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MINIMUM-R_Z MOVING-WEIGHTED-AVERAGE FORMULAS

ELIAS S. W. SHIU

ABSTRACT

The coefficients of the minimum-R_z moving-weighted-average formulas are derived using matrix algebra and the method of Lagrange multipliers.

I. INTRODUCTION

Thirty-seven years ago Dr. T. N. E. Greville ([7], [8]) determined the coefficients of the symmetric and asymmetric minimum-R_z moving-weighted-average formulas by manipulating certain orthogonal polynomials. In this paper, we shall derive these coefficients using matrix algebra. An advantage of our matrix formula is that the coefficients can be easily obtained with *APL*.

II. FORMULATION

Consider the class of graduation formulas of the form

$$u_x = \sum_{s=-m}^{n} a_s \cdot u''_{x+s}.$$

Then

$$\begin{aligned}\Delta^z u_x &= \sum_{s=-m}^{n} a_s \cdot \Delta^z u''_{x+s} \\ &= \underline{a}^T K \underline{u}''_x,\end{aligned}$$

where

$$\begin{aligned}\underline{a} &= (a_{-m}, \ldots, a_o, \ldots, a_n)^T, \\ \underline{u}''_x &= (u''_{x-m}, \ldots, u''_x, \ldots, u''_{x+n+z})^T\end{aligned}$$

and K is the $(m + 1 + n)$ row by $(m + 1 + n + z)$ column differencing matrix of order z ([9], p. 51; [11], p. 43). For column vectors $\underline{x}$ and $\underline{y}$, let the inner product $\underline{x}^T\underline{y}$ be denoted by $<\underline{x}, \underline{y}>$. Thus,

$$\begin{aligned}\Delta^z u_x &= <\underline{a}, K\underline{u}''_x> \\ &= <K^T\underline{a}, \underline{u}''_x>.\end{aligned}$$

The progression of the graduated values $\{u_x\}$ is considered to be smooth if their zth differences are numerically small ([9], p. 9). By the Cauchy-Schwarz inequality,

$$|\Delta^z u_x| \leq \|K^T \underline{a}\| \cdot \|\underline{u}_x''\|,$$

where $\| \ \|$ denotes the Euclidean norm. Hence, in general, if we minimize $\|K^T \underline{a}\|$, we minimize $|\Delta^z u_x|$.

A moving-weighted-average formula is usually required to reproduce polynomials up to, say, degree d. Let $\underline{\iota}$ denote the column vector $(\underbrace{0, \ldots, 0}_{m}, 1, \underbrace{0, \ldots, 0}_{n})^T$ and for a polynomial p, let $\underline{p}$ denote $(p(-m), \ldots, p(0), \ldots, p(n))^T$; it is thus required that

$$<\underline{a}, \underline{p}> = <\underline{\iota}, \underline{p}>$$

for all polynomials p of degree d or less. If P denotes the $(n + 1 + m)$ by $(1 + d)$ matrix $[\underline{p}_0\ \underline{p}_1 \ldots \underline{p}_d]$, where $\{p_i\}$ is a basis for all polynomials of degree d or less, then the requirement becomes

$$P^T \underline{a} = P^T \underline{\iota}. \tag{1}$$

III. LAGRANGE MULTIPLIERS

We now have the following

PROBLEM: Minimize $\|K^T \underline{a}\|$ subject to equation (1). Observe that $\|K^T \underline{a}\|^2 = <K^T \underline{a}, K^T \underline{a}> = \binom{2z}{z} R_z^2$, and the vector $\underline{a}$ that minimizes $\|K^T \underline{a}\|^2$ also minimizes $\|K^T \underline{a}\|$. (Also note that $\binom{2z}{z} = <K^T \underline{\iota}, K^T \underline{\iota}>$.) By the method of Lagrange multipliers ([6], Appendix; [26], p. 9; [20], p. 73; [23], p. 87; cf. [4], p.3, Problem B) the problem is to find the critical point of the function

$$l(\underline{a}, \underline{\lambda}) = <K^T \underline{a}, K^T \underline{a}> + <P^T(\underline{a} - \underline{\iota}), \underline{\lambda}>,$$

where $\underline{\lambda}$ is the vector of multipliers.

