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THE BOUNDARY OF THE Q-NUMERICAL RANGE OF SOME TOEPLITZ NILPOTENT MATRIX

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Abstract. In this note we compute the boundary of some generalized numerical range $W_q(A)$ of a 4×4 Toeplitz nilpotent matrix A. We also provide a program to plot $W_q(A)$ by using "Mathematica".

Celebrating the contribution of Professor Kichi-Suke Saito to Mathematics in long years.

1. Introduction

Let A be a bounded linear operator on a complex Hilbert space H. The numerical range of A is defined and denoted by

$$W(A) = \{\langle A\xi, \xi\rangle : \xi \in H, ||\xi|| = 1\} \tag{1.1}$$

(cf. [7], page 93, [10]). In 1919, Hausdorff [11] proved the convexity of this range. The numerical radius $w(A)$ of A is defined as

$$\sup\{|\langle A\xi, \xi\rangle| : \xi \in H, ||\xi|| = 1\}.$$

The various interesting results are known for the radius $w(A)$ and the numerical radius norms on the operator spaces (cf. [12], [16], [21]). In this note we mainly treat the case H is a finite-dimensional space $\mathbb{C}^n$ of column vectors with the standard inner product $\langle \xi, \eta\rangle = \eta^*\xi$. In this setting, the numerical range satisfies

$$\sigma(A) = \{\lambda \in \mathbb{C} : \det(\lambda I_n - A) = 0\} \subset W(A),$$

$$W(A + \lambda I_n) = \{\lambda + z : z \in W(A)\},$$

$$W(A) = \cap_{0\le\theta\le 2\pi}\{z \in \mathbb{C} : \Re(ze^{-i\theta}) \le \lambda_1(\Re(e^{-i\theta}A))\},$$

where $\Re(B) = (1/2)(B + B^*)$ and $\lambda_1(G)$ is the largest eigenvalue of a Hermitian matrix G.

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Goldberg and Strauss [9] introduced the C-numerical range $W_C(A)$ of A as

$$W_C(A) = \{\mathrm{tr}(CU^*AU) : U^*U = I_n\} \tag{1.2}$$

where C is an arbitrary $n \times n$ matrix. Cheung and Tsing [5] proved the star-shapedness of $W_C(A)$ with respect to the point $1/n\,\mathrm{tr}(C)\mathrm{tr}(A)$. By using this property Glaser et al [8] developed a numerical algorithm to plot the boundary of $W_C(A)$ and applied it to NMR techniques. If C is a rank one orthogonal projection, the range $W_C(A)$ is reduced to the classical numerical range $W(A)$. In the case A, C are normal matrices, the range $W_C(A)$ is characterized as

$$W_C(A) = \{\sum_{i,j=1}^{n} a_i c_j w_{ij} : (w_{ij}) \in \Omega_n\},$$

where $\sigma(A) = \{a_1, a_2, \ldots, a_n\}$, $\sigma(C) = \{c_1, c_2, \ldots, c_n\}$ and

$$\Omega_n = \{(|u_{ij}|^2 : (u_{ij})\,\text{is an}\, n \times n\,\text{unitary matrix}\}.$$

The above Ω_n is a typical set of entrywise nonnegative matrices. In the paper [18], nonnegative square roots of entrywise nonnegative matrices are closedly studied. By using the above characterization, the boundary of the range $W_C(A)$ for 3×3 normal matrices are closely analyzed (cf. [15]). Tsing [19] proved the convexity of $W_C(A)$ in the case C is a rank one matrix. We consider the 2-dimensional space V containing the ranges $C(\mathbb{C}^n)$, $C^*(\mathbb{C}^n)$.We assume that $||C|| = 1$. Then the operator C restricted to V is unitarily similar to

$$\begin{bmatrix} q & \sqrt{1-|q|^2} \\ 0 & 0 \end{bmatrix}$$

for some $q \in \mathbb{C}$ with $|q| \leq 1$. Using this characterization, the range $W_C(A)$ for a rank-one matrix C is characterized as

$$W_q(A) = \{\eta^* A\xi : \xi, \eta \in \mathbb{C}^n, \xi^*\xi = \eta^*\eta = 1, \eta^*\xi = q\}. \tag{1.3}$$

