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1992 J. Phys. A: Math. Gen. 25 635

(http://iopscience.iop.org/0305-4470/25/3/020)

J. Phys. A: Math. Gen. 25 (1992) 635-648. Printed in the UK

On the inverse eigenvalue problem for matrices

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Received 23 April 1991, in final form 9 October 1991

Abstract. The inverse eigenvalue problem for matrices is studied with the objective of obtaining an efficient method for correcting energy levels in atomic systems, though the results are applicable to any eigenvalue problem. The approach is a development of earlier work by S Friedland. The diagonal elements of a real symmetric matrix with given off-diagonal elements are adjusted to yield a given spectrum. We discuss cases where there are real solutions and no real solutions, with particular emphasis on the latter. Problems of slow convergence arise. We demonstrate the cause of this slow convergence, give a geometrical interpretation of the problem and show how it can be avoided. Also the matrices encountered arise from complex calculations and are subject to error. We develop an error analysis that permits us, among other things, to judge whether corrections in any particular case are justified in view of anticipated errors in the given computed off-diagonal matrix elements. Finally, the method is demonstrated in an application to certain sets of levels in 12 times ionized (neon-like) titanium.

1. Introduction

A difficulty arises in the computation of the wavefunctions of complex atoms which can be explored and alleviated by a discussion of the additive inverse eigenvalue problem. The difficulty can be explained as follows. In computing the electronic structure of an atom, one expands the atom's state vector on a convenient algebraic basis and the expansion coefficients are determined by solving the eigenvalue problem for a certain matrix—the Hamiltonian matrix. In many cases of interest, the diagonal elements of the Hamiltonian differ by quantities that are comparable to the magnitudes of one or more off-diagonal elements. This leads to expansion coefficients of the state vector being comparable in size (i.e. the state vector is not dominated by one basis vector with small admixtures of others). Also the expansion coefficients depend sensitively on errors in the closely spaced diagonal elements and perhaps on errors in the off-diagonal elements as well. This sensitive dependence on approximate computed matrix elements implies possibly unacceptable errors in the atomic properties computed using the atomic state vector—properties such as the radiative transition rates between states.

The obvious resolution, namely greatly increasing the computational accuracy of the diagonal matrix elements, is not feasible for many complex atoms and would be very inefficient for others. Instead, we consider the application of a correction method to obtain accurate state vectors. For this, we point out that the eigenvalues of the Hamiltonian matrix correspond to the energy levels of the atom and these can be measured to a very high degree of accuracy. We therefore invert the eigenvalue problem

0305-4470/92/030635+14$04.50

using these known eigenvalues to obtain corrected diagonal matrix elements for the Hamiltonian. Hence, diagonalizing the corrected Hamiltonian matrix, we obtain corrected state vectors as well as other corrected properties such as radiative transition rates.

Previous articles give more detail on the physical problem and on one method of solving this inverse eigenvalue problem (Luke 1985). In the present work we investigate a different method of solution. This method is efficient and can be automated. It provides some understanding of the important case where there is no real matrix of physical interest with the computed off-diagonal elements and the given observed eigenvalues. (The physical Hamiltonian operator is Hermitian hence its diagonal elements must be real.) Furthermore the present approach allows us to analyse numerically the effect of errors in the off-diagonal elements in a practical straightforward way. This analysis, among other things, can reveal whether a real set of diagonal elements can be obtained within the error range of the off-diagonal elements. It will also reveal in any given case how sensitively the state vector depends on errors in the Hamiltonian matrix. This is clearly important if we are to know the sensitivity of calculated physical properties to errors in the computed Hamiltonian matrix.

In the next section, we describe precisely the mathematical problem under consideration. Then we describe the case where there is a real solution of interest to the inverse eigenvalue problem and following that we discuss in more detail the case where the solution of interest is complex. Finally we give some results and summarize our conclusions.

2. Statement of the problem

We consider the additive inverse eigenvalue problem: given a real symmetric n-dimensional matrix $\mathbf{A}$ with zero diagonal elements, find a real diagonal matrix, $\mathbf{D}$, such that $\mathbf{A}+\mathbf{D}$ has a given set of real eigenvalues, $\boldsymbol{\omega} = (\omega_1, \ldots, \omega_n)^T$. In the applications considered here, the case in which two or more eigenvalues are exactly equal does not occur.

As stated by Friedland (1977), there are almost always $n!$ solutions for $\mathbf{D}$ if complex solutions are allowed. The number of real solutions for $\mathbf{D}$ in a particular application varies from 0 to $n!$. We are always interested in a particular real solution whose eigenvectors approximate most closely those which are physically observed. This solution may not exist owing to errors in the elements of $\mathbf{A}$. Nevertheless, there may be a nearby complex solution. Thus the following modified additive inverse eigenvalue problem is of physical interest and is studied in this paper.

Find real diagonal matrices $\mathbf{D}$ such that $\|\boldsymbol{\lambda} - \boldsymbol{\omega}\|^2 = \Sigma_1^n (\lambda_j - \omega_j)^2$ is a minimum where $\boldsymbol{\lambda} = (\lambda_1, \ldots, \lambda_n)^T$ is the set of eigenvalues of $\mathbf{A}+\mathbf{D}$. Without loss of generality, we will take the observed eigenvalues to be ordered $\omega_i > \omega_{i+1}$ and take $\Sigma_i \omega_i = 0$ which implies the trivial constraint $\mathrm{Tr}\,\mathbf{D} = 0$. It follows that $\{\lambda_i\}$ will satisfy $\Sigma_i \lambda_i = 0$. We also take $\{\lambda_i\}$ to be ordered $\lambda_i > \lambda_{i+1}$ as in Friedland (1977).

We will consider the two cases when the minimum of $\|\boldsymbol{\lambda} - \boldsymbol{\omega}\|$ has a zero or a non-zero value and refer to these in the following as case 1 and case 2.

Case 1. To determine $\mathbf{D}$ when $\boldsymbol{\lambda} = \boldsymbol{\omega}$, the most efficient algorithm is based on Newton's method (see e.g. Biegler-Konig 1981, Friedland *et al* 1987). We start with an initial estimate $\mathbf{D}^0$ and compute the estimates $\mathbf{D}^i$, $i = 1, 2, \ldots$ Assuming that $\mathbf{D}^i$ is known, the

eigenvalues $\boldsymbol{\lambda}^i = (\lambda_1^i, \ldots, \lambda_n^i)^T$ and normalized eigenvectors $\boldsymbol{X}_k^i$ are computed:

$$(\mathbf{A}+\mathbf{D}^i)\boldsymbol{X}_k^i = \lambda_k^i \boldsymbol{X}_k^i. \tag{1}$$

We use the notation $\mathbf{D}^i = \text{diag}\,(d_j^i)$, $\boldsymbol{d}^i = (d_1^i, \ldots, d_n^i)^T$.

