

ON SOME p -ALMOST HADAMARD MATRICES

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Abstract. Let $M(n, \mathbb{R})$ be the space of all real valued $n \times n$ matrices and $O(n, \mathbb{R})$ be the orthogonal group. A square matrix $H_n \in M(n, \mathbb{R})$ is called “almost Hadamard” if $U_n := H_n/\sqrt{n}$ is orthogonal, and locally maximizes the 1-norm on $O(n, \mathbb{R})$. The matrix H_n is “ p -almost Hadamard” if it maximizes the p -norm on $O(n, \mathbb{R})$ for $p \in [1, 2)$ and minimizes the p -norm on $O(n, \mathbb{R})$ for $p \in (2, \infty]$. In this work, we consider the Conjecture 4.4 stated in [8] and discuss its truth content. For $n \in \mathbb{N} \setminus \{2\}$, we show that the matrix

$$K_n := \frac{1}{\sqrt{n}} \begin{pmatrix} 2-n & 2 & \cdots & 2 \\ 2 & 2-n & \cdots & 2 \\ \vdots & \vdots & \ddots & \vdots \\ 2 & 2 & \cdots & 2-n \end{pmatrix}$$

is p -almost Hadamard, for any $p \in (2, \infty)$ such that

$$(p-1)[(n-2)^{2p} + (n-2)^2 2^{p-2} + 2^2(n-2)^{p-2}] > (n-2)^p + 2^p(n-1).$$

We also establish that for any $p \in [1, 2)$ and $n \in \mathbb{N} \setminus \{2\}$, K_n is p -almost Hadamard and hence the Conjecture is valid for this case. Finally, we give some particular examples of p -almost Hadamard matrices of different orders, incorporating conference and weighing matrices.

1. Introduction

Optimization problems involving orthogonal and unitary matrix constraints play an important role in the theory of engineering and technology, quantum information, physics and statistics; including linear and nonlinear eigenvalue problems, electronic structures computations, low-rank matrix optimization, polynomial optimization, subspace tracking, combinatorial optimization, sparse principal component analysis, etc (see [5, 1, 15, 21] for more details and references therein). These problems are difficult because the constraints are non-convex and the orthogonality constraints may lead to several local optimum and, in particular, many of these problems in special forms are non-deterministic polynomial-time hard (NP-hard). There is no assurance for obtaining the global optimizer, except for a few simple cases and hence is a tedious task for the numerical analysts to find a global optimum (see [21] for more details). The works [14, 10, 2, 3, 4], etc considered several optimization problems involving orthogonal matrix constrains.

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The concept of *almost* and *p-almost Hadamard matrices* introduced in [7, 8], is closely related to the optimization of a suitable cost functional over orthogonal groups. Some of the optimum values of this problem also have an interesting connection with the Hadamard, conference and weighing matrices. We explore these relationships in this work and give some concrete examples of *p-almost Hadamard matrices*. The complex Hadamard (Zeilinger) matrices are proved to be useful in several branches of quantum physics (see [20]). This connection also opens up various possibilities of application of the almost and *p-almost Hadamard matrices* to different problems in quantum physics.

Conjecture 4.4 in [8] states that the matrix $K_n := \frac{2}{\sqrt{n}}\mathbb{I}_n - \sqrt{n}I_n$, where \mathbb{I}_n is the $n \times n$ matrix with all entries 1 and I_n is the $n \times n$ identity matrix, is a *p-almost Hadamard matrix* for any $p \in [1, \infty) - \{2\}$ and $n \in \mathbb{N}$. In this work, using multi-variable analysis tools, we prove that for $n \in \mathbb{N} \setminus \{2\}$, the matrix K_n is *p-almost Hadamard* for any $p \in (2, \infty)$ satisfying (see Proposition 6)

$$(p - 1) [(n - 2)2^p + (n - 2)^2 2^{p-2} + 2^2(n - 2)^{p-2}] > (n - 2)^p + 2^p(n - 1).$$

We also establish that the matrix K_n is *p-almost Hadamard* for any $p \in (1, 2)$ and $n \in \mathbb{N} \setminus \{2\}$ (see Proposition 7 and Remark 11), and hence the Conjecture 4.4 in [8] holds true for this case. In particular, one can also obtain that K_n is almost Hadamard for all $n \in \mathbb{N} \setminus \{2\}$ (see Corollary 1). With the help of Hadamard, conference and weighing matrices, we give some particular examples of *p-almost Hadamard matrices* for various orders (see Propositions 3 and 4).

2. Mathematical preliminaries

In this section, we give some mathematical preliminaries needed to establish the main results for this paper. We denote $M(n, \mathbb{R})$, the vector space of all real valued $n \times n$ matrices over \mathbb{R} .

2.1. Real Hadamard, conference and weighing matrices

Let us first give the definition and characterizations of real Hadamard, conference and weighing matrices.

DEFINITION 1. For every positive integer n , the *orthogonal group* $O(n, \mathbb{R}) \subset M(n, \mathbb{R})$ is the group of $n \times n$ real orthogonal matrices M_n with the group operation of matrix multiplication, satisfying

$$M_n M_n^T = I_n = M_n^T M_n,$$

where M_n^T is the transpose of M_n .

Because the determinant of an orthogonal matrix is either 1 or -1 , the orthogonal group has two components. The component containing the identity I_n is the *special orthogonal group* $SO(n, \mathbb{R})$. That is,

$$SO(n, \mathbb{R}) = \{M_n \in O(n, \mathbb{R}) : \det(M_n) = 1\},$$

and is a normal subgroup of $O(n, \mathbb{R})$ and $O(n, \mathbb{R})/SO(n, \mathbb{R}) \cong \mathbb{Z}_2$. It should also be noted that $SO(n, \mathbb{R}) = \det^{-1}(\{1\})$ is an open, connected subset of $O(n, \mathbb{R})$, and both $O(n, \mathbb{R})$ and $SO(n, \mathbb{R})$ are smooth submanifolds of the n^2 -dimensional Euclidean space.

DEFINITION 2. (Real Hadamard matrix) A *real Hadamard matrix* H_n of order n is defined as an $n \times n$ square matrix with entries from $\{1, -1\}$ such that

$$H_n H_n^T = nI_n.$$

The following theorem discusses the existence of real Hadamard matrices.

THEOREM 1. (Theorem 4.4, [18]) *If a real Hadamard matrix of order n exists, then $n = 1, 2$ or $n \equiv 0 \pmod{4}$.*

CONJECTURE 1. (The Hadamard conjecture, [17]) *If $n \equiv 0 \pmod{4}$, then there is a real Hadamard matrix of order n .*

Two Hadamard matrices of order n are said to be *equivalent* if and only if one can be transformed into the other by using the following operations,

- (1) multiply any row or column by -1 , and
- (2) interchange two rows or two columns.

If H_{n_1} is a Hadamard matrix of order n_1 and H_{n_2} is a Hadamard matrix of order n_2 , then $H_{n_1} \otimes H_{n_2}$ is a Hadamard matrix of order $n_1 n_2$, where $H_{n_1} \otimes H_{n_2}$ denotes the Kronecker product of the matrices H_{n_1} and H_{n_2} .

Let $\mathcal{H}(n, \mathbb{R})$ be the set of $n \times n$ matrices with ± 1 entries. The *Hadamard inequality* is given by

$$\det(M_n) \leq \left(\prod_{i=1}^n \sum_{j=1}^n a_{ij}^2 \right)^{1/2} \leq n^{n/2},$$

where $M_n = (a_{ij})_{i,j=1}^n \in \mathcal{H}(n, \mathbb{R})$. It should be noted that the equality holds only for Hadamard matrices.

DEFINITION 3. (Real conference matrix) A *real conference matrix* of order $n > 1$ is an $n \times n$ matrix C_n with diagonal entries 0 and off-diagonal entries ± 1 which satisfies

$$C_n C_n^T = (n - 1)I_n.$$

A conference matrix $C_n = (c_{ij})_{i,j=1}^n$ is a *symmetric conference matrix* if $c_{ij} = c_{ji}$ for all $1 \leq i, j \leq n$ and is a *skew-symmetric conference matrix* if $c_{ij} = -c_{ji}$ for all $1 \leq i, j \leq n$.

LEMMA 1. (Corollary 2.2, [11]) *Any real conference matrix of order $n > 2$ is equivalent, under multiplication of rows and columns by -1 , to a conference symmetric or to a skew-symmetric matrix according as $n \equiv 2 \pmod{4}$ or $n \equiv 0 \pmod{4}$.*

The following theorem gives the existence of symmetric conference matrices. The existence theorem for skew-symmetric conference matrices is same as Theorem 1.

THEOREM 2. (Theorem 4.11, [18]) *If a symmetric conference matrix of order n exists, then $n \equiv 2 \pmod{4}$ and $n - 1$ is the sum of two integral squares or equivalently, the square free part of $n - 1$ must not contain a prime factor $\equiv 3 \pmod{4}$.*

DEFINITION 4. (Real weighing matrix) *A real weighing matrix $W_{n,k}$ is a square matrix with entries $0, \pm 1$ having k non-zero entries per row and column and inner product of distinct rows zero. Hence, $W_{n,k}$ satisfies $W_{n,k}W_{n,k}^T = kI_n$. The number k is called the *weight* of $W_{n,k}$.*

The determinant of $W_{n,k}$ is $\pm k^{n/2}$ and if n is odd, $[\det(W_{n,k})]^2 = k^n$ implies k must be a square. Note that a $W_{n,n}$, $n \equiv 0 \pmod{4}$, is a real Hadamard matrix of order n and a $W_{n,n-1}$, $n \equiv 2 \pmod{4}$, is equivalent to a symmetric conference matrix. Using this definition, the zero element is no more required to be on the diagonal, and hence $W_{n,n-1}$ is a relaxed definition of real conference matrices. The following theorem gives the existence of real weighing matrices.

THEOREM 3. (Proposition 23, [12]) *1. If n is odd, then a $W_{n,k}$ exists only if*

- (i) *k is a square and*
- (ii) *$(n - k)^2 - (n - k) + 1 \geq n$.*

2. If $n \equiv 2 \pmod{4}$, then for a $W_{n,k}$ to exist,

- (i) *$k \leq n - 1$ and*
- (ii) *k is the sum of two integral squares.*

It has been conjectured that $n \equiv 0 \pmod{4}$, then a $W_{n,k}$ exists for all $1 \leq k \leq n$ ([13]).

2.2. p -almost Hadamard matrices

Now we give the definition and characterizations of p -almost Hadamard matrices.

DEFINITION 5. Let $H_n \in M(n, \mathbb{R})$. We say that H_n is an ‘‘almost Hadamard matrix’’ if $U_n := H_n/\sqrt{n}$ is orthogonal and is a local maximum of the 1-norm on $O(n, \mathbb{R})$, i.e., U_n is a local maximum of $\|U_n\|_1 = \sum_{i,j=1}^n |U_{ij}|$, where U_{ij} is an entry of U_n .

Equivalently, $U_{ij} \neq 0$, and the matrix

$$S_n U_n^T, \text{ with } S_{ij} = \text{sgn}(U_{ij}) = \begin{cases} 1, & \text{if } U_{ij} > 0, \\ -1, & \text{if } U_{ij} < 0, \end{cases}$$

must be positive definite.

