Applied Numerical Mathematics 3 (1987) 339–345
North-Holland

A NOTE ON THE CAPACITANCE MATRIX ALGORITHM, SUBSTRUCTURING, AND MIXED OR NEUMANN BOUNDARY CONDITIONS

Dianne P. O'LEARY
Mathematical Analysis Division, National Bureau of Standards, Gaithersburg, MD 20899, U.S.A.; and Computer Science Department and Institute for Advanced Computer Studies, University of Maryland, College Park, MD 20742, U.S.A.

We develop in this work variants of the capacitance matrix algorithm which can be used to solve discretizations of elliptic partial differential equations when either the original system of equations or one which arises from substructuring has a rank-deficient matrix.

1. Introduction

The capacitance matrix algorithm is a variant of the Woodbury formula for updating the inverse of a modified matrix. It has been applied very successfully to the solution of finite difference or finite element problems arising from elliptic partial differential equations (see, for example, Hockney [6], Proskurowski and Widlund [11] and O'Leary and Widlund [9]). The standard algorithm requires that the discretization matrix and the related matrix for which a "fast" solver exists are nonsingular. We study in this work the case where one or both of these matrices are rank-deficient. The case in which one of the matrices is deficient has been studied previously by Buzbee, Dorr, George, and Golub [3]. The work presented here results in slightly different algorithms for this case and also handles the case in which both matrices are singular. Lewis and Rehm [8] and Proskurowski and Widlund [10,11] discuss alternate methods for computation with two singular matrices, based on conjugate gradients preconditioned by the related matrix. Astrakhantsev [2] studies another iterative method for this problem, and Gunzburger and Nicolaides [5] propose a direct factorization technique.

As a very simple example, consider the model problem

$$-u_{xx} - u_{yy} = f(x, y) \quad \text{on } \Omega,$$

where the region Ω consists of a union of rectangles, and appropriate boundary conditions (Dirichlet, Neumann, or mixed) are given (see Fig. 1). We discretize the problem into $Ax = b$ by either finite difference or finite element techniques.

In order to solve $Ax = b$ efficiently, it is tempting to take advantage of the fact that the matrix A is related to the matrix B corresponding to a direct sum of matrices for problems on rectangles ("substructures") each of which has either Dirichlet or Neumann boundary conditions on each side. Fast algorithms exist for the solution of such problems. To see the relationship between A

0168-9274/87/$3.50 © 1987, Elsevier Science Publishers B.V. (North-Holland)

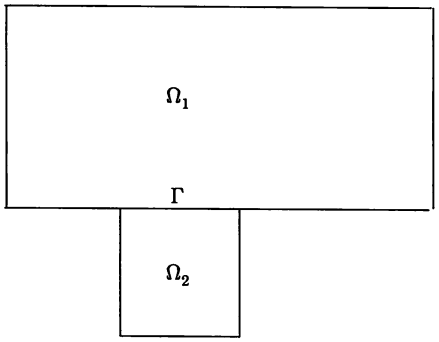

Fig. 1. The domain for the model problem.

and B, we order the equations and unknowns by considering first Ω_1, then Ω_2 and finally Γ. Then the matrix A has the structure

$$A = \begin{bmatrix} A_{11} & 0 & A_{13} \\ 0 & A_{22} & A_{23} \\ A_{31} & A_{32} & A_{33} \end{bmatrix}.$$

The matrix B corresponding to a discretization of the same partial differential equation over $\Omega_1 \cup \Gamma$ and over Ω_2 separately is

$$B = \begin{bmatrix} B_{11} & 0 & B_{13} \\ 0 & B_{22} & 0 \\ B_{31} & 0 & B_{33} \end{bmatrix},$$

where B_{22} is either equal to A_{22} or differs from it by a matrix of small rank corresponding to different boundary conditions along Γ, and B_{11} is equal to A_{11}. In this case, the two substructures are disjoint.

