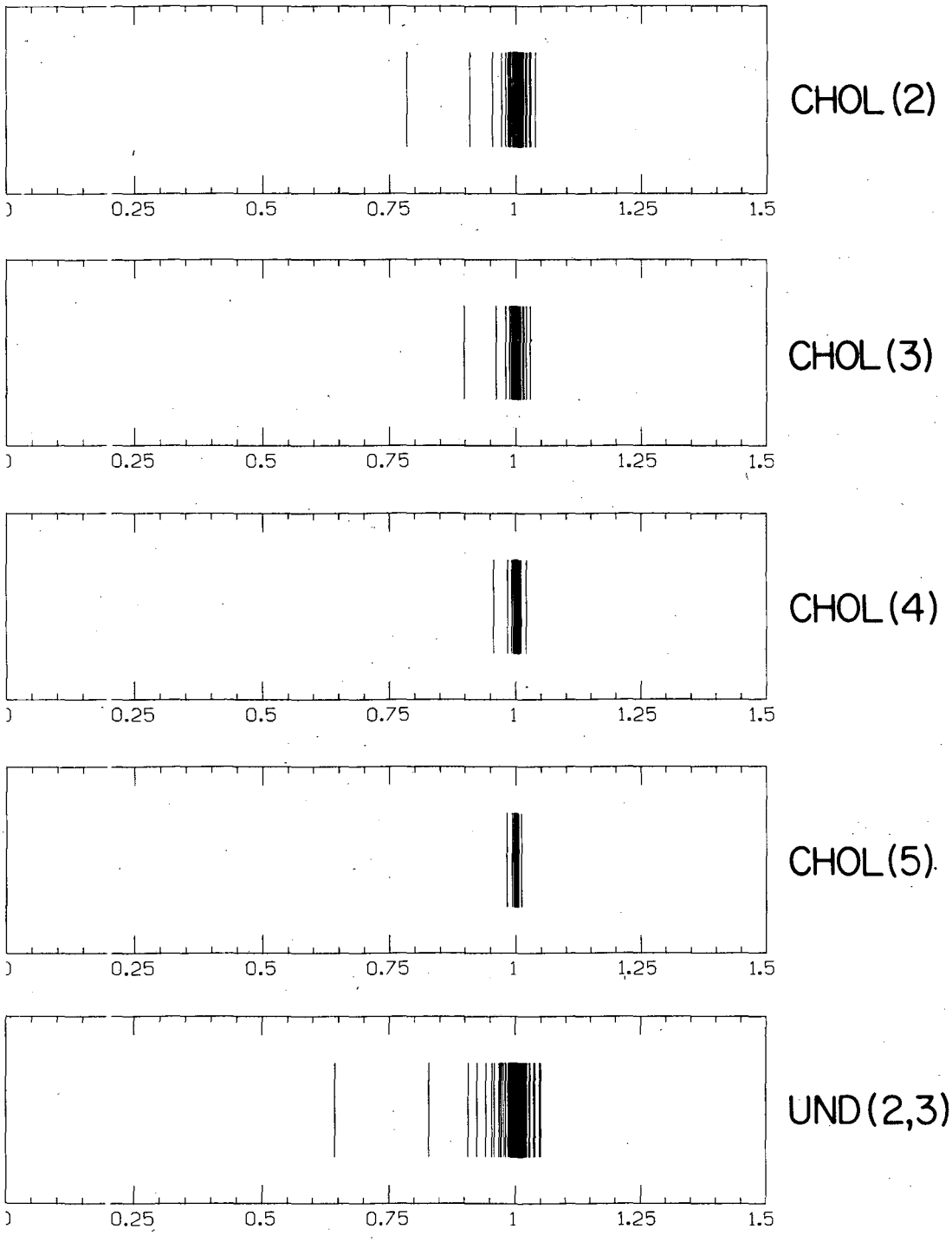


Fig. 2. *(cont.)*

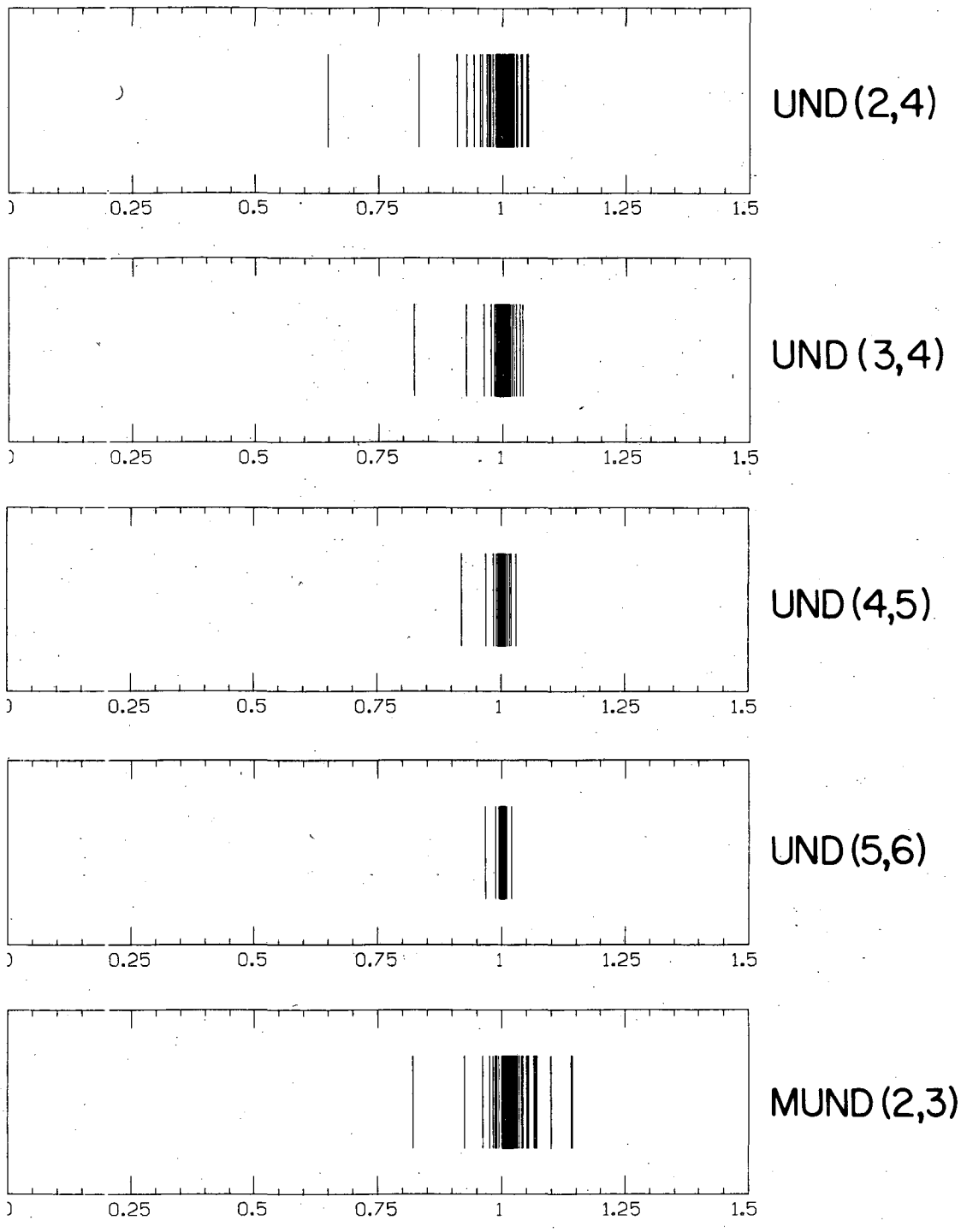

UND (2,4)
UND (3,4)
UND (4,5)
UND (5,6)
MUND (2,3)
0
0.25
0.5
0.75
1
1.25
1.5
XBL 832-8297

Fig. 2. *(cont.)*

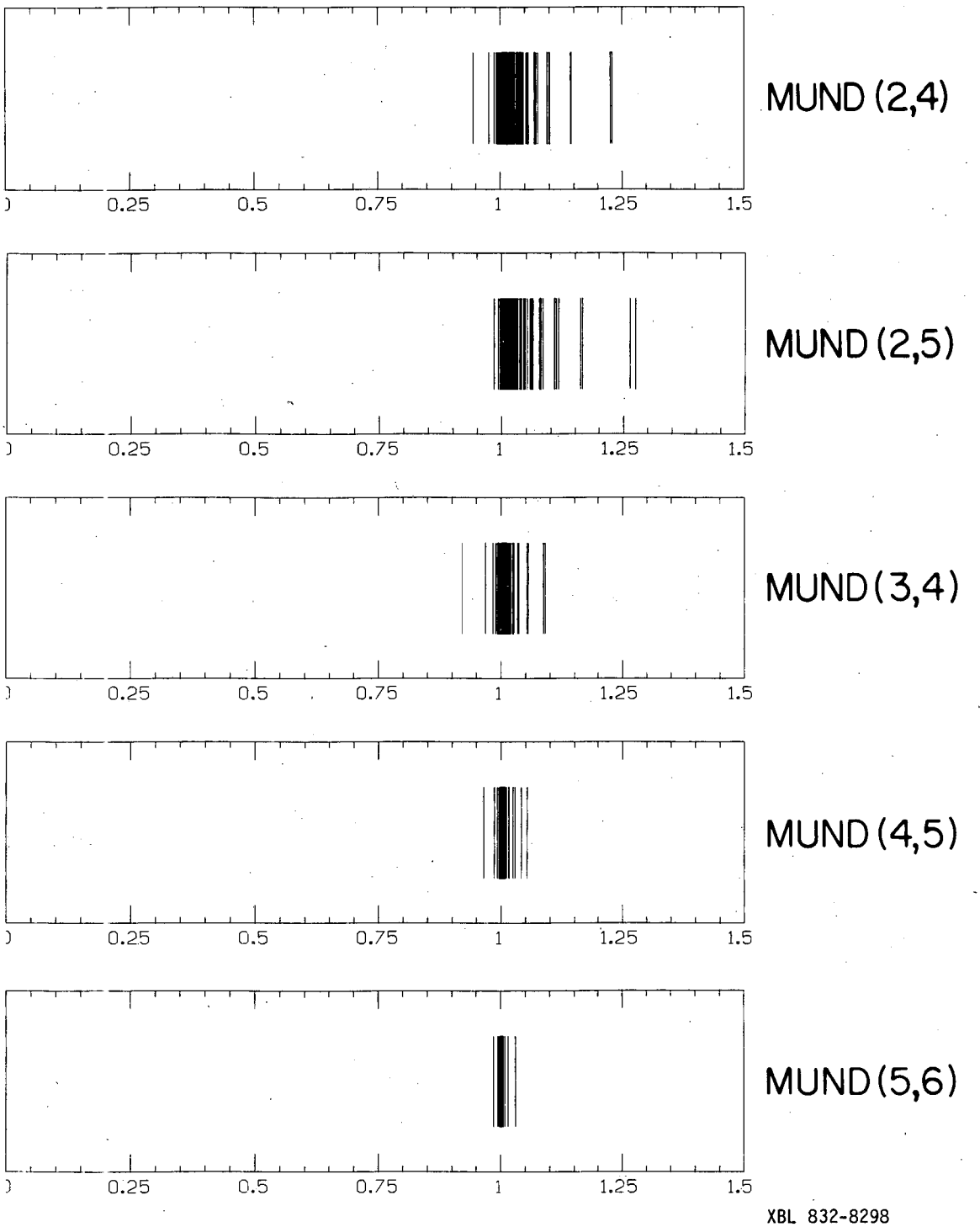

