Nihonkai Math. J.
Vol.7 (1996), 83-100

Set of 3×3 Orthostochastic Matrices

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Abstract. *A 3×3 matrix $(a_{i,j})$ is said to be orthostochastic if there exists a 3×3 unitary matrix $(u_{i,j})$ such that $a_{i,j}=|u_{i,j}|^2$ for every $1\leq i,j\leq 3$. Denote by O_3 the set of all 3×3 orthostochastic matrices. In this paper, the author characterizes the set O_3 and applies it to the determination of certain generalized numerical ranges of 3×3 complex diagonal matrices.*

1. Introduction and Results.

Let A_n be the affine space of all real $n\times n$ matrices whose all row and column sums are equal to 1. A matrix $(a_{i,j})\in A_n$ is said to be doubly stochasic if its entries are nonnegative. Denote by D_n the compact convex set of all $n\times n$ doubly stochastic matrices. An element $(a_{i,j})\in D_n$ is said to be orthostochasic if there exists an $n\times n$ unitary matrix $(u_{i,j})$ such that $a_{i,j}=|u_{i,j}|^2$ for every $1\leq i,j\leq n$. Denote by O_n the compact set of all $n\times n$ orthostochastic matrices. It is clear that $D_2=O_2=\{g\circ g: g\in SO(2)\}$ where $\circ$ denotes the Hadamard (Schur, entrywise) product. In this paper we treat the set O_3. Define two 3×3 matrices C_0, U_0 by

$$C_0=\begin{pmatrix}1/3 & 1/3 & 1/3\\ 1/3 & 1/3 & 1/3\\ 1/3 & 1/3 & 1/3\end{pmatrix}, \tag{1.1}$$

$$U_0=\sqrt{1/3}\begin{pmatrix}1 & 1 & 1\\ 1 & \omega & \omega^2\\ 1 & \omega^2 & \omega^4\end{pmatrix} \tag{1.2}$$

where $\omega=\exp(i2\pi/3)$. Then U_0 is a unitary matrix and $U_0\circ\overline{U_0}=C_0$. Thus C_0 is an element of O_3. The structure of the set O_3 is deeply related with properties of the

$c-$numerical range of a 3×3 complex diagonal matrix. Define a linear functional Ψ on the set $M_3(\mathbf{C})$ by

$$\Psi(\begin{pmatrix} x_{11} & x_{12} & x_{13} \\ x_{21} & x_{22} & x_{23} \\ x_{31} & x_{32} & x_{33} \end{pmatrix}) = x_{11} + x_{12} + x_{13} + x_{21} + x_{22} + x_{23} + x_{31} + x_{32} + x_{33}.$$

For 3×3 complex matrices C, A, define $W(C, A)$ by the relation

$$W(C, A) = \{tr(A\ U\ B\ U^*) : U \text{ is a 3 by 3 unitary matrix}\}. \tag{1.3}$$

The set $W(C, A)$ is said to be the *C-numerical range* of A. We easily see that $W(C, A) = W(A, C)$.

In the case $C = \mathrm{diag}\{c_1, c_2, c_3\}$ with $c = (c_1, c_2, c_3) \in \mathbf{C}^3$, the range $W(C, A)$ is denoted by $W_c(A)$. We easily obtain the relation

$$W_c(A) = \{c_1(A\xi_1, \xi_1) + c_2(A\xi_2, \xi_2) + c_3(A\xi_3, \xi_3) : \{\xi_1, \xi_2, \xi_3\} \text{ is an orthonormal basis of } \mathbf{C}^3\}. \tag{1.4}$$

$W_c(A)$ is said to be the *c-numerical range* of A. In the case $A = \mathrm{diag}\{a_1, a_2, a_3\}$ with $(a_1, a_2, a_3) \in \mathbf{C}^3$, we easily obtain the equation

$$W_c(\mathrm{diag}\{a_1, a_2, a_3\}) = \{\Psi(\begin{pmatrix} c_1a_1 & c_1a_2 & c_1a_3 \\ c_2a_1 & c_2a_2 & c_2a_3 \\ c_3a_1 & c_3a_2 & c_3a_3 \end{pmatrix} \circ X) : X \in O_3\}. \tag{1.5}$$

In [1] , Y. H. Au-Yeung and Y. T. Poon gave a necessary and sufficient condition for $(a_{i,j}) \in D_3$ to be orthostochastic. They also proved that 1) $\lambda C_0 + (1 - \lambda)(a_{i,j}) \in O_3$ for every $0 \leq \lambda \leq 1, (a_{i,j}) \in O_3$ and 2) $(\lambda/3)(c_1 + c_2 + c_3)(a_1 + a_2 + a_3) + (1 - \lambda)z \in W_c(\mathrm{diag}\{a_1, a_2, a_3\})$ for every $0 \leq \lambda \leq 1, z \in W_c(\mathrm{diag}\{a_1, a_2, a_3\})$.

