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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.

2. Iterative methods for large matrix diagonalisation

2.1. Background

Consider a real symmetric matrix A of order n . Let $\lambda_1, \lambda_2, \dots, \lambda_n$ be the eigenvalues of A and e_1, e_2, \dots, e_n be the corresponding orthonormal eigenvectors. Let $E = [e_1, e_2, \dots, e_n]$ and $\Lambda = \text{diag}(\lambda_1, \lambda_2, \dots, \lambda_n)$. Then $A = E\Lambda E^T$.

Let μ be a real number. Let $\alpha = \alpha(\mu)$ be the number of eigenvalues of A which are less than or equal to μ . Let $\beta = \beta(\mu)$ be the number of eigenvalues of A which are greater than or equal to μ . Let $\gamma = \gamma(\mu) = n - \alpha - \beta$ be the number of eigenvalues of A which are strictly between μ and μ . Let $\delta = \delta(\mu) = \alpha - \beta$ be the difference between the number of eigenvalues of A which are less than or equal to μ and the number of eigenvalues of A which are greater than or equal to μ . Let $\epsilon = \epsilon(\mu) = \beta - \alpha$ be the difference between the number of eigenvalues of A which are greater than or equal to μ and the number of eigenvalues of A which are less than or equal to μ .

Let $\mu_1, \mu_2, \dots, \mu_n$ be the eigenvalues of A arranged in ascending order. Let $\mu_{(k)}$ be the k th smallest eigenvalue of A . Let $\mu_{(k)}$ be the k th largest eigenvalue of A . Let $\mu_{(k)}$ be the k th smallest eigenvalue of A . Let $\mu_{(k)}$ be the k th largest eigenvalue of A .

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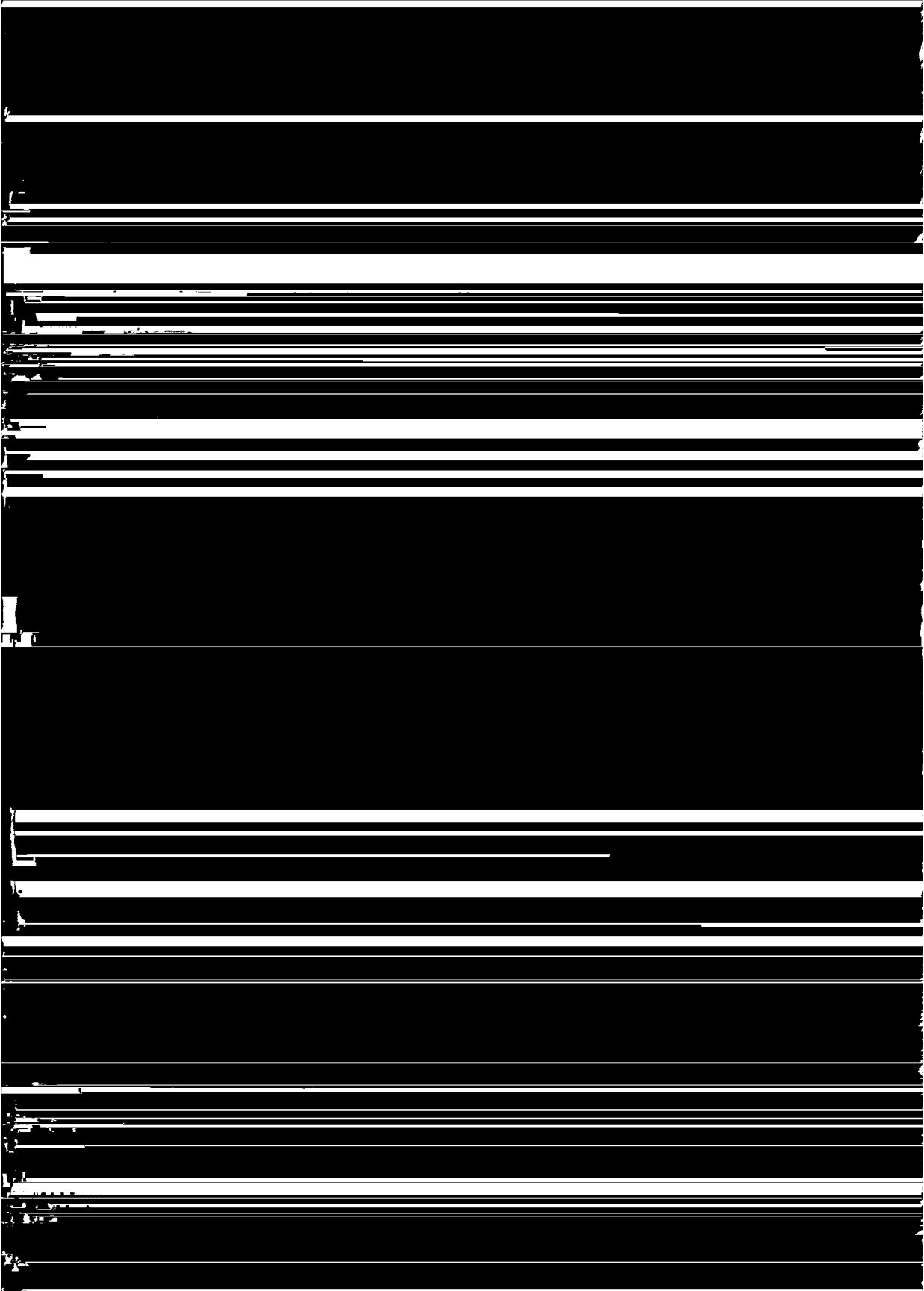
Using Consumer Information to Fight the Competition in the Child's Household

