The Moore-Penrose inverse of a vector: Coping with a sometimes tricky case differentiation

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1 Introduction

For any matrix $\boldsymbol{A} \in \mathbb{R}^{m \times n}$ a unique matrix $\boldsymbol{A}^{+} \in \mathbb{R}^{n \times m}$ exists, which satisfies the following four conditions

$$\boldsymbol{A}\boldsymbol{A}^{+}\boldsymbol{A} = \boldsymbol{A} \tag{1}$$

$$\boldsymbol{A}^{+}\boldsymbol{A}\boldsymbol{A}^{+} = \boldsymbol{A}^{+} \tag{2}$$

$$\left(\boldsymbol{A}^{+}\boldsymbol{A}\right)' = \boldsymbol{A}^{+}\boldsymbol{A} \tag{3}$$

$$\left(\boldsymbol{A}\boldsymbol{A}^{+}\right)' = \boldsymbol{A}\boldsymbol{A}^{+} \tag{4}$$

Note that $\boldsymbol{A}^{+}$ has the same dimension as $\boldsymbol{A}'$, the transpose of $\boldsymbol{A}$.

If $\boldsymbol{A}$ is square and nonsingular, its inverse $\boldsymbol{A}^{-1}$ exists. Obviously, in this case the above conditions (1) to (4) are satisfied when $\boldsymbol{A}^{-1}$ is substituted for $\boldsymbol{A}^{+}$. Hence, if $\boldsymbol{A}$ is a nonsingular matrix, we have $\boldsymbol{A}^{+} = \boldsymbol{A}^{-1}$.

2 Computation of the Moore-Penrose inverse of a vector

The Moore-Penrose inverse of a (column) vector $\boldsymbol{a} \in \mathbb{R}^n$ is given by

$$\boldsymbol{a}^+ = \begin{cases} \frac{1}{\boldsymbol{a}'\boldsymbol{a}}\boldsymbol{a}' & \text{if } \boldsymbol{a} \neq \boldsymbol{o} \\ \boldsymbol{o}' & \text{if } \boldsymbol{a} = \boldsymbol{o} \end{cases} \tag{5}$$

where $\boldsymbol{o}$ denotes the (n by 1) zero vector. Apparently, $\boldsymbol{a}^+$ is a row vector.

Since a vector is nothing else but a matrix with only one column, it should be declared in *Derive* as such. The following `MPIV` function has no problem computing the Moore-Penrose inverse of any vector which contains numbers only,

```
       MPIV(a) :=
         If DIM(a') = 1
            If (a'·a)↓1↓1 = 0
#1:            0·a'
               a'/(a'·a)↓1↓1
            "This is not a column vector!"
```

but might not be able to compute the Moore-Penrose inverse of a vector which has non-numeric elements. To illustrate this, we define the following set of vectors in *Derive*

$$\boldsymbol{a} = \begin{pmatrix} 0 \\ 2 \end{pmatrix}; \quad \boldsymbol{b} = \begin{pmatrix} x \\ 2 \end{pmatrix}; \quad \boldsymbol{c} = \begin{pmatrix} 0 \\ x \end{pmatrix}; \quad \boldsymbol{o} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

```
#2:   a := [0; 2]

#3:   b := [x; 2]

#4:   c := [0; x]

#5:   o := [0; 0]
```

Since $\boldsymbol{a}'\boldsymbol{a} = 4 \neq 0$, the Moore-Penrose inverse of $\boldsymbol{a}$ is

$$\boldsymbol{a}^+ = \tfrac{1}{\boldsymbol{a}'\boldsymbol{a}}\boldsymbol{a}' = \tfrac{1}{4}\begin{pmatrix}0 & 2\end{pmatrix} = \begin{pmatrix}0 & \tfrac{1}{2}\end{pmatrix}$$

As $\boldsymbol{b}'\boldsymbol{b} = x^2 + 4$, $\boldsymbol{b}'\boldsymbol{b} > 0$ for any $x \in \mathbb{R}$, such that

$$\boldsymbol{b}^+ = \tfrac{1}{\boldsymbol{b}'\boldsymbol{b}}\boldsymbol{b}' = \tfrac{1}{x^2+4}\begin{pmatrix}x & 2\end{pmatrix} = \begin{pmatrix}\tfrac{x}{x^2+4} & \tfrac{2}{x^2+4}\end{pmatrix}$$

As $\boldsymbol{c}'\boldsymbol{c} = x^2$, we have $\boldsymbol{c}'\boldsymbol{c} = 0$ for $x = 0$, and $\boldsymbol{c}'\boldsymbol{c} > 0$ otherwise. Therefore

$$\boldsymbol{c}^+ = \begin{cases} \tfrac{1}{\boldsymbol{c}'\boldsymbol{c}}\boldsymbol{c}' = \tfrac{1}{x^2}\begin{pmatrix}0 & x\end{pmatrix} = \begin{pmatrix}0 & \tfrac{1}{x}\end{pmatrix} & \text{if } x \neq 0 \\ \boldsymbol{o}' & \text{if } x = 0 \end{cases}$$

