Zamir, M. and **D. C. Bigelow**, 1984. "Cost of Departure from Optimality in Arterial Branching," Journal of Theoretical Biology, 109: 401-409.

Zamir, M., J. A. Medeiros and **T. K. Cunningham**, 1979. "Arterial Bifurcations in the Human Retina," Journal of General Physiology, 74: 537-548.

Zamir, M. and **J. A. Medeiros**, 1982. "Arterial Branching in Man and Monkey," Journal of General Physiology, 79: 353-360.

Chapter 10

The Invertibility of Distance Matrices

Michael F. Goodchild
Department of Geography
The University of Western Ontario
and
David M. Mark
Department of Geography
State University of New York at Buffalo

In informal discussion at a meeting at the Lincoln Land Institute in Boston in May, 1983, Charles Schwartz, of the National Geodetic Survey, US Department of Commerce, posed the following conjecture concerning distance matrices:

> **The Euclidean distance matrix for any set of distinct points in the plane can be inverted.**

By coincidence, a related conjecture with similar motivation appears to have been made at a conference in Italy by R. Franke (Franke, 1983). A paper by Micchelli (1986; see also Dyn, Goodman and Micchelli, 1986) proves the Franke conjecture (and perhaps by extension the Schwartz conjecture), although we frankly confess our inability to follow the mathematical argument. The purposes of the present paper are to introduce the Schwartz conjecture and its motivation to a broader audience, and to discuss its extension to a more general case. While we are unable to present proofs in the more general case, our analysis nevertheless yields interesting results.

This topic may appear impossibly arid and obscure for a volume such as this. But on deeper examination it seems to us extraordinarily appropriate, for two reasons. Throughout his long career William Warntz has been perhaps the discipline's strongest advocate of the fundamental importance of geometry to our understanding of the earth and the distribution of human and physical phenomena on its surface. Writing in 1971, Warntz and Wolff saw geometry and graphics as fundamental to geography, for which:

> "The heavy use of the various geometries seems assured. The distinctions between various systematic branches of geography diminish at the theoretical level as common spatial properties and dimensional problems are recognized despite their vast nonspatial dissimilarities...(B)ecause of the

lushness of the spatial logic of geometry, the incisive nature of graphics in portraying and discovering spatial relations, and the commitment of geography to the study of spatial patterns in the real world, the natural, but sometimes overlooked, affinities of these three disciplines can be a source of considerable intellectual richness and scientific development with obvious benefits to society through technology and planning." (Warntz and Wolff, 1971: 254-5).

Distance plays a fundamental role in the connections between location and geographical process; Tobler's "first law of geography: everything is related to everything else, but near things are more related than distant things" (Tobler, 1970) is nicely put by Gould (1970: 443-4):

> "Why we should expect independence in spatial observations which are of the slightest intellectual interest or importance in geographic research I cannot imagine. All our efforts to understand spatial pattern, structure and process have indicated that it is precisely the lack of independence - the interdependence - of spatial phenomena that allows us to substitute pattern, and therefore predictability and order, for chaos and apparent lack of interdependence of things in time and space".

The Schwartz conjecture seems to us to have much in common with many of the geometrical and combinatorial puzzles and conundrums for which Bill Warntz's teaching has been famous. Like the four-colour theorem it is simply stated, yet its analysis provides substantial mental stimulus; it has a geographical motivation, admittedly obscure; it deals with geometrical fundamentals; and yet it appears to defy simple proof.

DEFINITIONS

Matrix inversion is a fundamental procedure in linear algebra, and arises in a number of problems in multivariate statistics and spatial data handling. However, not all matrices can be inverted: a matrix can be inverted if and only if the **determinant** of the matrix is not zero (see, for example, Lang, 1971). A matrix which cannot be inverted is said to be **singular**. The determinant of a matrix can be computed recursively as follows:

Let the matrix be denoted by A, with dimensions n by n. Let the result of deleting the ith row and the jth column be an (n-1) by (n-1) matrix denoted by A_{ij}. Then the determinant of A is given by:

$$\mathrm{Det}(A) = (-1)^{i+1} a_{i1} \mathrm{Det}(A_{i1}) + \ldots + (-1)^{i+n} a_{in} \mathrm{Det}(A_{in}) \quad (1)$$

The procedure is applied to successively smaller and smaller matrices until only one row and column remain in each matrix.

