Reply to Letter to the Editor by S. Rehder and U. Zier on 'Logratio analysis and compositional distance' by J. Aitchison, C. Barceló-Vidal, J. A. Martín-Fernández and V. Pawlowsky-Glahn

The main thrust of the letter from Rehder and Zier seems to be that they are unconvinced that the 'measure of compositional distance' between two D-part compositions x and X, defined by Aitchison (1983; 1986, p.193) as

$$\Delta_S(x, X) = \left[\sum_{i=1}^{D} \left\{ \log \frac{x_i}{g(x)} - \log \frac{X_i}{g(X)} \right\}^2 \right]^{1/2}$$

where $g(\cdot)$ is the geometric mean, is a metric in the usual mathematical meaning within the algebraic-geometric structure of the d-dimensional unit simplex

$$S^d = \{ (x_1, \ldots, x_D): x_i > 0 \ (i = 1, \ldots, D), \ x_1 + \ldots + x_D = 1 \}$$

where $d = D - 1$. Clearly a first goal in responding to this lack of conviction is to spell out again in detail the nature of the simplex sample space as used in compositional data analysis and how the metric arises.

The algebraic-geometric vector space structure of the unit simplex. The fundamental operations of change in the simplex are those of perturbation and power transformation motivated and spelt out by Aitchison (1986, pp. 42 and 120). In their simplest forms these can be defined as follows. Given any two D-part compositions

$x, y \in S^d$ their *perturbation* is

$$x \oplus y = C(x_1 y_1, \ldots, x_D y_D)$$

where C is the well known closure operation; and given a D-part composition $x \in S^d$ and a real number a the *power transformed composition* is

$$a \otimes x = C(x_1^a, \ldots, x_D^a)$$

Note that we have used the operator symbols $\oplus$ and $\otimes$ to emphasize the analogy with the operations of translation and scalar multiplication of vectors in R^d. It is trivial to establish that these operations define a *vector or linear space* structure on S^d.

The unit simplex as a metric vector space. We shall not spell out all the trivial proofs which establish that $\Delta_S(x, y)$ as already defined is a metric on S^d in the standard mathematical sense. We simply note, for example, the power transformation property (the analogue of the scalar multiple property of Euclidean distance in R^d):

$$\Delta_S(a \otimes x, a \otimes y) = \left| a \right| \Delta_S(x, y)$$

which seems to have been the main property that has eluded Rehder and Zier. The other metric requirements, that $\Delta_S(x, y) \geq 0$, $= 0$ if and only if $x = y$, $\Delta_S(x, y) = \Delta_S(y, x)$, $\Delta_S(x, z) + \Delta_S(z, y) \geq \Delta_S(x, y)$ are simply established.

The fact that this metric has also desirable properties relevant and indeed logically necessary, such as scale, permutation and perturbation invariance and subcompositional dominance, for meaningful statistical analysis of compositional data

has already been spelt in detail, for example in Aitchison (1992) and will not be repeated here.

The unit simplex beyond its metric vector space structure. It is possible to go to even more mathematical sophistication for the unit simplex if either theoretical or practical requirements demand it. For example the norm $\| x \|$ and inner product $\langle x, y \rangle$ consistent with the metric Δ_S and sought by Rehder and Zier (2001) are simply provided by

$$\| x \|^2 = \Delta_S^2(x, e) = \sum_{i=1}^{D} \left(\log \frac{x_i}{g(x)} \right)^2$$

where e is the identity perturbation $(1, \ldots, 1)/D$; and

$$\langle x, y \rangle = \tfrac{1}{2}(\| x \|^2 + \| y \|^2 - \Delta_S^2(x, y)) = \sum_{i=1}^{D} \log \frac{x_i}{g(x)} \log \frac{y_i}{g(y)}$$

Further, it is easy to show that the unit simplex with all this structure is essentially a d-dimensional Hilbert space with all the mathematical properties and facilities associated with such a space. In particular, it assures us of the existence of an isometry between S^d and R^d (Berberian, 1961). Such an isometry is, for example, the clr transformation,

$$clr(x) = \left[\log \frac{x_1}{g(x)}, \ldots, \log \frac{x_D}{g(x)} \right]^T$$

which is defined between the simplex and the hyperplane V of R^D, orthogonal to the unit vector $(1,\ldots,1)$ and which goes through the origin. This hyperplane is a d-dimensional

subspace of R^D and it is easy to see that the clr transformation is an isometry between S^d and V, as it is an isomorphism and the scalar product in S^d is by definition exactly the same as the scalar product in R^D constrained to clr-transformed compositions.

