Computational Strategies for the Generation of Equivalence Classes of Hadamard Matrices

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Computational strategies are outlined for the construction of equivalence classes of Hadamard matrices. A proposed strategy involves comparison of nodal vectors of ordered Hadamard matrices. The techniques combined with the exhaustive generation of skew-Hadamard matrices generates equivalence classes of Hadamard matrices of order 16 and 28. Several types of equivalence are discussed.

1. INTRODUCTION

Hadamard matrices are useful in Hadamard transform spectroscopy and in the construction of optimal chemical designs.[1-8] The use of these matrices in spectroscopy has led to the advent of Hadamard transform spectroscopy[3] which employs spectroscopic multiplexing techniques and is a powerful tool for the analysis of complex spectra. Besides Hadamard matrices are useful in chemical designs and block designs. An optimal design is a method of accurately weighing a number of objects in groups rather than individually. This leads to an orthogonal set of equations that can be described by Hadamard matrices as illustrated in ref 3. The optimal weighing scheme finds applications both in chemical balance and in the multiplexing techniques pertinent to spectroscopy. These matrices also find applications in multisite Hadamard transform NMR spectroscopy.[1] We believe that these matrices would be potentially useful in stereochemistry. These matrices also find numerous other applications in disciplines such as computer science (error-correcting code), graph designs, tournaments, orthogonal arrays, projective planes, group theory, terminal networks, circuit theory, and coding theory.

A $n \times n$ Hadamard matrix, **H**, is defined as a square matrix composed of 1's and -1's such that

$$\mathbf{H}\mathbf{H}^{\mathrm{T}} = \mathbf{H}^{\mathrm{T}}\mathbf{H} = nI$$

where I is the $n \times n$ identity matrix and $\mathbf{H}^{\mathrm{T}}$ is the transpose of the Hadamard matrix **H**. Hadamard matrices are important because the rows of the **H**-matrix are orthogonal and they make the best balance designs.

Hadamard transform spectroscopy is a natural consequence of Hadamard matrices. In the spectroscopy of species exhibiting complex spectral components,[3] the total intensity of spectral components in a group can be measured instead of the intensity at each wavelength separately. The different wavelength components are multiplexes which leads to a more accurate determination of the spectra compared to the traditional method. The optimal multiplexing techniques are based on the Hadamard matrices. The advantage of the resulting Hadamard transform spectrum is that the mean square error per frequency component is reduced as much as the number of frequency components.

Construction of Hadamard matrices is a long-standing unsolved combinatorial problem.[9-14] The problem has been studied by several mathematicians over the years, and thus several theorems and techniques have been formulated for the construction of Hadamard matrices. In spite of such progress for certain special cases of Hadamard matrices, it is often difficult to construct all possible inequivalent $n \times n$ Hadamard matrices for large values of n. Exhaustive generation of Hadamard matrices of order $n \times n$ leads to 2^{n2} computations. For example, exhaustive generation of Hadamard matrices of order 100×100 would require generation of $2^{10\,000}$ possible 100×100 matrices and checking if the generated matrices are Hadamard. The latter procedure is a computationally intensive problem since such checkings involve matrix multiplications which are n^3 in order (100^3) for each such multiplication.

There are constructions in the mathematical literature which reduce the number of possibilities to a considerable extent for certain special classes of Hadamard matrices. For example, a procedure due to Williamson[20] reduces the number of possibilities from 2^{n2} to 2^{m2} or to a slightly smaller number where $m = 4n$. Even so, the number of possible matrices which need to be generated is roughly 4×2^{625} for all possible skew 100×100 matrices composed of 1's and -1's. The problem of classifying the generated matrices into equivalence classes is even a more difficult one because of the large number of operations that need to be performed to verify if two Hadamard matrices are equivalent or not.

The objective of this investigation is to consider computational strategies for the generation of equivalence classes of Hadamard matrices. While in a previous study[2] an efficient code in Fortran for *exhaustive* generation of Hadamard matrices was considered, no efforts were made to generate equivalence classes. This is because the computational steps required to classify the generated matrices into equivalence classes grow astronomically even for a small matrix. That is, the problem of determining if two Hadamard matrices are equivalent or not requires a factorial and exponential number of comparisons thereby making this problem computationally challenging and intriguing. For a few matrices such as 16×16 Hadamard matrices special techniques have been developed to show that there are five equivalence classes of 16×16 Hadamard matrices. In this study we show that the nodal vector can be a powerful tool for discriminating Hadamard matrices when used judiciously. We have applied this technique to generate equivalence classes of Hadamard matrices of orders 16×16 and 28×28. We also note that the Hadamard matrices have been used to characterize molecular orbitals.[22]

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Table 1. Number of Possible Exhaustive Solutions for skew-Hadamard Matrices up to Order 100[a]

$n = 4m$	decomposition	no. of solns found
12	$1^2 + 1^2 + 1^2 + 3^2$	1
20	$1^2 + 1^2 + 3^2 + 3^2$	3
28	$1^2 + 3^2 + 3^2 + 3^2$	15
28	$1^2 + 1^2 + 1^2 + 5^2$	6
36	$1^2 + 1^2 + 3^2 + 5^2$	3
44	$1^2 + 3^2 + 3^2 + 5^2$	30
52	$1^2 + 1^2 + 1^2 + 7^2$	28
52	$1^2 + 1^2 + 5^2 + 5^2$	62
60	$1^2 + 1^2 + 3^2 + 7^2$	28
60	$1^2 + 3^2 + 5^2 + 5^2$	32
68	$1^2 + 3^2 + 3^2 + 7^2$	40
76	$1^2 + 1^2 + 5^2 + 7^2$	45
76	$1^2 + 5^2 + 5^2 + 5^2$	114
84	$1^2 + 3^2 + 5^2 + 7^2$	42
84	$1^2 + 1^2 + 1^2 + 9^2$	62
92	$1^2 + 1^2 + 3^2 + 9^2$	66
100	$1^2 + 1^2 + 7^2 + 7^2$	0
100	$1^2 + 3^2 + 3^2 + 9^2$	66
100	$1^2 + 5^2 + 5^2 + 7^2$	>10

[a] These are maximum possible solutions treating mirror symmetry operation for the first row of A to produce equivalent solutions.

