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Davis–Wielandt shell and q-numerical range

Mao-Ting Chien [a,*,1], Hiroshi Nakazato [b]

[a] *Department of Mathematics, Soochow University, Taipei 11102, Taiwan, ROC*
[b] *Department of Mathematical System Science, Faculty of Science and Technology, Hirosaki University, Hirosaki 036-8561, Japan*

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Abstract

We describe the boundary of the q-numerical range of a square matrix using its Davis–Wielandt shell. The result is used to generate an algorithm for plotting the q-numerical range of the square matrix. Computations of the q-numerical ranges of a special class of matrices are explicitly given. © 2002 Elsevier Science Inc. All rights reserved.

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1. Introduction

Let M_n be the algebra of $n \times n$ complex matrices. For $A \in M_n$ and $q \in \mathbb{C}$ with $|q| \leqslant 1$, the q-numerical range of A is the set denoted and defined by

$$W_q(A) = \left\{x^*Ay\colon x, y \in \mathbb{C}^n, |x| = |y| = 1, x^*y = q\right\}.$$

The q-numerical radius $w_q(A)$ of A is the maximum modulus of any point in $W_q(A)$. If $q = 1$, $W_q(A)$ reduces to the (classical) numerical range which is usually denoted by

$$W(A) = \left\{x^*Ax\colon x \in \mathbb{C}^n, |x| = 1\right\}.$$

* Corresponding author. Tel.: +886-2-881-9471; fax: +886-2-881-1526.
Email-addresses: mtchien@math.scu.edu.tw (M.-T. Chien), nakahr@cc.hirosaki-u.ac.jp (H. Nakazato).

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Tsing [11] showed that $W_q(A)$ is a convex set, and $W_q(A)$ is the union of circular discs:

$$W_q(A) = \bigcup_x \left\{ z \in \mathbb{C}: |z - qx^*Ax| \leqslant \sqrt{1-q^2}(\|Ax\|^2 - |x^*Ax|^2)^{1/2} \right\}, \quad (1)$$

where x runs over all unit vectors. There are several important elementary facts about the q-numerical range, such as

(i) $W_q(\alpha A + \beta I_n) = \alpha W_q(A) + \beta q$,

(ii) $W_q(U^*AU) = W_q(A)$, U unitary,

(iii) $W_{qz}(A) = zW_q(A)$, $z \in \mathbb{C}$, $|z| = 1$.

Due to facts (i) and (iii), we may assume that $0 \leqslant q \leqslant 1$. For references on further properties and results on q-numerical range, see, for instance, [5,6].

The purpose of this paper is to describe the boundary of the q-numerical range of a square matrix by involving its Davis–Wielandt shell. The result can be used to generate an algorithm for plotting the q-numerical range of the square marix. Furthermore, we consider a special class of matrices, and explicitly compute the q-numerical ranges by means of the methods that are investigated.

2. Davis–Wielandt shell

Let $A \in M_n$. The Davis–Wielandt shell of A is defined by

$$DW(A) = \left\{ (x^*Ax, x^*A^*Ax): x \in \mathbb{C}^n, |x| = 1 \right\}.$$

A close relation between the q-numerical range and the Davis–Wielandt shell was proved by Li and Nakazato in [6]. We study the boundary of the q-numerical range along this direction. For normal matrices, the boundary property of the q-numerical range is characterized in [8], and is refined in [4].

For any $A \in M_n$, the upper boundary of $DW(A)$ is defined by

$$\partial_+ DW(A) = \left\{ (z, h(z)) \in \mathbb{C} \times \mathbb{R}: z \in W(A) \right\},$$

where

$$h(z) = \max \left\{ w \in \mathbb{R}: (z, w) \in DW(A) \right\}.$$

Then Tsing's circular union (1) can be written as follows:

$$W_q(A) = \bigcup_{z \in W(A)} \left\{ \xi \in \mathbb{C}: |\xi - q\,z| \leqslant \sqrt{1-q^2}\sqrt{h(z) - |z|^2} \right\}. \quad (2)$$

From (2),

$$\partial W_q(A) \subseteq \bigcup_{z \in W(A)} \left\{ \xi \in \mathbb{C}: |\xi - q\,z| = \sqrt{1-q^2}\sqrt{h(z) - |z|^2} \right\}. \quad (3)$$

Clearly, the quantity $\sqrt{h(z) - |z|^2}$ is useful in determining the q-numerical range. We define the function

$$\Phi(z) = \sqrt{h(z) - |z|^2}, \quad z \in W(A).$$

The functions $h(z)$ and $\Phi(z)$ are non-negative upper semi-continuous concave functions on $W(A)$ (cf. [6,8,11]). Recall that $A \in M_n$ is essentially Hermitian if $aA + bI$ is Hermitian for some $a, b \in \mathbb{C}$ such that $|a| = 1$, and it is known that A is essentially Hermitian if and only if $W(A)$ is a line segment (cf. [4]). If A is essentially Hermitian, then Φ is continuous on $W(A)$. If $W(A)$ has an interior point in $\mathbb{C}$, then Φ is continous on the interior $W(A)^\circ$ of $W(A)$ and Φ is continuous on a closed sectorial region $\{z_0 + r \exp(\mathrm{i}\theta)\colon \theta_1 \leqslant \theta \leqslant \theta_2, 0 \leqslant r \leqslant \epsilon\}$ containing in $W(A)$, where $0 < \theta_2 - \theta_1 < \pi, \epsilon > 0$. Furthermore, we show that:

Theorem 1.

(i) *The function Φ has a unique maximum point.*

(ii) *Suppose that Φ is continuously differentiable on a neighborhood U of $z_0 \in W(A)^\circ$ and* $\operatorname{grad}\Phi(z_0) = 0$. *Then the point z_0 is the unique maximum point of Φ.*

Proof. (i) If A is essentially Hermitian, we may assume that $W(A) = [a, b] \subset \mathbb{R}$, then we have

$$\Phi(ta + (1-t)b) = (b-a)\sqrt{t(1-t)}, \quad 0 \leqslant t \leqslant 1.$$

Hence the function Φ has a unique maximum point $(a + b)/2$. If A is not essentially Hermitian, then $W(A)$ has an interior point. Since Φ is bounded, we take a convergent sequence $\{z_n\colon n \in \mathbb{N}\} \subset W(A),\ z_n \to z_0$, and

$$\lim \Phi(z_n) = \sup\{\Phi(z)\colon z \in W(A)\}.$$

The upper semi-continuity of Φ assures that z_0 is a maximum point of Φ. Suppose that Φ has another maximum point at z_1. Since Φ is concave, it follows that $\Phi^2(z) = h(z) - |z|^2$ is constant on the line segment $[z_0, z_1]$. Hence the function $h(z)$ restricted to $[z_0, z_1]$ becomes

$$h(z) = |z|^2 + c, \quad z \in [z_0, z_1] \text{ for some constant } c.$$

But then, $h(z)$ is strictly convex on this line segment, a contradiction to the concaveness of $h(z)$.

