Hadamard Matrices, Quaternions, and the Pearson Chi-square Statistic

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Abstract

We present a symbolic decomposition of the Pearson chi-square statistic with unequal cell probabilities, by presenting Hadamard-type matrices whose columns are eigenvectors of the variance-covariance matrix of the cell counts. All of the eigenvectors have non-zero values so each component test uses all cell probabilities in a way that makes it intuitively interpretable.

When all cell probabilities are distinct and unrelated we establish that such decomposition is only possible when the number of multinomial cells is a small power of 2. For higher powers of 2, we show, using the theory of orthogonal designs, that the targeted decomposition is possible when appropriate relations are imposed on the cell probabilities, the simplest of which is when the probabilities are equal and the decomposition is reduced to the one obtained by Hadamard matrices. Simulations are given to illustrate the sensitivity of various components to changes in location, scale skewness and tail probability, as well as to illustrate the potential improvement in power when the cell probabilities are changed.

1 Introduction

Consider an i.i.d. sequence of random variables $\xi_0, \xi_1, \ldots, \xi_n$ of trials taking values in the set $1, \ldots, m$ with respective probabilities $p_1, \ldots, p_m$. These values can be the result of binning continuous random variables into $m$ multinomial cells. Let $k \geq 2$ be an integer and consider the sequence of dependent random vectors $\{X_i = (\xi_i, \ldots, \xi_{i+k-1})\}$ for $i = 0, \ldots, n$, where the index $i$ is taken modulo $n$, i.e. the sequence is wrapped around. Based on this overlapping sequence of dependent and identically distributed random vectors, a naive chi-square statistic can be formed as

$$V_k = \sum [C(\alpha) - nP(\alpha)]^2 /nP(\alpha),$$

where the sum is taken over all patterns $\alpha$ of size $k$ and $C(\alpha)$ is the frequency of $\alpha$ in the sequence $X_i$ while $P(\alpha)$ designates the probability of $\alpha$. $V_k$ mimics the Pearson chi-square statistic, but due to overlapping, it is obviously not asymptotically distributed as a chi-square random variable. I. J. Good [6] introduces the difference statistic $\nabla V_k = V_k - V_{k-1}$ and shows that it has an asymptotic chi-square distribution with $m^k - m^{k-1}$ degrees of freedom, when each component in the multinomial probability vector is equally $1/m$. Indeed, Good [6] also shows that $\nabla^2 V_k = \nabla V_k - \nabla V_{k-1}$ has a chi-square distribution. Marsaglia proposes $\nabla V_k$ as a test of uniformity for pseudo-random number sequences capable of detecting potential local correlations.

The idea of drawing information from the sequence $\{X_i\}$ is also exploited in the concept of approximate entropy, ApEn, introduced by Pincus [15]. ApEn has also been used as
a test of randomness as well as to quantify irregularity in medical time series in order to predict disorder in patients, see [16].

To thoroughly understand the difference statistic $\nabla V_k$ (and its relationship to approximate entropy), Alhakim [1] analyzes the asymptotic covariance matrix $B_k$ of the simple Markov chain $\{X_i\}$, obtaining the eigenvalues and a complete set of orthogonal eigenvectors for the equally likely multinomial probabilities. This spectral decomposition gives much insight about the information obtained by increasing the word size from $k-1$ to $k$. As an example, the kernel of $B_k$ is shown to have dimension $m^{k-1}$, which explains the degrees of freedom of the difference statistic. Also, each eigenvector is seen to provide a component test statistic of $\nabla V_k$ which is asymptotically chi-squared distributed with exactly one degree of freedom, thus obtaining a partitioning of $\nabla V_k$ into component tests that are asymptotically independent. More interestingly, the analysis in Alhakim [1] revealed exact relationships between component tests corresponding to word sizes $k$ and $k-1$. Following the diagram below with $k=4$, a component test corresponding to an eigenvector $v_4$ of $B_4$ with eigenvalue $\lambda = 4$ is deterministically the same as an component test with an appropriate eigenvector $v_3$ of $\lambda = 3$ of $B_3$, where $v_4$ can be obtained recursively from $v_3$. Inductively, this means that all components for $k = 4$ and $\lambda = 4$ correspond to components of $k = 1$ and $\lambda = 1$. Similarly, all components for $k = 4$ and $\lambda = 3$ correspond to components of $k = 2$ and $\lambda = 1$, etc. Two important implications are that

(a) The most significant components are those of the simple non-overlapping case of $k = 1$ which provide the components of the regular Pearson statistic. So it is not useful to use a test with $k = 2$ if the original test with $k = 1$ is failed.

(b) The only new information that one obtains when the word size is increased by one is within the eigenvectors corresponding to the lowest eigenvalue 1.

\[
\begin{array}{cccc}
  k = 1 & & 1 \\
  k = 2 & 1 & 2 \\
  k = 3 & 1 & 2 & 3 \\
  k = 4 & 1 & 2 & 3 & 4 \\
\end{array}
\]

We add to the previous points the fact that, for any $k$, orthogonal eigenvectors of $\lambda = 1$ can also be obtained recursively from orthogonal eigenvectors of $\lambda = 1$ with word size $k = 1$. It is worth mentioning that Alhakim et. al [2] generalizes the above results to sequences of random variables $\xi_i$ that follow any distribution (possibly continuous), including non-equally likely multinomial probability. Complete spectral analysis is also obtained with similar relations between eigenvectors. The above discussion thus suggests that a good set of orthogonal eigenvectors that partition the regular Pearson statistic is an essential requirement to get a complete and meaningful partitioning for higher $k$, both in the case of equally likely and general non-equally likely multinomial vectors. This is the main motivation and objective of the current paper.

The paper is organized as follows. We begin by introducing the classical partition problem in Section 2 then we establish the special case of equally likely cell probabilities using the non-constant columns of Hadamard matrices in Section 3. Section 4 deals with the
non-equally likely case. Section 5 introduces an orthogonal matrix that serves the purpose of Hadamard matrix for non-equilikely multinomial probability vectors. In Section 6 we construct some component vectors and perform power simulation illustrating the validity and utility of these components. Section 7 explains the limitations of the method and shows how to overcome these limitations by adding some restrictions on the cell probabilities. The last section is an appendix that includes some technical proof.

2 The Classical Partition Problem

The problem of decomposing the Pearson chi-square statistic into component tests that are asymptotically independent is a rather old problem. In fact, Pearson himself addressed this problem in his Editorial in 1917, see Lancaster [11], as an answer to the objection that $X^2$ is an omnibus, overall test. The importance of the decomposition is that each of the components provides a test of some particular aspect of the null distribution. However, the interpretation of these component tests depends largely on the choice of orthogonal scheme.

Several authors have worked on this problem. Lancaster [11] presents a general technique of getting various components based on different orthogonal polynomial schemes. Irwin [7] decomposes $X^2$ into independent components using Helmert matrices.

More recently, Anderson [3] presents an ad hoc decomposition based on 8-dimensional vectors, whose orthogonality guarantees the asymptotic independence. He proposes that his vectors provide component tests that can be used and interpreted individually as tests for location, symmetry, skewness and kurtosis. Therefore, when the chi-square test fails, the individual components provide information about what aspects of the null distribution leads to rejection. Furthermore, unlike the columns of a Helmert matrix (and all other decomposition matrices), the entries in Anderson’s vectors all have nonzero values, resulting in component tests that each use count statistics of all multinomial cells; a property that should improve the power of these components.

