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Calculation of Eigenvectors of Large Matrices

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A method of calculating eigenvectors by variance minimization is presented. The procedure of adjusting sequentially each component of a trial vector is discussed and it is shown that variance minimization and the MOR method both generate an approximate subspace of the true eigenspace. Procedures to deal with this subspace are given which both improve the MOR method and make the method of variance minimization suitable for obtaining non-extremal eigenvalues and eigenvectors of matrices with nearly degenerate eigenvalues.

1. INTRODUCTION

Complete diagonalization of a matrix **A** with rank N requires about N^3 multiplications [1] and involves cumbersome transformations when N is large.

When only a few eigenvectors and eigenvalues are required, it is useful to be able to calculate them individually. Also when **A** is large and sparse, it is desirable to restrict operations on **A** to the following two types:

1. Scalar product $v_i = (\mathbf{a}_i, \mathbf{X})$

where $\mathbf{a}_i$ is the ith column of **A** and **X** the trial vector.

2. Matrix-vector product $\mathbf{V} = (\mathbf{A}, \mathbf{X})$

which requires $\sim M$ multiplications, when A contains M nonzero elements.

The MOR method [3] operates under these requirements and is capable of efficiently giving the extremal eigenvalues and eigenvectors.

To obtain the other eigenvectors, each $(\mathbf{a}_i, \mathbf{X})$ must be corrected with a suitable linear combination of the ith component of the eigenvectors already generated [3]. This implicit deflation has undesirable consequences:

(1) MOR cannot give conveniently all eigenvectors because the implicit deflation will need much work for the intermediate eigenvectors.

(2) One cannot expect good accuracy for an eigenvector when the previous ones have themselves not been computed with equivalent accuracy.

It is therefore desirable to seek some property which can be improved without any knowledge of the eigenvectors. The variance, w, with respect to $\mathbf{X}$ is just such a quantity:

$$w = \{(\mathbf{AX} - \lambda X), (\mathbf{AX} - \lambda X)\}/(\mathbf{X}, \mathbf{X}) \geqslant 0$$

and $\lambda = (\mathbf{X}, \mathbf{AX})/(\mathbf{X}, \mathbf{X})$ is the Rayleigh quotient of X, which is extremized in MOR. When $\mathbf{X}$ is an eigenvector, it follows that $w = 0$, and λ is the eigenvalue. It can be shown that the inequality $w \gg (\lambda - \lambda_0)^2$ always holds [7], where λ_0 is the eigenvalue closest to λ. When λ_0 is the only eigenvalue such that $| \lambda - \lambda_0 | < \sqrt{w}$, one can be sure that the smaller w is, the closer $\mathbf{X}$ is to the corresponding eigenvector $\mathbf{X}_0$.

The variance concept has previously been used by Seidel [5], who solves the equation $\mathbf{AX} = \mathbf{Y}$ by minimizing the variance $\{(\mathbf{AX} - \mathbf{Y}), (\mathbf{AX} - \mathbf{Y})\}$. In his simplest procedure each component of $\mathbf{X}$ is adjusted in turn. This method is also adopted in MOR and the next step will be to attempt to minimize w in the same way.[1]

II. Minimizing Variance by Optimally Adjusting Components

The ith component x_i of $\mathbf{X}$ is to be changed by a quantity, α, such that

$$(dw/dx_i)_{x_i+\alpha} = 0 \qquad \text{and} \qquad (d^2w/dx_i^2)_{x_i+\alpha} > 0$$

Introduce the vector $\mathbf{V} = \mathbf{AX} - \lambda\mathbf{X}$ with ith component v_i, and the norm $r = (\mathbf{X}, \mathbf{X})$. Then the change $x_i \to x_i + \alpha$ produces the new (primed) values:

$$\begin{aligned} r' &= r + \alpha(2x_i + \alpha) \\ \lambda' &= \lambda + \alpha\{2v_i + \alpha(\mathbf{A}_{ii} - \lambda)\}/r' \\ w' &= (w + 2\alpha a + \alpha^2 b)/r' - (\lambda - \lambda')^2 \end{aligned}$$