One aim of this paper is to give a concrete parametrizations of O_3 and its boundary ∂O_3. Since each matrix $(a_{i,j}) \in A_3$ satisfies the conditions $a_{13} = 1 - a_{11} - a_{12}, a_{23} = 1 - a_{21} - a_{22}, a_{31} = 1 - a_{11} - a_{21}$, $a_{32} = 1 - a_{12} - a_{22}, a_{33} = a_{11} + a_{12} + a_{21} + a_{22} - 1$, we parametrize the entries $a_{11}, a_{12}, a_{21}, a_{22}$ of $(a_{i,j}) \in O_3$. We recall that a concrete parametrization of the rotation group $SO(3)$ is given by Eulerian angles, in other words, by using the Cartan decomposition $G = K\ A\ K$ of the group $G = SO(3)$ where K and A are isomorphic to $SO(2)$ (cf.[3] p.7). We prove the following theorem.

Theorem 1.1. *The compact set O_3 of all 3×3 orthostochastic matrices coincides with the set*

$$\{\lambda C_0 + (1-\lambda) g \circ g : 0 \leq \lambda \leq 1, g \in SO(3)\}, \tag{1.6}$$

and hence the set O_3 is parametrized as the following :

$$O_3 = \{ \begin{pmatrix} a_{11} & a_{12} & \cdot \\ a_{21} & a_{22} & \cdot \\ \cdot & \cdot & \cdot \end{pmatrix} \in A_3 : a_{11} = (\lambda/3) + (1-\lambda)x, a_{12} = (\lambda/3) + (1-\lambda)(1-x)t,$$

$$a_{21} = (\lambda/3) + (1-\lambda)(1-x)s,\ a22 = (\lambda/3) + (1-\lambda)\{x\ t\ s + (1-t)(1-s) +$$

$$2\epsilon\sqrt{x\ t\ (1-t)\ s\ (1-s)}\}, 0 \leq \lambda, x, t, s \leq 1,\ \epsilon \in \{+1, -1\}\}. \tag{1.7}$$

Another aim of this paper is to give a characterization of the range $W(C, A)$ for complex diagonal 3×3 matrices C, A which is more quantitative than that of [1]. For this aim, we prove the following theorem.

Theorem 1.2. *Suppose that C and A are 3 by 3 complex diagonal matrices. Then the equation*

$$W(C, A) = \{tr(C\ g\ A\ g^t) : g \in SO(3)\} \tag{1.8}$$

holds, where g^t denotes the transpose of the matrix g.

We shall determine the range $W(C, A)$ for 3×3 complex diagonal matrices A, C. If the eigenvalues a_1, a_1, a_3 of A lie on a straight line on the complex plane, then by results of [1] and [5], the range $W(C, A)$ is convex and coincides with the convex hull of the 6 points

$$\{a_1 c_{\sigma(1)} + a_2 c_{\sigma(2)} + a_3 c_{\sigma(3)} : \sigma \in S_3\}. \tag{1.9}$$

Therefore we may assume that $a_i \neq a_j$ for $1 \leq i < j \leq 3$ and the three points a_1, a_2, a_3 lie on a circle with radius $r \in (0, \infty)$ on the complex plane. Since $W(C, A) = W(A, C)$, we may assume that the eigenvalues c_1, c_2, c_3 of C also lie on a circle. By using rotations, translations and dilations, we may assume that $A = \mathrm{diag}\{a_1, a_2, a_3\}$ and $C = \mathrm{diag}\{c_1, c_2, c_3\}$ are elements of the group $SU(3)$ satisfying $a_i \neq a_j, c_i \neq c_j$ for $1 \leq i < j \leq 3$. To state the figure of the range $W(C, A)$, we introduce an algebraic curve. Define a simple closed curve Γ on the plane $\mathbf{C}$ by the equation

$$\Gamma = \{2 \ \exp(it) + \exp(-2\ i\ t) : 0 \leq t \leq 2\pi\}$$

$$= \{z = x + iy : (x, y) \in \mathbf{R}^2, (x^2 + y^2)^2 + 24xy^2 - 8x^3 + 18(x^2 + y^2) - 27 = 0\}. \tag{1.10}$$

The curve Γ is called a *deltoid*. We denote by D the closed domain surrounded by Γ:

$$D = \{2\ r\ \exp(it) + r\ \exp(-2\ i\ t) : 0 \leq t \leq 2\pi, 0 \leq r \leq 1\}.$$

Then we have the equation

$$D = \{\exp(is) + \exp(it) + \exp(iu) : (s, t, u) \in \mathbf{R}^3, s + t + u \equiv 0 \ \mathrm{mod}.2\pi\}. \tag{1.11}$$

For the point $z = \exp(is) + \exp(it) + \exp(iu)$ with $(s, t, u) \in \mathbf{R}^3, s + t + u \equiv 0 \ \mathrm{mod}.2\pi$ to belong the boundary Γ, it is necessary and sufficient that the condition

$$(\exp(it) - \exp(is))(\exp(it) - \exp(iu))(\exp(is) - \exp(iu)) = 0 \tag{1.12}$$

holds. We have the following theorem.

