OPTIMAL PRECONDITIONERS OF A GIVEN SPARSITY PATTERN

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Abstract.

We consider the problem of finding the symmetric positive definite preconditioner M of a given form – e.g., having nonzero elements only in specified positions – which minimizes the ratio of the largest to smallest eigenvalue of $M^{-1}A$, for a given symmetric positive definitive matrix A. We show how this problem can be expressed as one of minimizing a convex function and how an optimization code can be used to solve the problem numerically. Results are presented showing optimal preconditioners of various sparsity patterns and comparing these to preconditioners that have been proposed in the literature. Several conjectures are made, based on results from the optimization code.

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1. Introduction.

In recent years much research has focused on the problem of finding efficient preconditioners to use with various iterative methods for solving linear systems. Examples of preconditioners, or of iterative methods that can be viewed as using special preconditioners, include the incomplete Cholesky factorization [27], the SSOR preconditioner [33], multigrid methods [5], domain decomposition techniques [4], and many, many more.

An efficient preconditioner M for a matrix A must possess two properties: 1) Linear systems with coefficient matrix M must be relatively easy to solve; and 2) The matrix $M^{-1}A$ must "approximate" the identity.

Many of the preconditioners that have been proposed are easy to solve because of their sparsity or because they are products of known lower and upper triangular matrices with simple sparsity patterns.

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The sense in which $M^{-1}A$ should "approximate" the identity differs according to the iterative method to be used. For simple iterative refinement methods $(x^k = x^{k-1} + M^{-1}(b - Ax^{k-1}))$, the asymptotic convergence rate is determined by the spectral radius

$$\rho(I-M^{-1}A).$$

For fast asymptotic convergence, this quantity should be small.

When the matrices A and M are symmetric and positive definite, this basic iterative method can be accelerated through use of the Chebyshev or conjugate gradient iteration. For the Chebyshev or conjugate gradient methods, the ratio

$$\kappa(M^{-1}A) = \lambda_{\max}(M^{-1}A)/\lambda_{\min}(M^{-1}A)$$

of the largest to the smallest eigenvalue of $M^{-1}A$ enters into an upper bound for the error

$$||e^{k}||_{A}/||e^{0}||_{A} \leq 2[(\kappa^{1/2}-1)/(\kappa^{1/2}+1)]^{k}$$

where the A-norm of the error, $||e^k||_A$, is defined as $\langle e^k, Ae^k \rangle^{1/2}$. To make this bound small, κ should be close to 1. This bound is *sharp* for the Chebyshev method, in the sense that there is an initial guess for which the bound will be attained at every step. It is not sharp for the conjugate gradient method. A sharp error bound for the conjugate gradient method is more complicated [18], involving the distribution of all eigenvalues of $M^{-1}A$, but a condition number¹ $\kappa(M^{-1}A)$ close to 1 is *sufficient* to ensure fast convergence of this algorithm as well, even when the effects of finite precision arithmetic are taken into account [19]. Therefore, we will define "optimality" in terms of the condition number $\kappa(M^{-1}A)$ and minimization of this quantity will be our goal.

It is well-known that the largest eigenvalue of a symmetric matrix S is a convex function of the elements of S. Although the function is not differentiable at points where eigenvalues coalesce, (and one usually expects the minimum to occur at such a point), the problem of minimizing this function can be handled numerically using optimization techniques. If the elements of S are affine functions of a vector x of unknowns

$$S(x) = S_0 + \sum_{k=1}^m S_k x_k$$

then the largest eigenvalue of S(x) will be a convex function of x. Given the matrices S_k , k = 0, 1, ..., m an algorithm due to M. Overton [28] can be used to find the vector x for which the spectral radius of S(x) is minimal. The algorithm is asymptotically quadratically convergent and second derivatives are not required to obtain

¹ When referring to the condition number $\kappa(M^{-1}A)$, we actually mean the ratio of largest to smallest eigenvalue of $M^{-1}A$, or, the condition number in the 2-norm of $M^{-1/2}AM^{-1/2}$. Since the matrices we consider are all symmetric and positive definite, this should cause no confusion.

this quadratic convergence rate in many cases. The code uses a variant of Newton's method to minimize a related nonlinear but essentially differentiable function. In this paper, we report results using the Overton optimization code to find optimal preconditioners of a given sparsity pattern.

To see how the preconditioning problem can fit into this framework, we will need a few simple results. Given a symmetric positive definite matrix A and a sparsity pattern for the symmetric preconditioner M, we would like to find the matrix M of the given form which minimizes $\rho(I - M^{-1}A)$ or $\kappa(M^{-1}A)$, as explained above. The matrix $I - M^{-1}A$ is not symmetric, and its elements are not affine functions of the elements of M, but the following theorem relates the minimization of $\rho(I - M^{-1}A)$ to the minimization of the largest eigenvalue of $I - L^{-1}ML^{-T}$, where LL^{T} is a factorization (e.g., the Cholesky factorization) of A. We start with the following simple lemma.

LEMMA 1. For a given matrix Q with real nonnegative eigenvalues, the scalar c which minimizes $\rho(I - cQ)$ is

$$c = 1/\lambda_a(Q), \quad \lambda_a(Q) \equiv \frac{1}{2}(\lambda_{\min}(Q) + \lambda_{\max}(Q)),$$

where $\lambda_{\min}(Q)$ is the smallest and $\lambda_{\max}(Q)$ the largest eigenvalue of Q, and $\lambda_a(Q)$ is the arithmetic mean of these two.

PROOF: For c as defined above, the spectral radius of I - cQ is given by

$$\rho(I-cQ) = 1 - c\lambda_{\min}(Q) = c\lambda_{\max}(Q) - 1.$$

For any other scalar $c' \neq c$, one of the following two inequalities must hold:

 $c' < c \rightarrow 1 - c'\lambda_{\min}(Q) > 1 - c\lambda_{\min}(Q)$, or $c' > c \rightarrow c'\lambda_{\max}(Q) - 1 > c\lambda_{\max}(Q) - 1$, and so the spectral radius of I - c'Q must satisfy

$$\rho(I - c'Q) > \rho(I - cQ).$$

THEOREM 1. Let $A = LL^T$ be a factorization of the symmetric positive definite matrix A, and let M_1 and M_2 be two symmetric positive definite matrices such that

 $\rho(I - c_1 L^{-1} M_1 L^{-T}) < \rho(I - c_2 L^{-1} M_2 L^{-T}), \text{ where } c_i = 1/\lambda_a (L^{-1} M_i L^{-T}), i = 1,2.$ Then

