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HIGHER ORDER FRÉCHET DERIVATIVES OF MATRIX FUNCTIONS AND THE LEVEL-2 CONDITION NUMBER*

NICHOLAS J. HIGHAM[†] AND SAMUEL D. RELTON[†]

Abstract. The Fréchet derivative L_f of a matrix function $f: \mathbb{C}^{n \times n} \mapsto \mathbb{C}^{n \times n}$ controls the sensitivity of the function to small perturbations in the matrix. While much is known about the properties of L_f and how to compute it, little attention has been given to higher order Fréchet derivatives. We derive sufficient conditions for the k th Fréchet derivative to exist and be continuous in its arguments and we develop algorithms for computing the k th derivative and its Kronecker form. We analyze the level-2 absolute condition number of a matrix function (“the condition number of the condition number”) and bound it in terms of the second Fréchet derivative. For normal matrices and the exponential we show that in the 2-norm the level-1 and level-2 absolute condition numbers are equal and that the relative condition numbers are within a small constant factor of each other. We also obtain an exact relationship between the level-1 and level-2 absolute condition numbers for the matrix inverse and arbitrary nonsingular matrices, as well as a weaker connection for Hermitian matrices for a class of functions that includes the logarithm and square root. Finally, the relation between the level-1 and level-2 condition numbers is investigated more generally through numerical experiments.

Key words. matrix function, Fréchet derivative, Gâteaux derivative, higher order derivative, matrix exponential, matrix logarithm, matrix square root, matrix inverse, matrix calculus, partial derivative, Kronecker form, level-2 condition number, expm, logm, sqrtm, MATLAB

AMS subject classifications. 65F30, 65F60

1. Introduction. Matrix functions $f: \mathbb{C}^{n \times n} \mapsto \mathbb{C}^{n \times n}$ such as the matrix exponential, the matrix logarithm, and matrix powers A^t for $t \in \mathbb{R}$ are being used within a growing number of applications including model reduction [5], numerical solution of fractional partial differential equations [9], analysis of complex networks [13], and computer animation [35]. Increasingly the Fréchet derivative is also required, with recent examples including computation of correlated choice probabilities [1], registration of MRI images [6], Markov models applied to cancer data [14], matrix geometric mean computation [24], and model reduction [33], [34]. Higher order Fréchet derivatives have been used to solve nonlinear equations on Banach spaces by generalizing the Halley method [4, Sec. 3].

The Fréchet derivative of f at $A \in \mathbb{C}^{n \times n}$ is the unique function $L_f(A, \cdot)$ that is linear in its second argument and for all $E \in \mathbb{C}^{n \times n}$ satisfies

$$f(A + E) - f(A) - L_f(A, E) = o(\|E\|). \quad (1.1)$$

An important role of the Fréchet derivative is in the definition of condition numbers for matrix functions [20, Sec. 3.1], [26]. The absolute and relative condition numbers measure the sensitivity of $f(A)$ to small absolute and relative perturbations in A ,

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[†]School of Mathematics, The University of Manchester, Manchester, M13 9PL, UK (nick.higham@manchester.ac.uk, <http://www.maths.manchester.ac.uk/~higham>, samuel.relton@manchester.ac.uk, <http://www.maths.manchester.ac.uk/~srelton>).

respectively, and are defined by

$$\text{cond}_{\text{abs}}(f, A) := \lim_{\epsilon \rightarrow 0} \sup_{\|E\| \leq \epsilon} \frac{\|f(A + E) - f(A)\|}{\epsilon} = \max_{\|E\|=1} \|L_f(A, E)\|, \quad (1.2)$$

$$\text{cond}_{\text{rel}}(f, A) := \lim_{\epsilon \rightarrow 0} \sup_{\|E\| \leq \epsilon \|A\|} \frac{\|f(A + E) - f(A)\|}{\epsilon \|f(A)\|} = \max_{\|E\|=1} \|L_f(A, E)\| \frac{\|A\|}{\|f(A)\|}. \quad (1.3)$$

Associated with the Fréchet derivative is its Kronecker form: the unique matrix $K_f(A) \in \mathbb{C}^{n^2 \times n^2}$ such that for any $E \in \mathbb{C}^{n \times n}$ [20, eq. (3.17)]

$$\text{vec}(L_f(A, E)) = K_f(A) \text{vec}(E), \quad (1.4)$$

where vec is the operator stacking the columns of a matrix vertically from first to last. The condition numbers cond_{abs} and cond_{rel} can be estimated by applying a matrix norm estimator to the Kronecker matrix $K_f(A)$ [20, Alg. 3.22], which requires evaluating the Fréchet derivative in multiple directions E . This idea has been used in [2], [3], and [21] for the matrix exponential, the matrix logarithm, and matrix powers, respectively.

We will refer to cond_{abs} and cond_{rel} as level-1 condition numbers. Since the estimation of the condition number is itself subject to rounding errors it is important to know the condition number of the condition number, which we call the level-2 condition number. It has been shown by Demmel [11, Sec. 7] for matrix inversion, the eigenproblem, polynomial zero-finding, and pole assignment in linear control problems that the level-1 and level-2 (relative) condition numbers are equivalent; for matrix inversion D. J. Higham [18] obtains explicit constants in the equivalence. Cheung and Cucker [10] also derive tight bounds on the level-2 (relative) condition number for a class of functions that includes the matrix inverse. One purpose of our work is to investigate the connection between the level-1 and level-2 (absolute) condition numbers of general matrix functions.

The level-2 condition number is intimately connected with the second Fréchet derivative. There is little or no literature on higher Fréchet derivatives of matrix functions. Another goal of this work is to develop the existence theory for higher order derivatives and to derive methods for computing the derivatives. The computational aspects of estimating the norms of certain quantities involving higher order derivatives are considered in [22].

This work is organized as follows. In section 2 we define higher order Fréchet derivatives and summarize previous research into derivatives of matrix functions. In section 3 we obtain conditions for the existence and continuity of the k th order Fréchet derivative and also give an algorithm for computing it given only the ability to compute the matrix function f . The Kronecker matrix form of the k th order Fréchet derivative is discussed in section 4 and an algorithm is given for computing it. In section 5 we define and analyze the level-2 condition number. We derive an upper bound for general functions f in terms of the second Kronecker form. For the exponential function we show that the level-1 and level-2 absolute condition numbers are equal and that the level-2 relative condition number cannot be much larger than the level-1 relative condition number. We also derive an exact relation between the level-1 and level-2 absolute condition numbers of the matrix inverse, as well as a result connecting the two absolute condition numbers for Hermitian matrices for a class of functions that includes the logarithm and square root. Via numerical experiments we compare

the level-1 and level-2 condition numbers with different functions on unstructured matrices. Concluding remarks are given in section 6.

2. Higher order derivatives. The k th Fréchet derivative of $f : \mathbb{C}^{n \times n} \mapsto \mathbb{C}^{n \times n}$ at $A \in \mathbb{C}^{n \times n}$ can be defined recursively as the unique multilinear function¹ $L_f^{(k)}(A)$ of the matrices $E_i \in \mathbb{C}^{n \times n}$, $i = 1 : k$, that satisfies

$$\begin{aligned} L_f^{(k-1)}(A + E_k, E_1, \dots, E_{k-1}) - L_f^{(k-1)}(A, E_1, \dots, E_{k-1}) \\ - L_f^{(k)}(A, E_1, \dots, E_k) = o(\|E_k\|), \end{aligned} \quad (2.1)$$

where $L_f^{(1)}(A)$ is the first Fréchet derivative. Assuming $L_f^{(k)}(A)$ is continuous at A , we can view the k th Fréchet derivative as a mixed partial derivative

$$L_f^{(k)}(A, E_1, \dots, E_k) = \frac{\partial}{\partial s_1} \cdots \frac{\partial}{\partial s_k} \Big|_{(s_1, \dots, s_k)=0} f(A + s_1 E_1 + \cdots + s_k E_k), \quad (2.2)$$

as explained by Nashed [32, Sec. 9] in the more general setting of Banach spaces. From this equality it is clear that the order in which the derivatives are taken is irrelevant [8, p. 313], [16, Thm. 8], [30, Thm. 4.3.4], so the E_i can be permuted without changing the value of the Fréchet derivative. The k th Fréchet derivative of a matrix function also satisfies the sum, product, and chain rules (the proofs given in [20, Chap. 3] for the first Fréchet derivative are readily extended to higher order derivatives). Further information on higher order Fréchet derivatives in Banach spaces can be found in [12, Sec. 8.12], [25, Chap. 17], and [30, Sec. 4.3], for example.