(ii) We prove that z_0 is a maximum point of Φ, and is therefore the unique maximum point by (i). If there would exist a point $z_1 \in W(A)$ such that $\Phi(z_1) > \Phi(z_0)$, we choose $t_1 \in (0, 1)$ small enough, so that $z_2 = (1 - t_1)z_0 + t_1 z_1 \in U$. Then

$$\Phi(z_2) \geqslant (1 - t_1)\Phi(z_0) + t_1\Phi(z_1) > \Phi(z_0).$$

Consider the function

$$f(t) = \Phi((1-t)z_0 + t z_2), \quad 0 \leqslant t \leqslant 1.$$

By the mean value theorem, there exists a point $0 < t_2 < 1$ such that $f'(t_2) = f(1) - f(0) = \Phi(z_2) - \Phi(z_0) > 0$. Then $f'(0) > 0$ since f is concave. This contradicts $\operatorname{grad}\Phi(z_0) = 0$. $\square$

Motivated by the inclusion (3), we define

$$B_q(A) = \Big\{ z \in W(A)\colon\ qz + r\sqrt{1-|q|^2}\,\Phi(z) \in \partial W_q(A) \quad \text{for some } r \in \mathbb{C},\ |r| = 1 \Big\}.$$

We obtain the following characterization:

Theorem 2. *Let $A \in M_n$ and $0 < q < 1$. Then*

$$B_q(A) \cap \Big\{ (x+\mathrm{i}y) \in W(A)^\circ\colon\ \Phi \text{ is continuously differentiable on a neighborhood of } x+\mathrm{i}y \Big\}$$
$$\subset \Big\{ x+\mathrm{i}y \in W(A)^\circ\colon\ \Phi_x(x+\mathrm{i}y)^2 + \Phi_y(x+\mathrm{i}y)^2 = q^2/(1-q^2) \Big\}.$$

Proof. First we show that for each $\eta \in \mathbb{R}$, there exists a unique point $z_0 \in W_q(A)$ such that

$$\Re(z_0 \mathrm{e}^{-\mathrm{i}\eta}) = \max\Big\{ \Re(z\mathrm{e}^{-\mathrm{i}\eta})\colon z \in W_q(A) \Big\}.$$

The existence is trivial. Suppose that w_1 and w_2 are distinct in

$$S_\eta = \Big\{ w \in W_q(A)\colon \Re(w\mathrm{e}^{-\mathrm{i}\eta}) = \max\{\Re(z\mathrm{e}^{-\mathrm{i}\eta})\colon z \in W_q(A)\} \Big\}.$$

Then

$$\{sw_1 + (1-s)w_2\colon 0 \leqslant s \leqslant 1\} \subset S_\eta. \tag{4}$$

Assume that $z_1 \neq z_2$ are two points in $W(A)$ such that

$$w_j = qz_j + \sqrt{1-q^2}\,\mathrm{e}^{\mathrm{i}\eta}\Phi(z_j), \quad j = 1, 2. \tag{5}$$

By a result in [3] (see also [6, 3.2]) that Φ is strictly concave on $W(A)$, namely,

$$\frac{\Phi(x)+\Phi(y)}{2} < \Phi\left(\frac{x+y}{2}\right) \quad \text{for any } x, y \in W(A).$$

Together this concavity with (5), we obtain that

$$\Re\left(\left(q\frac{z_1+z_2}{2} + \sqrt{1-q^2}\,\mathrm{e}^{\mathrm{i}\eta}\Phi\left(\frac{z_1+z_2}{2}\right) \right) \mathrm{e}^{-\mathrm{i}\eta} \right) > \Re\left(\frac{w_1+w_2}{2}\mathrm{e}^{-\mathrm{i}\eta} \right),$$

a contradiction to (4) by taking $s = 1/2$, and thus we have the uniqueness.

If $z_0 \in B_q(A)$ and Φ is continuously differentiable on a neighborhood U of z_0, then the vector $(\Phi_x(z_0), \Phi_y(z_0)) \neq 0$. Otherwise we have $\mathrm{grad}(\Phi)(z_0) = 0$. Choose a real number θ such that

$$q\,z_0 + \sqrt{1-q^2}\,\mathrm{e}^{\mathrm{i}\theta}\Phi(z_0) \in \partial W_q(A). \tag{6}$$

Consider functions

$$g(t) = q\,(z_0 + t\mathrm{e}^{\mathrm{i}\theta}) + \sqrt{1-q^2}\mathrm{e}^{\mathrm{i}\theta}\Phi(z_0 + t\mathrm{e}^{\mathrm{i}\theta}) \tag{7}$$

and

$$g_1(t) = \mathrm{e}^{-\mathrm{i}\theta}(g(t) - g(0)) \tag{8}$$

for $t \in \mathbb{R}$ with $|t|$ being sufficient small. Observe that we may express $g_1(t)$ in terms of Φ:

$$g_1(t) = q\,t + \sqrt{1-q^2}\left(\Phi(z_0 + t\mathrm{e}^{\mathrm{i}\theta}) - \Phi(z_0)\right).$$

From condition (6), $g_1(0)$ is a local maximum of the function g_1. On the other hand, we find that $g_1'(0) = q > 0$, this is impossible. Therefore, there exist $a > 0$ and $\psi \in \mathbb{R}$ such that

$$(\Phi_x(z_0), \Phi_y(z_0)) = -a\,(\cos\psi, \sin\psi)). \tag{9}$$

It is known (cf. [5, Theorem 3]) that the boundary of $W_q(A)$ is a C^1-curve. Hence the boundary point

$$p = qz_0 + \sqrt{1-q^2}\mathrm{e}^{\mathrm{i}\,\eta}\Phi(z_0) \in \partial W_q(A) \quad \text{for some } \eta$$

has a unique tangent to $\partial W_q(A)$ which is written by

$$\left\{p + t\,\mathrm{e}^{\mathrm{i}\,(\eta+\pi/2)}: t \in \mathbb{R}\right\}.$$