This range satisfies $W_{cq}(A) = cW_q(A)$ for any $|c| = 1$. So we usually assume that $0 \leq q \leq 1$. If $q = 1$, the range $W_1(A)$ is reduced to $W(A)$. For $0 \leq q < 1$, the range $W_q(A)$ satisfies

$$q\sigma(A) \subset W_q(A), \quad W_q(A + \lambda I_n) = \{q\lambda + z : z \in W_q(A)\}.$$

Boundary points of the range $W(A)$ of an $n \times n$ matrix A lie on an algebraic curve of degree $\leq n(n-1)$ or its bitangents. Boundary points of $W_q(A)$ also lie on an algebraic curve. But its degree is supposed to be so high. In [6] Duan points out that the notion of numerical range and many of its variants such as local numerical range and q-numerical range play crucial role in characterizing the perfect distinguishability of quantum operations. Such applications bear new motivation to study the q-numerical range. For some more properties of the q-numerical range, we refer [1, 2, 3, 4]. We would expect some relation between the q-numerical ranges and the formula $[n]_q = 1+q+q^2+q^3+\ldots+q^{n-1} = (1-q^n)/(1-q)$ for $-1 < q < 1$. Some relations with the numerical radii and the series $[n]_q$ are known (cf. [20]). However no direct relation is known for $W_q(A)$ and $[n]_q$.

We also remark that $W_q(A)$ is a compact convex set of $\mathbb{C} \cong \mathbb{R}^2$. The convexity of this set is useful to analyze this range. The boundary of the unit ball of the 2-dimensional real vector space $\mathbb{R}^2$ with the ℓ^p-norm

$$||\{x_1, x_2\}||_p = (|x_1|^p + |x_2|^p)^{1/p}$$

for $1 < p < \infty$ lies on an algebraic curve if and only if p is a rational number. So the boundary curve is transcendental if p is irrational. Recently exact study of finite dimensional Banach space is developed extensively (cf. [17]). Some techniques used there would be useful to study the range $W_q(A)$. In 1984, Tsing [19] provided the following formula

$$W_q(A) = \{q\xi^* A\xi + \sqrt{1-q^2}w\sqrt{\xi^* A^* A\xi - |\xi^* A\xi|^2} : w \in \mathbb{C}, |w| \leq 1 \\ \xi \in \mathbb{C}^n, \xi^*\xi = 1\}. \tag{1.4}$$

The function

$$\phi(z) = \max\{\sqrt{\xi^* A^* A\xi - |\xi^* A\xi|^2} : \xi \in \mathbb{C}^n, \xi^*\xi = 1, \xi^* A\xi = z\}$$

($z \in W(A)$) is concave on $W(A)$. By using these properties, Tsing proved the convexity of $W_q(A)$. Based on Tsing's formula, C. K. Li [13] provides a Matlab program to plot $W_q(A)$ numerically. In Section 3, we provide a Mathematica program to plot $W_q(A)$. Its algorithm is basically same with Li's program. A performable algorithm to generate the polynomial $g(x, y)$ for which

$$\{(x, y) \in \mathbb{R}^2 : x + iy \in \partial W_q(A)\} \subset \{(x, y) \in \mathbb{R}^2 : g(x, y) = 0\},$$

$$\{(x, y) \in \mathbb{R}^2 : g(x, y) = 0\} \subset \{(x, y) \in \mathbb{R}^2 : x + iy \in W_q(A)\},$$

$$W_q(A) = \mathrm{Conv}(\{x + iy : (x, y) \in \mathbb{R}^2, g(x, y) = 0\})$$

is given in [2] (cf. [4]). We introduce a compact convex sets $\Gamma_0(A)$, $\Gamma(A)$ by

$$\Gamma_0(A) = \{(x_1, x_2, u) \in \mathbb{R}^3 : x_1 + ix_2 \in W(A), u^2 \leq \phi(x_1 + ix_2)^2\},$$

and

$$\Gamma(A) = \{(x_1, x_2, u_1, u_2) \in \mathbb{R}^4 : x_1 + ix_2 \in W(A), u_1^2 + u_2^2 \leq \phi(x_1 + ix_2)^2\}.$$

