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Numerical ranges and stability estimates

M.N. Spijker

*Department of Mathematics and Computer Science, University of Leiden, Niels Bohrweg 1,
2333 CA Leiden, Netherlands*

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Abstract

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This paper reviews various generalizations of the classical numerical range of a matrix, namely algebra numerical ranges and M -numerical ranges. Some new characterizations are given of these ranges.

The paper also discusses the relevance of numerical ranges to stability questions in numerical analysis. The focus is on the stability of one-step methods for the numerical solution of initial (boundary) value problems in ordinary and partial differential equations.

At the end of the paper three conjectures regarding stability estimates are formulated.

Keywords. Numerical range; field of values; Gerschgorin domain; stability analysis; numerical solution of initial value problems; linear algebra; numerical analysis; ordinary differential equations; partial differential equations.

1. Introduction

Let $A = (\alpha_{jk})$ be a square matrix of order s , with complex entries α_{jk} . The set of all eigenvalues λ of A is called the *spectrum* of A , and will be denoted by $\sigma[A]$.

This paper deals with so-called *numerical ranges* of A . Roughly speaking, a numerical range of A is a subset of the complex plane adjoined, in a systematic way, to A such that it encloses the spectrum of A . Denoting such a numerical range by $\tau[A]$ we thus have

$$\sigma[A] \subset \tau[A] \subset \mathbb{C}. \quad (1.1)$$

Already rather long ago, numerical ranges were used in the stability analysis of numerical processes. They have turned out to be useful tools in the numerical solution of initial value and initial boundary value problems for ordinary and partial differential equations. For instance the Lax–Wendroff condition for stability involves the so-called *classical numerical range*, defined by

$$\tau[A] = \{x^*Ax : x \in \mathbb{C}^s \text{ with } x^*x = 1\} \quad (1.2)$$

Correspondence to: M.N. Spijker, Department of Mathematics and Computer Science, University of Leiden, Niels Bohrweg 1, 2333 CA Leiden, Netherlands. E-mail: spijker@rulcri-leidenuniv.nl.

(cf. [11, Theorem 3; 19, pp. 88–89; 22, Theorem 5.4]). In the above x^* denotes the Hermitian adjoint of the column vector $x \in \mathbb{C}^s$.

In this paper we study generalizations of the classical numerical range, and we discuss the relevance of these generalizations to stability questions.

2. The algebra numerical range

Let $|x|$ be an arbitrary norm for vectors $x \in \mathbb{C}^s$, and let the corresponding induced matrix norm, for $s \times s$ matrices A , be given by

$$\|A\| = \sup\{|Ax| : x \in \mathbb{C}^s \text{ with } |x| = 1\}.$$

For $\gamma \in \mathbb{C}$ and $\rho \geq 0$ we introduce the disk

$$D[\gamma, \rho] = \{\zeta : \zeta \in \mathbb{C} \text{ with } |\zeta - \gamma| \leq \rho\}.$$

The matrix A is said to satisfy a *circle condition*, with respect to the disk $D[\gamma, \rho]$, if

$$\|A - \gamma I\| \leq \rho, \tag{2.1a}$$

where I denotes the $s \times s$ identity matrix.

Circle conditions provide a natural means to defining a set $\tau[A]$ satisfying (1.1). Suppose x is an eigenvector, with $|x| = 1$, corresponding to an eigenvalue λ of A , and suppose A satisfies a circle condition with respect to $D[\gamma, \rho]$. Then

$$|\lambda - \gamma| = |(\lambda - \gamma)x| = |(A - \gamma I)x| \leq \|A - \gamma I\| \leq \rho,$$

so that λ belongs to the disk $D[\gamma, \rho]$. The best enclosure of $\sigma[A]$ that can be obtained by using circle conditions thus equals the intersection of all disks with respect to which A satisfies a circle condition. Therefore, consider

$$\tau[A] = \bigcap D[\gamma, \rho], \tag{2.1b}$$

where the intersection is over all pairs γ, ρ for which (2.1a) holds.

The set $\tau[A]$ defined by (2.1) satisfies (1.1), and can be seen to be equal to the so-called algebra numerical range, well known in some parts of functional analysis (see [3, p. 42; 4, p. 35]). In the following we adopt this terminology and call the set $\tau[A]$ specified by (2.1) the *algebra numerical range* of A corresponding to the given norm on \mathbb{C}^s .

