Available online at www.sciencedirect.com
ScienceDirect
Linear Algebra and its Applications 428 (2008) 698–715
LINEAR ALGEBRA AND ITS APPLICATIONS
www.elsevier.com/locate/laa

Product of diagonal entries of the unitary orbit of a 3-by-3 normal matrix

Hiroshi Nakazato [a,*], Natália Bebiano [b], João da Providência [c]

[a] *Department of Mathematical Sciences, Hirosaki University, 036-8561 Hirosaki, Japan*
[b] *Mathematics Department, University of Coimbra, P 3001-454 Coimbra, Portugal*
[c] *Physics Department, University of Coimbra, P 3004-516 Coimbra, Portugal*

Received 16 August 2007; accepted 26 March 2008
Available online 15 May 2008
Submitted by M. Tsatsomeros

Abstract

Let N be a 3×3 normal matrix. We investigate the sets $W_k^{\Pi}(N) = \left\{\prod_{l=1}^{k}(UNU^*)_{ll} : U \in U(3)\right\}$, where $U(3)$ is the group of 3×3 unitary matrices and $1 \leqslant k \leqslant 3$. Geometric properties of these sets are studied, namely, star-shapedness and simple connectedness are investigated. A method for the numerical estimation of $W_k^{\Pi}(N)$ is also provided for normal matrices of size 3.

AMS classification: 47A12

Keywords: Orthostochastic matrix; Star-shapedness; Diagonal entries

1. Orthostochastic matrices

The special unitary group $SU(3)$ of degree 3 is the set of all 3×3 unitary matrices U with determinant 1, and plays an important role in many areas of physics and mathematics. One of its most famous applications is the description of the invariant properties (symmetries) in the quark theory. An $n \times n$ real matrix $A = (a_{lj})$ is said to be *orthostochastic* if it is expressed as

$$a_{lj} = |u_{lj}|^2$$

* Corresponding author.
E-mail address: nakahr@cc.hirosaki-u.ac.jp (H. Nakazato).

0024-3795/$ - see front matter
doi:10.1016/j.laa.2008.03.028

for some $n \times n$ unitary matrix $U = (u_{lj})$, where U can be chosen so that $\det(U) = 1$. An orthostochastic matrix is also called *unistochastic* in mathematical physics (cf. [2,5]). An orthostochastic matrix is *doubly stochastic*, that is, its entries are nonnegative and all its row and column sums equal 1. Throughout, we denote by $U(n)$ and $Ort(n)$ the sets of $n \times n$ unitary and orthostochastic matrices, respectively.

Consider the unitary similarity orbit of an $n \times n$ normal matrix N:

$$\{UNU^* : U \in U(n)\}$$

and the sets denoted and defined by

$$W_k^{\Pi}(N) = \left\{ \prod_{l=1}^{k} (UNU^*)_{ll} : U \in U(n) \right\}, \quad 1 \leqslant k \leqslant n. \tag{1}$$

Let $\lambda_1, \lambda_2, \ldots, \lambda_n$ be the eigenvalues of N. Obviously, we may assume $N = \operatorname{diag}(\lambda_1, \lambda_2, \ldots, \lambda_n)$ in (1). Moreover, having in mind that

$$\prod_{l=1}^{k} (UNU^*)_{ll} = \prod_{l=1}^{k} \sum_{j=1}^{n} |u_{lj}|^2 \lambda_j,$$

we can define $W_k^{\Pi}(N)$ equivalently by

$$W_k^{\Pi}(N) = \left\{ \prod_{l=1}^{k} \sum_{j=1}^{n} a_{lj} \lambda_j : (a_{lj}) \in Ort(n) \right\}.$$

The investigation of $W_k^{\Pi}(N)$, $k = 1, \ldots, n$, was firstly proposed by Marcus [7]. The main aim of this paper is the study of $W_k^{\Pi}(N)$ for 3×3 normal matrices. In the case $k = 1$, $W_1^{\Pi}(N)$ is the convex hull of $\lambda_1, \lambda_2, \ldots, \lambda_n$. In the case $n = 2$, every doubly stochastic matrix is orthostochastic. For $N = \operatorname{diag}(\lambda_1, \lambda_2)$ we get the line segment

$$W_2^{\Pi}(N) = \left[\lambda_1 \lambda_2, \left(\frac{\lambda_1 + \lambda_2}{2} \right)^2 \right].$$

In our investigation we use the structure theory of 3×3 orthostochastic matrices developed by Au-Yeung and Poon (cf. [1]). An indefinite metric version of this theory was presented in [11].

Let $SO(3)$ be the group of rotations in the 3-dimensional Euclidean space. The boundary of $Ort(3)$, denoted by $\partial Ort(3)$, coincides with the set of the Hadamard product of the rotation matrices by themselves, that is,

$$\begin{aligned} \partial Ort(3) &= \{(u_{lj}^2) : (u_{lj}) \in SO(3)\}, \\ Ort(3) &= \{(1-t)C_0 + t(u_{lj}^2) : 0 \leqslant t \leqslant 1, (u_{lj}) \in SO(3)\}, \end{aligned} \tag{2}$$

where

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

the so called *van der Waerden matrix* (cf. [2]). Since $Ort(3)$ is a compact connected set, $W_k^{\Pi}(N)$ is a compact connected subset of $\mathbf{C}$. Let A_3 be the real affine space of the 3×3 real matrices with all row and column sums equal to 1, and denote by $D(n)$ the semi-group of all $n \times n$ doubly stochastic matrices. The boundary of $Ort(3)$ in $D(3)$ is characterized by a polynomial function $F : A_3 \to \mathbf{R}$ (cf. Eq.(17)). If $A = (a_{lj}) \in \partial Ort(3)$ satisfies $a_{lj} > 0$ for $l, j = 1, 2, 3$ and V is a sufficiently small neighborhood of A in A_3, then $\partial Ort(3) \cap V$ is a C^∞-differentiable manifold. If $a_{lj} = 0$ for some $1 \leqslant l, j \leqslant 3$, then $\partial Ort(3) \cap V$ is viewed as a doubly ruled surface on a face of $D(3)$ (cf. [2]).

A subset S of the Euclidean space $\mathbf{R}^n$ is said to be *star-shaped* with s_0 as a star center if $(1 - t)s_1 + ts_0 \in S$ for every point $s_1 \in S$ and $0 \leqslant t \leqslant 1$. Star-shaped sets are simply connected ([12]). In [3], it was shown that $W_3^\Pi(\mathrm{diag}(1 + 6i, 1 - 6i, 1, 1))$ has a hole and so it is not simply connected. The study of the shapes of these sets are the main aim of our investigation.

This note is organized as follows. In Section 2, we study the star-shapedness of $W_k^\Pi(N)$ for N normal of size 3 with zero trace and for N a 3×3 normal matrix with co-linear eigenvalues. The main result of Section 3 is Theorem 3.1, which provides a method to determine numerically $W_k^\Pi(N)$ when N is normal of size 3. The method is described in Section 4. In Section 5, we give an illustrative example, proposing a methodology for the computation of the boundary of $W_k^\Pi(N)$.

2. Preliminary results

As a simple consequence of the star-shapedness of $Ort(3)$, we have the following theorem.

Theorem 2.1. *Let N be a 3×3 normal matrix with zero trace. Then $W_k^\Pi(N)$ is star-shaped with 0 as a star center for $k = 1, 2, 3$.*

Proof. Let $z \in W_k^\Pi(N)$. Then there exists $(u_{lj}) \in SU(3)$ such that

$$z = \prod_{l=1}^{k} \sum_{j=1}^{n} |u_{lj}|^2 \lambda_j.$$

By Au-Yeung and Poon's theory, we have

$$(1 - t)C_0 + t(|u_{lj}|^2) \in Ort(3), \quad 0 \leqslant t \leqslant 1.$$

Thus, the following homogeneity relation holds:

$$\prod_{l=1}^{k} \sum_{j=1}^{n} ((1 - t)/3 + t|u_{lj}|^2)\lambda_j = t^k \prod_{l=1}^{k} \sum_{j=1}^{n} |u_{lj}|^2 \lambda_j = t^k z \in W_k^\Pi(N).$$

From the star-shapedness of the set $Ort(3)$ with respect to C_0, it follows that $W_k^\Pi(N)$ is star-shaped relatively to the star center 0. □

Remark. As can be easily seen, the set $W_1^\Pi(N)$ is convex for every normal matrix N. This result was generalized by Tsing in [13] and later on in [4] in the context of the theory of numerical ranges. We conjecture the star-shapedness of $W_k^\Pi(N)$ for N an arbitrary 3×3 normal matrix.

