THE FRECHET DIFFERENTIAL OF A PRIMARY MATRIX FUNCTION

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Let \( X \) be a given complex matrix of order \( n \). If \( f(z) \) is analytic at the eigenvalues of \( X \), one may define the primary matrix function \( f(X) \) with stem function \( f(z) \) by using any of several well-known methods: for instance, canonical forms, power series, or interpolating polynomials [9]. The Frechet differential of the primary matrix function \( f \) at \( X \), evaluated for the "increment" \( H \), is written \( df(X; H) \) and is defined [1, p. 143] to be the unique linear function of \( H \) which satisfies

\[
\| f(X + H) - f(X) - df(X; H) \| = o(\| H \|).
\]

If \( H \) commutes with \( X \) it is known [6] that \( df(X; H) = Hf^{(1)}(X) \). (Throughout this paper, \( f^{(k)}(X) \) denotes the primary matrix function with stem function \( f^{(k)}(z) \).) Several attempts have been made to find a similarly satisfying expression for the differential under less restrictive conditions [7; 11], but these have had only partial success because of the reliance on canonical forms to represent \( f(X) \). The results of these investigations and the important role of commutativity motivate the following.

Definition. The successive commutes, or inner derivatives, of \( H \) with respect to \( X \) are defined by:

\[
H^{(0)} = H \quad \text{and} \quad H^{(k)} = H - DX - XH^{(k-1)} \quad \text{for} \quad k \geq 1.
\]

In [12] Roth investigated commutes in detail, and some additional information will be found in [3].

As we shall be dealing with linear functions on matrices, it is convenient to use some notation and results of Neudecker [4]. Let the columns of the \( n \times n \) matrix \( H \) be \( h_1, h_2, \ldots, h_n \). We define an isomorphism between the \( n \times n \) matrices and the \( n^2 \times 1 \) matrices by \( \text{vec} \ H = [h_1^T, h_2^T, \ldots, h_n^T]^T \). It can be shown that

\[
\text{vec}(XH) = (I \times X) \text{vec} H, \quad \text{vec}(HX) = (X^T \times I) \text{vec} H
\]

where \( \times \) denotes the Kronecker product. By induction, we find that \( \text{vec} H^{(k)} = (X^T \times I - I \times X)^k \text{vec} H \) with the convention that the zeroth power of a square matrix is the identity.

In this notation, it is easy to prove that

\[
e^{-X}He^X = \sum_{n=0}^{\infty} \frac{1}{n!} H^{(n)}.
\]

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**Proof.** \(\text{vec}(e^{-XHe^X}) = \left[ (e^X)^T \times e^{-X} \right] \text{vec} H.\) But \((e^X)^T \times e^{-X} = \exp(X^T \times I - I \times X).\)

(See [4].) Thus,

\[
\text{vec}(e^{-XHe^X}) = \sum_{n=0}^{\infty} \frac{1}{n!} (X^T \times I - I \times X)^n \text{vec} H = \sum_{n=0}^{\infty} \frac{1}{n!} \text{vec} H^{(n)}.
\]

A second identity which will be needed is

\[
(2) \quad X^{r-1}H + X^{r-2}HX + \ldots + HX^{r-1} = \sum_{s=1}^{r} \binom{r}{s} X^{r-s}H^{(s-1)}
\]

The proof of (2) will be found in reference [3].

This latter formula, in fact, is the Frechet differential of the function \(f(X) = X^r.\) For, if \((X + H)^r - X^r\) is expanded, the terms which are linear in \(H\) are precisely the left-hand side of (2). From this point, we may pass to the first representation for a Frechet differential.

**Theorem 1.** Let \(f(z) = \sum_{n=0}^{\infty} a_n(z - c)^n\) be analytic in a disk of centre \(c\) and radius \(R.\) Let \(\rho + \sigma < R,\) where \(\rho\) and \(\sigma\) are respectively the spectral radii of \(X - cI\) and \(X^T \times I - I \times X.\) Then

\[
df(X; H) = \sum_{s=1}^{\infty} \frac{1}{s!} f^{(s)}(X) H^{(s-1)}.
\]

**Proof.** We may safely assume that \(c = 0\) and that a norm has been chosen to make \(||X|| = \rho + \epsilon < R - \sigma.\) Define \(g(x) = \sum_{r=1}^{\infty} |a_r| x^r,\) and take \(H\) so small that this series converges at \(|x| = ||X|| + ||H||.\) Then the series for \(f(X + H)\) converges absolutely, and

\[
f(X + H) - f(X) = \sum_{r=1}^{\infty} a_r[(X + H)^r - X^r] = \sum_{r=1}^{\infty} a_r[X^{r-1}H + X^{r-2}HX + \ldots + HX^{r-1}] + o(||H||).
\]