In a generic case the boundaries of Γ_0, Γ are algebraic hypersurfaces of degree $N = 2n(n-1)^2$. Define an orthogonal projection Π_q of $\mathbb{R}^4$ onto $\mathbb{C} \cong \mathbb{R}^2$ by

$$\Pi_q(x_1, x_2, u_1, u_2) = (qx_1 + \sqrt{1-q^2}u_1) + i(qx_2 + \sqrt{1-q^2}u_2). \tag{1.5}$$

Then Tsing's formula is rewritten as

$$W_q(A) = \Pi_q(\Gamma(A)).$$

A general theory of algebraic varieties tell us that the degree of the boundary of $W_q(A)$ is $\leq N(N-1)^2$ (cf. [3]). This upper bound is not sharp for $n = 3$. The above formula provides a principle to compute the equation $g(x, y) = 0$ of the boundary $W_q(A)$. The q-numerical range of some typical 3×3 matrices are given in [3]. Numerical experiments suggest us that the degree of the boundary equation $g(x, y)$ for a generic 3×3 unitarily irreducible matrix is 24. It is rather hard to compute the polynomial $g(x, y)$ for a generic unitarily irreducible 4×4 matrix A by using a standard personal computer. As a first step to treat a generic 4×4 matrix, we treat the following Toeplitz nilpotent matrix

$$N = \begin{bmatrix} 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \end{bmatrix}. \tag{1.6}$$

2. Equation of the boundary

The standard method to generate the function $\phi = \phi_A$ on the numerical range $W(A)$ for an $n \times n$ matrix is given by the formula

$$\phi_A(z) = \sqrt{h(z) - |z|^2},$$

$$h(z) = \max\{s : (z, s) \in W(A, A^*A)\}$$

where

$$W(A, A^*A) = \{(z, s) \in \mathbb{C} \times \mathbb{R} : z = \xi^* A \xi, s = \xi^* A^* A \xi, \xi \in \mathbb{C}^n, \xi^* \xi = 1\}.$$

We shall generate a real polynomial $L_{0,A}(X, Y, Z)$ for which the equation $L_{0,A}(X, Y, Z) = 0$ holds for a generic point $(X + iY, Z)$ of the boundary of $W(A, A^*A)$. As it is mentioned in [2], the algebraic surface $L_{0,A}(X, Y, Z) = 0$ is characterized as the dual surface of the algebraic surface $G_A(x, y, z, 1) = 0$ defined by

$$G_A(x, y, z, t) = \det(x\Re(A) + y\Im(A) + zA^*A + tI_n),$$

where $\Re(A) = (A + A^*)/2$, $\Im(A) = (A - A^*)/(2i)$. By using Sylvester's resultant, we can compute the polynomials G_N and $L_{0,N}$ for the Toeplitz matrix N defined by (1.6).

Theorem 2.1. *Suppose that N is the 4×4 Toeplitz matrix given by* (1.6). *Then the polynomials G_N and $L_{0,N}$ are given by the following:*

$$\begin{array}{rcl} 4G_N(x,y,z,1) & = & x^2y^2 + y^4 - x^2z^2 - y^2z^2 - 4x^2z - 8y^2z \\ & & +4z^3 - 4x^2 - 4y^2 + 16z^2 + 16z + 4, \\ L_{0,N}(X,Y,Z) & = & 256(20X^{12} + \ldots + 20X^2Y^{10} + \ldots \\ & & +116X^2Y^8Z^2 + \ldots + 4Z^{12}) + \ldots - 52X^2Z - 16Y^2Z \\ & & +X^2 + Y^2 + 12Z^2 - Z. \end{array}$$

