Section 1
ORIENTATION

1 Representation of Structure in Similarity Data: Problems and Prospects*

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Editors note

The first part of this article, which was Professor Shepard's Presidential address to the Psychometric Society, being an introductory excursus such as is customary on such occasions, has been omitted from the present volume.

On the basis of extensive first-hand experience with non-metric multidimensional scaling and examination of a large number of reports by other investigators using this type of method, I believe the following six problems to be most in need of further attention.

1. The problem of attaining the globally minimum departure from monotonicity (primarily the problem of avoiding merely local minima).
2. The problem of achieving a meaningful substantive interpretation of the spatial configuration.
3. The problem of determining the proper number of dimensions for the coordinate embedding space.
4. The problem of avoiding undesirable loss or extraneous imposition of structural information (especially the so-called problem of "degeneracy").
5. The problem of determining the form of the underlying metric (particularly the form of the rule governing how differences along two or more underlying dimensions combine to yield the overall similarity between two objects).
6. The problem of representing discrete or categorical structure (in view of the fact that the scaling model assumes a continuous underlying coordinate space).

I proceed, now, to consider each of these six problems in turn. For each I shall attempt, under the subheading *"Problem,"* to define and to illustrate the nature of the problem and some of its aspects and then, under the subheading *"Prospects,"* to suggest some directions in which I think a way of overcoming that problem might profitably be sought.

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1. Attaining the Globally Minimum Departure from Monotonicity

Problem

All existing methods for nonmetric multidimensional scaling use some variant of the steepest descent or gradient method to minimize the chosen measure of departure from monotonicity. This is not because gradient methods guarantee either quick or certain achievement of the desired minimum; they do not. The choice is dictated, rather, by the present lack of a viable alternative for this particular class of large and nonlinear numerical problems. In fact the gradient method has two rather frustrating properties. First, convergence tends to become quite slow as a minimum point is approached—unless, perhaps, recourse is taken to second-order methods. But, owing to the enormously greater demands that second-order methods place on computer memory, they are apt to be prohibitive, except in the case of a relatively small matrix of data or of an exceptionally large computer. Second, entrapment in an undesired, merely local minimum is not unlikely—unless the initial configuration is constructed so as to fall (with sufficiently high probability) within the vicinity of the desired global minimum. But to ensure this is to solve, by some other means, a very large part of the problem of optimization itself.

The problem of entrapment in merely local minima is the more troublesome of the two because, rather than merely resulting in a delayed attainment of the absolute minimum, it can result in a failure to attain that minimum at all. I must confess to having underestimated the seriousness of the problem when, in previous papers, I have glibly remarked that, if a local minimum is suspected, one can always try a number of random starting configurations and simply take, as the absolute minimum solution, the one that (repeatedly) turns up with the same smallest value of departure from monotonicity ("stress"). Unfortunately, according to recent much more extensive experience (particularly by my former student and colleague Phipps Arabie), although the absolute minimum *is* often attained within the first four or five random starts, to be quite safe at least 20 different starts should be used if a Euclidean solution is sought. (Indeed, in the case of one set of data, the globally optimum Euclidean solution failed to emerge at all until the 26th random try!) And, as we shall see, in the case of severely non-Euclidean metrics such as the so-called city-block or dominance metrics, the situation is very much worse.

Ironically, local minima pose especially prevalent and therefore irksome obstacles to the attainment of the optimum configuration in what might otherwise seem to be the simplest case; viz., that of a one-dimensional space. Theoretical analysis confirms what has become clear from practical experience. Evidently, a point that is initially situated on the wrong side of some other points can gradually work its way around those other points in a space of two or more dimensions but, when confined to a single line, is unable to move through those points owing to forces of mutual repulsion. Even in published studies, one-dimensional solutions have been presented

that I can show to correspond to such merely local minima.

A widely advocated remedy for the problem of local minima is, of course, the use of rationally constructed initial configurations instead of configurations generated either arbitrarily or purely at random. Generally, such rational starting configurations have been obtained by procedures derived from the classical metric approach to multidimensional scaling perfected by Torgerson [1952]. The hope is that such metric solutions will be sufficiently close to the global minimum for the nonmetric method to avoid entrapment in other merely local minima (cf., Young and Torgerson [1967]). Possibly such procedures will eventually be modified to the point where they can be demonstrated to be uniformly satisfactory. However, in the experience of my associates and myself (*e.g.*, [Arabie, 1973] and [Arabie & Boorman, 1973]), the ability of available procedures of this type to circumvent local minima has so far been disappointing—particularly so in cases of non-Euclidean metrics, one-dimensional spaces, and the highly nonlinear relations between similarity and distance that are characteristic of the types of behavioral data with which I have often been concerned (*viz.*, those of confusion [Shepard, 1957b, 1972c], association [Shepard, 1957a], or reaction time [Shepard, *et al.*, in press]).

Incidentally, the prevalence of the local-minimum problem implies that conclusions drawn from "Monte Carlo" investigations (*e.g.*, of stress, dimensionality, or alternative methods and programs) should be received with caution unless adequate assurances are provided that the reported statistics are not contaminated by the undetected occurrence of suboptimal solutions. I believe that Arabie [1973] is justified in suggesting (a) that several studies purportedly comparing different *methods* (*viz.*, M-D-SCAL, TORSCA, and SSA) succeeded only in demonstrating the undesirability of a certain type of initial configuration (*viz.*, the arbitrary *L*-shaped configuration used in early versions of M-D-SCAL), and (b) that the stress values reported even in some of the most useful Monte Carlo studies [Klahr, 1969; Stenson and Knoll, 1969] are inflated to an unknown extent.

Prospects

In the absence of a promising alternative to the gradient method for minimizing the chosen measure of departure from good fit, the judicious selection or construction of the initial configuration does seem to offer the best hope for ensuring convergence to the desired global minimum. However, since it is not yet clear which of a number of possible ways of doing this will eventually prove most uniformly efficient and successful, several quite different possibilities should be pursued. Currently, these appear to divide into two general classes. In one, the construction of an initial configuration that is sufficiently close to the globally minimum configuration is attempted within the space of specified, low dimensionality in which a solution is being sought. In the other, a completely unbiased configuration is first constructed in a space that is either sufficiently high-dimensional [Shepard, 1962a] or non-dimensional [Cunningham & Shepard, 1974] to make this possible and, then, a smooth and presumably trap-free mapping of this unbiased con-

figuration is attempted down into the specified low-dimensional target space.

With respect to the first of these two classes, several quite different approaches to the construction of a rational starting configuration appear worthy of further exploration. Within the spirit of those already in existence, is the approach—apparently first considered by Torgerson himself (personal communication)—in which a metric multidimensional scaling procedure based upon a parametrically specified, smooth functional relation between similarity and distance is alternated with a reestimation of the parameters of the functional relation. Then, when this preliminary iterative process becomes suitably stationary, the resulting configuration can be used to start the iterative process of the nonmetric method itself. Alternatively, some combinatorial method of arriving at an optimal assignment or permutation of the objects with respect to points in a pre-established configuration or ordering might prove desirable--particularly when the target space has only one dimension or, possibly, has a Minkowski power metric of one of the two limiting forms ($r = 1$ or $r = \infty$). Finally, there is the related possibility of building up the starting configuration by finding a near-optimum placement for each point individually as the points are added to the configuration, one at a time. In particular, if each successive point is allowed to migrate in from an extra dimension orthogonal to the space in which the rest of the configuration is confined, there should be no reason for any point to become trapped on the wrong side of any other points.

The technique of dimensional compression that I incorporated in my original method of "analysis of proximities" [Shepard, 1962a] belongs in the second of the two above-mentioned general classes of methods for generating initial configurations. It can however be regarded as carrying out the just-described point-by-point inward migration—but on all n points simultaneously. Such a way of looking at that method may help, moreover, to clarify why that method is not susceptible to entrapment in unwanted local minima. To start with, the n points are arranged as the vertices of a regular simplex in $n - 1$ dimensions. This is a completely unbiased configuration in which all $n(n - 1)/2$ interpoint distances are equal. As iteration proceeds, the variance of the distances is systematically increased by stretching distances that should be large and shrinking distances that should be small. The net effect is that each point migrates towards its optimum location within the hyperplane of the $(n - 2)$ dimensional simplex defined by the other $n - 1$ points in such a way as to instate and maintain the desired rank order of the distance from that point to each of the $n - 1$ other points. Clearly, there is again no reason for any point to become trapped in an inappropriate region. Experience reinforces our theoretical expectation that this process becomes stationary when all points have mutually gravitated into close proximity of the lowest dimensional hyperplane within which a good monotone fit to the similarity data is still possible. Rotation to principal axes then enables elimination of the superfluous dimensions, leaving us with the desired coordinates for the dimensionally-reduced and trap-free starting configuration.

Although this method requires that the n points be initially embedded

in a space of $n - 1$ dimensions, the efficiency of the method and its invulnerability to entrapment may more than offset the disadvantage of having to carry along $n(n - 1)$ coordinates during these preliminary iterations. I know of no case in which this procedure has led to a merely local minimum. And, illustrative of its efficiency, for the first significant set of data analyzed by this method (*viz.*, Ekman's [1954] data on the judged similarities among 14 spectral colors), a highly satisfactory, virtually two-dimensional starting configuration was achieved in just two iterations [Shepard, 1962b].

A final alternative, which has close conceptual relations to the approach just considered, is offered by the method of "maximum variance nondimensional scaling" recently developed by my student, Jim Cunningham, and myself [Cunningham & Shepard, 1974]. This method finds that set of (generalized) distances among the n points such that (a) the distances satisfy only the metric axioms (positivity, symmetry, and triangle inequality) and such that (b) an appropriate balance is achieved between maximization of the variance of those distances and approximation to a monotone relation of the distances to the given similarity data. The distances are not required to satisfy the much stronger conditions entailed by embedding the points in a coordinate space of the Euclidean, Minkowskian, or any other variety. Owing to its coordinate-free and nondimensional nature, the obtained representation is, like the high-dimensional representation just considered, not subject to entrapment in merely local minima. But, owing to the device of maximizing variance, the obtained distances tend, where possible, toward consistency with a low-dimensional representation. Accordingly, purely linear metric multidimensional scaling based upon those distances should yield a near-optimum initial configuration for nonmetric multidimensional scaling. Unfortunately, convergence has so far proved to be rather slow with this method. So it remains to be seen whether the efficiency of this approach can be improved to the point where it becomes a practical competitor of my original method of dimensional compression.

2. Achieving a Meaningful Substantive Interpretation

Problem

The substantive interpretation of a spatial configuration obtained by multidimensional scaling is usually a matter of paramount importance. Typically, in fact, such an interpretation is *the* end result which the investigator is seeking and which, to the extent that it is meaningful and enlightening, justifies the often rather costly computations from which it derives. In addition to its importance for its own sake, moreover, the interpretability of the configuration often plays a crucial role in determining whether the obtained solution is valid and, particularly, whether it has been embedded in a space of the appropriate number of dimensions.

In view of its importance, it is distressing to see that this matter of interpretation is still sometimes neglected or mishandled in some way. In some cases, a spatial configuration of some number of dimensions has simply been presented without any compelling interpretation. For, even when an

acceptably small measure of departure from monotonicity (stress) is achieved, in the absence of such an interpretation one can not determine (a) that the number of dimensions retained is appropriate or (b) that the configuration itself is valid (and not heavily determined by some mixture of random fluctuations in the data, degeneracy, and/or a merely local minimum).

In the worst cases, an overriding preoccupation with the reduction of stress to some desired level has led to solutions in four or more dimensions (a) where the configuration can not be visually apprehended and is probably not statistically reliable anyway, and even (b) where attempts at substantive interpretation, if any, have often been based solely on the coordinates for the points as they are printed out with respect to the unrotated axes of the solution. Such an approach to interpretation fails to appreciate two facts: First, except in certain special cases of non-Euclidean metrics, (o of methods of individual difference scaling [Carroll, 1972a] beyond the scope of this paper), the axes of the obtained configuration are entirely arbitrary. And second, even when appropriately rotated, axes do not necessarily offer the most interpretable features of a configuration.

Prospects

What seems to be most immediately needed, are efforts to educate potential users of multidimensional scaling concerning such matters as substantive interpretation, rotation of axes, and minimization of stress versus minimization of dimensionality. This paper is in part intended as one such effort. Some specific suggestions that may be helpful to some users are the following: First, always try for a solution in a space of three or, preferably, fewer dimensions where the spatial structure of the entire configuration can be seen and interpreted directly (rather than through the coordinates of the points on arbitrary axes). Second, when a representation in three or more dimensions can be shown to be both reliable and desirable, try objective methods for finding the most interpretable, rotated axes through the resulting high-dimensional space. (An excellent survey of such objective methods has been prepared by Carroll [1972b]. Less complete and up-to-date, though perhaps more readily available, is my own brief overview [Shepard, 1972b, pp. 39–43].) Third, search for *any* interpretable features of the spatial configuration—including clusters and circular orderings, as well as the linear ordering provided by (rotated) rectilinear axes.

Some concrete examples may help to illustrate the usefulness of searching for interpretable features other than axes. In fact the first significant application of nonmetric multidimensional scaling (again, my reanalysis of Ekman's [1954] data on 14 spectral colors, [Shepard, 1962b]) led to a quasi-circular configuration (similar to that presented in Fig. 7D) in which there was a perfect agreement between the ordering of the points around the circle and the ordering of the corresponding colors with respect to wave length. In this and some subsequent, quite different applications, interpretation in terms of a circular dimension (akin to Guttman's [1954] "circumplex") seems as inviting as interpretation in terms solely of rectilinear dimensions.

In Fig. 1 I exhibit the two-dimensional result of a nonmetric analysis

of data (which I had originally collected in 1953) on the strengths of mental associations among 16 familiar kinds of animals. Subjects were asked simply to list as many kinds of animals as they could think of in ten minutes. For the 16 most frequently listed kinds, I used, as a measure of the associative distance between the two items in each pair, a nonlinear average of the numbers of intervening items between those two items in the lists returned by the individual subjects.

In a first attempt to analyze association data by multidimensional scaling, I then applied the metric method described by Torgerson [1952, 1958] to these distance-like numbers in order to obtain a spatial representation for the 16 kinds of animals [see Shepard, 1957a]. At that time I obtained a three-dimensional representation in which [following Osgood, Suci, and Tannenbaum 1957] I tentatively interpreted the three axes, after appropriate rotation, as dimensions of size, potency, and activity. However, even though similar three-dimensional configurations were independently recovered from the data for two random subsets of the subjects, and even though subsequent studies have independently come up with a dimension of size and a dimension (of "predacity") that is obviously related to potency [see Rips, *et al.*, 1973], I did not at the time feel that the interpretations of the three axes sufficiently enlightening to warrant publication of the three-dimensional spatial configuration itself.

More recently, I have reanalyzed the very same set of measures of associative distance by nonmetric methods of multidimensional scaling and hierarchical clustering (using, specifically, M-D-SCAL [Kruskal, 1964a, b], HICLUS [Johnson, 1967], and embedding the clustering into the spatial representation as advocated in Shepard [1972c]). The two-dimensional solution (Fig. 1) provided a satisfactory monotone fit to the association data and, also, was consistent with the (nondimensional) clustering result—as is indicated by the fact that the obtained clusters could be uniformly represented by smooth, convex, nonoverlapping contours. The principal point that I wish to make here, however, is that the way in which the points representing the kinds of animals cluster together in the spatial representation appears to be far more readily and compellingly interpreted than the order in which those points project onto any axes passing through this spatial representation. In some cases, the specific interpretative label printed in the figure may be open to dispute; *e.g.*, the label "Jungle Beasts" for lion, tiger, and elephant. But in every case the concept—as opposed to the verbal label—is, I hope, clear. Other examples in which clusters as well, possibly, as axes seem particularly susceptible to substantive interpretation will be presented in connection with later issues (see Figs. 8 and 13).

3. Determining the Proper Number of Dimensions

Problem

In my opinion, widespread practices and recommendations concerning the determination of dimensionality are tending to detract from the use-

fulness of multidimensional scaling. I believe that users, more often than not, are inclined to err in the direction of extracting too many dimensions. This inclination seems to be attributable to certain prevalent misconceptions about the nature of nonmetric multidimensional scaling and about the implications of Monte Carlo studies.

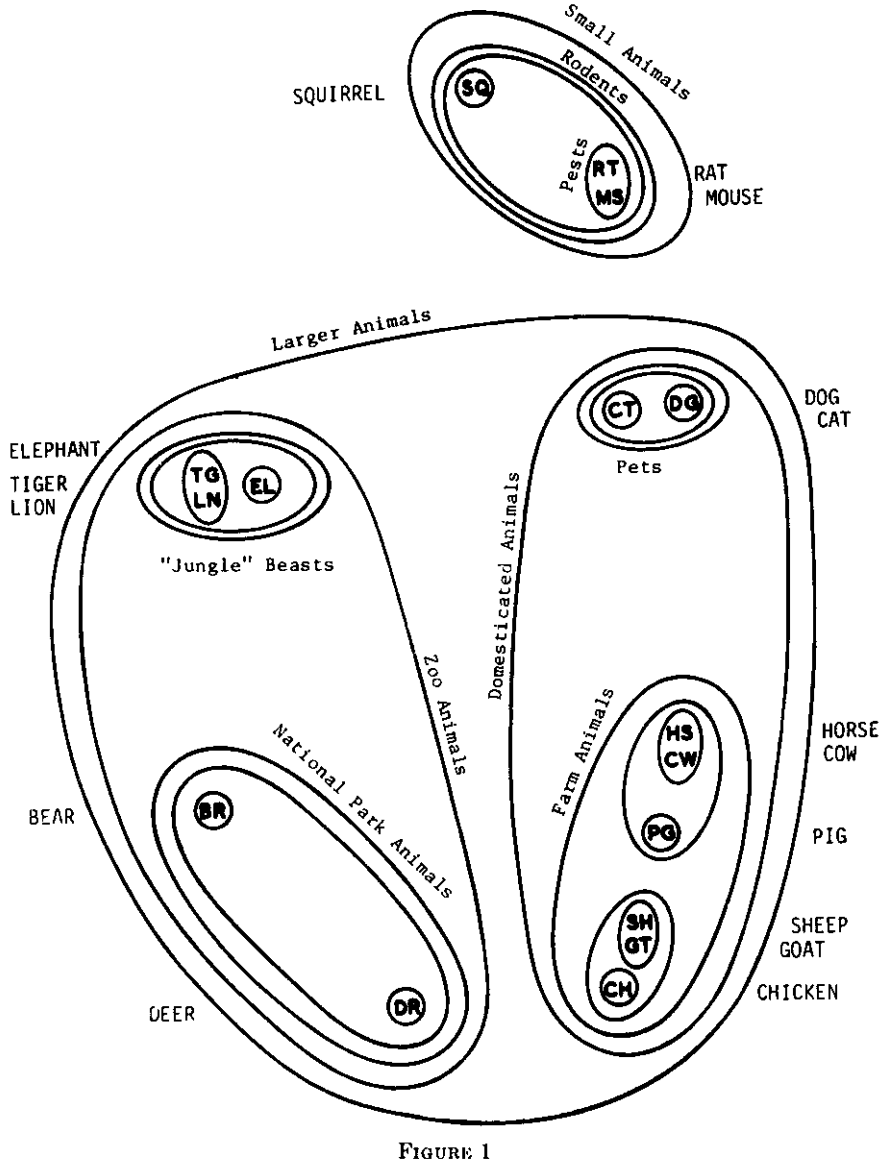

FIGURE 1

Two-dimensional spatial representation of the concepts of 16 animals, with embedded hierarchical clustering, based upon measures of association from a free-recall experiment by Shepard [1957a].