Define two functions $h(t)$ and $h_1(t)$ by replacing θ with η in (7) and (8), respectively,

$$h(t) = q(z_0 + \mathrm{e}^{\mathrm{i}\eta}) + \sqrt{1-q^2}\mathrm{e}^{\mathrm{i}\eta}\Phi(z_0 + \mathrm{e}^{\mathrm{i}\eta}), \tag{10}$$

and

$$h_1(t) = \mathrm{e}^{\mathrm{i}\eta}(h(t) - h(0))$$

for $t \in \mathbb{R}$. Then $h_1(t)$ assumes its local maximum at $t = 0$, and thus $h'(0) = 0$. It follows from (10) that

$$\frac{\mathrm{d}}{\mathrm{d}t}\Big|_{t=0}\Phi(z_0 + t\,\mathrm{e}^{\mathrm{i}\,\eta}) = -\frac{q}{\sqrt{1-q^2}}. \tag{11}$$

Note that the region

$$\left\{z \in W(A): \Phi(z) \geqslant \Phi(z_0)\right\}$$

is a convex set. By the implicit function theorem, there exists a C^1-curve Γ in a neighborhood U of z_0 such that

$$\Gamma = \left\{z \in U: \Phi(z) = \Phi(z_0)\right\},$$

and the tangent of Γ at z_0 is given by

$$\{z_0 + s\mathrm{e}^{\mathrm{i}(\psi+\pi/2)}: s \in \mathbb{R}\}.$$

Moreover,

$$\left\{q\, z + s \exp(\mathrm{i}\,\eta)\sqrt{1-q^2}\,\Phi(z): z \in \Gamma, 0 \leqslant s \leqslant 1\right\}$$
$$= \left\{q\, z + s \exp(\mathrm{i}\,\eta)\sqrt{1-q^2}\,\Phi(z_0): z \in \Gamma, 0 \leqslant s \leqslant 1\right\} \subset W_q(A).$$

If η and ψ are not congruent mod 2π, there would exist a point $z_1 \in W_q(A)$ near p such that $\Re(z_1\mathrm{e}^{-\mathrm{i}\,\eta}) > \Re(p\mathrm{e}^{-\mathrm{i}\,\eta})$, a contradiction to the assumption on p. Thus $\eta = \psi$ mod 2π, and the conclusion follows from (9) and (11). □

The following result is obtained in [8], it is also an immediate consequence of Theorem 2.

Corollary 3. *Let* $A = \mathrm{diag}(\alpha_1, \alpha_2, \alpha_3) \in M_3$ *be a unitary matrix with distinct diagonals. Then*

$$B_q(A) \cap \mathrm{conv}\{\alpha_1, \alpha_2, \alpha_3\}^\circ = \left\{z:\ z \in \mathrm{conv}\{\alpha_1, \alpha_2, \alpha_3\}^\circ, |z| = q\right\}.$$

Proof. In this case, $\Phi(z) = (1-|z|^2)^{1/2}$, and

$$\left\{(x+\mathrm{i}y): \Phi_x(x+\mathrm{i}y)^2 + \Phi_y(x+\mathrm{i}y)^2 = \frac{q^2}{(1-q^2)}\right\}$$
$$= \left\{(x+\mathrm{i}y): x^2+y^2 = q^2\right\}.$$

On the other hand, if $z = q\mathrm{e}^{\mathrm{i}\theta} \in \mathrm{conv}\{\alpha_1, \alpha_2, \alpha_3\}^\circ$ for some θ, then

$$qz + \sqrt{1-q^2}\mathrm{e}^{\mathrm{i}\theta}\,\Phi(z) = q^2\mathrm{e}^{\mathrm{i}\theta} + (1-q^2)\mathrm{e}^{\mathrm{i}\theta} = \mathrm{e}^{\mathrm{i}\theta} \in \partial W_q(A). \qquad \square$$

In the following, we compute the region in Theorem 2 for some concrete matrices.

Example 1. Let

$$A = \begin{pmatrix} 0 & \alpha \\ \beta & 0 \end{pmatrix}, \quad 0 < \beta < \alpha.$$

By the well-known elliptic theorem for the classical numerical range, we have

$$W(A) = \left\{x+\mathrm{i}y: (x,y)^2, ((\alpha+\beta)/2)^{-2}\ x^2 + ((\alpha-\beta)/2)^{-2}\ y^2 \leqslant 1\right\}.$$

It is shown in [9], see also [3,8], that

$$\Phi(x+\mathrm{i}y) = \Big((\alpha^2+\beta^2)/2 - (x^2+y^2)$$
$$+(1/2)(\alpha^2-\beta^2)\sqrt{1-4(\alpha+\beta)^{-2}\,x^2 - 4(\alpha-\beta)^{-2}\,y^2}\Big)^{1/2}.$$

Hence

$$\Phi_x(x+\mathrm{i}y)^2+\Phi_y(x+\mathrm{i}y)^2=4\frac{(\alpha-\beta)^2x^2+(\alpha+\beta)^2y^2}{(\alpha^2-\beta^2)^2-4(\alpha-\beta)^2x^2-4(\alpha+\beta)^2y^2}.$$

Furthermore, for $0<q<1$,

$$\Phi_x\left(q\,\frac{\alpha+\beta}{2}\,\cos\theta+\mathrm{i}q\,\frac{\alpha-\beta}{2}\,\sin\theta\right)^2$$
$$+\Phi_y\left(q\,\frac{\alpha+\beta}{2}\cos\theta+\mathrm{i}q\frac{\alpha-\beta}{2}\,\sin\theta\right)^2=\frac{q^2}{1-q^2},$$

and thus we have

$$B_q(A)=\left\{q\,\frac{\alpha+\beta}{2}\,\cos\theta+\mathrm{i}q\,\frac{\alpha-\beta}{2}\,\sin\theta\colon 0\leqslant\theta\leqslant 2\pi\right\}.$$

