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A NEW CLASS OF MOVING-WEIGHTED-AVERAGE GRADUATION FORMULAS

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I. ABSTRACT

This paper has two related purposes: first, to introduce a new class of Moving Weighted Average (MWA) graduation formulas where the coefficients are determined in accordance with the relative emphasis placed on smoothness and fit by the graduator, similar to the Whittaker-Henderson graduation method, and second, to consider the question posed by Greville in the part 5 study note on graduation regarding what value of n to use when graduating by MWA formula.

II. MINIMUM R_z^2 FORMULAS

When graduating by the MWA method, it has been customary to define a measure of roughness associated with the MWA formula. If $a_{-n},\cdots,a_n$ are the coefficients of the formula, the measure of roughness R_z^2 is defined as:

$$R_z^2 = \sum_{s=-n-z}^{n} (\Delta^z a_s)^2 \div \binom{2z}{z}$$, where a_s is taken to be 0 for $s=\pm(n+1),\cdots,\pm(n+z)$. Among all MWA formulas of order n which reproduce cubics, there exists one whose associated value of R_z^2 is a minimum among all possible values of R_z^2. This graduation formula is called the minimum R_z^2 formula of order n.

Proposition 1: Fix z, and let r_n be the value of R_z^2 associated with the minimum R_z^2 formula of order n. Then $\{r_n\}$ forms a non-increasing sequence.

Proof: Let $a_{-n},\cdots,a_n$ be the coefficients of the minimum R_z^2 formula of order n. Consider the MWA formula of order n+1 whose coefficients are $0,a_{-n},\cdots,a_n,0$. Cubics will be reproduced by this formula since the formula with $a_{-n},\cdots,a_n$ as coefficients reproduces cubics. It is easily seen that the value of R_z^2 associated with the formula with coefficients $0,a_{-n},\cdots,a_n,0$ is the same as the value of R_z^2 associated with the formula with coefficients $a_{-n},\cdots,a_n$, namely r_n. Now since r_{n+1} is the smallest value of R_z^2 that can be associated with any cubic-reproducing order n+1 MWA formula, it follows that $r_{n+1} \leq r_n$, and so the sequence $\{r_n\}$ is non-increasing.

This proposition shows that if the overriding concern is with the smoothness of the graduated values, the best value of n to use when graduating by minimum R_z^2 formulas is the largest one that the raw data will permit.

III. A MEASURE OF FIT IS INTRODUCED

When performing a graduation, the closeness of the graduated values to the raw data, referred to as fit, should always be considered. The fact that minimum R^2 formulas reproduce cubics provides some

assurance of fit if we assume that the "underlying law" that the variable under consideration follows can be closely approximated by a cubic. However, the most obvious numerical measure of fit between the raw data $\left\{u_x''\right\}$ and the graduated values $\left\{u_x\right\}$ is $\sum_x (u_x-u_x'')^2$. Since under the MWA method $u_x = \sum_{s=-n}^{n} a_s u''_{x+s}$, it is true that $(u_x-u_x'')^2 = (\sum_{s=-n}^{n} a_s u''_{x+s} - u_x'')^2 =$

$$(\sum_{\substack{s=-n \\ s\neq 0}}^{n} a_s u''_{x+s} + (a_0-1)\, u_x'')^2. \qquad (1)$$

Consider for a moment how the measure of roughness R_z^2 was obtained in the part 5 study note on graduation. First the equation

$$(\Delta^z u_x)^2 = \left(\sum_{s=-n-z}^{n} (\Delta^z a_s)\, u''_{x+z+s}\right)^2 \qquad (2)$$

was deduced. Then, to get a measure of the size of the right-hand side of equation (2) which was independent of the particular $\left\{u_x''\right\}$ under consideration, the sum of the squares of the coefficients of the u'''s was considered, namely: $\sum_{s=-n-z}^{n} (\Delta^z a_s)^2$ (3)

Finally the expression (3) was divided by $\binom{2z}{z}$ in order to make the value of R_z^2 be 1 for the identity MWA formula.

Consider again the measure of fit given by expression (1) above. It is possible to duplicate the construction of R_z^2 and define a measure of fit associated with a MWA formula which is independent of the particular u'''s under consideration by taking the sum of the squares of the coefficients of the u'''s in expression (1), namely:

$$F = \sum_{\substack{s=-n \\ s\neq 0}}^{n} a_s^2 + (1-a_0)^2 \qquad (4)$$

The key step in both the construction of R_z^2 and the construction of F above involves proceeding from an exact expression of the quantity under consideration to an expression which only represents the size of the quantity under consideration but which is independent of the raw data. In both cases the exact expression is of the form $\left(\sum_{s=-k}^{k} x_s y_s\right)^2$, and the expression used to represent the exact one is $\sum_{s=-k}^{k} (x_s)^2$. What we hope is that there is a correlation between the size of the exact expression $\left(\sum_{s=-k}^{k} x_s y_s\right)^2$ and the substituted expression $\sum_{s=-k}^{k} (x_s)^2$. The following proposition relates the size of these two quantities.

Proposition 2: $\sum_{s=-k}^{k} (x_s y_s)^2 \leq M^2 \ (2k+1)^2 \sum_{s=-k}^{k} (x_s)^2$ for any choice of real x_s's and y_s's, where $M = \max_{-k \leq s \leq k} |y_s|$.

Proof: The proof is contained in Appendix I.

Remarks: The above proposition provides some justification for both the minimum R_z^2 graduation method and the graduation method that will be introduced in this paper. In non-mathematical language, it says that by making the expression $\sum_{s=-k}^{k}(x_s)^2$ small, one forces the expression $\sum_{s=-k}^{k}(x_s y_s)^2$ to be less than or equal to a multiple of something small. However, it definitely does not imply that the minimum value of the expression $\sum_{s=-k}^{k}(x_s y_s)^2$ will be taken on when the expression $\sum_{s=-k}^{k}(x_s)^2$ takes on its minimum value.