Next, the matrix $\mathbf{J}^i = [(x_{jk}^i)^2]^T$ is formed where x_{jk}^i is the jth component of $\boldsymbol{X}_k^i$ and $[x_{ij}]$ denotes the matrix whose ij component is x_{ij}. The elements of the rows of $\mathbf{J}$ are thus the squares of the components of the normalized eigenvectors. The sum of the elements in any column or row of $\mathbf{J}$ is unity which characterizes a doubly stochastic matrix. The rows of $\mathbf{J}$ have the physical significance that the ijth element gives the probability that a system in the ith physical state, an eigenstate, will be in the jth algebraic basis state.

The $(i+1)$ estimate, $\boldsymbol{d}^{i+1} = \boldsymbol{d}^i + \Delta\boldsymbol{d}^i$, is then determined by solving

$$\mathbf{J}^i \Delta\boldsymbol{d}^i = \boldsymbol{\omega} - \boldsymbol{\lambda}^i \tag{2}$$

as shown by Friedland *et al* (1987). If the initial estimate is sufficiently close to the correct root, the sequence $\{\mathbf{D}^i\}$ is quadratically convergent.

Case 2. In the case of a non-zero minimum for $\|\boldsymbol{\omega} - \lambda\|$, the calculation of the above $\Delta\boldsymbol{d}^i$ becomes highly unstable because $\mathbf{J}^i$ becomes singular as we discuss shortly.

It is shown by Friedland (1977) that if we define a different increment $\Delta\boldsymbol{d}^i$ by

$$\Delta\boldsymbol{d}^i = (\mathbf{J}^i)^T(\boldsymbol{\omega} - \boldsymbol{\lambda}^i) \tag{3}$$

then $\|\boldsymbol{\lambda}^{i+1} - \boldsymbol{\omega}\| < \|\boldsymbol{\lambda}^i - \boldsymbol{\omega}\|$ for $\Delta\boldsymbol{d}^i \neq \mathbf{0}$. With this algorithm, the eigenvalue $\boldsymbol{\lambda}^i$ is closer to the given eigenvalue $\boldsymbol{\omega}$ after each iteration. This approach usually works well although, as we shall discuss later, in some cases the convergence of $\{\mathbf{D}_i\}$ can be remarkably slow.

In this section we describe a different approach from Friedland's which allows us to remove the problem of slow convergence and achieve the objective described in the introduction. As we noted there, investigating this case is of particular interest in this work. We seek an efficient algorithm to obtain the real point $\boldsymbol{d}^*$ corresponding to a set of eigenvalues $\boldsymbol{\lambda}^*$ where $\|\boldsymbol{\lambda}^* - \boldsymbol{\omega}\|$ is a minimum. We also seek to illustrate the effect on $\boldsymbol{d}^*$ and on $\{\boldsymbol{X}_k^*\}$ of fluctuations in the matrix $\mathbf{A}$ and to estimate the changes in $\mathbf{A}$ that will lead to the real spectrum $\boldsymbol{\omega}$ for the matrix $\mathbf{A}+\mathbf{D}^*$. As a further benefit, we will obtain a geometrical interpretation of our method and of Friedland's.

A useful device for this study is the singular value decomposition of $\mathbf{J}^i$ (Press *et al* 1986, Noble and Daniel 1988). There exist orthogonal matrices $\mathbf{U}^i$, $\mathbf{V}^i$ and a diagonal matrix $\mathbf{W}^i$ with (distinct in our case) non-negative elements such that

$$\boldsymbol{J}^i = \mathbf{U}^i\mathbf{W}^i(\mathbf{V}^i)^T. \tag{4}$$

$\mathbf{U}^i$, $\mathbf{V}^i$ and $\mathbf{W}^i$ have a number of interesting properties that are useful in our study. We describe them now. In the following, we will use the notation $\boldsymbol{U}_j^i$, $\boldsymbol{V}_j^i$ for the jth columns of $\mathbf{U}^i$, $\mathbf{V}^i$ respectively. Also let $\alpha_j^i = W_{jj}^i$. For convenience, we order α_j^i so that $\alpha_j^i \geqslant \alpha_{j+1}^i \geqslant 0$. Since $\mathbf{J}^i$ is doubly stochastic, $\alpha_1^i = 1$ (Minc 1988). In our case, α_j^i are distinct and, when $\mathbf{J}^i$ is singular, $\alpha_n^i = 0$. Examples where more than one $\alpha_j^i \to 0$ can be given. They do not arise in the present work, however, and will not be considered in the present analysis. Note also that

$$\mathbf{J}^i\boldsymbol{V}_j^i = \alpha_j^i\boldsymbol{U}_j^i \tag{5}$$

which follows from equation (4), postmultiplying both sides by $\mathbf{V}^i$ and using the fact that the columns of $\mathbf{V}^i$ form an orthonormal set.

Using this singular value decomposition of $\boldsymbol{J}^i$, equation (3) becomes

$$\begin{aligned}\Delta \boldsymbol{d}^i &= \mathbf{V}^i \mathbf{W}^i (\mathbf{U}^i)^T (\boldsymbol{\omega} - \boldsymbol{\lambda}^i) \\ &= \sum_j \alpha_j^i ((\boldsymbol{U}_j^i)^T (\boldsymbol{\omega} - \boldsymbol{\lambda}^i)) \boldsymbol{V}_j^i . \end{aligned} \tag{6}$$

If we premultiply both sides of equation (6) by $\mathbf{J}^i$ we have, from equation (5),

$$\mathbf{J}^i \Delta \boldsymbol{d}^i = \sum_j (\alpha_j^i)^2 ((\boldsymbol{U}_j^i)^T (\boldsymbol{\omega} - \boldsymbol{\lambda}^i)) \boldsymbol{U}_j^i \tag{7}$$

which redues to equation (2) if $(\alpha_j^i)^2$ is replaced by 1. Thus $\Delta \boldsymbol{d}^i$ can be regarded as a modified Newton step. We return to the question of convergence later.

Recall that in the case of present interest, $\Delta \boldsymbol{d}^i \to \mathbf{0}$ while $\| \boldsymbol{\omega} - \boldsymbol{\lambda}^i \|$ approaches a non-zero minimum. We see from equation (6), therefore, that $\alpha_n^i \to 0$, $\boldsymbol{U}_j^i$ becomes orthogonal to $\boldsymbol{\omega} - \boldsymbol{\lambda}^i$ for $j < n$, and $\boldsymbol{U}_n^i$ becomes parallel to $\boldsymbol{\omega} - \boldsymbol{\lambda}^i$ since both become perpendicular to the set of vectors $\boldsymbol{U}_j^i$, $j < n$. Also, we may expand $\boldsymbol{\omega} - \boldsymbol{\lambda}^i$ in the basis $\{\boldsymbol{U}_j^i\}$

$$\boldsymbol{\omega} - \boldsymbol{\lambda}^i = \sum_j C_j \boldsymbol{U}_j^i . \tag{8}$$

(Note that $C_1 = 0$. This arises from the fact that $\alpha_1^i = 1$ and equation (5) is satisfied by $\boldsymbol{U}_1^i = \boldsymbol{V}_1^i = n^{-1/2}(1, 1, 1, \ldots, 1)^T$ which is orthogonal to all vectors of interest in $\boldsymbol{\lambda}$ and $\boldsymbol{d}$ spaces because of the summation constraints on ω_j and λ_j noted earlier.) Convergence implies that $C_j \to 0$ for $j = 2, \ldots, n-1$ and $\boldsymbol{\omega} - \boldsymbol{\lambda}^i \to C_n^* \boldsymbol{U}_n^*$.

