大型线性方程组的迭代求解

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摘要: 将求解大型标准特征值问题的 Davidson 方法推广到求解大型线性方程组. 推广后的方法既可以用于求解对称问题, 又可以用于求解非对称问题. 数值计算结果显示, 该方法对这两类问题的求解分别优于共轭梯度方法和双共轭梯度方法.

关键词: 线性方程组; Davidson 方法; 共轭梯度方法; 双共轭梯度方法

中图分类号: O641

Iterative Solution of Large-Scale Linear Equations

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Abstract: The Davidson's method originally developed for eigenvalue problems was extended to solve large-scale linear equations. It can be used for symmetrical and nonsymmetrical matrices. Numerical results presented in this study demonstrate that the present scheme is much more effective than conjugate gradient method and biconjugate gradient method for symmetrical and nonsymmetrical problems, respectively.

Key Words: Linear equations; Davidson's method; Conjugate gradient method; Biconjugate gradient method

Linear systems of equations are associated with many problems^[1–6] in physics, chemistry, engineering, and geophysics. The typical examples in quantum mechanical calculations are related to problems encountered in the linear coupled Hartree-Fock equations^[9] and coupled-cluster method^[10], in computing nonlinear optical properties of correlated conjugated systems^[11,12], and surface charges of a solvent cavity that nominally encloses the solute in dielectric continuum theory^[13].

For small systems there are well-established direct algorithms^[1–6] such as Gaussian elimination to obtain an accurate solution of a set of linear equations. However, for large dimensional systems iterative approaches^[1–3] are usually more efficient in terms of the computer storage and the computational speed. Among them the conjugate gradient method (CGM)^[1–3,14] and biconjugate gradient method (BCGM)^[9] are often exploited to find a solution for a symmetrical and positive definite matrix and a nonsymmetrical matrix, respectively. The generalized minimum residual method^[2,15–17]

is another general purpose method. Its performance is more or less equivalent to the CGM and BCGM. More iterative techniques could be found from Refs.[1–3].

Davidson's method^[18,19] is a very effective approach for a large-scale standard eigenvalue problem. Lenthe and Pulay^[20] pointed out that expansion vectors in Davidson's method could be truncated to two vectors without significant reduction in the speed of convergence as the dimension of the subspace became large. Davidson's method has been extended to calculate a few lowest eigenvalues and corresponding eigenvectors of large generalized eigenvalue problem^[21,22]. It is the purpose of this study to derive an analogues version of the Davidson's method for solution of linear equations. Numerical results were presented and compared with the conjugate gradient method for symmetrical systems and also with the biconjugate gradient method for nonsymmetrical systems.

Received: May 29, 2009; Revised: July 16, 2009; Published on Web: August 27, 2009.

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The project was supported by the National Natural Science Foundation of China (20473011, 20773011).

国家自然科学基金(20473011, 20773011)资助项目

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1 Theory

A set of linear equations has the following matrix form:

$$\mathbf{A}\mathbf{x}=\mathbf{b} \quad (1)$$

where $\mathbf{A}$ is an $n \times n$ matrix, $\mathbf{x}$ and $\mathbf{b}$ are n -dimensional vectors. The elements of $\mathbf{A}$, $\mathbf{x}$, and $\mathbf{b}$ are denoted as a_{ij} , x_j , and b_j ($i, j=1, 2, \dots, n$), respectively. Corresponding to Eq.(1), there always exists a function $f(\mathbf{x})$

$$f(\mathbf{x})=\frac{1}{2}\mathbf{x}^T\cdot\mathbf{A}\cdot\mathbf{x}-\mathbf{x}^T\cdot\mathbf{b} \quad (2)$$

where T means a transpose of a vector or a matrix. For a symmetric and positive definite matrix $\mathbf{A}$, the solution of Eq.(1) is equivalent to the vector which minimizes the function in Eq.(2). This leads directly to the conjugate gradient method^[1-3,14]. If $\mathbf{A}$ is not symmetrical, a biconjugate gradient scheme^[3] is usually exploited instead.

The gradient of the function $f(\mathbf{x})$ in Eq.(2) is

$$\nabla f=\mathbf{A}\cdot\mathbf{x}-\mathbf{b} \quad (3)$$

provided that $\mathbf{A}$ is symmetrical. If ∇f is equal to zero, we obtain Eq.(1). This means that the solution of Eq.(1) corresponds to a stationary point of the function $f(\mathbf{x})$. The j th component of the gradient is

$$\frac{\partial f}{\partial x_j}=\sum_{k=1}^n a_{jk}x_k-b_j \quad (4)$$

Similar to the derivation of correction vector in the Davidson's method^[18], if the element x_j of the vector $\mathbf{x}$ is changed to $x_j+\delta_j$, keeping its other elements constant, Eq.(4) becomes

$$\left.\frac{\partial f}{\partial x_j}\right|_{x_j=x_j+\delta_j}=\sum_{k=1}^n a_{jk}x_k-b_j+a_{jj}\delta_j \quad (5)$$

If the right side of Eq.(5) is set equal to zero, we get a new vector δ with its component δ_j defined as

$$\delta_j=(b_j-\sum_{k=1}^n a_{jk}x_k)/a_{jj} \quad (6)$$

The vector δ is an improved vector for iterative solutions of Eq.(1). The numerator of the right side of Eq.(6) is actually a negative component of the gradient ∇f , i.e., the steepest descent search direction. In the above derivation, it is assumed that the matrix $\mathbf{A}$ is symmetrical. However, numerical results as discussed below show that the vector δ also works well for nonsymmetrical matrices.

