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ON THE DIFFERENTIALS OF CERTAIN MATRIX FUNCTIONS

DAVID L. POWERS

1. Introduction. In [**5**], Rinehart showed that if X is an $n \times n$ complex matrix with distinct eigenvalues, then a suitably defined diagonalizing matrix P and the diagonal matrix Λ of eigenvalues in $P^{-1}XP = \Lambda$ are both Hausdorff differentiable functions in an open set containing X. Furthermore, if the scalar function $f(z)$ is analytic at the eigenvalues of X, then the primary matrix function $f(X)$ is Hausdorff differentiable, and its differential may be represented in terms of the differentials of P and Λ [**4**]. Rinehart noted that the actual computation of differentials was difficult and *ad hoc*. This difficulty clearly arises because of the definition given for the diagonalizing matrix. Therefore, our aim in this note is to give a different definition of the diagonalizing matrix, one which simplifies the computations.

2. Preliminaries. It will be useful to employ the notation $\mathfrak{D}(M)$ for the matrix made from M by replacing all off-diagonal elements with zeros. For instance, if $M = [m_{ij}]$, then $\mathfrak{D}(M) = \operatorname{diag}\{m_{11}, \ldots, m_{nn}\}$.

Define E_j to be the $n \times n$ matrix which has a 1 in the (j, j) position and zeros elsewhere. $\mathfrak{D}(M) = \sum_{j=1}^{n} E_j M E_j$ is another representation for the operator $\mathfrak{D}$.

We shall also need the commuting reciprocal inverse [**2**] (a generalized inverse) denoted by a superscript c. An $n \times n$ matrix M has a commuting reciprocal inverse if and only if zero is a root of multiplicity 1 or 0 in the minimum equation. In the case of multiplicity 0, $M^c = M^{-1}$. In either case, M^c may be realized as the primary function $g(M)$, where $g(0) = 0$, $g(z) = z^{-1}$, otherwise. The properties of M^c are: $MM^c = M^cM$, $MM^cM = M$, $M^cMM^c = M^c$, and $(P^{-1}MP)^c = P^{-1}M^cP$, for any non-singular P.

3. Definitions and differentials of P, Λ, and $f(X)$. The specification of the diagonalizing matrix P is of primary importance; thus we begin with a lemma concerning such matrices. Let $\mathfrak{G}$ be the set of $n \times n$ matrices $M = [m_{ij}]$ which have disjoint Geršgorin disks. That is, $\Delta_i(M) \cap \Delta_j(M) = \emptyset$ $(i \neq j)$, where

$$\Delta_i(M) = \left\{z \colon |z - m_{ii}| \leqq \sum_{j \neq i} |m_{ij}|\right\}.$$

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It is easily verified that $\mathfrak{G}$ is an open set containing all diagonal matrices with distinct eigenvalues.

LEMMA. *There exists a unique matrix-valued function $Y(M)$ defined for all M in $\mathfrak{G}$ having the following properties:*
(a) *$Y(M)$ is non-singular,*
(b) *$Y(M)$ diagonalizes M,*
(c) *$Y(M)$ is a continuous function of M,*
(d) *$Y(M) = I$ if M is diagonal,*
(e) *$\mathfrak{D}(Y(M)) = I$ for all M.*

Proof. Let M in $\mathfrak{G}$ be given and let μ_j be the eigenvalue of M contained in $\Delta_j(M)$. Consider the equations

$$(1a) \qquad (M - \mu_j I)y_j = 0,$$

$$(1b) \qquad e_j^T y_j = 1,$$

in which y_j is an $n \times 1$ matrix to be found and e_j is the jth column of the identity.

Equation (1a) has a solution which is unique up to a scalar multiplier. If the elements of y_j are y_{ij}, $i = 1, \ldots, n$, then $y_{jj} \neq 0$; for otherwise μ_j would lie in some Geršgorin disk $\Delta_i(M)$ with $i \neq j$, which is impossible. Thus equation (1b) provides a normalizing condition for the eigenvector y_j of M.

If the jth equation of (1a) is replaced by (1b), the resulting $n \times n$ system has a coefficient matrix which is diagonally dominant. Moreover, each entry in this coefficient matrix depends continuously on M, and consequently the same is true for y_j.

We define $Y(M)$ to be the matrix whose jth column is y_j. Properties (c), (d), and (e) follow from the properties of the columns; (a) and (b) are satisfied since the columns of $Y(M)$ are eigenvectors corresponding to the distinct eigenvalues of M. Also, it is clear that $Y(M)$ is uniquely defined.

