**THE EFFECT OF INCOMPLETE DECOMPOSITION
PRECONDITIONING ON THE CONVERGENCE OF
CONJUGATE GRADIENTS**

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IMA Preprint Series # 944

April 1992

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March 10, 1992

1 Introduction

The ICCG method, for the iterative solution of the large sparse linear system $Ax = b$ (A is symmetric positive definite) consists of the preconditioning of the system, using an incomplete Choleski decomposition K of the matrix A , and the subsequent iterative solution of this system by the conjugate gradients method. For the construction of an incomplete Choleski decomposition it is, in addition, desirable that A be an M -matrix (see, e.g., [12]).

If A is not an M -matrix then it may be necessary to take measures in order to prevent the incomplete decomposition algorithm from failing or from leading to unstable decompositions.

The improvement of the convergence behaviour of the preconditioned conjugate gradient method, as observed in practice, can only be partly understood from a reduction of the condition number. A favourable distribution of the eigenvalues appears to be an important factor. For a simple model problem we shall derive approximations for relevant eigenvalues of the preconditioned matrix $K^{-1}A$ that will help to explain the convergence behaviour.

It should be mentioned that the model problem has two disadvantages: such problems can be solved much more efficiently by certain other methods (e.g., Fast Poisson Solvers or Multigrid), and in more realistic cases (e.g., with strongly varying coefficients) often a much more impressive improvement of the convergence behaviour is observed [6].

In this paper we will first give the algorithm for conjugate gradients, together with some of the main properties of the method. Then we will for a model problem analyse the effects of preconditioning. Throughout this paper we will assume exact arithmetic.

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2 The conjugate gradient method

For the solution of the linear system $Ax = b$, with A a symmetric and positive definite n by n matrix, the conjugate gradient (CG) method can be used. This method may be represented in various alternative forms, of which we have selected the following one:

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 $x_0$  = initial guess;  $r_0 = b - Ax_0$ ;
 $p_{-1} = 0$ ;  $\beta_{-1} = 0$ ;
 $\rho_0 = (r_0, r_0)$ 
for  $i = 0, 1, 2, \dots$ 
     $p_i = r_i + \beta_{i-1}p_{i-1}$ ;
     $q_i = Ap_i$ ;
     $\alpha_i = \frac{\rho_i}{(p_i, q_i)}$ 
     $x_{i+1} = x_i + \alpha_i p_i$ ;
     $r_{i+1} = r_i - \alpha_i q_i$ ;
    if  $x_{i+1}$  accurate enough then quit;
     $\rho_{i+1} = (r_{i+1}, r_{i+1})$ ;
     $\beta_i = \frac{\rho_{i+1}}{\rho_i}$ ;
end;
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For a discussion on the CG method and its main properties we refer to [2], [3], [4] and [9]. We recall the following properties:

1. The CG method minimizes $\|x_i - x\|_A \equiv (x_i - x, A(x_i - x))^{\frac{1}{2}}$ for all i , among all algorithms of the form

$$x_i = x_0 + Q_{i-1}(A)A(x - x_0), \quad (1)$$

where $Q_{i-1}(A)$ is an $(i-1)$ -st degree polynomial in A .

Note: many well-known iteration methods can be written in this form, e.g., Richardson iteration, Chebyshev iteration.

2. Iteration (1) can be rewritten as

$$x_i - x = (I - AQ_{i-1}(A))(x_0 - x) = P_i(A)(x_0 - x), \quad (2)$$

with $P_i(0) = 1$. If we exploit the optimality property, then by selecting for P_i a shifted and normalized Chebyshev polynomial, we obtain the well-known upperbound for the error in A -norm ([1],[3]):

$$\|x_i - x\|_A \leq 2 \left(\frac{\sqrt{\kappa_2} - 1}{\sqrt{\kappa_2} + 1} \right)^i \|x_0 - x\|_A, \quad (3)$$

where κ_2 is the condition number of A with respect to the 2-norm. This upperbound is often quite realistic in the early phase of the iteration process, but it turns out to be very pessimistic on the long run since it does not account for the so-called superlinear convergence behaviour [2], [9].