First, many users tend to place undue emphasis on the numerical value of the measure of departure from monotonicity (stress) to the virtual exclusion of much more important considerations of the statistical stability and substantive interpretability of the obtained configuration. In part, this may stem from an unfortunate tendency of users to accept, a bit too literally, the evaluative labels ("excellent," "good," "fair," and "poor") that Kruskal [1964a] once associated with particular numerical levels of stress. (Nobody likes to submit for publication a result that is only "fair" or "poor"!) Second, Monte Carlo studies, which generally recommend the extraction of more rather than fewer dimensions, are often limited in one or both of two respects: (a) they place excessive emphasis on approximating an underlying (artificially constructed) configuration (which the unprocessed similarity data themselves already do quite well!), while they disregard the more important considerations of stability and accessibility to substantive interpretation, and (b) they report mean stress values that in some cases may be inflated owing to the undetected occurrence of suboptimal solutions. Third, there has been a pervasive failure, even among otherwise sophisticated investigators, to recognize the guises under which a basically one-dimensional case can appear to the unwary to be two- or even three-dimensional.

As just one illustration of this last phenomenon, I present in Fig. 2A a two-dimensional representation that Levelt, Van de Geer, and Plomp [1966] obtained by a nonmetric analysis of the judged similarities among 15 aurally presented musical intervals. They attempted (without striking success, I feel) to give substantive interpretations to the two orthogonal dimensions of this representation and even to the third dimension of a three-dimensional solution as well. (Their interpretive effort included the fitting of a parabola—displayed, here, by the dashed curve—to the two-dimensional configuration.) To me, however, two aspects of this solution strongly suggest that the data should be represented in a one-dimensional space. First, the points fall essentially on a *C*-shaped curve that is very similar to the semicircular configuration that, under the permissible monotone transformations of the interpoint distances is equivalent to a one-dimensional straight line [Shepard, 1962a, p. 130]. And second, the ordering of the points around this curve (as indicated by the solid curve terminating in an arrowhead) agrees nearly perfectly with an obvious physical property of the intervals—namely, their separation in terms of number of intervening half-tones on the musical scale.

A completely independent solution, shown in Fig. 2B, is based upon similarity data that a former student of mine, Christopher Wickens, collected for his 1967 undergraduate honors thesis at Harvard before either of us knew of the study by Levelt *et al.* Although Wickens' experiment included only 12 of the 15 intervals investigated by Levelt *et al.*, the overall *C*-shaped nature of the two configurations in two-dimensional space is quite striking.

In analyses of many different sets of data that were known to be basically one-dimensional, I have found that two-dimensional solutions, when attempted, characteristically can assume either the simple *C*-shape (illustrated

in Fig. 2) or the inflected *S*-shape, and that solutions in higher-dimensional spaces are even more various. (Note for example that, just as a semicircle in two dimensions is monotonely equivalent to a straight line in one, a helix in three dimensions is, in the same sense, monotonely equivalent to both.) Evidently, by bending away from a one-dimensional straight line, the configuration is able to take advantage of the extra degrees of freedom provided by additional dimensions to achieve a better fit to the random fluctuations in the similarity data. In some published applications, moreover, the possibility of the more desirable one-dimensional result was mistakenly dismissed because the undetected occurrence of a merely local minimum (which is especially likely in one-dimension) made the one-dimensional solution appear to yield an unacceptibly poor monotone fit and/or substantive interpretation.

Prospects

With the exception of my own original method, all methods of nonmetric multidimensional scaling require the user to specify, in advance, the number of dimensions of the space in which the solution is to be sought. When in doubt, the user must obtain solutions, separately, in spaces of different numbers of dimensions (perhaps 3, 2, and 1) and then use criteria such as goodness of fit, statistical stability, and substantive interpretability to choose among the resulting solutions [Shepard, 1972a, pp. 9–10]. In order to take maximum advantage of this approach and to avoid the specific pitfalls mentioned above, I believe it to be highly desirable (a) to recognize the importance of the criteria of stability and interpretability (including the special advantages of visually accessible two-dimensional representations and the embedded clusterings to which they particularly lend themselves), (b) to strive toward more careful Monte Carlo studies and, hopefully, more illuminating mathematical analyses, and (c) to be vigilant for configurations (especially *C*-shaped or *S*-shaped ones in two dimensions) which strongly indicate the attainability of an acceptable one-dimensional solution.

The possibility of a one-dimensional solution can also be determined by an examination of the matrix of similarity data itself. If and only if the underlying structure is truly one-dimensional, a permutation of the rows and columns of the matrix can be found such that, except for random fluctuations, the entries decrease monotonically with distance from the principal diagonal (as in the generalized "simplex" of Guttman [1955]). Fig. 3 displays such a premuted version of the matrix of data reported by Levelt, *et al.* [1966] and upon which the spatial representation in Fig. 2A was based. To assist visualization, the heaviness of the cell entries has been chosen, here, in accordance with their numerical magnitudes. Notice that, except for minor fluctuations in seemingly isolated cells, these cell entries do tend to shade off quite uniformly as we move from the diagonal to the lower left corner. This is in contrast to the matrix of similarities among spectral colors reported by Ekman [1954], in which the similarities systematically increased again toward the lower left corner and in which monotonicity could only be maintained by a two-dimensional configuration in which the

two ends of the *C*-shape (corresponding to red and violet) necessarily approached each other to form the familiar "color circle." (See Shepard [1962b] and the present Fig. 7D.)

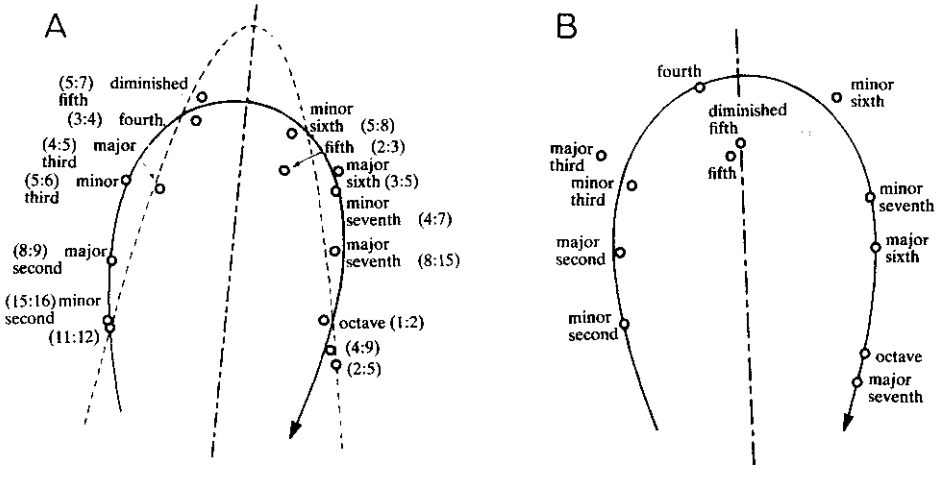

FIGURE 2

Two-dimensional spatial representations of musical intervals, obtained by Levelt, Van de Geer, and Plomp [1966] (A) and by Wickens (B), on the basis of independent sets of judged similarities.

All of the preceding recommendations are with respect to the (almost universally adopted) approach of obtaining solutions in spaces of specified dimensionalities and then using various external criteria to choose among the resulting configurations. An entirely different approach, attempted in my original method [Shepard, 1962a], is to use constraints internal to the data themselves to determine the proper number of dimensions objectively. I still believe that such an approach is feasible, particularly in cases of relatively noise-free data, and that it avoids a number of problems, particularly the just-considered problems of inherently low-dimensional configurations appearing as curved structures in higher-dimensional spaces and of entrapment in merely local minima.

The first compelling demonstration of the possibility of determining the true number of underlying dimensions objectively was that illustrated in Fig. 2 of my original report [Shepard, 1962b, p. 223]. That figure showed that, by means of the above-mentioned device of stretching large distances relative to small, an initially regular simplex in 14 dimensions flattened down into a stationary configuration of 15 points that was virtually two-dimensional and essentially identical to the true underlying structure from which the input data were monotonically derived. And, again, this process of dimensional compression was sufficiently effective that the true number of underlying dimensions could be estimated after only three iterations.

Even more striking demonstrations of the potential power of this ap-

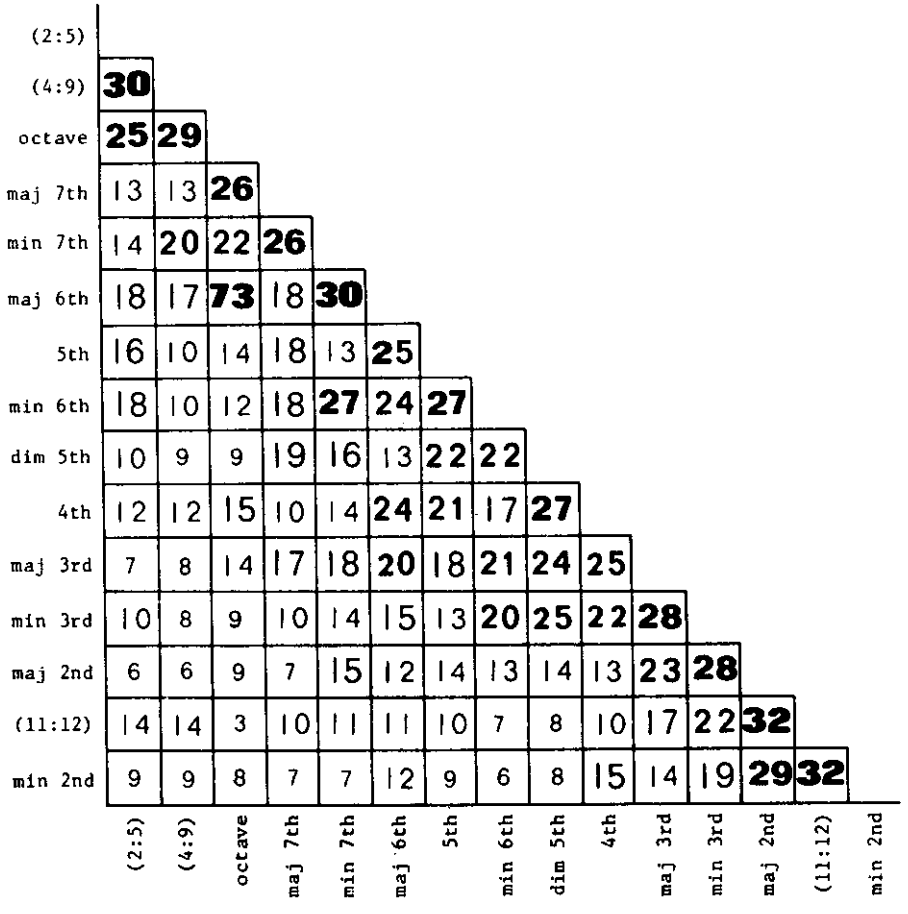

FIGURE 3

Rearranged version of the matrix of similarities among musical intervals obtained by Levelt *et al.* [1966].

proach have arisen from subsequent attempts to extend the approach to permit the determination of the "intrinsic dimensionality" of curved structures in general [Bennett, 1969; Shepard & Carroll, 1966]. Fig. 4 presents the results of two tests of a method of this type, for "conformal reduction of nonlinear data structure," that I developed at the Bell Laboratories with the collaboration of Jih-Jie Chang. The method uses essentially the same sort of differential stretching of distances as my original 1962 method but differs from that method in that the requirement of monotonicity between the original data and the final distances is enforced only locally rather than globally. The method is quite similar to that developed by Bennett [1965, 1969] except for the definition of the local neighborhood around each point. In our method each neighborhood is defined (a) with respect to distances between points in the (evolving) configuration rather than with respect to the (fixed) set of data, and (b) according to an exponential-decay weighting

function of these distances rather than according to an arbitrary discontinuous cutoff.

As can be seen from the nine successive stages of the iterative process shown in Fig. 4A, the abandonment of global monotonicity permitted a configuration of 19 points in the form of a circle with a gap (similar to the configurations in Figs. 2 and 7D and to Guttman's [1954] "circumplex") to open out into a straight line. The iterative process achieved stationarity with this perfectly one-dimensional configuration; there were no further changes with continued iteration. A similar evolution is shown in Fig. 4B for an intrinsically two-dimensional configuration of 49 points on a sphere. As can be seen from the portrayed two-dimensional projections, the initially spherical configuration (1), flattened out into shapes successively resembling a deep bowl (2), a parabolic microwave antenna (3), a shallow platter (4), and a perfectly flat disk (5). The striking degree of flatness of this final, stationary configuration is exhibited more clearly in view 5a, which shows the final configuration (of step 5) rotated into an edge-on orientation.

The maintenance of monotonicity, locally, ensured that the flattening in both cases, despite the global distortion, preserved local structure and hence was essentially "conformal." This is attested to by the evenness of the spacing of the points in the final configuration (9) that evolved from the 19 points on the circle, and by the systematically expanding regularity of the final configuration (5) that evolved from the 49 points on the sphere. This last regularity is most evident in view 5b, which shows the same configuration (of views 5 and 5a) rotated into a flat-on orientation. (The views in this figure are reproduced from the Shepard–Chang computer-generated movie "Illustrations of Conformal Mapping" which was first shown during an invited address before the 1966 meeting of the American Psychological Association [Shepard, 1966a].)

In the two examples presented in Fig. 4, the data were error free and the usual requirement of global monotonicity was relaxed. Nevertheless, the success of this objective method for dimensional reduction, together with the success of my original method from which this method derives (and in which global monotonicity was required with real and therefore fallible data) encourages me to believe that true underlying dimensionality is in principle determinable by automatic, objective methods.

4. Avoiding Loss or Imposition of Structure

Problem

Ironically, although we always seek to minimize the chosen measure of departure from monotonicity, special difficulties are apt to arise whenever the stress is zero or close to zero. Zero-stress solutions, in particular, are generally either *nonunique*—and to that extent introduce some degree of extraneous structure that is not contained in the data, or *degenerate*—and therefore fail to preserve some structure that *is* contained in the data. The

problem of nonuniqueness is the less troublesome. One can always evaluate the degree of uniqueness of a solution by using several different starting configurations. Moreover, what the finding that substantially different solutions are obtainable with the same zero stress really indicates is that either the number of objects being scaled should be increased or the number of dimensions of the embedding space should be decreased. The problem of degeneracy, however, is sometimes bothersome enough to motivate a search for methodological innovations.

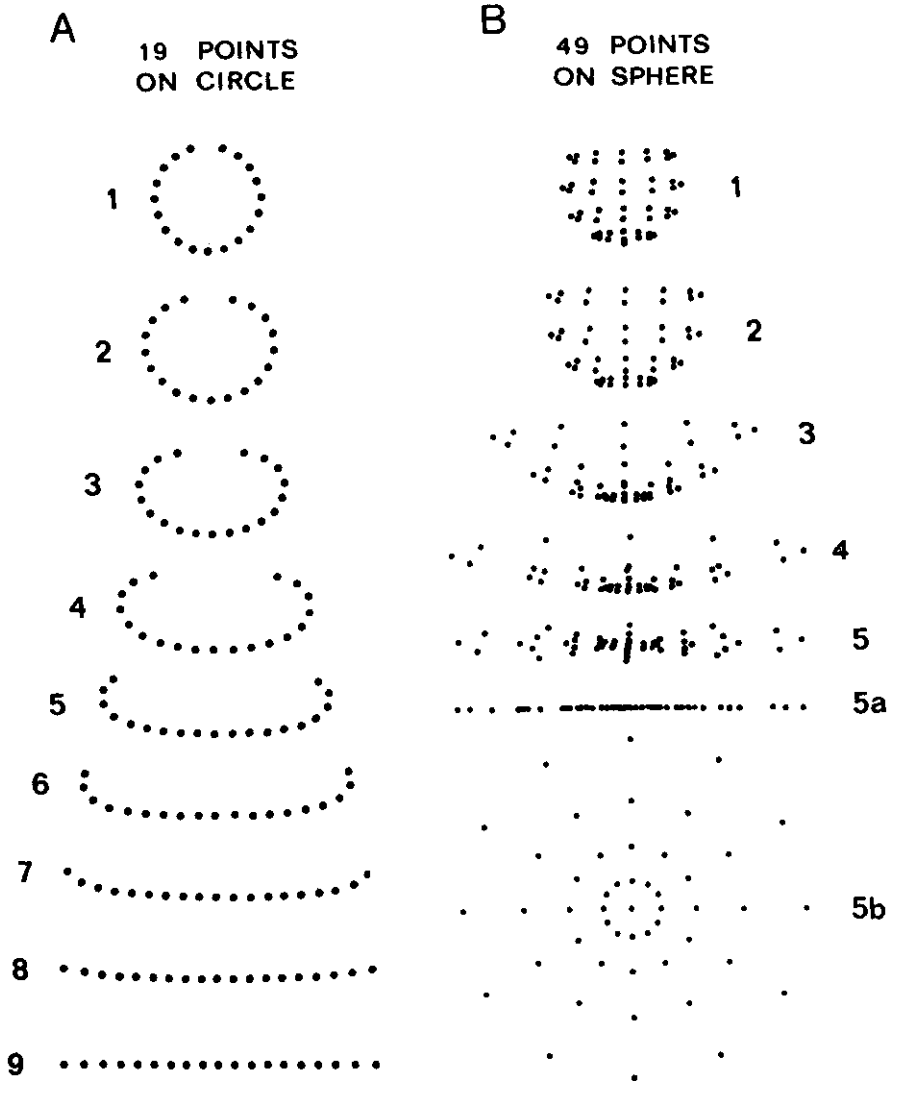

FIGURE 4

Successive stages in Shepard-Chang conformal reduction of 19 points on the perimeter of a circle (A) and of 49 points on the surface of a sphere (B) into flat spaces of the appropriate intrinsic dimensionalities.