We denote the l_p -norm of $x \in \mathbb{C}^s$ (cf. e.g. [10]) by $|x|_p$, and the corresponding induced matrix norm, for $s \times s$ matrices A , by $\|A\|_p$.

In case the norm $\|\cdot\|$ occurring in (2.1a) equals the norm $\|\cdot\|_2$, then the algebra numerical range, defined by (2.1), coincides with the classical numerical range (1.2) (cf. Section 5).

As a further example, consider the case where $\|\cdot\|$ in (2.1a) equals $\|\cdot\|_\infty$. For any $s \times s$ matrix $A = (\alpha_{jk})$ we denote, for $1 \leq j \leq s$, by $D_j[A]$ the so-called *Gerschgorin disk*,

$$D_j[A] = D[\alpha_{jj}, \rho_j], \quad \text{with } \rho_j = \sum_{k \neq j} |\alpha_{jk}|.$$

Further, for arbitrary subsets $V \subset \mathbb{C}$, we denote the *convex hull* of V , i.e. the intersection of all convex W with $V \subset W \subset \mathbb{C}$, by

$$\text{conv}(V).$$

With these notations, the algebra numerical range corresponding to $\|\cdot\|_\infty$ allows the following representation,

$$\tau[A] = \text{conv}(D_1 \cup D_2 \cup \dots \cup D_s) \tag{2.2}$$

(cf. Section 5).

3. The M -numerical range

Let an arbitrary constant $M \geq 1$ be given. The algebra numerical range can be generalized by replacing (2.1a) with the *generalized circle condition*

$$\|(A - \gamma I)^k\| \leq M\rho^k \quad \text{for } k = 1, 2, 3, \dots \tag{3.1a}$$

Suppose again x to be an eigenvector, with $|x| = 1$, corresponding to an eigenvalue λ of A , and suppose A satisfies (3.1a). Then

$$|\lambda - \gamma|^k = |(A - \gamma I)^k x| \leq \|(A - \gamma I)^k\| \leq M\rho^k$$

for $k = 1, 2, 3, \dots$. This still implies that λ belongs to the disk $D[\gamma, \rho]$. The best enclosure of $\sigma[A]$ obtainable from relations of the form (3.1a) thus equals the intersection of all disks with respect to which A satisfies the generalized circle condition (3.1a). Therefore, we introduce

$$\tau[A] = \bigcap D[\gamma, \rho], \tag{3.1b}$$

where the intersection is now over all pairs γ, ρ for which (3.1a) holds.

The set $\tau[A]$ defined by (3.1) satisfies (1.1). It is called the M -numerical range of A with respect to the norm $|\cdot|$, and was introduced in Lenferink and Spijker [12].

If we want to express the dependence of $\tau[A]$ on M , we write

$$\tau[A] = \tau[A, M],$$

Clearly $\tau[A, 1]$ equals the algebra numerical range (2.1).

For arbitrary $M \geq 1$, arbitrary $s \times s$ matrix A and arbitrary norm $|x|$ for $x \in \mathbb{C}^s$, we have the following five properties of the M -numerical range.

$$\tau[A, M] \text{ is a closed, bounded and convex subset of } \mathbb{C}, \tag{3.2}$$

$$\tau[\zeta_0 I + \zeta_1 A, M] = \zeta_0 + \zeta_1 \cdot \tau[A, M] \quad \text{for all } \zeta_0, \zeta_1 \in \mathbb{C}, \tag{3.3}$$

$$\tau[A, M_2] \subset \tau[A, M_1] \quad \text{for } 1 \leq M_1 \leq M_2, \tag{3.4}$$

$$\text{conv}(\sigma[A]) \subset \tau[A, M], \tag{3.5}$$

$$\lim_{M \rightarrow \infty} \tau[A, M] = \text{conv}(\sigma[A]). \tag{3.6}$$

The first four properties (3.2)–(3.5), follow easily from the definition (3.1). Property (3.6) can be proved by using the spectral radius formula (cf. [12, p. 262]).

From (3.4)–(3.6) we see that the set $\tau[A, M]$ with $M > 1$ has a potential for enclosing $\sigma[A]$ more tightly than the set $\tau[A, 1]$. This is one of the gains in the generalization (3.1).