Theorem 1.3. *Suppose that* $A = \mathrm{diag}\{a_1, a_2, a_3\}, C = \mathrm{diag}\{c_1, c_2, c_3\}$ *are elements of the group* $SU(3)$ *with* $a_i \neq a_j, c_i \neq c_j$ *for* $1 \leq i < j \leq 3$. *Set*

$$V_+ = \{a_1c_1 + a_2c_2 + a_3c_3, a_1c_2 + a_2c_3 + a_3c_1, a_1c_3 + a_2c_1 + a_3c_2\},$$

$$V_- = \{a_1c_1 + a_2c_3 + a_3c_2, a_1c_3 + a_2c_2 + a_3c_1, a_1c_2 + a_2c_1 + a_3c_3\}.$$

Then the boundary $\partial W(A, C)$ *of the range* $W(A, C)$ *in the plane* $\mathbf{C}$ satisfies the inclusion

$$\partial W(A, C) \subset \Gamma \cup \{tz_1 + (1-t)z_2 : 0 \leq t \leq 1, z_1 \in V_+, z_2 \in V_-\}. \tag{1.13}$$

Remark. *We assume that the assumptions of Theorem 1.3 hold. Then, for every* $z_1 \in V_+, z_2 \in V_-$ *the straight line* $L(z_1, z_2)$ *passing through* z_1, z_2, *i.e.,*

$$L(z_1, z_2) = \{tz_1 + (1-t)z_2 : t \in \mathbf{R}\}$$

is a tangent line of the deltoid Γ *at some non-singular point of* Γ *or at one of 3 cusps of* Γ.

2. Parametrization of the set of 3 x 3 orthostochastic matrices.

In this section we shall prove Theorems 1.1 and 1.2. First we observe the condition (*) of Au-Yeung and Poon in [1, p.70]. We use the following equation for real numbers a, b, c:

$$a^4 + b^4 + c^4 - 2a^2b^2 - 2b^2c^2 - 2c^2a^2 = (a+b+c)(a-b-c)(b-c-a)(c-a-b). \tag{2.1}$$

The following simultaneous inequalitities for non-negative real numbers a, b, c,

$$a \leq b + c, \ (2.2)\ b \leq c + a, \ (2.3)\ c \leq a + b \ (2.4)$$

are equivalent to the inequality

$$a^4 + b^4 + c^4 - 2a^2b^2 - 2b^2c^2 - 2c^2a^2 \leq 0. \tag{2.5}$$

We define a polynomial function F on A_3 by

$$F\left(\begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix}\right)$$

$$= a_{11}^2\, a_{12}^2 + a_{21}^2\, a_{22}^2 + a_{31}^2\, a_{32}^2 - 2\, a_{11}\, a_{12}\, a_{21}\, a_{22} - 2a_{11}\, a_{12}\, a_{31}\, a_{32} - 2a_{21}\, a_{22}\, a_{31}\, a_{32}. \quad (2.6)$$

Then the function F is expressed as the following :

$$F = F(a_{11}, a_{12}, a_{21}, a_{22})$$

$$= a_{11}^2\, a_{22}^2 + a_{12}^2\, a_{21}^2 - 2\, a_{11}\, a_{12}\, a_{21}\, a_{22} - 2\, a_{11}\, a_{22}(a_{11} + a_{22}) - 2\, a_{12}a_{21}(a_{12} + a_{21})$$

$$-2\,(a_{11}\, a_{12}\, a_{21} + a_{11}\, a_{12}\, a_{22} + a_{11}\, a_{21}\, a_{22} + a_{12}\, a_{21}\, a_{22}) + a_{11}^2 + a_{12}^2 + a_{21}^2 + a_{22}^2$$

$$+2\,(a_{11}\, a_{12} + a_{11}\, a_{21} + a_{12}\, a_{22} + a_{21}\, a_{22} + 2\, a_{11}\, a_{22} + 2\, a_{12}\, a_{21})$$

$$-2(a_{11} + a_{12} + a_{21} + a_{22}) + 1. \quad (2.7)$$

Lemma 2.1. (cf.[1], Theorem 3) If $(a_{r,s}) \in O_3$ and $0 \leq \alpha < 1$, then the matrix $\alpha \cdot (a_{r,s}) + (1-\alpha) \cdot C_0$ satisfies the strict inequality

$$\sqrt{(\alpha\; a_{\ell,j} + (1-\alpha)/3)\;(\alpha\; a_{\ell,k} + (1-\alpha)/3)}$$

$$< \sum_{1 \leq i \leq 3, i \neq \ell} \sqrt{(\alpha\; a_{i,j} + (1-\alpha)/3)\;(\alpha\; a_{i,k} + (1-\alpha)/3)} \quad (2.8)$$

for every $1 \leq \ell \leq 3, 1 \leq j \neq k \leq 3$.

