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Note

A Method for the Solution of the Inverse Eigenvalue Problem

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In this note we present a numerical method for the solution of the inverse eigenvalue problem which frequently arises in chemistry and physics, *e. g.* in the analysis of infrared and NMR spectra. The problem is to find the values of the parameters $p_1 \ldots p_m$ so that the symmetric n by n matrix

$$A = A_0 + \sum_{i=1}^{m} p_i A_i$$

possesses the given eigenvalues $\lambda_1 \ldots \lambda_n$.

The majority of the known methods for the solution of this problem are iterative methods where one successively tries to improve the parameters in order that the calculated eigenvalues approach the given ones[1]. In all of these methods m must not exceed n. In many practical cases, therefore, the number of parameters has to be artificially reduced.

To deal with the general case we suggest the following method. First, we diagonalize the matrix

$$A^{(o)} = A_0 + \sum_{i=1}^{m} p_i^{(o)} A_i = L^{(o)} \Lambda^{(o)} \tilde{L}^{(o)}$$

where $p_i^{(o)}$ are the initial parameters. Next, we calculate the matrix

$$B = L^{(o)} \Lambda \tilde{L}^{(o)}$$

where $\Lambda = \text{diag}\ (\lambda_1 \ldots \lambda_n)$. In order to obtain the next approximation to the parameters we solve the over- determined system of linear equations in which matrix B is equated to the initial matrix A expressed in terms of the parameters p_i. This leads to the equations

$$(A_0 + \sum_{i=1}^{m} p_i A_i)_{jk} = B_{jk},\ j = 1, \ldots n,\ k = 1, \ldots j.$$

This is a system of $1/2\ n\ (n + 1)$ equations in m unknowns. We must assume that $m \leqq 1/2\ n\ (n + 1)$. By the least square method we find the first approximate value of the parameters $p_i^{(1)}$ and repeat the process until the differences between the corresponding parameters in two consecutive cycles are suffi-

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ciently small. It is advisable that the calculated eigenvalues and eigenvectors are ordered so that correct correspondence to the given values may be obtained.

The method has been tested for the determination of the force constants in H_2O and HOCl. In the case of H_2O we have obtained results close to the known values[2] (Table) providing that we chose the two most significant force constants close to the correct ones.

TABLE

	$p_i^{(0)}$	$p_i^{(1)}$	exact[2] (mdyne A^{0-1})
f_r	8.0	8.45	8.45
f_{rr}	0	— 0.09	— 0.09
f	1	0.75	0.79
f_r	0.1	0.26	0.26

The same feature has been observed in the case of HOCl where we have obtained for the interaction force constant the value recommended by Fadini[3].

In several tests that we have made, the convergence of the method has proved to be very rapid. We are aware that in the case $m > n$ the number of solutions to the problem is, in general, infinite. Nevertheless, the results obtained with plausible initial approximations are always acceptable.

The numerical computations were made on the *Elliott 503* computer of the University of Surrey, London.

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IZVLEČEK

Metoda za reševanje inverznega problema lastnih vrednosti

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Za reševanje inverznega problema lastnih vrednosti je opisana metoda, katere osnova je uporaba lastnih funkcij namesto lastnih vrednosti, v iteraciski proceduri. Metodo smo testirali na izračunu potencialnega polja vibracij molekul H_2O in HOCl.

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