

A new method for diagonalising large matrices

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of eigenvalues sought: even if only the lowest few eigensolutions are needed, the computational effort involved is close to that required for *all* eigensolutions.

There are many problems of physical interest for which such difficulties with the CH method can become acute. Many quantum mechanical Hamiltonian problems require only the lowest few eigensolutions to very large matrices whose elements $\langle \phi_i | \mathbf{H} | \phi_j \rangle$ are easy to calculate, but which possess no simple systematics (e.g. they are not diagonally dominant or sparse). Such is the case, for example, in ground-state electronic structure calculations for molecules, solids and surfaces, where our relative ignorance of what constitutes a physically motivated basis set (14) often leads to the

2. Iterative methods for large matrix diagonalisation

2.1. Background

Consider a real $n \times n$ matrix A with elements a_{ij} . Let λ be a real eigenvalue of A and x a corresponding real eigenvector. Then

$$Ax = \lambda x$$

Let $\lambda_1, \lambda_2, \dots, \lambda_n$ be the eigenvalues of A and x_1, x_2, \dots, x_n be the corresponding eigenvectors. Then the matrix X formed by the eigenvectors as columns and the diagonal matrix Λ formed by the eigenvalues as diagonal elements, satisfy the equation

$$AX = X\Lambda$$

where X is the matrix of eigenvectors and Λ is the diagonal matrix of eigenvalues. This equation can be written as

$$A - \Lambda = X^{-1}(A - \Lambda)X$$

where X^{-1} is the inverse of the matrix X . The matrix $X^{-1}(A - \Lambda)X$ is a matrix whose elements are all zero except for the elements on the diagonal which are all zero.

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Using Consumer Information to Fight the Competition in the Child's Household

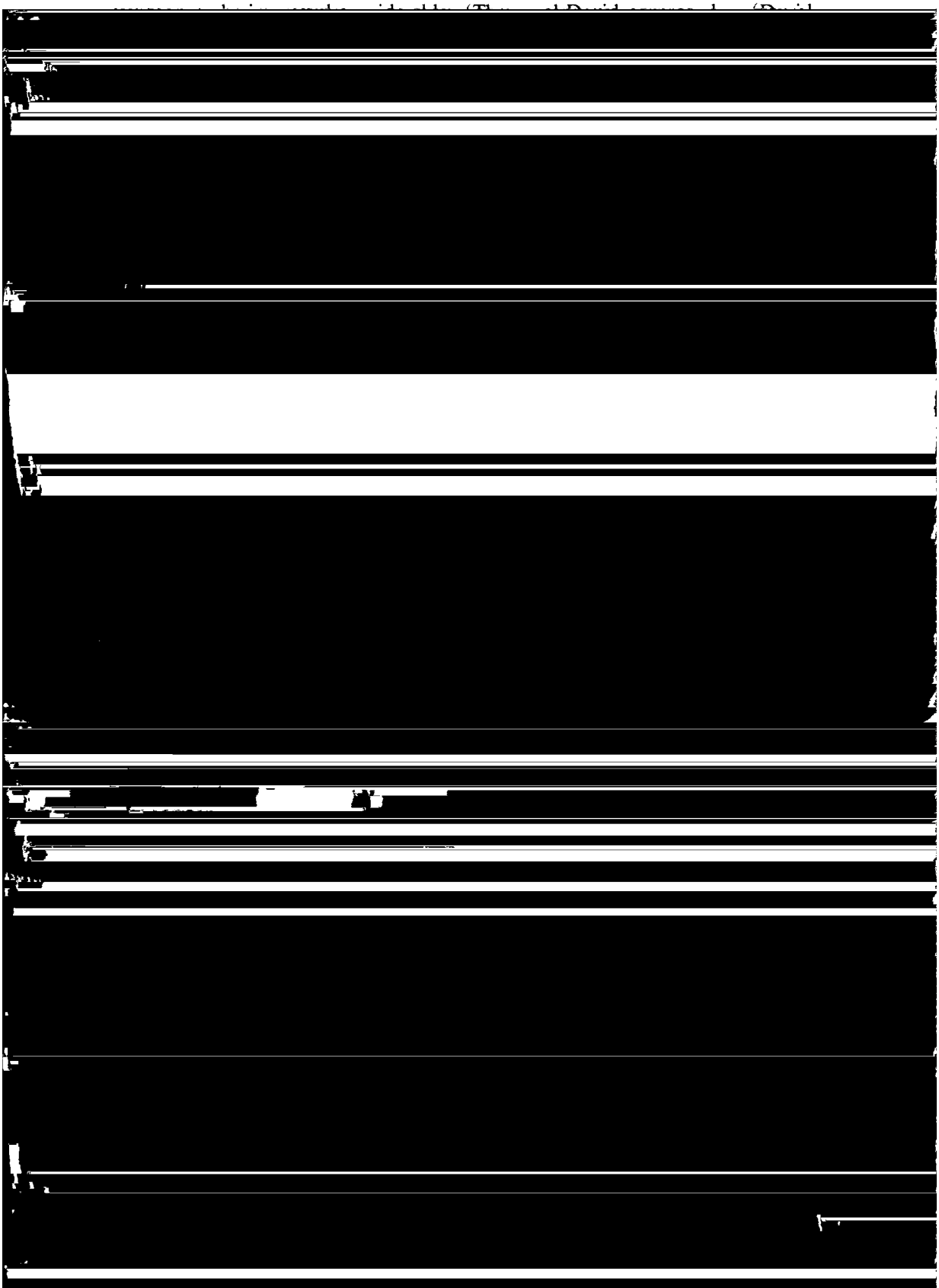
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where we have used the linearity of the residual operator. Unfortunately, the formal solution

