A BIVARIATE EXTENSION OF THE CROUZEIX-PALENCE RESULT WITH AN APPLICATION TO FRÉCHET DERIVATIVES OF MATRIX FUNCTIONS

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Abstract. A result by Crouzeix and Palencia states that the spectral norm of a matrix function $f(A)$ is bounded by $K = 1 + \sqrt{2}$ times the maximum of $f$ on $W(A)$, the numerical range of $A$. The purpose of this work is to point out that this result extends to a certain notion of bivariate matrix functions; the spectral norm of $f\{A, B\}$ is bounded by $K^2$ times the maximum of $f$ on $W(A) \times W(B)$. As a special case, it follows that the spectral norm of the Fréchet derivative of $f(A)$ is bounded by $K^2$ times the maximum of $f'$ on $W(A)$. An application to the convergence analysis of certain Krylov subspace methods and the extension to functions in more than two variables are discussed.

1. Introduction

The numerical range of a matrix $A \in \mathbb{C}^{n \times n}$ is the set

$$W(A) := \{v^*Av : v \in \mathbb{C}^n, \|v\|_2 = 1\},$$

where we let $\| \cdot \|_2$ denote the Euclidean norm of a vector and the spectral norm of a matrix. Consider the matrix function $f(A)$ for an analytic function $f : \Omega \subset \mathbb{C} \to \mathbb{C}$ with $W(A) \subset \Omega$. A result by Crouzeix and Palencia [5] shows that

$$\|f(A)\|_2 \leq (1 + \sqrt{2}) \max_{z \in W(A)} |f(z)|.$$  

The purpose of this work is to point out that an analogous result holds for a certain notion of multivariate matrix functions.

To provide some intuition on the multivariate matrix functions considered in this work, let us first consider the bivariate polynomial $p(x, y) = 1 + xy + ...$
For matrices $A \in \mathbb{C}^{m \times m}$ and $B \in \mathbb{C}^{n \times n}$, evaluating $p$ in the commuting matrices $I \otimes A$, $B \otimes I$ gives
\[ p\{A, B\} := I + B \otimes A + B^2 \otimes A^3 \in \mathbb{C}^{mn \times mn}, \]
where $\otimes$ denotes the usual Kronecker product. Equivalently, $p\{A, B\}$ can be viewed as the linear operator on $\mathbb{C}^{n \times n}$ defined by $p\{A, B\} : X \mapsto X + AXB^T + A^3X(B)^T$, where $B^T$ is the complex transpose of $B$. For a general bivariate function $f$ analytic on a domain $\Omega \subset \mathbb{C} \times \mathbb{C}$ containing the Cartesian product of the eigenvalues of $A$ and $B$, we define
\[ (2) \quad f\{A, B\} := -\frac{1}{4\pi^2} \oint_{\Gamma_A} \oint_{\Gamma_B} f(x, y)(yI - B)^{-1} \otimes (xI - A)^{-1} \, dy \, dx, \]
for closed contours $\Gamma_A$ and $\Gamma_B$ enclosing the eigenvalues of $A$ and $B$, respectively, and satisfying $\Gamma_A \times \Gamma_B \subset \Omega$. As explained in [11], this definition represents a special case of the well established notion of evaluating a multivariate holomorphic function in elements from a commutative Banach algebra; see, e.g., [3] for an introduction. The definition (2) is also closely related to the notion of double operator integrals [15].

