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SOLUTION OF THE PERTURBED EIGENVALUE EQUATION BY THE LOW-RANK PERTURBATION METHOD*

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Abstract

In its simplest form, the low-rank perturbation (LRP) method solves the perturbed matrix eigenvalue equations $A\Psi \equiv (B + V)\Psi = \varepsilon\Psi$, where A, B and V are nth-order Hermitian matrices, and where the eigenstates and the eigenvalues of the unperturbed matrix B are known. The method can be applied to arbitrary perturbations V, but it is numerically most efficient if the rank ρ of V is "small". A special case of low-rank perturbations are localized perturbations (e.g. replacement of one atom with another, creation and destruction of a chemical bond, local interaction of large molecules, etc.). In the case of local perturbations with a fixed localizability l, the operation count for the calculation of a single eigenvalue and/or a single eigenstate is $O(l^2n)$. In the more general case of a delocalized perturbation with a fixed rank ρ, the operation count for the derivation of all eigenvalues and/or all eigenstates is $O(\rho^2n^2)$. For large n, the performance of the LRP method is hence at least one order of magnitude better than the performance of other methods. The obtained numerical results demonstrate that the LRP method is numerically reliable, and that the performance of the method is in accord with predicted operation counts.

1. Introduction

This is a preliminary report on the low-rank perturbation (LRP) method. A more comprehensive account of this method will be given elsewhere [1].

The LRP method deals with the solution of the perturbed eigenvalue equation

$$A\Psi_i \equiv (B + V)\Psi_i = \varepsilon_i \Psi_i, \tag{1}$$

where A, B and V are n order matrices, and where the solution of the unperturbed eigenvalue equation

$$B\,\Phi_i = \lambda_i \Phi_i \tag{2}$$

is known.

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More generally, the LRP method treats the generalized perturbed eigenvalue equation

$$\boldsymbol{A}\Psi_i \equiv (\boldsymbol{B} + \boldsymbol{V})\Psi_i = \varepsilon_i(\boldsymbol{S} + \boldsymbol{P})\Psi_i, \tag{3}$$

where the corresponding (generalized) unperturbed eigenvalue equation is

$$\boldsymbol{B}\,\Phi_i = \lambda_i \boldsymbol{S}\,\Phi_i. \tag{4}$$

In this general formulation matrices $\boldsymbol{B}$, $\boldsymbol{V}$, $\boldsymbol{S}$ and $\boldsymbol{P}$ can be non-Hermitian, with the only restriction that matrix $\boldsymbol{S}$ be nonsingular and that matrix $\boldsymbol{S}^{-1/2}\boldsymbol{B}\boldsymbol{S}^{-1/2}$ be nondefective [1]. By definition, a matrix is nondefective if it has a complete set of eigenvectors [2]. In the present paper, only relations (1) and (2) will be treated.

Unlike the standard perturbation approach, the accuracy and the operation count of the LRP method does not depend on the norm of the perturbation $\boldsymbol{V}$. A critical parameter is the rank ρ of $\boldsymbol{V}$, and if this parameter is "small" with respect to n, the method is fast and efficient. Special cases of low-rank perturbations are local perturbations. If the perturbation $\boldsymbol{V}$ is local, then at most l columns and l rows of $\boldsymbol{V}$ contain nonzero elements. With a suitable permutation of rows and columns, all nonzero matrix elements of $\boldsymbol{V}$ are contained in an l-by-l submatrix of $\boldsymbol{V}$. By definition, the quantity l is the "localizability" of $\boldsymbol{V}$. One easily finds that $\rho \leq l$.

Local perturbations are common in various quantum chemical problems. Depending on the quantum chemical model, a replacement of an atom with another, creation and destruction of a chemical bond, local interactions of large molecules, etc., are all examples of local perturbations. In the case of a local perturbation with a fixed localizability l, the operation count for a calculation of a single eigenstate and/or eigenvalue scales as $O(l^2n)$. In the more general case of a delocalized perturbation with a fixed rank ρ, the operation count for the derivation of all eigenvalues and/or all eigenstates scales as $O(\rho^2n^2)$ [1].