IV. A Practical Solution to the Number of Terms Question

If the measure of fit F defined above in equation (4) is accepted as a valid one, it is possible to analyze minimum R_z^2 formulas from a different point of view. As in the Whittaker-Henderson graduation method, the expression F+kS can be considered, where F is as defined above in equation (4), $k(\geq 0)$ is up to the discretion of the graduator, and $S = R_z^2 \times \binom{2z}{z}$, i.e.

$$S = \sum_{s=-n-z}^{n} (\Delta^z a_s)^2. \qquad (5)$$

Of course z is also up to the discretion of the graduator.

A practical solution to the number of terms question posed by Greville is now possible when minimum R_z^2 formulas are being considered. A computer can be programmed to calculate the coefficients of the minimum R_z^2 formulas for all values of n that would be practical for the data under consideration. Values of z and k could be chosen by the graduator, and the value of F+kS could be calculated for the coefficients generated by the computer. The value of n which resulted in the smallest value of F+kS would be considered the best value of n to use for the given values of z and k. The above procedure was performed for $2 \leq n \leq 11$, z = 1,2,3,4, and values of k in the range .1 to 20.0. The "best" value of n in each case is shown in Table I.

V. A New Class of MWA Formulas is Contemplated

If one accepts the numerical measure of fit defined in equation (4) as a valid one, then there is no reason why this measure should be applied only to minimum R_z^2 formulas. One approach would be to assign values to z and k and calculate coefficients which would minimize the quantity F+kS for the chosen values of z and k. When this approach was tried, it was found that the resulting MWA formulas would not necessarily reproduce constants. Considerations of fit make the reproduction of low degreee polynomials by MWA formulas a desirable characteristic when the variable under consideration can be closely approximated by low degree polynomials. Therefore, the initial approach was modified by considering the measure F+kS only for those MWA formulas which reproduce cubics. It was found that once z, k, and n are chosen, there is a unique MWA formula of order n which reproduces cubics and which has the minimum value of F+kS among all order n cubic-reproducing MWA formulas. The mathematics behind this approach, along with a method for calculating the unique coefficients, will now be developed.

VI. A New Class of MWA Formulas

For a MWA formula of degree n with coefficients $a_{-n}, \cdots, a_n,$ the measure of fit F defined by equation (4) can be expressed in matrix notation as: $F = (\vec{a} - \vec{e})^T (\vec{a} - \vec{e})$ (6)
where $\vec{a}$ is the vector $\begin{pmatrix} a_{-n} \\ \vdots \\ a_n \end{pmatrix}$ and $\vec{e}$ is the vector $\begin{pmatrix} 0 \\ \vdots \\ 1 \\ \vdots \\ 0 \end{pmatrix}$, of length 2n+1, consisting of all zeros except a 1 in the n+1'st position. Also, the measure of smoothness S defined by equation (5) can be expressed as $S = \vec{a}^T K^T K \vec{a}$ (7)
where $\vec{a}$ is as above and K is the (2n+1+z) x (2n+1) matrix which, when multiplied on the right by $\vec{a}$, gives the 2n+1+z values of $\Delta^z a_s$ for s = -n-z,$\cdots$,n. (An exact description of the matrix K is given in the appendix.) Note that this K is not exactly of the same form as the K used in the Whittaker-Henderson graduation method discussed in the part 5 study note on graduation. In the Whittaker-Henderson method, the matrix K allows one to calculate the n-z z'th differences of a set of n values, whereas the matrix K referred to above allows one to calculate 2n+z+1 z'th differences from 2n+1 values, plus z zeroes catenated on either end of the 2n+1 values. For example, for n = 3 and z = 2, the matrix K used in equation (7) would be:

proposition, contained in Appendix 2, the method for calculating the coefficients of this MWA formula is developed. This method will be summarized now.

Let n, z, and k be given. Let K be the matrix used in equation (7) of the previous section. Let A be the following $(2n+3) \times (2n+3)$ matrix:

$$A = \left[\begin{array}{ccccc|cc}
 & & & & & 1 & (-n)^2 \\
 & & & & & 1 & (-n+1)^2 \\
 & & 2(I+kK^TK) & & & \vdots & \vdots \\
 & & & & & 1 & (n-1)^2 \\
 & & & & & 1 & (n)^2 \\ \hline
1 & 1 & \cdots & 1 & 1 & 0 & 0 \\
(-n)^2 & (-n+1)^2 & \cdots & (n-1)^2 & n^2 & 0 & 0
\end{array}\right]$$

i.e. the upper left $2n+1 \times 2n+1$ submatrix of A is the matrix $2(I+kK^TK)$, where I is the $2n+1 \times 2n+1$ identity matrix; the $2n+2$'nd column of A consists of $2n+1$ one's and 2 zeros; the $2n+3$'rd column of A consists of the sequence $(-n)^2$, $(-n+1)^2$, $\cdots$, $(n-1)^2$, n^2, and two zeros; and the $2n+2$'nd row and $2n+3$'rd row are equal to the $2n+2$'nd column and the $2n+3$'rd column respectively.

The key fact used to calculate the coefficients $a_{-n}, \cdots, a_n$ of the MWA formula of proposition 3 is that the following matrix equation holds:

$$A \begin{pmatrix} a_{-n} \\ \vdots \\ a_n \\ \lambda \\ \mu \end{pmatrix} = \vec{f} \qquad (11)$$

where $\vec{f}$ is the vector of length $2n+3$ consisting of all zeros except a 2 in the $n+1$'st position and a 1 in the $2n+2$'nd position. The variables λ and μ in equation (11) above were introduced to guarantee the reproduction of cubics. Since the matrix A is always invertible (proved in Appendix 2), one just has to calculate A^{-1} and then multiply it on the right by $\vec{f}$. The first 2n+1 entries of this product are the values of $a_{-n},\cdots,a_n$.