Assuming additionally that $f$ is analytic in a domain containing $W(A) \times W(B)$, our main result (see Theorem 3.1) states that
\[ (3) \quad \|f\{A, B\}\|_2 \leq (1 + \sqrt{2})^2 \|f\|_{W(A) \times W(B)}, \]
where $\|f\|_{W(A) \times W(B)}$ denotes the maximum of $|f|$ on $W(A) \times W(B)$. The constant $(1 + \sqrt{2})^2$ in (3) is worse than the one in (1) but it is in fact not possible to reduce the constant in (3) to $1 + \sqrt{2}$. To see this, let $A = B = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}$ and $f(x, y) := xy$. Because the numerical range of $A$ is a disc centered at zero with radius $1/2$, we have $\|f\|_{W(A) \times W(B)} = 1/4$. On the other hand, $\|f\{A, B\}\|_2 = \|B \otimes A\|_2 = 1$, which shows that the constant in (3) must be at least 4. This is entirely analogous to the univariate bound (1) for which the constant is known to be at least 2 and, in fact, conjectured to be exactly 2; see [11, 8, 9, 14] for recent progress in this direction.

In Section 4 we will see that the result (3) easily extends to functions in more than two variables; with a constant that (necessarily) grows exponentially with the number of variables.

Our result (3) has important implications in a variety of applications, including norm estimates for derivatives of matrix functions and the convergence analysis of certain Krylov subspace methods; see Sections 5 and 6 respectively.

Related work. When $f(x, y) = g(x + y)$ for some univariate function $g$, a result by Starke [17, Corollary 3.2] combined with (1) implies (3), in fact with the lower constant $1 + \sqrt{2}$; see also [12, Remark 1]. Existing results for general functions include work by Gil’, such as [7, Theorem 1.1], and [12, Lemma 3]. These bounds are significantly more complicated than (3) and depend on additional quantities, such as the distance to normality of $A$ and/or $B$.

It is simple to see that (3) holds with constant 1 when $A, B$ are both normal. This becomes more subtle when replacing the spectral norm by
other Schatten norms, a question that has been studied extensively in the literature on double and multiple operator integrals [16].

The von Neumann inequality is a variant of (1), which states that \( \| f(A) \|_2 \leq \| f \|_D \) for \( \| A \|_2 \leq 1 \), assuming that \( f \) is analytic on the open unit disk \( \mathbb{D} \) and continuous on \( \overline{\mathbb{D}} \). This result has been extended in various ways to multivariate functions; see [2, Sec. 37.4] for a survey. In particular, applying the seminal result by Ando [1] to the commuting matrices \( I \otimes A, B \otimes I \) one obtains

\[
(4) \quad \| f\{A, B\} \|_2 \leq \| f \|_{D \times D}, \quad \text{if } \| A \|_2 \leq 1 \text{ and } \| B \|_2 \leq 1.
\]

Let us note that such a result also holds for functions in more than two variables, in the sense defined in Section 4, because the involved matrices are doubly commuting [13, Sec. 1.5.9 (g)].

2. Norm estimates for matrix-valued mappings

Our proof of (3) is based on the matrix-valued version of (1), which is equivalent to stating that \( W(A) \) is not only a \( (1 + \sqrt{2}) \)-spectral set but in fact a complete \( (1 + \sqrt{2}) \)-spectral set for \( A \). The existence of such a matrix-valued version is stated without proof in [5]. Given the centrality of this result in our derivation, we feel it worthwhile to include a detailed proof.

Consider a smooth, bounded, convex domain \( \Omega \subset \mathbb{C} \) and a matrix-valued function \( F : \Omega \to \mathbb{C}^{m \times p} \) that is (element-wise) analytic in \( \Omega \) and admits a continuous extension to \( \overline{\Omega} \). We will work with the maximum of the matrix 2-norm:

\[
\| F \|_{\Omega} := \sup_{z \in \Omega} \| F(z) \|_2.
\]

The function defined by

\[
G(z) = \frac{1}{2\pi i} \oint_{\partial \Omega} F^*(\sigma) \frac{d\sigma}{\sigma - z}
\]

is clearly analytic in \( \Omega \) and, by applying [5, Lemma 2.1] to each entry of \( G \), it also admits a continuous extension to \( \overline{\Omega} \).

