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Revisiting the Geometry of a Ternary Diagram With the Half-Taxi Metric[1]

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An alternative definition of distance is presented for observations plotted in a ternary diagram and, more generally, for observations in a compositional data set. This definition, which conforms to the triangular coordinate system of the ternary diagram, is compared to other distance measures, and is shown to be tied to the covariance structure of compositional data. Angular differences are also discussed briefly in an Appendix.

KEY WORDS: compositional data, taxicab or city block metric, theory of random graphs, partial correlation, correspondence analysis.

INTRODUCTION

Geologists are probably the scientists most familiar with examples of compositional data, where all the responses are nonnegative and sum to one for each observation. Although there are many examples of such multivariate data in geology and chemistry, they are also found in other areas of research. A marketing example is given by DeSarbo, Ramaswamy, and Lenk (1993), where the responses for a sample of households are the proportions of television viewing time of national networks. The proportions or percentages in a compositional data set are sometimes referred to as the intensive variables, which result from normalizing the raw counts or masses (the extensive variables) of a parent data set by dividing by the total count or mass for each observation. The proportions then contain only information about relative magnitudes and so, as noted by Greenacre (1984), this transformation tends to emphasize the shape rather than the magnitude of the outcomes. However, there are other reasons for converting to proportions, such as when a nuisance variable affects the amounts, but not the relative amounts, of an outcome of interest.

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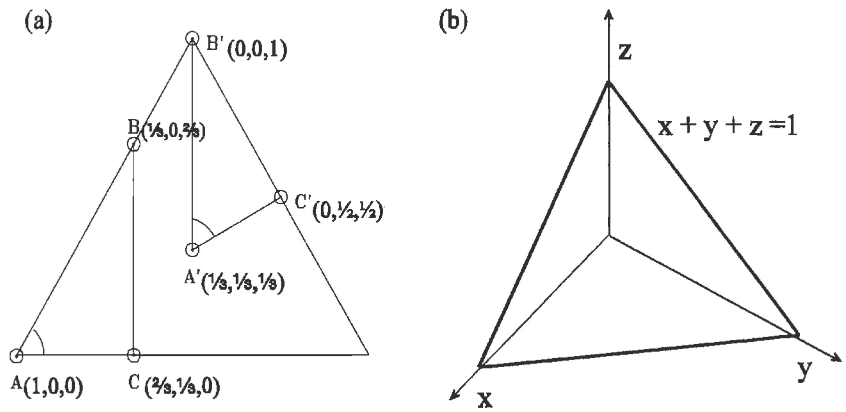


Figure 1. (A) Reference triangle for the ternary diagram, where the coordinates (t_1, t_2, t_3) are the proportions. The smaller triangles within the diagram provide a counterexample to the side-angle-side property. Using the half-taxi metric, which is introduced in the second section of the text, $\angle BAC = \angle B'A'C' = 60°$, $d(A, B) = d(A', B') = 2/3$ and $d(A, C) = d(A', C') = 1/3$; however, $2/3 = d(B, C) \neq d(B', C') = 1/2$. (B) A representation of the reference triangle in Cartesian space, where its interior is the intersection of the plane $x + y + z = 1$ and the positive octant (i.e., all coordinates positive). It is also possible to view the reference triangle as the result of an affine transformation.

It has long been the practice of geologists to present compositional data with three components in a ternary diagram, a two-dimensional graph with a triangular coordinate system. An early example of its use is found in a paper by Reid (1902). The interior of the ternary diagram can be regarded as that part of the plane $x + y + z = 1$ which lies in the positive octant (Fig. 1). Compositional data with four parts can be displayed within a tetrahedron, also referred to as a quaternary diagram. Compositional data with n parts can, at least in theory, be displayed in an $(n - 1)$-dimensional simplex with n vertices.

An indication that the ternary diagram is becoming more widely applied is its inclusion in standard statistical packages, such as JMP® (SAS Institute, 1995) and SigmaPlot® (SPSS Inc., 2000). However, geologists and others have long questioned the meaning of patterns in ternary diagrams, which could be explained by the closure imposed on the variables. For example, compositional data with just two components t_1 and t_2 has perfect negative correlation between the components, because they are complementary (i.e., $t_2 = 1 - t_1$). Chayes (1971) has shown that, for data with three components, correlations are completely determined by the variances, and he has also shown that there is a bias toward negative correlation. Drawing upon Chayes' work, Butler (1979) has shown how linear trends and curvilinear trends in ternary plots are tied to the covariance structure. These facts are related to the spurious correlations that result from forming ratios of random variables (Chayes, 1971; Pearson, 1897).