An *essentially Hermitian* matrix is a normal matrix with co-linear eigenvalues.

Theorem 2.2. *If N is an $n \times n$ essentially Hermitian matrix, then $W_k^\Pi(N)$ is the continuous image of a compact convex polyhedron in an $(n - 1)$-dimensional affine space.*

Proof. We *claim* that

$$W_k^{\Pi}(N) = \left\{ \prod_{l=1}^{k} \left(\sum_{j=1}^{n} a_{lj}\lambda_j \right) : (a_{lj}) \in D(n) \right\}. \tag{3}$$

It suffices to show that

$$\left\{ \left(\sum_{j=1}^{n} a_{lj}\lambda_j \right)_{l=1}^{n} : (a_{ij}) \in Ort(n) \right\} = \left\{ \left(\sum_{j=1}^{n} a_{lj}\lambda_j \right)_{l=1}^{n} : (a_{lj}) \in D(n) \right\}. \tag{4}$$

Indeed, since N is essentially Hermitian its eigenvalues lie on a straight line in the Gaussian plane. If the straight line passes through the origin, (4) is a consequence of Theorem B.6, p. 24 of [8] (cf. [6]).

So we assume now that the straight line does not pass through the origin. By using a scalar multiplication $N \mapsto cN$ for some $c \neq 0$, we may consider $\Im(\lambda_j) = 1$, $j = 1, \ldots, n$ and so $\lambda_j = \Re(\lambda_j) + \mathrm{i}$, $j = 1, \ldots, n$. Thus

$$\sum_{j=1}^{n} a_{lj}\lambda_j = \mathrm{i} + \sum_{j=1}^{n} a_{lj}\Re(\lambda_j), \quad l = 1, \ldots, n$$

for every $(a_{lj}) \in D(n)$. Hence (4) is rewritten as

$$\left\{ \left(\mathrm{i} + \sum_{j=1}^{n} a_{lj}\Re(\lambda_j) \right)_{l=1}^{n} : (a_{ij}) \in Ort(n) \right\} = \left\{ \left(\mathrm{i} + \sum_{j=1}^{n} a_{lj}\Re(\lambda_j) \right)_{l=1}^{n} : (a_{ij}) \in D(n) \right\}.$$

The above equation follows from Theorem B.6, p. 24 of [8] and so we obtain (3).

By (3), $W_k^{\Pi}(N)$ is the continuous image of the compact convex polyhedron $D(n)$ in an $(n-1)^2$-dimensional affine space. Next, we show that we can express $W_k^{\Pi}(N)$ as the continuous image of a compact convex polyhedron in an $(n-1)$-dimensional affine space. By using a scalar multiplication, without loss of generality we may consider $\Re(\lambda_j) = 1$, $j = 1, 2, \ldots, n$, and so for $1 \leqslant p \leqslant n-1$ we have

$$\begin{aligned}\sum_{j=1}^{n} a_{pj}(1 + \mathrm{i}\Im(\lambda_j)) &= 1 + \mathrm{i}\sum_{j=1}^{n} a_{pj}\Im(\lambda_j) \\ &= 1 + \mathrm{i}\Im(\lambda_n) + \mathrm{i}\sum_{j=1}^{n-1} a_{pj}(\Im(\lambda_j) - \Im(\lambda_n)),\end{aligned}$$

while for $p = n$ we get

$$\begin{aligned}\sum_{j=1}^{n} a_{nj}(1 + \mathrm{i}\Im(\lambda_j)) &= 1 + \mathrm{i}\Im(\lambda_n) + \mathrm{i}\sum_{j=1}^{n-1} a_{nj}(\Im(\lambda_j) - \Im(\lambda_n)) \\ &= 1 + \mathrm{i}\Im(\lambda_n) + \mathrm{i}\sum_{j=1}^{n-1}(\Im(\lambda_j) - \Im(\lambda_n)) \\ &\quad - \mathrm{i}\sum_{p=1}^{n-1}\sum_{j=1}^{n-1} a_{pj}(\Im(\lambda_j) - \Im(\lambda_n)).\end{aligned}$$

Define the following projection:

$$P((a_{lj})) := \left(\sum_{j=1}^{n-1}(\Im(\lambda_j) - \Im(\lambda_n))a_{1j}, \ldots, \sum_{j=1}^{n-1}(\Im(\lambda_j) - \Im(\lambda_n))a_{n-1,j}\right).$$

Then $W_k^{\Pi}(N)$ is expressed as the continuous image of $P(D(n))$, which is a convex polyhedron. By Birkhoff's theorem, $P(D(n))$ coincides with the convex hull of the images of all permutation matrices under P. □

Example 1. As an application of Theorem 2.2, we characterize $W_3^{\Pi}(N)$ for $N = \mathrm{diag}(1 + \mathrm{i}a, 1 - \mathrm{i}a, 1, 1)$ with $a > 0$. We easily find

$$W_3^{\Pi}(N) = \left\{\prod_{p=1}^{3}(1 + \mathrm{i}a\ (a_{p1} - a_{p2})) : (a_{lj}) \in D(4)\right\}.$$

The vertices of the convex polyhedron

$$\Delta = \{(a_{11} - a_{12}, a_{21} - a_{22}, a_{31} - a_{32}) : (a_{lj}) \in D(4)\}$$

are

$$\begin{aligned}&\{(1, 0, 0), (-1, 0, 0), (0, 1, 0), (0, -1, 0), (0, 0, 1), (0, 0, -1)\}\\ &\quad \cup \{(1, -1, 0), (-1, 1, 0), (1, 0, -1), (-1, 0, 1), (0, 1, -1), (0, -1, 1)\}\end{aligned}$$

and it clearly contains the line segment $\{(t, t, t) : -1/3 \leqslant t \leqslant 1/3\}$. We can write

$$W_3^{\Pi}(N) = \{(1 + \mathrm{i}ax)(1 + \mathrm{i}ay)(1 + \mathrm{i}az) : (x, y, z) \in \Delta\}.$$

Let $a \geqslant 3\sqrt{3}$. Then the curve $z(t) = (1 + \mathrm{i}t)^3$, $-\sqrt{3} \leqslant t \leqslant \sqrt{3}$, or equivalently,

$$\{(X, Y) \in \mathbf{R}^2 : -8 \leqslant X \leqslant 1,\ 27Y^2 - (X + 8)^2(1 - X) = 0\}$$

is contained in $W_3^{\Pi}(N)$. We *claim* that this curve is part of the boundary of $W_3^{\Pi}(N)$. It suffices to prove that if x, y, z are real numbers and $X = \Re((1 + 3\mathrm{i}x)(1 + 3\mathrm{i}y)(1 + 3\mathrm{i}z))$ is such that $-8 \leqslant X \leqslant 1$, then $Y = \Im((1 + 3\mathrm{i}x)(1 + 3\mathrm{i}y)(1 + 3\mathrm{i}z))$ satisfies the inequality

$$27Y^2 \geqslant (X + 8)^2(1 - X).$$

We easily find that $X = 1 - 9(xy + xz + yz)$, $Y = 3(x + y + z) - 27xyz$, and we determine the extreme values of Y for $X = x_0$. So we consider the Lagrange function $\Phi = Y - \lambda(X - x_0)$, where $0 \neq \lambda \in \mathbf{R}$ is the Lagrange multiplier. The extremal points are the solutions of the simultaneous equations

$$\begin{aligned}&3 - 27yz + 9\lambda(y + z) = 0,\\ &\frac{3 - 27yz}{y + z} = \frac{3 - 27xy}{x + y} = \frac{3 - 27xz}{x + z}.\end{aligned}$$

Straightforward calculations show that the extreme values of Y occur for $x = y = z$. The parametric equations of the boundary are given by

$$X(t) = 1 - 27t^2, \quad Y(t) = 9t - 27t^3, \quad t \in \left[-\frac{\sqrt{3}}{3}, \frac{\sqrt{3}}{3}\right]$$

and the claim follows.

Theorem 2.3. *Let* $N = \mathrm{diag}(\lambda_1, \lambda_2, \lambda_3)$ *be an essentially Hermitian matrix. Then* $W_k^{\Pi}(N)$ *is simply connected for* $k = 1, 2, 3$.

