CORRECTING MOMENT SEQUENCES FOR ERRORS ASSOCIATED WITH ADVECTIVE TRANSPORT

Here the goal is to adjust a single moment or, in the worse case, a few moments to correct for errors associated with advective transport so as to obtain a valid (i.e., physically consistent) moment set.

1. Difference tables

A useful approach to data analysis is based on the construction of difference tables. These are especially useful for spoting isolated errors in an ordered sequence of data (Lanczos, 1988), which is just what the moment correction problem requires. Construction of a difference table is simple and self-evident from inspection of the individual tables included in Table 1. Table 1a shows a difference table constructed for a sequence of six moments μ_k. The first column gives the moment index, *k*. The second column gives the 'data' to be evaluated, a sequence of values of $\ln \mu_k$. The i^{th}-order difference column is labeled d_i. Column 3 contains the first-order differences, d_1, which are differences of the elements in column 2. Column 4 contains the second-order differences, d_2, which are just the first-order differences of the elements in column 3, etc. The convexity requirement, a necessary condition for a valid moment sequence (Feller, 1971) is satisfied if and only if the second-order differences are non-negative. In Table 1a the higher-order differences vanish because for this case the $\ln \mu_k$ were assigned as a quadratic function of *k*. Thus the moments of Table 1a follow the pattern of the moments of a lognormal distribution: $\ln \mu_k = \ln \mu_0 + km + (ks)^2 / 2$ where μ_0 (particles per cc) is the normalization, *m* is the logarithm of the ratio of the count median radius (which is equal to the logarithm of the geometric mean radius) to the unit of length, and *s* is the logarithm of the geometric standard deviation (Hinds). Even multimodal distributions can have moments which follow the quadratic form (White, 1990; McGraw et al., 1995).

In general we cannot expect that $\ln \mu_k$ will have quadratic form, however it is reasonable to expect that $\ln \mu_k$ will be smooth function of index *k* and moment

interpolation methods have been developed that exploit smoothness in $\ln \mu_k$ (Frenklach, 2002; Diemer, 2002). In Table 1b the third moment has been changed and the modified sequence violates the required convexity condition. This violation is evident from the appearance of negative elements in the column of second-order differences, d_2. Note how the error propagates with amplified oscillation in sign through the higher-order differences. Here one sees the useful property of a difference table for spotlighting errors in sequence of data through inspection of higher-order differences (Lanczos, 1988). For sequences of six moments, we find that the third-order differences can be used to both attribute the error (i.e. identify the index of the miss-assigned moment) and provide an optimal correction in the sense of minimizing the sum of the squared differences of the elements in column d_2 so as to restore smoothness. (Note that the sum of squared differences of elements in column d_2 is just the squared magnitude of the vector $\mathbf{a} = \{-3, 9, -9\}$, in Table 1b, containing the third-order differences listed in column d_3. For the quadratic case the third-order differences vanish and $|\mathbf{a}|^2 = 0$).

k	$\ln\mu_k$	d_1	d_2	d_3	d_4	d_5
0	0	1	2	0	0	0
1	1	3	2	0	0	n
2	4	5	2	0	n	n
3	9	7	2	n	n	n
4	16	9	n	n	n	n
5	25	n	n	n	n	n

a

k	$\ln\mu_k$	d_1	d_2	d_3	d_4	d_5
0	0	1	2	-3	12	-30
1	1	3	-1	9	-18	n
2	4	2	8	-9	n	n
3	6	10	-1	n	n	n
4	16	9	n	n	n	n
5	25	n	n	n	n	n

b

Table 1. Moment sequences and first-order to fifth-order differences ('n' means no entry): (a) $\ln \mu_k$ is quadratic in index *k*. (b) Same as (a) except that the third moment has been changed resulting in a failure of the convexity criterion as evidenced by the negative entries in column d_2.

