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A NOTE ON THE SCALAR HAFFIAN

HEINZ NEUDECKER
Cesaro, Schagen
Department of Economics
University of Amsterdam*

In this note a uniform transparent presentation of the scalar Haffian wil be given. Some well-known results will be generalized.
A link will be established between the scalar Haffian and the derivative matrix as developed by Magnus and Neudecker.

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*Roetersstraat 11, 1018 WB Amsterdam, The Netherlands, e-mail: heinz@fee.uva.nl

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1. INTRODUCTION

Haff (1977, 1979a, 1979b, 1980) introduced a scalar function based on the derivatives of the elements of a **square** matrix function $F(X)$ with respect to the elements of a **symmetric** argument matrix X. We shall name it the scalar Haffian. It was used by Haff in various applications in multivariate statistical analysis. Several authors, among others Konno (1988, 1991), Leung (1994) and Leung & Ng (1998) made use of it later. The exposition and notation vary over authors and time, the derivations tend to be obscure and sometimes unnecessarily complicated.

In this note we shall attempt to give a uniform transparent presentation of the scalar Haffian, and generalize some of the well-known results.

Basic is a differentiable **square** matrix function $F(X)$, shortly F, which depends on a **symmetric** matrix X. Both matrices are of the same dimension. A strategic rôle is being played by a square matrix $\nabla = (d_{ij})$ of differential operators $d_{ij} := \frac{1}{2}(1+\delta_{ij})\frac{\partial}{\partial x_{ij}}$, where δ_{ij} is the Kronecker delta ($\delta_{ii} = 1, \delta_{ij} = 0$ for $i \neq j$).

In the work mentioned earlier the symbol D is used instead of ∇. We prefer ∇, because D will denote the so-called duplication matrix which will be extensively used. The matrix ∇ is being applied to F and ultimately produces the scalar Haffian $\mathrm{tr}\nabla F$, where «tr» stands for the trace operator. Haff uses $D^*F_{(1/2)}$ to denote this function, with $F_{(1/2)} := 1/2(F - F_d)$, F_d being the diagonal matrix obtained from the diagonal of F. The scalar Haffian $\mathrm{tr}\nabla F$ will be studied in this note. It will be related to the derivative matrix $\frac{\partial f}{\partial x'}$ as developed by Magnus and Neudecker (1999).

In the exposition frequent use will be made of matrix vectorization, Kronecker products, the duplication matrix D and the commutation matrix K. For these concepts and some of their properties see Magnus and Neudecker (1979, 1980, 1999).

2. THE SCALAR HAFFIAN

Consider a differentiable **square** matrix function $F(X)$ with **symmetric** matrix argument X, both of dimension m. The application of $\nabla = (d_{ij})$, a (square) matrix of differential operators $d_{ij} := 1/2(1+\delta_{ij})\frac{\partial}{\partial x_{ij}}$ to F yields ∇F from which follows $\mathrm{tr}\nabla F$, the scalar Haffian.

Clearly

$$\begin{aligned}
\mathrm{tr}\nabla F &= \sum_{ij} d_{ij} f_{ji} = \sum_i d_{ii} f_{ii} + \sum_{j\neq i} d_{ij} f_{ji} \\
&= \sum_i \frac{\partial f_{ii}}{\partial x_{ii}} + \frac{1}{2}\sum_{j\neq i} \frac{\partial f_{ji}}{\partial x_{ij}} = \sum_i \frac{\partial f_{ii}}{\partial x_{ii}} + \frac{1}{2}\sum_{j<i} \frac{\partial (f_{ij} + f_{ji})}{\partial x_{ij}}
\end{aligned}$$

$$= \quad \sum_i \frac{\partial g_{ii}}{\partial x_{ii}} + \sum_{j<i} \frac{\partial g_{ij}}{\partial x_{ij}} = \mathrm{tr}\,\frac{\partial g}{\partial x'} \quad \text{where}$$

$$g_{ii} := f_{ii}, \quad g_{ij} := 1/2(f_{ij} + f_{ji})$$

$$g := (g_{11} \cdots g_{m1} g_{22} \cdots g_{m2} \cdots g_{mm})' \qquad (j < i)$$

$$x := (x_{11} \cdots x_{m1} x_{22} \cdots x_{m2} \cdots x_{mm})'.$$

The expression $\frac{\partial g}{\partial x'}$ is the Magnus-Neudecker derivative for the vector function $g(x)$, with $x := v(X)$, $g := v(G)$ and $G := 1/2(F + F')$.

We have thus established the identity

(1) $$\mathrm{tr}\nabla F = \mathrm{tr}\frac{\partial g}{\partial x'}$$

for the scalar Haffian $\mathrm{tr}\nabla F$ and the Magnus-Neudecker derivative matrix $\frac{\partial g}{\partial x'}$.