Recall that $\boldsymbol{\lambda}^* = (\lambda_1^*, \ldots, \lambda_n^*)^T$ is the vector yielding a minimum for $\| \boldsymbol{\omega} - \boldsymbol{\lambda} \|$ and we denote the solution obtained using equation (6) corresponding to $\boldsymbol{\lambda}^*$ by $\boldsymbol{d}^* = (d_1^*, \ldots, d_n^*)^T$ where d_i^* are all real. $\mathbf{J}$ is singular at $\boldsymbol{\lambda} = \boldsymbol{\lambda}^*$ and there is a surface in $\boldsymbol{\lambda}$ space through $\boldsymbol{\lambda}^*$ on which $\det(\mathbf{J}) = 0$ and a corresponding surface in $\boldsymbol{d}$ space through $\boldsymbol{d}^*$. Denote these surfaces by S_λ and S_d. S_λ has the property that if $\boldsymbol{\lambda}$ moved across it towards $\boldsymbol{\omega}$, $\boldsymbol{d}$ would become complex. Our iteration procedure automatically avoids this region where $\boldsymbol{d}$ is complex, thus the Hamiltonian matrix is real symmetric at all times. The surface S_d has the property that as $\boldsymbol{d}$ moves across it, $\boldsymbol{\lambda}$ is reflected from the surface S_λ thus ensuring that $\boldsymbol{d}$ remains real.

As a consequence of $\| \boldsymbol{\omega} - \boldsymbol{\lambda} \|$ being a minimum at $\boldsymbol{\lambda} = \boldsymbol{\lambda}^*$, $\boldsymbol{\omega} - \boldsymbol{\lambda}^*$ is normal to S_λ. Referring to equation (8) and the discussion following it, therefore, we see that $\boldsymbol{U}_n^i$ approximates the normal to S_λ and the limiting vector $\boldsymbol{U}_n^*$ is the exact normal to S_λ at $\boldsymbol{\lambda} = \boldsymbol{\lambda}^*$. We demonstrate that $\boldsymbol{V}_n^i$ and $\boldsymbol{V}_n^*$ are the approximate and exact normals, respectively, to S_d at $\boldsymbol{d}^*$ using the following first-order analysis. Using equation (6), we can write

$$\begin{aligned}\Delta \boldsymbol{d}^i &= \sum_j \alpha_j^i ((\boldsymbol{U}_j^i)^T [\boldsymbol{\omega} - \boldsymbol{\lambda}^* + \boldsymbol{\lambda}^* - \boldsymbol{\lambda}^i]) \boldsymbol{V}_j^i \\ &\simeq \alpha_n^i C_n^* \boldsymbol{V}_n^i + \sum_{j=2}^{n-1} \alpha_j^i ((\boldsymbol{U}_j^i)^T [\boldsymbol{\lambda}^* - \boldsymbol{\lambda}^i]) \boldsymbol{V}_j^i \end{aligned} \tag{9}$$

if $\boldsymbol{\lambda}^i$ is on the singular surface, S_λ. The first term drops out (since α_n^i equals zero on the surface), $\boldsymbol{d}^i$ is on the singular surface S_d, and the vector $\Delta \boldsymbol{d}^i = \boldsymbol{d}^* - \boldsymbol{d}^i$ has the form $\sum_{j=2}^{n-1} \beta_j^i \boldsymbol{V}_j^i$ where we have used the fact that the vector $\boldsymbol{\lambda}^* - \boldsymbol{\lambda}^i$ has no first-order component in the $\boldsymbol{U}_n^i$ direction. Thus, the set $\{\boldsymbol{V}_j^i\}$, $j = 2, n-1$, defines the tangent plane to the surface S_d and the remaining vector, $\boldsymbol{V}_n^i$, defines the normal.

The increments in the iterative solution of the problem are related to the foregoing vectors as follows. It is convenient to decompose the increments $\Delta\boldsymbol{\lambda}^i$, $\Delta\boldsymbol{d}^i$ into normal and tangential components: $\Delta\boldsymbol{\lambda}^i = \Delta\boldsymbol{\lambda}_n^i + \Delta\boldsymbol{\lambda}_t^i$ where $\boldsymbol{\lambda}^{i+1} = \boldsymbol{\lambda}^i + \Delta\boldsymbol{\lambda}^i$ and similarly for the $\boldsymbol{d}$ increments. Then $\Delta\boldsymbol{\lambda}_n^i$ is the projection of $\Delta\boldsymbol{\lambda}^i$ in the $\boldsymbol{U}_n^i$ direction, that is, in the direction normal to the surface, S_λ. Also, $\Delta\boldsymbol{\lambda}_t^i$ is the projection in the direction normal to $\boldsymbol{U}_n^i$, that is, in the direction tangential to the surfaces S_λ, approximately. Remarks corresponding to the foregoing can be made for the $\boldsymbol{d}$ increments, replacing $\boldsymbol{U}^i$ by $\boldsymbol{V}^i$ and S_λ by S_d. This follows from equation (6) as we have seen.

We use this geometrical picture to describe our computational method for obtaining $\boldsymbol{d}^i$. Our approach to an efficient solution is the following. Start with an initial estimate $\boldsymbol{d}^0$ and use Newton's method, equation (2), until $|\det(\mathbf{J}^i)|$ is smaller than some preassigned number so that we are close to the singular surfaces. Note that Newton's method is unstable for sufficiently small $|\det(\mathbf{J}^i)|$. To remove this instability, we compute $\Delta\boldsymbol{d}_n^i$ and $\Delta\boldsymbol{d}_t^i$ separately using the singular value decomposition of $\mathbf{J}^i$.

