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# Note

## Acceleration of the Convergence in Nesbet's Algorithm for Eigenvalues and Eigenvectors of Large Matrices

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A few years ago Nesbet [1] introduced an algorithm for the determination of eigenvalues and eigenvectors of large symmetric matrices. The algorithm has recently been modified by Shavitt [2] for efficient application to sparse symmetric matrices and extended by Bender and Shavitt [3] to cover extremal eigenvalues of nonsymmetric matrices. A well-known property of the Rayleigh quotient [4] is exploited, namely, that if we have estimates $\mathbf{b}$ and $\mathbf{c}$ for corresponding left and right eigenvectors of a normal (4) matrix $\mathbf{A}$, and if the absolute errors in $\mathbf{b}$ and $\mathbf{c}$ are of order $\epsilon$, then the generalized Rayleigh quotient $E = (\mathbf{b}^T\mathbf{A}\mathbf{c})/(\mathbf{b}^T\mathbf{c})$ gives an estimate of the corresponding eigenvalue, accurate to order $\epsilon^2$. When the matrix is non-normal, Wilkinson [4] has shown that $E$ may still provide a good estimate of the eigenvalue; the error in this case is of order $\epsilon^2/(\mathbf{b}^T\mathbf{c})$ and in practice one is unlikely to be concerned with cases where $(\mathbf{b}^T\mathbf{c})$ is small since the eigenvalue problem is not then a priori well-posed [5]. In the most general version of the algorithm [3] we start with trial vectors $\mathbf{b}$ and $\mathbf{c}$ and compute $E$ as an estimate of the eigenvalue, the next trial values of $\mathbf{b}$ and $\mathbf{c}$ being generated by applying one step of the simple Gauss–Seidel (GS) iterative process [6] to the matrix $\mathbf{A} - E\mathbf{I}$ (where $\mathbf{I}$ is the unit matrix). It is at this point that the convergence can be improved. Knowing that in the solution of linear equations the *extrapolated* GS (or successive over-relaxation (SOR)) method can frequently be made to converge faster than the basic GS scheme, we found it natural to investigate the effect of replacing the single GS iteration in Nesbet's algorithm by an SOR iteration. In this paper we show how this modification may very simply be incorporated in the iterative scheme given by Bender and Shavitt [3] and we discuss the results of applying the modified algorithm to some matrices which arise in the statistical mechanics of lattice systems.

## THE SOR METHOD

Both GS and SOR are members of the same class of iterative methods for the solution of sets of linear equations. To solve the set of equations $\mathbf{Ax} = \mathbf{b}$ we split the matrix $\mathbf{A}$ into the form $\mathbf{A} = \mathbf{M} - \mathbf{N}$ and then iterate as follows:

$$\mathbf{x}_0 \text{ arbitrary},$$
$$\mathbf{Mx}_{m+1} = \mathbf{Nx}_m + \mathbf{b}, \qquad m = 1, 2, 3, \ldots. \tag{1}$$

In practice the splitting of $\mathbf{A}$ is chosen to make the solution of (1) simple or even trivial.[1] The GS method is defined by the splitting

$$\begin{aligned} \mathbf{M} &= \mathbf{D} - \mathbf{E}, \\ \mathbf{N} &= \mathbf{F}, \end{aligned} \tag{2}$$

where $\mathbf{D}$ is diagonal and $\mathbf{E}$, $\mathbf{F}$ are, respectively, strictly lower and upper triangular matrices. However, this particular splitting of $\mathbf{A}$ is just one member of the one-parameter family of splittings defined by

$$\begin{aligned} \mathbf{M}(\omega) &= (1/\omega)(\mathbf{D} - \omega\mathbf{E}), \\ \mathbf{N}(\omega) &= (1/\omega)\{(1 - \omega)\,\mathbf{D} + \omega\mathbf{F}\}. \end{aligned} \tag{3}$$

SOR is the iterative scheme defined by the splitting (3) and it can be shown [6] that SOR *may* converge when $0 < \omega < 2$. If $\omega = 1$ we retrieve the basic GS scheme, but it is frequently found that with the choice of an alternative value of $\omega$ (usually between 1 and 2) we achieve faster convergence to the solution of a set of linear equations.