Now let X_0 be any $n \times n$ complex matrix with distinct eigenvalues, and let P_0 be any non-singular matrix which diagonalizes X_0, namely $P_0^{-1}X_0P_0 = \operatorname{diag}\{\lambda_1^0, \lambda_2^0, \ldots, \lambda_n^0\}$. Then for all matrices X in some neighbourhood of X_0, $P_0^{-1}XP_0$ lies in $\mathfrak{G}$. For such X we define $Q(X) = Y(P_0^{-1}XP_0) - I$ and $P(X) = P_0(I + Q(X))$. As a consequence of the lemma, $P(X)$ is the unique matrix which:
(a) diagonalizes X;
(b) satisfies $P_0^{-1}P(X) = I + Q(X)$ with $\mathfrak{D}(Q(X)) = 0$;
(c) is a continuous function of X and equals P_0 at $X = X_0$.
Also, because of the properties of the diagonalizing matrix, the diagonal matrix of eigenvalues, $\Lambda(X) = P^{-1}(X)XP(X)$, is a uniquely defined and continuous function of X in some neighbourhood of X_0.

The Hausdorff differentials of P and Λ may now be calculated from their defining equation. We use the notation dX for an "increment" in X; dP and $d\Lambda$

represent the Hausdorff (or Fréchet) differentials of P and Λ at the point X, evaluated for increment dX. Also, the argument X of the functions $P(X)$, $Q(X)$, and $\Lambda(X)$ will be suppressed during calculations.

The defining equations for P and Λ are

$$P^{-1}P = I, \qquad P^{-1}XP = \Lambda = \operatorname{diag}\{\lambda_1, \lambda_2, \ldots, \lambda_n\}.$$

On differentiating these, we find first that $d(P^{-1}) = -P^{-1}(dP)P^{-1}$, and second that

$$-P^{-1}(dP)P^{-1}XP + P^{-1}(dX)P + P^{-1}X(dP) = d\Lambda.$$

Now set $P^{-1}(dP) = G$, so that the equation above becomes

$$-G\Lambda + P^{-1}(dX)P + \Lambda G = d\Lambda. \tag{2}$$

Evidently, the matrix $d\Lambda$ must be diagonal, and since $\Lambda G - G\Lambda$ has zeros on its diagonal, we conclude that

$$d\Lambda = \mathfrak{D}(P^{-1}(dX)P). \tag{3}$$

The matrix $G = [g_{ij}]$ may now be determined. Equations (2) and (3) together yield

$$G\Lambda - \Lambda G = P^{-1}(dX)P - d\Lambda = K = [k_{ij}].$$

The off-diagonal elements of G are thus

$$g_{ij} = k_{ij}(\lambda_j - \lambda_i)^{-1} \qquad (i \neq j). \tag{4}$$

The diagonal elements of G are determined from the normalizing condition:

$$(I + Q)G = P_0^{-1}PP^{-1}dP = P_0^{-1}dP = dQ.$$

Since $\mathfrak{D}(dQ) = 0$, we must have $\mathfrak{D}(G) = -\mathfrak{D}(QG)$, which in terms of the elements of G means that

$$g_{ii} = -\sum_{j \neq i} q_{ij}g_{ji}. \tag{5}$$

(It should be mentioned that the formulas for G were inspired by the so-called method of Collar and Jahn, a technique for improving approximate eigenvectors [**1**].)

It is now a simple matter to establish expressions for dP and $d\Lambda$ which display their character as Hausdorff differentials. (The representations are not unique.) First, equation (3) may be rewritten immediately as

$$d\Lambda = \sum E_j P^{-1}(dX)PE_j. \tag{6}$$

Equations (4) and (5) may be rewritten as

$$G - \mathfrak{D}(G) = \sum (\lambda_j I - \Lambda)^c K E_j,$$

$$\mathfrak{D}(G) = -\sum E_j QGE_j = -\sum E_j Q(G - \mathfrak{D}(G))E_j = -\sum E_j Q(\lambda_j I - \Lambda)^c K E_j,$$

and these two combined yield

$$G = \sum (I - E_jQ)(\lambda_j I - \Lambda)^c K E_j. \tag{7}$$

Finally, an expression for dP is

$$\begin{aligned} dP &= \sum P(I - E_jQ)(\lambda_j I - \Lambda)^c P^{-1}(dX)PE_j \\ &= \sum P(I - E_jQ)P^{-1}(\lambda_j I - X)^c(dX)PE_j. \end{aligned} \tag{8}$$

THEOREM. *If X is sufficiently close to the matrix X_0 and if $P(X)$, $\Lambda(X)$, and $Q(X)$ are defined as above, then the Hausdorff or Fréchet differentials of P and Λ are given by* (6) *and* (8).

With the above definitions for P and Λ and the relations for their differentials, it is now easier to compute the differential of a primary matrix function $f(X)$. We restate a theorem given by Rinehart [**4**].