**Lemma 2.1.** For the function \( G \) defined above, it holds that \( \| G \|_{\Omega} \leq \| F \|_{\Omega} \).

**Proof.** Given arbitrary vectors \( u \in \mathbb{C}^m \), \( v \in \mathbb{C}^p \) with \( \| u \|_2 = \| v \|_2 = 1 \), we can apply [5] Lemma 2.1 to the scalar functions

\[
u^*G(z)v = \frac{1}{2\pi i} \oint_{\partial \Omega} v^*F(\sigma)u \frac{d\sigma}{\sigma - z}
\]

and \( v^*F(z)u \) to obtain \( |u^*G(z)v| \leq \| v^*F(\sigma)u \|_{\Omega} \leq \| F \|_{\Omega} \). By taking the supremum over all such \( u, v \) we obtain \( \| G(z) \|_2 \leq \| F \|_{\Omega} \). \( \square \)

For a matrix \( A \in \mathbb{C}^{n \times n} \) with eigenvalues contained in \( \Omega \), we define \( F(A) \) by replacing the function \( f_{ij}(z) \) at each entry \((i, j)\) of \( F(z) \) by the corresponding matrix function \( f_{ij}(A) \):

\[
F(A) = \begin{bmatrix}
f_{11}(A) & \cdots & f_{1p}(A) \\
\vdots & \ddots & \vdots \\
f_{m1}(A) & \cdots & f_{mp}(A)
\end{bmatrix}.
\]
Using the Cauchy integral formula and the Kronecker product $\otimes$, we can write
\[ F(A) = \frac{1}{2\pi i} \oint_{\partial \Omega} F(\sigma) \otimes (\sigma I - A)^{-1} \, d\sigma. \]
and, in turn,
\[ G(A) = \frac{1}{2\pi i} \oint_{\partial \Omega} F(\sigma)^* \otimes (\sigma I - A)^{-1} \, d\sigma. \]

**Lemma 2.2.** Assume that $W(A) \subset \Omega$. Then the matrices $F(A), G(A)$ defined above satisfy $\|F(A) + G(A)^*\|_2 \leq 2\|F\|_\Omega$.