The above degree 12 *polynomial $L_{0,N}(X,Y,Z)$ has* 135 *terms.*

Proof. By direct computations (by using some computer software), we can obtain the explicit expression of the polynomial $G_N(x,y,z,1)$. For every non-zero vector $(x_0,y_0,z_0) \in \mathbb{R}^3$, we consider the support plane $\Pi(x_0,y_0,z_0)$ of the convex set $W(N,N^*N) \subset \mathbb{C} \times \mathbb{R}^2 \cong \mathbb{R}^3$ defined by

$$\Pi(x_0,y_0,z_0) = \{(x,y,z) \in \mathbb{R}^3 : x_0x + y_0y + z_0z = M(x_0,y_0,z_0)\},$$

$$M(x_0,y_0,z_0) = \max\{x_0x + y_0y + z_0z : (x+iy,z) \in W(N,N^*N)\}.$$

The value $M(x_0,y_0,z_0)$ is the maximum of the eigenvalues of the Hermitian matrix $x_0\Re(N) + y_0\Im(N) + z_0N^*N$. Thus the boundary of $W(N,N^*N)$ is obtained as the convex hull of the dual surface of the algebraic surface $G_N(x,y,z,1) = 0$. This polynomial satisfies

$$G_N(-x_0,-y_0,-z_0,M(x_0,y_0,z_0)) = 0.$$

The defining polynomial $L_{0,N}(X,Y,Z) = 0$ of the dual surface of the algebraic surface $G_N(x,y,z,1) = 0$ is obtained by the elimination of the indeterminates x,y from the equations

$$H(X,Y,Z,x,y) = Z^3G_N(x,y,-\frac{xX}{Z} - \frac{yY}{Z} - \frac{1}{Z},1) = 0,$$

$$H_x = \frac{\partial H}{\partial x} = 0, \quad H_y = \frac{\partial H}{\partial y} = 0.$$

We can elimate the indeterminates x,y by successive usage of Sylvester's determinants. We take the simple factor $J(X,Y,Z,y)$ of the resultant of $H(X,Y,Z,x,y)$ and H_x. Then we take the simple factor $L_{0,N}$ of the resultant of $J(X,Y,Z,y)$ and $J_y(X,Y,Z,y)$ with respect to y. In this way we obtain the equation of the dual surface of $G_N(x,y,z,1) = 0$. To perform this process, Lagrange's interpolation is effective, especially in the second elimination. □

By using the equation $L_{0,A}(X,Y,Z) = 0$ of the boundary of the simultaneous numerical range $W(A,A^*A)$, the equation of the boundary of the convex set $\Gamma(A)$ is given by

$$L_{0,A}(x_1,x_2,x_1^2 + x_2^2 + u_1^2 + u_2^2) = 0.$$

We use the orthogonal projection Π_q of $\mathbb{R}^4$ onto the plane $\mathbb{C} \cong \mathbb{R}^2$ given by (1.5). The algorithm to compute the equation of the boundary of $W_q(A)$ is given by the following. We substitute

$$x_1 = \frac{1}{q}(x - \sqrt{1-q^2}u_1), \quad x_2 = \frac{1}{q}(y - \sqrt{1-q^2}u_2)$$

into the polynomial

$$L(x, y, u_1, u_2) = L_{0,A}(x_1, x_2, x_1^2 + x_2^2 + u_1^2 + u_2^2).$$

The polynomial $g(x, y)$ vanishing on the boundary of $W_q(A)$ is obtained by the successive eliminations of u_1, u_2 from the equations

$$M(x, y, u_1, u_2) = L(1/q(x - \sqrt{1-q^2}u_1), 1/q(y - \sqrt{1-q^2}u_2), u_1, u_2),$$

$$M_{u_1}(x, y, u_1, u_2) = 0, M_{u_2}(x, y, u_1, u_2) = 0.$$

We provide the equation of the boundary of $W_q(N)$ for $q = 1599/1601$, $\sqrt{1-q^2} = 80/1601$. This value of q is obtained by a Pythagorean triple $(1599, 80, 1601)$ for which $80/1601$ is rather small.

Theorem 2.2. *Suppose that N is the 4×4 nilpotent matrix given by* (1.6) *and $q = 1599/1601$. Then every point $x + iy$ of the boundary of $W_q(N)$ $((x, y) \in \mathbb{R}^2)$ satisfies the equation $g(x, y) = 0$ for the following degree* 40 *polynomial with* 253 *terms*

$$\begin{aligned}
&g(x,y) = 2^{26} \cdot 1601^{40}\, (x^2+y^2)^{14}\, (2563201x^2 + 6400y^2)^2\, (6400x^2 + 2563201y^2)^4 \\
&+2^{25} \cdot 13 \cdot 1601^{38}\, (x^2+y^2)^{12}\, (2563201x^2 + 6400y^2)(6400x^2 + 2563201y^2)^2 \\
&\cdot(3301687627081318085120 0x^8 - 1326548367335133886936910 8x^6y^2 \\
&-3673981984582525074276824 7x^4y^4 - 4328970570066311850852480 1x^2y^6 \\
&-124358510381267802592000y^8) + \ldots \\
&+2^{14} \cdot 3^{46} \cdot 5^4 \cdot 13^{36} \cdot 41^{36} \cdot (811 \cdot 2473 \cdot 120721 \cdot 284689)^2.
\end{aligned}$$