We mention that some authors prefer to denote the k th Fréchet derivative by $D^k f(A)(E_1, \dots, E_k)$. Our notation has the advantage of being consistent with the notation in the matrix function literature for the first Fréchet derivative (1.1).

Previous research into higher derivatives of matrix functions has primarily focused on different types of derivative. Mathias [29] defines the k th derivative of a matrix function by

$$\frac{d^k}{dt^k} \Big|_{t=0} f(A(t)), \quad (2.3)$$

where $A(t) : \mathbb{R} \mapsto \mathbb{C}^{n \times n}$ is a k times differentiable path at $t = 0$ with $A(0) = A$. When $A'(0) = E$, the first derivative of f along the path $A(t)$ is equivalent to the first Fréchet derivative (assuming the latter exists) but this agreement does not hold for higher order derivatives.

Najfeld and Havel [31] investigate a special case of Mathias' type of derivative that corresponds to $A(t) = A + tV$. They find that [31, Thm. 4.13]

$$f \left(\begin{bmatrix} A & V & & \\ & \ddots & \ddots & \\ & & A & V \\ & & & A \end{bmatrix} \right) = \begin{bmatrix} f(A) & D_V^{[1]} f(A) & \cdots & \frac{D_V^{[q]} f(A)}{q!} \\ & f(A) & \ddots & \vdots \\ & & \ddots & D_V^{[1]} f(A) \\ & & & f(A) \end{bmatrix}, \quad (2.4)$$

¹We write $L_f^{(k)}(A)$ as a shorthand for $L_f^{(k)}(A, \cdot, \dots, \cdot)$ when we want to refer to the mapping at A and not its value in a particular set of directions.

where the argument of f is a block $q \times q$ matrix and $D_V^{[k]} f(A) = \left. \frac{d^k}{dt^k} \right|_{t=0} f(A(t))$. This is a generalization of the formula for evaluating a matrix function on a Jordan block [20, Def. 1.2].

There is also a componentwise derivative for matrix functions (including the trace and determinant etc.) which Magnus and Neudecker summarize in [28, pp. 171–173]. Athans and Schweppe apply this type of derivative to the matrix exponential in [7].

3. Existence and computation of higher Fréchet derivatives. One approach to investigating the existence of higher order Fréchet derivatives is to generalize the series of results for the first Fréchet derivative found in [20, Chap. 3]. However, this yields a somewhat lengthy development. Instead we present an approach that leads more quickly to the desired results and also provides a scheme for computing the Fréchet derivatives.

We first state three existing results on which we will build. Let \mathcal{D} be an open subset of \mathbb{C} and denote by $\mathbb{C}^{n \times n}(\mathcal{D}, p)$ the set of matrices in $\mathbb{C}^{n \times n}$ whose spectrum lies in \mathcal{D} and whose largest Jordan block is of size p .

THEOREM 3.1 (Mathias [29, Lem. 1.1]). *Let f be $p - 1$ times continuously differentiable on \mathcal{D} . Then f exists and is continuous on $\mathbb{C}^{n \times n}(\mathcal{D}, p)$.*

THEOREM 3.2. *Let f be $2p - 1$ times continuously differentiable on \mathcal{D} . Then for $A \in \mathbb{C}^{n \times n}(\mathcal{D}, p)$ the Fréchet derivative $L_f(A, E)$ exists and is continuous in both A and $E \in \mathbb{C}^{n \times n}$.*

Proof. This is a straightforward strengthening of [20, Thm. 3.8] (which has $p = n$) with essentially the same proof. \square

THEOREM 3.3 (Mathias [29, Thm. 2.1]). *Let f be $2p - 1$ times continuously differentiable on \mathcal{D} . For $A \in \mathbb{C}^{n \times n}(\mathcal{D}, p)$,*

$$f \left(\begin{bmatrix} A & E \\ 0 & A \end{bmatrix} \right) = \begin{bmatrix} f(A) & L_f(A, E) \\ 0 & f(A) \end{bmatrix}. \quad (3.1)$$

We need the Gâteaux derivative of f at A in the direction E (also known as the directional derivative), which is defined by

$$G_f(A, E) = \left. \frac{d}{dt} \right|_{t=0} f(A + tE) = \lim_{\epsilon \rightarrow 0} \frac{f(A + \epsilon E) - f(A)}{\epsilon}. \quad (3.2)$$

Gâteaux differentiability is a weaker notion than Fréchet differentiability: if the Fréchet derivative exists then the Gâteaux derivative exists and is equal to the Fréchet derivative. Conversely, if the Gâteaux derivative exists, is linear in E , and is continuous in A , then f is Fréchet differentiable and the Gâteaux and Fréchet derivatives are the same [8, Sec. X.4], [32, Sec. 8, Rem. 3].

Now define the sequence $X_i \in \mathbb{C}^{2^i n \times 2^i n}$ by

$$X_i = I_2 \otimes X_{i-1} + \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix} \otimes I_{2^{i-1}} \otimes E_i, \quad X_0 = A, \quad (3.3)$$

where \otimes is the Kronecker product [17], [27, Chap. 12]. Thus, for example, $X_1 = \begin{bmatrix} A & E_1 \\ 0 & A \end{bmatrix}$ and

$$X_2 = \begin{bmatrix} A & E_1 & E_2 & 0 \\ 0 & A & 0 & E_2 \\ 0 & 0 & A & E_1 \\ 0 & 0 & 0 & A \end{bmatrix}. \quad (3.4)$$

We will need the following lemma, which is a corollary of [23, Thm. 3.2.10.1] and [29, Lem. 3.1].

LEMMA 3.4. *If the largest Jordan block of $A \in \mathbb{C}^{n \times n}$ is of size p then the largest Jordan block of X_k is of size at most $2^k p$.*

Now we can give our main result, which generalizes Theorems 3.2 and 3.3.

THEOREM 3.5. *Let f be $2^k p - 1$ times continuously differentiable on \mathcal{D} . Then for $A \in \mathbb{C}^{n \times n}(\mathcal{D}, p)$ the k th Fréchet derivative $L_f^{(k)}(A)$ exists and $L_f^{(k)}(A, E_1, \dots, E_k)$ is continuous in A and $E_1, \dots, E_k \in \mathbb{C}^{n \times n}$. Moreover, the upper right $n \times n$ block of $f(X_k)$ is $L_f^{(k)}(A, E_1, \dots, E_k)$.*

Proof. Our proof is by induction on k , with the base case $k = 1$ given by Theorems 3.2 and 3.3. Suppose the result holds for some m between 1 and $k - 1$. To prove that it holds for $m + 1$ consider

$$f(X_{m+1}) = f \left(\begin{bmatrix} X_m & I_{2^m} \otimes E_{m+1} \\ 0 & X_m \end{bmatrix} \right), \quad (3.5)$$

which exists by Lemma 3.4 and Theorem 3.1. If we apply (3.1) to $f(X_{m+1})$ we see that its upper-right quarter is

$$L_f(X_m, I_{2^m} \otimes E_{m+1}) = \lim_{\epsilon \rightarrow 0} \frac{f(X_m + \epsilon(I_{2^m} \otimes E_{m+1})) - f(X_m)}{\epsilon}, \quad (3.6)$$

since the Fréchet derivative equals the Gâteaux derivative.