Proof. In the case $k = 1$, it is well known that the set is a closed line segment, so we concentrate on the cases $k = 2, 3$. Assume that $\lambda_1 = 1 + ia_1$, $\lambda_2 = 1 + ia_2$, $\lambda_3 = 1 + ia_3$ with $a_1 > a_2 > a_3$. Let $\widetilde{\Delta}$ be the hexagon in the Euclidean plane with vertices $(a_1 - a_3, 0)$, $(a_2 - a_3, 0)$, $(0, a_1 - a_3)$, $(0, a_2 - a_3)$, $(a_1 - a_3, a_2 - a_3)$, $(a_2 - a_3, a_1 - a_3)$:

$$\widetilde{\Delta} = \left\{ \left(\frac{t+s}{2}, \frac{t-s}{2}\right) : a_2 - a_3 \leqslant t \leqslant a_1 + a_2 - 2a_3, \right.$$
$$\left. |s| \leqslant (a_1 - a_3) - |t - (a_1 - a_3)| \right\},$$

and let

$$\check{\Delta} = \left\{ \left(\frac{t+s}{2}, \frac{t-s}{2}\right) : a_2 - a_3 \leqslant t \leqslant a_1 + a_2 - 2a_3, \right.$$
$$\left. 0 \leqslant s \leqslant (a_1 - a_3) - |t - (a_1 - a_3)| \right\}.$$

For $(x, y) \in \widetilde{\Delta}$, consider the functions defined by

$$g(x, y) := (1 + \mathrm{i}a_3 + \mathrm{i}x)(1 + \mathrm{i}a_3 + \mathrm{i}y),$$
$$f(x, y) := (1 + \mathrm{i}a_3 + \mathrm{i}x)(1 + \mathrm{i}a_3 + \mathrm{i}y)(1 + \mathrm{i}(a_1 + a_2 - a_3) - \mathrm{i}x - \mathrm{i}y).$$

Then

$$W_2^{\Pi}(N) = \{g(x, y) : (x, y) \in \widetilde{\Delta}\} = \{g(x, y) : (x, y) \in \check{\Delta}\}$$

because $g(x, y)$ is symmetric in x, y. We also have

$$W_3^{\Pi}(N) = \{f(x, y) : (x, y) \in \widetilde{\Delta}\}.$$

We analyze the symmetries of $W_3^{\Pi}(N)$. The function $f(x, y)$ is invariant on $\widetilde{\Delta}$ under the transformations

$$(x, y) \mapsto (a_1 + a_2 - 2a_3 - x - y, y), \quad (x, y) \mapsto (x, a_1 + a_2 - 2a_3 - x - y),$$
$$(x, y) \mapsto (y, x)$$

and under their compositions

$$(x, y) \mapsto (a_1 + a_2 - 2a_3 - x - y, x), \quad (x, y) \mapsto (y, a_1 + a_2 - 2a_3 - x - y).$$

We take a fundamental domain Δ' of the group of these transformations. For instance, we may take Δ' as the quadrilateral with vertices $((a_1 + a_2 - 2a_3)/2, (a_1 + a_2 - 2a_3)/2)$, $(a_1 - a_3, a_2 - a_3)$,$(a_1 - a_3, (a_2 - a_3)/2)$, $((a_1 + a_2 - 2a_3)/3, (a_1 + a_2 - 2a_3)/3)$.

The Jacobians of $g(x, y)$ and $f(x, y)$ are

$$\frac{\partial\Re(g)}{\partial x}\frac{\partial\Im(g)}{\partial y} - \frac{\partial\Re(g)}{\partial y}\frac{\partial\Im(g)}{\partial x} = x - y$$

and

$$(x-y)(a_1+a_2-2a_3-x-2y)(a_1+a_2-2a_3-2x-y),$$

respectively. These Jacobians have constant sign in the interior of the domains $\check{\Delta}$ and Δ', respectively. Hence, the maps g and f are local homeomorphisms. We show that they are also global homeomorphisms. Suppose that $g(x,y)=g(x',y')$ for some $(x,y),(x',y')\in\widetilde{\Delta}$. Comparing the real and the imaginary parts of g, we have $x+y=x'+y'$, $xy=x'y'$ and so $(x',y')=(x,y)$ or $(x',y')=(y,x)$. Suppose that $f(x_1,y_1)-f(x_2,y_2)=0$. The resultant of the real and imaginary parts of this equation with respect to y_2 is

$$(x_2-x_1)^2(x_2-y_1)^2(a_1+a_2-2a_3-x_1-y_1-x_2)^2=0.$$

If $x_2=a_1+a_2-2a_3-x_1-y_1$, then the real part of $f(x_1,y_1)-f(x_2,y_2)$ is $(y_2-x_1)(y_2-y_1)$, and so $y_2=y_1$ or $y_2=x_1$. Thus, if (x_1,y_1), (x_2,y_2) belong to the same fundamental domain, then the real parts of $f(x_1,y_1)$ and $f(x_2,y_2)$ coincide. The cases $x_2=x_1$ and $x_2=y_1$ may be similarly treated, and by a limiting process we may treat the case $\lambda_j=\lambda_k$ for some $1\leqslant j<k\leqslant 3$. Thus, the result follows. □

In the sequel, we shall consider the differentiable map

$$\Lambda_k: T=(t_{lj})\in A_3\mapsto \prod_{l=1}^{k}\left(\sum_{j=1}^{3}t_{ij}\lambda_j\right)\in\mathbf{C}\cong\mathbf{R}^2,\quad k=2,3.$$

For $N=\mathrm{diag}(1+\mathrm{i}a_1,1+\mathrm{i}a_2,1+\mathrm{i}a_3)$, we determine the boundary of $W_k^{\Pi}(N)$ under the condition $a_1>a_2>a_3$. For $k=2$, four line segments on the lines

$$\Im(Z)=a_2+a_3,\quad \Re(Z)=-a_3\Im(Z)+a_3^2+1, \tag{5}$$

$$\Re(Z)=-a_1\Im(Z)+a_1^2+1,\quad \Im(Z)=a_1+a_2 \tag{6}$$

belong to the boundary. The second and the third line segments of the above list intersect at the point $A_0=(1+\mathrm{i}a_1)(1+\mathrm{i}a_3)$. The line segment on $y=x$, which is contained in the boundary of $\check{\Delta}$, generates the parabola

$$\Re(Z)=-\frac{\Im(Z)^2}{4}+1. \tag{7}$$

This parabola is contained in $\partial W_2^{\Pi}(N)$, and intersects the first line segment in (5) and the second in (6) at

$$A_1=\left(1+\mathrm{i}\frac{a_2+a_3}{2}\right)^2,\quad A_2=\left(1+\mathrm{i}\frac{a_1+a_2}{2}\right)^2,$$

respectively. The tangent lines to the parabola (7) at these points are

$$\Re(Z)=-\frac{a_2+a_3}{2}(\Im(Z)-(a_2+a_3))+1-\left(\frac{a_2+a_3}{2}\right)^2,$$

$$\Re(Z)=-\frac{a_1+a_2}{2}(\Im(Z)-(a_1+a_2))+1-\left(\frac{a_1+a_2}{2}\right)^2,$$

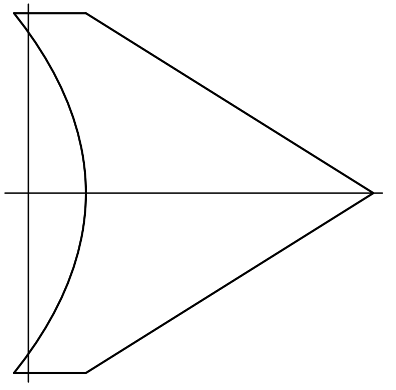

Fig. 1. $W_2^{\Pi}(N)$ for $N = \mathrm{diag}(1+\mathrm{i}, 1, 1-\mathrm{i})$.

respectively. Since

$$-a_1 < -\frac{a_1+a_2}{2} < -\frac{a_2+a_3}{2} < -a_3,$$

the intersection of these tangents is an interior point of $W_2^{\Pi}(N)$ (see Fig. 1).

