Derivations, derivatives and chain rules

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Abstract

For a smooth function f on the space of bounded operators in a Hilbert space, we obtain formulas for the nth order commutator $[[[f(A),X],X],\dots,X]$ in terms of the Fréchet derivatives $D^n f(A)$. We illustrate the use of these formulas in obtaining bounds for norms of generalised commutators $f(A)X - Xf(B)$ and their higher order analogues.

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1. Introduction

Let $\mathscr{B}(\mathscr{H})$ be the space of bounded linear operators on a Hilbert space $\mathscr{H}$. Let f be a function mapping $\mathscr{B}(\mathscr{H})$ into itself. If f is n times (Fréchet) differentiable, we write $D^n f(A)$ for the nth derivative of f at the point A. The first derivative $Df(A)$ is a linear operator on $\mathscr{B}(\mathscr{H})$. Its action is given as

$$Df(A)(B) = \lim_{t\to 0} \frac{f(A+tB) - f(A)}{t} = \left.\frac{\mathrm{d}}{\mathrm{d}t}\right|_{t=0} f(A+tB). \tag{1.1}$$

The second derivative $D^2f(A)$ can be identified with a linear map from $\mathscr{B}(\mathscr{H}) \times \mathscr{B}(\mathscr{H})$ into $\mathscr{B}(\mathscr{H})$. Its action is described as

$$\begin{aligned} D^2f(A)(B_1, B_2) &= \lim_{t\to 0} \frac{Df(A+tB_2)(B_1) - Df(A)(B_1)}{t} \\ &= \frac{\partial^2}{\partial t_1 \partial t_2}\bigg|_{t_1=t_2=0} f(A + t_1B_1 + t_2B_2). \end{aligned} \tag{1.2}$$

Higher order derivatives are defined inductively. We have

$$\begin{aligned} &D^nf(A)(B_1, \ldots, B_n) \\ &\quad = \lim_{t\to 0} \frac{D^{n-1}(A+tB_n)(B_1, \ldots, B_{n-1}) - D^{n-1}f(A)(B_1, \ldots, B_{n-1})}{t} \\ &\quad = \frac{\partial^n}{\partial t_1 \cdots \partial t_n}\bigg|_{t_1=\cdots=t_n=0} f(A + t_1B_1 + \cdots + t_nB_n). \end{aligned} \tag{1.3}$$

Thus $D^nf(A)$ is a multilinear map from the n fold product $\mathscr{B}(\mathscr{H}) \times \cdots \times \mathscr{B}(\mathscr{H})$ into $\mathscr{B}(\mathscr{H})$. It is symmetric in the variables $B_1, \ldots, B_n$.

A brief summary of basic properties of these derivatives may be found in [1].

Every element A of $\mathscr{B}(\mathscr{H})$ induces a *derivation* on $\mathscr{B}(\mathscr{H})$. This is the linear operator defined as

$$\delta(A)(X) = [A, X] = AX - XA. \tag{1.4}$$

We will denote by $\delta^{[2]}(A)$ the (nonlinear) map on $\mathscr{B}(\mathscr{H})$ defined as

$$\delta^{[2]}(A)(X) = [\delta(A)(X), X] = [[A, X], X]. \tag{1.5}$$

We define, inductively, $\delta^{[n]}(A)$ as

$$\delta^{[n]}(A)(X) = \left[\delta^{[n-1]}(A)(X), X\right]. \tag{1.6}$$

In this paper we establish formulas that relate the quantities $D^nf(A)$ and $\delta^{[n]}(f(A))$. These formulas should be of interest in the calculus of operator functions.

In our earlier work [2–5], we have identified classes of functions f on $\mathbb{R}$ for which the map induced on self-adjoint operators in $\mathscr{H}$ satisfies the relation $\|D^nf(A)\| = \|f^{(n)}(A)\|$, where $f^{(n)}$ is the (ordinary) nth derivative of the real function f. For such functions, our formulas lead to bounds for the norms $\|\delta^{[n]}(f(A))\|$.