In comparison, standard diagonalization methods (Householder, Givens, Jacobi, etc.) require $O(n^3)$ operations for the derivation of all eigenvalues and/or all eigenstates. There are some other methods (power method, Lanczos, Davidson, etc.) which are more efficient if only a few selected eigenvalues and/or eigenstates are required. However, unless a few extreme eigenvalues are required, these methods are also $O(n^3)$. Concerning the operation count of the various perturbation expansion methods, it strongly depends on the order of the approximation. If most matrix elements $\langle\Phi_i|V|\Phi_j\rangle$ are nonzero, already a second-order perturbation expansion requires $O(n^2)$ operations for the calculation of a single eigenvalue and $O(n^3)$ operations for the calculation of a single eigenstate. In either case, the operation count of the LRP method for large n is substantially smaller.

2. The method

Each perturbation V can be written in the form

$$V = \sum_{s=1}^{m} \omega_s |u_s\rangle\langle v_s|, \tag{5}$$

where $\omega_s \neq 0$. In general, vectors $|u_s\rangle$ and/or vectors $\langle v_s|$ are linearly dependent. However, any linear dependence of these vectors can be easily eliminated [1], and hence the perturbation V can, without loss of generality, be represented in the form (5), where $m = \rho$ is the rank of V. Note also that (5) does not explicitly require V to be Hermitian. Hence, the following results apply to arbitrary V [1], although we will be mostly interested in the Hermitian case.

Many different forms (5) of the same perturbation V are possible. For example, if V is Hermitian, parameters ω_s can be chosen to be nonzero eigenvalues of V and vectors $|u_s\rangle = |v_s\rangle$ to be the corresponding eigenstates. This is a "diagonal" representation of V and it automatically ensures $m = \rho$.

There is another representation which is convenient if the localizability l of the perturbation V is small. In this case, at most l components of vectors $|u_s\rangle$ and $|v_s\rangle$ are nonzero. One can choose vectors $\langle v_s|$ to be unit row vectors and one can normalize vectors $|u_s\rangle$ with $\omega_s = 1$:

$$V = \sum_{s=1}^{l} |u_s\rangle\langle v_s| . \tag{5a}$$

With such a choice, vectors $|u_s\rangle$ coincide with nonvanishing columns of V. This is a "column-wise" representation of V, and there is a similar row-wise representation. In general, $\rho \leq l$. However, $\rho < l$ only if columns of V are linearly dependent, and thus usually $\rho = l$.

In the LRP method, it is convenient to distinguish "cardinal" and "singular" eigenvalues and eigenstates. If the eigenvalue ε_0 of the perturbed eigenvalue equation (1) differs from all the eigenvalues λ_i of the unperturbed eigenvalue equation (2), it is cardinal [1]. Otherwise, i.e. if $\varepsilon_0 \in \{\lambda_i\}$, it is "singular". The corresponding eigenstates are in the same way partitioned into cardinal and singular, respectively [1]. Singular solutions are essentially accidental, and the perturbed eigenvalue equation (1) usually has either no singular solution or only a few such solutions. Cardinal solutions are much more important, and in many cases they are the only solutions of (1).

We first consider cardinal solutions [1]:

THEOREM 1 (CARDINAL EIGENVALUES AND EIGENSTATES)

Let $A = B + V$ be an nth-order Hermitian matrix, the sum of Hermitian matrices B and V. Further, let λ_i and Φ_i be, respectively, the eigenvalues and the corresponding

orthonormalized eigenstates of $\boldsymbol{B}$, and let the perturbation $\boldsymbol{V}$ be represented in the form (5). Then,

(a) Each cardinal eigenvalue ε_0 of $\boldsymbol{A}$ is a root of the LRP equation

$$\mathcal{D}(\varepsilon) \equiv |S_{sp}(\varepsilon) - \delta_{sp}/\omega_s| = 0, \qquad s,p = 1,\ldots,m, \tag{6a}$$

where

$$S_{sp}(\varepsilon) = \sum_{i=1}^{n} \frac{\langle \upsilon_s|\Phi_i\rangle\langle\Phi_i|\boldsymbol{u}_p\rangle}{\varepsilon - \lambda_i}, \qquad s,p = 1,\ldots,m. \tag{6b}$$

Inversely, each root $\varepsilon_0 \notin \{\lambda_i\}$ of the LRP equation (6) is a cardinal eigenvalue of $\boldsymbol{A}$.