2. HADAMARD MATRICES AND THEIR EQUIVALENCES

We shall start with an illustration of Hadamard matrix. Consider the following 8 × 8 matrix which is Hadamard.

$$\mathbf{H}_8 = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & -1 & 1 & -1 & 1 & -1 \\ 1 & 1 & -1 & -1 & 1 & 1 & -1 & -1 \\ 1 & -1 & -1 & 1 & 1 & -1 & -1 & 1 \\ 1 & 1 & 1 & 1 & -1 & -1 & -1 & -1 \\ 1 & -1 & 1 & -1 & -1 & 1 & -1 & 1 \\ 1 & 1 & -1 & -1 & -1 & -1 & 1 & 1 \\ 1 & -1 & -1 & 1 & -1 & 1 & 1 & -1 \end{bmatrix}$$

A skew-Hadamard matrix $\mathbf{H}$ is defined as $\mathbf{H} = S + I$ where S is a skew-symmetric matrix composed of +1 and −1 such that

$$S_{ji} = -S_{ij} \quad i \neq j$$

An example of a skew-Hadamard matrix is shown below.

$$\mathbf{H}_4 = \begin{bmatrix} 1 & 1 & 1 & 1 \\ -1 & 1 & 1 & -1 \\ -1 & -1 & 1 & 1 \\ -1 & 1 & -1 & 1 \end{bmatrix}$$

Significant developments pertaining to basic theorems and techniques for Hadamard matrices can be found in the monographs of Wallis et al.,[13] Agaian,[11] and the book of Harwit and Sloane.[3] All Hadamard matrices must be of order $4n$, where n is a positive integer with the exception of 1 × 1 and 2 × 2 Hadamard matrices. The determinant of a Hadamard or skew-Hadamard $n \times n$ matrix can be seen to be $\sqrt{n^n}$.

Let us now consider several relations which define equivalence classes for Hadamard matrices. Two Hadamard matrices $\mathbf{H}_1$ and $\mathbf{H}_2$ are said to be **H**-equivalent if there exists monomial permutation matrices **P** and **Q** containing +1 or −1 (signed permutations) such that

Table 2. Five Inequivalent Hadamard Matrices of Order 16 × 16

Hall's Class I Matrix

1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
1	1	1	1	1	1	1	1	−1	−1	−1	−1	−1	−1	−1	−1
1	1	1	1	−1	−1	−1	−1	1	1	1	1	−1	−1	−1	−1
1	1	1	1	−1	−1	−1	−1	−1	−1	−1	−1	1	1	1	1
1	1	−1	−1	1	1	−1	−1	1	1	−1	−1	1	1	−1	−1
1	1	−1	−1	1	1	−1	−1	−1	−1	1	1	−1	−1	1	1
1	1	−1	−1	−1	−1	1	1	1	1	−1	−1	−1	−1	1	1
1	1	−1	−1	−1	−1	1	1	−1	−1	1	1	1	1	−1	−1
1	−1	1	−1	1	−1	1	−1	1	−1	1	−1	1	−1	1	−1
1	−1	1	−1	1	−1	1	−1	−1	1	−1	1	−1	1	−1	1
1	−1	1	−1	−1	1	−1	1	1	−1	1	−1	−1	1	−1	1
1	−1	1	−1	−1	1	−1	1	−1	1	−1	1	1	−1	1	−1
1	−1	−1	1	1	−1	−1	1	1	−1	−1	1	1	−1	−1	1
1	−1	−1	1	1	−1	−1	1	−1	1	1	−1	−1	1	1	−1
1	−1	−1	1	−1	1	1	−1	1	−1	−1	1	−1	1	1	−1
1	−1	−1	1	−1	1	1	−1	−1	1	1	−1	1	−1	−1	1

Hall's Class II Matrix

1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
1	1	1	1	1	1	1	1	−1	−1	−1	−1	−1	−1	−1	−1
1	1	1	1	−1	−1	−1	−1	1	1	1	1	−1	−1	−1	−1
1	1	1	1	−1	−1	−1	−1	−1	−1	−1	−1	1	1	1	1
1	1	−1	−1	1	1	−1	−1	1	1	−1	−1	1	1	−1	−1
1	1	−1	−1	1	1	−1	−1	−1	−1	1	1	−1	−1	1	1
1	1	−1	−1	−1	−1	1	1	1	1	−1	−1	−1	−1	1	1
1	1	−1	−1	−1	−1	1	1	−1	−1	1	1	1	1	−1	−1
1	−1	1	−1	1	−1	1	−1	1	−1	1	−1	1	−1	1	−1
1	−1	1	−1	1	−1	1	−1	−1	1	−1	1	−1	1	−1	1
1	−1	1	−1	−1	1	−1	1	1	−1	1	−1	−1	1	−1	1
1	−1	1	−1	−1	1	−1	1	−1	1	−1	1	1	−1	1	−1
1	−1	−1	1	1	−1	−1	1	1	−1	−1	1	−1	1	1	−1
1	−1	−1	1	1	−1	−1	1	−1	1	1	−1	1	−1	−1	1
1	−1	−1	1	−1	1	1	−1	1	−1	−1	1	1	−1	−1	1
1	−1	−1	1	−1	1	1	−1	−1	1	1	−1	−1	1	1	−1

Hall's Class III Matrix

1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
1	1	1	1	1	1	1	1	−1	−1	−1	−1	−1	−1	−1	−1
1	1	1	1	−1	−1	−1	−1	1	1	1	1	−1	−1	−1	−1
1	1	1	1	−1	−1	−1	−1	−1	−1	−1	−1	1	1	1	1
1	1	−1	−1	1	1	−1	−1	1	1	−1	−1	1	1	−1	−1
1	1	−1	−1	1	1	−1	−1	−1	−1	1	1	−1	−1	1	1
1	1	−1	−1	−1	−1	1	1	1	1	−1	−1	−1	−1	1	1
1	1	−1	−1	−1	−1	1	1	−1	−1	1	1	1	1	−1	−1
1	−1	1	−1	1	−1	1	−1	1	−1	1	−1	1	−1	1	−1
1	−1	1	−1	1	−1	1	−1	−1	1	−1	1	−1	1	−1	1
1	−1	1	−1	−1	1	−1	1	1	−1	−1	1	1	−1	−1	1
1	−1	1	−1	−1	1	−1	1	−1	1	1	−1	−1	1	1	−1
1	−1	−1	1	1	−1	−1	1	1	−1	−1	1	−1	1	1	−1
1	−1	−1	1	1	−1	−1	1	−1	1	1	−1	1	−1	−1	1
1	−1	−1	1	−1	1	1	−1	1	−1	1	−1	−1	1	−1	1
1	−1	−1	1	−1	1	1	−1	−1	1	−1	1	1	−1	1	−1