To resolve these complications for interpretation, several transformations have been proposed for compositional data. Many of them are reviewed by Aitchison (1986), who himself has suggested a log-ratio transformation which has been widely applied in conjunction with standard statistical methods. One example is its application in a principal components analysis (Aitchison, 1983). However, because the log-ratio transformation is not defined for a composition if any component is zero, alternative transformations (Baxter, Cool, and Heyworth, 1990; Underhill and Peisach, 1985) have been suggested which use correspondence analysis. One effect of the log-ratio and other transformations is to give more equal weight to the variables, and so prevent gross differences between compositions from dominating an analysis.

Although more attention has been given to the covariance structure, researchers have also addressed the question of how differences might be defined for compositional data in general, and the ternary diagram in particular. For example, Philip and Watson (1988) and Stanley (1990) define an angular measure of difference, and Aitchison (1992) uses the log-ratio transformation with Euclidean distance. The choice of such a measure is certainly relevant to applications like cluster analysis and outlier detection. For the cluster analysis of compositional data, DeSarbo, Ramaswamy, and Lenk (1993) compare a maximum likelihood approach to a method which utilizes the Aitchison transformation, and with respect to outlier detection, Barceló, Pawlowsky, and Grunsky (1996) discuss the use of the log-ratio transformation and Box-Cox transformations.

An exhaustive review of compositional data analysis is not given here, but, generally speaking, previous research has focused on using various transformations in tandem with standard statistical methods. In contrast, this paper presents an alternative definition of distance without yet suggesting how it might be applied. Instead, it goes back to a more elementary position, in order to determine whether a better understanding of the underlying geometry can increase our comprehension of various aspects of compositional data.

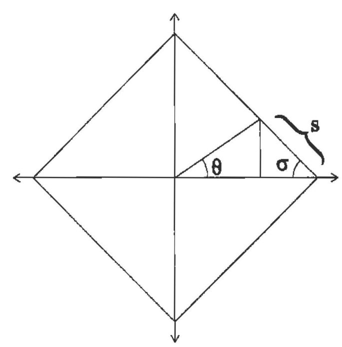
HALF-TAXI DISTANCE

A convenient way of defining a two-dimensional geometry for a surface, say the Cartesian plane, is to define an inner product on it. The standard inner product for the plane is the dot product of Euclidean geometry, and it single-handedly determines definitions of distances, angles, and trigonometric functions. Short of an inner product, we can at least provide for what we mean by distance by defining a metric on the surface. A metric function d, a generalization of our concept of distance, satisfies the following properties for any points

p, q, and r:

$$\begin{aligned} &d(p, p) = 0 && \text{(reflexive property)} \\ &d(p, q) = d(q, p) && \text{(symmetric property)} \\ &d(p, q) + d(q, r) \geq d(p, r) && \text{(triangle inequality)} \end{aligned}$$

The best-known example of a metric for the Cartesian plane is the Euclidean definition of distance, namely $d(p, q) = [\sum(p_i - q_i)^2]^{1/2}$ for points p and q with coordinates (p_1, p_2) and (q_1, q_2). Another example is the taxicab or city-block metric (Krause, 1986) where distance is defined as $d(p, q) = \sum |p_i - q_i|$. Because differences are squared, Euclidean distance gives greater weight to the components with large differences. On the other hand, contributions of the different components are more equitable for the taxicab metric. For instance, points with coordinates (4, 4) and (7, 1) have the same taxicab distance, but not the same Euclidean distance, from the origin (0, 0). The taxicab metric can also be referred to as the diamond metric, because a taxicab "circle" (i.e., the locus of points equidistant from a specified point) is diamond-shaped in this geometry, in contrast to the familiar circle of Euclidean geometry. Taxicab geometry has some interesting parallels with Euclidean geometry (Fig. 2). An introduction is given by Krause (1986), who indicates how it might be applied to city planning. In contrast to Euclidean distance, the taxicab metric depends somewhat on the direction of one point relative to another. In other words, the distance from a fixed point is anisotropic (i.e., not isotropic). Figuratively speaking, within the taxicab



θ′ = (s / radius)

so s = θ′ <in taxicab radians>

= θ · (π_taxi / 180°) <in degrees>

= θ / 45° <because π_taxi = 4>

But ½ = cos(45°) = cos(σ)

= (1 - cos(θ)) / s

= (1 - cos(θ)) / (θ / 45°)