For $k = 3$, the two line segments on the lines

$$\Im(Z) = a_1\Re(Z) + (a_1^2+1)(a_2+a_3), \tag{8}$$

$$\Im(Z) = a_3\Re(Z) + (a_3^2+1)(a_1+a_2) \tag{9}$$

belong to $\partial W_3^{\Pi}(N)$, and its intersection is the point $(1+\mathrm{i}a_1)(1+\mathrm{i}a_2)(1+\mathrm{i}a_3)$. Another part of $\partial W_3^{\Pi}(N)$ is a portion of the following cubic curve:

$$3(3\Im(Z') - (a_1+a_2+a_3)\Re(Z'))^2 - 4\Re(Z')^3 = 0, \tag{10}$$

where

$$Z' = Z - \left(1+\mathrm{i}\frac{a_1+a_2+a_3}{3}\right)^3.$$

The cubic arc corresponds to a line segment on the line $y = x$, which is contained in $\partial\Delta'$. The cubic arc has a cusp at

$$Z_0 = \Lambda_3(C_0) = \left(1+\mathrm{i}\frac{a_1+a_2+a_3}{3}\right)^3 \tag{11}$$

and the tangent to the curve at this point with equation

$$\begin{aligned}&9(a_1+a_2+a_3)\Re(Z) - 27\Im(Z) + 2(a_1+a_2+a_3)\\&\quad\times(a_1^2+a_2^2+a_3^2+2a_1a_2+2a_1a_3+2a_2a_3+9) = 0,\end{aligned} \tag{12}$$

intersects one of the line segments of $\partial W_3^{\Pi}(N)$ in (8) and (9) at

$$Z_1 = \left(1+\mathrm{i}\frac{a_1+a_2+a_3}{3}\right)(1+\mathrm{i}a_3)\left(1+\mathrm{i}\frac{2a_1+2a_2-a_3}{3}\right) \tag{13}$$

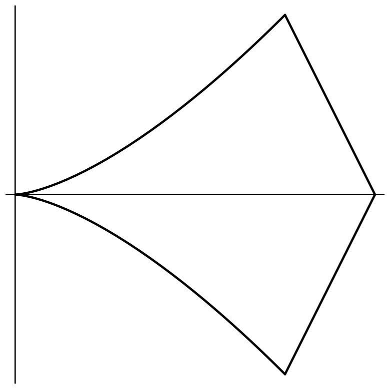

Fig. 2. $W_3^{\Pi}(N)$ for $N = \mathrm{diag}(1+\mathrm{i}, 1, 1-\mathrm{i})$.

if $(a_1 + a_3)/2 \geqslant a_2$, and at

$$Z_2 = \left(1 + \mathrm{i}\frac{a_1 + a_2 + a_3}{3}\right)(1 + \mathrm{i}a_1)\left(1 + \mathrm{i}\frac{2a_2 + 2a_3 - a_1}{3}\right) \tag{14}$$

if $(a_1 + a_3)/2 \leqslant a_2$. The cubic arc intersects the line segments in (8) and (9) at

$$Z_3 = (1 + \mathrm{i}a_1)\left(1 + \mathrm{i}\frac{a_2 + a_3}{2}\right)^2, \quad Z_4 = (1 + \mathrm{i}a_3)\left(1 + \mathrm{i}\frac{a_1 + a_2}{2}\right)^2,$$

respectively. The tangent lines to the cubic arc (10) at these points intersect the straight line (12) at

$$W_3 = (1 + \mathrm{i}(a_1 + a_2 + a_3)/3)(1 + \mathrm{i}(a_2 + a_3)/2)(1 + \mathrm{i}(4a_1 + a_2 + a_3)/6),$$
$$W_4 = (1 + \mathrm{i}(a_1 + a_2 + a_3)/3)(1 + \mathrm{i}(a_1 + a_2)/2)(1 + \mathrm{i}(a_1 + a_2 + 4a_3)/6).$$

In the case $(a_1 + a_3)/2 \geqslant a_2$, we have

$$W_3 = Z_0 + t_3\,(Z_1 - Z_0), \quad W_4 = Z_0 + \frac{1}{4}(Z_1 - Z_0)$$

with

$$t_3 := \frac{((a_1 - a_2) + (a_1 - a_3))^2}{4((a_1 - a_3) + (a_2 - a_3))^2} \tag{15}$$

being $t_3 \geqslant \frac{1}{4}$ and $1 - t_3 \geqslant 0$. If $(a_1 + a_3)/2 \leqslant a_2$, we find

$$W_3 = Z_0 + \frac{1}{4}(Z_2 - Z_0), \quad W_4 = Z_0 + t_4\,(Z_2 - Z_0)$$

with

$$t_4 := \frac{((a_1 - a_3) + (a_2 - a_3))^2}{4((a_1 - a_2) + (a_1 - a_3))^2} \tag{16}$$

being $t_4 \geqslant \frac{1}{4}$ and $1 - t_4 \geqslant 0$ (see Fig. 2).

One could conjecture that $W_k^{\Pi}(N)$ is star-shaped relatively to $\Lambda_k(C_0)$. The following example shows that this guess fails. Consider $W_k^{\Pi}(N)$ for $k = 2, 3$. Then $\Lambda_k(C_0) = 1$ for $k = 2, 3$. The point 1 belongs to the parabola (7) and it is the cusp of the cubic arc (10). The line segment $[3/4 + \mathrm{i}, 1]$ intersects $W_2^{\Pi}(N)$ only at its endpoints. A similar situation holds for every point of the cubic arc (10).

We show that $(1 + \mathrm{i}a_1)(1 + \mathrm{i}a_2)(1 + \mathrm{i}a_3)$ is not generally a star center of $W_3^{\Pi}(N)$. In fact, let $a_1 = 4, a_2 = 0, a_3 = -1$. The point $(1 - t)(2 + 2\mathrm{i}) + t(5 + 3\mathrm{i})$ does not belong to $W_3^{\Pi}(N)$ if t is a sufficiently small positive number. Thus, these candidates are not generally star centers of the set.

By the local concaveness of the cubic curve (10) and of the parabola (7), and having in mind the previous discussion, we obtain the following.

Theorem 2.4. *Let* $N = \mathrm{diag}(1 + \mathrm{i}a_1, 1 + \mathrm{i}a_2, 1 + \mathrm{i}a_3)$, *where* $a_1 \geqslant a_2 \geqslant a_3$ *and* $a_1 > a_3$. *For* Z_0, Z_1, Z_2 *in* (11), (13), (14), *respectively, the following holds*:

(i) $W_2^{\Pi}(N)$ *is star-shaped with a star center* $(1 + \mathrm{i}a_1)(1 + \mathrm{i}a_3)$, *and* $\partial W_2^{\Pi}(N)$ *is constituted by four line segments in* (5) *and* (6) *and an arc of the parabola in* (7).

(ii) *If* $(a_1 + a_3)/2 \geqslant a_2$, *then* $W_3^{\Pi}(N)$ *is star-shaped with a star center* $Z_0 + t_0(Z_1 - Z_0)$, *where* $t_3 \leqslant t_0 \leqslant 1$ *for* t_3 *in* (15).

(iii) *If* $(a_1 + a_3)/2 \leqslant a_2$, *then* $W_3^{\Pi}(N)$ *is star-shaped with a star center* $Z_0 + t_0(Z_2 - Z_0)$, *where* $t_4 \leqslant t_0 \leqslant 1$ *for* t_4 *in* (16).

In the cases (ii) *and* (iii), $\partial W_3^{\Pi}(N)$ *is constituted by two line segments in* (8) *and* (9) *and an arc of the cubic in* (10).

3. Critical points and critical values

In this section, we treat the general case of the eigenvalues $\lambda_1, \lambda_2, \lambda_3$ not lying on a straight line. The rank of the Jacobian matrix of the differentiable map Λ_k is 2 at the regular points and is less than or equal to 1 at the critical points. We consider $a_{11}, a_{12}, a_{21}, a_{22}$ as independent coordinates of A_3. If $W_k^{\Pi}(N)$ is simply connected, then the following theorem provides a method to determine this set numerically. If $W_k^{\Pi}(N)$ is not simply connected, it also gives important information.

Theorem 3.1. *Suppose that the eigenvalues* $\lambda_1, \lambda_2, \lambda_3$ *of* N *do not lie on a straight line. Then the image of the interior of* $Ort(3)$ *in* A_3 *under* Λ_k *is an open subset of the Gaussian plane* $\mathbf{C}$ *for* $k = 2, 3$. *Hence, the boundary of* $W_k^{\Pi}(N)$ *is contained in the image of* $\partial Ort(3)$ *under the map* Λ_k *for* $k = 2, 3$.

To prove this theorem we need the following four lemmas.

Lemma 3.1. *Suppose that the eigenvalues* $\lambda_1, \lambda_2, \lambda_3$ *of* N *do not lie on a straight line. Then the map* Λ_2 *has a unique* (*and hence isolated*) *critical point in the affine space* A_3. *The critical point* (a_{lj}) *satisfies* $a_{21} = a_{11},\ a_{22} = a_{12}, \sum_{j=1}^{3} a_{1j}\lambda_j = 0$, *and the critical value is* 0.