Hall's Class IV Matrix

1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
1	1	1	1	1	1	1	1	−1	−1	−1	−1	−1	−1	−1	−1
1	1	1	1	−1	−1	−1	−1	1	1	1	1	−1	−1	−1	−1
1	1	1	1	−1	−1	−1	−1	−1	−1	−1	−1	1	1	1	1
1	1	−1	−1	1	1	−1	−1	1	1	−1	−1	1	1	−1	−1
1	1	−1	−1	1	1	−1	−1	−1	−1	1	1	−1	−1	1	1
1	1	−1	−1	−1	−1	1	1	1	1	−1	−1	−1	−1	1	1
1	1	−1	−1	−1	−1	1	1	−1	−1	1	1	1	1	−1	−1
1	−1	1	−1	1	−1	1	−1	1	−1	1	−1	1	−1	1	−1
1	−1	1	−1	1	−1	−1	1	1	−1	−1	1	−1	1	−1	1
1	−1	1	−1	−1	1	1	−1	−1	1	−1	1	1	−1	−1	1
1	−1	1	−1	−1	1	−1	1	−1	1	1	−1	−1	1	1	−1
1	−1	−1	1	1	−1	1	−1	−1	1	−1	1	−1	1	1	−1
1	−1	−1	1	1	−1	−1	1	−1	1	1	−1	1	−1	−1	1
1	−1	−1	1	−1	1	1	−1	1	−1	1	−1	−1	1	−1	1
1	−1	−1	1	−1	1	−1	1	1	−1	−1	1	1	−1	1	−1

Hall's Class V Matrix

1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
1	1	1	1	1	1	1	1	−1	−1	−1	−1	−1	−1	−1	−1
1	1	1	1	−1	−1	−1	−1	1	1	1	1	−1	−1	−1	−1
1	1	1	1	−1	−1	−1	−1	−1	−1	−1	−1	1	1	1	1
1	1	−1	−1	1	1	−1	−1	1	1	−1	−1	1	1	−1	−1
1	1	−1	−1	1	1	−1	−1	−1	−1	1	1	−1	−1	1	1
1	1	−1	−1	−1	−1	1	1	1	−1	1	−1	1	−1	1	−1
1	1	−1	−1	−1	−1	1	1	−1	1	−1	1	−1	1	−1	1
1	−1	1	−1	1	−1	1	−1	1	1	−1	−1	−1	−1	1	1
1	−1	1	−1	1	−1	1	−1	−1	−1	1	1	1	1	−1	−1
1	−1	1	−1	−1	1	−1	1	1	−1	−1	1	−1	1	1	−1
1	−1	1	−1	−1	1	−1	1	−1	1	1	−1	1	−1	−1	1
1	−1	−1	1	1	−1	−1	1	1	−1	1	−1	−1	1	−1	1
1	−1	−1	1	1	−1	−1	1	−1	1	−1	1	1	−1	1	−1
1	−1	−1	1	−1	1	1	−1	1	−1	−1	1	1	−1	−1	1
1	−1	−1	1	−1	1	1	−1	−1	1	1	−1	−1	1	1	−1

$$\mathbf{H}_2 = \mathbf{P}\mathbf{H}_1\mathbf{Q}$$

The above equivalence means that two Hadamard matrices are equivalent if one can be obtained from the other by (1) a permutation of rows or columns or both, (2) by changing the sign of a row or column, or (3) a combination of operations in (1) and (2).

The second operation may not always be a physically feasible operation in some applications as this may produce a physically different configuration. This is the case with chirality and NMR spin functions. The sign change will lead to switching of R with S for a chiral center and these are not equivalent. Hence, some times it may be necessary to restrict the equivalence based only on permutation matrices containing +1 which will restrict the equivalence to operation (1). This would in general lead to more equivalence classes of Hadamard matrices.

There are several other types of equivalences discussed in the mathematical literature. Another equivalence relation is called the z-equivalence and is somewhat stronger than the **H**-equivalence considered above. Two Hadamard matrices are said to be integer-equivalent or z-equivalent if there exists integral matrices **P** and **Q** with determinant ± 1 such that

$$\mathbf{H}_2 = \mathbf{P}\mathbf{H}_1\mathbf{Q}$$

The z-equivalence is tantamount to a combination of the operations listed above:

(i) Reorder rows or columns.

(ii) Add an integer multiple of a row to another row or an integer multiple of a column to another.

(iii) Multiply a row with a minus sign or a column with a minus sign.

Evidently, z-equivalence implies **H**-equivalence. Two Hadamard matrices are said to be Seidel equivalent if the Hadamard matrix $\mathbf{H}_2$ can be obtained from $\mathbf{H}_1$ by a combination of the following operations.

(i) Interchange row i with row j and interchange column i with column j.

(ii) Multiply both row i and column i by -1.

We define two Hadamard matrices to be automorphic equivalent if

$$\mathbf{H}_1 = \mathbf{P}^{\mathrm{T}}\mathbf{H}_2\mathbf{P}$$

where **P** is a permutation matrix which includes the possibility of the permutation being a signed permutation. In this case

$$|\mathbf{H}_1 - \lambda I| = |\mathbf{H}_2 - \lambda I|$$

where the determinants are the characteristic polynomials of the two Hadamard matrices. The characteristic polynomials of Hadamard matrices[21] and the corresponding polynomials of graphs[15-18] have been considered before. Evidently the automorphism and seidel equivalences are weaker equivalences, while the z-equivalence is the strongest equivalence. That is under z-equivalence one would obtain the minimum number of equivalence classes, while under the seidel and automorphic equivalences more equivalence classes are generated.

Table 3. Generation of Nodal Pattern of the Binary-Fipped and Ordered Hall's Matrices as a Function of Iterations

Nodal Pattern of the Hadamard Matrix No. 1
iteration 1
0 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15
iteration 2
0 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15
convergence in nodal pattern reached

Nodal Pattern of the Hadamard Matrix No. 2
iteration 1
0 1 2 3 4 5 6 7 9 9 10 10 12 13 14 15
iteration 2
0 1 2 3 4 5 6 7 9 9 10 10 12 13 14 15
convergence in nodal pattern reached

Nodal Pattern of the Hadamard Matrix No. 3
iteration 1
0 1 2 3 4 5 6 7 9 10 10 11 11 12 14 15
iteration 2
0 1 2 3 4 5 6 7 9 10 10 11 11 12 14 15
convergence in nodal pattern reached

Nodal Pattern of the Hadamard Matrix No. 4
iteration 1
0 1 2 3 4 5 6 7 10 10 11 11 11 12 12 15
iteration 2
0 1 2 3 4 5 6 7 10 10 11 11 11 12 12 15
convergence in nodal pattern reached

Nodal Pattern of the Hadamard Matrix No. 5
iteration 1
0 1 2 3 6 7 9 9 9 10 10 10 10 11 11 12
iteration 2
0 1 2 3 6 7 9 9 9 10 10 10 10 11 11 12
convergence in nodal pattern reached

No. of Equivalence Classes of Nodal Patterns Is 5
class no. 1 contains solution 1
class no. 2 contains solution 2
class no. 3 contains solution 3
class no. 4 contains solution 4
class no. 5 contains solution 5

3. EXHAUSTIVE GENERATION OF HADAMARD MATRICES

The author[2] developed a computer code for the exhaustive generation of Hadamard matrices of any order using the Williamson-type construction[20] which is described below. This method generates skew-Hadamard matrices without any consideration of equivalences. Before we consider the generation of equivalence classes first we describe the Williamson construction of Hadamard matrices of certain order.