Mind that $\nabla F \neq \frac{\partial g}{\partial x'}$! In fact ∇F is another useful concept also developed and applied by Haff.

See Haff (1981, 1982). Obviously the scalar Haffian can then also be obtained from ∇F. We shall name ∇F the matrix Haffian. It will be examined in another paper.

An attractive alternative expression for the scalar Haffian is $\mathrm{tr}\,\frac{\partial v(F+F')}{\partial v'(X)}$ which shows immediately that

(2) $$\mathrm{tr}\nabla F' = \mathrm{tr}\nabla F.$$

When F is **symmetric**

(3) $$\mathrm{tr}\nabla F = \mathrm{tr}\,\frac{\partial f}{\partial x'}$$

where $f := (f_{11} \cdots f_{m1} f_{22} \cdots f_{m2} \cdots f_{mm})' = v(F)$.

Proof

In the creation of (1) we now have $f_{ij} = f_{ji}$, , hence $g = f$.

□

3. A GENERAL RESULT

Instead of deriving umpteen specific scalar Haffians we shall establish a general result from which other specific results can be derived.

Theorem

For symmetric X and square constant matrices P and Q

$$\mathrm{tr}\,\nabla PXQ' = 1/2(\mathrm{tr}\,P)\,\mathrm{tr}\,Q + 1/2\,\mathrm{tr}\,PQ.$$

Proof

Take $F := PXQ'$. Again $G := 1/2(F+F')$. Then

$$\mathrm{dvec}\,G = 1/2(\mathrm{dvec}\,F + \mathrm{dvec}\,F') = 1/2(I_{m^2} + K_{mm})\mathrm{dvec}\,F,$$

and

$$\begin{aligned} \mathrm{dg} &= 1/2D_m^+(I_{m^2} + K_{mm})\mathrm{dvec}\,F = D_m^+\,\mathrm{dvec}\,F \\ &= D_m^+\,\mathrm{vec}\,P(dX)Q' = D_m^+(Q\otimes P)\mathrm{dvec}\,X \\ &= D_m^+(Q\otimes P)D_m\,dx. \end{aligned}$$

Hence

$$\frac{\partial g}{\partial x'} = D_m^+(Q\otimes P)D_m.$$

Therefrom

$$\begin{aligned} \mathrm{tr}\,\nabla F &= \mathrm{tr}\,D_m^+(Q\otimes P)D_m = \mathrm{tr}\,D_m D_m^+(Q\otimes P) \\ &= 1/2\mathrm{tr}(I_{m^2} + K_{mm})(Q\otimes P) = 1/2\mathrm{tr}(Q\otimes P) + 1/2\mathrm{tr}\,K_{mm}(Q\otimes P) \\ &= 1/2(\mathrm{tr}\,P)\mathrm{tr}\,Q + 1/2\mathrm{tr}\,QP = 1/2(\mathrm{tr}\,P)\mathrm{tr}\,Q + 1/2\mathrm{tr}\,PQ. \end{aligned}$$

We used various results from Magnus and Neudecker (1999, pp. 30, 47 and 49) and Magnus and Neudecker (1979, Theorem 3.1, xiv).

□

Corollary

For any function $F = F(X)$ such that $dF = P(dX)Q'$, the scalar Haffian is

$$\mathrm{tr}\,\nabla F = 1/2(\mathrm{tr}\,P)\mathrm{tr}\,Q + 1/2\mathrm{tr}\,PQ.$$

With the help of this corollary we can now derive scalar Haffians in practice.

4. VARIOUS SCALAR HAFFIANS

$(i)\quad \mathrm{tr}\,\nabla PX^{-1}Q' = -1/2(\mathrm{tr}\,PX^{-1})\mathrm{tr}\,QX^{-1} - 1/2\mathrm{tr}\,PX^{-1}QX^{-1}.$

Proof

Now $F := PX^{-1}Q'$ and $dF = P(dX^{-1})Q' = -PX^{-1}(dX)X^{-1}Q'$.