For the equivalence between the two conditions in Definition 5, we refer the readers to see [6, 7]. Using the Cauchy-Schwarz inequality, we have

$$\begin{aligned} \|U_n\|_1 &= \sum_{i,j=1}^n |U_{ij}| \\ &\leq n \left(\sum_{i,j=1}^n |U_{ij}|^2 \right)^{1/2} = n\sqrt{n}, \end{aligned}$$

since U_n is orthogonal and we know that $\sum_{i,j=1}^n |U_{ij}|^2 = n$. Let us now define

$$\|U_n\|_p^p := \sum_{i,j=1}^n |U_{ij}|^p.$$

DEFINITION 6. A matrix $H_n \in M(n, \mathbb{R})$ such that $U_n = H_n/\sqrt{n}$ is orthogonal is called:

- (1) p -almost Hadamard ($p < 2$), if U_n locally maximizes the p -norm on $O(n, \mathbb{R})$.
- (2) p -almost Hadamard ($p > 2$), if U_n locally minimizes the p -norm on $O(n, \mathbb{R})$.

REMARK 1. Strictly speaking, one should use the terminology “real p -almost Hadamard matrices” instead of “ p -almost Hadamard matrices”, as the matrices under our consideration are real orthogonal matrices.

PROPOSITION 1. Let $U_n \in O(n, \mathbb{R})$, and let $p \in [1, \infty] \setminus \{2\}$.

- (1) If $p < 2$, then $\|U_n\|_p \leq n^{2/p-1/2}$, with equality if and only if $H_n = \sqrt{n}U_n$ is Hadamard.
- (2) If $p > 2$ then $\|U_n\|_p \geq n^{2/p-1/2}$, with equality if and only if $H_n = \sqrt{n}U_n$ is Hadamard.

For a proof Proposition 1, see Proposition 7.1, [6] or Proposition 2.1, [8]. It should be noted that for $p = 1, 4, \infty$, we obtain $\|U_n\|_1 \leq n\sqrt{n}$, $\|U_n\|_4 \geq 1$, $\|U_n\|_\infty \geq 1/\sqrt{n}$ and in all cases equality holds if and only if the rescaled matrix $H_n = \sqrt{n}U_n$ is Hadamard. As we discussed earlier, given an exponent $p \neq 2$ and a number $n \in \{2\} \cup 4\mathbb{N}$, where the Hadamard conjecture holds, the Hadamard matrices of order n are the best examples of p -almost Hadamard matrices. That is, $H_n \in M(n, \mathbb{R})$ are “optimal”, in the sense that the rescaled matrix $U_n = H_n/\sqrt{n}$ is a global maximum/minimum of the p -norm on $O(n, \mathbb{R})$, for $p \in [1, \infty] \setminus \{2\}$.

2.3. Complex Hadamard matrices

Next, we consider the complex Hadamard matrices and discuss about the existence of such matrices.

DEFINITION 7. For every positive integer n , the $n \times n$ unitary group $U(n, \mathbb{C})$ is the group of $n \times n$ unitary matrices with the group operation of matrix multiplication, satisfying

$$U_n U_n^* = U_n^* U_n = I_n,$$

where U_n^* is the conjugate transpose of U_n .

The $n \times n$ special orthogonal group is

$$SU(n, \mathbb{C}) = \left\{ U_n \in U(n, \mathbb{C}) : \det(U_n) = 1 \right\}.$$

Note that unitary and special unitary groups are smooth manifolds, compact and path-connected.

DEFINITION 8. A complex Hadamard matrix H_n is an $n \times n$ matrix with complex entries of modulus 1 such that $H_n H_n^* = n I_n$.

Thus a complex Hadamard matrix H_n is having unimodular entries such that $\frac{1}{\sqrt{n}} H_n$ is unitary.

LEMMA 2. For every $n \geq 1$, there exists a complex Hadamard matrix of order n .

Proof. The Fourier matrix

$$[F_n]_{ij} = e^{2\pi i(i-1)(j-1)/n}, \quad i, j = 1, \dots, n, \tag{1}$$

where $i = \sqrt{-1}$, is an example of a complex Hadamard matrix of order n . \square

The following are complex Hadamard matrices of orders $n = 1, 2$ and 3 , respectively:

$$F_1 = [1], \quad F_2 = \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}, \quad F_3 = \begin{pmatrix} 1 & 1 & 1 \\ 1 & \omega & \omega^2 \\ 1 & \omega^2 & \omega \end{pmatrix}, \tag{2}$$

where $\{1, \omega, \omega^2\}$ are the cube roots of unity. In general, F_n is given by the scaled Vandermonde's matrix:

$$F_n = \begin{pmatrix} 1 & 1 & 1 & \dots & 1 \\ 1 & \omega & \omega^2 & \dots & \omega^{n-1} \\ 1 & \omega^2 & \omega^4 & \dots & \omega^{2(n-1)} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & \omega^{n-1} & \omega^{2(n-1)} & \dots & \omega^{(n-1)^2} \end{pmatrix}.$$

For more details on the complex Hadamard matrices, the interested readers may refer to [19].

3. The optimization problem

The main objective of this work is to find p -almost Hadamard matrices of different orders and thus we formulate it as a constrained optimization problem (see Definition 6). For notational simplification, we use the symbols A, B, G, I, W, X, Y, Z , etc as $n \times n$ matrices. We also use the symbols $A^{i,j}$ for matrices and a_{ij} for matrix entries. The general minimization problem (see [21]) over the real orthogonal matrices can be formulated as:

$$\min_{X \in \mathbb{R}^{n \times n}} \mathcal{F}(X), \text{ such that } X^T X = I, \tag{3}$$

where $\mathbb{R}^{n \times n} := M(n, \mathbb{R})$, I is the $n \times n$ identity matrix and $\mathcal{F}(\cdot) : \mathbb{R}^{n \times n} \rightarrow \mathbb{R}$ is a twice continuously differentiable function. The feasible set $\mathcal{M}_n := \{X \in \mathbb{R}^{n \times n} : X^T X = I\}$ is often referred to as the *Stiefel Manifold*.

Given a differentiable function, $\mathcal{F}(\cdot) : \mathbb{R}^{n \times n} \rightarrow \mathbb{R}$, the gradient of \mathcal{F} with respect to X is denoted by $G := \mathcal{D}\mathcal{F}(X) = \left(\frac{\partial \mathcal{F}(X)}{\partial X_{ij}}\right)_{i,j=1}^n$. The derivative of \mathcal{F} at X in the direction Z is defined as

$$\mathcal{D}\mathcal{F}(X)[Z] := \lim_{t \rightarrow 0} \frac{\mathcal{F}(X + tZ) - \mathcal{F}(X)}{t} = \langle \mathcal{D}\mathcal{F}(X), Z \rangle.$$

Here $\langle \cdot, \cdot \rangle$ denotes the Euclidean inner product between two matrices and is defined by

$$\langle A, B \rangle := \sum_{j,k=1}^n a_{jk} b_{jk} = \text{Tr}(A^T B), \text{ for all } A = (a_{ij})_{i,j=1}^n, B = (b_{ij})_{i,j=1}^n \in \mathbb{R}^{n \times n},$$

where $\text{Tr}(A)$ is the trace of A , i.e., the sum of the diagonal elements of A . We use $\nabla \mathcal{F}$ for gradients in tangent planes. Given a feasible point X and the gradient G , we define a skew-symmetric matrix A as either

$$\left. \begin{aligned} A &:= GX^T - XG^T \text{ or} \\ A &:= (P_X G)X^T - X(P_X G)^T, \text{ where } P_X := \left(I - \frac{1}{2}XX^T\right). \end{aligned} \right\} \tag{4}$$

REMARK 2. We know that $SO(n, \mathbb{R})$ is the connected component of the identity in $O(n, \mathbb{R})$. The subsets of $SO(n, \mathbb{R})$, whose members are connected to the identity by paths (path-connected component). Let us now find $Z \in \mathcal{T}_X \mathcal{M}_n := \{Z \in \mathbb{R}^{n \times n} : X^T Z + Z^T X = \mathbf{0}\}$, which is the tangent space of \mathcal{M}_n at X .

Let $\gamma : (-a, a) \rightarrow SO(n, \mathbb{R})$, $a \in \mathbb{R}$ be a smooth curve with $\gamma(0) = I$. Since, it is a curve in $SO(n, \mathbb{R})$, for each s , we have $\gamma(s)\gamma(s)^T = I$. Let us differentiate this relation with respect to s to obtain

$$\gamma'(s)\gamma(s)^T + \gamma(s)\gamma'(s)^T = \mathbf{0}.$$

For $s = 0$, we have $\gamma'(0) + \gamma'(0)^\top = \mathbf{0}$, so that $\gamma'(0)$ is skew-symmetric. Hence, every tangent vector to $\text{SO}(n, \mathbb{R})$ at \mathbf{I} is a skew-symmetric matrix. Since $\mathcal{T}_\mathbf{I} \mathcal{M}_n^{\text{SO}} \subset \mathfrak{so}(n, \mathbb{R})$, where

$$\mathcal{M}_n^{\text{SO}} := \left\{ \mathbf{X} \in \mathbb{R}^{n \times n} : \mathbf{X}^\top \mathbf{X} = \mathbf{I}, \det(\mathbf{X}) = 1 \right\},$$

and $\mathfrak{so}(n, \mathbb{R})$ denotes the $n \times n$ skew-symmetric matrices, and both are vector spaces of dimension $\frac{n(n-1)}{2}$, they must be equal.

In general, the tangent space of a matrix $\mathbf{X} \in \text{SO}(n, \mathbb{R})$ is given by

$$\mathcal{T}_\mathbf{X} \mathcal{M}_n^{\text{SO}} = \left\{ \mathbf{X}\mathbf{A} : \mathbf{A} \in \mathfrak{so}(n, \mathbb{R}) \right\},$$

where the dimension of $\mathcal{T}_\mathbf{X} \mathcal{M}_n^{\text{SO}}$ is $\frac{n^2-n}{2}$. This means that any tangent vector at \mathbf{X} is \mathbf{X} times some skew-symmetric matrix. Since $\text{SO}(n, \mathbb{R})$ is a connected component of $\text{O}(n, \mathbb{R})$ containing \mathbf{I} , the group $\text{SO}(n, \mathbb{R})$ has the same tangent space at the neutral element \mathbf{I} , because all members of $\text{O}(n, \mathbb{R})$ near the identity are members of $\text{SO}(n, \mathbb{R})$. Thus we denote $\mathcal{T}_\mathbf{X} \mathcal{M}_n^{\text{SO}} = \mathcal{T}_\mathbf{X} \mathcal{M}_n^{\text{O}} := \mathcal{T}_\mathbf{X} \mathcal{M}_n$.

Following [21], we next state the first and second order optimality conditions for the optimization problem (3) in the following lemmas. Since the matrix $\mathbf{X}^\top \mathbf{X} = \mathbf{I}$ is symmetric, the Lagrangian multiplier Λ corresponding to $\mathbf{X}^\top \mathbf{X} = \mathbf{I}$ is a symmetric matrix. The Lagrangian function for the optimization problem (3) is given by

$$\mathcal{L}(\mathbf{X}, \Lambda) = \mathcal{F}(\mathbf{X}) - \frac{1}{2} \text{Tr} \left(\Lambda \left(\mathbf{X}^\top \mathbf{X} - \mathbf{I} \right) \right). \tag{5}$$

Let us now give the first order necessary condition and second order necessary and sufficient conditions of optimality for the problem (3).