As a rough index of the *non*degeneracy of a solution, I would propose the ratio of the number of distinct values of distances among the n points to the total number of distances (*viz.*, $n(n-1)/2$). Thus, if no two distances are tied we have a totally nondegenerate solution, while if all $n(n-1)/2$ distances are tied we have a totally degenerate solution (namely, the regular simplex in $n-1$ dimensions). Typically, because we require a solution in fewer than $n-1$ dimensions, a zero-stress solution is not totally degenerate by this index, and the distances assume one of two or three different values.

As an illustration, Fig. 5A shows a degenerate solution that occurred when I analyzed data long ago sent to me by A. Howard, on the judged similarities among eight gustatory stimuli. The stimuli collapsed into the

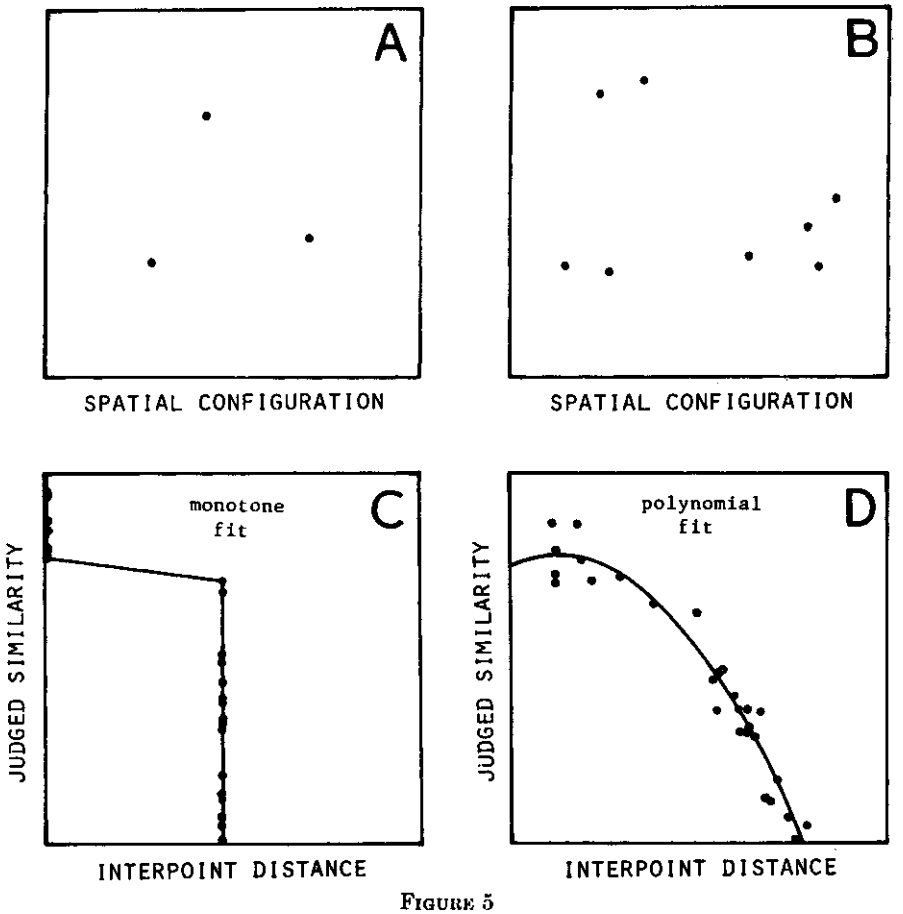

FIGURE 5

Degenerate (A) and nondegenerate (B) configurations for eight gustatory stimuli, based upon the "nonmetric" and "metric" assumptions that the relation of the similarity data to the interpoint distances has the form of a merely monotone function (C) or the form of a polynomial of low degree (D), respectively.

three vertices of an equilateral triangle and, so, there were just two values of distance: zero, for pairs of points located at the same vertex, and a fixed

larger value, for pairs of points located at two different vertices. This degeneracy arose because the stimuli divided into three groups such that all of the similarities within any group were greater than any of the similarities between any two groups. The consequence is that much structural information is lost in the spatial solution. We learn only that the stimuli strongly cluster into the three groups; we learn nothing about either the relationships among these three groups or the relationships among the stimuli within any one of these groups. Correspondingly, the function relating the given similarities and the recovered distances assumes the implausible and uninformative shape of the single, discontinuous step shown in Fig. 5C. Although the fit is perfect (*i.e.*, the stress is zero), the representation is too degenerate to be of much use.

In Fig. 6 I display all maximally degenerate four-point configurations in two dimensions; *i.e.*, all two-dimensional configurations in which the distances among the four points take on only two distinct values. The smaller distances are represented by the heavier lines connecting pairs of points—unless those distances are zero, in which case the two or three coincident points are represented by concentric circles. (These configurations may be regarded as two-dimensional analogues of the one-dimensional "corner sequences" defined by Abelson and Tukey [1959].) Of the many strongly degenerate two-dimensional configurations that I have obtained in the analysis of real and artificial data, regardless of the number of points all

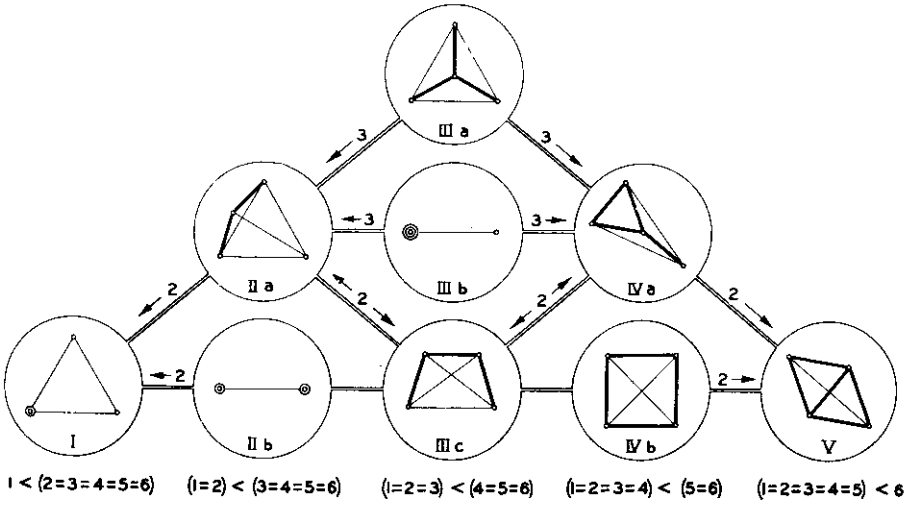

FIGURE 6
The nine degenerate four-point configurations in two dimensions, for which the six interpoint distances take on just two distinct values (as indicated along the bottom).

have taken one or another of the nine forms shown in Fig. 6. In cases of extreme degeneracy, apparently, the additional points usually collapse onto these same few vertices. Thus, the eight-point configuration shown in Fig. 5A corresponds to the equilateral triangular degeneracy labeled "I" at the

left in Fig. 6. Therefore, whenever the points in an obtained solution cluster close to the vertices of one of the highly symmetric configurations exhibited in Fig. 6, one should suspect the occurrence of a rather marked degeneracy. In practice, the true extent of this degeneracy is often not immediately obvious because the criterion (*e.g.*, of low stress) for terminating the iterative process is attained before the clusters complete their collapse into the vertices. Even so, the tendency of the monotonicity diagram (see Fig. 5C) toward a discontinuous function of one or two steps will usually suffice as a signal of impending degeneracy.

Closely related to the problem of true degeneracy, in which a large proportion of the interpoint distances are tied, is the problem of quasidegeneracy, in which many of the monotone values being brought into a mutual best fit with the distances, if not the distances themselves, are tied. Actually, some degree of quasidegeneracy in this sense is always present in solutions obtained by nonmetric methods (although it may be negligible when the number of points is large and the data are sufficiently error-free [Shepard, 1966b]). It shows up in the zigzag or step-like shape that is characteristic of the best-fitting monotone functions obtained by nonmetric multidimensional scaling (see Fig. 7A). Roughly, the more pronounced the individual steps appear, the greater is the quasidegeneracy of the solution.

To the extent that we are interested in the functional form of the relation between the similarity data and metric distances (as in the study of stimulus generalization), such quasidegeneracy is undesirable for two related reasons; one substantive and one statistical. Substantively, the step-like function is unappealing if, as I assume, we generally believe that the true underlying relationship has some smooth functional form (such as the exponential decay form expected under some circumstances on theoretical grounds [Shepard, 1958a]). Statistically, the zigzag function is unreliable in the sense that, when we analyze a new set of similarity data for the same set of objects, we find that the individual zigs and zags of the function shift about in a quite unpredictable manner. The presumption, therefore, is that these individual zigs and zags do not represent any reliable or substantively meaningful phenomenon but, rather, reflect the attempt of the large number of degrees of freedom of a merely monotone function to fit the random fluctuations peculiar to each individual set of data.

Prospects

In order to minimize the likelihood of true degeneracy or of marked quasidegeneracy, researchers should try, whenever possible, to select objects for nonmetric scaling (a) that are not obviously grouped into a few psychologically compact clusters, and (b) that are not fewer than about ten in total number, for a two-dimensional solution, or more, for a higher-dimensional solution [Shepard, 1966b]. (A distressing number of two- and even three-dimensional solutions have been published in which, despite the inclusion of only six to eight objects, no evidence is provided that the configuration has a reasonable degree of metric determinacy and is not a prematurely

arrested case of convergence toward a degeneracy.) Whether or not it is actually included in the published report, the monotonicity diagram (Figs. 5C and 7A) should be examined for step-like evidences of degeneracy and the results reported.

When true degeneracy does occur (as illustrated in Figs. 5A and 6), one currently has recourse to one or both of two further kinds of analysis in order to achieve a representation that preserves more of the structure in the similarity data. One can reapply the nonmetric analysis, separately, to the submatrix of similarities for the objects corresponding to each collapsed cluster containing enough points to make this worthwhile. If this does not lead to a further (hierarchically deeper) degeneracy, additional information can thereby be recovered about the internal structure of such a subset—though not about the relation of that subset to any other. Alternatively, if a representation of the overall structure of the entire set of objects is still desired, one must resort to metric methods, which depend upon stronger assumptions concerning the functional form of the monotone relation between similarity and distance. Sometimes, a combination of both approaches is quite successful. (See, for example, Fig. 18 and accompanying discussion in Shepard, *et al.* [in press].)

The present Figs. 5B and 5D illustrate the use of stronger, metric assumptions to overcome degeneracy. Here, the very same set of data already analyzed nonmetrically in Figs. 5A and 5C were reanalyzed using a program for "polynomial fitting in the analysis of proximities" that I developed in an early attempt to deal with the problem of degeneracy [Shepard, 1964b]. (Subsequently, of course, Kruskal and others have generalized their programs to provide for the fitting of polynomial or other parametric functions, also.) Notice that, although the fit is no longer perfect (as it should not be with fallible data), the spatial configuration preserves structural information about all eight of the stimuli (Fig. 5B), and (apart from a minor deviation from monotonicity, to be considered shortly) the relation between similarity and distance approximates a more plausible, smooth functional form—specifically, in this case, a quadratic (Fig. 5D).

The fitting of smooth, parametric functions rather than jagged, merely monotonic functions also permits us to circumvent the lesser problem of quasidegeneracy. This is illustrated in Fig. 7. The upper two panels (*A* and *B*) are both based upon measures of the tendency of pigeons trained to respond to each of a number of spectral colors to generalize that response to each of the other colors. These data, collected by Guttman and Kalish [1956], are of the sort for which the question of the functional form of the "gradient of stimulus generalization" is of central interest [Shepard, 1965]. From this standpoint, the function obtained by applying my polynomial-fitting program—in this case an exponential-like quartic curve (Fig. 7B) seems to be both substantively more plausible and statistically more reliable than the function obtained by nonmetric multidimensional scaling (Fig. 7A).

The lower panels (*C* and *D*) present a reanalysis of Ekman's [1954] data

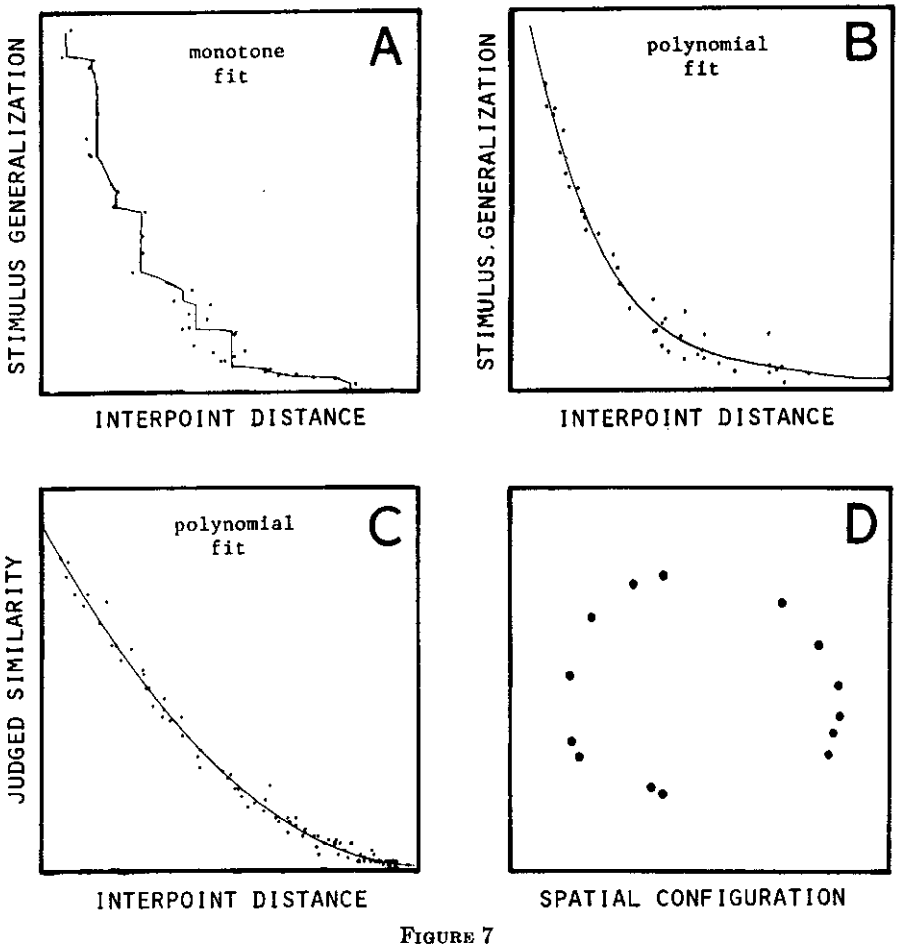

FIGURE 7

Measures of stimulus generalization between spectral colors, obtained for pigeons by Guttman and Kalish [1956], plotted against interpoint distances obtained by multidimensional scaling on the assumption of a merely monotone (A) or a polynomial (B) relation between similarity and distance; and a plot for a similar polynomial analysis of Ekman's [1954] judged similarities among 14 spectral colors (C) together with the quasicircular spatial configuration obtained by that analysis (D).

on the similarities among spectral colors as judged by human subjects. The quasicircular configuration obtained for the 14 colors by means of the polynomial-fitting program (Fig. 7D) is virtually identical to the nondegenerate one I originally obtained by a nonmetric analysis [Shepard, 1962b, p. 236]. Moreover, the obtained relationship between judged similarity and Euclidean distance between points in this configuration (Fig. 7C) exhibits a strikingly good fit to a smooth and plausible monotone decreasing function. Evidently, such a metric method of analysis can yield quite satisfactory results whether or not there is a problem of degeneracy or of quasidegeneracy.

One drawback of polynomial-fitting programs, of course, is that it is difficult to ensure that the resulting polynomial will be monotone over the

range covered. Thus, a departure from monotonicity is evident in Fig. 5D and, although not included in the figure, a nonmonotonic upswing occurs just beyond the right-hand border of Fig. 7B. Kruskal (personal communication) has suggested the strategy of simultaneously minimizing departures from monotonicity and from a polynomial of specified degree (a possibility that is provided in recent versions of his program, *e.g.*, M-D-SCAL 5M). But, even with this strategy, I have found that the fitted polynomial can still become markedly nonmonotone in the range of the data.

In order to ensure monotonicity, one can of course iterate into a best fit with a parametric function of some other general type that can be more easily constrained to strict monotonicity. Since confusion and generalization data seem in general to decay exponentially with interstimulus distance [Shepard, 1958, a, b, 1965, 1972c], Jih-Jie Chang and I developed a gradient method for optimally adjusting, simultaneously, the coordinates of a spatial configuration and the parameters of an exponential decay function relating the similarity data to the interpoint distances [Chang & Shepard, 1966]. In Fig. 8 the results of applying this exponential-fitting method to Miller and Nicely's [1955] data on confusions among 16 consonants (*A*) is contrasted with the results of a nonmetric (M-D-SCAL) analysis of the same data (*B*). The closed curves show the embedded results of hierarchical clustering [Johnson, 1967] applied to the same data, as previously explained for Fig. 1. (See Shepard [1972c] for the full substantive interpretation of this configuration.)