Proof. The equation $g(x, y) = 0$ of the boundary of $W_{1599/1601}(N)$ is obtained by the successive eliminations of u_1, u_2 from the equations $M(x, y, u_1, u_2) = 0$ and $M_{u_1} = 0$, $M_{u_2} = 0$. We take the simple factor $K(x, y, u_2)$ of the resultant of $M(x, y, u_1, u_2)$ and $M_{u_1}(x, y, u_1, u_2)$ with respect to u_1. The total degree of $m(x, y, u_2)$ with respect to x, y is 40. The polynomial $g(x, y)$ is obtained as a simple factor of the resultant of $K(x, y, u_2)$ and $K_{u_2}(x, y, u_2)$ with respect to u_2. These processes essentially coincide with those in [2]. □

By using the above polynomial $g(x, y)$, we shall determine some characteristic invariants of $W_q(N)$ for $q = 1599/1601$. We determine the least rectangle R containing $W_{1599/1601}(N)$ with edges parallel to the real and imaginary axes. Since N is a real matrix, the range $W_q(N)$ is symmetric with respect to the real axis. The numerical range $W(A)$ is symmetric with respect to the imaginary axis and the function $\phi(x+iy)$ satisfies $\phi(-x+iy) = \phi(x+iy)$. Hence the range $W_q(N)$ is symmetric with respect to the imaginary axis. So the values

$$M_x = \max\{\Re(z) : z \in W_q(A)\}, \quad M_y = \max\{\Im(z) : z \in W_q(A)\}$$

are attained respectively on half-lines $\{x : x > 0\}, \{iy : y > 0\}$. The value M_x for $q = 1599/1601$ is the maximum real root of a simple factor

$$\begin{aligned} p(x) = {} & 172659566698038165790771204x^8 - 690638266792152663163084816x^7 \\ & +1035526290327212459458841624x^6 - 689344937209103057305728016x^5 \\ & +214154580429043752468444805x^4 - 8514557676709384978427520 2x^3 \\ & +4270791337192984163838560 1x^2 + 804299421253508966448 00x \\ & -535990422765690745632 00 \end{aligned}$$

of the polynomial $g(x,0)$. The polynomial $p(-x)$ is also a simple factor of $g(x,0)$. The value M_y for $q = 1599/1601$ is the maximum real root of a simple factor

$$\begin{aligned} q(y) = {} & 138127653358430532632616963 2y^8 + 1381276533584305326326169632y^7 \\ & -1383863192750404538040883232y^6 - 1388174291360569890898739232y^5 \\ & +511297035462706296012556812y^4 + 343702202310090276474886408y^3 \\ & -172120143173202689945619204y^2 - 4825796527521053798688 00y \\ & +427351678437883822451072 01 \end{aligned}$$

of the polynomial $g(0,y)$. The polynomial $q(-y)$ is also a simple factor of $g(0,y)$. The values M_x, M_y are approximately given by

$$M_x \sim 1.0350266, \quad M_y \sim 0.75321029.$$

In Figure 1, we provide a graphic of the curve $g(x,y) = 0$. The outer arc of this figure represents the boundary of $W_{1599/1601}(N)$.