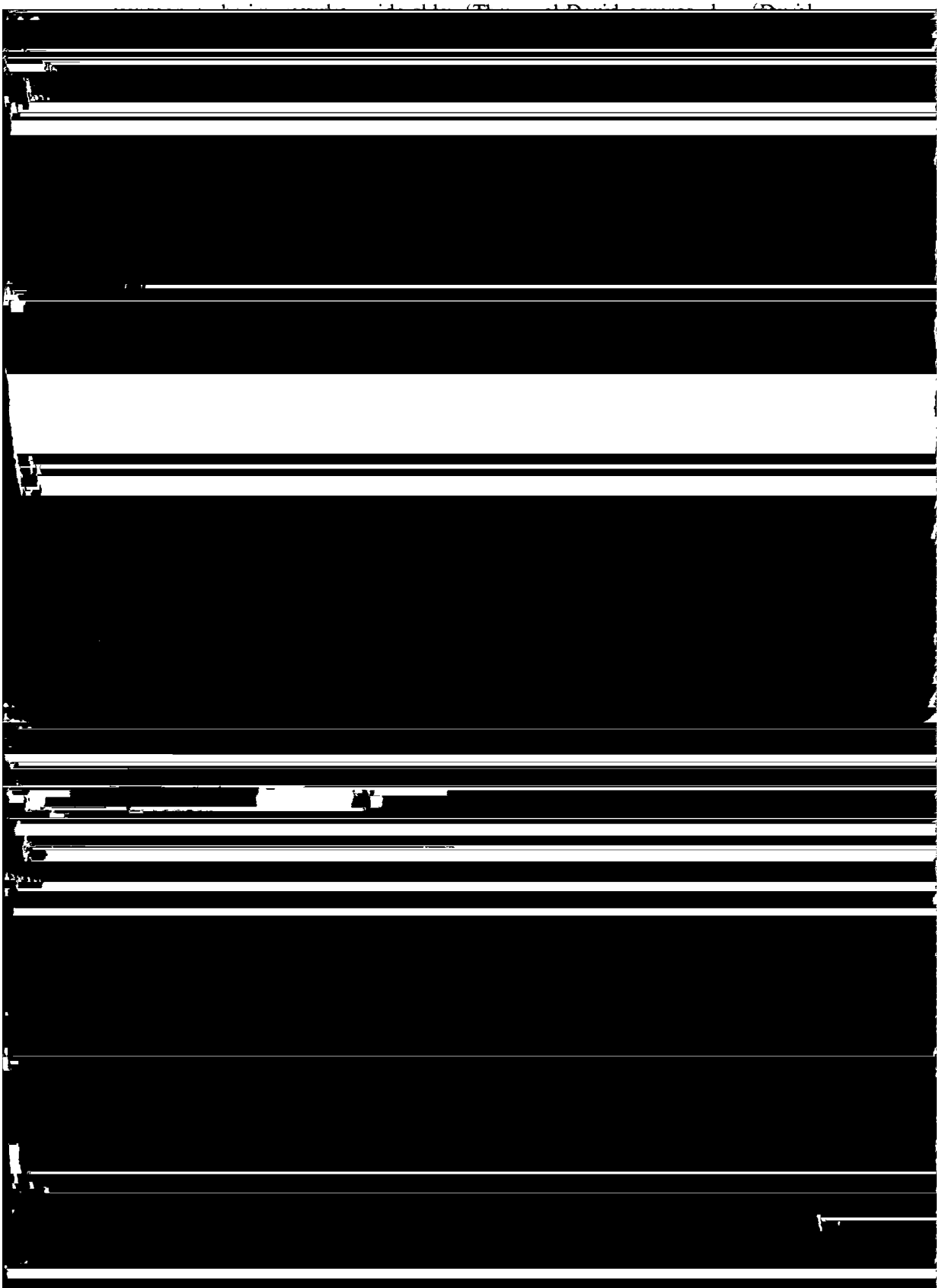
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where we have used the linearity of the residual operator. Unfortunately, the formal solution