MUND (2,4)
MUND (2,5)
MUND (3,4)
MUND (4,5)
MUND (5,6)
0.25
0.5
0.75
1
1.25
1.5
XBL 832-8298

Fig. 2. *(cont.)*

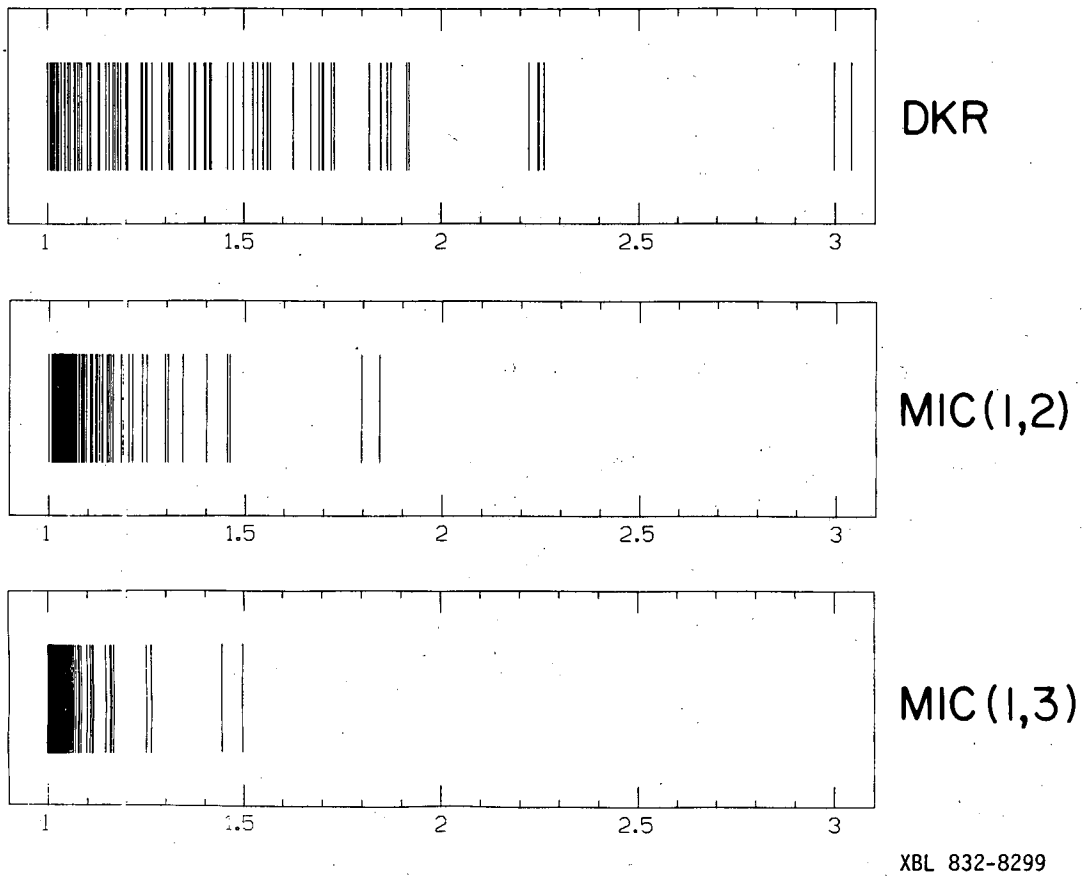


Fig. 3. *Spectra of $M^{-1}A$ for modified preconditionings. Test problem 1. $N = 100$.*