Proof For simplicity we assume that $j = 1, k = 2$. By the condition $0 \leq \alpha < 1$, the inequality in [1, p.73, lines 3,4] is replaced by strict one:

$$\sum_{1 \leq p \leq 3, p \neq \ell} (\alpha\ a_{p,1} + (1-\alpha)/3)\ (\alpha\ a_{p,2} + (1-\alpha)/3)$$

$$+2\ \sqrt{(\alpha\ a_{p,1} + (1-\alpha)/3)}\ \sqrt{(\alpha\ a_{p,2} + (1-\alpha)/3)}$$

$$\cdot \sqrt{(\alpha\ a_{q,1} + (1-\alpha)/3)}\ \sqrt{(\alpha\ a_{q,2} + (1-\alpha)/3)}$$

$$> \sum_{1 \leq p \leq 3, p \neq \ell} [[\alpha^2\ a_{p,1}\ a_{p,2} + \{(\alpha\ (1-\alpha))/3\}(a_{p,1} + a_{p,2}) + \{(1-\alpha)/3\}^2]$$

$$+2\ \alpha^2\ \sqrt{a_{p,1}\ a_{p,2}\ a_{q,1}\ a_{q,2}}].$$

Here $1 \leq p < q \leq 3, p \neq \ell, q \neq \ell$. The proof of Lemma 2.4 is complete.

For every $(b_{11}, b_{12}, b_{21}, b_{22}) \in \mathbf{R}^4 \setminus \{(0,0,0,0)\}$, we set

$$B(b_{11}, b_{12}, b_{21}, b_{22}) = \begin{pmatrix} b_{11} & b_{12} & -(b_{11} + b_{12}) \\ b_{21} & b_{22} & -(b_{21} + b_{22}) \\ -(b_{11} + b_{21}) & -(b_{12} + b_{22}) & b_{11} + b_{12} + b_{21} + b_{22} \end{pmatrix}.$$

Then, by [1] Theorem 1 and [1] Theorem 3, there exits $0 < \lambda = \lambda(b_{11}, b_{12}, b_{21}, b_{22}) < \infty$ such that

$$\{t \in \mathbf{R} : t \geq 0, C_0 + t\ B(b_{11}, b_{12}, b_{21}, b_{22}) \in O_3\} = \{t \in \mathbf{R} : 0 \leq t \leq \lambda\}. \qquad (2.9)$$

Thus we obtain the following proposition by combining Lemma 2.1 and Theorems 1 and 3 of [1].

Proposition 2.2. *Suppose that F is the polynomial function on the space A_3 given by (2.6). Then the sets O_3 and ∂O_3 are characterized as the following:*

$$O_3 = \{ \begin{pmatrix} a_{11} & a_{12} & \cdot \\ a_{21} & a_{22} & \cdot \\ \cdot & \cdot & \cdot \end{pmatrix} \in D_3 : F(a_{11}, a_{12}, a_{21}, a_{22}) \leq 0\} \tag{2.10}$$

and

$$\partial O_3 = \{ \begin{pmatrix} a_{11} & a_{12} & \cdot \\ a_{21} & a_{22} & \cdot \\ \cdot & \cdot & \cdot \end{pmatrix} \in D_3 : F(a_{11}, a_{12}, a_{21}, a_{22}) = 0\}. \tag{2.11}$$

Next we shall prove that $\partial O_3 = \{g \circ g : g \in SO(3)\}$.

Proposition 2.3. *Every point of $\{g \circ g : g \in SO(3)\}$ belongs to the boundary of O_3 in the space A_3.*

Proof The set $\{g \circ g : g \in SO(3)\}$ is represented as the following (cf.[3], p.7):

$$\{g \circ g : g \in SO(3)\} = \{ \begin{pmatrix} a_{11} & a_{12} & \cdot \\ a_{21} & a_{22} & \cdot \\ \cdot & \cdot & \cdot \end{pmatrix} \in A_3 : a_{11} = u_1^2,\ a_{12} = (1-u_1^2)(1-u_2^2),$$

$$a_{21} = (1-u_1^2)(1-u_3^2),\ a_{22} = u_1^2\,(1-u_2^2)(1-u_3^2) + u_2^2\,u_3^2 - 2\,u_1\,u_2\,u_3\,v_2\,v_3$$

$$\text{for some } u_1, u_2, u_3, v_1, v_2, v_3 \in \mathbf{R} \text{ satisfying } u_1^2 + v_1^2 = u_2^2 + v_2^2 = u_3^2 + v_3^2 = 1\}. \tag{2.12}$$

In the expression of F, we substitute $a_{i,j}$ $(1 \leq i, j \leq 2)$ by their expressions appearing in (2.11):

$$(1/4)F(a_{i,j}\ (u_1,u_2,u_3,v_1,v_2,v_3))$$

$$= (u_1^2\ u_2^2\ u_3^2 - 2u_1^4u_2^2u_3^2 + u_1^6u_2^2u_3^2)v_2^2\ v_3^2 - (u_1^2\ u_2^2\ u_3^2 - 2u_1^4u_2^2u_3^2 + u_1^6\ u_2^2\ u_3^2)$$

$$+(u_1^2\ u_2^2\ u_3^2 - 2u_1^4u_2^2u_3^2 + u_1^6\ u_2^2\ u_3^2)\ u_2^2 + (u_1^2\ u_2^2\ u_3^2 - 2u_1^4u_2^2u_3^2 + u_1^6\ u_2^2\ u_3^2)\ u_3^2$$

$$-(u_1^2\ u_2^2\ u_3^2 - 2u_1^4u_2^2u_3^2 + u_1^6\ u_2^2\ u_3^2)\ u_2^2\ u_3^2.$$

Since $v_j^2 = 1 - u_j^2$ $(j = 2, 3)$, we obtain the conclusion

$$F(a_{i,j}\ (u_1,u_2,u_3,v_1,v_2,v_3)) = 0.\ (2.13)$$

By Proposition 2.2 and the equation (2.12), we obtain the assertion of Proposition 2.3. The proof of Proposition 2.3 is complete.