Solving for cos(θ), we have

cos(θ) = 1 - (θ / 90°) for 0 ≤ θ ≤ 180°

Figure 2. The unit circle of taxicab geometry, $|x| + |y| = 1$, is shown in the $x - y$ plane. The ratio of the circumference of the unit circle to its diameter is $\pi_{\text{taxi}} = 4$ for the taxicab metric. The derivation at right demonstrates that, for an angle with θ degrees, $\cos(\theta) = 1 - (\theta/90°)$ on the interval (0°, 180°). Akça and Kaya (1997) have also shown that $\cos(\theta) = -3 + (\theta/90°)$ on the interval (180°, 360°). Therefore, the cosine function in taxicab space is a linear function of the angle. Additional derivations would show that $\sin(\theta) + \cos(\theta) = 1$, which is analogous to $\sin^2(\theta) + \cos^2(\theta) = 1$, a familiar trigonometric identity of Euclidean geometry.

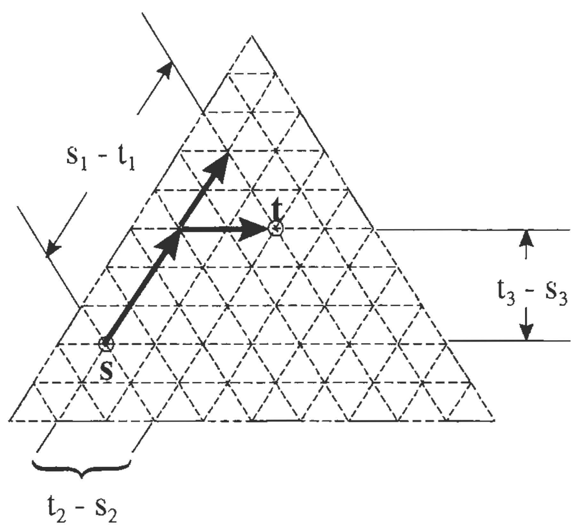


Figure 3. An illustration of the equivalence of Equations (1) and (3), where the compositions s and t have been arbitrarily chosen so that $s_1 > t_1$, $t_2 > s_2$, and $t_3 > s_3$.

space our Euclidean ruler appears to shrink or expand as we point it in different directions.

The Euclidean definition of distance is viewed as natural, due to assumptions that we make about the physical space in which we live. We now define a distance which can be viewed as natural to the ternary diagram, given certain assumptions. We define two compositions in a ternary diagram as being "close" if their proportions overlap considerably for corresponding components. Mathematically, this means that we define the distance between compositions s and t as

$$d(s,t) = 1 - [\min(s_1,t_1) + \min(s_2,t_2) + \min(s_3,t_3)] \tag{1}$$

where $\min(s_i, t_i)$ is the minimum value for the ith components. In Figure 3, s and t have been chosen arbitrarily so that $s_1 > t_1$, $t_2 > s_2$, and $t_3 > s_3$. If we now regard $d(s,t)$ as the distance of the shortest path over the triangular coordinate lines, then

$$d(s,t) = (t_2 - s_2) + (t_3 - s_3) = s_1 - t_1 \tag{2}$$

$$\text{so that } d(s,t) = \frac{1}{2}[(s_1 - t_1) + (t_2 - s_2) + (t_3 - s_3)]$$

$$= \frac{1}{2}[|s_1 - t_1| + |s_2 - t_2| + |s_3 - t_3|]$$

It also follows from (2) that

$$\begin{aligned} d(s,t) &= (t_2 - s_2) + (t_3 - s_3) \\ &= t_2 + t_3 - s_2 - s_3 \\ &= 1 - t_1 - s_2 - s_3 \\ &= 1 - \min(s_1, t_1) - \min(s_2, t_2) - \min(s_3, t_3) \end{aligned}$$

Therefore, this illustrates that definition (1) is equivalent to

$$d(s,t) = \frac{1}{2}[|s_1 - t_1| + |s_2 - t_2| + |s_3 - t_3|] \tag{3}$$

which is a rescaled version of the taxicab metric. (A formal proof of equivalence for all dimensions uses mathematical induction.)

Because the "half-taxi" distance is proportional to the taxicab metric, it is also a metric, and it is natural to assume that other properties are transferred to it. However, its unit circle is not a diamond. To illustrate this, we can view the ternary diagram in terms of the reference triangle found in the positive octant of Cartesian space (see Fig. 1), but under the taxicab metric. The taxicab equivalent of a sphere is an octahedron. The Euclidean sphere has the nice property of having the same shape in all directions, so that each nontrivial slice is a circle. However, the shape of the octahedron is not the same in all directions. The plane containing the reference triangle is parallel to one of the faces of the octahedron, and a slice in this direction is a hexagon (Fig. 4).