Boero et al [4] notices that these vectors are obtained from the nonconstant rows of a Hadamard matrix. They then show how to use a Hadamard matrix, when the number of multinomial classes, $k$, is a power of 2, to obtain a full set of $k-1$ asymptotically independent components that include those of Anderson. Indeed, Boero et al [4] establishes the result for the equiprobable case and proves that those components are not asymptotically independent in the non-equiprobable case, thus disputing a claim by Anderson about the generality of his component tests. They also show that, when 8 cells are used, three of the four vectors that relate to location, skewness and kurtosis–as described by Anderson–are in fact 4-dimensional rather than 8-dimensional. That is, the same information can be provided by partitioning the support into 4 cells rather than 8. Then more vectors with new information come up as we increase the number of cells (and therefore the dimension) to the next power of 2.

This paper obtains a decomposition in the general case of non-equiprobable cells with the constraint that each component uses all cell counts, as in the Hadamard decomposition. This is desirable because, in regard to higher tests described in the introduction, using orthogonal vectors with many zeros would yield scarce vectors of higher order, which in turn give higher order component tests that use very few counts and are extremely hard to interpret.
Interestingly, it is shown that, when no two cell probabilities are assumed to be a priori related (i.e. taken as different indeterminate variables), this approach is only possible when the number of cells is 4, 8 or the trivial case of 2. This is due to reasons that pertain to limitations on the possible dimension of division algebras over the field of real numbers. For cell counts that are a higher power of 2, the situation is remedied by using the theory of orthogonal designs. Indeed, this theory explains why the cases 2, 4, and 8 are constructible without further assumptions, and also provides constructions for higher powers by imposing relations between cell probabilities. To the best of the author’s knowledge, orthogonal designs have not been used in the chi-square partitioning problem. We will discuss this construction and also show, via simulation that the power of various components can be drastically improved by varying the cell probabilities.

3 The Equiprobable Case

The classical goodness-of-fit chi-square test statistic of Pearson is performed by dividing the range of a variable into \( k \) bins that are mutually exclusive classes, thus making a multinomial model with respective cell probability vector, say, \( \mathbf{p} = (p_1, \ldots, p_k) \), calculated based on the hypothesized null distribution. For simplicity of presentation here, we will assume that the null distribution is completely specified, so that the above cell probabilities are known exactly and do not need to be estimated.

We will denote the transpose of a matrix \( \mathbf{A} \) by \( \mathbf{A}' \) and a diagonal matrix by \( \mathbf{D}(\mathbf{c}) \), where \( \mathbf{c} = (c_1, \ldots, c_k)' \) and \( D_{ii} = c_i \). Likewise, \( D^{1/2}(\mathbf{c}) \) denotes a diagonal matrix with diagonal entries given by \( \sqrt{c_i} \) and \( D^{-1/2}(\mathbf{c}) \) is its inverse when all \( c_i \)'s are distinct from zero.

For a sample of size \( n \), the test works by comparing the observed cell frequency vector \( \mathbf{m} = (m_1, \ldots, m_k) \) to the expected vector \( \mu = np \) via the test statistic \( X^2 = \sum_{i=1}^{k} \frac{(m_i - np_i)^2}{np_i} \) which has an asymptotic chi-square distribution with \( k - 1 \) degrees of freedom. This asymptotic distribution is based on the multivariate central limit theorem that states that the multinomial vector has an approximate multi-normal distribution with mean \( np \) and variance-covariance matrix with diagonal entries \( np_i(1 - p_i) \) and off-diagonal entries \( \Sigma_{ij} = -np_ip_j \). Thus the normalized vector

\[
\mathbf{x} = \frac{\mathbf{m} - \mu}{\sqrt{n}} = \sqrt{n}(\hat{\mathbf{p}} - \mathbf{p})
\]

has an asymptotic multinormal distribution \( \mathcal{N}(\mathbf{0}, \Sigma) \), where \( \Sigma = \text{diag}(\sigma_{ij}), \sigma_{ii} = p_i(1 - p_i) \) and \( \sigma_{ij} = -p_ip_j \) for \( i \neq j \), and \( \hat{p} \) is the vector of relative frequencies. It is, of course, well-known that \( \Sigma \) is singular with rank \( k - 1 \).

We note that \( \Sigma \) can be represented as \( (\mathbf{D}(\mathbf{p}) - \mathbf{pp}') \). In the equiprobable case, \( i.e., \) when \( p_i = 1/k \) for all \( i = 1, \ldots, k \), \( \Sigma \) reduces to the form \( \frac{1}{k}(\mathbf{I}_k - \mathbf{1}\mathbf{1}'/k) \), where \( \mathbf{I}_k \) is the \( k \times k \) identity matrix and \( \mathbf{1} \) is a \( k \times 1 \) vector of ones.

Since \( \Sigma \) is positive semi-definite, it can be diagonalized. If the eigenvalues are \( \lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_k \), we can write

\[
\Sigma = \Gamma'\Lambda\Gamma, \quad (3.1)
\]
where $\Lambda = D (\lambda_1, \cdots, \lambda_k)'$ and $\Gamma$ is the matrix whose rows are orthonormal eigenvectors of $\Sigma$ corresponding respectively to the ordered eigenvalues.

Although $\Sigma$ is diagonalizable, the presence of a zero eigenvalue makes it rank deficient. In this case, one would typically calculate any generalized inverse $\Sigma^{-}$ of $\Sigma$ and thus use as test statistic the quadratic form $(\sqrt{n}(\hat{p} - p)')\Sigma^{-}(\sqrt{n}(\hat{p} - p))$ which is asymptotically distributed as $\chi^2_{k-1}$.

Tanabe and Saga [17] provides a treatise on the symbolic Cholesky decomposition of $\Sigma$ and a formula for its generalized inverse. Watson [18] gives sharp inequalities for the eigenvalues in terms of the cell probabilities as well as exact and efficient formulae for calculating the eigenvectors, which also lead to a formula for the generalized inverse, under general conditions on the $p_i$s.

In the equiprobable case, Boero et al [4] use the fact that $(I_k - 11'k)$ is an idempotent matrix (and hence is a weak inverse of itself) to represent the Pearson statistic as

$$X^2 = (\sqrt{n}(\hat{p} - p)'(I_k - 11'k)(\sqrt{n}(\hat{p} - p))/ (1/k). \quad (3.2)$$

In the case $k = 2^l$, they use a Hadamard matrix (without the constant row) to produce $(k - 1)$ asymptotically independent components of $X^2$, giving a theoretical basis to the seemingly ad hoc selection of vectors in Anderson [3]. Despite the elegance, Boero et al [4] does not justify the use of Hadamard matrices in the above procedure. In the following paragraphs, we will explain their inherent relevance in the diagonalization, thus setting the stage for a generalization of this procedure to the non-equiprobable case.