2. **Description of the algorithm**

Because corruption of moment sequences through advection tends to be infrequent, it is likely that this is due improper asignment of one, or at worse a few of the moments in the sequence. Accordingly, we want to adjust only *these* moments. It is known that a gross error in a single data point, e.g. the kind of error that can lead to the inconsistency of a moment sequence, tends to result in large and oscillatory values of the higher-order differences (Lanczos) (see Table 1). The following minimum square gradient algorithm restores a valid moment sequence by adjusting that moment , μ_{k*}, which after adjustment maximizes smoothness through minimization of $|\mathbf{a}|^2$. To illustrate the method, we begin by first determining the response of $|\mathbf{a}|^2$ to change in an arbitrary moment μ_k and next determine $k*$. (In actual calculations these steps are reversed as described below.) Consider a change in the k^{th} moment from an initial value $\mu_k(0)$ to a final value $\mu_k(1)$. Note by inspection of the difference table that if $\mu_k(1) = c_k \mu_k(0)$ or, equivalently, $\ln \mu_k(1) = \ln c_k + \ln \mu_k(0)$, then $\mathbf{a}_1 - \mathbf{a}_0 = (\ln c_k)\mathbf{b_k}$ where $\mathbf{a}_0$ and $\mathbf{a}_1$ are, respectively, the initial and final vectors of third-orer differences and the "response vectors" $\mathbf{b_k}$ give the change in the vector of third-order differences to a unit increment in $\ln \mu_k$. The latter are as follows:

$$\mathbf{b_0} = \{-1, 0, 0\}; \mathbf{b}_1 = \{3, -1, 0\}; \mathbf{b}_2 = \{-3, 3, -1\}; \mathbf{b}_3 = \{1, -3, 3\}; \mathbf{b}_4 = \{0, 1, -3\}; \mathbf{b}_5 = \{0, 0, 1\}, \tag{2.1}$$

which are related to the entries in the Pascal triangle except for oscillations in sign (Lanczos, 1988). Next consider the value of c_k (actually $\ln c_k$) for which $|\mathbf{a}_1|^2 = |\mathbf{a}_0 + (\ln c_k)\mathbf{b_k}|^2$ is minimized. Inspection of Fig. 1 shows that minimization is achieved for the condition that $\mathbf{a}_0 + (\ln c_k)\mathbf{b_k}$ is orthogonal to $\mathbf{b_k}$. The value of c_k that satisfied this condition is:

$$\ln c_k = -\cos(\mathbf{a}_0, \mathbf{b_k}) \frac{|\mathbf{a}_0|}{|\mathbf{b_k}|} = -\frac{(\mathbf{a}_0 \bullet \mathbf{b_k})}{|\mathbf{b_k}|^2} \tag{2.2a}$$

where

$$\cos(\mathbf{a}_0, \mathbf{b_k}) = \frac{(\mathbf{a}_0 \bullet \mathbf{b_k})}{|\mathbf{a}_0|\,|\mathbf{b_k}|} \tag{2.2b}$$

is the cosine of the angle formed between the vectors $\mathbf{a}_0$ and $\mathbf{b_k}$. The resulting minimum squared amplitude satisfies:

$$|\mathbf{a}_1|^2 = |\mathbf{a}_0 + \ln c_k \mathbf{b_k}|^2 = |\mathbf{a}_0|^2\left[1 - \cos^2(\mathbf{a}_0, \mathbf{b_k})\right] \tag{2.3}$$

which is the smallest reduction achievable by changing μ_k alone (Fig. 1).

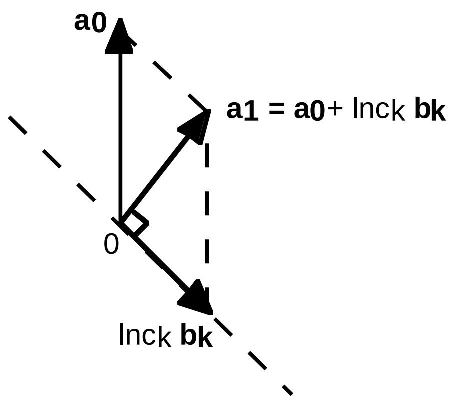

Figure 1: Disposition of the third order difference vectors before and after correction, $\mathbf{a}_0$ and $\mathbf{a}_1 = \mathbf{a}_0 + \ln c_k \mathbf{b_k}$ respectively.

