Critical loci of the 4×4 unistochastic map

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ABSTRACT Let $U(4)$ be the unitary group formed by the unitary matrices of order 4, and let $D(4)$ be its subgroup of diagonal matrices. The compact set U_4 of unistochastic matrices, determined by the squared moduli entries of unitary matrices, is contained in the famous Birkhoff polytope B_4. It is of great interest, and our main goal, to determine the shape of U_4, and in particular its boundary. For this purpose, the bicoset space $D(4)\backslash U(4)/D(4)$ will be viewed as the preimage of U_4 under the unistochastic map $\Phi_4 : U(4) \to U_4$, defined as $\Phi_4(U) := U \circ \bar{U}$, where $\circ$ denotes the Hadamard or entrywise product. The investigation of the critical loci of this map is crucial for our purposes, since every boundary point of U_4 is the image of a critical point. Using a standard parametrization of the bicoset space $D(4)\backslash U(4)/D(4)$, we provide a criterion for a point of the bicoset space to be a critical point. We also present an algorithm to decide the unistochascity of a given bistochastic matrix, and we analyze the unistochascity of the bistochastic matrix obtained multiplying by 1/34 the magic square engraved in Dürer‘s celebrated *Melancolia I*.

Dedicated to Albrecht Dürer by his Mathematical Contributions

Key words: bistochastic matrix, unistochastic matrix, critical point, Jacobian

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1 Introduction

A real square matrix $B = (B_{ij})_{i,j=1}^{N}$ is *bistochastic* if it has non-negative entries that add up to 1 in every row and column. The convex set $\mathbf{B}_N$ of all bistochastic matrices of order N is called the *Birkhoff's polytope*, named after Birkhoff's famous result in 1949 stating that the set of all the extreme points of $\mathbf{B}_N$ is the set of permutation matrices of order N, representing the *symmetric group of degree* N, $\mathfrak{S}_N$. This set contains the closed subset $\mathbf{U}_N$ of *unistochastic* matrices. A bistochastic matrix of order N is unistochastic if its entries are the squared moduli entries of some unitary matrix $U = (U_{ij})_{i,j=1}^{N} \in \mathcal{U}(N)$, the *unitary group* formed by the unitary matrices of order N. Denote by Δ_N the $(N-1)$-dimensional probability simplex in $\mathbb{R}^N$. The transformation of Δ_N into itself defined as $Y = BX$ for $X \in \Delta_N$, performed by a bistochastic matrix B, is *quantized* if B is unistochastic. Since $\mathcal{U}(N) \subset M_N(\mathbb{C}) = \mathbb{R}^{2N}$ is an algebraic set and $U \mapsto \Phi_N(U) = U \circ \overline{U}$ is a polynomial map, then $\mathbf{U}_N$ is a semi-algebraic set and its boundary in $\mathbf{B}_N$ is also semi-algebraic [2]. Hence there is a non-zero real polynomial P in B_{ij} $(i, j = 1, 2, \dots, N-1)$ for which

$$\partial\mathbf{U}_N \subset \{B \in \mathbf{B}_N : P((B_{ij})_{i,j=1}^{N-1}) = 0\},$$

with $\partial\mathbf{U}_N$ the boundary of $\mathbf{U}_N$. In this paper, we develop a differential geometrical approach to investigate $\partial\mathbf{U}_N$ for $N = 4$. Notice that in the case $N = 2$, the two sets $\mathbf{B}_N$ and $\mathbf{U}_N$ coincide. For $N = 3$, Au-Yeung and Poon [1] characterized the set $\mathbf{U}_3$ by using the *bracelet* conditions on the products of the square roots $\sqrt{B_{ij}}$, with B_{ij} the entries of $B = (B_{ij})_{i,j=1}^{3} \in \mathbf{U}_3$ (cf. [12]).

In this paper we mainly study the polynomial map Φ_4 from $\mathcal{U}(4)$ into $\mathbf{U}_4 \subset \mathbf{B}_4 \subset \mathbb{M}_4(\mathbb{R})$. This map Φ_4 is a (real) analytic map and hence a $C^{(\infty)}$-map from the 16-dimensional compact Lie group $\mathcal{U}(4)$ into the 9-dimensional affine space of 4×4 real matrices $B = (B_{ij})_{i,j=1}^{4}$ satisfying

$$\sum_{k=1}^{4} B_{ik} = \sum_{k=1}^{4} B_{kj} = 1, \;\; 1 \le i, j \le 4.$$

For any $g \in \mathcal{U}(4)$, by using an analytic coordinate system $(X_1, \dots, X_{16})$ around g, we consider the 9×16-Jacobian matrix

$$J(g) = \{\frac{\partial Y_i}{\partial X_j}\Big|_g : i = 1, 2, \dots, 9, j = 1, 2, \dots, 16\}$$

for

$$Y_1 = (\Phi_4)_{1,1}, Y_2 = (\Phi_4)_{1,2}, Y_3 = (\Phi_4)_{1,3}, Y_4 = (\Phi_4)_{2,1}, Y_5 = (\Phi_4)_{2,2},$$

$$Y_6 = (\Phi_4)_{2,3}, Y_7 = (\Phi_4)_{3,1}, Y_8 = (\Phi_4)_{3,2}, Y_9 = (\Phi_4)_{3,3}.$$

For a generic point g of $\mathcal{U}(4)$, the matrix rank of the map $J(g)$ is 9.

If the matrix rank of $J(g)$ for $g \in \mathcal{U}(4)$ is less than or equal to 8, such a point g is said to be a *critical point* of the unistochastic map Φ_4. We remark that if the rank of $J(g)$ is 9, the point $\Phi(g)$ is an interior point of $\mathbf{U}_4$ in the 9-dimensional affine space spanned by $\mathbf{B}_4$. So the condition for $g \in \mathcal{U}(4)$ to be a critical point of Φ_4 is a necessary condition for $\Phi_4(g)$ to be a boundary point of $\mathbf{U}_4$. Our main aim is to investigate the shape of the set $\mathbf{U}_4$. The study of the critical points of Φ_4 is an adequate and efficient tool for this purpose. The set $\mathbf{U}_4$ is a compact connected subset of the Birkhoff polytope $\mathbf{B}_4$, and the determination of its boundary $\partial\mathbf{U}_4$ is a crucial subject to answer our problem. The unistochastic map Φ_4 satisfies the following invariance for any angles θ_j's and η_k's

$$\Phi_4(D_\theta g D_\eta) = \Phi_4(g),$$

where

$$D_\theta = \mathrm{diag}(\exp(i\theta_1), \exp(i\theta_2), \exp(i\theta_3), \exp(i\theta_4)),$$
$$D_\eta = \mathrm{diag}(\exp(i\eta_1), \exp(i\eta_2), \exp(i\eta_3), \exp(i\eta_4)).$$

Based on this invariance, Φ_4 is often restricted to the unitary matrices $U = (U_{ij})_{i,j=1}^4$ for which the 7 entries $U_{11}, U_{12}, U_{13}, U_{14}, U_{21}, U_{31}, U_{41}$ in the first row and column are real (or more strictly, non-negative).

We mention some articles treating our subject or related topics. The articles [18], [3], [4] and [15] have been published in recent years. A numerical algorithm is presented in [16] to provide a criterion for a given 4×4 bistochastic matrix to be, or not to be, unistochastic (cf. [8], [14]). In the present paper, we provide an alternative method (cf. [4]). Many articles, e.g. [5], published in the last century are related to our subject.

Our main motivation to study $\mathbf{U}_N$ arised from our interest in generalized *numerical ranges*, namely the *C-numerical range* $W_C(A)$, defined by

$$W_C(A) = \{\mathrm{tr}(CUAU^*) : U \in \mathcal{U}(N)\}.$$

For two $N \times N$ complex diagonal matrices $C = \mathrm{diag}(a_1, a_2, \ldots, a_N)$ and $A = \mathrm{diag}(c_1, c_2, \ldots, c_N)$,it can be easily verified that this range may be rewritten as

$$W_C(A) = \{\sum_{i,j=1}^{N} a_i c_j B_{ij} : (B_{ij}) \in \mathbf{U}_N\}$$

(cf. [13]). We are also interested in its analogue for Krein space operators ([7]) and the numerical range of an operator and its related topics ([10], [17]). The relevance of $\mathbf{U}_N$ in quantum physics is another main motivation to study this subject.

The remaining of the paper is organized as follows. In Section 2, we present a parametrization of the unitary group $U(4)$, which is efficient to treat the bicoset space $D(4)\backslash U(4)/D(4)$ and the unistochastic map Φ_4. In Section 3, some special critical points of the unistochastic map Φ_4 are exhibited. The main theorem of this paper is stated in Section 4. In this theorem, the necessary and the sufficient condition for a point in the bicoset space to be a critical point of Φ_4 is obtained. The proof of the main theorem is given in Section 5. In Section 6, a numerical criterion for a bistochastic matrix to be unistochastic is provided. Here, we consider a 4×4 bistochastic matrix B for which $34B$ is the 4×4 magic square of the German artist Albrecht Dürer (1471-1528) engraved in his work *Melancolia I* in 1514:

$$34B = \begin{pmatrix} 16 & 3 & 2 & 13 \\ 5 & 10 & 11 & 8 \\ 9 & 6 & 7 & 12 \\ 4 & 15 & 14 & 1 \end{pmatrix}.$$

Moreover, we address and answer the question of the unistochasticy of B. In Section 7, we present examples of a boundary point and of an inner point of the set of unistochastic matrices, which are the images of some critical points of Φ_4.

2 An efficient parametrization of the unitary group $U(4)$

Our parametrization of the 16-dimensional Lie group $U(4)$ is based on some parametrization of the bicoset space $D(4)\backslash U(4)/D(4)$. To start, we parametrize this bicoset space or the set of its representatives, the space of 4×4 unitary matrices $(U_{ij})_{i,j=1}^4$ with real first row $U_{11}, U_{12}, U_{13}, U_{14}$ and real first column U_{21}, U_{31}, U_{41}. As a first step, we parametrize the first row by the spherical coordinates on the unit sphere $\mathbf{S}^3$:

$$\begin{aligned} &U_{11} = \cos t_1,\ U_{12} = (\sin t_1)(\cos t_2), \\ &U_{13} = (\sin t_1)(\sin t_2)(\cos t_3),\ U_{14} = (\sin t_1)(\sin t_2)(\sin t_3), \end{aligned}$$

where t_1, t_2, t_3, t_4 are real parameters. Let $E_1 = (U_{11}, U_{12}, U_{13}, U_{14})$ be the row vector with the above defined entries. We consider the orthonormal basis of its orthogonal complement:

$$\begin{aligned} &E_2 = (-\sin t_1, (\cos t_1)(\cos t_2), (\cos t_1)(\sin t_2)(\cos t_3), (\cos t_1)(\sin t_2)(\sin t_3)), \\ &E_3 = (0, -\sin t_2, (\cos t_2)(\cos t_3), (\cos t_2)(\sin t_3)), \\ &E_4 = (0, 0, -\sin t_3, \cos t_3). \end{aligned}$$

Next, we parametrize a general unit vector H_2 of the complex vector space spanned by E_2, E_3, E_4 as follows:

$$H_2 = \exp(iu_1)(\cos s_1)E_2 + \exp(iu_2)(\sin s_1)(\cos s_2)E_3 + \exp(iu_3)(\sin s_1)(\sin s_2)E_4.$$

Thus, we get $H_2 = (-\exp(iu_1)(\cos s_1)(\sin t_1), \ldots)$. We choose the second row of the unitary matrix U as $H_2 = (U_{21}, U_{22}, U_{23}, U_{24})$. Following the requirement for U_{21} to be real, we may assume $u_1 = 0$. On this condition, we join the two following unit vectors H_3 and H_4, so that $\{H_2, H_3, H_4\}$ is an orthonormal basis of the space $\mathbf{C}E_2 + \mathbf{C}E_3 + \mathbf{C}E_4$:

$$H_3 = -\sin s_1 E_2 + \exp(iu_2)(\cos s_1)(\cos s_2)E_3 + \exp(iu_3)(\cos s_1)(\sin s_2)E_4,$$
$$H_4 = -\exp(iu_2)(\sin s_2)E_3 + \exp(iu_3)(\cos s_2)E_4.$$

Finally, we parametrize a general unit vector K_3 of the complex vector space spanned by H_3, H_4 as

$$K_3 = \exp(iu_4)(\cos s_3)H_3 + \exp(iu_5)(\sin s_3)H_4.$$

A unit vector in $\mathbf{C}H_3 + \mathbf{C}H_4$ orthogonal to K_3 is given by

$$K_4 = -\exp(iu_4)(\sin s_3)H_3 + \exp(iu_5)(\cos s_3)H_4,$$

up to a unit multiple. Writing $K_3 = (U_{31}, \dots, U_{34})$ and $K_4 = (U_{41}, \dots, U_{44})$, the respective entries U_{31}, U_{41} are

$$\exp(iu_4)(\sin t_1)(\sin s_1)(\cos s_3), \quad -\exp(iu_4)(\sin t_1)(\sin s_1)(\sin s_3).$$

