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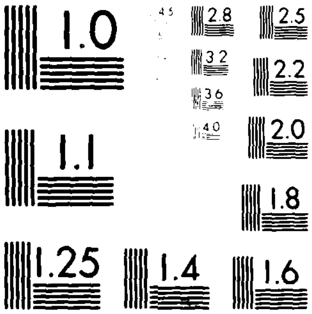

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The incomplete Cholesky decomposition and the subsequent iterative solution by the conjugate gradient method has been described recently by D. Kershaw [1]. The drawback of a triangular decomposition on a vector machine is the need for recursive computations. This paper proposes a method which eliminates the need for recursive computations. They are replaced by a number of non-recursive operations. This method can be utilized in the solution of potential equations in late time electrostatic codes.

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CONTENTS

A NON-RECURSIVE INCOMPLETE CHOLESKY DECOMPOSITION METHOD FOR THE SOLUTION OF LINEAR EQUATIONS WITH A SPARSE MATRIX

I. Introduction

The algorithm described in this paper is applicable to diagonally dominant matrices. It makes use of the fact that an incomplete Cholesky or LU decomposition which imposes a certain sparsity is actually an expansion in powers of off diagonal elements. It is therefore pointless to compute the elements of the tridiagonal matrices and the solution to infinite order by recursive procedures. It is self-consistent and sufficient to compute these quantities to the same order as the one introduced by the imposed sparsity of the tridiagonal decomposition.

The first section describes the method for symmetric matrices. The extension to non-symmetric matrices is achieved by iterating the solutions for the symmetric component of the matrix where the source terms contain the non-symmetric contributions from the previous iteration.

The second section gives the times and number of iterations used for a test case taken from a NRL electrostatic code. It involves the solution of an elliptic partial differential equation with variable coefficients in the two dimensions.

The third section gives some conclusions.

II. Algorithm

1) General considerations

The linear system of equations to be solved for the vector x can be written in the form

$$Mx = y \tag{1}$$

x,y are vectors of length N and Det(M) $\neq$ 0.

Manuscript submitted May 2, 1980

In order to explain the following concepts one must introduce the definition of weakly and strongly diagonally dominant matrices. A matrix A is defined to be weakly diagonally dominant if

$$W_{ij}(A) \equiv 1 - \frac{|A_{ij}|}{\min(|A_{ii}|,|A_{jj}|)} \geq 0 \qquad (2)$$

for all i,j;i $\neq$ j

A matrix A is defined to be strongly diagonally dominant if

$$S_j(A) \equiv 1 - \sum_{k\neq j} \Big(|A_{jk} A_{kj}/A_{kk}|\Big) / |A_{jj}| \geq 0 \qquad (3)$$

for all j.

Let L and U be two lower and upper triangular matrices respectively, subject to the following two conditions

a) $W(L^{-1}MU^{-1}) \geq W(M) \geq 0$ (4)

b) The inversions

$$z = L^{-1}y$$
$$x = U^{-1}z \qquad (5)$$

with z a vector of length N can be performed exactly.

Equation (1) can be transformed into

$$L^{-1}MU^{-1}(UX) = L^{-1}y \qquad (6)$$

It is obvious that Eq. (6) is easier to solve than Eq. (1). Any iteration scheme will use fewer iterations. One should also remark that neither L, U, or L^{-1}, U^{-1} have to be known, but only the results of L^{-1}, U^{-1} applied to a vector.

The real question is how one finds good matrices L, U with a minimum of operations, such that Eq. (6) can be solved with a few iterations. This is especially important in time-dependent problems where a good approximation to the solution is known from the previous timestep. It is clear that with more operations one could find a better L and U, thereby reducing the number of iterations needed to solve Eq. (6). The problem is to find an algorithm which minimizes the total number of operations.

For most physical problems (elliptic equations in two or three dimensions) the matrix M is sparse with an (average) bandwidth $B \ll N$. The number of operations Op should be

$$Op \approx B \cdot N\, f(N) \tag{7}$$

where f(N) is a weakly increasing function of N. Also, the algorithm should not contain recursive formula, which invoke scalar operations on a vector computer (ASC, CRAY, . . .) or parallel computer (ILLIAC).

2) Expansion in connections

In order that the following approximation for L and U be valid the matrix M must have two properties

a) the average bandwidth $B \ll N$

b) M must be expandable.

Condition b) will be explained now.