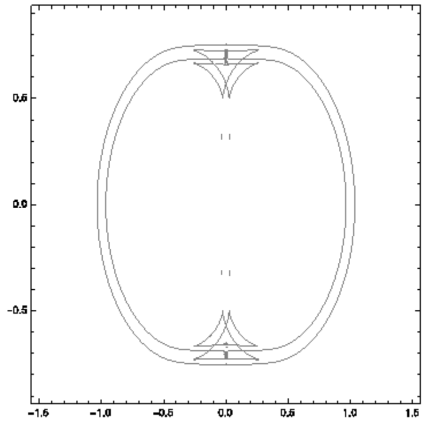

Figure 1: $\partial W_q(N)$ and its related envelope curve

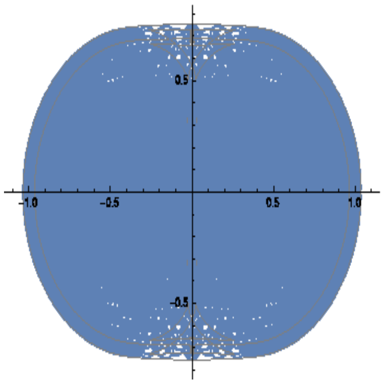

Figure 2

3. Numerical Approximation

We shall provide some codes to plot the q-numerical range of a complex matrix A by using “Mathematica”. Our codes depend on Tsing’s formula (1.4). We expect numerical experiments will be useful for further study. A program to plot the q-numerical range using “Matlab” was provided by [13]. Our program is viewed as its “Mathematica” version. For instance, we treat the matrix (1.6).

```
A = {{0, 1, 0, 1}, {0, 0, 1,0}, {0, 0, 0, 1}, {0, 0, 0, 0}};
A1 = Conjugate[Transpose[A]];
H = (1/2)(A+A1); G = (-I/2)(A-A1); K = A1.A
M1 = 200 ; M2 = 20; q = 1599/1601;
For [ k = 1, k < M1 + 1, k ++, t = k*2 Pi/M1;
T = Cos[t]*H + Sin[t]*G;
For[ m = 0, m < M2 + 1, m++, s = m*Pi/(2 M2);
```

```
TT = Cos[s]*T + Sin[s]*K + 5.0 IdentityMatrix[4];
MM = N[Eigenvectors[TT]][[1]];
M = Abs[MM]^2; W = Sqrt[Sum][M[[j]], {j, 1, 4 }]];
v = MM/W; u = Conjugate[v];
UU = {u}; LL = Transpose[{v}];
p = Re[UU.H. LL]; r = Re[UU. G. LL]; S = Re[UU. K. LL];
X = p[[1]][[1]]; Y = r[[1]][[1]]; Z = S[[1]][[1]]
ZZ = Sqrt[1 - q^2]*Sqrt[Z-X^2-Y^2];
XX = q*X; YY = q*Y]];
Q = Table[{XX[k,m],YY[k, m],ZZ[k,m]}, {k, 1, M1},{m, 0, M2}];
Q0 = Flatten[Q, 1];
Show[Table[ParametricPlot[ {Q0[[e]][[1]] +Q0[[e]][[3]]*Cos[x], Q0[[e]][[2]] +Q0[[3]]*Sin[x]
}, {x,0, 2Pi}, PlotRange → All, {e, M1*(M2+1) }]
```

In these codes, we may replace $M1, M2$ by other numbers. For finer approximations, we need longer computation time. In Figure 2, we merge the graphic produced by these codes and the graphic of the curve in Figure 1. In the above codes, we use the eigenvector of a Hermitian matrix $\cos s(\cos tH + \sin tG) + \sin sK$. In Mathematica's convention, a non-normalized eigenvector corresponding to the eigenvalue of a matrix with the largest modulus is chosen as the first eigenvector. We may meet a case the eigenvalues of the matrix satisfy

$$\lambda_1(\cos s(\cos tH + \sin tG) + \sin sK) \geq 0 > \lambda_n(\cos s(\cos tH + \sin tG) + \sin sK),$$

$$-\lambda_n(\cos s(\cos tH + \sin tG) + \sin sK) \geq \lambda_1(\cos s(\cos tH + \sin tG) + \sin sK) \geq 0,$$

where $\lambda_n(G)$ is the least eigenvalue of a Hermitian matrix G. We can avoid this inconvenience by adding some positive scalar matrix to the matrix

$$\cos s(\cos tH + \sin tG) + \sin sK.$$

In the definition of the vector W, the summation is done for $1 \leq j \leq n$, where the size of the matrix A is $n \times n$, in the above case $n = 4$.

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