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Short Paper

DECOMPOSITION OF SINGULAR LARGE SPARSE MATRIX BY ADDING DUMMY LINKS AND DUMMY DEGREES

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ABSTRACT

This paper proposes a simple scheme to decompose an nxn nonpositive definite matrix, A, associated with simultaneous equations, $A\,X = B$, into a triple-factors (lower triangular, diagonal, and upper triangular matrices), i.e., $\tilde{A} = L\,D\,U$, without interchanging rows or columns of A, but with A expanded with new rows and new columns to an mxm matrix $\tilde{A}$. Whenever a near-zero diagonal element, say $\bar{a}_{ii}$, is encountered and used as a pivoting element, an appropriate positive real number, say p, is added to this diagonal element, and a new term $-px_k$ is also added to the i-th equation, where x_k is a new variable called "dummy variable". If we also add a new equation $-px_i + px_k = 0$ to enforce the new added variable x_k equal to x_i then the modified i-th equation has the same effect as the original equation. Therefore, the original solution X can be found directly from the expanded solution of the modified expanded equation. The method is very useful in solving the following problems: (1) nonlinear problems near the limit state, (2) postbuckling analysis, (3) system equations with constraint conditions, and (4) getting eigenvectors from eigenvalues.

奇異大型稀疏矩陣之分解

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摘　要

本文提出一種分解奇異大型稀疏矩陣之方法。對於 n 元線性聯立式：$AX=B$，若其係數矩陣A爲奇異，或於矩陣分解時對角元素（設爲$\bar{a}_{ii}$）爲零，一般需做列或行調換，使做爲樞紐元素之該對角元素不爲零。但此動作會影響稀疏矩陣之元素儲存順序，而造成分解運算時之困難。本文所提方法不必做列或行調換，而是加一正值p於該對角元素 $\bar{a}_{ii}$，即於聯立式之第 i 式加入px_i使該

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樞紐元素不爲零。若新增一變數x_k令其等於x_i，則於第i式再加入$-px_k$可抵消前述加入px_i之影響。$x_k=x_i$之條件可於聯立式之後增列$-px_i+px_k=0$爲第k式而達成。原聯立式之解可直接由擴增聯立式之解直接取得。該法極適合於解下列諸問題：(1)接近極限狀態之非線性分析，(2)挫曲後之分析，(3)含束制條件之問題，(4)由特徵值求特徵向量。

INTRODUCTION

In order to preserve the sparseness of the matrix A in solving the following linear equations:

$$A\,X = B \tag{1a}$$

or

$$\begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{bmatrix} \tag{1b}$$

the matrix A is decomposed into a lower triangular matrix L, a diagonal matrix D, and an upper triangular matrix U, i.e., $A = L\,D\,U$. If a near-zero pivoting diagonal element is encountered, the interchanging of rows or columns may be required to make the diagonal pivoting element nonzero. This will, however, change the profile of the sparse matrix A and cause some difficulties in storing the matrix elements.

Sharifi and Popov [3] proposed a method to modify the matrix A to positive definite by adding a matrix $c\,B\,B^T$, where c is a positive constant. Therefore, they solve $\overline{X}$ from the following equation:

$$(A + c\,B\,B^T)\,\overline{X} = B \tag{2}$$

and then get the original solution X by

$$X = \overline{X}\,(1 - c\,B^T\,\overline{X})^{-1} \tag{3}$$

This method is very simple to apply but has the disadvantages of: (1) changing the matrix from sparse to dense for the arbitrary general constant vector B, and (2) losing the capability to solve for more than one constant vector B.

Stewart [4] also proposed a method to avoid interchanging rows and columns of the matrix by adding a positive number, c, to the diagonal element, a_{ii}, and solve $\overline{X}$ from the following equation:

$$(A + c\,e_i\,e_i^T)\,\overline{X} = B \tag{4}$$

where e_i is the i-th column of the identity matrix, and then getting the original solution X by using Sherman-Morrison-Woodbury formula [2] as follows:

$$X = \left(\overline{A}^{-1} - \frac{\overline{A}^{-1}\,e_i\,c\,e_i^T\,\overline{A}^{-1}}{c\,e_i^T\,\overline{A}^{-1}\,e_i - 1}\right) B \tag{5a}$$

$$= \overline{X} - \left(\frac{c\overline{x}_i}{c\,e_i^T\,\overline{A}^{-1}\,e_i - 1}\right)\overline{A}^{-1}\,e_i \tag{5b}$$

where $\overline{x}_i$ is the i-th element of the solution vector $\overline{X}$, $\overline{A} = A + c\,e_i\,e_i^T$, and $\overline{A}^{-1}\,e_i$ is the i-th column of the matrix $\overline{A}^{-1}$, which can be solved from the decomposed matrices of $\overline{A}$.