Since $\boldsymbol{o}'\boldsymbol{o} = 0$, the Moore-Penrose inverse of $\boldsymbol{o}$ is

$$\boldsymbol{o}^+ = \boldsymbol{o}'$$

Let us now see how the `MPIV` function copes with these vectors:

#6: $\text{MPIV(a)} = \left[\left[0, \dfrac{1}{2}\right]\right]$

#7: $\text{MPIV(b)} = \left[\left[\dfrac{x}{x^2+4}, \dfrac{2}{x^2+4}\right]\right]$

#8: $\text{MPIV(c)} = \text{IF}\left(x = 0,\ 0\cdot\begin{bmatrix}0\\x\end{bmatrix}',\ \begin{bmatrix}0\\x\end{bmatrix}'\cdot\left(\begin{bmatrix}0\\x\end{bmatrix}'\cdot\begin{bmatrix}0\\x\end{bmatrix}\right)^{-1}_{1,1}\right)$

#9: $\text{MPIV(o)} = [[0, 0]]$

The `MPIV` function finds $\boldsymbol{a}^+$, $\boldsymbol{b}^+$ and $\boldsymbol{o}^+$, but fails to compute the Moore-Penrose inverse of $\boldsymbol{c}$.

3 Computation of the Moore-Penrose inverse of a matrix

For the computation of the Moore-Penrose inverse of a matrix we apply Greville's method, which is an iterative algorithm that needs *n* steps for the computation of the Moore-Penrose inverse of an *m* by *n* matrix. The `MPI` function given below

```
       MPI(A, APLUS, aj, dt, c, bt, J) :=
         Prog
           APLUS := MPIV(A COL [1])
           J := 2
           Loop
             If J > DIM(A')
#2:             RETURN APLUS
             aj := A COL [J]
             dt := aj'·APLUS'·APLUS
             c := (IDENTITY_MATRIX(DIM(A)) - A COL [1, ..., J - 1]·APLUS)·aj
             bt := MPIV(c) + (1 - MPIV(c)·c)/(1 + dt·aj)·dt
             APLUS := APPEND(APLUS - APLUS·aj·bt, bt)
             J :+ 1
```

calls the `MPIV` function in each step. Hence, the `MPI` function might be unable to compute the Moore-Penrose inverse of a matrix if it has at least one non-numeric element. To illustrate this, we define the following four matrices in *Derive*

$$\boldsymbol{A}=\begin{pmatrix}1&0\\2&0\end{pmatrix};\quad \boldsymbol{B}=\begin{pmatrix}x&0\\2&0\end{pmatrix};\quad \boldsymbol{C}=\begin{pmatrix}1&0\\2&x\end{pmatrix};\quad \boldsymbol{D}=\begin{pmatrix}x&0\\0&0\end{pmatrix}$$

```
#3:    A := [ 1  0 ]
            [ 2  0 ]

#4:    B := [ x  0 ]
            [ 2  0 ]

#5:    C := [ 1  0 ]
            [ 2  x ]

#6:    D := [ x  0 ]
            [ 0  0 ]
```

The `MPI` function finds $\boldsymbol{A}^{+}$ and $\boldsymbol{B}^{+}$, but fails to compute the Moore-Penrose inverse of $\boldsymbol{C}$ and $\boldsymbol{D}$.

#7: $$\mathrm{MPI(A)} = \begin{bmatrix} \frac{1}{5} & \frac{2}{5} \\ 0 & 0 \end{bmatrix}$$

#8: $$\mathrm{MPI(B)} = \begin{bmatrix} \frac{x}{x^2+4} & \frac{2}{x^2+4} \\ 0 & 0 \end{bmatrix}$$

#9: $$\mathrm{MPI(C)} = \mathrm{APPEND}\left(\left[\left[-\frac{2\cdot x}{5}\right]\right]\cdot\left(\left(\mathrm{IF}\left(x = 0,\ 0\cdot\begin{bmatrix} -\frac{2\cdot x}{5} \\ \frac{x}{5} \end{bmatrix}',\ \begin{bmatrix} -\frac{2\cdot x}{5} \\ \frac{x}{5} \end{bmatrix}'\cdot\left(\left[\right.\right.\right.\right.\right.\right.$$