4. Characterizations of the M -numerical range

Below we shall formulate useful characterizations of the M -numerical range. We start with some definitions that are used in these characterizations.

Let V be an arbitrary convex subset of \mathbb{C} , and let $\zeta \in \mathbb{C}$. The *distance* from ζ to V is defined by

$$d(\zeta, V) = \inf\{|\zeta - \xi| : \xi \in V\}.$$

If ξ belongs to the *boundary* ∂V of V and

$$\operatorname{Re}\{e^{-i\theta}(\zeta - \xi)\} \leq 0 \quad \text{for all } \zeta \in V,$$

where θ is a real constant, then θ is said to be a *normal direction* to V at ξ .

We shall deal with the following four conditions on A with respect to $V \subset \mathbb{C}$.

- (I) $\tau[A, M] \subset V$;
- (II) $\zeta I - A$ is regular, and $\|(\zeta I - A)^{-k}\| \leq M \cdot [d(\zeta, V)]^{-k}$ for all $\zeta \notin V$ and $k = 1, 2, 3, \dots$;
- (III) $\|e^{\zeta A}\| \leq M e^{\operatorname{Re}(\xi \zeta)}$ whenever $\zeta \in \mathbb{C}$ and $\theta = -\arg(\zeta)$ is a normal direction to V at $\xi \in \partial V$;
- (IV) there exists a norm $|x|_0$ for $x \in \mathbb{C}^s$ such that the corresponding 1-numerical range satisfies

$$\tau_0[A, 1] \subset V$$

$$\text{and } |x| \leq |x|_0 \leq M|x| \quad (\text{for all } x \in \mathbb{C}^s).$$

Theorem 4.1. *Let $|x|$ be a given norm for $x \in \mathbb{C}^s$, and A a given $s \times s$ matrix. Let $M \geq 1$, and V an arbitrary nonempty closed and convex subset of \mathbb{C} . Let $\tau[A, M]$ be the M -numerical range of A with respect to the given norm on \mathbb{C}^s . Then conditions (I)–(IV) are equivalent to each other.*

Since $\tau[A, M]$ is evidently the smallest nonempty closed convex set $V \subset \mathbb{C}$ with property (I), the above theorem provides us with three new characterizations of the M -numerical range. We see that $\tau[A, M]$ equals the smallest nonempty closed convex $V \subset \mathbb{C}$ with property (II); and the same holds with regard to the properties (III) and (IV).

The above theorem is a variant to the closely related Theorem 2.1 in [12]. The above conditions (III) and (IV) are more transparent than analogous conditions occurring in [12].

Proof of Theorem 4.1. Theorem 2.1 in [12] amounts to the equivalence of four conditions on A , the first two of which agree with the above conditions (I) and (II). Further, a straightforward calculation shows that the third condition in [12] amounts to (III). Therefore, the above conditions (I), (II), and (III) are equivalent to each other.

Assume (IV). We shall prove (I). The matrix norm $\|\cdot\|_0$ induced by the norm $|\cdot|_0$, satisfies

$$\|B\| \leq M \cdot \|B\|_0 \quad \text{for all } s \times s \text{ matrices } B.$$

For any $\gamma \in \mathbb{C}$, $\rho \geq 0$ with

$$\|(A - \gamma I)^k\|_0 \leq \rho^k \quad \text{for } k = 1, 2, 3, \dots,$$

we thus also have

$$\|(A - \gamma I)^k\| \leq M\rho^k \quad \text{for } k = 1, 2, 3, \dots$$

Consequently

$$\tau[A, M] \subset \tau_0[A, 1] \subset V,$$

which implies (I).

Assume (III). We shall prove (IV) by defining, for $x \in \mathbb{C}^s$,

$$|x|_0 = \sup_{\xi, \zeta} e^{-\operatorname{Re}(\xi\zeta)} |e^{\zeta A} x|, \tag{4.1}$$

where the supremum is for all pairs ξ, ζ occurring in (III). Evidently, such pairs are characterized by the requirement

$$\xi \in \partial V \text{ and } \zeta = |\zeta| e^{-i\theta}, \text{ where } \theta \text{ is a normal direction to } V \text{ at } \xi. \tag{4.2}$$

With no loss of generality we assume $V \neq \mathbb{C}$, so that the set of pairs ξ, ζ satisfying (4.2) is nonempty.