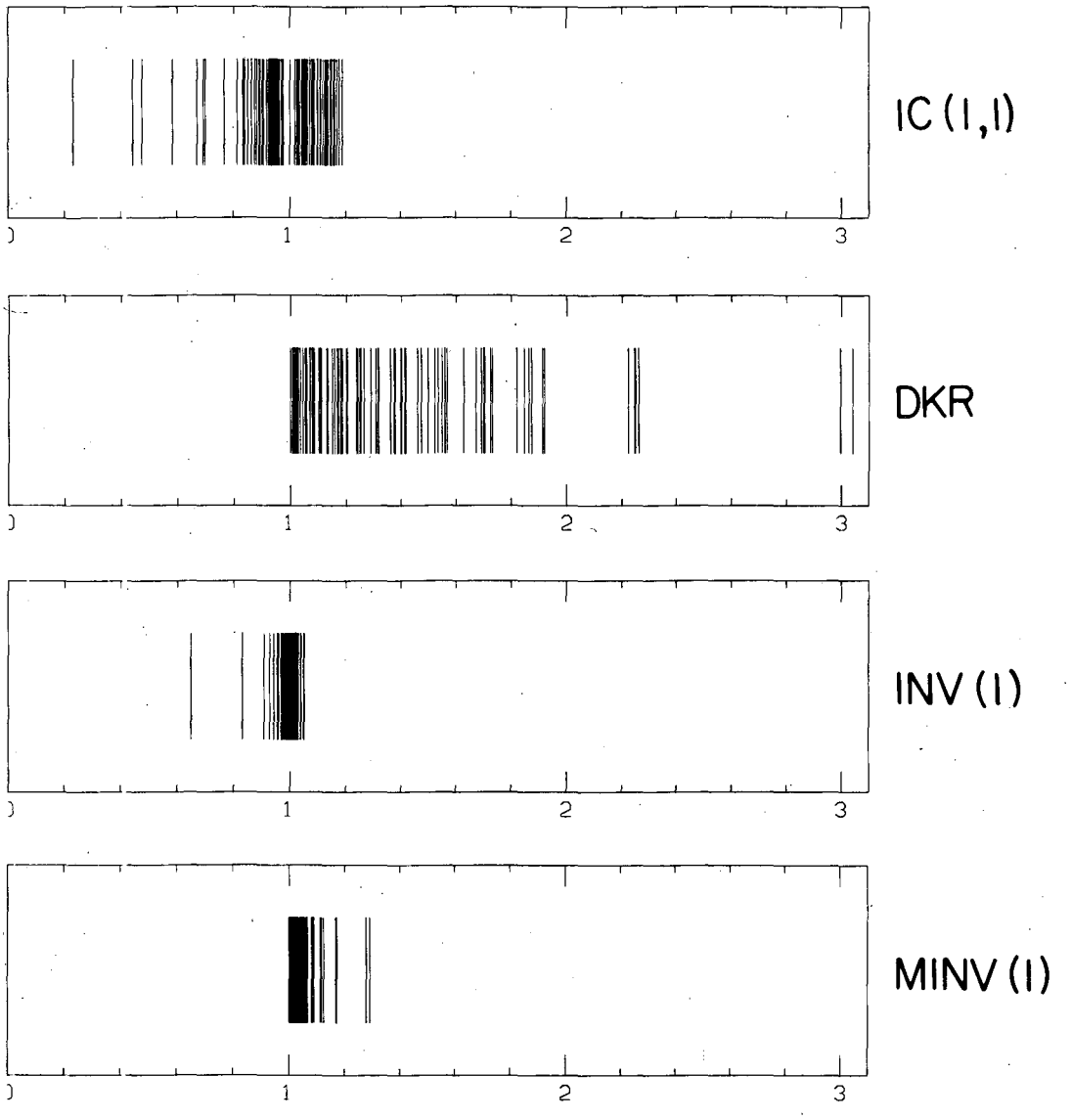


Fig. 4. *Spectra of $M^{-1}A$ for four preconditionings with comparable, minimal storage. Test problem 1.* $N = 100$.

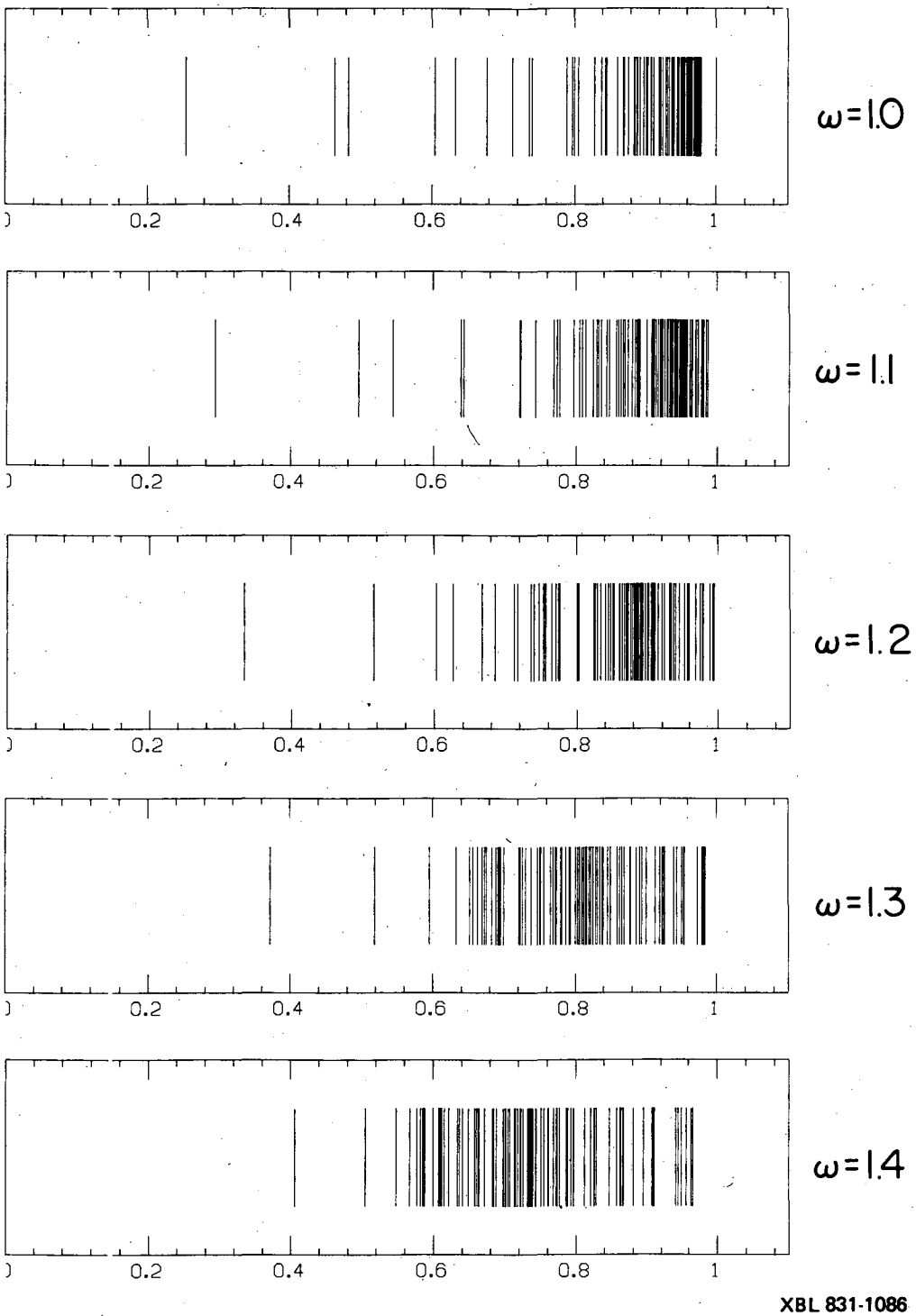


Fig. 5. *Spectra of $M^{-1}A$ for block SSOR preconditionings for different values of ω. Test problem 1. $N = 100$.*

