Research Article

The Fréchet Derivative of an Analytic Function of a Bounded Operator with Some Applications

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The main result in this paper is the determination of the Fréchet derivative of an analytic function of a bounded operator, tangentially to the space of all bounded operators. Some applied problems from statistics and numerical analysis are included as a motivation for this study. The perturbation operator (increment) is not of any special form and is not supposed to commute with the operator at which the derivative is evaluated. This generality is important for the applications. In the Hermitian case, moreover, some results on perturbation of an isolated eigenvalue, its eigenprojection, and its eigenvector if the eigenvalue is simple, are also included. Although these results are known in principle, they are not in general formulated in terms of arbitrary perturbations as required for the applications. Moreover, these results are presented as corollaries to the main theorem, so that this paper also provides a short, essentially self-contained review of these aspects of perturbation theory.

1. Introduction

Motivated by certain applications in numerical analysis and, in particular, statistics, this paper deals with the Fréchet derivative of an analytic function φ of a bounded linear operator T on a separable Hilbert space $\mathbb{H}$ (in the sense of the usual functional calculus), tangentially to the Banach space $\mathcal{L}$ of all bounded linear operators mapping $\mathbb{H}$ into itself. More precisely, a first order approximation to the difference

$$\varphi(\widetilde{T}) - \varphi(T), \quad \widetilde{T} = T + \Pi, \quad \Pi \in \mathcal{L}, \tag{1.1}$$

is obtained, including the order of magnitude of the remainder. An example of such a function φ is a generalized or regularized inverse of the square root

$$\varphi(\widetilde{T}) = (\alpha I + \widetilde{T})^{-1/2}, \quad \alpha > 0, \tag{1.2}$$

where I is the identity operator. Once the Fréchet derivative has been established (Section 2), it yields the asymptotic distribution of functions of certain random operators via an ensuing delta method : a well-known statistical technique (see Section 4).

Clearly $\widetilde{T}$ can be regarded as a perturbed version of T, and it is not surprising that perturbation methods are employed to obtain the desired result. The authors are aware of the possibility that the rather straightforward result on the Fréchet derivative might be hidden somewhere in the rich literature on perturbation theory [1–3]. Yet they have not been successful in identifying a reference that states the result in its present form, tailored to the applications they have in mind. Some remarks are particularly in order.

(a) The perturbations Π are typically of small norm but otherwise arbitrary bounded or Hermitian. In literature, they are often of the form

$$\Pi = \epsilon T_1 + \epsilon^2 T_2 + \cdots \tag{1.3}$$

for operators $T_1, T_2, \ldots$, and a small number ϵ. In statistics, there is no point in representing the perturbation in such a form.

(b) The perturbation Π and the operator T are not assumed to commute, because in our applications such an assumption would not in general be fulfilled. If the operators do commute, however, the Fréchet derivative would reduce to $\varphi'(T)$, in the sense of functional calculus with φ' the derivative of φ. In the case considered here, the actual Fréchet derivative and $\varphi'(T)$ may differ considerably.

(c) A central theme in perturbation theory concerns the perturbation of an isolated eigenvalue and corresponding eigenprojection (see, e.g, the references mentioned before). Some of the results are included, because they can be easily derived from the main result on the Fréchet derivative by choosing a special function φ (Section 3). In this way, the paper presents a concise and essentially self-contained review of some basic results in this area. They are again presented in terms of a general (Hermitian) perturbation Π, as being required for statistical application, in the same vein as, but somewhat more general than, Dauxois et al. [4].

As has already been mentioned in the beginning, $\mathbb{H}$ will be a separable Hilbert space and $\mathcal{L}$ the Banach space of all bounded linear operators mapping $\mathbb{H}$ into itself. The inner product on $\mathbb{H}$ will be denoted by $\langle \cdot, \cdot \rangle$ and the norm by $\| \cdot \|$. The norm on $\mathcal{L}$ will be written $\| \cdot \|_{\mathcal{L}}$, and the notation $\mathcal{L}_H$ and $\mathcal{C}_H$ will be used to denote the subspace of all Hermitian and all compact Hermitian operators, respectively.

We will exclusively deal with infinite dimensional Hilbert spaces and will not attempt to include the simpler finite dimensional case in our formulation. The Fréchet derivative for arbitrary perturbations is well known in the finite dimensional matrix case. This result and further references can be found in the recent monograph by Bhatia [5]. In the finite dimensional case, this derivative is also implicitly present in Theorem 2.1 of Ruymgaart and Yang [6] to obtain the asymptotic distribution of a function of a random matrix.

2. The Fréchet Derivative

Let us fix an arbitrary $T \in \mathcal{L}$ with spectrum $\sigma(T)$ and a bounded open region $\Omega \subset \mathbb{C}$ in the complex plane with smooth boundary $\Gamma = \partial\Omega$, such that

$$\sigma(T) \subset \Omega, \qquad \delta_\Gamma = \mathrm{dist}(\Gamma, \sigma(T)) > 0. \tag{2.1}$$

Furthermore, let us consider functions of type

$$\varphi : D \longrightarrow \mathbb{C}, \text{ analytic}, \tag{2.2}$$

where $D \supset \overline{\Omega}$ is an open neighborhood of $\overline{\Omega}$. Let us write

$$M_\Gamma = \max_{z \in \Gamma} |\varphi(z)| < \infty, \qquad L_\Gamma = \text{length of } \Gamma < \infty. \tag{2.3}$$