Another way to substructure is to allow the points in Γ to belong to both domains. In this case we have, for example

$$B = \begin{bmatrix} B_{11} & 0 & B_{13} \\ 0 & B_{22} & B_{23} \\ B_{31} & 0 & B_{33} \end{bmatrix},$$

and solutions of equations involving B require solving a problem on $\Omega_1 \cup \Gamma$ and then a problem on $\Omega_2 \cup \Gamma$ with data on Γ given. In this case, the substructures overlap.

In both the case of disjoint substructures and that of overlapping substructures, we can express A as $A = B + UZ^T$, where U and Z are matrices of rank at most a small multiple of the number of unknowns corresponding to Γ, and we can make use of fast solvers for B in order to efficiently solve equations involving A.

Such a strategy is complicated when the original problem has Neumann boundary conditions, leading to a matrix A which has a rank-deficiency of 1, and to a matrix B with a deficiency of 1 if the substructures are taken to overlap or a deficiency equal to the number of rectangles in Ω if the substructures are disjoint. Further, even if the original problem has mixed boundary

conditions, leading to a full-rank A, substructures with all Neumann boundary conditions lead to a rank-deficient B.

In this paper we derive formulas for the capacitance matrix algorithm when either A or B or both A and B are singular (Section 2), apply this to the model problem (Section 3), and discuss variants and extensions of the algorithm (Section 4).

2. The capacitance matrix algorithm

In this section we present the standard capacitance matrix algorithm, based on the Woodbury formula [7], and develop variants to handle rank-deficient matrices. This discussion is purely in terms of linear algebra. In Section 3, we apply these results to the model problem.

2.1. The standard algorithm

Let $\bar{A}$ and $\bar{B}$ be square nonsingular matrices of dimension n with $\bar{A} = \bar{B} + UZ^{\mathrm{T}}$. (Ordinarily, U and Z will be low-rank matrices.) One version of the capacitance matrix algorithm is as follows:

Algorithm 2.1. To solve $\bar{A}\bar{x} = \bar{b}$, compute $\bar{x} = \bar{G}(I - UC^{-1}Z^{\mathrm{T}}\bar{G})\bar{b}$, where $\bar{G} = \bar{B}^{-1}$ and $C = I + Z^{\mathrm{T}}\bar{G}U$.

If $U^{\mathrm{T}}U = I$, then an alternate formula for the capacitance matrix is $C = U^{\mathrm{T}}\bar{A}\bar{G}U$. This algorithm is useful in case there is an easy way to solve linear systems involving the matrix $\bar{B}$ but not an easy way for systems involving $\bar{A}$. It can be easily verified by substitution that the $\bar{x}$ defined by the capacitance matrix algorithm does indeed solve the problem $\bar{A}\bar{x} = \bar{b}$, assuming that $\bar{B}^{-1}$ and C^{-1} exist. Further, if $\bar{B}^{-1}$ exists, then C is nonsingular iff $\bar{A}$ is.

2.2. Algorithms involving singular matrices

Let the singular value decomposition of $\bar{A}$ be denoted by $\bar{A} = W_A \Sigma_A Y_A^{\mathrm{T}}$, where W_A and Y_A have orthonormal columns (denoted by w_i^A and y_i^A respectively) and Σ_A is diagonal with elements $\alpha_i > 0$. We will not assume that the α_i are ordered by size. Another way to write $\bar{A}$ is as

$$\bar{A} = \sum_{i=1}^{n} \alpha_i w_i^A \left(y_i^A\right)^{\mathrm{T}}.$$

Let A be a matrix related to $\bar{A}$ by

$$A = \sum_{i=1}^{m_A} \alpha_i w_i^A \left(y_i^A\right)^{\mathrm{T}},$$

where $m_A < n$. Thus, A is a matrix of rank m_A which differs from $\bar{A}$ by a matrix of rank $n - m_A$ aligned with the singular vectors.

The following simple lemma shows how to solve a consistent linear system $Ax = b$ using the capacitance matrix algorithm above.