Now consider $X_m + \epsilon(I_{2^m} \otimes E_{m+1})$, which is the matrix obtained from (3.3) with A replaced by $A + \epsilon E_{m+1}$. For ϵ sufficiently small the spectrum of $X_m + \epsilon(I_{2^m} \otimes E_{m+1})$ lies within \mathcal{D} by continuity of the eigenvalues. Hence we can apply the inductive hypothesis to both $f(X_m)$ and $f(X_m + \epsilon(I_{2^m} \otimes E_{m+1}))$, to deduce that their upper-right $n \times n$ blocks are, respectively,

$$L_f^{(m)}(A, E_1, \dots, E_m), \quad L_f^{(m)}(A + \epsilon E_{m+1}, E_1, \dots, E_m). \quad (3.7)$$

Hence the upper-right $n \times n$ block of (3.6), which is also the upper-right $n \times n$ block of $f(X_{m+1})$ is

$$\begin{aligned} [f(X_{m+1})]_{1n} &= \lim_{\epsilon \rightarrow 0} \frac{L_f^{(m)}(A + \epsilon E_{m+1}, E_1, \dots, E_m) - L_f^{(m)}(A, E_1, \dots, E_m)}{\epsilon} \\ &= \left. \frac{d}{dt} \right|_{t=0} L_f^{(m)}(A + t E_{m+1}, E_1, \dots, E_m), \end{aligned} \quad (3.8)$$

which is the Gâteaux derivative of the m th Fréchet derivative in the direction E_{m+1} . From our earlier discussion of the Gâteaux derivative we need to show that (3.8) is continuous in A and linear in E_{m+1} so that it is equal to the $(m + 1)$ st Fréchet derivative.

The continuity in A is trivial since f is sufficiently differentiable to be a continuous function of X_m by Theorem 3.1 and the map from $f(X_m)$ to its upper-right $n \times n$ block is also continuous. Now we show the linearity in E_{m+1} . Let us denote by σ the map from a matrix to its upper-right $n \times n$ block. Recalling that (3.8) is the upper right $n \times n$ block of (3.6), since the first Fréchet derivative is linear in its second

argument we have

$$\begin{aligned}
\left. \frac{d}{dt} \right|_{t=0} L_f^{(m)}(A + t(E + F), E_1, \dots, E_m) &= \sigma L_f(X_m, I_{2^m} \otimes (E + F)) \\
&= \sigma L_f(X_m, I_{2^m} \otimes E) + \sigma L_f(X_m, I_{2^m} \otimes F) \\
&= \left. \frac{d}{dt} \right|_{t=0} L_f^{(m)}(A + tE, E_1, \dots, E_m) \\
&\quad + \left. \frac{d}{dt} \right|_{t=0} L_f^{(m)}(A + tF, E_1, \dots, E_m),
\end{aligned}$$

which shows the required linearity. We have now shown that the Gâteaux derivative of the m th Fréchet derivative is equal to the $(m + 1)$ st Fréchet derivative. The proof follows by induction. \square

As an example, Theorem 3.5 shows that the second derivative $L_f^{(2)}(A, E_1, E_2)$ is equal to the $(1, 4)$ block of $f(X_2)$, where X_2 is given by (3.4). More generally, the theorem gives the following algorithm for computing arbitrarily high order Fréchet derivatives.

ALGORITHM 3.6. *Given $A \in \mathbb{C}^{n \times n}$, the direction matrices $E_1, \dots, E_k \in \mathbb{C}^{n \times n}$ and a method to evaluate the matrix function f (assumed sufficiently smooth), this algorithm computes $L = L_f^{(k)}(A, E_1, \dots, E_k)$.*

- 1 $X_0 = A$
- 2 for $i = 1:k$
- 3 $X_i = I_2 \otimes X_{i-1} + \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix} \otimes I_{2^{i-1}} \otimes E_i$
- 4 end
- 5 $F = f(X_k)$
- 6 Take L to be the upper-right $n \times n$ block of F .

Cost: Assuming that evaluating f at an $n \times n$ matrix costs $O(n^3)$ flops, applying f naively to X_k gives an overall cost of $O(8^k n^3)$ flops. Clearly this algorithm rapidly becomes prohibitively expensive as k grows, though exploiting the block structure of X_k could lead to significant savings in the computation.

To conclude this section we emphasize that the condition in Theorem 3.5 that f has $2^k p - 1$ derivatives, which stems from a bound on the worst possible Jordan structure of X_k , is not always necessary. It is easy to show there is always an E such that X_1 has a Jordan block of size $2p - 1$, so the condition is necessary for $k = 1$. However, in the appendix, we provide an example of a matrix A for which fewer than $4p - 1$ derivatives are required for the existence of $f(X_2)$. Determining the exact number of derivatives needed for the existence of $f(X_k)$ given the Jordan structure of A is an open problem.

4. Kronecker forms of higher Fréchet derivatives. The Kronecker form of the first Fréchet derivative is given by (1.4). The principal attraction of the Kronecker form is that it explicitly captures the linearity of the Fréchet derivative, so that standard linear algebra techniques can be applied and certain explicit formulas and bounds can be obtained. Indeed, in the Frobenius norm the absolute condition number (1.2) of a matrix function is

$$\text{cond}_{\text{abs}}(f, A) = \|K_f(A)\|_2, \quad (4.1)$$

as is easily shown from (1.4). For the 1-norm, $\text{cond}_{\text{abs}}(f, A)$ is within a factor n of $\|K_f(A)\|_1$ [20, Lem. 3.18], so for both the 1-norm and the 2-norm estimating $\text{cond}_{\text{abs}}(f, A)$ reduces to estimating a norm of $K_f(A)$.

In this section we derive a Kronecker form for the k th Fréchet derivative and show how it can be computed. We assume that the k th Fréchet derivative $L_f^{(k)}(A, E_1, \dots, E_k)$ is continuous in A , which allows reordering of the E_i , as noted in section 2.

To begin, since $L_f^{(k)}(A, E_1, \dots, E_k)$ is linear in E_k we have

$$\text{vec}(L_f^{(k)}(A, E_1, \dots, E_k)) = K_f^{(1)}(A, E_1, \dots, E_{k-1}) \text{vec}(E_k), \quad (4.2)$$

for some unique matrix $K_f^{(1)}(A, E_1, \dots, E_{k-1}) \in \mathbb{C}^{n^2 \times n^2}$. Since the E_i can be permuted within the k th Fréchet derivative it follows that the E_i can be permuted in (4.2). For example, using the third Fréchet derivative,

$$K_f^{(1)}(A, E_1, E_2) \text{vec}(E_3) = K_f^{(1)}(A, E_3, E_1) \text{vec}(E_2).$$

We can use this fact to show that $K_f^{(1)}(A, E_1, \dots, E_{k-1})$ is linear in each E_i .

LEMMA 4.1. *Assuming that $L_f^{(k)}(A)$ is continuous in A , $K_f^{(1)}(A, E_1, \dots, E_{k-1})$ is linear in each E_i .*

Proof. Using the definition (4.2) and the freedom to reorder the E_i within $K_f^{(1)}$ we write

$$\begin{aligned} & K_f^{(1)}(A, E_1, \dots, E_i + F_i, \dots, E_{k-1}) \text{vec}(E_k) \\ &= \text{vec}(L_f^{(k)}(A, E_1, \dots, E_i + F_i, \dots, E_{k-1}, E_k)) \\ &= K_f^{(1)}(A, E_1, \dots, E_{i-1}, E_{i+1}, \dots, E_{k-1}, E_k) \text{vec}(E_i + F_i) \\ &= K_f^{(1)}(A, E_1, \dots, E_{i-1}, E_{i+1}, \dots, E_{k-1}, E_k) (\text{vec}(E_i) + \text{vec}(F_i)) \\ &= (K_f^{(1)}(A, E_1, \dots, E_i, \dots, E_{k-1}) + K_f^{(1)}(A, E_1, \dots, F_i, \dots, E_{k-1})) \text{vec}(E_k). \end{aligned}$$

Since this is true for any matrix E_k , the matrices on the left and right-hand sides must be equal, and hence $K_f^{(1)}(A, E_1, \dots, E_{k-1})$ is linear in E_i . \square

Now since $K_f^{(1)}(A, E_1, \dots, E_{k-1})$ is linear in each E_i it is linear in E_{k-1} and so,

$$\text{vec}(K_f^{(1)}(A, E_1, \dots, E_{k-1})) = K_f^{(2)}(A, E_1, \dots, E_{k-2}) \text{vec}(E_{k-1}), \quad (4.3)$$

where $K_f^{(2)}(A, E_1, \dots, E_{k-2}) \in \mathbb{C}^{n^4 \times n^2}$. By the same argument as in the proof of Lemma 4.1 this matrix is also linear in each E_i and continuing this process we eventually arrive at $K_f^{(k)}(A) \in \mathbb{C}^{n^{2k} \times n^2}$, which we call the Kronecker form of the k th Fréchet derivative.