In effect, we note that the constant vector $1$ is an eigenvector of $\Sigma$ that corresponds to the simple eigenvalue 0. Since $\Sigma$ is symmetric and idempotent, it admits only the eigenvalues 0 and 1. It follows that any vector orthogonal to 1 is an eigenvector of $\lambda = 1$. Since all rows of a Hadamard matrix $H$ are orthogonal with constant norm $\sqrt{k}$, the diagonalization (3.1) is satisfied with $\Gamma = \frac{1}{\sqrt{k}}H$ (where $H$ is written in the standard form so that the first row of $H$ is the vector $1'$), and $\Lambda$ coincides with $\frac{1}{k}I_k$ except for $\Lambda_{11} = 0$.

If we now apply the transformation $y = \frac{1}{\sqrt{k}}Hx$, it follows from the general theory that $y$ converges to a centered multinormal distribution with variance-covariance matrix $\Lambda$. This and Equation (3.2) immediately lead to the decomposition $X^2 = y'y/(1/k)$.

4 The Non-Equiprobable Case

In this section we present a generalization to the above procedure in the non-equiprobable case, keeping the number of classes a power of 2. We remark here that the diagonalization in the equiprobable case of the previous section rests on the fact that $k\Sigma$ is idempotent. This property is lost in the general case. While 0 is always a simple eigenvalue, $\Sigma$ admits in general many other eigenvalues that depend on the cell probability vector $p$.

Indeed, Watson [18] establishes that, if $p_i \leq p_{i+1}$ for all $i$ then each of the $k - 1$ nonzero eigenvalues is squeezed between two consecutive $p_i$s, i.e., $p_1 \leq \lambda_1 \leq p_2 \leq \cdots \leq p_{k-1} \leq \lambda_{k-1} \leq p_k$. This immediately establishes that $\Sigma$ is idempotent if and only if all the $p_i$s are equal. The results in this section are outlined as follows. We first propose an appropriate transformation to the vector $x$ that will produce a vector whose variance-covariance matrix is idempotent. We
later proceed by providing a matrix of highly structured eigenvectors, symbolically defined in terms of $p$, and we characterize the cases when this matrix is orthogonal, which will then readily decompose the Pearson statistic.

**Theorem 4.1.** Let $y = D^{-1/2}(p)x$. Then $y$ converges in distribution to a multinormal distribution with an idempotent variance-covariance matrix $\Sigma^*$. Furthermore, the vector $\sqrt{p}$ defined as $(\sqrt{p_1}, \ldots, \sqrt{p_k})'$ is an eigenvector that spans the kernel of $\Sigma^*$.

It is worth noting that, componentwise, this transformation is a re-scaling of the already normalized multinomial frequencies. Namely, the coordinates of $y$ are $y_i = \frac{x_i}{\sqrt{p_i}} = \frac{m_i - np_i}{\sqrt{np_i}}$.

In the following Lemma, we will gather some simple facts that will be used in the proof of Theorem 4.1 and that can be checked by direct calculations.

**Lemma 4.2.** The following are true for any probability vector $p$.

(a) $D^{-1}(p)p = 1$.

(b) $p' D^{-1}(p)p$ is the scalar value 1.

(c) $D^{-1/2}(p)\sqrt{p} = 1$

(d) $D^{-1/2}(p)p = \sqrt{p}$

(e) $D^{1/2}(p)1 = \sqrt{p}$

**Proof of Theorem 4.1.** We first prove that $\Sigma^*$ is idempotent by direct multiplication. Observing that $\Sigma^* = D^{-1/2}(p)\Sigma D^{-1/2}(p)$, we get

$$\Sigma^{*2} = D^{-1/2}(p)(D(p) - pp')D^{-1/2}(p) \times D^{-1/2}(p)(D(p) - pp')D^{-1/2}(p) = D^{-1/2}(p)CD^{-1/2}(p)$$

where

$$C = D(p) - 2pp' + pp'D^{-1}(p)pp'.$$

The last expression in the last row is $pp'$ by Lemma 4.2(b). This shows that $\Sigma^{*2} = \Sigma^*$.

Next, consider $\Sigma^* \sqrt{p} = D^{-1/2}(p)(D(p) - pp')1 = D^{1/2}(p)1 - D^{-1/2}(p)p(p'1)$

$$= D^{1/2}(p)1 - D^{-1/2}(p)p = \sqrt{p} - \sqrt{p} = 0.$$ Where we have used parts (c), (d) and (e) of Lemma 4.2.

The fact that $\sqrt{p}$ is the only eigenvector of 0 plays a role similar to the vector 1 in the equiprobable case as outlined above. The next section shows how to construct an orthogonal matrix whose first column is $\sqrt{p}$ and, therefore, whose other columns are eigenvectors of $\Sigma^*$ all with eigenvalue 1. For now, suppose that $O$ is an orthogonal matrix with $\sqrt{p}$ as its first column. On one hand, $\Sigma^* = O'\Lambda O$, where $\Lambda$ coincides with $I_k$ except for $\Lambda_{11} = 1$. Letting $A$ be the submatrix of $O$ obtained by omitting the first column, it is immediate
that $A'A = I_{k-1}$ and $AA' = \Sigma^*$. Thus, $y'\Sigma^*y = y'AA'y = (A'y)'(A'y)$. On the other hand, with $D(p) = D$ and $D^{1/2}(p) = D^{1/2}$,

$$y'\Sigma^*y = \left(D^{-1/2}\left(\frac{m-\mu}{\sqrt{n}}\right)^\prime\right)^\prime D^{-1/2}(D - pp')D^{-1/2}\left(D^{-1/2}\left(\frac{m-\mu}{\sqrt{n}}\right)^\prime\right)$$

$$= \frac{1}{n}(m-\mu)^\prime D^{-1/2}\left(D^{-1/2}\Sigma D^{-1/2}\right)D^{-1/2}(m-\mu)$$

$$= \frac{1}{n}(m-\mu)^\prime (D^{-1} - D^{-1}pp'D^{-1})(m-\mu)$$

$$= \frac{1}{n}(m-\mu)^\prime D^{-1}(m-\mu) - \frac{1}{n}(m-\mu)^\prime D^{-1}pp'D^{-1}(m-\mu).$$

The first expression in the last row is clearly the Pearson statistic $X^2$. By Part (a) of Lemma 4.2, $(m-\mu)^\prime D^{-1}p$ is the zero vector, so that the second term collapses to zero. Hence we have obtained the partition $X^2 = (A'y)'(A'y)$. If we denote the columns of $A$ by $v_2 \cdots, v_k$, this partition can be expressed as

$$X^2 = \sum_{l=2}^{k} (v_l'y)^2,$$

where $v_l'y = \sum_{i=1}^{k} v_{li}\frac{(m_i - np_i)}{\sqrt{np_i}}$ and $v_{li}$ is the $i^{th}$ coordinate of $v_l$.

5 A Latin-Hadamard Matrix

As planned above, in this section we construct a matrix of orthogonal eigenvectors whose first column is $\sqrt{p}$, the generator of the kernel of $\Sigma^*$. To this end, we will first construct a square matrix with integer entries, whose special features will allow the construction we propose.