A connection of ν^{th} order is to be defined as

$$\epsilon_{ik}^{\nu+1} = \sum_{\substack{j \neq i \\ j \neq k}} \epsilon_{ij}^{\nu} M_{jk}/M_{jj} \; ; \; \nu \geq 1 \tag{8}$$

with

$$\epsilon_{ik}^{1} = M_{ik} \tag{9}$$

Then M is expandable if for all ν

$$|\epsilon_{ik}^{\nu+1}| \leq \max_j(|\epsilon_{ij}^{\nu}|,|M_{jk}|) \qquad (10)$$

It is obvious that the condition of strong diagonal dominance

$$S(M) > 0$$

is sufficient. Furthermore, if M is expandable then

$$W(M) > 0$$

M is weakly diagonally dominant. Therefore, the necessary and sufficient conditions for expandability lie somewhere between weak and strong diagonal dominance. The computation of L, U will be an expansion in the number of connections, thus avoiding recursion procedures. In general, given a recursion formula

$$\mu_i = \sigma_i + \varepsilon\mu_{i-1} \qquad i = 1,n \qquad (11)$$

with $o < \epsilon < 1$.

The iterative formula

$$\eta_i^{\nu} = \sigma_i + \epsilon\eta_{i-1}^{\nu-1} \qquad i = 1,n$$

$$\eta_i^{o} = \sigma_i \qquad (12)$$

will give the same results after n iterations. Terminating after the ν^{th} iteration gives the results to order $\epsilon^{\nu+1}$. All recursion formula which do occur will be replaced by an iteration with a very small ν. The matrices L, U will be computed to a certain order in the expansion in the number of connections. In order to explain this procedure the triangular decomposition is briefly described here without proof.

Let

$$1/D_j = L_{ii} = U_{ii} = M_{ii} - \sum_{k<i} L_{ik} D_k U_{ki}$$

$$L_{ii} = 0 \qquad j < i$$

$$L_{ii} = M_{ji} - \sum_{k<i} L_{jk} D_k U_{ki} \qquad j \geq i$$

$$U_{ji} = 0 \qquad j > i$$

$$U_{ji} = M_{ji} - \sum_{k>i} L_{jk} D_k U_{ki} \qquad j \leq i. \tag{13}$$

Then

$$M_{ij} = \sum_k L_{ik} D_k U_{kj} \tag{14}$$

and one can solve

$$z_i = D_i (y_i - \sum_{k<i} L_{ik} z_k)$$

$$x_i = z_i - \sum_{k>i} U_{ik} D_k x_k \tag{15}$$

directly.

The incomplete Cholesky or incomplete LU decomposition consists of imposing a specified sparsity on L, U. The order of approximation is

$$\eta = \nu_{(S)} + 1 \tag{16}$$

where $v_{(S)}$ is the highest possible connectivity given by the sparsity imposed on L and U (or η is first one neglected).

The recursion formulae in computing L, U (Eq. (13)) are reset by iteration to the order μ, which leaves an error of $0(\mu + 1)$. These iterations can be written as follows

$$\begin{aligned} 1/D_i^{\nu} &= M_{ji} - \sum_{k<i} L_{ik}^{\nu-1} D_k^{\nu-1} U_{ki}^{\nu-1} \\ L_{ji}^{\nu} &= M_{ji} - \sum_{k<i} L_{jk}^{\nu-1} D_k^{\nu-1} U_{ki}^{\nu-1} \qquad \nu = 1,\mu \\ U_{ji}^{\nu} &= M_{ji} - \sum_{k>i} L_{jk}^{\nu-1} D_k^{\nu-1} U_{ki}^{\nu-1} \end{aligned} \tag{17}$$

with

$$\begin{aligned} 1/D^{o} &= M_{ii} \\ L_{ji}^{o} &= M_{ji} \qquad j \geq i \\ U_{ji}^{o} &= M_{ji} \qquad j \leq i \\ z_i^{\nu} &= D_i^{\mu} (y_i - \sum_{k<i} L_{ik}^{\mu} z_k^{\nu-1}) \\ x_i^{\nu} &= z_i^{\mu} - \sum_{k>i} U_{ik} D_k^{\mu} x_k^{\nu-1} \qquad \nu = 1,\mu \end{aligned} \tag{18}$$

with

$$\begin{aligned} z_i^{o} &= D_i^{\mu} y_i \\ x_i^{o} &= z_i^{\mu} \end{aligned} \tag{19}$$

This procedure gives a matrix

$$L^{-1} MU^{-1}$$

whose off diagonal elements consists of errors of order $\nu_{(S)} + 1$ left by imposing a specified sparsity S, and errors of order $\mu + 1$ caused by resetting the recursion formula by iteration.