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

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





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

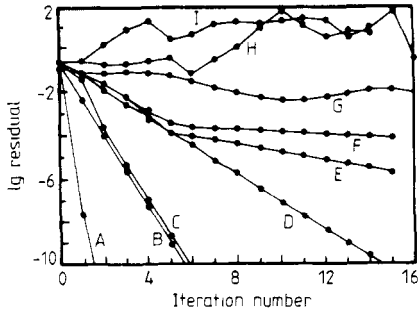


Figure 1. Iteration histories for the modified Nesbet matrix: A, block Davidson ($m = n = 4$), $\epsilon = 10^{-7}$; B, Davidson; C, DHS; D, E, F, simultaneous coordination relaxation for $m = 5$, $\epsilon = 10^{-7}$; G, symmetric Lanczos (equation 2.7); H, symmetric Lanczos (equation 2.8).

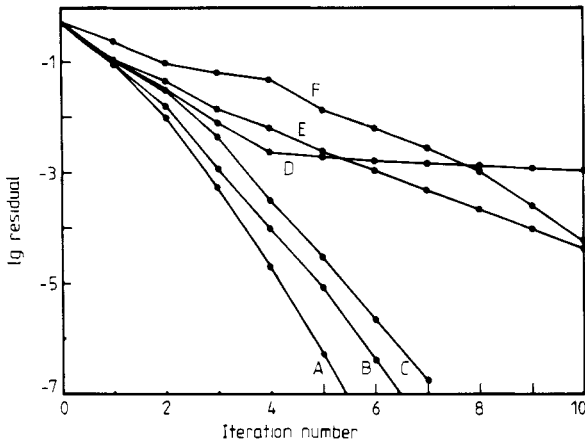


Figure 2. Iteration histories for the complex Hermitian 7x7 matrix: A, block Davidson