We can relate $K_f^{(k)}(A)$ to the k th Fréchet derivative by repeatedly taking vec of the k th Fréchet derivative and using $\text{vec}(AXB) = (B^T \otimes A) \text{vec}(X)$:

$$\begin{aligned} \text{vec}(L_f^{(k)}(A, E_1, \dots, E_k)) &= K_f^{(1)}(A, E_1, \dots, E_{k-1}) \text{vec}(E_k) \\ &= \text{vec}(K_f^{(1)}(A, E_1, \dots, E_{k-1}) \text{vec}(E_k)) \\ &= (\text{vec}(E_k)^T \otimes I_{n^2}) K_f^{(2)}(A, E_1, \dots, E_{k-2}) \text{vec}(E_{k-1}) \\ &= (\text{vec}(E_{k-1})^T \otimes \text{vec}(E_k)^T \otimes I_{n^2}) \text{vec}(K_f^{(2)}(A, E_1, \dots, E_{k-2})) \\ &= \dots \\ &= (\text{vec}(E_1)^T \otimes \dots \otimes \text{vec}(E_k)^T \otimes I_{n^2}) \text{vec}(K_f^{(k)}(A)). \end{aligned} \quad (4.4)$$

In the remainder of this section we give an algorithm to compute the Kronecker form. Consider $K_f^{(k)}(A)e_m$ where e_m is the m th unit vector, so that this product gives us the m th column of $K_f^{(k)}(A)$. We know from the above that this can be written as $\text{vec}(K_f^{(k-1)}(A, E_1))$, where $\text{vec}(E_1) = e_m$. Therefore to obtain the m th column of $K_f^{(k)}(A)$ we require $K_f^{(k-1)}(A, E_1)$ and as above we can find each column of this matrix as $K_f^{(k-1)}(A, E_1)e_p = \text{vec}(K_f^{(k-1)}(A, E_1, E_2))$ where E_2 is chosen so that $\text{vec}(E_2) = e_p$. Continuing in this way we obtain the following algorithm, of which [20, Alg. 3.17] is the special case with $k = 1$.

ALGORITHM 4.2. *The following algorithm computes the Kronecker form $K_f^{(k)}(A)$ of the k th Fréchet derivative $L_f^{(k)}(A)$.*

```

1  for  $m_1 = 1:n^2$ 
2      Choose  $E_1 \in \mathbb{R}^{n \times n}$  such that  $\text{vec}(E_1) = e_{m_1}$ .
3      for  $m_2 = 1:n^2$ 
4          Choose  $E_2 \in \mathbb{R}^{n \times n}$  such that  $\text{vec}(E_2) = e_{m_2}$ .
5          ...
6          for  $m_k = 1:n^2$ 
7              Choose  $E_k \in \mathbb{R}^{n \times n}$  such that  $\text{vec}(E_k) = e_{m_k}$ .
8              Compute  $L_f^{(k)}(A, E_1, \dots, E_k)$  using Algorithm 3.6.
9              Set the  $m_k$ th column of  $K_f^{(1)}(A, E_1, \dots, E_{k-1})$ 
              to  $\text{vec}(L_f^{(k)}(A, E_1, \dots, E_k))$ .
10             end
11             ...
12             Set the  $m_2$ th column of  $K_f^{(k-1)}(A, E_1)$  to  $\text{vec}(K_f^{(k-2)}(A, E_1, E_2))$ .
13         end
14         Set the  $m_1$ th column of  $K_f^{(k)}(A)$  to  $\text{vec}(K_f^{(k-1)}(A, E_1))$ .
15     end

```

Cost: $O(8^k n^{3+2k})$ flops, since line 8 is executed n^2 times for each of the k matrices E_i .

The cost of this method depends heavily upon k , which governs both the depth of the algorithm and the cost of evaluating the k th Fréchet derivative in line 8. However, even calculating the Kronecker form of the first Fréchet derivative costs $O(n^5)$ flops, so this algorithm is only viable for small matrices and small k . Nevertheless, the algorithm is useful for testing algorithms for estimating $\|K_f^{(k)}(A)\|$ and hence $\|L_f^{(k)}(A)\|$.

5. The level-2 condition number of a matrix function. It is important to understand how sensitive the condition number is to perturbations in A , since this will affect the accuracy of any algorithm attempting to estimate it, such as those in [2], [3], [21]. The quantity that measures this sensitivity is called the level-2 condition number.

The level-2 condition number is obtained by taking the absolute (or relative) condition number of the absolute (or relative) condition number, offering four possibilities. In this investigation we mainly limit ourselves to analyzing the absolute condition number of the absolute condition number,

$$\text{cond}_{\text{abs}}^{[2]}(f, A) = \lim_{\epsilon \rightarrow 0} \sup_{\|Z\| \leq \epsilon} \frac{|\text{cond}_{\text{abs}}(f, A + Z) - \text{cond}_{\text{abs}}(f, A)|}{\epsilon}, \quad (5.1)$$

where $\text{cond}_{\text{abs}}(f, X)$ is defined in (1.2). However in section 5.1 for the exponential we also consider the relative condition number of the relative condition number,

$$\text{cond}_{\text{rel}}^{[2]}(f, A) = \lim_{\epsilon \rightarrow 0} \sup_{\|Z\| \leq \epsilon \|A\|} \frac{|\text{cond}_{\text{rel}}(f, A+Z) - \text{cond}_{\text{rel}}(f, A)|}{\epsilon \text{cond}_{\text{rel}}(f, A)}. \quad (5.2)$$

We begin this section by deriving a bound for the level-2 absolute condition number for general functions f in the Frobenius norm. Using the second Fréchet derivative we have, from (1.2) and (2.1),

$$\text{cond}_{\text{abs}}(f, A+Z) = \max_{\|E\|=1} \|L_f(A, E) + L_f^{(2)}(A, E, Z) + o(\|Z\|)\|. \quad (5.3)$$

Therefore using the triangle inequality in the numerator of (5.1) we obtain

$$\begin{aligned} |\text{cond}_{\text{abs}}(f, A+Z) - \text{cond}_{\text{abs}}(f, A)| &= \left| \max_{\|E\|=1} \|L_f(A, E) + L_f^{(2)}(A, E, Z) + o(\|Z\|)\| \right. \\ &\quad \left. - \max_{\|E\|=1} \|L_f(A, E)\| \right| \\ &\leq \max_{\|E\|=1} \|L_f^{(2)}(A, E, Z) + o(\|Z\|)\|. \end{aligned}$$

Using this inequality in the definition of the level-2 condition number (5.1) we see

$$\begin{aligned} \text{cond}_{\text{abs}}^{[2]}(f, A) &\leq \lim_{\epsilon \rightarrow 0} \sup_{\|Z\| \leq \epsilon} \max_{\|E\|=1} \|L_f^{(2)}(A, E, Z/\epsilon) + o(\|Z\|)/\epsilon\| \\ &= \sup_{\|Z\| \leq 1} \max_{\|E\|=1} \|L_f^{(2)}(A, E, Z)\| \\ &= \max_{\|Z\|=1} \max_{\|E\|=1} \|L_f^{(2)}(A, E, Z)\|, \end{aligned} \quad (5.4)$$

where the supremum can be replaced with a maximum because we are working on a finite-dimensional vector space and the maximum is attained for $\|Z\| = 1$ because the second Fréchet derivative is linear in Z . We will see in subsection 5.2 that this upper bound is attained for the matrix inverse and the Frobenius norm. Note that the upper bound (5.4) can be thought of as $\|L_f^{(2)}(A)\|$.

