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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.

[redacted]

2. Iterative methods for large matrix diagonalisation

2.1. Background

[illegible]

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

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

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

[redacted]

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 [redacted]

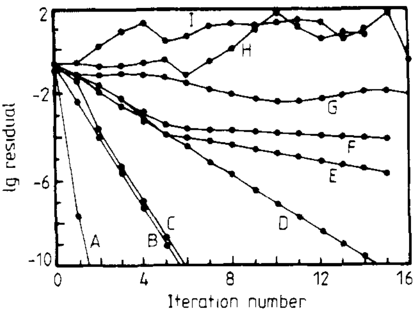
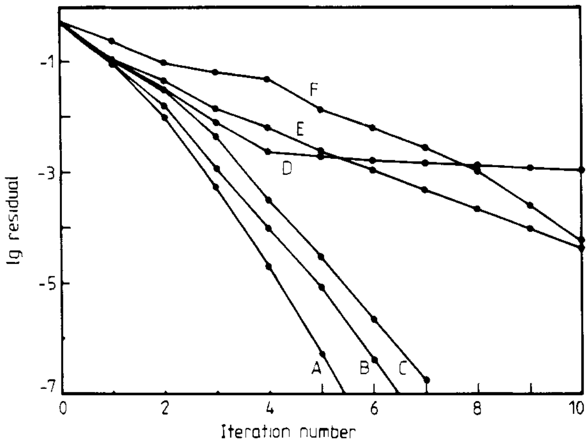
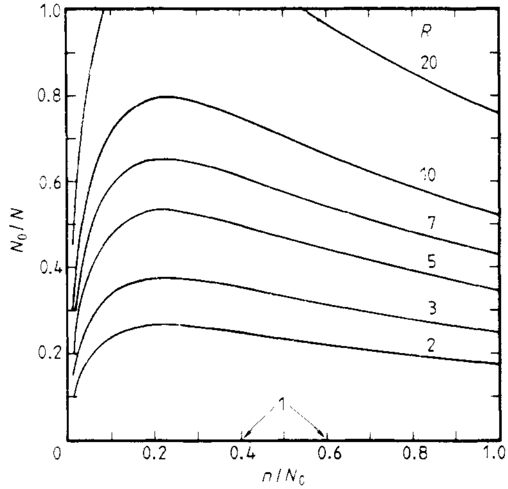


Figure 1. Iteration histories for the modified Nesbet matrix: A, block Davidson ($m = n = 4$), $\varepsilon = 10^{-7}$; B, Davidson; C, DIIS; D, E, F, simultaneous coordination relaxation for $m = 5$,



[redacted]



[redacted]

Acknowledgments

In preparing this paper, we have benefitted from notes by Paul Bendt and from Bendt [redacted]