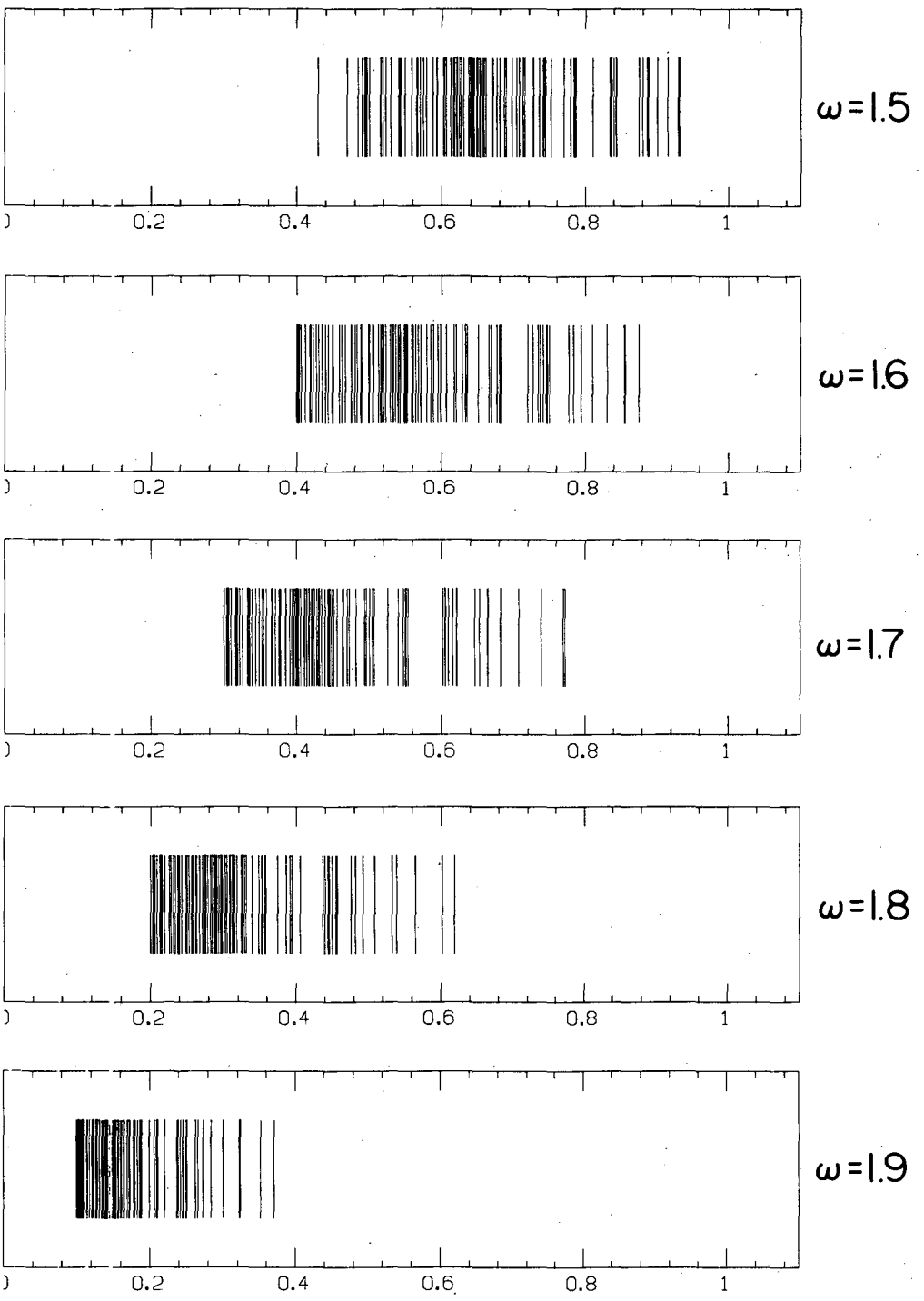


Fig. 5. *(cont.)*

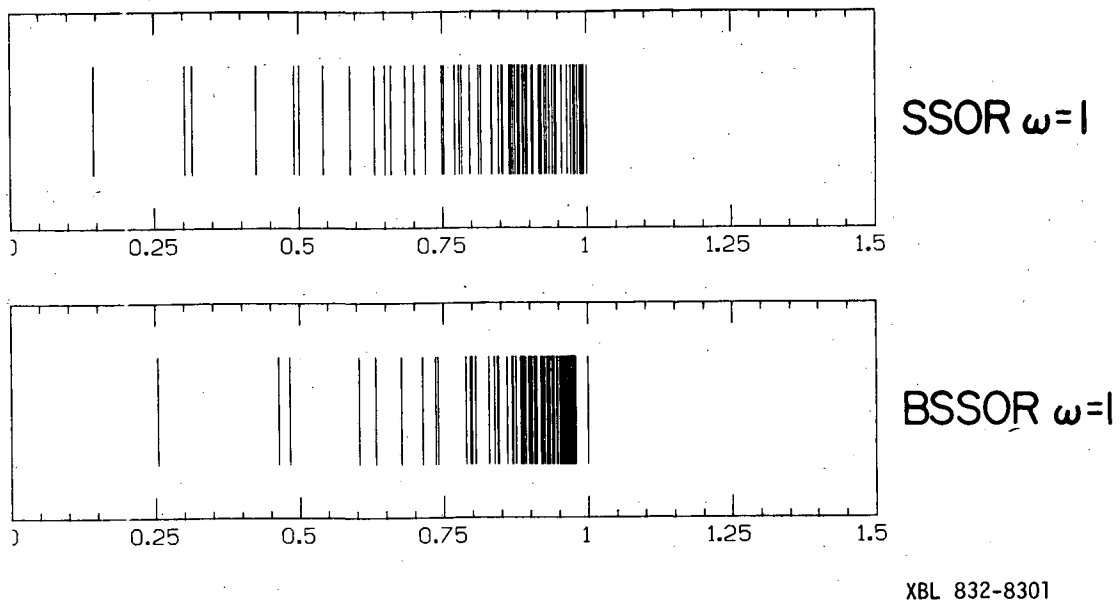


Fig. 6. *Spectra of $M^{-1}A$ for point and block SSOR preconditionings. Test problem 1.* $N = 100$.

The spectra for all of the methods shown in Fig. 2 are on the same scale for easy comparison. From the figure it is seen that for the block methods the eigenvalues are more clustered than for the point ones having the same storage requirements. The point modified methods are shown separately in Fig. 3, because the eigenvalue range for them is different than for the other methods. Fig. 4 shows on the same scale four methods with comparable storage: IC(1,1) and DKR, with one vector of storage, and INV(1) and MINV(1) with two. In Fig. 5 are given the spectra for block SSOR preconditioning for several values of ω. The smallest condition number occurs for $\omega = 1.5$. Figure 6 shows the well-known (cf. [9]) property that the eigenvalues are more clustered for block SSOR than for point SSOR preconditioning. Finally, Fig. 7, which is contained in the Appendix available separately from the authors, depicts enlargements showing the fine structure of the spectra of Figs. 2-6.

