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Generalized Complex Step Approximation to Estimate the First and Second Order Fréchet Derivative of Matrix Functions

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Abstract. Applications of Fréchet derivative emerge in the sensitivity analysis of matrix functions. Our work extends the generalized complex step approximation using the complex computation $f(A + e^{i\theta}hE)$ as a tool to matrix case, and combines it with finite difference formula to estimate the Fréchet derivative. We provide numerical results for the approximation to the first and the second order Fréchet derivative of the matrix exponential and matrix square root.

1. Introduction

Matrix functions such as matrix square root, matrix exponential, matrix logarithm and matrix sign functions are mappings from a set of matrices onto a set of matrices $f : \mathbb{C}^{n\times n} \to \mathbb{C}^{n\times n}$. They play an important role in a variety of applications such as the solution of fractional partial differential equations [11], quantum graphs [9], network analysis [10, 15, 24], exponential integrators [21] and computer animation [32]. In the computation of matrix functions A is subject to small perturbations where we can measure the effect of these perturbations by condition numbers. Since we can express the condition number by the Fréchet derivative we are interested in its computation. In addition to the sensitivity analysis the Fréchet derivative has applications in image reconstruction in tomography [31], the computation of choice probabilities [2], the analysis of carcinoma treatment [16], computing the matrix geometric mean and Karcher mean [22]. Second order Fréchet derivative is used in the extension of iterative methods to solve a nonlinear scalar equation to Banach spaces [8]. There are numerical algorithms evaluating the Fréchet derivative for the exponential [3, 23], logarithm [6], fractional power [12, 19]. Noferini gave an explicit expression for the Fréchet derivative of generalized matrix functions [30] by using Daleckiǐ-Kreǐn formula. Computation of higher order Fréchet derivatives was proposed in [20], in which the kth order Fréchet derivative and a Kronecker form of the kth Fréchet derivative cost $O(8^k n^3)$ and $O(8^k n^{3+2k})$, respectively.

Approximation to the derivatives of $f(x)$ using the complex arithmetic as a tool in scalar case was first introduced in [28, 29]. Trapp also compared the complex step (CS) approximation to the central difference formula in his work [33]. The complex step approach for the computation of higher order derivatives was given by [1, 25–27]. For the matrix case, our aim in this work is to extend the generalized complex step approximation using the formula $f(A + e^{i\theta}hE)$ to the computation of the first and second order Fréchet

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derivative of matrix functions and compare the approximations for different choice of θ values. In matrix case for $\theta = \pi/2$, the method was applied to approximate the first order Fréchet derivatives of matrix functions by Al-Mohy and Higham [5]. Higher order Fréchet derivatives are estimated by using the complex step approximation and mixed derivative in [7] with an efficient computation. We approximate the first Fréchet derivative using the imaginary parts of $f(A + e^{i\theta}hE)$ and test approaches for different θ values for the matrix exponential and the matrix square root. We also combine the method with finite difference formula to approximate the second order Fréchet derivative.

The paper is organized as follows. Section 2 reviews the first and the higher order Fréchet derivative of matrix functions and its relation to the condition number. Section 3 gives the generalized complex step approximation for the scalar and matrix cases. We also establish our main contribution extending the generalized complex step approximation to the higher order Fréchet derivatives of matrix functions with the approximation order and the computational cost for different choice of θ. Section 4 presents the numerical tests and provides results for the first and the second Fréchet derivative of the matrix exponential and the matrix square root. The final section gives the concluding remarks of our work.

2. Higher order Fréchet derivative

The Fréchet derivative of f at A is a linear map $L_f : \mathbb{C}^{n\times n} \to \mathbb{C}^{n\times n}$ such that

$$\|f(A+E) - f(A) - L_f(A,E)\| = o(\|E\|) \tag{1}$$

for all $E \in \mathbb{C}^{n\times n}$. Applying the vec operator to $L_f(A,E)$ gives

$$\mathrm{vec}(L_f(A,E)) = K_f(A)\mathrm{vec}(E), \tag{2}$$

where $K_f(A) \in \mathbb{C}^{n^2\times n^2}$ is called the Kronecker form of the Fréchet derivative and the vec operator stacks the columns of a matrix into one column vector. The absolute condition number of $f(A)$ is given by

$$\mathrm{cond}(f,A) = \lim_{\epsilon\to 0} \sup_{\|E\|\le\epsilon} \frac{\|f(A+E) - f(A)\|}{\epsilon}, \tag{3}$$

where $\|\cdot\|$ is any matrix norm. The condition number (3) can be expressed in terms of the norms of the Fréchet derivative.

$$\mathrm{cond}(f,A) = \max_{E\neq 0} \frac{\|L_f(A,E)\|}{\|E\|}.$$

When the Fréchet derivative of f at A exists, it is unique. In that case we have that [17, Thm. 3.1]

$$\mathrm{cond}(f,A) = \|L_f(A)\|.$$

If we specialize to the Frobenius norm we obtain

$$\mathrm{cond}(f,A) = \max_{E\neq 0} \frac{\|L_f(A,E)\|_F}{\|E\|_F} = \max_{E\neq 0} \frac{\|\mathrm{vec}(L_f(A,E))\|_2}{\|\mathrm{vec}(E)\|_2} = \|K_f(A)\|_2,$$

where we use the fact that for $A \in \mathbb{C}^{n\times n}$, $\|A\|_F = \|\mathrm{vec}(A)\|_2$.