In other respects the taxicab and half-taxi metrics are similar. For instance, taxicab geometry fails the side-angle-side property of Euclidean geometry. This property states that, if two sides and the included angle of one triangle are equal

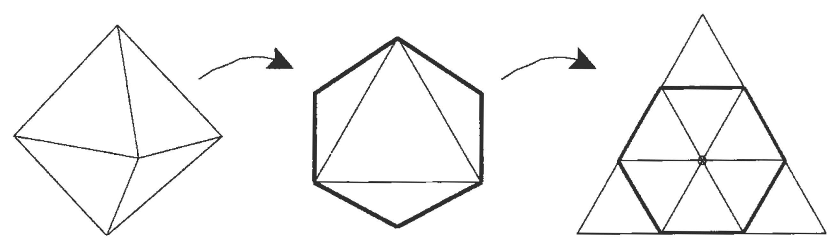


Figure 4. Two views of the octahedron, together with the ternary diagram, suggest the connection between a slice of the octahedron and the half-taxi circle. The first frame shows the octahedron from the side. The second frame presents an oblique view of the same octahedron, in order to suggest how a slice of it can be hexagonal. The final frame shows the ternary diagram and a half-taxi circle with radius 1/3 and center (1/3, 1/3, 1/3). The ratio of the circumference of the half-taxi circle to its diameter is $\pi_{\text{half-taxi}} = 3$.

to the corresponding parts of a second triangle, then they must be congruent. A counterexample for the half-taxi metric is shown in Figure 1.

The taxicab and the half-taxi metrics also have similar geometric interpretations. In examples given to describe taxicab geometry, the taxicab distance for any two points that lie on the rectangular grid is equivalent to the distance of a minimum path that follows the grid.

AITCHISON DISTANCE

As mentioned, the log-ratio transformation suggested by Aitchison has been widely applied to compositional data. For this transformation, the ith component t_i of a composition t is reexpressed as $\log(t_i/g(t))$, where $g(t)$ is the geometric mean of the composition. This is equivalent to centering the log-transformed components with respect to their mean. For the ternary diagram the log-ratio transformation is a mapping from the interior of the reference triangle to the plane. After the transformation is performed, the Euclidean metric can be applied to the transformed data, which resides in the unbounded plane. However, if we define the "Aitchison distance" for two points s and t as the composition of the log-ratio transformation with the Euclidean metric function, the resulting function

$$d(s,t) = \sqrt{\sum_i [\log(s_i/g(s)) - \log(t_i/g(t))]^2}$$

is applied directly to the ternary coordinates. We can then take a view similar to one found in Riemannian geometry (O'Neill, 1966, Chap. 7), and regard the ternary diagram as a surface which has a geometric structure induced by the Aitchison distance. This view is illustrated by Figure 5(A), which shows some contours of

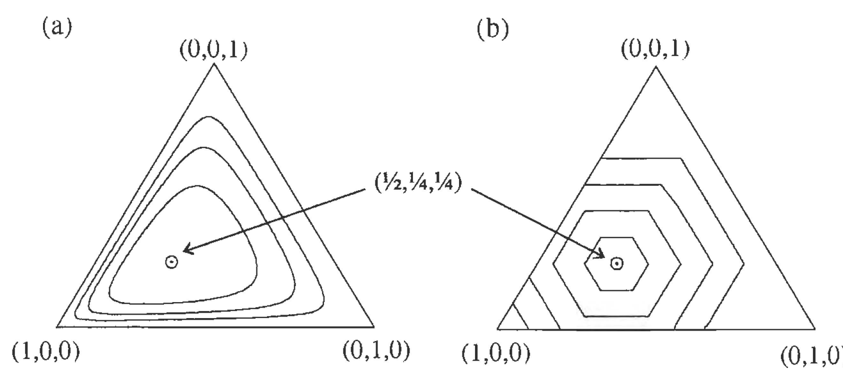
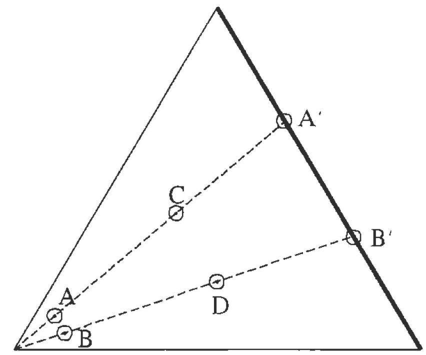