The Franke conjecture is stated by Micchelli (1986) as follows:

> **Given any set of n distinct points in the plane, form an n by n matrix C whose terms are given by** $c_{ij} = (1+d_{ij}^2)^{1/2}$, **where** d_{ij} **is the distance between points i and j. Then** $(-1)^{n-1}$ Det C > 0.

Since the distance terms can always be rescaled, the 1s in the definition of C ensure that all terms are positive, whereas the Schwartz conjecture requires diagonal terms to be zero.

CONTEXT OF THE PROBLEM

Spatial analysis often involves sets of points distributed over the surface of the earth, and it is common to compute the matrix of distances between all pairs of points in such sets. The result is a matrix which is square and symmetrical, with diagonal elements equal to zero; provided all the points are distinct, the elements off the diagonal are all strictly positive. Gatrell (1983) has reviewed the role of distance matrices and their analogs in spatial analysis.

Although it is not common to invert a distance matrix, or to be concerned with whether that operation is possible, inversion of related matrices is frequently necessary in carrying out spatial interpolation using one of a number of techniques known by different names in various disciplines, but most often in geography and geology as Kriging (Krige, 1951; David, 1977; Hanham and Chang, 1985; Olea, 1974). In order to see the motivation behind the Schwartz conjecture, we briefly review the essentials of Simple Kriging.

Suppose we have sampled a surface at a number of points located at (x_i, y_i), $i=1,\ldots,n$, the height of the surface measured at each of these points being denoted by z_i. We wish to estimate the height of the surface at points located between the sample points, and ultimately to construct an estimate of the entire surface.

Assume that the surface is statistically stationary, to the extent that the expected difference in height between pairs of points displaced **h** from each other is zero, and the variance between such pairs is a function of the distance of displacement:

$$E[z(\mathbf{x}) - z(\mathbf{x+h})] = 0 \quad (2)$$

$$Var[z(\mathbf{x}) - z(\mathbf{x+h})] = 2\Gamma(|\mathbf{h}|) \quad (3)$$

where $\Gamma(|\mathbf{h}|)$ is the semivariogram function and $|\mathbf{h}|$ denotes the length of the **h** vector, or the distance between the pair of points.

Given a set of sample points and an estimated semivariogram function, Simple Kriging attempts to estimate the height of the surface at some location **x** from a linear combination of the known values:

$$z^*(\mathbf{x}) = \sum_i \alpha_i \, z(\mathbf{x}_i) \quad (4)$$

where the α_i are weights to be determined. It can be shown that the weights which give unbiased and minimum variance estimates are given by:

$$[\Gamma(r_1),\Gamma(r_2),\ldots,\Gamma(r_n),1] = [\alpha_1,\alpha_2,\ldots,\alpha_n,\mu] \begin{vmatrix} \Gamma(d_{11}) & \Gamma(d_{12}) & \ldots & \Gamma(d_{1n}) & 1 \\ \Gamma(d_{21}) & \Gamma(d_{22}) & \ldots & \Gamma(d_{2n}) & 1 \\ . & . & \ldots & . & \\ \Gamma(d_{n1}) & \Gamma(d_{n2}) & \ldots & \Gamma(d_{nn}) & 1 \\ 1 & 1 & \ldots & 1 & 0 \end{vmatrix} \quad (5)$$

Solution of this set of linear equations requires the inversion of an (n+1) by (n+1) matrix: if the variogram is linear, as is frequently the case over the range of distances encountered, then it is necessary to be able to invert a matrix of distances, augmented by an additional row and column of 1s. Similar situations arise in other, related forms of spatial interpolation based on functions of distance.

DISTANCE MATRICES

A **distance matrix D** can be defined as a (square) real symmetric matrix in which the entry dij is equal to the distance from point i to point j. If the distance is given by:

$$d_{ij} = [(x_i-x_j)^2 + (y_i-y_j)^2]^{1/2} \quad (6)$$

then this is a **Euclidean** distance matrix.

The Euclidean distance is one example of what is termed a **metric space** (see, for example, Blumenthal, 1970). A distance measure and the associated space is termed metric if and only if the following four properties hold for the distance D(m,n) between points **m** and **n**:

(1) D(m,n) = 0 if and only if **m** and **n** coincide (nondegeneracy);

(2) D(m,n) > 0 (non-negativity);

(3) D(m,n) = D(n,m) (symmetry);

(4) D(m,n) + D(n,o) ≥ D(m,o) (triangle inequalities).