Proof. We may assume that $\lambda_1 \neq 0$ and by a scaling of N we may take $\lambda_1 = 1$. We consider the product

$$Z = \prod_{i=1}^{2}\left(\sum_{j=1}^{3} a_{ij}\lambda_j\right)$$

and its complex conjugate

$$\overline{Z} = \prod_{i=1}^{2}\left(\sum_{j=1}^{3} a_{ij}\overline{\lambda}_j\right).$$

Then the Jacobians

$$\frac{\partial Z}{\partial a_{11}}\frac{\partial \overline{Z}}{\partial a_{12}} - \frac{\partial Z}{\partial a_{12}}\frac{\partial \overline{Z}}{\partial a_{11}}$$

and

$$\frac{\partial Z}{\partial a_{21}}\frac{\partial \overline{Z}}{\partial a_{22}} - \frac{\partial Z}{\partial a_{22}}\frac{\partial \overline{Z}}{\partial a_{21}}$$

are given by

$$2\mathrm{i}\{(\Re(\lambda_3)-1)\Im(\lambda_2) - (\Re(\lambda_2)-1)\Im(\lambda_3)\}|(\lambda_1-\lambda_3)a_{21} + (\lambda_2-\lambda_3)a_{22} + \lambda_3|^2,$$

and

$$2\mathrm{i}\{(\Re(\lambda_3)-1)\Im(\lambda_2) - (\Re(\lambda_2)-1)\Im(\lambda_3)\}|(\lambda_1-\lambda_3)a_{11} + (\lambda_2-\lambda_3)a_{12} + \lambda_3|^2,$$

respectively. By the hypothesis, the three points $\lambda_1 = 1, \lambda_2, \lambda_3$ do not lie on a straight line, and so $(\Re(\lambda_3)-1)\Im(\lambda_2) - (\Re(\lambda_2)-1)\Im(\lambda_3) \neq 0$. Thus, the critical point (a_{lj}) necessarily satisfies the equations

$$(\lambda_1-\lambda_3)a_{l1} + (\lambda_2-\lambda_3)a_{l2} + \lambda_3 = 0, \quad l = 1, 2.$$

These equations originate a real linear system with four equations in $a_{11}, a_{12}, a_{21}, a_{22}$. The determinant of the matrix system is

$$((\Re(\lambda_3)-1)\Im(\lambda_2) - (\Re(\lambda_2)-1)\Im(\lambda_3))^2 \neq 0,$$

and so the linear system has a unique solution. This solution also satisfies

$$\frac{\partial Z}{\partial a_{ij}}\frac{\partial \overline{Z}}{\partial a_{pq}} - \frac{\partial Z}{\partial a_{pq}}\frac{\partial \overline{Z}}{\partial a_{ij}} = 0$$

for $(i, j, p, q) = (1, 1, 2, 1), (1, 1, 2, 2), (1, 2, 2, 1), (1, 2, 2, 2)$. Now, the lemma easily follows. □

Lemma 3.2. *Suppose that the eigenvalues $\lambda_1, \lambda_2, \lambda_3$ of N do not lie on a straight line. Then the image of an ϵ-neighborhood of the critical point of Λ_2 is a neighborhood of* 0 *in* **C** *for every* $\epsilon > 0$.

Proof. Near the critical point $(a_{11}^{(0)}, a_{12}^{(0)}, a_{11}^{(0)}, a_{12}^{(0)})$, we have

$$Z = \prod_{l=1}^{2}\left(\sum_{j=1}^{3} a_{lj}\lambda_j\right) = ((a_{11}-a_{11}^{(0)})(\lambda_1-\lambda_3) + (a_{12}-a_{12}^{(0)})(\lambda_2-\lambda_3))$$
$$\times((a_{21}-a_{11}^{(0)})(\lambda_1-\lambda_3) + (a_{22}-a_{12}^{(0)})(\lambda_2-\lambda_3)).$$

Since $\lambda_1-\lambda_3$, $\lambda_2-\lambda_3$ are linearly independent in the real linear space **C**, the above product describes a neighborhood of 0 in **C** when $(a_{lj}-a_{lj}^{(0)})$ ranges over an ϵ ball in $\mathbf{R}^4$ for every $\epsilon > 0$. □

Lemma 3.3. *If the eigenvalues $\lambda_1, \lambda_2, \lambda_3$ of N do not lie on a straight line, then a point in A_3 is a critical point of Λ_3 if and only if it is one of the following four points*:

(i) $a_{21} = a_{11}, a_{22} = a_{12}$ *and* $\sum_{j=1}^{3} a_{1j}\lambda_j = 0$,
(ii) $a_{31} = a_{11}, a_{32} = a_{12}$, *and* $\sum_{j=1}^{3} a_{1j}\lambda_j = 0$,
(iii) $a_{31} = a_{21}, a_{32} = a_{22}$, *and* $\sum_{j=1}^{3} a_{2j}\lambda_j = 0$,
(iv) $a_{11} = a_{12} = a_{21} = a_{22} = 1/3$, *that is*, $(a_{lj}) = C_0$.

The critical values are 0 *in the cases* (i), (ii), (iii) *and* $(\operatorname{tr} N/3)^3$ *in the case* (iv). *If two of the three points in* (i), (ii), (iii) *coincide, then all of them coincide. These three points coincide if and only if* $\operatorname{tr} N = 0$. *In this case all the four points coincide.*

Proof. We assume $\lambda_1 = 1$. Straightforward calculations show that

$$\frac{\partial Z}{\partial a_{11}}\frac{\partial \overline{Z}}{\partial a_{12}} - \frac{\partial Z}{\partial a_{12}}\frac{\partial \overline{Z}}{\partial a_{11}}$$
$$= 2\mathrm{i}((\Re(\lambda_3) - 1)\Im(\lambda_2) - (\Re(\lambda_2) - 1)\Im(\lambda_3))\,|(\lambda_1 - \lambda_3)a_{21} + (\lambda_2 - \lambda_3)a_{22} + \lambda_3|^2$$
$$\times |(\lambda_1 - \lambda_3)a_{31} + (\lambda_2 - \lambda_3)a_{32} - (\lambda_1 - \lambda_3)a_{11} - (\lambda_2 - \lambda_3)a_{12}|^2$$

and

$$\frac{\partial Z}{\partial a_{21}}\frac{\partial \overline{Z}}{\partial a_{22}} - \frac{\partial Z}{\partial a_{22}}\frac{\partial \overline{Z}}{\partial a_{21}}$$
$$= 2\mathrm{i}((\Re(\lambda_3) - 1)\Im(\lambda_2) - (\Re(\lambda_2) - 1)\Im(\lambda_3))\,|(\lambda_1 - \lambda_3)a_{11} + (\lambda_2 - \lambda_3)a_{12} + \lambda_3|^2$$
$$\times |(\lambda_1 - \lambda_3)a_{31} + (\lambda_2 - \lambda_3)a_{32} - (\lambda_1 - \lambda_3)a_{21} - (\lambda_2 - \lambda_3)a_{22}|^2.$$

Thus, the critical point $(a_{11}, a_{12}, a_{21}, a_{22})$ satisfies one of the conditions:

(a) $\sum_{j=1}^{3} a_{1j}\lambda_j = \sum_{j=1}^{3} a_{2j}\lambda_j = 0$,
(b) $\sum_{j=1}^{3} a_{1j}\lambda_j = \sum_{j=1}^{3} a_{3j}\lambda_j = 0$,
(c) $\sum_{j=1}^{3} a_{2j}\lambda_j = \sum_{j=1}^{3} a_{3j}\lambda_j = 0$,
(d) $\sum_{j=1}^{3} a_{1j}\lambda_j = \sum_{j=1}^{3} a_{2j}\lambda_j = \sum_{j=1}^{3} a_{3j}\lambda_j$.

Conversely, if one of the conditions (a), (b), (c) holds, then

$$\frac{\partial Z}{\partial a_{lj}}\frac{\partial \overline{Z}}{\partial a_{pq}} - \frac{\partial Z}{\partial a_{pq}}\frac{\partial \overline{Z}}{\partial a_{lj}} = 0$$

for $(l, j, p, q) = (1, 1, 2, 1), (1, 1, 2, 2), (1, 2, 2, 1), (1, 2, 2, 2)$. If the condition (d) holds, then it implies $a_{11} = a_{12} = a_{21} = a_{22} = 1/3$. □

Lemma 3.4. *If the eigenvalues $\lambda_1, \lambda_2, \lambda_3$ of N do not lie on a straight line, then the image of an ϵ-neighborhood of the critical point C_0 of Λ_3 is a neighborhood of the critical value* $(\operatorname{tr} N/3)^3$ *for every $\epsilon > 0$. The image of an ϵ-neighborhood of a critical point $(a_{11}^{(0)}, a_{12}^{(0)}, a_{21}^{(0)}, a_{22}^{(0)})$ of Λ_3 satisfying one of the conditions* (i), (ii), (iii) *of Lemma 3.3 is a neighborhood of* 0 *for every* $\epsilon > 0$.