LEMMA 3. (First order necessary condition, Lemma 1, [21]) *If \mathbf{X} is a local minimizer of the problem (3), then \mathbf{X} satisfies the first order optimality conditions,*

$$\mathcal{D}_\mathbf{X} \mathcal{L}(\mathbf{X}, \Lambda) = \mathbf{G} - \mathbf{X}\mathbf{G}^\top \mathbf{X} = \mathbf{0} \text{ and } \mathbf{X}^\top \mathbf{X} = \mathbf{I},$$

with the associated Lagrangian multiplier $\Lambda = \mathbf{G}^\top \mathbf{X}$. Define

$$\nabla \mathcal{F}(\mathbf{X}) := \mathbf{G} - \mathbf{X}\mathbf{G}^\top \mathbf{X}, \text{ and } \mathbf{A} := \mathbf{G}\mathbf{X}^\top - \mathbf{X}\mathbf{G}^\top. \tag{6}$$

Then, $\nabla \mathcal{F}(\mathbf{X}) = \mathbf{A}\mathbf{X}$. Moreover, $\nabla \mathcal{F}(\mathbf{X}) = \mathbf{0}$, if and only if $\mathbf{A} = \mathbf{0}$.

LEMMA 4. (Second order necessary condition, Theorem 12.5, [16], Lemma 2, [21]) *Suppose that $\mathbf{X} \in \mathcal{M}_n$ is a local minimizer for the problem (3). Then \mathbf{X} satisfies*

$$\text{Tr} \left(\mathbf{Z}^\top \mathcal{D} \left(\mathcal{D} \mathcal{F}(\mathbf{X}) \right) [\mathbf{Z}] \right) - \text{Tr} \left(\Lambda \mathbf{Z}^\top \mathbf{Z} \right) \geq 0, \text{ where } \Lambda = \mathbf{G}^\top \mathbf{X}, \tag{7}$$

for all $\mathbf{Z} \in \mathcal{T}_\mathbf{X} \mathcal{M}_n := \left\{ \mathbf{Z} \in \mathbb{R}^{n \times n} : \mathbf{X}^\top \mathbf{Z} + \mathbf{Z}^\top \mathbf{X} = \mathbf{0} \right\}$, which is the tangent space of \mathcal{M}_n at \mathbf{X} .

LEMMA 5. (Second order sufficient condition, Theorem 12.6, [16], Lemma 2, [21])
 Suppose that for $X \in \mathcal{M}_n$, there exists a Lagrange multiplier Λ such that the first order conditions are satisfied. Suppose also that

$$\text{Tr} \left(Z^\top \mathcal{D}(\mathcal{D}\mathcal{F}(X)) [Z] \right) - \text{Tr} \left(\Lambda Z^\top Z \right) > 0, \tag{8}$$

for any matrix $Z \in \mathcal{F}_X \mathcal{M}_n$. Then X is a strict local minimizer for the problem (3).

REMARK 3. For the corresponding maximization problem, Lemma 3 remains the same and the inequalities (7) and (8) in the second order necessary and sufficient conditions (Lemma 4 and Lemma 5) are reversed.

Since the orthogonality constraint is non-convex, the optimization problem (3) may lead to several local extrema, even if the cost functional is convex. Different optimization problems involving orthogonal matrix constraints can be found in [14, 21, 2, 3, 4], etc.

3.1. The optimization problem for p -almost Hadamard matrices

Let $p \in (2, \infty)$ and consider

$$\min_{X \in \mathbb{R}^{n \times n}} \sum_{i,j=1}^n |a_{ij}|^p, \text{ such that } \sum_{k=1}^n a_{ki} a_{kj} = \begin{cases} 1 & \text{if } i = j, \\ 0 & \text{if } i \neq j. \end{cases} \tag{9}$$

In this case, the derivative matrix G and the matrix A are given by

$$G := \left(\frac{\partial \mathcal{F}(X)}{\partial X_{ij}} \right)_{i,j=1}^n = p (|a_{ij}|^{p-2} a_{ij})_{i,j=1}^n, \tag{10}$$

and

$$A := GX^\top - XG^\top = p \left(\sum_{k=1}^n a_{ik} a_{jk} (|a_{ik}|^{p-2} - |a_{jk}|^{p-2}) \right)_{i,j=1}^n. \tag{11}$$

If there exists a matrix $X = M_n = (a_{ij})_{i,j=1}^n$ minimizes the function given in (9), then the first order necessary condition given in Lemma 3 becomes $GX^\top = XG^\top$ and hence for all i and j , we have

$$\sum_{k=1}^n a_{ik} a_{jk} (|a_{ik}|^{p-2} - |a_{jk}|^{p-2}) = 0. \tag{12}$$

In order to get the second order necessary and sufficient conditions given in Lemma 4 and Lemma 5, we first calculate $\mathcal{D}(\mathcal{D}\mathcal{F}(X)) [Z]$ as

$$\begin{aligned} \mathcal{D}(\mathcal{D}\mathcal{F}(X)) [Z] &= \text{Tr} \left(Z^\top \mathcal{D}\mathcal{F}(X) \right) = \sum_{i,j=1}^n z_{ij} \left(\frac{\partial (\mathcal{D}\mathcal{F}(X))_{ij}}{\partial X_{ij}} \right)_{i,j=1}^n \\ &= p(p-1) (z_{ij} |a_{ij}|^{p-2})_{i,j=1}^n, \end{aligned} \tag{13}$$

where $Z = (z_{ij})_{i,j=1}^n$. Hence, we find $\text{Tr} \left(Z^\top \mathcal{D}(\mathcal{D}\mathcal{F}(X)) [Z] \right)$ for all $Z \in \mathcal{F}_X \mathcal{M}_n$, as

$$\begin{aligned} \text{Tr} \left(Z^\top \mathcal{D}(\mathcal{D}\mathcal{F}(X)) [Z] \right) &= \sum_{i,j=1}^n z_{ij} (\mathcal{D}(\mathcal{D}\mathcal{F}(X)) [Z])_{ij} \\ &= p(p-1) \sum_{i,j=1}^n z_{ij}^2 |a_{ij}|^{p-2}, \end{aligned} \tag{14}$$

for all $Z \in \mathcal{F}_X \mathcal{M}_n$.

We define $A^{i,j} \in \mathfrak{so}(n)$, for $i \neq j$ and $i < j$, as a skew-symmetric matrix with 1 on the ij^{th} position and -1 on the ji^{th} position. Now, for any $Z^{i,j} \in \mathcal{F}_X \mathcal{M}_n$, $i \neq j$ and $i < j$, we have

$$\begin{aligned} \text{Tr} \left((Z^{i,j})^\top \mathcal{D}(\mathcal{D}\mathcal{F}(X)) [Z^{i,j}] \right) &= p(p-1) \sum_{k,l=1}^n (z_{kl}^{i,j})^2 |a_{kl}|^{p-2} \\ &= p(p-1) \sum_{k=1}^n [a_{ki}^2 |a_{kj}|^{p-2} + a_{kj}^2 |a_{ki}|^{p-2}], \end{aligned}$$

where $Z^{i,j} = (z_{kl}^{i,j})_{k,l=1}^n$. We also have

$$\text{Tr} \left(\Lambda (Z^{i,j})^\top Z^{i,j} \right) = p \left[\sum_{k=1}^n (|a_{ki}|^p + |a_{kj}|^p) \right],$$

where $\Lambda = G^\top X$ is the Lagrange multiplier. Finally, we obtain

$$\begin{aligned} \xi_{M_n}^{i,j} &:= \text{Tr} \left((Z^{i,j})^\top \mathcal{D}(\mathcal{D}\mathcal{F}(X)) [Z^{i,j}] \right) - \text{Tr} \left(\Lambda (Z^{i,j})^\top Z^{i,j} \right) \\ &= p \sum_{k=1}^n [(p-1)(a_{ki}^2 |a_{kj}|^{p-2} + a_{kj}^2 |a_{ki}|^{p-2}) - (|a_{ki}|^p + |a_{kj}|^p)]. \end{aligned} \tag{15}$$

For $p > 2$, M_n is a local minimum for the optimization problem (9) only if $\xi_{M_n}^{i,j} > 0$ for all $1 \leq i < j \leq n$.

REMARK 4. 1. For $1 < p < 2$, and if the entries of M_n are non-zero, then M_n is a local maximum for the optimization problem (9) only if $\xi_{M_n}^{i,j} < 0$ for all $1 \leq i < j \leq n$.

2. For $p = 2$, we know that $\sum_{i,j=1}^n a_{ij}^2 = n$, for any n . If we consider it as an optimization problem, then from (12), using the orthogonality, one can easily get that every orthogonal matrix $M_n \in \mathbb{R}^{n \times n}$ is a stationary point. Note also that $\xi_{M_n}^{i,j} = \mathbf{0}$, for all $1 \leq i < j \leq n$.

4. Some p -almost Hadamard matrices

In this section, first give some particular examples of p -almost Hadamard matrices of various orders using Hadamard, conference and weighing matrices. Then, we check the truth content of the Conjecture 4.4 in [8].

PROPOSITION 2. *If a real Hadamard matrix H_n exists, then $\frac{1}{\sqrt{n}}H_n$ is a stationary point of the minimization problem (9) and is a local minimum and also a global minimum.*

Proof. Let n be $1, 2$ or $\equiv 0 \pmod{4}$ and let us assume that a real Hadamard matrix H_n exists. We define $P_n := \frac{1}{\sqrt{n}}H_n$. Since the entries of H_n are ± 1 , we have the derivative matrix

$$G_n = \frac{p}{n^{\frac{p-2}{2}}}P_n, \text{ and } A_n = G_n P_n^T - P_n G_n^T = \mathbf{0}_n,$$

and the first order necessary condition is satisfied, so that P_n is a stationary point. Also, one can easily get

$$\xi_{P_n}^{i,j} = \frac{2p(p-2)}{n^{\frac{p-2}{2}}} > 0,$$

for each $Z^{i,j} \in \mathcal{T}_{P_n} \mathcal{M}_n$, $1 \leq i < j \leq n$ and $p > 2$. Hence P_n is a local minimum.

Let us now consider the sets:

$$\mathcal{A} := \left\{ X = (a_{ij})_{i,j=1}^n \in \mathbb{R}^{n \times n} : \sum_{j=1}^n a_{ij}^2 = 1, \text{ for } i = 1, \dots, n \right\},$$

$$\mathcal{B} := \left\{ X = (a_{ij})_{i,j=1}^n \in \mathbb{R}^{n \times n} : \sum_{j=1}^n a_{ij}^2 = 1, \text{ for } i = 1, \dots, n, \sum_{k=1}^n a_{ik}a_{jk} = 0, \text{ for } i \neq j \right\}.$$

Clearly the set $\mathcal{B} \subsetneq \mathcal{A}$. Now for each fixed $1 \leq i \leq n$, we consider the problem:

$$\min_{X \in \mathbb{R}^{n \times n}} \sum_{j=1}^n |a_{ij}|^p \text{ subject to } \sum_{j=1}^n a_{ij}^2 = 1. \tag{16}$$

That is, we are considering a minimization problem over the set \mathcal{A} . Using Lagrangian multipliers, one can easily obtain that one of the stationary points of the problem (16) is $M_n = (a_{ij})_{i,j=1}^n \in \mathcal{A}$ with $|a_{ij}|^2 = \frac{1}{n}$ for all $1 \leq j \leq n$. This is a local minimum, since the Hessian matrix is given by:

$$\mathcal{H} = p(p-2)\text{diag}(|a_{i1}|^{p-2}, \dots, |a_{in}|^{p-2}) = \frac{p(p-2)}{n^{\frac{p-2}{2}}}I_n,$$

and is positive definite for all $p > 2$. It is also a global minimum, since the cost functional and constraint both are convex. Since $\mathcal{B} \subsetneq \mathcal{A}$ and $P_n \in \mathcal{B}$ implies that there exists a global minimum for this problem in \mathcal{B} also. Thus, for any $M_n = (a_{ij})_{i,j=1}^n \in \mathcal{B}$, we have

$$\mathcal{F}(M_n) := \sum_{i,j=1}^n |a_{ij}|^p \geq \sum_{i=1}^n \sum_{j=1}^n \frac{1}{n^{p/2}} = \frac{1}{n^{p/2-2}} = \mathcal{F}(P_n).$$

Thus P_n is a global minimum and H_n is a p -almost Hadamard matrix. \square

REMARK 5. Since the matrix entries are nonzero, the above computation also shows that $P_n = \frac{1}{\sqrt{n}}H_n$ is a local minimum for $1 < p < 2$ and hence H_n is a p -almost Hadamard matrix, for $1 < p < 2$. Also H_n almost Hadamard for all n .

