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A MONTE CARLO INVESTIGATION OF THE STATISTICAL SIGNIFICANCE OF KRUSKAL'S NONMETRIC SCALING PROCEDURE*

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Recent advances in computer based psychometric techniques have yielded a collection of powerful tools for analyzing nonmetric data. These tools, although particularly well suited to the behavioral sciences, have several potential pitfalls. Among other things, there is no statistical test of the statistical significance of results yielded by Kruskal's nonmetric multidimensional scaling. The estimates, obtained from many randomly generated sets of data, reveal the relative frequency with which apparent structure is erroneously found in unstructured data. For a small number of points (i.e., six or seven) it is very likely that a good fit will be obtained in two or more dimensions when in fact the data are generated by a random process. The estimates presented here can be used as a bench mark against which to evaluate the significance of the results obtained from empirically based nonmetric multidimensional scaling.

1. Introduction

Recent developments in psychological scaling [Shepard, 1962a, 1962b; Kruskal, 1964a, 1964b; Lingoes, 1965] have yielded a collection of computer [illegible] circumstances where there is no appropriate metric, these new procedures provide powerful tools for the analysis of such data. They are being used with increasing frequency in a diverse range of applications, e.g., color vision, Morse Code perception [Shepard, 1963], tests [Russell & Gregson, 1966], college admissions [Klahr, 1968], marketing [Green, Carmone & Robinson, 1968].

However, the great strength of these new procedures must be tempered with careful application. Torgerson [1965, p. 381], in reviewing some of the advances in multidimensional scaling, says:

> The new procedures would . . . seem to offer nothing but advantages over the old; to require very little and to yield very much. Yet there are many problems connected with their use which . . . have not been at all obvious . . . . It is like doing a factor analysis. And like factor analysis, the methods always yield an answer. But it can be even more difficult to fully comprehend the meaning of that answer.

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Torgerson goes on to discuss several of the difficulties. One which he treats most extensively in his paper is the problem of the very nature of similarity itself. He shows that under certain circumstances the implicit models underlying the scaling technique are quite inappropriate. In particular, the similarity of one item to another often depends upon the context of the judgment, i.e., upon the other relevant items in the collection of things to be judged. The scaling models do not allow for this kind of variability in similarity judgments.

A second difficulty, the problem of multiple solutions (i.e., non-uniqueness [illegible] points we can be very sure that the solution is unique, and for 15 or more points we can be virtually certain that we have found the configuration which best fits the data.

Green [1966] suggests that "these . . . procedures need Monte Carlo and other computer runs to determine their properties. . . ." This paper deals [illegible] tistical significance of the results. We investigate, through Monte Carlo simulation, the following question: How likely are we to falsely reject the [illegible]

There are at present no statistical methods for testing the significance of the results generated by the scaling procedures. As a first step towards filling this [illegible] i.e., a good scaling solution) is found in randomly generated data. The results to be presented are based upon a series of attempts to scale randomly generated data. They can be used as a bench mark against which to assess the significance of empirical results.

2. Nonmetric Multidimensional Scaling

All multidimensional scaling procedures assume that there is an underlying structure—a spatial configuration of items, in which interpoint distances are inversely related to empirically determined proximity measures on those items. The goal of the procedures is to construct such a configuration from the inter-item proximity measures. For example, if the proximity measures are judgments of the relative similarity of pairs of stimuli, the scaling procedure would attempt to construct a spatial configuration in which [illegible] close together.

The three most widely used procedures—Shepard's [1962], Kruskal's [1964a, 1964b], and Lingoes' [1966]—are designed for the same purposes. That is, they yield essentially similar outputs, given the same input. Although the procedures achieve their desired result in different ways, for the purposes of our analysis it will suffice to discuss only one of them. Therefore, the re-

mainder of this paper will be based upon Kruskal's nonmetric multidimensional scaling procedure [1964a, 1964b].