2. The first derivative

We will show that under some conditions on f we have the formula

$$\delta(f(A)) = Df(A) \circ \delta(A). \tag{2.1}$$

In other words, we have

$$f(A)X - Xf(A) = Df(A)(AX - XA). \tag{2.2}$$

Theorem 2.1. *Let f be a holomorphic function on a complex domain Ω and let A be any operator whose spectrum is contained in Ω. Then relation* (2.2) *holds for all X.*

Proof. By the Riesz functional calculus, we can write

$$f(A) = \frac{1}{2\pi i}\int_{\gamma} f(z)(z - A)^{-1}\,dz, \tag{2.3}$$

where γ is a curve with winding number 1 around the spectrum of A. Note that, if $g(A) = A^{-1}$, then $Dg(A)(Y) = -A^{-1}YA^{-1}$ for all Y. Hence, from (2.3) we get

$$Df(A)(Y) = \frac{1}{2\pi i}\int_{\gamma} f(z)(z - A)^{-1}Y(z - A)^{-1}\,dz. \tag{2.4}$$

Put $Y = AX - XA$ in (2.4), note that

$$\begin{aligned}
&(z - A)^{-1}(AX - XA)(z - A)^{-1} \\
&\quad = (z - A)^{-1}(X(z - A) - (z - A)X)(z - A)^{-1} \\
&\quad = (z - A)^{-1}X - X(z - A)^{-1}.
\end{aligned}$$

This gives

$$\begin{aligned}
&Df(A)(AX - XA) \\
&\quad = \frac{1}{2\pi i}\left\{\left(\int_{\gamma} f(z)(z - A)^{-1}dz\right)X - X\left(\int_{\gamma} f(z)(z - A)^{-1}\,dz\right)\right\} \\
&\quad = f(A)X - Xf(A). \quad \square
\end{aligned}$$

We should remark that the argument we have used above works not just for $\mathscr{B}(\mathscr{H})$ but also for any Banach algebra. The identity (2.1) is, therefore, valid in these more general situations whenever f is a holomorphic function.

Self-adjoint operators play an important role in several applications. Here we can prove the identity (2.1) under less restrictive conditions on f.

Let I be any open interval on the real line, and let f be a funtion of class C^1 on I. If A is a self-adjoint operator on $\mathscr{H}$ whose spectrum is contained in I, we can define $f(A)$ via the spectral theorem. The derivative $Df(A)$ is then a linear map on the real linear space consisting of all self-adjoint operators. Note that $AX - XA$ is self-adjoint if X is skew-Hermitian.

Theorem 2.2. *Let f be a continuously differentiable function on an open interval I. Then relation* (2.2) *holds for all self-adjoint operators A with their spectra in I, and for all skew-Hermitian operators X.*

Proof. We have

$$\begin{aligned} f(A)X - Xf(A) &= \frac{\mathrm{d}}{\mathrm{d}t}\bigg|_{t=0} \mathrm{e}^{-tX} f(A)\mathrm{e}^{tX} \\ &= \frac{\mathrm{d}}{\mathrm{d}t}\bigg|_{t=0} f(\mathrm{e}^{-tX} A \mathrm{e}^{tX}) \\ &= \frac{\mathrm{d}}{\mathrm{d}t}\bigg|_{t=0} f(A + t[A,X] + \mathrm{O}(t^2)) \\ &= \frac{\mathrm{d}}{\mathrm{d}t}\bigg|_{t=0} f(A + t[A,X]) \\ &= Df(A)([A,X]). \end{aligned}$$

Note that the continuous differentiability of f was used in getting the fourth equality in this chain. □

For finite-dimensional spaces, we have an interesting consequence of Theorem 2.2.