Note that, in the configuration (*B*) obtained by the nonmetric analysis, only, there is an inconvenient partial degeneracy in which several points collapse together. Correspondingly, the fitted monotone function obtained by the nonmetric analysis manifested, again, a crude step-like shape (similar to that shown in Fig. 7A), whereas the fitted exponential function obtained by the metric analysis achieved an excellent fit (even better than that shown in Fig. 7B) and, in fact, accounted for some 99% of the variance of the confusion measures of similarity [Shepard, 1972c, p. 77]. Nevertheless, the exponential-fitting method is undesirably limited for general purposes, since many other types of similarity or dissimilarity data are not expected to bear an exponential relation to distance.

What may have seemed most remarkable in my original demonstrations of nonmetric scaling [Shepard, 1962b] was the extent to which a tightly constrained metric structure can be recovered from an analysis of merely ordinal relations in the data [cf., Shepard, 1966; Young, 1970]. It may seem odd, therefore, that I am now recommending consideration of methods that depend upon more than merely ordinal relations. Nevertheless, from the practical standpoint of trying to obtain results that are optimally meaningful and invariant under replication of the data as well as under reasonable (and therefore smooth) sorts of monotone transformations of the data, such a recommendation seems appropriate. The problem that remains, however, is to impose the desired condition of smoothness in some general and nonarbitrary way without having to specify a particular functional form—such

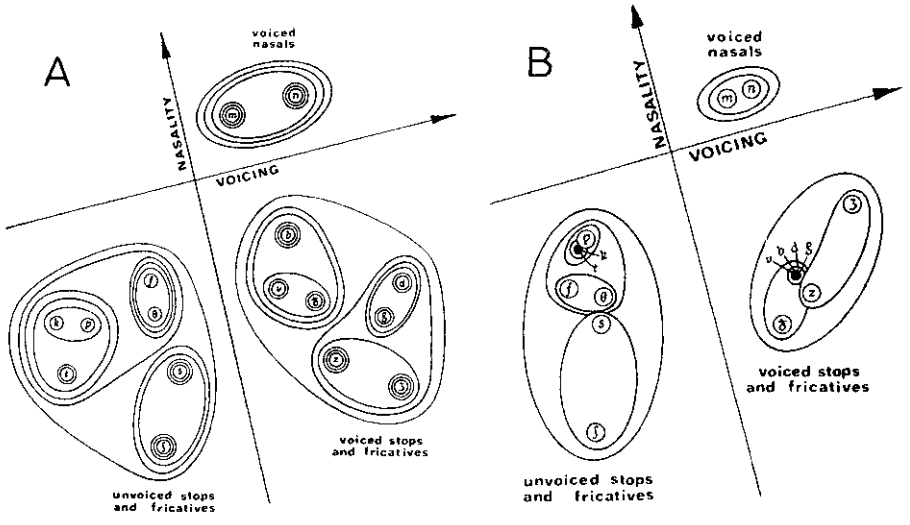

FIGURE 8

Two-dimensional spatial representations of 16 consonant phonemes obtained by multidimensional scaling on the assumptions that the relation of the confusion measures of similarity (obtained by Miller and Nicely [1955]) to the interpoint distances is exponential (A) or merely monotone (B), together with embedded hierarchical clusterings [see Shepard, 1972c].

as the polynomial (which can become nonmonotonic) or the exponential (which is often too restrictive).

Recently, with the collaboration of a student in computer science, Glen Crawford, I have been exploring a new approach to the problem of fitting functions which seems to provide a very natural and well-defined way of introducing general conditions such as convexity, concavity, or even "smoothness," as well as the condition of monotonicity. For each value x_i of an independent variable x (where the subscripts are assigned so that $x_1 < x_2 < \cdots < x_n$), we seek a theoretical estimate $\hat{y}_i$ that best fits the corresponding observed value y_i such that the theoretical values $\hat{y}_1, \hat{y}_2, \cdots, \hat{y}_n$ satisfy certain explicitly prescribed constraints on their weighted first- and second-order differences as required to ensure that the sequence of values is monotone, is convex or concave, and/or is locally linear, as desired. The method that we are currently testing (which we call "least-squares regression to a constrained-difference function") uses a gradient method with penalty functions to obtain a least-squares solution subject to the prescribed constraints.

The results of one test application of this method are displayed in Fig. 9. In Fig. 9A the best-fitting monotone decreasing function is indicated for a set of artificial data (a quadratic with added random error). The given data are represented by the open circles and the fitted function is represented by the connected small solid circles. Note, as before, the characteristically step-like shape of the best-fitting monotone function. By contrast, Fig. 9B

shows that, as soon as we use the method to impose just the condition of convexity in addition to the condition of monotonicity, the function fitted to the same data becomes very smooth. Moreover, the convex function also achieves a much closer fit to the true underlying (quadratic) function.

We plan to use this approach to curve fitting as the basis for a method of multidimensional scaling in which one will not have to assume a particular functional form for the relation between distance and similarity, but in which one can impose some further constraint beyond mere monotonicity (in order to obtain a functional relationship that is more plausible, more reliable, and less subject to degeneracy). In the most direct extension to multidimensional scaling, the fixed similarity values, s_{ij}, would be treated as the values of the independent variable x, while the to-be-varied distances, d_{ij}, would be treated as the values of the dependent variable y. However, other possibilities, e.g., turning the regression around, would also offer advantages, including that of being able to maximize the variance of the given similarity data accounted for by the spatial representation.

5. *Determining the Form of the Underlying Metric*

Problem

In addition to permitting the recovery of metric structure from merely ordinal data, the iterative procedures introduced in the original methods of nonmetric multidimensional scaling made possible the fitting of representations based upon non-Euclidean metrics. (See [Shepard, 1962b, p. 224] and, for the first actual implementation of this possibility, [Kruskal, 1964a, b].) Methods of this type are therefore used in the continuing investigation into the conditions under which psychological similarity is determined by alternative Euclidean or non-Euclidean rules of combination of differences along underlying psychological dimensions [see, *e.g.*, Arnold, 1971; Attneave, 1950; Cross, 1965; Hyman & Well, 1967, 1968; Shepard, 1964a; Shepard & Cermak, 1973; Thomas, 1968; Torgerson, 1958]. Unfortunately, difficulties both of a persistent practical sort and of a recently discovered theoretical nature raise doubts about the ways in which these methods are usually used for this purpose.

Methods of nonmetric multidimensional scaling generally seek Minkowski power-metric representations by iterating to a best fit after specifying a value for the power, r (where the most widely discussed metrics—the so-called "city-block," "dominance" and, of course, Euclidean varieties—correspond to the limiting values of $r = 1$, $r = \infty$, and the intermediate value of $r = 2$, respectively). Thus, if the appropriate value of r is (as in the typical case) not known in advance, the user is faced with the tedious and costly procedure of obtaining solutions, separately, for a number of representative values of r spaced out between 1 and some very large value. The user must then decide among the resulting set of solutions in some way (presumably on the basis of which solution achieves the lowest residual stress [*e.g.*, Kruskal

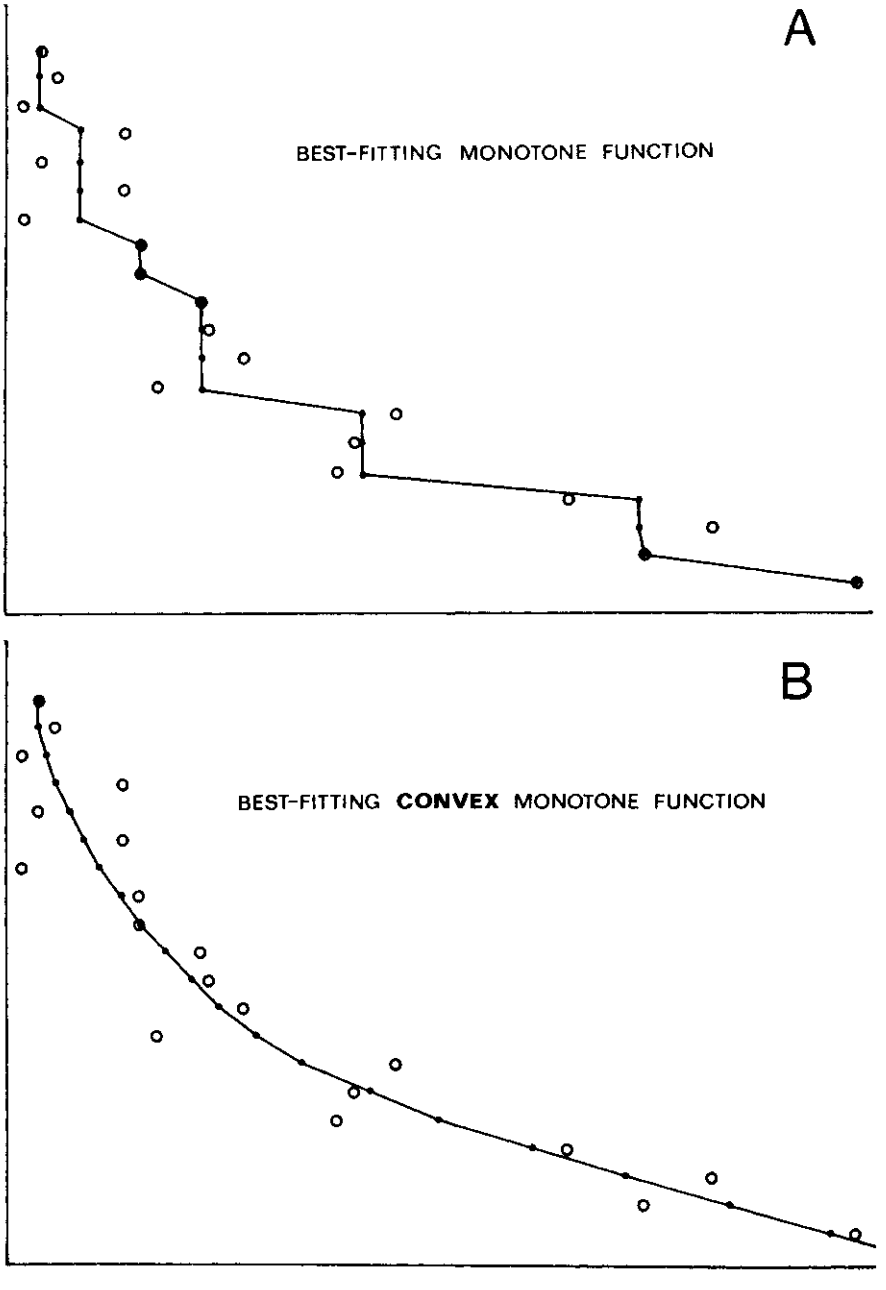

FIGURE 9

Identical artificially generated scatterplots with the best-fitting monotone decreasing function (A), and with the best-fitting monotone decreasing and convex function obtained by the Shepard-Crawford method of regression to a constrained difference function (B).

1964a, p. 24]).

From the practical standpoint, the cost of obtaining solutions separately

for many different values of r is apt to become prohibitive because problems of slow convergence and local minima are much more severe in the case of these non-Euclidean metrics. On the basis of his extensive attempts to obtain non-Euclidean solutions, Arabie (personal communication [see, also, Arabie & Boorman, 1973]) reports that, in three or more dimensions, random starting configurations are essentially useless. For this case, he recommends resorting to the incompletely validated strategy—apparently suggested, independently, by Arnold [1971] and Kruskal (personal communication)—of gradually working out from the Euclidean solution (for $r = 2$), by using the final configuration obtained for each value of r as the initial configuration for the next larger (or smaller) value of r. In the case of two dimensions, by contrast, Arabie reports that this (Arnold–Kruskal) strategy is generally unsuccessful and that one should therefore use random initial configurations (with perhaps as many as 100 different starts being required for each value of r in order to ensure attainment of the global minimum!).

Quite apart from this essentially practical problem, my own recent theoretical investigations have convinced me that the generally accepted practice of taking, as the correct metric, the one which yields the lowest residual departure from monotonicity is unfounded and probably leads to erroneous conclusions. Such a practice is based on the assumption, never explicitly justified, that values of stress are directly comparable across different values of r. I first came to question this assumption as a result of puzzling over the tendency (first noted by Arnold [1971] and, then, by Arabie and Boorman [1973]) of the points in spatial configurations conforming to the city-block or the dominance metric to be themselves disposed in a manner resembling the shape of the "unit sphere" for those particular metrics; that is, resembling the perimeter of a diamond or square, respectively, (in two dimensions) or the surface of an octahedron or cube, respectively, (in three). This led to the discovery of the purely geometrical fact that degeneracies and, hence, low values of stress are more prevalent for values of r close to 1 and, particularly so, for values of r approaching ∞.

The special nature of these extreme metrics (and a possible explanation for the puzzling phenomenon noted by Arnold and by Arabie and Boorman) is illustrated in Fig. 10, for the case of the city-block metric in two dimensions. In this case, the unit circle (*i.e.*, the set of all points equidistant from a given point) has the form of a diamond (or 45° square), as indicated by any one of the concentric dashed contours surrounding the point P. This implies that, for every point P, situated on a closed curve of the particular shape indicated by the solid curve, half of the remaining points on that same curve can be divided into three subsets (indicated by the heavier segments, a, b, and c) such that the distances from P to all points within any one of these subsets are tied. It follows that, if points (in finite number) are evenly distributed around the solid curve, no more than half of the interpoint distances will be distinct. According to the index of nondegeneracy proposed earlier, then, this situation is at least "half degenerate." But, as was illustrated in Fig. 5, whenever there is a choice between a more and a less degenerate

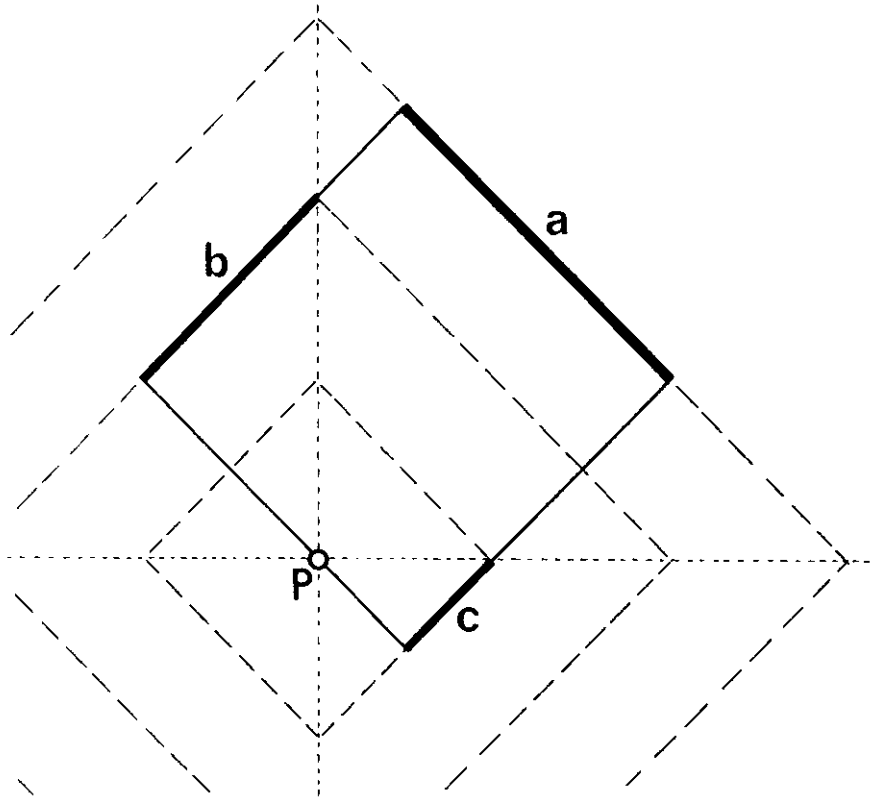

FIGURE 10
Demonstration of the prevalence of tied distances between points on an equidistance contour in the city-block metric.

configuration, the nonmetric method will move toward the more degenerate configuration, where the increased prevalence of ties permits the attainment of a lower value of stress.

When the point P coincides with any of the four corners of the solid curve, the three segments a, b, and c merge into one continuous region, which is coextensive with the two sides opposite P and within which *all* distances from P have the same value. Hence, a configuration of four points corresponding to these four corners has the completely degenerate property that all six interpoint distances have exactly the same value. This is in contrast to the Euclidean case, in which no more than three points (the vertices of an equilateral triangle) can be mutually equidistant, and in which a complete four-point degeneracy (the vertices of a regular tetrahedron) requires three dimensions.

In the case of higher-dimensional spaces, the contrast with the Euclidean metric becomes even more marked. Specifically, the maximum number of

points, m, that can be arranged in k dimensions, so that the points in all $m(m-1)/2$ pairs are separated by the same distance is given by $k+1$, by $2k$, and by 2^k in the cases of the Euclidean, city-block, and dominance metrics, respectively (where the points then coincide with the vertices of the regular simplex, the regular cross-polytope, and the hypercube, respectively). Thus, the number of points that can be mutually equidistant tends, with increasing dimensionality, to be twice as great for the city-block metric as for the Euclidean and to increase exponentially faster than either for the dominance metric. Even in just three dimensions, the number of points for which complete degeneracy is possible is 4, 6, and 8, for the Euclidean, city-block, and dominance metrics. Thus, while it is not true in the Euclidean case, with a dominance metric we know in advance that in only three dimensions we can fit any similarity data for eight objects whatever, and that the resulting spatial configuration will preserve none of the structural information in those data.

The same phenomenon emerges in partial as well as complete degeneracy. Thus, for 16 points at the vertices of a regular 3×3 lattice in two dimensions, the number of distinct values of interpoint distance is 9, 6, and only 3 for the Euclidean, city-block, and dominance metrics. Likewise, for 27 points at the vertices of a regular $2 \times 2 \times 2$ lattice in three dimensions, the number of distinct values of distance is 9, 6, and only 2 for the same three metrics. And, for 16 points at the vertices of a regular $1 \times 1 \times 1 \times 1$ lattice (or hypercube) in four dimensions, the number of distinct values of distance is 4, 4, and only 1. Quite generally, then, tied distances, degeneracies and, hence, lower levels of stress are easier to come by with non-Euclidean and, particularly, with the dominance metric. Consequently, while the finding that the lowest stress is attainable for $r = 2$ may be evidence that the underlying metric is Euclidean, the finding that a lower stress is attainable for a value of r that is much smaller or larger may be artifactual.

