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Note

Trace Orthogonal Hermitian Basis Matrices of Arbitrary Dimension

1. Introduction

An arbitrary $N \times N$ matrix $\mathbf{M}$ can be expressed as a linear combination of the N^2 basis matrices $\boldsymbol{\sigma}_n^{(N)}$

$$M = \sum_{n=1}^{N^2} M_n \boldsymbol{\sigma}_n^{(N)} \tag{1.1}$$

where M_n are (scalar) expansion coefficients (Fano [3], Pease [6]). If the $\boldsymbol{\sigma}_n^{(N)}$ are trace orthonormal, i.e.,

$$\operatorname{tr} \boldsymbol{\sigma}_n^{(N)} \boldsymbol{\sigma}_m^{(N)} = \delta_{nm} \tag{1.2}$$

then the expansion coefficients are given by

$$M_n = \operatorname{tr} \mathbf{M} \boldsymbol{\sigma}_n^{(N)} . \tag{1.3}$$

It is also common practice to require that the basis matrices be hermitian; so that if $\mathbf{M}$ be hermitian then the expansion coefficients M_n are real.

Although the usefulness of these basis matrices is unquestioned, the explicit representation of the $\boldsymbol{\sigma}_n^{(N)}$ is only known for $N = 2, 3$. The purpose of the present paper is to present an algorithm which permits the direct construction of these basis matrices for any N.

2. Off-Diagonal Basis Matrices

We will find it useful to employ a somewhat more elaborate notation involving two subscripts and rewrite Eq. (1.1) as

$$\mathbf{M} = \sum_{\alpha=1}^{N} \sum_{\beta=1}^{N} M_{\alpha\beta} \boldsymbol{\sigma}_{\alpha\beta}^{(N)}. \tag{2.1}$$

The trace orthogonality and hermitian conditions become

$$\operatorname{tr} \boldsymbol{\sigma}_{\alpha\beta}^{(N)} \boldsymbol{\sigma}_{\gamma\delta}^{(N)} = \delta_{\alpha\gamma}\delta_{\beta\delta} \tag{2.2}$$

$$\boldsymbol{\sigma}_{\alpha\beta}^{(N)} = (\boldsymbol{\sigma}_{\beta\alpha}^{(N)})^{+}. \tag{2.3}$$

The set of $N(N-1)/2$ matrices $\boldsymbol{\sigma}_{\alpha\beta}^{(N)}$ with $\alpha < \beta$ having elements

$$[\boldsymbol{\sigma}_{\alpha\beta}^{(N)}]_{jk} = \tfrac{1}{2}(\delta_{\alpha j}\delta_{\beta k} + \delta_{\alpha k}\delta_{\beta j}); \qquad j, k = 1,..., N \tag{2.4}$$

are hermitian since they are real symmetric. They satisfy the trace orthogonality condition, Eq. (2.2).

Another set of $N(N-1)/2$ basis matrices $\boldsymbol{\sigma}_{\alpha\beta}^{(N)}$ with $\alpha > \beta$ is

$$[\boldsymbol{\sigma}_{\alpha\beta}^{(N)}]_{jk} = (i/2)(\delta_{\alpha j}\delta_{\beta k} - \delta_{\alpha k}\delta_{\beta j}); \qquad j, k = 1,..., N. \tag{2.5}$$

These matrices are also trace orthogonal as well as hermitian.

It is easily demonstrated that each matrix corresponding to Eq. (2.4) is trace orthogonal to each matrix corresponding to Eq. (2.5). Finally, both sets of matrices are trace orthogonal to any diagonal matrix. Both sets of matrices possess zero diagonals and have only two nonzero elements.

To complete the set of hermitian basis matrices, we have to find the N diagonal matrices that are trace orthogonal subject to the requirement that one of these matrices be the unit matrix (suitably normalized by $N^{-1/2}$). However, this problem is precisely the same as that of finding $(N-1)$ vectors that are orthonormal to a vector having every element given by $N^{-1/2}$.