A procedure due to Williamson[20] generates a $4m \times 4m$ (m is an odd number) Hadamard matrix from circulant and back circulant matrices of order $m \times m$. This reduces the problem of constructing a $n \times n$ skew-Hadamard matrix to constructing four $m \times m$ matrices called **A**, **B**, **C**, and **D**, thereby reducing the number of combinatorial possibilities.

A matrix $\mathbf{A} = (a_{ij})$ of order m is said to be circulant if

$$a_{ij} = a_{1,j-i+1|m}$$

where $j - i + 1|_m$ stands for $j - \mathrm{i} + 1$ reduced modulo m.

Table 4. A 28 × 28 skew-Hadamard Matrix with a, b, c, d values of 1, 3, 3, 3[a]

1	1	0	1	0	1	0	1	1	0	1	1	0	1	1	1	1	0	0	1	1	1	1	1	0	0	1	1
0	1	1	0	1	0	1	1	0	1	1	0	1	1	1	1	0	0	1	1	1	1	1	0	0	1	1	1
1	0	1	1	0	1	0	0	1	1	0	1	1	1	1	0	0	1	1	1	1	1	0	0	1	1	1	1
0	1	0	1	1	0	1	1	1	0	1	1	1	0	0	0	1	1	1	1	1	0	0	1	1	1	1	1
1	0	1	0	1	1	0	1	0	1	1	1	0	1	0	1	1	1	1	1	0	0	1	1	1	1	1	0
0	1	0	1	0	1	1	0	1	1	1	0	1	1	1	1	1	1	1	0	0	1	1	1	1	1	0	0
1	0	1	0	1	0	1	1	1	1	0	1	1	0	1	1	1	1	0	0	1	1	1	1	1	0	0	1
0	0	1	0	0	1	0	1	1	0	1	0	1	0	1	1	1	0	0	1	1	0	0	0	1	1	0	0
0	1	0	0	1	0	0	0	1	1	0	1	0	1	1	1	0	0	1	1	1	0	0	1	1	0	0	0
1	0	0	1	0	0	0	1	0	1	1	0	1	0	1	0	0	1	1	1	1	0	1	1	0	0	0	0
0	0	1	0	0	0	1	0	1	0	1	1	0	1	0	0	1	1	1	1	1	1	1	0	0	0	0	0
0	1	0	0	0	1	0	1	0	1	0	1	1	0	0	1	1	1	1	1	0	1	0	0	0	0	0	1
1	0	0	0	1	0	0	0	1	0	1	0	1	1	1	1	1	1	1	0	0	0	0	0	0	0	1	1
0	0	0	1	0	0	1	1	0	1	0	1	0	1	1	1	1	1	0	0	1	0	0	0	0	1	1	0
0	0	0	1	1	0	0	0	0	0	1	1	0	0	1	1	0	1	0	1	0	1	1	0	1	1	0	1
0	0	1	1	0	0	0	0	0	1	1	0	0	0	0	1	1	0	1	0	1	1	0	1	1	0	1	1
0	1	1	0	0	0	0	0	1	1	0	0	0	0	1	0	1	1	0	1	0	0	1	1	0	1	1	1
1	1	0	0	0	0	0	1	1	0	0	0	0	0	0	1	0	1	1	0	1	1	1	0	1	1	1	0
1	0	0	0	0	0	1	1	0	0	0	0	0	1	1	0	1	0	1	1	0	1	0	1	1	1	0	1
0	0	0	0	0	1	1	0	0	0	0	0	1	1	0	1	0	1	0	1	1	0	1	1	1	0	1	1
0	0	0	0	1	1	0	0	0	0	0	1	1	0	1	0	1	0	1	0	1	1	1	1	0	1	1	0
0	0	0	1	1	0	0	1	1	1	0	0	1	1	0	0	1	0	0	1	0	1	1	0	1	0	1	0
0	0	1	1	0	0	0	1	1	0	0	1	1	1	0	1	0	0	1	0	0	0	1	1	0	1	0	1
0	1	1	0	0	0	0	1	0	0	1	1	1	1	1	0	0	1	0	0	0	1	0	1	1	0	1	0
1	1	0	0	0	0	0	0	0	1	1	1	1	1	0	0	1	0	0	0	1	0	1	0	1	1	0	1
1	0	0	0	0	0	1	0	1	1	1	1	1	0	0	1	0	0	0	1	0	1	0	1	0	1	1	0
0	0	0	0	0	1	1	1	1	1	1	1	0	0	1	0	0	0	1	0	0	0	1	0	1	0	1	1
0	0	0	0	1	1	0	1	1	1	1	0	0	1	0	0	0	1	0	0	1	1	0	1	0	1	0	1

[a] For simplicity all −1's are converted into 0. Thus all 0's must be interpreted as −1's in the above matrix.

Likewise, a matrix **B** of order m is said to be back circulant if

$$b_{ij} = b_{1,i+j-1|m}$$

Suppose that **A** is a circulant skew matrix containing +1 and −1 while **B**, **C**, and **D** are back-circulant matrices containing +1 and −1. Williamson's procedure produces a skew-Hadamard matrix from **A**, **B**, **C**, and **D** using the following construction:

$$\mathbf{H} = \begin{bmatrix} A & B & C & D \\ -B & A & D & -C \\ -C & -D & A & B \\ -D & C & -B & A \end{bmatrix}$$

Wallis et al.[13] have used the above technique to construct several Hadamard matrices. However, their procedure does not appear to be exhaustive while in the present study we develop algorithms and codes for exhaustive generation of these matrices. We accomplish this through bit-manipulation techniques but do not make any efforts to construct equivalence classes. All $n \times n$ Williamson-type matrices satisfy the equation

$$n = 4m = a^2 + b^2 + c^2 + d^2$$

where m is the order of the matrices **A**, **B**, **C**, and **D**, and a, b, c, and d are given by

$$a = \sum_{j=1}^{m} a_{1j}, \quad b = \sum_{j=1}^{m} b_{1j}, \quad c = \sum_{j=1}^{m} c_{1j}, \quad d = \sum_{j=1}^{m} d_{1j}$$

The matrices **A**, **B**, **C**, and **D** are determined once the first rows of the matrix **A**, **B**, **C**, and **D** are constructed since **A** is circulant while **B**, **C**, and **D** are back-circulant. The full skew-Hadamard matrix **H** is constructed as illustrated above.

We note that the first rows of **A**, **B**, **C**, and **D** also satisfy

$$a_{1,j} = -a_{1,m+2-j}, \quad b_{1,j} = b_{1,m+2-j}, \quad c_{1,j} = c_{1,m+2-j}, \quad d_{1,j} = d_{1,m+2-j}$$

$$a_{11} = b_{11} = c_{11} = d_{11} = 1$$

for $2 \le j \le m$

The above constraints reduce the maximum number of possibilities for each of the first rows of **A**, **B**, **C**, and **D** to $2^{(m-1)/2}$ so that the total number of solutions to be searched is $2^{2(m-1)}$.