(i) From equation (6), we let

$$\Delta\boldsymbol{d}_n^i = \gamma_n^i \alpha_n^i \boldsymbol{V}_n^i [(\boldsymbol{U}_n^i)^T (\boldsymbol{\omega} - \boldsymbol{\lambda}^i)] \tag{10}$$

where $\gamma_n^i \geq 1$ is a convergence factor. With $\gamma_n^i = 1$, $\Delta\boldsymbol{d}_n^i$ is the normal component of Friedland's $\Delta\boldsymbol{d}^i$ (equation (6)) and it is this term that contributes to the slow convergence of $\{\boldsymbol{d}^i\}$. More precisely, we use a linear interpolation of the values of $\det(\mathbf{J}^i)$ to estimate the convergence factor γ_n^i:

$$\begin{aligned} \gamma_n^i / \gamma_n^{i-1} &= |\det(\mathbf{J}^{i+1}) - \det(\mathbf{J}^i)| / |\det(\mathbf{J}^i) - \det(\mathbf{J}^{i-1})| \\ &= |\det(\mathbf{J}^i)| / |\det(\mathbf{J}^i) - \det(\mathbf{J}^{i-1})| \end{aligned} \tag{11}$$

where we use $\det(\mathbf{J}^{i+1}) = 0$ to obtain an estimate of the convergence factor that will take us to the singular surface. To avoid extreme values which could arise under some circumstances we apply the further constraint $1 \leq \gamma_n^i \leq 10^4$. This results in a great improvement in the rate of convergence compared with using $\gamma_n^i = 1$.

(ii) Approximate $\Delta\boldsymbol{\lambda}_t^i$, the projection of $(\boldsymbol{\omega} - \boldsymbol{\lambda}^i)$ in the plane through $\boldsymbol{\lambda}^i$ and normal to $\boldsymbol{U}_n^i$, as

$$\Delta\boldsymbol{\lambda}_t^i = \gamma_t [(\boldsymbol{\omega} - \boldsymbol{\lambda}^i) - \{(\boldsymbol{\omega} - \boldsymbol{\lambda}^i)^T \boldsymbol{U}_n^i\} \boldsymbol{U}_n^i] \tag{12}$$

where γ_t is a second convergence factor. This factor does not appear to have a dramatic effect on the convergence; we took $\gamma_t = 1$ in most cases.

$\Delta\boldsymbol{d}_t^i$ is estimated in the following way. With $\boldsymbol{\omega}$ replaced by $\boldsymbol{\lambda}^*$ in Newton's equation (2) we have

$$\boldsymbol{\lambda}^* - \boldsymbol{\lambda}^i = \mathbf{J}^i \Delta\boldsymbol{d}^i \tag{13}$$

where $\boldsymbol{\lambda}^* - \boldsymbol{\lambda}^i \simeq \Delta\boldsymbol{\lambda}_t^i$ and $\Delta\boldsymbol{d}^i \simeq \Delta\boldsymbol{d}_t^i$. Thus we solve

$$(\mathbf{U}^i \mathbf{W}^i (\mathbf{V}^i)^T) \Delta\boldsymbol{d}_t^i = \Delta\boldsymbol{\lambda}_t^i \tag{14}$$

which can be inverted to yield

$$\begin{aligned} \Delta\boldsymbol{d}_t^i &= \mathbf{V}^i (\mathbf{W}^i)^{-1} (\mathbf{U}^i)^T \Delta\boldsymbol{\lambda}_t^i \\ &= \mathbf{V}^i (\operatorname{diag}(1/\alpha_j)) (\mathbf{U}^i)^T \Delta\boldsymbol{\lambda}_t^i. \end{aligned} \tag{15}$$

Recall, however, that $\mathbf{J}^i = (\mathbf{U}^i \mathbf{W}^i (\mathbf{V}^i)^T)$ is very nearly singular so that these equations are ill conditioned. We obtain the least squares solution to the set of equations by setting $1/\alpha_n = 0$ in equation (15). This results in the solution $\Delta\boldsymbol{d}_t^i$ of minimum norm as discussed by Press *et al* (1986).

Note that as $\boldsymbol{d}^i$ crosses the surface S_d the sign of $\det(\mathbf{J}^i)$ as well as the sign of U_n^i or V_n^i changes. As a consequence of equation (10), $\Delta \boldsymbol{d}_n^i$ always points towards S_d, the surface on which the desired real solution lies.

3. Results and discussion

As we have noted, there are up to $n!$ solutions to the inverse eigenvalue problem though not all of these will be real. We wish to generate all real solutions and for each of the complex solutions we seek the 'solutions' $\boldsymbol{d}^*$ discussed in the last section. Additional conditions may be needed to choose the desired physical solution for the problem at hand. These depend on the particular problem and are not of primary interest in this work which emphasizes the mathematical and numerical problem of obtaining any solution in an efficient way.

We discuss the effect of this correction procedure for a model calculation on two different sets of four coupled energy levels in the Ti XIII ion—12 times ionized titanium. (This is not intended to provide a definitive set of results for this ion's energy levels but simply demonstrate the approach with realistic numerical data. The model calculations were performed as described in Luke 1985.) Calculations for the first set of states lead to both real and complex solutions for the inverse eigenvalue problem while those for the second lead only to complex solutions. These calculations will be referred by the designation of the states' total angular momentum and parity as (1+) and (2−) respectively.

Concerning the choice of initial values, $\boldsymbol{d}^0$, we have found that an effective way to generate solutions was to start with each of the $n!$ orderings of the given (observed) eigenvalues. Newton's method converges rapidly for real solutions. For complex solutions, convergence may be slow as we have noted. Also, the global situation is not yet well understood in the case of the complex solutions, case 2, which result in minima rather than zeros of $\|\boldsymbol{\omega} - \boldsymbol{\lambda}\|$. From studies involving varying the elements of the matrix $\mathbf{A}$, it is evident that the complex solutions evolve from coalescence of pairs of real solutions but higher degeneracies may occur. At present, we can report only that we have observed occasions where both one pair and more than one pair of the initial $\boldsymbol{d}^0$ vectors converged on the same minimum with eigenvalues, $\boldsymbol{\lambda}^*$.

Recall that initially the matrix $\mathbf{A}+\mathbf{D}$ is computed in a model of the physical system under consideration and this matrix is used to calculate a raw spectrum and set of eigenvectors. We then seek to correct these by the procedure we have described. A program has been written to perform the calculation of solutions automatically with minimum input of the elements of the matrix $\mathbf{A}$ and the observed eigenvalues, $\boldsymbol{\omega}$.

In figure 1, we display the upper triangle portion of the symmetric raw matrix, $\mathbf{A}+\mathbf{D}$ for each of the sets of states. Note that the diagonal elements are four orders of magnitude larger than the largest of the off-diagonal elements while the differences of these diagonal elements are comparable to the off-diagonal elements. In any practical calculation, relative errors in the matrix elements of a few per cent are modest and to be expected. Such relative errors are tolerable in the off-diagonal elements of $\mathbf{A}$ but in the large diagonal elements, whose differences are the significant quantities in the eigenvalue problem, they may lead to unacceptable errors in these differences and hence in the eigenvectors as discussed in the introduction.

In the following, we first discuss aspects of the real solutions (case 1) and then discuss the complex solutions (case 2).