The goal of the procedure is to find the spatial configuration of a set of points in which the rank order of the interpoint distances is maximally inversely correlated with the rank order of the corresponding inter-item similarity measures. It starts with an arbitrary configuration of points and iter- [illegible] order of the interpoint distances is exactly the opposite of the rank order of the similarity measures. When this [illegible] the data perfectly. As the dimensionality of the space is reduced and the solution becomes more highly constrained, we are apt to get some departures from perfect fit. Some of the distances may be "out of order." A measure of [illegible] developed by Kruskal [1964a]; it is quite similar to a residual sum of squares [illegible] Kruskal suggests that departure from perfect fit (stress = 0) be interpreted [illegible] We expect minimum stress to increase as the dimensionality decreases, starting in $n - 1$ space with zero stress.

The decision as to which configuration is the most appropriate representation of items rests upon scientific judgments and is not a direct output of the scaling technique. In most applications the decision is based upon the [illegible] configuration. Most users have used Kruskal's suggestions as to what constitutes an acceptable result in lieu of a rigorous statistical test for the significance of the stress. Although no appropriate statistical test exists at present, it is possible to obtain estimates of significance through the use of the techniques described in the next section.†

3. Procedure

In all applications of multidimensional scaling techniques the input [illegible] Whatever the metric for the raw data, the scaling procedure makes use of [illegible] simulate a wide range of empirical proximity measures on n stimuli simply by using a set of distinct values, one for each of the $n(n-1)/2$ pairs of n stimuli.

To the set of $n(n-1)/2$ distinct pairs of n hypothetical items we ran- [illegible]

†Since this work was done, a similar study by Stenson and Knoll [1969] has appeared covering a different range of parameters: $m = 1$ to 10 in steps of 1, and $n = 10$ to 60. For large n, there is much less variance in the final stress, and the averages based on 3 data sets are sufficient. For the small n studied in our paper, there is a need for more samples [illegible]

0 to 1. One hundred such sets of random proximities were generated for each value of $n = 6, 7, 8$ and 10; fifty sets each were generated for $n = 12$ and 16. Every one of the 500 sets was scaled by Kruskal's nonmetric multidimensional

values that control Kruskal's program were: minimum stress sought—zero; maximum number of iterations—75; type of proximity measure—dissimilarities; spatial metric—Euclidean.

4. Results

stress under conditions of pure noise that this study seeks to portray.

For each value of n we have plotted the cumulative distribution of the final stress values from one, two and three dimensional configurations in Figures 1 through 3 respectively. If an analytic expression could be developed for

of generating a family of curves quite similar to these empirical estimates.

In Table 1 we present some summary statistics for each value of n. The number of solutions less than or equal to Kruskal's "good" (.10) and "excellent" (.05) stress levels are included, along with the maximum, minimum, average and standard deviation of final stress values. Table 2 contains some selected

is a plot of the average final stress shown in Table 1.

5. Discussion

These data may provide some assistance in detecting and avoiding

For example, "good" solutions (i.e., stress $\leq$ .05) are often attainable for

for 8 points, 33 out of 100.) A small increase in the number of points (e.g., $n > 10$) provides a substantial reduction in the likelihood of this kind of

for a given number of points, stress increases with decreasing dimensionality.

One of the criteria that Kruskal suggests for selecting the appropriate dimensionality is an "elbow" in the plot of stress vs. dimensionality. [4] A

major decrease in the marginal improvement obtained by additional dimension. The lack of distinctive elbows in the plots in Figure 4 arises from the