For $k = 2^w$, define a matrix $S = [c_1, \cdots, c_k]$ with columns $c_i$ such that $c_1 = [1, \cdots, k]^\prime$, and for $i = 1, \cdots, 2^{w-1}$ let

$$c_{2i,2} = c_{2i-1,1}; \quad \text{and} \quad c_{2i-1,2} = c_{2i,1};$$

Now for $l = 0, \cdots, w - 1$, write $S$ in blocks of size $2^l \times 2^l$ matrices as

$$\begin{bmatrix}
S_{1,1}^l & \cdots & S_{1,2^{w-l}}^l \\
\vdots & \ddots & \vdots \\
S_{2^{w-l},1}^l & \cdots & S_{2^{w-l},2^{w-l}}^l
\end{bmatrix}$$

The first block column $S_{1,1}^l$ of $S$ has been defined. We fill in the rest of the matrix as follows. For each value of $l$, $l = 2, \cdots, w - 1$, we define the second column $S_{2,2}^l$ of block matrices as

$$S_{2,2}^l = S_{2,2-1}^l; \quad \text{and} \quad S_{2,2-1}^l = S_{2,1}^l;$$

for each $i = 1, \cdots, 2^{w-l}$. We note here that the second column can be defined in several ways, producing the same matrix up to a permutation of the rows. For example, the second
column $c_2$ can be defined as $[k, \cdots, 1]'$. The current construction is most convenient for recursive arguments due to its self-similarities, as apparent in Figure 1 where the upper left $2^w \times 2^w$ sub-matrix is one such matrix for $w = 1, \cdots, 4$.

$$\begin{pmatrix}
1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 & 10 & 11 & 12 & 13 & 14 & 15 & 16 \\
2 & 1 & 4 & 3 & 6 & 5 & 8 & 7 & 10 & 9 & 12 & 11 & 14 & 13 & 16 & 15 \\
3 & 4 & 1 & 2 & 7 & 8 & 5 & 6 & 11 & 12 & 9 & 10 & 15 & 16 & 13 & 14 \\
4 & 3 & 2 & 1 & 8 & 7 & 6 & 5 & 12 & 11 & 10 & 9 & 16 & 15 & 14 & 13 \\
5 & 6 & 7 & 8 & 1 & 2 & 3 & 4 & 13 & 14 & 15 & 16 & 9 & 10 & 11 & 12 \\
6 & 5 & 8 & 7 & 2 & 1 & 4 & 3 & 14 & 13 & 16 & 15 & 10 & 9 & 12 & 11 \\
7 & 8 & 5 & 6 & 3 & 4 & 1 & 2 & 15 & 16 & 13 & 14 & 11 & 12 & 9 & 10 \\
8 & 7 & 6 & 5 & 4 & 3 & 2 & 1 & 16 & 15 & 14 & 13 & 12 & 11 & 10 & 9 \\
9 & 10 & 11 & 12 & 13 & 14 & 15 & 16 & 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 \\
10 & 9 & 12 & 11 & 14 & 13 & 16 & 15 & 2 & 1 & 4 & 3 & 6 & 5 & 8 & 7 \\
11 & 12 & 9 & 10 & 15 & 16 & 13 & 14 & 3 & 4 & 1 & 2 & 7 & 8 & 5 & 6 \\
12 & 11 & 10 & 9 & 16 & 15 & 14 & 13 & 4 & 3 & 2 & 1 & 8 & 7 & 6 & 5 \\
13 & 14 & 15 & 16 & 9 & 10 & 11 & 12 & 5 & 6 & 7 & 8 & 1 & 2 & 3 & 4 \\
14 & 13 & 16 & 15 & 10 & 9 & 12 & 11 & 6 & 5 & 8 & 7 & 2 & 1 & 4 & 3 \\
15 & 16 & 13 & 14 & 11 & 12 & 9 & 10 & 7 & 8 & 5 & 6 & 3 & 4 & 1 & 2 \\
16 & 15 & 14 & 13 & 12 & 11 & 10 & 9 & 8 & 7 & 6 & 5 & 4 & 3 & 2 & 1
\end{pmatrix}$$

Figure 1: A $2^4 \times 2^4$ Latin square with the AB-BA property.

Several immediate properties that can be checked by induction make this matrix special. We first list a few such properties in the form of a lemma, then we state and prove a proposition that deals with the special feature that will allow us to turn $S$ into an orthogonal matrix by multiplying some entries by $-1$.

**Lemma 5.1.** The following assertions are true about $S$.

(a) $S$ is a Latin square.

(b) $S$ is symmetric with respect to both the first and second diagonals.

(c) $S$ can be defined recursively in $w$ as follows. For $w = 0$, let $S_0 = 1$. For an integer $w \geq 1$ let $S_w = \begin{bmatrix} A & B \\ B & A \end{bmatrix}$, where $A = S_{w-1}$ and $B = A + 2^{w-1}1_{2^{w-1}}1'_{2^{w-1}}$, and $1_{2^{w-1}}$ is the $2^{w-1}$-dimensional constant vector of ones.

**Proposition 5.2.** For dimension $k = 2^w$ and indices $1 \leq i_1, j_1, j_2 \leq k$, $j_1 \neq j_2$, if $S_{i_1,j_1} = a$ and $S_{i_1,j_2} = b$, then there exist an index $i_2 \neq i_1$, $1 \leq i_2 \leq k$ such that $S_{i_2,j_1} = b$ and $S_{i_2,j_2} = a$.

**Proof.** Let $S = \begin{bmatrix} A & B \\ B & A \end{bmatrix}$ as in Lemma 5.1. We will use an inductive argument. So, it suffices to assume that $a$ and $b$ are entries of $A$ and $B$ respectively. That is, for arbitrary indices $s_1, t_1$, and $t_2$, $1 \leq s_1, t_1, t_2 \leq 2^{w-1}$, let $A_{s_1,t_1} = a$ and $B_{s_1,t_2} = b$, where $t_1$ and $t_2$ need not be different. Since $S$ is a Latin square, there exists $s_2$ ($1 \leq s_2 \leq 2^{w-1}$) such that $S_{s_2+2^{w-1}-1,t_1} = b$. Referring to the block matrix composition of $S$, this means that $B_{s_2,t_1} = b$. Since the matrices $A$ and $B$ have the same structure and relative positions, by Lemma 5.1, it follows that $A_{s_1,t_2} = A_{s_2,t_1} = b'$ for some $b'$, $1 \leq b' \leq 2^{w-1}$. Applying the
inductive hypothesis to the matrix $A$, it is evident that $A_{s_2,t_2} = A_{s_1,t_1} = a$. To formally complete the proof we take $i_1 = s_1$, $j_1 = t_1$ and $i_2 = s_2 + 2^w - 1$, $j_2 = t_2 + 2^w - 1$.

We will refer to the property proven in the above proposition as the AB-BA property, and to every four entries that make up this property as AB-BA corners. This property potentially allows us, by appropriately inserting minus signs to certain entries, to come up with a matrix that has orthogonal columns. Namely, if among every four AB-BA corners exactly three are ‘colored’ by the same color (where the two available colors are ‘+’ and ‘−’) then all columns will be orthogonal. It turns out that this is possible only in few cases as stated in the following theorem.

**Theorem 5.3.** When $k = 2$, $4$ or $8$, there exists a matrix $H$ with orthogonal columns and orthogonal rows and that has the following properties

(a) $|H_{ij}| = S_{ij}$,

(b) The matrix $\tilde{H}$ defined componentwise by $\tilde{H}_{ij} = \text{sgn}(H_{ij})$ is a Hadamard matrix.

(c) The signs of entries of $H$ can be arranged so that all entries on the first row and first column are positive.

Furthermore, an orthogonal matrix with these properties is not possible for any other value of $k$.