There are several ways that one could solve the problem of determining a finite set of orthonormal vectors of which one vector corresponds to the diagonal of the unit matrix. This suggests the use of the Gram–Schmidt orthogonality procedure (Hildebrand [4]). However, to employ it one requires a set of linearly independent vectors of which one vector is the above mentioned unit vector. The approach via this method is tedious and time consuming. However, we have discovered a more direct method of construction which circumvents the iterative aspects of Gram–Schmidt. Our procedure is described in the next two sections.

3. Diagonal Basis Matrices

Before discussing the construction of the diagonal matrices, we present some ancillary material.

Suppose we have constructed the N_1^2 basis matrices for the $N_1 \times N_1$ case and the N_2^2 basis matrices for the $N_2 \times N_2$ case, then the set of $(N_1N_2)^2$ square matrices of dimension N_1N_2 obtained by calculating the *direct products* of these two sets of matrices also satisfy Eq. (2.2). The proof of the trace orthogonality condition is:

$$\begin{aligned}
\operatorname{tr}[\boldsymbol{\sigma}_{\alpha\beta}^{(N_1)} \otimes \boldsymbol{\sigma}_{\gamma\delta}^{(N_2)}][\boldsymbol{\sigma}_{\alpha_1\beta_1}^{(N_1)} \otimes \boldsymbol{\sigma}_{\gamma_1\delta_1}^{(N_2)}] &= \operatorname{tr}[\boldsymbol{\sigma}_{\alpha\beta}^{(N_1)}\ \boldsymbol{\sigma}_{\alpha_1\beta_1}^{(N_2)}] \otimes \operatorname{tr}[\boldsymbol{\sigma}_{\gamma\delta}^{(N_1)}\ \boldsymbol{\sigma}_{\gamma_1\delta_1}^{(N_2)}] \\
&= \operatorname{tr}[\boldsymbol{\sigma}_{\alpha\beta}^{(N_1)}\ \boldsymbol{\sigma}_{\alpha_1\beta_1}^{(N_2)}] \operatorname{tr}[\boldsymbol{\sigma}_{\gamma\delta}^{(N_1)}\ \boldsymbol{\sigma}_{\gamma_1\delta_1}^{(N_2)}] \qquad (3.1) \\
&= \delta_{\alpha\alpha_1}\delta_{\beta\beta_1}\delta_{\gamma\gamma_1}\delta_{\delta\delta_1}
\end{aligned}$$

where we have employed standard properties of direct matrix products (Wigner [5]). If in addition the two sets are hermitian, then so are the direct products. Consequently the only values of N we need consider are $N = 1, 2, 3, 5, 7, 11,...,$ the prime numbers.

With these facts in mind, let $p_1 = 1$, $p_2 = 2$, $p_3 = 3$, $p_4 = 5$, $p_5 = 7$, $p_6 = 11,...$ be the sequence of prime numbers. Suppose that the basis vectors of dimension p_m and all lesser dimensions $p_{m-1}, p_{m-2},..., p_1$ be known. Then it follows that the basis vectors of dimension $d_m = p_{m+1} - p_m$ are also known since all the factors of the difference between two primes of contiguous order are primes of lower order than the inferior prime; (Davenport [2]).

Let the known basis set of vectors for spaces of dimensions p_m and d_m be given by

$$\{\boldsymbol{\psi}_j(p_m)\}, \qquad j = 1, 2,..., p_m \tag{3.2}$$

$$\{\boldsymbol{\psi}_j(d_m)\}, \qquad j = 1, 2,..., d_m\ . \tag{3.3}$$

To obtain the next prime-ordered basis set (i.e., $N = p_{m+1}$) we will need the null vectors $\boldsymbol{\psi}_0(p_m)$ and $\boldsymbol{\psi}_0(d_m)$ in the p_m-dimensional and d_m-dimensional spaces, respectively. For notational convenience, we assign $\boldsymbol{\psi}_1(p_m)$ and $\boldsymbol{\psi}_0(d_m)$ to the vectors having every element given by $p_m^{-1/2}$ and $d_m^{-1/2}$, since we have already established that the unit matrix is one of the matrices in every trace orthogonal basis set.