The remainder on the right, containing terms of order two or higher in \(H,\) is bounded in norm by \(||H||^2 f''(\xi_1).\) The differential is transformed formally, using (2), as follows:

\[
df(X; H) = \sum_{r=1}^{\infty} a_r[X^{r-1}H + X^{r-2}HX + \ldots + HX^{r-1}] = \sum_{r=1}^{\infty} a_r \sum_{s=1}^{r} \binom{r}{s} X^{r-s}H^{(s-1)} = \sum_{r=1}^{\infty} \sum_{s=1}^{r} a_r \binom{r}{s} X^{r-s}H^{(s-1)} = \sum_{s=1}^{\infty} \frac{1}{s!} f^{(s)}(X) H^{(s-1)}.
\]
The rearrangement of the series is justified because, in the starred line, the inner sum is bounded in norm by \((s!)^{-1}g^{(s)}(\rho + \epsilon)\), and
\[
\lim \sup ||H_{(\epsilon - 1)}||^{1/\epsilon} \leq \sigma < R - \rho - \epsilon.
\]
A special case of (3) was discovered and used by Fer [2] in the iterative solution of the matrix equation: \(\dot{U} = H(t)U, \ U(0) = I\). He sets \(U = e^{XV}\), where
\[
X(t) = \int_{0}^{t} H(\tau)d\tau.
\]
Since
\[
(d/dt)f(X) = df(X; (d/dt)X) = df(X, H)
\]
(see [1]), the time derivative of \(e^{X}\) is found to be, using (1),
\[
(d/dt)e^{X} = e^{X} \sum_{s=1}^{\infty} \frac{1}{s!} H_{(s-1)}
\]
\[
= He^{X} - e^{X} \sum_{s=1}^{\infty} \frac{s}{(s + 1)!} H_{(s)}.
\]
Thus the matrix \(V(t)\) satisfies
\[
\dot{V} = \left[ \sum_{s=1}^{\infty} \frac{s}{(s + 1)!} H_{(s)} \right] V, \ V(0) = I
\]
in which the coefficient of \(V\) vanishes with \(t\) at \(t = 0\).

When \(H\) is required to satisfy some restriction relative to \(X\), the hypotheses on the function can be relaxed, as follows.

**Corollary 1** (Roth [12]). Let \(P\) be a nonsingular matrix such that \(P^{-1}XP = (\lambda_{1}I + N_{1}) \oplus \ldots \oplus (\lambda_{m}I + N_{m})\), where \(\lambda_{i} \neq \lambda_{j}\) if \(i \neq j\), and each \(N_{i}\) is nilpotent. If \(H\) is such that \(P^{-1}HP = H_{1} \oplus \ldots \oplus H_{m}\), where \(H_{i}\) is of the same order as \(\lambda_{i}I + N_{i}\), then \(H_{(k)} = 0\) for some \(k\). If \(f\) is analytic at the eigenvalues of \(X\), then
\[
df(X; H) = \sum_{i=1}^{k} \frac{1}{s!} f^{(s)}(X)H_{(s-1)}.
\]

It is easily shown that \(k \leq 2\mu - 1, \mu\) being the greatest of the multiplicities of roots of the minimum equation of \(X\). Thus for a diagonalizable \(X, k = 1\) and the assumption is that \(H\) commutes with \(X\).

A different sort of restriction on \(H\) can also provide a simplified representation for the differential.

**Lemma 1.** Let \(f\) be analytic at the eigenvalues of \(X\), and let \(H = MX - XM\) for some \(M\). Then
\[
df(X; H) = Mf(X) - f(X)M.
\]

**Proof.** Assume first that \(M\) is specified by
\[
vec M = (X^{T} \times I - I \times X)^{+} vec H
\]
where $+$ denotes the Moore-Penrose generalized inverse [5], so that $H$ and $M$ are of the same order as $H$ vanishes. Using the power series expansion for matrix exponentials, we find that
\[
\exp(-M)(X + H)\exp(M) = (I - M + - \ldots)(X + H)(I + M + \ldots) = X + H - MX + XM + o(||H||) = X + o(||H||).
\]

As $f(X)$ has a Frechet derivative [10], it satisfies a Lipschitz condition at $X$ [1, p. 155]. Hence
\[
f(X + H) = \exp(Mf(X + H)\exp(M))\exp(-M) = \exp(Mf(X)\exp(-M) + o(||H||)).
\]

Again employing the power series expansion for the exponential, and isolating the first order terms, yields
\[
f(X + H) - f(X) = f(X) + Mf(X) - f(X)M + o(||H||) = Mf(X) + o(||H||).
\]

Thus the lemma is proved for the special choice of $M$. In general, $M$ may be expressed as $M = M_1 + M_2$, where $M_1$ is as above and $M_2$ commutes with $X$; but then $M_2$ also commutes with $f(X)$. Hence the lemma holds in general.

Roth proves a similar theorem under more restrictive hypotheses and by different means [12]. For stem functions analytic in a sufficiently large region, application of (3) gives an alternate proof.