The kth order Fréchet derivative of $f : \mathbb{C}^{n\times n} \to \mathbb{C}^{n\times n}$ at $A \in \mathbb{C}^{n\times n}$ in the direction matrices $E_i \in \mathbb{C}^{n\times n}$, $i = 1 : k$, is defined as the unique multilinear operator $L_f^{(k)}(A)$ that satisfies

$$\|L_f^{(k-1)}(A+E_k, E_1, \cdots, E_{k-1}) - L_f^{(k-1)}(A, E_1, \cdots, E_{k-1}) - L_f^{(k)}(A, E_1, \cdots, E_k)\| = o(\|E_k\|), \tag{4}$$

where $L_f^{(0)}(A) = f(A)$ and $L_f^{(1)}(A, E_1)$ is the first order Fréchet derivative. For $E = E_j$, $j = 1 : k$, we denote the kth Fréchet derivative of f at E by $L_f^{(k)}(A,E)$; that is, $L_f^{(k)}(A,E) = L_f^{(k)}(A, E_1, E_2, \cdots, E_k)$. For simplicity let $\mathcal{E}_k$ denote the k-tuple $(E_1, E_2, \cdots, E_k)$ regardless of the order of E_k since the multilinear operator $L_f^{(k)}(A,\cdot)$ is symmetric. For the monomial X^r, where r is any nonnegative integer, write a recurrence for $L_{x^r}^{(k)}(A, \mathcal{E}_k)$.

Lemma 2.1 ([7, Lem. 2.1]). *The kth Fréchet derivative of X^r is given by*

$$L_{x^r}^{(k)}(A, E_1, E_2, \cdots, E_k) = AL_{x^{r-1}}^{(k)}(A, E_1, E_2, \cdots, E_k) + \sum_{j=1}^{k} E_j L_{x^{r-1}}^{(k-1)}(A, E_1, \cdots, E_{j-1}, E_{j+1}, \cdots, E_k) \quad (5)$$

with $L_{x^r}^{(k)}(A, E_1, E_2, \cdots, E_k) = 0$ if $k > r$.

To test our approximation we use the following theorem to compute the 'exact' first and second order Fréchet derivatives.

Theorem 2.2 ([20, Thm. 3.5]). *Let $A \in \mathbb{C}^{n\times n}$ whose largest Jordan block is of size p and whose spectrum lies in an open subset $\mathcal{D} \subset \mathbb{C}$. Let $f : \mathcal{D} \to \mathbb{C}$ be $2^k p - 1$ times continuously differentiable on an open $\mathcal{D}$. Then the kth Fréchet derivative $L_f^{(k)}(A)$ exists and $L_f^{(k)}(A, \mathcal{E}_k)$ is continuous in A and $E_1, E_2, \ldots, E_k \in \mathbb{C}^{n\times n}$. Moreover the upper right $n \times n$ block of $f(X_k)$ is $L_f^{(k)}(A, \mathcal{E}_k)$. The matrix X_k is defined recursively*

$$X_k = I_2 \otimes X_{k-1} + \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix} \otimes I_{2^{k-1}} \otimes E_k, \quad X_0 = A, \quad (6)$$

where the symbol $\otimes$ denotes the Kronecker product [17, Chap. 12] and I_m denotes the $m \times m$ identity matrix.

3. Generalized complex step approximation

3.1. Scalar case

We review the generalized complex step approximation [25] to estimate the first and the second order derivatives and extend it to the higher order derivatives. If $f(x)$ is a real function with real variables and is analytic then it can be expanded in a Taylor series

$$f(x + \mathrm{i}h) = f(x) + \mathrm{i}hf'(x) - h^2 \frac{f''(x)}{2!} - \mathrm{i}h^3 \frac{f^{(3)}(x)}{3!} + \cdots . \quad (7)$$

In Taylor series expansion $\mathrm{Im}(f(x + \mathrm{i}h))/h$ and $\mathrm{Re}(f(x + \mathrm{i}h))$ give an approximation to $f'(x)$ and $f(x)$, respectively with an approximation error $O(h^2)$. The approximation to $f'(x)$ using the imaginary part avoids the subtractive cancellation. Numerical results obtained by numerical algorithm design in metrology showed that the accuracy is obtained even with $h = 10^{-100}$ [13].

The following theorem states the generalized complex step approximation for the scalar case.

Theorem 3.1. *Let $f : \mathcal{D} \subset \mathbb{C} \to \mathbb{C}$ be an analytic function in an open subset $\mathcal{D}$. Assume that $x, h \in \mathbb{R}$. We also assume that $x + e^{\mathrm{i}\theta}h \in \mathcal{D}$. Then we approximate the kth order derivative of a function by the imaginary part of the $(k-1)$th order of derivative.*

$$f^{(k)}(x) = \frac{\mathrm{Im}\left(f^{(k-1)}(x + e^{\mathrm{i}\theta}h)\right)}{h \sin\theta} + O(h^2) \quad (8)$$

$$f^{(k-1)}(x) = \mathrm{Re}\left(f^{(k-1)}(x + e^{\mathrm{i}\theta}h)\right) + O(h^2). \quad (9)$$

Proof. Taking $e^{\mathrm{i}\theta}$ instead of i in the power series expansion (7) and differentiating repeatedly lead to

$$f^{(k-1)}(x + e^{\mathrm{i}\theta}h) = f^{(k-1)}(x) + e^{\mathrm{i}\theta}hf^{(k)}(x) + \frac{(e^{\mathrm{i}\theta}h)^2}{2!} f^{(k+1)}(x) + \cdots .$$

We derive equations (8) and (9) by equaling the imaginary and the real parts of $f^{(k-1)}(x+e^{\mathrm{i}\theta}h)$, respectively. □

For the first and the second order derivative approximations we can obtain the followings.

$$f'(x) \approx \frac{\mathrm{Im}\left[f(x+e^{\mathrm{i}\theta}h)\right]}{h\sin\theta}$$
$$f''(x) \approx \frac{\mathrm{Im}\left[f'(x+e^{\mathrm{i}\theta}h)\right]}{h\sin\theta}$$

In the next theorem we obtain an alternative form of the generalized complex step approximation for the scalar case.