Figure 5. Some contours of equal distance from the point (1/2, 1/4, 1/4) for (A) the Aitchison distance and (B) the half-taxi distance.

equal distance from the point (1/2, 1/4, 1/4). In other words, this displays some "Aitchison circles" with common center (1/2, 1/4, 1/4). The Aitchison distance, like the half-taxi distance, depends to some extent on direction, but the distance between two points depends more on location, that is, how close each point is to an edge of the ternary diagram. This is reminiscent of what occurs in models of hyperbolic geometry. Just as O'Neill (1966) suggests in his description of one such model, our Euclidean ruler appears to shrink as we approach an edge of the ternary diagram, and Aitchison circles become increasingly distorted (i.e., relative to Euclidean circles) as the center of a circle moves closer to an edge. Although a pair of points near an edge might appear to us to be the same distance apart as a pair of points near the center of the reference triangle, the distance between the first pair is larger if we use the scale of Aitchison distance.

Aitchison (1992) has compared some distance measures for compositional data with respect to various properties. Most of the distances, including the Aitchison distance, satisfy the property of being a metric. However, another property that he mentions is related to the important observation in Aitchison's work that ratios of components are invariant for a composition and its subcompositions. One of the strengths for using the Aitchison transformation is that it establishes a familiar relationship between compositions and subcompositions. For instance, when the log-ratio transformation is applied, the covariance structure of the transformed compositional data is completely determined by the covariance structure of its two-part subcompositions, which corresponds to the situation for multivariate normal data. This fact is related to what Aitchison calls subcompositional dominance, a property which highlights an interesting difference between the Aitchison and other distances. This calls for the requirement that the distance for subcompositions be no greater than the distance calculated for the full compositions. This condition is met by the Aitchison distance, and it is also met by Euclidean geometry, where a subcomposition results from orthogonal projection. However, a subcomposition in the ternary diagram can be found geometrically by using stereographic projection (Fig. 6).

If we were to view points A' and B' in Figure 6 as representing three-part compositions with one of the components equal to zero, then the Aitchison distance would be undefined, since this distance becomes unbounded when we consider points which are progressively nearer to the edge of the ternary diagram. However, when we view the line segment between the vertices (0, 1, 0) and (0, 0, 1) intrinsically (i.e., without reference to what is outside of it), then A' and B' can be regarded as two-part compositions which are obtained algebraically from A and B by dividing each of the last two components by their sum. The column with the Aitchison distances in Figure 6 shows that this distance is invariant under stereographic projection. However, the column with the half-taxi distances shows that, for subcompositions A' and B', the distances are larger than that for the full compositions A and B. Therefore, the half-taxi metric fails the requirement of subcompositional dominance.



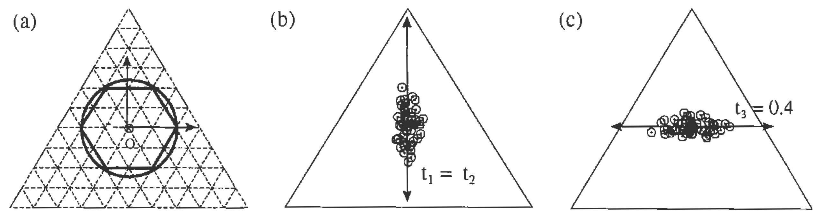
	Aitchison	Half-taxi
d(A,B)	0.98	0.05
d(C,D)	0.98	0.20
d(A′,B′)	0.98	0.33

Figure 6. The Aitchison and half-taxi distances for three sets of points. The subcompositions A' and B' can be found by stereographic projections of A and B, or points C and D. For the Aitchison distance between A' and B', we assume that the distance has been calculated for two-part compositions.

COVARIANCE AND DISTANCE

Although the situation is less definite for compositions with four or more components, Chayes (1971) has shown that the correlations between ternary variables are completely determined by their variances. Also, as already mentioned, there is a bias toward negative correlation. At least two of the three correlations between the ternary variables will be negative.

