Contents

CHAPTER 1 Introduction 1.1. Definition and Derivation of Principal Components 1.2. A Brief History of Principal Component Analysis	1 1 5
CHAPTER 2	
Mathematical and Statistical Properties of Population Principal	8
Components	٥
2.1. Optimal Algebraic Properties of Population Principal Components and	9
Their Statistical Implications	14
2.2. Geometric Properties of Population Principal Components	16
2.3. Principal Components Using a Correlation Matrix2.4. Principal Components with Equal and/or Zero Variances	21
CHAPTER 3	
Mathematical and Statistical Properties of Sample Principal	
Components	23
3.1 Optimal Algebraic Properties of Sample Principal Components	24
3.2. Geometric Properties of Sample Principal Components	27
3.3 Covariance and Correlation Matrices: An Example	32
3.4. Principal Components with Equal and/or Zero Variances	36
3.5 The Singular Value Decomposition	3
3.6 Probability Distributions for Sample Principal Components	39
3.7 Inference Based on Sample Principal Components	4
3.8. Principal Components for Patterned Correlation or Covariance	
Matrices	4

xii Contents

CHA	PTER 4	
Prin	cipal Components as a Small Number of Interpretable Variables:	
Som	e Examples	50
4.1.	Anatomical Measurements	51
4.2.	The Elderly at Home	55
4.3.	Spatial and Temporal Variation in Meteorology	58
4.4.	Properties of Chemical Compounds	60
4.5.	Stock Market Prices	61
	PTER 5	
Graj	phical Representation of Data Using Principal Components	64
5.1.	Plotting Data with Respect to the First Two (or Three) Principal	
	Components	65
	Principal Co-ordinate Analysis	71
	Biplots	75
	Correspondence Analysis	85
5.5.	Comparisons Between Principal Co-ordinates, Biplots, Correspondence	
	Analysis and Plots Based On Principal Components	88
5.6.	Methods for Graphical Display of Intrinsically High-Dimensional Data	89
	PTER 6	
Cho	osing a Subset of Principal Components or Variables	92
	How Many Principal Components?	93
	Choosing m, the Number of Components: Examples	103
	Selecting a Subset of Variables	107
6.4.	Examples Illustrating Variable Selection	110
	PTER 7	
Prin	cipal Component Analysis and Factor Analysis	115
7.1.	Models for Factor Analysis	116
	Estimation of the Factor Model	117
7.3.	Comparisons and Contrasts Between Factor Analysis and Principal	
	Component Analysis	122
	An Example of Factor Analysis	124
7.5.	Concluding Remarks	128
	PTER 8	
	cipal Components in Regression Analysis	129
	Principal Component Regression	130
8.2.	Strategies for Selecting Components in Principal Component	
	Regression	135
8.3.	Some Connections Between Principal Component Regression and	
	Other Biased Regression Methods	138
8.4.	Variations on Principal Component Regression	139
	Variable Selection in Regression Using Principal Components	143
	Functional and Structural Relationships	145
8.7.	Examples of Principal Components in Regression	147

CHAPTER 9 Principal Components Used with Other Multivariate Techniques 9.1. Discriminant Analysis 9.2. Cluster Analysis 9.3. Canonical Correlation Analysis	156 157 162 170
CHAPTER 10 Outlier Detection, Influential Observations and Robust Estimation	
of Principal Components	173
10.1. Detection of Outliers Using Principal Components	174
10.2. Influential Observations in a Principal Component Analysis	187
10.3. Robust Estimation of Principal Components	195
10.4. Concluding Remarks	198
CHAPTER 11	
Principal Component Analysis for Special Types of Data	199
11.1. Principal Component Analysis for Discrete Data	200
11.2. Principal Component Analysis for Non-independent and Time Series	205
Data Data	203
11.3. Principal Component Analysis for Compositional Data	212
11.4. Principal Component Analysis in Designed Experiments11.5. Common Principal Components in the Presence of Group Structure	212
and Comparisons of Principal Components	215
11.6. Principal Component Analysis in the Presence of Missing Data	219
11.7. Principal Components for Goodness-of-Fit Statistics	221
CHAPTER 12	
Generalizations and Adaptations of Principal Component Analysis	223
12.1. Generalized and Weighted Principal Component Analysis	224
12.2. Non-linear Principal Component Analysis	226
12.3. Non-centred Principal Component Analysis and Doubly-Centred	227
Principal Component Analysis	227
12.4. Discrete Coefficients for Principal Components and Sensitivity of	229
Principal Components	Litery
12.5. Principal Components in the Presence of Secondary or Instrumental	231
Variables 12.6. Alternatives to Principal Component Analysis for Non-normal	
Distributions	232
12.7. Three-Mode Principal Component Analysis	232
12.8. Concluding Remarks	233
APPENDIX	
Computation of Principal Components	235
A1. Numerical Calculation of Principal Components	235
A2. Principal Component Analysis in Computer Packages	240
References	247
Index	259