We have, for all $x \in \mathbb{C}^s$,

$$|x| \leq |x|_0 \leq M|x|.$$

Hence, by exploiting the equivalence of (I) and (III) with $M = 1$, we see that (IV) holds if

$$\|e^{\zeta A}\|_0 \leq e^{\operatorname{Re}(\xi\zeta)} \quad \text{for all } \xi \text{ and } \zeta \text{ satisfying (4.2)}. \tag{4.3}$$

Here $\|\cdot\|_0$ denotes the matrix norm induced by the norm (4.1).

Let ξ, ζ and ξ_0, ζ_0 be as in (4.2). Applying (4.1) it can be seen that, in order to establish (4.3), it is sufficient to prove the existence of ξ_1, ζ_1 , satisfying (4.2), with

$$\|e^{(\zeta + \zeta_0 - \zeta_1)A}\| \leq e^{\operatorname{Re}(\xi\zeta + \xi_0\zeta_0 - \xi_1\zeta_1)}. \tag{4.4}$$

We define $\zeta_1 = \zeta + \zeta_0$. A simple geometrical argument shows that $\zeta_1 = |\zeta_1| \exp(-i\theta_1)$, where θ_1 is a normal direction to V at some $\xi_1 \in \partial V$. With these choices for ξ_1, ζ_1 relation (4.4) is equivalent to

$$\operatorname{Re}\{(\xi_1 - \xi)\zeta\} + \operatorname{Re}\{(\xi_1 - \xi_0)\zeta_0\} \leq 0.$$

Since the pairs ξ, ζ and ξ_0, ζ_0 satisfy (4.2), and $\xi_1 \in V$, we have

$$\operatorname{Re}\{\zeta(\xi_1 - \xi)\} \leq 0, \quad \operatorname{Re}\{\zeta_0(\xi_1 - \xi_0)\} \leq 0.$$

This proves (4.4), and therefore also (IV).

The conditions (I)–(IV) have thus been shown to be equivalent. \square

5. Characterizations of the algebra numerical range

Below we shall establish a series of characterizations of the algebra numerical range, by applying Theorem 4.1 with $M = 1$. But, first we introduce some notations that will be used in these characterizations.

Let $|x|$ denote an arbitrary norm for vectors $x \in \mathbb{C}^s$, and let $\|A\|$ be the corresponding norm induced on the vector space $\mathbb{C}^{s,s}$ of all $s \times s$ matrices A . The dual space of \mathbb{C}^s can be identified with \mathbb{C}^s equipped with the *dual norm*

$$|y|^* = \sup\{|y^*x| : x \in \mathbb{C}^s \text{ with } |x| = 1\}$$

for column vectors $y \in \mathbb{C}^s$. Similarly, the dual space of $\mathbb{C}^{s,s}$ can be identified with $\mathbb{C}^{s,s}$ equipped with the *dual norm*

$$\|B\|^* = \sup\{|\text{tr}(BA)| : A \in \mathbb{C}^{s,s} \text{ with } \|A\| = 1\}$$

for $s \times s$ matrices B . Here

$$\text{tr}(C) = \gamma_{11} + \gamma_{22} + \dots + \gamma_{s,s}$$

denotes the *trace function* for $s \times s$ matrices $C = (\gamma_{jk})$.

We recall that the *logarithmic norm* of the $s \times s$ matrix A can be defined by the formula

$$\mu(A) = \inf\{t^{-1}(\|I + tA\| - 1) : t > 0\}$$

(cf. [1,6,21]).

We shall deal with the following six conditions on A with respect to $V \subset \mathbb{C}$.

- (i) $\tau[A] \subset V$;
- (ii) $\zeta I - A$ is regular, and $\|(\zeta I - A)^{-1}\| \leq [d(\zeta, V)]^{-1}$ for all $\zeta \notin V$;
- (iii) $\|e^{\zeta A}\| \leq e^{\text{Re}(\xi\zeta)}$ whenever $\zeta \in \mathbb{C}$ and $\theta = -\arg(\zeta)$ is a normal direction to V at $\xi \in \partial V$;
- (iv) $\mu(e^{-i\theta}A) \leq \text{Re}(e^{-i\theta}\xi)$ for all $\xi \in \partial V$ and normal directions θ to V at ξ ;
- (v) $y^*Ax \in V$ (for all $x, y \in \mathbb{C}^s$ with $y^*x = |x| = |y|^* = 1$);
- (vi) $\text{tr}(BA) \in V$ (for all $B \in \mathbb{C}^{s,s}$ with $\|B\|^* = \text{tr}(B) = 1$).