Now restricting ourselves to the Frobenius norm and recalling that $\|X\|_F = \|\text{vec}(X)\|_2$ we obtain

$$\begin{aligned} \text{cond}_{\text{abs}}^{[2]}(f, A) &\leq \max_{\|Z\|_F=1} \max_{\|E\|_F=1} \|L_f^{(2)}(A, E, Z)\|_F \\ &= \max_{\|Z\|_F=1} \max_{\|\text{vec}(E)\|_2=1} \|K_f^{(1)}(A, Z) \text{vec}(E)\|_2 \quad \text{by (4.2)} \\ &= \max_{\|Z\|_F=1} \|K_f^{(1)}(A, Z)\|_2 \\ &\leq \max_{\|Z\|_F=1} \|K_f^{(1)}(A, Z)\|_F \\ &= \max_{\|\text{vec}(Z)\|_2=1} \|K_f^{(2)}(A) \text{vec}(Z)\|_2 \quad \text{by (4.3)} \\ &= \|K_f^{(2)}(A)\|_2. \end{aligned} \quad (5.5)$$

For general functions f it is difficult to say more about the level-2 condition number. In the next few subsections we focus on the matrix exponential, inverse, and a class of functions containing both the logarithm and square root.

5.1. Matrix exponential. For the matrix exponential let us consider the level-2 absolute condition number in the 2-norm, for normal matrices

$$A = QDQ^*, \quad Q \text{ unitary, } D = \text{diag}(d_i). \quad (5.6)$$

Note first that for a normal matrix A , using the unitary invariance of the 2-norm we have $\|e^A\|_2 = \|e^D\|_2 = e^{\alpha(D)} = e^{\alpha(A)}$, where the spectral abscissa $\alpha(A)$ is the greatest real part of any eigenvalue of A .

Van Loan [36] shows that normality implies $\text{cond}_{\text{rel}}(\exp, A) = \|A\|_2$ and from (1.2) and (1.3) we therefore have $\text{cond}_{\text{abs}}(\exp, A) = e^{\alpha(A)}$.

To analyze the level-2 absolute condition number of the matrix exponential we require the following lemma.

LEMMA 5.1. *For a normal matrix A and an arbitrary matrix Z ,*

$$e^{\alpha(A) - \|Z\|_2} \leq \|e^{A+Z}\|_2 \leq e^{\alpha(A) + \|Z\|_2},$$

and for a given A both bounds are attainable for some Z .

Proof. To get the lower bound we recall from [20, Thm. 10.12] that $e^{\alpha(X)} \leq \|e^X\|_2$ for any matrix $X \in \mathbb{C}^{n \times n}$. We also know from [15, Thm. 7.2.2] that the eigenvalues of $A + Z$ are at most a distance $\|Z\|_2$ from those of A and so

$$e^{\alpha(A) - \|Z\|_2} \leq \|e^{A+Z}\|_2,$$

and it is easy to see that this inequality is attained for $Z = -\text{diag}(\epsilon, \dots, \epsilon)$.

For the upper bound, using the Lie–Trotter product formula [20, Cor. 10.7] gives

$$e^{A+Z} = \lim_{m \rightarrow \infty} (e^{A/m} e^{Z/m})^m.$$

Hence we have

$$\begin{aligned} \|e^{A+Z}\|_2 &= \lim_{m \rightarrow \infty} \|(e^{A/m} e^{Z/m})^m\|_2 \leq \lim_{m \rightarrow \infty} \|e^{A/m}\|_2^m \|e^{Z/m}\|_2^m \\ &= \lim_{m \rightarrow \infty} e^{\alpha(A/m)m} e^{\|Z/m\|_2 m} = e^{\alpha(A) + \|Z\|_2}. \end{aligned}$$

It is straightforward to show that $Z = \text{diag}(\epsilon, \dots, \epsilon)$ attains this upper bound, completing the proof. \square

We can now show that the level-2 absolute condition number of the matrix exponential is equal to the level-1 absolute condition number for normal matrices.

THEOREM 5.2. *Let $A \in \mathbb{C}^{n \times n}$ be normal. Then in the 2-norm $\text{cond}_{\text{abs}}^{[2]}(\exp, A) = \text{cond}_{\text{abs}}(\exp, A)$.*

Proof. By taking norms in the identity

$$L_{\text{exp}}(A + Z, E) = \int_0^1 e^{(A+Z)(1-s)} E e^{(A+Z)s} ds, \quad (5.7)$$

from [20, eq. (10.15)] we obtain

$$\begin{aligned} \text{cond}_{\text{abs}}(\exp, A + Z) &= \max_{\|E\|_2=1} \|L_{\text{exp}}(A + Z, E)\|_2 \\ &\leq \int_0^1 \|e^{(A+Z)(1-s)}\|_2 \|e^{(A+Z)s}\|_2 ds, \end{aligned}$$

and furthermore since scalar multiples of A are normal and $\alpha(sA) = s\alpha(A)$ for $s \geq 0$, we can apply Lemma 5.1 twice within the integral to get

$$\text{cond}_{\text{abs}}(\text{exp}, A + Z) \leq e^{\alpha(A) + \|Z\|_2}.$$

Also we can obtain the lower bound

$$\begin{aligned} \text{cond}_{\text{abs}}(\text{exp}, A + Z) &= \max_{\|E\|_2=1} \|L(A + Z, E)\|_2 \\ &\geq \|L_{\text{exp}}(A + Z, I)\|_2 \\ &= \left\| \int_0^1 e^{(A+Z)(1-s)} e^{(A+Z)s} ds \right\|_2 \\ &= \|e^{A+Z}\|_2 \geq e^{\alpha(A) - \|Z\|_2}, \end{aligned}$$

so that overall, combining these two inequalities,

$$e^{\alpha(A) - \|Z\|_2} \leq \text{cond}_{\text{abs}}(\text{exp}, A + Z) \leq e^{\alpha(A) + \|Z\|_2}. \quad (5.8)$$

With some further manipulation we can use these bounds to show that

$$\sup_{\|Z\|_2 \leq \epsilon} |\text{cond}_{\text{abs}}(\text{exp}, A + Z) - e^{\alpha(A)}| \leq e^{\alpha(A) + \epsilon} - e^{\alpha(A)}. \quad (5.9)$$

From the definition of the level-2 condition number (5.1) we have

$$\text{cond}_{\text{abs}}^{[2]}(\text{exp}, A) = \lim_{\epsilon \rightarrow 0} \sup_{\|Z\|_2 \leq \epsilon} \frac{|\text{cond}_{\text{abs}}(\text{exp}, A + Z) - e^{\alpha(A)}|}{\epsilon}.$$

Using the upper bound (5.9) on the numerator we see that

$$\text{cond}_{\text{abs}}^{[2]}(\text{exp}, A) \leq \lim_{\epsilon \rightarrow 0} \frac{e^{\alpha(A) + \epsilon} - e^{\alpha(A)}}{\epsilon} = e^{\alpha(A)}.$$

For the lower bound we use the fact that $\text{cond}_{\text{abs}}(\text{exp}, A + \epsilon I) = e^{\alpha(A) + \epsilon}$ (since $A + \epsilon I$ is normal) to obtain

$$\begin{aligned} \text{cond}_{\text{abs}}^{[2]}(\text{exp}, A) &\geq \lim_{\epsilon \rightarrow 0} \frac{|\text{cond}_{\text{abs}}(\text{exp}, A + \epsilon I) - e^{\alpha(A)}|}{\epsilon} \\ &= \lim_{\epsilon \rightarrow 0} \frac{e^{\alpha(A) + \epsilon} - e^{\alpha(A)}}{\epsilon} = e^{\alpha(A)}. \end{aligned}$$

This completes the proof, since $\text{cond}_{\text{abs}}(\text{exp}, A) = e^{\alpha(A)}$. \square

We can also show that the level-2 relative condition number cannot be much larger than the level-1 relative condition number for normal matrices. In the next result we exclude $A = 0$ because $\text{cond}_{\text{rel}}(\text{exp}, 0) = 0$ and so the computation of $\text{cond}_{\text{rel}}^{[2]}(\text{exp}, 0)$ involves division by 0 and is therefore undefined.