These same investigations disclosed some other curious properties of these non-Euclidean metrics. One is that the completely degenerate configuration for the city-block and dominance metrics (unlike the regular simplex for the Euclidean) give the misleading appearance of containing structural information. Thus, in the cubical degeneracy for the three-dimensional dominance metric, points separated by one edge of the cube appear to be related to each other in a way that points separated by two edges (or a face diagonal) or by three edges (or a body diagonal) do not. But, in fact, all pairs of points are related in the same way, and the interpoint distances are unchanged by any permutation of the assignment of points to vertices. Another fact of perhaps greater practical relevance is that, in the cases of the two-, three-, and four-dimensional lattices considered above, the rank order of the interpoint distances for the Euclidean metric (though divided into more levels) is entirely consistent with the rank order for the dominance metric (and differs, at most, by a reversal of one pair of adjacent values from that for the city-block metric). Thus, although it might seem quite natural to generate a set of stimuli by using every combination of values from among two, three, or four levels on each of four, three, or two physical

dimensions, respectively, nonmetric methods of analysis would be totally incapable of determining whether similarity data collected for such a set conformed with the Euclidean or dominance metrics (and would be extremely inefficient, at best, in revealing a better or worse correspondence to the city-block metric).

Finally, the limitations of the currently accepted practice of using nonmetric multidimensional scaling to test the appropriateness of the various Minkowski power metrics do not end with these practical and theoretical difficulties. There is the further limitation that this one-parameter class of so-called r-metrics is itself quite restricted. How much so may be seen from Fig. 11, which presents a hierarchy of some of the most thoroughly studied metric spaces, ranging from the most general, represented at the top, down to the most specific; represented at the bottom. Note that the class of Minkowski r-metric spaces occupies a relatively low position in this hierarchy. This is because the distance formula (displayed in the rectangle for that class of spaces) is extremely restrictive and, in fact, entails that the unit sphere in k dimensions has exactly $2k$ prominences for $r < 2$ and exactly 2^k prominences for $r > 2$.

Much more general, is the class of general Minkowski spaces in which the unit spheres may have any convex, centrally symmetric shape. The

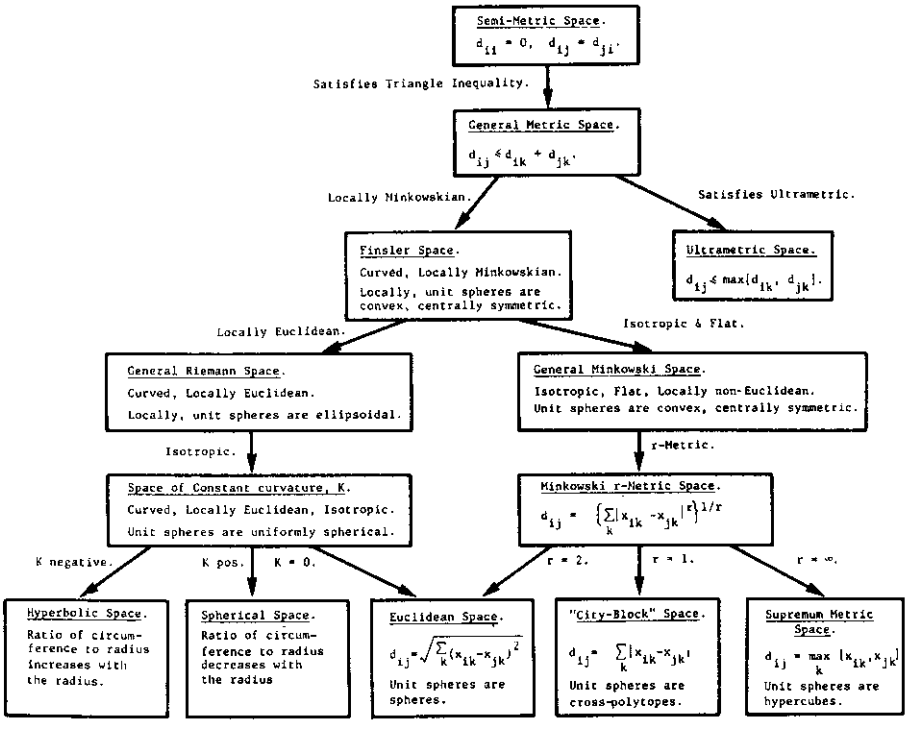

FIGURE 11
Hierarchy of some commonly considered metric and semimetric spaces.

conditions of symmetry and convexity of the unit spheres are connected with the distance axioms of symmetry and the triangle inequality, displayed in the top-most and next lower rectangles, respectively. An additional requirement, that these unit spheres be constant in size and shape throughout the space, entails that the general Minkowski space is isotropic and intrinsically flat. In this last respect, general Minkowski is, in turn, less general than Finsler space, in which these unit spheres can change continuously with location in the space. Thus, Finsler space permits both the locally non-Euclidean properties of flat Minkowski spaces and the globally non-Euclidean properties of intrinsically curved Riemann spaces (indicated on the left in Fig. 11). Finally, even Finsler space (along with all the more special cases arrayed below it) presupposes a continuous underlying coordinate space with its own intrinsic dimensionality and, so, is less general than the merely metric or semi-metric spaces. For, the constraints in these most general cases are defined solely in terms of interpoint distances and entail neither a specific dimensionality nor the embedability of a coordinate system. (For a fuller mathematical treatment of these various types of spaces see, *e.g.*, Beals, Krantz, and Tversky [1968]; Blumenthal [1959]; Busemann [1955]; and Rund [1959].)

Generally available methods for the analysis of similarity data have been designed to yield representations with metrics corresponding to only five of the thirteen boxes included in Fig. 11; namely, that of the ultrametric (as exemplified by Johnson's [1967] formulation of hierarchical clustering) and those of the Minkowski r-metric and, hence, the Euclidean, city-block, and dominance metrics (as already discussed). It is true (a) that general Riemann spaces and spaces of constant curvature have long been considered for representing, respectively, the perceived similarities among colors [*e.g.*, Silberstein, 1938; Silberstein & MacAdam, 1945] and the perceived distances among luminous points in a dark three-dimensional field [*e.g.*, Blank, 1958; 1959; Indow, in press; Luneburg, 1947, 1950]; (b) that general Minkowski spaces have been recognized as providing for the representation of considerably more diverse rules of combination than are representable just by the class of r-metrics [Shepard, 1964a]; and (c) that completely general metric spaces avoid the implication, possibly objectionable for the representation of semantic structure, of an underlying continuum. However, methods of multidimensional scaling have, up to now, not been fully extended to these cases.

Prospects

The strategy of obtaining Minkowski r-metric solutions for the same set of data using different values of r may still be useful in some cases. It apparently can provide evidence that the underlying metric is Euclidean or near-Euclidean. For those who wish to use this strategy, some savings in computation is possible owing to a kind of conjugate relationship that holds in certain cases between values of r above and below the Euclidean value of 2. Certainly in two dimensions there is no reason to seek optimum

solutions both for $r = 1$ and for $r = \infty$. These two limiting metrics are identical in two-dimensions, except for a 45° rotation and uniform dilation or contraction of the configuration as a whole. Moreover, for intermediate values of r, Koopman and Cooper [1974] have just reported numerical results suggesting that, if r and r^* stand in the relation $1/r + 1/r^* = 1$, an approximate conjugacy holds in two dimensions such that, for practical purposes, it may be unnecessary to obtain two-dimensional solutions for values of r both above and below 2. Additional support for this suggestion may be found in a result that Phipps Arabie (personal communication) has obtained in further analyses of Ekman's [1954] color data. Corresponding to the r-value of about 2.5 (or 5/2) for which Kruskal [1964a, p. 24] had found that stress was minimum for these data, Arabie found a corresponding, conjugate minimum stress at an r-value of about 5/3 (in accordance with $2/5 + 3/5 = 1$).

However, even in two dimensions, this conjugacy does not hold strictly except in the limiting case of $r = 1$ and $r^* = \infty$. Although the proof is too long to include here, I established some years ago that, for any value of r in the open interval between 1 and 2, there is no value, r^*, greater than 2 such that the r-metric and the r^*-metric are exactly equivalent except for a rotation and change of scale. And, from the already mentioned fact that the number of points that can be arranged to be mutually equidistant in k-dimensions is $2k$ for the city-block metric but 2^k for the dominance metric, it is clear that conjugacy for $k > 2$ does not even hold in the limiting cases in which r and r^* approach 1 and ∞.

In any case, the very serious limitations already noted in the use of Minkowski r-metric solutions to investigate the underlying rule of combination has led me to explore quite different approaches. One which appears to avoid the practical and theoretical difficulties discussed above and to offer considerable generality (at least for the two-dimensional case), is based upon results that I obtained with the collaborative help of Doug Carroll and Jih-Jie Chang [Shepard, 1966]. Basically, these results amount to a demonstration that purely Euclidean solutions can be surprisingly robust in the face of certain kinds of rather marked departures from the assumed Euclidean metric. As I shall argue, this means that one can determine the form of the underlying unit circle and, hence, the nature of an underlying (flat and isotropic) space even though the metric is of the general Minkowski type or of still more general merely semimetric types.

Our investigation was based upon a set of artificial data derived from a square array of 50 random points. The Euclidean distances among these points were converted into very non-Euclidean and, in fact, merely semimetric "distances" by differentially stretching or shrinking all distances depending upon the angular orientation of the line connecting each pair of points in accordance with the six-lobed unit circle shown in Fig. 12A. The resulting "metric" was essentially in the spirit of the general Minkowski metric. But, since the unit circle was nonconvex and had six rather than four prom-

inences the metric could not be approximated by any two-dimensional r-metric and was strictly speaking only a semimetric.

Nevertheless, when nonmetric multidimensional scaling (M-D-SCAL) was applied to these rather bizarre semimetric distances on the assumption that they were ordinary Euclidean distances, the obtained two-dimensional configuration achieved a close approximation to congruence with the randomly generated original configuration. For most of the individual points, the discrepancy in the recovered position of the point was small compared with the distance to even its nearest neighbor. When we then plotted, in polar coordinates, the ratio of the original (non-Euclidean) data to the recovered (Euclidean) distances as a function of the angle of the line between the two points in every pair, we obtained the scatterplot displayed in Fig. 12B. The six-lobed shape of the underlying unit circle reemerged quite clearly.

In the analysis of real data, of course, the similarity measures may be some unknown monotone function of the underlying (non-Euclidean) distances rather than those distances themselves. So, in general, it would not be appropriate merely to plot ratios as was done for Fig. 12B. Nevertheless, it should not be difficult to estimate, for each small angular interval, the (Euclidean) distance for which the function relating similarity to distance within that interval attains some specified level. I have outlined a procedure of this sort that, I am hopeful, will yield a good approximation to the desired unit circle. Depending upon whether the resulting plot is generally circular, square, or of some other (possibly even nonconvex) form, we could infer quite directly whether the metric is of the Euclidean, city-block (or dominance), or some other (perhaps merely semimetric) type.

The extension of existing methods of multidimensional scaling so as to yield solutions in spaces of constant curvature appears straightforward but, to my knowledge, has not been attempted. Perhaps the method that comes closest to being such an extension is the "nonmetric factor analysis" method,

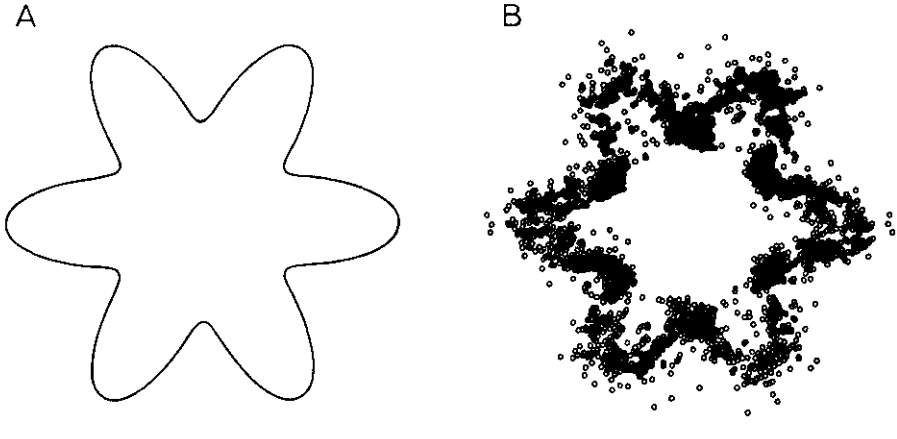

FIGURE 12
Six-lobed unit circle (A) and attempted reconstruction of that semimetric unit circle (B) on the basis of a Euclidean multidimensional scaling solution.

SSA-III, of Guttman and Lingoes [see Lingoes, 1972]. In this method scalar products of vectors, rather than distances, are brought into a best monotone fit with the similarity data. If the vectors were all constrained to be of the same length, the scalar products would become equivalent to distances on the surface of a hypersphere—a surface of constant positive curvature. Particularly since more recent findings regarding the binocular perception of luminous points in space have been in some ways inconsistent with Luneburg's [1947] model of visual space as a (hyperbolic) manifold of constant negative curvature [Foley, 1972], however, there has been no insistent demand for methods designed to yield representations in which the curvature is constrained to be constant, whether positive or negative.

Doug Carroll and I have pursued a quite different approach that appears to offer the appreciably greater generality of allowing for cases in which the intrinsic curvature of the underlying space may vary from region to region (as in general Riemann spaces) and, at the same time, the metric may behave locally as a general Minkowski metric or even as a still more general semimetric (such as that associated with the nonconvex unit circle illustrated above). Such an approach provides for the possibility that the underlying psychological space may be a kind of Finsler space or even some semimetric generalization of such a continuous space. This generality is achieved by abandoning the requirement that the triangle inequality be satisfied while retaining the requirement that the similarity between the objects represented by two points vary in an appropriately smooth and continuous manner with the positions of those points in the underlying space. The analysis itself is carried out by applying, to the given similarity data, a method of "parametric mapping" to optimize an index, developed by Carroll, for measuring departure from a smooth or "continuous" relation between the data and the coordinates for the points in the underlying parameter space [Shepard & Carroll, 1966].

As one test of this approach, again carried out with the collaborative assistance of Doug Carroll and Jih-Jie Chang [Shepard, 1968], the already-described square configuration of 50 random points was converted into a toroidal configuration by identifying opposite edges of the square and redefining distances so as to be non-Euclidean in two respects; local and global. The locally non-Euclidean structure was induced by stretching and shrinking each distance as a function of its angle in accordance with the six-lobed unit circle in Fig. 12A; and the globally non-Euclidean structure was secured by taking, as the distance between any two points, the shortest such distance within the surface of the torus (and so, where such a path is shorter, across what were previously bounding edges of the square). Finally, these doubly non-Euclidean distances were converted into artificial similarity measures by means of an exponential decay transformation.

Despite the intrinsic two-dimensionality of the underlying space, the best-fitting two-dimensional solution obtained by standard nonmetric multidimensional scaling (M-D-SCAL) failed (a) to achieve a good fit to the

data, (b) to achieve an accurate representation of any (either opened out or projected down) version of the toroidal configuration, and (c) to permit a recognizable reconstruction of the six-lobed unit circle. It was only by going to a four-dimensional space, within which the torus itself can be isometrically embedded, that a satisfactory fit was achieved. But, because the four-dimensional solution did not achieve a reduction to the correct intrinsic dimensionality of the toroidal surface itself, it was still not possible to reconstruct the unit circle and, hence, to infer the locally non-Euclidean form of the underlying metric.

The best-fitting two-dimensional solution obtained by the method of parametric mapping did, after some difficulties with apparently merely local minima, achieve what corresponded to an opened-out version of the toroidal surface (akin to those presented in Shepard and Carroll, [1966] and in Shepard and Cermak [1973]). Moreover, the construction of a scatterplot in the manner described for Fig. 12B again revealed the six-lobed form of the unit circle. Although in our experience the method of parametric mapping, even more than standard methods of nonmetric multidimensional scaling, is thus beset with problems of slow convergence and local minima, I believe that some of the suggestions made earlier for the construction of good initial configurations may substantially increase the effectiveness of the method. If so, the representation of similarities in terms of quite general semimetric but continuous coordinate spaces becomes a viable alternative.

In this just-considered generalization, the triangle inequality was abandoned while the notion of a continuous underlying coordinate space was retained. The method of "maximum variance nondimensional scaling" that Jim Cunningham and I have recently been exploring represents a very different kind of generalization in which the triangle inequality is made central while the requirement of an underlying coordinate space is relinquished [Cunningham & Shepard, 1974]. In order to obtain unique nontrivial solutions, the requirement of minimum dimensionality (which has no meaning in the absence of a continuous space) was replaced by a requirement of maximum variance of the distances (which does and which, according to the above-reported results on reduction of dimensionality, seems to have a very similar effect).

In test analyses with both real and artificial data, we found that, if we thus maximize the variance of the distances subject only to (a) the strict satisfaction of just the metric axioms (particularly the triangle inequality) and (b) adequate maintenance of monotonicity, we can in fact recover underlying Euclidean or non-Euclidean distances with considerable accuracy without any assumption or use of a coordinate embedding space. Since we are able to recover the underlying distances, we are also able to recover the form of the unknown function relating the similarity data to the distances. In fact, in a test with a rather exotically non-Euclidean metric (sum-over-path distances in a graph-theoretic tree), the sigmoid form of this (artificially imposed) functional relation was recovered with great precision, while a

straightforward application of standard nonmetric multidimensional scaling to the same artificial data gave a very poor fit and approximation to the sigmoid function. (Compare Figs. 3 and 4 in Cunningham & Shepard [1974].)