$$|\delta A\rangle = -(\mathbf{H} - E^{ap}\mathbf{S})^{-1}|R(|A^{ap}\rangle, E^{ap})\rangle \quad (2.8)$$

is no easier to solve than the original eigenproblem because of the need for matrix

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The expansion set $\{|b_i\rangle\}$ requires further explanation. Like the other basis expansion methods, DIIS uses a Newton step, equation (3.3), to generate a new vector $|\delta A\rangle$ which is then added to $\{|b_i\rangle\}$. The elements of this set are thus the $|\delta A\rangle$ generated in each of the preceding iterations, so that DIIS clearly incorporates information from the entire iteration history for the given eigenvector being refined. Since the vectors $\{|\delta A^{(i)}\rangle\}$ are

where

$$A_{ij} = \frac{1}{2}(\alpha_i + \alpha_j) \quad \text{for } i \neq j, \quad (2.1)$$

$$A_{ii} = \alpha_i \quad \text{for } i = 1, 2, \dots, n. \quad (2.2)$$

$$A_{ij} = \frac{1}{2}(\alpha_i - \alpha_j) \quad \text{for } i \neq j, \quad (2.3)$$

$$A_{ii} = \alpha_i \quad \text{for } i = 1, 2, \dots, n. \quad (2.4)$$

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$$A_{ii} = \alpha_i \quad \text{for } i = 1, 2, \dots, n. \quad (2.6)$$

$$A_{ij} = \frac{1}{2}(\alpha_i - \alpha_j) \quad \text{for } i \neq j, \quad (2.7)$$

$$A_{ii} = \alpha_i \quad \text{for } i = 1, 2, \dots, n. \quad (2.8)$$

$$A_{ij} = \frac{1}{2}(\alpha_i + \alpha_j) \quad \text{for } i \neq j, \quad (2.9)$$

$$A_{ii} = \alpha_i \quad \text{for } i = 1, 2, \dots, n. \quad (2.10)$$

$$A_{ij} = \frac{1}{2}(\alpha_i - \alpha_j) \quad \text{for } i \neq j, \quad (2.11)$$

