Journal of Statistical Research *ISSN 0256 - 422 X*
2012, Vol. 46, No. 1, pp. 19-30
Bangladesh

PARALLEL ANALYSIS TO DETERMINE THE NUMBER OF DIMENSIONS IN MULTIDIMENSIONAL SCALING ANALYSIS

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SUMMARY

Deciding on the number of latent factors or classes is a critical issue in statistical analyses such as factor analysis and finite mixture analysis. No new progress has been made in recent years with least-squares MDS analysis. In this paper, we proposed the use of parallel analysis, in addition to the conventionally used stress value, for determining the number of dimensionalities or profiles to retain in MDS analysis. Using two actual datasets, we demonstrated the approach. The results indicated that parallel analysis seemed to be viable in MDS model selection.

Keywords and phrases: multidimensional scaling, parallel analysis, model selection, the number of dimensions

1 Introduction

Model selection is an important first step in many statistical analyses. For example, in principal component analysis (PCA) or factor analysis (FA), one always needs to determine the number of components or factors that underlie the data, a critical task the researcher encounters when using these analytical techniques. What is typically believed is that an incorrect decision may lead to the either under-extraction (i.e., loss of information) or over-extraction (i.e., inclusion of spurious factors or components) of the data at hand. In the case of over-extraction, one tends to attach meaning to noise in the data, resulting in the interpretation of random variation that affects subsequent analyses. Another example is finite mixture modeling such as latent class analysis, factor mixture analysis, or growth mixture modeling. However, regardless types of analysis approaches used such as confirmatory-oriented approach with structural equation modeling or exploratory-oriented approach with multidimensional scaling analysis, a continuing issue is how to determine the numbers of latent classes (i.e., unobserved subgroups) in the data since latent classes are used for interpreting results and making inferences. In general, issues for determining the number of factors, components, or classes are known as model selection (e.g.,Schwarz, 1978).

Many empirical studies have devoted much effort to find statistical procedures that allow selecting the best model that represents the data. For statistical analyses employing maximum likelihood estimation, one of the most studied statistical procedures used for model selection is information criterion such as Akaike Information Criterion (AIC; Akaike, 1974), Bayesian information Criterion (BIC; Schwarz, 1978), or different variants of AIC or BIC related statistics. Another technique for model selection is likelihood ratio test such as Lo-Mendell-Rubin likelihood ratio test (Lo, Mendell, and Rubin, 2001), or bootstrap likelihood ratio test method (McLachlan and Peel, 2000). Although there is no common consensus yet with respect to which index is the best in determining the approximating model given the data, much of the progress has been made in the area of model selection.

In contrast, the development of model selection for statistical techniques that employ least squares estimations has not shown any noticeable progress, particularly for least-squares multidimensional scaling analysis (MDS). One reason may be that MDS models have not been widely used in social science research in recent years, and the utility of MDS analysis, although proven useful to researchers in different fields of science, including education, health, marketing, psychology, and sociology, is not well understood. However, MDS models have different applications, and it has been used to study such things as the perceptional structure of people (e.g., Goodrum, 2001; McWhirter, Palombi, and Garbin, 2000), vocational interest of college students (Johnson, 1995), test content and validity (Sireci and Geisinger, 1992), and cognitive organization of perceptions (Treat et al., 2002). More recently, MDS analysis has been developed for latent profile analysis (Davison, Gasser, and Ding, 1996; Ding, 2006; Kim, Davison, and Frisby, 2007) and exploratory growth mixture analysis (Ding, 2007a; Ding, 2007b). These developments, particularly exploratory growth modeling, have expanded our vision on how to explore growth heterogeneity underlying the data structure and provided complimentary analytical techniques to more confirmatory-based modeling approaches.

Regardless of any specific applications or purposes of MDS analysis, however, the first step in conducting MDS analyses is to determine the number of dimensions needed to characterize the distance data. This is the issue of model selection, an issue that has been studied in many other statistical modeling procedures as discussed previously. In the case of MDS analysis, there is a set of alternative distance models, each with a different number of dimensions, also called profiles, as potential approximations to the distance data. From the perspective of finite mixture modeling, different number of dimensions or profiles in MDS can be considered to summarize characteristics of subgroups in the data, with each subgroup showing a unique profile as measured by a particular set of variables. One generally does not know the proper number of dimensions or profiles, K, with which to represent the distance data for all possible pairs of v stimuli or v variables to be scaled. In other words, we seek a solution that parsimoniously approximates the distance data as closely as possible, and at the same time the model will provide a good summary of individual differences. In least-squares MDS, the most common measure for model selection is stress value (Kruskal, 1964a) or a closely related measure called S-Stress value (Young and Lewyckyi, 1988). No new progress has been made in this regard.