Let $\mathbb{H}$ be the space of all $n \times n$ Hermitian matrices. This is a real linear space with an inner product $\langle X, Y \rangle = \operatorname{tr} XY$. Given any A in $\mathbb{H}$ consider the following two subspaces of $\mathbb{H}$:

$$\mathscr{Z}_A = \{Y \in \mathbb{H} : [A, Y] = 0\},$$
$$\mathscr{C}_A = \{[A, X] : X^* = -X\}.$$

In other words, $\mathscr{Z}_A$ consists of all Hermitian matrices that commute with A and $\mathscr{C}_A$ consists of all commutators of A with skew-Hermitian matrices. We then have a direct sum decomposition

$$\mathbb{H} = \mathscr{Z}_A \oplus \mathscr{C}_A. \tag{2.5}$$

(This is verified easily using the cyclicity of the trace.) Now, if $Y \in \mathscr{Z}_A$, we can choose an orthonormal basis in which both A and Y are diagonal. This shows that $Df(A)(Y) = f'(A)Y$, where f' is just the ordinary derivative of f. In the complementary space $\mathscr{C}_A$ we have formula (2.2) for the action of $Df(A)$.

This observation leads to a simple and insightful proof of an important theorem in Loewner's theory of matrix monotone functions. This is explained below.

Let $f \in C^1(I)$ and let $f^{[1]}$ be the function on $I \times I$ defined as

$$f^{[1]}(\lambda, \mu) = \frac{f(\lambda) - f(\mu)}{\lambda - \mu} \quad \text{if } \lambda \neq \mu,$$
$$f^{[1]}(\lambda, \lambda) = f'(\lambda).$$

If A is a Hermitian matrix with eigenvalues $\lambda_1, \ldots, \lambda_n$ contained in I, let $f^{[1]}(A)$ denote the matrix whose i, j entries are $f^{[1]}(\lambda_i, \lambda_j)$. Then we have the following theorem.

Theorem 2.3. *Let $f \in C^1(I)$ and let A be a Hermitian matrix with all its eigenvalues in I. Then, for every Hermitian matrix H, we have*

$$Df(A)(H) = f^{[1]}(A) \cdot H, \tag{2.6}$$

where $\cdot$ denotes the Schur product (the entrywise product) of two matrices in an orthonormal basis in which A is diagonal.

Proof. First consider the special case when $H = [A, X]$ for some skew-Hermitian X. In this case (2.6) follows from (2.2). Then consider the case when H commutes with A. Combine the two cases to get the general case using the decomposition (2.5). □

Other proofs of Theorem 2.3 may be found in [1, p.124] and the references cited therein.

Remark 2.4. A third approach to formula (2.1) can be made via the exponential function and the Fourier transform. For this we need the well-known formula

$$\lim_{h \to 0} \frac{e^{t(A+hB)} - e^{tA}}{h} = \int_0^t e^{(t-s)A} B \, e^{sA} \, ds. \tag{2.7}$$

See [16] for a history of this formula. For the reader's convenience, we give a short proof of it. Since

$$\frac{d}{ds} e^{(t-s)X} e^{sY} = e^{(t-s)X} (Y - X) e^{sY},$$

we have

$$\int_0^t e^{(t-s)X} (Y - X) e^{sY} ds = e^{tY} - e^{tX}.$$

Hence,

$$\frac{e^{t(A+hB)} - e^{tA}}{h} = \int_0^t e^{(t-s)A} B e^{s(A+hB)} ds.$$

This gives (2.7).

Let f be any real integrable function on $\mathbb{R}$. Assume that the function $t\hat{f}(t)$, where $\hat{f}$ denotes the Fourier transform of f, is integrable. From the Fourier inversion formula

$$f(\xi) = \int_{-\infty}^{\infty} \hat{f}(t)\mathrm{e}^{\mathrm{i}t\xi}\,\mathrm{d}t,$$

we get

$$f(A) = \int_{-\infty}^{\infty} \hat{f}(t)\mathrm{e}^{\mathrm{i}tA}\,\mathrm{d}t. \tag{2.8}$$