Equation 2.3 shows that maximal smoothness is achieved by adjusting the moment, μ_{k*}, corresponding to that basis vector $\mathbf{b}_{\mathbf{k}*}$ which gives the largest $\cos^2(\mathbf{a}_0, \mathbf{b_k})$ for any moment index *k*. Thus by determining which *k* gives the maximum value of $\cos^2(\mathbf{a}_0, \mathbf{b_k})$, we obtain the index of the suspect moment, $k*$. That moment alone is corrected using the value of c_{k*} from Eq. 2.2a yielding an updated moment sequence. Recalling that $\mathbf{b_k}$ gives the third-order difference response to a unit change in $\ln \mu_k$, the actual change in the moment for $k = k*$ is:

$$\ln \mu_{k*}(1) = \ln \mu_{k*}(0) + \ln c_{k*} = \ln \mu_{k*}(0) - \frac{(\mathbf{a}_0 \cdot \mathbf{b}_{\mathbf{k}*})}{|\mathbf{b}_{\mathbf{k}*}|^2}. \qquad (2.4)$$

The other moments having $k \neq k*$ are unchanged. The new moment sequence gives the third-order difference vector $\mathbf{a}_1$ whose magnitude is in agreement with Eq. 2.3. The new moment sequence is in turn tested to insure that negative second-order differences have been removed. If not, the process repeated, replacing $\mathbf{a}_0$ by $\mathbf{a}_1$, and obtaining $\mathbf{a}_2$, etc. Equation 2.3 assures a reduction in the amplitude of the third order difference vector on each iteration. Thus the amplitude approaches zero after many interations, and $\ln \mu_k$ approaches a quadratic function of index k. In general, we do not anticipate that more than one or two passes through the algorithm wil be required in order to obtain a valid moment sequence.

3. Some examples

A single pass through the algorithm beginning with the moments of Table 1b restores the quadratic sequence of Table 1a. Here the maximum value of $\cos^2(\mathbf{a}_0, \mathbf{b}_\mathbf{k})$ in Eq. 2.3 is unity, which occurs for $k* = 3$. Thus $|\mathbf{a}_1| = 0$ for this case, which is the reason why a single pass through restores the quadratic sequence in $\ln \mu_k$. Note in Table 1b that the third-order difference vector is $\mathbf{a}_0 = \{-3, 9, -9\} = -3\mathbf{b}_\mathbf{3}$, which is understandable because $\mathbf{b}_\mathbf{3}$ gives the response to a unit change in $\ln \mu_3$ and in passing from Table 1a to Table 1b this quantity was changed by -3. To correct the third moment of Table 1b, we evaluate the right hand side of Eq. 2.2 to obtain

$$\ln c_3 = -(\mathbf{a}_0 \cdot \mathbf{b}_\mathbf{3}) / |\mathbf{b}_\mathbf{3}|^2 = -(-3\mathbf{b}_\mathbf{3} \cdot \mathbf{b}_\mathbf{3}) / |\mathbf{b}_\mathbf{3}|^2 = 3.$$

Finally from Eq. 2.4 we obtain $\ln \mu_3(1) = \ln \mu_3(0) + \ln c_3 = 6 + 3 = 9$ showing restoration of the moment sequence of Table 1a. In Table 2a, moments 3 and 5 both differ from those of Table 1a and convexity is not satisfied. After one pass through the algorithm

(Table 2b) the third moment has changed, but there is still a failure of convexity; although the sequence is smoother than before. After a second pass through the algorithm (Table 2c) the fifth moment has changed and convexity is satisfied for this and all subsequent iterations. The moment sequence of Table 2c passes all test and is readily invertable to get a set of three quadrature abscissas and three weights. The calculation would normally be stopped at this point and the updated moments (from Table 1e) taken as the corrected moments. However, here for the sake of illustration, we continue iteration. After eight interations (Table 2d) one sees clearly a reduction in higher-order differences, demonstrating convergence, and approach to quadratic form.

k	$\ln\mu_k$	d_1	d_2	d_3	d_4	d_5
0	0	1	2	-3	12	-33
1	1	3	-1	9	-21	n
2	4	2	8	-12	n	n
3	6	10	-4	n	n	n
4	16	6	n	n	n	n
5	22	n	n	n	n	n

a

k	$\ln\mu_k$	d_1	d_2	d_3	d_4	d_5
0	0	1	2	0.47368	-1.89472	1.736
1	1	3	2.47368	-1.42104	-0.15792	n
2	4	5.47368	1.05264	-1.57896	n	n
3	9.47368	6.52632	-0.52632	n	n	n
4	16	6	n	n	n	n
5	22	n	n	n	n	n