The resolvent

$$R(z) = (zI - T)^{-1}, \quad z \in \rho(T), \tag{2.4}$$

is analytic on the resolvent set $\rho(T) = [\sigma(T)]^c$, and the operator

$$\varphi(T) = \frac{1}{2\pi i} \oint_\Gamma \varphi(z) R(z) \, dz \tag{2.5}$$

is well defined. This relation establishes an algebra homomorphism [7, Section 17.2] which implies in particular that

$$\varphi(T)\psi(T) = (\varphi\psi)(T), \tag{2.6}$$

if $\psi : D \to \mathbb{C}$ is also analytic. In particular, we have

$$T = \frac{1}{2\pi i} \oint_\Gamma z R(z) dz. \tag{2.7}$$

The operators

$$\varphi'_T \Pi = \frac{1}{2\pi i} \oint_\Gamma \varphi(z) R(z) \Pi R(z) dz, \tag{2.8}$$

$$S_{\varphi,\Pi} = \frac{1}{2\pi i} \oint_\Gamma \varphi(z) R(z) (\Pi R(z))^2 (I - \Pi R(z))^{-1} dz \tag{2.9}$$

are well defined for every $\Pi \in \mathcal{L}$ sufficiently small. Note that according to Dunford and Schwartz [8, Lemma VII.6.11], there is a constant $0 < K < \infty$, such that

$$\left\| R(z) \right\|_{\mathcal{L}} \le \frac{K}{\delta_\Gamma}, \quad \forall z \in \Omega^c. \tag{2.10}$$

Theorem 2.1 (Fréchet Derivative). *Let $T \in \mathcal{L}$ and suppose that φ satisfies (2.2). Then φ maps the neighborhood $\{\widetilde{T} = T + \Pi : \Pi \in \mathcal{L}, \ \|\Pi\|_{\mathcal{L}} \le c\delta_\Gamma / K, \ \text{for some } 0 < c < 1\}$ into $\mathcal{L}$, when defined in the usual way of functional calculus. This mapping is Fréchet differentiable at T, tangentially to $\mathcal{L}$, with bounded derivative $\varphi'_T : \mathcal{L} \to \mathcal{L}$, as defined by (2.8). More specifically, we have*

$$\varphi(T + \Pi) = \varphi(T) + \varphi'_T \Pi + S_{\varphi,\Pi}, \tag{2.11}$$

where $S_{\varphi,\Pi}$ is defined in (2.9) and

$$\left\| \varphi'_T \Pi \right\|_{\mathcal{L}} \le \frac{1}{2\pi} M_\Gamma L_\Gamma \left(\frac{K}{\delta_\Gamma} \right)^2 \|\Pi\|_{\mathcal{L}}, \tag{2.12}$$

$$\left\| S_{\varphi,\Pi} \right\|_{\mathcal{L}} \le \frac{1}{2(1-c)\pi} M_\Gamma L_\Gamma \left(\frac{K}{\delta_\Gamma} \right)^3 \|\Pi\|_{\mathcal{L}}^2. \tag{2.13}$$

Proof. For φ to be well defined on the neighborhood, let us first show that

$$\sigma(\widetilde{T}) \subset \Omega, \quad \forall \Pi \in \mathcal{L} \ \text{with} \ \|\Pi\|_{\mathcal{L}} \le c\frac{\delta_\Gamma}{K}. \tag{2.14}$$

To verify this, note that by (2.10) we have $\|\Pi R(z)\|_{\mathcal{L}} < c$ for such Π. Consequently, the operator

$$\begin{aligned} R(z)(I - \Pi R(z))^{-1} &= R(z)\{(R(z)^{-1} - \Pi)R(z)\}^{-1} \\ &= (zI - T - \Pi)^{-1} = \widetilde{R}(z) \end{aligned} \tag{2.15}$$

is bounded for each $z \in \Omega^c$, which entails (2.14). Hence,

$$\varphi(\widetilde{T}) = \frac{1}{2\pi i} \oint_\Gamma \varphi(z) \widetilde{R}(z) \, dz \tag{2.16}$$

is well defined for Π with $\|\Pi\|_{\mathcal{L}} \le c\delta_\Gamma / K$.

Applying a Neumann series expansion [9, Section 5.2] to the inverse on the left in (2.15), we obtain

$$\begin{aligned} \widetilde{R}(z) &= R(z)\left\{ I + \Pi R(z) + (\Pi R(z))^2 + \cdots \right\} \\ &= R(z) + R(z)\Pi R(z) + R(z)(\Pi R(z))^2 (I - \Pi R(z))^{-1}, \end{aligned} \tag{2.17}$$

just as in Watson [10] for matrices. Term-wise integration yields (2.11).

The upper bounds in (2.12) and (2.13) are immediate from (2.8) and (2.9), respectively, by exploiting (2.3) and (2.15). The boundedness of φ'_T as a linear operator mapping $\mathcal{L}$ into itself follows at once from (2.12). □

Remark 2.2. It will be seen in Section 4 that for the applications we have in mind it is important that we do not require that T and Π commute. If they do, however, it is clear that the Fréchet derivative in (2.8) reduces to

$$\varphi'_T \Pi = \left\{ \frac{1}{2\pi i} \oint_\Gamma \varphi(z) R^2(z) dz \right\} \Pi. \tag{2.18}$$

It has been shown in Dunford and Schwartz [8, proof of Theorem VII.6.10] that

$$\frac{1}{2\pi i} \oint_\Gamma \varphi(z) R^2(z) dz = \frac{1}{2\pi i} \oint_\Gamma \varphi'(z) R(z) dz. \tag{2.19}$$

Combination of (2.11) with (2.18) and (2.19) yields

$$\varphi(T + \Pi) = \varphi(T) + \varphi'(T)\Pi + \mathcal{O}\big(\|\Pi\|_{\mathcal{L}}^2\big), \tag{2.20}$$

writing, for any $r > 0$,

$$\mathcal{O}\big(\|\Pi\|_{\mathcal{L}}^r\big), \quad \text{as } \|\Pi\|_{\mathcal{L}} \longrightarrow 0, \tag{2.21}$$

to indicate any quantity (operator, vector, number) whose norm or absolute value is of the given order. Note that in (2.20) the operator, $\varphi'(T)$ is to be understood in the sense of the usual functional calculus as in (2.5) with φ replaced by its derivative φ'.

In this situation of commuting operators, Dunford and Schwartz [8] obtain the Taylor expansion

$$\varphi(T + \Pi) = \sum_{n=0}^{\infty} \frac{\varphi^{(n)}(T)}{n!} \Pi^n, \tag{2.22}$$

which implies, of course, (2.20).