As an example, let z = 1, k = 1, and n = 1. The matrix A is:

$$\begin{bmatrix} 6 & -2 & 0 & 1 & 1 \\ -2 & 6 & -2 & 1 & 0 \\ 0 & -2 & 6 & 1 & 1 \\ 1 & 1 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 \end{bmatrix}$$

and A^{-1} is:

$$\begin{bmatrix} \frac{1}{12} & 0 & -\frac{1}{12} & 0 & \frac{1}{2} \\ 0 & 0 & 0 & 1 & -1 \\ -\frac{1}{12} & 0 & \frac{1}{12} & 0 & \frac{1}{2} \\ 0 & 1 & 0 & -6 & 8 \\ \frac{1}{2} & -1 & \frac{1}{2} & 8 & -13 \end{bmatrix},$$

$$\text{and } A^{-1}f = A^{-1}\begin{pmatrix} 0 \\ 2 \\ 0 \\ 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \\ 0 \\ -4 \\ 6 \end{pmatrix}$$

So for this case $a_{-1} = 0$, $a_0 = 1$, and $a_1 = 0$, i.e. $u_x = u_x''$, the identity MWA formula

VIII. EXAMPLES

As an example of graduation by the method introduced in the previous two sections, the twenty-five central values of the list of data on page 63of Miller's book Elements of Graduation were chosen as the ungraduated values. The value of z was chosen to be 2 for all graduations. This data was graduated by five methods: (1) Whittaker-Henderson Type A with k = 2, (2) minimum R_z^2 formula with n = 5, (3) minimum R_z^2 fromula with n = 10, (4) the method of this paper with

$k = 2$ and $n = 5$, and (5) the method of this paper with $k = 2$, and $n = 10$. The results of these graduations are shown in Table 2. All the MWA graduations done on this data used as many extra values of the data from page of Miller's book as necessary to get twenty-five graduated values. Notice how close the Whittaker-Henderson Type A graduation is to the graduations by the method of this paper.

One of the most appealing qualities of the MWA graduation method is its simplicity. No computers are necessary for its execution. It is true that determining the coefficients of the MWA formulas introduced in this paper is not computationally easy. However, once they are determined for particular values of z, n, and k, they can be used on any set of raw data without the need of a computer. For this reason, the coefficients of the MWA formulas produced by the method of this paper for $n = 5,10$ and $z = 1,2,3,4$ and $k = .5,1,2$ are shown in Table 3.

IX. CONCLUSION

Section VII gave the solution to the problem of finding coefficients $a_{-n}, \cdots, a_n$ of the MWA formula of order n which will minimize F+kS subject to the constraint of reproducing cubics. This formula will be referred to as the "minimum F+kS formula" of order n, even though this introduces ambiguity because the formula isn't determined until z is chosen.

Proposition 4: Fix z and k. Let m_n be the value of F+kS, where F and S are as previously defined, for the minimum F+kS formula of order n. Then $\{m_n\}$ is a non-increasing sequence.

Proof: The proof is essentially a repetition of the proof of proposition 1 and is left to the reader.

It is now possible to reconsider the question posed by Greville concerning the number of terms to use when graduating by MWA formulas in light of the new class of MWA formulas introduced in this paper. The main purpose for minimum F+kS formulas is to give the graduator control over the emphasis to be placed between smoothness and fit. Minimum R_z^2 formulas don't provide this option. However, proposition 4 implies that the value of the fit-smoothness measure will not increase if the value of n is increased. This would indicate that the graduator, when graduating by minimum F+kS formula, should choose the largest value of n which is convenient for the raw data under observation. However, there is a counterbalancing consideration. If there are t ungraduated values, graduating by a MWA formula of order n will produce only t-2n graduated values. Thus there is a trade-off between getting a small fit-smoothness measure and getting a lot of graduated values. To get t graduated values, extrapolation of the raw data is necessary, but this will introduce uncertainty into the final results.

The problem of what order MWA formula to use has not been solved by the introduction of minimum F+kS formulas. To solve the problem, an investigation into the extrapolation process is necessary to see whether it is better to use a high value of n with an associated low value of F+kS, or a low value of n with only a few extrapolated values necessary to get complete results.

TABLE I

Values of N in the Range $2 \leq N \leq 11$

Which Minimize F+kS for Minimum R_z^2 Formulas

k \ z	1	2	3	4
.1	2	2	2	3
.3	2	3	3	4
.5	2	3	4	4
.6	2	3	4	4
.7	3	3	4	4
.8	3	4	4	4
.9	3	4	4	5
1.0	3	4	4	5
1.5	4	4	5	5
2.0	5	5	5	5
2.5	6	5	5	5
3.0	6	5	5	6
3.5	7	6	6	6
4.0	8	6	6	6
5.0	9	6	6	6
6.0	9	7	6	6
8.0	11	7	7	7
10.0	11	8	7	7
12.0	11	8	7	7
15.0	11	9	8	7
20.0	11	10	8	8

TABLE 2

Example of Graduations by Various Methods

Age	(1) Raw Data	(2) Whittaker-Henderson	(3) Minimum R_z^2 (n=5)	(4) Minimum R_z^2 (n=10)	(5) Minimum F+kS (n=5)	(6) Minimum F+kS (n=10)
45	.00446	.00489	.00502	.00523	.00489	.00495
46	.00632	.00606	.00596	.00581	.00599	.00597
47	.00741	.00701	.00685	.00638	.00698	.00692
48	.00726	.00766	.00763	.00699	.00772	.00760
49	.00945	.00811	.00798	.00768	.00811	.00808
50	.00749	.00827	.00844	.00846	.00829	.00826
51	.00763	.00873	.00882	.00920	.00867	.00873
52	.01064	.00967	.00944	.00998	.00953	.00968
53	.00999	.01073	.01061	.01098	.01065	.01074
54	.01378	.01204	.01217	.01203	.01209	.01205
55	.00967	.01334	.01387	.01331	.01358	.01334
56	.01826	.01525	.01485	.01478	.01528	.01526
57	.01811	.01656	.01594	.01639	.01638	.01656
58	.01593	.01756	.01799	.01823	.01756	.01755
59	.01789	.01930	.01979	.02009	.01921	.01929
60	.01853	.02204	.02212	.02194	.02203	.02203
61	.03246	.02532	.02442	.02377	.02533	.02531
62	.02794	.02692	.02683	.02595	.02702	.02691
63	.01937	.02821	.02928	.02847	.02849	.02819
64	.04000	.03106	.03093	.03125	.03116	.03106
65	.02795	.03290	.03257	.03429	.03275	.03299
66	.03764	.03567	.03501	.03740	.03536	.03596
67	.04123	.03880	.03979	.04024	.03920	.03939
68	.03459	.04272	.04481	.04321	.04365	.04351
69	.05391	.04906	.04932	.04627	.04983	.04950

(1) From Miller, "Elements of Graduation", pg. 63.

