Ultrametric Simplices

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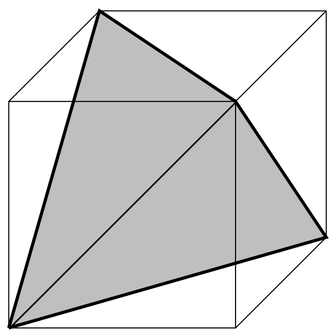

$$M = \begin{bmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{bmatrix}$$

$$M^\top M = \begin{bmatrix} 2 & 1 & 1 \\ 1 & 2 & 1 \\ 1 & 1 & 2 \end{bmatrix}$$

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Abstract

The main goal of this project is the study of ultrametric simplices whose vertices are vertices of the unit n-cube, which we will call ultrametric 0/1-simplices. We first consider ultrametric matrices. Following a paper from Varga and Nabben [14], we show that strictly ultrametric matrices are invertible, and their inverses are strictly diagonally dominant Stieljes matrices, and prove that any strictly ultrametric matrix of order n whose entries are integers can be written as the Gramian of a 0/1-matrix having at most $2n - 1$ distinct rows. We then characterize the geometrical properties of simplices in terms of linear algebra using the Gramians of their matrix representations. Using this characterization we show that ultrametric simplices are nonobtuse. Finally, we construct and implement an algorithm that generates a representative from each class of ultrametric 0/1-simplices modulo the symmetries of the n-cube for $3 \leq n \leq 12$. As a prelimary to this construction, we consider the problem of determining whether two 0/1-simplices differ a symmetry of the n-cube in a context of computational complexity theory, and prove in particular that this problem is polynomially reducible to that of graph isomorphism.

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Introduction

The well-known Hadamard inequality, named after the French mathematician Jacques Hadamard (1865-1963), gives an upper bound for the determinant of a 0/1-matrix of size $n \times n$. It is quite easy to show that this upper bound can be attained only when $n = 1$, $n = 2$ or $n - 3$ is divisible by 4. Whether the upper bound can in fact be attained for all these n, though, is not known. The Hadamard Conjecture [9] states that this is indeed the case, but after 120 years and plenty of attention [6, 8, 1, 10], no one has succeeded in proving this conjecture yet.

The entire problem translates very well to the study of simplices whose vertices are the vertices of the unit n-cube: the existence of a regular n-simplex whose vertices are vertices of the n-cube is equivalent to the existence of a 0/1-matrix of size $n \times n$ whose determinant is equal to the bound given by the Hadamard inequality. Regular simplices, however, are quite difficult to study. Because of this, we might be inclined to study a slightly larger class of simplices of which the regular ones are a subclass. This approach was taken by Brandts and Cihangir [11, 4], who studied acute simplices for this purpose. In this project, we will consider a slightly smaller class, namely that of the *ultrametric* simplices.

Our initial motivation for looking at ultrametric simplices is based on results by Varga and Nabben [14] which we will study in the first chapter. These results can be used firstly to show that ultrametric simplices are in particular nonobtuse. Secondly, they can be used to explicitly produce a congruent copy of a regular n-simplex based on a decomposition of ultrametric matrices, the vertices of which are corners of the unit k-cube for some $k \geq n$. It is our hope that through further study of this decomposition we might be able to 'improve' it, and enable it to provide a regular n-simplex inscribed in the n-cube, thus solving the Hadamard Conjecture.

Concretely, we will try to computationally generate a representative of each ultrametric n-simplex modulo symmetries of the n-cube, for small values of n. Based on the results of these computations, new conjectures about ultrametric simplices might be found. The generation of these simplices is non-trivial, and will require much preliminary work. In terms of pure mathematics, we must first study the properties of simplices, which we do in the second chapter. Chapters three and four will be oriented towards computer science. In the third chapter we will look at the computational complexity of determining whether two simplices are equivalent modulo symmetries of the n-cube in a theoretical setting. Then, in chapter four, we will work towards an efficient algorithm to actually generate the simplices and implement it. Finally, we shall provide the results of these computations.

1. Ultrametric Matrices

In this chapter we will study the properties of so-called ultrametric matrices. We find that they are invertible, and their inverses are quite special. Additionally, we cover the Varga-Nabben decomposition, which reduces a strictly ultrametric matrix to a linear combination of rank-one matrices in a very structured manner. The results of this chapter will form the foundation for our later chapter on simplices.

We start by defining ultrametricity for matrices in $\mathbb{R}^{3\times 3}$.

Definition 1.0.1 (Ultrametric Matrix)**.** A matrix $M \in \mathbb{R}^{3\times 3}$ is (strictly) *ultrametric* when

1. M is symmetric and has nonnegative entries.
2. The diagonal elements of M are (strictly) maximal in their rows.
3. The three entries above the diagonal do not have a unique minimum.

Example 1.0.1. Consider the symmetric matrices

$$M_1 = \begin{bmatrix} \pi & 3 & 3 \\ 3 & 5 & 4 \\ 3 & 4 & 8 \end{bmatrix}, \; M_2 = \begin{bmatrix} \pi & 3 & 0 \\ 3 & 5 & 0 \\ 0 & 0 & 8 \end{bmatrix}, \; M_3 = \begin{bmatrix} \pi & 3 & 3 \\ 3 & 2 & 4 \\ 3 & 4 & 8 \end{bmatrix}, \; M_4 = \begin{bmatrix} \pi & 3 & 1 \\ 3 & 5 & 4 \\ 1 & 4 & 8 \end{bmatrix}.$$

Checking the conditions, M_1 is strictly ultrametric, M_2 is ultrametric, M_3 is not ultrametric (since its second diagonal element is not maximal) and M_4 is also not ultrametric (since 1 is a unique minimum in the entries above the diagonal).

From here, we expand to the general case by looking at principal submatrices.

Definition 1.0.2 (Principal Submatrix)**.** Let $M = M_{ij} \in \mathbb{R}^{n\times n}$. For every permutation matrix $P \in \mathbb{R}^{n\times n}$ the matrix obtained by selecting the first k rows and columns of $P^\top MP$ is called a $k \times k$ principal submatrix of M.

Example 1.0.2. The stars ($\star$) in the following four matrices represent all possible 3×3 principal submatrices of a 4×4 matrix, the crosses ($\times$) indicate which entries are left out:

$$\begin{bmatrix} \star & \star & \star & \times \\ \star & \star & \star & \times \\ \star & \star & \star & \times \\ \times & \times & \times & \times \end{bmatrix}, \begin{bmatrix} \star & \star & \times & \star \\ \star & \star & \times & \star \\ \times & \times & \times & \times \\ \star & \star & \times & \star \end{bmatrix}, \begin{bmatrix} \star & \times & \star & \star \\ \times & \times & \times & \times \\ \star & \times & \star & \star \\ \star & \times & \star & \star \end{bmatrix}, \begin{bmatrix} \times & \times & \times & \times \\ \times & \star & \star & \star \\ \times & \star & \star & \star \\ \times & \star & \star & \star \end{bmatrix}.$$

Definition 1.0.3 (Ultrametric Matrix)**.** For $n \geq 3$, a matrix $M \in \mathbb{R}^{n\times n}$ is (strictly) ultrametric when all of its 3×3 principal submatrices are (strictly) ultrametric. For $n < 3$, any nonzero, nonnegative, symmetric, (strictly) diagonally dominant matrix is (strictly) ultrametric.

From the definition we can immediately deduce that $M \in \mathbb{R}^{n\times n}$ is (strictly) ultrametric if and only if $P^\top MP$ is (strictly) ultrametric for all permutation matrices $P \in \mathbb{R}^{n\times n}$. This, in turn, is the case if and only if $P^\top MP$ is (strictly) ultrametric for *some* permutation matrix $P \in \mathbb{R}^{n\times n}$. Additionally, it follows that M is (strictly) ultrametric if and only if all of its $k \times k$ principal submatrices are, for any $k \geq 3$. These facts will be important later on, and so we capture them in a lemma for future reference.

Lemma 1.0.4. *Let $M \in \mathbb{R}^{n\times n}$, and k an integer such that $3 \leq k \leq n$. The following are equivalent:*

1. *M is (strictly) ultrametric,*
2. *$P^\top MP$ is (strictly) ultrametric for all permutation matrices $P \in \mathbb{R}^{n\times n}$,*
3. *$P^\top MP$ is (strictly) ultrametric for some permutation matrix $P \in \mathbb{R}^{n\times n}$,*
4. *All $k \times k$ principal submatrices of M are (strictly) ultrametric.*

Finally, we define the *Gramian*, which we will need later on.

Definition 1.0.5 (Gramian)**.** Let $U \in \mathbb{R}^{n\times n}$. Then the matrix $U^\top U$ is called the *Gramian* of U.

1.1. The Inverse of an Ultrametric Matrix

In addition to ultrametric matrices, we define the class of Stieltjes matrices. Remember that a symmetric matrix $A \in \mathbb{R}^{n\times n}$ is called *positive definite* if for all nonzero $z \in \mathbb{R}^n$ the product $z^\top Az$ is positive. In similar ways A can be nonnegative, nonpositive and negative definite.

Definition 1.1.1 (Stieltjes Matrix)**.** A symmetric matrix $M \in \mathbb{R}^{n\times n}$ is called *Stieltjes*[1] if it is positive definite and all of its off-diagonal entries are nonpositive.

Proposition 1.1.2. *Let $S \in \mathbb{R}^{n\times n}$ be a Stieltjes matrix. Then S is invertible, and S^{-1} is symmetric and nonnegative.*

Proof. See [18] for a proof. □

[1]After the Dutch mathematician Thomas Joannes Stieltjes (1856 - 1894).

The converse of this statement does not hold in general for $n \geq 3$, in other words, for any $n \geq 3$ there exists a nonnegative, symmetric, invertible matrix whose inverse is not Stieltjes. To see this for $n = 3$, consider the matrix M_3 and its inverse M_3^{-1} given by

$$M_3 = \begin{bmatrix} 4 & 0 & 1 \\ 0 & 4 & 2 \\ 1 & 2 & 4 \end{bmatrix}, \; M_3^{-1} = \frac{1}{44}\begin{bmatrix} 12 & 2 & -4 \\ 2 & 15 & -8 \\ -4 & -8 & 16 \end{bmatrix}.$$

Then, for $n > 3$, consider the matrix M_n and its inverse M_n^{-1} given by

$$M_n = \begin{bmatrix} M_3 & 0 \\ 0 & I_{n-3} \end{bmatrix}, \; M_n^{-1} = \begin{bmatrix} M_3^{-1} & 0 \\ 0 & I_{n-3} \end{bmatrix}.$$

We see that M_n is again nonnegative and symmetric, but M_n^{-1} is not Stieltjes, since M_3^{-1} is not.

The next theorem tells us that ultrametricity is a sufficient condition for the converse of Theorem 1.1.2 to hold.

Theorem 1.1.3. *Let $M \in \mathbb{R}^{n\times n}$ be a strictly ultrametric matrix. Then $M = [m_{ij}]$ is invertible and $M^{-1} = [\mu_{ij}]$ is a strictly diagonally dominant Stieltjes matrix for which*

$$m_{ij} = 0 \iff \mu_{ij} = 0.$$

We shall follow a proof due to Varga and Nabben [14], which requires two lemmas. Firstly, write $e_n \in \mathbb{R}^n$ for the all-ones vector and $E_n := e_n e_n^\top$ for the $n \times n$ all-ones matrix. For any matrix M write $\min(M)$ for the value of a minimal element of M, and finally write $N_n := \{1, 2, \ldots, n\}$.

Lemma 1.1.4. *Let $M = [m_{ij}] \in \mathbb{R}^{n\times n}$ be a symmetric, nonnegative matrix. For $n > 1$, we have that M is ultrametric if and only if there exists a postive integer $k < n$ and a permutation matrix $P \in \mathbb{R}^{n\times n}$ such that*

$$P^\top\big(M - \min(M)E_n\big)P = \begin{bmatrix} C & 0 \\ 0 & D \end{bmatrix},$$

where $C \in \mathbb{R}^{k\times k}$ and $D \in \mathbb{R}^{(n-k)\times(n-k)}$ are both strictly ultrametric. We say that $M - \min(M)E_n$ is completely reducible*.*

We will give a proof of this lemma and look at some of its further implications in the next section. The second lemma we need is a general form of the Sherman-Morrison formula [2], which we will not derive here.

Lemma 1.1.5 (Sherman-Morrison Formula)**.** *Let $M \in \mathbb{R}^{n\times n}$ be an invertible matrix, and $x, y \in \mathbb{R}^n$ vectors such that $1 + v^\top M^{-1}u \neq 0$. Then $M + uv^\top$ is invertible and*

$$(M + uv^\top)^{-1} = M^{-1} - \frac{M^{-1}uv^\top M^{-1}}{1 + v^\top M^{-1}u}.$$

Now, we give a proof of the main theorem, following [14].

Proof of Theorem 1.1.3. We prove by induction on n. For $n = 1$, the statement is trivial. So assume that for some $n > 1$ the statement holds for all $m < n$, and let $M \in \mathbb{R}^{n\times n}$ be a strictly ultrametric matrix. Using Lemma 1.1.4, there exists a permutation matrix $P \in \mathbb{R}^{n\times n}$ such that

$$PMP^\top = \begin{bmatrix} C & 0 \\ 0 & D \end{bmatrix} + P(\min(M)E_n)P^\top = \begin{bmatrix} C & 0 \\ 0 & D \end{bmatrix} + \min(M)E_n,$$

where $C \in \mathbb{R}^{k\times k}$ and $D \in \mathbb{R}^{(n-k)\times(n-k)}$ for some $k > 0$. Using the induction hypothesis, both C and D are invertible and their inverses are strictly diagonally dominant Stieltjes matrices. But this means that if we set

$$A := \begin{bmatrix} C & 0 \\ 0 & D \end{bmatrix},$$

then A is invertible and A^{-1} is a strictly diagonally dominant Stieltjes matrix.

From the fact that A^{-1} is positive definite it follows that $e_n^\top A^{-1} e_n > 0$, and so $1 + \min(M)e_n^\top A^{-1}e_n$ is positive since $\min(M) \geq 0$. The Sherman-Morrison formula now gives us that

$$(PMP^\top)^{-1} = A^{-1} - \frac{\min(M)A^{-1}e_n e_n^\top A^{-1}}{1 + \min(M)e_n^\top A^{-1}e_n} = A^{-1} - c[A^{-1}e_n e_n^\top A^{-1}], \tag{1.1}$$

for some $c \geq 0$. Writing $p := A^{-1}e_n$, we have $p > 0$ and $cpp^\top = c[A^{-1}e_n e_n^\top A^{-1}]$, which means $c[A^{-1}e_n e_n^\top A^{-1}]$ is nonnegative definite, with nonnegative entries. So subtracting $c[A^{-1}e_n e_n^\top A^{-1}]$ from A^{-1}, which is Stieltjes, yields a matrix which has nonpositive off-diagonal entries.

To show that $(PMP^\top)^{-1}$ is strictly diagonally dominant, write $p = [p_1, p_2, \ldots, p_n]^\top$ and $|p| = \sum_i p_i > 0$ and consider the i-th entry of $(PMP^\top)^{-1}e_n$, which is the i-th row sum of $(PMP^\top)^{-1}$:

$$((PMP^\top)^{-1}e_n)_i = p_i - \frac{\min(M)|p|p_i}{1 + \min(M)|p|} = \frac{p_i}{1 + \min(M)|p|} > 0.$$

Since all the off-diagonal entries of $(PMP^\top)^{-1}$ are nonpositive, the fact that all of the row sums of $(PMP^\top)^{-1}$ are positive implies that $(PMP^\top)^{-1}$ is strictly diagonally dominant, and has positive diagonal elements. This immediately gives us that $(PMP^\top)^{-1}$ is positive definite, as $z^\top(PMP^\top)^{-1}z$ is surely positive for $z > 0$. So $(PMP^\top)^{-1}$ is Stieltjes, which means M^{-1} is Stieltjes as can easily be verified using

$$(PMP^\top)^{-1} = (P^\top)^{-1}M^{-1}P^{-1} = PM^{-1}P^\top.$$

Now, to conclude the proof we must show that the zero entries of M correspond precisely to the zero entries of M^{-1}. This follows from a relatively straightforward computation using Lemma 1.1.4, and considering the cases $\min(M) = 0$ and $\min(M) > 0$ seperately. Details can be found in [14]. □

1.2. The Varga-Nabben Decomposition

In this section we will focus on a decomposition of strictly ultrametric matrices. First, we give a proof of Lemma 1.1.4, following the proof given in [14].