Note that

$$\boldsymbol{C}^{+} = \begin{cases} \begin{pmatrix} 1 & 0 \\ -\frac{2}{x} & \frac{1}{x} \end{pmatrix} & \text{if } x \neq 0 \\ \begin{pmatrix} \frac{1}{5} & \frac{2}{5} \\ 0 & 0 \end{pmatrix} & \text{if } x = 0 \end{cases} \qquad \text{and} \qquad \boldsymbol{D}^{+} = \begin{cases} \begin{pmatrix} \frac{1}{x} & 0 \\ 0 & 0 \end{pmatrix} & \text{if } x \neq 0 \\ \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix} & \text{if } x = 0 \end{cases}$$

4 A way out

Let us consider the rank of the four vectors from section 2:

$$\mathrm{r}(\boldsymbol{a})=1,\quad \mathrm{r}(\boldsymbol{b})=1 \text{ for any } x\in\mathbb{R},\quad \mathrm{r}(\boldsymbol{c})=\begin{cases}1 & \text{if } x\neq 0\\ 0 & \text{if } x=0\end{cases},\quad \mathrm{r}(\boldsymbol{o})=0$$

Obviously, the rank of $\boldsymbol{c}$ depends on x. But in *Derive*

```
#10:    RANK(a) = 1
#11:    RANK(b) = 1
#12:    RANK(c) = 1
#13:    RANK(o) = 0
```

we get $\mathrm{r}(\boldsymbol{c})=1$, i.e. *Derive* does not make a case differentiation. Apparently, the single x value, which turns $\boldsymbol{c}$ into a zero vector, is neglected.

```
        MPIV0(a) :=
          If DIM(a') = 1
#1:          a'/(a'·a)↓1↓1
             "This is not a column vector!"
```

Let us now see how the `MPIV0` function copes with the four vectors:

$$\text{\#14:}\quad \mathrm{MPIV0}(a) = \left[\left[0,\ \frac{1}{2}\right]\right]$$

$$\text{\#15:}\quad \mathrm{MPIV0}(b) = \left[\left[\frac{x}{x^2+4},\ \frac{2}{x^2+4}\right]\right]$$

$$\text{\#16:}\quad \mathrm{MPIV0}(c) = \left[\left[0,\ \frac{1}{x}\right]\right]$$

$$\text{\#17:}\quad \mathrm{MPIV0}(o) = [[?,\ ?]]$$

The `MPIV0` function computes the Moore-Penrose inverse of $\boldsymbol{c}$ for $x\neq 0$. The special case $x=0$ is ignored. However, it is unable to compute the Moore-Penrose inverse of $\boldsymbol{o}$.

Let us now consider the rank of the four matrices from section 3:

$$\mathrm{r}(\boldsymbol{A})=1, \quad \mathrm{r}(\boldsymbol{B})=1 \text{ for any } x\in\mathbb{R}, \quad \mathrm{r}(\boldsymbol{C})=\begin{cases}2 & \text{if } x\neq 0\\ 1 & \text{if } x=0\end{cases}, \quad \mathrm{r}(\boldsymbol{D})=\begin{cases}1 & \text{if } x\neq 0\\ 0 & \text{if } x=0\end{cases}$$

Obviously, the value of x is crucial as to whether the second column of ***C***, and the first column of ***D***, are zero vectors or not. But in *Derive*

```
#11:                 RANK(A) = 1
#12:                 RANK(B) = 1
#13:                 RANK(C) = 2
#14:                 RANK(D) = 1
```

we get $\mathrm{r}(\boldsymbol{C})=2$, i.e. *Derive* again does not make a case differentiation. Apparently, the single x value, which turns the second column of ***C***, and the first column of ***D***, into zero vectors, is neglected.

The `MPIO` function is identical to the `MPI` function in section 3, except that it calls the `MPIVO` function instead of the `MPIV` function in lines 3 and 11. Let us now see how the `MPIO` function copes with the four matrices:

```
#15:        MPIO(A) = [ ?  ? ]
                      [ ?  ? ]

#16:        MPIO(B) = [ ?  ? ]
                      [ ?  ? ]

#17:        MPIO(C) = [  1    0 ]
                      [  2    1 ]
                      [- ─    ─ ]
                      [  x    x ]

#18:        MPIO(D) = [ ?  ? ]
                      [ ?  ? ]
```

The `MPIO` function computes the Moore-Penrose inverse of ***C*** for $x \neq 0$. The special case $x = 0$ is ignored. However, it is unable to compute the Moore-Penrose inverses of ***A***, ***B***, and ***D***.

Note that ***C*** is a nonsingular matrix for $x \neq 0$ such that $\boldsymbol{C}^{+} = \boldsymbol{C}^{-1}$. Computing the inverse of ***C*** in *Derive* generates the same matrix as the `MPIO` function, i.e. *Derive* is consistent in terms of disregarding the special case $x = 0$.

```
              -1     [  1    0 ]
#19:        C    =   [  2    1 ]
                     [- ─    ─ ]
                     [  x    x ]
```