(1.1)
$$\rho(I - \hat{c}_1 M_1^{-1} A) < \rho(I - \hat{c}_2 M_2^{-1} A), \text{ where } \hat{c}_i = 1/\lambda_a(M_i^{-1} A), i = 1, 2$$

and

(1.2)
$$\kappa(M_1^{-1}A) < \kappa(M_2^{-1}A).$$

PROOF: Because of the choice of c_1 and c_2 , we have

$$\rho(I - c_i L^{-1} M_i L^{-T}) = \frac{\lambda_{\max}(L^{-1} M_i L^{-T}) - \lambda_{\min}(L^{-1} M_i L^{-T})}{\lambda_{\max}(L^{-1} M_i L^{-T}) + \lambda_{\min}(L^{-1} M_i L^{-T})}, \quad i = 1, 2.$$

The eigenvalues of $L^{-1}M_iL^{-T}$, i = 1,2, are just the inverses of the eigenvalues of $L^TM_i^{-1}L$, or, of $M_i^{-1}A$. Hence we have

$$\rho(I - c_i L^{-1} M_i L^{-T}) = \frac{\lambda_{\max}(M_i^{-1} A) - \lambda_{\min}(M_i^{-1} A)}{\lambda_{\max}(M_i^{-1} A) + \lambda_{\min}(M_i^{-1} A)} = \frac{\kappa(M_i^{-1} A) - 1}{\kappa(M_i^{-1} A) + 1}.$$

Since $\frac{x-1}{x+1}$ is an increasing function of x for $x \ge 1$, the result (1.2) follows. Because of the choice of \hat{c}_1 and \hat{c}_2 , the right-hand side is equal to the spectral radius

of $I - \hat{c}_i M_i^{-1} A$, and so result (1.1) follows as well.

The symmetric matrix $I - L^{-1}ML^{-T}$ is an affine function of the elements of M. Theorem 1 shows that if M_1 minimizes the spectral radius of this matrix over all symmetric preconditioners M belonging to some set which also contains all positive scalar multiples of its members, then M_1 (or any positive scalar multiple of M_1) also minimizes the ratio of largest to smallest eigenvalue, $\kappa(M^{-1}A)$, and there is a scalar \hat{c}_1 such that $\hat{c}_1^{-1}M_1$ minimizes the spectral radius, $\rho(I - M^{-1}A)$, over this set. The scalar \hat{c}_1 is defined in Lemma 1.

In the following examples we find the matrix M in a given set which minimizes $\rho(I - L^{-1}ML^{-T})$. Theorem 1, together with the previous discussion, justifies referring to this matrix (or any positive scalar multiple of this matrix, since scalar factors do not affect the condition number) as an "optimal" preconditioner from the set for use with the Chebyshev method. It shows that the appropriate scalar multiple of this matrix is the "optimal" preconditioner from the set for use with iterative refinement. Other criteria are possible for defining a good preconditioner for the conjugate gradient method [e.g., 2, 3, 9, 22, 23, 29]. These ideas generally involve the minimization of a weighted Frobenius norm of the difference between the preconditioned matrix and the identity. They are easier to minimize than the condition number, but a small Frobenius norm is neither necessary nor sufficient to ensure fast convergence of the conjugate gradient method. The condition number is a reasonably simple measure, and if there is a matrix M in the set for which this measure is small, then the conjugate gradient method with this preconditioner will have guaranteed fast convergence.

This same idea of minimizing the condition number was actually pursued for a certain class of preconditioners much earlier by Concus and Golub [8]. They considered 1-D model problems and used a code by Fletcher [16] to find an optimal diagonal scaling of the Laplacian to use as a preconditioner.

2. Theoretical results.

There are few theoretical results concerning optimal preconditioners for most possible sparsity patterns. An exception is the case of diagonal and block diagonal preconditioners. Van der Sluis [30] proved the following theorem about diagonal scaling of a symmetric positive definite matrix A:

THEOREM (VAN DER SLUIS). Let D be the diagonal of the symmetric positive definite matrix A, and let \hat{D} be any other positive definite diagonal matrix. Then $\kappa (D^{-1/2}AD^{-1/2})$ satisfies

$$\kappa(D^{-1/2}AD^{-1/2}) \le m\,\kappa(\hat{D}A\hat{D}),$$

where m is the maximum number of nonzeros in any row of A.

Thus, D = diag(A) approximately minimizes $\kappa(M^{-1}A)$ over all diagonal preconditioners M. When the matrix A also possesses property-A, (that is, when A can be permuted into the form

$$A = \begin{pmatrix} D_1 & B \\ B^T & D_2 \end{pmatrix},$$

where D_1 and D_2 are diagonal matrices), a stronger result holds [17]:

THEOREM (FORSYTHE & STRAUSS). Using the above notation, if the symmetric positive definite matrix A has property-A, then $\kappa (D^{-1/2}AD^{-1/2})$ satisfies

$$\kappa(D^{-1/2}AD^{-1/2}) \le \kappa(\hat{D}A\hat{D})$$

In this case, then, D = diag(A) is the optimal diagonal preconditioner for the matrix A.

A generalization of the Van der Sluis theorem has also been proved for *block* diagonal preconditioners [7].

THEOREM (DEMMEL). Let D be the block diagonal of the symmetric positive definite matrix A, and let \hat{D} be any other symmetric positive definite block diagonal matrix with the same size blocks. Then $\kappa (D^{-1/2}AD^{-1/2})$ satisfies

$$\kappa(D^{-1/2}AD^{-1/2}) \le b\,\kappa(\hat{D}A\hat{D}),$$

where b is the number of blocks in D.

A result similar to that of Forsythe and Strauss has also been proved for block diagonal preconditioners [14], when the matrix A is *block* 2-cyclic and is permuted into the form

(2.1)
$$A = \begin{bmatrix} D_1 & C^T \\ C & D_2 \end{bmatrix}; \quad D_i = \begin{pmatrix} D_{i,1} & 0 & \dots & 0 \\ 0 & D_{i,2} & \dots & 0 \\ \vdots & \vdots & & \vdots \\ 0 & 0 & \dots & D_{i,r_i} \end{pmatrix}; \quad i = 1, 2$$

THEOREM (EISENSTAT, LEWIS, SCHULTZ). Let A be of the form (2.1), and let D be the block diagonal matrix whose diagonal blocks are $\{D_{1,1}, \ldots, D_{1,r_1}, D_{2,1}, \ldots, D_{2,r_2}\}$. Let \hat{D} be any other block diagonal matrix with the same size blocks. Then $\kappa (D^{-1/2}AD^{-1/2})$ satisfies

$$\kappa(D^{-1/2}AD^{-1/2}) \le \kappa(\hat{D}A\hat{D}).$$

A simple proof of these last two theorems is given in [15].