Proof of Lemma 1.1.4. First assume that M is strictly ultrametric. If $n = 2$, the result is trivial, so assume $n \geq 3$ and set

$$M' = [m'_{ij}] = M - \min(M)E_n \in \mathbb{R}^{n\times n}.$$

Clearly, M' is again symmetric and nonnegative, and $\min(M') = 0$. Furthermore, since we subtracted a multiple of the all-ones matrix, we have that

$$m_{ij} \leq m_{kl} \iff m'_{ij} \leq m'_{kl}, \text{ for all } i, j, k, l \in N_n.$$

It follows immediately that M' is a strictly ultrametric matrix. From this, using the fact that the diagonal elements of M' must be maximal in their rows, and $n > 1$, we know that some off-diagonal element of M' is equal to zero.

Using Lemma 1.0.4, we may assume without loss of generality that $m'_{1,n} = 0$, using a suitable permutation. Define

$$S_1 := \{j \in N_n : m'_{1,j} = 0\} \text{ and } S_2 := \{j \in N_n : m'_{1,j} > 0\}.$$

Then $n \in S_1$, and $1 \in S_2$, since M' is *strictly* ultrametric. Furthermore, by nonnegativity of M' we have $N_n = S_1 \cup S_2$ and since $S_1 \cap S_2 = \varnothing$ by definition, S_1 and S_2 partition N_n. Using this we may assume that

$$S_2 = \{1, 2, \ldots, r\} \text{ and } S_1 = \{r + 1, r + 2, \ldots, n\}$$

for some positive integer $k < n$, again using Lemma 1.0.4.

Now let $i \in S_1$ and $j \in S_2$. Consider the 3×3 principal submatrix of M' given by

$$A := \begin{bmatrix} a_{1,1} & a_{1,j} & a_{1,i} \\ a_{j,1} & a_{j,j} & a_{j,i} \\ a_{i,1} & a_{i,j} & a_{i,i} \end{bmatrix} = \begin{bmatrix} a_{1,1} & a_{1,j} & 0 \\ a_{j,1} & a_{j,j} & a_{j,i} \\ 0 & a_{i,j} & a_{i,i} \end{bmatrix}.$$

By ultrametricity of M' we must have that $a_{1,j} = 0$ or $a_{j,i} = 0$ to satisfy condition three of Definition 1.0.1. But $a_{1,j} > 0$ since $j \in S_2$, and so $a_{j,i} = 0 = a_{i,j}$, using the fact that M' is symmetric. But this implies that M' has the block structure

$$M' = \begin{bmatrix} C & 0 \\ 0 & D \end{bmatrix},$$

with $C \in \mathbb{R}^{k\times k}$ and $D \in \mathbb{R}^{(n-k)\times(n-k)}$. Noting that the blocks C and D in M' are principal submatrices of M', and using Lemma 1.0.4, we can conclude that C and D are strictly ultrametric. So M' has the desired form.

For the converse, it is enough to check that for strictly ultrametric $C \in \mathbb{R}^{k\times k}$, $D \in \mathbb{R}^{(n-k)\times(n-k)}$ and $c \geq 0$ the matrix

$$\begin{bmatrix} C & 0 \\ 0 & D \end{bmatrix} + cE_n$$

is strictly ultrametric, which follows quickly from the definitions. $\square$

Naturally, we can apply the above lemma to the resulting blocks C and D, and then again to the four resulting blocks of that decomposition and so forth until we are left with only 1×1 blocks, each of which must be positive. The process is best illustrated with an example. Consider the 4×4 strictly ultrametric matrix

$$M = \begin{bmatrix} 3 & 2 & 1 & 2 \\ 2 & 5 & 1 & 3 \\ 1 & 1 & 6 & 1 \\ 2 & 3 & 1 & 4 \end{bmatrix}$$

Then $\min(M) = 1$ and so using the lemma $M - E_4$ should be completely reducible. Using the notation from earlier, we have $S_1^M = \{3\}$ and $S_2^M = \{1, 2, 4\}$, and so $M - E_4$ should reduce to a 1×1 and a 3×3 block. Indeed, selecting the right permutation matrix P we have

$$P^\top(M - E_4)P = P^\top \begin{bmatrix} 2 & 1 & 0 & 1 \\ 1 & 4 & 0 & 2 \\ 0 & 0 & 5 & 0 \\ 1 & 2 & 0 & 3 \end{bmatrix} P = \begin{bmatrix} 2 & 1 & 1 & 0 \\ 1 & 3 & 2 & 0 \\ 1 & 2 & 4 & 0 \\ 0 & 0 & 0 & 5 \end{bmatrix} =: \begin{bmatrix} C & 0 \\ 0 & D \end{bmatrix}.$$

So let us continue to decompose C. We have $\min(C) = 1$, $S_1^C = \{1, 2\}$ and $S_2^C = \{3\}$, so $C - E_3$ reduces to a 2×2 and a 1×1 block. Indeed, selecting the right permutation P we have

$$P^\top(C - E_3)P = P^\top \begin{bmatrix} 1 & 0 & 0 \\ 0 & 2 & 1 \\ 0 & 1 & 3 \end{bmatrix} P = \begin{bmatrix} 3 & 1 & 0 \\ 1 & 2 & 0 \\ 0 & 0 & 1 \end{bmatrix} =: \begin{bmatrix} F & 0 \\ 0 & G \end{bmatrix}.$$

Lastly, $\min(F) = 1$, $S_1^F = \{2\}$, $S_2^F = \{1\}$ and

$$F - E_2 = \begin{bmatrix} 2 & 0 \\ 0 & 1 \end{bmatrix}.$$

If we use the notation that for any $S \subseteq N_n$ the vector $u(S) = [u_i]$, where $u_i = 1$ if $\in S$ and $u_i = 0$ otherwise, and e^i is the i-th standard basis vector for all $1 \leq i \leq n$, then we have decomposed M into seven rank one matrices as follows:

$$M = u(N_4)u(N_4)^\top + u(S_2^M)u(S_2^M)^\top + u(S_2^C)u(S_2^C)^\top + e^4(e^4)^\top + 5e^3(e^3)^\top + 2e^2(e^2)^\top + e^1(e^1)^\top,$$

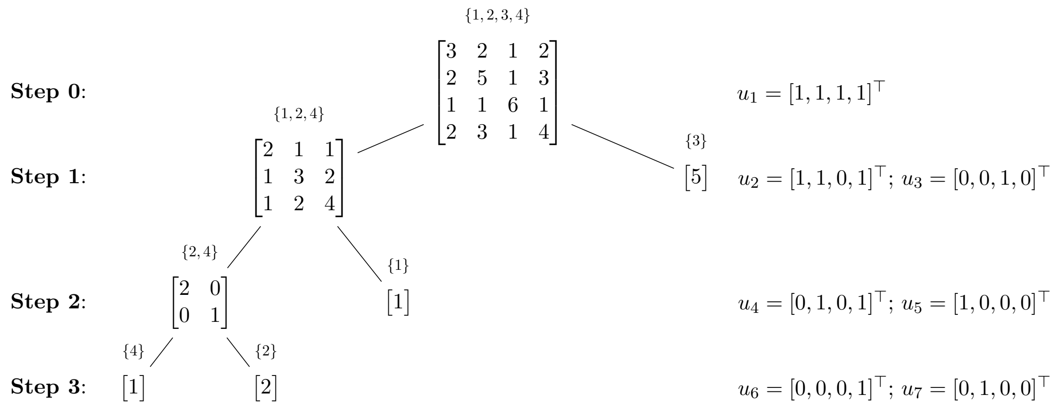


Figure 1.1.: The rooted tree associated with a 4×4 strictly ultrametric matrix.

or, more succinctly:

$$M = \sum_{i=1}^{7} \mu_i u_i u_i^\top, \tag{1.2}$$

for constants $\tau_i \in \mathbb{R}$ and u_i as described, where in this case $\tau_i > 0$ for all $1 \leq i \leq n$.

The entire process can be captured in a rooted binary tree quite nicely. The root node represents M itself. Inductively, the two children of each node represent the matrices C and D from the decomposition. The leaves of the tree represent the 1×1 blocks that cannot be reduced further. The tree associated to the decomposition of the example above is given in Figure 1.1. We have also given the corresponding vectors u_i in each step, as well as the sets that N_n is split up into.

From the example, we see that in the general case a strictly ultrametric $M \in \mathbb{R}^{n \times n}$ reduces to the linear combination of $2n-1$ rank one-matrices as in equation 1.2. Taking a closer look at the constants τ_i in this equation, we see that $\tau_i \geq 0$ whenever u_i corresponds to a decomposing step, since in this case it is the minimum of a strictly ultrametric (and thus nonnegative) matrix. On the other hand, $\tau_i > 0$ if it corresponds to one of the entries in the resulting diagonal matrix at the end of the decomposition, since the elements of that matrix are positive by Lemma 1.1.4. We summarize these findings in the following theorem.

Theorem 1.2.1 (Varga-Nabben)**.** *Let $M \in \mathbb{R}^{n \times n}$ be strictly ultrametric. Then there exist constants $\tau_i \geq 0$ such that*

$$M = \sum_{i=1}^{2n-1} \tau_i u_i u_i^\top,$$

where the vectors u_i have only zeroes and ones as elements and are derived from the rooted binary tree associated to M. Furthermore, all of the standard basis vectors of $\mathbb{R}^n$ are present in the decomposition and τ_i is positive whenever u_i is equal to one of these basis vectors. We refer to this decomposition as the Varga-Nabben decomposition of M.

Corollary 1.2.2. *If $M \in \mathbb{R}^{n\times n}$ is strictly ultrametric, then M is positive definite.*

Proof. By Theorem 1.2.1 M can be written as a nonnegative linear combination of positive definite matrices, and so M is nonnegative definite. Since this decomposition includes a positive diagonal matrix as well, M must be positive definite. $\square$

In conclusion of this section, we prove a theorem about the decomposition of a strictly ultrametric matrix $M \in \mathbb{R}^{n\times n}$ whose entries are all integers.

Theorem 1.2.3. *Let $M \in \mathbb{R}^{n\times n}$ be a strictly ultrametric matrix, all of whose entries are integers. Then there exists some $k \in \mathbb{N}$ and a matrix $U \in \mathbb{R}^{k\times n}$ whose entries are all either zero or one, such that U has at most $2n-1$ distinct rows and M is equal to the Gramian of U.*

Proof. Consider the Varga-Nabben decomposition

$$M = \sum_{i=1}^{2n-1} \tau_i u_i u_i^\top$$

of M. Per construction, all of the constants τ_i are nonnegative integers. Furthermore, $\sum_i \tau_i > 0$ and as such, we may write

$$M = \sum_{i=1}^{2n-1} \sum_{j=1}^{\tau_i} u_i u_i^\top.$$

Now, writing $\tau := \sum_i \tau_i$, consider the matrix $U \in \mathbb{R}^{\tau\times n}$ given by

$$U^\top = [\ \underbrace{u_1 \ \ \ldots \ \ u_1}_{\tau_1} \mid \underbrace{u_2 \ \ \ldots \ \ u_2}_{\tau_2} \mid \ldots \mid \underbrace{u_n \ \ \ldots \ \ u_n}_{\tau_n}\ ].$$

Note that the elements of U are all either zero or one, and that U has at most $2n-1$ distinct rows (since each row of U is equal to one of the $2n-1$ vectors from the rooted binary tree associated with M). Finally, the rules of matrix multiplication give us that $U^\top U = M$, or in other words that M is the Gramian of U, proving the theorem. $\square$

To illustrate the theorem above, consider again the 4×4 strictly ultrametric matrix M from before. Using the notation from Figure 1.1, we found that

$$M = u_1u_1^\top + u_2u_2^\top + 5u_3u_3^\top + u_4u_4^\top + u_5u_5^\top + u_6u_6^\top + 2u_7u_7^\top,$$

and so we have $M = U^\top U$, where

$$U^\top = \left[\begin{array}{c|c|ccccc|c|c|c|cc} 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 1 \\ 1 & 0 & 1 & 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 \end{array}\right].$$

2. 0/1-Simplices

We begin by defining *simplices.*

Definition 2.0.1 (n-simplex)**.** Let $k \geq n$. An n-simplex S is the convex hull of $v_0 = \mathbf{0} \in \mathbb{R}^k$ and n linearly independent vectors $v_1, \ldots, v_n \in \mathbb{R}^k$. We will refer to the v_i as the vectors *spanning* S, or as the *vertices* of S.

As is clear from the definition, an n-simplex is indeed an n-dimensional geometric object (i.e. is it is not contained in any $(n-1)$-dimensional hyperplane). If S is an n-simplex with vertices $v_0 = 0, v_1, \ldots, v_n$, then the convex hull of $n-1$ distinct vertices of S is called a *facet.* Notice that an n-simplex has $n+1$ facets, all of which are simplices themselves, with the exception of the facet F_0 spanned by $v_1, v_2, \ldots, v_n$. Translating F_0 along one of its vertices v_i, however, will result in a simplex F_0' spanned by the vertices $v_j - v_i$ and so F_0 is congruent to a simplex.

We are interested specifically in n-simplices whose vertices are the vertices of the n-dimensional unit cube in $\mathbb{R}^n$. Let us first introduce some notation. We define the unit n-cube as the set $I_n = [0,1]^n \subseteq \mathbb{R}^n$. We write $\mathbb{I} := \{0,1\}$, so that $\mathbb{I}^n = \{0,1\}^n$ is the set containing the vertices of I_n. Finally, we write $\mathbb{I}^{n\times n}$ for the set of matrices whose columns are vertices of I_n, that is the matrices with entries 0 and 1. We will call these 0/1-matrices.

Definition 2.0.2. A 0/1-n-simplex S is the convex hull of $v_0 = \mathbf{0}$ and n linearly independent vectors $v_1, \ldots, v_n \in \mathbb{I}^n$. A 0/1-$n$-simplex is, in particular, an n-simplex.

From here we will mostly limit ourselves to 0/1-simplices, although most of the theory we cover in the rest of this chapter also applies to the general case. In order to analyse simplices using linear algebra, we would like to represent them using a matrix. A fairly obvious choice would be to simply use the vertices of the simplex as columns, resulting in a $n \times (n+1)$-matrix. Since all simplices have $\mathbf{0}$ as a vertex though, we can do better than this.

Definition 2.0.3 (Matrix representation)**.** Let S be a 0/1-n-simplex. We say that $[m_1\ m_2\ \ldots\ m_n] = M \in \mathbb{I}^{n\times n}$ is a *matrix representation* of S if S is spanned by $\mathbf{0}$ and $m_1, m_2, \ldots, m_n$.

Note that each 0/1-simplex has at least one matrix representation, and that if M, N are both matrix representations of the same 0/1-simplex, then they have the same set of columns, or in other words, we have $M = NP$ for some permutation matrix P. Furthermore, if $M \in \mathbb{I}^{n\times n}$ is a matrix representation of some 0/1-n-simplex, then M is invertible. Conversely, if $M \in \mathbb{I}^{n\times n}$ is invertible, then it is a matrix representations of some 0/1-n-simplex S. This is S is unique and we will call it the simplex represented by M.

2.1. Symmetries of the n-Cube

Write $\mathcal{H}_n$ for the set of all symmetries of the n-cube, that is the set of all affine isometries $I^n \to I^n$. Then $\mathcal{H}_n$ is a group under composition with the identity as unit element, called the *hyperoctahedral* group.

Let $h \in \mathcal{H}$. Since h is an affine map, it is determined uniquely by the image of $\mathbf{0}$ and the standard basis vectors $\{e^i\}$ of $\mathbb{R}^n$. Now, because h is an isometry $I^n \to I^n$, we have $h(\mathbf{0}) \in \mathbb{I}^n$. Furthermore, for any $1 \leq i \leq n$, we know that $||h(\mathbf{0}) - h(e^i)|| = 1$, since $||0 - e^i|| = 1$. Since $\mathbb{I}^n$ has 2^n elements, and for each $v \in \mathbb{I}^n$ there are n distinct $w \in \mathbb{I}^n$ with $||v - w|| = 1$, we may conclude that $\mathcal{H}_n$ has order $2^n \cdot n!$. Additionally, we can give a set of generators of $\mathcal{H}_n$ by simply considering $h \in \mathcal{H}$ that permute the basis vectors, or map $\mathbf{0}$ to some $v \in \mathbb{I}^n$ in a suitable way. As is shown in [4], this results in the following proposition.