THEOREM 5.3. *Let $A \in \mathbb{C}^{n \times n} \setminus \{0\}$ be normal. Then in the 2-norm*

$$1 \leq \text{cond}_{\text{rel}}^{[2]}(\text{exp}, A) \leq 2 \text{cond}_{\text{rel}}(\text{exp}, A) + 1.$$

Proof. Combining the definition of the level-2 relative condition number (5.2) with the facts that $\text{cond}_{\text{rel}}(\exp, X) = \text{cond}_{\text{abs}}(\exp, X) \|X\|_2 / \|e^X\|_2$ for any $X \in \mathbb{C}^{n \times n}$, by (1.2) and (1.3), and $\text{cond}_{\text{rel}}(\exp, A) = \|A\|_2$ for normal A (mentioned at the beginning of this section), we have

$$\text{cond}_{\text{rel}}^{[2]}(\exp, A) = \lim_{\epsilon \rightarrow 0} \sup_{\|Z\|_2 \leq \epsilon \|A\|_2} \frac{|\text{cond}_{\text{abs}}(\exp, A + Z) \frac{\|A+Z\|_2}{\|e^{A+Z}\|_2} - \|A\|_2|}{\epsilon \|A\|_2}. \quad (5.10)$$

For the lower bound note that for any $X \in \mathbb{C}^{n \times n}$ we have $\|e^X\|_2 \leq \text{cond}_{\text{abs}}(\exp, X)$ [20, Lem. 10.15] and therefore taking $X = A + Z$ we obtain

$$\frac{\text{cond}_{\text{abs}}(\exp, A + Z) \frac{\|A+Z\|_2}{\|e^{A+Z}\|_2} - \|A\|_2}{\epsilon \|A\|_2} \geq \frac{\|A + Z\|_2 - \|A\|_2}{\epsilon \|A\|_2}.$$

Using this bound in (5.10) we see that

$$\begin{aligned} \text{cond}_{\text{rel}}^{[2]}(\exp, A) &\geq \lim_{\epsilon \rightarrow 0} \sup_{\|Z\|_2 \leq \epsilon \|A\|_2} \frac{\|A + Z\|_2 - \|A\|_2}{\epsilon \|A\|_2} \\ &= \lim_{\epsilon \rightarrow 0} \frac{(1 + \epsilon)\|A\|_2 - \|A\|_2}{\epsilon \|A\|_2} = 1, \end{aligned}$$

where the supremum is attained for $Z = \epsilon A$.

For the upper bound we first combine Lemma 5.1 and (5.8) to obtain

$$e^{-2\|Z\|_2} \leq \frac{\text{cond}_{\text{abs}}(\exp, A + Z)}{\|e^{A+Z}\|_2} \leq e^{2\|Z\|_2}.$$

After some further manipulation we obtain the bound

$$\frac{|\text{cond}_{\text{abs}}(\exp, A + Z) \frac{\|A+Z\|_2}{\|e^{A+Z}\|_2} - \|A\|_2|}{\epsilon \|A\|_2} \leq \frac{e^{2\|Z\|_2} - 1}{\epsilon} + e^{2\|Z\|_2} \frac{\|Z\|_2}{\epsilon \|A\|_2}.$$

Using this inequality in (5.10) we see that

$$\begin{aligned} \text{cond}_{\text{rel}}^{[2]}(\exp, A) &\leq \lim_{\epsilon \rightarrow 0} \sup_{\|Z\|_2 \leq \epsilon \|A\|_2} \left(\frac{e^{2\|Z\|_2} - 1}{\epsilon} + e^{2\|Z\|_2} \frac{\|Z\|_2}{\epsilon \|A\|_2} \right) \\ &= \lim_{\epsilon \rightarrow 0} \left(\frac{e^{2\epsilon \|A\|_2} - 1}{\epsilon} + e^{2\epsilon \|A\|_2} \right) \\ &= 2\|A\|_2 + 1 \\ &= 2 \text{cond}_{\text{rel}}(\exp, A) + 1, \end{aligned}$$

which completes the proof. \square

5.2. Matrix inverse. Assume now that A is a general nonsingular matrix. For the matrix inverse $f(A) = A^{-1}$, we have $L_f(A, E) = -A^{-1}EA^{-1}$. From the definition of the absolute condition number (1.2) we have

$$\text{cond}_{\text{abs}}(x^{-1}, A) = \max_{\|E\|=1} \|A^{-1}EA^{-1}\|,$$

so for any subordinate matrix norm we conclude from [3, Lem. 3.4] that

$$\text{cond}_{\text{abs}}(x^{-1}, A) = \|A^{-1}\|^2, \quad (5.11)$$

and that this maximum is attained for a rank-1 matrix E . However the level-2 absolute condition number is best analyzed in the Frobenius norm, which is not subordinate. The absolute condition number in the Frobenius norm is given by

$$\begin{aligned} \text{cond}_{\text{abs}}(x^{-1}, A) &= \max_{\|E\|_F=1} \|A^{-1}EA^{-1}\|_F \\ &= \max_{\|\text{vec}(E)\|_2=1} \|(A^{-T} \otimes A^{-1}) \text{vec}(E)\|_2 \\ &= \|(A^{-T} \otimes A^{-1})\|_2 = \|A^{-1}\|_2^2, \end{aligned} \quad (5.12)$$

which is also shown in [18, eq. (2.4)]. Using (5.12) in the definition of the level-2 absolute condition number (5.1) we have that in the Frobenius norm

$$\begin{aligned} \text{cond}_{\text{abs}}^{[2]}(x^{-1}, A) &= \lim_{\epsilon \rightarrow 0} \sup_{\|E\|_F \leq \epsilon} \frac{\| (A+E)^{-1} \|_2^2 - \|A^{-1}\|_2^2}{\epsilon}, \\ &= \lim_{\epsilon \rightarrow 0} \sup_{\|E\|_F \leq \epsilon} \frac{|\tilde{\sigma}_n^{-2} - \sigma_n^{-2}|}{\epsilon}, \end{aligned}$$

where σ_n and $\tilde{\sigma}_n$ are the smallest singular values of A and $A + E$, respectively. Now consider the singular value decomposition (SVD) $A = U\Sigma V^*$, where $\Sigma = \text{diag}(\sigma_1, \dots, \sigma_n)$ and $\sigma_1 \geq \dots \geq \sigma_n > 0$. We know from [15, Cor. 8.6.2] that $\tilde{\sigma}_n = \sigma_n + e$ where $|e| \leq \|E\|_2 \leq \|E\|_F \leq \epsilon$, and clearly the perturbation E that maximizes the numerator of the above equation moves σ_n closer to 0. Therefore when $\epsilon < \sigma_n$ the value of $\tilde{\sigma}_n$ that maximizes the numerator is $\tilde{\sigma}_n = \sigma_n - \epsilon$, which is attained by $E = U \text{diag}(0, \dots, 0, -\epsilon) V^*$, with $\|E\|_2 = \|E\|_F = \epsilon$. Continuing with this choice of E we see that

$$\text{cond}_{\text{abs}}^{[2]}(x^{-1}, A) = \lim_{\epsilon \rightarrow 0} \frac{|(\sigma_n - \epsilon)^{-2} - \sigma_n^{-2}|}{\epsilon} = \frac{2}{\sigma_n^3} = 2\|A^{-1}\|_2^3. \quad (5.13)$$

In fact the bound (5.4) on the level-2 absolute condition number is exact in this case. We can see this by maximizing the Frobenius norm of $L_{x^{-1}}^{(2)}(A, E, Z) = A^{-1}EA^{-1}ZA^{-1} + A^{-1}ZA^{-1}EA^{-1}$ using standard results.