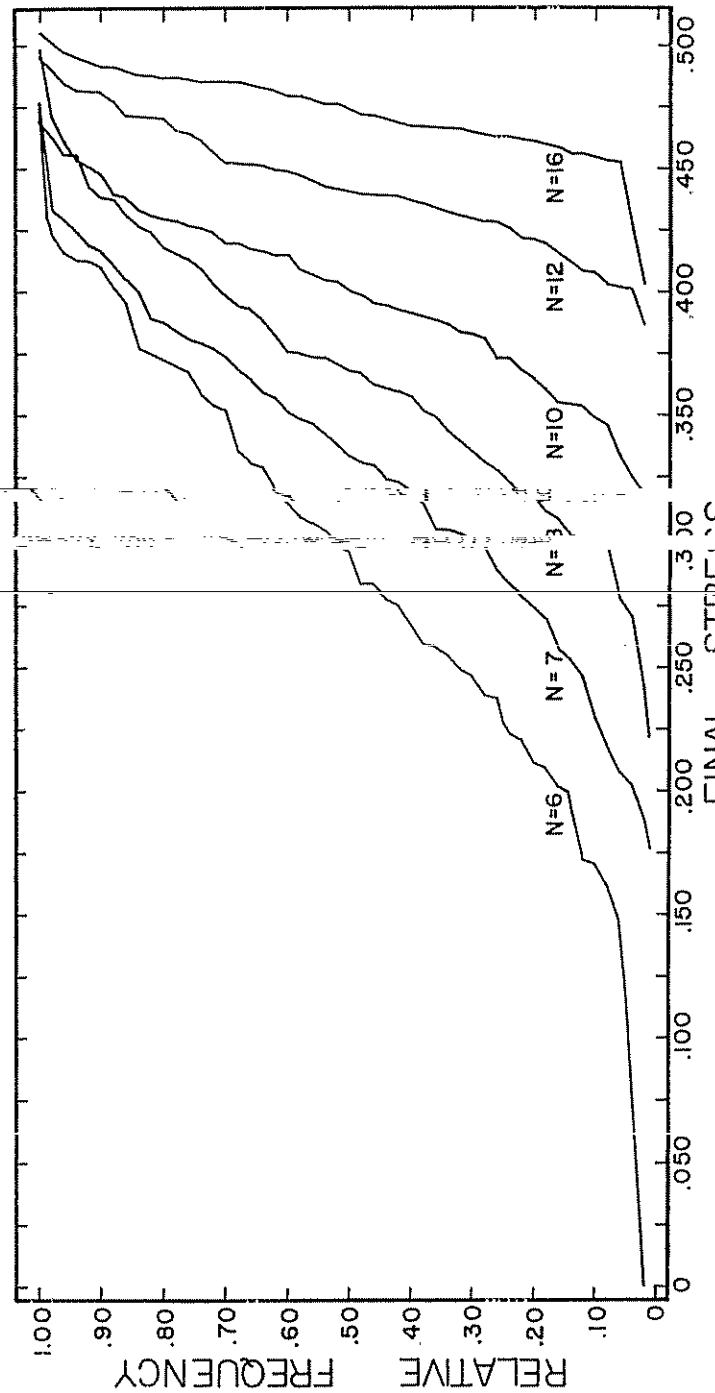

Fig. 1.--Cumulative distributions of relative frequency of final stress in a 1 dimensional configuration for 6, 7, 10, 12, and 16 points.