Following the requirement for U_{31}, U_{41} to be real, we may assume $u_4 = 0$, and so the representatives of $D(4)\backslash U(4)/D(4)$ are parametrized by the 9 real parameters $t_1, t_2, t_3,\ s_1, s_2, s_3$ and u_2, u_3, u_5. We unify the symbols to express the bicoset space by letting:

$$s_1 = t_4, s_2 = t_5, s_3 = t_6, u_5 = t_7, u_2 = t_8, u_3 = t_9.$$

By using these 9 real parameters $t_1, \dots, t_9$, we shall present the exact parametrization of the representatives of the bicoset space. For this purpose, we introduce the abbreviated notation $Cs_j = \cos t_j$, $Si_j = \sin t_j$ $(j = 1, 2, \dots, 9)$, and we get

$$U_{11} = Cs_1, U_{12} = Si_1Cs_2, U_{13} = Si_1Si_2Cs_3, U_{14} = Si_1Si_2Si_3,$$
$$U_{21} = -Si_1Cs_4, U_{31} = Si_1Si_4Cs_6, U_{41} = Si_1Si_4Si_6,$$
$$U_{22} = Cs_1Cs_2Cs_4 - Si_2Si_4Cs_5(Cs_8 + iSi_8), U_{23} = Cs_1Si_2Cs_3Cs_4$$
$$+Cs_2Cs_3Si_4Cs_5(Cs_8 + iSi_8) - Si_3Si_4Si_5(Cs_9 + iSi_9), U_{24}$$
$$= Cs_1Si_2Si_3Cs_4 + Cs_2Si_3Si_4Cs_5(Cs_8 + iSi_8) + Cs_3Si_4Si_5(Cs_9 + iSi_9),$$
$$U_{32} = -Cs_1Cs_2Si_4Cs_6 - Si_2Cs_4Cs_5Cs_6(Cs_8 + iSi_8) + Si_2Si_5Si_6 \cdot$$
$$(Cs_7 + iSi_7)(Cs_8 + iSi_8), U_{33} = -Cs_1Si_2Cs_3Si_4Cs_6$$
$$+Cs_2Cs_3Cs_4Cs_5Cs_6(Cs_8 + iSi_8) - Si_3Cs_4Si_5Cs_6(Cs_9 + iSi_9)$$
$$-Cs_2Cs_3Si_5Si_6(Cs_7 + iSi_7)(Cs_8 + iSi_8) - Si_3Cs_5Si_6(Cs_7 + iSi_7) \cdot$$
$$(Cs_9 + iSi_9),$$

$U_{34} = -Cs_1Si_2Si_3Si_4Cs_6 + Cs_2Si_3Cs_4Cs_5Cs_6(Cs_8 + iSi_8) + Cs_3 \cdot$
$Cs_4Si_5Cs_6(Cs_9 + iSi_9) - Cs_2Si_3Si_5Si_6(Cs_7 + iSi_7)(Cs_8 + iSi_8)$
$+Cs_3Cs_5Si_6(Cs_7 + iSi_7)(Cs_9 + iSi_9)$,
$U_{42} = Cs_1Cs_2Si_4Si_6 + Si_2Cs_4Cs_5Si_6(Cs_8 + iSi_8) + Si_2Si_5Cs_6 \cdot$
$(Cs_7 + iSi_7)(Cs_8 + iSi_8), U_{43} = Cs_1Si_2Cs_3Si_4Si_6 - Cs_2Cs_3Cs_4Cs_5Si_6 \cdot$
$(Cs_8 + iSi_8) + Si_3Cs_4Si_5Si_6(Cs_9 + iSi_9) - Cs_2Cs_3Si_5Cs_6(Cs_7 + iSi_7) \cdot$
$(Cs_8 + iSi_8) - Si_3Cs_5Cs_6(Cs_7 + iSi_7)(Cs_9 + iSi_9)$,
$U_{44} = Cs_1Si_2Si_3Si_4Si_6 - Cs_2Si_3Cs_4Cs_5Si_6(Cs_8 + iSi_8) - Cs_3Cs_4Si_5 \cdot$
$Si_6(Cs_9 + iSi_9) - Cs_2Si_3Si_5Cs_6(Cs_7 + iSi_7)(Cs_8 + iSi_8) + Cs_3Cs_5Cs_6 \cdot$
$(Cs_7 + iSi_7)(Cs_9 + iSi_9)$.

In the case $t_7 = t_8 = t_9 = 0$, the unitary matrix $U(t_1, \ldots, t_6, 0, 0, 0)$ is a real orthogonal matrix with determinant 1. The set of these matrices form the 6-dimensional Lie group $SO(4)$.

We denote a general element of the above parametrized bicoset space by $U(t_1, \ldots, t_9) = \{U_{ij} : i, j = 1, \ldots, 9\}$. Using this, we also parametrize the unitary group $U(4)$. Indeed, let

$$g = D(t_{10}, t_{11}, t_{12}, t_{13})U(t_1, \ldots, t_9)D(t_{14}, t_{15}, t_{16}, t_{17}),$$

where $D(s_1, s_2, s_3, s_4)$ is the 4×4 diagonal matrix defined as

$$\mathrm{diag}(\exp(is_1), \exp(is_2), \exp(is_3), \exp(is_4)).$$

Since $D(s, s, s, s)$ is a scalar matrix for any $s \in \mathbf{R}$, we have

$$D(s, s, s, s)U(t_1, \ldots, t_9) = U(t_1, \ldots, t_9)D(s, s, s, s),$$

and it follows that

$$\begin{aligned} &D(t_{10}, t_{11}, t_{12}, t_{13})U(t_1, \ldots, t_9)D(t_{14}, t_{15}, t_{16}, t_{17}) \\ &= D(t_{10} - t_{13}, t_{11} - t_{13}, t_{12} - t_{13}, 0)U(t_1, \ldots, t_9)D(t_{13} + t_{14}, \\ &t_{13} + t_{15}, t_{13} + t_{16}, t_{13} + t_{17}). \end{aligned}$$

Hence, we can parametrize the group $U(4)$ by 16 real parameters. Every element $g_0 \in U(4)$ has a neighborhood $\{g_0 \exp(X) : X + X^* = 0, ||X|| < \epsilon\}$ for small $\epsilon > 0$, where X is a 4×4 skew-Hermitian matrix, and so the space $\{g_0X : X + X^* = 0\}$ can be viewed as the tangent space of $U(4)$ at g_0. By using this system, we shall determine the condition for the parametrization

$$g = D(u_1, u_2, u_3, 0)U(t_1, \ldots, t_9)D(v_1, v_2, v_3, v_4), \tag{2.1}$$

to be a (faithful) local coordinate system in a small neighborhood.

Theorem 2.1 *The parametrization (2.1) is a local coordinate system in a small open set if and only if the condition* $\prod_{j=1}^{6}(\cos(t_j)_0)(\sin(t_j)_0) \neq 0$ *holds.*

Proof For small real numbers $h_1, \ldots, h_{16}$ and taking into account the relation

$$D(u_1 + h_{10}, u_2 + h_{11}, u_3 + h_{12}, 0)D(t_1 + h_1, \ldots, t_9 + h_9)D(v_1 + h_{13},$$
$$v_2 + h_{14}, v_3 + h_{15}, v_4 + h_{16})$$
$$= D(u_1, u_2, u_3, 0)D(h_1, h_2, h_3, 0)D(t_1 + h_1, \ldots, t_9 + h_9)D(h_{13}, h_{14},$$
$$h_{15}, h_{16})D(v_1, v_2, v_3, v_4),$$

the condition for the faithfulness of the parametrization in a small neighborhood of $g \in U(4)$ is reduced to the case $u_1 = u_2 = u_3 = 0$, $v_1 = v_2 = v_3 = v_4 = 0$, and so we may assume that $g \in D(4)\backslash U(4)/D(4)$. In this situation, we consider the elements

$$U(t_1, \ldots, t_9)^* D(h_{10}, h_{11}, h_{12}, 0)U(t_1 + h_1, \ldots, t_9 + h_9)U(h_{13}, h_{14}, h_{15}, h_{16})$$

in a neighborhood of the identity I_4. For each $1 \leq j \leq 16$, let $h_k = 0$ for $k \in \{1, \ldots, 16\}\backslash\{j\}$, and consider the derivative of the above matrix function at $h_j = 0$. We denote the 4×4 skew-Hermitian matrix so obtained by X_j. The faithfulness of the coordinates around $g = U(t_1, \ldots, t_9)$ is formulated as

$$\mathbf{R}X_1 + \mathbf{R}X_2 + \ldots + \mathbf{R}X_{16} = \{X : X \,\text{is a}\, 4 \times 4\text{matrix}, X + X^* = 0\}. \qquad (2.2)$$

We remark that

$$U(t_1, \ldots, t_9)^* U(t_1, \ldots, t_9)D(h_{13}, h_{14}, h_{15}, h_{16}) = D(h_{13}, h_{14}, h_{15}, h_{16}),$$

so that $\mathbf{R}X_{13} + \ldots + \mathbf{R}X_{16} = \{\text{diag}(ia_1, ia_2, ia_3, ia_4) : a_j \in \mathbb{R}\}$. We focus our attention on the above mentioned $(1, 2), (1, 3), (1, 4), (2, 3), (2, 4), (3, 4)$-entries of the skew Hermitian matrices $X_1, X_2, \ldots, X_{12}$ to examine the condition (2.2). We have

$$t_{10}X_{10} + t_{11}X_{11} + t_{12}X_{12} = i\, U(t_1, \ldots, t_9)^* \text{diag}(t_{10}, t_{11}, t_{12}, 0)U(t_1, \ldots, t_9),$$

where $i = \sqrt{-1}$. We shall denote the $(1, 2), \ldots, (3, 4)$-entries of the matrix X_j by $\tilde{X_j}$ using a row vector. We get

$$\tilde{X_3} = \{0, 0, 0, 0, 0, 1\}, \tilde{X_2} = \{0, 0, 0, \cos t_3, \sin t_3, 0\},$$

$$\tilde{X_1} = \{\cos t_2, \sin t_2 \cos t_3, \sin t_2 \sin t_3, 0, 0, 0\},$$

$$\tilde{X_4} = \{Cs_5 Si_1 S_2(Cs_8 + iSi_8), Si_1(-Cs_2 Cs_3 Cs_5(Cs_8 + iSi_8) + Si_3 Si_5(Cs_9 + iSi_9),$$
$$Si_1\{-Cs_2 Cs_5 Si_3(Cs_8 + iSi_8) - Cs_3 Si_5(Cs_9 + iSi_9)\},$$
$$Cs_1\{Cs_3 Cs_5(Cs_8 + \text{icos}(2\text{t}_2)Si_8 - Cs_2 Si_3 Si_5(Cs_9 + iSi_9)\},$$
$$Cs_1\{Cs_5 Si_3(Cs_8 + \text{icos}(2\text{t}_2)Si_8 + Cs_2 Cs_3 Si_5(Cs_9 + iSi_9)\},$$

$$Cs_1Si_2\{Cs_9Si_5 + i[Cs_2Cs_5\sin(2t_3)Si_8 + \cos(2t_3)Si_5Si_9]\},$$

$$\tilde{X_5} = \{0, 0, 0, Si_2Si_3(\cos(t_8-t_9)-i\sin(t_8-t_9), Cs_3Si_2(-\cos(t_8-t_9)+i\sin(t_8-t_9)),$$

$$Cs_2(\cos(t_8 - t_9) - i\cos(2t_3)\sin(t_8 - t_9))\},$$

$$\ldots,$$

$$\tilde{X_{10}} = \{iCs_1Cs_2Si_1, iCs_1Cs_3Si_1Si_2, iCs_1Si_1Si_2Si_3,$$

$$iCs_2Cs_3Si_1Si_2, iCs_2Si_1^2Si_2Si_3, iCs_3Si_1^2Si_2^2Si_3\}$$

$$\ldots.$$

Next, we take the Cartesian decomposition of each entry of $\tilde{X_j}$ and let

$$\check{X_j} = \{\Re(\tilde{X_j}), \Im(X_j)\},\ \ j = 1, \ldots, 12.$$

By using these row vectors, a 12×12 real matrix is obtained

$$M_0 = \{\check{X_9}, \check{X_3}, \check{X_8}, 16\check{X_7}, 8\check{X_6}, \check{X_5}, \check{X_4}, \check{X_1}, \check{X_1}, \check{X_{10}}, \check{X_{11}}, \check{X_{12}}\}.$$

This matrix has a rather complicated form. We compute its determinant by using some software (e.g. "Mathematica"). We obtain

$$\det(M_0) = 16 \times 8 \times Si_1^5Si_2^3Si_3Si_4^3Si_5Si_6Cs_1Cs_2Cs_3Cs_4Cs_5Cs_6.$$

Thus, we conclude that $\sin(2t_j) = 2\sin t_j \cos t_j \neq 0$ ($j = 1, 2, \ldots, 6$) is the necessary and the sufficient condition for the parametrization (2.1) to be a local coordinate system. □

Corollary 2.1 *If* $U((t_1)_0, \ldots, (t_9)_0) \in D(n)\backslash U(n)//D(n)$ *satisfies* $\sin(2(t_j)_0) \neq 0$ *(* $j = 1, 2, \ldots, 6$*) and the Jacobian* $\partial(Y_1, Y_2, \ldots, Y_9)/\partial(t_1, t_2, \ldots, t_9)$ *at* $U((t_1)_0, (t_2)_0, \ldots, (t_9)_0)$ *vanishes, then the matrix* $U((t_1)_0, \ldots, (t_9)_0)$ *is a critical point of the unistochastic map* Φ_4*. In the above*

$$Y_1 = (\Phi_4)_{1,1}, Y_2 = (\Phi_4)_{1,2}, Y_3 = (\Phi_4)_{1,3}, Y_4 = (\Phi_4)_{2,1}, Y_5 = (\Phi_4)_{2,2},$$

$$Y_6 = (\Phi_4)_{2,3}, Y_7 = (\Phi_4)_{3,1}, Y_8 = (\Phi_4)_{3,2}, Y_9 = (\Phi_4)_{3,3}.$$