b

k	$\ln\mu_k$	d_1	d_2	d_3	d_4	d_5
0	0	1	2	0.47368	-1.89472	3.315
1	1	3	2.47368	-1.42104	1.42098	n
2	4	5.47368	1.05264	-0.00006	n	n
3	9.47368	6.52632	1.05258	n	n	n
4	16	7.5789	n	n	n	n
5	23.5789	n	n	n	n	n

c

k	$\ln\mu_k$	d_1	d_2	d_3	d_4	d_5
0	-0.671818	1.67182	1.74917	-0.117472	-0.040598	0.07681
1	1	3.42099	1.6317	-0.15807	0.03622	n
2	4.42099	5.05269	1.47363	-0.12185	n	n
3	9.47368	6.52632	1.35178	n	n	n
4	16	7.8781	n	n	n	n
5	23.8781	n	n	n	n	n

d

Table 2. Moment sequences and first-order to fifth-order differences: (a) moments 3 and 5 differ from the quadratic sequence in $\ln\mu_k$, (b) result after a single pass through the algorithm, (c) result after two passes gives a physically consistent moment set, (d) result after eight pass showing near convergence to quadratic form.

4. Necessary and sufficient conditions for a valid moment set

The most common, and easiest to check for, signature of an invalid moment set is its failure to satisfy convexity. However, convexity is a necessary but not sufficient condition for physically consistent moments. The full (necessary and sufficient) condition is more complicated but is a well-known result that can be in terms of Gramian determinants derived form the moments (Gordon, Vorobyev). The first few determinants in the series are:

$$\left|\mu_0\right|, \quad \begin{vmatrix} \mu_0 & \mu_1 \\ \mu_1 & \mu_2 \end{vmatrix}, \quad \begin{vmatrix} \mu_0 & \mu_1 & \mu_2 \\ \mu_1 & \mu_2 & \mu_3 \\ \mu_2 & \mu_3 & \mu_4 \end{vmatrix}, \quad \cdots \tag{4.1}$$

The necessary and suffient conditions for a valid moment set are that each of these determinants be greater than zero. These conditions for the first few moments $\{\mu_0, \mu_1, \mu_2, \mu_3\}$ are equivalent to convexity. However, for the fourth moment Eq. 4.1 requires the more stringent condition:

$$\mu_4 \geq \frac{\left(\mu_4 \begin{vmatrix} \mu_0 & \mu_1 \\ \mu_2 & \mu_3 \end{vmatrix} - \mu_2 \begin{vmatrix} \mu_1 & \mu_2 \\ \mu_2 & \mu_3 \end{vmatrix}\right)}{\begin{vmatrix} \mu_0 & \mu_1 \\ \mu_1 & \mu_2 \end{vmatrix}} \tag{4.2}$$

Note that if second determinant of Eq. 4.1 vanishes the distribution function corresponding to these moments is simply monodisperse and Eq. 4.2, which divides by this determinant, cannot be used.

Consider, for example a moment sequence (see difference Table 3a below), which satisfies convexity but fails moment inversion. Moments 0-3 are fine, and the second-order differences are all positive, but the fourth moment fails to satisfy the inequality of Eq. 4.2. Specifically, we see from the initial moments that convexity requires $\ln\mu_4 \geq 9$ while Eq.4.2 requires $\ln\mu_4 \geq 9.20908$; thus within the narrow range $9 < \ln\mu_4 < 9.20908$

convexity will be satisfied even though the moment sequence is still unphysical and will fail the inversion test. The moment fix algorithm needs to include this possibility, which can be done using, for example, the computational flow scheme of Fig. 2. Only a single pass through the algorithm is required to obtain a valid moment set (Table 3b).

k	$\ln\mu_k$	d_1	d_2	d_3	d_4	d_5
0	0.	1.	1.	0.	-0.9	4.5
1	1.	2.	1.	-0.9	3.6	n
2	3.	3.	0.1	2.7	n	n
3	6.	3.1	2.8	n	n	n
4	9.1	5.9	n	n	n	n
5	15.	n	n	n	n	n

k	$\ln\mu_k$	d_1	d_2	d_3	d_4	d_5
0	0.	1.	1.	0.	0.	0.
1	1.	2.	1.	0.	0.	n
2	3.	3.	1.	0.	n	n
3	6.	4.	1.	n	n	n
4	10.	5.	n	n	n	n
5	15.	n	n	n	n	n

Table 3. Moment sequences and first-order to fifth-order differences: (a) these moments satisfy convexity but fail the moment inversion test, (b) after a single pass through the algorithm a valid moment set is obtained.