Specifically, Kruskal's Stress formula one (S_1) can be expressed as

$$S_1 = \sqrt{\frac{\sum(\hat{\delta}_{ij} - d_{ij})^2}{\sum d_{ij}^2}}, \tag{1.1}$$

where $\hat{\delta}_{ij}$ is disparities and d_{ij} is model estimated distance. In many MDS applications Stress is both the fit measure minimized by the estimation algorithm and the primary index used in model selection for models constructed in each of several spaces of varying dimensionalities. In least-squares MDS, Stress value is a normalized sum of squared discrepancies between the observed distance data points δ and the model derived data points d. The smaller the stress value, the better is the fit of the model to the data. Kruskal (1964b) suggests that a value of K (number of dimensions) be chosen which makes the stress value acceptably small. The benchmarks he suggested based on his experiences with simulation data were: .20 = poor fit, .10 = fair, .05 = good, .025 = excellent, 0 = perfect. In MDS analysis, this rule of thumb has often been used for selecting the number of dimensions. Such criteria, however, may lead to misuse by suggesting that only dimension or profile solutions with stress values less than .20 are acceptable (Borg and Groenen, 2005) and may lead to arbitrary decisions. For instance, it is difficult to decide whether a 3-dimensional model with a Stress value of .025 is a better model than a 4-dimensional model with a Stress value of .02. In addition, Stress is closely related to the proportion of error in the data, and it is possible that an MDS configuration is highly reliable over replications of data but with a high stress value (Borg and Groenen, 2005; Cox and Cox, 1992).

Sometimes a scree plot of Stress or eigenvalues against the number of dimensions is also used for visual inspection of elbow in the plot (Davison, 1983), similar to the use of scree plot in factor analysis. In this method, however, there sometimes is no clear cutoff point for elbow, leading to solution ambiguity and interpretation difficulty. This is because that in real data that do not conform exactly to the model or in which there is measurement or sampling error, elbow may be hard to discern. More importantly, a scree plot is simply a plot of Stress values, which may not provide more objective determination on the number of dimensions in MDS analysis.

So far, all the statistics used for model selection in least-squares MDS are based on a model-data fit approach; in other words, we are trying to identify a model with a statistic that shows the best fit between the model and the data. In this paper, we discussed a Monte Carlo method, called Parallel Analysis, as a statistical approach for MDS model-data fit measure in deciding the best approximating model for the data at hand. The idea was based on that of parallel analysis in factor analysis for determining number of factors to retain.

This paper was organized as follows. First, we introduced the basic principles of parallel analysis and its application in MDS analysis. Because parallel analysis was new in MDS, we discussed it more in detail. Second, we presented two examples of real datasets to illustrate the analytical approach proposed here. We used two studies that had a theoretically known dimensionality rather than artificial data. As indicated by Cudeck and Henly (2003), there were no true models to discover. Instead, a model was to summarize and formalize the behavioral processes and to make predictions even if the model was false. Any model selection procedures were to help researchers to make more objective decisions as to the best approximating model for such a purpose rather than find the true model. Thus, using real data rather than artificial data may provide a more realistic view of how parallel analysis could function in this regard. It should be noted that the main point of the paper was to illustrate parallel analysis as a potential model selection tool in MDS analysis. More in-depth studies of parallel analysis in MDS model selection were complex and warranted separate studies.