(*a*)	−303.8447983	0.5376508983E-1	0.5093650404E-1	0.2036445484E-5
		−303.8139624	−0.5883959266E-1	0.9587984935E-1
			−303.8425767	−0.4586297764E-1
				−304.0935668
(*b*)	−302.589297	0.5604554352E-1	0.6594756648E-1	0.5116233681E-4
		−302.55474604	−0.3137490645E-1	−0.8246505514E-1
			−302.5681623	0.6493929052E-1
				−302.7139037

Figure 1. Raw, computed Hamiltonian matrix $\mathbf{A}+\mathbf{D}$ for (*a*) (1+) levels and (*b*) (2−) levels.

The results for the real solutions from the correction procedure for the (1+) states are summarized in table 1. Here we obtain six real solutions corresponding to the observed spectrum, and for each solution we give the corrected diagonal elements required to obtain the observed spectrum as well as the resulting probabilities. The raw, calculated values for both quantities are also recorded. (The errors recorded for the probability vectors of solution A in table 1(*b*) will be discussed later.) For convenience, we have subtracted the trace from the diagonal elements. This has no effect on the eigenvalue problem of course but should be kept in mind when relative errors are considered.

Notice that in this particular model, for solution A which lies closest to the raw calculated solution, the distance $\|\boldsymbol{d}_{\text{raw}}-\boldsymbol{d}_{\omega}\|=0.025\,65$ and for all other solutions this distance is much larger. If no other information is available, this fact as well as the concomitant evidence from table 1(*b*), discussed below, would lead us to choose solution A as the preferred corrected solution for the (1+) ion levels. (Other information affecting the choice of solution might be the results of certain measurements on the behaviour of the ion in a magnetic field which can be predicted from a knowledge of the eigenvectors.)

If the original calculation is at all reasonable, the corrected results should lie reasonably near by, as indicated by both the diagonal matrix elements and the probability vectors and in this case this is seen to be so. Similarity, or otherwise, of corresponding probability vectors is of course significant. The components of the probability vectors are the squares of the components of the eigenvectors and they are listed in the same order as the corresponding eigenvalues. The physical character of the levels depends on the relative sizes of the components of the probability vectors. Thus we can see from table 1(*b*) that the different solutions give vectors for a given eigenvalue that will differ markedly from solution to solution.

We remark on one last point concerning this table. The eigenvalues and diagonal matrix elements are comparably scaled in magnitude. The former are generally known to a high degree of accuracy so it is significant that $\|\boldsymbol{\delta d}\| \gg \|\boldsymbol{\delta\lambda}\|$. The changes in probability vectors denoted by $\|\boldsymbol{\delta P}_i\|$ are also rather large, indicating rather large changes in physical behaviour of the corresponding states for the slight error or change in eigenvalues. There is a tendency to believe that if the calculated spectrum is 'fairly close' to the observed spectrum then the probabilities will be satisfactory. These results show that this may not be true. The composition of the levels may depend rather sensitively on the spectrum.

We consider next the question of sensitivity to fluctuations in off-diagonal elements—that is, elements of the matrix **A**. It is a simple matter using our code to apply perturbations to the elements of **A** in the neighbourhood of any solution, keeping the

Table 1. Case 1, real solutions to inverse eigenvalue problem. (*a*) Raw and corrected diagonal matrix elements and eigenvalues for (1+) levels in Ti XIII ion. (*b*) Raw and corrected probability vectors corresponding to eigenvalues in (*a*). The subscript ω designates corrected values.

(*a*)

	Raw	A	B	C	D	E	F	λ_{raw}	ω
d_1	0.053 93	0.069 43	0.080 47	0.146 89	0.136 96	0.103 76	0.065 72	0.164 25	0.166 29
d_2	0.084 76	0.092 35	−0.170 32	−0.167 03	−0.157 05	−0.152 75	−0.004 17	0.105 81	0.103 93
d_3	0.056 15	0.037 59	−0.027 77	−0.004 26	0.066 90	0.110 49	0.117 31	−0.042 44	−0.046 75
d_4	−0.194 84	−0.190 88	0.117 62	0.024 41	−0.046 82	−0.061 50	−0.178 86	−0.227 61	−0.223 47
$\|\delta d\|$†		0.025 65	0.412 85	0.351 80	0.295 62	0.282 18	0.109 74	$\|\delta\lambda\|$‡	0.00660

(*b*)

	Raw	A	B	C	D	E	F
P_1	0.031	0.059 ± 0.012	0.000	0.925	0.772	0.302	0.070
	0.661	0.713 ± 0.013	0.097	0.012	0.001	0.014	0.115
	0.230	0.151 ± 0.023	0.092	0.064	0.219	0.639	0.771
	0.078	0.077 ± 0.003	0.810	0.000	0.007	0.044	0.044
$\|\delta P_1\|$§		0.099	0.935	1.12	0.995	0.813	0.770
P_2	0.608	0.632 ± 0.011	0.895	0.009	0.153	0.601	0.653
	0.037	0.005 ± 0.006	0.018	0.158	0.164	0.140	0.312
	0.354	0.358 ± 0.011	0.086	0.247	0.465	0.154	0.000
	0.001	0.005 ± 0.002	0.001	0.586	0.217	0.106	0.035
$\|\delta P_2\|$		0.040	0.393	0.853	0.531	0.248	0.452
P_3	0.360	0.307 ± 0.021	0.062	0.041	0.052	0.072	0.272
	0.221	0.205 ± 0.006	0.052	0.001	0.068	0.111	0.411
	0.408	0.482 ± 0.027	0.745	0.642	0.297	0.195	0.226
	0.011	0.006 ± 0.002	0.140	0.316	0.582	0.623	0.090
$\|\delta P_3\|$		0.093	0.498	0.546	0.676	0.718	0.288
P_4	0.001	0.001 ± 0.000	0.043	0.026	0.022	0.025	0.005
	0.080	0.077 ± 0.003	0.832	0.829	0.766	0.736	0.163
	0.008	0.010 ± 0.001	0.077	0.047	0.018	0.012	0.002
	0.911	0.912 ± 0.003	0.048	0.097	0.194	0.227	0.831
$\|\delta P_4\|$		0.004	1.148	1.107	0.993	0.948	0.116

† Where $\|\delta d\| = \|d_{raw} - d_\omega\|$.
‡ $\|\delta\lambda\| = \|\lambda_{raw} - \omega\|$.
§ Where $\|\delta P_i\| = \|P_{i,raw} - P_{i,\omega}\|$.

matrix **A** symmetric, of course, and to calculate the resulting changes in various quantities of interest.

In the case of a real solution for **D** yielding the observed spectrum we are interested in the stability of the correction calculation with respect to errors in the computed elements of **A**. We have investigated this in two ways.

In appendix A, we outline a stability analysis based on computed norms for the quantities of interest. This approach leads to rather exaggerated error estmates as one would expect. Tighter error bounds derived directly from the calculations by applying specific perturbations can be obtained. Our procedure was to apply small perturbations to each of the elements of **A** in turn and to compute the resulting changes in probabilities. A relatively crude but convenient and conservative error estimate is then obtained by adding the absolute values of the changes in probabilities resulting from all the perturbations in A_{ij}. The changes in the probability vectors corresponding to the worst possible case, namely constructive addition of all perturbations—using a 1% shift in

each of the elements of **A**—are then noted and recorded in table 1(b) for solution A only, for illustration. The 'analytic' norm for this case resulted in a maximum error that was about 0.14 which is about five times larger than the largest of the 'numerical' error estimates.