Keeping the perturbation as before, we now restrict T to the class $\mathcal{C}_H$ of compact Hermitian operators. The bounded and countable spectrum consists of the number 0, whether an eigenvalue or not, and all the nonzero eigenvalues $\lambda_1, \lambda_2, \ldots \in \mathbb{R}$. In this work, we avoid technical issues related to $\lambda = 0$ being an eigenvalue, and assume that T is one-to-one, that is, $Tf = 0$ implies that $f = 0$. It is well known [7] that such a T can be represented as

$$T = \sum_{j=1}^{\infty} \lambda_j P_j, \tag{2.23}$$

where the P_j are the corresponding orthogonal eigenprojections onto the mutually orthogonal finite dimensional eigenspaces. These projections provide a resolution of the identity in $\mathbb{H}$, that is,

$$I_{\mathbb{H}} = \sum_{j=1}^{\infty} P_j. \tag{2.24}$$

The resolvent has the expansion

$$R(z) = \sum_{j=1}^{\infty} \frac{1}{z - \lambda_j} P_j, \quad z \in \rho(T). \tag{2.25}$$

Corollary 2.3. *Let the conditions of Theorem 2.1 be fulfilled for $T \in \mathcal{C}_H$ with expansion* (2.23). *In this case the Fréchet derivative* $\varphi'_T : \mathcal{L} \to \mathcal{L}$ *is given by*

$$\varphi'_T \Pi = \sum_{j} \varphi'(\lambda_j) P_j \Pi P_j + \sum_{j \neq k} \sum \frac{\varphi(\lambda_k) - \varphi(\lambda_j)}{\lambda_k - \lambda_j} P_j \Pi P_k, \quad \Pi \in \mathcal{L}. \tag{2.26}$$

Proof. Let us substitute the expansion (2.25) for $R(z)$ into the expression for $\varphi'_T \Pi$ in (2.8). Application of the partial fraction method yields

$$\begin{aligned}
\varphi'_T \Pi &= \sum_{j} \sum_{k} \left\{ \frac{1}{2\pi i} \oint_{\Gamma} \frac{\varphi(z)}{(z - \lambda_j)(z - \lambda_k)} dz \right\} P_j \Pi P_k \\
&= \sum_{j} \left\{ \frac{1}{2\pi i} \oint_{\Gamma} \frac{\varphi(z)}{(z - \lambda_j)^2} dz \right\} P_j \Pi P_j \\
&\quad + \sum_{j \neq k} \sum \left[\frac{1}{\lambda_k - \lambda_j} \frac{1}{2\pi i} \oint_{\Gamma} \left\{ \frac{\varphi(z)}{(z - \lambda_k)} - \frac{\varphi(z)}{(z - \lambda_j)} \right\} dz \right] P_j \Pi P_k.
\end{aligned} \tag{2.27}$$

The right-hand side of (2.27) reduces at once to the expression on the right in (2.26) by an application of Cauchy's integral formula. $\qquad\square$

Example 2.4. The function $\varphi(z) = z$, $z \in \mathbb{C}$, is analytic on the entire complex plane so that Corollary 2.3 applies. The Fréchet derivative in (2.26) now reduces to

$$\varphi'_T \Pi = \sum_{j} \sum_{k} P_j \Pi P_k = \Pi, \tag{2.28}$$

$\Pi \in \mathcal{L}$. Of course this result is immediate because in this simple case $\varphi(T + \Pi) = T + \Pi = \varphi(T) + \Pi$.

Example 2.5. Next let us, for $p > 0$, consider the function

$$\varphi_\alpha(z) = (\alpha + z)^{-p}, \quad \alpha > \delta_\Gamma > 0, \tag{2.29}$$

for $z \neq -\alpha$. Note that the choice of α ensures that the pole at $z = -\alpha$ remains outside the contour Γ. Clearly there exists an open region Ω of the type required, such that φ is analytic on some open neighborhood D of $\overline{\Omega}$. Hence Corollary 2.3 applies again. The operator $\varphi_\alpha(T) = (\alpha I + T)^{-p}$ represents a regularized or generalized inverse of Tikhonov type, according to whether T is injective or not. The Fréchet derivative in (2.26) now equals

$$\varphi'_{\alpha,T}\Pi = -p\sum_j \frac{1}{(\alpha + \lambda_j)^{p+1}}P_j\Pi P_j + \sum_{j \neq k}\sum \frac{(\alpha + \lambda_j)^p - (\alpha + \lambda_k)^p}{(\lambda_k - \lambda_j)(\alpha + \lambda_j)^p(\alpha + \lambda_k)^p}P_j\Pi P_k, \qquad (2.30)$$

for $\Pi \in \mathcal{L}$.

Remark 2.6. For $T \in \mathcal{C}_H$, T and Π commuting the double sum on the right in (2.26) cancels and we obtain

$$\varphi'_T\Pi = \sum_j \varphi'(\lambda_j)P_j\Pi, \qquad (2.31)$$

in accordance with (2.20). Apparently, the double sum is a correction term needed when T and Π do not commute.

3. Perturbation of Eigenvalues and Eigenvectors

Throughout this section, both T and Π are assumed to be Hermitian, so that also $T + \Pi \in \mathcal{L}_H$. In addition to this, we assume that

$$T \in \mathcal{L}_H \text{ has an isolated eigenvalue } \lambda_1, \qquad (3.1)$$

with one-dimensional eigenspace. Consequently, the eigenprojection can be written

$$P_1 = p_1 \otimes p_1, \quad \text{for some } p_1 \in \mathbb{H} \text{ with } \|p_1\| = 1, \qquad (3.2)$$

where for $a, b \in \mathbb{H}$ the operator $a \otimes b$ is defined by $(a \otimes b)x = \langle x, b\rangle a$, $x \in \mathbb{H}$.