Theorem 3.2. *Let $f : \mathcal{D} \subset \mathbb{C} \to \mathbb{C}$ be an analytic function in an open subset $\mathcal{D}$. Assume that $x, h \in \mathbb{R}$. We also assume that $x + e^{\mathrm{i}\theta}h \in \mathcal{D}$. Then we obtain the followings.*

$$f^{(k-1)}(x+e^{\mathrm{i}\theta}h) - f^{(k-1)}(x+e^{\mathrm{i}(\theta+\pi)}h) = 2\sum_{j=1}^{\infty}\frac{(e^{\mathrm{i}\theta}h)^{2j-1}}{(2j-1)!}f^{(k+2j-2)}(x) \tag{10}$$

$$f^{(k-1)}(x+e^{\mathrm{i}\theta}h) + f^{(k-1)}(x+e^{\mathrm{i}(\theta+\pi)}h) = 2\sum_{j=0}^{\infty}\frac{(e^{\mathrm{i}\theta}h)^{2j}}{(2j)!}f^{(k+2j)}(x) \tag{11}$$

Proof. Power series of $f(x+e^{\mathrm{i}\theta}h)$ and $f(x+e^{\mathrm{i}(\theta+\pi)}h)$ are given as follows.

$$f(x+e^{\mathrm{i}\theta}h) = f(x) + e^{\mathrm{i}\theta}hf'(x) + \frac{(e^{\mathrm{i}\theta})^2}{2!}h^2f''(x) + \frac{(e^{\mathrm{i}\theta})^3}{3!}h^3f^{(3)}(x) + \cdots$$
$$f(x+e^{\mathrm{i}(\theta+\pi)}h) = f(x) - e^{\mathrm{i}\theta}hf'(x) + \frac{(e^{\mathrm{i}\theta})^2}{2!}h^2f''(x) - \frac{(e^{\mathrm{i}\theta})^3}{3!}h^3f^{(3)}(x) + \cdots$$

Differentiating both sides of the power series repeatedly and then subtracting and adding these equations give respectively equations (10) and (11). □

For the first and the second derivative approximations we can deduce that

$$f'(x) \approx \frac{\mathrm{Im}\left[f(x+e^{\mathrm{i}\theta}h) - f(x+e^{\mathrm{i}(\theta+\pi)}h)\right]}{2h\sin\theta}$$
$$f''(x) \approx \frac{\mathrm{Im}\left[f(x+e^{\mathrm{i}\theta}h) + f(x+e^{\mathrm{i}(\theta+\pi)}h)\right]}{h^2\sin\theta}$$

We should note that in the alternative form the approximations are supposed to subtractive error.

3.2. Matrix case

Assume that A and E_i, $i = 1 : k$, are real matrices and f is a real function. Replacing the matrix E_k in the definition of the kth Fréchet derivative (4) by $e^{\mathrm{i}\theta}hE_k$, where h is a positive real number, and exploiting the linearity of the operator $L_f^{(k)}(A)$, we have

$$L_f^{(k-1)}(A+e^{\mathrm{i}\theta}hE_k, \mathcal{E}_{k-1}) - L_f^{(k-1)}(A, \mathcal{E}_{k-1}) - e^{\mathrm{i}\theta}hL_f^{(k)}(A, \mathcal{E}_k) = o(h).$$

Since $L_f^{(k)}(A, \mathcal{E}_k)$ is real, we obtain the CS approximation of $L_f^{(k)}(A, \cdot)$ via $L_f^{(k-1)}(A, \cdot)$ as

$$L_f^{(k)}(A, \mathcal{E}_k) = \lim_{h\to 0}\frac{\mathrm{Im}\Big(L_f^{(k-1)}(A+e^{\mathrm{i}\theta}hE_k, \mathcal{E}_{k-1})\Big)}{h\sin\theta}. \tag{12}$$

For a sufficiently small scalar h this yields

$$L_f^{(k-1)}(A,\mathcal{E}_{k-1}) \approx \mathrm{Re}\Big(L_f^{(k-1)}(A+e^{\mathrm{i}\theta}hE_k,\mathcal{E}_{k-1})\Big).$$

With stronger assumptions on f, the next theorem reveals the rate of convergence of the approximation as h goes to zero.

Theorem 3.3. *Let $f:\mathcal{D}\subset\mathbb{C}\to\mathbb{C}$ be an analytic function in an open subset $\mathcal{D}$ containing the spectrum of A. Assume that $A, E_i\in\mathbb{R}^{n\times n}$, $i=1:k$, f is real-valued at real arguments. Let h be a sufficiently small real number such that the spectrum of $A+e^{\mathrm{i}\theta}hE_k$ lies in $\mathcal{D}$. Then we get*

$$L_f^{(k)}(A,\mathcal{E}_k) = \frac{\mathrm{Im}\Big(L_f^{(k-1)}(A+e^{\mathrm{i}\theta}hE_k,\mathcal{E}_{k-1})\Big)}{h\sin\theta} + O(h^2) \tag{13}$$

$$L_f^{(k-1)}(A,\mathcal{E}_{k-1}) = \mathrm{Re}\Big(L_f^{(k-1)}(A+e^{\mathrm{i}\theta}hE_k,\mathcal{E}_{k-1})\Big) + O(h^2). \tag{14}$$