with $a = (\mathbf{a}_i, \mathbf{V}) - \lambda v_i$ and $b = \lambda^2 - 2\lambda\mathbf{A}_{ii} + (\mathbf{a}_i, \mathbf{a}_i)$. Instead of solving the quartic equation $dw'/d\alpha = 0$, w' is minimized by interpolating near α_0, a value for α for which $(dw'/d\alpha) = 0 + \theta(\alpha^2)$. Hence:

$$\alpha_0 = (x_i w - a)/\{b - w - 2(x_i^2 w + 2v_i^2 - a x_i)/r\}.$$

These equations show that the scalar products $(\mathbf{a}_i, \mathbf{V})$ and $(\mathbf{a}_i, \mathbf{X})$ have to be evaluated.

[1] The following arguments and speeding procedures can be also applied to the Seidel method (unpublished work).

The computational effort required by one iteration[2] may be twice as great as that required in MOR method, which only requires $(\mathbf{a}_i, \mathbf{X})$. However the present method, called W, needs no deflation with respect to the other vectors.

III. Usual Behaviour of the Components Relaxation Methods

The present work will not concern itself with diagonally dominating [4] matrices $|\mathbf{A}_{ij}| < |\mathbf{A}_{ii} - \mathbf{A}_{jj}|$. Instead it is preferred to consider matrices with nearly degenerate eigenvalues (N.D.E.). For the eigenvectors with eigenvalues belonging to N.D.E. clusters, convergence of MOR method can be very slow [3]. In Table I

TABLE I

Matrix and exact eigenvalue			Initial vector Rayleigh quotient	Initial vector Variance	Iteration number or Rayleigh quotient of iteration 200 with MOR	Iteration number or Rayleigh quotient of iteration 200 with W
$N = 20$ case 1	I	1.977662	1.95652	0.0742	13	49
	II	1.911146	1.83696	0.2560	37	1.911153
	III	1.801938	1.65074	0.4786	35	1.802015
	IV	1.652478	1.41260	0.6557	32	1.652525
	V	1.466104	1.13200	0.8110	32	1.466121
$\mathbf{A}_{ii} = 0.$						
$N = 40$ case 2	I	1.994132	1.97826	0.0376	42	1.994121
	II	1.976561	1.91848	0.1347	72	1.976076
	III	1.947391	1.82609	0.2687	1.947384	1.947353
	IV	1.906793	1.70652	0.4149	74	1.906249
	V	1.855005	1.57065	0.5874	83	1.855198
$N = 20$ case 3	I	4.270462	4.24383	0.0649	13	38
	II	3 527876	3.49866	0.0764	14	50
	III	2.940160	2.92373	0.0396	16	59
	IV	2.439539	2.40948	0.0415	18	98
	V[a]	2.026962	1.89708	0.0845	50	2.017525
$\mathbf{A}_{ii} = 3., 2.7, .. 0.3, 0., 0., 0., ..$						
$N = 40$ case 4	I	4.270462	Same as $N = 20$		13	38
	II	3.527876			14	50
	III	2.940160			16	59
	IV	2.439539			18	98
	V[a]	2.028264			108	2.017895

[a] Nearly degenerate with VI.

[2] We call "an iteration" a cycle of N steps. The corresponding computational time does not depend too much on the procedures which are discussed in this work.

TABLE II

	(50 × 50) Matrix given in section V					Matrix 2 of Table I	
		Iteration number or λ at iteration 100				Iteration number	
	Exact eigenvalue	MOR	MOREL	W	WEL	MOREL	WEL
I	−0.922401	47	26	−0.904277	31	18	29
II	−0.499910	49	39	−0.499077	64	27	47
III	−0.354915	62	40	−0.250166	140	27	62
IV	$5.736\ 10^{-7}$	43	33	$3.78\ 10^{-5}$	51	28	63
V	$3.805\ 10^{-4}$	77	48	$1.18\ 10^{-2}$	116	30	134