The region $\Omega \supset \sigma(T)$ will now be chosen in such a way that it has a connected component Ω_1 with the properties

$$\Omega_1 \cap \sigma(T) = \lambda_1, \quad \text{dist}(\Omega_1, \Omega \setminus \Omega_1) > 0. \qquad (3.3)$$

A special analytic function $\varphi_1 : D \to \mathbb{C}$ such that

$$\varphi_1(z) = 1, \quad z \in \Omega_1, \qquad \varphi_1(z) = 0, \quad z \in \Omega_0 = \Omega \setminus \Omega_1, \qquad (3.4)$$

will play an important role in the sequel. Note, for instance, that

$$\varphi_1(T) = P_1. \qquad (3.5)$$

For the Fréchet derivative of $\varphi_1(\widetilde{T})$ at T, a special expression can be obtained. Let us write

$$T = \lambda_1 P_1 + T_0, \tag{3.6}$$

where T_0 is Hermitian with spectrum $\sigma(T_0) \subset \Omega_0$. According to the spectral theorem, there exists a resolution of the identity $E(\lambda)$, $\lambda \in \sigma(T_0)$, such that

$$T_0 = \int_{\sigma(T_0)} \lambda \, dE(\lambda). \tag{3.7}$$

It should be noted that

$$P_1 E(\lambda) = E(\lambda) P_1 = O, \quad \forall \lambda \in \sigma(T_0), \tag{3.8}$$

where O is the zero operator, and that

$$R(z) = \frac{1}{z - \lambda_1} P_1 + \int_{\sigma(T_0)} \frac{1}{z - \lambda} dE(\lambda). \tag{3.9}$$

Let us define

$$Q_1 = \int_{\sigma(T_0)} \frac{1}{\lambda_1 - \lambda} dE(\lambda). \tag{3.10}$$

Lemma 3.1. *The Fréchet derivative of $\varphi_1(\widetilde{T})$ at T is given by*

$$\varphi'_{1,T} \Pi = P_1 \Pi Q_1 + Q_1 \Pi P_1, \quad \Pi \in \mathcal{L}_H. \tag{3.11}$$

Proof. This follows by substitution of (3.9) in the expression on the right in

$$\varphi'_{1,T} \Pi = \frac{1}{2\pi i} \oint_{\Gamma_1} R(z) \Pi R(z) dz, \quad \Gamma_1 = \partial \Omega_1, \tag{3.12}$$

for this derivative; see also (2.8). We thus obtain

$$\begin{aligned}
\varphi'_{1,T} \Pi &= \frac{1}{2\pi i} \oint_{\Gamma_1} \frac{1}{(z - \lambda_1)^2} P_1 \Pi P_1 dz \\
&\quad + \frac{1}{2\pi i} \oint_{\Gamma_1} \frac{1}{z - \lambda_1} P_1 \Pi \left\{ \int_{\sigma(T_0)} \frac{1}{z - \lambda} dE(\lambda) \right\} dz \\
&\quad + \frac{1}{2\pi i} \oint_{\Gamma_1} \left\{ \int_{\sigma(T_0)} \frac{1}{z - \lambda} dE(\lambda) \right\} \Pi \frac{1}{z - \lambda_1} P_1 dz \\
&\quad + \frac{1}{2\pi i} \oint_{\Gamma_1} \left\{ \int_{\sigma(T_0)} \frac{1}{z - \lambda} dE(\lambda) \right\} \Pi \left\{ \int_{\sigma(T_0)} \frac{1}{z - \mu} dE(\mu) \right\}.
\end{aligned} \tag{3.13}$$

By Cauchy's integral formula

$$\frac{1}{2\pi i}\oint_{\Gamma_1}\frac{1}{(z-\lambda_1)^2}\,dz = \varphi_1'(\lambda_1) = 0, \tag{3.14}$$

so that the first term on the right side in (3.13) is the zero operator. Regarding the second, note that

$$\frac{1}{2\pi i}\oint_{\Gamma_1}\frac{1}{(z-\lambda_1)(z-\lambda)}\,dz = \frac{1}{\lambda_1-\lambda}\left(\frac{1}{2\pi i}\oint_{\Gamma_1}\frac{1}{z-\lambda_1}\,dz - \frac{1}{2\pi i}\oint_{\Gamma_1}\frac{1}{z-\lambda}\,dz\right) = \frac{1}{\lambda_1-\lambda}, \tag{3.15}$$

because each $\lambda \in \sigma(T_0)$ lies outside the contour Γ_1. Consequently, the second term equals

$$P_1\Pi\left\{\frac{1}{2\pi i}\int_{\sigma(T_0)}\frac{1}{\lambda_1-\lambda}\,dE(\lambda)\right\} = P_1\Pi Q_1. \tag{3.16}$$

Similarly, the third term equals $Q_1\Pi P_1$. The last term cancels, because

$$\frac{1}{2\pi i}\oint_{\Gamma_1}\frac{1}{(z-\lambda)(z-\mu)}\,dz = 0, \tag{3.17}$$

since both λ and μ lie outside Γ_1. □

Some results about the perturbation of λ_1 and P_1 in a given direction as in (1.3) that are well known in literature [1, 2] can be partly recovered for perturbations in some neighborhood, in an essentially self-contained manner, as simple consequences of the results in Section 2.

Corollary 3.2. *Under the assumptions* (3.1), (3.2), *and for* $\Pi \in \mathcal{L}_H$ *sufficiently small, the operator* $\widetilde{T}$ *has an isolated eigenvalue* $\widetilde{\lambda}_1$ *with eigenprojection* $\widetilde{P}_1 = \widetilde{p}_1 \otimes \widetilde{p}_1$ *for some unit vector* $\widetilde{p}_1 \in \mathbb{H}$, *satisfying*

$$\widetilde{P}_1 = P_1 + P_1\Pi Q_1 + Q_1\Pi P_1 + \mathcal{O}\big(\|\Pi\|_{\mathcal{L}}^2\big), \tag{3.18}$$

where Q_1 *is defined in* (3.10).