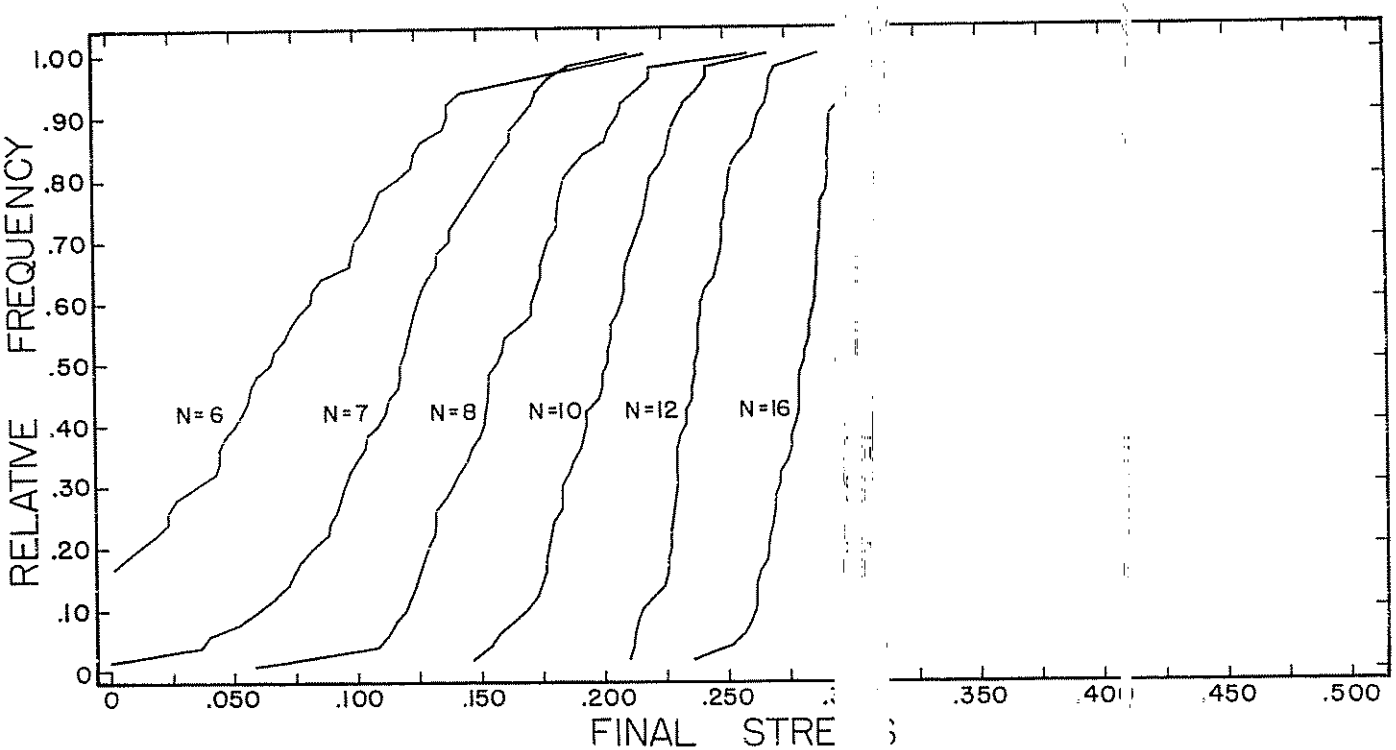

Fig. 2.--Cumulative distributions of rela frequency of final stress in a 2 dimensional configuration for 6, 7, 10, 12, and 16 poin s.