An interesting aspect of these extensions is that an inner product $\langle b, x \rangle$ can be expressed as

$$\sum_{i=1}^{D} \log \frac{b_i}{g(b)} \log \frac{x_i}{g(x)} = \sum_{i=1}^{D} a_i \log x_i$$

where $a_i = b_i / \log(b)$ $(i = 1, \ldots, D)$ and so $a_1 + \ldots + a_D = 0$; thus inner products play the role of logcontrasts, well established as the compositional 'linear combinations' required in many forms of compositional data analysis such as principal component analysis and investigation of subcompositions as concomitant or explanatory vectors (Aitchison and Bacon-Shone, 1984; Aitchison, 1986, Chapters 8 and 12).

On subcompositional dominance. Rehder and Zier seem to doubt the good sense of expecting a metric used for practical purposes to display subcompositional dominance. A scientist working with a full vector of measurements in R^d would be surprised to find that the use of a recommended metric produced a smaller scalar measure of difference between two vectors than another scientist comparing subvectors of these full vectors; and, of course, the Euclidean metric in R^d possesses such a property. Just consider a simple example such as two vectors $x = (x_1, x_2)$ and $y = (y_1, y_2)$ in real space. Everybody would be surprised if Euclidean distance in R^2 between x and y was smaller than Euclidean distance in R^1 between x_1 and y_1 or between x_2 and y_2. Since subcompositions are essentially the 'marginals' of compositional vectors we clearly expect a similar property of a compositional metric. A geologist with information only on the (MgO,

CaO, FeO) subcompositions derived from 10-part major oxides of limestone surely cannot see more variability then the scientist in possession of the full vectors.

The history of the compositional metric. The history of the metric may shed some light on the origins of some of the confusions that have arisen. Aitchison's (1983; 1986, p.193) original purpose in suggesting Δ_S as a suitable measure of compositional distance was to provide a measure which conformed with measures of variability derived from the usual covariance matrix approach, similar to the relationship for R^d between the sum of squared Euclidean distances between all pairs of data vectors and the trace of the estimated covariance matrix. For a N x D compositional data matrix X total variability as measured by the trace of the centered logratio covariance matrix is equal to

$$(N(N-1))^{-1}\sum_{m<n}^{D}\Delta_S^2(x_m,x_n)$$

so the metric Δ_S provides a similar conformity of intra- and inter-compositional measures of variability, a clearly desirable property. The attempt to further justify the metric arose from the argument in a series of letters (Aitchison 1989, 1990, 1991, 1992; Watson 1990, 1991; Watson and Philip 1989) over the claim by Watson and Philip that their 'angular measure' of difference between two D-part compositions, defined as rays in R_+^D, is the *unique* such measure. It is the fact that the reasoning used in Aitchison (1992) necessarily used the Watson and Philip perfectly valid sample space of rays in the positive orthant R_+^D and recognized compositions as equivalence or compositional classes that seems to have introduced confusion. For example, they do not recognize that criterion C2 of Aitchison (1992) has nothing to do with a *metric* scale invariance axiom, but is merely saying that any distance measure between two compositional

classes should not depend on which compositions within the class are used as representatives of the class. The metric property that Rehder and Zier are seeking has been discussed above. It is important to make the distinction between arguments relating to the ray space approach and the unit simplex approach in defining what are necessary requirements of a compositional metric. Both lead by motivated arguments to valid conclusions that our compositional metric is specially suited to compositional problems.