Figure 7(A) shows a half-taxi circle inscribed within a Euclidean circle. To make our comparisons easier, we can rescale the Euclidean metric, so that the distance between vertices is one unit (and not $\sqrt{2}$). When this is done, the distances from the center O to the vertices of the hexagon are the same for both the half-taxi metric and the rescaled Euclidean metric, and this corresponds to our visual impression of distance. However, the distance to a point on the ordinary circle, under the rescaled Euclidean metric, is also the same as the distance to a corresponding point on the side of the hexagon, under the taxi-cab metric. Therefore, we reach a side of the hexagon sooner relative to the circle, when we move from the center O in a direction away from the vertices. This suggests the dependence on direction for the half-taxi metric.



Half-taxi and Euclidean Circles (with common center at O)

Observations About the Line $t_1 = t_2$

$S.D.(t_1) = S.D.(t_2) = .05$
$S.D.(t_3) = .09$

$Corr(t_1,t_2) = .45$
$Corr(t_1,t_3) = -.86$
$Corr(t_2,t_3) = -.83$

Observations About the Line $t_3 = .4$

$S.D.(t_1) = S.D.(t_2) = .08$
$S.D.(t_3) = .03$

$Corr(t_1,t_2) = -.91$
$Corr(t_1,t_3) = -.17$
$Corr(t_2,t_3) = -.20$

Figure 7. (A) When we divide the Euclidean metric by $\sqrt{2}$, then the hexagon (under the half-taxi metric) and circle (under the rescaled Euclidean metric) have the same radius. A comparison of the metrics demonstrates how the half-taxi distance increases more rapidly moving in a direction away from the vertices of the hexagon. (B) and (C) Plots of computer-generated data, together with the standard deviations and rank correlations.

Figure 7(B) is a ternary plot of computer-generated data which lie near the line $t_1 = t_2$, which points away from the vertices of the hexagon of Figure 7(A). Figure 7(C) shows the results after rotating the data of Figure 7(B) about the centroid of the data. After this transformation, the resulting observations lie near the line $t_3 = 0.4$, which passes between two vertices of the hexagon. Below the figures are the standard deviations and the rank correlations. In Figure 7(B), the data lie along the direction of the vertex associated with t_3 (i.e., in other words, along the direction associated with changes in this variable). This is also the variable with the largest standard deviation, and, as noted above, this direction corresponds with relatively more rapid increases in half-taxi distance. The variable t_3 is also the variable which is most constrained by its correlations with the other two variables. Figure 7(C) shows the data cluster lying along a direction away from the same vertex. The relatively slower increases in taxicab distance in this direction now correspond to a new situation, where the variable t_3 has the smallest standard error and is the least constrained by the correlation structure. Therefore, an examination of these frames begins to suggest how half-taxi distances are connected to the covariance structure of data.

A FORMAL COMPARISON OF DISTANCES

Some researchers, such as McArdle (1991), have suggested that the theory of random graphs be applied at the beginning of an analysis, in order to determine whether enough structure is evident to pursue using one of the many clustering procedures.

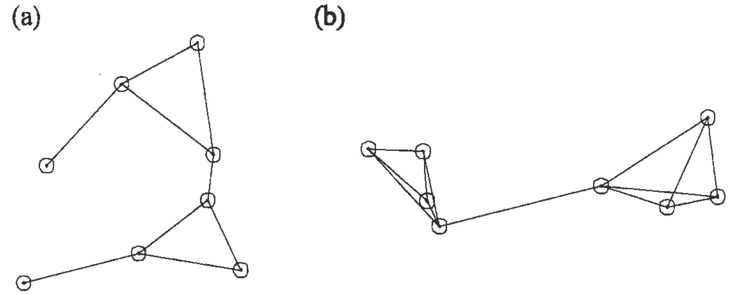


Figure 8. (A) Eight randomly-distributed points (or vertices) with a completed threshold graph composed of 9 links. (B) Eight points distributed in two clusters with a completed threshold graph with 13 links.

The basic idea can be illustrated by a threshold graph. To construct this graph, we start with a collection of points or vertices. The two closest points are linked first, then the next two closest points, and the process is complete when all the points or vertices are connected through a network of links. Figure 8(A) shows a completed threshold graph of eight randomly distributed points, and Figure 8(B) shows one for eight points which are distributed in two clusters. This illustrates that graphs with clusters of points tend to have a greater number of links in their completed threshold graphs. The idea has been formalized by Erdös and Rényi (1959), who give the probability of a random graph having at least the number of observed links, given the number of points or vertices. Ling and Killough (1976) have provided exact tables for data sets with up to 100 observations.