To illustrate consider a skew-Hadamard of order 12. Since the number 12 can be expressed as $1^2 + 1^2 + 1^2 + 3^2$, the sum of the first row entries are 1, 1, 1, and 3, respectively, for **A**, **B**, **C**, and **D**. Using the above relations for the first rows of **A**, **B**, **C**, and **D**, it can be seen that a solution for the first rows of **A**, **B**, **C**, and **D** is

first row of A	1	1	−1
first row of B	1	−1	−1
first row of C	1	−1	−1
first row of D	1	1	1

The matrices **A**, **B**, **C**, and **D** are determined once the first rows of **A**, **B**, **C**, and **D** are known and subsequently the entire Hadamard matrix. The result of the above solution is a skew-$\mathbf{H}_{12}$ matrix.

The author[2] used the bit-manipulation algorithms for generation of skew-Hadamard matrices exhaustively. The first step in this algorithm is to find possible integers a, b, c, and d satisfying

$$4m = a^2 + b^2 + c^2 + d^2$$

where m is an odd number and $a, b, c, d \ge 1$ are integers. Subsequently, the first rows of the matrices **A**, **B**, **C**, and **D**

Table 5. Fifteen Possible 28 × 28 Hadamard Matrices with $28 = 1^2 + 3^2 + 3^2 + 3^2$ Decomposition Obtained from Exhaustive Generation Using the Willaimson Method[a]

first rows of A, B, C, D						
			Solution No. 1			
1	1	−1	1	−1	1	−1
1	1	−1	1	1	−1	1
1	1	1	−1	−1	1	1
1	1	1	−1	−1	1	1
			Solution No. 2			
1	1	−1	1	−1	1	−1
1	1	1	−1	−1	1	1
1	1	−1	1	1	−1	1
1	1	1	−1	−1	1	1
			Solution No. 3			
1	1	1	−1	1	−1	−1
1	−1	1	1	1	1	−1
1	1	−1	1	1	−1	1
1	1	1	−1	−1	1	1
			Solution No. 4			
1	1	1	−1	1	−1	−1
1	1	−1	1	1	−1	1
1	−1	1	1	1	1	−1
1	1	1	−1	−1	1	1
			Solution No. 5			
1	−1	1	1	−1	−1	1
1	−1	1	1	1	1	−1
1	−1	1	1	1	1	−1
1	1	1	−1	−1	1	1
			Solution No. 6			
1	1	−1	1	−1	1	−1
1	1	1	−1	−1	1	1
1	1	1	−1	−1	1	1
1	1	−1	1	1	−1	1
			Solution No. 7			
1	1	1	−1	1	−1	−1
1	−1	1	1	1	1	−1
1	1	1	−1	−1	1	1
1	1	−1	1	1	−1	1
			Solution No. 8			
1	1	1	1	−1	−1	−1
1	−1	1	1	1	1	−1
1	1	−1	1	1	−1	1
1	1	−1	1	1	−1	1
			Solution No. 9			
1	1	1	−1	1	−1	−1
1	1	1	−1	−1	1	1
1	−1	1	1	1	1	−1
1	1	−1	1	1	−1	1
			Solution No. 10			
1	1	1	1	−1	−1	−1
1	1	−1	1	1	−1	1
1	−1	1	1	1	1	−1
1	1	−1	1	1	−1	1
			Solution No. 11			
1	1	1	−1	1	−1	−1
1	1	−1	1	1	−1	1
1	1	1	−1	−1	1	1
1	−1	1	1	1	1	−1
			Solution No. 12			
1	−1	1	1	−1	−1	1
1	−1	1	1	1	1	−1
1	1	1	−1	−1	1	1
1	−1	1	1	1	1	−1
			Solution No. 13			
1	1	1	−1	1	−1	−1
1	1	1	−1	−1	1	1
1	1	−1	1	1	−1	1
1	−1	1	1	1	1	−1
			Solution No. 14			
1	1	1	1	−1	−1	−1
1	1	−1	1	1	−1	1
1	1	−1	1	1	−1	1
1	−1	1	1	1	1	−1
			Solution No. 15			
1	−1	1	1	−1	−1	1
1	1	1	−1	−1	1	1
1	−1	1	1	1	1	−1
1	−1	1	1	1	1	−1

[a] Only the first rows of A,B, C, & D matrices are shown.

were constructed exhaustively compatible with the above solutions for *a*, *b*, *c*, and *d*. Then skew matrices are constructed in a solution space of

$$\max_2 = m_a m_b m_c m_d$$

possible solutions where m_a, m_b, m_c, and m_d are those solutions which satisfy the row-sum constraint. Williamson's theorem is used on these $\max_2$ solutions which states that if

$$\mathbf{AA}^{\mathrm{T}} + \mathbf{BB}^{\mathrm{T}} + \mathbf{CC}^{\mathrm{T}} + \mathbf{DD}^{\mathrm{T}} = 4mI$$

where I_m is a $m \times m$ identity matrix then the matrix **H** is Hadamard.

Bit-manipulation techniques[2] were used for both the generation of possible matrices and to verify if the above result is valid for each of the generated solutions. A code in Fortran '77 was developed for this propose. The code generated exhaustively Hadamard matrices up to order 100 × 100. Larger Hadamard matrices could be generated but not exhaustively in that constraints on the solution space had to be placed. Table 1 shows the number of exhaustive solutions thus found for the various decompositions for Hadamard matrices up to order 100 × 100. The code was found to be reasonably efficient in that all matrices up to order 76 × 76 took only a few seconds for exhaustive generation. Exhaustive generation of 100 × 100 matrices took several hours of CPU time, since the total number of "matrix multiplications" performed using bit-manipulation algorithms is of the order of $7.793\,441\,57 \times 10^{11}$ [$2510 \times 792^2 \times 495$]. Exhaustive generation of 92 × 92 Hadamard matrices which required $3.606\,35 \times 10^{10}$ matrix multiplications required 5.5 h of CPU time on a IBM RS6000/560 model.

4. COMPUTATIONAL TECHNIQUES FOR EQUIVALENCE CLASSES

The generation of **H**-equivalence classes from all possible $n \times n$ Hadamard matrices requires

$$(n!)^2 n^2$$

matrix multiplications where first $(n!)^2$ operations is for the interchanges of rows or columns, while n^2 is the number of possible row or column sign changes. Even for a 20 × 20 Hadamard matrix this amounts to

$$(20!)^2 20^2 \sim 2.3676 \times 10^{39}$$

matrix multiplications. Brute-force computational techniques can consume enormous amounts of computer time. We shall consider a few promising computational techniques.