Proof. In view of (3.5) and (3.11), application of (2.11) with $\varphi = \varphi_1$ yields $\varphi_1(\widetilde{T}) = P_1 + P_1\Pi Q_1 + Q_1\Pi P_1 + \mathcal{O}(\|\Pi\|_{\mathcal{L}}^2)$. Clearly $\varphi_1(\widetilde{T})$ is Hermitian, and because $\big(\varphi_1(\widetilde{T})\big)^2 = \varphi_1^2(\widetilde{T}) = \varphi_1(\widetilde{T})$ by (2.6), it is also idempotent so that it is in fact some projection $\widetilde{P}_1$, for example, it follows that $\|P_1 - \widetilde{P}_1\|_{\mathcal{L}} < 1$ for all Π sufficiently small, and hence the range of $\widetilde{P}_1$ must also have dimension 1 [11] so that $\widetilde{P}_1 = \widetilde{p}_1 \otimes \widetilde{p}_1$ for some $\widetilde{p}_1 \in \mathbb{H}$ with $\|\widetilde{p}_1\| = 1$.

Next, let $\chi(z) = z$, $z \in \mathbb{C}$, be the identity function. By (2.6), again, on the one hand we have $(\chi\varphi_1)(\widetilde{T})\widetilde{p}_1 = \widetilde{T}\widetilde{P}_1\widetilde{p}_1 = \widetilde{T}\widetilde{p}_1$, and on the other $(\varphi_1\chi)(\widetilde{T})\widetilde{p}_1 = \widetilde{P}_1\widetilde{T}\widetilde{p}_1 = (\widetilde{p}_1 \otimes \widetilde{p}_1)\widetilde{T}\widetilde{p}_1 = \langle\widetilde{T}\widetilde{p}_1, \widetilde{p}_1\rangle\widetilde{p}_1 = \widetilde{\lambda}_1\widetilde{p}_1$. Hence $\widetilde{p}_1$ is an eigenvector of $\widetilde{T}$ with eigenvalue $\widetilde{\lambda}_1$. □

Corollary 3.3. *Under the assumptions of Corollary 3.2, we have*

$$\tilde{p}_1 = p_1 + Q_1 \Pi p_1 + \mathcal{O}(\|\Pi\|_{\mathcal{L}}^2). \tag{3.19}$$

Proof. Let us first observe that $P_1 \Pi Q_1 p_1 = 0$ because of (3.8). Hence (3.18) yields $\tilde{p}_1 - p_1 = (\tilde{P}_1 - P_1)p_1 + r_1 + r_2 = Q_1 \Pi p_1 + r_1 + r_2 + \mathcal{O}(\|\Pi\|_{\mathcal{L}}^2)$, where

$$r_1 = P_1(\tilde{p}_1 - p_1), \qquad r_2 = (\tilde{P}_1 - P_1)(\tilde{p}_1 - p_1). \tag{3.20}$$

It suffices to show that $\|r_j\| = \mathcal{O}(\|\Pi\|_{\mathcal{L}}^2)$ for $j = 1, 2$. The idea of the proof can be found in Dauxois et al. [4].

Regarding r_1, note that $1 - \langle \tilde{p}_1, p_1 \rangle^2 = \|\langle \tilde{p}_1, p_1 \rangle \tilde{p}_1 - p_1\|^2 \leq \|\tilde{P}_1 - P_1\|_{\mathcal{L}}^2 = \mathcal{O}(\|\Pi\|_{\mathcal{L}}^2)$, once more using (3.18). Hence $\langle \tilde{p}_1, p_1 \rangle \to 1$, as $\|\Pi\|_{\mathcal{L}} \to 0$, and therefore $2 \geq 1 + \langle \tilde{p}_1, p_1 \rangle \geq 1$ for $\|\Pi\|_{\mathcal{L}}$ sufficiently small. This entails

$$\begin{aligned} \|r_1\| &= \|\langle \tilde{p}_1, p_1 \rangle \tilde{p}_1 - p_1\| = |1 - \langle \tilde{p}_1, p_1 \rangle| \\ &= \frac{\left| 1 - \langle \tilde{p}_1, p_1 \rangle^2 \right|}{|1 + \langle \tilde{p}_1, p_1 \rangle|} = \mathcal{O}(\|\Pi\|_{\mathcal{L}}^2). \end{aligned} \tag{3.21}$$

For r_2 we have

$$\begin{aligned} \|r_2\| &\leq \|\tilde{P}_1 - P_1\|_{\mathcal{L}} \|\tilde{p}_1 - p_1\| \\ &= \mathcal{O}(\|\Pi\|_{\mathcal{L}}) \sqrt{2(1 - \langle \tilde{p}_1, p_1 \rangle)} \\ &= \mathcal{O}(\|\Pi\|_{\mathcal{L}}) \sqrt{2\|r_1\|} = \mathcal{O}(\|\Pi\|_{\mathcal{L}}^2), \end{aligned} \tag{3.22}$$

as can be seen from (3.21). $\qquad\square$

Corollary 3.4. *Under the assumptions of Corollary 3.2, we have*

$$\tilde{\lambda}_1 = \lambda_1 + \langle \Pi p_1, p_1 \rangle + \mathcal{O}(\|\Pi\|_{\mathcal{L}}^2). \tag{3.23}$$

Proof. With the help of (3.19), we see that $\tilde{\lambda}_1 = \langle \tilde{T} \tilde{p}_1, \tilde{p}_1 \rangle = \langle (T + \Pi)(p_1 + Q_1 \Pi p_1), p_1 + Q_1 \Pi p_1 \rangle + \mathcal{O}(\|\Pi\|_{\mathcal{L}}^2)$. The result follows from a routine calculation combined with the equalities $\langle T p_1, p_1 \rangle = \lambda_1$, $\langle T p_1, Q_1 \Pi p_1 \rangle = \lambda_1 \langle p_1, Q_1 \Pi p_1 \rangle = \lambda_1 \langle Q_1 p_1, \Pi p_1 \rangle = 0$, and $\langle T Q_1 \Pi p_1, p_1 \rangle = \langle Q_1 \Pi p_1, T p_1 \rangle = \lambda_1 \langle Q_1 \Pi p_1, p_1 \rangle = \lambda_1 \langle \Pi p_1, Q_1 p_1 \rangle = 0$. For the last two equalities we assume that T and Q_1 are Hermitian and $Q_1 p_1 = 0$ by (3.8). $\qquad\square$