(b) Let ε_0 be a cardinal eigenvalue of $\boldsymbol{A}$. Then each eigenstate Ψ corresponding to this eigenvalue is of the form:

$$|\Psi\rangle = \sum_{i=1}^{n}\left[\sum_{p=1}^{m} \omega_p\langle\Phi_i|\boldsymbol{u}_p\rangle\langle\upsilon_p|\Psi\rangle/(\varepsilon_0 - \lambda_i)\right]|\Phi_i\rangle. \tag{7}$$

Moreover, the scalar products $\langle\upsilon_p|\Psi\rangle$ satisfy

$$\sum_{p=1}^{m}[\omega_p S_{sp}(\varepsilon_0) - \delta_{sp}]\langle\upsilon_p|\Psi\rangle = 0, \qquad s = 1,\ldots,m. \tag{8}$$

Inversely, each state Ψ of the form

$$\Psi = N\sum_{i=1}^{n}\Omega_i|\Phi_i\rangle,$$

$$\Omega_i = \left[\sum_{p=1}^{m}\omega_p\langle\Phi_i|\boldsymbol{u}_p\rangle C_p\right]/(\varepsilon_0 - \lambda_i), \tag{9a}$$

$$N^2 = 1/\sum_{i=1}^{n}\Omega_i^2,$$

where the coefficients C_p are the (nontrivial) solution of

$$\sum_{p=1}^{m}[\omega_p S_{sp}(\varepsilon_0) - \delta_{sp}]C_p = 0, \qquad s = 1,\ldots,m, \tag{9b}$$

is a normalized cardinal eigenstate of A corresponding to the eigenvalue ε_0. Moreover, the coefficients C_p are the scalar products $C_p = \langle v_p | \Psi \rangle$.

Relation (6) can be used to find all cardinal eigenvalues ε_i of the perturbed eigenvalue equation (1). The operation count for the derivation of these eigenvalues depends on the operation count for the construction of the determinant $\mathcal{D}(\varepsilon)$. If V is local, this operation count scales as $O(l^2 n)$, where l is a localizability of V [1]. Hence, if the localizability l is "small", a derivation of a single eigenvalue ε_i requires essentially $O(n)$ operations. If V is not local ($l \approx n$) but still has small rank ($\rho \ll n$), there is an overhead of $O(\rho n^2)$ operations which is required to calculate scalar products $\langle v_s | \Phi_i \rangle$ and $\langle \Phi_i | u_p \rangle$ in (6b). However, this calculation is performed only once, irrespective of how many eigenvalues of A are required. Hence, if the rank ρ is "small", a derivation of all cardinal eigenvalues of A requires essentially $O(n^2)$ operations.

Once a particular cardinal eigenvalue ε_0 is known, the corresponding eigenstate(s) can easily be obtained using relations (9). First, one solves (9b) for the unknown C_p. This is an m-order linear system, and provided m is "small" the coefficients C_p can be obtained quickly. Once C_p are known, one finds Ψ by simple insertion into (9a). The solution is unique and the function Ψ nondegenerate if (9b) has a unique solution. Otherwise, the function Ψ is degenerate. Depending on the application, one can choose either $m = \rho$ or $m = l \geq \rho$. The LRP method is hence fast if the rank ρ is small, and in particular if the localizability l is small.

The storage requirement of the LRP method is also favorable. If V is local, the storage requirement to store l components of each of n vectors Φ_i is nl. Next, one has to store $2nl$ scalar products $\langle v_s | \Phi_i \rangle$ and $\langle \Phi_i | u_p \rangle$. All the remaining storage requirement is relatively small. Thus, the storage requirement for vectors $|u_p\rangle$ is l^2, while the storage requirement for the eigenvalues λ_i is n. The total storage requirement is hence $O(nl)$. The storage requirement of direct approaches is at least n^2, since as an absolute minimum all matrix elements of the matrix A should be known. Since by assumption $l \ll n$, the LRP storage requirement is substantially smaller. This is also true for delocalized low-rank perturbation. If V is delocalized, a separate program, which uses relatively slow but large external memory, can generate scalar products $\langle v_s | \Phi_i \rangle$ and $\langle \Phi_i | u_p \rangle$. Once these scalar products are formed, the remaining storage requirement is essentially $2\rho n$.