The flow chart of Fig. 2 shows how both convexity and invertability can be separately handled in the correction algorithm. Furthermore, an inspection of the chart shows where diagnostic indicators can be placed to acquire statistics on the cases that convexity fails, that convexity passes but inversion fails, identify which moments tend to fail, number of passes through the algorithm required before a valid moment sequence is obtained, etc.

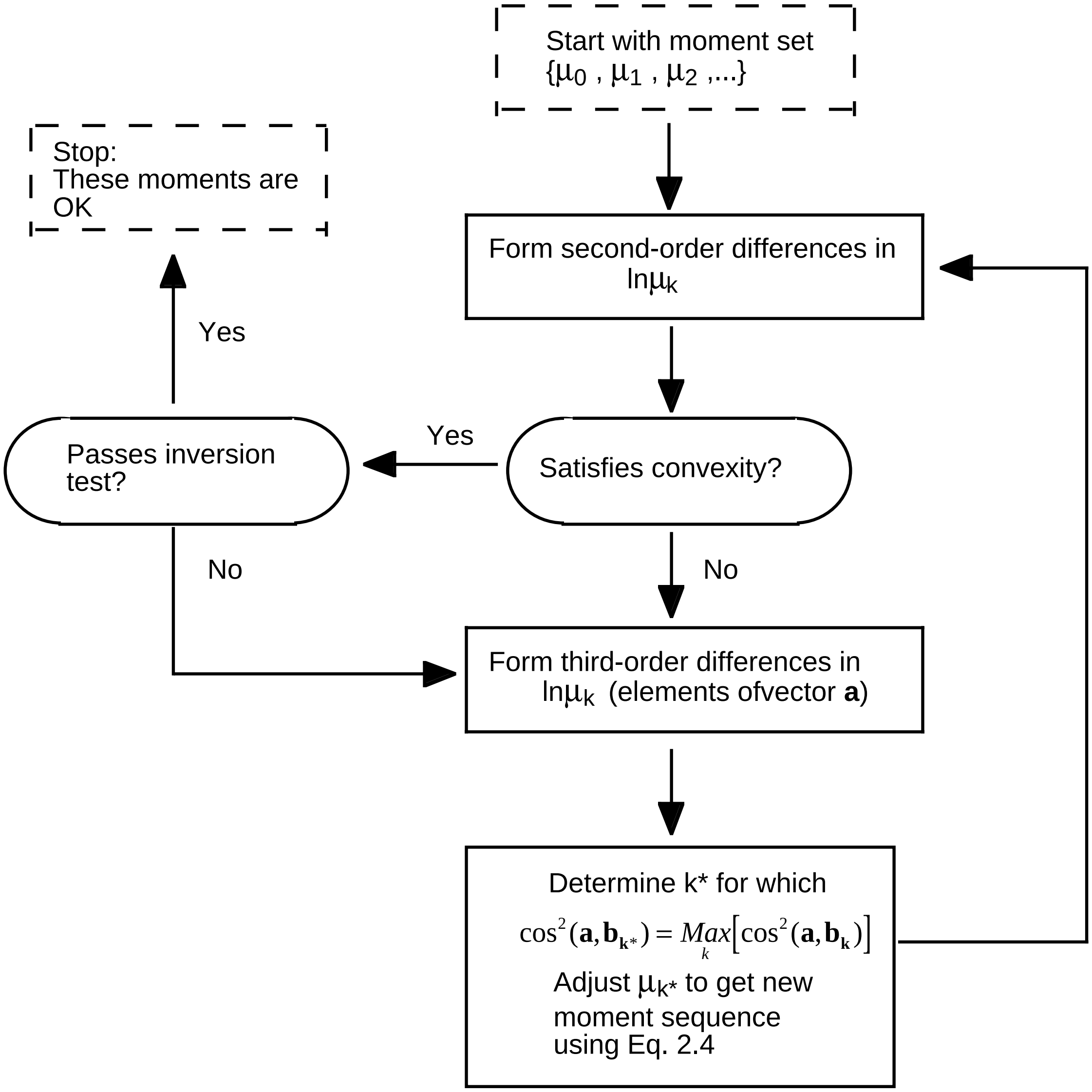

Figure 2: Flowchart of the computations used to generate a valid moment set.