Equating the derivative of l with respect to $\underline{a}$ with the zero vector (cf. [25]), we have

$$2KK^T \underline{a} = -P\underline{\lambda}, \tag{2}$$

or

$$\underline{a} = -\tfrac{1}{2}(KK^T)^{-1} P\underline{\lambda}. \tag{3}$$

(The matrix KK^T is invertible because K has full rank, but the matrix $K^T K$

is invertible only when $z = 0$, i.e., $K = I$.) In left-multiplying equation (3) by P^T, we get

$$-\tfrac{1}{2}P^T(KK^T)^{-1}P\underline{\lambda} = P^T\underline{a}$$
$$= P^T\underline{\iota} \qquad \because \text{equation (1)}.$$

Since P^T has full rank, the matrix $P^T(KK^T)^{-1}P$ is positive definite, hence invertible. Thus,

$$\underline{\lambda} = -2(P^T(KK^T)^{-1}P)^{-1}P^T\underline{\iota}. \tag{4}$$

The substitution of (4) into equation (3) gives

$$\underline{a} = (KK^T)^{-1}P(P^T(KK^T)^{-1}P)^{-1}P^T\underline{\iota}. \tag{5}$$

The following is an *APL* program for computing the coefficients of minimum-R_z exact-for-cubics *MWA* formulas.

```
    ∇MWA[□]∇
    ∇A← Z MWA MN;L;P;ZZ;C;SIGN;KK;X;□IO
[1] □IO←1
[2] L← +/1,MN
[3] P←((⍳L)−1+MN[1])∘.*0 1 2 3
[4] C←(0,⍳ZZ)!ZZ←2×Z
[5] SIGN←(ZZ+1)⍴1 ¯1
[6] KK←⌹(0,Z)↓(0,−Z)↓(L,L+ZZ)⍴(SIGN×C),L⍴0
[7] X← 1 0 0 0 ⌹(⍉P)+.×KK+.×P
[8] A←KK+.×P+.×X
    ∇
```

For instance, upon entering

```
 3 MWA 1 3
```

the computer returns

0.06118881119 0.7552447552 0.3671328671 ¯0.2447552448 0.0611888119.

Hence, we have the following five-term minimum-R_3 exact-for- cubics *MWA* formula (cf. [8], p. 13):

$$u_x = 0.0612\,u''_{x-1} + 0.7552u''_x + 0.3671u''_{x+1} - 0.2448u''_{x+2} + 0.0612u''_{x+3}.$$

IV. UNIQUENESS

Equation (5) can be used to prove Greville's theorem ([9], p. 13). To avoid confusion, we shall denote the right-hand side of equation (5) by $\underline{\hat{a}}$. The vector $\underline{\hat{a}}$ is independent of the basis matrix P, because

$$P(P^T(KK^T)^{-1}P)^{-1}P^T = (PS)((PS)^T(KK^T)^{-1}(PS))^{-1}(PS)^T \tag{6}$$

for each invertibile matrix S.

We now show that there is a unique polynomial q of degree $(2z + d)$ or less such that

$$\underline{\hat{a}} = (q(-m), \ldots, q(0), \ldots, q(n))^T,$$

and $q(s) = 0$ for $s = -(m + 1), \ldots, -(m + z), n + 1, \ldots, n + z$. By equation (2), $KK^T\underline{\hat{a}}$ is a polynomial vector of degree d or less. The matrix K^T is not a differencing matrix, but by multiplying K^T by $(-1)^z$ and adding z columns of appropriate numbers to each side of it, we can extend K^T to $\tilde{K}$, a differencing matrix of order z. The product $K\tilde{K}$ is a differencing matrix of order 2 z. Now extend $\underline{\hat{a}}$ by adding z zeros to both ends. Call this extended vector $\underline{\tilde{a}}$. Then clearly

$$(-1)^z K\tilde{K}\underline{\tilde{a}} = KK^T\underline{\hat{a}}.$$

Thus, $\underline{\tilde{a}}$ is a polynomial vector of degree $2z + d$ or less; i.e., there exists a polynomial q of degree $(2z + d)$ or less such that

$$\underline{\tilde{a}} = (q(-(m + z)), \ldots, q(n + z))^T.$$

For a slightly different argument, see ([4], page 10).

Such a polynomial q is necessarily unique ([9], p. 66) since (1) the $2z$ zeros specify $2z$ conditions and the reproducing criterion specifies another $(d + 1)$ independent conditions, and (2) there can be at most one such polynomial of degree $(2z + d)$ or less.