**Proof.** Without loss of generality, we may assume $\|F\|_\Omega = 1$. Set $S := F(A) + G(A)^*$. Using a counterclockwise oriented arclength parametrization $\sigma = \sigma(s)$ of $\Omega$, we obtain
\[
S = \frac{1}{2\pi i} \oint_{\partial \Omega} F(\sigma) \otimes [ (\sigma I - A)^{-1} \, d\sigma + (\bar{\sigma} I - A^*)^{-1} \, d\bar{\sigma} ]
= \oint_{\partial \Omega} F(\sigma) \otimes \mu(\sigma, A) \, ds,
\]
where $\mu(\sigma, A) = \frac{1}{4\pi} (\nu(\sigma I - A)^{-1} + \bar{\nu}(\sigma I - A^*)^{-1})$ and $\nu$ denotes the unit outward normal vector of $\partial \Omega$ at $\sigma$. As discussed in [21 Sec. 2], the matrix $\mu(\sigma, A)$ is Hermitian positive definite and satisfies
\[
\oint_{\partial \Omega} \mu(\sigma, A) \, ds = 2I.
\]
For matrices $X \in \mathbb{C}^{n \times p}, Y \in \mathbb{C}^{n \times m}$, we set $x = \text{vec}(X), y = \text{vec}(Y)$, let $\langle \cdot, \cdot \rangle_F$ denote the Frobenius inner product of matrices and derive
\[
|\langle Sx, y \rangle| = \left| \oint_{\partial \Omega} \langle \mu(\sigma, A)XF(\sigma)^T, Y \rangle_F \, ds \right| \leq \oint_{\partial \Omega} |\langle \mu(\sigma, A)XF(\sigma)^T, Y \rangle_F| \, ds
\leq \oint_{\partial \Omega} \langle \mu(\sigma, A)XF(\sigma)^T, XF(\sigma)^T \rangle_F^{1/2} \langle \mu(\sigma, A)Y, Y \rangle_F^{1/2} \, ds
\]
where we used the Cauchy-Schwarz inequality in the inner product $\langle \mu(\sigma, A), \cdot \rangle_F$. Combined with
\[
\langle \mu(\sigma, A)XF(\sigma)^T, XF(\sigma)^T \rangle_F = \text{trace}(\mu(\sigma, A)XF(\sigma)^T F(\sigma)^* X^*)
= \text{trace}(X^* \mu(\sigma, A)XF(\sigma)^* F(\sigma))
\leq \lambda_{\text{max}}(F(\sigma)^* F(\sigma)) \text{trace}(X^* \mu(\sigma, A)X)
\leq \text{trace}(X^* \mu(\sigma, A)X),
\]
we obtain
\[
|\langle Sx, y \rangle| \leq \oint_{\partial \Omega} \langle \mu(\sigma, A)X, X \rangle_F^{1/2} \langle \mu(\sigma, A)Y, Y \rangle_F^{1/2} \, ds
\leq \left( \oint_{\partial \Omega} \langle \mu(\sigma, A)X, X \rangle_F \, ds \right)^{1/2} \left( \oint_{\partial \Omega} \langle \mu(\sigma, A)Y, Y \rangle_F \, ds \right)^{1/2}
= \left( \oint_{\partial \Omega} \mu(\sigma, A) \, ds \, X, X \rangle_F \right)^{1/2} \left( \oint_{\partial \Omega} \mu(\sigma, A) \, ds \, Y, Y \rangle_F \right)^{1/2}
= 2\|X\|_F \|Y\|_F = 2\|x\|_2 \|y\|_2.
\]
This proves $\|S\|_2 \leq 2$. \qed
Theorem 2.3. Assume that $W(A) \subset \Omega$. Then
\[ \|F(A)\|_2 \leq (1 + \sqrt{2}) \|F\|_{W(A)} . \]

Proof. The result follows from Lemma 2.1 and Lemma 2.2 in a manner entirely analogous to the derivation in [14, Sec. 2]. □

3. Norm estimate for bivariate matrix functions

We now extend Theorem 2.3 to the bivariate case. For smooth, bounded, and convex domains $\Omega_A, \Omega_B \subset \mathbb{C}$ we consider a matrix valued function $F : \Omega_A \times \Omega_B \to \mathbb{C}^{m \times p}$ that is analytic in $\Omega_A \times \Omega_B$ and continuous on $\overline{\Omega_A} \times \overline{\Omega_B}$. For matrices $A \in \mathbb{C}^{n_A \times n_A}$ and $B \in \mathbb{C}^{n_B \times n_B}$ with the numerical ranges contained in $\Omega_A$ and $\Omega_B$, respectively, we define

\[ F\{A, B\} := -\frac{1}{4\pi^2} \oint_{\partial \Omega_A} \oint_{\partial \Omega_B} F(x, y) \otimes (yI - B)^{-1} \otimes (xI - A)^{-1} \, dy \, dx. \]

This includes (2) as a special case for $m = p = 1$.

Theorem 3.1. For the matrix $F\{A, B\}$ defined above it holds that
\[ \|F\{A, B\}\|_2 \leq (1 + \sqrt{2})^2 \|F\|_{W(A) \times W(B)} , \]

Proof. For $x \in \overline{\Omega_A}$, we let $F_x(y) := F(x, y)$. Inserting
\[ F_x(B) = \frac{1}{2\pi i} \oint_{\partial \Omega_B} F(x, y) \otimes (yI - B)^{-1} \, dy \]
into (5) yields
\[ F\{A, B\} = \frac{1}{2\pi i} \oint_{\partial \Omega_A} F_x(B) \otimes (xI - A)^{-1} \, dx . \]