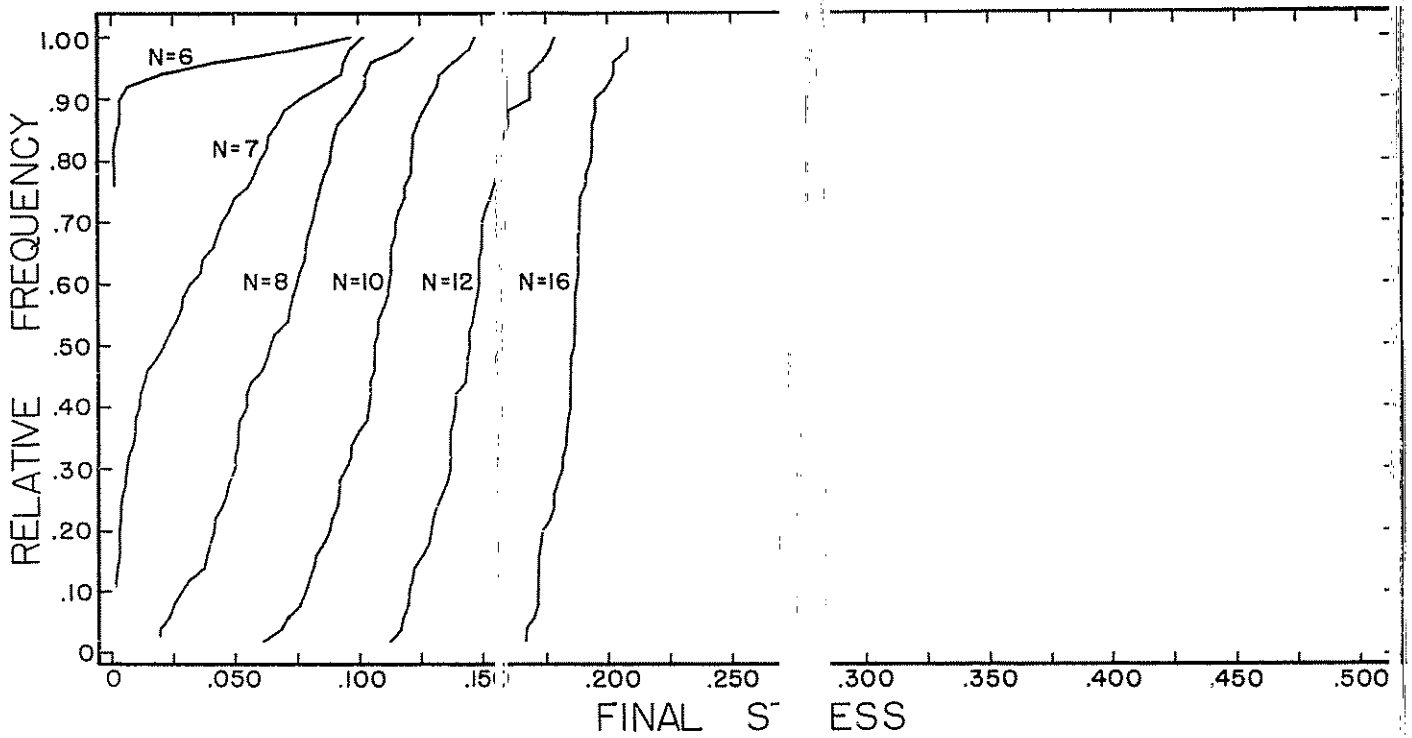

Fig. 3.--Cum lative distributions of lative frequency of final stress in a 3 dimens onal configuration for 7, 8, 10, 12, and 16 points.

TABLE 1

Summary Statistics From Monte Carlo Runs: Average, Standard Deviation, Max, Min, Good and Excellent Stress

	Number of Dimensions					
	1	2	3	4	5	
Number of "Good" Final Stresses	4	39	95	100	100	
Number of "Excellent" Final Stresses	4	27	95	100	100	
Average Final Stress	0.288	0.0 0	0.0	0.	0.	6 points
Standard Deviation of Final Stresses	0.097	0.0 3	0.0	0.	0.	100 sets
Maximum Final Stress	0.471	0. 8	0.0	0.001	0.	
Minimum Final Stress	0.	0.	0.	0.	0.	
Number of "Good" Final Stresses	0	7	74	100	100	
Number of "Excellent" Final Stresses	0	3	53	100	100	
Average Final Stress	0.332	0. 4	0.0	0.002	0.	7 points
Standard Deviation of Final Stresses	0.066	0. 3	0.0	0.005	0.	100 sets
Maximum Final Stress	0.477	0. 2	0.	0.025	0.00	
Minimum Final Stress	0.177	0.	0.	0.	0.	
Number of "Good" Final Stresses	0	0	33	9	0	
Number of "Excellent" Final Stresses	0	0	8	7	0	
Average Final Stress	0.368	0. 0	0.0	0.016	0.00	8 Points
Standard Deviation of Final Stresses	0.055	0. 4	0.0	0.018	0.00	100 sets
Maximum Final Stress	0.470	0. 0	0.	0.079	0.07	
Minimum Final Stress	0.222	0. 9	0.	0.	0.	
Number of "Good" Final Stresses	0	0	0	3	0	
Number of "Excellent" Final Stresses	0	0	0	3	0	
Average Final Stress	0.400	0. 1	0.	0.055	0.02	10 points
Standard Deviation of Final Stresses	0.038	0. 5	0.0	0.017	0.01	100 sets
Maximum Final Stress	0.498	0. 7	0.	0.096	0.05	
Minimum Final Stress	0.314	0. 2	0.0	0.008	0.	