If $(a_{p,q}) \in D_3$ satisfies $a_{11} = 1$, then there exists $\theta \in [0,\ \pi/2]$ for which

$$(a_{p,q}) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos^2\theta & \sin^2\theta \\ 0 & \sin^2\theta & \cos^2\theta \end{pmatrix}.$$

Therefore, it is sufficient for the completion of the proof of Theorem 1.1 to show the following.

Proposition 2.4. *If*

$$P = \begin{pmatrix} a_{11} & a_{12} & \cdot \\ a_{21} & a_{22} & \cdot \\ \cdot & \cdot & \cdot \end{pmatrix} \in \partial O_3$$

satisfies $0 \leq a_{11} < 1$, then $0 \leq a_{12} \leq 1 - a_{11}, 0 \leq a_{21} \leq 1 - a_{11}$ *and* a_{22} *satisfies*

$$(1-a_{11})^2 \cdot a_{22} = a_{11}\, a_{12}\, a_{21} + (1-a_{11}-a_{12})(1-a_{11}-a_{21}) + 2\, \epsilon\sqrt{a_{11}\, a_{12}\, a_{21}}$$

$$\sqrt{(1-a_{11}-a_{12})(1-a_{11}-a_{21})} \tag{2.14}$$

for some $\epsilon \in \{+1,-1\}$.

Proof Since $P \in D_3$, we have $0 \le a_{12} \le 1-a_{11}, 0 \le a_{21} \le 1-a_{11}$. By Proposition 2.2, we have the equation

$$(1-a_{11})^2 \cdot a_{22}^2 - 2\{a_{11}\, a_{12}\, a_{21} + (1-a_{11}-a_{12})(1-a_{11}-a_{21})\, a_{22}$$

$$+\{a_{12}^2\, a_{21}^2 - 2\, a_{12}^2\, a_{21} - 2\, a_{12}\, a_{21}^2 - 2\, a_{11}\, a_{12}\, a_{21}$$

$$+a_{11}^2 + 2\, a_{11}\, a_{12} + a_{12}^2 + a_{21}^2 + 2\, a_{11}a_{21} + 4\, a_{12}\, a_{21} - 2\, a_{11} - 2a_{12} - 2a_{21} + 1\} = 0.$$

We consider this as a quadratic equation of a_{22}. Since

$$\{a_{11}\, a_{12}\, a_{21} + (1-a_{11}-a_{12})(1-a_{11}-a_{21})\}^2 - (1-a_{11})^2\{a_{12}^2\, a_{21}^2 - 2\, a_{12}^2\, a_{21}$$

$$-2\, a_{12}\, a_{21}^2 - 4\, a_{11}\, a_{12}\, a_{21} + a_{11}^2 + 2\, a_{11}\, a_{12}$$

$$+a_{12}^2 + a_{21}^2 + 2\, a_{11}a_{21} + 4\, a_{12}\, a_{21} - 2\, a_{11} - 2a_{12} - 2a_{21} + 1\}$$

$$= 4a_{11}\, a_{12}\, a_{21}(1-a_{11}-a_{12})(1-a_{11}-a_{21}),$$

we have the equation (2.14). The proof of Proposition 2.4 is complete.

Thus we proved Theorem 1.1. By the relation (1.5), the range $W(C,A)$ for 3×3 diagonal matrices C, A is the image of the set O_3 under the real linear mapping of A_3 into $\mathbf{C}$. Thus Theorem 1.2 is immediately deduced from the relation $\partial O_3 = \{g \circ g : g \in SO(3)\}$.

3. Compact symmetric Riemannian space of Type AI

In this section we shall prove Theorem 1.3. We take a square root $B = \text{diag}\{b_1, b_2, b_3\} \in SU(3)$ of the matrix A, i.e., $b_i^2 = a_i$ $(1 \leq i \leq 3)$ and $b_1 b_2 b_3 = 1$. Since $a_i \neq a_j$ $(1 \leq i < j \leq 3)$, the relation

$$(b_i + b_j)(b_i - b_j) \neq 0 \tag{3.1}$$

holds for $1 \leq i < j \leq 3$. We obtain a fundamental equation

$$\text{tr}(A\ g\ C\ g^t) = \text{tr}(B\ g\ C\ g^t\ B)$$

for every $g \in SO(3)$. We consider the real analytic map Φ of the 3-dimensional Lie group $SO(3)$ into the plane $\mathbf{C} \simeq \mathbf{R}^2$:

$$g \mapsto \text{tr}(B\ g\ C\ g^t\ B).$$

We remark that for every $g \in SO(3)$ the element $B\ g\ C\ g^t\ B$ belongs to the 5-dimensinal compact symmetric Riemannian space

$$M = \{X : X \text{ is a 3 by 3 unitary matrix}, det(X) = 1, X^t = X\},$$

(cf. [2] p.451). Define a real analytic map ϕ of $SO(3)$ into M by the equation

$$\phi(g) = B\ g\ C\ g^t\ B.$$

Define a map τ of $M_3(\mathbf{C})$ into $\mathbf{C}$ by the equation $\tau(X) = \text{tr}(X)$. Then we have the relation $\Phi = \tau \circ \phi$.