$$A_{ii} = \alpha_i \quad \text{for } i = 1, 2, \dots, n. \quad (2.12)$$

$$A_{ij} = \frac{1}{2}(\alpha_i + \alpha_j) \quad \text{for } i \neq j, \quad (2.13)$$

$$A_{ii} = \alpha_i \quad \text{for } i = 1, 2, \dots, n. \quad (2.14)$$

$$A_{ij} = \frac{1}{2}(\alpha_i - \alpha_j) \quad \text{for } i \neq j, \quad (2.15)$$

$$A_{ii} = \alpha_i \quad \text{for } i = 1, 2, \dots, n. \quad (2.16)$$

$$A_{ij} = \frac{1}{2}(\alpha_i + \alpha_j) \quad \text{for } i \neq j, \quad (2.17)$$

$$A_{ii} = \alpha_i \quad \text{for } i = 1, 2, \dots, n. \quad (2.18)$$

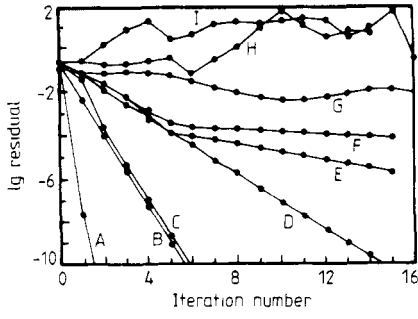


Figure 1. Iteration histories for the modified Nesbet matrix: A, block Davidson ($m = n = 4$), $\epsilon = 10^{-7}$; B, Davidson; C, DHS; D, E, F, simultaneous coordination relaxation for $m = 5$, $\epsilon = 10^{-7}$; G, H, symmetric Lanczos (equation 2.7).

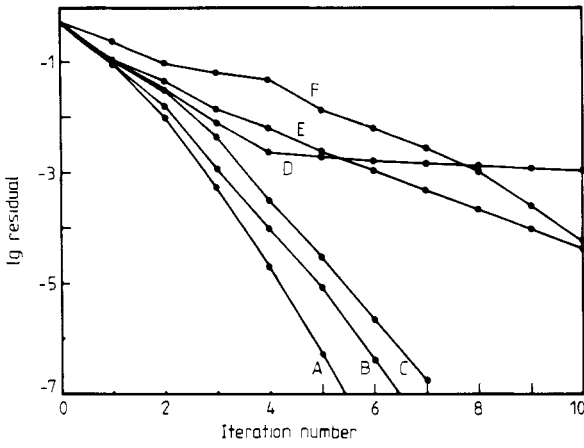


Figure 2. Iteration histories for the complex Hermitian 7x7 matrix: A, block Davidson