For many practical purposes, two drawbacks of this method may limit its general usefulness. First, although apparently not subject to local minima, so far it has tended to converge rather slowly and, so, to be relatively costly—particularly for large matrices. Second, it does not, of course, yield a spatial configuration in a two- or three-dimensional coordinate space of the sort that is usually sought for purposes of substantive interpretation. Nevertheless, it is of considerable theoretical interest as a demonstration of the possibility of recovering very general, merely metric representations—corresponding to the next to the top box in Fig. 11. Moreover, as already suggested, it should find some uses for the study of the form of the function relating distances, which are potentially very non-Euclidean, to similarity measures of various types (such as those of stimulus generalization or reaction time) and, possibly, for the generation of starting configurations for methods that are particularly susceptible to local minima. Finally, as I shall suggest in the next and final section, it may provide one basis for constructing more discrete, network-like or graph-theoretic representations such as have been proposed for certain, *e.g.*, semantic, domains.

6. Representing Discrete or Categorical Structure

Problem

Standard methods of multidimensional scaling and, in fact, nearly all of the methods discussed above have been based upon the assumption of an underlying space that is continuous and has a well-defined dimensionality. (The only exceptions discussed here were the two nondimensional methods of hierarchical clustering [Johnson, 1967] and maximum variance scaling [Cunningham & Shepard, in press].) Methods for mapping the data into a continuous coordinate space seem eminently appropriate for the investigation of domains of objects in which there is an underlying continuous physical variation—as there clearly is, for example, with colors which vary continuously in brightness, hue, and saturation; with tones which vary continuously in intensity, frequency, and duration; or even with facial expressions which also vary continuously (even though the physical dimensions of the variation are not yet completely specified). Experience indicates that, even when the stimuli vary only in discrete steps (as with the dot-and-dash signals of the Morse Code [Shepard, 1963a]), a representation within a continuous coordinate space is often quite satisfactory—particularly if the number of stimuli and number of steps of variation are not too small.

Other domains, particularly those of a more conceptual, linguistic, or semantic nature, appear to be inherently more discrete, categorical, or bipolar. With regard to the perception of speech, for instance, suggestive examples are provided by the empirical phenomenon of "categorical perception" [Liberman, Cooper, Shankweiler, & Studdert-Kennedy, 1967] and

by the related theoretical notion of "distinctive features" [Halle, 1964; Miller & Nicely, 1955]. And with regard to purely internal conceptual or semantic systems, inherently discrete structures seem to be the rule rather than the exception. Some especially clear-cut examples include the cognitive systems of kin terms [Haviland & Clark, 1974; Romney & D'Andrade, 1964], of linguistic marking [Clark, 1969, 1970; Greenberg, 1966], and of binary, componential, and algebraic structures in general [*e.g.*, Boyd, 1972; Lévi-Strauss, 1967]. I myself have several times argued that, although a frozen spatial configuration may well represent the perceived relations of pair-wise similarities among stimuli either on the average or else for any one individual at any one time, such a configuration does not exhaust the cognitive structure of a set of stimuli. In particular it may not adequately represent the ways in which different subjects or the same subject at different times may see subsets of the stimuli as grouped together or as having some property in common [Shepard, 1963b, 1964a; Shepard & Cermak, 1973; Shepard, Hovland & Jenkins, 1961].

It is of course true that subsets of scaled objects with strong mutual relations of similarity will tend to show up as visibly clustered groups of points even in the "continuous" spatial representations obtained by multidimensional scaling. Indeed, in their strongest form, such clusterings may take one of the more dramatic forms of complete degeneracy illustrated in Fig. 6. Moreover, objective methods of rotation or of affine transformation can bring out the discrete or discontinuous aspects of such a configuration more fully [Degerman, 1970; Kruskal, 1972; Torgerson, 1965]. Still, such basically continuous spatial representations, even when linearly transformed, do not (any more than transformations to simple structure in factor analysis) yield discrete subsets, as such, explicitly. Among other things, this makes it difficult to evaluate whether a seeming cluster is valid or reliable—in the sense that it would be if it repeatedly emerged, explicitly, in the analyses of independent sets of data.

It is also true that methods of hierarchical clustering [Jardine & Sibson, 1971; Johnson, 1967; Sokal & Sneath, 1963] do yield both explicit and categorical structures that, moreover, have been found to be quite useful and reliable in the representation of speech sounds (*e.g.*, see Fig. 8 and Shepard [1972c]) and of concepts (*e.g.*, see Fig. 1 and Shepard *et al.*, [in press]). However, the requirement that the clusters be hierarchically nested seems undesirably restrictive for many purposes. In Fig. 8A it means that, once just the back fricatives [z] and [ʒ] have been grouped with the unvoiced stops [d] and [g] (perhaps by virtue of their place of articulation), neither of these back fricatives can be grouped with either of the front fricatives [v] and [ð] (on the basis solely of their affrication). And in Fig. 1 it means that, once "cat" is grouped with the other household pet "dog," it can no longer be grouped with the other felines "lion" and "tiger." In short, although hierarchical systems can represent some of the discrete or categorical structure underlying a set of similarity data, it can not represent psychological properties, however salient, that correspond to overlapping subsets.

For the same reason, hierarchical systems can not represent parallel or analogical correspondences between the structures within two nonoverlapping subsets (such as the parallelism in articulation between the voiced and unvoiced consonants [Shepard, 1972c, p. 106]). The representation of such parallelisms requires the specification of connections (representable only as overlapping clusterings) between the subparts of disjoint clusters. And, finally, although a hierarchical clustering is equivalent to a graph-theoretic tree, arbitrary graph structures (containing closed paths or cycles) are precluded. So hierarchical representations can not, any more than continuous spatial representations, furnish the sorts of general graphs or networks currently being advocated for the representation of semantic structure [Anderson & Bower, 1973; Quillian, 1968; Rumelhart, Lindsay, & Norman, 1972].

Prospects

One already-noted limitation of maximum variance nondimensional scaling is that, because it drops the restrictive requirement that the distances be embedded in a coordinate space, it forfeits the pictorially presentable spatial configuration that has proved to be so useful in substantive applications of multidimensional scaling. Jim Cunningham and I are currently exploring a possible addition to this method of nondimensional scaling that we hope will be able to convert the obtained set of coordinate-free distances into a graph structure that will meet this need for a more picturable representation. If we succeed, the sort of general graph structure that is produced should also be much closer to the kind of discrete, network-like representations proposed for semantic memory. The distance estimates furnished by such maximum variance scaling appear ideally suited for the purposes of constructing a graph-theoretic representation because the maximization of variance together with the maintenance of the triangle inequality tends, wherever possible, to render distances additive—as they should be over a connected path through a graph. (Thus, as noted before, artificial data generated from sum-over-path distances were well fit by maximum variance nondimensional scaling but not by standard nonmetric multidimensional scaling.) As a first step toward the proposed addition, Cunningham [1974] has already reported encouraging results in the fitting of graphs of one particular type; namely, tree structures.

A last type of method for the representation of structure in similarity data to be considered here takes an entirely different approach. Although it is perhaps closest in spirit to the approach taken by Johnson [1967] in his formulation of hierarchical clustering, it departs from all methods for hierarchical clustering in abandoning the very strong restriction that the clusters never overlap. And, although it shares with both of the nondimensional methods mentioned (*viz.*, those of hierarchical clustering and maximum variance scaling) the abandonment of an underlying coordinate space, it goes beyond both of those methods in abandoning, also, the notion of distance.

As an initial basis for the exploratory development, with Phipps Arabie, of a method of this type, I chose a model according to which the perceived similarity between any two objects is a simple sum of the psychological weights associated with all and only those (discrete) properties that the two objects both share. Formally,

$$s_{ij} = \sum_{k=1}^{m} w_k p_{ik} p_{jk} ,$$

$$\text{where } p_{ik} = \begin{cases} 1 & \text{if object } i \text{ has property } k \\ 0 & \text{otherwise,} \end{cases}$$

and where w_k is a non-negative weight representing the psychological salience of property k.

The computational problem with which we are faced is that of finding a minimum set of m subsets of the objects and associated optimum weights such that the maximum possible variance of the similarities, s_{ij}, is accounted for. Although the model is closely related to the standard factor-analytic model, the restriction of the variables p_{ik} to binary values converts the computational problem into a much more difficult, combinatorial one. As we have currently developed it, the computer program, ADCLUS, for this type of additive cluster analysis [Arabie & Shepard, 1974] proceeds in two successive phases; a nonmetric and then a metric one. In the first phase, combinatorial methods are used to generate an ordered list of subsets with potentially positive weights that is invariant under monotone transformations of the data. In the second phase, a modified gradient method is then used to estimate optimum weights for these subsets and to eliminate all subsets for which the weights become sufficiently small.

As an illustration, Table 1 presents our nonhierarchical reanalysis of Miller and Nicely's [1955] data on the confusions among 16 consonant phonemes in the presence of white noise. These are the same data that have already been analyzed by a variety of more standard methods of multidimensional scaling and hierarchical clustering (see Fig. 8, Shepard [1972c] and, also, Wish and Carroll [in press]). In this case, approximately 99% of the variance was accounted for by the first 30 subsets (a representation that, in terms of number of parameters, is roughly comparable to the two-dimensional spatial solution which also accounted for about 99% of the variance). The first 16 subsets (roughly comparable to a one-dimensional solution) are listed in Table 1, in rank order according to their estimated weights. The obtained subsets appear to be readily interpretable except, possibly, for the four (ranked 3, 8, 10, and 13) for which the interpretations are given in parentheses. And the last three of these subsets, despite their uncertain interpretations, are very likely reliable in view of the facts (a) that the 8th (consisting of [b], [v], and [ð]) emerged repeatedly in hierarchical analyses of independent sets of data [Shepard, 1972c], (b) that the 13th (consisting of [p], [f], and [θ]) is, according to distinctive feature schemes, identical in structure to the 8th except for voicing, and (c) that the 10th

(consisting just of [b] and [v]) is contained entirely within the 8th. What these results, along with those in Shepard [1972c], seem to indicate is the need for some revision of the distinctive feature schemes on the basis of which the interpretations were attempted.

The results show a marked departure from a strictly hierarchical structure. The overlapping nature of the obtained subsets is apparent in Fig. 13, where the first 16 are embedded as closed curves in the spatial configuration used earlier for Fig. 8A. Note, for example, that the relatively back fricatives, [z] and [ʒ], now cluster both with the relatively back stops, [g], and [d], and *also* (through [z]) with the relatively front fricatives, [v] and [ð]. Likewise, the front unvoiced stop [p] clusters both with the other unvoiced stops, [t] and [k], and (as noted above) with the relatively front unvoiced fricatives, [f], [θ]. Finally, the overlapping clusters form chains connecting the four progressively further back unvoiced fricatives, [f], [θ], [s], and [ʃ], and, in parallel fashion, the four progressively further back voiced fricatives, [v], [ð], [z], and [ʒ], in a way that was not possible in the representation (Fig. 8) obtained by the hierarchical method.

The results of this early test application of this nonhierarchical method of additive cluster analysis encourage me to believe that methods based on models quite different from those underlying standard methods of multidimensional scaling can provide potentially useful, complementary information about the psychological structure underlying a set of objects. Our current efforts are being directed toward improving the efficiency of the iterative method used to adjust the weights and to eliminate unimportant

TABLE 1
Nonhierarchical Additive Cluster Analysis of Confusion Measures of Similarity Among 16 Consonants
(Data from Miller and Nicely [1955])

Rank	Weight	Elements of Subset	Interpretation
1st	.282	f θ	front unvoiced fricatives
2nd	.214	d g	back voiced stops
3rd	.196	p k	(unvoiced stops omitting t)
4th	.157	p t k	unvoiced stops
5th	.155	v ð	front voiced fricatives
6th	.129	m n	nasals
7th	.090	θ s	middle unvoiced fricatives
8th	.074	b v ð	(front voiced consonants)
9th	.071	s ʃ	back unvoiced fricatives
10th	.061	b v	(front voiced consonants)
11th	.050	d g z ʒ	back voiced consonants
12th	.044	z ð	middle voiced fricatives
13th	.044	p f θ	(front unvoiced consonants)
14th	.035	z ʒ	back voiced fricatives
15th	.033	v z ð	front & middle voiced fricatives
16th	.030	g z ʒ	back voiced consonants

subsets, and toward investigating the stability of the weights for independent sets of data and as more or fewer subsets are eliminated.

CONCLUSION

After struggling with the problem of representing structure in similarity data for over 20 years, I find that a number of challenging problems still remain to be overcome—even in the simplest case of the analysis of a single symmetric matrix of similarity estimates. At the same time, I am more optimistic than ever that efforts directed toward surmounting the remaining difficulties will reap both methodological and substantive benefits. The methodological benefits that I forsee include both an improved efficiency and a deeper understanding of "discovery" methods of data analysis. And the substantive benefits should follow, through the greater leverage that such methods will provide for the study of complex empirical phenomena—perhaps particularly those characteristic of the human mind.

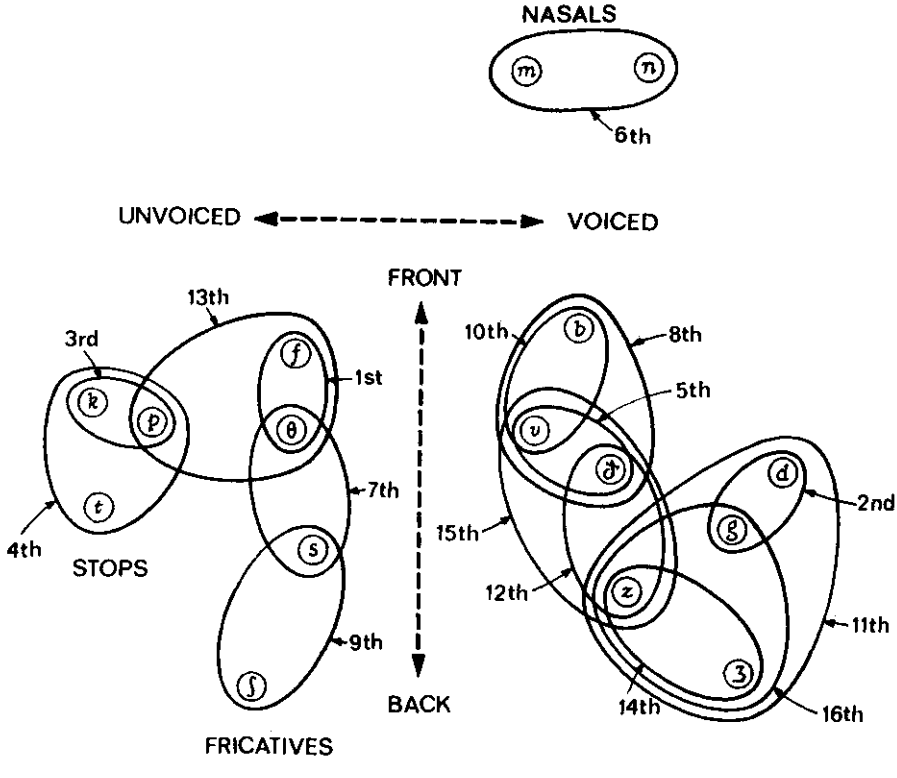

FIGURE 13

The first 16 clusters from Table 2, embedded in the two-dimensional spatial configuration (of Fig. 8A) representing the same confusion measures of similarity among the 16 consonant phonemes.

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2 Multidimensional Perceptual Models and Measurement Methods*

J. Douglas Carroll and Myron Wish

A. Properties of a Proximity Function

Given a measure of proximity, defined on pairs of stimuli, we might ask what properties this measure should have. Assuming that the stimuli can be described in terms of a finite set of underlying dimensions, let x_{jt} represent the value of stimulus j on dimension t, and $\mathbf{x}_j$ stand for the vector (or point in the multidimensional space) representing the jth stimulus. Let $p(\mathbf{x}_j, \mathbf{x}_k) = p_{jk}$ be the proximity between j and k. Consider now the properties this function should have.

First, it would seem that as two stimuli "approach" one another, their proximities to any third stimulus should approach one another. That is,

$$\mathbf{x} \rightarrow \mathbf{y} \quad \text{implies} \quad p(\mathbf{x}, \mathbf{z}) \rightarrow p(\mathbf{y}, \mathbf{z}) \qquad \text{for all } \mathbf{z} \tag{1}$$

(where $a \rightarrow b$ means a approaches b). This *continuity* assumption, of course, says nothing about how $p(\mathbf{x}, \mathbf{y})$ should behave as $\mathbf{x}$ and $\mathbf{y}$ approach one another. It would seem, however, that any reasonable proximity function should have the property that no stimulus can be more proximal to some other stimulus than to itself. This implies

$$p(\mathbf{x}, \mathbf{y}) \leq \min\,[p(\mathbf{x}, \mathbf{x}), \quad p(\mathbf{y}, \mathbf{y})] \tag{2}$$

Properties (1) and (2) would seem to be the least we would expect of any reasonable proximity measure. An additional property that might be assumed (but not always) is

$$p(\mathbf{x}, \mathbf{x}) = p(\mathbf{y}, \mathbf{y}) = p \qquad \text{for all } \mathbf{x} \text{ and } \mathbf{y}, \tag{3}$$

which says that all the "self-proximities" are the same. Equations (2) and (3) together imply that

$$p_{jk} \leq p_{ll} = p \qquad \text{for any } j, k, l. \tag{4}$$

[where $p_{jk} = p(\mathbf{x}_j, \mathbf{x}_k)$]

*reprinted from E. C. Carterette and M. Friedman, *Handbook of Perception*, **2**, 1974, pp. 395–412

We may also add the following symmetry assumption:

$$p_{jk} = p_{kj} \qquad \text{for all } j, k \tag{5}$$

which says that order is irrelevant to proximities. Although for certain kinds of stimuli (e.g., sequentially presented auditory stimuli) this may not be realistic, such a symmetry assumption seems quite reasonable for most stimulus domains.

If we define the dissimilarity (or antiproximity) between j and k as

$$\delta_{jk} = p - p_{jk}, \tag{6}$$

then the following hold for δ:

$$\delta_{jk} \geq \delta_{jj} = 0 \qquad \text{(positivity)} \tag{7}$$

$$\delta_{jk} = \delta_{kj} \qquad \text{(symmetry)}, \tag{8}$$

making δ a *semimetric*. A semimetric defined on a space satisfies continuity plus all the metric axioms except the triangle inequality.