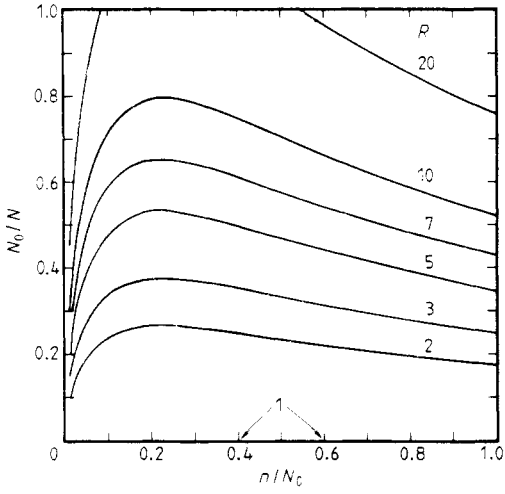
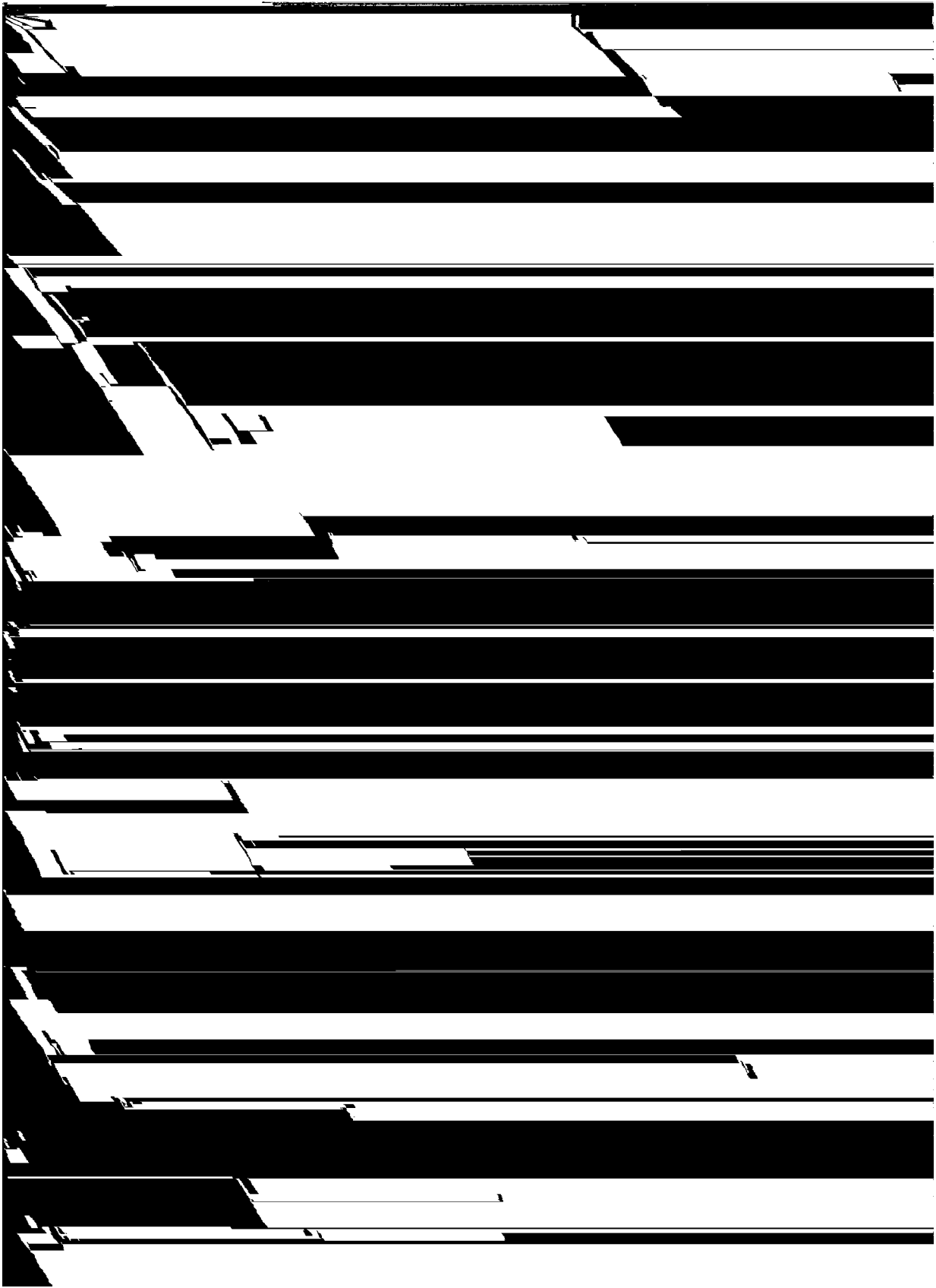


Fig. 4. Plot of N_0/N vs n/N_c for various values of P (see eq. (12)).



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