3. The vectors $r_0, \dots, r_i$ are mutually orthogonal and they satisfy the recurrence relation

$$Ar_j = -\frac{\beta_{j-1}}{\alpha_{j-1}}r_{j-1} + \left(\frac{1}{\alpha_j} + \frac{\beta_{j-1}}{\alpha_{j-1}}\right)r_j - \frac{1}{\alpha_j}r_{j+1}, \quad (4)$$

which describes essentially the Lanczos algorithm [8].

Let R_i denote the matrix with columns $r_0, \dots, r_i$, then the recurrence relation can be rewritten as

$$AR_i = R_i T_i - \frac{1}{\alpha_i} r_{i+1} e_{i+1}^T, \quad (5)$$

where $e_{i+1}^T = (0, \dots, 0, 1)$, the $(i+1)$ -st unit vector of dimension $i+1$, and T_i is a tridiagonal matrix of order $i+1$.

4. The eigenvalues of T_i are called the Ritz values of A with respect to the subspace spanned by $r_0, \dots, r_i$. These Ritz values approximate some eigenvalues of A increasingly well for increasing i . It has been observed that when an extremal eigenvalue has been sufficiently well approximated by a Ritz value, then the CG process converges faster from then on (superlinear convergence behaviour) [3]. This was further analyzed and quantified in [9].
5. More refined errorbounds for CG are given in [1] and [5]. These bounds take advantage from the distribution of the (extremal) eigenvalues.

CG is most often used in combination with a suitable splitting $A = K - R$, and then K^{-1} is called the preconditioner. We will assume that K is also positive definite.

A popular scheme that includes preconditioning can be obtained from the previous scheme as follows. First we remark that the CG method can be derived for any choice of the innerproduct. If we make the choice:

$$[x, y] \equiv (x, Ky),$$

where $(\cdot, \cdot)$ denotes the innerproduct: $(x, y) = \sum x_i y_i$, then it is easy to verify that $K^{-1}A$ is symmetric positive definite with respect to $[\cdot, \cdot]$:

$$[K^{-1}Ax, y] = (K^{-1}Ax, Ky) = (Ax, y) = (x, Ay) = [x, K^{-1}Ay].$$

Hence, we can formulate the CG procedure for solving the preconditioned system $K^{-1}Ax = K^{-1}b$, using the new $[\cdot, \cdot]$ -innerproduct.

Apparently, we are then minimizing

$$[x_i - x, K^{-1}A(x_i - x)] = (x_i - x, A(x_i - x)),$$

which leads to the remarkable result that for the preconditioned system we still minimize the error in A -norm, but now with A replaced by $K^{-1}A$ in (1).

In the following computational scheme for preconditioned CG, for the solution of $Ax = b$ with preconditioner K^{-1} , we have replaced the $[\cdot, \cdot]$ -innerproduct again by the familiar standard innerproduct. E.g., note that