**Proof.** In an appendix at the end of this paper, we we present a systematic way to color the entries by ‘+’ and ‘−’ in a way that guarantees that every column is orthogonal to the first column and every row is orthogonal to the first row. As it turns out, there are $2^{2^w - 1 - w}$ ways to make this happen. When $w = 1, 2, 3$ each of these colorings yields mutually orthogonal columns. (We will refer to such a matrix with orthogonal columns as a Latin-Hadamard matrix.) When $k = 4$, no such coloring makes all the columns mutually orthogonal. As the coloring is performed by first coloring the upper left quarter of the matrix, this already shows that no coloring is possible for $k \geq 4$. Now to see that there does not exist any colored matrix with $k = 4$ suppose one exists. Then necessarily the transpose is a colored matrix. In particular, every column is orthogonal to the first column and every row is orthogonal to the first row. Our exhaustive search shows that no such matrix with the latter property has all of its columns mutually orthogonal.

The above proof is a brute force argument, which does not reveal why the so-called Latin-Hadamard matrices do not exist in higher dimensions. In fact, the columns are all orthogonal if the equation

$$\alpha_{i,j} \cdot \alpha_{i,j+l} = -\alpha_{i+l,j} \cdot \alpha_{i+l,j+l'}$$

is satisfied for all $i$ and $j$ between 1 and $2^k$, $l \neq 0$ and $l' \neq 0$ such that $S_{i,j} = S_{i+l,j+l'}$ and $S_{i,j+l} = S_{i+l,j}$, and where the values of the $\alpha$s are defined via $H_{ij} = \alpha_{ij}S_{ij}$.

Indeed, the coloring scheme described in the appendix is performed with the only objective of making Equation 5.4 work for $i = 1$ and $j \neq 1$ or $i \neq 1$ and $j = 1$. That is, it only ensures that each column is orthogonal to the first column and each row is orthogonal to the first row. There is no guarantee that the numerous other equations of the form 5.4 for $i \neq 1$ and $j \neq 1$ are satisfied. For $k = 1, 2, 3$ a solution comes as a free gift. That is, we found a solution of an over-determined system by only considering some of the equations.
In Section 7 below we give another proof of Theorem 5.3 that better explains why the coloring scheme works only for \( k = 1, 2, 3 \). In the rest of this section we will describe how each colored matrix corresponding to \( w \leq 3 \) can be turned into an orthogonal matrix \( O \) that partitions the chi-square statistic in a way that each component test is a sum of differences of two cell frequencies in some order, where each cell frequency is used exactly once.

Figure 2 gives a matrix \( H \) of size 8, which also gives examples of lower sizes given by the upper left \( 2 \times 2 \) and \( 4 \times 4 \) sub-matrices respectively.

Interestingly, when \( k = 16 \), many pairs of vectors produced by our current construction are already orthogonal. Indeed the first eight columns (as well as the other eight) are all mutually orthogonal. Since different vectors are typically used as individual components, one is still able to use many of these vectors as independent component tests that can individually provide useful information.

\[
\begin{pmatrix}
+1 & +2 & +3 & +4 & +5 & +6 & +7 & +8 \\
+2 & -1 & -4 & +3 & +6 & -5 & +8 & -7 \\
+3 & +4 & -1 & -2 & +7 & -8 & -5 & +6 \\
+4 & -3 & +2 & -1 & +8 & +7 & -6 & -5 \\
+5 & -6 & -7 & -8 & -1 & +2 & +3 & +4 \\
+6 & +5 & +8 & -7 & -2 & -1 & +4 & -3 \\
+7 & -8 & +5 & +6 & -3 & -4 & -1 & +2 \\
+8 & +7 & -6 & +5 & -4 & +3 & -2 & -1
\end{pmatrix}
\]

Figure 2: A \( 8 \times 8 \) signed Latin square with orthogonal columns and rows.

Evidently, one can substitute the integers \( 1, \ldots, 2^w \), in the matrix \( H \), respectively with any set of \( 2^w \) real numbers and keep the orthogonality of the columns, thanks to the AB-BA property of the underlying matrix \( S \). Returning to the main problem of this paper, we are now ready to give an orthonormal matrix of eigenvectors of \( \Sigma^* \) when the number of categories in the multinomial model is a 2, 4 or 8. We present this matrix in the following corollary to Theorem 5.3.

**Corollary 5.4.** Consider the matrix \( O \) defined componentwise by the equation

\[
O_{ij} = \text{sgn}(H_{ij}) \cdot \sqrt{p_s}
\]

where \( s = |H_{ij}|, \) and \( p_s; s = 1, \ldots, 2^w \) are the components of the vector \( \sqrt{p} \) and \( H \) is as given in Theorem 7.3(c). Then the columns of \( O \) form a basis of orthonormal eigenvectors of \( \Sigma^* \), such that the first column is the zero eigenvector \( \sqrt{p} \).

All \( 4 \times 4 \) and \( 8 \times 8 \) Latin-Hadamard matrices are displayed in Table 2.

### 6 Power Simulation for Components

As an illustration, we will use the matrix on the left of the first row of \( 8 \times 8 \) matrices in Table 2 which displays all possible Latin-Hadamard matrices of dimensions \( 4 \times 4 \) and \( 8 \times 8 \). Since the columns of this matrix are orthogonal, the components of the Pearson statistic, given by the summands in Equation (4.3), are asymptotically independent chi-square statistics, each with one degree of freedom. Furthermore, each component can be
used individually as a separate test. Since the first column is an eigenvector of the zero
eigenvalue, it contains no information. Using the second column, we get the component
test, which we will call $T_2$,

$$\frac{1}{n}\left\{\sqrt{\frac{p_2}{p_1}}(m_1 - np_1) - \sqrt{\frac{p_1}{p_2}}(m_2 - np_2) + \sqrt{\frac{p_4}{p_3}}(m_3 - np_3) - \sqrt{\frac{p_3}{p_4}}(m_4 - np_4)
+ \sqrt{\frac{p_5}{p_6}}(m_5 - np_5) - \sqrt{\frac{p_6}{p_5}}(m_6 - np_6) + \sqrt{\frac{p_8}{p_7}}(m_7 - np_7) - \sqrt{\frac{p_7}{p_8}}(m_8 - np_8)\right\}^2$$

Noting that $T_2$, the square root of the above component test, is asymptotically normal, and
using $\hat{p}_i = \frac{m_i}{n}$, the statistic $T_2$ reduces as follows

$$\sqrt{T_2} = \sqrt{n}\left(\left(\sqrt{\frac{p_2}{p_1}}\hat{p}_1 - \sqrt{\frac{p_1}{p_2}}\hat{p}_2\right) + \left(\sqrt{\frac{p_4}{p_3}}\hat{p}_3 - \sqrt{\frac{p_3}{p_4}}\hat{p}_4\right)
+ \left(\sqrt{\frac{p_6}{p_5}}\hat{p}_5 - \sqrt{\frac{p_5}{p_6}}\hat{p}_6\right) + \left(\sqrt{\frac{p_8}{p_7}}\hat{p}_7 - \sqrt{\frac{p_7}{p_8}}\hat{p}_8\right)\right).$$