Proof. The analyticity of f on $\mathcal{D}$ implies that f has a power series expansion there. Thus in view of [5, Thm. 3.1], we have

$$\begin{aligned} f(A+e^{\mathrm{i}\theta}hE_k) &= \sum_{j=0}^{\infty}\frac{(e^{\mathrm{i}\theta}h)^j}{j!}L_f^{(j)}(A,E_k) \qquad (15)\\ &= f(A)+e^{\mathrm{i}\theta}hL_f(A,E_k)+\frac{(e^{\mathrm{i}\theta}h)^2}{2}L_f^{(2)}(A,E_k^{(2)})+O(h^3).\end{aligned}$$

Here $E_k^{(j)}$ denotes the j-tuple $(E_k,E_k,\dots,E_k)$. Since the power series converges uniformly to $f(A)$ on $\mathcal{D}$, we can repeatedly Fréchet differentiate the series (15) term by term in the directions $E_1,E_2,\dots,E_{k-1}$ and obtain

$$\begin{aligned} L_f^{(k-1)}(A+e^{\mathrm{i}\theta}hE_k,\mathcal{E}_{k-1}) &= L_f^{(k-1)}(A,\mathcal{E}_{k-1})+\sum_{j=1}^{\infty}\frac{(e^{\mathrm{i}\theta}h)^j}{j!}L_f^{(j+k-1)}(A,E_k^{(j)},\mathcal{E}_{k-1})\\ &= L_f^{(k-1)}(A,\mathcal{E}_{k-1})+e^{\mathrm{i}\theta}hL_f^{(k)}(A,\mathcal{E}_k)+\frac{(e^{\mathrm{i}\theta}h)^2}{2}L_f^{(k+1)}(A,E_{k-1}^{(2)},\mathcal{E}_{k-1})\\ &\quad +O(h^3)\end{aligned}$$

and (13) and (14) follow immediately by equaling the imaginary and real parts of the series, respectively. □

The following theorem extends Theorem 3.2 to the higher order Fréchet derivative of matrix functions.

Theorem 3.4. *Let $f:\mathcal{D}\subset\mathbb{C}\to\mathbb{C}$ be an analytic function in an open subset $\mathcal{D}$ obtaining the spectrum of A. Assume that $A,E_i\in\mathbb{R}^{n\times n}$, $i=1:k$, f is real-valued at real arguments. Let h be a sufficiently small real number such that the spectrum of $A+e^{\mathrm{i}\theta}hE_k$ and $A+e^{\mathrm{i}(\theta+\pi)}hE_k$ lie in $\mathcal{D}$. Then we obtain*

$$L_f^{(k-1)}(A+e^{\mathrm{i}\theta}hE_k,\mathcal{E}_{k-1})-L_f^{(k-1)}(A+e^{\mathrm{i}(\theta+\pi)}hE_k,\mathcal{E}_{k-1}) = 2\sum_{j=1}^{\infty}\frac{(e^{\mathrm{i}\theta}h)^{2j-1}}{(2j-1)!}L_f^{(k+2j-2)}(A,E_k^{(2j-2)},\mathcal{E}_k)$$

$$L_f^{(k)}(A+e^{\mathrm{i}\theta}hE_{k+1},\mathcal{E}_k)+L_f^{(k)}(A+e^{\mathrm{i}(\theta+\pi)}hE_{k+1},\mathcal{E}_k) = 2\sum_{j=0}^{\infty}\frac{(e^{\mathrm{i}\theta}h)^{2j}}{(2j)!}L_f^{(k+2j)}(A,E_k^{(2j)},\mathcal{E}_k).$$

Proof. Since the function f is analytic on $\mathcal{D}$ we can write the power series expansions.

$$f(A+e^{\mathrm{i}\theta}hE_k) = f(A)+e^{\mathrm{i}\theta}hL_f^{(1)}(A,E_k)+\frac{(e^{\mathrm{i}\theta})^2}{2!}h^2L_f^{(2)}(A,E_k^{(2)})+\frac{(e^{\mathrm{i}\theta})^3}{3!}h^3L_f^{(3)}(A,E_k^{(3)})+\cdots$$

$$f(A+e^{\mathrm{i}(\theta+\pi)}hE_k) = f(A)-e^{\mathrm{i}\theta}hL_f^{(1)}(A,E_k)+\frac{(e^{\mathrm{i}\theta})^2}{2!}h^2L_f^{(2)}(A,E_k^{(2)})-\frac{(e^{\mathrm{i}\theta})^3}{3!}h^3L_f^{(3)}(A,E_k^{(3)})+\cdots.$$

Taking the Fréchet derivative of power series expansions repeatedly and then subtracting/adding them, respectively yields the given equalities. □

3.3. Approximation to the first order Fréchet derivative

For the approximation to the first order Fréchet derivative we use equation (13)

$$\widehat{L}_f^{(1)}(A,\mathcal{E}_1) = \lim_{h\to 0} \frac{\operatorname{Im}\left(f(A+e^{\mathrm{i}\theta}hE_1)\right)}{h\sin\theta} \tag{16}$$

with different θ values. Taking $\theta = \pi/4$, $\theta = \pi/3$ and $\theta = \pi/2$ give the following approximations, which require one matrix function evaluation.

$$\begin{aligned}
\theta &= \pi/4, \quad \widehat{L}_f^{(1)}(A,\mathcal{E}_1) = \frac{2\operatorname{Im}\left(f(A+\mathrm{i}^{1/2}hE_1)\right)}{\sqrt{2}h} + O(h)\\
\theta &= \pi/3, \quad \widehat{L}_f^{(1)}(A,\mathcal{E}_1) = \frac{2\operatorname{Im}\left(f(A+\mathrm{i}^{2/3}hE_1)\right)}{\sqrt{3}h} + O(h)\\
\theta &= \pi/2, \quad \widehat{L}_f^{(1)}(A,\mathcal{E}_1) = \frac{\operatorname{Im}\left(f(A+\mathrm{i}hE_1)\right)}{h} + O(h^2)
\end{aligned}$$