The Euclidean distance as a compositional metric. In our view the Euclidean metric is completely unsuited to work in the simplex sample space (Martín-Fernández et al., 1998). The principal reason for this is that it does not match the algebraic-geometric structure of the simplex space in that it has no simple perturbation or power transformation properties. In particular it is not suited to subcompositional analyses; it does not satisfy the subcompositional dominance requirement.

Non-metric measures of difference. There seems to be an implication in the early part of Rehder and Zier's letter that there are useful non-metric measures of difference used in statistical analysis. We entirely agree and some of us have used such measures extensively in our work as, for example, in the use of the non-metric Kullback-Leibler directed divergence between two probability distributions (Aitchison, 1981) or between compositional data (Martin, 1998; Martín-Fernández et al., 1999). Our advocacy of the compositional metric is that it is perturbation and power friendly and conforms to established intra-compositional variability methodology.

The logratio transformation approach. The purpose of Aitchison (1982, 1986) as expositions on compositional data analysis was to attempt to convince statisticians that there was a valid methodology associated with simplex sample spaces. With the long-established success of transformation techniques, from the original McAlister's (1879) logarithmic transformation, through square-root, arcsin and other transformations in analysis of variance, through the more general normalizing and variance stabilizing Box-Cox transformations to those involved in the massive application of generalized linear models, it seemed natural to present the methodology in terms of such a transformation, from a simplex to a real space, and with the knowledge that there were available a whole gamut of standard multivariate methods and software for real vectors. In this context Rehder and Zier's disparagement of Aitchison's recipe for success, or summary of his methodology: 'Transform your compositional data into compatible logratios', seems to overlook the detailed analysis in Aitchison (1986) and subsequent publications. For example, it must be clear to any impartial reader that Aitchison (1986) was fully aware of difficulties that might arise from the use of the asymmetric logratio transformation alr. For example, in Chapters 5 and 8 he is meticulous in ensuring that his methods involving alr transformations are permutation invariant. Readers of these arguments would realize that the 'neutralizing' matrix H is introduced to ensure this invariance. It seems to us remarkable that, with the compositional metric Δ_S as already defined and its alr counterpart defined by

$$\Delta_S^2(x, y) = \{alr(x) - alr(y)\} H^{-1} \{alr(x) - alr(y)\}^T$$

Rehder and Zier persist in using an incorrect measure

$$\{alr(x) - alr(y)\}\,\{alr(x) - alr(y)\}^{T}$$

in their misplaced criticism of the correct metric.

In their remarks on the logarithmic transformation and lognormal distributions Zier and Rehder seem to be questioning the use of transformation techniques in general in statistical analysis, and by implication have a view that statisticians involved in such practice are naïve. To imply that a statistician transforming positive data logarithmically to R^1 and using normal distribution analysis will arrive at different statistical inferences from one staying in R_+^1 and using lognormal distribution analysis shows a lack of understanding of current and past statistical practice. Indeed they seem to be unaware of the huge literature, both theoretical and practical, on this subject over the last century. For the logarithmic transformation and the lognormal transformation their warning that $\log(E(X)) \neq E(\log(X))$ was recognized and resolved over a century ago by Galton (1879) and McAlister (1879) in their advocacy of the geometric mean as a 'measure of central tendency' for positive and positively skewed measurements. More recently concentration on the concept of *link functions* in generalized linear modeling addresses the same problem. The argument turns on what are such sensible 'measures of central tendency' for strange sample spaces. For compositional analysis the center

$$\xi = cen(x) = C[\exp\{E(\log(x))\}]$$

fulfils this purpose, and has a property analogous to that of the vector mean in real space: ξ minimizes $E\,(\Delta_S\,(x,\,\xi))$. Stay in the simplex and compute cen(x) or transform logratio-wise, to R^d, compute the standard mean vector and inverse transform back to the simplex and you are in agreement.