Example 2. Consider the matrix

$$A=\mathrm{diag}(\alpha_1,\alpha_2,\alpha_3),$$

where $\alpha_1,\alpha_2,\alpha_3$ are vertices of a non-degenerate triangle. We take $z_0\in\mathbb{C}$ so that

$$|\alpha_0-z_0|=|\alpha_2-z_0|=|\alpha_3-z_0|=R.$$

Then by Corollary 3

$$\left\{(x+\mathrm{i}y)\in W(A)^\circ\colon \Phi_x(x+\mathrm{i}y)^2+\Phi_y(x+\mathrm{i}y)^2\leqslant\frac{q^2}{(1-q^2)}\right\}$$
$$=\left\{(x+\mathrm{i}y)\in\mathrm{conv}\{\alpha_1,\alpha_2,\alpha_3\}^\circ\colon |x+\mathrm{i}y-z_0|\leqslant Rq\right\}. \tag{12}$$

By using this fact we can construct a 4×4 diagonal matrix A for which the set (12) is not convex. For instance, let

$$A=\mathrm{diag}(\alpha_1,\alpha_2,\alpha_3,\alpha_4),$$

where

$$\alpha_1=2/3,\alpha_2=-4/3,\alpha_3=\mathrm{i}\sqrt{20}/3,\alpha_4=-\mathrm{i}\sqrt{20}/3.$$

By [8, Theorem 1.1],

$$W_q(A)=\bigcup\left\{W_q(\mathrm{diag}(\alpha_{j_1},\alpha_{j_2},\alpha_{j_3}))\colon 1\leqslant j_1<j_2<j_3\leqslant 4\right\}.$$

We observe that

$$A_1=\frac{1}{2}\left(\mathrm{diag}(\alpha_1,\alpha_3,\alpha_4)+\frac{4}{3}I_3\right)$$

and

$$A_2=\frac{2}{3}\left(\mathrm{diag}(\alpha_2,\alpha_3,\alpha_4)-\frac{1}{6}I_3\right)$$

are 3×3 unitary matrices with distinct diagonals. Then the points $\alpha_1, \alpha_3, \alpha_4$ lie on the circle

$$(x + 4/3)^2 + y^2 = 4,$$

and the point α_2 is an interior point of this circle. Similarly, the points $\alpha_2, \alpha_3, \alpha_4$ lie on the circle

$$(x - 1/6)^2 + y^2 = 9/4,$$

and the point α_1 is an interior point of this circle. Hence, by Corollary 3,

$$\begin{aligned}&\left\{(x + \mathrm{i}y) \in W(A)^\circ\colon \Phi_x(x + \mathrm{i}y)^2 + \Phi_y(x + \mathrm{i}y)^2 \leqslant \frac{q^2}{(1 - q^2)}\right\}\\ &\quad = \left\{z = x + \mathrm{i}y\colon x > 0,\ z \in \operatorname{conv}\{\alpha_1, \alpha_3, \alpha_4\}, |z + 4/3| \leqslant 2q\right\}\\ &\qquad \cup \left\{z = x + \mathrm{i}y\colon x < 0,\ z \in \operatorname{conv}\{\alpha_2, \alpha_3, \alpha_4\}, |z - 1/6| \leqslant (3/2)q\right\}.\end{aligned}$$

It is obvious that this is not a convex set.

So far, we focused on those points $z \in W(A)^\circ$ at which Φ is differentiable. We now examine those non-differentiable points $z \in W(A)^\circ$ of Φ.

Lemma 4. *Suppose that $F(x, y, z) \in \mathbb{C}[x, y, z]$ is an irreducible polynomial with $\deg_z(F) \geqslant 1$ and $G(x, y, z) \in \mathbb{C}[x, y, z]$ satisfies one of the following two conditions*:

(i) *G is an irreducible polynomial with $\deg_z(G) \geqslant 1$ and satisfies $G \neq \lambda F$ for every $\lambda \in \mathbb{C}$,*

(ii) *$G = \partial F/\partial z$ and $\deg_z(G) \geqslant 1$.*

Then there exists a non-zero polynomial $L \in \mathbb{C}[x, y]$ such that

$$\begin{aligned}&\left\{(x, y) \in \mathbb{C}^2\colon\ F(x, y, z) = G(x, y, z) = 0 \text{ for some } z\right\}\\ &\quad \subset \left\{(x, y) \in \mathbb{C}^2\colon\ L(x, y) = 0\right\}.\end{aligned}$$

Proof. Suppose that the respective leading terms of F and G with respect to z are $a_n(x, y)$ and $b_m(x, y) \in \mathbb{C}[x, y]$. Then $a_n(x, y)\, b_m(x, y)$ is a non-zero polynomial. We take the resultant $R(x, y)$ of the polynomials $F(x, y, z)$ and $G(x, y, z)$ with respect to the indeterminate z (cf. [12, p. 21]). By conditions (i) or (ii), F and G have no common factor $K(x, y, z) \in \mathbb{C}[x, y, z]$ with $\deg_z(K) \geqslant 1$. Hence $R(x, y)$ is a non-zero polynomial. The field $\mathbb{C}$ is algebraically closed of characteristic 0. Hence for every fixed $(x, y) \in \mathbb{C}^2$ with $a_n(x, y)\, b_m(x, y) \neq 0$, the existence of z satisfying $F(x, y, z) = G(x, y, z) = 0$ is equivalent to $R(x, y) = 0$. Then $L = a_n\, b_m\, R$ is the polynomial required. □

Theorem 5. *Let $A \in M_n$ be a non-essentially Hermitian matrix. Then there exists a non-zero real polynomial $f(x, y)$ for which $h(z)$ and $\Phi(z)$ are real analytic on the open set*

$$\left\{z = x + \mathrm{i}y \in W(A)^\circ:\ (x, y) \in \mathbb{R}^2,\ f(x, y) \neq 0\right\}.$$

Moreover, the Hessians of $-\Phi^2$ and $-\Phi$ are strictly positive definite on U. If the vector field $\operatorname{grad}(|\operatorname{grad}\Phi|^2)$ *takes the value* $(0, 0)$ *at a point z_0 of U, then* $\operatorname{grad}\Phi(z_0) = 0$ *and z_0 is the maximum point of Φ.*