Above, we have discussed cardinal solutions of (1). Singular solutions are obtained by the following theorem [1]:

THEOREM 2 (SINGULAR EIGENVALUES AND EIGENSTATES OF A)

Let $\varepsilon_0 = \lambda_k$ be a singular eigenvalue of A. Further, let λ_k be a ν-degenerate eigenvalue of B, and let $\Phi_{k\kappa}$ ($\kappa = 1, \ldots, \nu$) be the corresponding orthonormalized eigenstates. Then:

(a) ε_0 is a root of the equation

$$\mathcal{D}^0(\varepsilon) \equiv \left| \begin{array}{c|c} S^0_{sp}(\varepsilon) - \delta_{sp}/\omega_s & \langle \upsilon_s | \Phi_{k\kappa} \rangle \\ \hline \langle \Phi_{k\kappa} | u_p \rangle & O \end{array} \right| = 0, \tag{10a}$$

where

$$S^0_{sp}(\varepsilon) = \sum_{i \neq k}^{n} \frac{\langle \upsilon_s | \Phi_i \rangle \langle \Phi_i | u_p \rangle}{\varepsilon - \lambda_i}, \quad s, p = 1, \ldots, m. \tag{10b}$$

Inversely, if the eigenvalue λ_k of $\boldsymbol{B}$ is a root of $\mathcal{D}^0(\varepsilon)$, then $\varepsilon_0 = \lambda_k$ is a singular eigenvalue of $\boldsymbol{A}$.

(b) Let $\varepsilon_0 = \lambda_k$ be a singular eigenvalue of $\boldsymbol{A}$. Then, each eigenstate Ψ corresponding to this eigenvalue is of the form

$$|\Psi\rangle = \sum_{i \neq k}^{n} \frac{\sum_{p=1}^{m} \omega_p \langle \Phi_i | u_p \rangle \langle \upsilon_p | \Psi \rangle}{(\varepsilon_0 - \lambda_i)} |\Phi_i\rangle + \sum_{\kappa=1}^{\nu} \langle \Phi_{k\kappa} | \Psi \rangle | \Phi_{k\kappa} \rangle. \tag{11}$$

Moreover, the scalar products $\langle \upsilon_p | \Psi \rangle$ and $\langle \Phi_{k\kappa} | \Psi \rangle$ satisfy

$$\sum_{p=1}^{m} [\omega_p S^0_{sp}(\varepsilon_0) - \delta_{sp}] \langle \upsilon_p | \Psi \rangle + \sum_{\kappa=1}^{\nu} \langle \upsilon_s | \Phi_{k\kappa} \rangle \langle \Phi_{k\kappa} | \Psi \rangle = 0, \quad s = 1, \ldots, m, \tag{12a}$$

$$\sum_{s=1}^{m} \omega_s \langle \Phi_{k\kappa} | u_s \rangle \langle \upsilon_s | \Psi \rangle = 0, \qquad \kappa = 1, \ldots, \nu. \tag{12b}$$

Inversely, each state Ψ of the form

$$|\Psi\rangle = \sum_{i \neq k}^{n} \Omega_i |\Phi_i\rangle + \sum_{\kappa=1}^{\nu} D_\kappa |\Phi_{k\kappa}\rangle,$$
$$\Omega_i = \left[\sum_{p=1}^{m} \omega_p \langle \Phi_i | u_p \rangle C_p \right] / (\varepsilon_0 - \lambda_i), \tag{13a}$$

where C_p and D_κ are the solution of

$$\sum_{p=1}^{m} [\omega_p S^0_{sp}(\varepsilon_0) - \delta_{sp}] C_p + \sum_{\kappa=1}^{\nu} \langle \upsilon_s \mid \Phi_{k\kappa} \rangle D_\kappa = 0, \quad s = 1, \ldots, m,$$

$$\sum_{p=1}^{m} \omega_p \langle \Phi_{k\kappa} \mid u_p \rangle C_p = 0, \qquad \kappa = 1, \ldots, \nu, \tag{13b}$$

is a singular eigenstate of A corresponding to the eigenvalue ε_0. Moreover, the coefficients C_p and D_κ are

$$C_p = \langle \upsilon_p \mid \Psi \rangle, \quad D_\kappa = \langle \Phi_{k\kappa} \mid \Psi \rangle. \tag{14}$$

For the sake of simplicity, we did not normalize the state Ψ in (13a). The normalization is trivial.

The above two theorems completely solve the eigenvalue equation (1). The first theorem refers to cardinal eigenvalues and eigenstates of A, while the second theorem refers to singular eigenvalues and eigenstates of A. These eigenvalues and eigenstates are expressed in terms of the eigenvalues and eigenstates of the unperturbed matrix B, and in terms of vectors $|u_s\rangle$ and $|\upsilon_s\rangle$ and quantities ω_s which define the perturbation V. Unlike the perturbation expansion method, the perturbation V is not required to be small, and the above relations apply to an arbitrary perturbation V. The method is, however, efficient if the rank ρ of V is small with respect to n. In particular, it is efficient if the localizability l of V is small.