Proof By considering the tangent space of $U(4)$ at the point $U(t_1, t_2, \ldots, t_9)$, the property

$$\Phi_4(D(u_1, u_2, u_3)U(t_1, t_2, \ldots, t_9)D(v_1, v_2, v_3, v_4)) = \Phi_4(U(t_1, t_2, \ldots, t_9))$$

implies that the point $U(t_1, \ldots, t_9)$ is a critical point of Φ_4 via the faithfulness of the coordinates $(t_1, t_2, \ldots, t_9)$ at that point. □

3 Some special critical points of the unistochastic map

Before using the previous coordinates $(t_1, t_2, \ldots, t_9)$ in the bicoset space $D(4)\backslash U(4)/D(4)$ to characterize the critical points of Φ_4, we develop a more primitive method to analyze the critical points of Φ_4 via a linear approximation of the expotential map $\exp(X)$ for a 4×4 skew-Hermitian matrix X. For a real parameter t and a 4×4 unitary matrix g, we have

$$\begin{aligned}\Phi_4(g \exp(tX)) &= (g + tgX + t^2/2gX^2 + \ldots) \circ (\overline{g} + t\overline{g}\overline{X} + t^2/2\overline{g}\overline{X}^2 + \ldots) \\ &= g \circ \overline{g} + 2t\Re(\overline{g} \cdot (gX)) + O(t^2),\end{aligned}$$

so that

$$(d\Phi_4)|_X(g) = 2\Re(\overline{g} \circ (gX)), \tag{3.1}$$

where $\Re(A)$ is the entrywise real part of the matrix $A = (A_{ij})_{i,j=1}^4$, that is, $\Re(A) = (\Re(A_{ij}))_{i,j=1}^4$. For any diagonal skew-Hermitian matrix $X = \mathrm{diag}(\sqrt{-1}b_{11}, \sqrt{-1}b_{22}, \sqrt{-1}b_{33}, \sqrt{-1}b_{44})$ (the b_{jj} are real), we have

$$\Phi_4(g \exp(tX)) = \Phi_4(g), (d\Phi_4)|_X(g) = 0.$$

Based on this fact, we consider the 4×4 skew Hermitian matrix in the form

$$X = \begin{pmatrix} 0 & a_{12} + ib_{12} & a_{13} + ib_{13} & a_{14} + ib_{14} \\ -a_{12} + ib_{12} & 0 & a_{23} + ib_{23} & a_{24} + ib_{24} \\ -a_{13} + ib_{13} & -a_{23} + ib_{23} & 0 & a_{34} + ib_{34} \\ -a_{14} + ib_{14} & -a_{24} + ib_{24} & -a_{34} + ib_{34} & 0 \end{pmatrix}, \tag{3.2}$$

with a_{ij} and b_{ij} real parameters (cf. [9]), and we analyze the 9×12 Jacobian matrix

$$\partial(Y_1, Y_2, \ldots, Y_9)/\partial(a_{12}, a_{13}, a_{14}, a_{23}, a_{24}, a_{34}, b_{12}, b_{13}, b_{14}, b_{23}, b_{24}, b_{34}).$$

The point g is a critical point of Φ_4 if and only if the matrix rank of this Jacobian matrix is less than 9.

Proposition 3.1 *If an entry U_{pq} of a 4×4 unitary matrix $U = (U_{ij})_{i,j=1}^4$ vanishes for some $1 \le p, q \le 4$, then U is a critical point of the unistochastic map Φ_4. Especially, if one of the 5 parameters t_1, t_2, t_3, t_4, t_6 satisfies $t_j \cong 0$ modulo $\pi/2$, or equivalently $Cs_j = 0$ or $Si_j = 0$, for some $j \in \{1, 2, 3, 4, 6\}$, then $U = U(t_1, t_2, \ldots, t_9)$ is a critical point of Φ_4.*

Proof By applying permutations on the indexes (i, j) with $U_{ij} = 0$, we may assume $1 \le i, j \le 3$ since the unistochasticity is invariant under such permutations. Then (3.1) implies that the (i, j)-entry of $\overline{U} \circ (UX)$ vanishes for any skew-Hermitian matrix X. It follows that one row of the Jacobian matrix $\partial(Y_1, \ldots, Y_9)/\partial(a_{12}, \ldots, b_{34})$ vanishes, and so the matrix rank of the Jacobian is less than 9. $\square$.

Proposition 3.2 *If two rows (or two columns) of a 4×4 unitary matrix U have real entries, then U is a critical point of Φ_4.*

Proof We may assume that the first and the second rows of U are real by considering some suitable permutations on rows and columns. We express the matrix U as

$$U = \begin{pmatrix} U_{11} & U_{12} & U_{13} & U_{14} \\ U_{21} & U_{22} & U_{23} & U_{24} \\ U_{31}+iV_{31} & U_{32}+iV_{32} & U_{33}+iV_{33} & U_{34}+iV_{34} \\ U_{41}+iV_{41} & U_{42}+iV_{42} & U_{43}+iV_{43} & U_{44}+iV_{44} \end{pmatrix},$$

where $U_{k\ell}$ and $V_{k\ell}$ are real numbers. By the property $\Phi_4(D(u_1,\ldots,u_4)\ U) = \Phi_4(U)$, we may assume that $V_{31} = V_{41} = 0$. We compute the $(1,1),(1,2),(1.3),$ $(2,1),(2,2),(2,3),\ (3,1),(3,2),(3,3)$-entries of the matrix $K = \Re[\overline{U} \circ UX]$ for the skew-Hermitian matrix (3.2). The $(1,1)$-entry of K is given by

$$C_1 = -U_{11}U_{12}a_{12} - U_{11}U_{13}a_{13} - U_{11}U_{14}a_{14}.$$

Similarly, the $(1,2),(1,3),(2,1),(2,2),(2,3),(3,1)$-entries of K are given by

$$\begin{aligned}
C_2 &= -U_{12}U_{11}a_{12} - U_{12}U_{13}a_{23} - U_{12}U_{14}a_{24},\\
C_3 &= U_{13}U_{11}a_{13} + U_{13}U_{12}a_{23} - U_{13}U_{14}a_{34},\\
C_4 &= -U_{21}U_{22}a_{12} - U_{21}U_{23}a_{13} - U_{21}U_{24}a_{14},\\
C_5 &= U_{22}U_{21}a_{12} - U_{22}U_{23}a_{23} - U_{22}U_{24}a_{24},\\
C_6 &= U_{23}U_{21}a_{13} + U_{23}U_{22}a_{23} - U_{23}U_{24}a_{34},\\
C_7 &= -U_{31}U_{32}a_{12} - U_{31}U_{33}a_{13} - U_{31}U_{34}a_{14}\\
&-U_{31}V_{32}b_{12} - U_{31}V_{33}b_{13} - U_{31}V_{34}b_{14},
\end{aligned}$$

It can be seen that the entries $C_1,\ldots,C_9$ are linear forms in the 12 variables $a_{12}, a_{13}, a_{14},\ a_{23}, a_{24}, b_{12}, b_{13}, b_{14}, b_{23}, b_{24}, b_{34}$. We consider the Jacobian matrix of Φ_4 as a 9×12 matrix, and we concentrate on its first 6 rows. We adopt the following numbering of the variables $X_1 = a_{12},\ X_2 = a_{13},\ X_3 = a_{14},\ X_4 = a_{23},$ $X_5 = a_{24},\ X_6 = a_{34}$. The entries $C_1,\ldots,C_6$ are linear forms in $X_1,\ldots,X_6$, and the 6×6 Jacobian determinant

$$[\partial(C_1,C_2,C_3,C_4,C_5,C_6)/\partial(X_1,X_2,X_3,X_4,X_5,X_6)]$$

is

$$(-U_{11})(U_{12})(U_{13})(-U_{21})(U_{22})(U_{23}) \times$$
$$\det(\begin{pmatrix} U_{12} & U_{13} & U_{14} & 0 & 0 & 0 \\ U_{11} & 0 & 0 & -U_{13} & -U_{14} & 0 \\ 0 & U_{11} & 0 & U_{12} & 0 & -U_{14} \\ U_{22} & U_{23} & U_{24} & 0 & 0 & 0 \\ U_{21} & 0 & 0 & -U_{23} & -U_{24} & 0 \\ 0 & U_{21} & 0 & U_{22} & 0 & -U_{24} \end{pmatrix}).$$

Applying Laplace development by the 6-th column of the above determinant, we conclude that the determinant is

$$(U_{12}U_{21} - U_{11}U_{22})(U_{14}U_{23} - U_{13}U_{24})(-U_{24}U_{14} + U_{14}U_{24}) = 0,$$

so that the forms $C_1, \ldots, C_6$ are linearly dependent and the matrix rank of Φ_4 at U is less than 9. □

As a consequence of Proposition 3.2, if $t_8 \cong 0$, $t_9 \cong 0$ modulo π, or equivalently $\sin t_8 = \sin t_9 = 0$, then the 4×4 unitary matrix $U(t_1, \ldots, t_9)$ given as the representative of a point of $D(4)\backslash U(4)/D(4)$ is a critical point of Φ_4.

By Theorem 2.1 and since $\Phi_4(D_1UD_2) = \Phi_4(U)$ for any 4×4 unitary matrix U and diagonal matrices D_1, D_2, we can provide a criterion for $U \in D(4)\backslash U(4)/D(4)$ to be a critical point of Φ_4 by using the coordinates $(t_1, t_2, \ldots, t_9)$ under the condition $(\cos t_j)(\sin t_j) \neq 0$ for $j = 1, 2, 3, 4, 5, 6$. By Proposition 3.1, if $(\cos t_j)(\sin t_j) = 0$ for some $j = 1, 2, 3, 4, 6$, then $U(t_1, \ldots, t_9)$ is a critical point. So the remaining delicate situations occur in the cases $(\cos t_5)(\sin t_5) = 0$ under $(\cos t_j)(\sin t_j) \neq 0$ for $j = 1, 2, 3, 4, 6$. We provide a special remark for these situations, considering separately the two cases (i) $\cos t_5 = 0$ and (ii) $\sin t_5 = 0$.

(i) Let $\cos t_5 = 0$. We can assume $\sin t_5 = 1$, by replacing t_7, t_9 by $t_7+\pi$, $t_9+\pi$ if necessary. Under this setting, the unitary matrix $U(t_1, \ldots, t_9)$ is parametrized as:

$$\begin{aligned}
U_{22} &= Cs_1Cs_2Cs_4, U_{23} = Cs_1Si_2Cs_3Cs_4 - Si_3Si_4(Cs_9 + iSi_9),\\
U_{24} &= Cs_1Si_2Si_3Cs_4 + Cs_3Si_4(Cs_9 + iSi_9),\\
U_{32} &= -Cs1Cs_2Si_4Cs_6 + Si_2Si_6(Cs_7 + iSi_7)(Cs_8 + iSi_8),\\
U_{33} &= -Cs_1Si_2Cs_3Si_4Cs_6 - Si_3Cs_4Cs_6(Cs_9 + iSi_9)\\
&\quad -Cs_2Cs_3Si_6(Cs_7 + iSi_7)(Cs_8 + iSi_8),\\
U_{34} &= -Cs_1Si_2Si_3Si_4Cs_6 + Cs_3Cs_4Cs_6(Cs_9 + iSi_9)\\
&\quad -Cs_2Si_3Si_6(Cs_7 + iSi_7)(Cs_8 + iSi_8),\\
U_{42} &= Cs_1Cs_2Si_4Si_6 + Si_2Cs_6(Cs_7 + iSi_7)(Cs_8 + iSi_8),\\
U_{43} &= Cs_1Si_2Cs_3Si_4Si_6 + Si_3Cs_4Si_6(Cs_9 + iSi_9)\\
&\quad -Cs_2Cs_3Cs_6(Cs_7 + iSi_7)(Cs_8 + iSi_8),\\
U_{44} &= Cs_1Si_2Si_3Si_4Si_6 - Cs_3Cs_4Si_6(Cs_9 + iSi_9)\\
&\quad -Cs_2Si_3Si_5Cs_6(Cs_7 + iSi_7)(Cs_8 + iSi_8).
\end{aligned}$$

Hence, the parameters t_7, t_8 can be unified by $t_7 + t_8$. In this situation, we assume $t_8 = 0$, or equivalently $Cs_8 = 1$, $Si_8 = 0$.