Hence, from (2.7) and (2.8) we get

$$Df(A)(B) = \mathrm{i}\int_{-\infty}^{\infty} \hat{f}(t)\left[\int_0^t \mathrm{e}^{\mathrm{i}(t-s)A}B\,\mathrm{e}^{\mathrm{i}sA}\,\mathrm{d}s\right]\mathrm{d}t. \tag{2.9}$$

Now note that

$$\begin{aligned}
&\mathrm{i}\int_0^t \mathrm{e}^{\mathrm{i}(t-s)A}(AX - XA)\mathrm{e}^{\mathrm{i}sA}\,\mathrm{d}s \\
&\quad = \mathrm{e}^{\mathrm{i}tA}\int_0^t \mathrm{e}^{-\mathrm{i}sA}\mathrm{i}(AX - XA)\mathrm{e}^{\mathrm{i}sA}\,\mathrm{d}s \\
&\quad = \mathrm{e}^{\mathrm{i}tA}(-\mathrm{e}^{-\mathrm{i}sA}X\mathrm{e}^{\mathrm{i}sA})|_0^t \\
&\quad = \mathrm{e}^{\mathrm{i}tA}X - X\mathrm{e}^{\mathrm{i}tA}.
\end{aligned} \tag{2.10}$$

From (2.8)–(2.10), we again obtain equality (2.2).

Remark 2.5. The operators $Df(A)$ and $\delta(A)$ commute; we have

$$Df(A) \circ \delta(A) = \delta(A) \circ Df(A). \tag{2.11}$$

Let us show this for functions f holomorphic on a complex domain. Using (2.4) we have

$$\begin{aligned}
Df(A)(AX) &= \frac{1}{2\pi\mathrm{i}}\int_\gamma f(z)(z-A)^{-1}AX(z-A)^{-1}\,\mathrm{d}z \\
&= A\frac{1}{2\pi\mathrm{i}}\int_\gamma f(z)(z-A)^{-1}X(z-A)^{-1}\,\mathrm{d}z \\
&= ADf(A)(X).
\end{aligned}$$

In the same way we can see that

$$Df(A)(XA) = Df(A)(X)A.$$

Hence

$$Df(A)([A,X]) = [A, Df(A)(X)].$$

This is equality (2.11).

Remark 2.6. We should point out that formula (2.1) can be found in works by other authors, sometimes implicitly and with a different emphasis. In several important papers Birman and Solomyak [6,7] have studied commutators $[f(A), X]$ and also derivatives $Df(A)$ in terms of Stieltjes double integral operators. Formula (2.1) can easily be inferred from their results. In a recent paper [18], Suzuki has proposed a scheme for "quantum analysis" in which he has found several relations expressing operator derivatives in terms of inner derivations. Formula (3.15) in this paper reads, in our notation, as

$$\delta(f(A)) = \delta(A) \circ Df(A). \tag{2.12}$$

This, in view of (2.11), is the same as (2.1). Brown and Vasudeva [9] have also discovered the relation (2.1).

Our approach is in line with our earlier work [1–5], and perhaps has some simplicity, and economy of notations as well as of proofs.

We should also point out that Hansen and Pedersen [13] have used Fourier transforms to study Fréchet derivatives of operator functions, as we did in Remark 2.4.

3. Higher derivatives

In this section we derive a basic formula that expresses $\delta^{[n]}(f(A))$ in terms of $D^j f(A)$ and $\delta^{[j]}(A)$, $1 \leqslant j \leqslant n$. This is analogous to the chain rule for the higher derivatives of a composite function $\varphi(x) = f(g(x))$. We will first carry out the computation for $n = 2$ and 3 in detail.

In Section 2 we derived (2.1) with different assumptions on f. When talking of $D^n f$, we can either assume that f is holomorphic, or it belongs to the class $C^n(I)$. In the first case our formulas are valid for all A; and more generally they are true in all Banach algebras. In the second case we restrict ourselves to self-adjoint operators. If we were to follow the approach using Fourier transforms in Remark 2.4, the requirement on f now would be the integrability of $t^n \hat{f}(t)$.