results are given obtained with MOR and W for 4 matrices with N.D.E. Symmetric tridiagonal matrices have been considered with $\mathbf{A}_{i,i\pm1} = 1$ and $\mathbf{A}_{ii} = 0$ in cases 1 and 2 or $\mathbf{A}_{ii} = 3$; 2.7; 2.4;...; 0.3; 0.; 0.; 0.;... in cases 3 and 4. The matrices are small: $N = 20$ for matrices 1 and 3, or $N = 40$ for 2 and 4. It was attempted to obtain the first 5 eigenvectors fulfilling a convergence criterion of $w < 10^{-7}$. The initial trial vectors were deduced from diagonalization of similar matrices with $N = 10$. It can be seen from columns 2 and 3 of Table 1 that the initial λ and w are good. Yet, columns 4 and 5 indicate that large numbers of iterations are required or no convergence is obtained (in this case, the λ value at the 200th iteration is given). W method always requires more iterations than MOR.

It was interesting to study the variation of the component of the ith eigenvector $\mathbf{X}_i$ in the trial vector $\mathbf{X}$ (i.e., $(\mathbf{X}_i, \mathbf{X})/(\mathbf{X}, \mathbf{X})$) as the iterative procedure progressed. In Figs. 1 and 2 the absolute value of the components greater than 0.01 ($\mathbf{X}_1$ excluded) are shown, for matrix 1 and an initial vector

$$\mathbf{X} = 2\mathbf{X}_1 + \tfrac{1}{3}(\mathbf{X}_3 + \mathbf{X}_5 + \cdots \mathbf{X}_{19}).$$

Two results are obtained: 1. Eigenvectors with initially zero components are introduced into the trial vector. This can be observed in Figs. 1 and 2 most noticeably in the cases of $\mathbf{X}_2$ and $\mathbf{X}_4$. This arises since modification of x_i introduces into $\mathbf{X}$ some weight of $\mathbf{e}_i$ (the vector with ith component equal to 1 and the rest all 0), and consequently some weight of all $\mathbf{X}_p$ which have a nonzero ith component. 2. Both W and MOR are inefficient in separating eigenvectors with N.D.E. This result appears in Figs. 1 and 2 where it is seen that only the first few eigenvectors have large components.

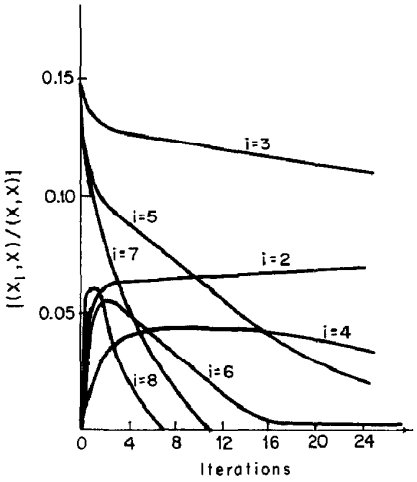

FIG. 1. Side components with W method

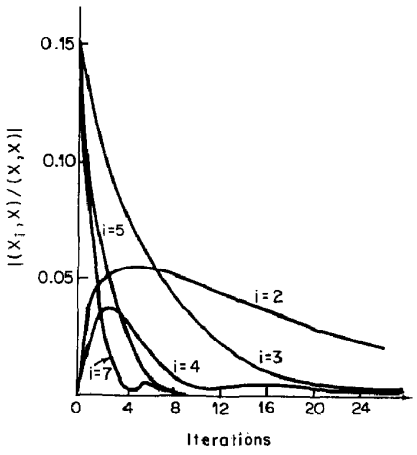

FIG. 2. Side components with *M.O.R.*

Let

$$\mathbf{X} = \mathbf{X}_i + \sum_{p \neq i} \epsilon_p \mathbf{X}_p .$$

For small ϵ_p, one obtains:

$$\lambda = \lambda_i + \sum_p \epsilon_p{}^2(\lambda_p - \lambda_i) + \theta(\epsilon^3)$$

and

$$w = \sum_p \epsilon_p^2(\lambda_p - \lambda_i)^2 + \theta(\epsilon^3)$$

Thus optimization of λ or w is clearly more sensitive to components which contribute most to $|\lambda - \lambda_i|$ or w. It follows that when there are several eigenvectors with eigenvalues close to the one required, adjustment of each component of $\mathbf{X}$ in turn will first mix them in, and then only eliminate them slowly.

