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Note

Determination of Eigenvectors of Symmetric Idempotent Matrices

I. Introduction

An explicit, detailed, and convenient algorithm has been developed recently [1] for constructing linear combinations of angular momentum eigenfunctions which transform according to the irreducible representations of the tetrahedral point group T_d. These "symmetry-adapted functions" or "tetrahedral harmonics" are useful in a wide variety of physical problems involving tetrahedral molecules such as methane. Many physical applications are discussed in Ref. [1].

The algorithm results from an application of the projection-operator technique [2]. In general, and especially for high values of the angular momentum quantum number J, the set of projected functions which transform according to a given row of a given rep may be linearly dependent. In this case, in earlier work [3], the functions were made orthogonal by the Gram-Schmidt procedure [4]. In Ref. [1], symmetric idempotent projection-operator matrices were constructed, and it was shown that the eigenvectors corresponding to eigenvalue 1 comprised *all* the required *orthonormal* tetrahedral harmonics.

The purpose of the present note is to show that a Cholesky factorization, with pivoting, on a symmetric idempotent matrix can produce an explicit, complete set of orthonormal eigenvectors corresponding to eigenvalue 1.

II. Determination of Eigenvectors

Let A be a real, symmetric idempotent matrix:

$$A^2 = A. \tag{1}$$

Do a Cholesky factorization [5] on A, with pivoting; that is, every interchange of rows is accompanied by an interchange of corresponding columns, so that diagonal elements remain so. The final result is that the matrix A is replaced by the matrix PAP^T, where P is some permutation matrix, and the factorization gives

$$PAP^T = LL^T, \tag{2}$$

where L is a lower trapezoidal matrix. (Actually, the permutations are not necessary, although they are permitted, for example, to get the largest pivot.)

Since A is idempotent, it follows that

$$LL^TLL^T = PAP^TPAP^T = PA^2P^T = PAP^T = LL^T. \tag{3}$$

Premultiplying by L^T and postmultiplying by L gives

$$L^TLL^TLL^TL = L^TLL^TL. \tag{4}$$

Now L is of maximal rank, and L^TL has the same rank and is hence nonsingular. Premultiply by $(L^TL)^{-1}$ and postmultiply by the same, and the result is

$$L^TL = I, \tag{5}$$

where I is the identity matrix.

Next, in Eq. (2), premultiply by P^T and postmultiply by L:

$$P^TPAP^TL = P^TLL^TL \tag{6}$$

or

$$AP^TL = P^TL, \tag{7}$$

where Eq. (5) has been used. Thus, the columns of P^TL comprise eigenvectors of A corresponding to eigenvalue 1. Also, since L is of maximal rank, so is P^TL. Then P^TL contains *all* the required eigenvectors.

Finally,

$$(P^TL)^T(P^TL) = L^TPP^TL = L^TL = I \tag{8}$$

which means that the columns of P^TL are *orthonormal.* This completes the proof.

III. Discussion

In the preceding section, we showed that a complete set of orthonormal eigenvectors, corresponding to eigenvalue 1, could be constructed by a Cholesky factorization, with pivoting, on the original symmetric idempotent matrix. Some thought has been given to carrying out this procedure numerically on a real, symmetric idempotent matrix. Although the Cholesky factorization is more commonly applied to nonsingular matrices, it is readily applicable to singular matrices as well. The computation is stable. The accumulation of rounding errors is no worse than in any other technique for calculating the eigenvectors. Finally, we note that unlike the usual case in which the eigenvectors must be "kept apart," the Cholesky factorization on an idempotent matrix leads to automatically orthonormal eigenvectors.

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