Proof. Since A is not essentially Hermitian, the range $W(A)$ contains interior points. By the fact that $h(z) - |z|^2$ is stricly concave on $W(A)^\circ$, it is positive on $W(A)^\circ$. Thus for an open subset V of $W(A)^\circ$, the continuous differentiability of h and Φ on V are equivalent. Since $\partial W(A)$ is a 1-dimensional semi-algebraic set, there exists a non-zero polynomial $g_1 \in \mathbb{R}[x, y]$ such that

$$\left\{(x, y) \in \mathbb{R}^2: x + \mathrm{i}y \in \partial W(A)\right\} \subset \left\{(x, y) \in \mathbb{R}^2: g_1(x, y) = 0\right\}.$$

By Proposition 2.1 in [10], the boundary of $DW(A)$ is a semi-algebraic set, and hence there exists a non-zero polynomial $F(x, y, z) \in \mathbb{R}[x, y, z]$ such that

$$\left\{(x, y, h(x + \mathrm{i}y)): (x, y) \in \mathbb{R}^2, x + \mathrm{i}y \in W(A)\right\}$$
$$\subset \left\{(x, y, z) \in \mathbb{R}^3: F(x, y, z) = 0\right\}.$$

We may assume that F is square free. Let $F = F_1 F_2 \cdots F_m$ be the irreducible decomposition of F in $\mathbb{C}[x, y, z]$. Then by Lemma 4, for $1 \leqslant j \neq k \leqslant m$, there exists a non-zero complex polynomial $f_{j,k}(x, y) \in \mathbb{C}[x, y]$ such that

$$\left\{(x, y) \in \mathbb{R}^2: x + \mathrm{i}y \in W(A)^\circ,\ F_j(x, y, z) = F_k(x, y, z) = 0 \text{ for some } z \in \mathbb{R}\right\}$$
$$\subset \left\{(x, y) \in \mathbb{R}^2: f_{j,k}(x, y) = 0\right\}$$
$$= \left\{(x, y) \in \mathbb{R}^2: \Re f_{j,k}(x, y) = \Im f_{j,k}(x, y) = 0\right\},$$

where both $\Re f_{j,k}$ and $\Im f_{j,k}$ are real polynomials and at least one of them is non-zero. Therefore, there exists a non-zero real polynomial $g(x, y)$ with the property that if $(x, y) \in \mathbb{R}^2$, $x + \mathrm{i}y \in W(A)$ and $g(x, y) \neq 0$, then the number of the set

$$\left\{j \in \{1, 2, \ldots, m\}, F_j(x, y, z) = 0 \text{ for some } z \in \mathbb{R}\right\}$$

is at most 1.

Let $x_0 + \mathrm{i}y_0 \in W(A)$ and $g(x_0, y_0) \neq 0$. Assume that $F_j(x_0, y_0, h(x_0, y_0)) = 0$. If $\frac{\partial F_j}{\partial z}(x_0, y_0, h(x_0, y_0)) \neq 0$, then, by the implicit function theorem, the equation $F_j(x, y, z) = 0$ for z has a unique solution near $(x_0, y_0, h(x_0, y_0))$, the function h is continuously differentiable and $F_j(x, y, h(x, y)) = 0$ near (x_0, y_0). If $\frac{\partial F_j}{\partial z}(x_0, y_0,$

$h(x_0, y_0)) = 0$, then by Lemma 4, there exists a non-zero real polynomial $f_j(x, y)$ such that

$$\left\{(x, y) \in \mathbb{R}^2\colon F_j(x, y, z) = \frac{\partial F_j}{\partial z}(x, y, z) = 0 \text{ for some } z \in \mathbb{R}\right\} \subset \left\{(x, y) \in \mathbb{R}^2\colon f_j(x, y) = 0\right\}.$$

Therefore the function $f = g f_1 f_2 \cdots f_m$ has the desired property for the first part of the theorem.

Next we prove the second part of the theorem. Since $\Phi^2(z) = h(z) - |z|^2$ and h is concave, the Hessian of $-\Phi^2$ is strictly positive definite on U. Set $\Psi = \Phi^2$. Then $\Psi(z) > 0$ for $z \in U \subset W(A)^\circ$. By a direct computation, we have

$$\begin{pmatrix} -\Phi_{xx} & -\Phi_{xy} \\ -\Phi_{yx} & -\Phi_{yy} \end{pmatrix} = (\Phi^{-3}/4) \begin{pmatrix} \Psi_x^2 & \Psi_x \Psi_x \Psi_y \\ \Psi_y \Psi_x & \Psi_y^2 \end{pmatrix} + (\Phi^{-1}/2) \begin{pmatrix} -\Psi_{xx} & -\Psi_{xy} \\ -\Psi_{yx} & -\Psi_{yy} \end{pmatrix}, \tag{13}$$

where the first matrix on the right-hand side of (13) is positive semi-definite. Hence the Hessian of Φ on U is also strictly positive definite.

If $\operatorname{grad}(|\operatorname{grad}\Phi|^2)(z_0) = 0$, then we have

$$\Phi_{xx}(z_0)\Phi_x(z_0) + \Phi_{xy}(z_0)\Phi_y(z_0) = 0,$$
$$\Phi_{yx}(z_0)\Phi_x(z_0) + \Phi_{yy}(z_0)\Phi_y(z_0) = 0,$$

and thus $\operatorname{grad}\Phi(z_0) = 0$. □

The results in this section are useful to generate an algorithm for plotting the q-numerical range of a square matrix. We briefly describe this algorithm which is a refinement of the result obtained in [11]. For a given matrix $A \in M_n$, consider the function

$$F(t, x, y, z) = \det(t I_3 + (x/2)(A + A^*) - \mathrm{i}(y/2)(A - A^*) + z A^* A).$$

Let $G(t, x, y, z) = 0$ be the dual surface of $F(t, x, y, z) = 0$. By Kippenhahn method (cf. [1]), the upper boundary $\partial_+ DW(A)$ lies on the rational surface

$$\left\{(x + \mathrm{i}y,\ z)\colon (x, y, z) \in \mathbb{R}^3, G(1, x, y, z) = 0\right\}.$$