Corollary 3.5. *Let $T \in \mathcal{C}_H$ be given by (2.23) and satisfy (3.2). Then (3.18) and (3.19) remain true with*

$$Q_1 = \sum_{j=2}^{\infty} \frac{1}{\lambda_1 - \lambda_j} P_j. \tag{3.24}$$

Proof. All nonzero eignvalues of T are isolated, in particular λ_1. It is immediate from (2.23) that $T_0 = \sum_{j=2}^{\infty} \lambda_j P_j$, and this leads to the special expression for Q_1 in (3.24). □

Remark 3.6. The assumption that Π be Hermitian is in fact not necessary. Of course, if we just require Π to be bounded, the perturbed operator $\widetilde{T}$ is not in general Hermitian anymore. In particular, a suitably modified version of Corollary 3.3 will now claim the existence of a pair of eigenvectors, $\widetilde{p}_1$ for $\widetilde{T}$ and $\widetilde{p}_1^*$ for $\widetilde{T}^*$, with expansions

$$\widetilde{p}_1 = p_1 + Q_1 \Pi p_1 + \mathcal{O}\big(\|\Pi\|_{\mathcal{L}}^2\big), \qquad \widetilde{p}_1^* = p_1 + Q_1 \Pi^* p_1 + \mathcal{O}\big(\|\Pi\|_{\mathcal{L}}^2\big), \tag{3.25}$$

as $\|\Pi\| \to 0$.

4. Applications

In this section, we will sketch three applications: two in statistics and one in numerical analysis.

4.1. Noisy Integral Equations

Let $K : L^2(0,1) \to L^2(0,1)$ be a compact injective integral operator, with measurable real kernel denoted by the same symbol without confusion. More specifically, input $f \in L^2(0,1)$ and output $g \in L^2(0,1)$ are related according to

$$g(s) = \int_0^1 K(s,t) f(t) dt. \tag{4.1}$$

In practice, only finitely many data regarding the output are available, usually blurred by random measurement error. If the data are collected according to a random design, we may think of the data set as of n independent copies $(X_1, Y_1), \ldots, (X_n, Y_n)$ of a pair (X, Y) of random variables, where

$$Y = g(X) + \epsilon = (Kf)(X) + \epsilon, \tag{4.2}$$

the design variable X has a Uniform $(0,1)$ distribution, the error variable ϵ has finite variance and zero mean, and where X and ϵ are stochastically independent.

It is the purpose to recover f from these data. It is expedient to "precondition" with the adjoint operator K^* and recover f from the equation

$$q = K^* g = K^* K f = Rf, \tag{4.3}$$

where R is compact, Hermitian, and strictly positive. Under suitable conditions,

$$\widehat{q}(t) = \frac{1}{n} \sum_{i=1}^n Y_i K^*(t, X_i) = \frac{1}{n} \sum_{i=1}^n Y_i K(X_i, t), \quad t \in [0, 1], \tag{4.4}$$

is an unbiased and $\sqrt{n}$-consistent estimator of q; see, for instance, van Rooij and Ruymgaart [12]. Since R^{-1} is unbounded, an estimator of the input f is obtained by applying a regularized inverse of R to $\widehat{q}$. Here we will use the Tikhonov type inverse

$$(\alpha I + R)^{-1} = \varphi_a(R), \quad \alpha > 0, \tag{4.5}$$

where $\varphi_\alpha(z) = (\alpha + z)^{-1}$; see also (2.29). This yields the input estimator

$$\widehat{f}_\alpha = \varphi_\alpha(R)\widehat{q}, \quad \alpha > 0. \tag{4.6}$$

To assess the quality of the estimator, one considers the mean integrated squared error (MISE)

$$\mathbb{E}\|\widehat{f}_\alpha - f\|^2. \tag{4.7}$$

The behavior of the MISE is well studied in literature.

Recently, there is an interest in certain econometric models where the operator K (or R) is unknown but can be estimated from the data. Let $\widehat{R}$ denote an estimator of R and assume that $\widehat{R}$ is also compact, Hermitian, and nonnegative. In this case, the input estimator

$$\widehat{\widehat{f}}_\alpha = \left(\alpha I + \widehat{R}\right)^{-1}\widehat{q} = \varphi_\alpha(\widehat{R})\widehat{q}, \quad \alpha > 0, \tag{4.8}$$

will be employed. One expects that estimation of R will increase the MISE, and naturally the question arises how much bigger the MISE of $\widehat{\widehat{f}}_\alpha$ will be than that of $\widehat{f}_\alpha$.

An upper bound for this increase of the MISE can be easily found from the results in Section 2. For large sample size n, $\widehat{R}$ will be close to R, and $\widehat{\Pi} = \widehat{R} - R$ can be considered as a small random perturbation of R. Writing $\varphi'_{\alpha,R}$ for the Fréchet derivative at R, we see from Theorem 2.1 that

$$\begin{aligned}
\widehat{\widehat{f}}_\alpha - f &= \left\{\varphi_\alpha(\widehat{R}) - \varphi_\alpha(R)\right\}\widehat{q} + \varphi_\alpha(R)\widehat{q} - f \\
&= (\varphi'_{\alpha,R}\widehat{\Pi})\widehat{q} + \widehat{f}_\alpha - f + \mathcal{O}(\|\widehat{\Pi}\|^2).
\end{aligned} \tag{4.9}$$

Apparently, $(\varphi'_{\alpha,R}\widehat{\Pi})\widehat{q}$ is an extra error term due to the estimation of R.