Lemma 2.2. *Suppose that the problem $Ax = b$ is consistent, i.e., $b^T w_i^A = 0$, $i = m_A + 1, \ldots, n$. Then if $\bar{A}\bar{x} = b$, then $\bar{x}$ also solves the system $A\bar{x} = b$.*

Proof. The solution to $\bar{A}\bar{x} = b$ is uniquely determined by

$$\bar{x} = \sum_{j=1}^{n} \frac{\gamma_j}{\alpha_j} y_j^A \quad \text{where} \quad b = \sum_{i=1}^{n} \gamma_i w_i^A,$$

and, by assumption, $\gamma_i = 0$ for $i = m_A + 1, \ldots, n$. Now,

$$A\bar{x} = \sum_{i=1}^{m_A} \alpha_i w_i^A \left(y_i^A\right)^T \sum_{j=1}^{n} \frac{\gamma_j}{\alpha_j} y_j^A = \sum_{i=1}^{m_A} \gamma_i w_i^A = b,$$

and the result is established. □

Now suppose that we also have a singular matrix B, related to $\bar{B}$ as A is related to $\bar{A}$:

$$\bar{B} = \sum_{i=1}^{n} \beta_i w_i^B \left(y_i^B\right)^T \quad \text{and} \quad B = \sum_{i=1}^{m_B} \beta_i w_i^B \left(y_i^B\right)^T.$$

Suppose further that B is the matrix for which linear systems are easy to solve. To use the capacitance matrix algorithm we need to be able to relate solutions of linear systems $By = d$ to those of $\bar{B}y = d$. The next lemma gives us this result.

Lemma 2.3. *Let s be a solution to the linear system $Bs = d$, where $d^T w_i^B = 0$ and $s^T y_i^B = 0$ for $i = m_B + 1, \ldots, n$. Then*

$$\bar{s} = s + \sum_{j=m_B+1}^{n} \frac{\delta_j}{\beta_j} y_j^B$$

solves $\bar{B}\bar{s} = \bar{d}$ where

$$\bar{d} = d + \sum_{i=m_B+1}^{n} \delta_i w_i^B.$$

Proof.

$$\bar{B}\bar{s} = \left(B + \sum_{i=m_B+1}^{n} \beta_i w_i^B \left(y_i^B\right)^T\right)\left(s + \sum_{j=m_B+1}^{n} \frac{\delta_j}{\beta_j} y_j^B\right)$$

$$= Bs + \sum_{i=m_B+1}^{n} \beta_i w_i^B \left(y_i^B\right)^T \sum_{j=m_B+1}^{n} \frac{\delta_j}{\beta_j} y_j^B = d + \sum_{i=m_B+1}^{n} \delta_i w_i^B = \bar{d},$$

as required. □

Therefore, the full capacitance matrix algorithm is as follows, where steps may be skipped if nonsingular matrices are involved.

Algorithm 2.4. To solve $Ax \approx b$, where A is a lower-rank version of $\bar{A}$, $\bar{A} = \bar{B} + UZ^T$, and B is a lower-rank version of $\bar{B}$, for which linear systems are easy to solve:

(1) Let $\bar{b}$ be the projection of b orthogonal to the null space of A^T.

(2) Let d be the projection of $\bar{b}$ orthogonal to the null space of B^T.

(3) Solve $\bar{B}\bar{s} = \bar{b}$ by solving $Bs = d$ (minimum norm solution) and computing

$$\bar{s} = s + \sum_{j=m_B+1}^{n} \frac{\left(\bar{b}^T w_j^B\right)}{\beta_j} y_j^B.$$

(4) Solve $Ct = Z^T\bar{s}$, where $C = I + Z^T\bar{B}^{-1}U$.

(5) Let $\bar{r} = \bar{b} - Ut$, and let r be the projection of $\bar{r}$ orthogonal to the null space of B^T.

(6) Solve $\bar{B}\bar{x} = \bar{r}$ by solving $Bx = r$ (minimum norm solution) and computing

$$\bar{x} = x + \sum_{j=m_B+1}^{n} \frac{\left(\bar{r}^T w_j^B\right)}{\beta_j} y_j^B.$$

(7) Now $\bar{x}$ solves $\bar{A}\bar{x} = \bar{b}$ and $A\bar{x} = \bar{b}$.