(ii) Let $\sin t_5 = 0$. We can assume $\cos t_5 = 1$, by replacing t_7, t_8 by $t_7 + \pi$, $t_8 + \pi$ if necessary. Under this setting, the unitary matrix $U(t_1, \ldots, t_9)$ is parametrized as:

$$\begin{aligned}
U_{22} &= Cs_1Cs_2Cs_4 - Si_2Si_4(Cs_8 + iSi_8), \\
U_{23} &= Cs_1Si_2Cs_3Cs_4 + +Cs_2Cs_3Si_4(Cs_8 + iSi_8), \\
U_{24} &= Cs_1Si_2Si_3Cs_4 + Cs_2Si_3Si_4(Cs_8 + iSi_8), \\
U_{32} &= -Cs1Cs_2Si_4Cs_6 - Si_2Cs_4Cs_6(Cs_8 + iSi_8), \\
U_{33} &= -Cs_1Si_2Cs_3Si_4Cs_6 + Cs_2Cs_3Cs_4Cs_5Cs_6(Cs_8 + iSi_8) \\
&\quad -Si_3Si_6(Cs_7 + iSi_7)(Cs_9 + iSi_9), \\
U_{34} &= -Cs_1Si_2Si_3Si_4Cs_6 + Cs_2Si_3Cs_4Cs_5Cs_6(Cs_8 + iSi_8) \\
&\quad +Cs_3Si_6(Cs_7 + iSi_7)(Cs_9 + iSi_9), \\
U_{42} &= Cs_1Cs_2Si_4Si_6 + Si_2Cs_4Si_6(Cs_8 + iSi_8), \\
U_{43} &= Cs_1Si_2Cs_3Si_4Si_6 - Cs_2Cs_3Cs_4Si_6(Cs_8 + iSi_8) \\
&\quad -Si_3Cs_6(Cs_7 + iSi_7)(Cs_9 + iSi_9), \\
U_{44} &= Cs_1Si_2Si_3Si_4Si_6 - Cs_2Si_3Cs_4Si_6(Cs_8 + iSi_8) \\
&\quad +Cs_3Cs_6(Cs_7 + iSi_7)(Cs_9 + iSi_9).
\end{aligned}$$

Thus, the parameters t_7, t_9 can be unified by t_7+t_9. In this situation, we assume $t_9 = 0$, or equivalently $Cs_9 = 1$, $Si_9 = 0$.

We shall assume that $\sin t_5 = 1$, $t_8 = 0$ in (i) and $\cos t_5 = 1$, $t_9 = 0$ in (ii), as the standard reduced form of U under the situation $(\cos t_5)(\sin t_5) = 0$. Using this form, we provide the criterion for $U \in D(4)\backslash U(4)/D(4)$ to be a critical point of Φ_4 in the statement (II) of our main theorem.

4 Main Theorem

Next, we state the main theorem of this paper.

Theorem 4.1 *(I) Assume that* $(\cos t_j)(\sin t_j) \neq 0$ *(* $j = 1, 2, 3, 4, 5, 6$*). Under this assumption, the point* $U \in D(4)\backslash U(4)/D(4)$*, represented as* $U = (t_1, t_2, \ldots, t_9)$ *by the parameters* $t_1, t_2, \ldots, t_9$*, is a critical point of the unistochastic map* Φ_4 *if and only if the main factor* MF *of the Jacobian* $J(U)$ *determined in the below vanishes at the point* $(t_1, t_2, \ldots, t_9) \in \mathbb{R}^9/[2\pi\mathbb{Z}]^9$*. For the 9-parameter system* $U = U(t_1, t_2, \ldots, t_9)$ *of the* 4×4 *matrix, the Jacobian determinant*

$$J(U) = \partial(B_{11}, B_{12}, B_{13}, B_{21}, B_{22}, B_{23}, B_{31}, B_{32}, B_{33})/\partial(t_1, t_2, t_3, t_4, t_5, t_6, t_7, t_8, t_9)$$

of the map Φ_4 *with respect to the variables*

$$B_{11} = \Phi_4(U)_{1,1}, B_{12} = \Phi_4(U)_{1,2}, B_{13} = \Phi_4(U)_{1,3}, B_{21} = \Phi_4(U)_{2,1}, B_{22} = \Phi_4(U)_{2,2}, B_{23} = \Phi_4(U)_{2,3}, B_{31} = \Phi_4(U)_{3,1}, B_{32} = \Phi_4(U)_{3,2}, B_{33} = \Phi_4(U)_{3,3}$$

has the factor

$$C_0 = -2^7(\sin^9 t_1)(\cos^2 t_1)(\sin^5 t_2)(\cos^2 t_2)(\sin^2 t_3)(\cos^2 t_3)$$

$$\cdot(\sin^5 t_4)(\cos^2 t_4)(\sin t_5)(\cos t_5)(\sin^2 t_6)(\cos^2 t_6). \qquad (4.1)$$

The main factor MF *of the Jacobian* $J(U)$ *divided by this factor* C_0 *is expressed as the following trigonometric polynomial in the* 9 *variables* $t_1, t_2, t_3, t_4, t_5, t_6$ *and* t_7, t_8, t_9*:*

$$\begin{aligned}
\mathrm{MF} \; = \; & [\alpha_{01}\sin t_8 + \alpha_{02}\sin t_9 + \alpha_{03}\sin(t_8+t_9) + \alpha_{04}\sin(t_8-t_9) \\
& +\alpha_{05}\sin(2t_8) + \alpha_{06}\sin(2t_9) + \alpha_{07}\sin(2t_8+t_9) + \alpha_{08}\sin(t_8+2t_9) \\
& +\alpha_{09}\sin(2t_8-t_9) + \alpha_{010}\sin(t_8-2t_9) + \alpha_{011}\sin(3t_8) \\
& +\alpha_{012}\sin(2t_8-2t_9) + \alpha_{013}\sin(3t_8-2t_9)] + [\alpha_{101}\sin t_7 + \alpha_{102}\cdot \\
& \sin(t_7+t_8) + \alpha_{103}\sin(t_7+t_9) + \alpha_{104}\sin(t_7-t_8) + \alpha_{105}\sin(t_7-t_9) \\
& +\alpha_{106}\sin(t_7+2t_8) + \alpha_{107}\sin(t_7+2t_9) + \alpha_{108}\sin(t_7+2t_8+t_9) \\
& +\alpha_{109}\sin(t_7+t_8+2t_9) + \alpha_{110}\sin(t_7+3t_8), \\
& +\alpha_{111}\sin(t_7-t_8+2t_9) + \alpha_{112}\sin(t_7+t_8-2t_9) + \alpha_{113}\sin(t_7-2t_8+t_9) \\
& +\alpha_{114}\sin(t_7+2t_8-t_9) + \alpha_{115}\sin(t_7-2t_8+2t_9) + \alpha_{116}\sin(t_7+2t_8-2t_9) \\
& +\alpha_{117}\sin(t_7+3t_8-2t_9) + \alpha_{118}\sin(t_7-3t_8+2t_9)] + [\alpha_{201}\sin(2t_7) \\
& +\alpha_{202}\sin(2t_7+t_8) + \alpha_{203}\sin(2t_7+t_9) + \alpha_{204}\sin(2t_7-t_8) \\
& +\alpha_{205}\sin(2t_7-t_9) + \alpha_{206}\sin(2t_7+2t_8) + \alpha_{207}\sin(2t_7+2t_9) \\
& +\alpha_{208}\sin(2t_7+t_8+t_9) + \alpha_{209}\sin(2t_7+t_8-t_9) + \alpha_{210}\sin(2t_7-t_8+t_9) \\
& +\alpha_{211}\sin(2t_7+3t_8) + \alpha_{212}\sin(2t_7+t_8+2t_9) + \alpha_{213}\sin(2t_7+2t_8+t_9) \\
& +\alpha_{214}\sin(2t_7+t_8-2t_9) + \alpha_{215}\sin(2t_7-t_8+2t_9) + \alpha_{216}\sin(2t_7+2t_8-t_9) \\
& +\alpha_{217}\sin(2t_7-2t_8+t_9) + \alpha_{218}\sin(2t_7+2t_8+2t_9) + \alpha_{219}\sin(2t_7-2t_8+2t_9) \\
& +\alpha_{220}\sin(2t_7+2t_8-2t_9) + \alpha_{221}\sin(2t_7+3t_8-2t_9) + \alpha_{222}\sin(2t_7-3t_8+2t_9)],
\end{aligned}$$

where the 53 *coefficients of the trigonometric polynomials* α_{pqr} *in* $t_1, \ldots, t_6$ *have at most degree* 15 *as polynomials in*

$$Cs_j = \cos t_j, \;\; Si_j = \sin t_j, \;\; j = 1, 2, 3, 4, 5, 6.$$

(II) Assume that $(\cos t_5)(\sin t_5) = 0$*,* $(\cos t_j)(\sin t_j) \neq 0$ *(* $1 \leq j \leq 6$*,* $j \neq 5$*), and that the unitary matrix* $U = U(t_1, \ldots, t_9)$ *has the standard reduced form in this situation for the parameters* t_8, t_9*. Then the main factor* MF *in (I) is expressed as*

$$\begin{aligned}
\mathrm{MF} \; = \; & \{Cs_1Cs_2Cs_4Si_7Si_9\}[-Si_2^2Cs_3Si_3Cs_4^2Cs_6Si_6Si_7Cs_9 \\
& -Cs_1Cs_2^2Si_2Cs_3^2Cs_4Si_4Cs_6Si_6Si_7 - Cs_1Si_2^3Cs_3^2Cs_4Si_4Cs_6Si_6Si_7 \\
& +Cs_1Si_2Si_3^2Cs_4Si_4Cs_6Si_6Si_7 + Cs_2^2Cs_3Si_3Si_4^2Cs_6Si_6Si_7Cs_9 \\
& +Cs_1^2Si_2^2Cs_3Si_3Si_4^2Cs_6Si6Si_7Cs_9 - Cs_1Cs_2Si_2Cs_3Si_3Cs_4^2Si_4C_s6^2Si_9 \\
& -Cs_1Cs_2Si_2Cs_3Si_3Si_4^3Cs_6^2Si_9 + Si_2^2Cs_3Si3Cs_4^2Cs_6Si_6Cs_7Si_9 \\
& -Cs_2^2Cs_3Si_3Si_4^2Cs_6Si_6Cs_7Si_9 + Cs_1^2Si_2^2Cs_3Si_3Si_4^2Cs_6Si_6Cs_7Si_9 \\
& +Cs_1Cs_2Si_2Cs_3Si_3Si_4Si_6^2Si_9]
\end{aligned}$$

in the case $\cos t_5 = 0$, *and*

$$\begin{aligned}
\mathrm{MF} &= \{Cs_3 Si_3 Cs_6 Si_6 Si_8\}[Cs_1 Si_2 Si_4 Si_7 - Cs_2 Cs_4 (Si_7 Cs_8 - Cs_7 Si_8)] \\
&\quad \cdot [Cs_1 (Cs_2^2 Si_4^2 + Si_2^2 Cs_4^2) Si_7 + Cs_2 Si_2 Cs_4 Si_4 (Si_7 Cs_8 - Cs_7 Si_8) \\
&\quad + Cs_1^2 Cs_2 Si_2 Cs_4 Si_4 (Si_7 Cs_8 + Cs_7 Si_8)]
\end{aligned}$$

in the case $\sin t_5 = 0$. *Further,* $U(t_1, \ldots, t_9)$ *is a critical point of* Φ_4 *if and only if the polynomial* MF *vanishes at this point.*

In the next subsection, we list the explicit expressions of the 53 coefficient polynomials α_{pqr}. We outline the computation of the Jacobian determinant $J(U)$ in the next section. We observe that in an expanded form of the MF in $Cs_1, Si_1, \ldots, Cs_9$, it has 362 terms.

4.2 List of Coefficients

In order to provide the exact expressions of the 53 coefficient polynomials of MF, we remark once more that if $t_7 = t_8 = t_9 = 0$, the point $U(t_1, \ldots, t_6, 0, 0, 0)$ is a critical point of Φ_4. We express it as the trigonometric polynomial in t_7, t_8, t_9 with coefficients α_{pqr}, which are polynomials in $Si_j = \sin t_j$ and $Cs_j = \cos t_j$ $(j = 1, 2, 3, 4, 5, 6)$:

$$\begin{aligned}
\mathrm{MF} &= \alpha_{01} \sin t_8 + \ldots + \alpha_{013} \sin(3t_8 - 2t_9) \\
&\quad + \alpha_{101} \sin t_7 + \ldots + \alpha_{118} \sin(t_7 - 3t_8 + 2t_9) \\
&\quad + \alpha_{201} \sin(2t_7) + \ldots + \alpha_{222} \sin(2t_7 - 3t_8 + 2t_9),
\end{aligned}$$

where the 53 polynomial coefficients α_{pqr} are given as follows:

$$\begin{aligned}
\alpha_{01} &= -Cs_3 Cs_5 Cs_6 Si_2 Si_3 Si_4 Si_6 \{Si2^2 (2Cs_1^2 Cs_4^2 Cs_5^2 + Cs_4^2 Si_5^2 \\
&\quad -2Cs_1^2 Cs_4^2 Si_5^2 - Cs_1^2 Si_4^2 Si_5^2 - Cs_5^2 Si_4^2 Si_5^2) + Cs_2^2 (Cs_1^2 Cs_4^2 Cs_5^2 \\
&\quad -2Cs_4^2 Cs_5^4 + 2Cs_1^2 Cs_5^2 Si_4^2 - 6Cs_1^2 Cs_4^2 Si_5^2 + Si_4^2 Si_5^2 - 2Cs_1^2 Si_4^2 Si_5^2 \\
&\quad +2Cs_4^2 Si_5^4)\}, \\
\alpha_{02} &= -Cs_2 Cs_6 Si_2 Si_4 Si_5 Si_6 (Cs_3^2 - Si_3^2)(-Cs_4^2 Cs_5^2 + 2Cs_1^2 Cs_4^2 Cs_5^2 \\
&\quad +Cs_1^2 Cs_5^2 Si_4^2 - 2Cs_1^2 Cs_4^2 Si_5^2 + Cs_5^2 Si_4^2 Si_5^2), \\
\alpha_{03} &= Cs_1 Cs_4 Cs_5 Cs_6 Si_4^2 Si_5 Si_6 (Cs_2^2 - Si_2^2)(Cs_3^2 - S_i 3^2), \\
\alpha_{04} &= Cs_1 Cs_4 Cs_5 Cs_6 Si_4^2 Si_5 Si_6 (Cs2^2 - Si2^2)(Cs3^2 - Si3^2)(Cs_5^2 - Si_5^2), \\
\alpha_{05} &= -Cs_1 Cs_2 Cs_3 Cs_4 Cs_5^2 Cs_6 Si_3 Si_6 (-Cs_4^2 Si_2^2 - Cs_2^2 Si_4^2 \\
&\quad +Si_2^2 Si_4^2 + Cs_1^2 Si_2^2 Si_4^2),
\end{aligned}$$