To find an upper bound for its MISE, let us first observe that (2.30) simplifies for $p = 1$ and yields

$$\varphi'_{\alpha,R}\widehat{\Pi} = -\sum_j\sum_k \frac{1}{(\alpha + \lambda_j)(\alpha + \lambda_k)}P_j\widehat{\Pi}P_k, \tag{4.10}$$

where now the λ_j and the P_j are the spectral characteristics of R. Let us write, for brevity,

$$\widehat{h} = \sum_k \frac{1}{\alpha + \lambda_k}P_k\widehat{q}, \tag{4.11}$$

and note that

$$\|\widehat{h}\|^2 \le \frac{1}{\alpha^2}\|\widehat{q}\|^2. \tag{4.12}$$

We thus arrive at

$$\mathbb{E}\left\|\left(\varphi'_{\alpha,R}\widehat{\Pi}\right)\widehat{q}\right\|^2 = \mathbb{E}\left\|\sum_j \frac{1}{\alpha + \lambda_j} p_j \widehat{\Pi}\,\widehat{h}\right\|^2 \le \frac{1}{\alpha^2}\mathbb{E}\|\widehat{\Pi}\|_{\mathscr{L}}^2 \|\widehat{h}\|^2 \le \frac{1}{\alpha^4}\mathbb{E}\|\widehat{\Pi}\|_{\mathscr{L}}^2 \|\widehat{q}\|^2. \tag{4.13}$$

Hence, under suitable assumptions, estimation of the kernel yields an extra term in the MISE of the input estimator which is of order α^{-4}. In the Russian literature, sharper bounds can be found; see in particular Bakushinsky and Kokurin [13, Section 2.2]. For results of this type in the statistical literature, obtained in a different manner, see, for instance, Hall and Horowitz [14] and Florens [15].

4.2. Some Asymptotics for Functional Canonical Correlations

Let X be a real random element in the Hilbert space $L^2(0,1)$ and assume that $\mathbb{E}\|X\|^4 < \infty$. Its mean $\mu \in L^2(0,1)$ and covariance operator $S : L^2(0,1) \to L^2(0,1)$ are well defined by the relations $\mathbb{E}\langle f, X\rangle = \langle f, \mu\rangle$, $\mathbb{E}\langle f, X - \mu\rangle\langle X - \mu, g\rangle = \langle f, Sg\rangle$ for all $f, g \in L^2(0,1)$. The operator S is known to be of finite trace and hence Hilbert-Schmidt and compact. It is also nonnegative Hermitian. Without real loss of generality, we will assume S to be injective, so that it will be strictly positive.

Next suppose that we are given a random sample $X_1, \ldots, X_n$ of independent copies of X. The usual estimators of μ and S are $\overline{X} = (1/n)\sum_{i=1}^n X_i$ and $\widehat{S} = (1/n)\sum_{i=1}^n (X_i - \overline{X}) \otimes (X_i - \overline{X})$, respectively, where $\widehat{S}$ shares all the properties of S, except that it cannot be injective because it has a finite dimensional kernel whose range has dimension at most $n - 1$.

Because $\widehat{S}$ cannot be injective, the finite dimensional definition of sample canonical correlation has to be modified, and some kind of smoothing or regularization is recommended in literature [16]. Regularization might even be useful when the population is considered, although S is injective [17]. This regularization yields Tikhonov type inverses in an expression for the canonical correlation .

For a precise definition, let $\mathbb{H}_1$ and $\mathbb{H}_2$ be two closed subspaces of $L^2(0,1)$ and I_j the orthogonal projection onto $\mathbb{H}_j$ ($j = 1, 2$). Let us write $S_{jk} = I_j S I_k$, and note that $I_j(\alpha I + S)I_k = S_{jk}$ for $j \ne k$. Similar notation will be used for $\widehat{S}$. The regularized squared principal canonical correlation for the population is now defined as

$$\rho^2 = \sup_{f_1, f_2 \ne 0} \frac{\langle f_1, S_{12}f_2\rangle^2}{\langle f_1, (\alpha I_1 + S_{11})f_1\rangle\langle f_2, (\alpha I_2 + S_{22})f_2\rangle}. \tag{4.14}$$

Its sample analogue $\widehat{\rho}^2$ is obtained by replacing the S_{jk} with $\widehat{S}_{jk}$ in (4.14). The supremum is actually a maximum, and pairs of maximizers will be denoted by f_1^*, f_2^*, and $\widehat{f_1^*}$, $\widehat{f_2^*}$,

respectively. The corresponding canonical variates then are

$$\langle X, f_j^* \rangle, \quad \langle X, \widehat{f_j^*} \rangle, \quad j = 1, 2. \tag{4.15}$$

For an alternative description of these canonical correlations, let us introduce the operator

$$R_1 = (\alpha I_1 + S_{11})^{-1/2} S_{12} (\alpha I_2 + S_{22})^{-1} S_{21} (\alpha I_1 + S_{11})^{-1/2}. \tag{4.16}$$

Interchanging the indices 1 and 2 yields R_2, and replacing S_{jk} with $\widehat{S}_{jk}$ yields $\widehat{R}_1$ and $\widehat{R}_2$. It can be seen that all these operators are Hilbert-Schmidt and strictly positive Hermitian. It will be assumed that R_j has the largest eigenvalue with one-dimensional eigenspace generated by f_j^* with $\|f_j^*\| = 1$. Under this condition, it has been shown in Cupidon et al. [18] that

$$\rho^2 = \text{largest eigenvalue of } R_j = \langle f_j^*, R_j f_j^* \rangle, \tag{4.17}$$

for $j = 1, 2$. A similar result holds true for $\widehat{\rho}^2$.