2 Basic Idea of Parallel Analysis in MDS

Originally parallel analysis was proposed to determine the number of factors that underlay the data in factor analysis (Horn, 1965) based on the generation of simulation data. It has been suggested that parallel analysis is a promising technique for model selection in factor analysis (Humphreys and Ilgen, 1969; Humphreys and Montanelli, 1975; Linn, 1968; Weng and Cheng, 2005) and is considered a better model-selection method in comparison with other methods such as eigenvalues-greater-than-one, scree plot, or minimum average partial test (Glorfeld, 1995; Zwick and Velicer, 1986). In factor analysis parallel analysis involves the factoring simulated variance-covariance matrix or correlation matrix (including tetrachoric or polychoric correlation) identical with respect to the number of variables and the number of cases as the original data matrix. Perhaps it is called parallel analysis for this reason. In a sense, parallel analysis is a Monte Carlo simulation procedure in which simulated eigenvalues are computed from normal random samples that mirror the real data at hand; in other words, parallel analysis not only models the same number of cases and variables as the original data, but also the same marginal distributions of the variables as well. In model building both over- and under-estimation may be made when the decision is based on a single sample of data (Humphreys and Montanelli, 1975). Thus, a Monte Carlo method provides a secondary useful criterion since a large number of parallel data sets are used, and in some cases rather than generating data, a permutation test approach is used in which individual variable values are mixed with one another to create the synthetic data. A factor is retained when the corresponding eigenvalue is greater than the mean or median of those computed from the simulated data. Glorfeld (1995) has also suggested to use the eigenvalue that corresponds to a particular percentile; in other words, a factor is retained when the associated eigenvalue is greater than, for instance, the 95th percentile of the distribution of eigenvalues from simulated data. It seems that most authors now only suggest using a particular percentile for parallel analysis, rather than the mean or median.

Given the sound rational and proved usefulness of parallel analysis in determining number of factors in the data (Buja and Eyuboglu, 1992; Glorfeld, 1995; Humphreys and Montanelli, 1975; Weng and cheng, 2005; Zwick and Velicer, 1986), it is feasible to adapt parallel analysis in MDS analysis for model selection, that is, number of dimensions or profiles to retain in MDS analysis. Since the idea of parallel analysis in factor analysis is based on the criterion of variance that can be accounted for by a specific number of factors in observed data with that in simulated data, this logic can also apply to MDS analysis, which has the same goal of explaining maximum amount of variance in the data by a specific number of dimensions or profiles. Thus, it seems reasonable that the method of parallel analysis can be used in MDS analysis. Although the mathematics of the method is not new, the approach is new for MDS analysis.

In factor analysis, eigenvalues are obtained from a correlation matrix, a covariance matrix, or a cross-product matrix. In MDS analysis, however, a distance matrix is typically used as input data. In order to obtain eigenvalues associated with each dimension, observed distance matrix D needs to be converted into an equivalent cross-product matrix and then eigenvalue of each dimension can be computed based on this transformed cross-product matrix (Abdi, 2007)[1]. Specifically, the cross-

[1]The proof is provided by Abdi (2007) on how distance matrix can be transformed into a cross-product matrix, which can

product matrix S can be obtained from distance matrix D as:

$$S = -\frac{1}{2} \in D \in^T, \tag{2.1}$$

where $\in = \mathtt{I} - 1m^T$ and m is called by Abdi (2007) a mass vector (i.e., a vector of 1/number of variables) whose v elements give the mass of the v rows of distance matrix, D, which is calculated between data points, y_i and y_j, for v variables as:

$$d_{ij} = \sqrt{\sum_{j=1}^{v} (y_i - y_j)^2}. \tag{2.2}$$

and this observed distance d_ij is assumed equal to distances δ_{ij} in m Euclidean space with coordinate x_{ik} and x_{jk}, which represents the configuration of variables in the geometric space, that is:

$$d_{ij} = \delta_{ij} = \sqrt{\sum_{k=0}^{m} (x_{ik} - x_{jk})^2}. \tag{2.3}$$

The elements of $\in$ are all positive and their sum is equal to one; that is, $m^T\mathtt{I} = 1$. The eigendecomposition of the cross-product matrix S gives:

$$S = U\Lambda U^T, \tag{2.4}$$

where $UU^T = I$ and is diagonal matrix of eigenvalues. Thus, one can compute eigenvalues of dimensions for both observed data at hand and those from simulated data. A dimension with corresponding eigenvalue that is greater than median or the 95th percentile of simulated eigenvalues will be retained. The parallel plot (Ledesma and Valero-Mora, 2007) can be used to graph the observed eigenvalues from the actual data and the estimated ones from the simulation data. The point at which the two lines of eigenvalues cross indicates the number of dimensions to retain in MDS analysis. Thus parallel analysis provides a more objective method to assess model-data fit in MDS.