$$
\begin{aligned}
\alpha_{06} &= -Cs_1Cs_2Cs_3Cs_4Cs_6Si_3Si_5^2Si_6(-Cs_4^2Si_2^2+Cs_2^2Si_4^2+Cs_1^2Si_2^2Si_4^2),\\
\alpha_{07} &= Cs_1^2Cs_2Cs_4^2Cs_5^2Cs_6Si_2Si_4Si_5Si_6(Cs_3^2-Si_3^2),\\
\alpha_{08} &= -Cs_1^2Cs_3Cs_4^2Cs_5Cs_6Si_2Si_3Si_4Si_5^2Si_6,\\
\alpha_{09} &= -Cs_2Cs_5^2Cs_6Si_2Si_4Si_5Si_6(Cs_3^2-Si_3^2)(Cs_1^2-Cs_4^2-Si_4^2Si_5^2),\\
\alpha_{010} &= Cs_3Cs_5Cs_6Si_2Si_3Si_4Si_5^2Si_6(-3Cs_1^2Cs_2^2Cs_4^2\\
&\quad -Cs_1^2Si_2^2+Cs_4^2Si_2^2+Cs_5^2Si_2^2Si_4^2-Cs_2^2Si_4^2Si_5^2),\\
\alpha_{011} &= Cs_1^2Cs_2^2Cs_3Cs_4^2Cs_5^3Cs_6Si_2Si_3Si_4Si_6,\\
\alpha_{012} &= -Cs_1Cs_2Cs_3Cs_4Cs_5^2Cs_6Si_3Si_4^2Si_5^2Si_6(2Cs_2^2-Si_2^2),\\
\alpha_{013} &= Cs_2^2Cs_3Cs_5^3Cs_6Si_2Si_3Si_4Si_4^2Si_5^2Si_6,\\
\alpha_{101} &= -Cs_1Cs_2Cs_3Cs_5Si_2^2Si_3Si_5(Cs_4^2-Si_4^2)(Cs_5^2-Si_5^2)(Cs_6^2-Si_6^2),\\
\alpha_{102} &= -Cs_3Cs_4Si_2Si_3Si_4Si_5(Cs_6^2-Si_6^2)(2Cs_1^2Cs_2^2Cs_5^2-Cs_2^2Cs_5\\
&\quad +Cs_1^2Cs_5^2Si_2^2-2Cs_1^2Cs_2^2Si_5^2-Cs_2^2Cs_5^2Si_5^2+Cs_5^2Si_2^2Si_5^2),\\
\alpha_{103} &= -Cs_2Cs_4Cs_5Si_2Si_4Si_5^2(Cs_3^2-Si_3^2)(Cs_6^2-Si_6^2)(Cs_1^2+Cs_5^2),\\
\alpha_{104} &= Cs_3Cs_4Cs_5^2Si_2Si_3Si_4Si_5(Cs_6^2-Si_6^2)(Cs_1^2-Cs_2^2-Si_2^2Si_5^2),\\
\alpha_{105} &= Cs_2Cs_4Cs_5Si_2Si_4Si_5^2(Cs_3^2-Si_3^2)(Cs_6^2-Si_6^2)(Cs_1^2-Cs5^2),\\
\alpha_{106} &= Cs_1Cs_2Cs_3Cs_5Si_2^2Si_3Si_5(Cs_4^2-Si_4^2)(Cs_6^2-Si_6^2),\\
\alpha_{107} &= -Cs_1Cs_2Cs_3Cs_5Si_2^2Si_3Si_5(Cs_4^2-Si_4^2)(Cs_6^2-Si_6^2),\\
\alpha_{108} &= Cs_1^2Cs_2Cs_4Cs_5Si_2Si_4Si_5^2(Cs_3^2-Si_3^2)(Cs_6^2-Si_6^2),\\
\alpha_{109} &= Cs_1^2Cs_3Cs_4Si_2Si_3Si_4Si_5(Cs_6^2-Si_6^2)(Cs_5^2Si_2^2-Cs_2^2Si_5^2),\\
\alpha_{110} &= Cs_1^2Cs_2^2Cs_3Cs_4Cs_5^2Si_2Si_3Si_4Si_5(Cs_6^2-Si_6^2),\\
\alpha_{111} &= -Cs_3Cs_4Cs_5^2Si_2Si_3Si_4Si_5(Cs_6^2-Si_6^2)(Cs_2^2Cs_5^2+Cs_1^2Si_2^2-Si_2^2Si_5^2),\\
\alpha_{112} &= -Cs_3Cs_4Si_2Si_3Si_4Si_5^3(Cs_6^2-Si_6^2)(Cs_1^2Cs_2^2-Cs_2^2Cs_5^2-Cs_5^2Si_2^2,\\
\alpha_{113} &= Cs_2Cs_4Cs_5^3Si_2Si_4Si_5^2(Cs_3^2-Si_3^2)(Cs_6^2-Si_6^2),\\
\alpha_{114} &= -Cs_2Cs_4Cs_5Si_2Si_4Si_5^2(Cs_3^2-Si_3^2)(Cs_6^2-Si_6^2)(Cs_1^2-Cs_5^2),\\
\alpha_{115} &= Cs_1Cs_2Cs_3Cs_5^3Si_2^2Si_3Si_5(Cs_4^2-Si_4^2)(Cs_6^2-Si_6^2),\\
\alpha_{116} &= -Cs_1Cs_2Cs_3Cs_5Si_2^2Si_3Si_5^3(Cs_4^2-Si_4^2)(Cs_6^2-Si_6^2),\\
\alpha_{117} &= -Cs_2^2Cs_3Cs_4Cs_5^2Si_2Si_3Si_4Si_5^3(Cs_6^2-Si_6^2),\\
\alpha_{118} &= Cs_2^2Cs_3Cs_4Cs_5^4Si_2Si_3Si_4Si_5(Cs_6^2-Si_6^2).\\
\alpha_{201} &= Cs_1Cs_2Cs_3Cs_4Cs_5^2Cs_6Si_2^2Si_3Si_5^2Si_6(2Cs_4^2-Si_4^2),\\
\alpha_{202} &= Cs_3Cs_5Cs_6Si_2Si_3Si_4Si_5^2Si_6(3Cs_1^2Cs_2^2Cs_4^2+Cs_1^2Si_4^2\\
&\quad -Cs_2^2Si_4^2-Cs_5^2Si_2^2Si_4^2+Cs_4^2Si_2^2Si_5^2),\\
\alpha_{203} &= -Cs_2Cs_5^2Cs_6Si_2Si_4Si_5Si_6(Cs_3^2-Si_3^2)(Cs_4^2Cs_5^2+Cs_1^2Si_4^2-Si_4^2Si_5^2),\\
\alpha_{204} &= -Cs_3Cs_4^2Cs_5^3Cs_6Si_2^3Si_3Si_4Si_5^2Si_6,\\
\alpha_{205} &= Cs_2Cs_4^2Cs_5^2Cs_6Si_2Si_4Si_5^3Si_6(Cs_3^2-Si_3^2),
\end{aligned}
$$

$$
\begin{aligned}
\alpha_{206} &= -Cs_1Cs_2Cs_3Cs_4Cs_6Si_3Si_5^2Si_6\{Cs_4^2Si_2^2+(-Cs_2^2+Cs_1^2Si_2^2)Si_4^2\},\\
\alpha_{207} &= -Cs_1Cs_2Cs_3Cs_4Cs_5^2Cs_6Si_3Si_6(Cs_4^2Si_2^2+Cs_2^2Si_4^2+Cs_1^2Si_2^2Si_4^2\\
&\quad -Cs_5^2Si_2^2Si_4^2-Si_2^2Si_4^2Si_5^2),\\
\alpha_{208} &= -Cs_1Cs_4Cs_5Cs_6Si_4^2Si_5Si_6(Cs_2^2-Si_2^2)(Cs_3^2-Si_3^2),\\
\alpha_{209} &= Cs_1Cs_4Cs_5Cs_6Si_4^2Si_5^3Si_6(Cs_2^2-Si_2^2)(Cs_3^2-Si_3^2),\\
\alpha_{210} &= Cs_1Cs_4Cs_5^3Cs_6Si_4^2Si_5Si_6(Cs_2^2-Si_2^2)(Cs_3^2-Si_3^2),\\
\alpha_{211} &= -Cs_1^2Cs_2^2Cs_3Cs_5Cs_6Si_2Si_3Si_4Si_5^2Si_6,\\
\alpha_{212} &= -Cs_1^2Cs_3Cs_5Cs_6Si_2Si_3Si_4Si_6(Cs_2^2Cs_4^2-Cs_4^2Cs_5^2Si_2^2\\
&\quad -Cs_2^2Cs_5^2Si_4^2+Cs_2^2Cs_4^2Si_5^2+Si_2^2Si_4^2Si_5^2),\\
\alpha_{213} &= Cs_1^2Cs_2Cs_6Si_2Si_4Si_5Si_6(Cs_3^2-Si_3^2)(Cs_5^2Si_4^2-Cs_4^2Si_5^2),\\
\alpha_{214} &= -Cs_3Cs_4^2Cs_5Cs_6Si_2Si_3Si_4Si_5^4Si_6,\\
\alpha_{215} &= Cs_3Cs_5^3Cs_6Si_2Si_3Si_4Si_6(Cs_1^2Cs_2^2Cs_4^2-Cs_2^2Cs_4^2Cs_5^2\\
&\quad -Cs_1^2Cs_4^2Si_2^2-Cs_1^2Cs_2^2Si_4^2+Si_2^2Si_5^2+Cs_2^2Si_4^2Si_5^2),\\
\alpha_{216} &= Cs_2Cs_6Si_2Si_4Si_5^3Si_6(Cs_3^2-Si_3^2)(Cs_1^2Cs_4^2-Cs_5^2),\\
\alpha_{217} &= Cs_2Cs_4^2Cs_5^4Cs_6Si_2Si_4Si_5Si_6(Cs_3^2-Si_3^2),\\
\alpha_{218} &= Cs_1^3Cs_2Cs_3Cs_4Cs_6Si_2^2Si_3Si_4^2Si_6,\\
\alpha_{219} &= Cs_1Cs_2Cs_3Cs_4Cs_5^4Cs_6Si_3Si_6(Cs_4^2Si_2^2+Cs_2^2Si_4^2-Si_2^2Si_4^2),\\
\alpha_{220} &= Cs_1Cs_2Cs_3Cs_4Cs_6Si_3Si_5^4Si_6(Cs_4^2Si_2^2-Cs_2^2Si_4^2),\\
\alpha_{221} &= Cs_2^2Cs_3Cs_5Cs_6Si_2Si_3Si_4Si_5^4Si_6,\\
\alpha_{222} &= Cs_2^2Cs_3Cs_4^2Cs_5^5Cs_6Si_2Si_3Si_4Si_6.
\end{aligned}
$$

Example 4.3 We exhibit the main factor MF in Theorem 4.1 in a special case. In the setting $\cos t_1 = \cos t_5 = 1/2$, $\sin t_1 = \sin t_5 = \sqrt{3}/2$, $\cos t_2 = -\cos t_4 = 1/\sqrt{3}, \sin t_2 = \sin t_4 = \sqrt{2/3}$, $\cos t_3 = \sin t_3 = \cos t_6 = -\sin t_6 = 1/\sqrt{2}$, $\cos t_7 = 0, \sin t_7 = 1$, $\cos t_8 = 1, \sin t_8 = 0$, $\cos t_9 = -1, \sin t_9 = 0$, the unitary matrix $U(t_1,\dots,t_9)$ satisfies

$$2U(t_1,\dots,t_9) = \begin{pmatrix} 1 & 1 & 1 & 1\\ 1 & -1 & 1 & -1\\ 1 & -i & -1 & i\\ 1 & i & -1 & -i \end{pmatrix}$$

and so

$$U(t_1,\dots,t_9)\circ\overline{U(t_1,\dots,t_9)} = \frac{1}{4}\begin{pmatrix} 1 & 1 & 1 & 1\\ 1 & 1 & 1 & 1\\ 1 & 1 & 1 & 1\\ 1 & 1 & 1 & 1 \end{pmatrix}.$$

Preserving the above assumption on t_j ($1 \le j \le 6$) and removing the assumption on t_7, t_8, t_9, the condition MF $= 0$ is rewritten as

$$\begin{aligned}
&7\sin t_8 - 2\sin(2t_8) - \sin(3t_8) + 9\sin(t_8 - 2t_9) - 6\sin(3t_8 - 2t_9) - 6\sin(2t_9)\\
&+9\sin(t_8 + 2t_9) + 6\sin(2t_7 - t_8) - 9\sin(2t_7 + t_8) - 6\sin(2t_7 + 2t_8)\\
&+9\sin(2t_7 + 3t_8) + 27\sin(2t_7 + t_8 - 2t_9) - 27\sin(2t_7 + 3t_8 - 2t_9)\\
&-2\sin(2t_7 + 2t_9) - \sin(2t_7 - 3t_8 + 2t_9) - 20\sin(2t_7 - t_8 + 2t_9)\\
&+15\sin(2t_7 + t_8 + 2t_9) + 8\sin(2t_7 + 2t_8 + 2t_9) = 0.
\end{aligned}$$