Some common metric spaces include those defined by the Minkowski metrics:

$$d_{ij} = [(x_i-x_j)^p + (y_i-y_j)^p]^{1/p} \quad (7)$$

for p≥1. Note that p=2 defines the Euclidean (or L_2) space, while p=1 is the well-known Manhattan or taxi-cab (L_1) space. There are many other metric spaces which do not belong to this class.

ANALYTICAL STUDIES

Three Points

The simplest non-trivial situation is the case of three distinct points in the plane. Let us denote the distance matrix for these points as:

$$\mathbf{D} = \begin{vmatrix} 0 & a & b \\ a & 0 & c \\ b & c & 0 \end{vmatrix}$$

Applying the determinant formula given above will show that the determinant of this matrix is just 2abc; since the points are distinct, property (1) of a metric space requires that none of a, b, and c can equal zero. Thus, the determinant cannot equal zero. In the 3-point case, we need not consider the triangle inequality or other distance metric properties in order to establish that the determinant cannot be zero and that the matrix is therefore always invertible; the nondegeneracy and symmetry properties are sufficient.

Four Points

The situation for four points is far more complicated. Again, for simplicity of notation, let the matrix be given by:

$$D = \begin{vmatrix} 0 & a & b & c \\ a & 0 & d & e \\ b & d & 0 & f \\ c & e & f & 0 \end{vmatrix}$$

The determinant of this matrix is:

$$\det[D] = (a^2f^2 + b^2e^2 + c^2d^2) - 2(abef + acdf + bcde) \quad (8)$$

Setting this equal to zero and solving the quadratic for a gives:

$$a = [be + cd \pm 2(bcde)^{1/2}] / f \quad (9)$$

To generate an example, we can set b=c=d=e=f=1; then the solutions for a are 0 or 4. Thus the real symmetric matrix:

$$D = \begin{vmatrix} 0 & 4 & 1 & 1 \\ 4 & 0 & 1 & 1 \\ 1 & 1 & 0 & 1 \\ 1 & 1 & 1 & 0 \end{vmatrix}$$

is singular (i.e., not invertible). Note, however, that this could not be a metric distance matrix, since the triangle inequality is violated by the triangles involving link 1-2; (4,1,1) cannot be the side lengths of a triangle in a metric space. This examples shows, however, that if a matrix is real and symmetric, has zeros on the diagonal, and is strictly positive off the diagonal, this is not sufficient to guarantee invertibility.

Geometric Solution

We can also examine four points geometrically. Since rotation and translation would not effect the distance matrix for the Euclidean metric, and since scaling would only multiply the matrix elements by a constant, we can place the four points in any convenient coordinate system. Let us denote the coordinates of the points by (x_i, y_i),

for i=1,...,4. Arbitrarily, place point number 4 at the origin, and point 3 on the x-axis at (1,0). Thus $x_4=y_4=y_3=0$ and $x_3=1$. Then, by definition, this sets f=1. Now, given that D(2,3)=d and D(2,4)=e, there are two possible locations in the plane for point 2. The equations for d and e are:

$$d^2 = (x_2-1)^2 + (y_2)^2 \quad \text{and}$$

$$e^2 = (x_2)^2 + (y_2)^2 \quad (10)$$

Solving these simultaneously for x_2 and y_2 gives:

$$x_2 = [e^2 - d^2 + 1] / 2 \quad \text{and}$$

$$y_2 = \pm [2(e^2+d^2+d^2e^2) - (e^4+d^4+1)]^{1/2} / 2 \quad (11)$$

We will arbitrarily take the positive y_2 solution, which now fixes the coordinate transformation.