V. MINIMUM R_z

The minimum value of R_z^2 is given by $\|K^T\underline{\hat{a}}\|^2/\binom{2z}{z}$ or equivalently $(\|K^T\underline{\hat{a}}\|/\|K^T\underline{\iota}\|)^2$. It follows immediately from equation (5) that this minimum value also equals

$$\frac{\underline{\iota}^T P(P^T(KK^T)^{-1}P)^{-1}P^T\underline{\iota}}{\underline{\iota}^T KK^T\underline{\iota}}.$$

If we apply equation (5) again, the numerator of the last expression becomes $\underline{\iota}^T KK^T \underline{\hat{a}}$, which is $(-1)^z \delta^{2z} \hat{a}_o$. This result was first derived by Greville ([7], p. 257).

It is interesting to note that the problem:

$$\text{Minimize } \|K^T \underline{a}\|^2 \text{ subject to } P^T \underline{a} = P^T \underline{\iota}$$

is equivalent to the problem ([22], p. 234, Theorem 12.1.II):

Find $\underline{a}$ such that

$$\text{(i) } KK^T \underline{a} \in \text{Kernel } (P^T)^\perp$$
$$\text{and (ii) } P^T \underline{a} = P^T \underline{\iota}.$$

The equivalence is a consequence of the identity ([2], p. 64; [23], p. 49)

$$\text{Kernel } (P^T)^\perp = \text{Range } (P),$$

which shows that condition (i) and equation (2) imply each other.

VI. SYMMETRIC FORMULAS

Let us consider the case where $n = m$. Define $\underline{\ddot{a}} = (\hat{a}_n, \ldots, \hat{a}_o, \ldots, \hat{a}_{-n})^T$. It is obvious that $\|K^T \underline{\ddot{a}}\|^2 = \|K^T \underline{\hat{a}}\|^2$. Furthermore, $< \underline{\ddot{a}}, \underline{p} > = p(0)$, because $p(-s)$, as a polynomial in s, has the same degree as $p(s)$. Thus, by the uniqueness of $\underline{\hat{a}}$,

$$\underline{\ddot{a}} = \underline{\hat{a}}.$$

Hence, the graduation formula is symmetric.

Since $\underline{\hat{a}}$ is an even polynomial vector, $<\underline{\hat{a}}, \underline{p}> = 0 = p(0)$ for each odd polynomial p. Therefore, we only need to require the graduation formula to reproduce even polynomials. Consequently, formula (5) can be simplified as

$$\underline{\hat{a}} = (KK^T)^{-1} E (E^T (KK^T)^{-1} E)^{-1} E^T \underline{\iota}, \tag{7}$$

where the column vectors of the matrix E constitute a basis for all the even polynomial vectors of degree d or less. For a symmetric *MWA* formula, the maximum degree of reproduction, d, is an odd number, and the matrix E consists of $(d + 1)/2$ columns.

VII. PARTITIONED MATRICES

The technique of partitioned matrices provides an alternative method to derive the results above.

Equations (1) and (2) can be combined as a single matrix equation (cf. [2], p. 124, No. 36):

$$\begin{bmatrix} 2KK^T & P \\ P^T & O \end{bmatrix} \begin{bmatrix} \underline{\hat{a}} \\ \underline{\lambda} \end{bmatrix} = \begin{bmatrix} \underline{0} \\ P^T \underline{\iota} \end{bmatrix} \tag{8}$$

To obtain formula (5) we invert the matrix in the left-hand side of equation (8) using the following result ([20], p. 68; [2], p. 197, No. 9).

LEMMA 1 (*Schur's Identity*). Let $M = \begin{bmatrix} A & B \\ C & D \end{bmatrix}$, where A and D (thus M) are square matrices. If M and A are invertible, then

$$M^{-1} = \begin{bmatrix} H & -A^{-1}BG^{-1} \\ -G^{-1}CA^{-1} & G^{-1} \end{bmatrix}, \tag{9}$$

where $$G = D - CA^{-1}B,$$

and $$H = A^{-1} + A^{-1}BG^{-1}CA^{-1}.$$

Proof. Let $L = \begin{bmatrix} I & O \\ -CA^{-1} & I \end{bmatrix}$ and $R = \begin{bmatrix} I & -A^{-1}B \\ O & I \end{bmatrix}$; then

$$LMR = \begin{bmatrix} A & O \\ O & G \end{bmatrix}.$$

Since LMR is a product of invertible matrices, G^{-1} exists.