3) Example

As an example the five point difference formula for an elliptic equation in two dimensions is taken. M at one point, j,k is then

$$M = \begin{array}{ccc|c} & -\mu_y & & k-1 \\ -\mu_x & 1 & -\mu_x & k \\ & -\mu_y & & k+1 \\ \hline j-1 & j & j+1 & \end{array} \tag{20}$$

Then imposing the same sparsity on L and U and for $\nu = 1,2$ gives:

$$L^{(\nu)} = \begin{array}{ccc|c} & 0 & & k-1 \\ 0 & 1/D^{(\nu)} & -\mu_x & k \\ & -\mu_y & & k+1 \\ \hline j-1 & j & j+1 & \end{array} \tag{21}$$

$$U^{(\nu)} = \begin{array}{ccc|c} & -\mu_y & & k-1 \\ -\mu_x & 1/D^{(\nu)} & 0 & k \\ & 0 & & k+1 \\ \hline k-1 & k & k+1 & \end{array} \tag{22}$$

with $D^{(1)} = 1 \qquad D^{(2)} = \dfrac{1}{1-\mu_x{}^2-\mu_y{}^2}$ (23)

This yields:

$$(L^{-1}MU^{-1})^{(1)} = \begin{array}{ccccc|c} 0 & 0 & -\mu_y^2 & 0 & 0 & k-2 \\ 0 & -2\mu_x\mu_y & 0 & -\mu_x\mu_y & 0 & k-1 \\ -\mu_x^2 & 0 & 1-\mu_x^2\mu_y^2 & 0 & -\mu_x^2 & k \\ 0 & -\mu_x\mu_y & 0 & -2\mu_x\mu_y & 0 & k+1 \\ 0 & 0 & -\mu_y^2 & 0 & 0 & k+2 \\ \hline j-2 & j-1 & j & j+1 & j+2 & \end{array} \qquad (24)$$

This is not a good approximation to a unity matrix. Therefore, one more iteration step has to be taken;

$$(L^{-1}MU^{-1})^{(2)} =$$

$$\begin{array}{ccccccc|c} 0 & 0 & 0 & -\mu_y^3 & 0 & 0 & 0 & k-3 \\ 0 & 0 & -3\mu_y^2\mu_x & 0 & -\mu_y^2\mu_x & 0 & 0 & k-2 \\ 0 & -3\mu_y\mu_x^2 & 0 & -\mu_y\mu_x^2 & -\mu_y\mu_x & -\mu_y\mu_x^2 & 0 & k-1 \\ -\mu_x^3 & 0 & -\mu_y^2\mu_x & 1 & -\mu_y^2\mu_x & 0 & -\mu_x^3 & k \\ 0 & -\mu_y\mu_x^2 & -\mu_y\mu_x^2 & -\mu_y\mu_x^2 & 0 & -3\mu_y\mu_x^2 & 0 & k+1 \\ 0 & 0 & -\mu_y^2\mu_x & 0 & -3\mu_y^2\mu_x & 0 & 0 & k+2 \\ 0 & 0 & 0 & -\mu_y^3 & 0 & 0 & 0 & k+3 \\ \hline j-3 & j-2 & j-1 & j & j+1 & j+2 & j+3 & \end{array}$$

This is a much better approximation to the unity matrix correct to terms of third order, except for the off diagonal terms $\mu_x\mu_y$ caused by the sparsity imposed on L and U. A complete recursion would give only the expansion of those off diagonal terms. A third order $(L^{-1}MU^{-1})^{(3)}$ with the inclusion of these off diagonal elements will give 4th order accuracy.

4) The conjugate gradient method

A short description of the conjugate gradient method which is used to solve the equation

$$L^{-1}MU^{-1}(Ux) = L^{-1}y \tag{26}$$

is given for completeness. The procedure is taken from Kershaw's [1] paper where further references can be found. It minimizes (x, Mx-y). For other norms see the paper by Petravic [2]. The conjugate gradient method can only be applied to symmetric matrices. The handling of asymmetric matrices will be discussed in the next paragraph.