Similar analysis applies to the position of point 1. D(1,3)=b and D(1,4)=c, giving:

$$b^2 = (x_1-1)^2 + (y_1)^2 \quad \text{and}$$

$$c^2 = (x_1)^2 + (y_1)^2 \quad (12)$$

Solving these simultaneously for x_1 and y_1 gives:

$$x_1 = [c^2 - b^2 + 1] / 2 \quad \text{and}$$

$$y_1 = \pm [2(c^2+b^2+b^2c^2) - (c^4+b^4+1)]^{1/2} / 2 \quad (13)$$

Since all the degrees of freedom in the coordinate transformation have been removed, there are two possible locations for point 1. Since a=D(1,2), there are thus two possible values for a, given the other five interpoint distances. If it can be shown that this and equation 9 can never be satisfied by the same set of values for (b,c,d,e,f), then this would constitute a proof that all 4 x 4 Euclidean distance matrices are invertible. It would not necessarily apply to other metric spaces, nor does it generalize in any obvious way to cases of more than 4 points.

SIMULATION STUDIES

One approach is simply to search for counter-examples by means of simulation. Failure to find a counter-example by this method would, of course, not prove the Schwartz conjecture, but such an approach could disprove it by discovering such a counter-example. Otherwise, the procedure increases the veracity of the conjecture. All of the simulations reported below were conducted using 60-bit floating point precision on a Cyber 840 at CSIRONET, Canberra, Australia.

The problem of finding a set of distinct points in the plane whose distance matrix is singular can be re-cast as follows. Consider a set of n-1 distinct points at fixed locations in the plane. Then, let (x,y) be the position of the n-th point, and Det(x,y) be the determinant of the distance matrix for the set of n points when point n is located at (x,y). Det(x,y) will be zero when (x,y) coincides with any of the first (n-1) points; if it is zero anywhere else, then the conjecture will be false. In the latter case, there may be regions of the plane in which Det(x,y)<0, and others where Det(x,y)>0; the boundary between these regions (the zero-set of Det(x,y)) would provide counter-examples to the conjecture. Thus, if for any particular n, the sign of the determinant is invariant, the conjecture gains further support. Of course, even if this can be proved, a complete proof of the conjecture would also have to show that there are no other points in the plane at which Det(x,y)=0, and further that this holds for all possible distinct sets of (n-1) points.

To begin the simulation studies, we distributed sets of random points over the unit square, computed Euclidean distance matrices for the points, and then computed determinants. The matrices analyzed involved sets of n=4,5,...,9 points. For each n, 1,000 replications were conducted; in no case was a distance matrix found to be singular. Of course, numerical properties of discrete representations of real numbers on computers make values of exactly zero extremely unlikely. However, in all of the simulations, the sign of the determinant was invariant for each value of n; the determinant was always negative for even n and positive for odd n. The fact that the sign is constant for each n strongly suggests that singular distance matrices for sets of n<10 distinct points in the plane are impossible. In addition, the sign is consistent with the Franke conjecture. Of course, we can state with complete confidence only that singular distance matrices are very unlikely.

In the analytical section above, we derived a 4 by 4 real symmetric matrix, with zeros on the diagonal and no zeros off the diagonal, which nevertheless was singular. We observed, however, that the matrix violated the triangle inequality property of metric spaces. To explore this aspect of the conjecture, further simulation studies were conducted. In these simulations, we focussed on observing the sign of the determinant.

The basic analyses involved 1,000 replications for each n between 4 and 9, inclusive. First, matrices of size n by n were filled with random numbers uniformly distributed in

the interval from 0 to 1; in each case, the numbers of cases with positive and negative determinants were approximately equal. However, if the diagonal was zeroed, the results were as follows:

sign	n=4	5	6	7	8	9
+	68	851	258	659	384	574
-	932	149	742	341	616	426

For each n, there is a preponderance of matrices with determinants having the same sign as for actual distance matrices of the same size; however, there is a clear trend toward equal numbers of positive and negative determinants with increasing n.

If symmetry is imposed on the matrix by replacing each term d_{ij} by $(d_{ij}+d_{ji})/2$ (in addition to a zeroed diagonal), the results are more complex:

sign	n=4	5	6	7	8	9
+	406	201	753	571	236	585
-	594	799	247	429	764	415

The meaning of this pattern is unclear.

