

Preface

A set of multivariate data can be expressed as a table, i.e., a matrix, of individuals (rows) by variables (columns), with the variables interrelated. Statistical procedures for analyzing such data sets are generally referred to as multivariate data analysis. The demand for this kind of analysis is increasing in a variety of fields. Each procedure in multivariate data analysis features a special purpose. For example, predicting future performance, classifying individuals, visualizing inter-individual relationships, finding a few factors underlying a number of variables, and examining causal relationships among variables are included in the purposes for the procedures.

The aim of this book is to enable readers who may not be familiar with matrix operations to understand major multivariate data analysis procedures in matrix forms. For that aim, this book begins with explaining fundamental matrix calculations and the matrix expressions of elementary statistics, followed by an introduction to popular multivariate procedures, with chapter-by-chapter advances in the levels of matrix algebra. The organization of this book allows readers without knowledge of matrices to deepen their understanding of multivariate data analysis.

Another feature of this book is its emphasis on the model that underlies each procedure and the objective function that is optimized for fitting the model to data. The author believes that the matrix-based learning of such models and objective functions is the shortest way to comprehend multivariate data analysis. This book is also arranged so that readers can intuitively capture for what purposes multivariate analysis procedures are utilized; plain explanations of the purposes with numerical examples precede mathematical descriptions in almost all chapters.

The preceding paragraph featured three key words: purpose, model, and objective function. The author considers that capturing those three points for each procedure suffices to understand it. This consideration implies that the mechanisms behind how objective functions are optimized must not necessarily be understood. Thus, the mechanisms are only described in appendices and some exercises.

This book is written with the following guidelines in mind:

- (1) Not using mathematics except matrix algebra
- (2) Emphasizing singular value decomposition (SVD)
- (3) Preferring a simultaneous solution to a successive one

Although the exceptions to (1) are found in Appendix A6, where differential calculus is used, and in some sections of Part III and Chap. 15, where probabilities are used, those exceptional parts only occupy a limited number of pages; the majority of the book is matrix-intensive. Matrix algebra is also exclusively used for formulating the optimization of objective functions in Appendix A4. For matrix-intensive formulations, ten Berge's (1983, 1993) theorem is considered to be the best starting fact, as found in Appendix A4.1.

Guideline (2) is due to the fact that SVD can be defined for any matrix, and a number of important properties of matrices are easily derived from SVD. In the former point, SVD is more general than eigenvalue decomposition (EVD), which is only defined for symmetric matrices. Thus, EVD is only mentioned in Sect. 6.2. Further, SVD takes on an important role in optimizing trace and least squares functions of matrices: The optimization problems are formulated with the combination of SVD and ten Berge's (1983, 1993) theorem, as found in Appendix A4.2 and Appendix A4.3.

Guideline (3) is particularly concerned with principal component analysis (PCA), which can be formulated as minimizing $\|\mathbf{X} - \mathbf{FA}'\|^2$ over PC score matrix \mathbf{F} and loading matrix \mathbf{A} for a data matrix \mathbf{X} . In some of the literature, PCA is described as obtaining the first component, the second, and the remaining components in turn (i.e., per column of \mathbf{F} and \mathbf{A}). This can be called a successive solution. On the other hand, PCA can be described as obtaining \mathbf{F} and \mathbf{A} matrix-wise, which can be called a simultaneous solution. This is preferred in this book, as the above formulation is actually made matrix-wise and the simultaneous solution facilitates understanding PCA as a reduced rank approximation of \mathbf{X} .

This book is appropriate for undergraduate students who have already learned introductory statistics, as the author has used preliminary versions of the book in a course for such students. It is also useful for graduate students and researchers who are not familiar with the matrix-intensive formulations of multivariate data analysis.

I owe this book to the people who can be called the "matricians" in statistics, more exactly, the ones taking matrix-intensive approaches for formulating and developing data analysis procedures. Particularly, I have been influenced by the Dutch psychometricians, as found above, in that I emphasize the theorem by Jos M.F. ten Berge (Professor Emeritus, University of Groningen). Yutaka Hirachi of Springer has been encouraging me since I first considered writing this book. I am most grateful to him. I am also thankful to the reviewers who read through drafts of this book. Finally, I must show my gratitude to Yoshitaka Shishikura of the publisher Nakanishiya Shuppan, as he readily agreed to the use of the numerical examples in this book, which I had originally used in that publisher's book.

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