B. The Triangle Inequality

All we need add to such a semimetric to make it a *metric* (and thus, to make the stimulus space a *metric space*) is the triangle inequality. The triangle inequality states

$$d_{jl} \leq d_{jk} + d_{kl} \qquad \text{for all } j, k, l \qquad \text{(triangle inequality)} \tag{9}$$

where the d's are interpreted as *distances* between the entities referred to by the subscripts. If d satisfies properties (7), (8), and (9) (the metric axioms), it is a metric.

Since the proximities and thus the dissimilarities, δ, are assumed to be measured only ordinally, it is quite reasonable to assume that, among the class of permissible monotonic functions, there is at least one that will transform them into distances. In fact, it is trivial to do this for any finite set of points, simply by defining the monotone function by adding a suitably large constant to the mixed δ's (leaving the unmixed equal to 0). The smallest constant that will work is

$$c_{\min} = \max_{j,k,l} (\delta_{jl} - \delta_{jk} - \delta_{kl}) \tag{10}$$

so that we may define d by

$$d_{jk} = \delta_{jk} + c_{\min} \qquad \text{for } j \neq k; \tag{11}$$

$$d_{jj} = 0 \qquad \text{for all } j. \tag{12}$$

Of course, any larger constant $c > c_{\min}$ would also convert the δ's into d's satisfying the triangle inequality, but $c_{\min}$ is the smallest one that will do the job. In fact $c_{\min}$ is one of the estimates of the additive constant used to convert *comparative* (interval scale) distances into (ratio scale) dis-

tances in the now classical metric scaling procedures described in Torgerson (1958). This particular method of estimating the constant was justified by assuming that some set of three points lie exactly on a straight line in the multidimensional space. It seems simpler to us to justify it as the smallest additive constant guaranteeing satisfaction of the triangle inequality.

Thus we see that even this fairly trivial monotone function can convert essentially any set of dissimilarities into "distances" (i.e., numbers that at least satisfy the metric axioms). It is not unreasonable, therefore, to suppose that a more interesting function might be available to do this. As Shepard (1962a,b) has pointed out, the existence of a monotone function that assures satisfaction of the triangle inequality is not, in general, a very interesting condition—not, that is, without some other constraint. Shepard speaks of "low dimensionality" as being the right additional condition. This is not terribly interesting, either, unless the underlying metric (which is assumed monotonically related to proximities or antiproximities) is assumed to be Euclidean or a member of some fairly limited family of metrics. There is a kind of trading relation between dimensionality and complexity of the metric assumed. By assuming a sufficiently complex metric (which could still be continuously related to parameters of the stimulus space) one could obtain low-dimensional solutions in which distances relate monotonically to any proximities whatever. Thus, if we are considering the possibility of very general metric spaces, it would seem that Shepard's condition of low dimensionality must necessarily be supplemented by a condition of "simplicity of metric." After describing and illustrating some multidimensional scaling methods, we shall discuss some non-Euclidean metrics that have been considered in psychology.

C. Violations of the Metric Axioms

Let us assume we have a matrix of antiproximities (e.g., dissimilarities) for n stimuli or other entities. In the typical situation there is only a half-matrix, without diagonal, of data values. By imposing the constraint $\delta_{jk} = \delta_{kj}$, and treating the diagonals of the matrix (the δ_{jj}'s) as all tied at a value less than any of the nondiagonal δ's, the rest of the matrix could be filled in.

When the physical identity of a stimulus is not obvious (e.g., degraded acoustical or visual stimuli), it is common to collect proximities data associated with the diagonal cells (which indicate the dissimilarity between each stimulus and itself). In some cases it makes sense to collect data on both the (jk) and (kj) pairs—for example, when order effects are likely to occur. Systematic nonsymmetries (or any nonsymmetry not accountable for by chance) may cast doubt on the existence of an underlying metric space, since they imply violations of the symmetry axiom. Likewise, the failure of the self-dissimilarities to be equal to each other and less than any nondiagonal dissimilarities violates the positivity axiom of Eq. (7).

In some situations it is appropriate to take out row and column effects before analyzing the matrix of interactions by multidimensional scaling. An example of this is Coombs's (1964, 1971) analysis of journal citation data. The rationale for removing the main effects, is that differences in

the overall number of citations made or received by a journal may distort the multidimensional representation of relatedness among the journals. In many instances the matrix of interactions will be more symmetric than the original data matrix.

If the violations of the metric axioms are severe, it is likely (but not certain) to be unreasonable and unproductive to seek a multidimensional representation of the data. Some indications of severe violations might be that the diagonal values were of about the same magnitude as the nondiagonal values, or that the rank ordering of proximity values in a row was unrelated to the ordering in the corresponding column. In most instances, however, the violations of the metric axioms are mild enough to justify a multidimensional scaling analysis. The simplest way to deal with nonsymmetries is to fit a multidimensional model to the nonsymmetric matrix, thereby providing a space for the symmetric part of the data. In effect the distance model could be regarded as a first approximation, and the nonsymmetries could be studied separately. For example, Wish (1967a,b) explored the nonsymmetries in matrices of confusions among Morse code signals and related rhythmic patterns, discovering that the probability of a "same" response to a pair of sequentially presented signals was greater when the shorter of the pair was presented first. The systematic nature of the nonsymmetries provides some information about the way such signals are stored and about the judgmental process.

Another approach to the problem of nonsymmetric matrices is to symmetrize the matrix by averaging the (jk) and (kj) entries. This might be expected to cancel out any significant order effects, leaving only the data that can be accounted for by an asymmetric distance model. A good example of this approach is provided by Shepard's (1957) analysis of stimulus generalization data. He proposed a rational model involving response bias to account both for asymmetries and for discrepancies in the diagonals, or self proximities. While this is an oversimplification, in essence, Shepard assumed that the observed probability p_{jk} of the response appropriate to stimulus k being given when stimulus j was presented is given by

$$p_{jk} = w_j^{(s)} w_k^{(r)} \pi_{jk}, \tag{13}$$

where $w_j^{(s)}$ and $w_k^{(r)}$ are weights associated with the jth stimulus and the kth response, respectively; and π_{jk} is a symmetric proximity measure satisfying (4) and (5), and assumed to be related by a decreasing monotonic function to distances in a metric space. (The monotonic function was assumed to be a negative exponential in Shepard's work, while the space was assumed to be Euclidean.)

Since, without loss of generality it is possible to assume the common value of π_{jj} and π_{kk} to be 1, Eq. (13) implies that

$$\pi_{jk} = p_{jk}p_{kj}/p_{jj}p_{kk}. \tag{14}$$

This method of symmetrizing was used by Shepard in his analysis of the Miller–Nicely data on confusions between consonant phonemes (to be discussed later in this chapter).

Another way to take into account the lack of symmetry and of maximality of the diagonal values (in a proximity matrix) is to treat the matrix

as a conditional rather than as an unconditional proximity matrix. A row (column) conditional proximity matrix is one in which the order within a given row (column) is meaningful, but proximities in different rows (columns) are not comparable. Such a matrix generally arises when the row and column elements have different meanings or play different roles—for example, in a stimulus identification experiment in which the rows are associated with stimuli and the columns with responses, or when the entries in a row (column) indicate the rank order of similarity to the standard stimulus associated with that row (column). In terms of formal assumptions, the proximity matrix is row-conditional if and only if proximities are related to distances by

$$M_j(p_{jk}) \cong d_{jk}, \tag{15}$$

with M_j monotone nonincreasing.

The difference here is that we are assuming a different monotonic function for each j (corresponding to a row of the proximity matrix). A column-conditional matrix would be obtained by replacing M_j with $M_k{}^*$ in Eq. (15). In the unconditional case, there would just be a single unsubscripted M. The stimulus generalization paradigm that Shepard utilized could also be regarded as producing a row-conditional proximity matrix, although under Shepard's model, a suitable transformation of the matrix leads to an unconditional matrix.

Versions 4 and 5 of Kruskal's MDSCAL (Kruskal & Carmone, 1969) and certain programs in the Guttman and Lingoes series (Lingoes, 1966) have the facility to analyze row or column conditional proximity matrices, in effect fitting a different monotone function to each row (column). In principle, these programs can even handle data matrices in which the rows and columns represent distinct sets of elements—for example, stimuli and responses, or individuals and stimuli (as in the multidimensional unfolding model—see Coombs, 1964). A multidimensional scaling analysis of such a matrix would provide a "joint space" in which there was a point in the space for each row and for each column. The multidimensional space could conceivably reveal what kinds of stimulus–response or order effects were occurring. At one extreme, the jth row point and the jth column point may be very close together, suggesting no biases. At the other extreme, the column points may be related in a very systematic way to the row points, as, for example, by a tendency to shift in a specified direction. It should be pointed out, however, that there are difficulties in practice in determining a "nondegenerate" multidimensional space from such an "off-diagonal" or "corner matrix" (or from any matrix in which there are large blocks of missing data—see Carroll, 1972; Kruskal; 1972; Kruskal & Carroll, 1969).

Perhaps a more elegant way to account for nonsymmetries is to build them into the metric space model (see, e.g., Nakatani, 1972). This amounts, in one sense, to redefining distances in the space so as to drop the symmetry axiom of Eq. (5). In another sense, it might be viewed simply as superimposing an additional process onto the basic metric space

model. This is the way Shepard apparently conceived of his response bias model—as a way of *preserving* the notion of symmetric distances rather than as defining asymmetric distances. The kind of bias parameters Shepard assumes could be introduced explicitly into the model, however, rather than simply being canceled out by averaging, thus creating a composite "asymmetric distance" model.

Kruskal (personal communication) has experimented with a model that provides for a nonsymmetric distance function. In this model the jth row point is related to the jth column point by a "drift vector," corresponding to a fixed shift in one direction. In a variant of the model, the appended vector might be the one pointing from one of the points toward (or away from) a specific fixed point in the space. This could be thought of as implying a kind of regression toward a stereotype or schema corresponding to the fixed point.

Keeping in mind the possibility of violations of the metric axioms, and other potential problems such as missing data, we shall restrict our attention for the moment to the standard case of a half-matrix (without diagonal) in which there are no missing entries. However, we do not necessarily restrict our attention to cases in which the metric axioms are satisfied. We shall, in fact, consider a sequence of increasingly general classes of proximity models, ranging from a very specific metric (the Euclidean) through various non-Euclidean metrics, to semimetrics (in which the triangle inequality is dropped) and finally the case in which all that is assumed is that similarity or proximity is *continuously* related to perceptual parameters. Cutting across this hierarchy is another distinction—that between so-called metric and nonmetric models and analyses, in which the proximities are treated as being on an interval (or stronger) scale, versus being merely ordinally measured.

METRIC, NONMETRIC, AND "CONTINUITY" SCALING

The distinction between metric and nonmetric multidimensional scaling was first made by Coombs (1958) and later elaborated by Kruskal (1964a), who used the term *nonmetric multidimensional scaling* to mean much the same as Shepard's (1962a,b) term *analysis of proximities*. The term has to do with the strength of the assumed scale properties of the data (proximities or antiproximities). In Stevens's terms, if the data are assumed to be measured on a ratio or interval scale, the analysis is (or ought to be) a metric one. If the data are assumed merely ordinal, then the analysis is (or ought to be) nonmetric.

For an analysis to be metric it is not necessary that the original data be linearly related to distances; only that they be convertible to at least interval scale distances by some known transformation. For example, Shepard's (1957) assumption of a negative exponential connecting proximities to distances meant that a logarithmic transformation would carry the (suitably symmetrized) proximities into ratio scale distances.

What might be called the "classical" metric method of multidimensional

scaling is the one described in Torgerson's (1958) book. The theoretical basis for this was supplied by Young and Householder (1938), who proved a theorem that enabled determination of the minimum dimensionality of the space required to accommodate a given set of Euclidean distances among n points. A by-product of this theorem was a method of constructing the space, and indeed, of determining whether the distances could be accommodated in any Euclidean space. This constructive method was used by Richardson (1938) to implement the first known application of multidimensional scaling (see also Klingberg, 1941). The method essentially lay fallow until the early 1950s, when methodological improvements by Torgerson (1958), Messick and Abelson (1956) and others, together with the advent of high-speed digital computers, made it feasible to deal with fairly large data sets in cases of reasonably high dimensionality. This classical metric method can be outlined as follows:

Similarities data were first collected by one of several means, the most popular being the *complete method of triads* (in which the subject judges whether stimulus A is more like B or C for every triad A, B, C of stimuli) or the methods of equal appearing or of successive intervals (in both of which every pair of stimuli is placed in one of a series of ordered categories). These data were then typically put through one of the Thurstone-type undimensional scaling procedures to produce interval scale measures of distances (which were called comparative distances).

Since ratio scale distances were needed, the problem of estimating the "additive constant" arose. A number of methods were worked out for estimating this constant, the simplest (and possibly the best in a number of ways) being the estimate $c_{\min}$ defined in Eq. (10), which, as discussed earlier, is the smallest constant guaranteeing satisfaction of the triangle inequality. Some methods of data collection (e.g., Helm, 1964; Indow, 1960a,b) could plausibly be assumed to lead directly to ratio scale distances, so that many of these steps would be avoided. Once ratio scale distances were obtained, one proceeded to convert them to *scalar products*. Torgerson and others derived equations for calculating (estimated) scalar products around an origin placed at the centroid (or center of gravity) of all n points. (The Young–Householder results required placing the origin at one of the points, and getting scalar products of vectors from that point to the $n - 1$ remaining ones. This solution was unsatisfactory both esthetically and statistically.)

The simplest way to describe the conversion from Euclidean distances to scalar products is that one *double centers* the matrix whose general entry is $-1/2d_{ij}^2$. Double centering is equivalent to taking out both row and column effects in analysis of variance, leaving interaction numbers. In this case, the interaction numbers are the scalar products. The scalar product between stimuli j and k, usually called b_{jk} is defined as

$$b_{jk} = \sum_{t=1}^{m} x_{jt}x_{kt}. \tag{16}$$

In matrix notation, this can be written as

$$B = XX', \tag{17}$$

where B is the $n \times n$ matrix of scalar products and X is the (initially unknown) $n \times m$ matrix of coordinates of the n points in m dimensions. This equation looks a great deal like the fundamental equation of factor analysis, the main difference being that B replaces R (the correlation matrix). The matrix B can, in fact, be viewed as analogous to a covariance matrix, and methods closely related to factor analysis (or its statistical cousin, principal components analysis) can be used to determine the X matrix of appropriate dimensionality that best accounts for the scalar products. See Torgerson (1958) for further details.

A. Other Metric Scaling Techniques

In addition to this classical metric multidimensional scaling, there are other metric methods that are closely related to the newer nonmetric methods, in that they utilize computer-implemented iterative numerical procedures to fit a specified metric model to the data. This really amounts simply to replacing the monotone function central to the nonmetric methods with some specified function (linear, polynomial of some degree, or other) which may or may not be monotone.

Kruskal's MDSCAL, for example, allows use of polynomial functions up to degree 4 (including linear functions either with or without the constant term). The program used by Shepard to analyze the Miller–Nicely data (to be discussed subsequently) incorporated the explicit requirement that the function converting distances into proximities be a negative exponential. These approaches are metric in the general sense that interval-scale properties of the data are used. Of course, as functions with increasing numbers of parameters are used, this distinction becomes less and less meaningful; with enough parameters almost anything can be fit. (A monotone function, in a sense, has as many parameters as data points, but with strong inequality constraints on the values these parameters may legitimately assume.)

B. Nonmetric Multidimensional Scaling

The term *nonmetric multidimensional scaling* was first introduced by Coombs (1958), who had something in mind which is a little different from what is now called nonmetric scaling. The method Coombs and his co-workers proposed was based on nonmetric (i.e., merely ordinal) proximities data. It was nonmetric, too, in the sense that the space determined was not, in any well-defined sense, a metric space, since the values of stimuli on dimensions were defined only ordinally. There was, thus, no way to calculate interpoint distances, even if a specific metric such as the Euclidean was assumed. To do this, one would need to know the monotone

function (different for each dimenison) transforming the rank order coordinates into at least interval scale coordinates. In this sense, i.e., that both data and solution are nonmetric, Coombs's procedure could be termed "doubly nonmetric."

It was Shepard (1962a,b) who first showed (by producing a computer algorithm) that it was possible to produce essentially metric solutions from such purely nonmetric (or ordinal) proximities data. These latter were metric in the dual sense that coordinates were defined up to interval scale and that the space *was* indeed a (Euclidean) metric space.

Shepard's method, which he called "analysis of proximities," started out with the n stimuli arranged in what might be called the "maximum entropy" configuration (a regular simplex in $n - 1$ dimensions—the multidimensional generalization of the equilateral triangle in two dimensions or the regular tetrahedron in three). He then introduced two processes, one tending to decrease dimensionality and the other to increase agreement with the data (in an ordinal sense). The dimensionality-reducing process is now primarily of historical interest. The approach to dimensionality estimation now almost universally used entails finding solutions in a number of different dimensionalities, and using the dimensionality versus goodness-of-fit curves in some way to judge how many dimensions are appropriate for the data. Shepard's notion, on the other hand, was to start in the highest possible dimensionality, but to impose forces tending to reduce that dimensionality to the smallest possible. Once that dimensionality was estimated, the best configuration in that smallest dimensionality was determined. The process he used to decrease the dimensionality (what he called the β process) was based on the idea of increasing large distances and decreasing small ones (one can see intuitively that this would tend to straighten out, say, a two-dimensional set of points on an arc of a circle into a one-dimensional set whose locus is a straight line). When this had seemingly reduced dimensionality as much as possible, the points were then projected exactly into a space of the "right" dimensionality, and the other, or α process, was continued in this "right" dimensionality (without the β process). The α process (which was used together with the β process in the first phase, and then alone) quite simply tended to increase distances between points that were too close together (relative to the ordinal proximities data) and to decrease distances between points too far apart. It did this by setting up what can be conceived as force vectors from each point, oriented either toward or away from each of the $n - 1$ other points. If the rank order of the distance were greater than (less than) that of the corresponding dissimilarity, the vector would be pointed away from (toward) the other point. The magnitude of the vector was proportional to the magnitude of the discrepancy. If the two rank orders agreed exactly, the force vector had zero magnitude, which is the same as saying there was no force vector in this case. These $n - 1$ force vectors (some possibly with zero magnitude) were then summed for each point, producing a resolution vector that could be thought of as the resolution of all the attractive and repulsive

forces operating on that point. Each point was allowed to move in the direction of its resolution force vector a distance proportional to the magnitude of the force (the constant of proportionality being the α of the α-process, which corresponds to what numerical analysts would call the step-size), and these new force vectors were computed. This process was continued until, ideally, the system was in perfect equilibrium (i.e., all force vectors had zero magnitude). Since this state of perfect equilibrium is seldom actually reached, however, in any such iterative procedure, some criterion of being close enough to equilibrium must be used.