3. Application to the model problem

We illustrate the capacitance matrix algorithm by applying it to two examples: the model problem with all Neumann boundary conditions, and the model problem with mixed boundary conditions. We will assume that there is a fast way to solve either problem over region $\Omega_1 \cup \Gamma$ and over Ω_2.

Example 3.1. In the Neumann case, the matrix A is equal to the matrix B corresponding to the Laplacian over the two disjoint rectangles with all Neumann boundary conditions, plus a correction:

$$A = B + \begin{bmatrix} 0 & 0 \\ 0 & E \\ I & 0 \end{bmatrix} \begin{bmatrix} 0 & 0 \\ A_{32}^T & A_{22}^T - B_{22}^T \\ 0 & A_{23}^T \end{bmatrix}^T,$$

and E is a matrix of unit vectors in the positions of the boundary points of Ω_2 along Γ. For each point on Γ, or adjacent to it in Ω_2, the left correction matrix has a unit vector in that direction as a column. The corresponding row of the right correction matrix is the difference between the corresponding row of A and that of B. The correction matrices have dimensions $n \times 2p$, where n is the total number of unknowns and p is the number of unknowns corresponding to Γ.

The matrix A has the property that $Ae = 0$, where e is the vector of all ones. (In terms of the original differential equation, this corresponds to the fact that any constant solves the homogeneous equation.) Similarly, $Be_1 = 0$ and $Be_2 = 0$, where

$$e_1 = \begin{bmatrix} e \\ 0 \\ e \end{bmatrix}, \qquad e_2 = \begin{bmatrix} 0 \\ e \\ 0 \end{bmatrix}.$$

A nonsingular form of the matrix B can be created by adding rank-one terms corresponding to

the zero eigenvalues: $\bar{B} = B - c_1 e_1 e_1^T - c_2 e_2 e_2^T$. The constants should be chosen within an interval containing the nonzero eigenvalues of B. Let $\bar{A} = A + c_0 e e^T$. Now, note that $\bar{A} = \bar{B} + UZ^T$, where

$$U = \begin{bmatrix} 0 & 0 & c_1 e & 0 \\ 0 & E & 0 & c_2 e \\ I & 0 & c_1 e & 0 \end{bmatrix}, \quad Z = \begin{bmatrix} 0 & 0 & (1 + c_0/c_1)e & (c_0/c_2)e \\ A_{32}^T & A_{22}^T - B_{22}^T & (c_0/c_1)e & (1 + c_0/c_2)e \\ 0 & A_{23}^T & (1 + c_0/c_1)e & (c_0/c_2)e \end{bmatrix}^T.$$

We define the result $\bar{v} = G\bar{u}$ as follows:

For each rectangle (i.e., substructure):

(1) Let $\bar{u}_i$ be the subvector of $\bar{u}$ with the n_i components corresponding to this rectangle, and let $\mu_i = \bar{u}_i^T e/n_i$ and $u_i = \bar{u}_i - \mu_i e$, so that u_i has mean zero.

(2) Solve the differential equation on the rectangle with all Neumann boundary conditions and discrete right-hand side function u_i, yielding a vector v_i with mean zero.

(3) Let $\bar{v}_i = v_i + c_i \mu_i e$.

For this example problem, the capacitance matrix algorithm is:

Algorithm 3.2.

(1) Compute $\bar{b} = b - (b^T e/n)e$. This forces the right-hand side $\bar{b}$ to have mean zero, ensuring that the problem is consistent.

(2) Form $s = G\bar{b}$.

(3) Multiply Z^T times s.

(4) Solve $Ct = Z^T s$. This can be accomplished by explicitly forming and factoring the capacitance matrix $C = I + Z^T GU$, or by using an iterative method such as preconditioned conjugate gradients, which requires matrix-vector products Cp but does not explicitly require the matrix C.

(5) Form $r = \bar{b} - Ut$.

(6) Form $x = Gr$.

(7) If a solution with mean zero is required, replace x by $x - (x^T e/n)e$.