$$\rho_{i+1} = [K^{-1}r_{i+1}, K^{-1}r_{i+1}] = (r_{i+1}, K^{-1}r_{i+1}),$$

and $K^{-1}r_{i+1}$ is the residual corresponding to the preconditioned system

$$K^{-1}Ax = K^{-1}b.$$

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 $x_0$  = initial guess;  $r_0 = b - Ax_0$ ;
 $p_{-1} = 0$ ;  $\beta_{-1} = 0$ ;
Solve  $w_0$  from  $Kw_0 = r_0$ ;
 $\rho_0 = (r_0, w_0)$ 
for  $i = 0, 1, 2, \dots$ 
     $p_i = w_i + \beta_{i-1}p_{i-1}$ ;
     $q_i = Ap_i$ ;
     $\alpha_i = \frac{\rho_i}{(p_i, q_i)}$ 
     $x_{i+1} = x_i + \alpha_i p_i$ ;
     $r_{i+1} = r_i - \alpha_i q_i$ ;
    if  $x_{i+1}$  accurate enough then quit;
    Solve  $w_{i+1}$  from  $Kw_{i+1} = r_{i+1}$ ;
     $\rho_{i+1} = (r_{i+1}, w_{i+1})$ ;
     $\beta_i = \frac{\rho_{i+1}}{\rho_i}$ ;
end;
```

Note that this formulation, which is quite popular, has the advantage that the preconditioner needs not to be split into two factors, and it is also avoided to backtransform solutions and residuals, as is necessary when one applies CG to $L^{-1}AL^{-1T}y = L^{-1}b$ (for $K = LL^T$).

3 The model problem

We consider the Poisson equation

$$-\Delta u = f, \tag{6}$$

over the unit square in $\mathbb{R}^2$, with Dirichlet boundary conditions. Standard 5-point finite difference discretization with stepsize $\frac{1}{m+1}$ in both directions will be used, which leads to a linear system with m^2 unknowns and with a matrix A , as given in (7). An equivalent analysis can be done for unequal stepsizes and this leads to essentially the same results, but it makes most of the formulas less

transparent.

$$A = \begin{pmatrix} A_1 & C_1 & & & \\ C_1 & A_2 & C_2 & & \\ & C_2 & A_3 & \ddots & \\ & & \ddots & \ddots & \ddots \\ & & & \ddots & C_{m-1} & C_{m-1} \\ & & & & C_{m-1} & A_m \end{pmatrix} \quad (7)$$

with

$$A_j = \begin{pmatrix} a_{1,j} & b_{1,j} & & & \\ b_{1,j} & a_{2,j} & b_{2,j} & & \\ & b_{2,j} & a_{3,j} & \ddots & \\ & & \ddots & \ddots & \ddots \\ & & & \ddots & b_{m-1,j} & b_{m-1,j} \\ & & & & b_{m-1,j} & a_{m,j} \end{pmatrix}, \quad (8)$$

$$C_j = \begin{pmatrix} c_{1,j} & & & \\ & c_{2,j} & & \\ & & \ddots & \\ & & & c_{m,j} \end{pmatrix}. \quad (9)$$

The values for $a_{i,j}$, $b_{i,j}$ and $c_{i,j}$ are: $a_{i,j} = 4$, $b_{i,j} = -1$, $c_{i,j} = -1$.
The eigenvectors of A are given by

$$v_{i,j}^{k,\ell} = \sin \frac{ik\pi}{m+1} \sin \frac{j\ell\pi}{m+1}, \quad 1 \leq i, j, k, \ell \leq m, \quad (10)$$

where $v_{i,j}^{k,\ell}$ is the (i, j) -th component of $v^{k,\ell}$, corresponding to the i -th gridpoint on the j -th gridline (there are m gridlines with m gridpoints each).

The eigenvalue corresponding to $v^{k,\ell}$ is

$$\lambda^{k,\ell} = 4 - 2 \cos \frac{\pi k}{m+1} - 2 \cos \frac{\pi \ell}{m+1}. \quad (11)$$

Throughout this paper the incomplete decomposition of A will be the following splitting:

$$A = K - R \quad \text{with} \quad K = (L + \tilde{D})\tilde{D}^{-1}(\tilde{D} + L^T), \quad (12)$$

where K is defined by

1. $\text{diag}\left((L + \tilde{D})\tilde{D}^{-1}(\tilde{D} + L^T)\right) = \text{diag}(A) \equiv D$
2. L is a lower triangular matrix, whose subdiagonal elements equal those of A
3. $\tilde{D}$ is a diagonal matrix whose diagonal elements equal those of L .

If, according to the notation in (8), the diagonal elements of $\tilde{D}$ are denoted by $d_{i,j}$, then they can be computed recursively from

$$d_{i,j} = a_{i,j} - \frac{b_{i-1,j}^2}{d_{i-1,j}} - \frac{c_{i,j-1}^2}{d_{i,j-1}} \quad (13)$$

(Convention: Here, and elsewhere in this paper, terms involving factors with an index 0 or $m+1$ should be omitted).

For any vector u we have

$$(Ru)_{i,j} = \frac{b_{i,j-1}c_{i,j-1}}{d_{i,j-1}}u_{i+1,j-1} + \frac{b_{i-1,j}c_{i-1,j}}{d_{i-1,j}}u_{i-1,j+1}. \quad (14)$$

This incomplete decomposition belongs to the class of incomplete Choleski decompositions [7]; it is the standard decomposition with no fill-in. The existence of these and other incomplete decompositions was proven for M -matrices in [7]. For the model problem it is straightforward to prove from the recurrence relations (13) that

$$0 < \frac{1}{d_{i,j}} < \frac{1}{d} \quad \text{with } d = 2 + \sqrt{2}. \quad (15)$$

4 Eigenvalues of the preconditioned matrix

