http://mmg.tversu.ru ISSN 2311-1275

Mathematical Modelling and Geometry

Volume 2, No 1, p. 10 – 26 (2014)

Iterative methods for calculations of extreme eigenvalues of large symmetric matrices

A. V. Mitin

The Chemistry Department, Moscow State University, 119991 Moscow, Russia

e-mail: mitin@phys.chem.msu.ru

Received 14 January 2014, in final form 12 February. Published 13 February 2014.

Abstract. It is shown that the iterative methods for the calculation of the extreme eigenvalues and corresponding eigenvectors of the generalized symmetric matrix eigenvalue problem can be divided into two general classes that differ from each other in the method of combining the Krylov subspace with iterations. The paper demonstrates unused possibilities in the development of iterative methods. Correspondingly, many new iterative methods are presented. Difficult problems related to the classification of some methods are also considered.

Keywords: Generalized matrix eigenvalue problem, Iterative methods

PACS numbers: 02.60.Dc

This work is supported by RFBR grant No 14-01-00420

1. Introduction

The generalized eigenvalue problem

$$AX = \lambda BX, \tag{1}$$

with real symmetric matrices A, B and a positive definite matrix B, is one of the main problems of computational linear algebra [1], which appears in many fields of natural and engineering sciences. For example, it arises in quantum mechanical calculations of the electronic and rotational-vibrational states of atoms and molecules using different methods [2, 3, 4, 5, 6], as well as in numerous engineering applications related to vibrations of constructions [7, 8, 9, 10]. The precision of such calculations strongly depends on the dimension of the matrices in Eq. (1) and usually increases with the matrix dimension. The dimension of the matrices in modern calculations may substantially exceed 10^4 and in many cases only extreme eigenvalues and corresponding eigenvectors are required.

The methods for calculating the eigenvalues of matrices can be divided into two groups: the methods for calculating all eigenvalues with corresponding eigenvectors and those for calculating the extreme eigenvalues with corresponding eigenvectors. The methods of the first group are applicable for matrices of dimensions not greater than 10^4 using modern computers, while for the methods of the second group the dimension of matrices is limited mainly by the available computational resources.

In the present paper we consider only iterative methods for calculating the extreme eigenvalues. It will be shown that such methods can be classified in accordance with two general algorithms, which differ from each other in the incorporation of the Krylov subspace with iterations. Classification of all known iterative methods is probably impossible, because of the great number of publications related to the topic during the last decades. However, the most important types of iterative methods, presented in the books [1, 11, 12, 13, 14, 15] and reviews [16, 17, 18, 19], as well as some methods published later will be taken into account. The analysis of these algorithms reveals unused possibilities in the development of iterative methods which allows the proposal of many new methods. The problems arising in the classification of the vectors, which form a basis of the Krylov subspace, will also be discussed.

2. General algorithms of projection and projection-iterative methods

The development of iterative methods for the determination of eigenvalues and corresponding eigenvectors of Eq. (1) has been initiated after the formulation of the Rayleigh-Ritz variational principle [20, 21, 22]. This principle transforms the algebraic generalized eigenvalue problem (1) into a variational problem for the Rayleigh functional

$$\rho(X) = \frac{(X, AX)}{(X, BX)}\,, \tag{2}$$

and thus the eigenvalue problem (1) is reduced to the determination of the minimum points of the Raylegh functional (2).

The analysis of the Rayleigh-Ritz variational principle have led to the proof of the Courant-Hilbert-Fischer minimax theorem [23, 24], the Hyleraas-Undheim-McDonald variational theorem [25, 26], as well to the proof of the fact that the approximate eigenvectors are close to the exact ones [27, 28]. These theorems have founded the basis of projection methods.

Further development of the Ritz variational method was continued by Bubnov [29] and Galerkin [30], where a projection method for solving the general variational problem was proposed and employed in practical calculations.

An important step towards to the modern projective methods was made by Krylov [31] who demonstrated that the vectors $X, B^{-1}AX, ..., (B^{-1}A)^{N-1}X$ form a system of linear independent basis vectors in the space associated with the $B^{-1}A$ matrix of the order of N for the problem (1).

The simple power and relaxation methods [32, 33, 34, 35, 36] were the first successful iterative algorithms that have been developed for the determination of extreme eigenvalues of Eq. (1). It is difficult to decide when the power method has been introduced. Probably, this is due to the fact that the simple power method naturally follows from the good approximation of the eigenvector corresponding to the largest absolute eigenvalue of the $B^{-1}A$ matrix by the vector $(B^{-1}A)^k X$ for sufficiently large k.

An important projection method has been developed by Lanczos [37] for the case of the unit matrix B. In fact, Lanczos has shown that the usual orthogonalization of the Krylov basis vectors yields a different set of basis vectors of the same space and that the original matrix has the tridiagonal form in this basis. For this reason, Lanczos method initially has been considered only as a tridiagonalization method of a real symmetric matrix. Later, however, it was found [38] that this method could be successfully used also for calculating of the extreme eigenvalues of real symmetric matrices. This property of the Lanczos method follows from the nature of the basis vectors in this method, which are consequent orthogonal gradients of the Rayleight functional (2).

The first projection-iterative algorithm for the calculation of extreme eigenvalues of Eq. (1) with the unit matrix B was developed by Karush [39]. In this method the orthogonal basis vectors introduced by Lanczos [37] were used to form a projection of the original matrix onto Krylov subspace.