Proposition 2.1.1. *Write $e^0 := \mathbf{0}$. For $1 \leq i < n, v \in \mathbb{I}^n$, define affine isometries $\phi_i, \xi_v : I^n \to I^n$ by*

$$\phi_i(e^j) = \begin{cases} e_{j+1} & \text{if } j = i, \\ e_{j-1} & \text{if } j = i+1, \\ e_j & \text{otherwise.} \end{cases} \quad \text{and } \xi_v(e^j) = \begin{cases} v + e^j & \text{if } v^\top e^j = 0, \\ v - e^j & \text{if } v^\top e^j = 1. \end{cases}$$

Then ϕ_i, ξ_v generate $\mathcal{H}_n$.

Essentially, these generators are just reflections in properly chosen $(n-1)$-dimensional hyperplanes, as can be seen for $n = 2$ in the following example.

Example 2.1.1. For $n = 2$ we have $\mathcal{H}_2$, the set of symmetries of the square I_2, with vertices $\{\mathbf{0}, e^1, e^2, e_2\}$. Using the notation of Proposition 2.1.1, it is generated by the maps $\phi_1, \xi_{e^1}, \xi_{e^2}$ and ξ_{e_2}. As can be seen in Figure 2.1, these maps correspond to reflections in the lines

$$\begin{aligned} l_1 &= \operatorname{Span}(e_2), \\ l_2 &= \operatorname{Span}(e^2) + \frac{1}{2}e^1, \\ l_3 &= \operatorname{Span}(e^1) + \frac{1}{2}e^2, \\ l_4 &= \operatorname{Span}(e^1 - e^2) + e^1 = \operatorname{Span}(e^2 - e^1) + e^2, \end{aligned}$$

respectively.

If S, T, and U are 0/1-n-simplices such that $S = H_1(T)$ and $T = H_2(Q)$ for some $H_1, H_2 \in \mathcal{H}_n$, then $S = H_3(T)$, where $H_3 := (H_1 \circ H_2) \in \mathcal{H}_n$. This observation leads to an equivalence relation on 0/1-n-simplices.

Definition 2.1.2. Let S_1 and S_2 be two 0/1-n-simplices. We say they are *0/1-equivalent* if $S_1 = H(S_2)$ for some $H \in \mathcal{H}_n$. We shall write $S_1 \simeq_{01} S_2$.

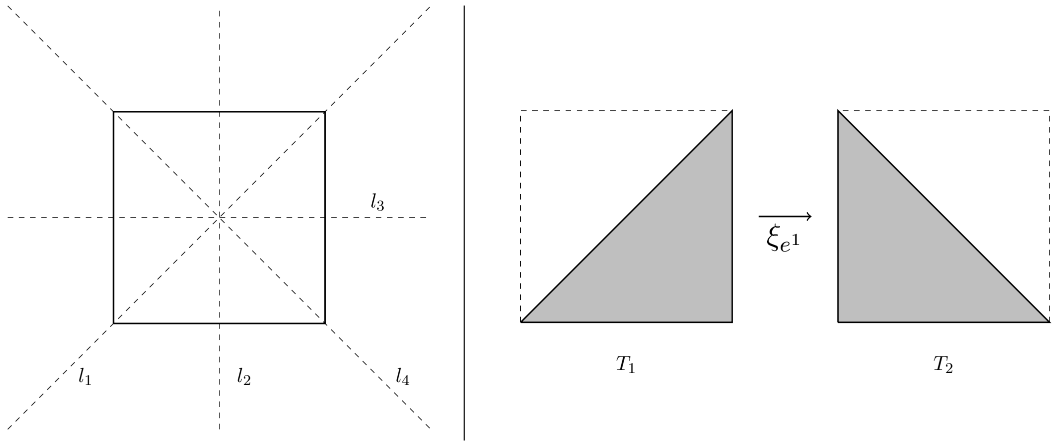


Figure 2.1.: The generators of $\mathcal{H}_2$ (left) and an example of two 0/1-equivalent simplices (right).

If S and T are two 0/1-simplices such that $S = H(T)$ for some $H \in \mathcal{H}_n$, then S and T are congruent. The converse does not always hold, as an example in [19] shows.

This equivalence on simplices induces an equivalence relation on invertible 0/1-matrices very naturally. If $M, N \in \mathbb{I}^{n\times n}$ are invertible, and S_M, S_N are the simplices they represent, we say that M and N are 0/1-equivalent if and only if $S_M \simeq_{01} S_K$, and we write $M \simeq_{01} N$. It follows immediately that if two simplices have 0/1-equivalent matrix representations, then they are 0/1-equivalent themselves.

Example 2.1.2. The triangles T_1, spanned by $[0,0]^\top, [0,1]^\top, [1,0]^\top \in \mathbb{I}^2$ and T_2, spanned by $[0,0]^\top, [0,1]^\top, [1,1]^\top \in \mathbb{I}^2$ are both 0/1-2-simplices. As can be seen in Figure 2.1, we have $T_2 = \xi_{e^1}(T_1)$ so that $T_1 \simeq_{01} T_2$. Since we have matrix representations

$$M_1 = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix},\ M_2 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \text{ for } T_1, \text{ and}$$
$$M_3 = \begin{bmatrix} 1 & 0 \\ 1 & 1 \end{bmatrix},\ M_4 = \begin{bmatrix} 0 & 1 \\ 1 & 1 \end{bmatrix} \text{ for } T_2,$$

it follows immediately that $M_1 \simeq_{01} M_2 \simeq_{01} M_3 \simeq_{01} M_4$.

To end this section, we tie 0/1-equivalence of simplices to 0/1-equivalence of their matrix representations in a new way, that will be of great practical use later on. For this purpose we will need the xor-operator, which we will define now.

Definition 2.1.3 (The xor-operator)**.** Let $p, q \in \mathbb{I}$. We define $\mathrm{xor} : \mathbb{I} \times \mathbb{I} \to \mathbb{I}$ by

$$\mathrm{xor}(p,q) = \mathrm{xor}(q,p) = \begin{cases} 1 & \text{if } p \neq q, \\ 0 & \text{if } p = q. \end{cases}$$

Additionally, letting $m, k \in \mathbb{I}^n$, we define $\mathrm{xor} : \mathbb{I}^n \times \mathbb{I}^n \to \mathbb{I}^n$ elementwise by

$$\mathrm{xor}(m,k)_i = \mathrm{xor}(m_i, k_i).$$

Finally, letting $M \in \mathbb{I}^{n\times n}$, with columns m_i, and $m \in \mathbb{I}^n$, we define $\mathrm{xor} : \mathbb{I}^{n\times n} \times \mathbb{I}^n \to \mathbb{I}^{n\times n}$ by

$$\mathrm{xor}(M, m) = \begin{bmatrix}\mathrm{xor}(m_1, m) & \mathrm{xor}(m_2, m) & \dots & \mathrm{xor}(m_n, m)\end{bmatrix}.$$

Proposition 2.1.4. *Let $M, N \in \mathbb{I}^{n\times n}$ then $M \simeq_{01} N$ if and only if there exist permutation matrices $P, Q \in \mathbb{R}^{n\times n}$, and a column m_i of M such that*

$$N = P \cdot \mathrm{xor}(M, m_i) \cdot Q \text{ or } N = PMQ.$$

Using the set of generators for $\mathcal{H}_n$ from Proposition 2.1.1 the following two lemmas prove the proposition above.

Lemma 2.1.5. *Let S be a 0/1-n-simplex with matrix representation M, and let $v \in \mathbb{I}^n$. Then, using the notation from Proposition 2.1.1, we have that $\xi_v(S)$ is a 0/1-n-simplex if and only if v is a vertex of S. When this is the case,* $\mathrm{xor}(M, v)$ *is a matrix representation of $\xi_v(S)$.*

Proof. Suppose that v is not a vertex of S. Then by definition of ξ_v, the origin is not an element of $\xi_v(S)$ and so $\xi_v(S)$ is not a 0/1-n-simplex. On the other hand, if v *is* a vertex of S, then $\xi_v(S)$ contains the origin since $\xi_v(v) = \mathbf{0}$. Furthermore, ξ_v maps the vertices of S to $\mathbb{I}^n$, and since ξ_v is an affine isometry, this means that $\xi_v(S)$ is indeed a 0/1-n-simplex. It follows quite quickly from the definition that $\xi_v(w) = \mathrm{xor}(w, v)$, which in turn immediately implies that $\mathrm{xor}(M, v)$ is a matrix representation of $\xi_v(S)$. $\square$

Lemma 2.1.6. *Let S be a 0/1-n-simplex with matrix representation M, and let $1 \leq i \leq n$. Then, using the notation from Proposition 2.1.1, we have that $\phi_i(S)$ is a 0/1-n-simplex and PM is a matrix representation of $\phi_i(S)$, for some permutation matrix P.*

Proof. Since $\phi_i(S)$ is a linear isometry, $\phi_i(S)$ is surely a 0/1-n-simplex. Furthermore, it is immediately clear from the definition that if P_i is the permutation matrix corresponding to the cycle $(i\ i+1)$ we have $\phi_i(v) = P_i v$ for all $v \in \mathbb{R}^n$. This in turn implies that PM is a matrix representation of $\phi_i(S)$. $\square$

2.2. The Gramian of a 0/1-Simplex

So far, matrix representations of 0/1-simplices have aided us only in determining 0/1-equivalence. We will be able to use them to describe the geometrical properties of 0/1-simplices in much more detail following methodology of Brandts et al. [12].

Let S be a 0/1-n-simplex with matrix representation $M \in \mathbb{I}^{n\times n}$. The n facets F_j, $1 \leq j \leq n$, of S that contain $\mathbf{0}$, then, can be given by taking the convex hull of $\mathbf{0}$ and the columns of M, except for the j-th one. If we write $M_j \in \mathbb{I}^{n\times(n-1)}$ for M without its j-th column, we have $F_j \subseteq \mathrm{Span}(M_j)$, which is an $n-1$ dimensional hyperplane in $\mathbb{R}^n$.

We define the *height* h_j of S relative to F_j as the Euclidian distance between m_j and $\text{Span}(M_j)$ (i.e. $||m_j - \text{Proj}_{\text{Span}(M_j)}(m_j)||$). Since M is invertible, there exists a matrix $Q \in \mathbb{R}^{n\times n}$ with columns q_i such that $Q = (M^{-1})^\top$, or in other words $Q^\top M = I_n$.

We write $e_n^i \in \mathbb{R}^n$ for the i-th basis vector of $\mathbb{R}^n$, and $e_n \in \mathbb{R}^n$ for the all-ones vector. Since M_j misses the j-th column of M, $q_j^\top M_j = 0$ ($q_j^\top M$ would be equal to e^j). So q_j is orthogonal to $\text{Span}(M_j)$. Furthermore, $q_j^\top m_j = 1$ and so q_j points towards m_j. For these reasons, we call q_j an *inward normal* of F_j.

Proposition 2.2.1. *Using the same notation as above,* $||q_j|| = h_j^{-1}$ *for all* $1 \leq j \leq n$.

Proof. We have

$$h_j = ||m_j - \text{Proj}_{\text{Span}(M_j)}(m_j)|| = \frac{m_j^\top q_j}{||q_j||} = \frac{1}{||q_j||}. \qquad \square$$

It remains to find an inward normal for the facet F_0, the convex hull of the columns of M.

Proposition 2.2.2. *Using the same notation as above, the vector* $q_0 = -Qe_n$ *is an inward normal of* F_0. *Furthermore,* $h_0^{-1} = ||q_0||$.

Proof. We first define a new simplex $\hat{S}$ by shifting S along m_1, so $\hat{S}$ is the simplex spanned by $\mathbf{0}, -m_1, m_2 - m_1, m_3 - m_1, \ldots, m_n - m_1$. Although $\hat{S}$ is no longer a 0/1-simplex, it is congruent to S. The facet $\hat{F}_0$ of $\hat{S}$ that corresponds to F_0 is spanned by $\mathbf{0}$ and the vectors $m_j - m_1$, $1 < j \leq n$. We have

$$e_n^\top Q(p_1 - p_j) = e_n^\top(e_n^1 - e_n^j) = 1 - 1 = 0$$

and

$$m_i^\top Qe_n = (e_n^1)^\top e_n = 1,$$

showing that $-Qe_n$ is orthogonal to $\hat{F}_0$ and $|| - Qe_n||$ is the inverse of the height of $\hat{F}_0$ relative to $\hat{S}$. Since $\hat{S}$ is just a translated copy of S, the same holds in S. $\square$

Using the inward normals, we can define the *dihedral angles* between the facets of a simplex. To be safe, we first recall the definition of angles between vectors.

Definition 2.2.3 (Angle)**.** Let $v, w \in \mathbb{R}^n$, then the *angle* γ between v and w is defined as

$$\gamma = \cos^{-1}\Big(\frac{v^\top w}{||v||||w||}\Big) \in [0, \pi).$$

Definition 2.2.4 (Dihedral angles)**.** Let S be a $0/1$-n-simplex with facets F_j and inward normals q_j for $0 \leq j \leq n$, and let $\gamma_{ij} \in (0, \pi)$ be the angle between q_i and q_j. Then we define the *dihedral angle* $\alpha_i j$ between F_i and F_j as

$$\alpha_{ij} = \pi - \gamma_{ij} \in (0, \pi).$$

Furthermore, if $\alpha_{ij} < \frac{1}{2}\pi$ we say α_{ij} is *acute*, if $\alpha = \frac{1}{2}\pi$ we say α_{ij} is *right* and if $\alpha_{ij} > \frac{1}{2}\pi$ we say α_{ij} is *obtuse*.

In accordance with the above definition, we say a simplex is *acute* when all of its dihedral angles are acute, *non-obtuse* when none of its dehedral angles are obtuse and *obtuse* if at least one of its dihedral angles is obtuse.

The main point of this section is to show that qualitive information about the dihedral angles of S can be derived from the Gramian of Q very easily.

Theorem 2.2.5. *Let S be a 0/1-n-simplex with matrix representation $M \in \mathbb{I}^{n\times n}$, and let $Q = (M^{-1})^\top$. Then every off-diagonal entry g_{ij} of $G := Q^\top Q$ corresponds to the dihedral angle α_{ij} in the sense that*

$$\alpha_{ij} \text{ is } \begin{cases} \text{acute if } g_{ij} < 0, \\ \text{right if } g_{ij} = 0, \\ \text{obtuse if } g_{ij} > 0. \end{cases}$$

In the opposite way, the i-th row sum $g_i := \sum_j g_{ij}$ of G corresponds to the dihedral angle $\alpha_{0,i}$, so

$$\alpha_{0,i} \text{ is } \begin{cases} \text{acute if } g_i > 0, \\ \text{right if } g_i = 0, \\ \text{obtuse if } g_i < 0. \end{cases}$$

Proof. Using the same notation as before we have

$$g_{ij} = q_i^\top q_j = ||q_i||||q_j|| \cos \gamma_{ij} = ||q_i||||q_j|| \cos(\pi - \alpha_{ij}) = -||q_i||||q_j|| \cos(\alpha_{ij}),$$

and so in particular the sign of g_{ij} is opposite to the sign of $\cos(\alpha_{ij})$, which proves the first part of the theorem. For the second part, note that for $j > 1$

$$g_i = e_n^j G e_n = -q_j^\top q_0 = ||q_0||||q_j|| \cos(\alpha_{0,j}),$$

and so by the same reasoning the second part of the theorem holds. $\square$

The following example illustrates the definitions and results above.

Example 2.2.1. Consider again the 0/1-2-simplex S spanned by $\mathbf{0}$ and the columns of

$$M = \begin{bmatrix} 1 & 1 \\ 0 & 1 \end{bmatrix}.$$

Then M is of course a matrix representation of S. We compute

$$Q := (M^{-1})^\top = \begin{bmatrix} 1 & 0 \\ -1 & 1 \end{bmatrix} \text{ and } G := Q^\top Q = \begin{bmatrix} 2 & -1 \\ -1 & 1 \end{bmatrix}.$$

We find inward normals $q_0 = -Qe_2 = -[1, 0]^\top$, $q_1 = [1, -1]^\top$ and $q_2 = [0, 1]^\top$. Since $g_{1,2} < 0$, we have an acute angle between F_1 and F_2. Since $g_1 > 0$, we have an acute angle between F_0 and F_1. Finally, since $g_2 = 0$, we have a right angle between F_0 and F_2. Figure 2.2 confirms that these findings are indeed correct.