Using random number generators, a series of computer simulations of ternary diagrams were produced for both 20 and 50 points, and the median number of links was calculated for the half-taxi, Aitchison, and Euclidean distances. The results are similar for the half-taxi and Euclidean metrics, but much more structure is perceived using the Aitchison distance (Table 1). Therefore, it appears that the

Table 1. Median Number of Links for Random Graphs With 20 and 50 Points

Number of points	Half-taxi	Aitchison	Euclidean
20	46 (0.07)	71 (0.001)	48 (0.05)
50	176 (0.02)	360 (<0.001)	181 (0.02)

Note. The median number of links for 50 computer simulations of ternary diagrams is shown for each distance measure and for both 20 or 50 points. The associated probability for the median number of links, given that a random graph has this number of points, is shown in parentheses (Ling and Killough, 1976).

Aitchison distance tends to introduce a substantially larger amount of spurious structure into an analysis.

DISCUSSION

Hexagons are not new to compositional data analysis. Hexagonal confidence regions or dispersion fields have been suggested in papers by Philip, Skilbeck, and Watson (1987); Valloni and Maynard (1981); and Ingersoll (1978). However, those hexagons are generally irregular, and the sides not usually parallel to the sides of half-taxi circles. The property of anisotropy is also not new to geological research. Grunsky and Agterberg (1992) consider anisotropic relationships in their spatial factor analysis.

Previous sections have suggested that different aspects of compositional data are revealed by different choices of distance. For instance, the results have indicated that the determination that an observation is an outlier may depend on its proximity to an edge of the ternary diagram (Aitchison distance), or the orientation of an observation with respect to the centroid of data (half-taxi distance). In spite of these results, we cannot yet say anything definite about the relative merits of the metrics with respect to data analysis. The simple interpretation of the half-taxi metric is appealing, but it is not yet clear what benefit it can provide over other metrics. Its connection with the covariance structure may be better understood when we work in higher dimensions. There is a more refined dependence between distance and direction in three dimensions. The half-taxi sphere is a cuboctahedron, a polyhedron with 14 faces and 12 vertices. It is composed of alternating triangular and squared faces, where the half-taxi distance tends to increase more quickly in the direction of the square faces than in the direction of the triangular faces.

The property of subcompositional dominance makes the Aitchison distance attractive for many standard statistical methods. However, the results using the theory of random graphs have shown that, because of its dependence on location, the Aitchison distance is more likely to introduce spurious patterns into a cluster analysis. However, it is still possible that, in practice, it will reveal interesting structures in data. The results only indicated the degree of structure which is detected for data with minimal structure. Ideally, we would also like to compare the metrics with respect to nonrandom data, but the theory of random graphs is probably a poor tool for detecting the variety of possible structures. The choice of a metric will be at least as difficult as the choice of one of the many competing clustering procedures. The theory of random graphs is associated with the single-linkage clustering method and, although Jardine and Sibson (1971) have shown that the single-linkage method is mathematically attractive, there is still no clear preference for it in practice. It might be more promising to compare the various metrics by using a more robust method like projection pursuit, which has different indices to reflect the different properties of skewness, central mass, or group structures (Bolton and Krzanowski, 1999).

Other metrics might also be worth considering, including variations of the half-taxi metric. Another possibility is the chi-square distance found in correspondence analysis. This is a weighted Euclidean distance which is proportional to the χ^2 statistic. Variables which have smaller mean proportions are given greater weight in its calculation. In general, the chi-square "circle" is an ellipse where the minor axis points toward the vertices identified with the components with the smallest mean responses.

We have not discussed definitions for angular differences, but an Appendix presents one geometric approach. The exploration of angular differences is a potentially important area of research, because of its connection to definitions of correlation, and its resulting implications for dimension-reducing techniques. However, this research could also be more difficult. The instability of the correlation coefficient is well-known among data analysts. Some have complained of it being a mixture of "random" and "systematic" error, and Tukey (1969) has referred to it as the "enemy of generalization." However, definitions of distance and correlation are not unrelated. Nelson (1998) has shown that a correlation can be defined in terms of moments of inertia, which in turn depend on how distance has been defined. Therefore, a consideration of distance measures might be relevant to this research, and the Appendix draws attention to this.

This paper is somewhat exploratory, and the results are not yet very deep with respect to implications for data analysis. The presentation here has focused on a model-free examination of the geometry of the ternary diagram to determine if, by going back to first principles and regaining some control over the geometry, we might obtain a better understanding of some aspects of compositional data. Additional work is necessary to better assess the relative contributions of information which result from the varying methods of analysis. As long as the relative strengths are not well understood, the situation which Chayes (1971) described three decades ago will be somewhat unchanged: we will see the nonsense in taking at face value the meaning of certain patterns, and yet not be certain that we can always make sense of ternary diagrams.