(2) Type A, with z=2 and k=2.

(3) The value of z is 2. To get the graduated values at ages 45-49 and 65-69, values of the raw data were used for ages 40-44 and 70-74.

(4) The value of z is 2. To get the graduated values at ages 45-54 and 60-69, values of the raw data were used for ages 30-44 and 70-79.

(5) z=2 and k=2. To get the graduated values at ages 45-49 and 65-69, values of the raw data were used for ages 40-44 and 70-74.

(6) z=2 and k=2. To get the graduated values at ages 45-54 and 60-69, values of the raw data were used for ages 30-44 and 70-79.

Table 3

Values of Minimum F+kS Coefficients

A. n = 5, z = 1

s	k = .5	k = 1	k = 2
-5	-.0141889413	-.0229251389	-.0322171146
-4	-.0063118852	-.0088011393	-.0104318083
-3	.0106668370	.0230123562	.0376965794
-2	.0483681026	.0782860103	.1062473592
-1	.1662397521	.1936914537	.2080781474
0	.5904522696	.4734729158	.3812536740
1	.1662397521	.1936914537	.2080781474
2	.0483681026	.0782860103	.1062473592
3	.0106668370	.0230123562	.0376965794
4	-.0063118852	-.0088011393	-.0104318083
5	-.0141889413	-.0229251389	-.0322171146

B. n = 5, z = 2

s	k = .5	k = 1	k = 2
-5	-.0066450661	-.0145207363	-.0223633258
-4	-.0144004685	-.0184295859	-.0206526587
-3	-.0074587477	.0071097381	.0222572379
-2	.0569777432	.0882945393	.1125545426
-1	.2357519042	.2407259820	.2389923725
0	.4715492697	.3936401257	.3384236630
1	.2357519042	.2407259820	.2389923725
2	.0569777432	.0882945393	.1125545426
3	-.0074587477	.0071097381	.0222572379
4	-.0144004685	-.0184295859	-.0206526587
5	-.0066450661	-.0145207363	-.0223633258

Table 3 (Continued)

C. n = 5, z = 3

	k		
s	.5	1	2
-5	-.0046127052	-.0125138164	-.0188274610
-4	-.0202222597	-.0234060740	-.0250918283
-3	-.0137706862	.0031063058	.0165507815
-2	.0753977821	.1011567923	.1186799653
-1	.2612188337	.2547586729	.2484788826
0	.4039780707	.3537962389	.3204193198
1	.2612188337	.2547586729	.2484788826
2	.0753977821	.1011567923	.1186799653
3	-.0137706862	.0031063058	.0165507815
4	-.0202222597	-.0234060740	-.0250918283
5	-.0046127052	-.0125138164	-.0188274610

D. n = 5, z = 4

	k		
s	.5	1	2
-5	-.0068646435	-.0133010324	-.0175338170
-4	-.0237418974	-.0259180269	-.0271069906
-3	-.0093801195	.0051427948	.0146396719
-2	.0928407231	.1110966109	.1222851642
-1	.2645446275	.2565426446	.2511595706
0	.3652026194	.3328740180	.3131128018
1	.2645446275	.2565426446	.2511595706
2	.0928407231	.1110966109	.1222851642
3	-.0093801195	.0051427948	.0146396719
4	-.0237418974	-.0259180269	-.0271069906
5	-.0068646435	-.0133010324	-.0175338170

Table 3 (Continued)

E. n = 10, z = 1

s	k = .5	k = 1	k = 2
-10	-.0022830516	-.0040976375	-.0069856103
-9	-.0021810780	-.0043048780	-.0078257211
-8	-.0015102405	-.0031082969	-.0056322903
-7	-.0007363297	-.0013507183	-.0017171469
-6	.0000936537	.0009259616	.0037520947
-5	.0012574969	.0044388777	.0116682271
-4	.0039133500	.0113813309	.0244308467
-3	.0124160256	.0276160896	.0471461515
-2	.0430266245	.0685381574	.0901800404
-1	.1564347371	.1744697770	.1743410625
0	.5791376239	.4509826732	.3412846913
1	.1564347371	.1744697770	.1743410625
2	.0430266245	.0685381574	.0901800404
3	.0124160256	.0276160896	.0471461515
4	.0039133500	.0113813309	.0244308467
5	.0012574969	.0044388777	.0116682271
6	.0000936537	.0009259616	.0037520947
7	-.0007363297	-.0013507183	-.0017171469
8	-.0015102405	-.0031082969	-.0056322903
9	-.0021810780	-.0043048780	-.0078257211
10	-.0022830516	-.0040976375	-.0069856103

F. n = 10, z = 2

s	k = .5	k = 1	k = 2
-10	.0000390811	.0002940140	.0003859604
-9	.0001884168	.0005015347	.0000494714
-8	.0003952726	.0001272898	-.0017276045
-7	.0001960243	-.0016891817	-.0052481953
-6	-.0016870936	-.0058376715	-.0096397030
-5	-.0069382620	-.0114547015	-.0112068455
-4	-.0138738428	-.0118043885	-.0013339547
-3	-.0069332740	.0113137469	.0342156277
-2	.0571976292	.0878941450	.1102952224
-1	.2357098438	.2365912648	.2245472245
0	.4714124092	.3881278959	.3193255934
1	.2357098438	.2365912648	.2245472245
2	.0571976292	.0878941450	.1102952224
3	-.0069332740	.0113137469	.0342156277
4	-.0138738428	-.0118043885	-.0013339547
5	-.0069382620	-.0114547015	-.0112068455
6	-.0016870936	-.0058376715	-.0096397030
7	.0001960243	-.0016891817	-.0052481953
8	.0003952726	.0001272898	-.0017276045
9	.0001884168	.0005015347	.0000494714
10	.0000390811	.0002940140	.0003859604