The first equality in Theorem 3.4 leads to

$$\bar{L}_f^{(1)}(A,\mathcal{E}_1) = \lim_{h\to 0} \frac{\operatorname{Im}\left(f(A+e^{\mathrm{i}\theta}hE_1) - f(A-e^{\mathrm{i}\theta}hE_1)\right)}{2h\sin\theta}.$$

Substituting $\theta = \pi/4$, $\theta = \pi/3$ and $\theta = \pi/2$ gives the following approximations.

$$\begin{aligned}
\theta &= \pi/4, \quad \bar{L}_f^{(1)}(A,\mathcal{E}_1) = \frac{\operatorname{Im}\left(f(A+\mathrm{i}^{1/2}hE_1) - f(A+\mathrm{i}^{5/2}hE_1)\right)}{\sqrt{2}h} + O(h^2)\\
\theta &= \pi/3, \quad \bar{L}_f^{(1)}(A,\mathcal{E}_1) = \frac{\operatorname{Im}\left(f(A+\mathrm{i}^{2/3}hE_1) - f(A+\mathrm{i}^{8/3}hE_1)\right)}{\sqrt{3}h} + O(h^4)\\
\theta &= \pi/2, \quad \bar{L}_f^{(1)}(A,\mathcal{E}_1) = \frac{\operatorname{Im}\left(f(A+\mathrm{i}hE_1) - f(A-\mathrm{i}hE_1)\right)}{2h} + O(h^2)
\end{aligned}$$

The estimation $\bar{L}_f^{(1)}(A,\mathcal{E}_1)$ with $\theta = \pi/3$ provides $O(h^4)$ approximation error but it requires two matrix function evaluations.

Table 1: The approximation to the first order Fréchet derivative of $f(A)$ in the direction E_1 for different values of θ.

θ	$\widehat{L}_f^{(1)}(A,\mathcal{E}_1)$	$\bar{L}_f^{(1)}(A,\mathcal{E}_1)$
$\pi/4$	$\frac{2\operatorname{Im}\left(f(A+\mathrm{i}^{1/2}hE_1)\right)}{\sqrt{2}h}$	$\frac{\operatorname{Im}\left(f(A+\mathrm{i}^{1/2}hE_1) - f(A+\mathrm{i}^{5/2}hE_1)\right)}{\sqrt{2}h}$
$\pi/3$	$\frac{2\operatorname{Im}\left(f(A+\mathrm{i}^{2/3}hE_1)\right)}{\sqrt{3}h}$	$\frac{\operatorname{Im}\left(f(A+\mathrm{i}^{2/3}hE_1) - f(A+\mathrm{i}^{8/3}hE_1)\right)}{\sqrt{3}h}$
$\pi/2$	$\frac{\operatorname{Im}\left(f(A+\mathrm{i}hE_1)\right)}{h}$	$\frac{\operatorname{Im}\left(f(A+\mathrm{i}hE_1) - f(A-\mathrm{i}hE_1)\right)}{2h}$

3.4. Approximation to the second order Fréchet derivative

To approximate the second order Fréchet derivative $L_f^{(2)}(A, \mathcal{E}_2)$ we first take equation (13) with different θ values.

$$\theta = \pi/4, \qquad \widehat{L}_f^{(2)}(A, \mathcal{E}_2) = \frac{2\,\mathrm{Im}\left(L_f^{(1)}(A + \mathrm{i}^{1/2} h E_2, E_1)\right)}{\sqrt{2}h} + O(h)$$

$$\theta = \pi/3, \qquad \widehat{L}_f^{(2)}(A, \mathcal{E}_2) = \frac{2\,\mathrm{Im}\left(L_f^{(1)}(A + \mathrm{i}^{2/3} h E_2, E_1)\right)}{\sqrt{3}h} + O(h)$$

$$\theta = \pi/2, \qquad \widehat{L}_f^{(2)}(A, \mathcal{E}_2) = \frac{\mathrm{Im}\left(L_f^{(1)}(A + \mathrm{i} h E_2, E_1)\right)}{h} + O(h^2)$$

We combine the finite difference formula with the generalized complex step approximation (16) in the following lemma.

Lemma 3.5. *Suppose f, A, E_1 and E_2 satisfy the assumptions of Theorem 2.2. Then*

$$L_f^{(2)}(A, \mathcal{E}_2) = \lim_{(h_1,h_2)\to(0,0)} \frac{\mathrm{Im}\Big(f(A + e^{\mathrm{i}\theta} h_1 E_1 + h_2 E_2) - f(A + e^{\mathrm{i}\theta} h_1 E_1 - h_2 E_2)\Big)}{2 h_1 h_2 \sin\theta}. \tag{17}$$

Proof. Using finite difference formula and (16), we obtain

$$\begin{aligned} L_f^{(2)}(A, \mathcal{E}_2) &= \frac{L_f^{(1)}(A + h_2 E_2, E_1) - L_f^{(1)}(A - h_2 E_2, E_1)}{2h_2} + O(h_2^2) \\ &= h_2^{-1}\left(\frac{\mathrm{Im}\Big(f(A + e^{\mathrm{i}\theta} h_1 E_1 + h_2 E_2)\Big)}{h_1 \sin\theta} - \frac{\mathrm{Im}\Big(f(A + e^{\mathrm{i}\theta} h_1 E_1 - h_2 E_2)\Big)}{2h_1 \sin\theta}\right) + O(h_2^2) \\ &= \lim_{(h_1,h_2)\to(0,0)} \frac{\mathrm{Im}\Big(f(A + e^{\mathrm{i}\theta} h_1 E_1 + h_2 E_2) - f(A + e^{\mathrm{i}\theta} h_1 E_1 - h_2 E_2)\Big)}{2 h_1 h_2 \sin\theta}. \end{aligned}$$