Bauer [40] was the first to recognize that the iterations in the simple power method could be performed not only with a single vector, but also with a block of orthogonal vectors. Such simple improvement results in significant improvement of convergence of iterations.

A successful projection method for the calculation of extreme eigenvalues of Eq. (1) with the unit B matrix was developed by Davidson [41]. In contrast to the Lanczos method, it uses the nonorthogonal relaxation system of vectors [34, 42] with update of the new approximated eigenvector after each multiplication of the

original matrix by the vector. The new vector is then used for the calculation of the correction vector needed for the extension of the Krylov subspace. This results in significant improvement of the computational efficiency of the Davidson method as compared to the Lanczos method.

Finally, Liu [43] made the last step to the general algorithm of the projection and projection-iterative methods known now. He has proposed a block generalization of the Davidson algorithm by introducing Bauer's idea into the Davidson algorithm.

The analysis of these iterative methods shows that the iterations in them can be implemented using one of two general algorithms presented below.

Algorithm 1. Block projection method

Step 1. For the required m-th extreme eigenvalue define a set of k orthogonal vectors, which approximate the first eigenvectors X_1,X_2,...,X_k ($k \geq m$), and a set of orthogonal vectors Y_1,Y_2,...,Y_l. Form AV_1,AV_2,...,AV_{k+l}; BV_1,BV_2,...,BV_{k+l} and $F_{ij} = (AV_i, V_j)$, $S_{ij} = (BV_i, V_j)$, $i, j = 1, ..., k+l$, where $V_i = X_i$ for $i = 1, ...k$ and $V_i = Y_i$ for $i = k+1, ..., k+l$.

Step 2. Solve $Fd = \epsilon Sd$; select l eigenvalues ϵ_j, $j = m+1, ..., m+l$ with corresponding eigenvectors $d^j = (d_1^j, ..., d_{k+l}^j)^t$ of this equation starting from the m-th eigenvalue.

Step 3. Form l vectors $Z^j = \sum_{i=1}^{k+l} d_i^j V_i$ and residual vectors $R_j = AZ^j - \epsilon_j BZ^j$ and check the convergence using $\|R_j\|$.

Step 4. Define a new set of vectors $Y_{k+l+i}, i = 1, ..., l$, by using vectors Z^j obtained at *Step 3*.

Step 5. Orthonormalize $Y_{k+l+1}, Y_{k+l+2}, ..., Y_{k+2l}$ to $V_l, V_2, ..., V_{k+l}$ and use them for the extension of $\{V_i\}_{i=1}^{k+l}$.

Step 6. Put $k = k + l$. Form $F_{ij} = (AV_i, V_j)$ and $S_{ij} = (BV_i, V_j)$ for new i, j and return to *Step 2*.

Algorithm 2. Block projection-iterative method

Step 1. Define a set of k orthogonal vectors, which approximate the first eigenvectors X_1,X_2,...,X_k ($k \geq m$), where m is the number of required extreme eigenvalue. Define the Krylov subspace dimension $N = k * M$, where M is an integer number.

Step 2. Calculate the orthogonal basis vectors of the Krylov subspace $\{V_i\}, i = 1, ..., N$.

Step 3. Form AV_1,AV_2,...,AV_N; BV_1,BV_2,...,BV_N and $F_{ij} = (AV_i, V_j)$, $S_{ij} = (BV_i, V_j)$, $i, j = 1, ..., N$.

Step 4. Solve $Fd = \epsilon Sd$. Select the extreme eigenvalues ϵ_j, $j = 1, ..., k$ with corresponding eigenvectors $d^j = (d_1^j, ..., d_N^j)^t$.

Step 5. Form k vectors $Z^j = \sum_{i=1}^{N} d_i^j V_i$ and residual vectors $R_j = AZ^j - \epsilon_j BZ^j$. Check the convergence using $\|R_j\|$.

Step 6. Orthogonalize $Z_1, Z_2, ..., Z_k$. Return to *Step 1* and use $\{Z_i\}$ instead of the initial set of vectors.

The methods of both classes are intended for calculating the m-th extreme eigenvalue or a group of extreme eigenvalues and corresponding eigenvectors of

Eq. (1). It should be emphasized that the methods of both classes are projection methods. The difference between them arises from different incorporation of the Krylov subspace with iterations. Thus, in the first class of methods the iterations are needed to calculate the new vectors for an extension of the Krylov subspace, which is used for approximating the extreme part of the spectrum, while in the second class of methods a Krylov subspace of fixed dimension is used to calculate the new approximate vectors. The block versions of these methods permit to calculate degenerate eigenvalues and corresponding eigenvectors of Eq. (1).

Note also, that the vectors at *Step 1* and *Step 5* of **Algorithm 1** and at *Step 2* and *Step 6* of **Algorithm 2** can be mutually orthogonalized with respect to the matrix B, instead of usual orthogonalization, together with corresponding reduction of the generalized eigenvalue problem to a usual eigenvalue problem at *Step 2* and *Step 4*, respectively. Practically the dimension of the Krylov subspace in *Algorithm 1* is restricted by a certain value and the methods are restarted when the current dimension of the Krylov subspace reaches the limit.