The rational curve has an implicit expression $w = \Phi(x + \mathrm{i}y)$ satisfying

$$H(x, y, w) \equiv G(1, x, y, x^2 + y^2 + w^2) = 0. \tag{14}$$

By the implicit function theory, we have the equations

$$\frac{\partial w}{\partial x} = -\frac{H_x(1, x, y, w)}{H_w(x, y, w)}, \quad \frac{\partial w}{\partial y} = -\frac{H_y(1, x, y, w)}{H_w(x, y, w)},$$

and hence

$$\left(\frac{\partial w}{\partial x}\right)^2 + \left(\frac{\partial w}{\partial y}\right)^2 = \frac{H_x(1, x, y, w)^2 + H_y(1, x, y, w)^2}{H_w(1, x, y, w)^2}.$$

The equation in Theorem 2 becomes

$$H_x(1, x, y, z)^2 + H_y(1, x, y, z)^2 - q^2/(1-q^2)\, H_w(1, x, y, z)^2 = 0. \tag{15}$$

Next we find the curve $K(x, y) = 0$ representing $B_q(A)$ which can be achieved by eliminating the variable w from Eqs. (14) and (15). Then every boundary point of $W_q(A)$ is expressed as

$$q\,(x_0 + \mathrm{i}y_0) + \sqrt{1-q^2}\,\exp(\mathrm{i}\theta)\,\Phi(x_0 + \mathrm{i}y_0),$$

for some $x_0 + \mathrm{i}y_0 \in W(A)$ with $K(x_0, y_0) = 0$. The following example illustrates the described algorithm for computing the boundary of the q-numerical range.

Example 3. Consider the 3×3 nilpotent matrix

$$A = \begin{pmatrix} 0 & 1 & 1 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix}.$$

This matrix was given in [2], and was shown that $W(A)$ is the convex hull of a cardioid. We compute that

$$\begin{aligned} &F(t, x, y, z) \\ &\quad = 4\det(tI_3 + (x/2)(A + A^*) - \mathrm{i}(y/2)(A - A^*) + zA^*A) \\ &\quad = 4t^3 - 3tx^2 + x^3 - 3ty^2 + xy^2 + 12t^2z - 4txz - x^2z - y^2z + 4tz^2. \end{aligned}$$

The dual surface $G(t, x, y, z) = 0$ of $F(t, x, y, z) = 0$ is given by the following quartic polynomial:

$$\begin{aligned} G(t, x, y, z) = {} & t^2x^2 + 4tx^3 + 20x^4 + t^2y^2 + 4txy^2 + 36x^2y^2 + 16y^4 \\ & - t^3z - 4t^2xz - 24tx^2z + 24x^3z - 20ty^2z + 24xy^2z \\ & + 4t^2z^2 - 24txz^2 + 24x^2z^2 + 24y^2z^2 - 23tz^3 + 2xz^3 + 9z^4. \end{aligned}$$

The rational surface

$$\left\{(x + \mathrm{i}y,\ z)\colon (x, y, z) \in \mathbb{R}^3, G(1, x, y, z) = 0\right\}$$

containing the upper boundary $\partial_+ DW(A)$ is parametrized by

$$\begin{aligned} x &= -\frac{-3 + 6s^2 + s^4 - 8su + 2u^2 - 2s^2u^2 + u^4}{3 + 6s^2 + 3s^4 - 16su + 10u^2 - 6s^2u^2 + 3u^4}, \\ y &= \frac{-8(-s + u)v}{3 + 6s^2 + 3s^4 - 16su + 10u^2 - 6s^2u^2 + 3u^4}, \\ z &= \frac{(1 + s^2 - u^2)(5 + s^2 - u^2)}{3 + 6s^2 + 3s^4 - 16su + 10u^2 - 6s^2u^2 + 3u^4}, \end{aligned}$$

where $s = u\,t + \sqrt{3+u^2}(1-t)$, $u = \cos\theta$, $v = \sin\theta$ and (θ, t) runs over the rectangle $\{(\theta, t)\colon -\pi/2 \leqslant \theta \leqslant \pi/2,\ 0 \leqslant t \leqslant 1\}$. The values $\Phi^2(x+\mathrm{i}y) = z - x^2 - y^2$ are parametrized by

$$\Phi^2(x+\mathrm{i}y) = \frac{2\,(1+s^2-u^2)^3\,(3+s^2-u^2)}{(3+6s^2+3s^4-16s\,u+10u^2-6s^2\,u^2+3u^4)^2}.$$

On the other hand, by using the Mathematica software for the algebraic resultant elimination of (14) and (15), we have

$$\begin{aligned} K(x,y) = {} & 223\,389 + 6\,311\,034x + 80\,606\,961x^2 + 614\,046\,456x^3 \\ & + 3\,085\,957\,422x^4 + 10\,570\,898\,604x^5 + 23\,894\,495\,422x^6 \\ & + 28\,685\,321\,136x^7 - 13\,083\,233\,427x^8 - 121\,117\,956\,966x^9 \\ & - 204\,227\,302\,239x^{10} - 95\,004\,009\,000x^{11} + 168\,927\,128\,424x^{12} \\ & + 273\,611\,545\,920x^{13} + 123\,125\,195\,664x^{14} + 10\,512\,585y^2 \\ & + 216\,978\,696\,xy^2 + 1\,955\,648\,628\,x^2y^2 + 9\,918\,540\,024x^3y^2 \\ & + 29\,134\,549\,626x^4y^2 + 36\,348\,112\,944x^5y^2 \\ & - 68\,307\,170\,940x^6y^2 - 386\,465\,976\,792x^7y^2 \\ & - 672\,250\,911\,651x^8y^2 - 257\,010\,845\,400x^9y^2 \\ & + 860\,396\,307\,192x^{10}y^2 + 1\,340\,696\,575\,008x^{11}y^2 \\ & + 615\,625\,978\,320x^{12}y^2 + 128\,364\,246y^4 + 1\,613\,072\,748xy^4 \\ & + 7\,314\,311\,754\,x^2y^4 + 4\,831\,291\,728x^3y^4 \\ & - 94\,191\,742\,242x^4y^4 - 439\,439\,167\,332x^5y^4 \\ & - 793\,507\,344\,246x^6y^4 - 139\,445\,884\,368x^7y^4 \\ & + 1\,752\,313\,944\,528x^8y^4 + 2\,626\,670\,840\,832x^9y^4 \\ & + 1\,231\,251\,956\,640x^{10}y^4 - 93\,649\,778y^6 \\ & - 3\,689\,597\,232xy^6 - 42\,755\,420\,700x^2y^6 - 203\,952\,232\,152x^3y^6 \\ & - 379\,475\,837\,766x^4y^6 + 173\,687\,329\,296x^5y^6 \\ & + 1\,783\,835\,274\,672x^6y^6 + 2\,571\,948\,531\,648x^7y^6 \\ & + 1\,231\,251\,956\,640x^8y^6 - 3\,787\,615\,971y^8 - 29\,861\,084\,646xy^8 \\ & - 46\,296\,778\,203x^2y^8 + 212\,688\,975\,096x^3y^8 \\ & + 907\,678\,302\,408x^4y^8 + 1\,258\,613\,111\,232x^5y^8 \\ & + 615\,625\,978\,320x^6y^8 + 7\,695\,324\,729y^{10} \\ & + 61\,562\,597\,832xy^{10} + 184\,687\,793\,496x^2y^{10} \\ & + 246\,250\,391\,328x^3y^{10} + 123\,125\,195\,664x^4y^{10}. \end{aligned}$$