Thus

$$L_f^{(2)}(A, \mathcal{E}_2) \approx \frac{\mathrm{Im}\Big(f(A + e^{\mathrm{i}\theta} h_1 E_1 + h_2 E_2) - f(A + e^{\mathrm{i}\theta} h_1 E_1 - h_2 E_2)\Big)}{2 h_1 h_2 \sin\theta}$$

for sufficiently small real scalars h_1 and h_2. $\square$

The parameter h_1 can be chosen as small as desired. However, the parameter h_2 is a finite difference step and it has to be chosen carefully.

We obtain approximations to the second Fréchet derivative substituting $\theta = \pi/4$, $\pi/3$ and $\pi/2$ into equation (17).

$$\theta = \pi/4, \qquad \bar{L}_f^{(2)}(A, \mathcal{E}_2) \approx \frac{\mathrm{Im}\Big(f(A + \mathrm{i}^{1/2} h_1 E_1 + h_2 E_2) - f(A + \mathrm{i}^{1/2} h_1 E_1 - h_2 E_2)\Big)}{\sqrt{2} h_1 h_2}$$

$$\theta = \pi/3, \qquad \bar{L}_f^{(2)}(A, \mathcal{E}_2) \approx \frac{\mathrm{Im}\Big(f(A + \mathrm{i}^{2/3} h_1 E_1 + h_2 E_2) - f(A + \mathrm{i}^{2/3} h_1 E_1 - h_2 E_2)\Big)}{\sqrt{3} h_1 h_2}$$

$$\theta = \pi/2, \qquad \bar{L}_f^{(2)}(A, \mathcal{E}_2) \approx \frac{\mathrm{Im}\Big(f(A + \mathrm{i} h_1 E_1 + h_2 E_2) - f(A + \mathrm{i} h_1 E_1 - h_2 E_2)\Big)}{2 h_1 h_2}$$

Table 2: The approximation to $L_f^{(2)}(A, E_1, E_2)$ for different values of θ.

θ	$\widehat{L}_f^{(2)}(A,\mathcal{E}_2)$	$\bar{L}_f^{(2)}(A,\mathcal{E}_2)$
$\pi/4$	$\dfrac{2\,\mathrm{Im}\left(L_f^{(1)}(A+\mathrm{i}^{1/2}hE_2,E_1)\right)}{\sqrt{2}h}$	$\dfrac{\mathrm{Im}\left(f(A+\mathrm{i}^{1/2}h_1E_1+h_2E_2)-f(A+\mathrm{i}^{1/2}h_1E_1-h_2E_2)\right)}{\sqrt{2}h_1h_2}$
$\pi/3$	$\dfrac{2\,\mathrm{Im}\left(L_f^{(1)}(A+\mathrm{i}^{2/3}hE_2,E_1)\right)}{\sqrt{3}h}$	$\dfrac{\mathrm{Im}\left(f(A+\mathrm{i}^{2/3}h_1E_1+h_2E_2)-f(A+\mathrm{i}^{2/3}h_1E_1-h_2E_2)\right)}{\sqrt{3}h_1h_2}$
$\pi/2$	$\dfrac{\mathrm{Im}\left(L_f^{(1)}(A+\mathrm{i}hE_2,E_1)\right)}{h}$	$\dfrac{\mathrm{Im}\left(f(A+\mathrm{i}h_1E_1+h_2E_2)-f(A+\mathrm{i}h_1E_1-h_2E_2)\right)}{2h_1h_2}$

4. Numerical results

We will compare the approaches given in Table 1 and Table 2. We use MATLAB R2020b on a machine with Core i7 to run the experiments. For the matrix exponential we take `A = gallery('lesp',10)`, and take E_1 and E_2 to be random matrices of the same size. For the matrix square root we choose random 10×10 matrices with no eigenvalues on $\mathbb{R}^-$. The matrix functions $f(X_1)$ and $f(X_2)$ in equation (6) are evaluated using [20, Alg. 3.6]. As stated in Theorem 2.2 the upper-right 10×10 block of $f(X_1)$ and $f(X_2)$ gives the 'exact' first and the second Fréchet derivative, respectively, namely,

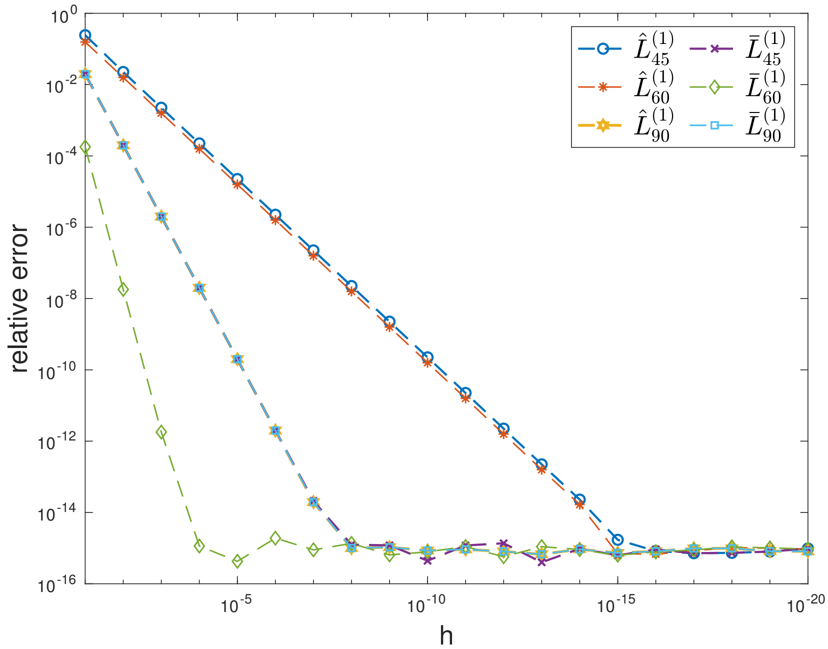
$$[f(X_1)]_{1n} = L_f(A,E_1) \qquad [f(X_2)]_{1n} = L_f^{(2)}(A,E_1,E_2).$$