PROPOSITION 3. *If a conference matrix C_n of order n exists, then the matrix $R_n := \frac{1}{\sqrt{n-1}}C_n$ is a strict local minimum to the problem (9), for $p \in (\frac{2n-3}{n-2}, \infty), n > 2$.*

Proof. Let $n > 2$ be even and assume that a conference matrix C_n of order n exists and let $R_n = \frac{1}{\sqrt{n-1}}C_n$. Since the entries of C_n are $0, \pm 1$ and 0 occurs only along the diagonal, we have

$$G_n = \frac{P}{(n-1)^{\frac{p-2}{2}}}R_n \text{ and } A_n = G_nR_n^\top - R_nG_n^\top = \mathbf{0}_n.$$

Thus it is immediate that (12) is satisfied and R_n is a stationary point. Now, we have

$$\xi_{R_n}^{i,j} = \frac{2p}{(n-1)^{\frac{p}{2}}} [n(p-2) - 2p + 3]. \tag{17}$$

Note that $\xi^{ij} > 0$ only if $n > \frac{2p-3}{p-2}$ and we know that $\lim_{p \rightarrow \infty} \frac{2p-3}{p-2} = 2$. Thus, $\frac{1}{\sqrt{n-1}}C_n$ is a strict local minimum to the problem (9), for all $p \in (\frac{2n-3}{n-2}, \infty)$. \square

REMARK 6. Since R_n is a local minimum to the problem (9), the matrix $\tilde{R}_n := \frac{\sqrt{n}}{\sqrt{n-1}}C_n$ is p -almost Hadamard, for all $p > \frac{2n-3}{n-2}$ and $n > 2$.

PROPOSITION 4. *If a weighing matrix $W_{n,k} = (w_{ij})_{i,j=1}^n$ exists for some $1 \leq k \leq n$, then the orthogonal matrix $S_{n,k} := \frac{1}{\sqrt{k}}W_{n,k}$ is a stationary point to the minimization problem (9). Also if*

$$\beta_{ij} = \sum_{l=1}^n w_{li}^2 w_{lj}^2, \underline{\beta} = \min_{i,j} \beta_{ij} \text{ and } \bar{\beta} = \max_{i,j} \beta_{ij}, \text{ for } 1 \leq i < j \leq n,$$

then we have $S_{n,k}$ is

- (i) a strict local minimum if $\underline{\beta} > \frac{k}{p-1}$,
- (ii) a strict local maximum if $\bar{\beta} < \frac{k}{p-1}$,
- (iii) a saddle point if $\beta_{ij} \geq \frac{k}{p-1}$ and $\beta_{ij} \leq \frac{k}{p-1}$ for some i and j .

Proof. If a weighing matrix $W_{n,k} = (w_{ij})_{i,j=1}^n$ exists for some $1 \leq k \leq n$, then the orthogonal matrix $S_{n,k} = \frac{1}{\sqrt{k}}W_{n,k}$ is a stationary point to the minimization problem (9), since the entries of weighing matrices are $0, \pm 1$ and

$$G_{n,k} = \frac{P}{k^{\frac{p-2}{2}}}S_{n,k} \text{ and } A_{n,k} = G_{n,k}S_{n,k}^\top - S_{n,k}G_{n,k}^\top = \mathbf{0}_n.$$

Also, $S_{n,k}$ is a strict local minimum if $\underline{\beta} > \frac{k}{p-1}$, a strict local maximum if $\overline{\beta} < \frac{k}{p-1}$, and a saddle point if $\beta_{ij} \geq \frac{k}{p-1}$ and $\beta_{ij} \leq \frac{k}{p-1}$ for some i and j , since

$$\xi_{S_{n,k}}^{i,j} = \frac{2p}{k^{\frac{p}{2}}} ((p-1)\beta_{ij} - k),$$

for $1 \leq i < j \leq n$. Hence the matrix $S_{n,k}$ is a strict local minimum if $\underline{\beta} > \frac{k}{p-1}$. \square

REMARK 7. The matrix $\widetilde{S}_{n,k} := \frac{\sqrt{n}}{\sqrt{k}} W_{n,k}$ is a p -almost Hadamard matrix for all $p \in (\frac{k}{\beta}, \infty)$. Since some of the matrix entries are zero, at this moment, we cannot say anything about the case for $1 < p < 2$.

PROPOSITION 5. The matrix $T_{n_1 n_2} := \frac{1}{\sqrt{n_1}} H_{n_1} \otimes M_{n_2}$ is a strict local minimum of the optimization problem (9) of order $n_1 n_2$ if M_{n_2} is a strict local minimum of the optimization problem (9) of order n_2 .

Proof. For $p \in (2, \infty)$, from Proposition 2, we know that $\frac{1}{\sqrt{n_1}} H_{n_1}$ is a global minimum of the optimization problem (9) of order n_1 . If the matrix $M_{n_2} = (a_{ij})_{i,j=1}^{n_2}$ is a strict local minimum of the optimization problem (9) of order n_2 , then we know that

$$\sum_{k=1}^{n_2} a_{ik} a_{jk} (|a_{ik}|^{p-2} - |a_{jk}|^{p-2}) = 0$$

for all $1 \leq i, j \leq n_2$, and

$$\xi_{M_{n_2}}^{i,j} = p \sum_{k=1}^{n_2} [(p-1)(a_{ki}^2 |a_{kj}|^{p-2} + a_{kj}^2 |a_{ki}|^{p-2}) - (|a_{ki}|^p + |a_{kj}|^p)] > 0,$$

for $1 \leq i < j \leq n_2$. Now, we consider the matrix $T_{n_1 n_2} := \frac{1}{\sqrt{n_1}} H_{n_1} \otimes M_{n_2} = (c_{ij})_{i,j=1}^{n_1 n_2}$. Since the entries of H_{n_1} are ± 1 , one can easily get

$$\sum_{k=1}^{n_1 n_2} c_{ik} c_{jk} (|c_{ik}|^{p-2} - |c_{jk}|^{p-2}) = \frac{1}{n_1^{p/2-1}} \sum_{k=1}^{n_2} a_{ik} a_{jk} (|a_{ik}|^{p-2} - |a_{jk}|^{p-2}) = 0,$$

for all $1 \leq i, j \leq n_1 n_2$. Thus $T_{n_1 n_2}$ is a stationary point of the optimization problem (9) of order $n_1 n_2$. Also, we have $\xi_{T_{n_1 n_2}}^{i,j}$ is either

$$\xi_{T_{n_1 n_2}}^{i,j} = p \frac{1}{n_1^{p/2-1}} \sum_{k=1}^{n_2} [(p-1)(a_{ki}^2 |a_{kj}|^{p-2} + a_{kj}^2 |a_{ki}|^{p-2}) - (|a_{ki}|^p + |a_{kj}|^p)] > 0,$$

or

$$\xi_{T_{n_1 n_2}}^{i,j} = \frac{p(p-2)}{n_1^{p/2-1}} \sum_{k=1}^{n_2} [|a_{ki}|^p + |a_{kj}|^p] > 0,$$

for $1 \leq i < j \leq n_1 n_2$. Thus $T_{n_1 n_2}$ is a strict local minimum of the optimization problem (9) of order $n_1 n_2$. \square

4.1. The matrix K_n

Let us now verify the truth content of the Conjecture 4.4 in [8]. We begin with the following proposition:

PROPOSITION 6. For $p > 2$, the orthogonal matrix

$$Q_n = \frac{1}{n} \begin{pmatrix} -(n-2) & 2 & \cdots & 2 \\ 2 & -(n-2) & \cdots & 2 \\ \vdots & \vdots & \ddots & \vdots \\ 2 & 2 & \cdots & -(n-2) \end{pmatrix} = \frac{K_n}{\sqrt{n}}, \tag{18}$$

is always a stationary point of the minimization problem (9). For $n \in \mathbb{N} \setminus \{2\}$, Q_n is a strict local minimum for

$$(p-1) [(n-2)2^p + (n-2)^2 2^{p-2} + 2^2(n-2)^{p-2}] > (n-2)^p + 2^p(n-1). \tag{19}$$

That is, for $n \in \mathbb{N} \setminus \{2\}$, K_n is p -almost Hadamard for all $p \in (2, \infty)$ satisfying (19).

Proof. For the orthogonal matrix given in (18), the matrix

$$A_n = G_n Q_n^\top - Q_n G_n^\top = \mathbf{0}_n,$$

where $G_n = \frac{p}{n^{p-1}} \begin{pmatrix} -(n-2)^{p-1} & 2^{p-1} & \cdots & 2^{p-1} \\ 2^{p-1} & -(n-2)^{p-1} & \cdots & 2^{p-1} \\ \vdots & \vdots & \ddots & \vdots \\ 2^{p-1} & 2^{p-1} & \cdots & -(n-2)^{p-1} \end{pmatrix} = G_n^\top$ and $Q_n^\top = Q_n$

and $G_n Q_n = Q_n G_n$. Thus, Q_n is always a stationary point of the minimization problem (9).

It can also be calculated that

$$\left. \begin{aligned} \text{Tr}(\Lambda_n(Z^{i,j})^\top Z^{i,j}) &= \frac{2p}{n^p} [(n-2)^p + 2^p(n-1)], \\ \text{Tr}((Z^{i,j})^\top \mathcal{D}(\mathcal{D}\mathcal{F}(Q_n)) [Z^{i,j}]) &= \frac{2p(p-1)}{n^{p-1}} [(n-2)^2 2^{p-2} + 2^2(n-2)^{p-2} + (n-2)2^p], \\ \text{and } \xi_{Q_n}^{i,j} &= \frac{2p}{n^p} \left\{ (p-1) [(n-2)^2 2^{p-2} + 2^2(n-2)^{p-2}] \right. \\ &\quad \left. + (n-2)2^p - (n-2)^p - 2^p(n-1) \right\}, \end{aligned} \right\}$$

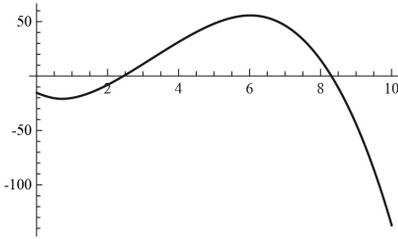
for each $Z^{i,j} \in \mathcal{T}_X \mathcal{M}_n$, $1 \leq i < j \leq n$. Hence, $\xi_{Q_n}^{i,j} > 0$ for the condition given in (19) and is a strict local minimum for the minimization problem (9), for $n \geq 3$. For $n = 2$, $\xi_{Q_n}^{i,j} < 0$, for all $p \in (2, \infty)$, and Q_n is a strict local maximum. Hence, for $n \geq 3$, K_n is p -almost Hadamard for all $p \in (2, \infty)$ satisfying (19). \square

REMARK 8. 1. For $p = 2$, Q_n is always a stationary point by Remark 4 (2) and $\xi_{Q_n}^{i,j} = \mathbf{0}$, for all $1 \leq i < j \leq n$.

