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On constructing Hermitian unitary matrices with prescribed moduli [1]

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Abstract

The problem of reconstructing the phases of a unitary matrix with prescribed moduli is of a broad interest to people working in many applications, e.g in the circuit theory, phase shift analysis, multichannel scattering, computer science (e.g in the theory of error correcting codes, design theory). We propose efficient algorithms for computing Hermitian unitary matrices for given symmetric bistochastic matrices $A(n \times n)$ for $n = 3$ and $n = 4$. We mention also some results for matrices of arbitrary size n.

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1 Introduction

We will study the set of unistochastic matrices which is a subset of the set of bistochastic matrices. We say that a matrix $A \in \mathbb{R}^{n\times n}$ is bistochastic (doubly stochastic) if all its entries are nonnegative real numbers and all its row sums and column sums are equal to 1. A unistochastic matrix is a bistochastic matrix whose entries are the squares of the absolute values of the entries of some unitary matrix U. We recall that a matrix $B \in \mathbb{C}^{n\times n}$ is Hermitian if $B = B^*$, i.e. $b_{ij} = \overline{b_{ji}}$ for $i, j = 1, \ldots, n$. A matrix $U \in \mathbb{C}^{n\times n}$ is unitary if $U^*U = I$. A matrix $Q \in \mathbb{R}^{n\times n}$ is orthogonal if $Q^TQ = I$. We say that a symmetric bistochastic matrix $A \in \mathbb{R}^{n\times n}$ is H-unistochastic if there exists a Hermitian unitary matrix $U \in \mathbb{C}^{n\times n}$ such that $a_{ij} = |u_{ij}|^2,\ i, j = 1, \ldots, n$. If U is real (so U is orthogonal) then A is called H-orthostochastic.

Perhaps the van der Waerden matrix (W_n) is the most famous unistochastic matrix. Its elements are all equal to $\frac{1}{n}$. For example, for $n = 4$ there exists an orthogonal preimage U ($2U$ is called an Hadamard matrix):

$$W_4 = \frac{1}{4}\begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \end{bmatrix}, \quad U = \frac{1}{2}\begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & -1 \\ 1 & 1 & -1 & -1 \\ 1 & -1 & -1 & 1 \end{bmatrix}$$

so W_4 is even orthostochastic (and also H- orthostochastic). However, it is easy to verify that W_3 is not H-unistochastic!

Hadamard's Conjecture (still open!) says that for $n > 2$ the Hadamard matrices exist when $n = 4k$ and only for such n, see W.Tadej et al. [5] for explicit examples of the Hadamard matrices.

We consider the following research problems.

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- I. Given a bistochastic matrix $A \in \mathbb{R}^{n\times n}$ check if there exists a unitary matrix $U \in \mathbb{C}^{n\times n}$ such that $a_{ij} = |u_{ij}|^2,\ i,j = 1,\dots,n$ (so A is unistochastic).
- II. Given a symmetric bistochastic matrix $A \in \mathbb{R}^{n\times n}$ check if there exists a Hermitian unitary matrix $U \in \mathbb{C}^{n\times n}$ such that $a_{ij} = |u_{ij}|^2,\ i,j = 1,\dots,n$ (so A is H-unistochastic).

For $n = 2$ every bistochastic matrix A is symmetric and is orthostochastic (U can be chosen to be orthogonal). We have

$$A = \begin{bmatrix} c^2 & s^2 \\ s^2 & c^2 \end{bmatrix}, \quad U = \begin{bmatrix} c & s \\ s & -c \end{bmatrix}, \quad c = \cos\Theta, \quad s = \sin\Theta$$

Given a 3×3 bistochastic matrix A it is easy to check whether it is unistochastic or not (see e.g [2]). We get

$$A = \begin{bmatrix} a_1^2 & b_1^2 & c_1^2 \\ a_2^2 & b_2^2 & c_2^2 \\ a_3^2 & b_3^2 & c_3^2 \end{bmatrix}, \quad U = \begin{bmatrix} a_1 & b_1 & c_1 \\ a_2 & b_2 e^{i\Phi} & \dots \\ a_3 & b_3 e^{i\Psi} & \dots \end{bmatrix}, \quad 0 \le a_i, b_i, c_i \le 1$$

Therefore the problem is to form a triangle from 3 line segments of given lengths $L_i = a_i b_i,\ i = 1,2,3$. Then A is unistochastic if and only if the chain-link conditions are fulfilled: $|L_2 - L_3| \le L_1 \le L_2 + L_3$. In this case

$$\cos\Phi = \frac{L_3^2 - L_2^2 - L_1^2}{2L_1L_2}, \quad \cos\Psi = \frac{L_2^2 - L_1^2 - L_3^2}{2L_1L_3}, \quad \cos(\Phi - \Psi) = \frac{L_1^2 - L_2^2 - L_3^2}{2L_2L_3}$$

Some methods for constructing unitary preimages to 3×3 bistochastic matrices are discussed in [3].