There appears to be little known theoretically about optimal preconditioners of more general sparsity patterns; e.g., tridiagonal or banded. There is, however, a useful theorem due to Varga [31] for comparing "regular splittings" which, in some cases, enables one to determine the optimal preconditioner among all regular splittings of a given sparsity pattern. (More general, but less simple, versions of this theorem can be found in [10].)

DEFINITION. For $n \times n$ real matrices A, M, and N, A = M - N is a regular splitting of the matrix A if M is nonsingular with $M^{-1} \ge 0$, and $N \ge 0$.

THEOREM (VARGA). Let $A = M_1 - N_1 = M_2 - N_2$ be two regular splittings of A, where $A^{-1} > 0$. If $N_2 \ge N_1 \ge 0$, (and neither N_1 nor $N_2 - N_1$ is the null matrix), then

$$1 > \rho(M_2^{-1}N_2) > \rho(M_1^{-1}N_1) > 0.$$

This theorem implies that among all regular splitting matrices M of a given bandwidth, for example, the optimal one for minimizing the spectral radius of $I - M^{-1}A$ is M = band(A). This matrix is closer element-wise to A than is any other member of the class, and so, by the theorem, is a better splitting, or, preconditioner. As will be shown in the following examples, however, there may be better banded preconditioners outside the class of regular splittings. This theorem is quite general and important to remember. Unfortunately, however, many of the most effective preconditioners are not regular splittings, and so it is of limited applicability.

It should also be noted that because the set of regular splittings does not contain all positive scalar multiples of its members, the matrix, say, \overline{M} , from some class of regular splittings, which minimizes $\rho(I - M^{-1}A)$ over that class does *not* necessarily minimize $\kappa(M^{-1}A)$. The hypotheses of Varga's theorem, together with the assumption that A, M_1 , and M_2 are symmetric and positive definite, do *not* imply $\kappa(M_1^{-1}A) \leq \kappa(M_2^{-1}A)$. Only if the matrices M_1 and c_2M_2 – where c_2 minimizes $\rho(I - cM_2^{-1}A)$, as explained in Lemma 1 – only if these matrices satisfy the hypotheses of Varga's theorem would it also follow, from Theorem 1, that $\kappa(M_1^{-1}A) \leq \kappa(M_2^{-1}A)$. With a weaker assumption about the matrix M_2 , however, it can be shown that $\kappa(M_1^{-1}A) < 2 \kappa(M_2^{-1}A)$.

THEOREM 2. Let A, M_1 , and M_2 be symmetric positive definite matrices satisfying the hypotheses of Varga's theorem, and suppose the largest eigenvalue of $M_2^{-1}A$ is greater than or equal to 1. (This would be the case, for example, if A and M_2 have at least one diagonal element equal, since then the symmetric matrix N_2 would have a zero diagonal element and hence $M_2^{-1}N_2$ would have a nonpositive eigenvalue.) Then the ratios of largest to smallest eigenvalues of $M_1^{-1}A$ and $M_2^{-1}A$ satisfy

$$\kappa(M_1^{-1}A) < 2\kappa(M_2^{-1}A).$$

PROOF: Since the elements of $M_2^{-1}N_2$ are nonnegative, the Perron-Frobenius

theorem states that its spectral radius is equal to its (algebraically) largest eigenvalue:

$$\rho(M_2^{-1}N_2) = \rho(I - M_2^{-1}A) = 1 - \lambda_{\min}(M_2^{-1}A).$$

The result $\rho(M_1^{-1}N_1) < \rho(M_2^{-1}N_2)$ from Varga's theorem implies

 $1 - \lambda_{\min}(M_1^{-1}A) < 1 - \lambda_{\min}(M_2^{-1}A) \text{ and } \lambda_{\max}(M_1^{-1}A) - 1 < 1 - \lambda_{\min}(M_2^{-1}A),$

or, equivalently,

$$\lambda_{\min}(M_1^{-1}A) > \lambda_{\min}(M_2^{-1}A) \text{ and } \lambda_{\max}(M_1^{-1}A) < 2 - \lambda_{\min}(M_2^{-1}A).$$

Dividing the second inequality by the first gives

$$\kappa(M_1^{-1}A) < \kappa(M_2^{-1}A)(2 - \lambda_{\min}(M_2^{-1}A))/\lambda_{\max}(M_2^{-1}A) < 2\kappa(M_2^{-1}A)$$

with the last inequality holding because $\lambda_{\max}(M_2^{-1}A) \ge 1$, and $\lambda_{\min}(M_2^{-1}A) > 0$ since $\rho(M_2^{-1}N_2) < 1$.

A somewhat more general result can be proved for symmetric matrices.

DEFINITION. A splitting A = M - N is said to be a weak regular splitting of the matrix A if M is nonsingular with $M^{-1}N \ge 0$.

We then get the following comparison theorem.

THEOREM 3. Suppose A and M are symmetric positive definite matrices such that A = M - N is a weak regular splitting of A. Let $M_Q = M + Q$ for some symmetric matrix Q such that $v^T Q v \ge 0$ whenever $v \ge 0$ (e.g., for a positive semi-definite matrix Q or for a matrix Q with nonnegative elements). Then

$$\rho(M^{-1}N) \le \rho(M_Q^{-1}N_Q)$$

where $A = M_Q - N_Q$.