In the following sections, we employed two actual studies to demonstrate how one could employ parallel analysis in determining the number of dimensions or profiles to retain in MDS. The first data was on student math achievement over a four-year period, and the second data was on student reported vocational interest as assessed via Strong-Campbell Interest Inventory (Campbell and Hansen, 1985). All the analyses were performed using SAS software package.

3 Examples

3.1 Profiles of Strong-Campbell vocational interest

The data in this example were from the Minnesota Vocational Assessment Clinic at the University of Minnesota. The sample used here contained 328 participants with no missing values. The reason

also be transformed back to distance matrix.

for using the *Strong-Campbell Interest Inventory* in this paper was that the instrument has a well-known two-dimensional MDS structure (Hogan, 1983; Prediger, 1982). The variables were measures of the six General Occupational Themes of the *Strong-Campbell Interest Inventory* (Campbell and Hansen, 1985): Realistic (practical, hands-on, action-oriented), Investigative (abstract, analytical, and theory-oriented), Artistic (imaginative and preferences for literary, musical, or artistic activities), Social (preferences for helping, teaching, treating, counseling, or serving others through personal interaction), Enterprising (preferences for persuading manipulating, or directing others), and Conventional (preferences for establishing or maintaining orderly routines, applications of standards). According to Holland (1973), these six measures form a two-dimensional hexagonal model. While Holland did not name the two dimensions, others did, and the theoretical patterns of these interests are: (1) highest scores on the Realistic and Investigative scales and lowest scores on the Enterprising and Social scales and (2) highest scores on the Artistic scale and lowest scores on the Conventional scale (e.g., Hogan, 1983).

The parallel analysis was performed using the actual sample and 1,000 random samples drawn from $N(0, \sigma^2)$ that mirrored the actual sample with respect to sample size and the number of variables. In the analysis, eigenvalues were computed using cross-product matrix converted from distance matrix based on Equation (2.1). The eigenvalues greater than the 95^{th} percentile from 1,000 random samples were obtained and used as a comparison baseline. The parallel plot of the 95th percentile simulated eigenvalues along with the observed eigenvalues from the actual data was used in model selection. Figure 1 shows the parallel plot. In the plot, the dimension with eigenvalue greater than the point at which the two lines crossed each other was retained. As can be seen in Figure 1, two dimensions had eigenvalue that was greater than the 95th percentile of simulated eigenvalues, suggesting a two-dimensional model fit the data. In contrast, the stress value was .013, .009, .005, and .001 for a one-, two-, three- and four-dimensional solution, respectively. Based on the cutoff point suggested by Kruskal (1964b), the stress value below .025 indicates an excellent fit of the model. Accordingly, all three models could provide an excellent fit for the current data, leading to an ambiguity with respect to the appropriate number of dimensions to retain. Similarly, the Bayesian dimension selection criterion, MDSIC, from Bayesian MDS analysis (Oh and Raftery, 2001; Okada and Shigemasu, 2009) of one to four dimensions was 144.38, 136.21, 128.81, and 121.53, respectively. This set of MDSIC values suggested a four-dimensional MDS model since it had the smallest value.

Based on these findings, the result from parallel analysis was consistent with the theoretical expectation of two-dimensional MDS structure. Dimensionalities more than two led to non-interpretable dimensions, which were illustrated in Figure 2. Figure 2 shows a configuration of four-dimensionality vocational interests. The interesting part of Figure 2 was that dimensions 1 and 2 represented the vocational interest suggested by Hogan (1983), with Dimension 1 being highest scores on the Realistic and Investigative scales and lowest scores on the Enterprising and Social scales and Dimension 2 being highest scores on the Artistic scale and lowest scores on the Conventional scale. It seemed that MDS parallel analysis identified these two nontrivial dimensionalities underlying the data structure. On the other hand, Dimensionalities of 3 and 4 did not suggest any interpretable vocational interest patterns, reflecting perhaps random noise in the data. Thus, we would