This method may cause problems if the denominator in Eq. (5) is zero, which may happen when matrix A is singular. And the method is rather complicated if more than one diagonal element is modified.

The method proposed in this paper not only modifies the diagonal elements but also adds new variables and new equations, such that the modified equations have the same solution as the original equations for the original variables. Therefore the matrix decomposition and the substitutions are simple and straightforward. If the matrix is modified only by adding some numbers to the diagonal elements, as proposed by Stewart, then the modified equations will have different solution from the original equations. Therefore the original solution can not be obtained directly.

THE ALGORITHM

It is clear that the following augmented equations have the same solution as the original Eq. (1) for the original n-variables:

$$\begin{bmatrix} a_{11} & \cdots & a_{1i} & \cdots & a_{1j} & \cdots & a_{1n} & & \\ \vdots & \ddots & \vdots & \ddots & \vdots & \ddots & \vdots & & \\ a_{i1} & \cdots & a_{ii}+p_1 & \cdots & a_{ij} & \cdots & a_{in} & -p_1 & \\ \vdots & \ddots & \vdots & \ddots & \vdots & \ddots & \vdots & & \\ a_{j1} & \cdots & a_{ji} & \cdots & a_{jj}+p_2 & \cdots & a_{jn} & & -p_2 \\ \vdots & \ddots & \vdots & \ddots & \vdots & \ddots & \vdots & & \\ a_{n1} & \cdots & a_{ni} & \cdots & a_{nj} & \cdots & a_{nn} & & \\ & & -p_1 & & & & & p_1 & \\ & & & & -p_2 & & & & p_2 \end{bmatrix} \begin{bmatrix} x_1 \\ \vdots \\ x_i \\ \vdots \\ x_j \\ \vdots \\ x_n \\ x_{n+1} \\ x_{n+2} \end{bmatrix} = \begin{bmatrix} b_1 \\ \vdots \\ b_i \\ \vdots \\ b_j \\ \vdots \\ b_n \\ 0 \\ 0 \end{bmatrix} \tag{6}$$

The p_k is added to the diagonal only when a near-zero diagonal element is to be used as a pivoting element.

To get the physical meaning of the modification, we use a structure system as an example. In structural terminology, a truss element called a dummy link with the stiffness matrix $\begin{bmatrix} p & -p \\ -p & p \end{bmatrix}$ is added to the original structural system. The dummy link connects a system degree to a new degree, which is not in the original system and therefore called a dummy degree. If no loading is applied to the dummy degree, the displacement of the dummy degree must be equal to the displacement of the linked system degree, and the displacement of the system degree will not be affected by the added dummy link and the dummy degree.

CHOICE OF P

In this section, we will discuss how to choose the magnitude of the p. During the computation of the decomposed diagonal element d_{jj}, i.e.,

$$d_{jj} = a_{jj} - \sum_{k=1}^{j-1} l_{jk} d_{kk} u_{kj} \tag{7}$$

we can get the maximum intermediate value, $\tilde{d}_{jj}$, from the following equation:

$$\tilde{d}_{jj} = max\ (|\ a_{jj} - \sum_{k=1}^{i-1} l_{jk} d_{kk} u_{kj}\ |,\ i=1,2,\ \ldots,\ j) \tag{8}$$

where l_{jk}, d_{kk} and u_{kj} are the elements in the decomposed lower triangular matrix $\boldsymbol{L}$, diagonal matrix $\boldsymbol{D}$, and upper triangular matrix $\boldsymbol{U}$. And if

$$|\ d_{jj}\ | = \alpha \cdot \tilde{d}_{jj} \cdot 2^{-s},\ \ 2^{-1} \le \alpha < 1 \tag{9}$$

we can say that the new d_{jj} has lost (at least) s-bits (binary digits). Therefore, we can choose $p = \tilde{d}_{jj}$ for adding to the diagonal element d_{jj}, and this will maximize the accuracy of the pivoting element and minimize the truncation error of the diagonal element d_{jj}. For this p, it will truncate the s least significant bits of d_{jj}, which is just the inaccurate part of d_{jj}.