We change h from 10^{-1} to 10^{-20} in the approximations and show the effect of the choice of h to the relative error evaluated by

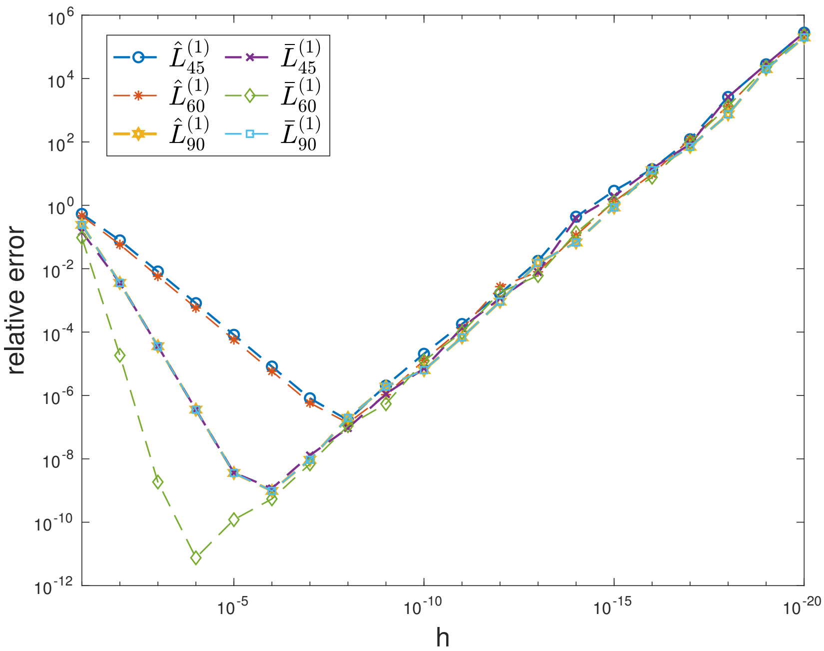
$$\frac{\|\,[f(X_k)]_{1n} - \tilde{L}_f^{(k)}(A,\mathcal{E}_k)\|_2}{\|\,[f(X_k)]_{1n}\,\|_2}, \quad k = 1,2$$

where $\tilde{L}_f^{(k)}(A,\mathcal{E}_k)$ represents the approximated kth Fréchet derivative. The approximation $\tilde{L}_f^{(k)}(A,\mathcal{E}_k)$ denotes either $\widehat{L}_f^{(k)}(A,\mathcal{E}_k)$ or $\bar{L}_f^{(k)}(A,\mathcal{E}_k)$, in which the matrix exponential and its first order Fréchet derivative are computed by MATLAB `expm` function and `expm_frechet` based on the algorithms of Al-Mohy and Higham [4, Alg. 5.1] and [3, Alg. 6.4], respectively. In the approximations to evaluate the matrix square root we use `sqrtm` MATLAB function based on the method [14] and its first order Fréchet derivative $L_f(A,E)$, is the solution to the Sylvester equation, $XL + LX = E$ with $X = A^{1/2}$, that is solved by `sylvsol` from [18]. In the legend of the figure the subscript values 45, 60 and 90 refer to the θ values of $\pi/4$, $\pi/3$ and $\pi/2$, respectively. Figure 1(a) and Figure 1(b) give the approximation to the first order Fréchet derivative $\tilde{L}_f^{(1)}$ computed by $\widehat{L}_f^{(1)}(A,\mathcal{E}_1)$ and $\bar{L}_f^{(1)}(A,\mathcal{E}_1)$ in the direction of E_1 for the matrix exponential and the matrix square root, respectively. Although computing $\bar{L}_f^{(1)}(A,\mathcal{E}_1)$ for $\theta = \pi/3$ is subject to subtractive error it gives better approximation for large values of h. For small h all the approaches give the same accuracy for the matrix exponential. In the matrix square root the best accuracy is obtained for $h = 10^{-4}$ and $\theta = \pi/3$.

The second experiment is presented in Figure 2 and Figure 3, in which the second order Fréchet derivative $\tilde{L}_f^{(2)}(A,\mathcal{E}_2)$ of the matrix exponential and the square root are approximated by the formulas in Table 2 in the direction of $\mathcal{E}_2 = (E_1, E_2)$. In the top part of Figure 2 we fix $h_2 = 10^{-8}$ and take $h_1 = 10^{-r}$, $r = 1 : 20$. It seems the accuracy is the same for h_1 values smaller than 10^{-15} in $\widehat{L}_f^{(2)}(A,\mathcal{E}_2)$ approximations. For the approximation $\bar{L}_f^{(2)}(A,\mathcal{E}_2)$ the accuracy is the same for h_1 smaller than 10^{-8}. In the bottom part of Figure 2 we



(a) Matrix exponential



(b) Matrix square root

Figure 1: Relative error for the first order Fréchet derivative of matrix functions according to the change in h.

fix $h_1 = 10^{-16}$ and $h_2 = 10^{-r}$, $r = 1:20$. Obviously while the change in h_2 does not effect the approximation $\widehat{L}_f^{(2)}(A, \mathcal{E}_2)$ the relative error of $\bar{L}_f^{(2)}(A, \mathcal{E}_2)$ grows rapidly with the decrease in h_2.