For the model problem (the discretized Poisson problem) we can derive quite accurate bounds on the eigenvalues of the preconditioned matrix. In this section we will discuss the bound for the largest eigenvalue only, the derivation for the bounds on the smallest eigenvalues follows similar ideas and will be omitted here.

The preconditioned matrix $K^{-1}A$ is a product of two symmetric positive definite matrices and hence its eigenvalues are positive real. The splitting $A = K - R$, as defined above, defines a regular splitting [7], and therefore the spectrum of $K^{-1}A$ is contained in the interval $(0, 2)$. This result guarantees the convergence of the basic iteration $x_i = x_{i-1} + K^{-1}(b - Ax_{i-1})$, but it does not explain the success of preconditioning in the conjugate gradient process. To that end we need more refined bounds.

Note that if λ is an eigenvalue of $K^{-1}A$, then 0 must be in the spectrum of $\lambda K - A$ (denoted by $\sigma(\lambda K - A)$). The main idea is to split from $\lambda K - A$ a

positive definite part as large as possible. This will help us to bound $\sigma(\lambda K - A)$ from below. It is easy to verify that

$$\begin{aligned}\lambda K - A &= \frac{1}{\lambda} \left[((1 - \lambda)\tilde{D} - \lambda L)\tilde{D}^{-1}((1 - \lambda)\tilde{D} - \lambda L^T) - (1 - 2\lambda)\tilde{D} - \lambda D \right] \\ &= \frac{1}{\lambda} [W(\lambda) + V(\lambda)]\end{aligned}\tag{16}$$

with $V(\lambda) = -(1 - 2\lambda)\tilde{D} - \lambda D$. Since $W(\lambda)$ is symmetric non-negative definite, the diagonal matrix $V(\lambda)$ cannot be positive definite if we want to have $\lambda K - A$ singular. For our model problem this leads immediately to the condition that

$$\lambda \leq \frac{d}{2d - 4} = (1 + \sqrt{2})/2 \approx 1.20711.\tag{17}$$

For the 30 by 30 model problem the true largest eigenvalue of the preconditioned matrix has been computed to be ≈ 1.20455 . This is remarkably close to the derived upperbound.

By slightly more complicated techniques also bounds for some of the smallest eigenvalues of $K^{-1}A$ can be derived (this will be published elsewhere). These eigenvalue approximations can be used to bound the number of preconditioned CG steps necessary to reduce the residual by at least 10^{-12} . To that goal we used Chebychev-type bounds, as proposed in [5]. This approach led to a prediction of 51 iterations at most, if we used only the information for the five smallest eigenvalues and the upperbound for the largest one [11]. The position of all the other eigenvalues is irrelevant for obtaining that bound on the number of iterationsteps. Would we have used the exact locations of the required eigenvalues, then that would have led to a predicted 50 iterationsteps. In actual computation we have seen as many as 44 iterationsteps for some random generated right-hand sides.

We see that only the largest eigenvalue as well as the position of a few of the smallest eigenvalues is really necessary for getting a realistic upperbound on the number of iterationsteps (at least for the required reduction factor for the residuals). Here we have taken the 30 by 30 model problem as an example. In the next section we will discuss the convergence behaviour of CG for more general sizes.

5 A discussion on the convergence of ICCG

In the previous section we have argued that at least for the 30 by 30 model problem the number of iterationsteps for preconditioned CG could be predicted quite accurately. A natural question is, of course, whether this situation is typical for what happens when the size (m) is much larger. In this section we

will shed light on this matter.

For m large, the bounds on the smallest eigenvalues, as sketched in the previous section, turn out to be rather close. Hence, denoting the eigenvalues of $K^{-1}A$ as $\lambda_1 \leq \lambda_2 \leq \lambda_3 \leq \dots$, we have for an increasing number of successive smallest eigenvalues (as m increases):

$$\lambda_1 \approx \frac{d}{2}\lambda^{1,1}, \lambda_2 \approx \lambda_3 \approx \frac{d}{2}\lambda^{1,2} = \frac{d}{2}\lambda^{2,1}, \lambda_4 \approx \frac{d}{2}\lambda^{2,2}, \dots \quad (18)$$

Since $\lambda_{\max}(A) \approx 8$ and $\lambda_{\max}(K^{-1}A) \approx 1.207$, we have for the condition number $\kappa_2(A)$ of A