3. Further developments of iterative methods

Lanczos method [37] permits to transform the symmetric dense matrix A of the eigenvalue problem

$$AX = \lambda X, \tag{3}$$

into a tridiagonal unsymmetric matrix. This is not convenient from the computational point of view. Therefore, in [44, 38, 45, 46] the variants of the Lanczos methods were considered that yield a symmetric tridiagonal matrix. Taking into account the results of these studies, an extension of the Lanczos method on the generalized eigenvalue problem (1) has been proposed in [12] and independently in [47]. In these papers it was shown that Eq. (1) in the space of basis vectors

$$\begin{aligned} &P_0 = X_0 \\ &SP_1 = AP_0 - \lambda_0 SP_0 \\ &SP_{i+1} = AP_i - \lambda_i SP_i - \beta_i SP_i, \ (i = 1, 2, ..., N-2), \end{aligned} \tag{4}$$

where

$$\begin{aligned} &\alpha_i = (AHP_i, P_i)/(SP_i, P_i), \ (i = 0, 1, ..., N-1) \\ &\beta_i = (AP_i, P_{i-1})/(SP_{i-1}, P_{i-1}), \ (i = 1, 2, ..., N-1), \end{aligned}$$

transforms into the eigenvalue problem (3) A being a tridiagonal matrix.

The convergence of the iterative method is very important in calculations of the selected eigenvalues of Eq. (1). The analysis of *Algorithm 1* and *Algorithm 2* shows that the properties of the basis vectors of the Krylov subspaces, used for the calculation of projections of the original matrices, to a large extent determine the convergence of the iterative methods. The system of basis vectors (4) is a system of orthogonal gradient vectors. Numerical experiments [33, 1, 34, 42] with single vector iterative methods for Eq. (3) show that with relaxation vectors the

convergence of iterations is better than with gradient vectors. Taking this result into account, Davidson proposed the method [41] that uses the relaxation vectors. The generalization of Davidson's method for Eq. (1) was presented in [48] together with the projection-iterative method. The basis vectors in these methods are calculated in accordance with the following equation

$$X_{l,j+1} = (A - \rho(X_j)B)X_{l,j}/(\rho(X_j)B_{l,l} - A_{l,l}) \ ,$$

where the fist index corresponds to a vector element, while the second one shows the iteration number. The algorithms of these two methods correspond to *Algorithm 1* and *Algorithm 2* presented above with no block generalization.

It is well known in the numerical analysis, that the iterative methods, derived by using the Newton-Raphson approach, display nearly quadratic convergence [49]. On the other hand, the methods mentioned above do not possess quadratic convergence near the solutions. This fact stimulates further developments and modifications of the new and known methods with the main aim of improving the convergence of iterations [50]. In Ref. [51] it was found that the correction vector [34, 42] used in Davidson method [41] often has the direction close to the initial one. This results in convergence problem in the Davidson method. To improve the Davidson method it was proposed to use the approach introduced by Jacobi that implies the calculation of a correction vector in an orthogonal space. Following this way, the Jacobi-Davidson method has been developed [51, 52, 53]. In this method a new correction vector U is calculated from the equation

$$(I - XX^+)(A - \epsilon I)(I - XX^+)U = -R \ , \tag{5}$$

where $R = (A-\epsilon I)X$ is a residual vector, while ϵ and X are current approximations for the eigenvalue and eigenvector of Eq. (3), respectively. Numerical tests of this method show that it converges faster than quadratically at the end of iterations. This fact is confirmed by the proof that the Jacobi-Davidson correction vector has the second-order property [52]. Thus the Jacobi-Davidson method can be considered as a Newton-type method. However, it was not clear which functional could be used for the derivation of the correction vector (5).

In this connection in [54] it was noted that the Lagrange functional

$$L(X, \lambda) = X^t AX - \lambda(X^t BX - 1) \ , \tag{6}$$

whose stationary points correspond to the eigenvalues of Eq. (1), can be used to obtain the Newton-type correction vector. Then the application of Newton-Raphson approach to the functional (6) yields the equation for correction vector δX

$$(A - \lambda B)\delta X - \delta\lambda BX = -(A - \lambda B)X \ , \tag{7}$$

where

$$\delta\lambda = \frac{X^t B(A - \lambda B)^{-1}(A - \lambda B)X}{X^t B(A - \lambda B)^{-1}BX} \ . \tag{8}$$

The Lagrange correction vector defined by equations (6) and (7) is exactly the Jacobi-Davidson correction vector in an equivalent form (Eq. (16) in [51]) or the Olsen correction vector [55]. Hence, the Jacobi-Davidson and Olsen methods can be treated as Newton-Raphson-type methods for the Lagrange functional. The derivation of the correction vector (6), (7) in [54] provides an independent proof of the second-order property of the Jacobi-Davidson correction vector, initially given in [52].

The Lagrange correction vector given above, allows the development of the block Newton-Lagrange method for the calculation of selected extreme eigenvalues of Eq. (1), presented in [54]. In this method, the Ritz eigenvalues for evaluation of λ and diagonal A_D and B_D matrices in $(A - \lambda B)^{-1}$ were used in the formulas for correction vector (7) and (8).