Theorem 5.1. *Let $A \in \mathbb{C}^{s,s}$, and $|x|$ be an arbitrary norm for $x \in \mathbb{C}^s$. Let $\tau[A]$ be the corresponding algebra numerical range defined by (2.1), and assume V is a nonempty closed and convex subset of \mathbb{C} . Then conditions (i)–(vi) are equivalent to each other.*

This theorem provides us, in a similar way as Theorem 4.1, with five characterizations of $\tau[A]$ that are different from (2.1). We see that $\tau[A]$ is the smallest nonempty closed and convex set $V \subset \mathbb{C}$ with any of the properties (ii)–(vi).

Such a characterization based on (ii) was essentially used by Glazman and Ljubič [9] to define a generalization of the classical numerical range (1.2), and similarly (iv) and (vi) were used as a definition by Söderlind [20] and Bonsall and Duncan [2–4], respectively.

In the subsequent proof it will be convenient to use the notations

$$\mathcal{F}[A] = \{y^*Ax : x, y \in \mathbb{C}^s \text{ with } y^*x = |x| = |y|^* = 1\}, \tag{5.1}$$

$$\mathcal{E}[A] = \{\text{tr}(BA) : B \in \mathbb{C}^{s,s} \text{ with } \text{tr}(B) = \|B\|^* = 1\}. \tag{5.2}$$

Proof of Theorem 5.1. Since $\tau[A] = \tau[A, 1]$, an application of Theorem 4.1 with $M = 1$ yields the equivalence of the conditions (i), (ii), and (iii).

The equivalence of (iii) and (iv) is an immediate consequence of well-known properties of the logarithmic norm (cf. e.g. [21]).

Deutsch [7, p. 451] proved that condition (ii) is equivalent to the inclusion $\mathcal{F}[A] \subset V$. Therefore, (ii) and (v) are equivalent.

From [3, p. 42] or [4, p. 35] it can be seen that $\tau[A] = \mathcal{F}[A]$. Hence (i) and (vi) are equivalent. \square

Let us denote the algebra numerical range corresponding to the l_p -norm on \mathbb{C}^s by

$$\tau_p[A].$$

The expressions for $\tau_2[A]$ and $\tau_\infty[A]$ given in Section 2 are easily obtained by combining the material of Nirschl and Schneider [16] with the fact that the above conditions (i) and (v) are equivalent. Further, the expression for $\tau_\infty[A]$ allows us to compute $\tau_1[A]$, since one easily sees that

$$\tau_1[A] = \tau_\infty[A^T],$$

where A^T is the transpose of A .

We finally consider the case where Q is a regular $s \times s$ matrix, and $|x|'$ and $|x|$ are two norms on \mathbb{C}^s with

$$|x|' = |Qx| \quad \text{for all } x \in \mathbb{C}^s.$$

The algebra numerical ranges $\tau'[A]$ and $\tau[A]$ corresponding to the norms $|x|'$ and $|x|$, respectively are easily seen to be related to each other by the formula

$$\tau'[A] = \tau[QAQ^{-1}].$$

6. Numerical ranges and stability analysis

In the following we deal with the numerical process

$$u_n = \phi(hA)u_{n-1} \quad \text{for } n = 1, 2, 3, \dots \tag{6.1}$$

Here $u_n \in \mathbb{C}^s$ are numerical approximations computed successively from (6.1), starting from a given $u_0 \in \mathbb{C}^s$. Further, $h > 0$ is the so-called *stepsize* and A is an $s \times s$ matrix. With $\phi(s)$ we denote a given rational function with $\phi(0) = \phi'(0) = 1$. We assume $\phi(\zeta) = P(\zeta)/Q(\zeta)$, where $P(\zeta)$ and $Q(\zeta)$ are polynomials without common zero, and define $\phi(hA) = P(hA)[Q(hA)]^{-1}$ whenever the matrix $Q(hA)$ is regular.