The nodes of molecular orbitals are known to be invariant characteristics of the MOs. That is, the number of nodes of a MO does not depend on the labeling of the atoms or the vertices of the graph associated with the MO. Furthermore, the energy characteristics of a MO depend on the number of nodes. In a preliminary study the relationship between the nodal pattern of the Hadamard matrices and molecular orbitals was considered.[22] This provides the motivation for the following computational technique to analyze Hadamard matrices and generate their equivalence classes.

Let the number of nodes in the *i*th row the Hadamard matrix be defined by the number of sign changes for the successive entries in that row. More precisely the number

Table 6. Nodal Vectors of 15 Solutions Corresponding to 28 × 28 Williamson Hadamard Matrices Before and After Binary Flips and Ordering

Hadamard Matrix for Solution 1
Nodal pattern before arranging the matrix
10 11 11 11 12 12 12 12 13 13 13 13 14 14 14 14 14 14 14 15 15 15 15 15 15 15 16 16
Nodal pattern after arranging the matrix
0 1 3 7 11 12 13 13 13 13 13 14 14 14 14 14 15 16 16 16 16 17 17 18 18 19 20 21

Hadamard Matrix for Solution 2
Nodal pattern before arranging the matrix
10 11 11 11 12 12 12 13 13 13 13 13 14 14 14 14 14 14 14 14 15 15 15 15 15 15 16 16
Nodal pattern after arranging the matrix
0 1 3 7 11 12 13 13 13 13 13 14 14 14 14 14 15 16 16 16 16 17 17 18 18 19 20 21

Hadamard Matrix for Solution 3
Nodal pattern before arranging the matrix
11 11 12 12 12 13 13 13 13 13 13 13 14 14 14 14 14 14 14 14 14 14 14 15 15 15 15 15
Nodal pattern after arranging the matrix
0 1 3 7 9 11 12 12 13 14 14 14 14 14 15 15 15 16 16 16 17 17 18 18 18 19 19 21

Hadamard Matrix for Solution 4
Nodal pattern before arranging the matrix
12 12 12 12 13 13 13 13 13 13 13 13 13 13 14 14 14 14 14 14 14 14 14 14 15 15 15 15
Nodal pattern after arranging the matrix
0 1 3 7 10 10 11 12 13 13 14 14 14 14 15 15 15 16 16 17 17 17 18 18 19 19 20 20

Hadamard Matrix for Solution 5
Nodal pattern before arranging the matrix
11 11 12 12 12 12 13 13 13 13 13 13 13 13 14 14 14 14 14 14 14 14 15 15 15 15 16 16
Nodal pattern after arranging the matrix
0 1 3 7 9 11 12 13 14 14 14 14 15 15 15 15 15 16 16 16 17 17 17 18 18 18 18 20

Hadamard Matrix for Solution 6
Nodal pattern before arranging the matrix
10 11 11 11 12 12 12 13 13 13 13 13 14 14 14 14 14 14 14 14 15 15 15 15 15 15 16 16
Nodal pattern after arranging the matrix
0 1 3 7 11 12 12 12 13 13 13 14 14 14 15 15 15 16 16 16 16 17 17 18 18 19 19 22

Hadamard Matrix for Solution 7
Nodal pattern before arranging the matrix
12 12 12 13 13 13 13 13 13 13 13 13 13 13 14 14 14 14 14 14 14 14 14 14 14 15 15 15
Nodal pattern after arranging the matrix
0 1 3 7 10 10 11 12 13 13 14 14 14 14 15 15 15 16 16 17 17 17 18 18 19 19 20 20

Hadamard Matrix for Solution 8
Nodal pattern before arranging the matrix
11 11 12 12 12 13 13 13 13 13 13 13 13 13 14 14 14 14 14 14 14 14 14 14 15 15 16 17
Nodal pattern after arranging the matrix
0 1 3 7 8 11 11 13 14 14 14 15 15 15 15 15 16 16 16 16 16 17 17 18 18 18 19 20

Hadamard Matrix for Solution 9
Nodal pattern before arranging the matrix
11 11 11 11 12 12 12 13 13 13 14 14 14 14 14 14 14 14 14 14 14 15 15 15 15 15 15 15
Nodal pattern after arranging the matrix
0 1 3 7 9 11 12 12 13 14 14 14 14 14 15 15 15 16 16 16 17 17 18 18 18 19 19 21

Hadamard Matrix for Solution 10
Nodal pattern before arranging the matrix
11 11 11 11 12 12 12 12 12 13 13 13 14 14 14 14 14 14 14 14 15 15 15 15 15 15 16 17
Nodal pattern after arranging the matrix
0 1 3 7 8 11 11 12 13 14 14 15 15 15 16 16 16 16 16 16 17 17 17 17 18 18 19 20

Hadamard Matrix for Solution 11
Nodal pattern before arranging the matrix
11 11 12 12 12 12 13 13 13 13 13 13 14 14 14 14 14 14 14 14 14 14 15 15 15 15 15 15
Nodal pattern after arranging the matrix
0 1 3 7 9 11 12 12 13 14 14 14 14 14 15 15 15 16 16 16 17 17 18 18 18 19 19 21

Hadamard Matrix for Solution 12
Nodal pattern before arranging the matrix
12 12 12 12 12 12 13 13 13 13 13 13 13 13 13 13 14 14 14 14 14 14 15 15 15 15 16 16
Nodal pattern after arranging the matrix
0 1 3 7 9 11 12 13 14 14 14 14 15 15 15 15 15 16 16 16 17 17 17 18 18 18 18 20

Hadamard Matrix for Solution 13
Nodal pattern before arranging the matrix
12 12 12 12 12 12 12 13 13 13 13 13 13 13 14 14 14 14 14 14 14 15 15 15 15 15 15 15
Nodal pattern after arranging the matrix
0 1 3 7 10 10 11 12 13 13 14 14 14 14 15 15 15 16 16 17 17 17 18 18 19 19 20 20

Hadamard Matrix for Solution 14
Nodal pattern before arranging the matrix
12 12 12 12 12 12 12 13 13 13 13 13 13 13 13 13 14 14 14 14 14 14 15 15 15 15 16 17
Nodal pattern after arranging the matrix
0 1 3 7 8 11 11 13 14 14 14 15 15 15 15 15 16 16 16 16 16 17 17 18 18 18 19 20

Hadamard Matrix for Solution 15
Nodal pattern before arranging the matrix
12 12 12 12 12 13 13 13 13 13 13 13 13 13 13 13 14 14 14 14 14 14 14 15 15 15 16 16
Nodal pattern after arranging the matrix
0 1 3 7 9 11 12 13 14 14 14 14 15 15 15 15 15 16 16 16 17 17 17 18 18 18 18 20

Table 7. Equivalences of Hadamard Matrices of Order 28 × 28 as Characterized by Their Nodal Patterns

class no.	solutions
1	1 2
2	3 9 11
3	4 7 13
4	5 12 15
5	6
6	8 14
7	10

[a] No. of equivalence classes of nodal patterns is 7.

of nodes of the ith row of the Hadamard matrix is defined as

$$n_i = \sum_{j=1}^{n-1} \mathrm{sign}(\mathbf{H}_{ij}\mathbf{H}_{i,j+1})$$

where the sign function is defined as

$$\begin{aligned}\mathrm{sign}(\mathbf{H}_{i,j}\mathbf{H}_{i,j+1}) &= 1 \text{ if } \mathbf{H}_{ij}\mathbf{H}_{i,j+1} < 0 \\ &= 0 \text{ if } \mathbf{H}_{ij}\mathbf{H}_{i,j+1} > 0\end{aligned}$$

That is, the sign function keeps track of the number of times the sign changes occur in proceeding successively from the first column to the last column of the *i*th row of the Hadamard matrix.