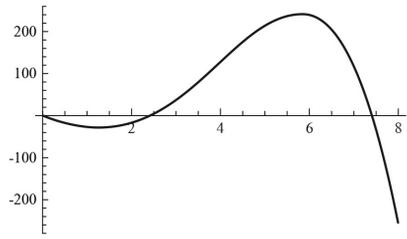
2. Let us define

$$f(p, n) := (p - 1) [(n - 2)2^p + (n - 2)^2 2^{p-2} + 2^2(n - 2)^{p-2}] - (n - 2)^p - 2^p(n - 1).$$

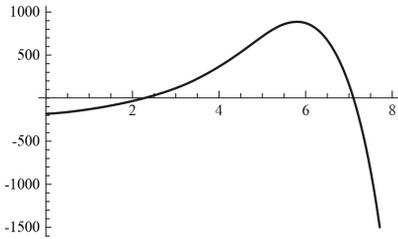
For $p = 2$, we have $f(n, 2) = 0$, for all $n \geq 2$. For $p = 3, \dots, 8$ and $n \geq 0$, the plots are given below (n on the x -axis and $f(p, n)$, for $p = 3, \dots, 8$ on the y -axis):



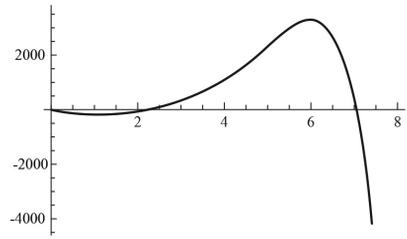
(a) $f(3, n) = -n^3 + 10n^2 - 12n - 16$.



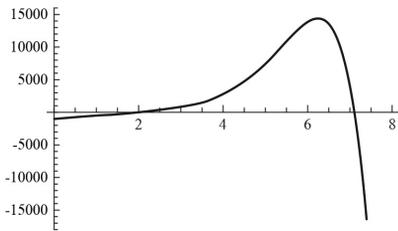
(b) $f(4, n) = -n^4 + 8n^3 - 32n$.



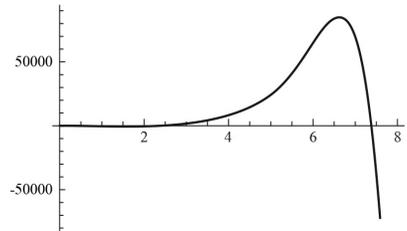
(c) $f(5, n) = -n^5 + 10n^4 - 24n^3 + 16n^2 + 80n - 192$.



(d) $f(6, n) = -n^6 + 12n^5 - 40n^4 + 320n^2 - 512n$.



(e) $f(7, n) = -n^7 + 14n^6 - 60n^5 + 40n^4 + 400n^3 - 1056n^2 + 1344n - 1280$.



(f) $f(8, n) = -n^8 + 16n^7 - 84n^6 + 112n^5 + 560n^4 - 2688n^3 + 5736n^2 - 4096n$.

Figure 1: Plots of $f(p, n)$, $n = 3, \dots, 8$.

From the Figure 1, it is clear that K_n is 3-almost Hadamard for all $n = 3, \dots, 8$, and 4-, ..., 8-almost Hadamard for all $n = 3, \dots, 7$.

REMARK 9. One can write $f(\cdot, \cdot)$ as

$$f(p, n) = 2^{p-2} [(n^2 - 4)p - (n^2 + 4n - 8)] + (n - 2)^{p-2} [4p - (n^2 - 4n + 8)]. \quad (20)$$

From this expression, it is also clear that $f(p, n) > 0$ for all

$$p > \max \left\{ \frac{n^2 + 4n - 8}{n^2 - 4}, \frac{n^2 - 4n + 8}{4} \right\} = \frac{n^2 - 4n + 8}{4}, \tag{21}$$

for $n > 4$. Thus, for $n > 4$, K_n is p -almost Hadamard for all p satisfying (21).

REMARK 10. It can also be proved that Q_n is a global minimum for $n = 3$ (see [10, 3] for more details). The Rény and Tsallis entropy for orthogonal matrices defined in [3] has an interesting connection with the p -almost Hadamard matrices. Both of them have same stationary points and same local (global) minima.

PROPOSITION 7. For $p \in (1, 2)$, the orthogonal matrix Q_n is always a stationary point of the maximization problem

$$\max_{X \in \mathbb{R}^{n \times n}} \sum_{i,j=1}^n |a_{ij}|^p, \text{ such that } \sum_{k=1}^n a_{ki}a_{kj} = \begin{cases} 1 & \text{if } i = j, \\ 0 & \text{if } i \neq j, \end{cases} a_{ij} \neq 0 \text{ for all } 1 \leq i, j \leq n. \tag{22}$$

For $n \in \mathbb{N} \setminus \{2\}$, Q_n is a strict local maximum for

$$(p - 1) [(n - 2)2^p + (n - 2)^2 2^{p-2} + 2^2(n - 2)^{p-2}] < (n - 2)^p + 2^p(n - 1). \tag{23}$$

That is, K_n is p -almost Hadamard for all $n \in \mathbb{N} \setminus \{2\}$ and $p \in (1, 2)$ satisfying (23).

Proof. A similar calculation in the Theorem 6 yields Q_n is a stationary point of the problem (22). Since the entries of Q_n are nonzero, we have

$$\xi_{Q_n}^{i,j} = \frac{2p}{n^p} \left\{ (p - 1) [(n - 2)^2 2^{p-2} + 2^2(n - 2)^{p-2} + (n - 2)2^p] - (n - 2)^p - 2^p(n - 1) \right\},$$

for each $Z^{i,j} \in \mathcal{T}_X \mathcal{M}_n$, $1 \leq i < j \leq n$. Hence for $n \in \mathbb{N} \setminus \{2\}$, Q_n is a local maximum and K_n is p -almost Hadamard for $p \in (1, 2)$ satisfying (23). \square

REMARK 11. For $1 < p < 2$, from the definition of $f(\cdot, \cdot)$ in (20), it is clear that

$$\begin{aligned} f(p, n) &= 2^{p-2} [(n^2 - 4)p - (n^2 + 4n - 8)] + (n - 2)^{p-2} [4p - (n^2 - 4n + 8)] \\ &< 2^{p-2} [(n^2 - 4)2 - (n^2 + 4n - 8)] + (n - 2)^{p-2} [8 - (n^2 - 4n + 8)] \\ &= (n^2 - 4n) (2^{p-2} - (n - 2)^{p-2}) < 0 \end{aligned}$$

for all $n > 4$. Thus K_n is p -almost Hadamard for all $1 < p < 2$ and $n \in \mathbb{N} \setminus \{2\}$ (see below for the cases $n = 3$ and 4), and hence the Conjecture 4.4 in [8] holds true for all $p \in (1, 2)$.

Indeed it is proved in Lemma 3.1, [6] that if $M_n = (a_{ij})_{i,j=1}^n \in O(n, \mathbb{R})$ locally maximizes the 1-norm, then $a_{ij} \neq 0$ for any $1 \leq i, j \leq n$. Thus, we also have

COROLLARY 1. K_n is almost Hadamard for all $n \in \mathbb{N} \setminus \{2\}$.

Proof. Since the matrix entries are non-zero, by taking $p = 1$ in (23) and using the fact that [1] is a Hadamard matrix, we find K_n is almost Hadamard for all $n \in \mathbb{N}$. \square

Let us now discuss the p -almost Hadamard property of K_n , for $n = 3, \dots, 9$ using the results obtained in Propositions 6 and 7.

Case (i). For $n = 3$, we know that

$$f(p, 3) = (5p - 13)2^{p-2} + (4p - 5). \quad (24)$$

Note that $f(1, 3) = -3$, $f(2, 3) = 0$ and $f(3, 3) = 11$. We also have $f'(p, 3) = 2^{p-2}[(5p - 13)\ln 2 + 5] + 4 > 0$ for all $p > 1$ and so $f(\cdot, 3)$ is an increasing function for all $p > 1$. Hence K_3 is p -almost Hadamard for all $p \in (1, 2) \cup (2, \infty)$.

Case (ii). For $n = 4$, K_4 is nothing but a real Hadamard matrix of order 4. We also have $f(p, 4) = (p - 2)2^{p+1} > 0$ for all $p \in (2, \infty)$ and < 0 for all $p \in (1, 2)$. Hence K_4 is p -almost Hadamard for all $p \in (1, 2) \cup (2, \infty)$.

Case (iii). For $n = 5$, we obtain

$$f(p, 5) = (21p - 37)2^{p-2} + (4p - 13)3^{p-2}.$$

It is clear from the above expression that $f(p, 5) > 0$ for all $p > 13/4 = 3.2500$. But graphically, one can show that $f(p, 5) > 0$ for all $p \in (2, \infty)$ and hence K_5 is p -almost Hadamard for all $p \in (1, 2) \cup (2, \infty)$ (see Figure 2 below).

Case (iv). For $n = 6$, we have

$$f(p, 6) = (8p - 13)2^p + (p - 5)4^{p-1}.$$

It is immediate from the above expression that $f(p, 6) > 0$ for all $p > 5$. One can show graphically that $f(p, 6) > 0$ for all $p \in (2, \infty)$ and hence K_6 is p -almost Hadamard for all $p \in (1, 2) \cup (2, \infty)$ (see Figure 2 below).

Case (v). For $n = 7$, we obtain

$$f(p, 7) = (45p - 69)2^{p-2} + (4p - 29)5^{p-2}.$$

It is clear from the above expression that $f(p, 7) > 0$ for all $p > 29/4 = 7.2500$. From the graph below (see Figure 3), it is clear that $f(p, 7) > 0$ for all $p \in (2, \infty)$ and hence K_7 is p -almost Hadamard for all $p \in (1, 2) \cup (2, \infty)$.