However, for a given 4×4 bistochastic matrix A it is not easy to check whether it is unistochastic or not! There are only partial results, so it is reasonable to try to develop efficient algorithms to check whether a given bistochastic matrix $A(n\times n)$ is unistochastic or not. We focus our attention only on symmetric bistochastic matrices and their Hermitian unitary preimages.

2 New results

For simplicity define a matrix

$$M = (m_{ij})_{i,j=1,\dots,n}, \quad \text{where} \quad m_{ij} = \sqrt{a_{ij}}, \quad i,j = 1,\dots,n$$

Notice that without loss of generality we can seek a Hermitian unitary matrix $U(n\times n)$ in the dephased form, i.e. such that the first row and the first column of U are the same as the first row and the first column of M. It is obvious because if U is not dephased, we can find a unitary diagonal matrix D such that the matrix $\hat{U} = \pm DUD^*$ satisfies these conditions and it is still Hermitian.

Given a 3×3 symmetric bistochastic matrix A it is easy to check whether it is H-unistochastic or not.

Notice that we can assume that the diagonal elements of A are ordered in such a way that $a_{11} \le a_{22} \le a_{33}$. If $a_{p_1p_1} \le a_{p_2p_2} \le a_{p_3p_3}$ for some permutation $\{p_1, p_2, p_3\}$ of $\{1,2,3\}$, then we can permute rows and columns of A. Define a permutation matrix $P = [e_{p_1}, e_{p_2}, e_{p_3}]$, where $I = [e_1, e_2, e_3]$. Then $\tilde{A} = P^TAP$ has the desired property. Note also that A is H-unistochastic iff $\tilde{A}$ is H-unistochastic. That is, U is a unitary preimage for A iff P^TUP is a unitary preimage for $\tilde{A}$.

As it was said above, we can assume that a Hermitian unitary U has the dephased form

$$U = \begin{bmatrix} \sqrt{a_{11}} & \sqrt{a_{12}} & \sqrt{a_{13}} \\ \sqrt{a_{12}} & \sqrt{a_{22}}\,(s_1) & \sqrt{a_{23}}\ (z) \\ \sqrt{a_{13}} & \sqrt{a_{23}}\ (\overline{z}) & \sqrt{a_{33}} \quad (s_2) \end{bmatrix}, \quad s_1, s_2 \in \{-1, 1\}, \quad z \in \mathcal{C}, \quad |z| = 1$$

Theorem 2.1. *Let $A(3 \times 3)$ be a symmetric bistochastic matrix, $0 < a_{i,j} < 1$ for all i, j and $a_{11} \le a_{22} \le a_{33}$. Then A is H-unistochastic if and only if the following matrix*

$$U = \begin{bmatrix} \sqrt{a_{11}} & \sqrt{a_{12}} & \sqrt{a_{13}} \\ \sqrt{a_{12}} & \sqrt{a_{22}}(s) & \sqrt{a_{23}}(-s) \\ \sqrt{a_{13}} & \sqrt{a_{23}}(-s) & \sqrt{a_{33}}(s) \end{bmatrix}$$

where $s = -1$ or $s = 1$, is orthogonal.

Now we consider the case $n = 4$. Assume that all the elements of a symmetric bistochastic matrix A are nonzero. We show that our problem can be reduced to the linear system of equations.

Write $A(4 \times 4)$ and U as follows

$$A = \begin{bmatrix} m_1^2 & a_2^2 & a_3^2 & a_4^2 \\ a_2^2 & m_2^2 & b_3^2 & b_4^2 \\ a_3^2 & b_3^2 & m_3^2 & c_4^2 \\ a_4^2 & b_4^2 & c_4^2 & m_4^2 \end{bmatrix}, \quad U = \begin{bmatrix} m_1 & a_2 & a_3 & a_4 \\ a_2 & m_2(s_2) & b_3(z_1) & b_4(z_2) \\ a_3 & b_3(\overline{z_1}) & m_3(s_3) & c_4(z_3) \\ a_4 & b_4(\overline{z_2}) & c_4(\overline{z_3}) & m_4(s_4) \end{bmatrix}$$

where $s_k \in \{-1, 1\}$ and $z_k \in \mathcal{C}, |z_k| = 1$. Here $0 < a_k, b_k, c_k, m_k < 1$ is assumed in order to avoid trivial cases.

By the orthogonality of the first column of U and the columns $2, 3, 4$ we obtain

$$\begin{aligned} &m_1 a_2 + a_2 m_2(s_2) + a_3 b_3(z_1) + a_4 b_4(z_2) = 0 \\ &m_1 a_3 + a_2 b_3(\overline{z_1}) + a_3 m_3(s_3) + a_4 c_4(z_3) = 0 \\ &m_1 a_4 + a_2 b_4(z_2) + a_3 c_4(z_3) + a_4 m_4(s_4) = 0 \end{aligned}$$

We can assume that the signs s_k are prescribed, in an algorithm we have to check all the combinations of signs (± 1).

