

Contents

1	INTRODUCTION	1
1.1	Data Matrices and Scatter Diagrams, 3	
1.2	Some Definitions and Other Preliminaries, 8	
1.3	Aim and Scope of This Book, 11	
2	CLASSIFICATION BY CLUSTERING	13
2.1	Introduction, 13	
2.2	Nearest-Neighbor Clustering, 15	
2.3	Farthest-Neighbor Clustering, 22	
2.4	Centroid Clustering, 25	
2.5	Minimum Variance Clustering, 32	
2.6	Dissimilarity Measures and Distances, 40	
2.7	Average Linkage Clustering, 63	
2.8	Choosing Among Clustering Methods, 72	
2.9	Rapid Nonhierarchical Clustering, 76	
	Appendix: Apollonius's Theorem, 78	
	Exercises, 79	
3	TRANSFORMING DATA MATRICES	83
3.1	Introduction, 83	
3.2	Vector and Matrix Multiplication, 85	

- 3.3 The Product of a Data Matrix and its Transpose, 102
- 3.4 The Eigenvalues and Eigenvectors of a Square Symmetric Matrix, 116
- 3.5 The Eigenanalysis of XX' and $X'X$, 126
- Exercises, 129

4 ORDINATION

133

- 4.1 Introduction, 133
- 4.2 Principal Component Analysis, 136
- 4.3 Four Different Versions of PCA, 152
- 4.4 Principal Coordinate Analysis, 165
- 4.5 Reciprocal Averaging or Correspondence Analysis, 176
- 4.6 Linear and Nonlinear Data Structures, 188
- 4.7 Comparisons and Conclusions, 197
- Exercises, 199

5 DIVISIVE CLASSIFICATION

203

- 5.1 Introduction, 203
- 5.2 Constructing and Partitioning a Minimum Spanning Tree, 205
- 5.3 Partitioning a PCA Ordination, 211
- 5.4 Partitioning RA and DCA Ordinations, 218
- Exercises, 221

6 DISCRIMINANT ORDINATION

223

- 6.1 Introduction, 223
- 6.2 Unsymmetric Square Matrices, 224
- 6.3 Discriminant Ordination of Several Sets of Data, 230
- Exercises, 237

CONTENTS

xi

ANSWERS TO EXERCISES

239

GLOSSARY

247

BIBLIOGRAPHY

257

INDEX

261