From (5.12) and (5.13) we obtain the following result.

THEOREM 5.4. *For nonsingular $A \in \mathbb{C}^{n \times n}$,*

$$\text{cond}_{\text{abs}}^{[2]}(x^{-1}, A) = 2 \text{cond}_{\text{abs}}(x^{-1}, A)^{3/2}. \quad (5.14)$$

This difference between the level-1 and level-2 absolute condition numbers for the inverse is intriguing since D. J. Higham [18, Thm. 6.1] shows that the relative level-1 and level-2 relative condition numbers for the matrix inverse are essentially equal for subordinate norms.

5.3. Hermitian matrices. The previous two sections gave relationships between the level-1 and level-2 absolute condition numbers for the exponential and the inverse. Interestingly these correspond closely to relationships between the first and second derivatives of the respective scalar functions: for $f(x) = e^x$, $|f''| = |f'|$ and

for $f(x) = x^{-1}$, $|f''| = |2(f')^{3/2}|$. It is therefore natural to wonder whether analogous relations, such as $\text{cond}_{\text{abs}}^{[2]}(\log, A) = \text{cond}_{\text{abs}}(\log, A)^2$ and $\text{cond}_{\text{abs}}^{[2]}(x^{1/2}, A) = 2 \text{cond}_{\text{abs}}(x^{1/2}, A)^3$, hold for suitable classes of A . The next result, which applies to Hermitian matrices and a class of functions that includes the logarithm and the square root, provides a partial answer.

THEOREM 5.5. *Let $A \in \mathbb{C}^{n \times n}$ be Hermitian with eigenvalues λ_i arranged so that $\lambda_1 \geq \dots \geq \lambda_n$ and let $f : \mathbb{R} \rightarrow \mathbb{R}$ be such that $f(A)$ is defined and f has a strictly monotonic derivative. Then in the Frobenius norm,*

$$\text{cond}_{\text{abs}}(f, A) = \max_i |f'(\lambda_i)|. \quad (5.15)$$

Moreover, if the maximum in (5.15) is attained for a unique i , say $i = k$ (with $k = 1$ or $k = n$ since f' is monotonic), then

$$\text{cond}_{\text{abs}}^{[2]}(f, A) \geq |f''(\lambda_k)|. \quad (5.16)$$

Proof. Using [20, Cor. 3.16] we see that $\text{cond}_{\text{abs}}(f, A) = \max_{i,j} |f[\lambda_i, \lambda_j]|$, where $f[\lambda_i, \lambda_j]$ is a divided difference. But $f[\lambda_i, \lambda_j] = f'(\theta)$ for some θ on the closed interval between λ_i and λ_j [20, eq. (B.26)], and since f' is monotonic it follows that $|f[\lambda_i, \lambda_j]| \leq \max(|f'(\lambda_i)|, |f'(\lambda_j)|)$, with equality for $i = j$, and (5.15) follows.

We can write $A = Q\Lambda Q^*$, where Q is unitary and $\Lambda = \text{diag}(\lambda_1, \dots, \lambda_n)$. Now define $Z = QDQ^*$, where D differs from the zero matrix only in that $d_{kk} = \epsilon$, so that the eigenvalues of $A + Z$ are λ_i , for $i \neq k$, and $\lambda_k + \epsilon$. Then, by the assumption on k , for sufficiently small ϵ the maximum of $|f'|$ over the eigenvalues of $A + Z$ is $|f'(\lambda_k + \epsilon)|$. Therefore using this Z in (5.1) we obtain

$$\begin{aligned} \text{cond}_{\text{abs}}^{[2]}(f, A) &\geq \lim_{\epsilon \rightarrow 0} \left| \frac{\text{cond}_{\text{abs}}(f, A + Z) - \text{cond}_{\text{abs}}(f, A)}{\epsilon} \right| \\ &= \lim_{\epsilon \rightarrow 0} \left| \frac{|f'(\lambda_k + \epsilon)| - |f'(\lambda_k)|}{\epsilon} \right| \\ &= \left| \lim_{\epsilon \rightarrow 0} \frac{f'(\lambda_k + \epsilon) - f'(\lambda_k)}{\epsilon} \right| \\ &= |f''(\lambda_k)|. \quad \square \end{aligned}$$

Note that when applying this result to the matrix logarithm and square root we require A to be Hermitian positive definite, since these functions are not defined for matrices with negative eigenvalues.

5.4. Numerical experiments. We have a full understanding of the relationship between the level-1 and level-2 absolute condition numbers for the matrix inverse but our results for the matrix exponential, logarithm and square root are applicable only to normal or Hermitian matrices. We now give a numerical comparison of $\text{cond}_{\text{abs}}(f, A)$ and $\text{cond}_{\text{abs}}^{[2]}(f, A)$ for the matrix exponential, logarithm, and square root using unstructured matrices in the Frobenius norm.

Our test matrices are taken from the Matrix Computation Toolbox [19] and the MATLAB gallery function and we use 5×5 matrices because the cost of computing the first and second Kronecker forms using Algorithm 4.2 is $O(n^5)$ and $O(n^7)$ flops,

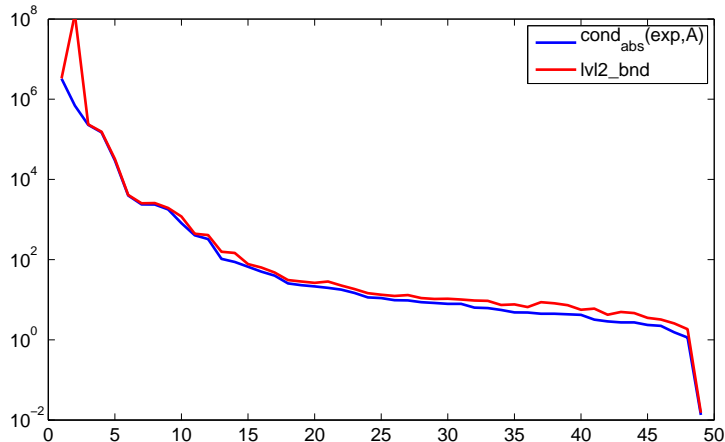


FIG. 5.1. Level-1 absolute condition number and `lv12_bnd` for the matrix exponential in the Frobenius norm sorted by decreasing value of $\text{cond}_{\text{abs}}(\exp, A)$.

respectively. Most of the matrices are neither normal nor Hermitian, so our previous analyses (except for the inverse) do not apply. The matrix exponential and logarithm are computed using the algorithms from [2] and [3] and the square root is computed using the MATLAB function `sqrtn`. All experiments are performed in MATLAB 2013a.

For arbitrary matrices we are unable to compute the level-2 condition number exactly so instead we use the upper bound (5.5) which we refer to as `lv12_bnd` in this section. Experiments comparing `lv12_bnd` to the exact level-2 condition number for the inverse showed that they agreed reasonably well over our test matrices: the mean and maximum of the factor by which `lv12_bnd` exceeded the level-2 condition number were 1.19 and 2.24 times, respectively. In 66% cases the overestimation factor was less than 1.2. The level-1 condition number can be computed exactly in the Frobenius norm using [20, Alg. 3.17].

Figure 5.1 compares the level-1 condition number and `lv12_bnd` for the matrix exponential on the 49 test matrices for which the matrix exponential did not overflow. The values are sorted in decreasing order of $\text{cond}_{\text{abs}}(\exp, A)$. Note that in each case `lv12_bnd` is greater than or equal to the level-1 condition number. We see that the two lines are almost equal for arbitrary matrices in the Frobenius norm, with the most serious disagreement on the first few ill conditioned problems. This suggests that for the matrix exponential it may be possible to show that the level-1 and level-2 condition numbers are equal or approximately equal for a wider class of matrices than just the normal matrices, to which Theorem 5.2 applies.