The orthonormal basis set of vectors in the p_{m+1}-dimensional space now can be constructed by the following recursion relations:

$$\boldsymbol{\psi}_{1+j}(p_{m+1}) = \boldsymbol{\psi}_j(p_m) \oplus \boldsymbol{\psi}_0(d_m), \qquad j = 2,..., p_m \tag{3.4}$$

$$\boldsymbol{\psi}_{m+j}(p_{m+1}) = \boldsymbol{\psi}_0(p_m) \oplus \boldsymbol{\psi}_j(d_m), \qquad j = 2,..., d_m \tag{3.5}$$

and the indicial equations

$$\psi_1(p_{m+1}) = (p_m/p_{m+1})^{1/2}\, \psi_1(p_m) \oplus (d_m/p_{m+1})^{1/2}\, \psi_1(d_m) \tag{3.6}$$

$$\psi_2(p_{m+1}) = (d_m/p_{m+1})^{1/2}\, \psi_1(p_m) \oplus (-1)(p_m/p_{m+1})^{1/2}\, \psi_1(d_m) \tag{3.7}$$

where $\oplus$ denotes the *direct sum*. Note that the first indicial equation yields the vector corresponding to the normalized unit matrix as we will verify by direct manipulation. From a heuristic viewpoint, we are enlarging the space of allowable vectors by combining the lower dimension vectors via a direct sum operation, so that vectors of dimensions N_1 and N_2 yield vectors of dimension $(N_1 + N_2)$.

To use this algorithm, we need only know the vectors for $m = 1$ (i.e., $p_1 = 1$), since everything can be generated inductively from them. They are

$$\psi_0(1) = 0, \qquad \psi_1(1) = 1. \tag{3.8}$$

The vector $\psi_1(1)$ is the basis set for the one-dimensional space (i.e., $m = 1, p_1 = 1$), $\psi_0(1)$ is the above-mentioned null vector.

To compute the next order, that is $p_2 = 2$, we use the recursion relations in which $d_1 = p_2 - p_1 = 1$. Equation (3.4) yields

$$\psi_1(2) = \left(\frac{1}{2}\right)^{1/2} |\, 1\, | \oplus \left(\frac{1}{2}\right)^{1/2} |\, 1\, | = \frac{1}{\sqrt{2}} \begin{vmatrix} 1 \\ 1 \end{vmatrix} \tag{3.9}$$

the normalized unit vector. Equation (3.5) yields

$$\psi_2(2) = \left(\frac{1}{2}\right)^{1/2} |\, 1\, | \oplus (-1)\left(\frac{1}{2}\right)^{1/2} |\, 1\, | = \frac{1}{\sqrt{2}} \begin{vmatrix} 1 \\ -1 \end{vmatrix}. \tag{3.10}$$

Consequently, the diagonal basis matrices for $N = 2$ are

$$\sigma_{11} = \frac{1}{\sqrt{2}} \begin{vmatrix} 1 & 0 \\ 0 & 1 \end{vmatrix}, \qquad \sigma_{22} = \frac{1}{\sqrt{2}} \begin{vmatrix} 1 & 0 \\ 0 & -1 \end{vmatrix}. \tag{3.11}$$

The off-diagonal matrices corresponding to Eqs. (2.4) and (2.5) are

$$\sigma_{12} = \frac{1}{\sqrt{2}} \begin{vmatrix} 0 & 1 \\ 1 & 0 \end{vmatrix}, \qquad \sigma_{21} = \frac{1}{\sqrt{2}} \begin{vmatrix} 0 & -i \\ i & 0 \end{vmatrix}. \tag{3.12}$$

These four basic matrices are proportional to the well-known Pauli spin matrices. The numerical factor arises from our choice of normalization, Eq. (2.2).