Table 3 (Continued)

G. n = 10, z = 3

s	k = .5	k = 1	k = 2
-10	-.0004514093	.0002195679	.0014960255
-9	-.0000690936	.0016634367	.0034740727
-8	.0020611345	.0035899642	.0031521751
-7	.0044560592	.0025413062	-.0026444710
-6	.0018193295	-.0059511426	-.0144730171
-5	-.0117133044	-.0213550554	-.0257761678
-4	-.0300634165	-.0291286614	-.0197869197
-3	-.0188682012	.0025661333	.0262599852
-2	.0774910720	.1048338437	.1239660063
-1	.2686789336	.2607686531	.2466570678
0	.4133177921	.3605039087	.3153504860
1	.2686789336	.2607686531	.2466570678
2	.0774910720	.1048338437	.1239660063
3	-.0188682012	.0025661333	.0262599852
4	-.0300634165	-.0291286614	-.0197869197
5	-.0117133044	-.0213550554	-.0257761678
6	.0018193295	-.0059511426	-.0144730171
7	.0044560592	.0025413062	-.0026444710
8	.0020611345	.0035899642	.0031521751
9	-.0000690936	.0016634367	.0034740727
10	-.0004514093	.0002195679	.0014960255

H. n = 10, z = 4

s	k = .5	k = 1	k = 2
-10	-.0013996913	-.0003372530	.0014752155
-9	-.0012595359	.0016868639	.0048872356
-8	.0035179276	.0061884184	.0067332015
-7	.0096364120	.0068339370	.0006073341
-6	.0057424110	-.0052040967	-.0164571202
-5	-.0169516101	-.0288984769	-.0353969770
-4	-.0431373474	-.0409863321	-.0319849216
-3	-.0228077995	-.0005504051	.0220147245
-2	.0944060042	.1166659522	.1323909726
-1	.2795671771	.2700481900	.2573711852
0	.3853721045	.3491064046	.3167182993
1	.2795671771	.2700481900	.2573711852
2	.0944060042	.1166659522	.1323909726
3	-.0228077995	-.0005504051	.0220147245
4	-.0431373474	-.0409863321	-.0319849216
5	-.0169516101	-.0288984769	-.0353969770
6	.0057424110	-.0052040967	-.0164571202
7	.0096364120	.0068339370	.0006073341
8	.0035179276	.0061884184	.0067332015
9	-.0012595359	.0016868639	.0048872356
10	-.0013996913	-.0003372530	.0014752155

Appendix I

This appendix contains the proof of Proposition 2.

Proposition 2: $\left(\sum_{s=-k}^{k} x_s y_s\right)^2 \leq M^2 (2k+1)^2 \sum_{s=-k}^{k} (x_s)^2$ for any choice of real x_s's and y_s's, where $M = \max_{-k \leq s \leq k} |y_s|$.

Proof: $\left(\sum_{s=-k}^{k} x_s y_s\right)^2 = \left(\left|\sum_{s=-k}^{k} x_s y_s\right|\right)^2 \leq \left(\sum_{s=-k}^{k} |x_s|\,|y_s|\right)^2 \leq M^2 \left(\sum_{s=-k}^{k} |x_s|\right)^2$

Now $\sqrt{\sum_{s=-k}^{k} (x_s)^2} \geq |x_i|$ for each i s.t. $-k \leq i \leq k$. Letting i run through all integer values from -k to k produces 2k+1 inequalities, which we can add up, giving $(2k+1)\sqrt{\sum_{s=-k}^{k} (x_s)^2} \geq \sum_{i=-k}^{k} |x_i| = \sum_{s=-k}^{k} |x_s|$. Squaring each side we obtain $(2k+1)^2 \left(\sum_{s=-k}^{k} (x_s)^2\right) \geq \left(\sum_{s=-k}^{k} |x_s|\right)^2$. Thus $M^2\left(\sum_{s=-k}^{k} |x_s|\right)^2 \leq M^2 (2k+1)^2 \left(\sum_{s=-k}^{k} (x_s)^2\right)$, and so $\left(\sum_{s=-k}^{k} x_s y_s\right)^2 \leq M^2 (2k+1)^2 \sum_{s=-k}^{k} (x_s)^2$.

Appendix 2

This appendix contains the proof of Proposition 3.

Proposition 3: Let n, z, and k be given, with $k \geq 0$. Let F and S be as defined in equations (4) and (5). Then there exists a unique MWA formula of order n which reproduce cubics and which has the smallest value of F+kS of all order n MWA Formulas which reproduce cubics.

Remarks: The proof will show that the coefficients $a_{-n}, \cdots, a_n$ of this unique MWA formula satisfy $A\begin{pmatrix} a_{-n} \\ \vdots \\ a_n \end{pmatrix} = \vec{f}$ where A and $\vec{f}$ are defined in Section VII of this paper, and, since A is an invertible matrix (shown below), this equation can be used to find the coefficients of the unique MWA formula.

Proof of Proposition 3: The proof has three main sections. In Section I coefficients $a_{-n}, \cdots, a_n$ will be defined. In Section II, it will be shown that the MWA formula with these coefficients is symmetric and reproduces cubics. In Section III it will be shown that the MWA formula with these coefficients has the minimum value of F+kS among all order n cubic-reproducing MWA formulas, and that it is unique in this respect.

Section I

In order to define the appropriate coefficients, we need

Lemma 1: The matrix A defined by equation (10) in Section VII is invertible.