Now the boundary of $W_q(A)$ can be obtained by plotting

$$q\,(x+\mathrm{i}y) + \sqrt{1-q^2}\,\exp(\mathrm{i}\theta)\,\Phi(x+\mathrm{i}y),$$

where $x + \mathrm{i}y \in W(A)$ runs over the curve $K(x, y) = 0$.

3. Unilateral shift

Suppose that $A_n \in M_n$ is the unilateral shift matrix

$$A_n = \begin{pmatrix} 0 & 1 & 0 & \dots & 0 \\ 0 & 0 & 1 & \dots & 0 \\ \dots & \dots & \dots & \dots & \dots \\ 0 & \dots & \dots & \dots & 1 \\ 0 & 0 & 0 & \dots & 0 \end{pmatrix}.$$

It is well known, see for example [1, 3.1], that $W_q(A_n)$ is a circular disc centered at the origin with radius $w_q(A_n)$. In their paper [6], Li and Nakazato showed that for $n = 3$ and $1/2 \leqslant q \leqslant 1$,

$$w_q(A_n) = (1/8)\left(27 + 18q - 13q^2 + (9 + 7q)\left((1 - q)(9 + 7q)\right)^{1/2}\right)^{1/2}.$$

It seems complicated to formulate $w_q(A_n)$ for general n and q. However, we have the following special result.

Theorem 6. *Let $A \in M_n$ and $0 < q < 1$. Then $w_q(A) = \|A\|$ if and only if $(q, 1) \in DW(A/\|A\|)$.*

Proof. If $(q, 1) \in DW(A/\|A\|)$, then there exists a unit vector $\xi \in \mathbb{C}^n$ such that $q\|A\| = \xi^* A\xi$ and $\|A\|^2 = |A\xi|^2$. Clearly, $w_q(A) \leqslant \|A\|$. On the other hand, by (1), we have

$$w_q(A) \geqslant \left| q\, \xi^* A\xi + \sqrt{1 - q^2}\sqrt{|A\xi|^2 - |\xi^* A\xi|^2} \right| = \|A\|,$$

and thus $w_q(A) = \|A\|$.

Conversely, suppose $w_q(A) = \|A\|$. Again, by (1), there exists a unit vector $x \in \mathbb{C}^n$ such that

$$\|A\| = w_q(A) = \left| qx^* Ax + \sqrt{1 - q^2}\sqrt{|Ax|^2 - |x^* Ax|^2} \right|. \tag{16}$$

By Cauchy–Schwartz inequality, we have

$$\begin{aligned} \|A\| = w_q(A) &\leqslant |qx * Ax| + \sqrt{1 - q^2}\sqrt{|Ax|^2 - |x^* Ax|^2} \\ &\leqslant \sqrt{q^2 + (\sqrt{1 - q^2})^2}\sqrt{|x^* Ax|^2 + (|Ax|^2 - |x^* Ax|^2)} \\ &= |Ax| \leqslant \|A\|. \end{aligned}$$

This shows that the equality holds for Cauchy–Schwartz inequality. Hence there exists a constant c such that

$$x^*Ax = cq, \tag{17}$$

$$\sqrt{|Ax|^2 - |x^*Ax|^2} = c\sqrt{1-q^2}. \tag{18}$$

Substituting (17) into (18), we have

$$c = |Ax|. \tag{19}$$

Substituting (17)–(19) into (16), we obtain $c = \|A\|$. Then (17) becomes $x^*Ax = q\|A\|$, and thus (18) becomes $|Ax|^2 = \|A\|^2$, i.e., $(q, 1) \in DW(A/\|A\|)$. □

As a consequence of Theorem 6, we have the following result for certain range of q.

Corollary 7. *Let $A_n \in M_n$ be the unilateral shift matrix, and let $0 \leqslant q \leqslant \cos(\pi/n)$. Then $w_q(A_n) = 1$.*

Proof. By [7], $W(A_{n-1})$ is a circular disc centered at the origin with radius $\cos(\pi/n)$. If $0 \leqslant q \leqslant \cos(\pi/n)$, q lies in the circular disc $W(A_{n-1})$ and thus there exists a unit vector $x = [x_2, x_3, \ldots, x_n] \in \mathbb{C}^{n-1}$ such that $x^*A_{n-1}x = q$. Set the unit vector $v = [0, x_2, x_3, \ldots, x_n] \in \mathbb{C}^n$. Then $v^*A_nv = q$ and $|A_nv|^2 = 1$. Thus $(q, 1) \in DW(A)$, and the conclusion follows from Theorem 6. □

Although the general formula of $w_q(A_n)$ is probably very complicated for arbitrary q, but it is not so difficult to compute numerically the function $w_q(A_n)$ for $0 < q < 1$. We give an algorithm that implements the computation of this function.