Similarly, the sixth and eighth vectors yield the asymptotically normal component tests

$$T_6 = \sqrt{n}\left(\left(\sqrt{\frac{p_6}{p_1}}\hat{p}_1 - \sqrt{\frac{p_1}{p_6}}\hat{p}_6\right) + \left(\sqrt{\frac{p_5}{p_2}}\hat{p}_2 - \sqrt{\frac{p_2}{p_5}}\hat{p}_5\right)
- \left(\sqrt{\frac{p_8}{p_3}}\hat{p}_3 - \sqrt{\frac{p_3}{p_8}}\hat{p}_8\right) + \left(\sqrt{\frac{p_7}{p_4}}\hat{p}_4 - \sqrt{\frac{p_4}{p_7}}\hat{p}_7\right)\right),$$

and

$$T_8 = \sqrt{n}\left(\left(\sqrt{\frac{p_8}{p_1}}\hat{p}_1 - \sqrt{\frac{p_1}{p_8}}\hat{p}_8\right) - \left(\sqrt{\frac{p_7}{p_2}}\hat{p}_2 - \sqrt{\frac{p_2}{p_7}}\hat{p}_7\right)
+ \left(\sqrt{\frac{p_6}{p_3}}\hat{p}_3 - \sqrt{\frac{p_3}{p_6}}\hat{p}_6\right) + \left(\sqrt{\frac{p_5}{p_4}}\hat{p}_4 - \sqrt{\frac{p_4}{p_5}}\hat{p}_5\right)\right).$$

Notice that the mutual weighted differences between pairs of sample proportions make
it relatively easier to interpret many individual components. Suppose a null hypothesis
specifies a distribution $F$ and subdivide its support into 8 bins with probabilities $p_1, \ldots, p_8$
labeled from left to right. Generally, the first three vectors (second, third and fourth) deal
with local changes in the distribution while the other four vectors compare bins from the
opposite sides of the support. In particular, in the examples above, $T_2$ compares consecutive
bins, so it is sensitive to the rate at which a distribution increases or decays; while $T_8$ is
sensitive to a change in location.

To illustrate the significance of this partition into component tests, the table below shows
results of power simulation when the null distribution is assumed to be $N(0, 1)$. The actual
data is generated from several distributions with a change from standard normal along a
location shift, an increase in variance or an increase in the tail. From each distribution
in the table, 10000 samples of size \( n = 200 \) were generated from the distribution named in the first column. The real axis was divided into eight sub-domains whose standard normal probabilities from left to right are equal to the specified multinomial vector. The table estimates the power of the overall chi-square statistic as well as all the components provided by the columns of the upper left matrix in Table 2. It is worth noting that various components behave drastically differently. The middle two rows (in the upper part of the table) investigate the power with respect to location shift. Components \( T_4 \) and \( T_8 \) are the only components that are sensitive to this location shift, with \( T_8 \) outperforming the \( X^2_P \). One can also compare the power of the equally likely case (Case (a)) to the other cases. The most important remark is that the choice of the multinomial vector directly affects the power of various components; notice how Case (c) allows all components to pick up some nontrivial power. The lower part of the table compares gamma generated values with given shape and scale parameters to a null normal model with matched mean and standard deviation. This case is meant to check which component is sensitive to skewness and it clearly shows the superiority of each component test to the global statistic \( X^2_P \). Components \( T_3 \) and \( T_5 \) consistently show a higher sensitivity. Most remarkably, changing the probability vector can greatly increase the power of the same component test. For example, Component \( T_4 \) becomes sensitive to skewness when the probability vector is not uniform. Similarly, \( T_8 \) picks up a lot of power against fat tails (Cauchy and t distribution) when the probability vector (c) is used. This is also observed with \( N(0,1.3) \) data.

7 Connections with Algebra

In the first subsection we give an explanation to the non-existence of valid colorings for size 16 and higher. We then show, in Subsection 7.2 how to remedy this issue by taking some of probability values to be equal, using the theory of orthogonal designs.

7.1 Division Algebras Connections

An algebra over a field is a vector space that is equipped with a bilinear multiplication operator. Three well-known algebras over the field of real numbers are the two dimensional algebra of complex numbers, the four dimensional algebra of quaternions, and the eight dimensional non-associative algebra of octonions. The octonions are constructed from the quaternions in a way similar to the construction of the quaternions from the complex numbers, and the construction of the latter from the real numbers. This sort of construction can be repeated indefinitely via a classical doubling procedure called the Cayley-Dickson construction. The next algebra produced by doubling the octonions is the less known algebra of sedenions, which has been mostly neglected by mathematicians, perhaps because it is not a division algebra. That is, in this algebra the equations \( ax = b \) and \( xa = b \) need not have a solution in \( x \). Equivalently, there exist zero divisors in the sedenions algebra, i.e., there are elements \( a \neq 0 \) and \( b \neq 0 \) but \( ab = 0 \). This is not possible in the first three algebras above.

Usually the multiplication operation in an algebra is defined via a multiplication table for elements of a basis. As an illustration, the basis elements of quaternions are denoted by \( 1, i, j, k \). Multiplication of quaternions is defined by \( i^2 = j^2 = k^2 = -1, ij = k, jk = i, \)
ki = j, ji = −k, kj = −i, ik = −j. Denoting 1, i, j and k by e₁, e₂, e₃ and e₄ respectively, the multiplication table can be seen as a 4 x 4 matrix.

\[
\begin{pmatrix}
  e₁ & e₂ & e₃ & e₄ \\
  e₁ & +e₁ & +e₂ & +e₃ & +e₄ \\
  e₂ & +e₂ & −e₁ & +e₄ & −e₃ \\
  e₃ & +e₃ & −e₄ & −e₁ & +e₂ \\
  e₄ & +e₄ & +e₃ & −e₂ & −e₁
\end{pmatrix}
\]

Note that the resulting 4 x 4 matrix consists of an orthogonal matrix with the AB-BA property. A similar phenomenon is noticed if we write the multiplication table of octonions. The multiplication table of the sedenions also has the AB-BA property but the columns are no more orthogonal.

A classical theorem in algebra, Hurwitz Theorem, states that the only division algebras over the field of real numbers are the algebras of real numbers, complex numbers, quaternions and octonions, see [8], [9] for example. The connection to our problem is estab-
Table 2: All possible orthogonal $4 \times 4$ and $8 \times 8$ Latin-Hadamard matrices. Here $\hat{p}_i$ denotes $\sqrt{p_i}$, for typographical reasons.
lished by seeing that the existence of zero divisors is associated with the existence of two columns that are not orthogonal. In effect, let \( e_1, \ldots, e_{16} \) be a basis of a 16-dimensional algebra generated by a coloring of our matrix. Suppose also that \( e_1 \) is the unit element while the rest are the imaginary roots of \(-1\). de Marrais [12] shows that the zero divisors are only of the form \( e_i \pm e_j \) for some \( i, j \neq 1 \), see also [14]. Consider some basis elements \( k_1, k_2, l_1, l_2 \) all different from unity and suppose that \( k_1 l_1 = \alpha_{11} e_a, k_1 l_2 = \alpha_{12} e_b, k_2 l_1 = \alpha_{21} e_b, k_2 l_2 = \alpha_{22} e_{a'}, \) where the \( a' \)'s are \pm 1. Since the multiplication table without the signs makes a Latin square, note that \( a \neq b, a \neq b', a' \neq b \) and \( a' \neq b' \). If \( a \neq a' \) or \( b \neq b' \) then one can readily check that none of the four products \((k_1 \pm k_2)(l_1 \pm l_2)\) can be zero. For \( a = a' \) and \( b = b' \), \((k_1 - k_2)(l_1 + l_2) = 0 \) if and only if \( \alpha_{11} = \alpha_{22} \) and \( \alpha_{12} = -\alpha_{21} \). Likewise, \((k_1 + k_2)(l_1 + l_2) = 0 \) if and only if \( \alpha_{11} = -\alpha_{22} \) and \( \alpha_{12} = -\alpha_{21} \). In both scenarios, and using our terminology, we do not obtain a ‘correct’ coloring of the AB-BA corners. In other words, the existence of a (complete) coloring of the multiplication table is equivalent to the non-existence of zero divisors. Hence, the non-existence of a Latin-Hadamard matrix of order 16 or above rests on the deeper truth stated by the Hurwitz theorem. The next section shows that this issue can be remedied.