In any case start with the relation

$$\delta(f(A))(X) = Df(A)(\delta(A)(X)), \tag{3.1}$$

to get

$$\begin{aligned}\delta^{[2]}(f(A))(X) &= \delta(Df(A)(\delta(A)(X)))(X) \\ &= D(Df(A)(\delta(A)(X)))(\delta(A)(X)).\end{aligned} \tag{3.2}$$

We evaluate the operator $D(Df(A)(\delta(A)(X)))$ from first principles. For any Y in $\mathscr{B}(\mathscr{H})$, we have by definition,

$$
\begin{aligned}
&D(Df(A)(\delta(A)(X)))(Y)\\
&\quad=\lim_{t\to 0}\frac{1}{t}\{Df(A+tY)(\delta(A+tY)(X))-Df(A)(\delta(A)(X))\}\\
&\quad=\lim_{t\to 0}\frac{1}{t}\{Df(A+tY)(\delta(A)(X))+tDf(A+tY)(\delta(Y)(X))\\
&\qquad-Df(A)(\delta(A)(X))\}\\
&\quad=\lim_{t\to 0}\frac{1}{t}\{[Df(A+tY)-Df(A)](\delta(A)(X))+tDf(A+tY)(\delta(Y)(X))\}\\
&\quad=D^2f(A)(\delta(A)(X),Y)+Df(A)(\delta(Y)(X)).
\end{aligned}
\tag{3.3}
$$

Putting $Y=\delta(A)(X)$ and substituting (3.3) in (3.2), we obtain the following:

$$
\delta^{[2]}(f(A))(X)=D^2f(A)(\delta(A)(X),\delta(A)(X))+Df(A)(\delta^{[2]}(A)(X)). \tag{3.4}
$$

This is the desired formula for $n=2$.

From this one gets

$$
\begin{aligned}
\delta^{[3]}(f(A))(X)&=\delta(D^2f(A)(\delta(A)(X),\delta(A)(X)))(X)\\
&\quad+\delta(Df(A)(\delta^{[2]}(A)(X)))(X).
\end{aligned}
\tag{3.5}
$$

We will use (2.1) to calculate, one by one, the two terms on the right hand side of this equation. The first term can be written as

$$
D(D^2f(A)(\delta(A)(X),\delta(A)(X)))(\delta(A)(X)). \tag{3.6}
$$

We evaluate this from first principles. For any Y, we have

$$
\begin{aligned}
&D(D^2f(A)(\delta(A)(X),\delta(A)(X)))(Y)\\
&\quad=\lim_{t\to 0}\frac{1}{t}\{D^2f(A+tY)(\delta(A+tY)(X),\delta(A+tY)(X))\\
&\qquad-D^2f(A)(\delta(A)(X),\delta(A)(X))\}\\
&\quad=\lim_{t\to 0}\frac{1}{t}\{\left[D^2f(A+tY)-D^2f(A)\right](\delta(A)(X),\delta(A)(X))\\
&\qquad+2tD^2f(A+tY)(\delta(A)(X),\delta(Y)(X))\\
&\qquad+t^2D^2f(A+tY)(\delta(Y)(X),\delta(Y)(X))\}\\
&\quad=D^3f(A)(\delta(A)(X),\delta(A)(X),Y)+2D^2f(A)(\delta(A)(X),\delta(Y)(X)).
\end{aligned}
$$

Hence, the quantity (3.6) is equal to

$$D^3 f(A)(\delta(A)(X), \delta(A)(X), \delta(A)(X)) + 2D^2 f(A)(\delta(A)(X), \delta^{[2]}(A)(X)). \tag{3.7}$$