THEOREM (Rinehart [**4**]). *If the scalar function $f(z)$ is analytic at the eigenvalues of X_0, then for all X sufficiently close to X_0 the primary matrix function $f(X)$ is differentiable and its Hausdorff or Fréchet differential is given by*

$$df = P(X)[Gf(\Lambda) + f'(\Lambda)d\Lambda - f(\Lambda)G]P^{-1}(X), \tag{9}$$

where $f'(\Lambda)$ is the primary function $f'(z)$ evaluated at the diagonal matrix $\Lambda = \Lambda(X)$.

It should be noted that since $f(\Lambda)$ is diagonal, the expression $Gf(\Lambda) - f(\Lambda)G$ has zeros on the diagonal, and G may be replaced by $G - \mathfrak{D}(G)$.

4. Fréchet derivatives. The computations of formulas become simpler and the formulas themselves more interesting when calculations are carried out in terms of tensor products. For $n \times n$ matrices A, B, and X, let $A \times B$ be the partitioned matrix $[a_{ij}B]$, and let X_v be the $n^2 \times 1$ column

$$[x_{11}, \ldots, x_{n1}, x_{12}, \ldots, x_{n2}, \ldots, x_{1n}, \ldots, x_{nn}]^{\mathrm{T}}.$$

The following rules hold [**3**]:

$$\begin{aligned} (AXB)_v &= (B^{\mathrm{T}} \times A)X_v, \\ (\mathfrak{D}(X))_v &= DX_v, \qquad \text{where } D = E_1 \oplus \ldots \oplus E_n. \end{aligned}$$

In this notation, equations (2) and (3) become

$$(\Lambda \times I - I \times \Lambda)G_v = (P^{-1}(dX)P - d\Lambda)_v, \tag{2'}$$

$$(d\Lambda)_v = D(P^{-1}(dX)P)_v. \tag{3'}$$

Since $D(\Lambda \times I - I \times \Lambda) = (\Lambda \times I - I \times \Lambda)D = \mathbf{0}$, we have

$$(\Lambda \times I - I \times \Lambda)(I - D)G_v = (I - D)(P^{-1}(dX)P)_v.$$

Also, by the definition of the commuting reciprocal inverse,

$$(\Lambda \times I - I \times \Lambda)^c D = \mathbf{0}$$

(in fact, D is the projector of $\Lambda \times I - I \times \Lambda$ associated with its zero eigenvalues); therefore the solution of the equation above is

$$(4') \qquad (I - D)G_v = (\Lambda \times I - I \times \Lambda)^c (P^{-1}(dX)P)_v.$$

The normalizing condition for the diagonal elements of G was $\mathfrak{D}(G) = -\mathfrak{D}(QG) = -\mathfrak{D}(QG - Q\mathfrak{D}(G))$ or in tensor form:

$$DG_v = -D(I \times Q)(I - D)G_v.$$

This equation combined with (4′) yields

$$(10) \qquad G_v = [I - D(I \times Q)][\Lambda \times I - I \times \Lambda]^c (P^{-1}(dX)P)_v.$$

To further simplify these equations, we introduce $\Pi = P^{\mathrm{T}} \times P^{-1}$; then (6) and (8) become:

$$(6') \qquad (d\Lambda)_v = D\Pi(dX)_v,$$

$$\begin{aligned}(8') \qquad (dP)_v &= (I \times P)[I - D(I \times Q)][\Lambda \times I - I \times \Lambda]^c \Pi(dX)_v \\ &= (I \times P)[I - D(I \times Q)]\Pi[X^{\mathrm{T}} \times I - I \times X]^c (dX)_v.\end{aligned}$$

The differential of f takes a most interesting form. We use the fact that the diagonal of G plays no role in (9), so that

$$\begin{aligned}(df(X))_v &= \Pi^{-1}[Gf(\Lambda) - f(\Lambda)G + f'(\Lambda)d\Lambda]_v \\ &= \Pi^{-1}[f(\Lambda) \times I - I \times f(\Lambda)][\Lambda \times I - I \times \Lambda]^c \Pi(dX)_v \\ &\qquad + \Pi^{-1}[I \times f'(\Lambda)]D\Pi(dX)_v \\ &= \{[f^{\mathrm{T}}(X) \times I - I \times f(X)][X^{\mathrm{T}} \times I - I \times X]^c \\ &\qquad + [I \times f'(X)]\Pi^{-1}D\Pi\}(dX)_v.\end{aligned}$$

The first term in brackets may be interpreted as a generalized difference quotient operating in a subspace; for, the factor $I - \Pi^{-1}D\Pi$ may be inserted before the plus sign without changing the result, and $\Pi^{-1}D\Pi$ is the projector onto the null space of $X^{\mathrm{T}} \times I - I \times X$.

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Clarkson College of Technology,
Potsdam, New York