Example 3.3. As a second example, consider the model problem of Fig. 1 with Neumann boundary conditions on $\Omega_1 \cup \Gamma$ but at least one Dirichlet segment on Ω_2. The correction matrices are somewhat simplified in this case:

$$U = \begin{bmatrix} 0 & 0 & c_0 e \\ 0 & E & 0 \\ I & 0 & c_0 e \end{bmatrix}, \quad Z = \begin{bmatrix} 0 & 0 & e \\ A_{32}^T & A_{22}^T - B_{22}^T & 0 \\ 0 & A_{23}^T & e \end{bmatrix}^T.$$

For the first rectangle, the result for $\bar{v} = G\bar{u}$ is defined as above by first projecting the right-hand side and by later correcting the mean; for the second rectangle, the linear system has a nonsingular matrix and no projection is necessary. The capacitance matrix algorithm is the same as for the all Neumann problem above, except that steps (1) and (7) are omitted and $\bar{b} = b$.

4. Further discussion

The algorithm in the previous section is well suited for parallel processing. Coarse grain

parallelism can be achieved by assigning the work for each substructure to a separate processor. Finer grain parallelism can result from using parallel solvers for solving Laplace's equation on each substructure (see, for example [1]). The work in multiplying by U and Z can be similarly divided.

The model problem from Fig. 1 has corners which can give rise to nonsmooth solutions. To better resolve the solution, standard techniques can be used, such as refining the mesh near the corners or adding an appropriate function to the basis set.

The use of a direct or an iterative method for solving the capacitance matrix equation (step (4) above) involves a trade-off between storage space and solution time. In two dimensions, either option is reasonable, but the size of the capacitance matrix and its lack of sparsity often forces the use of an iterative method in three-dimensional problems; see the discussion in [9]. For certain simple problems, it may be possible to determine the singular value decomposition of C in terms of Fourier vectors, leading to a more efficient implementation [4].

References

[1] L. Adams and R. Voigt, A methodology for exploiting parallelism in the finite element process, in: J. Kowalik, ed., *Proceedings of NATO Workshop on High Speed Computations*, F.R.G., NATO ASI Series *F7* (Springer, Berlin, 1984) 373–392.

[2] G.P. Astrakhantsev, Method of fictitious domains for a second-order elliptic equation with natural boundary conditions, *USSR Comput. Maths. Math. Phys. 18* (1978) 114–121.

[3] B.L. Buzbee, F.W. Dorr, J.A. George and G.H. Golub, The direct solution of the discrete Poisson equation on irregular regions, *SIAM. J. Numer. Anal. 8* (1971) 722–736.

[4] T.F. Chan, Analysis of preconditioners for domain decomposition, Yale University Computer Science Department Rept. YALEU/DCS/RR-408, New Haven, CT, 1985.

[5] M.D. Gunzburger and R.A. Nicolaides, On substructuring algorithms and solution techniques for the numerical approximation of partial differential equations, in: J.C. South, Jr. and M.Y. Hussaini, eds. *Advances in Numerical and Applied Mathematics*, ICASE Rept. 86-18, NASA Langley Research Center, Hampton, VA (1986) 165–195.

[6] R.W. Hockney, The potential calculation and some applications, *Meths. Comput. Phys. 9* (1970) 135–211.

[7] A.S. Householder, *The Theory of Matrices in Numerical Analysis* (Blaisdell, New York, 1964); reprinted by (Dover, New York, 1975).

[8] J.G. Lewis and R.G. Rehm, The numerical solution of a nonseparable elliptic partial differential equation by preconditioned conjugate gradients, *J. Res. Nat. Bur. Standards 85* (1980) 367–390.

[9] D.P. O'Leary and O. Widlund, Capacitance matrix methods for the Helmholtz equation on general three dimensional regions, *Math. Comp. 33* (1979) 849–879.

[10] W. Proskurowski and O. Widlund, A finite element-capacitance matrix method for the Neumann problem for Laplace's equation, *SIAM J. Sci. Statist. Comput. 1* (1980) 410–425.

[11] W. Proskurowski and O. Widlund, On the numerical solution of Helmholtz's equation by the capacitance matrix method, *Math. Comp. 30* (1976) 433–468.