Table 7 gives the number of iterations required to solve the test problem for different convergence criteria. For these cases the initial approximation was $x^0 \equiv 0$, and the solution was the same smooth vector as for Tables 3 and 4 with $N = 2500$.

Table 7

Number of iterations for different convergence criteria.
Test problem 1, $x^0 \equiv 0$.

M	Number of iterations			
	$\frac{\|r^k\|_\infty}{\|r^0\|_\infty} \le 10^{-6}$	$\|x-x^k\|_\infty \le 10^{-6}$	$\|x-x^k\|_2 \le 10^{-6}$	$\|x-x^k\|_A \le 10^{-6}$
I	117	99	114	110
IC(1,1)	38	31	36	35
IC(1,2)	26	22	26	24
IC(1,3)	21	19	22	20
IC(2,4)	16	14	16	15
DKR	25	18	22	21
MIC(1,2)	18	14	17	16
MIC(1,3)	18	16	18	17
SSOR $\omega = 1.$	44	37	43	41
SSOR $\omega = 1.7$	22	17	20	19
BSSOR $\omega = 1.$	36	28	34	32
BSSOR $\omega = 1.7$	18	15	18	16
BDIA	27	24	28	26
POL(1,-1)	23	20	24	22
INV(1)	19	16	19	18
MINV(1)	13	9	11	11
CHOL(1)	20	18	21	19
CHOL(2)	15	13	16	14
CHOL(3)	12	11	13	12
CHOL(4)	10	9	10	10
CHOL(5)	9	8	9	8
UND(2,3)	19	16	19	18
UND(3,4)	14	13	15	14
UND(4,5)	12	10	12	11
UND(5,6)	9	8	10	9
MUND(2,3)	15	14	16	15
MUND(2,4)	13	11	13	12
MUND(2,5)	12	9	11	10
MUND(3,4)	12	11	13	12
MUND(3,5)	11	9	11	10
MUND(4,5)	10	9	10	10
MUND(4,6)	9	8	9	9
MUND(5,6)	9	8	9	8

From these results, it appears that, at least for the test problem with a smooth solution, the relative norm of the residual gives a good stopping

criterion.

In Table 8 we give results for $N = 2500$ for the same smooth solution as for previous tables, with two different choices of the starting vector, $x^0 \equiv 0$ and x^0 consisting of random numbers in [-1,1]. The stopping criterion is $\|r^k\|_\infty / \|r^0\|_\infty \leq 10^{-6}$.

Table 8

Number of iterations for $\|r^k\|_\infty / \|r^0\|_\infty \leq 10^{-6}$ for different starting vectors. Test problem 1.

M	# of its.	
	$x^0 = 0$	x^0 random
I	117	109
IC(1,1)	38	33
IC(1,2)	26	21
IC(1,3)	21	17
IC(2,4)	16	12
DKR	25	23
MIC(1,2)	18	17
MIC(1,3)	18	14
SSOR $\omega = 1.$	44	40
SSOR $\omega = 1.7$	22	21
BSSOR $\omega = 1.$	36	28
BSSOR $\omega = 1.7$	18	16
BDIA	27	22
POL(1,-1)	23	18
INV(1)	19	15
MINV	13	11
CHOL(1)	20	16
CHOL(2)	15	12
CHOL(3)	12	9
CHOL(4)	10	8
CHOL(5)	9	7
UND(2,3)	19	15
UND(3,4)	14	11
UND(4,5)	12	9
UND(5,6)	9	7
MUND(2,3)	15	12
MUND(2,4)	13	10
MUND(2,5)	12	9
MUND(3,4)	12	10
MUND(3,5)	11	8
MUND(4,5)	10	8
MUND(4,6)	9	7
MUND(5,6)	9	7

The initial approximation x^0 random appears to give better results. This feature will be developed in a subsequent study.

From the tables one can conclude that for this test problem block methods give better results than point ones. The most promising block method is MINV(1). Since the setup time for constructing M was not included in the tables,

it is of interest to consider it, as it can be of importance if only one problem is to be solved or only a few iterations taken. Table 9 gives the effect of including the setup time for three of the preconditionings for the $N = 2500$ test problem. Times are in CPU seconds for an IBM 3081 computer.

Table 9

Setup time and total time in CPU seconds for $\|r^k\|_\infty / \|r^0\|_\infty \leq 10^{-6}$.
Test problem 1.

M	setup time	total time
IC(1,1)	0.163	1.37
INV(1)	0.178	0.963
MINV(1)	0.415	0.723

Even if the setup times are included, MINV(1) still gives considerable improvement for this problem.

5.3 Second test problem

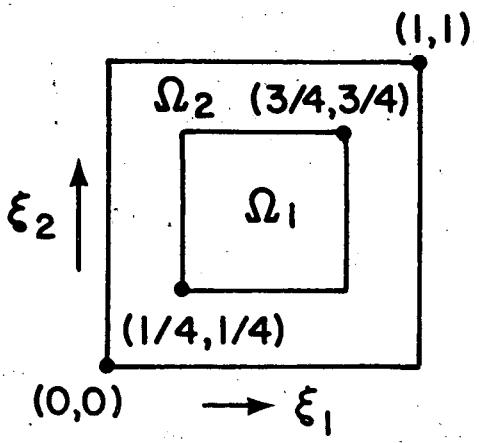
We solve the linear system obtained by the standard five point discretization of the problem

$$-\frac{\partial}{\partial \xi_1}\left(\lambda(\xi_1,\xi_2)\,\frac{\partial u}{\partial \xi_1}\right)-\frac{\partial}{\partial \xi_2}\left(\lambda(\xi_1,\xi_2)\,\frac{\partial u}{\partial \xi_2}\right)=f \qquad \text{in the unit square } (0,1)\times(0,1)$$

$$u=0 \quad \text{on} \quad \partial\Omega\,,$$

for the discontinuous λ depicted in Fig. 8.

The solution is the same smooth one used for the first test problem, the starting



$$\lambda = \begin{cases} 1000 & , \ (\xi,\eta) \in \Omega_1 \\ 1 & , \ (\xi,\eta) \in \Omega_2 \end{cases}$$

Fig. 8. *Test problem 2*

vector is random, and the stopping criterion is $\|r^k\|_\infty / \|r^0\|_\infty \leq 10^{-6}$.

Table 10 gives the results for the number of iterations, the work required, and an estimate of the condition number as obtained from the conjugate gradient parameters. The values $\omega = 1.6$ for SSOR and $\omega = 1.5$ for BSSOR are the observed optimal ones to the nearest 0.1.

Table 10

Number of iterations, total work per point, and estimated condition number of $M^{-1}A$. Test problem 2, $N = 2500, \|r^k\|_\infty / \|r^0\|_\infty \leq 10^{-6}$.