The Newton-type correction vector can also be obtained by applying the Newton-Raphson approach to the Rayleight functional (2). This was demonstrated in [56], where the following equation for correction vector δX was obtained

$$(A - \rho(X)B - BXG^{+} - G(BX)^{+})\delta X = -G \,, \tag{9}$$

where $G = (A - \rho(X)B)X$, and the block Newton-Rayleigh method using this correction vector was proposed. The correction vector given by (9) is orthogonal to the current gradient vector G. It is clear because X is a solution of the homogeneous system of linear equations

$$(A - \rho(X)B - BXG^{+} - G(BX)^{+})\delta X = 0$$

and, hence, Eq. (9) has a solution when δX is orthogonal to G.

All three correction vectors calculated from Eqs. (5), (7), and (9) possess the second-order property. Therefore, the iterative methods that used them [51, 54, 56] demonstrate the convergence higher than quadratic at the end of iterations, because they use a few such correction vectors for calculating the new ones. However, the numerical complexity of calculating the correction vectors from the solutions of systems of linear equations is proportional to $\sim N^3$ and thus it is comparable with the calculation of all eigevalues and eigenvectors of Eq. (1) by using other methods. This results in a limitation on the maximal dimension of matrices for which the extreme eigenvalues can be calculated.

In this connection let us consider approximations which reduce the numerical complexity of solutions of linear equation systems (5), (7), and (9). The simplest diagonal approximation for matrices in these equations were proposed in [56, 54] and three block diagonal methods: Jacobi-Davidson, Newton-Rayleight, and Newton-Lagrange have been proposed. The correction vectors in them are calculated in accordance with the following formulas

$$\delta X_{i,j+1} = -G_{i,j}/[(A_{ii} - \epsilon_j B_{ii})\left(I_{ii} - B_{ii}(X_{i,j})^2\right)^2] \,,$$

$$\delta X_i = -G_i/(A_{ii} - \rho B_{ii} - B_{ii}X_iG_i - G_iB_{ii}X_i) \,,$$

$$\delta X_{i,j} = (G_{i,j} - \delta\epsilon_i (BX^i)_j)/(A - \epsilon_i B)_{jj} \ ,$$

where

$$\delta\epsilon_i = [(X^i)^t B(A_D - \epsilon_i B_D)^{-1}(A - \epsilon_i B)X^i]/[(X^i)^t B(A_D - \epsilon_i B_D)^{-1} BX^i] \ .$$

Another approach for the simplification of the solutions of Eqs. (5), (7), and (9) consists in using band submatrices instead of the full matrices in the left-hand side of these equations. It permits the development of the block-band methods, i.e., Jacobi-Davidson, Newton-Rayleight, and Newton-Lagrange, presented in [56, 54].

A simplification of solutions can also be reached by using the skeleton matrix (SM) approximation for left-hand matrices in (5), (7), and (9). It can be formulated as follows: *only those matrix elements of matrices are taken into account whose absolute values are greater than a predefined threshold (Thr).* From this definition it follows that the full Newton-Raphson equation is recovered when $Thr = 0$. Hence, the predefined threshold (Thr) changes the complexity and the precision of the solution of the Newton-Raphson equation from the simplest diagonal matrices to the full ones. The block methods: Jacobi-Davidson, Newton-Rayleight, and Newton-Lagrange with SM approximation were proposed in [56, 54].

4. Test calculations

Accurate numerical tests of the new methods mentioned above with the aim to determine their performance in different cases is a difficult problem. Therefore, the few tests presented below have to be considered only as a first step in this direction.

The consideration of the correction vectors in the methods presented above shows that a double effect is caused by the approximations used in the solution of the Newton-Raphson equations. On the one hand, it leads to increasing the number of iterations, which are needed to calculate the required eigenvalue and the corresponding eigenvector. But on the other hand, it reduces the computational complexity of calculations of the new correction vectors and, therefore, the iterations become less expensive. For this reason, all tested methods are naturally divided into three groups: the Newton-Raphson-type methods with highest convergence at the end of iterations; the fastest diagonal type iterative methods that display the slowest convergence; and the methods with SM approximation.

The following notations will be used below: NL is for the Newton-Lagrange method; NR is for the Newton-Rayleigh method; JD is for the Jacobi-Davidson method; D is for the Davidson method; and R is for the residual method. An additional letter B will be used for the block version of these methods, while the additional letters D and SM denote the diagonal method and the method with the skeleton matrix approximation. In all numerical tests the iterations for calculating eigenvalues and the iterations for solving the system of linear equations were terminated when the Euclidean norm of the residual vector was smaller than 10^{-10}. The Euclidean norm of the final residual vector, the number of required iterations, and the number of the matrix-vector (MV) multiplications are presented in tables

Table 1: Example 1. Convergence on the norm of the residual vector for different methods.