### 7.2 Trade-Offs Via Orthogonal Designs

We have seen that a Latin-Hadamard matrix allows for component tests that compare pairs of sample proportions in various ways. When the number of bins is 16 or a higher power of two, we are faced with the impossibility of having division algebras over the real numbers. However, this can be overcome if we are willing to assume some prior relations between the bin probabilities \( p_1, \ldots, p_{16} \). An obvious example that we already discussed is when we assume that all of them are equal, in which case Hadamard matrices clearly exist for all pure powers of two.

It turns out that we have discussed the two extreme cases: when all cell probabilities are equal and when all are different. The latter case is thought to occur when no a priori relations are assumed between the cell probabilities. In both cases we have insisted that each component test uses all cell counts, by requiring that the matrix has no zero entries.

The mathematical apparatus to study cases other the two mentioned above is the theory of orthogonal designs which we will briefly define next.

**Definition 7.1.** Given any integer \( n \), we can write \( n = 2^a \cdot b \) for some integers \( a \) and \( b \) where \( b \) is odd. Writing \( a = 4c + d; 0 \leq d < 4 \), Radon’s function is defined as \( \rho(n) = 8c + 2^d \).

It is worth noting that \( \rho(n) = n \) if \( n = 1, 2, 3, 4 \). Also \( \rho(16) = 9, \rho(32) = 10, \rho(64) = 12, \) etc.

**Definition 7.2.** An orthogonal design of order \( n \) and type \( (s_1, \ldots, s_l) \) \((s_i > 0 \text{ and } 0 < l \leq n \) is an integer) on the commuting variables \( x_1, \ldots, x_l \) is an \( n \times n \) matrix \( A \) with entries from \( \{0, \pm x_1, \ldots, \pm x_l\} \) such that

\[
AA^t = \left( \sum_{i=1}^{l} s_i x_i^2 \right) I_n
\]

That is, the columns of \( A \) are orthogonal and each column has exactly \( s_i \) entries of type \( \pm x_i \). Radon’s Theorem states the following.
Radon’s Theorem. Let $A$ be an orthogonal design of order $n$ and type $(s_1, \ldots, s_l)$ on the variables $x_1, \ldots, x_l$. Then $\rho(n) \geq l$.

It follows by this theorem, and the remark that $\rho(n) = n$ if and only if $n = 1, 2, 4, 8$, that we can only find orthogonal designs of order $n$ and $n$ variables when $n$ takes one of the four values, $1, 2, 4, 8$.

For a chi-square decomposition with relations between class probabilities that are less restrictive than those of Section 3 we make use of orthogonal designs with nonzero entries. I. Kotsireas and C. Koukouvinos [10] obtain an orthogonal design of order 16 using the algebra of sedenions. They start with 16 indeterminate variables $A, B, \ldots, P$, and imitate a construction by Becker and Weispfenning [5] of Hadamard matrices using quaternions. As a result of this direct imitation, they obtain a $16 \times 16$ matrix whose entries are polynomial functions in the indeterminate variables and with identical diagonal entries. To obtain the orthogonal design they set all non-diagonal entries to zero and thus obtain a system of 42 equations. Applying a Gröbner basis technique, they obtain an equivalent but reduced set of equations. Each solution of this reduced system yields a $16 \times 16$ orthogonal design. They show computationally that all solutions boil down an at-most-9-variable orthogonal design. They report an explicit orthogonal design matrix, which we show with $\sqrt{p_1}, \ldots, \sqrt{p_9}$ as the indeterminate variables (with $p_i$ denoting $\sqrt{p_i}$).

$\left( \begin{array}{cccccccccc} p_1 & p_2 & p_3 & p_4 & p_5 & p_6 & p_7 & p_8 & p_9 & p_{10} \\ -p_2 & p_1 & -p_4 & p_3 & -p_6 & p_5 & -p_7 & -p_8 & -p_9 \\ -p_3 & p_4 & p_1 & -p_2 & -p_5 & p_6 & -p_7 & -p_8 & -p_9 \\ -p_4 & -p_3 & p_2 & p_1 & -p_5 & -p_6 & p_7 & -p_8 & -p_9 \\ -p_5 & p_6 & p_7 & p_8 & p_9 & p_1 & -p_2 & -p_3 & -p_4 \\ -p_6 & -p_5 & p_8 & p_9 & p_1 & p_2 & p_3 & p_4 & -p_5 \\ -p_7 & -p_8 & -p_9 & p_1 & p_2 & -p_3 & -p_4 & -p_5 & p_6 \\ -p_8 & p_7 & p_6 & p_5 & p_4 & -p_3 & -p_2 & -p_1 & p_9 \\ -p_9 & p_8 & -p_7 & -p_6 & -p_5 & -p_4 & -p_3 & -p_2 & -p_1 \\ -p_{10} & -p_9 & -p_8 & -p_7 & -p_6 & -p_5 & -p_4 & -p_3 & -p_2 & -p_1 \end{array} \right)$

The transpose of this matrix is exactly what we need to decompose the chi-square statistic. The columns are all orthogonal and the entries still enjoy the AB-BA property, and with all non-zero probabilities allowing for each component test to use all multinomial cell counts.

The method above can be extended to higher Cayley-Dickson algebras via similar calculations. Moreover, it can be applied to every multiplication table provided by our colored matrices.

8 Appendix

In this appendix we show how to ‘color’ a $2^k \times 2^k$ matrix $S_k$ with the AB-BA property (given in Proposition 5.2) in a way that produces orthogonal columns, thus proving Theorem 5.3. This is done in two steps. First we present a systematic procedure to color the entries so that in every set of four AB-BA corners, exactly one is colored with a distinct color (i.e. one ‘+’ and three ‘−’s or one ‘−’ and three ‘+’s). In practice, the matrix is completely colored before checking all AB-BA corners. Therefore, once all entries are colored, we need to check that all columns are orthogonal. The steps detailed below yield all possible cases.
For $w = 1, \cdots , k$ we will represent $S_w$ as a block matrix $\begin{bmatrix} A_1 & B_1 \\ B_2 & A_2 \end{bmatrix}$, as in Lemma 5.1(c), with indices introduced for easy referencing.