In the top part of Figure 3 we again fix $h_2 = 10^{-8}$ and choose $h_1 = 10^{-r}$, $r = 1:20$. The approximations using the first order Fréchet derivative with the complex step approximation provide better accuracy. For around $h_1 = 10^{-8}$ the approximation $\widehat{L}_f^{(2)}(A, \mathcal{E}_2)$ give the same results for different θ values. As seen from the bottom part of Figure 3, where $h_1 = 10^{-8}$ is fixed the drop in finite difference parameter h_2 destroys the accuracy in $\bar{L}_f^{(2)}(A, \mathcal{E}_2)$. It is apparent from the tables that since the approximation $\widehat{L}_f^{(2)}(A, \mathcal{E}_2)$ does not depend on h_2 the change in h_2 does not affect it in both Figure 2 and Figure 3.

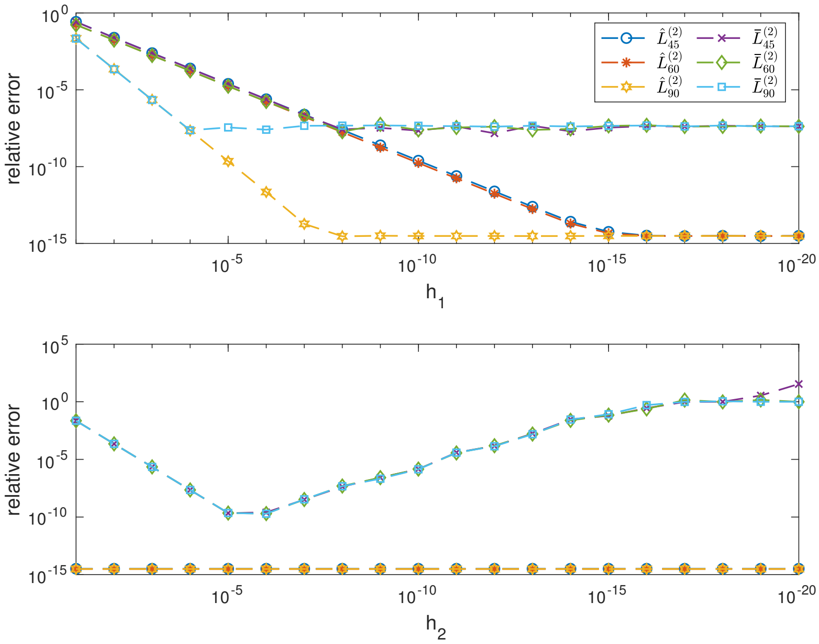


Figure 2: Relative error for the second order Fréchet derivative of matrix exponential according to the change in h_1 and h_2.

5. Concluding remarks

Theoretical analysis for the generalized complex step approximation using the complex computation $f(A + e^{i\theta}hE)$ to approximate the first and the second order Fréchet derivative of matrix exponential and matrix square root is presented. Generalized complex step approximation is also combined with the finite difference formula. For different θ values the computations are compared in terms of the accuracy and the computational cost. Our findings reveal that the approximation $\bar{L}_f^{(1)}(A, \mathcal{E}_1)$ that combines the complex step approximation with the finite difference method to the first order Fréchet derivative gives better accuracy for $\theta = \pi/3$. In the estimation of the second order Fréchet derivative using the generalized complex step approximation with the first order Fréchet derivative provides better accuracy since the error in finite difference formula combined with the generalized complex step approximation is magnified by the decrease of the finite difference step h_2.

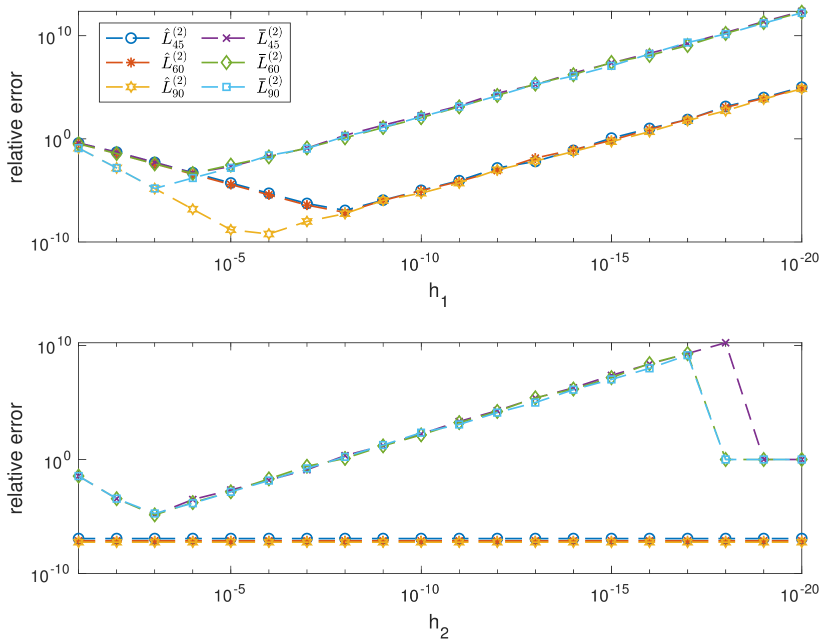


Figure 3: Relative error for the second order Fréchet derivative of matrix square root according to the change in h_1 and h_2.

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