The second term on the right hand side of (3.5) can be written, using (2.1), as

$$D(Df(A)(\delta^{[2]}(A)(X)))(\delta(A)(X)). \tag{3.8}$$

Once again, we evaluate this from first principles. We have for any Y,

$$\begin{aligned}
&D(Df(A)(\delta^{[2]}(A)(X)))(Y) \\
&= \lim_{t\to 0} \frac{1}{t}\{Df(A+tY)(\delta^{[2]}(A+tY))(X) - Df(A)(\delta^{[2]}(A)(X))\} \\
&= \lim_{t\to 0} \frac{1}{t}\{[Df(A+tY) - Df(A)](\delta^{[2]}(A)(X)) + tDf(A+tY)(\delta^{[2]}(Y)(X))\} \\
&= D^2 f(A)(\delta^{[2]}(A)(X), Y) + Df(A)(\delta^{[2]}(Y)(X)).
\end{aligned}$$

Hence, the quantity (3.8) is equal to

$$D^2 f(A)(\delta^{[2]}(A)(X), \delta(A)(X)) + Df(A)(\delta^{[3]}(A)(X)). \tag{3.9}$$

Combining (3.5)–(3.9) we get

$$\begin{aligned}
\delta^{[3]}(f(A))(X) = {} & D^3 f(A)(\delta(A)(X), \delta(A)(X), \delta(A)(X)) \\
& + 3D^2 f(A)(\delta^{[2]}(A)(X), \delta(A)(X)) \\
& + Df(A)(\delta^{[3]}(A)(X)).
\end{aligned} \tag{3.10}$$

This is the desired formula for $n = 3$.

We can continue this process to obtain expressions for $\delta^{[n]}(f(A))(X)$, each time using (2.1) and then evaluating the derivatives $D^n f(A)$. This requires some intricate book-keeping. It is possible to reduce the problem to some familiar combinatorial problems. The simplest method, and the most natural one, seems to be the connection between the process of obtaining expressions like (3.4) and (3.10) and the one of finding successive derivatives of composite functions. Consider a composite of two functions of a single variable

$$\varphi(x) = f(g(x)).$$

We have

$$\varphi'(x) = f'(g(x))g'(x), \tag{3.11}$$

$$\varphi''(x) = f''(g(x))g'(x)^2 + f'(g(x))g''(x), \tag{3.12}$$

$$\begin{aligned}
\varphi'''(x) = {} & f'''(g(x))g'(x)^3 + 2f''(g(x))g''(x)g'(x) \\
& + f''(g(x))g'(x)g''(x) + f'(g(x))g'''(x).
\end{aligned}$$

So,

$$\varphi'''(x) = f'''(g(x))g'(x)^3 + 3f''(g(x))g''(x)g'(x) + f'(g(x))g'''(x). \qquad (3.13)$$

We should first note a formal analogy between the expressions (3.11)–(3.13) on the one hand and (2.1), (3.4), and (3.10) on the other. Formally, if we replace the expression $\varphi^{(n)}(x)$ by $\delta^{[n]}(f(A))(X)$ and an expression of the form $f^{(m)}(g(x))g^{(i)}(x)g^{(j)}(x)g^{(k)}(x)$ by $D^m f(A)(\delta^{[i]}(A)(X), \delta^{[j]}(A)(X), \delta^{[k]}(A)(X))$, we see that the relations (3.11)–(3.13) are converted to (2.1),(3.4) and (3.10). We should also note that the numerical coefficients in the two sets of relations arise in exactly the same way.

This observation is the basis for the following theorem, a chain rule for derivations.

Theorem 3.1. *For all positive integers n,*

$$\delta^{[n]}(f(A))(X) = \sum_{r=1}^{n} \sum_{\mathbf{m},\mathbf{j}} c(n,r,\mathbf{m},\mathbf{j}) D^r f(A)(\langle \delta^{[j_1]}(A)(X)\rangle^{m_1}, \ldots, \langle \delta^{[j_k]}(A)(X)\rangle^{m_k}), \qquad (3.14)$$

where for positive integers r, n *with* $r \leqslant n$, $\mathbf{m}$ *and* $\mathbf{j}$ *are multiindices,* $\mathbf{m} = (m_1, \ldots, m_k)$, $\mathbf{j} = (j_1, \ldots, j_k)$, $k \geqslant 1$, *with positive integer entries satisfying*