Case (vi). For $n = 8$, we find

$$f(p, 8) = (15p - 22)2^p + 4(p - 10)6^{p-2}.$$

It should be noted from the above expression that $f(p, 8) > 0$ for all $p > 10$. Now, it can be easily seen that $f(3, 8) = 16 > 0$ and $f(4, 8) = -256 < 0$, and $f(9, 8) = -1061888 < 0$ and $f(10, 8) = 131072 > 0$. Thus there are two zero of $f(\cdot, 8)$, one lies between 3 and 4, and the other between 9 and 10. We find both zeros of $f(\cdot, 8)$

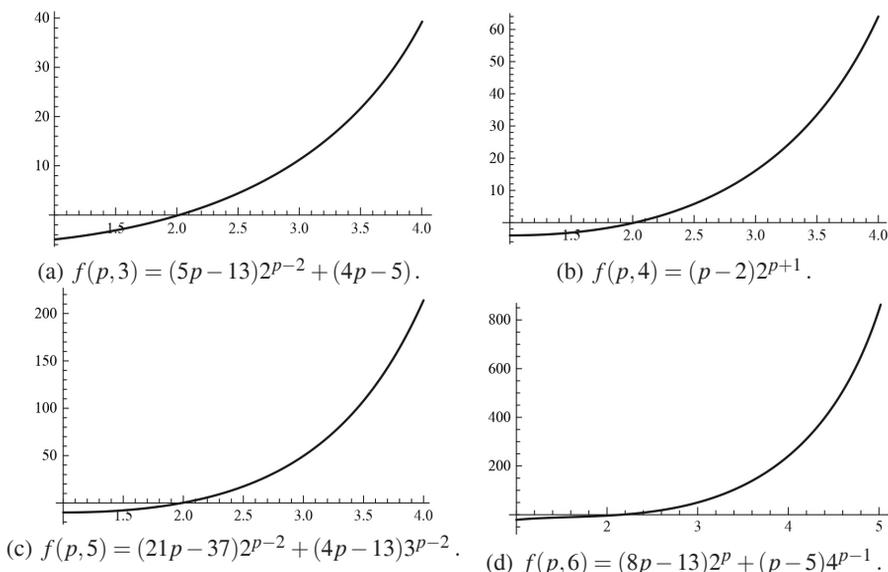


Figure 2: Plots of $f(p, n)$, $p = 3, \dots, 6$.

using the Newton-Raphson method. We define the iterative scheme for $g(x) = (15x - 22)2^x + 4(x - 10)6^{x-2}$ as

$$\begin{aligned}
 x_{n+1} &= x_n - \frac{g(x_n)}{g'(x_n)} \\
 &= \frac{[(15x_n^2 - 22x_n) \ln 2 + 22]2^{x_n} + 4[\ln 6(x_n^2 - 10x_n) + 10]6^{x_n-2}}{[(15x_n - 22) \ln 2 + 15]2^{x_n} + 4[\ln 6(x_n - 10) + 1]6^{x_n-2}}.
 \end{aligned}$$

With an initial approximation, $x_0 = 3.5$, one can get the first zero ≈ 3.2595 , and using $x_0 = 9.5$, the second zero ≈ 9.9801 . Thus K_8 is p -almost Hadamard for all $p \in (1, 2) \cup (2, 3.2595) \cup (9.9801, \infty)$.

Case (vii). For $n = 9$, we get

$$f(p, 9) = (77p - 109)2^{p-2} + (4p - 53)7^{p-2}.$$

It can be easily seen from the above expression that $f(p, 9) > 0$ for all $p > 53/4 = 13.2500$. One can get that $f(2.5, 9) = 4.3195 > 0$ and $f(3, 9) = -43 < 0$, and $f(13, 9) < 0$ and $f(14, 9) > 0$. Thus there are two zero of $f(\cdot, 9)$, one lies between 2.5 and 3, and the other between 13 and 14. Once again, we use the Newton-Raphson method to find both zeros of $f(\cdot, 9)$. Let us define the iterative scheme for $g(x) = (77x - 109)2^{x-2} + (4x - 53)7^{x-2}$ as

$$x_{n+1} = \frac{[(77x_n^2 - 109x_n) \ln 2 + 109]2^{x_n-2} + [\ln 7(4x_n^2 - 55x_n) + 53]7^{x_n-2}}{[(77x_n - 109) \ln 2 + 77]2^{x_n-2} + [\ln 7(4x_n - 53) + 4]7^{x_n-2}}.$$

With an initial approximation, $x_0 = 2.75$, one can obtain the first zero ≈ 2.6294 . Using the initial approximation $x_0 = 13.5$, we get the second zero ≈ 13.2498 . Thus K_9 is p -almost Hadamard for all $p \in (1, 2) \cup (2, 2.6294) \cup (13.2498, \infty)$.

In Figure 3 below, the sub figures (c) and (d) represent $n = 8$ case, and the values of p ranging from 1 to 4 in Figure (c) and 4 to 10 in Figure (d). For large values of n also, one can compute the validity of p -almost Hadamard property of K_n in this way.

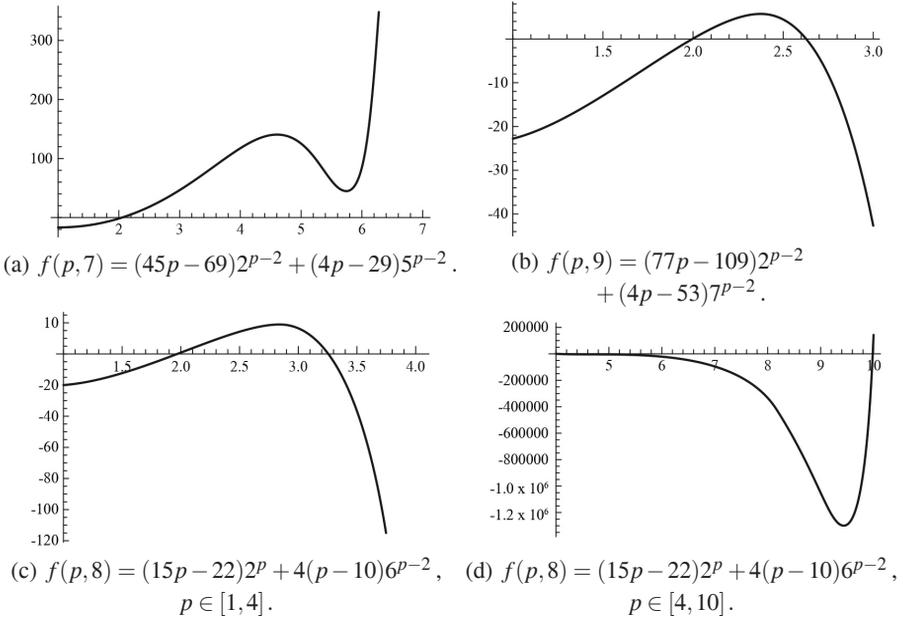


Figure 3: Plots of $f(p, n)$, $p = 7, 9, 8$.

4.2. Optimization problems with unitary matrix constraints

For a complex matrix $X = M_n = (a_{ij})_{i,j=1}^n$, let us consider the optimization problem

$$\min_{X \in \mathbb{C}^{n \times n}} \sum_{i,j=1}^n |a_{ij}|^p, \text{ such that } XX^* = I_n, \tag{25}$$

for $p \in (2, \infty)$. This is a minimization problem over unitary matrices. The global minimizer of (25) is a complex Hadamard matrix

$$M_n = \left(\frac{1}{\sqrt{n}} \right) F_n, \tag{26}$$

where F_n is the matrix, $F_n = \begin{pmatrix} 1 & 1 & 1 & \cdots & 1 \\ 1 & \omega & \omega^2 & \cdots & \omega^{n-1} \\ 1 & \omega^2 & \omega^4 & \cdots & \omega^{2n-2} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & \omega^{n-1} & \omega^{2n-2} & \cdots & \omega^{(n-1)^2} \end{pmatrix}$, a special case of the Van-

dermonde matrix, and ω is the n^{th} root of unity ($\omega \neq 1$). Thus F_n is complex p -almost Hadamard for all $p \in (2, \infty)$ and hence there exists a complex p -almost Hadamard matrix for all $p \in (2, \infty)$.

4.3. Examples

We have seen some of the p -almost Hadamard matrices in the subsection 4.1 using Propositions 6 and 7. Now we list some more p -almost Hadamard matrices of various orders using Propositions 2, 3, 4 and 5.

Case (i). $n = 1$ and $n = 2$: The following matrices are p -almost Hadamard for all $p \in [1, 2) \cup (2, \infty)$:

$$H_1 = [1] \text{ and } H_2 = \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix},$$

since they are Hadamard matrices. In fact, these are the only (equivalent) p -almost Hadamard matrices for these cases.

Case (ii). $n = 3$: We have already seen that K_3 is p -almost Hadamard for all $p \in (1, 2) \cup (2, \infty)$. The optimization problem considered in Proposition 3.2, [10] suggests that the matrix

$$N_3 = \frac{1}{2} \begin{pmatrix} 1 & -\sqrt{2} & 1 \\ \sqrt{2} & 0 & -\sqrt{2} \\ 1 & \sqrt{2} & 1 \end{pmatrix}.$$

is also a candidate for the local minimum of the optimization problem (9). It is in fact true since the condition (12) is satisfied. For the second order necessary and sufficient conditions, we have three different cases. For $i = 1, j = 2$ and $i = 2, j = 3$ in (15), we obtain

$$f_1(p) := \xi_{N_3}^{1,2} = \xi_{N_3}^{2,3} = p \left(\frac{1}{2}\right)^{p/2} \left[(p-4) + \frac{(2p-3)}{2^{p/2-1}} \right].$$

We next consider the function

$$g(x) = (x-4) + \frac{2(2x-3)}{2^{x/2}}, \text{ so that } g'(x) = \frac{2^{x/2} + 4 - (2x-3)\ln 2}{2^{x/2}} > 0,$$

for all $x > 0$. Note that $g(2) = -1$ and $g(3) = 1.1213$, so that the only zero of $g(\cdot)$ lies between 2 and 3. We use the Newton-Raphson method to find the zero of $g(\cdot)$. The iterative scheme is given by

$$x_{n+1} = x_n - \frac{g(x_n)}{g'(x_n)} = \frac{4(x_n + 2^{x_n/2}) - (2x_n - 3)(2 + x_n \ln 2)}{2^{x_n/2} + 4 - (2x_n - 3)\ln 2}.$$

For $x_0 = 2.5$, we get $x_1 = 2.4234$, $x_2 = 2.4151$, $x_3 = 2.4151$, etc. Thus the approximate value of the zero is given by $x \approx 2.4151$. Thus $f_1(p) > 0$ for all $p \in (2.4151, \infty)$. Now, for $i = 1$, $j = 3$, we find

$$f_2(p) := \xi_{N_3}^{1,3} = 2p(p-2) \left(\frac{1}{2}\right)^{p/2} \left[1 + \frac{1}{2^{p/2-1}}\right] > 0,$$

for all $p > 2$. Thus, $\tilde{N}_3 := \sqrt{3}N_3$ is p -almost Hadamard for all $p \in (2.4151, \infty)$.

Case (iii). $n = 4$: A Hadamard matrix H_4 exists and is p -almost Hadamard for all $p \in (1, 2) \cup (2, \infty)$. For example

$$H_4 = \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & -1 \\ 1 & 1 & -1 & -1 \\ 1 & -1 & -1 & 1 \end{pmatrix} = H_2 \otimes H_2 = 2K_4,$$

is a p -almost Hadamard matrix. We now consider the matrix

$$\tilde{R}_4 = \frac{2}{\sqrt{3}} \begin{pmatrix} 0 & 1 & 1 & 1 \\ 1 & 0 & -1 & 1 \\ 1 & 1 & 0 & -1 \\ 1 & -1 & 1 & 0 \end{pmatrix} = \frac{2}{\sqrt{3}}C_4.$$

From (17), it is clear that \tilde{R}_4 is a p -almost Hadamard matrix for all $p \in (2.5, \infty)$.

Case (iv). $n = 5$: In the previous subsection, we have shown that K_5 is p -almost Hadamard for all $p \in (1, 2) \cup (2, \infty)$.