Although the above relations are formulated for Hermitian matrices, they are in fact valid for more general cases [1]. In particular, the perturbation V can be arbitrary non-Hermitian, as suggested by the explicitly nonsymmetric representation (5). In this general non-Hermitian case, one should carefully distinguish between left and right eigenstates [1].

The possibility to represent the perturbation V in many different forms (5) gives a substantial flexibility to the LRP method [1]. Due to this possibility, there is no need for a preliminary diagonalization of V. This is especially important if the LRP method is used to derive isoenergy surfaces [3]. It is also important from a more general point of view. Since the representation (5) is explicitly nonsymmetric, the method can be easily generalized to non-Hermitian and nonsymmetric matrices [1].

It should be noted that the eigenvalue problem with a low-rank perturbation has also been treated by some other authors, although not in such a general form. Dr. G.H. Golub pointed out to the present author that similar problems have been studied in the mathematical literature [4–7]. In the case of Hermitian matrices, where in addition $|u_s\rangle = |\upsilon_s\rangle$, a formula equivalent to (6) has apparently been stated for the first time by Beattie and Fox [4], and independently by Arbenz and Golub [5]. Subject to the same limitations, these latter authors have also derived a formula apparently equivalent to relations (10). Formulae obtained by these authors are much more abstract, and they

explicitly apply only to the Hermitian case and to the symmetric representation of the perturbation $\boldsymbol{V}$. Substantially more restrictive formulae have previously been derived by some authors [6,7]. A comprehensive list of relevant references in the mathematical literature can be found in ref. [5].

Recently, Dr. D.J. Klein communicated to the author that a similar problem has also been considered in the chemical literature [8–11]. Thus, Koster and Slater treat the motion of electrons in a perturbed periodic lattice [8,9]. They explicitly use translational symmetry and Wannier functions. A similar problem was treated by Lax [10]. Löwdin [11] has a slightly more general treatment. However, his approach requires an explicit evaluation of the resolvent $(\boldsymbol{B} - \lambda \boldsymbol{I})^{-1}$ associated with the unperturbed Hermitian matrix $\boldsymbol{B}$. Unless this resolvent can be easily calculated, his approach is impractical. In addition, all these papers are restricted to local perturbations and they do not consider more general low-rank perturbations. It is interesting that although these papers were published much earlier, they were apparently unknown to the authors in the mathe-matical literature. Thus, in the recent paper by Arbenz and Golub [5], which contains quite a comprehensive list of references, these papers were not cited.

3. Numerical results

In order to check the accuracy and the efficiency of the LRP method, a computer program was written by the author, and applied to random matrices. The program was written in C and run on the personal computer NEC Multispeed.

Matrices $\boldsymbol{B}$ of order $n = 20$ through $n = 200$ in increments of 10 were considered. Matrix elements of these matrices were created as random numbers in the interval $(-10.0, 10.0)$. Perturbations $\boldsymbol{V}$ were also constructed as random matrices. A nonsymmetric representation (5) was explicitly used; this avoids the need to diagonalize $\boldsymbol{V}$. For the sake of simplicity, perturbations $\boldsymbol{V}$ were chosen to be local with a localizability $l = \rho$. The choice of local perturbations decreases the time needed to calculate matrix elements $\langle \upsilon_s | \Phi_i \rangle$ and $\langle \Phi_i | \boldsymbol{u}_p \rangle$. Otherwise, it is of no consequence for the performance of the LRP method. Perturbations having rank $\rho = 1$ up to and including $\rho = 7$ were considered.