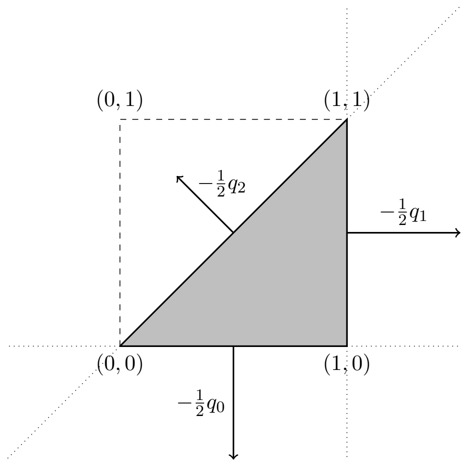


Figure 2.2.: A depiction of S from example 2.2.1. Outward normals are drawn at half size for clarity

.

We end this section by properly naming the matrix $Q^\top Q$ from before and noting that it is equal to the inverse of the Gramian of M for later reference.

Definition 2.2.6 (Simplex Gramian)**.** Let S be a 0/1-n-simplex with matrix representation M Then, setting $Q = (M^{-1})^\top$, the matrix $Q^\top Q$ is called a *Gramian* of S.

Remark 2.2.1. In the same notation as the definition above, we have that

$$Q^\top Q = M^{-1}(M^{-1})^\top = (M^\top M)^{-1}.$$

2.3. Ultrametric and Regular Simplices

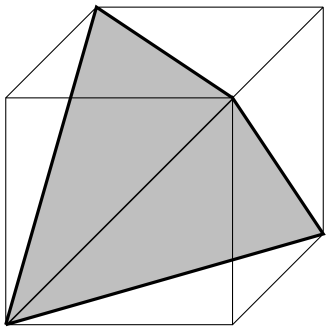
For any two distinct vertices v, w of a simplex S, $(v - w) \in \mathbb{R}^n$ is called an *edge* of S (between v and w). For $n \geq 2$, a 0/1-n-simplex S is called *regular*[1] if all of its edges are of length $\frac{1}{2}\sqrt{2n+2}$. This property can be expressed in terms of the Gramian of a matrix representation of S.

Proposition 2.3.1. *Let S be a 0/1-n-simplex and let M be a matrix representation of S. Define $R_n = [r_{ij}]$ by*

$$r_{ij} = \begin{cases} \frac{1}{2}(n+1) & \text{if } i = j, \\ \frac{1}{4}(n+1) & \text{if } i \neq j. \end{cases}$$

Then S is regular if and only if $M^\top M = R_n$.

[1] Generally, a simplex is called regular if all of its edges are of the same (unspecified) length. In the case of 0/1-simplices, though, this length is determined uniquely by n, and so for the sake of simplicity we fix the edge length in the definition.



$$M = \begin{bmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{bmatrix}$$

$$M^\top M = \begin{bmatrix} 2 & 1 & 1 \\ 1 & 2 & 1 \\ 1 & 1 & 2 \end{bmatrix}$$

Figure 2.3.: A regular 0/1-3-simplex with a matrix representation and Gramian.

Proof. Suppose that S is regular. Consider the edges of S between $\mathbf{0}$ and some vertex $v \neq \mathbf{0}$ of S. We have

$$\frac{1}{2}(n+1) = \big(\frac{1}{2}\sqrt{2n+2}\big)^2 = ||\mathbf{0} - v||^2 = ||v||^2 = \sqrt{v^\top v},$$

We conclude that the diagonal entries m_{ii} of M satisfy $m_{ii} = r_{ii}$. Now consider an edge between two distinct vertices $v, w \neq \mathbf{0}$ of S. We have

$$\frac{1}{2}(n+1) = ||v-w||^2 = (v-w)^\top(v-w) = v^\top v - 2v^\top w + w^\top w = (n+1) - 2v^\top w,$$

and so $v^\top w = \frac{1}{4}(n+1)$, which implies that the off-diagonal entries m_{ij} of M satisfy $m_{ij} = r_{ij}$. So $M = R_n$.

Reversing this argument, we see that S is regular if $M = R_n$, proving the proposition. $\square$

Figure 2.3 illustrates the proposition above for $n = 3$. We can deduce immediately that if $n+1$ is not divisible by four a regular 0/1-n-simplex cannot exist, since the entries of $M^\top M$ are integers. The question remains then, if there does exist a regular 0/1-n-simplex whenever $n \equiv 3 \mod 4$. The answer to this deceptively simple question is unknown, although it has been studied for over a 100 years, primarily in the equivalent form of the *Hadamard Conjecture*, which is expanded upon in Appendix A.

Apparently it is very difficult to say something about regular simplices directly. Instead, we could try to consider a slightly larger class of simplices of which the regular ones are a subclass. It is at this point that we finally arive at the namesake of this project, the *ultrametric simplices.* Note that the matrix R_n from Proposition 2.3.1 is, in particular, ultrametric (see Definition 1.0.3). This motivates the following definition.

Definition 2.3.2 (Ultrametric simplex)**.** Let S be a 0/1-simplex. Then S is called *ultrametric* if S has a Gramian which is ultrametric.

We write $\mathrm{Ult}^{n\times n} \subseteq \mathbb{I}^{n\times n}$ for the set of all 0/1-matrices of order n that represent an ultrametric simplex. It can be shown that if two 0/1-simplices S and T are 0/1-equivalent, then S is ultrametric if and only if T is. This is done by Cihangir [4] by very precisely expressing ultrametricity of a simplex as being a geometrical property. This characterization goes beyond the scope of this project, though.

What we *will* show here, by making use of our findings in Chapter 1, is that ultrametric matrices are, in particular, nonobtuse.

Corollary 2.3.3. *If S is an ultrametric 0/1-simplex, then S is nonobtuse. If, in addition, none of the vertices of S are orthogonal, S is acute.*

Proof. Let S be an ultrametric 0/1-simplex and let $M \in \mathbb{I}^{n\times n}$ be one of its ultrametric matrix representations. Using Theorem 1.1.3, we know that $G = (M^\top M)^{-1}$ is strictly diagonally dominant and Stieltjes. So all of the off-diagonal entries of G are nonpositive, and all of its row-soms are positive. Now, using Theorem 2.2.5 we conclude that S is nonobtuse. If none of the vertices of S are orthogonal, we have $M^TM > 0$. Using the second part of Theorem 1.1.3, this means that the off-diagonal entries of G are negative, which, by Theorem 2.2.5, implies that S is acute. □

Since Cihangir considers acute 0/1-simplices in [4], it will be convenient for us to restrict to acute ultrametric 0/1-simplices. From now on, we assume that ultrametric simplices are acute as well, or in other words that their Gramians do not contain any zeroes.

Remember that using the Varga-Nabben decomposition defined in Chapter 1, we are able to write any ultrametric matrix whose entries are integers as the Gramian of some 0/1-matrix. In particular, we could use the decomposition to find a 0/1-matrix M_n such that $M_n^\top M_n = R_n$. The problem is, of course, that this M_n need not necessarily be *square*, and as such might not be a matrix representation of a 0/1-n-simplex. Instead, the Varga-Nabben decomposition provides us with an n-simplex whose vertices lie in $\mathbb{I}^k$ for some $k \geq n$ that is congruent to the regular 0/1-n-simplex (if it exists). The hope is that through further study of ultrametric 0/1-simplices, we might be able to improve upon the Varga-Nabben decomposition and eventually find a way to write R_n as the Gramian of an $M \in \mathbb{I}^{n\times n}$, thus finding a regular 0/1-n-simplex.

2.4. Minal Representatives

The next half of this project will be dedicated to computationally generating a representative of each 0/1-equivalence class of ultrametric 0/1-n-simplices for small values of n. In particular we wish to find the amount of different classes that exists for each n. Through these explicit examples, more general conjectures might be found. For practical reasons, it will be convenient to define which representative of each class we wish to find. For this purpose we define the *column representation* of a 0/1-matrix.

Definition 2.4.1 (Column representation)**.** Let $M \in \mathbb{I}^{n\times n}$. Then the *column representation* of M is equal to

$$[1, 2, \ldots, 2^n] \cdot M.$$

In other words, it is a row vector containing the decimal representations of the binary numbers given by the columns of M.

We can now define a well-ordering $<_{01}$ on $\mathbb{I}^{n\times n}$ by setting $M <_{01} N$ if and only if the column representation of M is smaller than that of N in terms of lexicographical ordering. Using this ordering, we define the *minimal representative*.

Definition 2.4.2 (Minimal representative)**.** Let E be a 0/1-equivalence class of 0/1-n-simplices, and let $\mathcal{M} \subseteq \mathbb{I}^{n\times n}$ be the set of 0/1-matrices that represent a simplex in E. Then the *minimal representative* of E is the minimal element of $\mathcal{M}$ under $<_{01}$.

For later reference, we also define the *row representation* of a 0/1-matrix.

Definition 2.4.3 (Row representation)**.** Let $M \in \mathbb{I}^{n\times n}$. Then the *row representation* of M is equal to

$$M \cdot \begin{bmatrix} 2^n \\ \dots \\ 2 \\ 1 \end{bmatrix}.$$

In other words, it is a column vector containing the decimal representations of the binary numbers given by the rows of M.

Example 2.4.1. Consider the regular simplices S_1, S_2 represented by

$$M_1 = \begin{bmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{bmatrix},\ M_2 = \begin{bmatrix} 1 & 0 & 1 \\ 0 & 1 & 1 \\ 1 & 1 & 0 \end{bmatrix},$$

respectively. Since M_2 can be obtained from M_1 by swapping the first and second row, we have $S_1 \simeq_{01} S_2$. The row representations of of M_1 and M_2 are

$$M_1 \cdot \begin{bmatrix} 4 \\ 2 \\ 1 \end{bmatrix} = \begin{bmatrix} 3 \\ 5 \\ 6 \end{bmatrix} \text{ and } M_2 \cdot \begin{bmatrix} 4 \\ 2 \\ 1 \end{bmatrix} = \begin{bmatrix} 5 \\ 3 \\ 6 \end{bmatrix}.$$

The column representations of M_1 and M_2 are

$$[1, 2, 4] \cdot M_1 = [6, 5, 3] \text{ and } [1, 2, 4] \cdot M_2 = [5, 6, 3],$$

and so $M_2 <_{01} M_1$ which means in particular that M_1 is not the minimal representative of the 0/1-equivalence class of S_1, S_2.

Before we discuss concrete algorithms and computational results (which we will do in Chapter 4), we will first consider the problem of determining whether two 0/1-matrices are 0/1-equivalent, a crucial element of any further computations, in a context of complexity theory. In this way we will have a general idea of what we might expect later on.

3. Complexity of the 0/1-equivalence problem

The goal of this chapter is to put the problem of determining whether two matrices are 0/1-equivalent into context in terms of complexity. Concretely, we will prove that this problem is easier than determining whether two graphs are isomorphic. In other words, our problem reduces to the well-known problem of graph isomorphism. Before we elaborate on what it is we mean by this exactly, let us first give some basic definitions and results regarding graphs and isomorphisms between them.

3.1. Graphs and Graph Isomorphisms

A graph G is an ordered pair (V, E), where V is a finite, ordered set which elements represent the vertices of G, and E is a set of unordered pairs of distinct elements of V which represent the edges of G. We shall denote $V(G)$ and $E(G)$ for these sets, respectively. The *order* $\operatorname{ord}(G)$ of the graph is $|V|$, the amount of vertices. We say two vertices $v, w \in V$ are *adjacent* when $\{v, w\} \in E$. The *degree* of a vertex is equal to the amount of vertices adjacent to it. The *index* $i(v)$ of a vertex v is its position in the ordering on V. We write $\mathcal{G}$ for the class of all graphs.

A practical way to represent graphs is by their *adjacency matrix.*

Definition 3.1.1 (Adjacency Matrix)**.** Let G be a graph of order k, and let $\{v_i : 1 \leq i \leq k\}$ be its vertex set. Then the *adjacency matrix* $M(G) \in \mathbb{I}^{k\times k}$ of G is the unique matrix such that

$$M(G)_{i,j} = \begin{cases} 1 & \text{if } v_i, v_j \text{ adjacent,} \\ 0 & \text{otherwise.} \end{cases}$$

Note that the adjaceny matrix of a graph is symmetric and all of its diagonal elements are zero and that two graphs which are not equal may have the same adjacency matrix.

In the above definition a renaming or reordering of the vertices of a graph would yield a new graph that is structurally identical to the original, but not equal to it. To capture this structural equivalence, we introduce the notion of a *graph isomorphism.*

Definition 3.1.2 (Graph Isomorphism)**.** Let G and H be two graphs. Then a bijective function $f : V(G) \to V(H)$ is called a *graph isomorphism* when

$$v, w \text{ adjacent in } G \iff f(v), f(w) \text{ adjacent in } H$$

for all $v, w \in V(G)$. If such a function exists, we say that G and H are *(graph) isomorphic*, and we write $G \simeq H$.

It is trivial to show that $\simeq$ is indeed an equivalence relation on graphs.

Definition 3.1.3 (Associated permutation)**.** Let G and H be two graphs, and let $f : G \to H$ be a graph isomorphism. Then G and H have the same order, say k, so we can denote $V = \{v_i : 1 \leq i \leq k\}, W = \{w_i : 1 \leq i \leq k\}$ for their vertex sets. The graph isomorphism f induces a permutation $\sigma : \{1, 2, \dots, k\} \to \{1, 2, \dots, k\}$ by $\sigma(i) = j \iff f(v_i) = w_j$.

Crucial to our later analysis is the fact that the concept of graph isomorphism can be translated to adjacency matrices very naturally.

Proposition 3.1.4. *Let G and H be two graphs. Write $M := M(G)$ and $N := M(H)$ for their adjacency matrices. Then*

$$G \simeq H \iff N = P^\top MP,$$

for some permutation matrix P.

Proof. Denote $V = \{v_i : 1 \leq i \leq |V(G)|\}$, $W = \{w_i : 1 \leq i \leq |V(H)|\}$ for the vertex sets of G and H.

Suppose $G \simeq H$. Let $f : V \to W$ be a graph isomorphism and σ its associated isomorphism. Let P be the permutation matrix corresponding to σ and consider $P^\top MP$. We have that

$$\begin{aligned}(P^\top MP)_{i,j} = 1 &\iff M_{\sigma^{-1}(i),\sigma^{-1}(j)} = 1,\\ &\iff f^{-1}(w_i), f^{-1}(w_j) \text{ are adjacent},\\ &\iff w_i, w_j \text{ are adjacent.}\end{aligned}$$

And so $P^\top MP = N$, the adjacency matrix of H.

Now suppose $N = P^\top MP$ for some permutation matrix P, and let σ be the corresponding permutation. It is easy to see that the function $f : G \to H$ given by $f(v_i) = w_{\sigma(j)}$ is a graph isomorphism. $\square$

We will now take a look at a few subclasses of graphs that we will need later on. Consider a graph G with vertex set V. If a division of V into two disjoint subsets V_1 and V_2 exist such that all edges of G run between a vertex from V_1 and a vertex from V_2 we say G is *bipartite*, or that G is a *bigraph* and we write $G = (V_1 \cup V_2, E)$. We write $\mathcal{G}_{bp} \subseteq \mathcal{G}$ for the class of all bipartite graphs. If, in addition, $i(v) < i(w)$ whenever $v \in V_1$ and $w \in V_2$, we say G is *biordered.* We write $\mathcal{G}_{bi} \subseteq \mathcal{G}_{bp}$ for the class of all biordered graphs.

The reason we are interested in biordered graphs is the very particular form of their adjacency matrices, which follows immediately from their definition.

Proposition 3.1.5. *Let G be a biordered graph of order k, and let $m = |V_1|, n = |V_2|$. Then its adjacency matrix $M(G)$ is of the form*

$$M(G) = \begin{bmatrix} 0 & A \\ A^\top & 0 \end{bmatrix}$$

for some $A \in \mathbb{I}^{m\times n}$. Conversely, any graph with an adjacency matrix of the above form is biordered.

Definition 3.1.6 (Associated Biordered Graph)**.** For any matrix $A \in \mathbb{I}^{k\times k}$ we write $\mathcal{B}_A$ for the unique biordered graph G with vertex set $\{1, 2, \ldots, 2k\}$ and adjacency matrix

$$M(G) = \begin{bmatrix} 0 & A \\ A^\top & 0 \end{bmatrix}.$$

Any graph isomorphism respects bipartiteness. However, in order to ensure biorderedness is respected a restriction is required.