We research the rank of the Jacobian matrix of the map Φ at every $g \in SO(3)$. For almost every $g \in SO(3)$, the rank is equal to 2. We say that g is a *critical point* if the rank at g is less than 2. If $\Phi(g)$ is a boundary point of $W(A,C)$, then the point g is necessarily critical. We obtain the following theorem.

Theorem3.1. *Suppose that $C = \mathrm{diag}\{c_1, c_2, c_3\}$ and $B = \mathrm{diag}\{b_1, b_2, b_3\}$ are elements of $SU(3)$ satisfying the relations $(b_i + b_j)(b_i - b_j) \neq 0$, $c_i \neq c_j$ for $1 \leq i < j \leq 3$. Set $X = X(g) = B\ g\ C\ g^t\ B$, $X = \{x_{ij} = x_{ij}(g) : 1 \leq i, j \leq 3\}$ for every $g \in SO(3)$. Then an element $g \in SO(3)$ is a critical point of the map Φ, if and only if the three complex numbers x_{12}, x_{13}, x_{23} lie on a straight line passing through the origin 0 on the complex plane* **C**. *Moreover for the points x_{12}, x_{13}, x_{23} to enjoy this condition, it is necessary and sufficient that one of the following conditions holds: 1) The matrix $g = \{g_{pq} : 1 \leq p, q \leq 3\}$ has an entry g_{ij} for which $g_{ij} = 1$ or $g_{ij} = -1$; 2) Some eigenvalue of the unitary matrix X has multiplicity ≥ 2.*

Proof We shall prove the first half of Theorem 3.1. We consider $\{Y_g : Y$ is a 3×3 skew symmetric real matrix$\}$ as the tangent space of $SO(3)$ at g. Here Y_g is a differential operator defined by $Y_g(f) = \lim_{s \to 0} 1/s[f(\exp(s\,Y)g) - f(g)]$ for every differentiable function f on $SO(3)$. Since the symmetric space M is a closed submanifold of the linear space $M_3(\mathbf{C}) \simeq \mathbf{R}^{18}$, we consider the tangent space of M at $X \in M$ as a real linear subspace of $M_3(\mathbf{C})$. Then we have the following relation:

$$\{d\phi(g)(Y_g) : Y \text{ is a } 3 \times 3 \text{ skew symmetric real matrix}\}$$

$$= \{\lim_{s \to 0} 1/s(B \exp(s\ Y)g\ C\ g^t \exp(-s\ Y)B - B\ g\ Cg^t\ B) : Y \text{ is } \ldots\}$$

$$= \{Z\ X(g) + X(g)\ Z^t : Z = (z_{ij}) \text{ is a skew} - \text{Hermitian } 3 \times 3 \text{ matrix with}$$

$$z_{11} = z_{22} = z_{33} = 0,\ z_{12} = b_1 \overline{b_2} x,\ z_{13} = b_1 \overline{b_3} y, z_{23} = b_2 \overline{b_3} u$$

$$\text{for some real numbers } x, y, u\}.$$

Here we used the relation $B\ Y = Z\ B, -Y\ B = B\ Z^t$. The 3×3 skew-Hermitian matrix $Z = (z_{ij})$ is calculated as the following:

$$Z = B\ Y\ B^{-1}$$

$$= \begin{pmatrix} b_1 & 0 & 0 \\ 0 & b_2 & 0 \\ 0 & 0 & b_3 \end{pmatrix} \begin{pmatrix} 0 & x & y \\ -x & 0 & u \\ -y & -u & 0 \end{pmatrix} \begin{pmatrix} \overline{b_1} & 0 & 0 \\ 0 & \overline{b_2} & 0 \\ 0 & 0 & \overline{b_3} \end{pmatrix}$$

$$= \begin{pmatrix} 0 & b_1\overline{b_2}x & b_1\overline{b_3}y \\ -b_2\overline{b_1}x & 0 & b_2\overline{b_3}u \\ -b_3\overline{b_1}y & -b_3\overline{b_2}u & 0 \end{pmatrix}.$$

For $X = X(g) = (x_{ij})$, we have the equation

$$\mathrm{tr}(Z\ X + X\ Z^t) = 2\ i(\Im(z_{12})x_{12} + \Im(z_{13})x_{13} + \Im(z_{23}x_{23})$$

$$= 2\ i(\Im(b_1\overline{b_2})xx_{12} + \Im(b_1\overline{b_3})yx_{12} + \Im(b_2\overline{b_3})ux_{23})$$

where (x, y, u) runs over $\mathbf{R}^3$ as Y runs over the Lie algebra of $SO(3)$. Since the eigenvalues of B satisfy (3.1), we have

$$\Im(b_1\overline{b_2}) \neq 0, \Im(b_1\overline{b_3}) \neq 0, \Im(b_2\overline{b_3}) \neq 0.$$

Therefore for $g \in SO(3)$ to be critical it is necessary and sufficient that the rank of the real linear map $(x, y, u) \mapsto xx_{12}(g) + yx_{13}(g) + ux_{23}(g)$ of $\mathbf{R}^3$ into $\mathbf{C}$ is less than 2. Thus the first half of Theorem 1.3 follows from this.