Processes of the form (6.1) occur in the numerical solution of *ordinary differential equations*. Consider the initial value problem

$$\frac{d}{dt}U(t) = AU(t), \quad t \geq 0, \quad U(0) = u_0.$$

Any Runge–Kutta method applied to such a problem reduces to a process of the form (6.1). In this case $u_n \approx U(nh)$ for $n = 1, 2, 3, \dots$. Note that initial value problems of the above type may arise when the method of semi-discretization is applied to initial boundary value problems in linear *partial differential equations*. The dimension s of the system of ordinary differential equations is then related to the discretization of the space variables in the partial differential equation, and can attain (arbitrarily) large values.

Process (6.1) is called *stable* if any numerical errors introduced at some stage of the calculations are propagated in a mild fashion. Such a mild error propagation is equivalent to a mild growth of $\|\phi(hA)^n\|$ when n (or s) increases. Here $\|\cdot\|$ again denotes a matrix norm induced by a vector norm on \mathbb{C}^s .

Recently useful *stability estimates* were derived of the form

$$\|\phi(hA)^n\| \leq \gamma \cdot s^p n^q \quad \text{for } n \geq 1, s \geq 1, \quad (6.2)$$

(see [5,8,13–15,17,18]). Here p and q are nonnegative with $p + q \leq 1$, and γ is of moderate size.

In order to outline the conditions imposed on hA in the papers just mentioned, we introduce the *stability region*

$$S = \{\zeta: \zeta \in \mathbb{C} \text{ with } |\phi(\zeta)| \leq 1\},$$

and a set V satisfying

$$V \subset S. \quad (6.3)$$

The conditions in [5,8,13–15,17,18] are essentially of the form

$$\zeta I - hA \text{ is regular and } \|(\zeta I - hA)^{-1}\| \leq M \cdot [d(\zeta, V)]^{-1} \quad \text{for all } \zeta \notin V. \quad (6.4)$$

Under additional technical assumptions, for which we refer to the above papers, conditions (6.3) and (6.4) were proved to imply (6.2) with

$$\gamma = M \cdot \gamma_0,$$

where γ_0 only depends on ϕ and V (and not on n , s , or hA).

A relation between stability estimates and numerical ranges becomes clear by an inspection of condition (6.4). By virtue of Theorem 4.1 we can make the following two observations.

- (1) If V is any set with $\tau[hA, M] \subset V$, then (6.4) is fulfilled.
- (2) In order to determine a set V as in (1) we only have to find a finite number of pairs γ_j, ρ_j such that (3.1a) holds (with A , γ , and ρ replaced by hA , γ_j , and ρ_j). Clearly the set $V = \bigcap_j D[\gamma_j, \rho_j]$ is as required.

In [12,14] stability estimates were derived essentially along the lines of these two observations. For instance, a matrix A standing for a discrete version of the differential operator d^2/dx^2 was shown to satisfy (6.4) with $\|\cdot\| = \|\cdot\|_\infty$ and with a (lens-shaped) region V being equal to the intersection of two disks as in observation (2).

7. Some open problems

Below we formulate three conjectures related to the material of the preceding sections. The notations are as above, and we deal with *arbitrary* norms $|x|$ for $x \in \mathbb{C}^s$.

Conjecture 1. For each ϕ and $\rho \geq 0$ there is a γ such that

$$\|\phi(hA)^n\| \leq \gamma \sqrt{s} \quad \text{for } n = 1, 2, 3, \dots,$$

whenever $D[-\rho, \rho] \subset S$ and $A \in \mathbb{C}^{s,s}$ satisfies the circle condition $\|hA + \rho I\| \leq \rho$.

Conjecture 2. For each ϕ and $\rho \geq 0$ there is a γ such that

$$\|\phi(hA)^n\| \leq \gamma M \sqrt{n} \quad \text{for } n = 1, 2, 3, \dots,$$

whenever $\tau[hA, M] \subset D[-\rho, \rho] \subset S$.

Conjecture 3. There is a universal constant γ such that

$$\|B^n\| \leq \gamma M \sqrt{s} \quad \text{for } n = 1, 2, 3, \dots,$$

whenever $B \in \mathbb{C}^{s,s}$ satisfies $\tau[B, M] \subset D[0, 1]$.

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