<u>Proof</u>: Assume $A\vec{x} = 0$. We will show that $\vec{x} = \vec{0}$. Let $x = \begin{pmatrix} w_{-n} \\ \vdots \\ w_n \\ \beta \end{pmatrix}$. Now the matrix A can be expressed as:

$$+ \; 2k \left[\begin{array}{ccccc|cc} & & K^T K & & & 0 & 0 \\ & & & & & 0 & 0 \\ & & & & & \vdots & \vdots \\ & & & & & 0 & 0 \\ & & & & & 0 & 0 \\ \hline 0 & 0 & \cdots & 0 & 0 & 0 & 0 \\ 0 & 0 & \cdots & 0 & 0 & 0 & 0 \end{array}\right]$$

$$+ \left[\begin{array}{cccc|cc} & & & & 1 & (-n)^2 \\ & & & & 1 & (-n+1)^2 \\ & & 0 & & \vdots & \vdots \\ & & & & 1 & (n-1)^2 \\ & & & & 1 & n^2 \\ \hline 1 & 1 & \cdots \; 1 & 1 & 0 & 0 \\ (-n)^2 & (-n+1)^2 & \cdots \; (n-1)^2 & n^2 & 0 & 0 \end{array}\right]$$

Therefore

$$\vec{x}^T Ax = 2\,\vec{x}^T \left[\begin{array}{ccccc|cc} & & I & & & 0 & 0 \\ & & & & & \vdots & \vdots \\ & & & & & 0 & 0 \\ & & & & & 0 & 0 \\ \hline 0 & 0 & \cdots & 0 & 0 & 0 & 0 \\ 0 & 0 & \cdots & 0 & 0 & 0 & 0 \end{array}\right] \vec{x}$$

$$+ \; 2k\,\vec{x}^T \left[\begin{array}{ccccc|cc} & & K^T K & & & 0 & 0 \\ & & & & & 0 & 0 \\ & & & & & \vdots & \vdots \\ & & & & & 0 & 0 \\ & & & & & 0 & 0 \\ \hline 0 & 0 & \cdots & 0 & 0 & 0 & 0 \\ 0 & 0 & \cdots & 0 & 0 & 0 & 0 \end{array}\right] \vec{x}$$

$$+ \; \vec{x}^T \left[\begin{array}{c|cc} & 1 & (-n)^2 \\ & 1 & (-n+1)^2 \\ 0 & \vdots & \vdots \\ & 1 & (n-1)^2 \end{array}\right. \vec{x}$$

$$= 2 \sum_{i=-n}^{n} w_i^2 + 2k \sum_{i=-n-z}^{n} (\Delta^z w_i)^2 + 2\alpha \sum_{i=-n}^{n} w_i + 2\beta \sum_{i=-n}^{n} i^2 w_i$$

where in calculating the Δ^z in the last expression it is assumed that $w_s = 0$ for $s = \pm(n+1), \cdots \pm(n+z)$ as usual. Now since $A\vec{x} = \vec{0}$, it is true that $\vec{x}^T A\vec{x} = 0$, so $0 = 2 \sum_{i=-n}^{n} w_i^2 + 2k \sum_{i=-n-z}^{n} (\Delta^z w_i)^2 + 2\alpha \sum_{i=-n}^{n} w_i + 2\beta \sum_{i=-n}^{n} i^2 w_i$

Now because $A\vec{x} = \vec{0}$, the last two elements of $A\vec{x}$ must both be 0, so $\sum_{i=-n}^{n} w_i = 0 = \sum_{i=-n}^{n} i^2 w_i$.

Thus the above equation reduces to:

$$0 = 2 \sum_{i=-n}^{n} w_i^2 + 2k \sum_{i=-n-z}^{n} (\Delta^z w_i)^2.$$

Since $k \geq 0$, this implies that $w_i = 0$ for $-n \leq i \leq n$. So now all we have to prove is that $\alpha = 0$ and $\beta = 0$. Now since $A\vec{x} = 0$, the first two elements of $A\vec{x}$ must both be 0, so since we have already shown that $w_i = 0$ for $-n \leq i \leq n$, we have

$$\alpha + (-n)^2 \beta = 0 \text{ and}$$
$$\alpha + (-n+1)^2 \beta = 0.$$

These two equations imply that $\alpha = \beta = 0$, so $\vec{x} = \vec{0}$ and A is invertible.

It is now possible to define the appropriate coefficients for the proposition.

Definition 1: let $(a_{-n}, \cdots, a_n, \lambda, \mu)$ be defined as the unique solution for $\vec{x}$ in the equation $A\vec{x} = \vec{f}$ where $\vec{f}$ is the vector of length 2n+3 defined in Section VII, i.e. $\vec{f}$ has all elements 0 except a "2" in the n+1'st position and a "1" in the 2n+2'nd position.

This solution exists and is unique by Lemma 1. The MWA formula we will be considering is

$$U_x = \sum_{s=-n}^{n} a_s U''_{x+s}$$

where the a's are given in definition 1.

Section II: In order to prove that the above formula reproduces cubics and is symmetric, we need

Lemma 2: The matrix K^TK is symmetric about the lower left to upper right diagonal as well as the upper left to lower right diagonal.

Proof: First we need a complete description of the matrix K. I claim that K satisfies:

$$K_{xy} = \begin{cases} 0 \text{ if } x-y<0 \\ (-1)^{x-y}\binom{z}{x-y} \text{ if } 0\leq x-y\leq z \\ 0 \text{ if } z<x-y \end{cases}$$

This can be written compactly as $(-1)^{x-y}\binom{z}{x-y}$ if it is agreed that $\binom{a}{b} = 0$ for $b<0$ or $b>a$.

To see the validity of the above expression, consider that the x'th row of K by definition gives the coefficients of the a's in the expansion of $\Delta^z a_{-n-z-1+x}$, so since $\Delta^z a_{-n-z-1+x} = \sum_{i=0}^{z} (-1)^{z-i} \binom{z}{i} a_{-n-z-1+x+i}$, we have that $K_{xy} = (-1)^i\binom{z}{i}$ where $-n-z-i+x+i = -n-1+y$, which implies that $i = z-(x-y)$ so $K_{xy} = (-1)^{(z-(z-(x-y)))}\binom{z}{z-(x-y)} = (-1)^{x-y}\binom{z}{x-y}$.