Replacing then P by $-PX^{-1}$ and Q' by $X^{-1}Q'$ in the Corollary, one immediately obtains

$$\mathrm{tr}\,\nabla PX^{-1}Q' = -1/2(\mathrm{tr}\,PX^{-1})\mathrm{tr}\,QX^{-1} - 1/2\mathrm{tr}\,PX^{-1}QX^{-1}.$$

□

$(ii)\quad \mathrm{tr}\,\nabla PXQXR' = 1/2(\mathrm{tr}\,P)\mathrm{tr}\,RXQ' + 1/2\mathrm{tr}\,PRXQ' + 1/2\mathrm{tr}\,PXQR + 1/2(\mathrm{tr}\,R)\mathrm{tr}\,PXQ.$

Proof

As $F := PXQXR'$ and $dF = P(dX)QXR' + PXQ(dX)R'$ we have to make the following substitutions:

$$\begin{cases} P & \longrightarrow & P \\ Q' & \longrightarrow & QXR' \end{cases} \quad \text{and} \quad \begin{cases} P & \longrightarrow & PXQ \\ Q' & \longrightarrow & R' \end{cases}$$

This then leads to the scalar Haffian

$$\mathrm{tr}\,\nabla PXQR' = 1/2(\mathrm{tr}\,P)\mathrm{tr}\,RXQ' + 1/2\mathrm{tr}\,PRXQ' + 1/2(\mathrm{tr}\,R)\mathrm{tr}\,PXQ + 1/2\mathrm{tr}\,PXQR.$$

□

$$\begin{aligned}(iii)\quad \mathrm{tr}\,\nabla PX^{-2}Q' &= = -1/2(\mathrm{tr}\,PX^{-1})\,\mathrm{tr}\,QX^{-2} - 1/2(\mathrm{tr}\,PX^{-2})\,\mathrm{tr}\,QX^{-1} \\ &- \quad 1/2\,\mathrm{tr}\,PX^{-1}QX^{-2} - 1/2\,\mathrm{tr}\,PX^{-2}QX^{-1}.\end{aligned}$$

Proof

In this case $F := PX^{-2}Q'$ and

$$\begin{aligned} dF &= P(dX^{-2})Q' = P(dX^{-1})X^{-1}Q' + PX^{-1}(dX^{-1})Q' \\ &= -PX^{-1}(dX)X^{-2}Q' - PX^{-2}(dX)X^{-1}Q'. \end{aligned}$$

We shall make the following substitutions

$$\begin{cases} P & \longrightarrow & -PX^{-1} \\ Q' & \longrightarrow & X^{-2}Q' \end{cases} \quad \text{and} \quad \begin{cases} P & \longrightarrow & -PX^{-2} \\ Q' & \longrightarrow & X^{-1}Q' \end{cases}$$

and get the above given result. □

$$
\begin{aligned}
(iv) \qquad \mathrm{tr}\nabla PX^3Q' \;&=\; 1/2(\mathrm{tr}\,P)\mathrm{tr}\,QX^2 + 1/2\,\mathrm{tr}\,PQX^2 + 1/2(\mathrm{tr}\,PX)\mathrm{tr}\,QX \\
&+\; 1/2\,\mathrm{tr}\,PXQX + 1/2\,\mathrm{tr}\,PX^2Q + 1/2(\mathrm{tr}\,Q)\mathrm{tr}\,PX^2.
\end{aligned}
$$

Proof

Now $F := PX^3Q'$, hence

$$dF = P(dX)X^2Q' + PX(dX)XQ' + PX^2(dX)Q',$$

which leads to the substitutions

$$\begin{cases} P & \longrightarrow & P \\ Q' & \longrightarrow & X^2Q' \end{cases}, \begin{cases} P & \longrightarrow & PX \\ Q' & \longrightarrow & XQ' \end{cases} \quad \text{and} \quad \begin{cases} P & \longrightarrow & PX^2 \\ Q' & \longrightarrow & Q' \end{cases}$$

Hence the scalar Haffian obtains.

□

NOTES

1. Haff (1979a, 1980), Konno (1988) and Leung (1994) considered $\mathrm{tr}\,\nabla XQ'$ and $\mathrm{tr}\,\nabla PX$, with occasionally positive definite Q and X.

2. Clearly the Theorem also holds for symmetric P, Q and PXQ'.

3. $\mathrm{tr}\,\nabla X^{-1}Q'$ was derived by Haff (1979a), $\mathrm{tr}\,\nabla X^{-1}$ was given by Haff (1980) for positive definite X.

4. $\mathrm{tr}\,\nabla X^2Q'$ was derived by Haff (1979a), the identical $\mathrm{tr}\,\nabla QX^2$ was found by Konno (1991). In fact these are special cases of (*ii*).

5. Konno (1988) gave $\mathrm{tr}\,\nabla XQX$, with positive definite X. Leung (1994) and Leung & Ng (1998) considered $\mathrm{tr}\,\nabla XQX$ with symmetric, even positive definite Q.

6. Haff (1980) presented $\mathrm{tr}\,\nabla X^{-2}$ for positive definite X.

7. Konno (1991), gave $\mathrm{tr}\,\nabla X^3$ for positive definite X.

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