The stay-in-the-simplex approach. In some respects in the development of our statistical methodology for compositional data analysis we wish we had avoided the transformation approach and remained solidly in the simplex with all our arguments. N. I. Fisher , in the discussion of Aitchison (1982), made the comment that 'one is ultimately better off working within the confines of the original geometry [of the sample space] and with techniques particular thereto.' For compositional data analysis this is readily achieved and we are currently presenting and working on research to achieve this. A simple example may suffice to give the flavor of such an approach. The singular value decomposition, which is at the heart of any multivariate analysis, takes the following form. Any N x D compositional data matrix X with nth row composition x_n can be decomposed in a perturbation-power form as follows

$$x_n = \xi \oplus (u_{n1}s_1 \otimes \beta_1) \oplus \ldots \oplus (u_{nR} s_R \otimes \beta_R)$$

where ξ is the center of the data set, the s's are positive 'singular values' in descending order of magnitude, the β's are compositions, R is a readily defined rank of the compositional data set and the u's are power components specific to each composition. This decomposition is intimately connected with logcontrast principal component analysis, questions of the dimensionality of the data set, compositional biplots, differential perturbation processes (Aitchison and Thomas, 1998), and to compositional regression analysis. It is clear that while mathematically sophisticated scientists may find such an approach attractive, it may be some time before the mathematical training of scientists makes such concepts attractive to the less numerate.

Convex mixture models. Rehder and Zier claim that 'most of the processes like mixing in the original space are linear.' We can find no evidence for this statement. If

conservation of mass is induced in support of this, we would be forced to ask the question in what way can compositional data ever support a conservation-of-mass hypothesis: *compositions carry no information about mass*. The process producing the compositional data could be otherwise, for example metamorphic, metasomatic, weathering, in which case the differential perturbation model may be more instructive in determining the nature of the process. We are happy to accept that compositions can be analyzed *within models which assume conservation of mass* and indeed have done so ourselves, for example in the analysis of pollution sources through the study of convex linear combinations of compositions in Aitchison and Bacon-Shone (1999).

The additive nature of such modeling does not mean that basic principles of compositional data analysis are thereby neglected. For example our approach to the so-called endmember problem where a set of say C endmember compositions $\beta_1, \ldots, \beta_C$ is sought such that each composition x_n $(n = 1, \ldots, N)$ of the data set can be expressed as a convex linear combination ξ_n of $\beta_1, \ldots, \beta_C$, uses as criterion of success the magnitude of

$$\sum_{n=1}^{N} \Delta_S^2 (x_n, \xi_n)$$

while monitoring the magnitude of

$$\sum_{b<c} \Delta_S^2 (\xi_b, \xi_c)$$

Algorithms for such a process are now readily available and, for example, provide a criterion which could be compared with the fit of a differential perturbation process in assessing whether a mixture or perturbation process is more realistic to explain the compositional variability.

Scale invariance. It is unfortunate that the words scale and scalar enter into this discussion with three different meanings, in the compositional scale invariance argument that leads to the advocacy of compositional analysis in terms of ratios, in terms of a desirable property of compositional equivalence classes and in one of the axioms in the mathematical definition of a metric. We apologize for any confusion that we have caused in this overuse of the terms and would encourage any introduction of terminology, which removes this confusion. As far as its compositional meaning is concerned we hold fast to ensuring that a, possibly the, safe way to ensure sensible interpretation of compositional variability is to express compositional problems in terms of ratios of components. In our view a problem is compositional if and only if it can be expressed in terms of such ratios. In other words, the problem does not arise, as Rehder and Zier imply, from the compositional scale invariance criterion; it is resolved by the scale invariance criterion.

Granulometric data as compositional data and histograms. Granulometric data obtained by sieving techniques are not histograms, as commonly defined, but are weight (or volume) $\times$ diameter profiles. Mathematically they are third moment distributions of the basic grain diameter distribution, a fact apparently first noted by Hatch (1933); see also Aitchison and Brown (1956) for further details and its relation to the Kolmogorov (1941) breakage model. Thus it could be argued that fitting a probability distribution to such an object is every bit as weird as considering the profile as a composition. Indeed to move from a weight $\times$ diameter profile to a diameter histogram is nothing more than a perturbation operation. For example if the weight $\times$ diameter profile has H diameter intervals $I_1, \ldots, I_H$, with centers $d_1, \ldots, d_H$ and with associated proportional weights

$p_1, \ldots, p_H$, then on the assumption of uniform specific gravity, the diameter histogram $q_1, \ldots, q_H$ is approximated by the perturbation $[d_1^{-3}, \ldots, d_H^{-3}] \oplus [p_1, \ldots, p_H]$. A consequence of the perturbation invariance property of the compositional metric Δ_S is that the distance between profiles is the same as between histograms, a clearly desirable property.