Results of the LRP calculation were verified by an independent Householder-QL diagonalization of $\boldsymbol{A}$. For matrices of order $n = 20$ through $n = 90$, the Householder-QL calculation was performed in double precision. For these matrices, the LRP eigenvalues and eigenstates agree with the Householder-QL eigenvalues and eigenstates approximately up to all fifteen significant figures. For matrices of order $n = 100$ through $n = 120$, the Householder-QL calculation was performed in single precision. For these matrices, the LRP eigenvalues and eigenstates agree with the Householder-QL eigenvalues and eigenstates approximately up to all seven significant figures in single precision. Matrices of order $n > 120$ were too large to be diagonalized on the personal computer (with the present compiler, which limits a single data item to maximum 64K of memory). For these matrices, the LRP eigenstates were verified in an independent

manner. In the case of Hermitian matrices, eigenstates satisfy $\langle \Psi_k | \Psi_l \rangle = 0$ whenever $\varepsilon_k \neq \varepsilon_l$. This relation was verified, and it was found that the normalized LRP eigenstates Ψ_k and Ψ_l satisfy $\langle \Psi_k | \Psi_l \rangle \approx 10^{-15}$. This also verifies the corresponding eigenvalues since, unless these eigenvalues are equally reliable, eigenstates Ψ_k and Ψ_l cannot be orthogonal (except possibly accidentally).

The performance of the LRP method was checked by monitoring times needed to calculate a single eigenvalue and/or a single eigenstate. The results are shown in figs. 1 and 2. Times (in seconds) needed to calculate a single eigenvalue by the LRP method

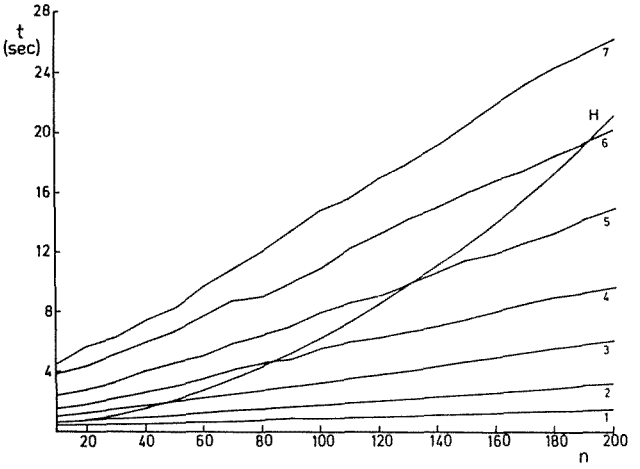

Fig. 1. Times needed to calculate a single eigenvalue by the LRP method. Lines 1 through 7 correspond to perturbations having rank 1 through 7. Line H corresponds to the hypothetical "per eigenvalue" Householder-QL calculation.

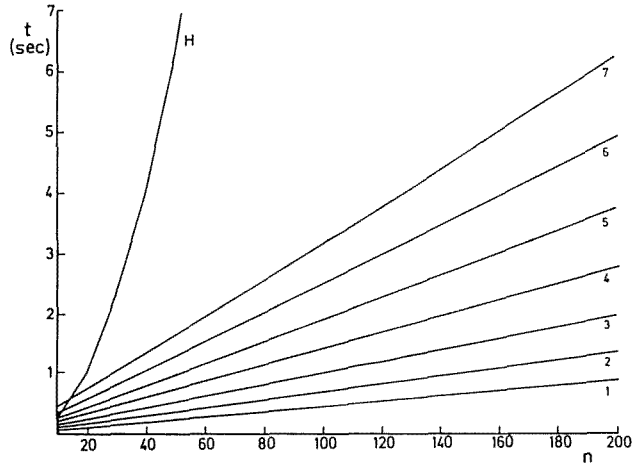

Fig. 2. Times needed to calculate a single eigenstate by the LRP method. Lines 1 through 7 correspond to perturbations having rank 1 through 7. Line H corresponds to the hypothetical "per eigenstate" Householder-QL calculation.

are shown in fig. 1. These times are plotted as a function of the degree n of matrices $\boldsymbol{B}$ and $\boldsymbol{V}$. Lines 1 through 7 correspond to perturbations having rank 1 through 7. Line H is drawn for comparison. This line corresponds to the "per eigenvalue" Householder-QL calculation. In the Householder-QL method (presently the best method for the derivation of all eigenvalues or all eigenvalues and all eigenstates of a real symmetric matrix), one obtains simultaneously all eigenvalues of $\boldsymbol{A}$. "Per eigenvalue" Householder-QL times are times needed to derive all eigenvalues of $\boldsymbol{A}$ divided by the number n of these eigenvalues. The corresponding times (in seconds) needed to calculate a single eigenstate are shown in fig. 2. These times are also plotted as a function of the degree n of matrices $\boldsymbol{B}$ and $\boldsymbol{A}$. Lines 1 through 7 correspond to perturbations having rank 1 through 7. Line H corresponds to the hypothetical "per eigenstate" Householder-QL calculation. "Per eigenstate" Householder-QL time is the time needed to obtain all eigenstates of $\boldsymbol{A}$, diminished by the time needed to obtain all eigenvalues of $\boldsymbol{A}$, and divided by the number n of these eigenstates.