$$m_1 + \cdots + m_k = r,$$
$$j_1 > j_2 > \cdots j_k \geqslant 1,$$
$$m_1 j_1 + \cdots + m_k j_k = n,$$

for $1 \leqslant i \leqslant k$, *the symbol* $\langle \delta^{[j_i]}(A)(X)\rangle^{m_i}$ *stands for* $\delta^{[j_i]}(A)(X), \ldots, \delta^{[j_i]}(A)(X)$, (*repeated* m_i *times*), *and*

$$c(n,r,\mathbf{m},\mathbf{j}) = \frac{n!}{(j_1!)^{m_1}(j_2!)^{m_2}\cdots(j_k!)^{m_k} m_1! m_2! \cdots m_k!}. \qquad (3.15)$$

Proof. The proof relies on the analogy pointed out before stating the theorem. We have to figure out what the coefficients $c(n,r,\mathbf{m},\mathbf{j})$ in the expansion (3.14) ought to be. If $\varphi(x) = f(g(x))$ is any composite function, we have a similar expression for the nth derivative

$$\varphi^{(n)}(x) = \sum_{r=1}^{n} \sum_{\mathbf{m},\mathbf{j}} c(n,r,\mathbf{m},\mathbf{j}) f^{(r)}(g(x))(g^{(j_1)}(x))^{m_1} \cdots (g^{(j_k)}(x))^{(m_k)}. \qquad (3.16)$$

It can be checked that performing a differentiation on each term in (3.16) has the same effect as applying a derivation $\delta(f(A))$ on the corresponding term in (3.14) and then evaluating it using the relation (2.1). We leave the details of this to the reader. So, the coefficients $c(n, r, \mathbf{m}, \mathbf{j})$ in (3.14) and (3.16) are the same. For the latter identity, these are known to be given by (3.15). See [12, p. 34; 17, pp. 38–40].

4. Norms of commutators

An important application of the results in this paper, and the motivation for our study, is the following question in perturbation theory: given a function f on $\mathscr{B}(\mathscr{H})$, how to find bounds for $\|f(A) - f(B)\|$ in terms of $\|A - B\|$. More generally, one may ask for bounds for the generalised commutator $\|f(A)X - Xf(B)\|$ in terms of $\|AX - XB\|$. See [1, Ch. 9; 6–8,10,11,14,15].

Formula (2.2) readily gives such a bound. We have

$$\|f(A)X - Xf(A)\| \leqslant \|Df(A)\| \; \|AX - XA\|. \tag{4.1}$$

If f is holomorphic on a complex domain Ω this inequality holds for all A with spectra in Ω, and all X. If $f \in C^1(I)$, this holds for all self-adjoint operators A with spectra in I, and for all self-adjoint X.

There is a familiar device by which the inequality (4.1) can be extended. Given operators A, B and X on $\mathscr{H}$, consider the operators

$$\begin{pmatrix} A & 0 \\ 0 & B \end{pmatrix}$$

and

$$\begin{pmatrix} 0 & X \\ 0 & 0 \end{pmatrix}$$

on $\mathscr{H} \oplus \mathscr{H}$.

Then note that

$$\begin{pmatrix} A & 0 \\ 0 & B \end{pmatrix}\begin{pmatrix} 0 & X \\ 0 & 0 \end{pmatrix} - \begin{pmatrix} 0 & X \\ 0 & 0 \end{pmatrix}\begin{pmatrix} A & 0 \\ 0 & B \end{pmatrix} = \begin{pmatrix} 0 & AX - XB \\ 0 & 0 \end{pmatrix}.$$

From this and (4.1) we get

$$\|f(A)X - Xf(B)\| \leqslant \|Df(A \oplus B)\| \quad \|AX - XB\|, \tag{4.2}$$

where f is any holomorphic function on a domain Ω, A, B are operators, with their spectra in Ω, X is any operator, and $A \oplus B$ stands for the operator

$$\begin{pmatrix} A & 0 \\ 0 & B \end{pmatrix}$$

on $\mathscr{H} \oplus \mathscr{H}$.