Proof. Firstly, suppose that $\operatorname{tr} N = 0$. In this case, the four critical points of Λ_3 coincide. By the assumption, the complex numbers λ_1, λ_2 are linearly independent over the reals, and so $2\lambda_1 + \lambda_2, \lambda_1 + 2\lambda_2$ are also linearly independent. By setting $a_{21} - 1/3 = -2x$, $a_{22} - 1/3 = -2y$, $a_{11} - 1/3 = x$, $a_{12} - 1/3 = y$, we have

$$Z = -2\{(2\lambda_1 + \lambda_2)x + (\lambda_1 + 2\lambda_2)y\}^3.$$

Hence, the image of an ϵ-neighborhood of a critical point under Λ_3 is a neighborhood of the critical value 0 for sufficiently small $\epsilon > 0$ and hence for every $\epsilon > 0$.

Now, we assume $\operatorname{tr} N \neq 0$. In this case, by setting $a_{21} = 1/3$, $a_{22} = 1/3$, $a_{11} - 1/3 = x$, $a_{12} - 1/3 = y$, we have

$$27Z - (\operatorname{tr} N)^3 = -9\operatorname{tr} N((\lambda_1 - \lambda_3)x + (\lambda_2 - \lambda_3)y)^2 + \text{cubic terms in } x, y.$$

Thus, the image of an ϵ-neighborhood of C_0 under Λ_3 is a neighborhood of $(\operatorname{tr} N/3)^3$ for every $\epsilon > 0$.

Let $(a_{lj}^{(0)})$ be the critical point satisfying the condition (i) of Lemma 3.3. Then

$$\begin{aligned} Z = {} & \{(\lambda_1 - \lambda_3)(a_{11} - a_{11}^{(0)}) + (\lambda_2 - \lambda_3)(a_{12} - a_{12}^{(0)})\} \\ & \times \{(\lambda_1 - \lambda_3)(a_{21} - a_{21}^{(0)}) + (\lambda_2 - \lambda_3)(a_{22} - a_{22}^{(0)})\} \\ & \times \{\lambda_1 + \lambda_2 - (\lambda_1 - \lambda_3)(a_{11} - a_{11}^{(0)} + a_{21} - a_{21}^{(0)}) \\ & - (\lambda_2 - \lambda_3)(a_{12} - a_{12}^{(0)} + a_{22} - a_{22}^{(0)})\}. \end{aligned}$$

By setting $a_{11} - a_{11}^{(0)} = a_{21} - a_{21}^{(0)} = x$, $a_{12} - a_{12}^{(0)} = a_{22} - a_{22}^{(0)} = y$, we have

$$Z = (\lambda_1 + \lambda_2)\{(\lambda_1 - \lambda_3)x + (\lambda_2 - \lambda_3)y\}^2 + \text{cubic terms in } x, y,$$

in the case $\lambda_1 + \lambda_2 \neq 0$ and

$$Z = -2\{(\lambda_1 - \lambda_3)x + (\lambda_2 - \lambda_3)y\}^3$$

in the case $\lambda_1 + \lambda_2 = 0$. Hence, the image of an ϵ-neighborhood of the point $(a_{lj}^{(0)})$ under Λ_3 is a neighborhood of the critical value 0 for every $\epsilon > 0$. The critical point satisfying the condition (ii) or (iii) of Lemma 3.3 can be treated similarly. □

The proof of Theorem 3.1 follows straightforwardly from the previous four lemmas.

4. Numerical approximation

In this section, we provide a method to describe $W_k^{\Pi}(N)$ numerically in the case $\lambda_1, \lambda_2, \lambda_3$ do not lie on a straight line. By Theorem 3.1, the boundary of $W_k^{\Pi}(\operatorname{diag}(\lambda_1, \lambda_2, \lambda_3))$ is realized by the image of Λ_k on $\partial Ort(3)$, and by (2) we should use a convenient parametrization of this set. The orthogonal group $SO(3)$ is locally isomorphic to the simply connected Lie group $SU(2)$, the subgroup of $U(2)$ whose matrices have determinant 1. The group $SU(2)$ is isomorphic to the group of all pure imaginary quarternions $a_1 i + a_2 j + a_3 k$ with modulus 1. It is given as a linear Lie group by

$$SU(2) = \left\{ U = \begin{pmatrix} a_1 + \mathrm{i}a_2 & -b_1 + \mathrm{i}b_2 \\ b_1 + \mathrm{i}b_2 & a_1 - \mathrm{i}a_2 \end{pmatrix} \in \mathbf{C}^{2\times 2} : a_1^2 + a_2^2 + b_1^2 + b_2^2 = 1 \right\}$$

and a continuous homomorphism ϕ of $SU(2)$ onto $SO(3)$ is given by

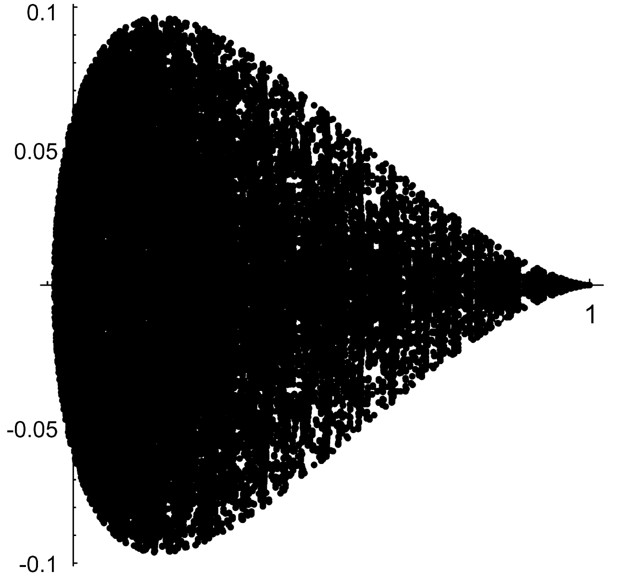

Fig. 3. $W_3^{\Pi}(\mathrm{diag}(1, (-1+\sqrt{3}i)/2, (-1-\sqrt{3}i)/2))$.

$$\phi(U) := \begin{pmatrix} a_1^2 - a_2^2 - b_1^2 + b_2^2 & -2a_1a_2 + 2b_1b_2 & 2a_1b_1 + 2a_2b_2 \\ 2a_1a_2 + 2b_1b_2 & a_1^2 - a_2^2 + b_1^2 - b_2^2 & 2a_2b_1 - 2a_1b_2 \\ -2a_1b_1 + 2a_2b_2 & 2a_2b_1 + 2a_1b_2 & a_1^2 + a_2^2 - b_1^2 - b_2^2 \end{pmatrix}.$$

The above homomorphism ϕ is a linear representation of the adjoint action of the group $SU(2)$ on its Lie algebra. The entries $a_{11}, a_{12}, a_{21}, a_{22}$ of a point of $\partial Ort(3)$ are parametrized as

$$a_{11} = (a_1^2 - a_2^2 - b_1^2 + b_2^2)^2, \quad a_{22} = (a_1^2 - a_2^2 + b_1^2 - b_2^2)^2,$$
$$a_{12} = 4(a_1^2a_2^2 + b_1^2b_2^2) - 8a_1a_2b_1b_2, \quad a_{21} = 4(a_1^2a_2^2 + b_1^2b_2^2) + 8a_1a_2b_1b_2.$$

Thus

$$\begin{aligned} &\{\Lambda_k((a_{lj})) : (a_{lj}) \in \partial Ort(3)\} \\ &\quad = \{\Lambda_k(a_{lj}(a_1^2, a_2^2, b_1^2, b_2^2, a_1a_2b_1b_2)) : a_1^2 + a_2^2 + b_1^2 + b_2^2 = 1, a_1a_2b_1b_2 \geqslant 0\} \\ &\quad \cup \{\Lambda_k(a_{lj}(a_1^2, a_2^2, b_1^2, b_2^2, a_1a_2b_1b_2)) : a_1^2 + a_2^2 + b_1^2 + b_2^2 = 1, a_1a_2b_1b_2 \leqslant 0\}. \end{aligned}$$

We may use other parametrizations of $\partial Ort(3)$, such as that one based on Euler's angles to express rotations (cf. [10]).