Thus, $M^{-1} = R \begin{bmatrix} A^{-1} & O \\ O & G^{-1} \end{bmatrix} L$, proving equation (9).

VIII. CENTROSYMMETRIC MATRICES

The technique of partitioned matrices can be further exploited to show that when $m = n$, the vector $\underline{\hat{a}}$ is an even polynomial vector and equation (7) holds.

DEFINITION ([21], p. 19; [1], p. 124). A square matrix is called *centrosymmetric* if it is symmetric about its center; that is, $C = (c_{ij})$ is a centrosymmetric matrix of order $r \times r$ if

$$c_{ij} = c_{r+1-i,\ r+1-j}.$$

It is easy to see that the matrix KK^T is centrosymmetric; for an explicit calculation, see Lemma 2 of [5], or page 25 of [17]. We shall show that the matrix

$$Q = P(P^T (KK^T)^{-1}P)^{-1}P^T \tag{10}$$

is also centrosymmetric.

Let J denote the square matrix with 1's on the secondary diagonal and 0's elsewhere, that is,

$$J = \begin{bmatrix} 0 & \dots & 0 & 1 \\ 0 & \dots & 1 & 0 \\ \cdot & & & \\ \cdot & & & \\ \cdot & & & \\ 1 & \dots & 0 & 0 \end{bmatrix}.$$

Left-multiplication by J reverses the order of the rows of a matrix, and right-multiplication by J reverses the columns. Thus, a matrix C is centrosymmetric if and only if $C = JCJ$ and if and only if C commutes with J. It follows immediately that the inverse of a centrosymmetric matrix is centrosymmetric, and the sums and products of centrosymmetric matrices are also centrosymmetric.

We say a vector $\underline{x}$ is *symmetric* if $\underline{x} = J\underline{x}$; *skew-symmetric* if $\underline{x} = -J\underline{x}$. If C is a centrosymmetric matrix, then $C\underline{x}$ is symmetric if $\underline{x}$ is symmetric and $C\underline{x}$ is skew-symmetric if $\underline{x}$ is skew-symmetric.

LEMMA 2. For $m = n$, the matrix Q defined by equation (10) is centrosymmetric.

Proof. Recall that by equation (6) the matrix Q is independent of the choice of basis. Since $n = m$, we can choose a basis matrix P such that P can be partitioned as $[E\ F]$, where the matrices E and F consist of symmetric and skew-symmetric column vectors, respectively. Thus,

$$P^T(KK^T)^{-1}P = \begin{bmatrix} E^T \\ F^T \end{bmatrix} (KK^T)^{-1} [E\ F]$$

$$= \begin{bmatrix} E^T(KK^T)^{-1}E & O \\ O & F^T(KK^T)^{-1}F \end{bmatrix}$$

Hence,

$$Q = [E\ F] \begin{bmatrix} (E^T(KK^T)^{-1}E)^{-1} & O \\ O & (F^T(KK^T)^{-1}F)^{-1} \end{bmatrix} \begin{bmatrix} E^T \\ F^T \end{bmatrix}$$

$$= E(E^T(KK^T)^{-1}E)^{-1}E^T + F(F^T(KK^T)^{-1}F)^{-1}F^T . \tag{11}$$

Since $E = JE$ and $F = -JF$,

$$Q = JQJ,$$

that is, Q is centrosymmetric.

A consequence of Lemma 2 is that the matrix $(KK^T)^{-1}Q$ is centrosymmetric. Since the vector $\underset{\sim}{\iota}$ is symmetric ($m = n$),

$$\underset{\sim}{\hat{a}} = (KK^T)^{-1}Q\underset{\sim}{\iota}$$

is a symmetric vector. Thus, the entries of $\underset{\sim}{\hat{a}}$ are the values of an even polynomial. Furthermore, the equation

$$F^T\underset{\sim}{\iota} = \underset{\sim}{0}$$

and equation (11) immediately give equation (7).

IX. REMARKS

1. *MWA* graduation can be considered from the standpoint of reduction of random errors ([9], p.22). For extensive statistical treatments of *MWA* graduation, the reader is referred to the recent papers [3], [14] and [16]. These papers also discuss *MWA* formulas which reproduce functions other than polynomials. Also see [19].