M	# its.	work/N	$\kappa(M^{-1}A)$
DIAG	137	1507	
IC(1,1)	47	705	46770
IC(1,2)	30	570	17062
IC(1,3)	25	525	11102
IC(2,4)	18	450	5668
DKR	32	480	40
MIC(1,2)	23	437	26
MIC(1,3)	20	420	24
SSOR $\omega = 1.$	55	880	66162
SSOR $\omega = 1.6$	36	576	16620
BSSOR $\omega = 1.$	41	779	33929
BSSOR $\omega = 1.5$	23	437	14777
BDIA	34	646	21489
POL(1,-1)	28	532	14182
INV(1)	22	418	8790
MINV(1)	17	323	20
CHOL(1)	24	456	10288
CHOL(2)	18	378	5531
CHOL(3)	14	350	3307
CHOL(4)	12	348	2154
CHOL(5)	10	330	1490
UND(2,3)	22	418	8946
UND(3,4)	17	357	4762
UND(4,5)	14	350	2876
UND(5,6)	12	348	1899
MUND(2,3)	19	361	5825
MUND(2,4)	17	323	3472
MUND(2,5)	16	304	2135
MUND(3,4)	15	315	3355
MUND(3,5)	14	294	2135
MUND(3,6)	14	294	1379
MUND(4,5)	12	300	2136
MUND(4,6)	12	300	1416
MUND(5,6)	11	319	1451
LJAC	111	1554	

The very large condition numbers for most of the entries result from the small first eigenvalue, which is isolated from the others. Thus the number of

iterations does not change much, for example, from IC(1,1), which has a small isolated eigenvalue, to DKR, which has all eigenvalues greater than one. It is the distribution of the other eigenvalues that is important. In terms of work per point, block methods give better results than point ones. Again MINV(1) seems a good compromise between efficiency and storage. This example shows that block methods can be effective for problems with coefficients having large jump discontinuities.

5.4 Third test problem

We consider

$$-\Delta u + \sigma u = f \qquad \text{in } \Omega \text{ the unit square}$$

$$\frac{\partial u}{\partial n}\Big|_{\partial\Omega} = 0$$

to examine the effect of Neumann boundary conditions. We take $\sigma = 1$ with f smooth, x^0 random, $h = 1/49$, and $\|r^k\|_\infty / \|r^0\|_\infty \leq 10^{-6}$. The obtained results are given in Table 11. The value $\omega = 1.7$ for SSOR and BSSOR is the observed optimal one for each case to the nearest 0.1. The relative merits of the different preconditionings are almost the same for this case as for the Dirichlet boundary conditions.

Table 11

Number of iterations and total work per point for $\|r^k\|_\infty / \|r^0\|_\infty \leq 10^{-6}$. Test problem 3, $N = 2500$.

M	# its.	work/N
I	195	2145
DIAG	189	2079
IC(1,1)	58	870
IC(1,2)	35	665
IC(1,3)	29	609
IC(2,4)	22	550
DKR	35	525
MIC(1,2)	24	456
MIC(1,31)	21	441
SSOR $\omega = 1.$	68	1088
SSOR $\omega = 1.7$	42	672
BSSOR $\omega = 1.$	49	931
BSSOR $\omega = 1.7$	39	741
BDIA	41	779
POL(1,-1)	32	608
INV(1)	26	494
MINV(1)	19	361
CHOL(1)	29	551
CHOL(2)	21	441
CHOL(3)	19	475
CHOL(4)	15	435
CHOL(5)	12	396
UND(2,3)	26	494
UND(3,4)	20	420
UND(4,5)	16	400
UND(5,6)	14	406
MUND(2,3)	23	437
MUND(2,4)	21	399
MUND(2,5)	18	342
MUND(3,4)	19	399
MUND(3,5)	16	336
MUND(3,6)	14	294
MUND(4,5)	15	375
MUND(4,6)	14	350
MUND(5,6)	13	377
LJAC	135	1890

5.5 Fourth test problem

$$-\frac{\partial}{\partial \xi_1}\left(\lambda_1 \frac{\partial u}{\partial \xi_1}\right) - \frac{\partial}{\partial \xi_2}\left(\lambda_2 \frac{\partial u}{\partial \xi_2}\right) + \sigma u = f \qquad \text{in } \Omega \text{ the unit square}$$

$$\left.\frac{\partial u}{\partial n}\right|_{\partial\Omega} = 0 .$$

We solve this problem for $\sigma = 0.01$, $\lambda_1 = 100$, $\lambda_2 = 1$, and $h = 1/49$. The right-hand side is zero except for

$$f(4,4) = 1. \ , \quad f(4,28) = -0.3 \ , \quad f(15,16) = -2.$$
$$f(24,5) = 0.5 \ , \quad f(40,10) = 1.5 \ , \quad f(45,2) = -1. \ .$$

This problem, which is of practical interest in multiphase displacement in porous media, was suggested to us by M. Karakas and T. Lasseter. It is particularly favorable for block preconditioning, because line ordering of the mesh points in the ξ_1 direction can be used to capture the strongly one-dimensional nature of the problem. The results for x^0 random and $\|r^k\|_\infty / \|r^0\|_\infty \leq 10^{-6}$ are given in Table 12. The values $\omega = 1.7$ for SSOR and $\omega = 1.0$ for BSSOR are the observed optimal ones to the nearest 0.1.

Table 12

Number of iterations and total work per point for $\|r^k\|_\infty / \|r^0\|_\infty \leq 10^{-6}$.
Test problem 4, $N = 2500$.

M	# its.	work/N
IC(1,1)	28	420
IC(1,2)	25	475
IC(1,3)	26	546
IC(2,4)	24	600
DKR	42	630
MIC(1,2)	30	570
MIC(1,3)	24	504
SSOR $\omega = 1.$	115	1840
SSOR $\omega = 1.7$	80	1280
BSSOR $\omega = 1.$	12	228
BDIA	12	228
POL(1,-1)	12	228
INV(1)	11	209
MINV(1)	9	171
CHOL(1)	15	285
CHOL(2)	12	252
CHOL(3)	11	275
CHOL(4)	10	290
CHOL(5)	10	330
UND(2,3)	12	228
UND(3,5)	11	231
UND(4,5)	11	275
UND(5,6)	10	290
MUND(2,3)	13	247
MUND(2,4)	11	209
MUND(2,5)	10	190
MUND(3,4)	11	231
MUND(3,5)	10	210
MUND(3,6)	11	231
MUND(4,5)	10	250
MUND(4,6)	10	250
MUND(5,6)	10	290
LJAC	31	434

From the tables we see that

(i) As expected, the block methods give significantly better results than the point ones.

(ii) It does not pay to increase the number of diagonals retained in the approximations to the Δ_i^{-1}. This observation corresponds to the property for this problem that the inverse of the matrix A and its Cholesky factors contain almost all their larger elements clustered around the three main diagonals.

Fig. 9 depicts the spectra for some block methods and one point method for this problem for $N = 100$. The block methods show relatively few distinct eigenvalues, the remainder being clustered in a small interval near 1.

5.6 Fifth test problem

This example, which is frequently used in the literature, was presented in [21]. The problem is to solve

$$-\frac{\partial}{\partial \xi_1}\left(\lambda_1 \frac{\partial u}{\partial \xi_1}\right) - \frac{\partial}{\partial \xi_2}\left(\lambda_2 \frac{\partial u}{\partial \xi_2}\right) + \sigma u = 0 \quad \text{in } \Omega = (0,2.1)\times(0,2.1)$$

$$\frac{\partial u}{\partial n}\Big|_{\partial\Omega} = 0 .$$

The domain is shown in Fig. 10 and depicts the values of the coefficients, which are discontinuous. The solution is $u \equiv 0$.

We take $h = 1/42$, x^0 a vector with random elements in [-1,1], and stopping criterion $\|x^k\|_\infty \le 10^{-6}$. The results are given in Table 13. The values $\omega = 1.7$ for SSOR and $\omega = 1.5$ for BSSOR are the observed optimal ones to the nearest 0.1.