In Fig. 3, we present a numerical approximation of $W_3^{\Pi}(N)$ for $N = \mathrm{diag}(1, (-1+\sqrt{3}\mathrm{i})/2, (-1-\sqrt{3}\mathrm{i})/2))$. Having in mind Theorems 2.1 and 3.1, we find $W_3^{\Pi}(N) = \{\Lambda_3((a_{lj})) : (a_{lj}) \in \partial Ort(3)\}$.

5. An example

An efficient and general method to compute the equation of the boundary of $W_k^{\Pi}(N)$ is not available in general, but only in simple cases. One might guess that every boundary point of $N = \mathrm{diag}(1, (-1+\sqrt{3}i)/2, (-1-\sqrt{3}i)/2))$ is realized as a point of

$\{\Lambda_k((a_{lj})) : (a_{lj}) \in \partial Ort(3) \cap \partial D(3)\}$.

If such a property held, it would be useful. However, the answer to this question is negative, as may be shown considering

$$W_2^{\pi}((\mathrm{diag}(1, \mathrm{i}, 0)) = \{(a_{11} + \mathrm{i}a_{12})(a_{21} + \mathrm{i}a_{22}) : (a_{ij}) \in Ort(3)\}.$$

This set is contained in the upper half-plane $\Im(Z) \geqslant 0$, and due to its invariance under the transformation $(a_{11}, a_{12}, a_{21}, a_{22}) \mapsto (a_{22}, a_{21}, a_{12}, a_{11})$, it is symmetric relatively to the imaginary axis. It can be easily seen that $-1/4 \leqslant \Re(Z) \leqslant 1/4$ and $\Im(Z) \leqslant 1$ for every $Z \in W_2^{\Pi}(\mathrm{diag}(1, i, 0))$. Let (a_{lj}) be an arbitrary point of $\partial Ort(3)$ satisfying $a_{lj} > 0$ $(l, j = 1, 2, 3)$. The equation of $\partial Ort(3)$ is (cf. [9])

$$\begin{aligned} &F(a_{11}, a_{12}, a_{21}, a_{22}) \\ &\quad = a_{11}^2 a_{22}^2 + a_{12}^2 a_{21}^2 - 2a_{11}a_{22}a_{12}a_{21} - 2a_{11}a_{22}(a_{11} + a_{22}) - 2a_{12}a_{21}(a_{12} + a_{21}) \\ &\qquad - 2(a_{11}a_{12}a_{21} + a_{11}a_{12}a_{22} + a_{11}a_{21}a_{22} + a_{12}a_{21}a_{22}) + a_{11}^2 + a_{12}^2 + a_{21}^2 + a_{22}^2 \\ &\qquad + 2(a_{11}a_{12} + a_{11}a_{21} + a_{12}a_{22} + a_{21}a_{22} + 2a_{11}a_{22} + 2a_{12}a_{21}) \\ &\qquad - 2(a_{11} + a_{12} + a_{21} + a_{22}) + 1 = 0. \end{aligned} \tag{17}$$

For $X = a_{11}a_{21} - a_{12}a_{22}$, $Y = a_{11}a_{22} + a_{12}a_{21}$, $(a_{lj}) \in Ort(3)$, consider the Jacobians

$$\begin{aligned} D_1 &= \frac{\partial(F, X, Y)}{\partial(a_{11}, a_{12}, a_{21})}, \quad D_2 = \frac{\partial(F, X, Y)}{\partial(a_{11}, a_{12}, a_{22})}, \\ D_3 &= \frac{\partial(F, X, Y)}{\partial(a_{11}, a_{21}, a_{22})}, \quad D_4 = \frac{\partial(F, X, Y)}{\partial(a_{12}, a_{21}, a_{22})}. \end{aligned}$$

A point $(a_{lj}) \in \partial Ort(3)$ is a critical point of the function $(a_{lj}) \mapsto Z = (a_{11} + ia_{12})(a_{21} + ia_{21})$ if and only if $D_1 = D_2 = D_3 = D_4 = 0$. Then we get

$$\begin{aligned} D_1 - D_2 + D_3 - D_4 &= 2(a_{11}a_{21} + a_{12}a_{22})(a_{11}a_{22} - a_{12}a_{21})(a_{11} + a_{12} - a_{21} - a_{22}) \\ &= 0. \end{aligned}$$

Since $a_{11}a_{21} + a_{12}a_{22} > 0$, at a critical point we have

$$a_{11}a_{22} = a_{12}a_{21}, \tag{18}$$

or

$$a_{11} + a_{12} = a_{21} + a_{22}. \tag{19}$$

By simple calculations, we can conclude that under the assumption $a_{ij} > 0$, every critical point (a_{lj}) satisfies Eq. (19), that is, $a_{13} = a_{23}$. We solve (19) in a_{22}, substitute the solution in (17) and obtain

$$\begin{aligned} &(a_{11} + a_{12})^2(a_{11} - a_{21})^2 - 4(a_{11} + a_{12})(a_{11}^2 + a_{11}a_{12} - a_{11}a_{21} + a_{12}a_{21}) \\ &\quad + 6a_{11}^2 + 4a_{12}^2 + 10a_{11}a_{12} - 2a_{11}a_{21} + 2a_{12}a_{21} - 4a_{11} - 4a_{12} + 10. \end{aligned} \tag{20}$$

By the condition $a_{21} \leqslant 1$, the solution of (20) in a_{21} is given on the quadrilateral

$$\left\{(a_{11}, a_{12}) \in \mathbf{R}^2 : 0 \leqslant a_{11}, 0 \leqslant a_{12}, \frac{1}{2} \leqslant a_{11} + a_{12} \leqslant 1\right\}.$$

Using this solution, we can determine the part of $W_2^{\Pi}(\mathrm{diag}(1, \mathrm{i}, 0))$ corresponding to the condition $a_{11} + a_{12} = a_{21} + a_{22}$:

$$\Gamma_0 = \{(a_{11} + \mathrm{i}a_{12})(a_{21} + \mathrm{i}a_{22}) : (a_{ij}) \in \partial Ort(3), a_{11} + a_{12} = a_{21} + a_{22}\}. \tag{21}$$

This set is a simply connected closed region bounded by four arcs. By the elimination method (cf. [14]), we can compute the equations of these boundary arcs. The boundary is a simple closed curve consisting of four irreducible algebraic arcs: the parabolic arcs

$$\Re(Z) = \Im(Z)^2 - \frac{1}{4}, \quad \Re(Z) = -\Im(Z)^2 + \frac{1}{4}, \quad 0 \leqslant \Im(Y) \leqslant \left(\sqrt{2} - 1\right)\Big/ 2, \tag{22}$$

the parabolic arc

$$\Im(Z) = -2\Re(Z)^2 + \frac{1}{8}, \quad -1/4 \leqslant \Re(Z) \leqslant 1/4$$

and an arc of the deltoid

$$\begin{aligned} G(\Re(Z), \Im(Z)) = \{\Re(Z)^2 + \Im(Z)^2\}^2 + 14\Re(Z)^2\Im(Z) \\ - 2\Im(Z)^3 + 11\Re(Z)^2 + 2\Im(Z) - 1 = 0. \end{aligned}$$

This arc intersects the arcs in (22) at $(\pm(\sqrt{2} - 1)/2, (\sqrt{2} - 1)/2)$. Under the condition $a_{22} = a_{11} + a_{12} - a_{21}$, the polynomials D_1, D_2, D_3, D_4 are respectively rewritten as

$$\begin{aligned} D_1 &= 2(a_{11} + a_{12} - a_{21})(1 - a_{11} - a_{12}) \\ &\quad \times (a_{11} - a_{21})(a_{12}^2 + a_{11}a_{12} + a_{11}a_{21} - a_{12}a_{21} + a_{11} + a_{12} - 1), \\ D_2 &= -2a_{21}(1 - a_{11} - a_{12})(a_{11} - a_{21}) \\ &\quad \times (a_{12}^2 + a_{11}a_{12} + a_{11}a_{21} - a_{12}a_{21} + a_{11} + a_{12} - 1), \\ D_3 &= -2a_{12}(1 - a_{11} - a_{12})(a_{11} - a_{21}) \\ &\quad \times (a_{12}^2 + a_{11}a_{12} + a_{11}a_{21} - a_{12}a_{21} + a_{11} + a_{12} - 1), \\ D_4 &= 2a_{11}(1 - a_{11} - a_{12})(a_{11} - a_{21})(a_{12}^2 + a_{11}a_{12} + a_{11}a_{21} - a_{12}a_{21} + a_{11} + a_{12} - 1). \end{aligned}$$

Thus, under the conditions $a_{ij} > 0$ for $i, j = 1, 2, 3$, each of the conditions $D_1 = 0$, $D_2 = 0$, $D_3 = 0$, $D_4 = 0$ is equivalent to

$$(a_{11} - a_{21})(a_{12}^2 + a_{11}a_{12} + a_{11}a_{21} - a_{12}a_{21} + a_{11} + a_{12} - 1) = 0. \tag{23}$$

The critical values corresponding to the condition $a_{11} = a_{21}$ are the parabolic arc $\Im(Z) = -2\Re(Z)^2 + (1/8)$. The deltoid part and the parabolic arcs $\pm\Re(Z) = \Im(Z)^2 - (1/4)$ intersect at the annihilating points of the second factor of (23).