TA[illegible]E 1--Contin[illegible]

	Nu[illegible]r o[illegible] Dimensions					
	1	2	3	4	5	
Number of "Good" Final [illegible]ses	0	0	0	1	16	12 poi[illegible] 50 set[illegible]
Number of "Excellent" F[illegible] Stresses	0	0	0	0	0	
Average Final Stress	0.4[illegible]4	0.240	0.144	0.0[illegible]38	0.057	[illegible]nts
Standard Deviation of F[illegible] Stresses	0.0[illegible]5	0.017	0.016	0.0[illegible]16	0.015	[illegible]s
Maximum Final Stress	0.4[illegible]6	0.288	0.178	0.1[illegible]31	0.089	
Minimum Final Stress	0.3[illegible]7	0.210	0.112	0.0[illegible]49	0.027	
Number of "Good" Final [illegible]ses	0	0	0	0	0	16 poi[illegible] 50 set[illegible]
Number of "Excellent" F[illegible] Stresses	0	0	0	0	0	
Average Final Stress	0.4[illegible]3	0.279	0.185	0.1[illegible]30	0.096	[illegible]nts
Standard Deviation of F[illegible] Stresses	0.0[illegible]3	0.014	0.010	0.0[illegible]11	0.011	[illegible]s
Maximum Final Stress	0.5[illegible]5	0.300	0.207	0.1[illegible]52	0.127	
Minimum Final Stress	0.4[illegible]4	0.237	0.166	0.1[illegible]06	0.074	

TABLE 2

Selected Percentile Points From Cumulative Distributions of Final Stress

		Percentile 5	10	25	50	75	90	95	
Dimensions	1	.121	.171	.227	.296	.363	.410	.415	6 points 100 sets
	2	.000	.000	.023	.065	.107	.138	.148	
	3	.000	.000	.000	.000	.000	.004	.020	
	4	.000	.000	.000	.000	.000	.000	.000	
Dimensions	1	[illegible]	.230	[illegible]	.334	[illegible]	.417	.427	7 points 100 sets
	2	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	
	3	.000	.000	.004	.021	.056	.077	.094	
	4	.000	.000	.000	.000	.000	.006	.009	
	5	.000	.000	.000	.000	.000	.000	.000	
Dimensions	1	.276	.298	.326	.396	.412	.439	.456	8 points 100 sets
	2	.111	.120	.132	.157	.183	.206	.215	
	3	.022	.028	.046	.064	.084	.100	.104	
	4	.000	.000	.002	.010	.023	.042	.050	
	5	.000	.000	.000	.000	.001	.005	.007	
Dimensions	1	.333	.349	.373	.401	.427	.440	.461	[illegible] 100 sets
	2	.153	.169	.180	.202	.216	.232	.246	
	3	.060	.078	.092	.107	.119	.129	.136	
	4	.027	.035	.044	.054	.067	.077	.079	
	5	.004	.009	.018	.024	.032	.040	.050	
Dimensions	1	.402	.408	.429	.441	.465	.481	.485	[illegible] 50 sets
	2	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	
	3	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	
	4	.071	.072	.075	.086	.094	.109	.118	
	5	.032	.037	.047	.057	.063	.078	.085	
Dimensions	1	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	16 points [illegible]
	2	.257	.261	.270	.282	.289	.293	.298	
	3	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	
	4	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	
	5	.077	.083	.089	.096	.102	.112	.119	

averaging of many curves, some with quite distinctive elbows at different dimensionalities. Thus Figure 4 should not obscure the fact that pure noise [illegible] may give the spurious appearance of a true dimensionality.