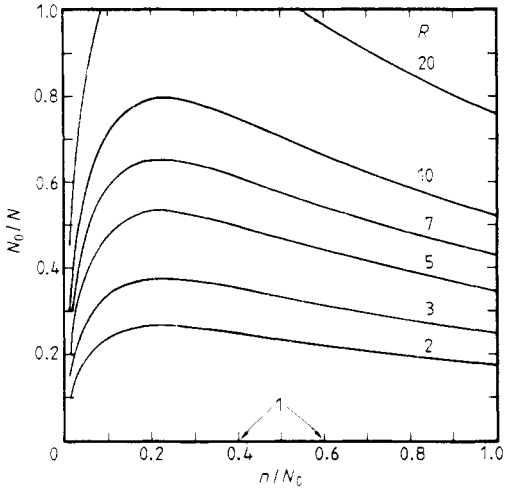
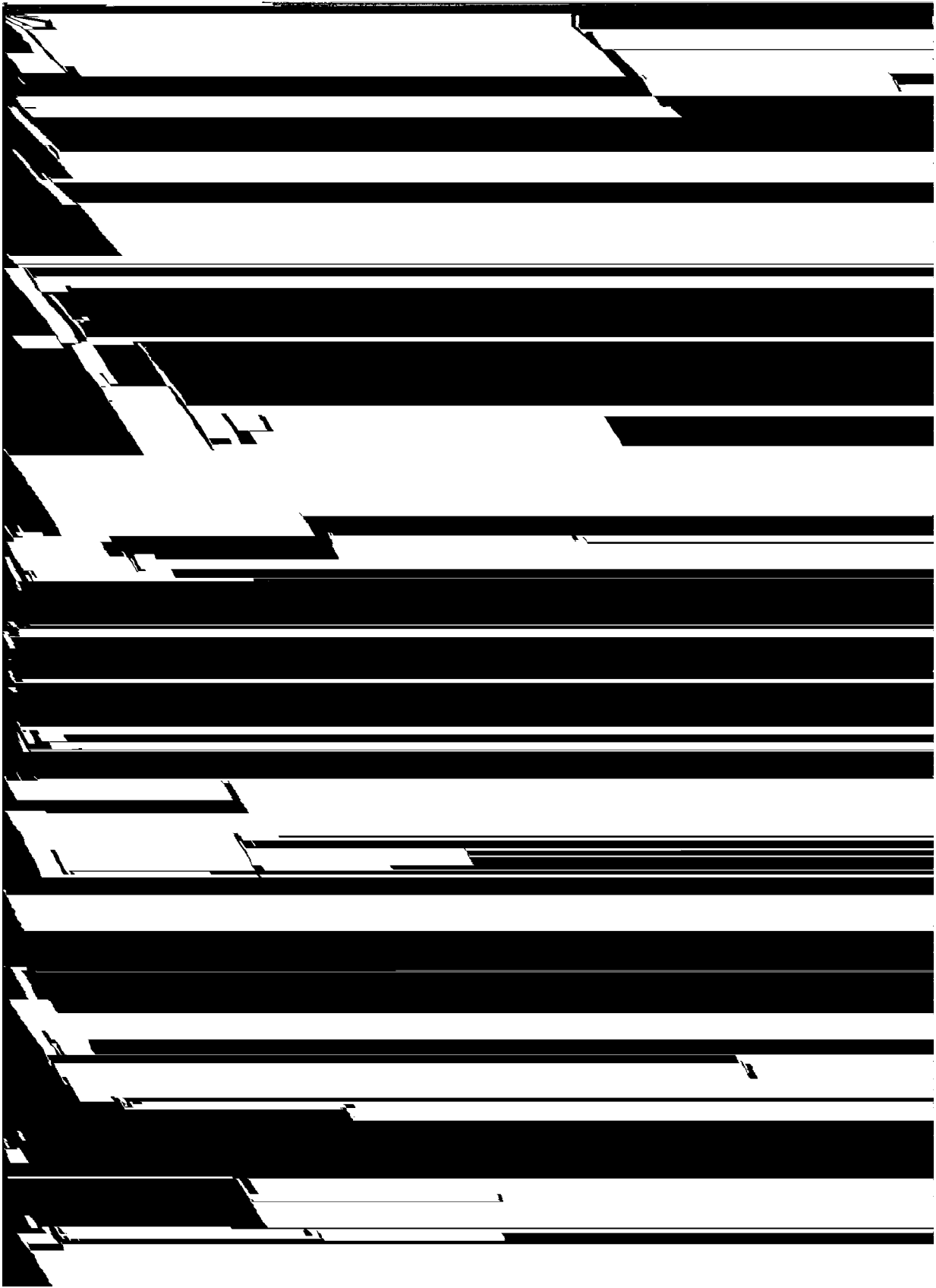


Fig. 4. Plot of N_0/N versus n/N_c for various values of P (1.2)



Acknowledgments

In preparing this paper, we have benefitted from notes by Paul Bendt and from Bendt and Zunger (1982b). We gratefully acknowledge R Nesbet for pointing out NRCC