Note that the correct number of bits, s, may be larger than that from Eq. (9), if the dominate terms of $l_{jk}d_{kk}u_{kj}$ has lost some bits. To account for these errors, we must trace the error of every element. This will require a considerable amount of working space and computations. Therefore, in practice, we do not make any effort to trace the accuracy of each element. The simplest thing we can do is to keep every pivoting element as accurate as possible.

Next, we must point out that, if the original matrix is singular, i.e., $t = n - rank\ (A) > 0$, then it will have a $t \times t$ null submatrix in the lower right corner of the three decomposed matrices $\boldsymbol{L}$, $\boldsymbol{D}$ and $\boldsymbol{U}$. In that case, if we try to modify the first zero element in the decomposed diagonal matrix by adding p, then after eliminating, the zero will appear in the newly added last diagonal and it still have a $t \times t$ null submatrix. Therefore, we need not make any modification to the diagonal elements in the last $t \times t$ null submatrix.

APPLICATION EXAMPLES

To illustrate the applications of the proposed method, two numerical examples are shown in this section.

Example 1:

An important application is to solve system equations including constrained equations. The general formulations can be stated as:

$$\text{Minimize } \pi = \frac{1}{2}\ \Delta^T \boldsymbol{K}\, \Delta - \Delta^T \boldsymbol{F} \tag{10a}$$

$$\text{Subject to} \quad \boldsymbol{G}\, \Delta - \boldsymbol{H} = 0 \tag{10b}$$

where K is a $n \times n$ stiffness matrix, Δ is a displacement vector, F is a loading vector, G is a $m \times n$ matrix, and H is a constant vector. This is equivalent to find the stationary point of the Lagrangian:

$$L\ (\Delta,\ \Lambda) = \frac{1}{2}\ \Delta^T K \Delta\ -\ \Delta^T F\ +\ \Lambda^T\ (G\ \Delta\ -\ H) \tag{11}$$

from the following stationary conditions:

$$\begin{bmatrix} K & G^T \\ G & 0 \end{bmatrix} \begin{bmatrix} \Delta \\ \Lambda \end{bmatrix} = \begin{bmatrix} F \\ H \end{bmatrix} \tag{12}$$

where the Lagrange multiplier λ_i represents a load factor of the constraint force vector g^i, i.e., the i-th column of G^T.

The difficulty with this problem is that the matrix K may be singular, and the system matrix is typically non-positive definite. A procedure had been proposed by Chang and Lin [1] to solve this problem, but it is too complicated to implement.

To keep the example small, we will just analyze a structure with only one truss element, and the structure is subject to the constraint condition of $\delta_1 + \delta_2 = 0$, where δ_1 and δ_2 are the displacements of the end nodes of the truss element. The equation to solve this problem is

$$\begin{bmatrix} 1 & -1 & 1 \\ -1 & 1 & 1 \\ 1 & 1 & 0 \end{bmatrix} \begin{bmatrix} \delta_1 \\ \delta_2 \\ \lambda \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} \tag{13}$$

The 3x3 matrix A is expanded to a 4x4 matrix $\tilde{A}$ and decomposed as

$$\begin{bmatrix} 1 & -1 & 1 & 0 \\ -1 & 1+1 & 1 & -1 \\ 1 & 1 & 0 & 0 \\ 0 & -1 & 0 & 1 \end{bmatrix} = \begin{bmatrix} 1 & & & \\ -1 & 1 & & \\ 1 & 2 & 1 & \\ & -1 & -.4 & 1 \end{bmatrix} \begin{bmatrix} 1 & & & \\ & 1 & & \\ & & -5 & \\ & & & .8 \end{bmatrix} \begin{bmatrix} 1 & -1 & 1 & \\ & 1 & 2 & -1 \\ & & 1 & -.4 \\ & & & 1 \end{bmatrix} \tag{14}$$

By forward and backward substitutions, the solution for the expanded constant vector $\tilde{B} = [1,0,0,0]^t$ is $\tilde{X} = [0.25,\ -.25,\ .5,\ -.25]^t$, and then the original solution is $X = [0.25,\ -.25,\ .5]^t$.