Iter.	DNL	DNR	DJD	D	NL	NR	JD
1	0.168+03	0.168+03	0.168+03	0.168+03	0.168+03	0.168+03	0.168+03
2	0.718+02	0.870+00	0.710+00	0.723+02	0.382+00	0.711+02	0.711+02
3	0.418+02	0.548+00	0.770+00	0.636+02	0.923-01	0.358+02	0.358+02
4	0.110+02	0.629-01	0.206+00	0.237+02	0.165-01	0.247+02	0.247+02
5	0.162+01	0.173-01	0.592-01	0.173+02	0.641-03	0.617+01	0.617+01
6	0.300+00	0.175-02	0.794-02	0.138+02	0.477-04	0.228+01	0.228+01
7	0.648-01	0.954-04	0.115-02	0.417+01	0.274-05	0.698+00	0.698+00
8	0.134-01	0.120-04	0.925-04	0.547+00	0.138-06	0.491-02	0.491-02
9	0.134-02	0.787-06	0.898-05	0.164+01	0.670-08	0.183-09	0.182-09
10	0.134-03	0.474-07	0.521-06	0.847+00	0.298-09	0.936-10	0.136-09
11	0.105-04	0.212-08	0.381-07	0.528+00	0.122-10		0.118-09
12	0.710-06	0.121-09	0.172-08	0.153+01			0.108-09
13	0.484-07	0.426-11	0.101-09	0.294+01			0.981-10
14	0.275-08		0.377-11	0.670+01			
15	0.147-09			0.611+00			
16	0.554-11			0.447+00			

to demonstrate the convergence and the computational complexity of the different methods in the test calculations.

Example 1. The largest eigenvalue of the matrix whose non-zero elements are defined as $A_{i,j} = i$ for $i = j$; $A_{i,j} = 0.5$, for $j = i - 1, j = i + 1$; $A_{i,j} = 0.5$ for $i = 1, j = N$, and $i = N, j = 1$ was calculated by different methods. The dimension of the matrix was equal to 1000. The initial vector was defined as $(1.0, 0.01, ..., 0.01)^t$. The results of the test calculations obtained for four diagonal and three full methods are given in Table 1. The Newton-Rayleigh method shows overall the best performance. And the overall performance of the Newton-Lagrange method is better compared to that of the Jacobi-Davidson method. However, at the beginning the Newton-Lagrange method demonstrates the best performance due to using the approximations mentioned above. The stagnation of the Jacobi-Davidson method observed in this test calculation can be attributed to rounding errors arising from the projector operators used in this method. The performances of the diagonal DJD, DNR, and DNL methods do not differ significantly from those of the full methods. This means that the diagonal methods can be extremely efficient in some cases. Among the diagonal methods the convergence of the diagonal Newton-Rayleigh method is the fastest. The convergence of the diagonal Jacobi-Davidson method comes at the second, and the diagonal Newton-Lagrange method at the third place. The Davidson method required as many as 54 iterations in this test.

Example 2. In this example the 15 lowest eigenvalues and corresponding eigen-

Table 2: Example 2. Number of iterations and matrix-vector multiplications for different methods.

Method	Iter.	MV mult.
Block Newton-Lagrange (BNL)	6	66
Block Newton-Rayleigh (BNR)	6	59
Block Jacobi-Davidson (BJD)	8	73
With SM approximation ($Thr = 0.005$)		
Block Newton-Lagrange ($BNLSM$)	12	140
Block Newton-Rayleigh ($BNRSM$)	12	134
Block Jacobi-Davidson ($BJDSM$)	14	149
Block Residual ($BRSMS$)	13	143
Diagonal		
Block Diagonal Newton-Lagrange ($BDNL$)	25	275
Block Diagonal Newton-Rayleigh ($BDNR$)	25	275
Block Diagonal Jacobi-Davidson ($BDJD$)	24	276
Block Davidson (BD)	25	276

vectors of the matrix of dimension 5564 arising in an ADC calculation [57] of the excitation spectrum of the H_2O molecule have been calculated by using three full block methods, four block methods with SM approximation, and four block diagonal methods. The results of these test calculations are presented in Table 2. In this test the block Newton-Lagrange and the block Newton-Rayleigh methods show the best performance in the number of iterations, the block Newton-Rayleigh method being superior to the Newton-Lagrange method with respect to the number of matrix-vector multiplications. All block diagonal methods show similar performance. The performance of the methods with SM approximations are between those of the block full methods and block diagonal methods. The Newton-Rayleigh and the Newton-Lagrange methods are seen to be superior to the block residual and the block Jacobi-Davidson methods with respect to the number of iterations and matrix-vector multiplications.

Example 3. In this test, the lowest 10 eigenvalues of the *case*39 matrix of dimension 40216 from the sparse matrix collection of University of Florida (http://www.cise.ufl.edu/research/sparse/matrices/) have been calculated. Only four block diagonal methods were used in this test because the *case*39 matrix is a very sparse matrix with the number of non-zero elements less than 0.07%. The obtained results are presented in Table 3. In this test the block diagonal Newton-Lagrange method has required the smallest number of iterations and it was the second in the number of the matrix-vector multiplications. The block diagonal Newton-Rayleigh method was the second in the number of iterations and it has required the smallest number of the matrix-vector multiplications. The performance of the block diagonal Jacobi-Davidson and block Davidson methods were not as good as the former two methods.

Table 3: Example 3. Number of iterations and matrix-vector multiplications for different methods.