In the more special situation $t_7 = 0$, the above equation is rewritten as

$$k_8(k_8 - 3k_9)(3 + k_8k_9)(1 + 2k_8k_9 - k_9^2) = 0,$$

by using $k_8 = \tan(t_8/2)$, $k_9 = \tan(t_9/2)$, and so this equation has the following 4 solutions in $k_8 = \tan(t_8/2)$:

$$\tan(t_8/2) = 0, \tan(t_8/2) = 3\tan(t_9/2), \tan(t_8/2) = -3/\tan(t_9/2) = -3\cot(t_9/2)$$

and

$$\tan(t_8/2) = -(1 - k_9^2)/(2k_9) = -\cot(t_9).$$

5 Proof of the main theorem

We shall prove the assertion (I) of Theorem 4.1. For this purpose, we compute the Jacobian determinant of the 9×9 matrix

$$\partial(B_{11}, B_{12}, B_{13}, B_{21}, B_{22}, B_{23})/\partial(t_1, t_2, t_3, t_4, t_5, t_6, t_7, t_8, t_9).$$

We use the notation

$$\begin{aligned}
&J_{1j} = \partial B_{11}/\partial t_j, J_{2j} = \partial B_{12}/\partial t_j, J_{3j} = \partial B_{13}/\partial t_j,\\
&J_{4j} = \partial B_{21}/\partial t_j, J_{5j} = \partial B_{22}/\partial t_j, J_{6j} = \partial B_{23}/\partial t_j,\\
&J_{7j} = \partial B_{31}/\partial t_j, J_{8j} = \partial B_{32}/\partial t_j, J_{9j} = \partial B_{33}/\partial t_j.
\end{aligned}$$

As shown below, a partial triangular property of the Jacobian matrix essentially reduces the computation of the Jacobian determinant to the determinant of a 4×4 submatrix.

By the relation $B_{11} = \cos^2 t_1$, we have

$$J_{11} = -2(\sin t_1)(\cos t_1), J_{12} = J_{13} = J_{14} = J_{15} = J_{16} = J_{17} = J_{18} = J_{19} = 0.$$

By the relation $B_{12} = (\sin^2 t_1)(\cos^2 t_2)$, we find

$$J_{22} = -2(\sin^2 t_1)(\sin t_2)(\cos t_2), J_{23} = J_{24} = J_{25} = J_{26} = J_{27} = J_{28} = J_{29} = 0.$$

By the relation $B_{13} = (\sin^2 t_1)(\sin^2 t_2)(\cos^2 t_3)$, we have

$$J_{33} = -2(\sin^2 t_1)(\sin^2 t_2)(\sin t_3)(\cos t_3), J_{34} = J_{35} = J_{36} = J_{37} = J_{38} = J_{39} = 0.$$

By the relation $B_{21} = (\sin^2 t_1)(\sin^2 t_4)$, we get

$$J_{44} = -2(\sin^2 t_1)(\sin t_4)(\cos t_4), J_{45} = J_{46} = J_{47} = J_{48} = J_{49} = 0.$$

By the relation $B_{31} = (\sin^2 t_1)(\sin^2 t_4)(\cos^2 t_6)$, we obtain

$$J_{76} = -2(\sin^2 t_1)(\sin^2 t_4)(\sin t_6)(\cos t_6), J_{75} = J_{77} = J_{78} = J_{79} = 0.$$

Hence, the Jacobian determinant of the 9×9 matrix is, up to a ± 1 factor, given by

$$2^5(\sin^9 t_1)(\cos t_1)(\sin^3 t_2)(\cos t_2)(\sin t_3)(\cos t_3)(\sin^3 t_4)(\cos t_4)(\sin t_6)(\cos t_6)$$

$$\times \det(\begin{pmatrix} J_{55} & J_{57} & J_{58} & J_{59} \\ J_{65} & J_{67} & J_{68} & J_{69} \\ J_{85} & J_{87} & J_{88} & J_{89} \\ J_{95} & J_{97} & J_{98} & J_{99} \end{pmatrix}).$$

Now, by the relation

$$\begin{aligned} B_{32} &= (\cos^2 t_1)(\cos^2 t_2)(\cos^2 t_4) + (\sin^2 t_2)(\sin^2 t_4)(\cos^2 t_5) \\ &\quad -2(\cos t_1)(\sin t_2)(\cos t_2)(\sin t_4)(\cos t_4)(\cos t_5)(\cos t_8), \end{aligned}$$

we find

$$J_{57} = J_{59} = 0.$$

On the other hand, by the relation

$$\begin{aligned} B_{23} &= (\cos^2 t_1)(\sin^2 t_2)(\cos^2 t_3)(\cos^2 t_4) + (\cos^2 t_2)(\cos^2 t_3)(\sin^2 t_4)(\cos^2 t_5) \\ &\quad +(\sin^2 t_3)(\sin^2 t_4)(\sin^2 t_5) + 2(\cos t_1)(\sin t_2)(\cos^2 t_3)(\sin t_4)(\cos t_4) \cdot \\ &\quad (\cos t_5)(\cos t_8) - 2(\cos t_1)(\sin t_2)(\sin t_3)(\cos t_3)(\sin t_4)(\cos t_4)(\sin t_5) \cdot \\ &\quad (\cos t_9) - 2(\cos t_2)(\sin t_3)(\cos t_3)(\sin^2 t_4)(\sin t_5)(\cos t_5)\cos(t_8 - t_9), \end{aligned}$$

we get

$$J_{67} = 0.$$

Finally, by the relation

$$\begin{aligned} B_{32} = {} & (\cos^2 t_1)(\cos^2 t_2)(\sin^2 t_4)(\cos^2 t_6) + (\sin^2 t_2)[(\cos^2 t_4)(\cos^2 t_5)(\cos^2 t_6) \\ & +(\sin^2 t_5)(\sin^2 t_6) - 2(\cos t_4)(\sin t_5)(\cos t_5)(\sin t_6)(\cos t_6)(\cos t_7)] \\ & +(\cos t_1)(\sin[2t_2])(\sin t_4)(\cos t_6)[(\cos t_4)(\cos t_5)(\cos t_6)(\cos t_8) \\ & -(\sin t_5)(\sin t_6)\cos(t_7 + t_8)], \end{aligned}$$

we obtain

$$J_{89} = 0.$$

Henceforth, the computation of the main factor of the Jacobian $\det(J_{ij})$ is reduced to

$$
\begin{aligned}
\mathrm{MF}_0 &= \det\left(\begin{pmatrix} J_{55} & 0 & J_{58} & 0 \\ J_{65} & 0 & J_{68} & J_{69} \\ J_{85} & J_{87} & J_{88} & 0 \\ J_{95} & J_{97} & J_{98} & J_{99} \end{pmatrix}\right) \\
&= \det\left(\begin{pmatrix} J_{58}J_{65} - J_{55}J_{68} & 0 & J_{69} \\ J_{58}J_{85} - J_{55}J_{88} & J_{87} & 0 \\ J_{58}J_{95} - J_{55}J_{98} & J_{97} & J_{99} \end{pmatrix}\right) \\
&= -J_{55}J_{69}J_{88}J_{97} + J_{55}J_{69}J_{87}J_{98} - J_{55}J_{68}J_{87}J_{99} \\
&\quad -J_{58}J_{69}J_{87}J_{95} + J_{58}J_{69}J_{85}J_{97} + J_{58}J_{65}J_{87}J_{99}.
\end{aligned}
$$

The exact computation of the above polynomial MF_0 shows that this polynomial has the factor

$$
\begin{aligned}
&(\cos t_1)(\sin^2 t_2)(\cos t_2)(\sin t_3)(\cos t_3) \\
&\cdot(\sin^2 t_4)(\cos t_4)(\sin t_5)(\cos t_5)(\sin t_6)(\cos t_6).
\end{aligned}
$$

Thus, the factor C_0 of the Jacobian $J(U)$ given by (4.1) is deduced.The constant -2^7 is arranged so that the expression of the coefficient polynomials α_{pqr} in $Cs_1, Si_1, \ldots, Cs_6, Si_6$ are integers.

Next, we list the non identically vanishing 12 entries of the above 4×4 matrix. For simplicity of notation, we use the symbols $Cs_j = \cos t_j$, $Si_j = \sin t_j$:

$$
\begin{aligned}
J_{55} &= -2Si_2Si_4Si_5\{-Cs_1Cs_2Cs_4Cs_8 + Cs_5Si_2Si_4\}, \\
J_{58} &= 2Cs_1Cs_2Cs_4Cs_5Si_2Si_4Si_8, \\
J_{65} &= -2Si_4[Cs_1Cs_3Cs_4Cs_5Cs_9Si_2Si_3 + Cs_5(Cs_2^2Cs_3^2 - Si_3^2)Si_4Si_5 \\
&\quad +Cs_2Cs_3Cs_8\{Cs_5^2Cs_9Si_3Si_4 + Si_5(Cs_1Cs_3Cs_4Si_2 - Cs_9Si_3Si_4Si_5)\} \\
&\quad +Cs_2Cs_3Si_3Si_4(Cs_5^2 - Si_5^2)Si_8Si_9], \\
J_{68} &= -2Cs_2Cs_3Cs_5Si_4\{Cs_1Cs_3Cs_4Si_2Si_8 - Cs_9Si_3Si_4Si_5Si_8 \\
&\quad +Cs_8Si_3Si_4Si_5Si_9\}, J_{69} = 2Cs_3Si_3Si_4Si_5\{-Cs_2Cs_5Cs_9Si_4Si_8 \\
&\quad +Cs_1Cs_4Si_2Si_9 + Cs_2Cs_5Cs_8Si_4Si_9\}, \\
J_{85} &= -2Si_2[Si_2\{Cs_4^2Cs_5Cs_6^2Si_5 + Cs_4Cs_6Cs_7(Cs_5^2 - Si_5^2)Si_6 - Cs_5Si_5Si_6^2\} \\
&\quad +Cs_1Cs_2Cs_6Si_4(Cs_4Cs_6Si_5 + Cs_5Cs_7Si_6)Cs_8 \\
&\quad -Cs_1Cs_2Cs_5Cs_6Si_4Si_6Si_7Si_8], J_{87} = 2Cs_6Si_2Si_5Si_6\{Cs_4Cs_5Si_2Si_7 \\
&\quad +Cs_1Cs_2Si_4Si_7Cs_8 + Cs_1Cs_2Cs_7Si_4Si_8\}, J_{88} = -2Cs_1Cs_2Cs_6Si_2Si_4\,\cdot \\
&\quad \{-Cs_8Si_5Si_6Si_7 + Cs_4Cs_5Cs_6Si_8 - Cs_7Si_5Si_6Si_8\},
\end{aligned}
$$

$$
\begin{aligned}
J_{95} &= -2[Cs_2^2Cs_3^2\{Cs_4^2Cs_5Cs_6^2Si_5 + Cs_4Cs_6Cs_7(Cs_5^2 - Si_5^2)Si_6 - Cs_5Si_5Si_6^2\} \\
&\quad +Si_3\{Cs_4^2Cs_5Cs_6^2Si_5 + Cs_4Cs_6Cs_7(Cs_5^2 - Si_5^2)Si_6 - Cs_5Si_5Si_6^2\} \\
&\quad +Cs_1Cs_3Cs_6Si_2Si_4Cs_4Cs_5Cs_6Cs_9 + Cs_1Cs_3Cs_6Si_2Si_4Si_5Si_6 \cdot \\
&\quad (-Cs_7Cs_9 + Si_7Si_9) - Cs_2Cs_3\{-Cs_4^2Cs_6^2Si_3(Cs_5^2 - Si_5^2)(Cs_8Cs_9 \\
&\quad +Si_8Si_9) + Cs_4Cs_6Si_5\{Cs_1Cs_3Cs_6Cs_8Si_2Si_4 + 4Cs_5Cs_7Si_3Si_6 \cdot \\
&\quad (Cs_8Cs_9 + Si_8Si_9)\} + Si_6Cs_1Cs_3Cs_5Cs_6Si_2Si_4(Cs_7Cs_8 - Si_7Si_8) \\
&\quad +Si_3Si_6^2(Cs_5^2 - Si_5^2)(Cs_8Cs_9 + Si_8Si_9)\}], \\
J_{97} &= 2Cs_6Si_6[Si_5\{Cs_2^2Cs_3^2Cs_4Cs_5Si_7 - Cs_4Cs_5Si_3^2Si_7 - Cs_1Cs_2Cs_3^2Si_2Si_4 \cdot \\
&\quad (Cs_8Si_7 + Cs_7Si_8)\} + Cs_3Si_3Cs_9\{-Cs_1Cs_5Si_2Si_4Si_7 + Cs_2Cs_4Cs_5^2 \cdot \\
&\quad (Cs_8Si_7 - Cs_7Si_8) - Cs_2Cs_4S_i5^2(Cs_8Si_7 + Cs_7Si_8)\} + Cs_3Si_3Si_9 \cdot \\
&\quad \{-Cs_1Cs_5Cs_7Si_2Si_4 + Cs_2Cs_4Si_5^2(Cs_7Cs_8 - Si_7Si_8) + Cs_2Cs_4Cs_5^2 \cdot \\
&\quad (Cs_7Cs_8 + Si_7Si_8)\}], \\
J_{98} &= 2Cs_2Cs_3[Cs_5\{Cs_1Cs_3Cs_4Cs_6^2Si_2Si_4Si_8 + Si_3Si_5(Cs_4^2Cs_6^2 - Si_6^2) \cdot \\
&\quad (Cs_9Si_8 - Cs_8Si_9)\} + Cs_6Si_6Cs_7\{-Cs_1Cs_3Si_2Si_4Si_5Si_8 \\
&\quad +Cs_4Si_3(Cs_5^2 - Si_5^2)(Cs_9Si_8 - Cs_8Si_9)\} - Cs_6Si_6Si_7\{Cs_1Cs_3Cs_8 \cdot \\
&\quad Si_2Si_4Si_5 + Cs_4Si_3(Cs_8Cs_9 + Si_8Si_9)\}], \\
J_{99} &= -2Cs_3Si_3[Cs_1Cs_4Cs_6^2Si_2Si_4Si_5Si_9 + Cs_2Cs_5Si_5(Cs_4^2Cs_6^2 - Si_6^2) \cdot \\
&\quad (Cs_9Si_8 - Cs_8Si_9) + Cs_6Si_6Cs_7\{Cs_1Cs_5Si_2Si_4Si_9 + Cs_2Cs_4 \cdot \\
&\quad (Cs_5^2 - Si_5^2)(Cs_9Si_8 - Cs_8Si_9)\} + Cs_1Cs_5Cs_6Cs_9Si_2Si_4Si_6Si_7 \\
&\quad -Cs_2Cs_4Cs6Si_6Si_7(Cs_8Cs_9 + Si_8Si_9)].
\end{aligned}
$$