This allows us to view $F\{A, B\}$ as the evaluation of the matrix valued function $F_B(x) := F_x(B)$ in $A$, that is, $F\{A, B\} = F_B(A)$. Using Theorem 2.3 twice gives
\[ \|f\{A, B\}\|_2 \leq (1 + \sqrt{2}) \sup_{x \in \Omega_A} \|F_B(x)\|_2 = (1 + \sqrt{2}) \sup_{x \in \Omega_A} \|f_x(B)\|_2 \leq (1 + \sqrt{2})^2 \sup_{x \in \Omega_A} \|f(x, y)\|_2 . \]

As this inequality holds for any $\Omega_A, \Omega_B$ containing $W(A), W(B)$, the statement of the theorem follows by continuity. □

4. Extension to multivariate functions

The result of Theorem 3.1 extends without difficulty to functions in more than two variables. Let $\Omega_i \subset \mathbb{C}$ be smooth, bounded, and convex domains for $i = 1, \ldots, d$ and consider a function $F(x_1, \ldots, x_d) \in \mathbb{C}^{m \times p}$ that is analytic in $\Omega_1 \times \cdots \times \Omega_d$. For matrices $A_i \in \mathbb{C}^{n_i \times n_i}$ with eigenvalues contained in $\Omega_i$, we define recursively
\[ F\{A_1, \ldots, A_d\} = \frac{1}{2\pi i} \oint_{\partial \Omega_1} F_{x_1}(A_2, \ldots, A_d) \otimes (x_1I - A)^{-1} \, dx_1, \]
where \( F_{x_i}(x_2, \ldots, x_d) := F(x_1, x_2, \ldots, x_d) \). Applying the technique from the proof of Theorem 3.1 recursively, we obtain

\[
\|F(A_1, \ldots, A_d)\|_2 \leq (1 + \sqrt{2})^d \|F\|_{W(A_1) \times \cdots \times W(A_d)}.
\]

provided that \( W(A_1) \subset \Omega_1, \ldots, W(A_d) \subset \Omega_d \).

A straightforward extension of the example from the introduction shows that the constant in (6) must be at least \( 2^d \); hence, the exponential growth with respect to \( d \) is unavoidable. On the other hand, the constant can be decreased to \( (1 + \sqrt{2})^{d-k} \) if one assumes that there are \( k \) normal matrices among \( A_1, \ldots, A_d \).

5. Application to derivatives of matrix functions

The Fréchet derivative of the matrix function \( f(A) \) is the linear operator \( Df(A) : \mathbb{C}^{n \times n} \to \mathbb{C}^{n \times n} \) satisfying

\[
f(A + \Delta) = f(A) + Df(A)\{\Delta\} + O(\|\Delta\|_2^2)
\]

for all \( \Delta \in \mathbb{C}^{n \times n} \) of sufficiently small norm. The norm \( \|Df(A)\|_2 \) induced by the Frobenius norm is the (absolute) condition number of \( f(A) \), an important quantity to assess the effect of perturbations (e.g., due to roundoff error) on matrix functions [10, Chap. 3]. Most existing bounds for \( |W(A)| \) proceed via diagonalizing \( A \) and inevitably involve the squared condition number of the eigenvector matrix; see, e.g., [10, Theorem 3.15]. A notable exception is Corollary 3.2 in [6], which derives a bound in terms of the pseudospectrum of \( A \). The following corollary presents a bound in terms of the maximum of the derivative on the numerical range.