An immediate application of the Lemma can be made to the approximation of $f(Z)$ if $Z = [z_{ij}]$ has distinct diagonal entries. Set $X = \text{diag}\{z_{11}, \ldots, z_{nn}\}$, so $f(Z) \approx f(X) + df(X; Z - X) = [\phi_{ij}]$. The elements $\phi_{ij}$ are given by $\phi_{ii} = f(z_{ii})$ and, for $i \neq j$,
\[
\phi_{ij} = \frac{f(z_{ii}) - f(z_{jj})}{z_{ii} - z_{jj}}.
\]

This approximation would have been useful in [13] where $Z$ is a Ritz matrix and $f(z) = (z)^{-\frac{1}{2}} \tanh(z^{\frac{1}{2}})$.

We shall now show that the two different restrictions on $H$ mentioned in the Corollary and Lemma 1 are complementary.

**Lemma 2.** For any matrix $H$ of order $n$, there exist matrices $L$ and $M$ satisfying:
\[H = L + MX - XM, \text{ and } L_{(i)} = 0 \text{ for some } k.\]

**Proof.** Let $P^{-1}XP = (\lambda_1I + N_1) \oplus \ldots \oplus (\lambda_mI + N_m)$ as in Corollary 1. Let $P^{-1}HP = [H_{ij}], P^{-1}LP = [L_{ij}], P^{-1}MP = [M_{ij}]$ be partitioned conformally with $P^{-1}XP$. In order that $L_{(i)} = 0$ for some $k$, $L_{ij} = 0$ ($i \neq j$) is necessary and sufficient [12]. The equations to be satisfied are thus:

\[
\begin{align*}
M_{ij}(\lambda_jI + N_j) - (\lambda_iI + N_i)M_{ij} &= H_{ij} \quad (i \neq j), \\
L_{ii} &= H_{ii} - M_{ii}N_i + N_iM_{ii}.
\end{align*}
\]
The submatrices \( M_{i,j} \) are, in fact, arbitrary but we shall take them to be 0. Equation (4) determines \( M_{i,j} \) uniquely, since \( \lambda_i \neq \lambda_j \) for \( i \neq j \) [4]. We also note that \( M \) is of the same order as \( H \) when \( H \) vanishes.

By combining the Lemmas and the Corollary, and using the linearity of the Frechet differential, one easily proves the principal representation below.

**Theorem 2.** Let \( f(z) \) be analytic at the eigenvalues of \( X \). Let \( H = L + MX - XM, \) where \( L_{(k)} = 0 \) for some \( k \). Then

\[
\frac{df(X;H)}{dt} = Mf(X) - f(X)M + \sum_{i=1}^{\infty} \frac{1}{i!} f^{(i)}(X) L_{(i-1)}. 
\]

Several derivatives for functions of matrices have been defined by limit processes [8; 10]. It is also possible to obtain the Frechet differential via a limit.

**Theorem 3.** For sufficiently small \( \epsilon \neq 0 \), let \( S = S(\epsilon) \) be defined by \( SX - XS + \epsilon S = H \), and let \( f(z) \) be analytic at the eigenvalues of \( X \). Then

\[
\frac{df(X;H)}{dt} = \lim_{\epsilon \to 0} \left[ Sf(X) - f(X)S + \epsilon \sum_{i=1}^{3n-1} \frac{1}{i!} f^{(i)}(X) S_{(i-1)} \right].
\]

**Proof.** For \( \epsilon \neq 0 \) and sufficiently small, \( S \) exists and is unique. By substitution one verifies that

\[
S(\epsilon) = M - \sum_{m=1}^{3n-1} (-\epsilon)^{-m} L_{(m-1)} + O(\epsilon)
\]

where \( L \) and \( M \) are as in Lemma 2, and that the quantity in brackets in (6) is \( df(X;H) + O(\epsilon) \). The upper limit in the sums may be reduced if more is known about the matrix \( X \).

The Frechet derivative, that is, the linear function \( H \to \frac{df(X;H)}{dt} \), may be realized as a matrix of order \( n^2 \) if \( H \) and \( df(X;H) \) are replaced by their images under "vec". We replace \( X^T \times X - I \times X \) by \( \Delta \) for brevity.

**Theorem 4.** Under the conditions of Theorem 1, 2, or 3, the Frechet derivative of \( f \) at \( X \) is

\[
\left( \text{Th} \ 1 \right) \quad \sum_{i=1}^{\infty} \frac{1}{i!} [I \times f^{(i)}(X)] \Delta^{i-1},
\]

\[
\left( \text{Th} \ 2 \right) \quad [f(X^T) \times I - I \times f(X)] \Gamma
\]

\[
+ \sum_{i=1}^{k} \frac{1}{i!} [I \times f^{(i)}(X)] \Delta^{i-1} \Pi
\]

where \( \Gamma \) is any matrix having the property that \( \Delta^{k+1} \Gamma = \Delta^k \) for some integer \( k \), and \( \Pi = I - \Delta \Gamma \), or

\[
\left( \text{Th} \ 3 \right) \quad \lim_{\epsilon \to 0} \left\{ \left[ f(X^T) \times I - I \times f(X)
\right.ight.
\]

\[
+ \epsilon \sum_{i=1}^{3n-1} \frac{1}{i!} (I \times f^{(i)}(X)) \Delta^{i-1} \right\} (\Delta + \epsilon I)^{-1}.
\]
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