We shall prove the latter half of Theorem 1.3. We suppose that the element $X = X(g) = (x_{ij})$ of M satisfies the condition

$$x_{12} = q\ k_{12}, x_{13} = q\ k_{13}, x_{23} = q\ k_{23}$$

for some complex number q with $|q| = 1$ and real numbers k_{12}, k_{13}, k_{23}. We consider the two cases (I) At least two of $k_{1,2}, k_{1,3}, k_{2,3}$ are nonzero and (II) Two of $k_{1,2}, k_{1,3}, k_{2,3}$ are zero. First we prove that in the case (I), one eigenvalue of $X = X(g)$ has multiplicity ≥ 2. We set $V = q^{-1}\ X$ and $\beta_{ii} = q^{-1}\ b_{ii}$ $(1 \leq i \leq 3)$. Then V is a 3×3 symmetric unitary matrix. For instance we assume that $k_{12} \neq 0, k_{23} \neq 0$. The case $k_{12} \neq 0, k_{13} \neq 0$ and the case $k_{13} \neq 0, k_{23} \neq 0$ can be treated similarily. Since V is unitary, we have the equations

$$\beta_{11}k_{12} + k_{12}\overline{\beta_{22}} + k_{13}k_{23} = 0, \tag{3.2}$$

$$\beta_{22}k_{23} + k_{23}\overline{\beta_{33}} + k_{12}k_{13} = 0. \tag{3.3}$$

By (3.2) and (3.3), we have the relations

$$k_{12}\Im(\beta_{11}+\overline{\beta_{22}}) = \Im(-k_{13}k_{23}) = 0, \tag{3.4}$$

$$k_{23}\Im(\beta_{22}+\overline{\beta_{33}}) = \Im(-k_{12}k_{13}) = 0. \tag{3.5}$$

Since $k_{12} \neq 0, k_{23} \neq 0$, the equations (3.4) and (3.5) impliy

$$\Im(\beta_{11}) = \Im(\beta_{22}) = \Im(\beta_{33}). \tag{3.6}$$

Thus there exists a real number k with $-1 \leq k \leq 1$ for which the unitary matrix V is expressed as

$$V = \Re(V) + i\ k\ I_3.$$

Where $\Re(V)$ is a 3×3 real symmetric matrix and commutes with the matrix $k\ I_3$. Therefore eigenvalues of V are $(1-k^2)^{1/2} + i\ k$ or $-(1-k^2)^{1/2} + i\ k$. Thus one eigenvalue of V and hence of X has multiplicity ≥ 2.

Second we prove that in the case (II), some entry of the matrix $g \in SO(3)$ is equal to 1 or -1. We assume that $k_{12} = k_{13} = 0$. The case $k_{12} = k_{23} = 0$ and the case $k_{13} = k_{23} = 0$ can be treated similarily. By the assumption the matrix $X = X(g)$ is expressed as follows:

$$X = B\ g\ C\ g^t\ B$$

$$= \begin{pmatrix} x_{11} & 0 & 0 \\ 0 & x_{22} & x_{23} \\ 0 & x_{23} & x_{33} \end{pmatrix}.$$

Thus the symmetric matrix $g\ C\ g^t$ is represented as

$$g\ C\ g^t = \begin{pmatrix} s_{11} & 0 & 0 \\ 0 & s_{22} & s_{23} \\ 0 & s_{23} & s_{33} \end{pmatrix},$$

for some complex numbers $s_{11}, s_{22}, s_{33}, s_{23}$. Then s_{11} is an eigenvalue of the unitary matrix C. We set

$$S = \begin{pmatrix} s_{22} & s_{23} \\ s_{23} & s_{33} \end{pmatrix}.$$

Then the matrix S is symmetric and unitary. Thus $S^* = \overline{S}$ and $SS^* = S^*S = I_2$ and hence $\Re(S) = (S + \overline{S})/2$ and $\Im(S) = (S - \overline{S})/(2\,i)$ are commuting 2×2 real symmetric matrices. Hence there exists a 2×2 real symmetric matrix S_1 for which $\Re(S), \Im(S)$ are expressed in the form

$$\Re(S) = f(S_1),\ \Im(S) = h(S_1),$$

where f and h are polynomials with real coefficients in one variable. We choose a real number θ for which $c = \cos\theta, s = \sin\theta$ satisfy

$$\begin{pmatrix} c & s \\ -s & c \end{pmatrix} S_1 \begin{pmatrix} c & -s \\ s & c \end{pmatrix}$$

$$= \begin{pmatrix} t_1 & 0 \\ 0 & t_2 \end{pmatrix}$$

for some real numbers t_1, t_2. Then we have

$$\begin{pmatrix} c & s \\ -s & c \end{pmatrix} \begin{pmatrix} s_{22} & s_{23} \\ s_{23} & s_{33} \end{pmatrix} \begin{pmatrix} c & -s \\ s & c \end{pmatrix}$$

$$= \begin{pmatrix} \xi_1 & 0 \\ 0 & \xi_2 \end{pmatrix}$$

for some complex numbers ξ_1, ξ_2 with $|\xi_1| = |\xi_2| = 1$. Thus there exists a permutation $\sigma \in S_3$ for which