PROOF. Let $\lambda_{\min}(M^{-1}A)$ and $\lambda_{\min}(M_Q^{-1}A)$ denote the smallest eigenvalues of $M^{-1}A$ and of $M_Q^{-1}A$, respectively. Since $M^{-1}N$ has nonnegative elements, the Perron-Frobenius theorem states that its spectral radius is equal to its (algebraically) largest eigenvalue. Hence we have

$$\rho(M^{-1}N) = \rho(I - M^{-1}A) = 1 - \lambda_{\min}(M^{-1}A).$$

If \bar{v} is the eigenvector corresponding to the largest eigenvalue of $M^{-1}N$, then the Perron-Frobenius theorem also states that the elements of \bar{v} are nonnegative. Hence $\lambda_{\min}(M^{-1}A)$ also satisfies

$$\lambda_{\min}(M^{-1}A) = \frac{\bar{v}^T A \bar{v}}{\bar{v}^T M \bar{v}} \ge \frac{\bar{v}^T A \bar{v}}{\bar{v}^T M \bar{v} + \bar{v}^T Q \bar{v}} \ge \min_{v \neq 0} \frac{v^T A v}{v^T M_Q v} = \lambda_{\min}(M_Q^{-1}A),$$

and from this the desired result follows:

$$\rho(M_Q^{-1}N_Q) = \rho(I - M_Q^{-1}A) \ge 1 - \lambda_{\min}(M_Q^{-1}A) \ge 1 - \lambda_{\min}(M^{-1}A) = \rho(M^{-1}N).$$

Theorem 3 shows that while the optimal preconditioner of a given sparsity pattern may not be a regular splitting or even a weak regular splitting, it cannot be of the form M + Q, where M is a weak regular splitting and Q is as described in the theorem. To have a possibility of improving upon the optimal weak regular splitting, one must add a matrix Q such that v^TQv can be negative when v is nonnegative.

Other work on iterative methods has focussed on preconditioners that are "optimal" in a different sense from that being considered here [e.g., 1,2]. Multigrid methods and algebraic multilevel methods, for example, are "optimal" in the sense that the preconditioned matrix has condition number O(1), independent of the size mesh from which the linear system was obtained (assuming that the linear system comes from a finite element approximation to an elliptic partial differential equation). In this paper, to be considered "optimal", a preconditioner of the form of the multigrid or algebraic multilevel preconditioner, must not only give a condition number O(1), but the constant must be as small as possible, too.

3. Experimental results for the 5-point Laplacian.

In the following sections we report experimental results using the Overton optimization code [28] to find the matrix M of a given form which minimizes $\rho(I - L^{-1}ML^{-T})$, for a given matrix $A = LL^{T}$. According to Theorem 1, an appropriate scalar multiple of this matrix also minimizes $\rho(I - M^{-1}A)$ and any scalar multiple of this matrix minimizes $\kappa(M^{-1}A)$ over all matrices M of the given form. The matrix A was taken to be the 5-point Laplacian on a square with Dirichlet boundary conditions:

(3.1)
$$\mathbf{A} = \begin{bmatrix} D_1 & E_1 & & \\ E_1^T & D_2 & & \\ & \ddots & \ddots & \\ & \ddots & \ddots & E_{m-1} \\ & & E_{m-1}^T & D_m \end{bmatrix},$$

$$D_i = \begin{pmatrix} 4 & -1 & & \\ -1 & & & \\ & & -1 & \\ & & -1 & 4 \end{pmatrix}, \quad E_i = \begin{pmatrix} -1 & & \\ & & \\ & & -1 \end{pmatrix}, \quad i = 1, \dots, m.$$

In most cases, the matrix M was taken to have a fixed sparsity pattern, e.g.

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diagonal or tridiagonal. The matrix $I - L^{-1}ML^{-T}$ can then be expressed in the form

$$I - L^{-1}ML^{-T} = I - \sum_{k=q} M_{kq} V^{(k,q)},$$

where the sum is over all indices (k, q) such that M_{kq} is allowed to be nonzero, and the matrices $V^{(k,q)}$ are given by

$$(V^{(k,q)})_{ij} = (L^{-1})_{ik}(L^{-1})_{jq}, \qquad i, j = 1, \dots, n.$$

The matrices I and $-V^{(k,q)}$, $(k,q) \in \{$ indices of free elements of $M \}$, are the input to the optimization code.

In some cases, slightly different forms for M were considered. For example, in one experiment, we found the matrix M^{-1} having the same sparsity pattern as A, for which $\rho(I - L^T M^{-1}L)$ was minimal. This is equivalent to minimizing $\rho(I - M^{-1}A)$, and from Theorem 1, this also minimizes $\kappa(M^{-1}A)$ over all matrices M^{-1} with the given sparsity pattern. The elements of $L^T M^{-1}L$ are again linear functions of the free elements of M^{-1} , and so $\rho(I - L^T M^{-1}L)$ can be minimized with the same optimization code.

Another preconditioning problem considered was one involving not A but the Schur complement C in A of a block corresponding to a dividing line in the center of the square domain:



If nodes in Ω_1 are numbered first, then nodes in Ω_2 , and finally nodes on the boundary Γ_3 , then the matrix A takes the form

(3.2)
$$A = \begin{bmatrix} K_{11} & 0 & K_{13} \\ 0 & K_{22} & K_{23} \\ K_{13}^T & K_{23}^T & K_{33} \end{bmatrix}$$

The Schur complement of K_{33} in A is defined as

(3.3)
$$C = K_{33} - K_{13}^T K_{11}^{-1} K_{13} - K_{23}^T K_{22}^{-1} K_{23},$$

and the problem of solving a linear system with coefficient matrix A can be reduced to one of solving a smaller linear system with coefficient matrix C. This the is basis of many domain decomposition methods [6]. One still needs a good preconditioner for the matrix C, and here we considered preconditioners with a given sparsity pattern; e.g., tridiagonal, as well as certain other forms; e.g., Toeplitz. Again, the matrix C was factored in the form LL^T , and the function $\rho(I - L^{-1}ML^{-T})$ was minimized. This is a convex function of the nonzero elements of M (when M is restricted to have a certain sparsity pattern) or of the values on each diagonal of M (when M is restricted to be Toeplitz).

Many of the most efficient preconditioners M are easy to solve not because they themselves have a special sparsity pattern, but because they are of the form KK^T , where K is a lower triangular matrix with a simple sparsity pattern; e.g., that of the lower triangle of A. The problem of finding the matrix K of a given form which minimizes $\rho(I - L^{-1}KK^TL^{-T})$ is more difficult than the previously described problems, however, because the matrix

$$(3.4) I - L^{-1}KK^{T}L^{-T}$$

is not an affine function of the elements of K. Moreover, its spectral radius is not a convex function of K, and the function may have local minima.

The optimization code is easily modified to handle the case of matrix elements which are nonlinear functions of the unknowns, but there is no guarantee that the solution it finds will be the *global* minimum. Still, it will be shown in the numerical examples that the optimization code is able to find preconditioners of the form (3.4), where K has a fixed sparsity pattern, that are significantly better than many currently used preconditioners. We considered matrices K having the same sparsity as the lower triangle of A, and compared the preconditioner KK^T returned by the optimization code with the incomplete Cholesky decomposition [27], the modified incomplete Cholesky decomposition [21], and the SSOR preconditioner [33].