When $\mathbf{A}$ is almost diagonal, the procedure is more efficient because each $\mathbf{e}_i$ can introduce only a few $\mathbf{X}_p$ into $\mathbf{X}$, and the separation of eigenvalues is better.

In conclusion, W and MOR produce an approximate subspace of eigenvectors with N.D.E., the dimension of which depends on how much the small components $\mathbf{X}_p$ with a large $|\lambda_p - \lambda_i|$ contribute to w or $(\lambda - \lambda_i)$.

Procedures designed to extract the required eigenvector from this approximate subspace are now discussed.

IV. Extrapolation Procedures

Let $\mathbf{X}^{(0)}$ and $\mathbf{X}^{(1)}$ be the vectors produced by two successive iterations. When one adds to $\mathbf{X}^{(1)}$ some multiple of $(\mathbf{X}^{(1)} - \mathbf{X}^{(0)})$ such that λ or w is optimized, this clearly is an extrapolation procedure. However when applied to the above examples, poor results are obtained: $(\mathbf{X}^{(1)} - \mathbf{X}^{(0)})$ can be considered to be a vector belonging to the approximate subspace, and since this subspace is of more than two dimensions, two vectors are not enough. A multiple extrapolation procedure has therefore been tried. Even in this case convincing results were not obtained, since the vectors $(\mathbf{X}^{(i+1)} - \mathbf{X}^{(i)})$ thus introduced contain large weights of eigenvectors unimportant to $\mathbf{X}^{(i)}$.

It is therefore necessary to investigate other procedures for generating better vectors from the approximate subspace.

V. Iterated Vector Method

Since interest may be centered upon any particular eigenvector, the simplest iterated vectors generated by the power method [9] are not used. Instead consider the vectors:

$$\mathbf{X};\ \mathbf{X}^{(1)} = \mathbf{AX} - \frac{(\mathbf{X}, \mathbf{AX})}{(\mathbf{X}, \mathbf{X})}\mathbf{X};\ldots;\ \mathbf{X}^{(m)} = \mathbf{AX}^{(m-1)} - \sum_{i=1}^{m-1} \frac{(\mathbf{X}^{(i)}, \mathbf{AX}^{(m-1)})}{(\mathbf{X}^{(i)}, \mathbf{X}^{(i)})}\mathbf{X}^{(i)}.$$

These vectors are orthogonal to each other. When one uses the property

$(\mathbf{Y}, \mathbf{AX}) = (\mathbf{X}, \mathbf{AY})$, it can be seen that the expression for $\mathbf{X}^{(p+1)}$ can be reduced to

$$\mathbf{X}^{(p+1)} = \mathbf{AX}^{(p)} - \frac{(\mathbf{X}^{(p)}, \mathbf{AX}^{(p)})}{(\mathbf{X}^{(p)}, \mathbf{X}^{(p)})} \mathbf{X}^{(p)} - \frac{(\mathbf{X}^{(p)}, \mathbf{X}^{(p)})}{(\mathbf{X}^{(p-1)}, \mathbf{X}^{(p-1)})} \mathbf{X}^{(p-1)}.$$

These vectors are clearly identical to those proposed by Hestenes and Karush [2] or Lanczos [8]. We now look for the linear combination of these $(m + 1)$ vectors with the least variance.

It has proved efficient to calculate the linear combination $\mathbf{Y}$ of these $(m + 1)$ vectors such that $w(\lambda)$ is minimized, where:

$$w(\lambda) = (\bar{\mathbf{A}}\mathbf{Y}, \bar{\mathbf{A}}\mathbf{Y})/(\mathbf{Y}, \mathbf{Y}) \qquad \text{with} \qquad \bar{\mathbf{A}} = \mathbf{A} - \lambda(\mathbf{X})\,\mathbf{I}.$$

The solution of this variational problem [6] is given by simple manipulation of matrices of rank $(m + 1)$ and the resulting linear combination has almost the least variance.

In the following examples, this procedure is taken to be equivalent to m iterations, since the multiplications $\mathbf{AX}^{(p)}$ form the main part of the computational effort when $m \ll N$.

Subsequently $m \leqslant 9$ and calculations were performed in double precision on the IBM 370-165 computer. The complete procedures, called WEL and MOREL, contain the following steps:

(1) A few iterations (usually 10) of MOR or W are performed. When convergence is fast, this is the only step required.