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & c & s \\ 0 & -s & c \end{pmatrix} (g\ C\ g^t) \begin{pmatrix} 1 & 0 & 0 \\ 0 & c & -s \\ 0 & s & c \end{pmatrix}$$

$$= \begin{pmatrix} c_{\sigma(1)} & 0 & 0 \\ 0 & c_{\sigma(2)} & 0 \\ 0 & 0 & c_{\sigma(3)} \end{pmatrix}.$$

Since $c_1 \neq c_2, c_1 \neq c_3, c_2 \neq c_3$, we obtain the relation

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & c & s \\ 0 & -s & c \end{pmatrix} g \in W, \qquad (3.7)$$

where W is a finite subgroup of $SO(3)$ defined by the following :

$$H = \{\mathrm{diag}(h_1, h_2, h_3) : h_1, h_2, h_3 \text{ are real numbers}\},$$

$$W = \{k \in SO(3) : k\ h\ k^t \in H \text{ for every } h \in H\}.$$

Then for every $k \in W$, $k \circ k$ is a permutation. Hence by the relation (3.7), an entry of the first row of the matrix g is equal to 1 or -1.

We shall show the converse. Suppose that $X = X(g) \in M$ has a multiple eigenvalue. Then the eigenvalues of $X(g)$ satisfy the condition (1.12) and hence the point $\mathrm{tr}(X(g))$ is a boundary point of the closed domain D. Since $M \subseteq SU(3)$, $\{\mathrm{tr}(U) : U \in M\} \subseteq D$. Thus g is a critical point of the map Φ. Next we suppose that an entry of the matrix $g = (g_{ij}) \in SO(3)$ is equal to 1 or -1. For instance we assume that $g_{11} = -1$. Other cases can be treated similarily. By using $c = \cos\theta, s = \sin\theta$ for some suitable $\theta \in \mathbf{R}$, g is expressed as

$$g = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -c & s \\ 0 & -s & -c \end{pmatrix}.$$

Thus we have

$$g\ C\ g^t = \begin{pmatrix} c_1 & 0 & 0 \\ 0 & c^2c_2 + s^2c_3 & c\ s(c_2 - c_3) \\ 0 & c\ s(c_2 - c_3) & c^2c_3 + s^2c_2 \end{pmatrix},$$

$$X(g) = B\ g\ C\ g^t\ B = \begin{pmatrix} a_1c_1 & 0 & 0 \\ 0 & \cdot & b_2b_3c\ s(c_2 - c_3) \\ 0 & \cdot & \cdot \end{pmatrix}.$$

Hence the points $x_{12}(g) = 0, x_{13}(g) = 0, x_{23}(g)$ lie on a straight line passing through the origin 0 on the complex plane $\mathbf{C}$. Thus g is a critical point of Φ. The proof of Theorem 3.1 is complete.

We shall prove Theorem1.3. Since $\partial W(C,A) \subseteq \{\Phi(g) : g$ is a critical point of $\Phi\}$ and $\{\Phi(g) : X(g)$ has a multiple eigenvalue$\} \subseteq \Gamma$, it is sufficient to show the inclusion

$$\{\Phi(g) : g \in SO(3) \text{ has an entry equal to 1 or } -1\}$$

$$\subseteq \{tz_1 + (1-t)z_2 : 0 \le t \le 1, z_1 \in V_+, z_2 \in V_-\}.$$

This inclusion follows from the equation

$$\{g \circ g : g \in SO(3) \text{ has an entry equal to 1 or } -1\} = \{t\, P + (1-t)Q : P \text{ is an even}$$

$$3 \times 3 \text{ permutation matrix}, Q \text{ is an odd } 3 \times 3 \text{ permutation matrix}\}.$$

The proof of Theorem 1.3 is complete.

An analogous assertion to Theorem 1.3 in a special case $C = A$ was already announced by the author in [4].

Acknowledgement. The author would like to express his thanks to the referee for his (or her) valuable suggestions on the proof of Theorem 1.1. The usage of the factorization (2.1) is due to the referee.

References

1. Au-Yeung Y.H., Poon Y.T., 3 × 3 orthostochastic matrices and the numerical ranges, Linear Alg.Appl.27(1979) pp. 69-79.

2. Helgason S.,"Differential Geometry, Lie Groups, and Symmetric Spaces", Academic Press, 1978, Orland, San Diego, New York.

3. Naimark M.A.,"Linear representations of the Lorentz group", Pergamon Press, 1964, Oxford, London.

4. Nakazato H., the generalized numerical range and its boundary, R.I.M.S. Koukyuuroku 903 (1995) pp. 30-39.

5. Westwick R., A theorem of numerical range, Lin. and Multi. 2 (1975) pp. 311-315.

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Received April 14, 1995 Revised July 25, 1996