Experiments that have been carried out so far are for *very* small problems. It is planned to continue this work on larger problems when the optimization code has been ported to larger and faster machines. It should be stressed that this is not meant as a practical means for finding a good preconditioner for a given problem. It is *much* easier to solve the linear system than it is to find the optimal preconditioner of a given class. Rather, the optimization code is meant to provide insight into the properties of preconditioners and to be used as a test of conjectures about optimal preconditioners. If the optimal preconditioner of a certain form for a given problem does *not* give rise to a preconditioner of that form (unless such preconditioners can exhibit other desirable properties, such as tight clustering of most of the eigenvalues). On the other hand, if the code shows that there is a good preconditioner of the given form, then it still may or may not be possible to compute such a preconditioner in a reasonable amount of time.

3.1. Diagonal preconditioning for A.

As a check on the code, we first tried computing the optimal *diagonal* preconditioner for the matrix A of (3.1). According to the Forsythe and Strauss theorem of Section 2, this is simply D = diag(A). Indeed, even from very far off initial guesses, the code always converged to M = diag(A) and indicated that it had successfully found the minimum. This gave us confidence to try problems for which the answers were not known.

3.2. Tridiagonal preconditioning for A.

By numbering the odd block-rows and block-columns first and the even ones last, the matrix A of (3.1) can be permuted into block 2-cyclic form, without changing the diagonal blocks. It follows from the Eisenstat, Lewis, Schultz theorem of Section 2, that the optimal block diagonal preconditioner for A is $D = block \ diag(A)$. This matrix is also tridiagonal. It also follows from Varga's theorem that among *regular splittings* this is the optimal tridiagonal preconditioner. The optimization code was used to compute the best *tridiagonal* preconditioner for A (which is not necessarily a regular splitting), and it was found to be slightly better than the block diagonal matrix D. Fig. 1 shows condition numbers for A, $D^{-1}A$, and $M^{-1}A$, where M is the optimal tridiagonal preconditioner, plotted against h^{-2} . From the figure, it appears that all of these matrices have condition number $O(h^{-2})$, and based on these results we make the following conjecture:

CONJECTURE 1. Let A_h be the 5-point Laplace matrix of (3.1), for grid size h, and let M_h be any symmetric positive definite tridiagonal preconditioner for A_h . Then the condition number $\kappa(M_h^{-1}A_h)$ of the preconditioned matrix satisfies

$$\kappa(M_h^{-1}A_h) \ge O(h^{-2})$$

Based on these results we conclude that tridiagonal preconditioners for A cannot be very effective, in terms of giving a small condition number, for small values of h. Additional experiments were performed to find optimal preconditioners of slightly larger bandwidths, but again they appeared to give condition numbers for the preconditioned matrix that were $O(h^{-2})$.

The elements of the optimal tridiagonal preconditioner for different values of h are listed in Table 1. The tridiagonal matrix given in the table has been multiplied by an appropriate constant so that it minimizes $\rho(I - M^{-1}A)$ (although the code actually computes the tridiagonal matrix which minimizes $\rho(I - A^{-1}M)$). Only half of the elements of each diagonal are listed because the preconditioners are persymmetric (symmetric about their northeast to southwest diagonal), as would be expected due to the symmetry of the problem. This restriction was not enforced on the class of matrices from which the optimal one was to be found, and so it gives



further evidence that the optimization code is functioning correctly. Also given in Table 1 are some of the eigenvalues of the preconditioned iteration matrices $I - M^{-1}A$. Note that for all problems sizes, the largest and smallest eigenvalues of the preconditioned iteration matrix each have multiplicity 2. Based on this evidence we make the following conjecture:

CONJECTURE 2. Let A_h be the 5-point Laplace matrix of (3.1) for grid size h, and let M_h be the optimal tridiagonal preconditioner for A_h . If $\lambda_1 \leq \lambda_2 \leq \ldots \leq \lambda_{n-1} \leq \lambda_n$ are the eigenvalues of $M_h^{-1}A_h$, then the largest and smallest eigenvalues satisfy

$$\lambda_1 = \lambda_2, \quad \lambda_{n-1} = \lambda_n$$

3.3. Approximation to A^{-1} with same sparsity as A.

Upon computing the inverse of the matrix A of (3.1), one finds that the larger elements of the inverse are on or near diagonals in which A has nonzeros. In fact, it is shown in [11] that elements of A^{-1} decay exponentially away from these diagonals. It therefore seems reasonable to consider an approximation M^{-1} to A^{-1} , which has nonzero entries only in the diagonals where A has nonzeros. If an effective preconditioner of this form could be found, it would result in a highly vectorizable or parallelizable algorithm, since "solving" the preconditioner would now just mean multiplying by a sparse matrix. The optimization code was used to find the matrix M^{-1} having nonzeros only in the five diagonals where A has nonzeros, for which

h = 1/5		h = 1/6		h = 1/7	
eigenvalues -0.634, -0.634, -0.255, -0.230, 0.020, 0.070, 0.314, 0.375, 0.437 0.487, 0.634, 0.634		eigenvalues -0.732, -0.732, -0.406, -0.400, -0.034, -0.031, 0.507, 0.575, 0.593, 0.610, 0.732, 0.732		eigenvalues -0.798, -0.798, -0.539, -0.508, -0.188, -0.182, 0.671, 0.679, 0.692, 0.699, 0.798, 0.798	
diagonal	subdiagonal	diagonal	subdiagonal	diagonal	subdiagonal
4.4111 4.7698 5.0153 5.2966 4.9314 4.9285 4.9806 5.1583 5.1583 :	$\begin{array}{c} -1.2754 \\ -1.6842 \\ -1.8785 \\ -1.1143 \\ -1.5857 \\ -1.6675 \\ -1.7323 \\ -1.2442 \\ -1.7323 \\ \vdots \end{array}$	4.5383 5.1029 5.7456 6.1396 6.3366 5.6482 5.6718 5.8645 6.0232 6.2313 6.0631 5.9260 5.9285 5.9260 	$\begin{array}{c} -1.3198 \\ -1.8296 \\ -2.3460 \\ -2.4573 \\ -1.4563 \\ -1.9397 \\ -2.4873 \\ -2.2516 \\ -2.2930 \\ -1.7199 \\ -2.1707 \\ -2.1821 \\ -2.1821 \\ \vdots \end{array}$	4.6009 5.2721 6.2098 7.0826 7.5027 7.5623 6.4873 6.4556 6.7498 7.1391 7.3354 7.4991 7.1410 7.0021 7.0845 7.1929 7.2359 7.3990 	$\begin{array}{c} -1.3366\\ -1.8816\\ -2.5799\\ -3.0903\\ -3.1271\\ -1.8487\\ -2.3507\\ -2.4075\\ -2.7103\\ -2.9591\\ -2.9480\\ -2.2456\\ -2.6953\\ -2.7208\\ -2.8095\\ -2.8707\\ -2.8434\\ -2.3548\\ -2.8434\\ -2.3548\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.8434\\ -2.84$

 Table 1. Optimal tridiagonal preconditioners for A.