With a slight modification, this argument can be applied to the situation when $f \in C^1(I)$ and A, B are self-adjoint operators with spectra in I. Note that for any X, the operator

$$\begin{pmatrix} 0 & X^* \\ X & 0 \end{pmatrix}$$

is self-adjoint, and

$$\begin{pmatrix} A & 0 \\ 0 & B \end{pmatrix}\begin{pmatrix} 0 & X \\ X^* & 0 \end{pmatrix} - \begin{pmatrix} 0 & X \\ X^* & 0 \end{pmatrix}\begin{pmatrix} A & 0 \\ 0 & B \end{pmatrix} = \begin{pmatrix} 0 & AX - XB \\ BX^* - X^*A & 0 \end{pmatrix}.$$

If X is also self-adjoint then the norm of the operator on the right hand side is $\|AX - XB\|$. So, inequality (4.2) follows in this case too from (4.1).

This still leaves the problem of finding the norm $\|Df(A)\|$. In our earlier work [2–5], we have found interesting examples of functions on the interval $[0, \infty)$ and on the real line, for which

$$\|Df(A)\| = \|f'(A)\|, \tag{4.3}$$

where f' is the ordinary derivative of f on $\mathbb{R}$.

The class of functions satisfying (4.3) is denoted by $\mathscr{D}$. From the inequality (4.2) we see that for all $f \in \mathscr{D}$ we have

$$\|f(A)X - Xf(B)\| \leqslant \|f'\|_\infty \, \|AX - XB\|, \tag{4.4}$$

where $\|f'\|_\infty$ stands for the supremum norm of the function f'. In particular, we have for all $f \in \mathscr{D}$,

$$\|f(A) - f(B)\| \leqslant \|f'\|_\infty \, \|A - B\|. \tag{4.5}$$

Inequalities like these are much sought after in perturbation theory. Some comments are, therefore, in order.

Farforovskaya [10] and McIntosh [15] constructed examples of functions f on an interval I, with a bounded derivative f', and self-adjoint operators A, B with spectra in I, such that an estimate of the form

$$\|f(A) - f(B)\| \leqslant c\|f'\|_\infty \, \|A - B\| \tag{4.6}$$

can not be true for any constant c. It was shown by Birman and Solomyak [7] that an inequality of the form (4.6) does hold under some smoothness requirements on f'. See [11] for a recent exposition of such results. Explicit constants that make the inequality (4.6) work are rarely known. Our inequality (4.4) is of some interest in this context.

We should also point out that an interesting estimate can be derived from the formula (2.9). Since e^{itA} is unitary for all t and self-adjoint A, we get from (2.2) and (2.9) the estimate

$$\|f(A)X - Xf(B)\| \leqslant \|t\hat{f}(t)\|_1 \; \|AX - XB\|.$$

If $\hat{f'}$ is an integrable function, then using the above inequality for functions in the Schwartz class and a standard approximation argument, we can derive the inequality

$$\|f(A)X - Xf(B)\| \leqslant \|\hat{f'}\|_1 \; \|AX - XB\|. \tag{4.7}$$

This inequality has been obtained earlier by Boyadzhiev [8].

In the same way we can obtain estimates for higher order commutators from the results in this paper using our characterisation of functions of class $\mathscr{D}_n$ defined by the property

$$\|D^n f(A)\| = \|f^{(n)}(A)\|.$$

See [5]. Thus, for example, if $f \in \mathscr{D}_1 \cap \mathscr{D}_2$, then from (3.4) we obtain the inequality

$$\|\delta^{[2]}(f(A))(X)\| \leqslant \|f''\|_\infty \|\delta(A)(X)\|^2 + \|f'\|_\infty \|\delta^{[2]}(A)(X)\|. \tag{4.8}$$

Similar inequalities can be written down for higher order derivations using our results.

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