Definition 3.1.7 (Biordered graph isomorphism)**.** Let $G = (V_1 \cup V_2, E)$ and $H = (W_1 \cup W_2, F)$ be biordered graphs. Then a graph isomorphism $f : V(G) \to V(H)$ is called *biordered* when $f(V_1) = W_1$ and $f(V_2) = W_2$. If such an f exists we say that G and H are biorderedly graph isomorphic, and we write $G \simeq_{bi} H$

As can be easily verified from the definition, $\simeq_{bi}$ is an equivalence relation on the biordered graphs. Just like before the concept of biordererd graph isomorphism can be translated to adjacency matrices.

Proposition 3.1.8. *Let $G = (V_1 \cup V_2, E)$ and $H = (W_1 \cup W_2, F)$ be two biordered graphs. Write $M := M(G)$ and $N := M(H)$ for their adjacency matrices, and let $m = |V_1|, n = |V_2|$. We have*

$$G \simeq_{bi} H \iff N = \begin{bmatrix} P^\top & 0 \\ 0 & Q^\top \end{bmatrix} M \begin{bmatrix} P & 0 \\ 0 & Q \end{bmatrix}$$

for certain permutation matrices $P \in \mathbb{R}^{m\times m}$, $Q \in \mathbb{R}^{n\times n}$.

Proof. This follows quickly using Proposition 3.1.4 and the fact that any biordered isomorphism $f : G \to H$ must satisfy $f(V_1) = W_1$ and $f(V_2) = W_2$, which ensures that the permutation matrix associated to f is of the proper form. □

As a corollary, we can tie $\simeq_{bi}$ to 0/1-equivalence on 0/1-matrices.

Corollary 3.1.9. *Let $A, B \in \mathbb{I}^{n\times n}$. Then there exist permutation matrices $P, Q \in \mathbb{R}^{n\times n}$ such that $A = PBQ$ if and only if $\mathcal{B}_A \simeq_{bi} \mathcal{B}_B$.*

Proof. Suppose that $A, B \in \mathbb{I}^{n\times n}$ and $A = PBQ$ for certain permutation matrices $P, Q \in \mathbb{R}^{n\times n}$. Then

$$M(\mathcal{B}_A) = \begin{bmatrix} 0 & A \\ A^\top & 0 \end{bmatrix} = \begin{bmatrix} 0 & PBQ \\ Q^\top B^\top P^\top & 0 \end{bmatrix} = \begin{bmatrix} P & 0 \\ 0 & Q^\top \end{bmatrix} M(\mathcal{B}_B) \begin{bmatrix} P^\top & 0 \\ 0 & Q \end{bmatrix},$$

and so by Proposition 3.1.8 we get $\mathcal{B}_A \simeq_{bi} \mathcal{B}_B$. Reversing this reasoning gives the converse. □

3.2. Computational Complexity

A decision problem is a problem in which a 'yes or no' question must be answered based on some input. An example of this is 'given a natural number p, determine if p is a prime', or 'given two complex numbers z_1 and z_2, determine whether $|z_1| = |z_2|$'. We can formalize this concept as a triple consisting of a class of mathematical objects $\mathcal{U}$ (representing the possible inputs) together with a function $s : \mathcal{U} \to \mathbb{N}$ (representing the *size* of each input) and a class $\mathrm{Y} \subseteq \mathcal{U}$ (representing the inputs which should result in an answer of 'yes').

Example 3.2.1. Write $\mathbb{I}^{*\times*} = \bigcup_{n\in\mathbb{N}} \mathbb{I}^{n\times n}$. In the case of the 0/1-equivalence problem, we have

$$\mathcal{U} = \mathbb{I}^{*\times*} \times \mathbb{I}^{*\times*},\ \mathrm{Y} = \{(M,N) \in \mathcal{U} : M \simeq_{01} N\}$$

and $s : (M,N) \mapsto \max(\dim(M), \dim(N))$.

Example 3.2.2. In the case of the graph isomorphism problem, we have

$$\mathcal{U} = \mathcal{G} \times \mathcal{G},\ \mathrm{Y} = \{(G,H) \in \mathcal{U} : G \simeq H\}$$

and $s : (G,H) \mapsto \max(\mathrm{ord}(G), \mathrm{ord}(H))$.

Example 3.2.3. If $P = (\mathcal{U}, s, \mathrm{Y})$ is a decision problem, then $(\mathcal{U},\ s,\ \mathcal{U} - \mathrm{Y})$ is a decision problem as well, called co-P.

Complexity theory involves determining the *(computational) complexity* of these decision problems (amongst many other things). Intuitively, the complexity of a problem is the amount of basic arithmetic operations needed to solve it, relative to the size of the given input. What this means exactly is not trivial and requires knowledge of theoretical models of computation like automata and Turing machines that lies outside of the scope of this project. See [15] for an introductory text.

For now, if $P = (\mathcal{U}, s, \mathrm{Y})$ is a decision problem, we say that P is solvable in polynomial time if there exists a polynomial p such that it takes at most $p(s(x))$ basic operations to determine whether $x \in \mathrm{Y}$, for all $x \in \mathcal{U}$. In the same vein, if S is some class, we will say that a function $f : \mathcal{U}_1 \to S$ is *polynomially computable* if there exists some polynomial p, dependent only on f, such that it requires at most $p(s(x))$ basic operations to compute $f(x)$ for all $x \in \mathcal{U}_1$.

Traditionally, solving a problem in polynomial time is considered efficient in complexity theory. As such, if we can solve a problem P_1 by first perfoming a polynomial amount of basic operations and then solving another problem P_2, we could say P_1 is, in a sense, *easier* than P_2. This idea is formalized as a *Karp reduction.*

Definition 3.2.1 (Karp Reduction)**.** Let $P_1 = (\mathcal{U}_1, s_1, \mathrm{Y}_1)$, $P_2 = (\mathcal{U}_2, s_2, \mathrm{Y}_2)$ be two decision problems. We say that P_1 *Karp reduces* to P_2 if there exists a polynomially computable function $f : \mathcal{U}_1 \to \mathcal{U}_2$ such that

$$x \in \mathrm{Y}_1 \iff f(x) \in \mathrm{Y}_2,\ \forall x \in \mathcal{U}_1.$$

Karp reductions are a little bit too restrictive, however, for our purposes. So we define *Cook* reductions as well.

Definition 3.2.2 (Cook Reduction)**.** Let P_1, P_2 be two decision problems. We say that P_1 *Cook reduces* to P_2 if P_1 can be solved in polynomial time when we assume that P_2 can be solved in polynomial time.

Intuitively, we have that P_1 Cook reduces to P_2 if we can efficiently solve P_1 given an efficient solution of P_2. Contrary to Karp reductions, Cook reductions allow for multiple invocations of this solution, as well as usage of 'No'-answers. Proving that P_1 Cook reduces to P_2 is often done by explicitely giving a polynomial time algorithm that solves P_1, which may depend on solving P_2. We give an example of this by proving that Karp reductions are indeed more restrictive than Cook reductions.

Proposition 3.2.3. *Let $P_1 = (\mathcal{U}_1, s_1, \mathrm{Y}_1)$, $P_2 = (\mathcal{U}_2, s_2, \mathrm{Y}_2)$ be two decision problems and suppose P_1 Karp reduces to P_2. Then P_1 Cook reduces to P_2*

Proof. We know that P_1 Karp reduces to P_2, so there exists a polynomially computable function $f : \mathcal{U}_1 \to \mathcal{U}_2$ such that $x \in \mathcal{U}_1 \iff f(x) \in \mathcal{U}_2$, for all $x \in \mathcal{U}_1$. We can define an algorithm $\mathcal{A}$ that solves P_1 as follows:

function $\mathcal{A}$(x)
  $y \leftarrow f(x)$
  if $y \in \mathrm{Y}_2$ **then return** yes
  else return no

This algorithm computes $f(x)$, which can be done in polynomial time, and solves P_2 once. So P_1 Cook reduces to P_2. □

Using reductions, we can define an equivalence relation on the class of all decision problems. We will think of equivalent problems as 'equally difficult'.

Definition 3.2.4 (Cook Equivalent)**.** We say two problems are *Cook equivalent* when they Cook reduce to one another.

A nice property of polynomials is that they are closed under addition, multiplication and composition. Using this, Cook equivalence does indeed define an equivalence relation.

The study of the equivalence classes under this relation plays a central role within the field of complexity analysis. The well-known **P=NP** problem relates to this directly. The **P** refers to the equivalence class of a trivial problem, that is the class of all problems solvable in polynomial time. The **NP** refers to the set of all problems for which it is possible to verify a 'yes'-answer in polynomial time. Intuitively, a decision problem is in **NP** when it is possible to give an argument that shows the given answer is correct which can be verified in polynomial time (finding such an argument, however, might not be easy). It is currently unknown whether **P** does indeed equal **NP**. The general consensus is that this is probably not the case, but no proof has been found to back this up (although not for lack of trying).

Another famous equivalence class, known as **GI**, is that of the graph isomorphism problem. It is quite clear that $\mathbf{GI} \subseteq \mathbf{NP}$, since we can simply provide the isomorphism. As we shall see in the next section, the problem of determining whether two matrices are 0/1-equivalent reduces to a problem in **GI**.

3.3. Reduction of 0/1-Equivalence to Graph Isomorphism

Reducing the 0/1-equivalence problem to the graph isomorphism problem is not trivial. Instead of trying to give a reduction directly, we will work towards one in four steps, using the following five decision problems:

1. P_1, the graph isomorphism problem.

2. P_2, the bipartite graph isomorphism problem, which is just the graph isomorphism problem restricted to the bipartite graphs.

3. P_3, the biordered graph isomorphism problem, given by $P_3 = (\mathcal{G}_{bi} \times \mathcal{G}_{bi},\ (G, H) \mapsto \max(\mathrm{ord}(G), \mathrm{ord}(H)),\ \mathrm{Y}_3)$, where
$$\mathrm{Y}_3 = \{(G, H) \in \mathcal{G}_{bi} \times \mathcal{G}_{bi} : G \simeq_{bi} H\}.$$

4. P_4, the simplified 0/1-equivalence problem, given by $P_4 = (\mathbb{I}^{*\times *} \times \mathbb{I}^{*\times *},\ (M, N) \mapsto \max(\dim(M), \dim(N)),\ \mathrm{Y}_4)$, where
$$\mathrm{Y}_4 = \{(M, N) \in \mathbb{I}^{*\times *} \times \mathbb{I}^{*\times *} : N = PMQ,\ \text{for permutation matrices } P, Q\}.$$

5. P_5, the 0/1-equivalence problem.

Our goal is to prove that P_5 Cook reduces to P_1. In order to do so, we shall prove equivalence between each of the successive problems P_1, P_2, P_3, P_4, and then give a reduction from P_5 to P_4.

Lemma 3.3.1. *P_1 and P_2 are Cook equivalent.*

Proof. We follow a proof due to Booth and Colbourn [13]. First off, note that since P_2 is a restriction of P_1, we have a trivial Karp reduction from P_2 to P_1 by taking $f : \mathcal{G}_{bi} \to \mathcal{G}$ the embedding.

For a graph $G = (V, E)$, we define the seperation graph $S(G) = (V \cup S, F)$, where $S = \{v_e : e \in E\}$ contains a vertex for each edge of G, and

$$F = \{(v, v_e) \in V \times S : e \text{ has } v \text{ as an endpoint}\}.$$

The seperation graph is clearly bipartite (with bipartite sets V and S). Furthermore, a quick check will show that $S(G) \simeq S(H) \iff G \simeq H$ for all $G, H \in \mathcal{G}$. Finally, the function $g : \mathcal{G} \times \mathcal{G} \to \mathcal{G}_{bp} \times \mathcal{G}_{bp}$ defined by $(G, H) \mapsto (S(G), S(H))$ is polynomially computable, since $|E| \leq |V|^2 = \mathrm{ord}(G)^2$ for all $G \in \mathcal{G}$. We conclude that P_1 Karp reduces to P_2 using g.

Since Karp reductions induce Cook reductions, we can conclude P_1 and P_2 are Cook equivalent. □

For the next few reduction, it will be convenient to note that if $G = (V, E)$ is a bipartite graph, it is possible to find $V_1, V_2 \subseteq V$ that partition V such that no edges run between V_1 and V_2 in polynomial time with respect to $\mathrm{ord}(G)$. The procedure is quite simple: start by colouring a randomly chosen vertex of G blue. Then, colour all uncoloured neighbours of blue vertices red. After this, colour all uncoloured neighbours of red vertices blue. Repeat until there are no uncoloured neighbours of coloured vertices left. At this point, if there are uncoloured vertices left (which can be the case if G is not connected), colour a random uncoloured vertex blue and repeat.

It is easy to check that this procedure will colour all vertices in polynomially many steps (namely $\mathrm{ord}(G)$ many), and that setting $V_1 = \{\text{blue vertices}\}$ and $V_2 = \{\text{red vertices}\}$ yields the required partition. Using this new knowledge, we may assume throughout when dealing with bipartite graphs that V_1 and V_2 are known.

Lemma 3.3.2. *P_3 Cook reduces to P_2.*

Proof. Since a biordered graph is, in particular, bipartite, we can apply a solution to the bipartite graph isomorphism problem directly to a pair of biordered graphs G, H. The problem with this is, though, that the existence of a graph isomorphism between G and H does not necessarily imply the existence of a *biordered* graph isomorphism.

Consider for a biordered graph $G = (V_1 \cup V_2, E)$ the graph $G' = (V_1 \cup V_2 \cup \{v'\}, E')$, defined by adding one vertex to V_2, and connecting it to all of the vertices in V_2. See Figure 3.1 for illustration. Naturally, G' is bipartite. Furthermore, for any two biordered graphs G, H we have

$$G \simeq_{bi} H \iff G \simeq H \text{ and } G' \simeq H'.$$

To see this, write $G' = (V_1 \cup V_2, E)$, $H' = (W_1 \cup W_2, F)$, and notice that since $|V_1| \neq |W_2|$ a graph isomorphism $g : G' \to H'$ must satisfy $g(V_1) = W_1$. If we define $f : \mathcal{G}_{bi} \to \mathcal{G}_{bp}$ by

$$f(G) = G',$$

we can define an algorithm that solves P_3 as follows:

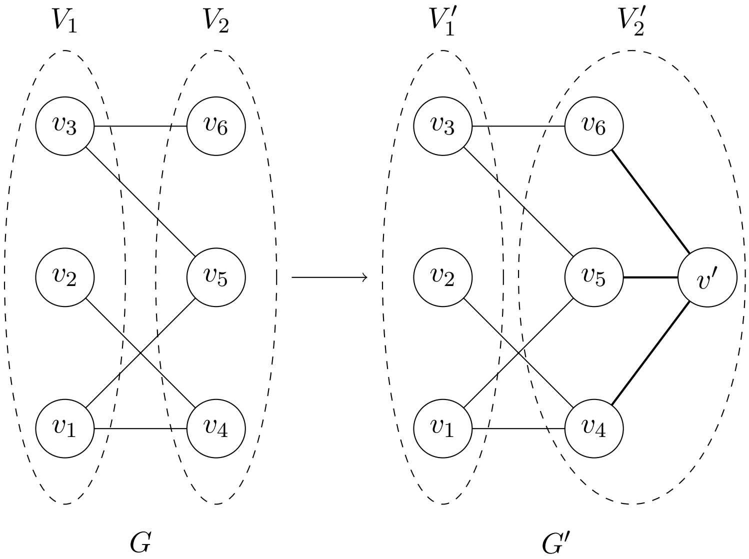


Figure 3.1.: A biordered graph G with its extension as in the proof of Lemma 3.3.2.

function $\mathcal{A}$(G, H)
    if $(G, H) \in \mathrm{Y}_2$ **then**
        if $(f(G), f(H)) \in \mathrm{Y}_2$ **then**
            return yes
        else
            return no
    else
        return no

Since f is clearly polynomially computable, this algorithm gives us a Cook reduction from P_3 to P_2. □

Lemma 3.3.3. *P_2 Cook reduces to P_3.*

Proof. Let $G = (V_1 \cup V_2, E)$, $H = (W_1 \cup W_2, F)$ be bipartite graphs. Cleary, we can find biordered graphs that are isomorphic to G and H, respectively, in polynomial time, and so we may assume without loss of generality that G and H are biordered. Now define $H' = (W_2 \cup W_1, F)$, which is just H with the order of its vertices reversed. It is not hard to see that

$$G \simeq H \iff G \simeq_{bi} H \text{ or } G \simeq_{bi} H'.$$

Because of this, we can construct a polynomial time algorithm that solves P_2 using a solution to P_3, and so P_2 Cook reduces to P_3. □

Lemma 3.3.4. *P_3 and P_4 are Cook equivalent.*

Proof. The function $f : \mathbb{I}^{*\times *} \times \mathbb{I}^{*\times *} \to \mathcal{G}_{bi} \times \mathcal{G}_{bi}$ defined by $(M, N) \mapsto (\mathcal{B}_M, \mathcal{B}_N)$ is polynomially computable (since $\mathrm{ord}(\mathcal{B}_M) = 2\dim(M)$ for all $M \in \mathbb{I}^{*\times *}$). So by corollary 3.1.9 P_4 Karp reduces to P_3 using f.