 $\kappa(M^{-1}A)$ was as small as possible.

This turned out to be a more difficult problem for the optimization code, than either of the previous two cases. Using a very coarse mesh, h = 1/3, the optimization code returned a solution with the following caveat:

"Apparently optimal (or very nearly optimal) with non-unique solution (since a Lagrange matrix nearly singular)".

The eigenvalues of the matrix $I - M^{-1}A$, for the computed matrix M^{-1} , were all equal in magnitude, with three being positive and one negative. Upon restarting the code from a different initial guess, it returned with the same warning message but a different optimal M^{-1} . For this newly computed matrix M^{-1} , the eigenvalues of $I - M^{-1}A$, were again all equal in magnitude, and of the same magnitude as those previously computed, but this time three were negative and one positive. The elements of the two different optimal matrices M^{-1} are given in Table 2.

For smaller values of h, the problem appears to have a unique solution. The code was able to find and identify as such the optimal M^{-1} , for h = 1/5. For h = 1/4, 1/6,

eigenvalues - 1.429, 1.429, 1.429, 1.429			eigenvalues 		
diag	1st subdiag	2nd subdiag	diag	1st subdiag	2nd subdiag
2.857e-01 2.500e-01 2.500e-01 2.857e-01	7.143e-02 3.571e-02 7.143e-02	7.143e-02 7.143e-02	2.857e-01 3.214e-01 3.214e-01 2.857e-01	7.143e-02 3.571e-02 7.143e-02	7.143e-02 7.143e-02

Table 2. Two "optimal" matrices M^{-1} with same sparsity pattern as A (h = 1/3).

and 1/7, attempts at finding the minimum resulted in the code halting with the message

"radius too small"

indicating that its trust region radius had been reduced below the machine precision and it had been unable to find a descent direction. Restarting, in the case h = 1/4, resulted in the code finding approximately the same "solution", but this time giving the message "Apparently optimal (or very nearly optimal) with non-unique solution." In the case h = 1/6, several restarts resulted in the code finding approximately the same "solution", but still halting because the trust region radius was too small. A restart in the case h = 1/7, however, resulted in the code finding a significantly different approximation and identifying it as optimal. The spectral radius of $I - M^{-1}A$ for this "truly" optimal M^{-1} was .680, compared to .685 for the M^{-1} at which it stopped the first time because of a too small radius. It is believed that the spectral radii returned by the code, for the different sizes of h, are all near optimal, though the actual matrices M^{-1} may be significantly further from the optimal ones.

An approximation to A^{-1} that has been suggested in the literature [13, 22] is the following. If we write A in the form

$$A = D^{1/2}(I - G)D^{1/2}$$

where D is a diagonal matrix, and if the spectral radius of G is less than 1 (which it is for this problem), then A^{-1} is given by

$$A^{-1} = D^{-1/2}(I + G + G^2 + ...)D^{-1/2}.$$

An approximation to A^{-1} is obtained by retaining just a finite number of terms in the infinite Neumann series above. The approximation can be improved by multiplying each term retained by a appropriate constant [22]. If only one term is retained, then this approximation has the same sparsity pattern as A. Thus, A^{-1} can be approximated by

$$(3.3.1) M_1^{-1} \equiv D^{-1/2} (c_0 I + c_1 G) D^{-1/2}.$$

When A is the 5-point Laplacian, the optimal constants are just $c_0 = c_1 = 1$. The condition number of A, that of $M_1^{-1}A$, where M_1^{-1} is defined by (3.3.1), and



that of $M^{-1}A$, where M^{-1} is the optimal preconditioner having nonzeros only in diagonals where A has nonzeros (or, at least, the preconditioner returned by the optimization code) are plotted in Fig. 2. Note that the condition number of $M_1^{-1}A$ is almost the same as that of $M^{-1}A$ for all values of h! It should be noted, however, that in cases where the code was able to find a matrix which it identified as optimal, it was significantly different from the matrix in (3.3.1). The condition number of the preconditioned matrix was very nearly the same, but the eigenvalues of the optimally preconditioned matrix tended to cluster somewhat more at the ends and less in the middle. For the h = 1/5 case, for example, for the optimal M^{-1} , the matrix $I - M^{-1}A$ had 5 eigenvalues equal to -.474, 3 eigenvalues equal to +.474, and no repetitions among the remaining interior eigenvalues. Using the matrix of (3.3.1), $I - M_1^{-1}A$ had 4 eigenvalues equal to -.486, 4 equal to -.393, 2 equal to -.344, 4 equal to -.022, and 2 equal to +.486.

It is known that a polynomial preconditioner of the form (3.3.1) can reduce the number of conjugate gradient steps (over the number required with just the diagonal matrix D as preconditioner) by no more than a factor of 2 (one plus the degree of the polynomial in G) [13]. It is also known that when A is the 5-point Laplacian, for small values of h, the condition number of the matrix $M_1^{-1}A$ is approximately 1/4 that of A. This is not apparent from Fig. 2, however, because only very coarse grid sizes are shown. Because the asymptotic behavior of preconditioner (3.3.1) cannot be predicted from the figure, we are wary of predicting the behavior of the optimally preconditioned matrix based on these results. From the figure, it would appear that

the condition number of the optimally preconditioned matrix is still $O(h^{-2})$, but testing on larger problems is needed to see if this trend continues.