Method	Iter.	MV mult.
Block Diagonal Newton-Lagrange ($BDNL$)	13	125
Block Diagonal Newton-Rayleigh ($BDNR$)	16	119
Block Diagonal Jacobi-Davidson ($BDJD$)	34	158
Block Davidson (BD)	24	137

5. Conclusions

During the last years, a significant progress was reached in the development of efficient methods for calculating extreme eigenvalues of Eq. (1). The methods possessing higher than quadratic convergence at the end of iterations were developed. They are based on using correction vectors with second-order properties. It was shown that the vectors (5), (7), and (9) can be considered as Newton-Raphson vectors. However, these vectors can also be derived by employing other methods. Thus, the vector (5) was obtained by introducing the Jacobi approach into the Davidson method. It was derived, also, in an equivalent form by using the perturbation theory of the second order. Additionally, it can be noted that the Jacobi-Davidson correction method can be directly obtained by supposing that the orthogonal variation of eigenvector $X + (I + XX^+)\delta X$ has to provide a zero variation of the residual vector $\delta R(X + (I + XX^+)\delta X) = 0$. This leads to the equation for the Jacobi-Davidson correction vector

$$(A - \lambda B)(I + XX^+)\delta X = -(A - \lambda B)X \ ,$$

which transforms to the expression for Jacobi-Davidson correction vector after symmetrization of the left-hand-side matrix. This derivation has an advantage over the other ones, because it does not use any approximations.

The numerical tests show that the convergence of the block Newton-Lagrange method is between that of the block Newton-Rayleigh and the block Jacobi-Davidson methods. The convergence of the block-diagonal Newton-Lagrange method is slightly better than that of the Davidson and the block-diagonal Jacobi-Davidson methods, matching that of the block-diagonal Newton-Rayleigh method. The convergences of the methods with the SM approximation are between those of the corresponding full methods and their diagonal versions. The threshold of the SM approximation permits to tune the convergence behavior of a method from the full to the diagonal version.

The test calculations in *Example 1* show that the convergence of the diagonal methods can be only a little worse than that of the full ones. This means that in some cases the diagonal methods could significantly outperform the full methods, because in the latter ones a solution of the Newton-Raphson linear equations system is required. Therefore, the investigations of the convergence rates of different

methods are an important field of further research. Refs. [58, 59] give examples of such studies, where analytic estimations of the convergence rates were obtained for some iterative methods.

References

[1] Faddeev D. K. and Faddeeva V. N., *Computational Methods of Linear Algebra*, English Translation, Freeman, San Francisco, 1963

[2] McWeeny R. and Sutcliffe B. T. *Methods of Molecular Quantum Mechanics*, Academic Press, London, New York, 1969

[3] Shavitt I. *The method of configuration interaction*, in: Methods of Electronic Structure Theory, edited by Shaefer III H. F., Plenum Press, New York, 1977, pp. 189–275

[4] Ram-Mohan L. R. *Finite Element and Boundary Element Applications in Quantum Mechanics*, Oxford University Press, London, New York, 2002

[5] Fischer C. F. *The Hartree-Fock Method for Atoms. A Numerical Approach*, Wiley, New York, 1977

[6] Wilson E. B., Decius J. C., and Cross P. C. *Molecular Vibrations*, McGrow-Hill, New York,1955

[7] Bathé K.-J. and Wilson E. *Numerical Methods in Finite Element Analysis*, Prentice Hall, Englewood Cliffs, N.J., 1976

[8] Zienkiewicz O. C. and Taylor R. L. *The Finite Element Method. Basis Formulation and Linear Problems*, Fourth Edition, Vol. 1. McGraw-Hill, London, 1989

[9] Zienkiewicz O. C. and Taylor R. L. *The Finite Element Method. Solid and Fluid Mechanics. Dynamics and Non-Linearity*, Fourth Edition, Vol. 2. McGraw-Hill, London, 1989

[10] Senhi N. S. *Large Order Structural Eigenanalysis Techniques: Algorithms for Finite Element Systems*, Fourth Edition, Ellis Horwood, Chichester, Halsted Press, New York, 1989

[11] Wilkinson J. H. *The Algebraic Eigenvalue Problem*, Clarendon Press, Oxford, 1965

[12] Parlett B. N. *The Symmetric Eigenvalue Problem*, Prentice-Hall Inc., Englewood Cliffs, 1980

[13] Golub G. H. and Van Loan C. F. *Matrix Computations*, Johns Hopkins, Baltimore, 1983

[14] Cullum J. K. and Wiloughby R. A. *Lanczos Algorithms for Large Symmetric Eigenvalue Computations. Theory*, Vol. 1, Birkhaeuser, Boston, 1985

[15] Saad Y. *Numerical Methods for Large Eigenvalue Problems*, Halsted Press-John Wiley & Sons Inc., New York, 1992

[16] Stewart G. S. *A bibliographical tour of the large, sparse generalized eigenvalue problem*, in: Sparse Matrix Computations, edited by Bunch J. R. and Ross D. J., (Academic Press, New York, 1976), pp. 113–130

[17] Davidson E. R. *Matrix eigenvector methods*, in: Methods in Computational Molecular Physics, edited by Dierksen G. H. F., Wilson S., (D. Reidel, Dordrecht, 1983), pp. 95–113

[18] Parlett B. N. *The software scene in the extraction of eigenvalues from sparse matrices*, SIAM J. Sci. Stat. Comput. 1984, **5**, pp. 590–604

[19] Davidson E. R. *Super-matrix method*, Comput. Phys. Commun., 1989, **53**, pp. 49–60

[20] Rayleigh J. W. *In Finding the Correction for the Open End of an Organ-Pipe*, Phil. Trans. 1870, **161**, p. 77