For the other direction, remember that for any biordered graph G of order k we have

$$M(G) = \begin{bmatrix} 0 & A \\ A^\top & 0 \end{bmatrix}.$$

for some $A \in I^{n\times m}$, $n + m = k$, by Proposition 3.1.5. Write $A(G)$ for this A. Define $g : \mathcal{G} \times \mathcal{G} \to \mathbb{I}^{*\times *} \times \mathbb{I}^{*\times *}$ by $(G, H) \mapsto (A(G), A(H))$. Then g is polynomially computable, and so by Corollary 3.1.9 P_3 Karp reduces to P_4 using g.

Since Karp reductions induce Cook reductions, we can conclude P_1 and P_2 are Cook equivalent. □

Lemma 3.3.5. P_5 *Cook reduces to* P_4.

Proof. Writing m_i for the columns of a matrix M, and considering Proposition 2.1.4, the following algorithm solves P_5:

```
function A(M, N)
    k ← dim(M)
    for 0 ≤ i ≤ k do
        if i = 0 then
            T ← M
        else
            T ← xor(M, m_i)
        if (T, N) ∈ P_4 then
            return yes
    return no
```

In essence, we simply apply xor for each column of M, which is not a problem since there are only polynomially many of those (in fact, exactly $\dim(M)$ many). Apart from this, the algorithm uses only polynomially many operations, the most complex of which is xor, which runs in $\mathcal{O}(\dim(M)^2)$. □

As a corollary of the lemmas above, we find that the 0/1-equivalence problem Cook reduces to that of graph isomorphism. The question remains open whether these two problems are Cook equivalent. The problem is that we need to determine for arbitrary $M, N \in \mathbb{I}^{k\times k}$ whether

$$M = PNQ,$$

for certain permutation matrices P, Q, using only answers to P_5. Sadly, we were not able to do this, and so we end this chapter with a conjecture.

Conjecture 3.3.1. P_4 Cook reduces to P_5, and, as a corollary, the 0/1-equivalence problem is Cook equivalent to the problem of graph ismorphism.

4. Computations and Results

The primary goal of this chapter is to construct a two-step algorithm that finds the minimal representative of each 0/1-equivalence class of ultrametric 0/1-n-simplices for given n, as well as consider an implementation of this algorithm using MatLab and C. Furthermore, we will briefly analyse some computational results. Step one of the algorithm consists of finding a subset $U = U(n) \subset \mathrm{Ult}^{n \times n}$ that contains the minimal representative of each equivalence class of ultrametric 0/1-n-simplices, amongst many non-minimal representatives. In step two, then, these non-minimal representatives are removed. In the next two sections we will cover the two steps seperately.

4.1. Generating Ultrametric Simplices

A very straightforward approach to finding a satisfactory U would be to simply check for each matrix M in $\mathbb{I}^{n \times n}$ whether its Gramian is ultrametric. The problem with this approach is the enormously large amount of elements in $\mathbb{I}^{n \times n}$: there are n^2 entries, each of which is either 0 or 1, meaning that $|\mathbb{I}^{n \times n}| = 2^{(n^2)}$. As Table 4.1 shows, $\mathbb{I}^{n \times n}$ would have too many elements to realistically consider for $n \geq 7$.

n	1	2	3	4	5	6	7
$\lvert\mathbb{I}^{n \times n}\rvert$	2	16	512	65536	33554432	68719476736	56294995342131

Table 4.1.: The growth of $|\mathbb{I}^{n \times n}|$

We can avoid a lot of possibilities by making use of the fact that ultrametricity is a very *local* property of a matrix: $M \in \mathbb{I}^{n \times n}$ has an ultrametric Gramian if and only if for each triple of columns m_1, m_2, m_3 of M the matrix $[m_1\ m_2\ m_3]$ has an ultrametric Gramian, as follows directly from Definition 1.0.3. This observation justifies a new strategy to find a suitable U: start by finding a set U_3 consisting of all $M \in \mathbb{I}^{n \times 3}$ that have an ultrametric Gramian and then extend these M using columns that preserve ultrametricity.

This strategy is a sizeable improvement upon the naive one, but it still has a large flaw. Although we only need minimal representatives of ultrametric simplices, we will find *all* of them. To decrease time spent both constructing U and filtering it later on, it would be useful to do some basic *prefiltering* by not including those $M \in \mathbb{I}^{n \times n}$ which are clearly not minimal. The first part of this prefiltering will consist of reducing U_3 to just those elements that are 'minimal':

Lemma 4.1.1. *Let $M \in I^{n \times n}$ be a minimal representative of some 0/1-equivalence class of simplices, and write $\{m_i\}$ for the columns of M. Then the matrix $M' \in I^{n \times 3}$*

consisting of the first three columns of M is minimal in the sense that

$$M' \leq_{01} P \cdot \mathrm{xor}(M', v) \cdot Q$$

for all permutation matrices P, Q and $v \in \{0, m_1, m_2, m_3\}$.

In addition to reducing the size of U_3, we may drastically decrease the amount of extensions that need to be considered at each step using the following two lemmas:

Lemma 4.1.2 (Block property). *Let $M \in I^{n\times n}$ be a minimal representative of some 0/1-equivalence class of simplices. Then*

1. *The entries of the column representation of M are ascending.*
2. *The entries of the row representation of M are descending.*

Proof. Write $M = [m_{ij}]$. For the first part, note that if the column representation of M is ascending, a simple column permutation would yield an $N \simeq_{01} M$ with $N <_{01} M$. For the second part, assume that the row representation of M is not descending. Then there exists a least $i < n$ such that the i-th row of M is 'smaller' than the $(i+1)$-th row, but this, as a simple check shows, implies that applying a permutation that swaps rows i and $i+1$ would yield an $N \simeq_{01} M$ with $N <_{01} M$. □

Lemma 4.1.3 (SRE property). *Let $M \in I^{n\times n}$ be a minimal representative of some 0/1-equivalence class of simplices. Then for each $k > 1$ the amount of ones in the first column of M is smaller than or equal to the amount of ones in the k-th column.*

Proof. Suppose there exists a $k > 1$ such that the k-th column of M contains fewer ones than the first column. Then swapping the first and the k-th column, and applying a row permutation such that the new first column will be of the form

$$n_1^\top = [\ \underbrace{1 \ \ \ldots \ \ 1}_{k} \,|\, \underbrace{0 \ \ \ldots \ \ 0}_{n-k}\ ].$$

would yield an $N \simeq_{01} M$ that has a 'smaller' first column than M. So $N <_{01} M$. □

Finally, we make use of a property of minimal $M \in \mathbb{I}^{n\times 3}$ with an ultrametric Gramian that is expanded upon in [4]: the first two columns of such an M will represent what is known as a *minimal acute triangle*. We will not expand on this further here, see [11] for a full characterization. For now, what is important is that we may find all minimal $M \in \mathbb{I}^{n\times 3}$ that have an ultrametric Gramian by considering the set of all minimal acute triangles, which can be generated very efficiently [11], and extending them with some column that respects both the block property and the SRE property. A MatLab implementation that does exactly this is given in `UMT.m` (see Appendix B).

The matrices found by `UMT.m` still have to be filtered in accordance with Lemma 4.1.1. This is done by looping over each of them, and discarding them whenever they are not minimal. To check if an $M \in \mathbb{I}^{n\times 3}$ is minimal, the following algorithm is used:

function CHECK_MINIMAL(M)
  for $0 \leq i \leq 3$ **do**
    if $i = 0$ **then**
      $T \leftarrow M$
    else
      $T \leftarrow \text{xor}(M, m_i)$
    for P an $n \times n$ permutation matrix **do**
      $T' \leftarrow PT$
      Sort the columns of T' in ascending order
      if $T' <_{01} M$ **then**
        return false
  return true

A MatLab implementation that uses this algorithm to filter the set generated by `UMT.m` can be found in `FilterUMT.m` (see Appendix B). Table 4.2 illustrates the difference (pre)filtering makes on the size U_3.

n	3	4	5	6	7	8	9
$\|U_3(n)\|$ (no filtering)	1	6	31	131	451	1389	4057
$\|U_3(n)\|$ (prefiltering)	1	4	12	33	77	160	306
$\|U_3(n)\|$ (full filtering)	1	4	10	23	47	88	156

Table 4.2.: The size of $|U_3|$ without any filtering, with prefiltering and with full filtering

Now that we have a set of minimal $M \in \mathbb{I}^{n\times 3}$ with ultrametric Gramians, it remains to extend these matrices, respecting the block property and the SRE property. This results in the following recursive algorithm:

function UMS(n)
  UMS $\leftarrow$ empty list
  min_UMT $\leftarrow U_3$
  for $s \in$ min_UMT **do**
    extend(s)
function EXTEND(s)
  if $\dim(s) = n$ **then**
    add s to UMS
  else
    for $t \in \mathbb{I}^{n\times n}$ **do**
      if [s t] has an ultrametric Gramian and satisfies block/SRE property **then**
        extend([s t])

Table 4.3 illustrates the difference prefiltering using the block/SRE property makes on the size of U, assuming that U_3 is filtered fully.

Checking ultrametricity and the block/SRE property of $[s\ t]$ can be optimized slightly by making use of earlier computations. These optimizations are all quite trivial, and so we will not cover them here. An implementation of this algorithm in MatLab can be

n	3	4	5	6	7	8
$\|U(n)\|$ (no filtering)	1	2	18	312	7248	247290
$\|U(n)\|$ (prefiltering)	1	1	3	14	67	313

Table 4.3.: The size of $|U|$ without any filtering and with prefiltering.

found in `UMS.m`, and an implementation in C can be found in `UMS.c` (see Appendix B). We chose to implement this algorithm in C for speed, Figure 4.1 shows the computation time versus n for both implementations on an Intel i5 processor. The implementation in C is much faster than the one in MatLab, it can feasably compute $U(n)$ for $n = 12$, whereas the MatLab implementation will not go beyond $n = 10$.

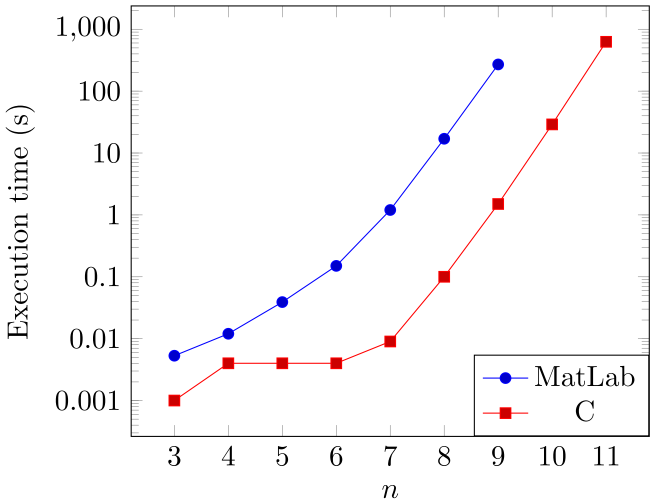


Figure 4.1.: Execution time versus n for the MatLab and C implementation of the algorithm that finds $U(n)$.

4.2. Filtering for Minimality

Given U, we need to filter out its non-minimal elements. We can do this by first sorting U in ascending order with respect to $<_{01}$, so that we have $U = \{u_1, u_2, \ldots, u_k\}$ for some $k \in \mathbb{N}$, with $u_i <_{01} u_j$ whenever $i < j$. Then, we can loop over the elements of U in ascending order, removing u_i from U if there is a u_j left with $j < i$ and $u_i \simeq_{01} u_j$:

function FILTER(U)
  $k \leftarrow |U|$
  sort U in ascending order
  for $i \in \{1, 2, \ldots, k\}$ **do**
    for $j \in \{1, 2, \ldots, i-1\}$ **do**
      if u_j minimal and $u_i \simeq_{01} u_j$ **then**
        remove u_i from U
        break

It remains to find a way to determine whether $u_i \simeq_{01} u_j$. Here we can make use of our findings in Chapter 3, by transforming the reduction we gave from 0/1-equivalence to graph isomorphism into a practical algorithm. We define for any $M \in \mathbb{I}^{n \times n}$ with columns m_i the set

$$\mathcal{G}(M) := \{(\mathcal{B}_{\text{xor}(M,v)})' : v \in \{0, m_1, m_2, \ldots, m_n\}\},$$

where $(\mathcal{B}_M)'$ is the extension of the biordered graph associated with M as in Lemma 3.3.2 and Figure 3.1. Now we have (see Lemma 3.3.2):

$$M \simeq_{01} N \iff \exists G \in \mathcal{G}(M) \text{ s.t. } G \simeq (\mathcal{B}_N)'.$$

Using the above notation, we get the following algorithm:

function 0/1EQUIVALENT(M, N)
  $H \leftarrow (\mathcal{B}_N)'$
  for $G \in \mathcal{G}(M)$ **do**
    if $G \simeq H$ **then**
      return true
  return false

In the worst case, this algorithm requires n solutions of the graph isomorphism problem, for input of order $2n + 1$.

An implementation based on the two algorithms above in C can be found in `FilterUMS.c` (see Appendix B). To determine graph isomorphism, we made use of the igraph library [5].

4.3. Results

We were able to find the set $U_{min} = U_{min}(n)$ of minimal representatives for all $3 \leq n \leq 12$. Table 4.4 shows the growth of $|U_{min}(n)|$ as n increases. Comparing with Table 4.1, we can see that minimal representatives of ultrametric simplices are incredibly rare. It appears that $|U(n)|$ grows roughly as 2^n, altough this might ofcourse just be the case for small n. Sadly, the sequence $U_{min}(n)$ did not appear in the Online Encyclopedia for Integer Sequences [17].

We give matrix depictions of the set $U_{min}(n)$ for $3 \leq n \leq 9$ below. Matrix depictions of $U_{min}(n)$ for $n \geq 10$ would take up too much space. Column representations of $U_{min}(n)$ for $3 \leq n \leq 12$ can be provided digitally, please email the author (lfh.slot@gmail.com).

n	3	4	5	6	7	8	9	10	11	12
$\|U_{min}(n)\|$	1	1	2	6	13	27	64	148	327	725
$\|A_{min}(n)\|$	1	1	2	6	13	29	67	162	392	-

Table 4.4.: The size of $|U_{min}|$ and $|A_{min}|$

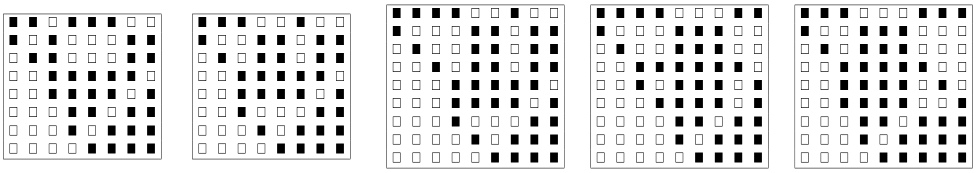


Figure 4.2.: Minimal $M \in \mathbb{I}^{8\times 8} \cup \mathbb{I}^{9\times 9}$ that have acute, but not ultrametric Gramians.

It might be interesting to compare our results with those of Cihangir [4], who found the set $A_{min} = A_{min}(n)$ of minimal representatives of *acute* 0/1-n-simplices for $3 \leq n \leq 9$. The growth of $|A_{min}(n)|$ is also shown in Table 4.4. Obviously, $|U_{min}(n)| \leq |A_{min}(n)|$ for all n. Apparently all acute 0/1-simplices are also ultrametric for $3 \leq n \leq 7$, since we have $|U_{min}(n)| < |A_{min}(n)|$ only for $n \geq 8$. Figure 4.2 depicts the minimal $M \in \mathbb{I}^{8\times 8} \cup \mathbb{I}^{9\times 9}$ that represent acute simplices, but do not have ultrametric Gramians. Sadly, we were not able to find any interesting patterns within the data, so we will leave our discussion of the results at this.