Let the zero order approximation vector r and p be defined by

$$\begin{aligned} r^{(o)} &= y - Mx^{(o)} \\ p^{(o)} &= (LL^T)^{-1} r^{(o)} \end{aligned} \tag{27}$$

where $x^{(o)}$ is an approximation to the solution x. Compute two auxiliary vectors as

$$\begin{aligned} q^{(\lambda)} &= Mp^{(\lambda)} \\ s^{(\lambda)} &= (LL^T)^{-1} r^{(\lambda)} \end{aligned} \tag{28}$$

and two scalar products

$$\begin{aligned} \alpha^{(\lambda)} &= (r^{(\lambda)}, s^{(\lambda)}) \\ \beta^{(\lambda)} &= (p^{(\lambda)}, q^{(\lambda)}) \end{aligned} \tag{29}$$

The next iteration vectors are then given by

$$x^{(\lambda+1)} = x^{(\lambda)} + \frac{\alpha^{(\lambda)}}{\beta^{(\lambda)}} p^{(\lambda)}$$

$$r^{(\lambda+1)} = r^{(\lambda)} - \frac{\alpha^{(\lambda)}}{\beta^{(\lambda)}} p^{(\lambda)} \tag{30}$$

$$p^{(\lambda+1)} = s^{(\lambda+1)} + \frac{\alpha^{(\lambda+1)}}{\alpha^{(\lambda)}} p^{(\lambda)}$$

5) Non-symmetric matrices

Non-symmetric matrices M arise in physical problems from different sources: gradients that can also be present in elliptic equations, non-separable coordinate systems and most important from Neumann boundary conditions. The method proposed by Kershaw [1] did not work very well in test problems. It consists essentially of multiplying

$$L^{-1}MU^{-1}(Ux) = L^{-1}y \tag{31}$$

by the transposed matrix $(L^{-1}MU^{-1})^T$ and then solving the resulting linear system. One can easily see that off diagonal elements are multiplied essentially by two. Therefore, the convergence of the conjugate gradient method is slowed. Even worse is to take M^TM. Then the condition of expandability is not fullfilled for elliptic equations. The method used here is to solve for the asymmetry by iteration. Let

$$M_s = \frac{1}{2}(M + M^T)$$

$$\delta M = \frac{1}{2}(M - M^T) \tag{32}$$

Let σ denote the iteration for the asymmetry, then

$$M_s x^{(\sigma)} = y - \delta M x^{(\sigma-1)} \tag{33}$$

One can go one step further and correct $x^{(\sigma-1)}$ as used in the above equation. Let

$$r^{(\sigma)} = S - Mx^{(\sigma)} - \delta M\tilde{x}^{(\sigma-1)} \tag{34}$$

Then

$$M_s(r^{\sigma} + \delta x) = 0$$

or

$$M_s\delta x = - r^{(\sigma)} \tag{35}$$

Now use LL^T in above equation and define

$$\tilde{x}^{(\sigma)} = x^{(\sigma)} - (LL^T)^{-1} r^{(\sigma)} \tag{36}$$

for the right hand side of Eq. (33).

III. Numerical results

Test runs have been made with an elliptic equation which arises in numerical simulations of electrostatic plasma flow:

$$\left(\frac{\partial}{\partial x}\ \sigma\,\frac{\partial}{\partial x} + \frac{\partial}{\partial y}\ \sigma\,\frac{\partial}{\partial y}\right) f = \frac{\partial\sigma}{\partial x} \qquad 0 < x,y < 1 \tag{37}$$

$$\sigma = 1 + \beta\cdot\exp\left[-\left(\frac{x-x_o}{\ell_x}\right)^2 - \left(\frac{y}{\ell_y}\right)\right]$$

The partial differential equation was translated into a five point formula in two different ways; a) by leaving σ inside of the second derivative and b) by taking the differentiation of σ out of the second derivatives and treating the first derivatives of σ separately.

$$\frac{1}{dx^2}\left[(\sigma_{j+1,k}+\sigma_{j,k})(f_{j+1,k}-f_{j,k})-(\sigma_{j,k}+\sigma_{j-1,k})(f_{j,k}-f_{j-1,k})\right]$$

$$+\frac{1}{dy^2}\left[(\sigma_{j,k+1}+\sigma_{j,k})(f_{j,k+1}-f_{j,k})-(\sigma_{j,k}+\sigma_{j,k-1})(f_{j,k}-f_{j,k-1})\right]$$

$$=\frac{1}{2dx}(\sigma_{j+1,k}-\sigma_{j-1,k}) \qquad (38)$$

while b) gives

$$\frac{1}{dx^2}\left[(f_{j+1,k}-2f_{j,k}+f_{j-1,k})+\frac{1}{4\sigma_{j,k}}(\sigma_{j+1,k}-\sigma_{j-1,k})(f_{j+1,k}-f_{j-1,k})\right]$$

$$+\frac{1}{dy^2}\left[(f_{j,k+1}-2f_{j,k}+f_{j,k-1})+\frac{1}{4\sigma_{j,k}}(\sigma_{j,k+1}-\sigma_{j,k-1})(f_{j,k+1}-f_{j,k-1})\right]$$

$$=\frac{1}{2\sigma_{j,k}dx}(\sigma_{j+1,k}-\sigma_{j-1,k}). \qquad (39)$$

Version a) is symmetric; b) is not.