We determine the part of $W_2^{\Pi}(\mathrm{diag}(1, i, 0))$ corresponding to the intersection of $\partial Ort(3)$ with the nine faces of $D(3)$. Let

$$\Gamma_1 = \{(a_{11} + \mathrm{i}a_{12})(a_{21} + \mathrm{i}a_{22}) : (a_{ij}) \in \partial Ort(3), a_{31} = 0\}$$

and

$$\Gamma_2 = \{(a_{11} + \mathrm{i}a_{12})(a_{21} + \mathrm{i}a_{22}) : (a_{ij}) \in \partial Ort(3), a_{32} = 0\},$$

that satisfy $\Gamma_2 = \{-\overline{Z} : Z \in \Gamma_1\}$. The condition $a_{31} = 0$ implies $a_{11}a_{12} - a_{22} + a_{11}a_{22} = 0$. Then $a_{11} = 0$ implies $a_{22} = 0$ and so $a_{11}a_{21} - a_{12}a_{22} = 0$. If $a_{11} > 0$, then $a_{12} = a_{22}(1 - a_{11})/a_{11}$, $a_{12} + a_{22} = a_{22}/a_{11}$ and so $a_{22} \leqslant a_{11}$. It follows that

$$a_{11}a_{21} - a_{12}a_{22} = \frac{(a_{11} - a_{22})(a_{11} + a_{22})(1 - a_{11})}{a_{11}} \geqslant 0.$$

The set Γ_1 consists of parabolic arcs

$$\Re(Z) = \frac{(a_{11}^2 - a_{11})\Im(Z)^2 - 4a_{11}^6 + 12a_{11}^5 - 16a_{11}^4 + 12a_{11}^3 - 5a_{11}^2 + a_{11}}{(2a_{11}^2 - 2a_{11} + 1)^2},$$

$0 \leqslant \Im(Z) \leqslant 1$, $0 \leqslant a_{11} \leqslant 1$ for $0 \leqslant \Im(Z) \leqslant 1/2$, $0 \leqslant a_{11} \leqslant (1 - \sqrt{2\Im(Z) - 1})/2$. We determine the envelope of these arcs by the elimination method, and we obtain the quartic curve:

$$\Re(Z)^2\Im(Z)^2 + \Im(Z)^4 - 8\Re(Z)^3 - 10\Re(Z)\Im(Z)^2 + 12\Re(Z)^2 - 2\Im(Z)^2 - 6\Re(Z) + 1 = 0$$

for $\sqrt{3}/6 \leqslant \Im(Z) \leqslant 1$, and the parabola

$$\Re(Z) = -\Im(Z)^2 + \frac{1}{4}$$

for $0 \leqslant \Im(Z) \leqslant \sqrt{6} \leqslant \sqrt{3}/6$. The part of these arcs corresponding to $(\sqrt{2} - 1)/2 < \Im(z) < 1$ is contained in the interior of (21).

The set $\Gamma_1 \cup \Gamma_2$ contains

$$\{Z : -1/4 < \Re(Z) < 1/4, 0 \leqslant \Im(Z) < -2\Re(Z)^2 + (1/8)\},$$

which does not intersect (21). The other part of $\Gamma_1 \cup \Gamma_2$ is contained in (21).

We also have

$$\begin{aligned}
&\{(a_{11} + \mathrm{i}a_{12})(a_{21} + \mathrm{i}a_{22}) : (a_{ij}) \in \partial Ort(3), a_{11}a_{12}a_{21}a_{22} = 0\} \\
&\quad = \{Z : 0 \leqslant \Im(Z) \leqslant 1, |\Re(Z)| \leqslant (1 - \Im(Z))^2/4\} \subset \Gamma_1 \cup \Gamma_2, \\
&\{(a_{11} + \mathrm{i}a_{12})(a_{21} + \mathrm{i}a_{22}) : (a_{ij}) \in \partial Ort(3), a_{13}a_{23} = 0\} = \{\mathrm{i}t : 0 \leqslant t \leqslant 1\} = \Gamma_1 \cap \Gamma_2, \\
&\Gamma_3 = \{(a_{11} + \mathrm{i}a_{12})(a_{21} + \mathrm{i}a_{22}) : (a_{ij}) \in \partial Ort(3), a_{33} = 0\} \\
&\quad = \{Z : -1/4 \leqslant \Re(Z) \leqslant 1/4, 0 \leqslant \Im(Z) \leqslant -2\Re(Z)^2 + (1/8)\}.
\end{aligned}$$

The simply connected closed region

$$\begin{aligned}
\Gamma_0 \cup \Gamma_3 = &\{Z : 0 \leqslant \Im(Z) \leqslant (\sqrt{2} - 1)/2, |\Re(Z)| \leqslant 1/4 - \Im(Z)^2\} \\
&\cup \{Z : (\sqrt{2} - 1)/2 \leqslant \Im(Z) \leqslant 1, \ G(\Re(Z), \Im(Z)) \leqslant 0\}
\end{aligned}$$

contains the set $\Gamma_1 \cup \Gamma_2$. By Theorem 3.1, we conclude that $\Gamma_0 \cup \Gamma_3$ contains $\partial W_2^{\Pi}(N)$ and it is contained in $W_2^{\Pi}(N)$. By the simple connectedness of the region $\Gamma_0 \cup \Gamma_3$, we conclude that it coincides with $W_2^{\Pi}(\mathrm{diag}(1, \mathrm{i}, 0))$.

Acknowledgements

The authors acknowledge the referees careful reading of the manuscript and valuable suggestions.

References

[1] Y.H. Au-Yeung, Y.T. Poon, 3 × 3 orthostochastic matrices and the convexity of generalized numerical ranges, Linear Algebra Appl. 27 (1979) 69–79.

[2] I. Bengtsson, A. Ericsson, M. Kuś, W. Tadej, K. Życzkowski, Birkhoff's polytope and unistochastic matrices, $N = 3$ and $N = 4$, Comm. Math. Phys. 259 (2005) 307–324.

[3] N. Bebiano, C.K. Li, J. da Providência, Product of diagonal elements of matrices, Linear Algebra Appl. 178 (1993) 185–200.
[4] W.-S. Cheung, N.-K. Tsing, The *C*-numerical range of matrices is star-shaped, Linear and Multilinear Algebra 41 (1996) 245–250.
[5] P. Diţă, Separation of unistochastic matrices from the double stochastic ones: recovery of a 3×3 unitary matrix from experimental data, J. Math. Phys. 47 (8) (2006) 24, 083510.
[6] M. Goldberg, E.G. Straus, Elementary inclusion relations for generalized numerical ranges, Linear Algebra Appl. 18 (1977) 1–24.
[7] M. Marcus, Derivations, Plüker relations, and the numerical range, Indiana Univ. Math. J. 22 (1972–1973) 1137–1149.
[8] A.W. Marshall, I. Olkin, Inequalities: Theory of Majorization and Its Applications, Academic Press, San Diego, New York, 1979.
[9] H. Nakazato, Set of 3×3 orthostochastic matrices, Nihonkai Math. J. 7 (1996) 83–100.
[10] M.A. Naimark, Linear Representation of the Lorentz Group, Pergamon Press, Oxford, London, 1964.
[11] H. Nakazato, N. Bebiano, J. da Providência, *J*-orthostochastic matrices of size 3×3 and numerical ranges of Krein space operators, Linear Algebra Appl. 407 (2005) 211–232.
[12] I.M. Singer, J.A. Thorpe, Lecture Notes on Elementary Topology and Geometry, Springer, New York, 1996.
[13] N.-K. Tsing, On the shape of generalized numerical ranges, Linear and Multilinear Algebra 10 (1981) 173–182.
[14] B.L. van der Waerden, Algebra, Springer, New York, Berlin, Heidelberg, 1991.