It is thus clear from the table that these numerical norms yield more realistic bounds than the analytical norms, though we note that the purpose of calculating these is not to obtain accurate error estimates so much as to show where the problem is ill-conditioned. This does not occur in the present example where this procedure leads to perturbations in the larger probabilities—which are the physically significant ones—of only about 5% or less; however, if very large errors in probabilities were to result from perturbations in **A** this would clearly warn the user to anticipate serious uncertainties in such properties as transition rates between states that depend on the probabilities.

We next consider some aspects of complex solutions, case 2. These are the instances where the set of diagonal matrix elements yielding the observed spectrum is complex but one can calculate a set of real diagonal elements, denoted by $\boldsymbol{d}^*$, that yield an approximation of the observed spectrum $\boldsymbol{\lambda}$, denoted $\boldsymbol{\lambda}^*$, as described earlier in section 2.

In table 2(a) we record the optimum sets of diagonal matrix elements, $\boldsymbol{d}^*$, obtained as described in section 2, along with the corresponding eigenvalues for the four case 2 solutions obtained by our procedure. These results refer again to the (1+) levels. In table 2(b) we give the raw and corrected probabilities for each of the solutions that were found and, for solution G which is the one closest to the calculated (raw) solution, we give the fluctuations induced by an accumulation of 1% fluctuations in the elements of **A** as was done in table 1(b) for the real solutions.

This solution G is markedly closer to the raw, calculated one than any of the others though it is substantially further than the real solution A as we can see from the norms $\|\boldsymbol{\delta d}\|$ and $\|\boldsymbol{\delta P}_i\|$ quoted in tables 1 and 2. It is also the case 2 solution that gives the set of eigenvalues, $\boldsymbol{\lambda}^*$, closest to the observed values. The errors on the probabilities indicate that this solution is comparable in stability to the real solution, A.

It is, of course, not necessarily the case that the corrected solution corresponding to the observed spectrum that is closest to the raw solution is a real solution as in the foregoing set of levels, and indeed there may be no real solutions. Such is the situation for the present calculation of four coupled (2−) levels in Ti XIII where we are therefore forced to consider a complex nearby solution, $\boldsymbol{d}^*$, as the one best suited for use in calculating corrected atomic properties.

We record in table 3 our results for the case 2 solutions found for these (2−) levels. We see from the $\|\boldsymbol{\delta\lambda}_\omega\|$ values in table 3 that the approximate solution B comes closest to the observed eigenvalues followed by D and then A. There would be a modest perturbation of the matrix **A** that would cause B to be real, in fact, while leaving A 'complex'. Nevertheless A is still the preferred approximation to the physical problem. That this is the case becomes apparent from examining the relation of the diagonal matrix elements, d_i, and more importantly the probability vectors, $\boldsymbol{P}_i$. Approximate solution A is clearly the one that evolves from the original calculation. The probability vectors of A are similar to the raw vectors while those of B and D are entirely different. That a complex solution, $\boldsymbol{d}_\omega$, evolved from the raw calculation (with a real solution perhaps occurring elsewhere) is an accident of the closeness of the real-complex boundary surface (S_λ) to this solution, not a reflection on the accuracy or relevance of this complex solution.

Table 2. Case 2 solutions to inverse eigenvalue problem. (*a*) Raw and corrected diagonal matrix elements and eigenvalues for (1+) levels in Ti XIII ion. (*b*) Raw and corrected probability vectors corresponding to eigenvalues in (*a*).

(*a*)

	Raw	G	H	I	J	λ_{raw}	ω
d_1	0.053 93	0.031 11	0.140 60	−0.045 81	0.094 10		
d_2	0.084 76	0.068 88	0.000 77	−0.169 33	0.039 56		
d_3	0.056 15	0.089 08	0.039 02	0.113 29	−0.195 64		
d_4	−0.194 84	−0.189 08	−0.180 39	0.101 86	0.061 98		
$\|\delta d^*\|$†		0.043 48	0.122 75	0.407 19	0.364 71		
λ_1^*		0.166 14	0.167 63	0.188 58	0.172 48	0.164 25	0.166 29
λ_2^*		0.101 77	0.113 25	0.079 70	0.103 14	0.105 81	0.103 93
λ_3^*		−0.044 41	−0.056 92	−0.043 13	−0.052 21	−0.042 24	−0.046 75
λ_4^*		−0.223 50	−0.223 95	−0.225 15	−0.223 41	−0.227 61	−0.223 47
$\|\delta\lambda_r^*\|$‡		0.006 44	0.017 20	0.035 78	0.013 85		
$\|\delta\lambda_\omega\|$§		0.003 19	0.013 87	0.033 16	0.008 29		

(*b*)

	Raw	G	H	I	J
P_1	0.031	0.000 ± 0.000	0.881	0.007	0.137
	0.661	0.472 ± 0.018	0.052	0.078	0.444
	0.230	0.454 ± 0.021	0.066	0.467	0.018
	0.078	0.074 ± 0.003	0.001	0.448	0.402
$\|\delta P_1\|$¶		0.295	1.061	0.730	0.456
P_2	0.608	0.519 ± 0.014	0.001	0.115	0.784
	0.037	0.210 ± 0.018	0.417	0.028	0.004
	0.354	0.266 ± 0.008	0.481	0.437	0.051
	0.001	0.005 ± 0.001	0.102	0.420	0.161
$\|\delta P_2\|$		0.214	0.734	0.652	0.387
P_3	0.360	0.478 ± 0.014	0.116	0.776	0.043
	0.221	0.225 ± 0.009	0.382	0.083	0.502
	0.408	0.275 ± 0.015	0.449	0.067	0.024
	0.011	0.022 ± 0.003	0.053	0.074	0.431
$\|\delta P_3\|$		0.178	0.298	0.559	0.709
P_4	0.001	0.002 ± 0.000	0.002	0.102	0.036
	0.080	0.093 ± 0.004	0.149	0.811	0.050
	0.008	0.005 ± 0.001	0.004	0.030	0.907
	0.911	0.899 ± 0.000	0.844	0.058	0.006
$\|\delta P_4\|$		0.018	0.096	1.128	1.276

† Where $\|\delta d^*\| = \|d_{raw} - d^*\|$.
‡ $\|\delta\lambda_r^*\| = \|\lambda_{raw} - \lambda^*\|$.
§ $\|\delta\lambda_\omega^*\| = \|\omega - \lambda^*\|$.
¶ Where $\|\delta P_i\| = \|P_{i,raw} - P_i^*\|$.