One experiment was performed in which the approximation to A^{-1} was allowed to have nonzeros in extra diagonals – the same diagonals in which the second degree polynomial preconditioner

$$M_2^{-1} \equiv c_0 I + c_1 G + c_2 G^2$$

has nonzeros. In this case, the code again stopped with the message "radius too small," so it is not known how close it came to finding the optimal preconditioner of the given sparsity pattern. Still, the matrix M^{-1} returned by the optimization code was considerably better than the polynomial preconditioner M_2^{-1} with the optimal coefficients, c_0 , c_1 , c_2 . For h = 1/5, the spectral radius of $I - M^{-1}A$ was .208, compared to .260 for $I - M_2^{-1}A$.

3.4. Preconditioners for the Schur complement C.

In this set of experiments we found optimal preconditioners of various forms for the Schur complement matrix C defined in (3.3). The condition number of the matrix C is $O(h^{-1})$ and, in fact, its entire eigendecomposition can be derived using Fourier analysis [6]. Based on this, one can determine analytically the optimal Toeplitz tridiagonal preconditioner [31,7] (since any Toeplitz tridiagonal matrix has the same eigenvectors as C), and it can be shown that this preconditioned matrix has condition number $O(h^{-1/2})$. With the optimization code, we were able to determine the optimal tridiagonal preconditioner, without requiring that it be Toeplitz. This turned out to be a relatively easy problem for the optimization code, with the code returning a solution which it identified as optimal, for all values of h tested. It was observed, however, that especially for the smaller values of h, the optimal tridiagonal preconditioner for C was very nearly Toeplitz. In Fig. 3 are plotted the condition numbers of C, of $K_{33}^{-1}C$, where K_{33} is as defined in (3.2), of $T^{-1}C$, where T is the optimal Toeplitz tridiagonal preconditioner for C, and of $M^{-1}C$, where M is the optimal tridiagonal preconditioner for C, returned by the optimization code. Note that the curves for $\kappa(T^{-1}C)$ and for $\kappa(M^{-1}C)$ are almost identical. In Fig. 3b, these two curves only are plotted versus $h^{-1/2}$. Based on this evidence, we make the following conjecture:

CONJECTURE 3. Let C_h be the Schur complement matrix corresponding to a center dividing line for the 5-point Laplace matrix on a grid of size h, as defined in (3.3). Let M_h be any symmetric positive definite tridiagonal preconditioner for C_h . Then the condition number $\kappa(M_h^{-1}C_h)$ of the preconditioned matrix satisfies

$$\kappa(M_h^{-1}C_h) \ge O(h^{-1/2}).$$



Fig. 3. Tridiagonal Preconditioners for C



Fig. 3b. Tridiagonal Preconditioners for C

3.5. Preconditioners of the form KK^T , where K has the same sparsity as the lower triangle of A.

Several well-known preconditioners - e.g., the incomplete Cholesky (IC) and modified incomplete Cholesky (MIC) decompositions [26,21], and the symmetric successive overrelaxation (SSOR) preconditioner [33] – are of the form KK^{T} , where K is a lower triangular matrix with the same sparsity pattern as the lower triangle of A. As mentioned earlier, the problem of finding the optimal preconditioner of this form is not one of minimizing a convex function, and so the "solution" returned by the optimization code may not be the global minimum. The code can, however, be used to find a local minimum for the spectral radius of (3.4), when K is restricted to have the same sparsity pattern as the lower triangle of A. This also turned out to be a difficult problem for the optimization code, and in all cases, it reached a point at which it could go no further because its trust region radius had been reduced below the precision of the machine. Still, the preconditioner KK^T returned by the optimization code was significantly better than those proposed in the literature. Condition numbers for the matrix preconditioned by the IC decomposition, the MIC decomposition, and the SSOR preconditioner are plotted in Fig. 4, along with that of the matrix preconditioned by KK^{T} , where K is the matrix returned by the



Fig. 4. Preconditioners of the form KK^T ; K Has Sparsity of Lower Tri(A)

optimization code. It remains to be seen how much further this condition number can be reduced.

4. Experimental results for other diffusion-type operators.

To determine if other diffusion-type elliptic operators could be preconditioned more or less effectively than the Laplacian, we attempted to compute optimal preconditioners of some of these same forms for several other operators. The problems were all of the form

$$\nabla \cdot \rho \nabla u = f$$
, on $(0, 1) \times (0, 1)$,
 $u(x, 0) = u(x, 1) = u(0, y) = u(1, y) = 0$,

where the diffusion coefficient ρ was varied. The values of ρ considered were:

(a)
$$\rho(x, y) = 1$$
 (as in the previous section)

(b)
$$\rho(x, y) = .01 + x^2 + y^2$$

(c)
$$\rho(x, y) = \begin{cases} 1 & \text{if } x < .5\\ 100 & \text{if } x \ge .5 \end{cases}$$

(d)
$$\rho(x, y) = \begin{cases} 1 & \text{if } x < .5 \text{ and } y < .5 \\ 10^4 & \text{if } x \ge .5 \text{ and } y < .5 \\ 10^{-4} & \text{if } x < .5 \text{ and } y \ge .5 \\ 5 & \text{if } x \ge .5 \text{ and } y \ge .5 \end{cases}$$

To avoid ambiguity in differencing around the discontinuities in ρ , a continuous piecewise linear finite element approximation was used to generate the matrix A corresponding to each of these operators.

4.1. Diagonal preconditioners for A.

Although a highly-varying diffusion coefficient, such as that in (d), results in a very badly conditioned finite difference or finite element matrix, it has long been known that a simple diagonal scaling could greatly reduce the condition number. In Fig. 5 are plotted the condition numbers of the matrices for these four problems, after they have been scaled by their diagonals. According to the Forsythe & Strauss theorem, this is the optimal diagonal preconditioner for these matrices. Note from the figure that after diagonal scaling, the condition numbers for all of these matrices are nearly the same, with case (b) actually being somewhat better conditioned than the Laplacian (a). In cases (c) and (d), this condition number jumps slightly when the mesh size 1/h is not even. In this case, the finite element equations are a poor



Fig. 5. Diagonally Preconditioned Elliptic Operators

approximation to the differential equation, anyway, because the discontinuity of ρ , and hence ∇u , occurs within a mesh cell.

It is also interesting to note that, although the optimal diagonal preconditioners for these problems are known, the optimization code had a great deal of difficulty in finding the solutions for cases (c) and (d). For the h = 1/4 grid, starting from an initial guess that was equal to twice the true solution, the code required 272 iterations to find the optimal diagonal preconditioner for case (c), compared to just 12 for case (b). In case (d), the code was stopped after 600 iterations when only negligible improvement had been made over the initial guess. The reasons for this difficulty are currently being investigated to determine if some rescaling or other modification of the problem can make the optimization job easier.