In order to distinguish it from Shepard's rather different algorithm, Kruskal borrowed Coombs's term nonmetric multidimensional scaling to describe his procedure. It is important to realize that it is the proximities data that are nonmetric in this case, not the solution. Some authors, notably Beals, Krantz, and Tversky (1968) call this ordinal rather than nonmetric scaling. This nomenclature, although possibly more appropriate, is not favored by usage. Green and Carmone (1970) have called methods such as those of Shepard and Kruskal nonmetric, whereas they call Coombs's procedure fully nonmetric (to emphasize that both data and solution are nonmetric).*

Kruskal's (1964) MDSCAL method improved Shepard's method in two important ways: (1) The notion of optimizing an explicitly defined measure of goodness (or badness) of fit was introduced; (2) an explicit numerical method, the method of gradients, or steepest descent was used.† Kruskal called his goodness-of-fit measure STRESS, defined in his original paper as

$$\text{STRESS} = \left[\frac{\Sigma_j \Sigma_k (d_{jk} - \hat{d}_{jk})^2}{\Sigma_j \Sigma_k d_{jk}^2} \right]^{1/2}, \tag{18}$$

where the d's are distances in the underlying metric space, and the $\hat{d}$'s are related to proximities data by a nonincreasing monotonic function. This formula for STRESS is now called STRESSFORM1. Another STRESS formula, called STRESSFORM2 has now been incorporated as the standard form. STRESSFORM2 differs only in the normalization factor in the denominator (under the radical). It is normalized by dividing by $\Sigma_j \Sigma_k (d_{jk} - \bar{d})^2$ rather than $\Sigma_j \Sigma_k d_{jk}^2$, where $\bar{d}$ is the mean of the d_{jk}'s.

* The first author of this paper (Carroll) has used the term "fully nonmetric" elsewhere (e.g., Carroll & Chang, 1970; Carroll, 1972) to distinguish a technique whose solutions are completely invariant under monotone transformation of the data and which guarantees (at least "in principle") a perfect solution (one where rank order of distances agrees perfectly with that of the data) when one is possible. This was contrasted with what was called a "quasi-nonmetric" procedure, where one or the other (or both) of these conditions is only approximately true. This usage of the term should not be confused with that of Green and Carmone (1970). Perhaps this terminological difficulty could be resolved by calling the Coombs procedure "doubly nonmetric," as was suggested earlier.

† It has very recently been discovered by Kruskal and Carroll that Shepard's algorithm could in fact be characterized as a gradient method optimization of an explicitly defined measure of fit. This was not known at the time (1964), however. Furthermore, the measure of fit Shepard used as criterion in his method was different from the criterion being optimized.

Given a particular metric in the underlying space (Euclidean, say) *and* a particular dimensionality (say m), the objective was rigorously defined as that of minimizing STRESS over the class of all m-dimensional spaces (with the appropriate metric) *and* over the class of all nonincreasing monotonic functions. Formally, we can think of STRESS as a function of X, the coordinate matrix, and of M, the monotonic function converting proximities into distances. If we represent that function as $S(X, M)$, we can set our task as the minimization over all X and M of STRESS $= S(X, M)$. Phrased in this way, this seems like a formidable task. However, Kruskal was able to take advantage of one very important simplification, which is expressed in the following seductively simple-looking formula

$$\min_{X,M} S(X, M) = \min_{X} [\min_{M} S(X, M)],$$

whose import is that if we can find a way to find the M minimizing S for a fixed X, then we are a long way toward our goal of minimizing S over X *and* M. It turns out that there is a well-defined and *finite* algorithm for finding the best M, given a specified X. Since the X matrix implies a set of distances, we could just as well assume that a set of fixed distances is given. The problem is to define the $\hat{d}$'s as a monotone function M of the δ's (the proximity, or antiproximity values) that minimize STRESS as defined in (18). Since the $\hat{d}$'s do not enter into the denominator, this is, in fact, equivalent to finding the g that minimizes the numerator; i.e., that produces the best least squares approximation to the $\hat{d}$'s. This problem of *least squares monotone* regression was first solved by van Eeden (1957a,b) and others (Bartholomew, 1959; Barton & Mallows, 1961; Miles, 1959) and was adopted by Kruskal (1964) to solve this problem of finding the best M. Since M could now easily be solved for any X, we can in effect redefine STRESS as a function of X alone; i.e.,

$$\text{STRESS} = S(X) = [\min_{M} S(X, M)],$$

so that the seemingly simpler problem now arises of finding X minimizing $S(X)$. The numerical method that Kruskal used to solve the problem actually turns out to be nearly equivalent to the α process described for Shepard's analysis of proximities. The major (and critically important) difference is that the algebraic magnitude of the discrepancy for points i and j is effectively defined to be proportional to $d_{ij} - \hat{d}_{ij}$. (This is not immediately obvious from Kruskal's gradient formula, but it can be established by some algebraic manipulation. The effective step-size, however, is changed somewhat.)

C. An Illustrative Application of Multidimensional Scaling

Before discussing further issues and details we would like to illustrate multidimensional scaling by an application to some data from Miller and Nicely's (1955) study of confusions among English consonants. The subjects in Miller and Nicely's experiment listened to female speakers read one-syllable stimuli, such as *pa, ta,* and *ka,* from randomized lists, and

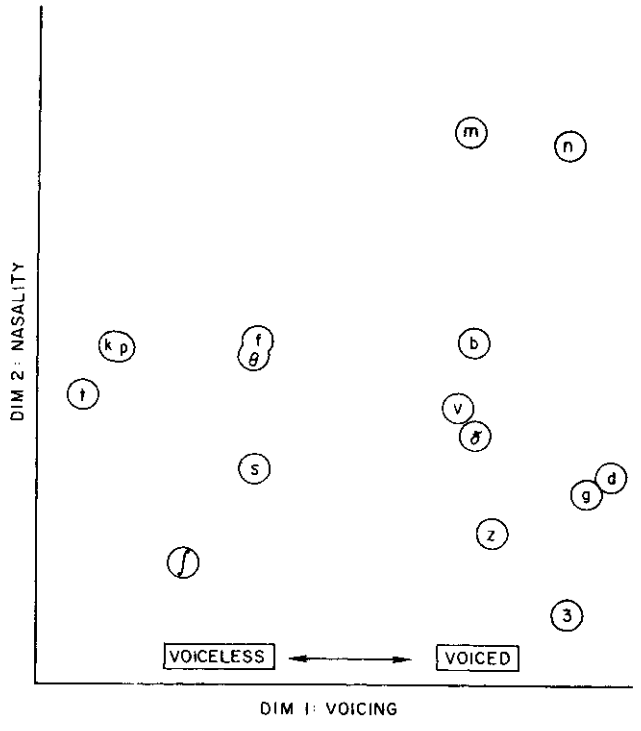

FIG. 1. Two-dimensional space from Shepard's (1973) analysis of data (see Table I) from Miller and Nicely's (1955) study of confusions among consonants.

wrote down the consonant they heard after each syllable was spoken. There were 17 experimental sessions in each of which the speech transmission circuit was degraded in a different way. In addition to the standard condition, which had a frequency response from 200 to 6500 Hz and a signal-to-noise ratio of 18 dB, there were five noise conditions (signal-to-noise ratio decreased from 12 dB to −12 dB in 6-dB steps), six low-pass filtering conditions (in which frequencies above a specified cutoff were filtered out) and five high-pass filtering conditions (in which the frequencies below a specified cutoff were filtered out).

Shepard (1973)* analyzed the pooled symmetrized matrix from the noise conditions, shown in Table I, by a variant of multidimensional scaling described earlier, in which an exponential rather than a monotonic fit was required. (Almost identical results were obtained by using a monotonic function; moreover, the best fitting monotonic function turned out to be very close to an exponential decay curve.) The two-dimensional (rotated) space obtained for these data is shown in Fig. 1. Shepard assigned the interpretation "voicing" to the horizontal dimension, since it distinguishes the voiced consonants (those, which, when spoken, produce vocal cord

* Despite the 1973 reference, the paper was actually written in 1965.

TABLE I

p	—															
t	.229	—														
k	.432	.241	—													
f	.101	.057	.077	—												
θ	.124	.079	.084	.423	—											
s	.052	.050	.063	.066	.157	—										
ʃ	.038	.050	.047	.030	.048	.115	—									
b	.022	.013	.018	.046	.045	.024	.012	—								
d	.025	.022	.020	.025	.041	.031	.033	.058	—							
g	.013	.016	.030	.015	.039	.033	.021	.069	.342	—						
v	.016	.022	.020	.035	.040	.023	.020	.210	.059	.054	—					
ð	.028	.016	.018	.032	.031	.026	.018	.145	.094	.120	.338	—				
z	.025	.023	.025	.018	.033	.035	.017	.055	.106	.139	.080	.161	—			
ʒ	.019	.017	.019	.007	.017	.022	.012	.027	.089	.125	.029	.033	.136	—		
m	.025	.022	.021	.016	.019	.017	.012	.038	.024	.032	.030	.034	.121	.016	—	
n	.017	.018	.020	.012	.018	.013	.011	.024	.032	.030	.022	.028	.016	.030	.151	—
	p	t	k	f	θ	s	ʃ	b	d	g	v	ð	z	ʒ	m	n

vibration) from their voiceless cognates. The interpretation "nasality" given to the vertical dimension reflects the fact that the two nasals, *m* and *n*, are separated from the other consonants.

Even though only two distinctive features (voicing and nasality) are explicitly mentioned in the labels for dimensions, Shepard does point out that some information regarding affrication and place of articulation is preserved in the two-dimensional space. For example, the stops are generally at opposite extremes of dimension 1, with the fricatives in between.

Shepard further clarified this configuration in particular, and the Miller and Nicely data in general, by applying Johnson's (1967) hierarchical clustering procedure to the same confusion matrix (Table I).

Johnson's hierarchical clustering procedure starts with the finest possible clustering (each point a separate "cluster") and proceeds to "merge" the two stimuli with the highest proximity value. (In case there is a tie for the most proximal pair, all pairs of points with the common value are merged simultaneously.) The newly merged cluster is treated as a separate point, so there are now (in general) $n - 1$, rather than n points. Distances must then be calculated between this point and the others. In the "maximum" method (used by Shepard) the distance of a cluster to another point (which may be another cluster) is taken to be the largest of the distances (smallest proximity) between the merged points; in the minimum method, it is the smallest distance (largest proximity). This process now continues, but with $n - 1$ points instead of n, and does not end until all points are merged into a single large cluster. This process of continual merging produces a hierarchical clustering, which can be represented as a tree. The tree generated in this way for the Miller–Nicely data is shown in Fig. 2. The height of different nodes of the tree is then defined as the distance between the two points merged at that node. In the maximum method, this can also be shown to be the diameter of the largest cluster in the clustering, where diameter is defined as the largest distance between a pair of points in that cluster. If this process is applied to proximities rather than distances or antiproximities, the heights would be replaced by proximity levels that get smaller as one goes up the hierarchy. In Fig. 2, the heights have, in fact, been replaced by these proximity levels, and the tree is inverted so larger proximities are at the top. Perhaps in this case we should refer to the "depth" rather than "height" of the clusterings.

Figure 3 shows an embedding of results for five clustering levels (minimum intracluster proximity of .40, .20, .10, 05, and .025) in the multidimensional space for these data. These contours were drawn manually by Shepard. It is quite important to note, however, that they *could* be so drawn; without overlapping or crossing of cluster boundaries, and with all the clusters appearing to be reasonably compact and connected. Since the two analyses (multidimensional scaling and hierarchical clustering) were done quite independently, there was no guarantee that this would happen. That it did tends to increase the credibility of both analyses, while also being quite helpful in interpretation of the multidimensional scaling solution.

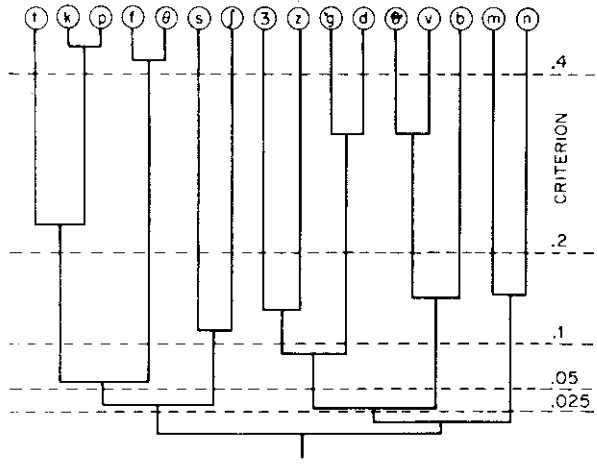

FIG. 2. Hierarchical clustering from Shepard's (1973) analysis of data (see Table I) from Miller and Nicely's (1955) study of confusions among consonants. Clusters at five levels (.40, .20, .10, .05, and .025) are indicated by dashed horizontal lines.

As indicated by the three outermost curves, the clustering at the .025 level partitions the consonants into three broad clusters—the nasals, the voiced nonnasals, and the voiceless consonants. At the .05 level the voiceless and voiced consonants both subdivide, making five clusters in all. As the minimum intracluster value increases from .10 to .20 to .40, the number of clusters increases from 7 to 11 to 14. Twelve of the clusters at the .40 level contain a single consonant; the only two-element clusters at the .40 level are *p*, *k* (proximity = .432) and f, θ (proximity = .423).

Shepard also did separate hierarchical clusterings of the confusion matrices for each of the 17 experimental conditions. At the levels of each hierarchical clustering at which there were six clusters and five clusters, exactly the same clusters appeared for the four intermediate noise conditions (6, 0, −6, and −12 dB). In the two extreme conditions, the confusion rate was too low (at 12 dB) or too high (−18 dB) for stable clusters to be defined. The consistency in these and other clustering results led Shepard to conclude that "although signal-to-noise ratio is a powerful determiner of overall level of confusion, it has little or no effect on the internal *pattern* of those confusions [Shepard, 1973]."

Whereas the clustering results for the low-pass filtering conditions were quite similar to those for the noise conditions, the clusterings for the high-pass filtering conditions were so different that they could not be embedded very well in the multidimensional space based on the "noise" conditions (see Shepard, 1973). The correspondence between results for the noise and low-pass filtering conditions is consistent with the fact (Miller & Nicely, 1955, p. 350) that the higher frequencies are more susceptible to

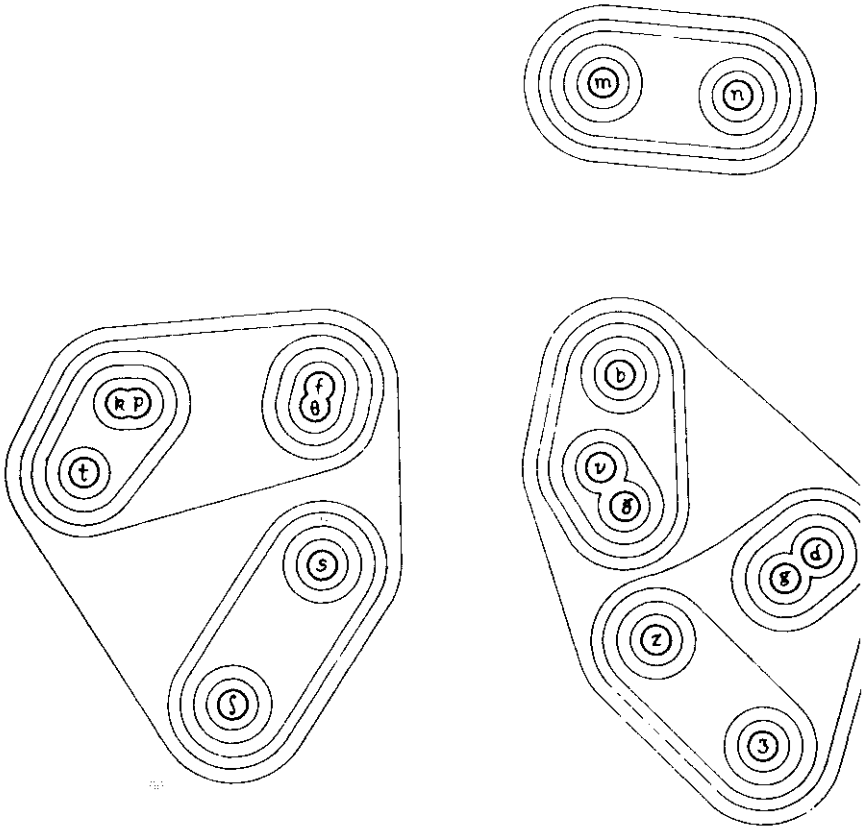

FIG. 3. Embedding of clusters from a hierarchical clustering analysis (Fig. 2) in the two-dimensional space (Fig. 1) for the same data (Table I). At a clustering level (lowest intracluster proximity) of .025, there are three clusters; while at a clustering level of .40, there are 14 clusters.

masking by broadband, or white, noise, since the sound energy is generally weaker in the higher frequencies. In Chapter 13 in this volume (Wish & Carroll, 1974), we describe a later analysis of the Miller–Nicely data (Wish, 1970a), which gives more information about the confusion structure for high-pass filtering conditions and which allows for more direct and sensitive comparisons of the data for different kinds and degrees of acoustical degradations.