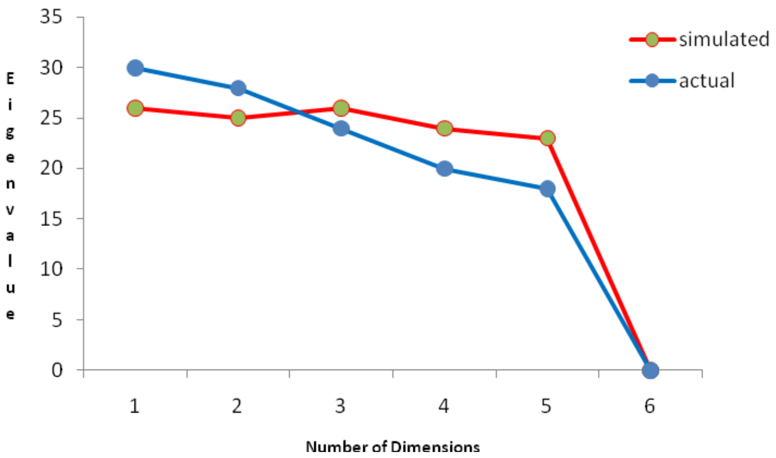

Figure 1: Parallel plot for vocational interest data. The first two profiles have eigenvalues greater than the 95th percentile of the simulated eigenvalues.

retain these two dimensions for interpretation and for subsequent analyses such as examining how these two profiles were associated with some personality variables.

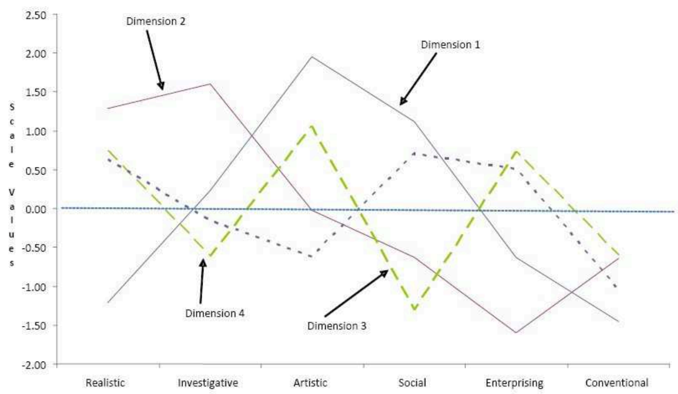

Figure 2: Four profiles of vocational interests.

3.2 Profiles of student math achievement patterns

In this second example, we presented a dataset that contained student math achievement over a four-year period. The data in this example were individual test scores from the SAT 9 mathematics test administered between 1997 and 2000 to a cohort of 337 grade 3 students in a school district from a southwestern state in the U.S. These students in grade 3 cohort were tested at 3rd, 4th, 5th, and 6th grade. Specifically from 1997 to 2000, students in the sample were annually tested in mathematics using the standardized, nationally norm-referenced Stanford Achievement Test, 9th edition (SAT-9 Math) as part of a larger effort to monitor the progress of elementary school students toward mastering mathematics knowledge from one year to the next. The SAT-9 is a widely used achievement test published by Harcourt Brace Educational Measurement in the U.S. It was designed to measure achievement in the curriculum content commonly taught in grades 1 through 9 throughout the United States. The test results of SAT-9 Math were also used as an indicator that students were making Annual Yearly Progress, AYP. For the purpose of comparing a student's progress from one year to the next, the test scores were vertically scaled across multiple measurements so that the scores were comparable over time.

The research question was: how did student math achievement change over these four years? Did all of them have increased math achievement, how much was the increase? Were there any improvements needed to be made? These questions had practical implications for the school district in terms of its school improvement plan and teaching and learning interventions. To address these issues related to growth, we conducted MDS profile growth analysis to explore the growth profiles underlying the data. Using MDS for growth modeling were investigated by Ding and his associates (Ding, Davison, and Petersen, 2005) and it was shown to be a viable alternative for studying change and growth. As in Example 1, the first task was to determine the number of growth profiles that might best approximate the data. The result from parallel analysis with 1,000 simulated samples indicated that model with one growth profile fit the data under the inquiry. Figure 3 shows the parallel plot of the analysis, and one profile clearly had an eigenvalue greater than the 95th percentile of simulated eigenvalues. In contrast, the Stress value from MDS analysis of one- to three-dimensions was .011, .007, and .003, respectively, providing no clear indication of appropriate number of dimensions based on the cutoff point of .025 as suggested by Kruskal (1964a). The Bayesian dimension selection criterion, MDSIC, was 132.21, 115.68, and 109.52 for one- to three-dimension, respectively, indicating a three-dimensional MDS structure, which was inconsistent with what we expected.