First we color all entries of the first column and first row by ‘+’. The following remarks are crucial. Since the diagonal entries all have value 1, the y must obviously be colored by ‘-’. The diagonal entries of $B$ are all equal to $2^{w-1} + 1$. Hence, for $i = 1, \cdots , 2^{w-1}$,

$$S_{1,2^{w-1}+1} = S_{i,2^{w-1}+i},$$
$$S_{1,2^{w-1}+i} = S_{i,2^{w-1}+1}.$$

Since the two entries on the left are already colored with ‘+’, and since these four entries form AB-BA corners, the two entries on the right must have distinct colors. Similarly, the four entries $S_{i,1}, S_{i,2^{w-1}+i}, S_{2^{w-1}+1,i}$ and $S_{2^{w-1}+1,2^{w-1}+i}$ form a $2 \times 2$ submatrix whose entries are AB-BA corners. Since the first and third are colored by ‘+’ (as they belong to the first column), it is evident that $S_{i,2^{w-1}+i}$ and $S_{2^{w-1}+1,2^{w-1}+i}$ must have different colors.

In a like manner, by alternately using the first row and the first column to color a new entry, we see that the sequence of entries

$$S_{i,2^{w-1}+1}, S_{i,2^{w-1}+i}, S_{2^{w-1}+1,i}, S_{2^{w-1}+1,2^{w-1}+i}, S_{2^{w-1}+i,2^{w-1}+1}, S_{i,2^{w-1}+1}.$$

must have alternating colors. Notice that by doing this we cycle back to the first entry, and that the sign allocation is consistent because the number of different entries in the sequence is even (namely 6.)

The above remarks suggest a recursive strategy to color the $2^k \times 2^k$ matrix $S_k$ by coloring the $2^w \times 2^w$ upper left submatrix progressively as $w$ increases from 2 to $k$.

(1) Base Case: Since the first column and first row are all colored with ‘+’, and consequently the diagonal entries that are not on the first row are colored with ‘-’, the $2 \times 2$ upper left submatrix is colored.

(2) Recursive Step: Suppose the $2^{w-1} \times 2^{w-1}$ upper left submatrix is colored, for some $w > 2$. We choose an arbitrary color for each entry $S_{i,2^{w-1}+1}, i = 2, \cdots , 2^{w-1}$. By the remark given above, each entry just colored leads to coloring a total of six entries. Noting that two of these entries belong to the $(2^{w-1} + 1)^{st}$ row and two entries belong to the $(2^{w-1} + 1)^{st}$ column, it follows in particular—that the $(2^{w-1} + 1)^{st}$ row and the $(2^{w-1} + 1)^{st}$ column are colored completely. Next, we are ready to color the entries of block $B_2$. For $i = 1, \cdots , 2^{w-1}$ and $j = 2, \cdots , 2^{w-1}$, if the entry $S_{2^{w-1}+i,j}$ has not been colored, we observe that the absolute value of this entry exists in the first column of $B_1$, which is the $(2^{w-1} + 1)^{st}$ column of $S_w$. Hence, for an appropriate $i'$ in $\{1, \cdots , 2^{w-1}\}, S_{i',2^{w-1}+1} = S_{2^{w-1}+i,j}$. It follows, by the AB-BA property, that

$$S_{i',j} = S_{2^{w-1}+i,2^{w-1}+1}.$$

Since exactly three of the above four entries are colored, the fourth will be colored accordingly.

At this point, using the fact that diagonal entries are ‘-1’, and that the matrix $S_{2^k}$ is symmetric, all uncolored entries of $B_1$ are colored as follows. For $i = 2, \cdots , 2^{w-1}$, $j = 2, \cdots , 2^{w-1}$

$$S_{i,2^{w-1}+j} = -S_{2^{w-1}+j,i}.$$
Lastly, once $A_1$, $B_1$, and $B_2$ are all colored, coloring $A_2$ is immediate. This concludes the construction.

To count the number of potential colorings of a $2^k \times 2^k$ matrix, observe that we start choosing random colors when $w = 2$ to $w = k$. We get $(2^1 - 1) + \cdots + (2^{k-1} - 1) = 2^k - (k+1)$. Therefore the number of potential colorings is $2^{2^k - (k+1)}$.

Our scheme for coloring need not produce all orthogonal columns. So further checking is needed. It turns out that the 2 colorings of $S_2$ and the 16 colorings of $S_3$ all yield matrices with orthogonal columns. However, none of the 2048 colorings of $S_4$ gives all orthogonal columns.

References

[1] Alhakim, A., On the eigenvalues and Eigenvectors of an Overlapping markov Chain. Probability Theory and Related Fields, 128, pp. 589-605, (2004).

[2] Alhakim, A., J. Kawczakand S. Molchanov, On the Class of Nilpotent Markov Chains, I., the Spectrum of Covariance Operator. Markov Processes and Related Fields, 10, pp. 629-652, (2004).

[3] G. Anderson , Simple tests of distributional form, Journal of Econometrics, 62, pp. 265-276, (1994).

[4] G. Boero, J. Smith, K. Wallis, Decompositions of Pearson’s Chi-square tests, Journal of Econometrics, 123, pp. 189-193, (2004).

[5] T. Becker and V. Weispfenning, Gröbner bases. A computational Approach to commutative algebra, Graduate texts in Mathematics 141, Springer-Verlag, New York, 1993.

[6] Good, I.J., (1953) The serial test for sampling numbers and other tests of randomness. In Proceedings of Cambridge Phylosophical Society, 49, 276-284.

[7] J. Irwin, A note on the subdivision of $\chi^2$ into components, Biometrica, 36, No. 1/2, pp. 130-134, (1949).

[8] N. Jacobson, Basic Algebra, Vol. 1, 2nd Edition, Dover Publications, 2009.

[9] I.L. Kantor, A.S. Solodovnikov, Hypercomplex Numbers, An Elementary Introduction to Algebra. Springer Verlag 1989.

[10] I. Kotsireas, C. Koukouvinos, Orthogonal Designs Via Computational Algebra, Journal of Combinatorial Designs, 14(5), pp. 351-362, (2006).

[11] H.O. Lancaster, The Chi-Squared Distribution. Wiley Publications in Statistics, 1969.

[12] R.P.C. de Marrais, The 42 Assessors and the Box-Kites they fly: Diagonal Axis-Pair Systems of Zero-Divisors in the Sedenions’ 16 Dimensions. arXiv:math/0011260v1 [math.GM].
[13] G. Marsaglia. A Current View of Random Number Generators. Computer Science and Statistics, Elsevier Science Publisher B.V. North-Holland. (1985).

[14] G. Moreno, The zero divisors of the Cayley-Dickson algebras over the real numbers, Bol. Soc. Mat. Mex., (1997).

[15] Pincus, S., Approximate entropy as a measure of system complexity. Proc. Nati. Acad. Sci. Vol. 88, pp. 2297-2301, (1991).

[16] Pincus, S., Singer, B.H., Randomness and Degrees of Irregularity, Proc. Nati. Acad. Sci., Vol 93, pp. 2083-2088, (1996).

[17] Tanabe, K., Sagae, M., An Exact Cholesky decomposition of the generalized inverse of the variance-covariance matrix of the multinomial distribution with applications, Journal of the Royal Statistical Society B, 54 No 1, pp. 211-219, (1992).

[18] Watson, Goeffrey S., Spectral decomposition of the covariance matrix of the multinomial, Journal of the Royal Statistical Society B, 58 No 1, pp. 289-291, (1996).