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

MMG *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

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

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