In the case of Hadamard matrices, columns also represent the orthogonal vectors and thus the nodal patterns for column vectors could be defined as

$$n_j^{\mathrm{T}} = \sum_{i=1}^{n-1} \mathrm{sign}(\mathbf{H}_{ij}\mathbf{H}_{i+1,j})$$

where the sign function has the same meaning as above.

The nodal (row) vector for a Hadamard matrix can be brought to an ordered form (n_1, n_2, . . . n_m) such that $n_m \geq n_{m-1} \geq \ldots n_1 = 0$. For any Hadamard matrix it is always possible to bring it to a form called the normalized matrix in which the first row and first column contain only +1's. Thus the n_1 components of both row and column nodal vectors can be made to zeros.

The nodal vectors of two inequivalent Hadamard matrices must be different, but the converse is not true as we show here. The problem is that the row nodal vectors change if the columns of the Hadamard matrices are permuted. The row nodal vector is invariant to interchange of rows and multiplying any row by −1. However, multiplying a column by −1 and permuting the columns could change the row nodal vector and vice versa. For smaller Hadamard matrices, it is possible to bring the matrix into a standard representation such that the first row contains no nodes, the second row contains one node, the third row contains two nodes, etc. Beyond the third row it may not always be possible to bring it in this form for all Hadamard matrices.

The nodal vector pattern and ordering can be illustrated with five equivalence classes of 16 × 16 Hadamard matrices shown in Table 2. These are called Hall's class of Hadamard matrices, and there are exactly five H-equivalence classes of 16 × 16 Hadamard matrices. The matrices shown in Table 2 are ordered not only with respect to first row but also other rows in that the binary numbers obtained by changing −1 to 0 in rows and columns are ordered. The corresponding row nodal vectors are shown in Table 3.

A computational algorithm based on the nodal vector generation and ordering of the Hadamard matrix can be utilized to generate the nodal vector patterns which can be compared for the classification of the generated Hadamard matrices into equivalence classes. The procedure is rigorous if the Hadamard matrix can be brought into a completely ordered form with respect to both rows and columns. In practice this is hard to accomplish for large Hadamard matrices especially in determining if two large Hadamard matrices are H-equivalent or not. Note that Z-equivalence is even more difficult but automorphic-equivalence is easier to ascertain.

Let us consider a 28 × 28 Hadamard matrix generated using Williamson's technique. The **A**, **B**, **C**, and **D** matrices which correspond to one of the solutions for $1^2 + 3^2 + 3^2 + 3^2$ were generated. The entire matrix is shown in Table 4. This solution was obtained using our exhaustive Hadamard matrix generation. There are 14 other such solutions. Table 5 shows all 15 generated solutions in compact form in terms of the first rows of **A**, **B**, **C**, and **D**. It was not determined how many of these solutions are equivalent.[2]

Our algorithm first maps all −1 entries into 0. Then each row of the Hadamard matrix is treated as a binary number. The entries in columns of a given row are packed, and a packed REAL*8 label is generated. The REAL*8 representation is adequate for up to 64 × 64 matrix, but for larger matrices we employ arrays of REAL*8 words. That is each row is split into several REAL*8 words. In order to take into consideration the negation operation (that is, multiplying any row by −1) we first invoke the binary flipping technique. This technique would change each bit to its complement. For example, a word with

n	$n-1$	...	6	5	4	3	2	1
0	1	...	0	1	0	1	0	1

will be changed to

n	$n-1$		6	5	4	3	2	1
1	0	...	1	0	1	0	1	0

Note that for a $n \times n$ Hadamard matrix bits $n + 1$ to the left most bit are cleared to zero in the representation. First the original binary row and the flipped binary row are compared. If the flipped binary row generates a larger packed label, then the flipped label is used in the representation compared to the original representation. The binary flipping technique thus accounts for multiplying a row by −1.

The next step in our algorithm is to arrange the packed row labels in a descending order. This brings the rows of the Hadamard matrix into an ordered and flipped form. Note that this corresponds to interchange of rows, multiplying the rows by −1, or a combination of both.

The binary flipping followed by ordering technique is now applied to the columns of the Hadamard matrix. The columns are ordered subsequent to row ordering and flipping. The row nodal vector is computed following the ordering and flipping technique.

It is important to recognize that the row nodal vector changes when the columns of the Hadamard matrix are

Table 8. Row Nodal Vector Patterns as a Function of Iteration for the Hadamard Matrix in Table 4

Nodal Vectors of the Hadamard Matrix for Solution 1
iteration no. 1
0 1 3 7 11 12 13 13 13 13 13 14 14 14 14 14 15 16 16 16 16 17 17 18 18 19 20 21
iteration no. 2
0 1 3 7 11 12 12 12 12 13 13 14 14 14 14 15 15 15 16 16 17 18 18 19 19 19 19 20
iteration no. 3
0 1 3 7 10 10 12 12 13 13 14 14 15 15 15 15 15 16 16 17 17 17 18 18 18 18 19 20
iteration number 4
0 1 3 7 10 10 12 13 13 13 13 14 15 15 15 15 16 16 16 16 17 17 17 18 18 18 20 20
iteration number 5
0 1 3 7 12 13 13 13 14 14 14 14 15 15 15 15 15 16 16 16 16 16 17 17 17 18 18 18
iteration number 6
0 1 3 7 11 12 13 13 14 14 14 14 14 14 15 15 15 15 15 16 16 17 17 18 18 18 19 20
iteration number 7
0 1 3 7 11 12 13 14 14 14 14 14 14 15 15 15 16 16 16 16 16 16 17 17 17 17 17 21
iteration number 8
0 1 3 7 11 11 12 13 13 13 14 14 14 14 15 15 15 16 16 16 17 17 17 18 18 18 20 20
iteration number 9
0 1 3 7 10 11 12 12 12 13 13 13 13 14 14 14 15 16 17 17 17 18 18 18 19 20 20 21
iteration number 10
0 1 3 7 11 12 13 13 14 14 14 14 14 15 15 15 15 16 16 16 16 17 17 17 18 18 18 19