Table 1 shows the scale values of math achievement over a four-year period. This profile showed that the students in the grade 3 cohort had a linear increase in math achievement from 1997 to 2000, with percentage of increase being 40% in the 1998, 31% in 1999, and 29% in 2000, respectively.

Table 1: Scale Values of Math Achievement of Students in a Grade 3 Cohort

Time	Scale Vales
1997	-1.42
1998	-0.35
1999	0.49
2000	1.28

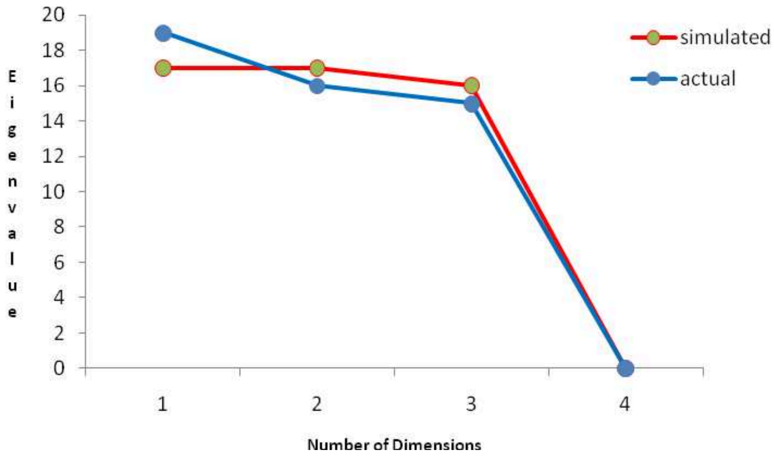

Figure 3: Parallel plot for math achievement data. The first profile has eigenvalue greater than the 95^{th} percentile of the simulated eigenvalues.

4 Conclusion

In the paper, we suggested using parallel analysis as a MDS model-data fit criterion for determining the number of dimensions or profiles that underlie the data in MDS analysis. Our results based on two real datasets revealed that parallel analysis seemed to provide a more objective method than stress value in this regard. In both examples, results from parallel analysis provided clear evidence on number of dimensions or profiles to retain in MDS, whereas Stress value did not provide such a clear indication of appropriate number of dimensions to retain. In general, the advantage of parallel analysis is that it should provide more objective criterion for model selection than stress value and other available methods to determine appropriate MDS solutions. In view of that, this paper describes a new approach that may serves as a catalyst for stimulating further investigations.

In the current study, parallel analysis for MDS was performed using a SAS macro. SAS is a commonly used statistical analysis package and the macro for MDS parallel analysis was easy to use. The programming of such a macro is not extensive, and when SAS is not available, the macro can also be programmed into R statistical language, which is free statistical software.

The implication of the current study for practice is that although parallel analysis is one of the recommended criteria for determining the appropriate number of factors in factor analysis, it has not been utilized and fully investigated in MDS analysis. Given the limited choice of model selection criteria in MDS analysis, the results of the study provide preliminary evidence of parallel analysis as a potential method for model selection, adding one more tool for deciding on the number of dimensions. Research should employ this criterion, along with Stress value and other available methods to determine appropriate MDS solutions. In view of that, this paper describes a new approach that may serves as a catalyst for stimulating further investigations.

However, model selection is complex, involving issues of model parsimony, interpretability, practicality, as well as philosophical perspective on the role of model. There are several points that are worth noting. First, Abidi's method for converting distance matrix to cross-product matrix is proposed for metric data. The key difference between metric and nonmetric MDS is how the observed distance is assumed to be related to the model-derived distance. But the basic logic with respect to variance explained by the dimensionality is the same for both models. Thus, the parallel analysis may also be applicable to nonmetric MDS. Second, in the current study we used the 95th percentile when comparing the eigenvalues of the observed cross-product matrix with that of the simulated ones. However, there is a need to examine the conditions in which the 95th percentile may be preferred over median when comparing the eigenvalues of the observed cross-product matrix with that of the simulated ones. Third, given the complexity of model selection, the suitability of employing parallel analysis in MDS needs to be further examined using more sophisticate methods such as simulation studies.

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