Let $A \in M_n$ be a strictly upper triangular whose associated non-directed graph is a tree or a union of trees. Set

$$H = (1/2)(A + A^*) \quad \text{and} \quad G = A^*A.$$

For $3\pi/2 < t < 2\pi$, the maximum eigenvalue of

$$\cos t\, H - \sin t\, G \tag{20}$$

is denoted by $a(t)$. Replacing t by $s + 3\pi/2$ and denoting $A(s)$ the value $a(t + 3\pi/3)$, the matrix (20) becomes

$$(\sin s)H + (\cos s)G.$$

For $0 \leqslant s, s + \Delta s < \pi/2$, there correspond two tangent lines of $W(H + \mathrm{i}G)$:

$$\left\{x + \mathrm{i}y\colon (x, y) \in \mathbb{R}^2, x\cos s + y\sin s = A(s)\right\} \tag{21}$$

and

$$\left\{x + \mathrm{i}y\colon (x, y) \in \mathbb{R}^2, x\cos(s + \Delta s) - y\sin(s + \Delta s) = A(s + \Delta s)\right\}. \tag{22}$$

Then the intersection $x_0 + \mathrm{i}y_0$ of the two lines (21) and (22) is given by

$$x_0 = \frac{1}{\sin(\Delta s)}(A(s + \Delta s)\cos s - A(s)\cos(s + \Delta s)),$$
$$y_0 = \frac{1}{\sin(\Delta s)}(-A(s + \Delta s)\sin s + A(s)\sin(s + \Delta s)).$$

The graph of the function $h(x)$ on the interval $[0, w(A)]$ is numerically approximated by connecting the line segments with end points (x_k, y_k) and (x_{k+1}, y_{k+1}), $k = 1, 2, \ldots, K - 2$, where

$$\begin{aligned} x_k = {} & \frac{1}{\sin(\pi/(2K))}(A((k+1)\pi/(2K))\cos((k\pi)/(2K)) \\ & - A(k\pi/(2K))\cos((k+1)\pi/(2K)), \\ y_k = {} & \frac{1}{\sin(\pi/(2K))}(-A((k+1)\pi/(2K))\sin(k\pi/(2K)) \\ & + A(k\pi/(2K))\sin((k+1)\pi/(2K)). \end{aligned}$$

Then the derivative $h'(x_k)$ is approximated by

$$s_k = \frac{y_{k+1} - y_k}{x_{k+1} - x_k},$$

and the derivative $\Phi'(x_k)$ is given by

$$u_k = (1/2)\frac{h'(x_k) - 2x_k}{\sqrt{h(x_k) - x_k^2}} = (1/2)\frac{s_k - 2x_k}{\sqrt{y_k - x_k^2}}.$$

Now since

$$\Phi'(x) = \frac{-q}{\sqrt{1 - q^2}}, \quad 0 < x < w(A), \ \ 0 < q < 1,$$

we have

$$q = -\frac{\Phi'(x)}{\sqrt{1 + \Phi'(x)^2}}.$$

Thus the correspondence approximation value q_k of q is given by

$$q_k = -\frac{u_k}{\sqrt{1 + u_k^2}},$$

and the approximation value w_k of the q-numerical radius $w_q(A)$ is therefore given by

$$w_k = q_k x_k + \sqrt{1 - q_k^2}\sqrt{y_k - x_k^2}.$$

We may plot (q_k, w_k), $k = 1, 2, \ldots, K - 2$, to obtain a numerical graph of $w = w_q(A)$.

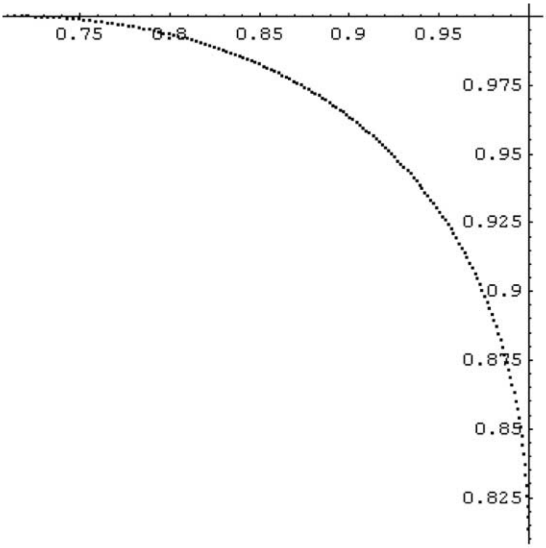

Fig. 1.

For example, we consider the matrix

$$A = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \end{pmatrix}.$$

By Corollary 7, $w_q(A) = 1$ for $0 \leqslant q \leqslant \cos\frac{\pi}{4}$. The graphics shown in Fig. 1 was produced by running a Mathematica program that implements the computation of $w_q(A)$ by means of this algorithm for $\cos\frac{\pi}{4} \leqslant q \leqslant 1$.

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References

[1] M.T. Chien, H. Nakazato, Boundary generating curves of the c-numerical range, Linear Algebra Appl. 294 (1999) 67–84.
[2] D. Keeler, L. Rodman, I. Spitkovsky, The numerical range of 3 × 3 matrices, Linear Algebra Appl. 252 (1997) 115–139.

[3] C.K. Li, Some convexity theorems for the generalized numerical range, Linear Multilinear Algebra 40 (1996) 235–240.
[4] C.K. Li, q-Numerical ranges of normal and convex matrices, Linear Multilinear Algebra 43 (1998) 377–384.
[5] C.K. Li, P.P. Metha, L. Rodman, A generalized numerical range: The range of a constrained sesquilinear form, Linear Multilinear Algebra 37 (1994) 25–50.
[6] C.K. Li, H. Nakazato, Some results on the q-numerical range, Linear Multilinear Algebra 43 (1998) 385–409.
[7] M. Marcus, B.N. Shure, The numerical range of certain 0,1-matrices, Linear Multilinear Algebra 7 (1979) 111–120.
[8] H. Nakazato, The boundary of the range of a constrained sesquilinear form, Linear Multilinear Algebra 40 (1995) 37–43.
[9] H. Nakazato, The C-numerical range of a 2×2 matrix, Sci. Rep. Hirosaki University 41 (1994) 197–206.
[10] H. Nakazato, Y. Nishikawa, M. Takaguchi, On the bounary of c-numerical range of a matrix, Linear Multilinear Algebra 39 (1995) 231–240.
[11] N.K. Tsing, The constrained bilinear form and the C-numerical ranges, Linear Algebra Appl. 56 (1984) 195–206.
[12] R.J. Walker, Algebraic Curves, Dover, New York, 1950.