## MODIFICATION OF THE ALGORITHM

The most general current version of the algorithm was given by Bender and Shavitt [3] and we now show how their scheme may be modified to incorporate SOR in the iterative solution of the eigenvalue problem

$$\begin{aligned} \mathbf{Ac} &= E\mathbf{c}, \\ \mathbf{bA} &= E\mathbf{b}. \end{aligned} \tag{4}$$

Given estimates $\mathbf{b}$ and $\mathbf{c}$ for the right and left eigenvectors we guess initially that the eigenvalue is

$$E \equiv N/D = (\mathbf{b}^T\mathbf{Ac})/(\mathbf{b}^T\mathbf{c}). \tag{5}$$

[1] The requirement that the iterative scheme converges leads to restrictions on the choice of splitting. This problem is discussed by Varga [6].

Bender and Shavitt modify **b**, **c** and $E$ thus:

$$\sigma_\mu = \sum_{\lambda=1}^{n} A_{\mu\lambda} c_\lambda - E c_\mu , \tag{6}$$

$$\sigma_\mu' = \sum_{\lambda=1}^{n} b_\lambda A_{\lambda\mu} - E b_\mu , \tag{7}$$

$$\Delta c_\mu = \sigma_\mu/(E - A_{\mu\mu}), \tag{8}$$

$$\Delta b_\mu = \sigma_\mu'/(E - A_{\mu\mu}), \tag{9}$$

$$\Delta D = (\Delta b_\mu)\, c_\mu + b_\mu(\Delta c_\mu) + (\Delta b_\mu)(\Delta c_\mu), \tag{10}$$

$$\Delta E = \Delta b_\mu \sigma_\mu/(D + \Delta D) \equiv \Delta c_\mu \sigma_\mu'/(D + \Delta D). \tag{11}$$

Equations (8) and (9) are the results of a single GS iteration on the Eqs. (4). Equation (10) is obvious. Equation (11) may be verified by evaluating the Rayleigh quotient

$$E + \Delta E = ((\mathbf{b} + \Delta\mathbf{b})^T \mathbf{A}(\mathbf{c} + \Delta\mathbf{c}))/((\mathbf{b} + \Delta\mathbf{b})^T (\mathbf{c} + \Delta\mathbf{c})). \tag{12}$$

To incorporate SOR into the algorithm we have only to replace Eqs. (8), (9), and (11) by

$$\Delta c_\mu = \omega\sigma_\mu/(E - A_{\mu\mu}), \tag{8'}$$

$$\Delta b_\mu = \omega\sigma_\mu'/(E - A_{\mu\mu}), \tag{9'}$$

$$\Delta E = (\Delta b_\mu)\, \sigma_\mu(2 - \omega)/(D + \Delta D). \tag{11'}$$

These equations are obtained in a similar manner to (8), (9), and (11).

## Use of the Modified Algorithm

The algorithm, modified to incorporate SOR, was tested by the author on some sequences of matrices $\{\mathbf{K}_m\}$, which arise in a problem in lattice statistics [7]. The matrices are irreducible and the matrix elements, all nonnegative, are functions of the real positive variable $z$; the quantities of physical interest derive from the eigenvalue of maximum modulus (necessarily real and positive) and its derivatives with respect to $z$. Denoting by $E$, **b**, **c**, respectively, the maximum eigenvalue and the corresponding left and right eigenvectors of $\mathbf{K}_m$, and by $\mathbf{K}_m'$ the matrix whose elements are the derivatives of the elements of $\mathbf{K}_m$, we can easily show that

$$dE/dz = (\mathbf{b}^T \mathbf{K}_m' \mathbf{c})/(\mathbf{b}^T \mathbf{c}). \tag{13}$$

TABLE I

Properties of the Matrices $\mathbf{K}_m$

| $m$ | Dimension of $\mathbf{K}_m$ | Percentage of nonzero elements |
|---|---|---|
| 2 | 3 | 55.6 |
| 4 | 5 | 44 |
| 6 | 10 | 28 |
| 8 | 19 | 20.2 |
| 10 | 41 | 14.1 |
| 12 | 97 | 9.1 |
| 14 | 241 | 6.1 |