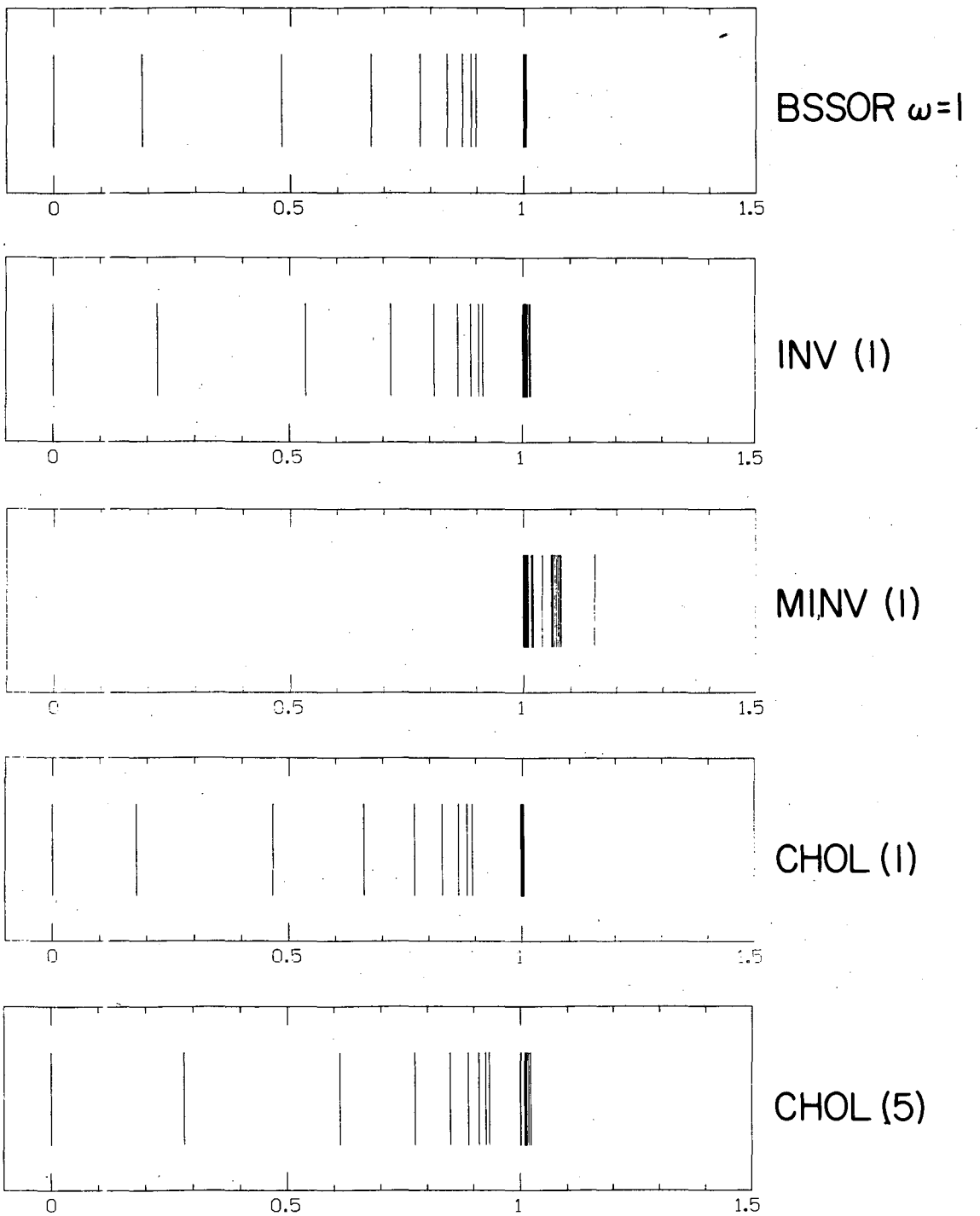


Fig. 9. *Spectra of $M^{-1}A$ for some block preconditionings. Test problem 4.* $N = 100$.

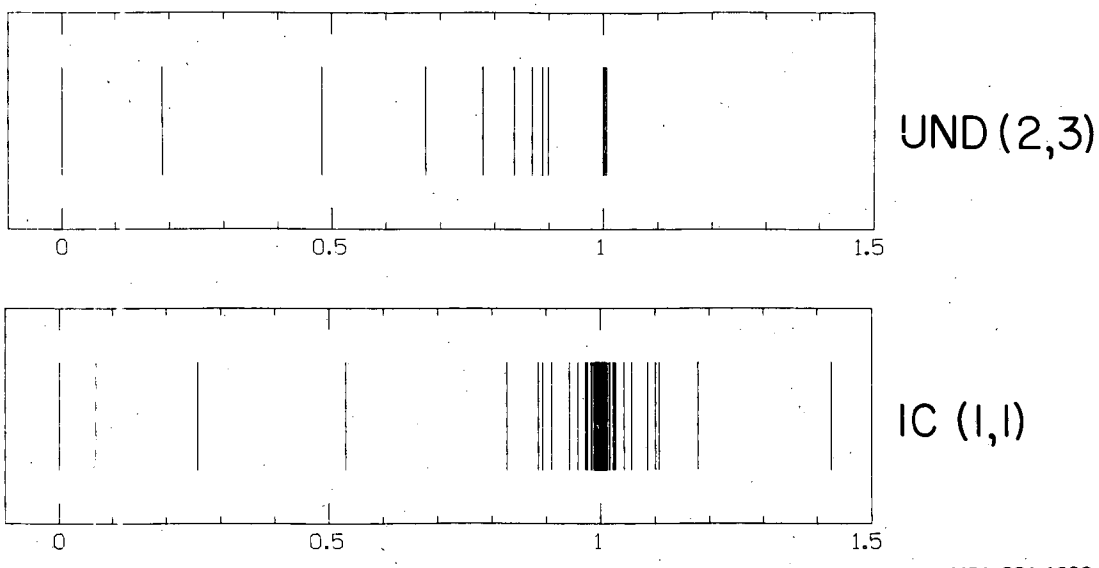


Fig. 9. *(cont.)*

	λ_1	λ_2	σ
Ω_1	1.	1.	0.02
Ω_2	2.	2.	0.03
Ω_3	3.	3.	0.05

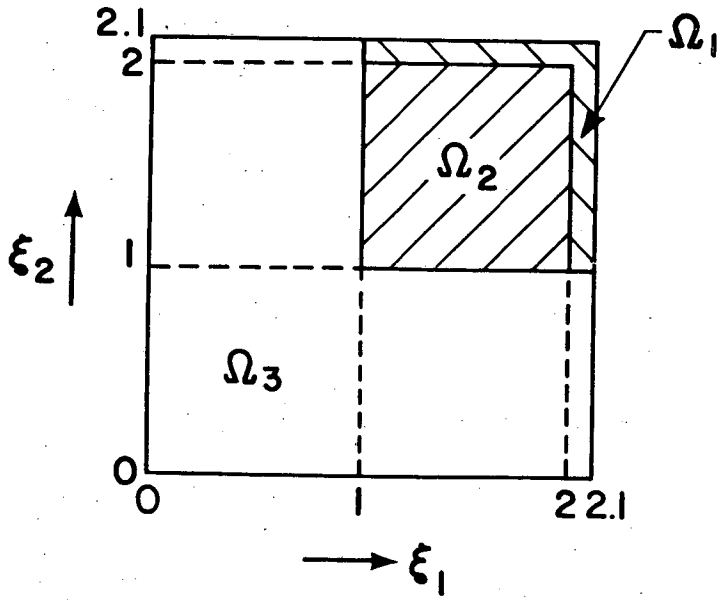


Fig. 10. *Test problem 5*

Table 13 indicates that for this problem the larger the number of diagonals retained, the lower the work required for convergence. This holds both for point and block methods. Generally, the block methods are slightly better.

Table 13

Number of iterations and total work per point for $\|x^k\|_\infty \leq 10^{-6}$.
Test problem 5, $N = 1849$.