Test runs have been made with β from 10^4 to .1, ℓ_x, ℓ_y from .1 to .5. The number of points in x and y has been varied between 25 and 100. The rms error:

$$\text{rms} \equiv \sqrt{\frac{(Mx-s)^2}{s^2}} \text{ varied between } 10^{-3} \text{ and } 10^{-5}.$$

The general experience gained by the test runs can be summarized as follows.

1) The need for double precision on the ASC (the ASC has a 32-bit word). The reason seems to be that the orthogonalization has to be achieved with high precision.

2) A simple-minded iterative scheme with single precision worked well only for a low accuracy and relatively small $n \leq 30$. The scheme eventually did converge but with a great number of iterations.

3) The use of recursion rather than iteration for the incomplete LU decomposition for a specific approximation did not (essentially) change the convergence rate.

4) The use of $\mu = 3$, $\nu_{(S)} = 2$ compared to $\mu = 2$, $\nu_{(S)} = 1$ decreases the number of iterations in about the same ratio as the number of operations per point increases. Therefore, the total time remained essentially constant.

5) The use of recursion in the second index (allowing partial vectorization on a vector-computer) only decreased slightly the number of iterations. It seems to be more appropriate - at least in the test cases run - to use the same approximation in the x and y directions. There may be asymmetric cases where this will not be true.

Timing

The number of operations per point is:

Scalar products	2
Compute x,r,p	6
q = Mp	9
Total	17
rms error	11

The number of operations for $x = (LL^T)^{-1}$ depends on the approximation. Let nsca be the equivalent number of vector operations for one scalar operation; then the ratio of operations for the equivalent number for a recursive procedure becomes for $\mu = 2$, $\nu_{(S)} = 1$, for $\mu = 3$, $\nu_S = 2$

$$r_1 = \frac{38}{4\text{nsca} + 24} \qquad r_2 = \frac{58}{4\text{nsca} + 26}$$

This gives for nsca = 20 (≈ factor for the ASC)

$$r_1 = .37 \qquad\qquad r_2 = .55$$

The iterative procedure can be vectorized over the whole array. For the recursive procedure the remaining vectorization can be only achieved for an inner loop, thus increasing the setup times compared to the iterative procedure. Also the more efficient use of two pipes on the ASC machine decreases the ratio further. Test runs have shown for $\mu = 2$, $\nu_S = 1$ an overall savings of about a factor of 5.

The total number of iterations N_i seems to be proportional to

$$N_i \approx (N_x N_y)^{3/2}$$

The dependence of N_i on the error reduction rate seems to be more complicated, roughly speaking 5 iterations per factor 10, such that the convergence factor is $f_{red} = (.1)^{1/5}$. In contrast to ADI and other methods the convergence factor seems to be more or less constant and independent of the error itself.

Imposing the Neumann boundary condition $\frac{\partial f}{\partial y} = 0$ at $y = \pm 1$ introduces an asymmetric matrix M. The number of iterations about the asymmetry is on average two. The program imposes at each iteration an error limit which is about 1/2 the error of the asymmetry. It thereby avoids unnecessary iterations for the symmetric solutions. Test runs have shown that the number of iterations (computing time) increases by about 50%, when compared to the same problem using Dirichlet boundary conditions.

In time dependent problems the computing time depends to a large extent on the guess of f_o. Crude time dependent calculations where the center of the exponential function is simply shifted and f_o is set to the previous solution, gives a reduction of about 3 - 10 over that given by $f_o = 0$, depending on the required rms error and Nx, Ny. The relationships for N_i and f_{red} still hold approximately. The reduction is about 10 for higher accuracy and lower for a lower accuracy because the change in f is the same.

S. Zalesak has used the scheme extensively in his electrostatic code. For small error (rms = 10^{-3}) and bad approximations the code runs about as fast as a vectorized ADI. For higher accuracy (10^{-4}) and a good approximation the code runs about two times faster than ADI with an accuracy of 10^{-3}. ADI did not converge after a reasonable number of iterations for a rms error of 10^{-4}.

IV. Conclusion

A vectorized incomplete Cholesky description scheme for the solution of large linear systems for sparse matrices has been developed. The vectorization is achieved by systematically replacing recursive formulae by non-recursive expansions in connection strength, both in the incomplete LU decomposition and in applying $(LU)^{-1}$ to a vector. The conjugate gradient method assures convergence. The saving in computing time over the recursive solution on a vector machine is about a factor five.

V. Acknowledgement

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