Figure 5.2 compares the level-1 condition number and `lv12_bnd` for the matrix logarithm over the 49 test matrices for which the matrix logarithm and its condition number are defined, sorted by decreasing values of $\text{cond}_{\text{abs}}(\log, A)$. In black we have plotted the square of the level-1 condition number; we see that it bears a striking similarity to the level-2 condition number, consistent with Theorem 5.5, since $|f''(\lambda)| = |f'(\lambda)|^2$.

Our final experiment compares the level-1 condition number and `lv12_bnd` for the matrix square root on the 51 test matrices where the square root and its condition number are defined, again sorted by decreasing values of $\text{cond}_{\text{abs}}(x^{1/2}, A)$. Figure 5.3

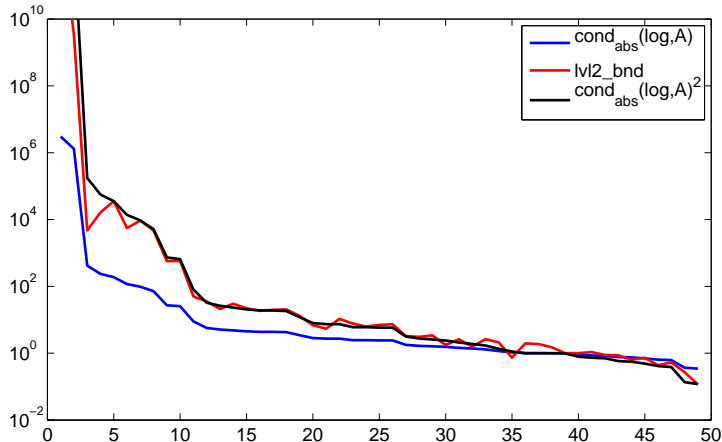


FIG. 5.2. Level-1 absolute condition number and 1v12.bnd for the matrix logarithm in the Frobenius norm sorted by decreasing value of $\text{cond}_{\text{abs}}(\log, A)$. The black line is $\text{cond}_{\text{abs}}(\log, A)^2$.

shows two plots with the same data but with different y-axes so the fine details can be seen. In black we have plotted $2 \text{cond}_{\text{abs}}(x^{1/2}, A)^3$ which, consistent with Theorem 5.5, provides a reasonable estimate of 1v12.bnd except for the first few problems, which are very ill conditioned.

6. Concluding remarks. We have derived sufficient conditions for the existence and continuity of higher order Fréchet derivatives of matrix functions as well as methods for computing the k th Fréchet derivative and its Kronecker form. These lay the foundations for further investigation of higher order Fréchet derivatives and their use in applications. In [22] we apply this work to develop an efficient algorithm for estimating the condition number of Fréchet derivatives of matrix functions.

We have also investigated the level-2 condition number for matrix functions, showing that in a number of cases the level-2 condition number can be related to the level-1 condition number, through equality, a functional relationship, or a bound. It is an interesting open question whether stronger results can be proved, but our numerical experiments give some indication that this may be possible.

Acknowledgements. We thank Stefan Güttel and Daniel Kressner for helpful discussions regarding the appendix.

Appendix. The necessity of the conditions in Theorem 3.5. As mentioned at the end of section 3, our assumption in Theorem 3.5 that f has $2^k p - 1$ derivatives is not necessary for the existence of the k th Fréchet derivative. Our method of proof employs X_k and to evaluate $f(X_k)$ we need f to have $p_k - 1$ continuous derivatives, where p_k is the size of the largest Jordan block of X_k (see Theorem 3.1). From Theorem 3.4 we know that $p_k \leq 2^k p$ where p is the size of the largest Jordan block of A ; this is the bound used in Theorem 3.5, but it is possible for X_k to have smaller Jordan blocks. The following example shows that for a specially chosen A only $4p - 2$ derivatives are needed for the existence of $f(X_2)$.

Take $A = J$ where $J \in \mathbb{C}^{n \times n}$ is a Jordan block of size n with eigenvalue 0. We first show that $\text{rank}(X_2) \leq n - 2$. Note from (3.4) that the first column of X_2 is 0 and the $(n+1)$ st and $(2n+1)$ st columns have at most n nonzero elements corresponding to the first columns of E_1 and E_2 , respectively. Since A has 1s on its first superdiagonal

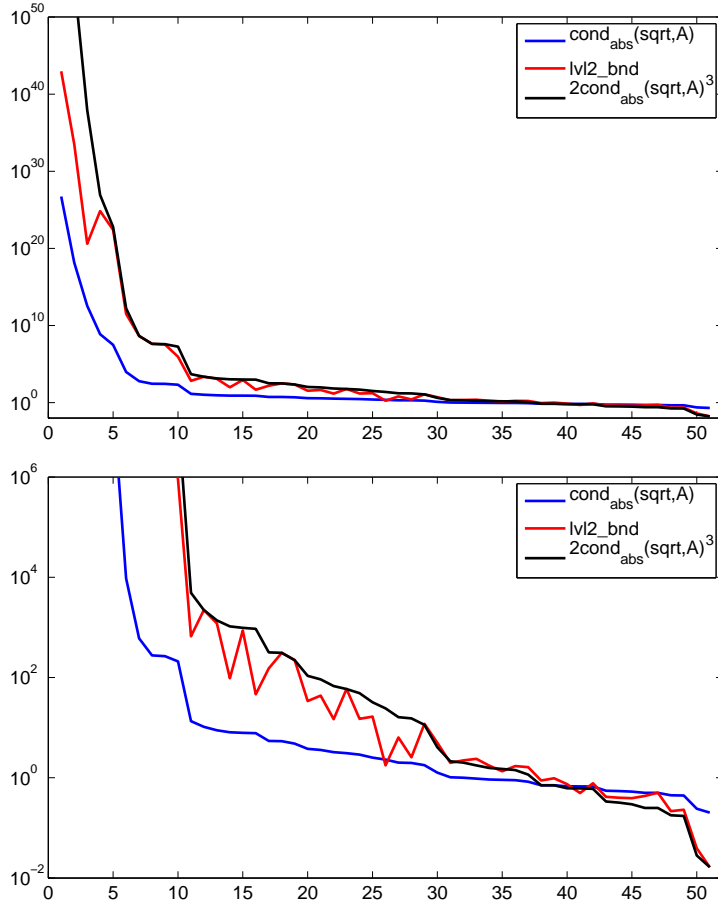


FIG. 5.3. *Top: Level-1 absolute condition number and 1v12_bnd for the matrix square root in the Frobenius norm sorted by decreasing value of $\text{cond}_{\text{abs}}(\log, A)$. The black line is $2 \text{cond}_{\text{abs}}(x^{1/2}, A)^3$. Bottom: Zoomed view of same data with narrowed y-axis.*

we see that columns $2:n$ are the unit vectors e_1, \dots, e_{n-1} and they span all but the last element of the $(n+1)$ st and $(2n+1)$ st columns. Therefore if $[E_1]_{n,1} = 0$ or $[E_2]_{n,1} = 0$ the respective column can be written as a linear combination of columns $2:n$. On the other hand if both are nonzero then we can write the $(2n+1)$ st column as a linear combination of columns $2:n+1$. Thus there are at most $n-2$ linearly independent columns in X_2 and so $\text{rank}(X_2) \leq n-2$.

This means that X_2 has at least two Jordan blocks and therefore the largest Jordan block is of size at most $4n-1$, meaning $4n-2$ derivatives of f are sufficient for the existence of $f(X_2)$ by Theorem 3.1, which is slightly weaker than the requirement in Theorem 3.5 (with $k=2$ and $p=n$) of $4n-1$ derivatives.

The general problem of determining the Jordan structure of X_k given the Jordan structure of A remains open. Indeed the minimum number of derivatives required for the existence of the k th Fréchet derivative is also unknown; this number is potentially less than the number of derivatives required for the existence of $f(X_k)$.

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