Especially, these 12 entries are degree 1 polynomials in Cs_9, Si_9. A similar property holds for Cs_8, Si_8 and also for Cs_7, Si_7. With respect to $Cs_7, Si_7, Cs_8, Si_8, Cs_9, Si_9$, terms like $Si_7Cs_8Cs_9$ appear in MF, and the degree of the polynomial MF with respect to Cs_9, Si_9 is 2, and so the equation MF $= 0$ is expressed as a quartic equation in $\tan(t_9/2)$ with coefficients expressed by Cs_j, Si_j ($j = 1, \ldots, 8$).

The exact computation of the polynomial MF by substituting the above expressions of J_{ij} $(i = 5, 6, 8, 9, j = 5, 7, 8, 9)$ can be performed by using some computer software like "Mathematica". This computation is performed by a usual lap-top personal computer in a few minutes.

Next, we shall prove the assertion (II) of Theorem 4.1. The exact expression of the polynomial MF in the case $(\cos t_5)(\sin t_5) = 0$ can be easily obtained by computation with some software, like "Mathematica". The criterion for the point U to be a critical point of Φ_4 provided in (I) under the condition $(\cos t_5)(\sin t_5) \neq 0$, is extended to its limit by using the MF since the critical points form a closed subset of $D(4)\backslash U(4)//D(4)$. □

We remark the relation among Theorem 4.1 and Propositions 3.1 and 3.2.

In the case $\sin t_7 = \sin t_9 = 0$, the unitary matrix $U(t_1, \ldots, t_9)$ is not necessarily a critical point of Φ_4. In this situation, the main factor MF of Theorem 4.1 is a constant multiple of

$$(\sin^2 t_1)(\sin t_2)(\cos^2 t_2)(\sin t_3)(\cos t_3)(\sin t_4)(\cos t_5)(\sin^3 t_8)$$
$$\{(\cos t_4)(\cos t_5)(\sin t_6)(\cos t_7) + (\sin t_5)(\cos t_6)\}\{(\cos t_4)(\cos t_5)$$
$$(\cos t_6) - (\sin t_5)(\sin t_6)(\cos t_7)\}.$$

If $(\cos t_4)(\cos t_5)(\cos t_6) - (\sin t_5)(\sin t_6)(\cos t_7) = 0$, then the third row of the unitary matrix $U(t_1, \ldots, t_9)$ is real. Similarly, if $(\cos t_4)(\cos t_5)(\sin t_6)(\cos t_7) + (\sin t_5)(\cos t_6) = 0$, the fourth row is real. So that Proposition 3.2 implies that $U(t_1, \ldots, t_9)$ is a critical point. If $\sin t_7 = \sin t_8 = 0$, the first and second columns of $U(t_1, \ldots, t_9)$ are real, while if $\sin t_8 = \sin t_9 = 0$, the first and second rows of $U(t_1, \ldots, t_9)$ are real. Henceforth, the point $U(t_1, \ldots, t_9)$ is a critical point in these two situations by Proposition 3.2. Theorem 4.1 would provide a method to find critical points of Φ_4.

6 Numerical criterion for a bistochastic matrix to be unistochastic

In Section 1, we posed a question on Dürer's 4×4 magic square. In this section we shall provide a numerical criterion for a given 4×4 bistochastic matrix $B = (B_{ij})_{i,j=1}^4$ to be unistochastic. The principle of the criterion is simple. The matrix B is unistochastic if and only if the equation $B = \Phi_4(U)$ holds for some $U(t_1, t_2, \ldots, t_9)$ with real parameters $t_1, t_2, \ldots, t_9$. Firstly, we remark that a generic 4×4 unitary matrix U with real first row and column has several parameter expressions by real parameters $0 \leq t_1, t_2, \ldots, t_9 \leq 2\pi$. In fact, we can confirm the following 4 facts, used in the sequel.

I The points $(t_1, t_2, t_3, t_4, t_5, t_6, t_7, t_8, t_9) \in \mathbb{R}^9$ and $(-t_1, t_2 + \pi, t_3, t_4 + \pi, -t_5, t_6, t_7, t_8, t_9)$ correspond to the common unitary matrix

$$U(t_1, \ldots t_9) = U(-t_1, t_2 + \pi, \ldots).$$

II The points $(t_1, t_2, t_3, t_4, t_5, t_6, t_7, t_8, t_9) \in \mathbb{R}^9$ and $(t_1, -t_2, t_3 + \pi, -t_4, t_5, t_6 + \pi, t_7, t_8, t_9)$ correspond to the same unitary matrix

$$U(t_1, \ldots, t_9) = U(t_1, -t_2, t_3 + \pi, -t_4, t_5, t_6 + \pi, t_7, t_8, t_9).$$

III The points $(t_1, t_2, t_3, t_4, t_5, t_6, t_7, t_8, t_9) \in \mathbb{R}^9$ and $(t_1, -t_2, t_3 + \pi, t_4, t_5, t_6, t_7, t_8 + \pi, t_9 + \pi)$ correspond to the common unitary matrix

$$U(t_1, \ldots, t_9) = U(t_1, -t_2, \ldots, t_9 + \pi).$$

IV The points $(t_1, t_2, t_3, t_4, t_5, t_6, t_7, t_8, t_9) \in \mathbb{R}^9$ and $(t_1, t_2, t_3, -t_4, t_5, t_6 + \pi, t_7, t_8 + \pi, t_9 + \pi)$ correspond to the common unitary matrix

$$U(t_1, \ldots, t_9) = U(t_1, \ldots, -t_4, \ldots, t_9 + \pi).$$

We assume that a 4×4 matrix U is given and satisfies the conditions

$$U_{11} > 0, U_{12} > 0, U_{13} > 0, U_{14} > 0, U_{21} > 0, U_{31} > 0, U_{41} > 0.$$

Then, there are just 8 quintet systems $0 \leq t_1, t_2, t_3, t_4, t_6 < 2\pi$ satisfying

$$\begin{aligned}
&U_{11} = \cos t_1, U_{12} = (\sin t_1)(\cos t_2), U_{13} = (\sin t_1)(\sin t_2)(\cos t_3),\\
&U_{14} = (\sin t_1)(\sin t_2)(\sin t_3), U_{21} = -(\sin t_1)(\cos t_4),\\
&U_{31} = (\sin t_1)(\sin t_4)(\cos t_6), U_{41} = -(\sin t_1)(\sin t_4)(\sin t_4).
\end{aligned}$$

Denoting such a quintet system by

$$(i) : (T_1, T_2, T_3, T_4, T_6),$$

the remaining 7 quintet systems are given by

$$\begin{aligned}
&(ii) : (T_1, -T_2, T_3 + \pi, -T_4, T_6 + \pi),\\
&(iii) : (T_1, -T_2, T_3 + \pi, T_4, T_6),\\
&(iv) : (T_1, T_2, T_3, -T_4, T_6 + \pi),\\
&(v) : (-T_1, T_2 + \pi, T_3, T_4 + \pi, T_6),\\
&(vi) : (-T_1, -T_2 + \pi, T_3 + \pi, -T_4 + \pi, T_6 + \pi),\\
&(vii) : (-T_1, -T_2 + \pi, T_3 + \pi, T_4 + \pi, T_6),\\
&(viii) : (-T_1, T_2 + \pi, T_3, -T_4 + \pi, T_6 + \pi).
\end{aligned}$$

If a unitary matrix U with positive first row and column is realized by $(T_1, T_2, T_3, t_5, T_6, t_7, t_8, t_9)$, then it is also realized by $(T'_1, T'_2, \dots, T'_6)$ in (ii) -(viii) with suitable (t'_5, t'_7, t'_8, t'_9), by (I),(II),(III),(IV). In fact, the sequence $(t'_5, \dots, t'_9)$ is given by

$$\begin{aligned}
&(i) : (t_5, t_7, t_8, t_9), \quad (ii) : (t_5, t_7, t_8, t_9),\\
&(iii) : (t_5, t_7, t_8 + \pi, t_9 + \pi), \quad (iv) : (t_5, t_7, t_8 + \pi, t_9 + \pi),\\
&(v) : (-t_5, t_7, t_8, t_9), \quad (vi) : (-t_5, t_7, t_8, t_9)\\
&(vii) : (-t_5, t_7, t_8 + \pi, t_9 + \pi), \quad (viii) : (-t_5, t_7, t_8 + \pi, t_9 + \pi),
\end{aligned}$$

We take the limits in the above situation:

$$U_{11} \geq 0, U_{12} \geq 0, \dots, U_{41} \geq 0.$$

Next, we judge whether a given 4×4 bistochastic matrix B is unistochastic or not. We take just one quintet system $(T_1, T_2, T_3, T_4, T_6)$ satisfying

$$\begin{aligned}
&\sqrt{B_{11}} = \cos T_1, \sqrt{B_{12}} = (\sin T_1)(\cos T_2), \sqrt{B_{13}} = (\sin T_1)(\sin T_2)(\cos T_3),\\
&\sqrt{B_{14}} = (\sin T_1)(\sin T_2)(\sin T_3),\\
&\sqrt{B_{21}} = -(\cos T_1)(\cos T_4), \sqrt{B_{31}} = (\sin T_1)(\sin T_4)(\cos T_6),\\
&\sqrt{B_{41}} = -(\sin T_1)(\sin T_4)(\sin T_6).
\end{aligned}$$

We solve numerically the simultaneous equations in $0 \le t_5, t_7, t_8, t_9 < 2\pi$:

$$B_{ij} = |U(T_1, T_2, T_3, T_4, t_5, T_6, t_7, t_8, t_9)|^2$$

for $(i, j) = (2, 2), (2, 3), (3, 2), (3.3)$. If one real solution (t_5, t_7, t_8, t_9) exists, then B is unistochastic. If there is no real solution, then B is not unistochastic.

We have other transformations on the points $(t_1, t_2, \ldots, t_9)$, which yield a common point $U(t_1, t_2, \ldots, t_9)$. By exact computations, we can confirm the following.

(V) For a fixed $(t_1, t_2, t_3, t_4, t_6) \in \mathbb{R}^5$, the two points $(t_5, t_7, t_8, t_9) \in \mathbb{R}^4$ and $(-t_5 + \pi, t_7 + \pi, t_8 + \pi, t_9)$ correspond to the common unitary matrix $U(t_1, t_2, \ldots, t_9)$.

(VI) For a fixed $(t_1, t_2, t_3, t_4, t_6) \in \mathbb{R}^5$, the two points $(t_5, t_7, t_8, t_9) \in \mathbb{R}^4$ and $(-t_5, t_7 + \pi, t_8, t_9 + \pi)$ correspond to the common unitary matrix $U(t_1, t_2, \ldots, t_9)$.

The following fact is also useful to study the map Φ_4.

(VII) The point $(t_1, t_2, t_3, t_4, t_5, t_6, -t_7, -t_8, -t_9) \in \mathbb{R}^9$ corresponds to the complex conjugate of $U(t_1, \ldots, t_6, t_7, t_8, t_9)$, and so

$$\Phi_4(U(t_1, \ldots, t_6, -t_7, -t_8, -t_9)) = \Phi_4(U(t_1, \ldots, t_9)).$$

By (i)-(viii) and (I)-(VII), we may assume that $0 < t_j < \pi/2$ for $j = 1, 2, 3$ and $\pi/2 < t_4 < \pi$, $-\pi/2 < t_6 < 0$ to examine whether B is unistochastic or not. In a generic case, there are 8 real solutions (t_5, t_7, t_8, t_9), if real solutions exist. If we restrict solutions as $0 < t_5 < \pi/2$, the solutions are restricted as (t_7, t_8, t_9) and $(-t_7, -t_8, -t_9)$.

Next,we answer our question concerning Dürer's magic square.