Two questions are now of primary interest: we can ask as in the real case whether the solutions are stable with respect to fluctuations in the elements of **A** as before in the real case. Also, although the computed off-diagonal matrix **A** does not yield a real solution near the point in question, we can ask what change in the elements of **A** will allow a real solution near that point. In other words we enquire as to whether the solution A which yields a non-zero minimum of $\|\lambda - \omega\|$ would be a reasonable

Table 3. Case 2 solutions to inverse eigenvalue problem. (*a*) Raw and corrected diagonal matrix elements and eigenvalues for (2−) levels of Ti XIII ion. (*b*) Raw and corrected probability vectors corresponding to eigenvalues of (*a*).

(*a*)

	Raw	A	B	C	D	E	λ_{raw}	ω
d_1^*	0.020 43	0.017 93	0.062 72	−0.103 41	0.071 37	0.073 10		
d_2^*	0.048 90	0.047 71	0.039 83	0.057 39	−0.097 98	0.004 28		
d_3^*	0.038 20	0.037 90	−0.004 72	0.069 66	−0.008 38	−0.105 99		
d_4^*	−0.107 54	−0.103 54	−0.097 83	−0.023 64	0.035 00	0.028 61		
$\|\delta d^*\|$†		0.004 87	0.061 70	0.153 09	0.216 00	0.209 98		
λ_1^*		0.123 15	0.123 25	0.155 69	0.125 03	0.129 85	0.123 19	0.123 40
λ_2^*		0.101 08	0.102 11	0.075 25	0.102 55	0.101 11	0.102 69	0.103 45
λ_3^*		−0.072 04	−0.073 39	−0.085 35	−0.075 51	−0.079 13	−0.070 50	−0.074 60
λ_4^*		−0.152 19	−0.151 97	−0.145 59	−0.152 07	−0.151 83	−0.155 39	−0.152 24
$\|\delta\lambda_r^*\|$‡		0.003 90	0.004 52	0.046 11	0.006 29	0.011 58		
$\|\delta\lambda_\omega^*\|$§		0.003 50	0.001 84	0.044 70	0.002 08	0.008 23		

(*b*)

	Raw	A	B	C	D	E
P_1	0.002	0.001 ± 0.001	0.511	0.001	0.325	0.254
	0.522	0.509 ± 0.028	0.433	0.364	0.021	0.399
	0.305	0.314 ± 0.034	0.009	0.384	0.345	0.011
	0.171	0.176 ± 0.005	0.047	0.252	0.309	0.336
$\|\delta P_1\|$¶		0.017	0.608	0.195	0.613	0.439
P_2	0.523	0.519 ± 0.017	0.203	0.188	0.490	0.588
	0.160	0.171 ± 0.032	0.207	0.381	0.188	0.010
	0.316	0.310 ± 0.014	0.429	0.424	0.001	0.169
	0.000	0.000 ± 0.000	0.160	0.007	0.319	0.223
$\|\delta P_2\|$		0.013	0.378	0.415	0.450	0.321
P_3	0.475	0.480 ± 0.018	0.285	0.007	0.110	0.066
	0.207	0.204 ± 0.006	0.257	0.156	0.004	0.566
	0.318	0.315 ± 0.015	0.452	0.099	0.626	0.002
	0.001	0.001 ± 0.001	0.006	0.738	0.260	0.366
$\|\delta P_3\|$		0.007	0.238	0.902	0.580	0.727
P_4	0.000	0.000 ± 0.000	0.000	0.805	0.074	0.092
	0.111	0.115 ± 0.007	0.104	0.100	0.787	0.025
	0.061	0.062 ± 0.006	0.109	0.093	0.028	0.817
	0.828	0.823 ± 0.005	0.787	0.003	0.110	0.065
$\|\delta P_4\|$		0.006	0.064	1.153	0.989	1.082

† Where $\|\delta d^*\| = \|d_{raw} - d^*\|$.
‡ Where $\|\delta\lambda_r^*\| = \|\lambda_{raw} - \lambda^*\|$.
§ $\|\delta\lambda_\omega^*\| = \|\omega - \lambda^*\|$.
¶ Where $\|\delta P_i\| = \|P_{i,raw} - P_i^*\|$.

approximation for the physical state given that the computed **A** is subject to modest errors.

For the first question, we record in table 3 the changes in probability vectors resulting from perturbations in **A**. This information corresponds to that in table 2 for the real solutions and it appears that these solutions are again fairly stable. Constructive

addition of the results of 1% shifts in the elements of **A** lead to maximum probability shifts of 0.03 roughly, so there is no sign of significant ill-conditioning.

Concerning the second question, we note that in complex cases, when **D**, $\boldsymbol{\lambda}^*$, and the eigenvectors are known, it is possible to perturb **A** to $\mathbf{A}+\Delta\mathbf{A}$ in such a way that the eigenvectors, hence the probabilities, are unchanged and the eigenvalues of the new matrix $\mathbf{D}+\mathbf{A}+\Delta\mathbf{A}$ are $\boldsymbol{\omega}$, the observed eigenvalues. For this perturbation we have

$$\mathbf{D}+\mathbf{A}+\Delta\mathbf{A}=[x_{jk}](\mathrm{diag}(\omega_i))[x_{jk}]^T \tag{16}$$

and hence

$$\Delta\mathbf{A}=[x_{jk}](\mathrm{diag}(\omega_i-\lambda_i^*))[x_{jk}]^T. \tag{17}$$

This perturbation is interesting in that it gives the change in **A** that yields a matrix with the observed spectrum, $\boldsymbol{\omega}$, and the same eigenvectors or equivalently the same probabilities as those of the corrected matrix $\mathbf{A}+\mathbf{D}^*$ which results from the non-zero optimum of $\|\boldsymbol{\lambda}-\boldsymbol{\omega}\|$. If the resulting changes in **A** are within the expected range of its errors in a given calculation, the non-zero optimum can justifiably be used for calculating eigenvectors and resulting physical properties for the system.

We record in table 4 some relevant numerical results, namely the fluctuations in the elements of **A** required to produce a real solution that is very close to the 'optimum' solution, A, and has as described in the foregoing the same eigenvectors but with the observed eigenvalues. In this example, at least, the perturbations on **A** are very small—less than 3% changes in the larger elements, which are the significant ones for mixing levels, yield a real solution in place of A. We also see from table 3 that the probability vectors are reasonably stable in the neighbourhood of the solution A. In this case, therefore, it is acceptable to use the eigenvectors from solution A as corrected vectors for the problem.