To show that K^TK is symmetric about the lower left to upper right diagonal, it is necessary and sufficient to show that $(K^TK)_{ij} = (K^TK)_{2n+2-j,\ 2n+2-i}$ since K^TK is a $2n+1 \times 2n+1$ matrix. Now $(K^TK)_{ij} = \sum_{t=1}^{2n+z+1} K^T{}_{it} K_{tj} = \sum_{t=1}^{2n+z+1} K_{ti} K_{tj}$, and $(K^TK)_{2n+2-j,2n+2-i} = \sum_{t=1}^{2n+z+1} K_{t,2n+2-j} K_{t,2n+2-i}$. Using the above description for K_{xy} we get:

$$(K^TK)_{ij} = \sum_{t=1}^{2n+z+1} (-1)^{t-i}\binom{z}{t-i}(-1)^{t-j}\binom{z}{t-j} = (-1)^{i+j} \sum_{t=1}^{2n+z+1} \binom{z}{t-i}\binom{z}{t-j} \qquad (12)$$

and $(K^TK)_{2n+2-j,2n+2-i} = (-1)^{i+j} \sum_{t=1}^{2n+z+1} \binom{z}{t-(2n+2-j)} \binom{z}{t-(2n+2-i)}$.

Transform the last summation by letting $s = 2n+2+z-t$. We get $(K^TK)_{2n+2-j,\ 2n+2-i}$

$$= (-1)^{i+j} \sum_{s=1}^{2n+z+1} \binom{Z}{j+z-s} \binom{Z}{i+z-s} = (-1)^{i+j} \sum_{s=1}^{2n+Z+1} \binom{Z}{s-j} \binom{Z}{s-i}. \quad (13)$$

Since the right hand sides of equations (12) and (13) are identical except for the name of the dummy variable, we have that

$$(K^TK)_{ij} = (K^TK)_{2n+2-j,\ 2n+2-i}$$

and hence K^TK is symmetric about both diagonals.

<u>Remark</u>: Since the upper left $(2n+1) \times (2n+1)$ part of the matrix A is $2(I + kK^TK)$, lemma 2 implies that

$$A_{tx} = A_{2n+2-x,\ 2n+2-t}$$

for $1 \le t \le 2n+1$ and $1 \le x \le 2n+1$.

We are now ready to prove that the MWA formula

$$U_x = \sum_{s=-n}^{n} a_s \, U''_{x+s}$$

where the a's are given in Definition 1 is symmetric. To do this we shall show that the vector $\begin{pmatrix} a_n \\ \vdots \\ a_{-n} \\ \lambda \\ \mu \end{pmatrix}$, i.e. the vector with the a's reversed but with λ and μ in the same position, is a solution for $\vec{x}$ in the equation $A\vec{x} = \vec{f}$. Since we know that $\begin{pmatrix} a_{-n} \\ \vdots \\ a_n \\ \lambda \\ \mu \end{pmatrix}$ is the unique solution to this equation, we will have shown that $a_{-s} = a_s$ for $1 \le s \le n$, and hence that the MWA formula under consideration is symmetric.

<u>Lemma 3</u>: $\begin{pmatrix} a_n \\ \vdots \\ a_{-n} \\ \lambda \\ \mu \end{pmatrix}$ is a solution for $\vec{x}$ in the equation $A\vec{x} = \vec{f}$.

<u>Proof</u>: To verify that $A\begin{pmatrix} a_n \\ \vdots \\ a_{-n} \\ \lambda \\ \mu \end{pmatrix} = \vec{f}$, it is necessary to verify 2n+3 linear equations; namely, that $A_t\begin{pmatrix} a_n \\ \vdots \\ a_{-n} \\ \lambda \\ \mu \end{pmatrix} = f_t$ where A_t is the t'th row of A,

for $1 \le t \le 2n+3$. The last two of these are immediate since $\sum_{i=n}^{-n} a_i = \sum_{i=-n}^{n} a_i = 1$ and $\sum_{i=n}^{-n} i^2 a_i = \sum_{i=-n}^{n} i^2 a_i = 0$. To get the other $2n+1$ equations, we will show that $\begin{pmatrix} a_n \\ \vdots \\ a_{-n} \\ \lambda \\ \mu \end{pmatrix}$ satisfies the equation represented by the t'th row of A because $\begin{pmatrix} a_{-n} \\ \vdots \\ a_n \\ \lambda \\ \mu \end{pmatrix}$ satisfies the equation represented by the $2n+2-t$'th row of A. Let's start with the equation we need to verify. The vector $\begin{pmatrix} a_n \\ \vdots \\ a_{-n} \\ \lambda \\ \mu \end{pmatrix}$ will satisfy the equation represented by the t'th row of A iff

$$\sum_{k=1}^{2n+1} A_{tk}\, a_{n+1-k} + \lambda + (n+1-t)^2 \mu = \begin{cases} 0 & \text{if } t \neq n+1 \\ 2 & \text{if } t = n+1 \end{cases}.$$

But since $\begin{pmatrix} a_{-n} \\ \vdots \\ a_n \\ \lambda \\ \mu \end{pmatrix}$ satisfies the equation represented by the $2n+2-t$ 'th row of A, we know that

$$\sum_{j=1}^{2n+1} A_{2n+2-t,j}\, a_{-n-1+j} + \lambda + (n+1-(2n+2-t))^2 \mu = \begin{cases} 0 & \text{if } t \neq n+1 \\ 2 & \text{if } t = n+1. \end{cases}$$

Now by the remark after lemma 2, we know that $A_{2n+2-t,j} = A_{j,2n+2-t} = A_{t,2n+2-j}$. Putting this into the above equation we have that

$$\sum_{j=1}^{2n+1} A_{t,2n+2-j}\, a_{-n-1+j} + \lambda + (t-(n+1))^2 \mu = \begin{cases} 0 & \text{if } t \neq n+1 \\ 2 & \text{if } t = n+1 \end{cases}$$

Let $k = 2n+2-j$. We then have

$$\sum_{k=1}^{2n+1} A_{tk}\, a_{n+1-k} + \lambda + (n+1-t)^2 \mu = \begin{cases} 0 & \text{if } t \neq n+1 \\ 2 & \text{if } t = n+1, \end{cases}$$

which is exactly what we wanted to verify. Thus $\begin{pmatrix} a_n \\ \vdots \\ a_{-n} \\ \lambda \\ \mu \end{pmatrix}$ is a solution to $A\vec{x} = \vec{f}$, and hence $a_s = a_{-s}$ for $1 \le s \le n$.