4.2. Preconditioners of the form $D\Delta D$, where Δ is the Laplacian and D is diagonal.

It was recently proved that the matrix A from an arbitrary second-order selfadjoint elliptic partial differential equation can be preconditioned by the matrix Δ corresponding to the Laplacian on the same grid and with the same boundary conditions so that the resulting preconditioned matrix has condition number O(1), independent of the mesh size [25]. Since the Laplacian is relatively easy to solve on a rectangular grid (and with an integral equation formulation, perhaps also on an irregular grid [26]), this might make an effective preconditioner. Unfortunately, however, the constant in the condition number bound can be quite large, and it is large for problems (c) and (d). One might ask if there is a simple modification of the



Fig. 6. Preconditioners of the Form DAD, for Elliptic Operators

Laplacian that would still be easy to solve and would give a condition number that is not only O(1) but has a small constant as well. The simplest idea is to scale the Laplacian by some diagonal matrix D and use the symmetric matrix $D\Delta D$ as the preconditioner. This is the same form of preconditioner that was studied by Concus and Golub [8], who determined the optimal such preconditioner for 1-D problems.

We used the optimization code to find the diagonal matrix D for which the spectral radius of $I - L^{-1}D \Delta D L^{-T}$ was as small as possible, and where $A = LL^{T}$ was the matrix arising from problems (b-d). Again, the optimization code had difficulty with problem (d), so we omitted this from our results. In Fig. 6 are plotted the condition numbers for problems (b) and (c), preconditioned by the optimally scaled Laplacian-type preconditioner, $D\Delta D$. Computations for case (c) were performed on somewhat finer grids than for case (b), as will be explained below. Although the condition number for each of these preconditioned matrices is bounded by a constant independent of h, we have not reached a small enough value of h to determine this constant. Clearly, problem (b) is very well-conditioned by the appropriate diagonal scaling of the Laplacian, and problem (c) is also reasonably well approximated by such a preconditioner, for the grid sizes shown.

The optimal diagonal matrix determined in problem (c) was especially interesting and has led to a new theorem about optimal preconditioners of this form. The proof of this result is too long to be included here but will appear in a following paper [20]. If nodes to the left of the discontinuity in ρ are numbered first, then nodes to the right of the discontinuity, and finally nodes on the discontinuity, then the optimal diagonal scaling for the Laplacian-type preconditioner, as determined by the optimization code, has the following form:

$$D = \begin{bmatrix} d_1 I & & \\ & d_2 I & \\ & & d_3 I \end{bmatrix},$$

where d_i , i = 1, 2, 3 are scalars and each block corresponds to one of the above mentioned subregions. Using this ordering of nodes, the matrix A arising from problem (c) has the form

$$A = \begin{bmatrix} c_1 K_{11} & 0 & c_1 K_{13} \\ 0 & c_2 K_{22} & c_2 K_{23} \\ c_1 K_{13}^T & c_2 K_{23}^T & c_3 K_{33} \end{bmatrix},$$

where the blocks $K_{i,j}$, i, j = 1, 2, 3 are the blocks of the Laplacian, and the constants c_i , i = 1, 2, 3 are

$$c_1 = 1, \quad c_2 = 100, \quad c_3 = 50.5.$$

The preconditioner $D\Delta D$ returned by the optimization code then has the form

(4.3.1)
$$A = \begin{bmatrix} d_1^2 K_{11} & 0 & d_1 d_3 K_{13} \\ 0 & d_2^2 K_{22} & d_2 d_3 K_{23} \\ d_1 d_3 K_{13}^T & d_2 d_3 K_{23}^T & d_3^2 K_{33} \end{bmatrix}$$

The scalars d_i , i = 1, 2, 3, are listed in Table 3, for grid sizes 1/h = 4, 6, 8. Seeing this pattern, we were able to go to finer grid sizes by restricting the preconditioner to be of the form (4.3.1), and having the optimization code determine only the best scalars d_i , i = 1, 2, 3. These are also listed in Table 3, for 1/h = 10, 16, and the corresponding condition numbers are plotted in Fig. 6. The condition number of the preconditioned matrix still has not reached its asymptotic limit, however, and one cannot determine from the numerical results alone what that limit is. Having seen these numerical results, however, we were able to prove the following theorem. For a more general statement and proof of this theorem, the reader is referred to [20].

THEOREM. For the problem (c) defined above, with grid size h, the optimal matrix D_h is of the form

$$\begin{bmatrix} d_{1,h}I_{1,h} & & \\ & d_{2,h}I_{2,h} & \\ & & & d_{3,h}I_{3,h} \end{bmatrix},$$

1/h	<i>d</i> ₁	<i>d</i> ₂	<i>d</i> ₃
4	1.97	16.92	13.52
6	1.94	14.60	12.77
8	1.91	13.05	12.08
10	1.89	11.98	11.49
16	1.88	10.05	10.05

Table 3. Constants defining the optimal preconditioner of the form $D\Delta D$.

where $d_{1,h}$, $d_{2,h}$, and $d_{3,h}$ are positive scalars and $I_{1,h}$, $I_{2,h}$, and $I_{3,h}$ are identity matrices corresponding to the left half of the domain, the right half of the domain, and the center dividing line, respectively. In the limit as h goes to zero, the scalars $d_{1,h}$, $d_{2,h}$, and $d_{3,h}$ all approach the same limit. Thus, in the limit as h goes to zero, the condition number of the optimally preconditioned matrix approaches that of the matrix preconditioned by the simple Laplacian, which is just $\rho_{max}/\rho_{min} = 100$.

Experiments with 1-D problems have shown that this limiting behavior may not be observed until the grid size is really very fine. (At grid size 1/h = 226, the condition number was still only about half of its asymptotic limit, and d_1 was not close to d_2 .) It is interesting to note, however, that at grid size 1/h = 16, in the 2-D problem, d_2 is already equal to d_3 . These two scalars match on relatively coarse grids, while it is only for much finer grids that the scalar d_1 approaches these two.

5. Conclusions.

We have demonstrated a very useful tool in the study of preconditioners. Again, an optimization code is not usually a practical method for finding a good preconditioner for a given problem, but rather it is intended to give insight into the properties of preconditioners and the forms of matrices that can or cannot be potentially effective preconditioners. Results from the code have led to several conjectures and a new theorem about preconditioners of various forms.

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