interchanged and flipped. Let us illustrate this in Table 6. Consider first the row nodal vector of the unordered raw matrix corresponding to the first solution in Table 5. The entire matrix for this solution is given in Table 4. The row nodal vector is (10, 11, 11, 11, 12, 12, 12, 12, 13, 13, 13, 13, 14, 14, 14, 14, 14, 14, 14, 15, 15, 15, 15, 15, 15, 15, 16, 16) such that the nodes themselves are arranged in an ascending order. The nodal pattern of the normalized and ordered Hadamard matrix obtained by binary flip followed by arrange techniques for both rows and columns once is (0, 1, 3, 7, 11, 12, 13, 13, 13, 13, 13, 14, 14, 14, 14, 14, 15, 16, 16, 16, 16, 17, 17, 18, 18, 19, 20, 21). This nodal pattern is substantially different from the nodal pattern of the row solution. Yet both Hadamard matrices are H-equivalent because one is generated from the other by binary flip and arrangement of both rows and columns and is thus H-equivalent to the matrix that we started with. This example clearly demonstrates that the nodal vectors of two H-equivalent Hadamard matrices can be different providing a proof for the theorem below.

Theorem: The row (column) nodal vectors of two H-equivalent Hadamard matrices need not be the same.

This is precisely why classification of Hadamard matrices is a very difficult problem. While the nodal patterns of two inequivalent Hadamard matrices must be different as exemplified by Hall's five equivalence classes of Hadamard matrices, the converse is evidently false.

As seen from Table 6, the nodal patterns of binary-flipped and ordered 15 28×28 Hadamard matrices generated by the Williamson construction can be compared. Although, the nodal patterns of raw Hadamard matrices of the first and second solutions are different, the row nodal vectors of binary-flipped and ordered Hadamard matrices is identical for both solutions to (0, 1, 3, 7, 11, 12, 13, 13, 13, 13, 13, 14, 14, 14, 14, 14, 15, 16, 16, 16, 16, 17, 17, 18, 18, 19, 20, 21). We believe that this is an exciting and encouraging finding. That is the Hadamard matrix corresponding to solutions 2 and 1 has been brought into the same representation through a series of judicious operations but without performing brute-force $(28!)^2 28^2$ permutational and binary-flip operations. Perhaps it is the first time an elegant procedure such as the nodal vector pattern combined with binary flips and ordering has shown that two 28×28 Hadamard matrices are H-equivalent.

The technique can be repeated for all 15 exhaustively generated solutions to classify the solutions into equivalence classes. The results are shown in Table 7. As seen from Table 7, the nodal pattern analysis of the ordered and binary-flipped 15 solutions of Hadamard matrices are classified into seven equivalence classes on the basis of the nodal vector pattern. Evidently, it is proven through this computational technique that the number of H-equivalent classes for 28×28 Hadamard matrices obtained from *Williamson construction* must be less than or equal to 7. The number obtained is an upperbound because it is conceivable that with respect to another binary flip-ordering the nodal vectors could become the same. However, the process was iterated some 1500 times computationally and yet the equivalence class pattern obtained in Table 6 did not change.

The nodal vector patterns obtained through repeating the same sequence of steps that is (1) row binary flip + row arrange and (2) column binary flip + arrange are not identical. This can be illustrated in Table 8 for 10 iterations for the first solution. The sequence should converge at some point in that the nodal vectors generated in subsequent iterations should be identical. However, let us recall that in general there are

$$(n!)^2 \times n^2$$

such operations. One could thus use up enormous amounts of computer time before exhaustive searches for equivalences are made.

In the event $b = c$ or $c = d$ in Williamson's construction, it was perceived by the author[2] that interchange of the matrix **B** with **C** if $b = c$ or **C** with **D** if $c = d$ could lead to equivalent solution. Let us examine this. The original matrix **H** can be written as

$$\mathbf{H} = \begin{bmatrix} \mathrm{A} & \mathrm{B} & \mathrm{C} & \mathrm{D} \\ -\mathrm{B} & \mathrm{A} & \mathrm{D} & -\mathrm{C} \\ -\mathrm{C} & -\mathrm{D} & \mathrm{A} & \mathrm{B} \\ -\mathrm{D} & \mathrm{C} & -\mathrm{B} & \mathrm{A} \end{bmatrix}$$

For example, interchange of **B** and **C** results in

$$\mathbf{H}' = \begin{bmatrix} A & C & B & D \\ -C & A & D & -B \\ -B & -D & A & C \\ -D & B & -C & A \end{bmatrix}$$

Interchanging rows or columns of the above matrix in blocks or multiplying any row or column by -1 produces $\mathbf{H}''$ shown below.

$$\mathbf{H}'' = \begin{bmatrix} A & B & +C & D \\ -B & A & -D & C \\ -C & D & A & -B \\ -D & C & B & A \end{bmatrix}$$

It can be seen that $\mathbf{H}''$ and $\mathbf{H}'$ are not the same in general. Consequently in general the proposal that interchange of **B** and **C** (if $b = c$) or **C** and **D** (if $c = d$) would lead to equivalent solutions is false.

5. CONCLUSION

In general the problem of classifying a set of exhaustive solutions obtained by Williamson's construction into equivalence classes is an unsolved problem. In this study we took up 15 possible 28×28 Hadamard matrices and developed efficient algorithms based on the nodal vector patterns to show that among the 15 solutions there are seven equivalence classes from the standpoint of nodal vectors. It was thus shown that there could be at most seven H-equivalence classes of 28×28 Hadamard matrices with the $1^2 + 3^2 + 3^2 + 3^2$ decomposition constructed using the Williamson theorem.

The general question of how many H-equivalence classes exist for Hadamard matrices and whether H-equivalences among the Hadamard matrices produced by the Williamson construction necessarily imply H-equivalences of all $n \times n$ Hadamard matrices remains unsolved. We have shown that the nodal vector patterns provide one promising avenue for further studies. However, we caution that the row nodal vector patterns are not invariant to binary-flips and permutations of columns. That is, we produced two H-equivalent Hadamard matrices related by these operations whose nodal vector patterns are different. If all $n \times n$ Hadamard matrices can be brought to a form that is perfectly row-ordered, column-ordered, and binary-flip-ordered, perhaps the nodal vector analysis could prove to be the ultimate solution to a long-standing unsolved problem. It is hoped that the current study would stimulate such studies.

We also point out in conclusion that the question of automorphic-equivalence of Hadamard matrices can be more easily handled based on the characteristic polynomials. However, this is going to be dependent on the technique used for constructing Hadamard matrices. Among the several combinatorial problems considered in the context of chemistry, in my opinion, Hadamard matrix generation and classification seems to be one of the most challenging unsolved problems.

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