We are now ready to prove that the MWA formula under consideration reproduces cubics. Recall that the four equations required for the reproduction of cubics are: $\sum a_s = 1$, $\sum s a_s = 0$, $\sum s^2 a_s = 0$, and $\sum s^3 a_s = 0$. Since we have just proved that $a_s = a_{-s}$ for the MWA formula under consideration, we are guaranteed that $\sum s a_s = 0 = \sum s^3 a_s$. However, we know that the a's satisfy $A\begin{pmatrix} a_{-n} \\ \vdots \\ a_n \\ \lambda \\ \mu \end{pmatrix} = \vec{f}$. The linear equations resulting from the last two rows of A in the above matrix equation are precisely what we need; namely, $\sum_{s=-n}^{n} a_s = 1$ and $\sum_{s=-n}^{n} s^2 a_s = 0$. Thus the MWA formula under consideration is symmetric and reproduces cubics.

Section III: We are now ready to prove that the MWA formula under consideration has the minimum value of F+kS among all order n MWA fromulas which reproduce cubics, and that it is the only MWA formula which reproduces cubics which has this minimum value. The basic idea of the proof is borrowed from the development in the part 5 study note on graduation on pages 53-54.

Let $u_x = \sum_{s=-n}^{n} b_s \; u_{x+s}$ be an arbitrary MWA formula of order n which reproduces cubics, so in particular $\sum_{s=-n}^{n} b_s = 1$ and $\sum_{s=-n}^{n} s^2 b_s = 0$. Let α and β be arbitrary variables. Let $\vec{w} = \begin{pmatrix} b_{-n} \\ \vdots \\ b_n \\ \alpha \\ \beta \end{pmatrix}$. Consider the expression E defined by:

[illegible]

Expanding the expression, we get (since $A^T = A$)

$$E = \vec{w}^T A \vec{w} - \vec{f}^T \vec{w} - \vec{w}^T \vec{f} + \vec{f}^T A^{-1} \vec{f}.$$

Now $\vec{w}^T A \vec{w} = 2 \sum_{s=-n}^{n} b_s^2 + 2k \sum_{s=-n-z}^{n} (\Delta^z b_s)^2 + 2 \sum_{s=-n}^{n} b_s + 2 \sum_{s=-n}^{n} s^2 b_s,$

as was seen in the proof of Lemma 1. Since $\sum_{s=-n}^{n} b_s = 1$ and $\sum_{s=-n}^{n} s^2 b_s = 0$, we have

$$\vec{w}^T A \vec{w} = 2\sum_{s=-n}^{n} b_s^2 + 2k\sum_{s=-n-z}^{n} (\Delta^z b_s)^2 + 2\alpha$$

$$= 2F+2kS + 2b_o^2 - 2(1-b_o)^2 + 2\alpha$$

$$= 2(F+kS) + 4b_o + 2\alpha - 2.$$

Also, $\vec{f}^{\,T} \vec{w} = \vec{w}^T \vec{f} = 2b_o + \alpha$.

So $E = 2(F+kS) + 4b_o + 2\alpha - 2 - (2b_o + \alpha) - (2b_o + \alpha) + \vec{f}^{\,T} A^{-1} \vec{f}$

$= 2(F+kS) -2 + \vec{f}^{\,T} A^{-1} \vec{f}.$

Notice that $-2 + \vec{f}^{\,T} A^{-1} \vec{f}$ is a constant, so finding b's which make F+kS a minimum is equivalent to finding b's and α and β which make E a minimum.

Now if A^{-1} were positive definite we would be done; however, it is not, since A has two diagonal elements which are 0. However, under the hypothesis that $\sum_{s=-n}^{n} b_s = 1$ and $\sum_{s=-n}^{n} s^2 b_s = 0$, it is true that the expression E is always non-negative. To see this, let $A\vec{w}-\vec{f}=\vec{v}$. Then $E = (A\vec{v})^T A^{-1} (A\vec{v})_n = \vec{y}^T A\vec{v}$.
Let $\vec{y} = \begin{pmatrix} c_{-n} \\ \vdots \\ c_n \\ p \\ q \end{pmatrix}$. Then $\vec{y}^T A\vec{y} = 2\sum_{i=-n}^{n} c_i^2 + 2k\sum_{i=-n-z}^{n} (\Delta^z c_i)^2 + 2p\sum_{i=-n}^{n} c_i +$
$2q\sum_{i=-n}^{n} i^2 c_i$ as in the proof of lemma 1. But since $A\vec{w}-\vec{f} = A\vec{y}$, we know, by looking at the last two elements of each side of this equation, that $\sum_{i=-n}^{n} b_i - 1 = \sum_{i=-n}^{n} c_i$ and $\sum_{i=-n}^{n} i^2 b_i = \sum_{i=-n}^{n} i^2 c_i$. But since $\sum_{i=-n}^{n} b_i = 1$ and $\sum_{i=-n}^{n} i^2 b_i = 0$, we know that $\sum_{i=-n}^{n} c_i = 0$ and $\sum_{i=-n}^{n} i^2 c_i = 0$. Thus

$$E = \vec{y}^T A\vec{y} = 2\sum_{i=-n}^{n} c_i^2 + 2k\sum_{i=-n-z}^{n} (\Delta^z c_i)^2$$

and so, since $k \geq 0$, E is always non-negative under the assumed hypothesis. In fact, we see from the above equation that E takes on its minimum value of 0 precisely when $c_i = 0$ for $-n \leq i \leq n$. Since the b's were not arbitrary