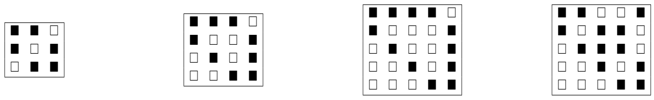


Figure 4.3.: The elements of $U_{min}(3) \cup U_{min}(4) \cup U_{min}(5)$.

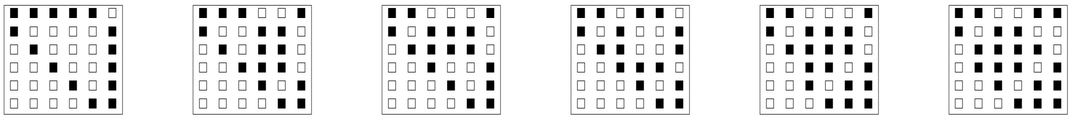


Figure 4.4.: The elements of $U_{min}(6)$.

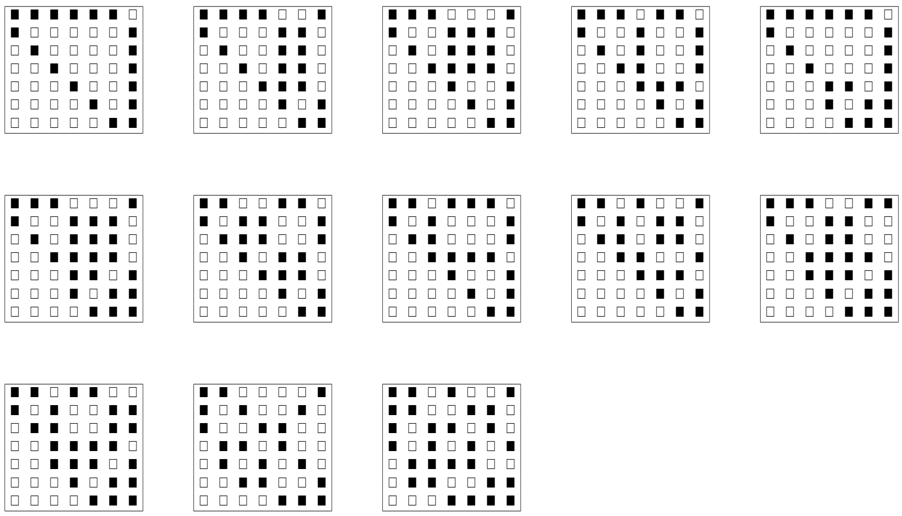


Figure 4.5.: The elements of $U_{min}(7)$.

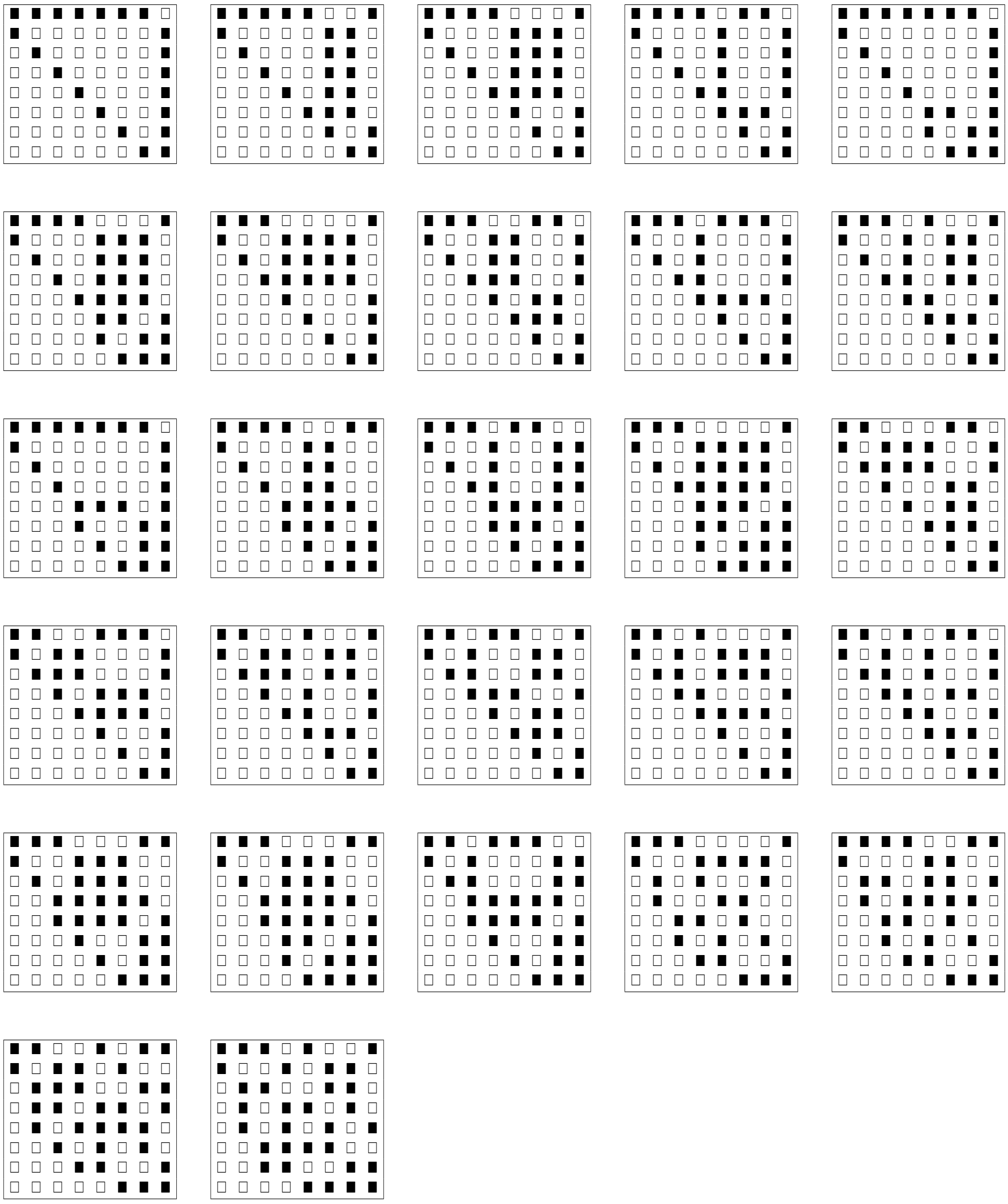


Figure 4.6.: The elements of $U_{min}(8)$.

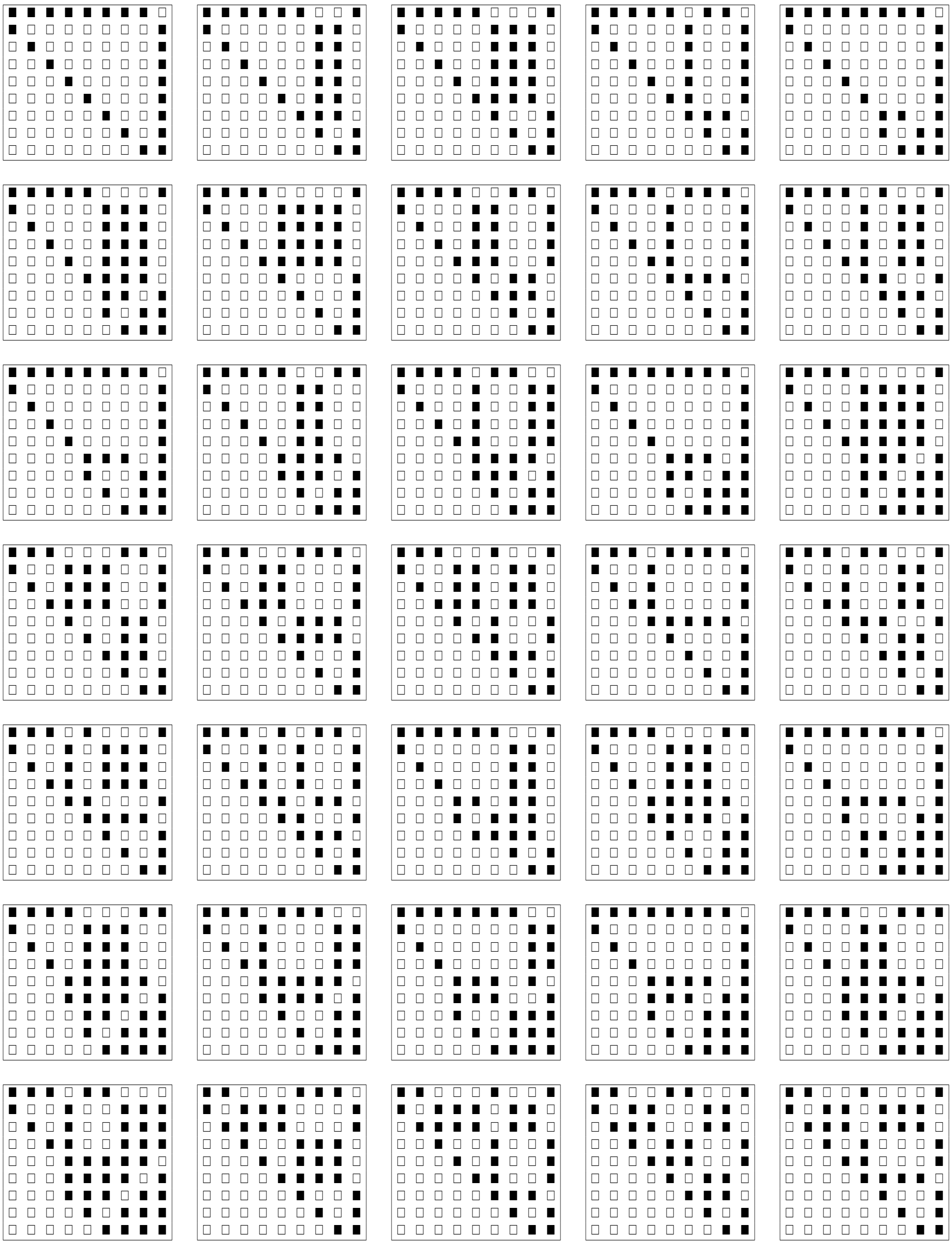


Figure 4.7.: The first 35 elements of $U_{min}(9)$.

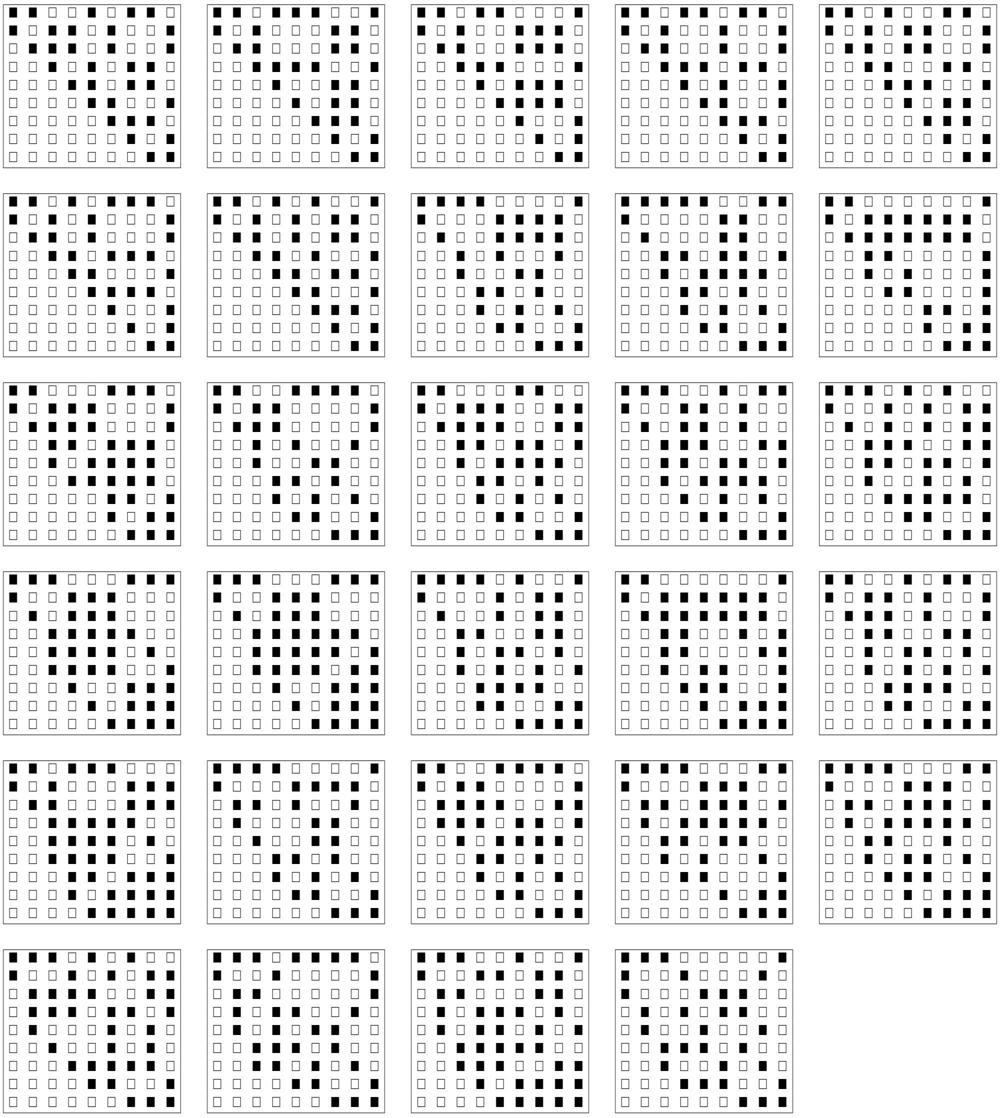


Figure 4.8.: The remaining 29 elements of $U_{min}(9)$.

Conclusion

In terms of pure mathematics, the main goal of this project was the study of ultrametric 0/1-simplices. In Chapter 1, we covered ultrametric matrices using work from Varga and Nabben [14]. In particular we saw that strictly ultrametric matrices have inverses that are strictly diagonally dominant and of Stieltjes type, and we gave a method to write any strictly ultrametric matrix of order n whose entries are integers as the Gramian of a 0/1-matrix with no more than $2n-1$ distinct rows. In Chapter 2, we built a linear algebra framework to analyse the geometrical properties of simplices based on the Gramians of their matrix representations. Furthermore, we covered 0/1-simplices and their equivalence classes under the symmetries of the n-cube. In particular, we gave a practical way to determine 0/1-equivalence of 0/1-simplices using their matrix representations. We combined the material from Chapters 1 and 2 to conclude that ultrametric simplices are non-obtuse, and explain the link between ultrametric 0/1-simplices and regular 0/1-simplices.

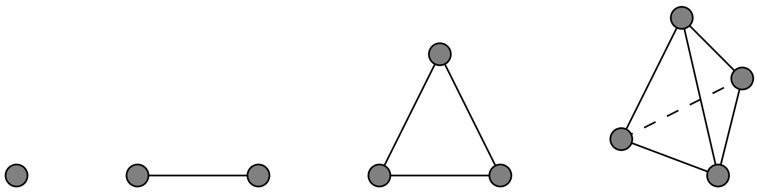
In terms of Computer Science, our first focus focus was the problem of determining whether two 0/1-simplices are 0/1-equivalent in the context of computational complexity theory. In Chapter 3, we covered some basic notions of graphs and graph isomorphism, and, using a series of polynomial reductions, proved that the 0/1-equivalence problem reduces to that of graph isomorphism. We then constructed an algorithm that finds a minimal representative of each 0/1-equivalence class of ultrametric simplices in Chapter 4. This algorithm works in two steps by first finding a set that contains all minimal representatives, and then filtering this set to contain only minimal representatives. For the first step we found some properties of ultrametric 0/1-simplices and their minimal representatives and used them to greatly increases the efficiency of our algorithm compared to a naive one. For the second step, we were able to adapt our reduction from Chapter 3 into a practical algorithm. Using an implementation in C, we found the set of minimal representatives for $3 \leq n \leq 12$.

Further research

At the end of the project, we see three major avenues for further research. Firstly, we are left with an open conjecture regarding the polynomial equivalence of the 0/1-equivalence problem and the problem of graph ismorphism. Secondly, our implementation of the algorithm to find minimal representatives could be parallelized rather nicely, which may allow succesful computation of the set of minimal representatives for larger n. Thirdly, though we were not able to find any interesting patterns within the generated data ourselves, we feel that further analysis might lay bare some structure of ultrametric 0/1-simplices that might be useful in their study, and the study of regular 0/1-simplices.