2. In the context of *MWA* formulas, formula (5) has been given by Borgan ([3], Theorem 3.4). The following is a more general result ([24], p. 60, 1.f.1(ii); [2], p. 125, No. 37). Let A be a positive definite $m \times m$ matrix,

B an $m \times k$ matrix and $\underline{u}$ a k-vector. Let S_- be any generalized inverse of $B^TA^{-1}B$.

Then

$$\inf_{\underline{x}} \{<A\underline{x}, \underline{x}>|B^T\underline{x} = \underline{u}\} = <S^-\underline{u}, \underline{u}>$$

and the infimum is attained at

$$\underline{\hat{x}} = A^{-1}BS^-\underline{u}.$$

3. The coefficients for minimum-R_3 and minimum-R_4 formulas can be found in [8]. On checking with our *APL* program we find that four tables in ([8], pp. 16-19, $n = 19, 21, 23, 25$) are incorrect.

One of the motivations for deriving the asymmetric minimum-R_z formulas was the graduation of end values ([7], p. 250). However, Greville ([9], p. 20; [12], pp. 75-76) has pointed out that such formulas are unsuitable for this purpose. Recent developments on the graduation of end values can be found in [11], [12], [13], [17] and [18].

4. If the asymmetric minimum-R_z formulas are not suitable for the graduation of end values, are there any reasons why we should study them? The following interesting result of Greville ([10], Section 8) provides a partial answer. For each z, there is a 5-term asymmetric exact-for-quadratics formula which has an R_z value smaller than that of the minimum-R_z 5-term symmetric formula.

5. The method of Lagrange multipliers is a powerful technique. For instance it can be applied to solve the three problems treated in [4] and derive the *MWA* formula proposed in [5].

Motivated by the Whittaker-Henderson graduation method, Gerritson [5] develops the *MWA* formula whose coefficients are obtained by minimizing

$$\|\underline{a} - \underline{\iota}\|^2 + k\|K^T\underline{a}\|^2, \; k > 0 \qquad \text{([5], Equation (8))}$$

subject to the constraint that

$$P^T\underline{a} = P^T\underline{\iota}. \qquad \text{([5], Equation (9))}$$

This minimization problem is a type "C" problem discussed in [4].

Equating the gradient vector (the derivative with respect to $\begin{bmatrix} \underline{a} \\ \underline{\lambda} \end{bmatrix}$) of the function

$$l(\underline{a}, \underline{\lambda}) = \|\underline{a} - \underline{\iota}\|^2 + k\|K^T\underline{a}\|^2 + <P^T(\underline{a} - \underline{\iota}), \underline{\lambda}>$$

to the zero vector and rearranging, we immediately have

$$\begin{bmatrix} 2(I + kKK^T) & P \\ P^T & O \end{bmatrix} \begin{bmatrix} \underline{a} \\ \underline{\lambda} \end{bmatrix} = \begin{bmatrix} 2\underline{\iota} \\ P^T\underline{\iota} \end{bmatrix},$$

which is equation (11) on page 8 of [5].

6. The matrix $(-1)^z KK^T$ is the subject of study in [15]. Lemma 5 of [15] gives a formula for the entries of the matrix $(-1)^z(KK^T)^{-1}$.

The matrix KK^T *corresponds* to the finite difference operator $(-1)^z\delta^{2z}$. We now conclude this paper by providing an interesting way to see this.

Let $m = n = +\infty$, so that we are dealing with doubly-infinite matrices. Let E denote the forward-shift matrix. The $(i, i+1)$-entries of E are 1's and all the other entries are 0's. Then

$$K = (E - I)^z.$$

The matrix E^T is the backward-shift matrix. Since we are working with doubly-infinite matrices,

$$E^T = E^{-1}.$$

Thus,

$$\begin{aligned} K^T &= ((E - I)^z)^T \\ &= ((E - I)^T)^z \\ &= (E^{-1} - I)^z \\ &= (-1)^z(I - E^{-1})^z. \end{aligned}$$

Hence,

$$KK^T\ (=K^TK) = (-1)^z\ ((E - I)\ (I - E^{-1}))^z$$

is the matrix for the finite-difference operator

$$(-1)^z(\Delta\nabla)^z = (-1)^z\delta^{2z}.$$

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