The 3×3 basis matrices follow from $m = 2$, $p_3 = 3$, and $d_2 = p_3 - p_2 = 1$. From the indicial equations we calculate

$$\psi_1(3) = \left(\frac{2}{3}\right)^{1/2} \left(\frac{1}{2}\right)^{1/2} \begin{vmatrix} 1 \\ 1 \end{vmatrix} \oplus \left(\frac{1}{3}\right)^{1/2} | 1 | = \frac{1}{\sqrt{3}} \begin{vmatrix} 1 \\ 1 \\ 1 \end{vmatrix} \tag{3.13}$$

$$\psi_2(3) = \left(\frac{1}{3}\right)^{1/2} \left(\frac{1}{2}\right)^{1/2} \begin{vmatrix} 1 \\ 1 \end{vmatrix} \oplus (-1)\left(\frac{2}{3}\right)^{1/2} | 1 | = \frac{1}{\sqrt{6}} \begin{vmatrix} 1 \\ 1 \\ -2 \end{vmatrix}. \tag{3.14}$$

The remaining vector $\psi_3(3)$ is obtained from the first recursion relation, Eq. (3.4)

$$\psi_3(3) = \psi_2(2) \oplus \psi_2(1) = \frac{1}{\sqrt{2}} \begin{vmatrix} 1 \\ -1 \\ 0 \end{vmatrix}. \tag{3.15}$$

Consequently the three diagonal matrices are:

$$\sigma_{11} = \frac{1}{\sqrt{3}} \begin{vmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{vmatrix}, \quad \sigma_{22} = \frac{1}{\sqrt{6}} \begin{vmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -2 \end{vmatrix}, \quad \sigma_{33} = \frac{1}{\sqrt{2}} \begin{vmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{vmatrix}. \tag{3.16}$$

The six off-diagonal matrices can be obtained from Eqs. (2.4) and (2.5); we omit their explicit representation. These nine basis matrices are proportional to the well-known $3 \times 3 \lambda_j$ matrices arising in elementary particle physics (Carruthers [1]). The numerical factor again arises from our normalization.

To obtain the 5×5 diagonal basis matrices, we use the recursion relations with $m = 3$, $p_4 = 5$, $d_3 = p_4 - p_3 = 2$. The reader can verify that Eq. 3.4 yields two matrices

$$\sigma_{33} = \frac{1}{\sqrt{6}} \begin{vmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & -2 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{vmatrix}, \qquad \sigma_{44} = \frac{1}{\sqrt{2}} \begin{vmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{vmatrix} \tag{3.17}$$

while Eq. 3.5 with $j = 2$ yields

$$\sigma_{11} = \frac{1}{\sqrt{2}} \begin{vmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & -1 \end{vmatrix}. \tag{3.18}$$

The two indicial equations yield

$$\sigma_{11} = \frac{1}{\sqrt{5}} \begin{vmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{vmatrix}, \qquad \sigma_{22} = \frac{1}{\sqrt{30}} \begin{vmatrix} 2 & 0 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 & 0 \\ 0 & 0 & 2 & 0 & 0 \\ 0 & 0 & 0 & -3 & 0 \\ 0 & 0 & 0 & 0 & -3 \end{vmatrix}. \tag{3.19}$$

The diagonal elements of the diagonal basis matrices for $N = 7$ are listed below:

$$\begin{aligned}
\sigma_{11} &= \frac{1}{\sqrt{7}}(1, 1, 1, 1, 1, 1, 1) \\
\sigma_{22} &= \frac{1}{\sqrt{70}}(2, 2, 2, 2, 2, -5, -5) \\
\sigma_{33} &= \frac{1}{\sqrt{30}}(2, 2, 2, -3, -3, 0, 0) \\
\sigma_{44} &= \frac{1}{\sqrt{6}}(1, 1, -2, 0, 0, 0, 0) \\
\sigma_{55} &= \frac{1}{\sqrt{2}}(1, -1, 0, 0, 0, 0, 0) \\
\sigma_{66} &= \frac{1}{\sqrt{2}}(0, 0, 0, 1, -1, 0, 0) \\
\sigma_{77} &= \frac{1}{\sqrt{2}}(0, 0, 0, 0, 0, 1, -1).
\end{aligned} \tag{3.20}$$

To derive matrices for larger prime numbers one simply applies the same procedure. We note that the entire algorithm is ideally suited for machine computation.

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