[21] Lord Rayleigh (Strutt J. W.) *On the calculation of the frequency of vibration of a system in its gravest mode, with an example from hydrodynamics*, Philos. Mag. 1899, **47**, pp. 566–572

[22] Ritz W. *Über einer neue Methode zur Lösung gewisser Variationsprobleme der mathematischen Physik*, J. Reine Angew. Math. 1909, **135**, pp. 1–61

[23] Courant R. and D. Hilbert D. *Methods of Mathematical Physics, Vol. 1*, Interscience, New York, 1953

[24] Fischer E. *Über Quadratische Formen mit reelen Koeffizienten*, Monatshefte für Mathematik und Physik 1905, **16**, pp. 234–249

[25] Hylleraas E. A. and B. Undheim B. *Numerische Berechnung der 2 S-Terme von Ortho- und Par-Helium*, Z. Phys. 1930, **65**, pp. 759–772

[26] McDonald J. K. L. *Successive approximations by the Rayleigh-Ritz variation method*, Phys. Rev. 1933, **43**, pp. 830–833

[27] Eckart C. *The theory and calculation of screening constants*, Phys. Rev. 1930, **36**, pp. 878–892

[28] Shull H. and Löwdin P.-O. *Variation theorem for excited states*, Phys. Rev. 1958, **110**, pp. 1466–1467

[29] Bubnov I. G. *Report on the works of Prof. Timoshenko which were awarded the Zhuranskii prize, Simposium of the Institute of Communication Engineers*, Sborn. Inst. Inzh. Putei Soobsch. Sankt Peterburg 1913 **81** (in Russian)

[30] Galerkin B. G. *Sterzni i plastinki. Rjadi v nekotorih voprosah yprygogo ravnovesija sterznei i plastinok*, Vestnik ingenerov 1915, **1**, pp. 897–908 (in Russian)

[31] Krylov A. N. *On the numerical solution of equations which in technical questions are determined by the frequency of small vibrations of material systems*, Izv. Acad.Nauk SSSR, VII Ser., Otd. Mat. Estest. 1931, issue **4**, pp. 491–539 (in Russian)

[32] Pellew A. and Southwell R. U. *Relaxation methods applied to engineering problems. VI. The natural frequencies of systems having restricted freedom*, Proc. Roy., Soc. (A) 1940, **175**, pp. 262–290

[33] Cooper J. L. B., *The solution of natural frequency equations by relaxation methods*, Quarterly of Applied Mathematics 1948, **6**, pp. 179–183

[34] Boys S. F. *Electronic wave functions. II. A calculation for the ground state of the beryllium atom*, Proc. Roy., Soc. (London) 1950, **A201**, pp. 125–137

[35] Crandall S. H. *On a relaxation method for eigenvalue problem*, J. Math. and Phys. 1951, **30**, pp. 140–145

[36] Crandall S. H. *Iterative procedures related to relaxation methods for eigenvalue problems*, Proc. Roy., Soc. (A) 1951, **A207**, pp. 416–423

[37] Lanczos C. *An iterative method for the solution of the eigenvalue problem of linear differential and integral operators*, J. Res. Natl. Bur. Stand. 1950, **45**, pp. 255–282

[38] Paige C. C. *Computational variants of the Lanczos method for the eigenproblem*, J. Inst. Math. Appl. 1972, **10**, pp. 373–381

[39] Karush W. *An iterative method for finding characteristic vectors of a symmetric matrix*, Pacif. J. Math. 1951, **1**, pp. 233–248

[40] Bauer F. L. *Das Verfahren der Treppeniteration und verwandte Verfahren zur Lösung algebraischer Eigenwertprobleme*, Z. Angew. Math. Phys. 1957, **8**, pp. 214–235

[41] Davidson E. R. *The iterative calculation of a few of the lowest eigenvalues and corresponding eigenvectors of large real-symmetric matrices*, J. Comp. Phys. 1975, **17**, pp. 87–94

[42] Nesbet R. K. *Algorithm for diagonalization of large matrices*, J. Chem. Phys. 1965, **43**, pp. 311–312

[43] Liu B. *The simultaneous expansion for solution of the lowest eigenvalues and corresponding eigenvectors of large real-symmetric eigenvectors of large real-symmetric matrices*, in: Numerical Algorithms in Chemistry: Algebraic Methods, Eds. Moler C. and Shavitt I., Lawrence Berkley Lab., Univ. of California, 1978, p. 49

[44] Paige C. C. *Practical use of the symmetric Lanczos process with reorthogonalisation*, BIT 1970, **10**, pp. 183–195

[45] Golub G. H. *Some uses of the Lanczos algorithm in numerical linear algebra*, in: Topics in Numerical Analysis, Ed. Miller J. H., London, New York, Academic Press, 1973, pp. 173–184

[46] Sebe T. and Nachamkin J. *Variational buildup of nuclear shell model bases*, Ann. Phys. 1969, **51**, pp. 100–123

[47] Mitin A. V. *Theoretical Investigations of the Low-Lying Electronic States of Diatomic Molecules. Molecules BeN, BC, and anion BeN^-*, Autoref. Diss. Kand. Nauk, Dolgoprudnyi, 1981 (in Russian)

[48] Mitin A. V. *Iterative methods for the calculation of a few of the lowest eigenvalues and corresponding eigenvectors of the $AX = \lambda BX$ equation with real symmetric matrices of large dimension*, J. Comput. Chem. 1994, **12**, pp. 747–751