Table 4. Elements of off-diagonal matrix **A** and the fluctuations required to produce a matrix $\mathbf{A}+\mathbf{D}$ with observed eigenvalues and the eigenvectors obtained from optimum solution A.

ij	$\mathbf{A}_{ij}$	$\delta\mathbf{A}_{ij}$
12	0.56E-1	0.15E-2
13	0.66E-1	0.19E-2
14	0.51E-4	−0.35E-4
23	−0.31E-1	−0.20E-3
24	−0.82E-1	−0.46E-4
34	0.65E-1	0.12E-3

The present calculation is of course somewhat unfortunate inasmuch as it is actually too accurate so that it is somewhat misleading. As we have pointed out, the corrected solution A is within the noise of a real corrected solution with the observed eigenvalues and the corrected eigenvectors. At the same time, from the fluctuations in the probabilities recorded in table 3, we see that even the raw solution does not differ significantly from the optimum corrected solution. One might as well use the raw results in this case it seems. Nevertheless, the point is obviously that in another calculation the corrected solution could move substantially away from the raw calculation so that the latter would not be useful. In this case, considerations analogous to those illustrated

in table 4 would be important in showing whether the optimum corrected solution was reasonable.

To conclude, we have described a method for applying inverse eigenvalue problem corrections to calculations in atomic systems. We have discussed questions of errors and shown how our approach can be used directly to judge the validity of the corrected solutions we obtain.

Acknowledgments

This work was supported by the Natural Sciences and Engineering Research Council of Canada.

Appendix A. Estimate of errors for case 1

Suppose we have obtained a solution of $\mathbf{A}+\mathbf{D}=\mathbf{X}\Omega\mathbf{X}^T$ where Ω is the diagonal matrix of eigenvalues and $\mathbf{X}$ is the matrix of eigenvectors. If we perturb $\mathbf{A}$ to $\mathbf{A}+\Delta\mathbf{A}$, reflecting errors in the computed $\mathbf{A}$ matrix, then perturbations $\Delta\mathbf{D}$ and $\Delta\mathbf{X}$ are induced in $\mathbf{D}$ and $\mathbf{X}$. We estimate $\Delta\mathbf{D}$ and $\Delta\mathbf{X}$ using the linearizing approach in 'method III' of Friedland *et al* (1987).

Let $\mathbf{X}+\Delta\mathbf{X}=\mathbf{X}\,\mathrm{e}^{\mathbf{Y}}$ where $\mathbf{Y}^T=-\mathbf{Y}$. Substituting into

$$(\mathbf{X}+\Delta\mathbf{X})^T(\mathbf{A}+\mathbf{D}+\Delta\mathbf{A}+\Delta\mathbf{D})(\mathbf{X}+\Delta\mathbf{X})=\Omega \tag{A1}$$

and expanding $\mathrm{e}^{\mathbf{Y}}$, so that $\Delta\mathbf{X}\simeq\mathbf{XY}$, we obtain the linearized form

$$\mathbf{X}^T(\mathbf{A}+\mathbf{D}+\Delta\mathbf{A}+\Delta\mathbf{D})\mathbf{X}\simeq\Omega+\mathbf{Y}\Omega-\Omega\mathbf{Y}. \tag{A2}$$

Hence

$$\mathbf{X}^T(\Delta\mathbf{A}+\Delta\mathbf{D})\mathbf{X}\simeq\mathbf{Y}\Omega-\Omega\mathbf{Y}. \tag{A3}$$

Upon equating diagonal and off-diagonal elements we obtain the following two equations:

$$\mathbf{J}\Delta\boldsymbol{d}=-[(\boldsymbol{X}_j)^T\Delta\mathbf{A}\boldsymbol{X}_j] \tag{A4}$$

and

$$Y_{ij}(\omega_j-\omega_i)=(\boldsymbol{X}_i)^T(\Delta\mathbf{A}+\Delta\mathbf{D})X_j. \tag{A5}$$

We also estimate an upper limit for the resulting perturbation in the probabilities. This is defined by

$$\begin{aligned}\Delta P_{ik}&=(X_{ik}+\Delta X_{ik})^2-(X_{ik})^2\simeq 2X_{ik}\Delta X_{ik}\\&=\sum_l 2X_{ik}X_{il}Y_{lk}\end{aligned} \tag{A6}$$

where Y_{lk} is given by equation (A5).

We assume the elements of $\mathbf{A}$ to be subject to a percentage error, P, so that

$$\Delta A_{ij}\simeq\pm\frac{P}{100}A_{ij}.$$

Without taking the specific structure of ΔA_{ij} into account, we now construct upper estimates for $\Delta \boldsymbol{d}$ and ΔP_{ik} as follows. Using equation (A4) and taking norms we obtain

$$\|\Delta \boldsymbol{d}\|_\infty = \|\mathbf{J}^{-1}\|_\infty \|(\boldsymbol{X}_j)^T \Delta \mathbf{A} \boldsymbol{X}_j\|_\infty .$$

Also

$$|(\boldsymbol{X}_j)^T \Delta \mathbf{A} \boldsymbol{X}_j| \leq \|(\boldsymbol{X}_j)\|_2 \|\Delta \mathbf{A}\|_2 \|\boldsymbol{X}_j\|_2 .$$

The eigenvectors $\boldsymbol{X}_j$ are normalized and for the symmetric matrix $\Delta \mathbf{A}$ we have

$$\|\Delta \mathbf{A}\|_2 \leq \|\Delta \mathbf{A}\|_1 = \|\Delta \mathbf{A}\|_\infty .$$

Therefore

$$|\boldsymbol{X}_j^T \Delta \mathbf{A} \boldsymbol{X}_j| \leq \|\Delta \mathbf{A}\|_\infty$$

and finally

$$\|\Delta \boldsymbol{d}\|_\infty \leq \|\boldsymbol{J}^{-1}\|_\infty \frac{P}{100} \|\mathbf{A}\|_\infty . \tag{A7}$$

Deriving a bound on ΔP_{ij} we have, using equation (A6),

$$\Delta P_{ik} = 2X_{ik} \mathbf{C}^T (\Delta \mathbf{A} + \Delta \mathbf{D}) \boldsymbol{X}_k \qquad \text{where } \mathbf{C} \equiv \mathbf{C}(i,k) = \sum_{l \neq k} \frac{\boldsymbol{X}_{il} (\boldsymbol{X}_l)^T}{\omega_k - \omega_l} .$$

Therefore

$$\begin{aligned} |\Delta P_{ik}| &\leq 2|X_{ik}| \, \|\mathbf{C}(i,k)\|_2 (\|\Delta \mathbf{A}\|_\infty + \|\Delta \mathbf{D}\|_\infty) \\ &\leq 2|X_{ik}| \, \|\mathbf{C}(i,k)\|_2 \frac{P}{100} (1 + \|J^{-1}\|_\infty) \|\mathbf{A}\|_\infty \end{aligned} \tag{A8}$$

where we have used equation (A7).

Note that $\|\mathbf{C}(i,k)\|_2$ can be simplified:

$$\|C(i,k)\|_2 = \left(\sum_{l \neq k} \frac{(X_{il})^2}{(\omega_k - \omega_l)^2} \right)^{1/2}$$

which is readily calculated.

The maximum error defined as $\mathrm{Max}_{i,k} \, |P_{ik}|$ can now be readily calculated.

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