The whole iterative scheme is described as follows. Start from a set of initial vectors $\{\mathbf{y}_1, \mathbf{y}_2, \dots, \mathbf{y}_l\}$, $1 \leq l < n$, they are assumed to be orthonormalized. The solution $\mathbf{x}$ of Eq.(1) can be expanded in this initial vector set as

$$\mathbf{x}=\sum_{k=1}^l \alpha_k \mathbf{y}_k \quad (7)$$

where α_k is the expansion coefficient to be determined. Substituting Eq.(7) into Eq.(1), after some manipulation, we get a new set of linear equations

$$\mathbf{G}\alpha=\mathbf{d} \quad (8)$$

where the matrix elements of $\mathbf{G}$ and $\mathbf{d}$ are as follows

$$g_{ij}=\mathbf{y}_i^T \mathbf{A} \mathbf{y}_j, d_i=\mathbf{y}_i^T \mathbf{b} \quad (i, j=1, 2, \dots, l) \quad (9)$$

The k th component of the vector α is the expansion coefficient α_k in Eq.(7). Since Eq.(8) is usually a small-scale linear equation,

it can be solved simultaneously with conventional numerical methods such as Gaussian elimination method^[1-3]. Once the expansion vector α is available, we then calculate the residue $\mathbf{r}$ corresponding to the approximate vector $\mathbf{x}$

$$\mathbf{r}=\mathbf{b}-\mathbf{A}\cdot\mathbf{x} \quad (10)$$

If the norm $\|\mathbf{r}\|$ of $\mathbf{r}$ is less than some convergence criterion such as 10^{-8} , the iterate process terminates. Otherwise, we get an improved vector δ through Eq.(6). If δ is not orthogonalized with the vectors $\{\mathbf{y}_1, \mathbf{y}_2, \dots, \mathbf{y}_l\}$, some types of orthogonalization procedure such as the Schmidt method^[22,23] should be carried out. The orthonormal vector is denoted as $\mathbf{y}_{l+1}$. Then we go back to Eq.(7) with $(l+1)$ vectors and repeat the computations in Eq.(8) and Eq.(10) until the convergence threshold is reached.

2 Numerical results

For convenience of comparison with the conjugated gradient method and biconjugate gradient method, we start with one initial vector which can be chosen as a unit vector and then begin the iteration. Eq.(6) is always used to get an improved vector δ even if matrix $\mathbf{A}$ is nonsymmetrical.

Four different examples are tested. The corresponding matrix elements of the first three examples are presented respectively below:

$$\begin{aligned} \text{(a)} \quad a_{ij} &= \frac{1}{1+i+j}; \\ \text{(b)} \quad a_{ij} &= a_{ji} = \begin{cases} \frac{i}{r} + \frac{j}{s}, & i > j \\ i, & i = j \end{cases} \quad \text{with } r \text{ and } s \text{ as parameters;} \\ \text{(c)} \quad a_{ij} &= \begin{cases} \frac{i}{r} + \frac{j}{s}, & i \neq j \\ i, & i = j \end{cases} \quad \text{with } r \text{ and } s \text{ as parameters.} \end{aligned}$$

Among them the first two matrices denoted as (a) and (b) are symmetrical. The matrices in the case (c) are nonsymmetrical. Before solving Eq.(1) the vector $\mathbf{b}$ is constructed by directly multiplying matrix $\mathbf{A}$ with the vector $\mathbf{x}$. Three types of the vector $\mathbf{x}$, $\{x_i=0.1, i=1, 2, \dots, n\}$, $\{x_i=0.5, i=1, 2, \dots, n\}$, and $\{x_i=i, i=1, 2, \dots, n\}$ are exploited. One purpose is to make sure that the program works correctly. Another one is to check the effect of the vector $\mathbf{b}$ on the convergence of the solution of Eq.(1).