Corollary 5.1. Let \( A \in \mathbb{C}^{n \times n} \) and consider an analytic function \( f : \Omega \to \mathbb{C} \) with \( W(A) \subset \Omega \). Then

\[
\|Df\{A\}\|_2 \leq (1 + \sqrt{2})^2 \|f'\|_{W(A)}.
\]

Proof. The divided difference

\[
f^{[1]}(x, y) := f[x, y] = \begin{cases} \frac{f(x) - f(y)}{x - y}, & \text{for } x \neq y, \\ f'(x), & \text{for } x = y, \end{cases}
\]

is analytic in \( \Omega \times \Omega \). Moreover, as explained in [11], the corresponding bi-variate matrix function \( f^{[1]}\{A, A^T\} \) is the (canonical) matrix representation of the linear operator \( Df(A) \). In turn, Theorem 3.1 gives

\[
\|Df\{A\}\|_2 = \|f^{[1]}\{A, A^T\}\|_2 \leq (1 + \sqrt{2})^2 \|f^{[1]}\|_{W(A) \times W(A)}.
\]

To simplify the last term, we note that for arbitrary \( x, y \in W(A) \), the line segment \( \gamma \) from \( x \) to \( y \) is contained in \( W(A) \) and thus

\[
|f(y) - f(x)| = \left| \int_{\gamma} f'(z)dz \right| \leq |y - x| \max_{z \in \gamma} |f'(z)|.
\]

Hence, \( |f^{[1]}(x, y)| \leq \sup_{z \in W(A)} |f'(z)| \) for all \( x, y \in W(A) \), which completes the proof. \( \square \)
6. Application to convergence analysis of Krylov subspace methods

As nicely explained in [2], norm bounds of the form (1) are an essential ingredient in deriving error bounds for approximations of matrix functions. Theorem 3.1 can serve the same purpose for bivariate matrix functions. To illustrate this, we consider the Arnoldi method from [12] for approximating the matrix-vector product \( f(A, B)c \), where \( c \) is the vectorization of a rank-one matrix: \( c = \text{vec}(c_A c_B^T) \) with \( c_A \in \mathbb{C}^m, c_B \in \mathbb{C}^n \).

The method from [12] applies \( k \) steps of the standard Arnoldi process to generate an orthonormal basis \( U_k \) of the \( k \)-dimensional Krylov subspaces \( K_k(A,c_A) \) and, similarly, an orthonormal bases \( V_\ell \) of \( K_\ell(B,c_B) \). It returns the approximation

\[
x_{k,\ell} = (V_\ell \otimes U_k)y_{k,\ell},
\]

which involves the reduced bivariate matrix function

\[
y_{k,\ell} = f\{U_k^* A U_k, V_\ell^* B V_\ell\}(V_\ell \otimes U_k)^* c.
\]

As explained in [12], this general framework unifies existing Krylov subspace methods for various types of matrix equations and the Fréchet derivative. Theorem 3.1 allows us to link the approximation error for \( y_{k,\ell} \) to a (bivariate) polynomial approximation problem.

Corollary 6.1. Consider an analytic function \( f : \Omega_A \times \Omega_B \to \mathbb{C} \) with \( W(A) \subset \Omega_A \) and \( W(B) \subset \Omega_B \). Then the approximation (7) returned by the Arnoldi method satisfies the error bound

\[
\| f\{A, B\} c - x_{k,\ell} \|_2 \leq 2(1 + \sqrt{2})^2 \| c \|_2 \inf_{p \in \Pi_{k-1,\ell-1}} \| f - p \|_{W(A) \times W(B)},
\]

where \( \Pi_{k,\ell} \) denote the set of all bivariate polynomials of degree at most \( (k, \ell) \).

Proof. The proof of Theorem 4.3 in [12] implies that

\[
\| f\{A, B\} c - x_{k,\ell} \|_F \leq (\| e\{A, B\} \|_2 + \| e\{U_k^* A U_k, V_\ell^* B V_\ell\} \|_2) \| c \|_2
\]

with \( e = f - p \) for arbitrary \( p \in \Pi_{k,\ell} \). Applying Theorem 3.1 to \( \| e\{A, B\} \|_2 \), \( \| e\{U_k^* A U_k, V_\ell^* B V_\ell\} \|_2 \) and noting that \( W(U_k^* A U_k) \subset W(A) \), \( W(V_\ell^* B V_\ell) \subset W(B) \) concludes the proof. \( \square \)

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