We have already stated in Aitchison et al (2000) that whether grain-size data is considered as grouped ordinal data and some class of univariate distributions is used to characterize each such 'histogram' or each histogram is considered a compositional vector is certainly an open question. In our view, in situations where the objective is to compare a number of weight $\times$ diameter profiles, until a satisfactory class of distributions giving good fits to the histogram emerges, the treatment of such data as compositional is certainly viable, with possibilities of inferring the nature of an underlying process through the study of possible differential perturbation processes.

Zier and Rehder put forward a challenge that they look forward to reading the first paper with the general advice: 'Follow Aitchison's simple principles of compositional data analysis, logtransform (presumably the intention is logratio transform) your histograms.' Anything that we write on the subject will certainly not be the first. Sediment compositions reported as (sand, silt, clay) compositions are just such weight $\times$ diameter profiles and have been traditionally treated as compositions for many decades. An example of a successful modeling as a differential perturbation process is to be found in Aitchison and Thomas (1998). They should also search the statistical literature more carefully. There is a huge statistical literature on the use of log odds (logratios of probabilities or frequencies) in statistical analysis, both Bayesian and non-Bayesian, for example in contingency table analysis, which often involve comparisons in effect of histograms, often with groupings on an ordinal scale; on the

use of likelihood ratios (again logratios of probabilities); in logistic regression where the basic transformation is a logratio of probabilities sometimes associated with an ordinal scale. There are also many studies in which subjects are invited to make probabilistic statements concerning a finite number of hypotheses. In studying variability between subjects or groups of subjects in such studies it is certainly useful to have available a measure of difference between probability statements and the compositional metric provides one such measure with sensible properties. For example, subcompositional coherence provides a necessary form of conditional probability coherence (Aitchison, 2001). Among other measures of differences between probability distributions or histograms some such as the Kullback-Leibler divergences involve logratios. Until such time as Rehder and Zier are prepared to make their criticism constructive by producing some overwhelmingly convincing measure of difference for histograms or some superior form of compositional data analysis we would encourage geologists to persevere with the current form of simplicial analysis.

The two major fallacies of Zier and Rehder (1998). Although Aitchison et al (2000) has already refuted the original claim by Zier and Rehder (1998) and now repeated in Rehder and Zier (2001), that their 'single example can disprove the logratio method', let us again point out the two major fallacies in their argument.

(1) The claim by Zier and Rehder (1998) that the logratio distance *they* use is not invariant is true *but* it is not the compositional metric we advocate, as we have already clearly pointed out in detail in Aitchison et al (2000). Moreover, the peculiar limiting properties they ascribe to the incorrect metric do not apply to the correct metric Δ_S . Specifically, if p is any perturbation, then

$$\Delta_S (x, p \oplus x) = \Delta_S (e, p) = \| p \|$$

which varies with p and $\to 0$ as $p \to e$, the identity perturbation.

(2) The other persistent argument is that the compositional metric Δ_S warps the vector space or distorts the Euclidean metric. This is a curious argument in view of the fact that it is Δ_S that is the natural metric associated with the $\oplus$ and $\otimes$ operations of the simplex vector space, so that the distorting culprit is the blind application of the non-metric Euclidean difference to a space for which it was never designed. This seems to be somewhat similar to a flat-earth approach to distance on the sphere, say $x^2 + y^2 + z^2 = r^2$. Would Rehder and Zier advocate the Euclidean metric $\sqrt{\{(x_1 - x_2)^2 + (y_1 - y_2)^2 + (z_1 - z_2)^2\}}$? We would prefer great circle distance

$$r \arccos\{(x_1 x_2 + y_1 y_2 + z_1 z_2)/r^2\}$$

in order to ensure that our aircraft has enough fuel for its practical purpose.

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