Finally, we required the random numbers to obey all triangle inequalities; these simulated matrices have all of the major properties of a distance matrix, but still may not be realizable as a set of distinct points in the Euclidean plane. To impose the constraints we simulated the upper triangle; the lower triangle follows from the symmetry constraint. The first row of the upper triangle was filled using independent random numbers, in the interval 0.0 to 1.0 as before. In the second and subsequent partial rows of the upper triangle there are constraints on the range of each element if the triangle inequalities are to be satisfied; these constraints are imposed by the cells already filled. Consider cell j,k, j<k. Examine all rows i<j<k; these will be located above row j. Then the value placed in cell j,k must be no larger than the sum of cells i,j and i,k, for all i<j. Similarly it must be no less than the absolute difference between the same two cells, again for all i less than j. This gives a range of feasible values for j,k, and a value can then be assigned by generating a random value in this range. In all of our trials the range of permissible values never vanished for any cell. Clearly the resulting values are not independent, but they are symmetrical, positive with zeroes on the diagonal and obey the triangle inequality.

The results for 1,000 trials at each value of n are:

sign	n=4	5	6	7	8	9
+	0	1000	1	990	22	899
-	1000	0	999	10	978	101

Thus, the addition of the triangle inequality constraint almost, but not quite, replicates the results for actual Euclidean distance matrices. A run of 10,000 trials at n=5 produced one negative determinant, but 100,000 trials at n=4 produced no positive ones. The unusual n=5 matrix had a determinant of -0.00497; by adjusting one off-diagonal element in a way which did not violate any triangle inequality, a matrix with a determinant with an absolute value of less than 10^{-7} was found. This matrix can be associated with a set of 5 points in Euclidean 4-space, but cannot be plotted in the plane. So we can reach one of two conclusions: either forcing the points into the Euclidean plane adds further constraints which guarantee invertibility, or the conjecture is false, but only very rarely.

CONCLUSIONS

As we noted at the outset, the Schwartz conjecture is simply stated, but to date no similarly simple mathematical proof of its truth has been found. Our simulations show that it is clearly not true of matrices which do not obey the rules of metrics, and it appears not to be true of metrics in general. Relaxing the requirement that terms be Euclidean distances between points in the plane, but maintaining the triangle inequality and other requirements of metrics produces matrices which violate the Schwartz conjecture with increasing frequency as the number of points increases. It is not clear from our simulations whether the Euclidean metric is necessary, or whether any metric in two-dimensional space would be sufficient. However, it seems unlikely that either requirement would be sufficient to distinguish between a rare condition and an impossible one, so as in the case of the four colour theorem we are left with the intuitive feeling that it might be possible to find a counter example. But our work offers no clues as to the likely configuration of points.

ACKNOWLEDGMENTS

We are grateful to Charles Schwartz for stimulating our interest in this problem and for bringing the Micchelli paper to our attention.

REFERENCES

Blumenthal, L.M., 1970. Theory and Applications of Distance Geometry. New York: Chelsea.

David, M., 1977. Geostatistical Ore Reserve Estimation. New York: Elsevier.

Dyn, N., T. Goodman and **C.A. Micchelli**, 1986. "On the spectrum of the matrix $|x_i - x_j|^\alpha$", Linear Algebra and its Applications, 80: 198-200.

Franke, R., 1983. "Lecture notes on global base mapping methods for scattered data". International Symposium on Surface Approximation, University of Milan, Gorgano, Italy.

Gatrell, A.C., 1983. Distance and Space: A Geographical Perspective. Oxford: Clarendon Press.

Gould, P.R., 1970. "Is statistix inferens the geographical name for a wild goose?", Economic Geography, 46: 439-48.

Hanham, R.Q. and **H.Y. Chang**, 1985. "Using Kriging to estimate missing spatial data in city planning: the example of housing conditions in Oklahoma City", Modeling and Simulation, 16 (Proceedings of the 16th Annual Pittsburgh Conference): 9-13.

Krige, D.G., 1951. "A statistical approach to some basic mine valuation problems on the Witwatersrand", Journal of the Chemical, Metallurgical and Mining Society of South Africa, 52: 119-39.

Lang, S., 1971. Linear Algebra. Reading, Mass.: Addison Wesley.

Micchelli, C.A., 1986. "Interpolation of scattered data: distance matrices and conditionally positive definite functions", Constructive Approximation, 2: 11-22.

Olea, R.A., 1974. "Optimal contour mapping using Universal Kriging", Journal of Geophysical Research, 79: 695-702.

Tobler, W.R., 1970. "A computer movie simulating urban growth in the Detroit region", Economic Geography, 46: 234-40.

Warntz, W. and **P. Wolff**, 1971. Breakthroughs in Geography. New York: Plume Books, New American Library.