M	# its.	work/N
IC(1,1)	74	1110
IC(1,2)	47	893
IC(1,3)	38	798
IC(2,4)	29	725
DKR	53	795
MIC(1,2)	36	684
MIC(1,3)	29	609
SSOR $\omega = 1.$	88	1408
SSOR $\omega = 1.7$	52	832
BSSOR $\omega = 1.$	65	1235
BSSOR $\omega = 1.5$	46	874
BDIA	52	988
POL(1,-1)	43	817
INV(1)	34	646
MINV(1)	25	475
CHOL(1)	36	684
CHOL(2)	28	588
CHOL(3)	22	550
CHOL(4)	19	551
CHOL(5)	16	528
UND(2,3)	34	646
UND(3,4)	26	546
UND(4,5)	21	525
UND(5,6)	18	522
MUND(2,3)	28	532
MUND(2,4)	25	475
MUND(2,5)	23	437
MUND(3,4)	23	483
MUND(3,5)	21	441
MUND(4,5)	19	475
MUND(4,6)	18	450
MUND(5,6)	17	493

In order to compare our methods with those presented by Meijerink and Van der Vorst [17] for this problem, we give the results in Table 14 for convergence criterion $\|r^k\|_2 \leq 10^{-6}$. For the IC methods, we obtain about the same results as in [17], within a few iterations. (The starting vectors are different -- our random numbers are between -1 and 1, while theirs are between 0 and 1.)

Table 14

Number of iterations and total work per point for $\|r^k\|_2 \leq 10^{-6}$.
Test problem 5, $N = 1849$.

M	# its.	work/N
IC(1,1)	79	1185
IC(1,2)	49	931
IC(1,3)	39	819
IC(2,4)	30	750
DKR	66	990
MIC(1,2)	43	817
MIC(1,3)	35	735
SSOR $\omega = 1.$	94	1504
SSOR ω_{opt}	56	896
BSSOR $\omega = 1.$	68	1292
BSSOR ω_{opt}	48	912
BDIA	55	1045
POL(1,-1)	45	855
INV(1)	36	684
MINV(1)	29	551
CHOL(1)	38	722
CHOL(2)	29	609
CHOL(3)	23	575
CHOL(4)	20	580
CHOL(5)	17	561
UND(2,3)	36	684
UND(3,4)	28	588
UND(4,5)	22	550
UND(5,6)	19	551
MUND(2,3)	30	570
MUND(2,4)	26	494
MUND(2,5)	24	456
MUND(3,4)	24	504
MUND(3,5)	22	462
MUND(4,5)	20	500
MUND(4,6)	19	475
MUND(5,6)	17	493

To compare point and block methods with the same storage, one can take, for example, IC(1,2) or MIC(1,2) and CHOL(2). It is clear that the block method is better. The situation is the same if more diagonals are taken. To get down to 16 iterations with point preconditioning Meijerink and Van der Vorst [17] use

IC(5,7), but approximately the same goal can be achieved with only six instead of 12 vectors of storage using the block preconditioning CHOL(5).

6. Concluding remarks

The above examples show that, for linear problems coming for finite-difference approximations of elliptic partial differential equations, the block preconditionings we have introduced can give better results for two dimensional problems than the corresponding point ones currently in use. The results are better also than for block SSOR preconditioning. Generally, for natural ordering of the unknowns, the modified methods give better results for our test problems than unmodified ones. Particularly attractive is the preconditioning INV(1) -- and its modified form MINV(1) -- because of the low storage requirements and rapid convergence. The results for three dimensional problems await further study. It would be of interest to explore the behavior of our block preconditioning methods on more general problems such as the ones arising from finite element approximation with node orderings leading to a block tridiagonal matrix.

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References

[1] E. Asplund, *Inverse of matrices $\{a_{ij}\}$ which satisfy $a_{ij} = 0$ for $j > i+p$*, Math. Scand., 7 (1959), pp. 57-60.

[2] A. Berman and R.J. Plemmons, *Non Negative Matrices in the Mathematical Sciences*, Academic Press, New York, 1979.

[3] P. Concus, G.H. Golub, and D.P. O'Leary, *A generalized conjugate gradient method for the numerical solution of elliptic partial differential equations*, in *Sparse Matrix Computations*, J.R. Bunch and D.J. Rose, eds., Academic Press, New York, 1976, pp. 309-332.

[4] R.W. Cottle, *Manifestations of the Schur complement*, Linear Algebra Appl., 8 (1974), pp. 120-211.

[5] S. Demko, *Inverses of band matrices and local convergence of spline projections*, SIAM J. Numer. Anal., 14 (1977), pp. 616-619.

[6] J.J. Dongarra, C.B. Moler, J.R. Bunch, and G.W. Stewart, *LINPACK User's Guide*, SIAM, Philadelphia, 1979.

[7] T. Dupont, R.P. Kendall, and H. Rachford, *An approximate factorization procedure for solving self adjoint elliptic difference equations*, SIAM J. Numer. Anal., 5 (1968), pp. 559-573.

[8] S. Eisenstat, *Efficient implementation of a class of preconditioned conjugate gradient methods*, SIAM J. Sci. Statist. Comput., 2 (1981), pp. 1-4.

[9] L.W. Ehrlich, *The block symmetric successive overrelaxation method*, SIAM J. Appl. Math., 12 (1964), pp. 807-826.

[10] D.K. Faddeev, *Properties of the inverse of a Hessenberg matrix*, in *Numerical Methods and Computational Issues*, 5 (1981), V.P. Ilin and V.N. Kublanovskaya, eds. (in Russian).

[11] A. George and J.W.H. Liu, *Algorithms for matrix partitioning and the numerical solution of finite element systems*, SIAM J. Numer. Anal., 15 (1978), pp. 297-327.

[12] G.H. Golub and G. Meurant, *Resolution numerique des grands systemes lineaires*, Note CEA N-2268, Commissariat a l'Energie Atomique - Limeil, France, 1981.

[13] I. Gustafsson, *A class of first order factorization methods*, BIT, 18 (1978), pp. 142-156.

[14] O.G. Johnson, C.A. Micchelli, and G. Paul, *Polynomial preconditioners for conjugate gradient calculations*, Tech. Rep., IBM Thomas J. Watson Research Center, Yorktown Heights, NY, 1982.

[15] D. Kershaw, *Inequalities on the elements of the inverse of a certain tridiagonal matrix*, Math. Comp., 24 (1970), pp. 155-158.

[16] J.A. Meijerink and H. Van der Vorst, *An iterative solution method for linear systems of which the coefficient matrix is a symmetric M-matrix*, Math. Comp., 31 (1977), pp. 148-162.

[17] J.A. Meijerink and H. Van der Vorst, *Guidelines for the usage of incomplete decompositions in solving sets of linear equations as they occur in practical problems*, J. Comput. Phys., 44 (1981), pp. 134-155.

[18] G. Meurant, *The Fourier method from the point of view of block Cholesky factorization*, Tech. Report, Commissariat a l'Energie Atomique - Limeil, France, 1983 (to appear).

[19] C. Moler, *MATLAB User's Guide*, Dept. of Computer Science, Univ. of New Mexico, Albuquerque, NM, 1981.

[20] R.R. Underwood, *An approximate factorization procedure based on the block Cholesky decomposition and its use with the conjugate gradient method*, Report NEDO-11386, General Electric Co., Nuclear Energy Div., San Jose, CA, 1976.

[21] R.S. Varga, *Matrix Iterative Analysis*, Prentice Hall, Englewood Cliffs, NJ, 1962.

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