Example 6.1 The 4×4 doubly stochastic matrix B obtained by the normalization of Dürer's magic square is not unistochastic.

In fact, we can show that there is no unitary matrix $U = U(t_1, \ldots, t_9) \in D(4)\backslash U(4)/D(4)$ satisfying

$$U(t_1, \ldots, t_4) \circ \overline{U(t_1, \ldots, t_4)} = \begin{pmatrix} 16/34 & 3/34 & 2/34 & 13/34 \\ 5/34 & 10/34 & 11/34 & 8/34 \\ 9/34 & 6/34 & 7/34 & 12/34 \\ 4/34 & 15/34 & 14/34 & 1/34 \end{pmatrix}.$$

Firstly, we solve numerically the simultaneous equations:

$$U_{11} = \cos t_1 = \sqrt{16/34}, U_{12} = (\sin t_1)(\cos t_2) = \sqrt{3/34},$$
$$U_{13} = (\sin t_1)(\sin t_2)(\cos t_3) = \sqrt{2/34},$$

$U_{14} = (\sin t_1)(\sin t_2)(\cos t_3) = \sqrt{13/34}$,
$U_{21} = -(\sin t_1)(\cos t_4) = \sqrt{5/34}, U_{31} = (\sin t_1)(\sin t_4)(\cos t_6) = \sqrt{9/34}$,
$U_{41} = (\sin t_1)(\sin t_4)(\sin t_6)$.

We use rational parameters $k_1, k_2, k_3, k_4, k_6 \in \mathbb{R}$ by the relations $k_1 = \tan(t_1/2)$, so that

$$\cos t_1 = \frac{1-k_1^2}{1+k_1^2}, \sin t_1 = \frac{2k_1}{1+k_1^2}.$$

Similarly, we set

$$\cos t_2 = \frac{1-k_2^2}{1+k_2^2}, \sin t_2 = \frac{2k_2}{1+k_2^2}, \cos t_3 = \frac{1-k_3^2}{1+k_3^2}, \sin t_3 = \frac{2k_3}{1+k_3^2},$$
$$\cos t_4 = -\frac{1-k_4^2}{1+k_4^2}, \sin t_4 = \frac{2k_4}{1+k_4^2}, \cos t_6 = \frac{1-k_6^2}{1+k_6^2}, \sin t_6 = -\frac{2k_6}{1+k_6^2}.$$

The simultaneous equations have 8 quintets of real solutions. One of these systems of solutions is numerically given by

$$k_1 = 0.4315595002904898, \quad k_2 = 0.6482315195103737,$$
$$k_3 = 0.6819400407827797, k_4 = 0.5565231378830596,$$
$$k_6 = 0.3027756377319944.$$

By the above facts (i) -(viii), we may restrict our attention to this solution. Based on this numerical solution we solve the simultaneous equations in t_5, t_7, t_8, t_9:

$$\begin{aligned}
B_{22} &= Cs_1^2Cs_2^2Cs_4^2 + Si_2^2Si_4^2(\cos^2 t_5) - 2Cs_1Cs_2Si_2Cs_4Si_4(\cos t_5)(\cos t_8) = \frac{10}{34},\\
B_{23} &= Cs_1^2Si_2^2Cs_3^2Cs_4^2 + Cs_2^2Cs_3^2Si_4^2(\cos^2 t_5) + Si_3^2Si_4^2(\sin^2 t_5) + 2Cs_1Cs_2Si_2 \cdot\\
&\quad Cs_3^2Cs_4Si_4(\cos t_5)(\cos t_8) - 2Cs_1Si_2Cs_3Si_3Cs_4Si_4(\sin t_5)(\cos t_9)\\
&\quad -2Cs_2Cs_3Si_3Si_4^2(\cos t_5)(\sin t_5)(\cos[t_8 - t_9]) = \frac{11}{34},\\
B_{32} &= Cs_1^2Cs_2^2Si_4^2Cs_6^2 + Si_2^2Si_6^2(\sin^2 t_5) + Si_2^2Cs_4^2Cs_6^2(\cos^2 t_5) + 2Cs_1Cs_2 \cdot\\
&\quad Si_2Cs_4Si_4Cs_6^2(\cos t_5)(\cos t_8) - 2Si_2^2Cs_4Cs_6Si_6(\cos t_5)(\sin t_5)(\cos t_7)\\
&\quad -2Cs_1Cs_2Si_2Si_4Cs_6Si_6(\sin t_5)(\cos[t_7 + t_8]) = \frac{6}{34},\\
B_{33} &= Cs_1^2Si_2^2Cs_3^2Si_4^2Cs_6^2 - 2Cs_1Cs_2Si_2Cs_3^2Cs_4Si_4Cs_6^2(\cos t_5)(\cos t_8)\\
&\quad +2Cs_1Si_2Cs_3Si_3Cs_4Si_4Cs_6^2(\sin t_5)(\cos t_9) + Cs_2^2Cs_3^2Cs_4^2Cs5^2Cs_6^2(\cos^2 t_5)\\
&\quad +Si_3^2Cs_4^2Cs_6^2(\sin^2 t_5) + Si_3^2Si_6^2(\cos^2 t_5) + Cs_2^2Cs_3^2Si_6^2 \cdot\\
&\quad (\sin^2 t_5) + 2Cs_1Si_2Cs_3Si_4Cs_6Si_6\{Cs_2Cs_3(\sin t_5)(\cos[t_7 + t_8])\\
&\quad +Si_3(\cos t_5)(\cos[t_7 + t_9])\} - 2Cs_2Cs_3Si_3(Cs_4^2Cs_6^2 - Si_6^2)(\cos t_5) \cdot\\
&\quad (\sin t_5)(\cos[t_8 - t_9]]) - 2Cs_2Cs_3Si_3Cs_4Cs_6Si_6(\cos^2 t_5)(\cos[t_7 + t_9 - t_8])\\
&\quad +2Cs_2Cs_3Si_3Cs_4Cs_6Si_6(\sin^2 t_5)(\cos[t_7 + t_8 - t_9]) = \frac{7}{34}.
\end{aligned}$$

By using the rational parameters k_5, k_7, k_8, k_9:

$$\cos t_j = \frac{1-k_j^2}{1+k_j^2}, \quad \sin t_j = \frac{2k_j}{1+k_j^2},$$

we solve the above simultaneous equations in the field of complex numbers, under the assumptions $k_1 = 0.431559...$, $\ldots$, $k_6 = 0.302775$. The equations have 8 distinct (numerical) solutions, none of which being real, like the following one:

$$k_5 = 0.00602669 + 1.97721i, k_7 = 0.630428 + 0.776301i,$$

$$k_8 = 0.0010087 - 0.759703i, k_9 = 0.222319 - 0.975767i.$$

Remark 6.2 The German artist Albrecht Dürer (1471-1528) published mathematical works in the latest years of his life. Some authors studied his mathematical contributions. We mention Fettis' paper [6], where his contributions to the theory of plane curves is analized, and Hughes' article [11] on his contributions to the approximate construction of regular polygons.

The following 4×4 unistochastic matrix is the normalization of a magic square

$$B = \begin{pmatrix} 5/13 & 4/13 & 3/13 & 1/13 \\ 2/13 & 4/13 & 3/13 & 4/13 \\ 4/13 & 2/13 & 5/13 & 2/13 \\ 2/13 & 3/13 & 2/13 & 6/13 \end{pmatrix}.$$

We can find a unitary matrix $U = U(t_1, \ldots, t_9)$ satisfying $\Phi_4(U) = B$ by a numerical method.

7 Examples of a boundary point and of an inner point of the set $\mathbf{U}_4$

We shall provide an example of a boundary point of $\mathbf{U}_4$, and an example of an inner point of $\mathbf{U}_4$ corresponding to the critical points of Φ_4.

Example 7.1 Let $\cos t_1 = 1/2$, $\sin t_1 = \sqrt{3}/2$, $\cos t_2 = -\cos t_4 = \cos t_7 = 1/\sqrt{3}$, $\sin t_2 = \sin t_4 = \sin t_= \sqrt{2/3}$, $\cos t_3 = \cos t_6 = \cos t_5 = \cos t_8 = 1/\sqrt{2}$, $\sin t_3 = -\sin t_6 = \sin t_5 = 1/\sqrt{2}$. Then the equation MF $= 0$ in Theorem 4.1 is expressed as

$$F(t_9) = (3 - 2\sqrt{2}) + (8 - 2\sqrt{2})\cos(2t_9) + (-5 + 10\sqrt{2})\sin(2t_9)$$

$$= \frac{1}{1+\tan^2(t_9)}\{-4\tan^2 t_9 + (-10 + 20\sqrt{2})\tan t_9 + (11 - 4\sqrt{2})\} = 0.$$

We can solve this equation as an algebraic equation in $\tan t_9$, and the four real solutions are:

$$(\cos t_9)_1 = \frac{5}{K}, (\sin t_9)_1 = \frac{-5+10\sqrt{2}-2\sqrt{70-30\sqrt{2}}}{K}$$

with

$$K = [530 - 220\sqrt{2} + (-80+20\sqrt{2})\sqrt{35-15\sqrt{2}}\ ]^{1/2},$$

$$(\cos t_9)_2 = \frac{5}{\tilde{K}}, (\sin t_9)_2 = \frac{-5+10\sqrt{2}+2\sqrt{70-30\sqrt{2}}}{\tilde{K}},$$

and

$$\tilde{K} = [530 - 220\sqrt{2} + (80-20\sqrt{2})\sqrt{35-15\sqrt{2}}\ ]^{1/2},$$

$$(\cos t_9)_3 = -(\cos t_9)_1, (\sin t_9)_3 = -(\sin t_9)_1,$$
$$(\cos t_9)_4 = -(\cos t_9)_2, (\sin t_9)_4 = -(\sin t_9)_2.$$

Approximate values of these solutions are

$$(\cos t_9)_1 \sim 0.96494286, \quad (\sin t_9)_1 \sim -0.26246005,$$

$$(\cos t_9)_2 \sim 0.24666287, \quad (\sin t_9)_2 \sim 0.96910135.44.$$

The corresponding two bistochastic matrices $B = (B_{ij})$ have entries

$$B_{11} = B_{12} = B_{13} = B_{21} = B_{31} = \frac{1}{4},$$

$$B_{22} = \frac{13}{36} \sim 0.36111111, \quad B_{32} = \frac{5-2\sqrt{2}}{36} \sim 0.060321469$$

commonly for the four solutions, and

$$\begin{aligned} B_{23} &= \frac{1}{36}(7 - 2\sqrt{6}(\sin t_9)_j), \\ B_{33} &= \frac{1}{36}\{11 + \sqrt{2} - (2\sqrt{3}+\sqrt{6})(\cos t_9)_j + (4\sqrt{3}+\sqrt{6})(\sin t_9)_j\} \end{aligned}$$

for $j = 1, 2$. Approximate values of $(B_{23})_j, (B_{33})_j$ are

$$(B_{23})_1 \sim 0.23016073, (B_{33})_1 \sim 0.11796295,$$

$$(B_{23})_2 \sim 0.062566455, (B_{33})_2 \sim 0.55676347.$$

At the two critical points $U(t_1, \ldots, t_8, (t_9)_j)$ $(j = 1, 2)$, the rank of $d\Phi_4$ is commonly 8. With respect to the inner product $\langle H_1, H_2 \rangle = \mathrm{tr}(H_1 H_2)$ of two 4×4 real matrices, the normal vectors N_j orthogonal to the tangent vectors $d\Phi_4(X)$ for $X \in M_4(\mathbb{C})$, such that $X + X^* = 0$, are (approximately up to a factor) given by

$$N_1 = (dB_{11}, dB_{12}, dB_{13}, dB_{21}, dB_{22}, dB_{23}, dB_{31}, dB_{32}, dB_{33})$$

$$\sim (1.0937850, 1.4859549, 1.5016907, 1.229821, 1.5551168,$$
$$1.5858860, 1.3784921, 0.870277261, 1)$$

and

$$N_2 = (dB_{11}, dB_{12}, dB_{13}, dB_{21}, dB_{22}, dB_{23}, dB_{31}, dB_{32}, dB_{33})$$
$$\sim (-0.16851123, 2.6998517, 4.3188399, -1.3035747,$$
$$1.0939334, 6.6567463, -2.0949601, -5.5329685, 1).$$

We shall judge whether the bistochastic matrix $B = (B_{k\ell})$ corresponding to $(t_9)_j$, $j = 1, 2$, is a boundary point or an inner point of $\mathbf{U}_4$ in the space of 4×4 bistochastic matrices. For this purpose, we use the criterion: (i) if both $B + \epsilon N_j$ and $B - \epsilon N_j$ are unistochastic matrices for a sufficiently small $\epsilon > 0$, then B is an inner point; (ii) if one of $B \pm \epsilon N_j$ is unistochastic and the other is not unistochastic, then B is a boundary point. As a practical method, we use the numerical approach in Section 4. For the matrix B corresponding to $(t_9)_1$ for $(\sin t_9)_1 \sim -0.262460$, we take $\epsilon = 1/100$. For the matrix B corresponding to $(t_9)_2$, we take $\epsilon = 1/200$. The numerical criterion shows that the matrix B is a boundary point for $(t_9)_1$,while the other matrix B for $(t_9)_2$ is an inner point. In fact, $B + N_1/100$ is unistochastic and $B - N_1/100$ is not unistochastic. The bistochastic matrices B corresponding to $(t_9)_3$ and $(t_9)_4$ can be similarly treated.

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