$$\kappa_2(A) \approx \frac{4(m+1)^2}{\pi^2}, \quad (19)$$

and for the condition number of $K^{-1}A$ we find

$$\kappa_2(K^{-1}A) \approx \frac{1.207}{4(2+\sqrt{2})}. \quad (20)$$

The rates of convergence of the CG algorithm for the unpreconditioned and the preconditioned case are then, according to (3)

$$r_A = \frac{\sqrt{\kappa_2(A)} - 1}{\sqrt{\kappa_2(A)} + 1} \approx 1 - \frac{2}{\sqrt{\kappa_2(A)}}, \quad (21)$$

and

$$r_{K^{-1}A} = \frac{\sqrt{\kappa_2(A)/\alpha} - 1}{\sqrt{\kappa_2(A)/\alpha} + 1} \approx 1 - \frac{2}{\sqrt{\kappa_2(A)}}\sqrt{\alpha}, \quad (22)$$

with $\sqrt{\alpha} \approx 3.3$.

We will further refer to the unpreconditioned process as CG and to the preconditioned process as ICCG.

We conclude that in the first phase of the iteration process, i.e., the phase in which the convergence behaviour can be described reasonably well by the condition number, a comparative accuracy will be achieved by ICCG within $\approx \sqrt{\alpha}$ times fewer iterations, and we note that this factor is independent of m . This corresponds quite nicely to what we see for the actual numbers of iterations when only moderate accuracies are required (say 10^{-6} or less).

Once the smallest Ritz value, associated with CG, has come close to the smallest eigenvalue of A (and even a modest degree of approximation suffices, see [9]), the convergence behaviour of CG will be more appropriately described by the "effective" condition number $8/\lambda^{1,2}$. Likewise, as soon as this happens for ICCG, the effective condition number for ICCG will be at most $1/\alpha$ times that value. Now we note that the length of the spectrum of $K^{-1}A$ is smaller than the

length of the spectrum of A , and on account of the estimates for the smallest eigenvalues we have

$$|\lambda_1 - \lambda_2| \approx \frac{d}{2} |\lambda^{1,1} - \lambda^{1,2}| \quad (23)$$

with $\frac{d}{2} > 1$).

Hence, in the terminology of Parlett [8], the smallest eigenvalue of $K^{-1}A$ has a larger gap ratio than the corresponding one of A . In addition the smallest eigenvalues of A and $K^{-1}A$ share almost the same eigenvectors (for m not too small), see [11]. Theorem 12-4-1 in [8] then indicates that we may expect the smallest eigenvalue of $K^{-1}A$ to be approximated to the same accuracy within fewer iterations than is the case for A .

Therefore we may expect ICCG to take sooner advantage of a reduced effective condition number (and, indeed: for $m = 30$ we find in practice that the first Ritz value for ICCG converges to 5 decimal places, within the first 15 iterations, whereas for CG this takes about 50 iterations).

A similar discussion about the subsequent phases might seem more complicated, because of the occurrence of almost double eigenvalues in ICCG, which leads to complications in the convergence of the Ritz values towards these close eigenvalues [10]. However, in [9] it has been shown that an almost double eigenvalue leads to only a modest delay in convergence of the (preconditioned) CG process, compared to the situation where the almost double eigenvalues have been replaced by one single eigenvalue.

Here we have focussed on the separation of the smallest eigenvalues. Note that we need much larger gaps at the upper end of the spectrum in order to obtain similar reductions in the effective condition number.

In conclusion we see that the successive phases of the iteration process for ICCG are entered within fewer iterations than the corresponding ones in CG. Since, in addition, in each phase of ICCG the convergence is $\approx \sqrt{\alpha}$ times faster than the corresponding phase of CG, it is clear that we should expect ICCG to be very much faster than CG for large values of m . Note that it is, contrary to popular belief, not so much the clustering of the eigenvalues near 1 which helps to explain the effect of preconditioning, but that this effect, at least for practical reductions of the error, can be largely explained by the reduction of the condition number and the improved relative separation of only a few of the smallest eigenvalues.

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