(2) The resulting vector is used to generate m "iterated vectors" and the best linear combination is taken as the new trial vector.

(3) If variance has decreased faster with these m iterations than with m cycles one returns to (2). If not, one returns to (1).

These procedures have been applied to matrix 2 of Table I and to a matrix

$$\mathbf{A}_{ij} = 4(N + 1 - i)(N + 1 - j)/(2N + 2 - i - j)^2$$
$$\text{where} \quad i \neq j = 1,\ldots, N \quad \text{and} \quad N = 50.$$

$\mathbf{A}_{ii} = 0;\ 0.5,\ 0.5;\ 1.,\ 1.,\ 1.;\ 1.5,\ 1.5,\ 1.5,\ 1.5;\ldots$

Using initial vectors derived from the first five eigenvectors of a similar $N = 10$ matrix, it is shown in table II that both WEL and MOREL are much faster than W and MOR.

Of course these matrices have many N.D.E. and in this kind of situation the 2^d Lanczos method [8] may be favoured. But the procedures described here give a regular decrease in w, so that they may be tried and then given up if convergence is too slow.

VI. Obtaining an Eigenvector with Eigenvalue Close to a Given Number

Given a number k, we wish to derive the eigenvector $\mathbf{X}_i$ with smallest possible $|\lambda_i - k|$. It can be shown easily that this eigenvector is the only solution to the condition:

$$w(k) = \{(\mathbf{AX} - k\mathbf{X}), (\mathbf{AX} - k\mathbf{X})\}/(\mathbf{X}, \mathbf{X}) = \text{minimum}.$$

On the other hand a condition requiring only the proximity of $\lambda(\mathbf{X})$ to k can generally be fullfilled with many solutions.

By analogous reasonings to those presented in Section II, minimization of $w(k)$ by adjustment correction of each component x_i of $\mathbf{X}$ requires correction factors α given by:

$$\alpha = (-B + \sqrt{B^2 - 4AC})/2A \qquad \text{with} \quad A = x_i(\mathbf{a}_i, \mathbf{a}_i) - (\mathbf{a}_i, \mathbf{V}),$$

$$B = (\mathbf{X}, \mathbf{X})(\mathbf{a}_i, \mathbf{a}_i) - (\mathbf{V}, \mathbf{V}) \quad \text{and} \quad C = (\mathbf{a}_i, \mathbf{V})(\mathbf{X}, \mathbf{X}) - x_i(\mathbf{V}, \mathbf{V}).$$

The notations are the same as in Section II except $\mathbf{V} = \mathbf{AX} - k\mathbf{X}$.

This new procedure, called WK, gives in semi-degenerate situations a linear combination of the eigenvectors possessing eigenvalues close to k. Therefore the iterated vector procedure outlined in Section V is needed.

The entire procedure, called WKEL, has been applied to a tridiagonal symmetric matrix ($N = 900$), with $\mathbf{A}_{i,i+1} = i$ and $\mathbf{A}_{ii} = i$ when $i \leqslant 100$ or $\mathbf{A}_{ii} = (i - 90)^2$ when $i > 100$. The eigenvalue closest to 200 and the corresponding eigenvector have been sought for. The initial trial vector was very poor ($\lambda \sim 10^4$). When submitted to 50 iterations of WKEL, this yelded a better vector ($\lambda \sim 200$) which was submitted to 400 cycles of WEL. The final λ was 202.3457. The matrix is very sparse, so that the entire computational time was only about 1/1000 of that required for complete diagonalization.

Conclusion

The examples given are all of matrices with near degeneracies (the two exceptions being matrices 3 and 4 in Table I). In such cases, neither MOR nor variance minimization converges quickly, even when supplemented with the iterated vectors procedure. Their main advantage however is that they do not need cumbersome transformations of the original matrix. There are many practical situations where the matrix is not too far from diagonality and in these case, variance minimization has the advantage that it can be used to obtain any eigenvector and not only the extremal ones. The versatility of the variance concept is also demonstrated by the possibility of obtaining eigenvectors with specific eigenvalue requirements.

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