The importance of these findings to a user of Kruskal's program rests [illegible] used to test *a priori* hypotheses about the dimensionality or spatial arrange-

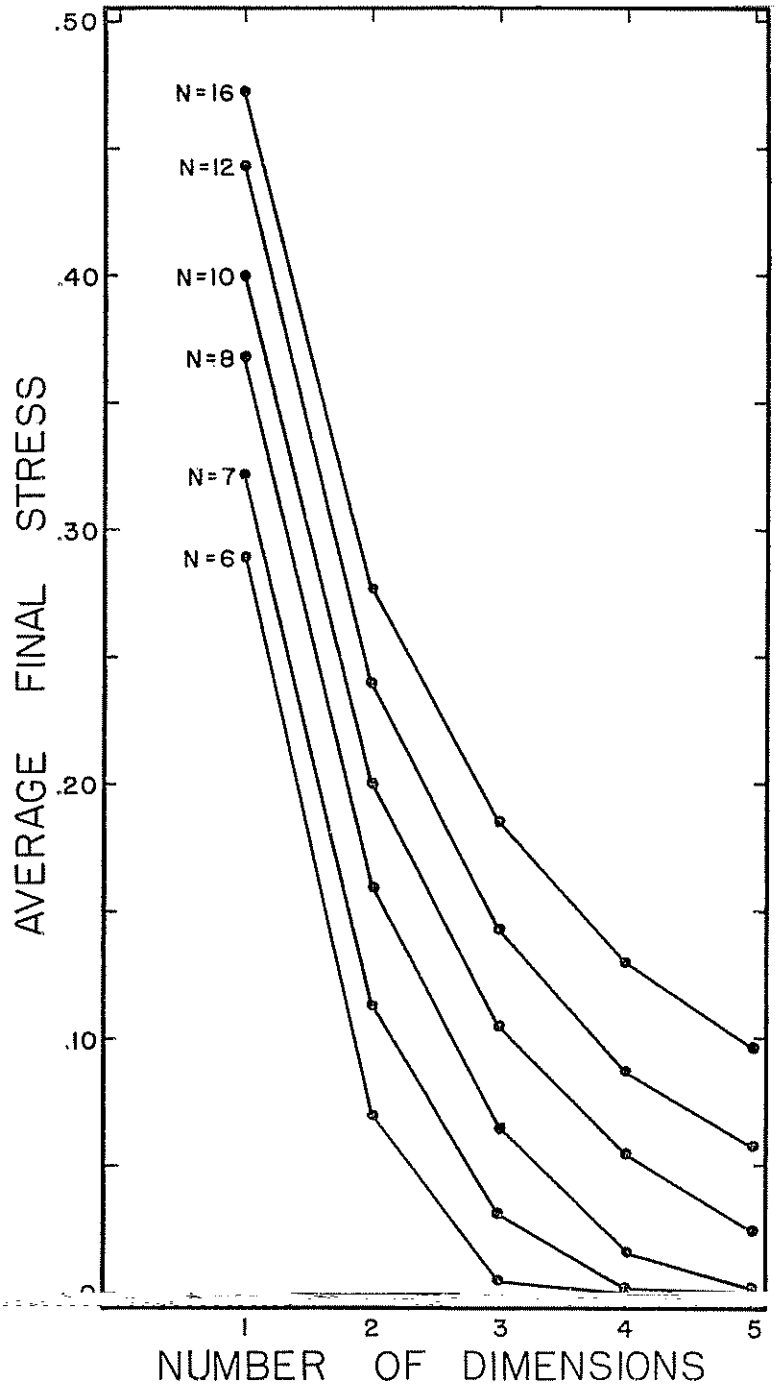

Fig. 4.--Average final stress vs. number of dimensions for 6, 7, 8, 10, 12, and 16 points.

ment of a stimulus set, then the significance criterion is but one of many pieces of evidence that can be used in interpreting results. However, if the scaling [illegible] about the configuration, then any results for only 8 or 9 points in 2 or 3 dimensions cannot be considered very convincing evidence for the existence of structure. For example, from Figure 3 it is evident that with eight points there are about 2 chances in 3 that pure noise could be accounted for in 3 dimensions with a stress less than .075. If the experimenter is at the design stage, then he can use these results as a lower bound on the number of stimuli he will need in a situation where he suspects a certain number of dimensions.

6. Conclusion

The scaling procedure discussed in this paper is one of a class of new techniques that are so powerful and convenient that they are being used as exploratory devices to see if any structure exists in a set of proximity measures [illegible] can be used as a benchmark [illegible] wide variety of multidimensional scaling applications.

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