Case (v). $n = 6$: We have already seen that K_6 is p -almost Hadamard for all $p \in (1, 2) \cup (2, \infty)$. From Proposition 3, it is clear that the matrix

$$\tilde{R}_6 = \frac{\sqrt{6}}{\sqrt{5}} \begin{pmatrix} 0 & 1 & 1 & 1 & 1 & 1 \\ 1 & 0 & 1 & -1 & -1 & 1 \\ 1 & 1 & 0 & 1 & -1 & -1 \\ 1 & -1 & 1 & 0 & 1 & -1 \\ 1 & -1 & -1 & 1 & 0 & 1 \\ 1 & 1 & -1 & -1 & 1 & 0 \end{pmatrix} = \frac{\sqrt{6}}{\sqrt{5}}C_6,$$

is a p -almost Hadamard matrix for $p \in (2.25, \infty)$. Now we consider the matrix

$$\tilde{S}_{6,4} = \frac{\sqrt{6}}{2} \begin{pmatrix} 1 & 1 & 1 & 1 & 0 & 0 \\ 1 & 1 & -1 & -1 & 0 & 0 \\ 1 & -1 & 0 & 0 & 1 & 1 \\ 1 & -1 & 0 & 0 & -1 & -1 \\ 0 & 0 & 1 & -1 & -1 & 1 \\ 0 & 0 & 1 & -1 & 1 & -1 \end{pmatrix} = \frac{\sqrt{6}}{2}W_{6,4}.$$

Note that for all $1 \leq i < j \leq 6$, β_{ij} is either 2 or 4 and hence $\underline{\beta} = 2$. Thus $\tilde{S}_{6,4}$ is p -almost Hadamard for all $p \in (3, \infty)$, using Proposition 4.

Let us now consider the matrix,

$$T_6 = \frac{1}{\sqrt{6}} \begin{pmatrix} -1 & 2 & 2 & -1 & 2 & 2 \\ 2 & -1 & 2 & 2 & -1 & 2 \\ 2 & 2 & -1 & 2 & 2 & -1 \\ -1 & 2 & 2 & 1 & -2 & -2 \\ 2 & -1 & 2 & -2 & 1 & -2 \\ 2 & 2 & -1 & -2 & -2 & 1 \end{pmatrix} = \frac{1}{\sqrt{6}} H_2 \otimes K_3.$$

Clearly the matrix T_6 is a stationary point of the minimization problem (9). Now, we need to verify the second order necessary and sufficient conditions given in (15). From, the structure of the matrix T_6 , we know that $\xi_{T_6}^{i,j}$ can be either

$$f_1(p) = \frac{4p}{6^{p/2}} [(5p - 13)2^{p-2} + (4p - 5)] = \frac{4p}{6^{p/2}} f(p, 3)$$

or

$$f_2(p) = \frac{4p(p-2)}{6^{p/2}} (1 + 2^p) > 0, \text{ for all } p > 2.$$

Note that in order for $f_1(p) > 0$, we need $(5p - 13)2^{p-2} + (4p - 5) > 0$, which is same as the case for $n = 3$ (see (24)). Combining both the cases, we have $\tilde{T}_6 := \sqrt{6}T_6$ is a p -almost Hadamard matrix for all $p \in [1, 2) \cup (2, \infty)$.

Similarly the matrix

$$N_6 = \frac{1}{2} \begin{pmatrix} 1 - \sqrt{2} & 1 & 1 - \sqrt{2} & 1 \\ \sqrt{2} & 0 - \sqrt{2} & \sqrt{2} & 0 - \sqrt{2} \\ 1 & \sqrt{2} & 1 & 1 & \sqrt{2} & 1 \\ 1 - \sqrt{2} & 1 & -1 & \sqrt{2} & -1 \\ \sqrt{2} & 0 - \sqrt{2} & -\sqrt{2} & 0 & \sqrt{2} \\ 1 & \sqrt{2} & 1 & -1 & -\sqrt{2} & -1 \end{pmatrix} = H_2 \otimes N_3,$$

is a stationary point of the optimization problem (9) for $n = 6$. Now, the possible values of $\xi_{N_6}^{i,j}$, for $1 \leq i < j \leq 6$ are given by:

$$f_1(p) = 2p \left(\frac{1}{2}\right)^{p/2} \left[(p - 4) + \frac{(2p - 3)}{2^{p/2-1}} \right] \text{ or}$$

$$f_2(p) = 4p(p - 2) \left(\frac{1}{2}\right)^{p/2} \left[1 + \frac{1}{2^{p/2-1}} \right] \text{ or}$$

$$f_3(p) = 4p(p - 2) \left(\frac{1}{2}\right)^p \left[1 + \frac{1}{2^{p/2}} \right] \text{ or}$$

$$f_4(p) = 8p(p - 2) \left(\frac{1}{2}\right)^p.$$

Note that $f_2(p), f_3(p), f_4(p) > 0$ for all $p > 2$, and $f_1(p) > 0$, for all $p \in (2.4151, \infty)$, by using case (ii). Thus $\tilde{N}_6 := \sqrt{6}N_6$ is p -almost Hadamard for all $p \in (2.4151, \infty)$.

Case (vi). $n = 7$: We have already shown that the matrix K_7 is p -almost Hadamard for all $p \in (1, 2) \cup (2, \infty)$. Let us now consider the matrix

$$\tilde{S}_{7,4} = \frac{\sqrt{7}}{2} \begin{pmatrix} 1 & 1 & 1 & 1 & 0 & 0 & 0 \\ 1 & -1 & 0 & 0 & 1 & 1 & 0 \\ 1 & 0 & -1 & 0 & -1 & 0 & 1 \\ 1 & 0 & 0 & -1 & 0 & -1 & -1 \\ 0 & 1 & -1 & 0 & 0 & 1 & -1 \\ 0 & 1 & 0 & -1 & 1 & 0 & 1 \\ 0 & 0 & 1 & -1 & -1 & 1 & 0 \end{pmatrix} = \frac{\sqrt{7}}{2} W_{7,4}.$$

For the above matrix, it can be easily seen that $\beta_{ij} = 2$ for all $1 \leq i < j \leq n$, so that $\underline{\beta} = 2$. Thus the matrix $\tilde{S}_{7,4}$ is p -almost Hadamard for all $p \in (1, 2) \cup (3, \infty)$.

Case (vii). $n = 8$: Remember from the previous subsection that K_8 is p -almost Hadamard for all $p \in (1, 2) \cup (2, 3.2595) \cup (9.9801, \infty)$. We now consider the following Hadamard matrix:

$$H_8 = \begin{pmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & -1 & 1 & -1 & 1 & -1 \\ 1 & 1 & -1 & -1 & 1 & 1 & -1 & -1 \\ 1 & -1 & -1 & 1 & 1 & -1 & -1 & 1 \\ 1 & 1 & 1 & 1 & -1 & -1 & -1 & -1 \\ 1 & -1 & 1 & -1 & -1 & 1 & -1 & 1 \\ 1 & 1 & -1 & -1 & -1 & -1 & 1 & 1 \\ 1 & -1 & -1 & 1 & -1 & 1 & 1 & -1 \end{pmatrix} = H_4 \otimes H_2.$$

Clearly H_8 is a p -almost Hadamard matrix for all $p \in (1, 2) \cup (2, \infty)$. By Proposition 3, the matrix

$$\tilde{R}_8 = \frac{2\sqrt{2}}{\sqrt{7}} \begin{pmatrix} 0 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 0 & 1 & -1 & -1 & 1 & 1 & -1 \\ 1 & -1 & 0 & 1 & 1 & -1 & 1 & -1 \\ 1 & 1 & -1 & 0 & 1 & 1 & -1 & -1 \\ 1 & 1 & -1 & -1 & 0 & -1 & 1 & 1 \\ 1 & -1 & 1 & -1 & 1 & 0 & -1 & 1 \\ 1 & -1 & -1 & 1 & -1 & 1 & 0 & 1 \\ 1 & 1 & 1 & 1 & -1 & -1 & -1 & 0 \end{pmatrix} = \frac{2\sqrt{2}}{\sqrt{7}} C_8.$$

is p -almost Hadamard for all $p \in (2.1667, \infty)$. For the matrix

$$\tilde{S}_{8,6} = \frac{2}{\sqrt{3}} \begin{pmatrix} 0 & 0 & -1 & 1 & -1 & -1 & 1 & 1 \\ 0 & 0 & -1 & -1 & 1 & -1 & 1 & -1 \\ -1 & 1 & 0 & 0 & -1 & -1 & -1 & -1 \\ -1 & -1 & 0 & 0 & -1 & 1 & 1 & -1 \\ -1 & -1 & -1 & -1 & 0 & 0 & -1 & 1 \\ 1 & -1 & -1 & 1 & 0 & 0 & -1 & -1 \\ 1 & 1 & -1 & -1 & -1 & 1 & 0 & 0 \\ 1 & -1 & 1 & -1 & -1 & -1 & 0 & 0 \end{pmatrix} = \frac{2}{\sqrt{3}} W_{8,6},$$

it is clear that $\underline{\beta} = 4$ and by Proposition 4, $\tilde{S}_{8,6}$ is p -almost Hadamard for all $p \in (2.5, \infty)$. Now we consider the matrix:

$$\tilde{S}_{8,5} = \frac{2\sqrt{2}}{\sqrt{5}} \begin{pmatrix} 1 & 1 & 1 & 1 & 1 & 0 & 0 & 0 \\ 1 & 1 & -1 & -1 & 0 & 1 & 0 & 0 \\ 1 & -1 & -1 & 1 & 0 & 0 & 1 & 0 \\ 1 & -1 & 1 & -1 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & -1 & -1 & -1 & -1 \\ 0 & 1 & 0 & 0 & -1 & -1 & 1 & 1 \\ 0 & 0 & 1 & 0 & -1 & 1 & 1 & -1 \\ 0 & 0 & 0 & 1 & -1 & 1 & -1 & 1 \end{pmatrix} = \frac{2\sqrt{2}}{\sqrt{5}} W_{8,5}.$$

It is immediate that $\underline{\beta} = 2$ and hence $\tilde{S}_{8,5}$ is p -almost Hadamard for all $p \in (3.5, \infty)$, by using Proposition 4.

REMARK 12. For $n = 9$, the matrices $K_3 \otimes K_3$, $3(N_3 \otimes N_3)$ and K_9 are p -almost Hadamard for some p . For $n = 10$, the matrices K_{10} , $H_2 \otimes K_5$, $\tilde{R}_{10} = \frac{\sqrt{10}}{3} C_{10}$ and $\tilde{S}_{10,8} = \frac{\sqrt{5}}{2} W_{10,8}$ are p -almost Hadamard for some p .

REMARK 13. It is also clear that if a weighing matrix $W_{n,k}$ exists, then it is p -almost Hadamard for all $k > [\frac{n}{2}]$, where $[\frac{n}{2}]$ is the integral part of $\frac{n}{2}$ and $p \in (\frac{k}{2} + 1, \infty)$, since the least possible value of $\underline{\beta}$ is 2.

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A. Finding the nearest orthonormal matrix

In the Appendix, we give a motivation for considering the orthogonal matrix given in (18). Let us start with an interesting optimization problem formulated in [14]. The optimization problem is to find the nearest orthogonal matrix to a given matrix. The problem can be stated as follows:

PROBLEM 1. Given a matrix M of order n , find the matrix Q of order n that minimizes the norm $\|M - Q\|_F^2$, subject to $Q^T Q = I$, where the norm chosen is the Frobenius norm, i.e., the sum of squares of elements of the matrix, or $\|X\|_F^2 = \text{Tr}(X^T X)$.