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APPENDIX: ANGULAR DIFFERENCES

One measure to describe the difference between two vectors is the angle between them or, in particular, the cosine of the angle, which is connected to definitions of correlation. Bryant (1984) illustrates how the simple Pearson correlation is defined in terms of finite-dimensional geometry. Suppose that $x_1, x_2, \ldots, x_n$ and $y_1, y_2, \ldots, y_n$ are the n observations for variables X and Y, expressed as deviations about the means. Then the simple correlation can be defined as the cosine of the angle between the vector **x** with coordinates $x_1, x_2, \ldots, x_n$ and vector **y** with coordinates $y_1, y_2, \ldots, y_n$. Kendall and Stuart (1977) have further shown that the partial correlation of variables X and Y, given Z, is equivalent to the cosine of the angle between the projections of vectors **x** and **y** on the plane which is orthogonal to **z**.

Defining the cosine of the angle between two observations in a ternary diagram is not straightforward, because inner products (and hence trigonometric functions) are not defined directly for oblique coordinate systems (Green and Carroll, 1976, Chap. 3). However, Figure 9 offers a geometric interpretation of a partial cosine function for two ternary compositions. Figure 9 shows a view which is similar to Figure 1, but we now regard the vertices of the reference triangle as the endpoints of three vectors.

A tangent vector consists of two parts: its vector part **v** and its point of application (O'Neill, 1966). The three unit vectors just described have their point of application at the origin. However, suppose that we have two compositions s and t with responses (s_1, s_2, s_3) and (t_1, t_2, t_3). We can then define the partial cosine of the last two components, given the first, to be equal to the cosine of the angle between the orthogonal projections of the vectors **v** and **w**, which are tangent to the vertex (1, 0, 0) and terminate at (s_1, s_2, s_3) and (t_1, t_2, t_3), respectively. Therefore, the partial cosine is the cosine of the angle between the orthogonal projections in the y-z plane, which are labeled $\mathbf{v}^*$ and $\mathbf{w}^*$ in Figure 9. However, it is not necessary to apply the usual Euclidean cosine function. One alternative is to use the taxicab cosine function (see Fig. 2) where

$$\cos_{\text{taxi}}(\theta) = \begin{cases} 1 - \frac{\theta}{90^\circ} & \text{if } 0^\circ \leq \theta \leq 180^\circ \\ -3 + \frac{\theta}{90^\circ} & \text{if } 180^\circ \leq \theta \leq 360^\circ \end{cases} \tag{4}$$

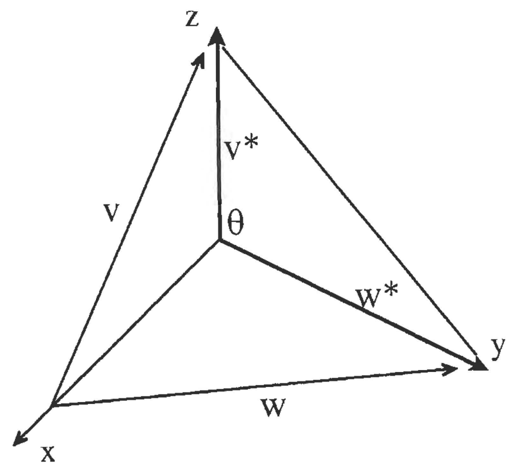

Figure 9. The partial cosine for the ternary diagram. The vectors **v** and **w** are tangent to the vertex (1, 0, 0,), and the partial cosine of the angle between the vectors is defined in terms of their orthogonal projections $\mathbf{v}^*$ and $\mathbf{w}^*$, which are tangent to the origin. In this example the partial cosine function for the angle between **v** and **w** is zero using Equation (4).

In a general definition for three-part compositions, the resulting vectors would be tangent to the vertex identified with the conditional component. We can also extend the idea to higher dimensions, even though the geometric interpretation will change somewhat. However, we are prevented from extending this definition to the factor space and thereby offering a possible definition for correlation between ternary variables, because the variables do not generally sum to one over all the compositions in a data set, and so the corresponding vectors do not generally lie within a ternary or simplex space. However, one solution would be to adopt the approach of correspondence analysis, and do a separate conversion to proportions for the variables (the columns) of the parent data set. This possibility may be investigated in future work.