Let $z_k = x_k + i y_k$ for $k = 1, 2, 3$. Then $x_k = re(z_k)$ can be computed as a unique solution of the following linear system of equation $Bx = f$, where $x = [x_1, x_2, x_3]^T$ and $f = [f_2, f_3, f_4]^T$, where $f_k = -a_k(m_1 + m_k(s_k))$ for $k = 2, 3, 4$. Here

$$B = \begin{bmatrix} a_3 b_3 & a_4 b_4 & 0 \\ a_2 b_3 & 0 & a_4 c_4 \\ 0 & a_2 b_4 & a_3 c_4 \end{bmatrix} = \begin{bmatrix} a_3 & a_4 & 0 \\ a_2 & 0 & a_4 \\ 0 & a_2 & a_3 \end{bmatrix} \begin{bmatrix} b_3 & 0 & 0 \\ 0 & b_4 & 0 \\ 0 & 0 & c_4 \end{bmatrix}$$

Then $\det(B) = -2\ (a_2 a_3 a_4)(b_3 b_4 c_4) \ne 0$, so there exists a unique solution x of the linear system $Bx = f$. We can compute it as follows $x = B^{-1} f$, where

$$B^{-1} = \frac{1}{2 a_2 a_3 a_4} \begin{bmatrix} \frac{1}{b_3} & 0 & 0 \\ 0 & \frac{1}{b_4} & 0 \\ 0 & 0 & \frac{1}{c_4} \end{bmatrix} \begin{bmatrix} a_2 a_4 & a_3 a_4 & -a_4^2 \\ a_2 a_3 & -a_3^2 & a_3 a_4 \\ -a_2^2 & a_2 a_3 & a_2 a_4 \end{bmatrix}$$

Now it is easy to compute y_k. We should check the conditions: $|x_k| \le 1$ for $k = 1, 2, 3$. Then we can compute y_k from the formulae

$$y_1 = \pm\ \sqrt{(1 - x_1)(1 + x_1)}, \quad y_2 = -\frac{a_3 b_3 y_1}{a_4 b_4}, \quad y_3 = \frac{a_2 b_3 y_1}{a_4 c_4}$$

Finally, we have to verify the orthogonality of the computed matrix U.

We have only some partial results for arbitrary size n. Notice that all the eigenvalues of a Hermitian unitary matrix $U \in \mathbb{C}^{n\times n}$ are real and equal to -1 or 1. There exists a unitary matrix $Q \in \mathbb{C}^{n\times n}$ such that $U = QDQ^*$, $Q^*Q = I$, where $D = diag(1, 1, \ldots, 1, -1, -1, \ldots, -1)$.

If we impose an additional condition on U, a Hermitian unitary preimage of A to be found, namely that $U = QDQ^*$ with $Q^*Q = I$ and $D = diag(1, 1, \ldots, 1, -1)$. Now it is not difficult to solve our problem! Notice that writing $D = I - 2 \quad diag(0, \ldots, 0, 1) = I - 2 \quad e_n e_n^T$, we obtain $U = I - 2 \quad (Qe_n)(Qe_n)^* = I - 2 \; q_n q_n^*$, so U is a reflection (Householder transformation).

Let $z = q_n$, $z = [z_1, z_2, \ldots, z_n]^T$. Then $U = I - 2\, zz^*$, where $z^*z = 1$. We assume that $a_{1,1} \neq 1$ (for otherwise the problem reduces to the case $(n-1)\times(n-1)$). Then we can choose z_1 being real and positive because U does not depend on scaling of z (if $z = \alpha u$ with $u^*u = 1$ and $|\alpha| = 1$, then $U = I - 2 \quad uu^*$). Moreover, if D is a unitary diagonal matrix then $DUD^* = I - 2\,(Du)(Du)^*$ is also a Householder matrix, so we can search for U in the dephased form. Then the desired Householder matrix U is real and must have the following form to have the correct moduli in the first row of U

$$U = I - \frac{pp^T}{(1 - m_{11})}, \quad p = [1 - m_{11}, -m_{12}, \ldots, -m_{1n}]^T$$

Notice that

$$p^T p = (1 - m_{11})^2 + m_{12}^2 + \ldots + m_{1n}^2 = 2(1 - m_{11})$$

so U is orthogonal ($U^T U = UU = I$). The only thing to do is to compute U and check the condition $|u_{ij}| = m_{ij} = \sqrt{a_{ij}}$ for $i, j = 1, \ldots, n$. How to improve the orthogonality of the computed U in floating point arithmetic? To improve the orthogonality of the columns of U we propose reorthogonalization. We apply QR decomposition to U. To compute QR decomposition we can use the Householder or Givens methods or special versions of Gram-Schmidt orthogonalization methods (see eg. [6]). Here is a code for MATLAB using the function qr (the Householder method):

```
[Q,R]=qr(U);
M=A.^(1/2); Z=Q./abs(Q); U=M.*Z; I=eye(n);
error_U=norm(I-U'*U));
error_A=norm(A-abs(U).*abs(U));
```

The numerical tests in MATLAB confirm the advantage of the proposed algorithms.

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