It has been derived in [14] that the nearest orthogonal matrix M is given by

$$Q = M(M^T M)^{-1/2}.$$

Since $M^T M$ is symmetric and positive semi-definite, it has non-negative real eigenvalues. If $M^T M$ is positive definite, we know that the inverse of the square root of $M^T M$ can be computed using eigenvalue-eigenvector decomposition. The matrix $(M^T M)^{-1/2}$ has the same eigenvectors as of $M^T M$, and eigenvalues are that of inverse of the square roots of the eigenvalues of $M^T M$. Hence, one can write

$$(M^T M)^{-1/2} = \frac{1}{\sqrt{\lambda_1}} \mathbf{e}_1 \mathbf{e}_1^T + \dots + \frac{1}{\sqrt{\lambda_n}} \mathbf{e}_n \mathbf{e}_n^T,$$

where λ_i for $i = 1, \dots, n$, are the eigenvalues and \mathbf{e}_i for $i = 1, \dots, n$, are the orthonormal set of eigenvectors of $M^T M$. The construction of $(M^T M)^{-1/2}$ fails if one of the n eigenvalues is zero. But it is possible however to pretend that eigenvalue is equal to one and then proceed (see [14] for more details).

Motivated from the above discussion, we now construct an orthogonal matrix nearest to the matrix $R_3 = \frac{1}{\sqrt{3}} \begin{pmatrix} -1 & 1 & 1 \\ 1 & -1 & 1 \\ 1 & 1 & -1 \end{pmatrix}$. It can be easily seen that

$$R_3^T R_3 = \frac{1}{3} \begin{pmatrix} 3 & -1 & -1 \\ -1 & 3 & -1 \\ -1 & -1 & 3 \end{pmatrix}.$$

The eigenvalues of $R_3^T R_3$ are $\frac{1}{3}, \frac{4}{3}$ and $\frac{4}{3}$ and the corresponding eigenvectors are

$$\mathbf{v}_1 = (1 \ 1 \ 1)^T, \quad \mathbf{v}_2 = (1 \ -1 \ 0)^T \quad \text{and} \quad \mathbf{v}_3 = (1 \ 0 \ -1)^T.$$

Using the Gram-Schmidt orthonormalization process, we obtain the orthonormal basis:

$$\mathbf{e}_1 = \frac{1}{\sqrt{3}} (1 \ 1 \ 1)^T, \quad \mathbf{e}_2 = \frac{1}{\sqrt{2}} (1 \ -1 \ 0)^T \quad \text{and} \quad \mathbf{e}_3 = \frac{1}{\sqrt{6}} (1, 1, -2).$$

Thus, we have

$$\begin{aligned} (\mathbf{R}_3^\top \mathbf{R}_3)^{-1/2} &= \frac{1}{\sqrt{\lambda_1}} \mathbf{e}_1 \mathbf{e}_1^\top + \frac{1}{\sqrt{\lambda_2}} \mathbf{e}_2 \mathbf{e}_2^\top + \frac{1}{\sqrt{\lambda_3}} \mathbf{e}_3 \mathbf{e}_3^\top \\ &= \frac{1}{\sqrt{3}} \begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{pmatrix} + \frac{1}{2\sqrt{3}} \begin{pmatrix} 2 & -1 & -1 \\ -1 & 2 & -1 \\ -1 & -1 & 2 \end{pmatrix} = \frac{1}{2\sqrt{3}} \begin{pmatrix} 4 & 1 & 1 \\ 1 & 4 & 1 \\ 1 & 1 & 4 \end{pmatrix}. \end{aligned}$$

The nearest orthogonal matrix to \mathbf{R}_3 is $\mathbf{Q}_3 = \mathbf{R}_3 (\mathbf{R}_3^\top \mathbf{R}_3)^{-1/2} = \frac{1}{3} \begin{pmatrix} -1 & 2 & 2 \\ 2 & -1 & 2 \\ 2 & 2 & -1 \end{pmatrix}$.

Now, we consider the matrix $\mathbf{R}_5 = \frac{1}{\sqrt{5}} \begin{pmatrix} -1 & 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & 1 & 1 \\ 1 & 1 & -1 & 1 & 1 \\ 1 & 1 & 1 & -1 & 1 \\ 1 & 1 & 1 & 1 & -1 \end{pmatrix}$. It is immediate

that $\mathbf{R}_5^\top \mathbf{R}_5 = \frac{1}{5} \begin{pmatrix} 5 & 1 & 1 & 1 & 1 \\ 1 & 5 & 1 & 1 & 1 \\ 1 & 1 & 5 & 1 & 1 \\ 1 & 1 & 1 & 5 & 1 \\ 1 & 1 & 1 & 1 & 5 \end{pmatrix}$. The eigenvalues of $\mathbf{R}_5^\top \mathbf{R}_5$ are $\frac{9}{5}$, $\frac{4}{5}$, $\frac{4}{5}$, $\frac{4}{5}$ and $\frac{4}{5}$, and

the corresponding eigenvectors are given by

$$\mathbf{v}_1 = \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \\ 1 \end{pmatrix}, \mathbf{v}_2 = \begin{pmatrix} 1 \\ -1 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \mathbf{v}_3 = \begin{pmatrix} 1 \\ 0 \\ -1 \\ 0 \\ 0 \end{pmatrix}, \mathbf{v}_4 = \begin{pmatrix} 1 \\ 0 \\ 0 \\ -1 \\ 0 \end{pmatrix} \text{ and } \mathbf{v}_5 = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \\ -1 \end{pmatrix}.$$

Once again using the Gram-Schmidt orthonormalization process, we obtain the orthonormal basis as

$$\left\{ \underbrace{\frac{1}{\sqrt{5}} \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \\ 1 \end{pmatrix}}_{\mathbf{e}_1}, \underbrace{\frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \\ 0 \\ 0 \\ 0 \end{pmatrix}}_{\mathbf{e}_2}, \underbrace{\frac{1}{\sqrt{6}} \begin{pmatrix} 1 \\ 1 \\ -2 \\ 0 \\ 0 \end{pmatrix}}_{\mathbf{e}_3}, \underbrace{\frac{1}{\sqrt{12}} \begin{pmatrix} 1 \\ 1 \\ 1 \\ -3 \\ 0 \end{pmatrix}}_{\mathbf{e}_4}, \underbrace{\frac{1}{20} \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \\ -4 \end{pmatrix}}_{\mathbf{e}_5} \right\}.$$

Hence, we have

$$\begin{aligned}
 (\mathbf{R}_5^\top \mathbf{R}_5)^{-1/2} &= \frac{1}{\sqrt{\lambda_1}} \mathbf{e}_1 \mathbf{e}_1^\top + \frac{1}{\sqrt{\lambda_2}} \mathbf{e}_2 \mathbf{e}_2^\top + \frac{1}{\sqrt{\lambda_3}} \mathbf{e}_3 \mathbf{e}_3^\top + \frac{1}{\sqrt{\lambda_4}} \mathbf{e}_4 \mathbf{e}_4^\top + \frac{1}{\sqrt{\lambda_5}} \mathbf{e}_5 \mathbf{e}_5^\top \\
 &= \frac{1}{3\sqrt{5}} \begin{pmatrix} 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 \end{pmatrix} + \frac{1}{2\sqrt{5}} \begin{pmatrix} 4 & -1 & -1 & -1 & -1 \\ -1 & 4 & -1 & -1 & -1 \\ -1 & -1 & 4 & -1 & -1 \\ -1 & -1 & -1 & 4 & -1 \\ -1 & -1 & -1 & -1 & 4 \end{pmatrix} \\
 &= \frac{1}{6\sqrt{5}} \begin{pmatrix} 14 & -1 & -1 & -1 & -1 \\ -1 & 14 & -1 & -1 & -1 \\ -1 & -1 & 14 & -1 & -1 \\ -1 & -1 & -1 & 14 & -1 \\ -1 & -1 & -1 & -1 & 14 \end{pmatrix}.
 \end{aligned}$$

The nearest orthogonal matrix to \mathbf{R}_5 is $\mathbf{Q}_5 = \frac{1}{5} \begin{pmatrix} -3 & 2 & 2 & 2 & 2 \\ 2 & -3 & 2 & 2 & 2 \\ 2 & 2 & -3 & 2 & 2 \\ 2 & 2 & 2 & -3 & 2 \\ 2 & 2 & 2 & 2 & -3 \end{pmatrix}$.

Now, we consider a general matrix $\mathbf{R}_n = \frac{1}{\sqrt{n}} \begin{pmatrix} -1 & 1 & \dots & 1 \\ 1 & -1 & \dots & 1 \\ \vdots & \ddots & \ddots & \vdots \\ 1 & 1 & \dots & -1 \end{pmatrix}$. Then, we have

$\mathbf{R}_n \mathbf{R}_n^\top = \frac{1}{n} \begin{pmatrix} n & n-4 & \dots & n-4 \\ n-4 & n & \dots & n-4 \\ \vdots & \vdots & \ddots & \vdots \\ n-4 & n-4 & \dots & n \end{pmatrix}$. The eigenvalues are given by $\frac{(n-2)^2}{n}, \underbrace{\frac{4}{n}, \dots, \frac{4}{n}}_{n-1}$.

The corresponding orthonormal eigenvectors are given by

$$\left\{ \underbrace{\frac{1}{\sqrt{n}} \begin{pmatrix} 1 \\ 1 \\ 1 \\ \vdots \\ 1 \\ 1 \end{pmatrix}}_{\mathbf{e}_1}, \underbrace{\frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \\ \vdots \\ 0 \\ 0 \\ 0 \end{pmatrix}}_{\mathbf{e}_2}, \underbrace{\frac{1}{\sqrt{6}} \begin{pmatrix} 1 \\ 1 \\ -2 \\ \vdots \\ 0 \\ 0 \end{pmatrix}}_{\mathbf{e}_3}, \dots, \underbrace{\frac{1}{\sqrt{n(n-1)}} \begin{pmatrix} 1 \\ 1 \\ 1 \\ \vdots \\ 1 \\ -(n-1) \end{pmatrix}}_{\mathbf{e}_n} \right\}.$$

Thus the matrix $(R_n^T R_n)^{-1/2}$ is given by

$$\begin{aligned} (R_n^T R_n)^{-1/2} &= \frac{1}{\sqrt{\lambda_1}} \mathbf{e}_1 \mathbf{e}_1^T + \dots + \frac{1}{\sqrt{\lambda_5}} \mathbf{e}_5 \mathbf{e}_5^T \\ &= \frac{1}{(n-2)\sqrt{n}} \begin{pmatrix} 1 & 1 & \dots & 1 \\ 1 & 1 & \dots & 1 \\ \vdots & \vdots & \ddots & \vdots \\ 1 & 1 & \dots & 1 \end{pmatrix} + \frac{1}{2\sqrt{n}} \begin{pmatrix} (n-1) & -1 & \dots & -1 \\ -1 & (n-1) & \dots & -1 \\ \vdots & \vdots & \ddots & \vdots \\ -1 & -1 & \dots & (n-1) \end{pmatrix} \\ &= \frac{1}{2(n-2)\sqrt{n}} \begin{pmatrix} (n^2 - 3n + 4) & -(n-4) & \dots & -(n-4) \\ -(n-4) & (n^2 - 3n + 4) & \dots & -(n-4) \\ \vdots & \vdots & \ddots & \vdots \\ -(n-4) & -(n-4) & \dots & (n^2 - 3n + 4) \end{pmatrix}. \end{aligned}$$

Let \mathbb{I}_n is the $n \times n$ matrix with all entries 1. The nearest orthogonal matrix to R_n is

$$Q_n = R_n (R_n^T R_n)^{-1/2} = \frac{1}{n} \begin{pmatrix} -(n-2) & 2 & \dots & 2 \\ 2 & -(n-2) & \dots & 2 \\ \vdots & \vdots & \ddots & \vdots \\ 2 & 2 & \dots & -(n-2) \end{pmatrix} = \frac{2}{n} \mathbb{I}_n - I_n.$$

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