The last example is the calculations of surface charges of the water cavity that nominally encloses the solute molecule CH_3CONH_2 ^[13]. The cavity is a solute electronic isodensity contour with the isodensity value as 0.001 atomic unit. It is not

Table 1 Number of iterations for solving Eq.(1) in case (a) with the present method and CGM

Size of matrix $\mathbf{A}$	The present method		CGM	
	10^{-6^*}	10^{-8^*}	10^{-6^*}	10^{-8^*}
$\{x_i=0.5, i=1, 2, \dots, n\}$				
1000	7	7	184	208
5000	7	8	419	472
$\{x_i=i, i=1, 2, \dots, n\}$				
1000	7	9	204	227
5000	9	9	461	515

* the convergence criterion for the iteration

Table 2 Number of iterations for solving Eq.(1) in case (b) with the present method and CGM

Parameter		The present method		CGM	
r^*	s^*	10^{-6**}	10^{-8**}	10^{-6**}	10^{-8**}
$n=1000, \{x_i=0.1, i=1, 2, \dots, n\}$					
10.0	20.0	13	15	161	195
10.0	100.0	16	18	190	218
$n=5000, \{x_i=0.1, i=1, 2, \dots, n\}$					
10.0	20.0	19	21	379	473
10.0	100.0	23	25	461	546
$n=1000, \{x_i=i, i=1, 2, \dots, n\}$					
10.0	20.0	17	19	219	245
10.0	100.0	19	21	229	254
$n=5000, \{x_i=i, i=1, 2, \dots, n\}$					
10.0	20.0	25	27	558	626
10.0	100.0	29	31	607	669

* r and s are the parameters of matrix A in case (b); ** the convergence criterion for the iteration; n : the size of matrix A

spherical. More details about this example and some related information can be found from Ref.[13] and references therein.

Quadruple precisions are used in all calculations below. The results for case (a) are listed in Table 1. The convergence criterion is 10^{-6} and 10^{-8} . As can be seen from the table, it takes only 7–9 iterations for the present method to get a convergent solution. But it takes 184–515 iterations for the conjugate gradient method to obtain the same results. Another advantage of the present method is that the number of iterates remains almost unchanged when the dimension of matrix A increases from 1000 to 5000. However, the number of iterates required for CGM is more than doubled.

The results for case (b) are presented in Table 2. In comparison with CGM, the advantage of the present method is still very significant though the differences are not as large as those in case (a). The next example is the nonsymmetrical case (c). The results are listed Table 3. The differences between the present method and BCGM are very large. The present method needs only 3 or 4 iterations to get convergent solutions while BCGM requires at

Table 3 Number of iterations for solving Eq.(1) in case (c) with the present method and BCGM

Parameter		The present method		BCGM	
r^*	s^*	10^{-6**}	10^{-8**}	10^{-6**}	10^{-8**}
$n=1000, \{x_i=0.1, i=1, 2, \dots, n\}$					
10.0	20.0	3	3	170	201
10.0	100.0	3	3	181	210
$n=5000, \{x_i=0.1, i=1, 2, \dots, n\}$					
10.0	20.0	3	3	388	465
10.0	100.0	3	3	409	480
$n=1000, \{x_i=i, i=1, 2, \dots, n\}$					
10.0	20.0	4	4	222	245
10.0	100.0	4	4	218	242
$n=5000, \{x_i=i, i=1, 2, \dots, n\}$					
10.0	20.0	4	4	532	589
10.0	100.0	4	4	526	580

* r and s are the parameters of matrix A in case (c); ** the convergence criterion for the iteration

Table 4 Number of iterations for solving Eq.(1) for the cavity surface charges of CH_3CONH_2 solvent with the present method and BCGM

Size of matrix A	The present method		BCGM	
	10^{-6*}	10^{-8*}	10^{-6*}	10^{-8*}
4002	30	40	35	58
5762	31	43	37	63

* the convergence criterion for the iteration

least 170 iterations. The maximum number of iterations for BCGM is 589 with the dimension of matrix A as 5000.

It is also found from the results in Tables 1, 2, and 3 that the vector b and the convergence threshold have almost no effect on the speed of convergence of the present method in terms of iterations, but do have some influence on the convergence of CGM and BCGM though the extents are not as large as the size of matrix A .

The surface charges of the water cavity that nominally encloses the solute molecule CH_3CONH_2 have been calculated with the so-called SS(V)PE (surface and simulation of volume polarization for electrostatics) method^[13,24,25] implemented in HONDO^[26]. The algebraic form of SS(V)PE method is a set of linear equations. The corresponding matrix is nonsymmetrical and diagonally dominant. The linear equations are solved with the present method and BCGM, respectively. The numerical results are listed in Table 4. The sizes of the matrix A are 4002 and 5762, respectively. It can be seen from Table 4 that the performances of the present method are also better than BCGM.

Some other types of well-conditioned matrices, for example, the configuration interaction matrices with dimensions larger than 100000, have also been investigated. The numerical results show that the present method is still superior to CGM.

3 Conclusions

The Davidson's method was extended to solve of large-scale linear equations. Numerical results in this study demonstrate that the present scheme is superior to the conjugate gradient method and the biconjugate gradient method for both symmetrical and nonsymmetrical cases, respectively. It seems that the present scheme is especially efficient for the nonsymmetrical and non-diagonal dominant matrices.

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