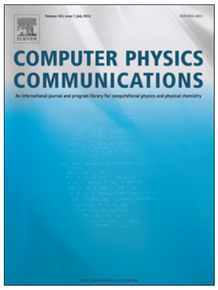
Accepted Manuscript



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J.H. Noble, M. Lubasch, J. Stevens, U.D. Jentschura

PII: S0010-4655(17)30196-0
DOI: http://dx.doi.org/10.1016/j.cpc.2017.06.014
Reference: COMPHY 6248

To appear in: *Computer Physics Communications*

Received date : 7 October 2013
Revised date : 9 June 2017
Accepted date : 17 June 2017

Please cite this article as: J.H. Noble, M. Lubasch, J. Stevens, U.D. Jentschura, Diagonalization of complex symmetric matrices: Generalized Householder reflections, iterative deflation and implicit shifts, *Computer Physics Communications* (2017), http://dx.doi.org/10.1016/j.cpc.2017.06.014

Diagonalization of Complex Symmetric Matrices: Generalized Householder Reflections, Iterative Deflation and Implicit Shifts

J. H. Noble[a], M. Lubasch[b], J. Stevens[a], U. D. Jentschura[a,*]

[a] *Department of Physics, Missouri University of Science and Technology, Rolla, Missouri 65409-0640, USA*
[b] *Clarendon Laboratory, Parks Road, Oxford OX1 3PU, United Kingdom*

Abstract

We describe a matrix diagonalization algorithm for complex symmetric (not Hermitian) matrices, $\underline{A} = \underline{A}^{\mathrm{T}}$, which is based on a two-step algorithm involving generalized Householder reflections based on the indefinite inner product $\langle \underline{u}, \underline{v} \rangle_* = \sum_i u_i\, v_i$. This inner product is linear in both arguments and avoids complex conjugation. The complex symmetric input matrix is transformed to tridiagonal form using generalized Householder transformations (first step). An iterative, generalized QL decomposition of the tridiagonal matrix employing an implicit shift converges toward diagonal form (second step). The QL algorithm employs iterative deflation techniques when a machine-precision zero is encountered "prematurely" on the super-/sub-diagonal. The algorithm allows for a reliable and computationally efficient computation of resonance and antiresonance energies which emerge from complex-scaled Hamiltonians, and for the numerical determination of the real energy eigenvalues of pseudo–Hermitian and $\mathcal{PT}$-symmetric Hamilton matrices. Numerical reference values are provided.

Keywords: Complex Symmetric Matrix Diagonalization; Indefinite Inner Product; Implicit Shift; Deflation Techniques

PROGRAM SUMMARY
Program Title: HTDQLS
Program Files doi: `http://dx.doi.org/10.17632/x24wjxtrsg.1`
Licensing provisions: GPLv3
Programming language: Fortran 90 using fixed form notation
Nature of problem: Calculating the eigenvalues and optionally the eigenvectors of complex symmetric (non-Hermitian), densely populated matrices.
Solution method: The complex symmetric (not Hermitian) input matrix is diagonalized in two steps. First step: The matrix is tridiagonalized via a series of $(n-2)$ generalized Householder reflections, where n is the rank of the input matrix. Second step: The tridiagonal matrix is diagonalized via a generalization of the "chasing the bulge" technique, which is an iterative process utilizing an initial implicitly shifted initial rotation followed by $(n-2)$ Givens rotations. This technique is an implementation of QL factorization, and converges roughly as $[(\lambda_i - \sigma_i)/(\lambda_{i+1} - \sigma_i)]^j$ where λ_i is the eigenvalue located in the (i,i) position of the final diagonal matrix and the eigenvalues are ordered $(|\lambda_1| < |\lambda_2| < \ldots < |\lambda_n|)$, and j is the iteration. The "educated guess" σ_i for the eigenvalue λ_i is obtained from the analytic determination of the eigenvalues of $(k \times k)$-submatrices of $\underline{A}$, in the vicinity of the ith element, where $k = 0, 1, 2, 3$ (here, $k = 0$ means that the implicit shift vanishes, $\sigma_i = 0$). The routine optionally calculates the rotation matrix $\underline{Z}$, such that $\underline{Z}^{-1}\, \underline{A}\, \underline{Z} = \underline{D}$ where $\underline{A}$ is the input matrix and $\underline{D}$ is the diagonal matrix containing the eigenvalues. The ith column of $\underline{Z}$ then is the eigenvector of $\underline{A}$ corresponding to the eigenvalue found at the element $\underline{D}(i,i)$, in the ith position on the diagonal of the matrix $\underline{D}$.
Unusual features:

*Corresponding author.
E-mail address: ulj@mst.edu, telephone +1-573-3416221, fax +1-573-3414715.