For fixed n, the LRP times should scale as ρ^2 [1]. This apparently contradicts the results in figs. 1 and 2, which do not scale as quickly. The discrepancy is due to the numerical overhead for low ρ. With increasing ρ, this discrepancy should disappear.

As expected [1], for each fixed rank ρ of the perturbation $\boldsymbol{V}$, LRP times are linear in n. The corresponding Householder-QL times are quadratic in n. The LRP method is hence superior to the Householder-QL method, provided n is sufficiently large.

If a single eigenvalue and/or eigenstate is required, the relative efficiency of the LRP method substantially increases. This is particularly true if $\boldsymbol{V}$ is localized, in which case the LRP calculation of a single eigenvalue and/or eigenstate is $O(n)$.

The Householder method is not very suitable for the calculation of a single eigenvalue and/or eigenstate. Usually, some other method, such as the power method, the Davidson algorithm, the Lanczos method, inverse iteration, perturbation expansion, etc., is more efficient. However, none of these methods are truly $O(n^2)$.

In the power method, one repeatedly calculates the action of the matrix $\boldsymbol{A}$ on previously obtained vectors. Each iteration hence requires $O(n^2)$ operations. However, the number of iterations needed to obtain a required accuracy increases with n. The total operation count is hence higher than $O(n^2)$. In addition, the power method can be directly applied only for the calculation of extreme eigenvalues of $\boldsymbol{A}$. In order to calculate an *arbitrary* eigenvalue ε_i by the power method, one has to replace the matrix $\boldsymbol{A}$ with the matrix $(\boldsymbol{A} - \lambda)^{-1}$ [12]. This requires the calculation of the matrix inverse, which is again $O(n^3)$ operations [2].

The Lanczos method seems to be more efficient than the power method. Each iterative step of this method requires $O(n^2)$ operations. In order to obtain all n eigenvalues, n iterations are required, which produces an operation count of $O(n^3)$. However, intermediate results usually converge to extreme eigenvalues already after a few iterations [12]. The Lanczos algorithm is hence faster that $O(n^3)$ if a few extreme eigenvalues are required. However, this method is again $O(n^3)$ if an *arbitrary* eigenvalue and/or eigenstate is required. The same restriction applies to the Davidson algorithm, which is also faster than $O(n^3)$ only if few extreme eigenvalues and/or eigenstates are required.

The perturbation approach is also at least $O(n^3)$ unless the perturbation V is so small that one can truncate the perturbation expansion with the second term. In conclusion, if an *arbitrary* eigenvalue and/or eigenstate is required and if the perturbation is local, the LRP method is faster than other approaches by two orders of magnitude.

4. Conclusions

The obtained numerical results demonstrate that the LRP method produces reliable eigenvalues and eigenstates of the perturbed matrix A. It is further shown that for each rank ρ of the perturbation V, the time needed to calculate all eigenvalues and/or all eigenstates by the LRP method is proportional to n^2, where n is the order of matrices B and A. If the perturbation V is in addition local, the time needed to calculate a single eigenvalue and/or eigenstate by the LRP method is proportional to n. For large n, these times are, respectively, one and two orders of magnitude faster than the corresponding times for other presently known methods.

The storage requirement of the LRP method is also favorable. The storage requirement of other approaches is usually at least n^2, since as an absolute minimum all matrix elements of the matrix A should be known. If V is localized, the LRP storage requirement is $O(ln)$. If V is delocalized but low rank, the numerically trivial but storage-wise large task to generate scalar products $\langle v_s | \Phi_i \rangle$ and $\langle \Phi_i | u_p \rangle$ can be performed using a slow external memory. The remaining storage requirement is then $O(\rho n)$. In both cases, this is substantially less than the storage requirement of other methods. Hence, one can use personal computers with relatively small RAM memory to perform LRP calculations on relatively large systems.

In conclusion, the LRP method is convenient for the treatment of large systems perturbed by a low-rank perturbation. Provided the rank of the perturbation is "small", it produces reliable numerical results, it is faster than other methods and, finally, it has a smaller storage requirement. The larger the system, the more pronounced the advantage of the LRP method (in comparison to other methods).

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