Populaire Samenvatting

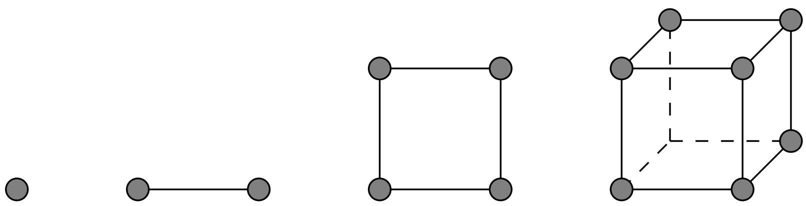
In dit project bekijken we *simplices*. Simplices zijn een veralgemenisering van driehoeken in meer dimensies. Een 0-simplex is gewoon een punt, een 1-simplex is een lijnstuk, een 2-simplex is een driehoek en een 3-simplex is een soort piramide met een driehoekig grondvlak, ook wel een *tetraëder* geheten. Zie onderstaande figuur.



Van links naar rechts: een 0-simplex, een 1-simplex, een 2-simplex en een 3-simplex.

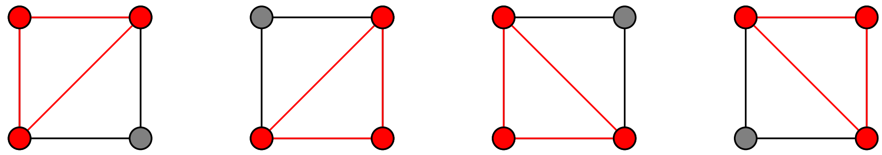
Het patroon is duidelijk: als n een positief geheel getal is, dan maak je een n-simplex door $n+1$ punten te kiezen in de n-dimensionale ruimte, en al die punten te verbinden met lijnstukken. Voor n groter dan 3 kunnen we hier natuurlijk geen plaatje meer van tekenen, maar het blijft mogelijk om simplices in hoge dimensies te bestuderen met behulp van *lineaire algebra*, een deelgebied van de wiskunde.

Net zoals driehoeken kunnen we ook vierkanten veralgemeniseren naar meer dimensies. We noemen die veralgemenisering de *n-kubus*. De 0-kubus is een punt, de 1-kubus een lijnstuk, de 2-kubus is het vierkant, de 3-kubus is een kubus en de 4-kubus staat beter bekend als de *hyperkubus*. Van de eerste vier n-kubussen kunnen we een plaatje tekenen, zie hieronder.



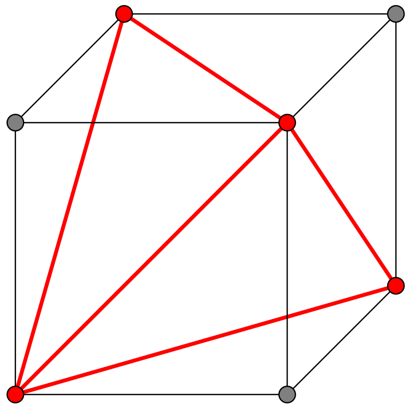
Van links naar rechts: de 0-kubus, de 1-kubus, de 2-kubus en de 3-kubus.

We zijn in het bijzonder geïnteresseerd in n-simplices waarvan de hoekpunten ook hoekpunten zijn van de n-kubus. We noemen deze 0/1-simplices. Voor $n = 2$ zijn er vier van deze 0/1-simplices, zoals in de figuur hieronder te zien is.
De vraag we ons mee bezig houden is de volgende: voor welke n bestaat er een *regelmatige* 0/1-simplex, dat is een 0/1-simplex waarvan alle zijden even lang zijn. Uit de figuur kunnen we al opmaken dat er voor $n = 2$ in elk geval niet zo'n 0/1-simplex bestaat, we



De vier 0/1-simplices voor $n = 2$.

hebben immers telkens twee zijden van lengte 1, en één zijde van lengte $\sqrt{2}$. Voor $n = 3$ bestaat er wél een regelmatige 0/1-simplex. Deze staat hieronder afgebeeld, en heeft zijden van lengte $\sqrt{2}$.



Een regelmatige 0/1-simplex voor $n = 3$.

Het is niet zo lastig om te bewijzen dat als n niet in de rij $3, 7, 11, 15, 19, \ldots$ voorkomt, er dan zeker geen regelmatige 0/1-simplex bestaat in de n-kubus. Het *vermoeden van Hadamard* stelt dat als n wel in deze rij voorkomt, er dan ook een regelmatige 0/1-simplex bestaat. Dit vermoeden werd zo'n 100 jaar geleden voor het eerst opgeschreven door de Franse wiskundige Jacques Hadamard (1865 - 1963) maar is nog steeds niet bewezen of ontkracht.

Het idee van dit project is om in plaats van direct regelmatige simplices te bestuderen te kijken naar een iets grote deelklasse, namelijk die van de *ultrametrische* simplices. De hoop is dat door beter begrip van deze subklasse uiteindelijk ook uitspraken gedaan kunnen worden over regelmatige simplices, en misschien het vermoeden van Hadamard zelfs wel kan worden opgelost.

A. The Hadamard Conjecture

As stated in section 2.3, the main reason to study ultrametric 0/1-simplices is to learn more about regular ones. In this section we will motivate our interest in regular 0/1-simplices by showing their connection to a somewhat famous conjecture of Hadamard regarding the determinant of matrices whose entries are either -1 or 1. In the following, we write $\mathbb{J} = \{-1, 1\}$, and use $'+'$ instead of 1 and $'-'$ instead of -1 when writing out matrices for clarity. Let us first state *Hadamard's inequality.*

Theorem A.0.1 (Hadamard's inequality)**.** *Let $M \in \mathbb{R}^{n \times n}$ with columns m_i. Then we have*

$$|\det(M)| \leq \prod_{i=1}^{n} ||m_i||.$$

Equality is attained if and only if the columns of M are orthogonal.

Proof. There exist many proofs of this theorem, see for instance [7]. We shall give a geometrical argument here to give an idea of what is going on. We know that $|\det(M)|$ is the volume of the parallelepiped spanned by the columns of M. But this volume is always smaller than or equal to the product of the lengths of the columns of M, which proves the first part of the theorem. For the second part, note that a parallelepided has maximal volume (with respect to the length of its sides) when it is a cuboid, or in other words, when its sides are orthogonal. □

For matrices in $\mathbb{J}^{n \times n}$ we get the following.

Corollary A.0.2. *Let $M \in \mathbb{J}^{n \times n}$. Then we have*

$$|\det(M)| \leq n^{\frac{1}{2}n}.$$

Equality is attained if and only if the columns of M are orthogonal.

Proof. Note that for any column m_i we have $||m_i|| = \sqrt{n}$. As such Hadamard's inequality gives us

$$|\det(M)| \leq \prod_{i=1}^{n} ||m_i|| = \prod_{i=1}^{n} \sqrt{n} = (\sqrt{n})^n = n^{\frac{1}{2}n}.$$

That equality is achieved if and only if M has orthogonal columns also follows directly from Hadamard's inequality. □

Matrices $H \in \mathbb{J}^{n\times n}$ whose columns are othogonal are called *Hadamard matrices*. Using the corrollary above, this is the same as saying $|\det H| = 2^{\frac{1}{2}n}$. Another equivalent condition is that $H^\top H = nI$, since this is obviously the case exactly when the columns of H are orthogonal and in $\mathbb{J}^n$. Furthermore, if H is Hadamard, any matrix that is the result of permutating rows and columns of H, multiplying rows or columns of H by -1 or transposing H is again Hadamard. This can be seen quite easily as each of these operations preserves orthogonality of the columns of H, and the resulting matrix is clearly again an element of $\mathbb{J}^{n\times n}$. Matrices that can be transformed into one another using these operations are called *Hadamard equivalent*.

We are interested in finding out for which n there exist a Hadamard matrix in $\mathbb{J}^{n\times n}$. For $n = 1, 2, 4$ it is quite easy to give an example, the following matrices for instance will do:

$$H_1 = \begin{bmatrix} + \end{bmatrix}, \; H_2 = \begin{bmatrix} + & - \\ + & + \end{bmatrix}, \; H_4 = \begin{bmatrix} + & - & + & - \\ + & + & + & + \\ + & - & - & + \\ + & + & - & - \end{bmatrix}$$

As a matter of fact, for any n that is a power of two we can construct a Hadamard matrix of order n.

Theorem A.0.3. *Let $k \geq 0$ and let $n = 2^k$ Then there exists a Hadamard matrix $H \in \mathbb{J}^{n\times n}$.*

Proof. We prove by induction on k. For $k = 0$ we have already given an example. Now suppose for some $k \geq 0$ there exists a Hadamard matrix H_k of order $n = 2^k$. We have $H_k^\top H_k = nI_n$. Now consider the matrix

$$H_{k+1} = \begin{bmatrix} H_k & H_k \\ H_k & -H_k \end{bmatrix} \in \mathbb{J}^{2n\times 2n}.$$

We have that

$$H_{k+1}^\top H_{k+1} = \begin{bmatrix} H_k^\top & H_k^\top \\ H_k^\top & -H_k^\top \end{bmatrix} \begin{bmatrix} H_k & H_k \\ H_k & -H_k \end{bmatrix} = \begin{bmatrix} nI_n + nI_n & nI_n - nI_n \\ nI_n - nI_n & nI_n + nI_n \end{bmatrix} = 2nI_{2n}.$$

So H_{k+1} is a Hadamard matrix of order $2n = 2^{k+1}$. □

The construction in the above proof is due to Sylvester [16]. As we shall now see, $\mathbb{J}^{n\times n}$ does not contain a Hadamard matrix for most n.

Theorem A.0.4. *For any $n > 2$ that is not divisible by 4, there does not exist a Hadamard matrix in $\mathbb{J}^{n\times n}$.*

Proof. We give a proof based on [3]. Let $n > 2$, and let $H \in \mathbb{J}^{n\times n}$ be a Hadamard matrix. By multplying some of the rows of H by -1 we can construct a new Hadamard matrix which has only ones in the first column. Orthogonality of the columns of this matrix implies that each of its other columns have exactly half of their entries equal to 1 and half of their entries equal to -1. Now by permuting rows we can construct a Hadamard matrix H' of the following form:

$$H' = \left[\begin{array}{cccc} + & + & + & \cdots \\ \cdots & \cdots & \cdots & \cdots \\ + & + & + & \cdots \\ \hline + & - & + & \cdots \\ \cdots & \cdots & \cdots & \cdots \\ + & - & + & \cdots \\ \hline + & + & - & \cdots \\ \cdots & \cdots & \cdots & \cdots \\ + & + & - & \cdots \\ \hline + & - & - & \cdots \\ \cdots & \cdots & \cdots & \cdots \\ + & - & - & \cdots \end{array}\right]$$

Each of the four blocks that the first three columns consist of must be of equal size to ensure orthogonality. As such, n is divisible by 4 and the theorem follows. □

Apart from the one we just saw, there are no known further restrictions on n. In fact, existence of Hadamard matrices has been proven for all n divisible by 4 no larger than 764, using a combination of techniques like Sylvester's and direct computation [6, 8]. Furthermore, proofs exists for several special cases, such as when n is a power of two, or when $n = q + 1$, where q is a prime power. No general proof is known, however, and so we are left with *Hadamard's conjecture.*

Conjecture A.0.1 (Hadamard's Conjecture)**.** There exists a Hadamard matrix of order n for each n divisible by 4.

So where do regular 0/1-simplices come in? As it turns out, the existence of a Hadamard matrix of order $n + 1$ is equivalent to the existence of a regular 0/1-simplex of dimension n.

Theorem A.0.5. *There exists a Hadamard matrix of order $n + 1$ if and only if there exists a regular 0/1-simplex of dimension n.*

We prove the statement as two seperate lemmas.

Lemma A.0.6. *Suppose there exists a regular 0/1-simplex of dimension n, then there exists a Hadamard matrix of order $n + 1$.*

Proof. Let $M \in \mathbb{I}^{n\times n}$ be a matrix representation of a regular 0/1-n-simplex, and let $A \in \mathbb{J}^{n\times n}$ be the result of changing all the zeroes in M to minus one. Now consider $H \in \mathbb{J}^{n+1\times n+1}$ given by

$$H = \left[\begin{array}{c|ccc} + & - & - & \cdots \\ \hline + & & & \\ + & & A & \\ \cdots & & & \end{array}\right].$$

We will show the columns h_i of H are orthogonal. Since M represents a regular simplex, we have

$$m_i^\top m_j = \begin{cases} \frac{1}{2}(n+1) & \text{if } i = j \\ \frac{1}{4}(n+1) & \text{if } i \neq j \end{cases}$$

This means that each column of M contains exactly $\frac{1}{2}(n+1)$ ones and $\frac{1}{2}(n-1)$ zeroes. This immediately gives us

$$h_1^\top h_i = \frac{1}{2}(n+1) - \frac{1}{2}(n-1) - 1 = 0,$$

for all $1 < i \leq n+1$. Furthermore, if $i \neq j$ we have $m_{ik} = m_{jk} = 1$ for exactly $\frac{1}{4}(n+1)$ different k. This leaves $\frac{1}{4}(n+1)$ ones in both m_i and m_j, so we have $m_{ik} \neq m_{jk}$ for $\frac{1}{2}(n+1)$ many k. So $m_{ik} = m_{jk} = 0$ in the remaining $\frac{1}{4}(n+1) - 1$ cases. But this means that for distinct $i, j > 1$ we have

$$h_i^\top h_j = \frac{1}{4}(n+1) - \frac{1}{2}(n+1) + (\frac{1}{4}(n+1) - 1) + 1 = 0.$$

So H is indeed a Hadamard matrix of order $n+1$.

□

Lemma A.0.7. *Suppose there exists a Hadamard matrix of order $n+1$, then there exists a regular 0/1-simplex of dimension n.*

Proof. We may assume the Hadamard matrix is of the form

$$H = \left[\begin{array}{c|ccc} + & - & - & \dots \\ \hline + & & & \\ + & & A & \\ \dots & & & \end{array}\right]$$

for some $[a_1\ a_2\ \dots\ a_n] = A \in \mathbb{J}^{n \times n}$. We can then define $[m_1\ m_2\ \dots\ m_n] = M \in \mathbb{I}^{n \times n}$ by changing all the minus ones in A to zero. Note that since $H = (n+1)I_{n+1}$, we have

$$a_i^\top a_j = \begin{cases} n & \text{if } i = j \\ -1 & \text{if } i \neq j \end{cases}$$

Since the columns of H are orthogonal, and the first column contains only ones, each of the columns of A contain $\frac{1}{2}(n+1)$ ones and $\frac{1}{2}(n+1) - 1$ minus ones. This immediately gives us that

$$m_i^\top m_i = a_i^\top a_i - (\frac{1}{2}(n+1) - 1) = n - \frac{1}{2}(n+1) + 1 = \frac{1}{2}(n+1).$$

Now for $i \neq j$, we have that

$$a_i^\top a_j = \#k \text{ such that } a_{ik} = a_{jk}.$$

Using this combined with the fact that the first entry of each column of H (except for the first one) is minus one, we find that $a_{ik} \neq a_{jk}$ for $\frac{1}{2}(n+1)$ different k and $a_{ik} = a_{jk} = -1$ for $\frac{1}{4}(n+1) - 1$ different k. So for $i \neq j$ we have that

$$m_i^\top m_j = a_i^\top a_j + \frac{1}{2}(n+1) - (\frac{1}{4}(n+1) - 1) = -1 + \frac{1}{2}(n+1) - \frac{1}{4}(n+1) + 1 = \frac{1}{4}(n+1).$$

This means $M^\top M$ corresponds to the Gramian of a regular 0/1-n-simplex and so M is a matrix representation of this simplex, which proves its existence. $\square$

B. Code

For a digital version of all code, please email the author (lfh.slot@gmail.com). In Chapter 4, references are made to `UMT.m`, `FilterUMT.m`, `UMS.m`, `UMS.c` and `FilterUMS.c`. These files have some dependencies, which have not been discussed but are included in the digital version, and well-documented through comments. For the C code, the library igraph [5] is also required. Please note that some of the files used, namely `MakeN.m` and `Acute01Triang.m` were written by Jan Brandts, and used with permission. The digital version also includes several `readme`-files that specify usage.

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