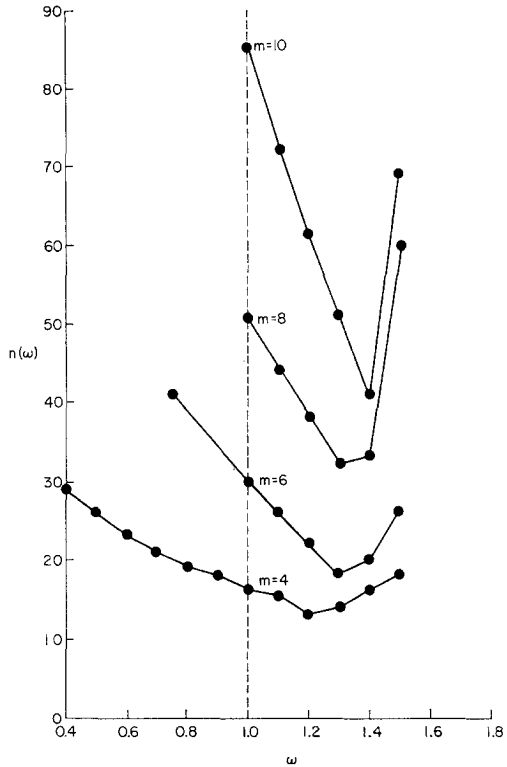


FIG. 1. Variation of $n(\omega)$, the number of iterations required for convergence with $\omega$, the SOR acceleration parameter for the matrices $\mathbf{K}_4$, $\mathbf{K}_6$, $\mathbf{K}_8$, $\mathbf{K}_{10}$. The original algorithm corresponds to $\omega = 1$.

Thus to compute $dE/dz$ we require (to high accuracy) a knowledge of **b** and **c** as well as of $E$.

For each value of $z$ we had a sequence of matrices, $\{\mathbf{K}_m : m = 2, 4, 6,...\}$, the dimension of the matrices increasing approximately exponentially with $m$ while the proportion of nonzero elements decreased slowly with $m$ (See Table I). We set $z = 1$ and studied the matrices $\mathbf{K}_4$ to $\mathbf{K}_{10}$. Using for **b** and **c** the deliberately poorly chosen starting vectors (1, 1,..., 1) and its transpose, we noted, for a number of values of $\omega$, the number of iterations $n(\omega)$ required before $\Delta b_\mu$ and $\Delta c_\mu$ were less than a certain tolerance ($10^{-6}$) for all $\mu$. To eliminate spurious effects due to the very inaccurate starting vectors, ten iterations with $\omega = 1$ were executed before setting $\omega$ to any other chosen value. The variation of $n(\omega)$ with $\omega$ is shown in Fig. 1 and it is clear that there is an optimum value of $\omega$ around $\omega = 1.4$ for which substantial acceleration of convergence is achieved. The work was repeated for a few different values of $z$ with the same results. Similar tests of the algorithm have been carried out on matrices arising from different problems in lattice statistics and have yielded the same qualitative conclusion, i.e., there is an optimum value of $\omega$ for which the convergence is substantially faster than with $\omega = 1$.

The obvious disadvantage of the modified algorithm is the lack of a simple method of estimating the optimum value of $\omega$. However, this can be overcome in two situations:

(i) If we have a family of matrices of increasing dimension a few test calculations on the smaller matrices may indicate a suitable value of $\omega$. (e.g., $\omega = 1.4$ proved satisfactory for the aforementioned matrices $\mathbf{K}_{12}$ and $\mathbf{K}_{14}$ over a wide range of values of $z$),

(ii) We are likely to be using the algorithm only for matrices which are too large to store in the core of the computer as an ordinary two-dimensional array (since otherwise methods based on similarity transformations are superior [4]), in which case each iteration may require a few seconds of computer time. In circumstances where the user may intervene during execution of the program, the value of $\omega$ may be changed if the convergence is slow. The author has found this "experimental" approach successful in dealing with a number of matrices of dimension greater than 250.

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