Example 2:

The second important application is to solve simultaneous equations with singular matrices. These may encountered in nonlinear analysis at limit states, or in eigenvector calculations from the eigenvalue. The applicability is very obvious. So we just illustrate a very simple numerical example as follows:

$$\begin{bmatrix} 0 & 1 & 1 \\ 1 & 1 & 0 \\ 1 & 0 & -1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix} \tag{15}$$

The 3x3 matrix A is expanded to a 5x5 matrix $\tilde{A}$ and decomposed as

$$\begin{bmatrix} 0+1 & 1 & 1 & -1 & \\ 1 & 1+1 & 0 & 0 & -1 \\ 1 & 0 & -1 & 0 & 0 \\ -1 & 0 & 0 & 1 & 0 \\ & -1 & 0 & 0 & 1 \end{bmatrix} =$$

$$\begin{bmatrix} 1 & & & & \\ 1 & 1 & & & \\ 1 & -1 & 1 & & \\ -1 & 1 & -\frac{2}{3} & 1 & \\ & -1 & \frac{1}{3} & 1 & 0 \end{bmatrix} \begin{bmatrix} 1 & & & & \\ & 1 & & & \\ & & -3 & & \\ & & & \frac{1}{3} & \\ & & & & 0 \end{bmatrix} \begin{bmatrix} 1 & 1 & 1 & -1 & \\ & 1 & -1 & 1 & -1 \\ & & 1 & -\frac{2}{3} & \frac{1}{3} \\ & & & 1 & 1 \\ & & & & 0 \end{bmatrix} \tag{16}$$

and the solution of the expanded equations can be solved from

$$\begin{bmatrix} 1 & 1 & 1 & -1 & \\ & 1 & -1 & 1 & -1 \\ & & 1 & -\frac{2}{3} & \frac{1}{3} \\ & & & 1 & 1 \\ & & & & 0 \end{bmatrix} \begin{Bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \\ x_5 \end{Bmatrix} = \begin{Bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{Bmatrix}$$

or

$$\begin{bmatrix} 1 & 1 & 1 & -1 \\ & 1 & -1 & 1 \\ & & 1 & -\frac{2}{3} \\ & & & 1 \end{bmatrix} \begin{Bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{Bmatrix} = -x_5 \begin{Bmatrix} 0 \\ -1 \\ \frac{1}{3} \\ 1 \end{Bmatrix} \tag{17}$$

By backward substitutions, the solution for the expanded equations is

$$\begin{Bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{Bmatrix} = -x_5 \begin{Bmatrix} 1 \\ -1 \\ 1 \\ 1 \end{Bmatrix} \quad \text{or} \quad \begin{Bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \\ x_5 \end{Bmatrix} = -x_5 \begin{Bmatrix} 1 \\ -1 \\ 1 \\ 1 \\ -1 \end{Bmatrix} \tag{18}$$

and then the original solution is $X = -x_2\,[1,\ -1,\ 1]^t$.

CONCLUSIONS

The method proposed in this paper has the following advantages:

(1) No interchange of rows or columns is required. Sparseness is preserved, thus making this method very suitable for large systems.

(2) By adding a suitable positive number to the near-zero diagonal element, the accuracy of the pivoting element can be retained.

(3) The method is so simple and straightforward that it can easily be implemented in the general solver of the large skyline matrix as a general and standard feature.

NOMENCLATURE

A	an $n \times n$ matrix
B	a constant vector
D	a diagonal matrix
e_i	the i-th column of the identity matrix I
F	a loading vector
G	an $m \times n$ matrix
H	a constant vector
K	a stiffness matrix
L	a lower triangular matrix
p	an added real number
U	an upper triangular matrix
X	a solution vector

Greek symbols

Δ	a displacement vector
Λ	a Lagrange multiplier vector

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