It is well known that the asymptotic distribution of the eigenvalues and eigenfunctions of a random operator can be derived from the asymptotic distribution of this random operator itself (see [10] for Euclidean spaces and [4] for Hilbert spaces). This technique is based on the results of Section 3. In the present situation, this means that we have to show the convergence in distribution of the suitably standardized $\widehat{R}_j$. Because all operators are Hilbert-Schmidt, it can be shown that

$$\mathcal{R}_j = \sqrt{n}(\widehat{R}_j - R_j) \xrightarrow{d} \mathcal{G}, \quad \text{as } n \longrightarrow \infty, \text{ in } \mathcal{L}. \tag{4.18}$$

Result (4.18) follows easily if convergence in distribution can be established for each of the factors defining $\widehat{R}_j$, for instance,

$$(\alpha I + \widehat{S}_{jj})^{-1/2} = \varphi_\alpha(\widehat{S}_{jj}), \tag{4.19}$$

where this time $\varphi_\alpha(z) = (\alpha + z)^{-1/2}$, compare (2.29). It is known [4] that

$$\sqrt{n}\{\widehat{S}_{jj} - S_{jj}\} \xrightarrow{d} \mathcal{G}_{jj}, \quad \text{as } n \longrightarrow \infty, \text{ in } \mathcal{L}_{\text{HS}}, \tag{4.20}$$

for some Gaussian random element $\mathcal{G}_{jj}$, where $\mathcal{L}_{\text{HS}}$ is the Hilbert space of all Hilbert-Schmidt operators mapping $\mathbb{H}$ into itself. Writing $\varphi'_{\alpha,j}$ for the Fréchet derivative evaluated at S_{jj} (Section 2) and exploiting the fact that the imbedding of $\mathcal{L}_{\text{HS}}$ is $\mathcal{L}$ are continuous, we obtain via a kind of delta-method [18, 19]

$$\sqrt{n}\{\varphi_\alpha(\widehat{S}_{jj}) - \varphi_\alpha(S_{jj})\} \xrightarrow{d} \varphi'_{\alpha,j} \mathcal{G}_{jj}, \quad \text{as } n \longrightarrow \infty, \text{ in } \mathcal{L} \tag{4.21}$$

the desired result. A combination of results like this for each of the factors of $\widehat{R}_j$ yields (4.18).

4.3. Solution of a Nonlinear Operator Equation

In Bakushinsky and Kokurin [13], the following problem is considered. Let $\mathbb{H}_1$ and $\mathbb{H}_2$ be Hilbert spaces and $F : \mathbb{H}_1 \to \mathbb{H}_2$ an operator, not necessarily linear. The (nonlinear) equation

$$F(x) = 0, \quad x \in \mathbb{H}, \tag{4.22}$$

is studied. Let x^* be a solution of (4.22) and introduce a set $\Omega = \{x \in \mathbb{H}_1 : \|x - x^*\|_1 \le r\}$, for some $r > 0$. It is assumed that F is Fréchet differentiable on Ω. If F'_x is the derivative at $x \in \Omega$ it is, moreover, assumed that

$$\left\| F'_x - F'_y \right\|_{\mathcal{L}(\mathbb{H}_1, \mathbb{H}_2)} \le L \|x - y\|_1, \quad x, y \in \Omega, \tag{4.23}$$

where $0 < L < \infty$ is a given number. Given an initial point $x_0 \in \Omega$ and a sequence $\{\alpha_n\}$, $\alpha_n > 0$, of regularization parameters, these authors show that, under some further conditions, the generalized Gauss-Newton method generates a sequence of points $\{x_n\}$ such that

$$\|x_n - x^*\| = \mathcal{O}(\alpha_n^p), \quad \text{for some } p \ge \frac{1}{2}. \tag{4.24}$$

In their proof of this result, the authors need a crucial upper bound. Under some additional assumptions, we want to derive this upper bound as an immediate consequence of Theorem 2.1. In order to relate the present problem to the setup of our paper, let us assume that $\mathbb{H}_1 = \mathbb{H}_2 = \mathbb{H}$, and note that

$$\left(F'_{x^*} \right)^* \left(F'_{x^*} \right) = T \in \mathcal{L}_H. \tag{4.25}$$

For x_n, let

$$\left(F'_{x_n} \right)^* \left(F'_{x_n} \right) = \tilde{T} \in \mathcal{L}_H, \tag{4.26}$$

and set

$$\tilde{T} = T + \tilde{T} - T = T + \Pi, \tag{4.27}$$

where obviously $\Pi \in \mathcal{L}_H$. It is not hard to see that (4.23) entails

$$\|\Pi\|_{\mathcal{L}} \le a \|x^* - x_n\|, \tag{4.28}$$

for some $0 < a < \infty$. Let Γ be the contour in (2.1) and D the corresponding domain. As in Bakushinsky and Kokurin [13], a function $\Theta(z, \alpha)$, $z \in D$, is employed in the iteration scheme, which is analytic on D.

Narrowing down the generality in Bakushinsky and Kokurin [13] somewhat further, so that the current conditions are satisfied, their proof of the convergence of the iterations requires an upper bound for the expression (in our notation)

$$
\begin{aligned}
\frac{1}{2\pi i}\oint_{\Gamma}\{1-\Theta(z,\alpha_n)\}\{R(z)-\tilde{R}(z)\}dz &= 1-\Theta(T,\alpha_n)-\{1-\Theta(\tilde{T},\alpha_n)\} \\
&= \Theta(\tilde{T},\alpha_n)-\Theta(T,\alpha_n).
\end{aligned}
\tag{4.29}
$$

Keeping n fixed, let us briefly write this last expression as $\Theta(\tilde{T})-\Theta(T)$. Now Theorem 2.1 applies with $\varphi=\Theta$, and application yields at once

$$
\begin{aligned}
\|\Theta(\tilde{T})-\Theta(T)\|_{\mathcal{L}} &\leq \|\Theta'_T(\tilde{T}-T)\|_{\mathcal{L}}+\mathcal{O}(\|\tilde{T}-T\|^2_{\mathcal{L}}) \\
&\leq b\|\tilde{T}-T\|_{\mathcal{L}}+\mathcal{O}(\|\tilde{T}-T\|^2_{\mathcal{L}}) \\
&\leq ab\|x^*-x_n\|+\mathcal{O}(\|x^*-x_n\|^2),
\end{aligned}
\tag{4.30}
$$

for some $0<b<\infty$, by (4.28).

Acknowledgments

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