[49] Bahvalov N. S., Zidkov N. P, and Kobelkov G. M. *Numerical methods*, Science, Moscow, 1987 (in Russian)

[50] Butscher W. and Kammer W. E. *Modification of Davidson's method for the calculation of eigenvalues and eigenvectors of large real-symmetric matrices: "Root homing procedure"*, J. Comput. Phys. 1976, **20**, pp. 313–325; Parlett B. N., *The Lanczos algorithm with selective orthogonalization*, Math. Comput. 1979, **33**, pp. 217–238; Ericsson T. and Ruhe A. *The spectral transformation Lanczos method for the numerical solution of large sparse generalized symmetric eigenvalue problems*, Math. Comput. 1980, **35**, pp. 1251–1268; Kalamboukis T. Z., *Davidson's algorithm with and without perturbation correction*, J. Phys. A: Math. Gen. 1980, **13**, pp. 57–62; Cullum J. and Wiloughby R. A. *Computing eigenvalues of very large symmetric matrices — An implementation of a Lanczos algorithm with no reorthogonalization*, J. Comput. Phys. 1981, **44**, pp. 329–358; van der Vorst H. A. *A generalized Lanczos scheme*, Math. Comput. 1982, **39**, pp. 559–561; Simon H. D. *Analysis of the symmetric Lanczos algorithm with reorthogonalization methods*, Linear Algebra Appl. 1984, **61**, pp. 101–131; Simon H. D. *The Lanczos algorithm with partial reorthogonalization*, Math. Comput. 1984, **42**, pp. 115–142; Kosugi N. *Modification of the Liu–Davidson method for*

obtaining one or simultaneously several eigensolutions of large real-symmetric matrix, J. Comput. Phys. 1984, **55**, pp. 426–436; Wood D. M. and Zunger A. *A new method for diagonalising large matrices*, J. Phys. A: Math. Gen. 1985, **18**, pp. 1343–1359; Morgan R. B. and Scott D. S. *Generalizations of Davidson's method for computing eigenvalues of sparse symmetric matrices*, SIAM J. Sci. Stat. Comput. 1986, **7**, pp. 817–825; Kress J. D., Woodruff S. W., and Parker G. A. and Pack R. T. *Some strategies for enhancing the performance of the block Lanczos method*, Comput. Phys. Comm. 1989, **53**, pp. 109–115; Parlett B. N. and Nour-Omid B. *Towards a block Lanczos program*, Comput. Phys. Comm. 1989, **53**, pp. 169–179; van Lenthe J. H. and Pulay P. *A Space-Saving Modification of Davidson's Eigenvector Algorithm*, J. Comput. Chem. 1990, **11**, pp. 1164–1168; Grimes R. G., Levis J. G., and Simon M. D. *A shifted block Lanczos algorithm for solving sparse symmetric generalized eigenproblems*, SIAM J. Matrix Anal. Appl. 1994, **15**, pp. 228–272; Crouzeix M., Philippe B., and Sadkane M. *The Davidson method*, SIAM J. Sci. Comput. 1994, **15**, pp. 62–76; Stathopoulos A., Saad Y., and Fischer C. F. *Robust preconditioning of large, sparse, symmetric eigenvalue problems*, J. Comput. Appl. Math. 1995, **64**, pp. 197–215

[51] Sleijpen G. L. G. and van der Vorst H. A. *A Jacobi–Davidson iteration method for linear eigenvalue problems*, SIAM J. Matrix Anal. Appl. 1996, **17**, pp. 401–425

[52] Sleijpen G. L. G., Booten J. G. L., Fokkema D. R., and van der Vorst H. A. *A Jacobi–Davidson type methods for generalized eigenproblems and polynomial eigenproblems*, BIT 1996, **36**, pp. 595–633

[53] Genseberger M. and Sleijpen G. L. G. *Alternative correction equation in the Jacobi–Davidson method*, Numer. Linear Algebra Appl. 1999, **6**, pp. 235–253

[54] Mitin A. V. *Lagrange type iterative methods for calculation of eigenvalues of generalized eigenvalue problem with large symmetric matrices*, Int. J. Quantum Chem. 2011, **111**, pp. 2545–2554

[55] Olsen J., Jørgensen P., and Simons J. *Passing the one-billion limit in full configuration-interaction (FCI) calculations*, Chem. Phys. Lett. 1990, **169**, pp. 463–472

[56] Mitin A. V. *New methods for calculations of the lowest eigenvalues of the real symmetric generalized eigenvalue problem*, J. Comput. Phys. 2000, **161**, pp. 653–667

[57] Schirmer J. *Beyond the random-pahse approximation: A new approximation scheme for the polarization propagator*, Phys. Rev. A 1982, **26**, pp. 2395–2416

[58] Knyazev A. V. and Skorokhodov A. L. *The rate of convergence of the method of steepest descent in a euclidean norm*, U.S.S.R. Comput. Maths. Math. Phys. 1988, **28**, pp. 195–196

[59] Knyazev A. V. and Skorokhodov A. L. *Preconditioned gradient-type iterative methods in a subspace for partial generalized symmetric eigenvalue problem*, SIAM J. Numer. Anal. 1994, **31**, pp. 1226–1239