

Contents

Preface	xii
1 What are compositional data, and why are they special?	1
1.1 Examples of compositional data	1
1.2 Why are compositional data different from other types of data?	2
1.3 Basic terminology and notation in compositional data analysis	3
1.4 Basic principles of compositional data analysis	5
1.5 Ratios and logratios	6
2 Geometry and visualization of compositional data	9
2.1 Simple graphics	9
2.2 Geometry in a simplex	12
2.3 Moving out of the simplex	14
2.4 Distances between points in logratio space	15
3 Logratio transformations	17
3.1 Additive logratio transformations	17
3.2 Centred logratio transformations	18
3.3 Logratios incorporating amalgamations	19
3.4 Isometric logratio transformations	19
3.5 Comparison of logratios in practice	21
3.6 Practical interpretation of logratios	23
4 Properties and distributions of logratios	25
4.1 Lognormal distribution	25
4.2 Logit function	27
4.3 Additive logistic normal distribution	27
4.4 Logratio variances and covariances	28

4.5 Testing for multivariate normality	30
4.6 When logratios are not normal	31
5 Regression models involving compositional data	33
5.1 Visualizing ratios as a graph	33
5.2 Using simple logratios as predictors	34
5.3 Compositions as responses – total logratio variance	37
5.4 Redundancy analysis	39
6 Dimension reduction using logratio analysis	41
6.1 Weighted principal component analysis	41
6.2 Logratio analysis	42
6.3 Different biplot scaling options	44
6.4 Constrained compositional biplots	46
7 Clustering of compositional data	49
7.1 Logratio distances between rows and between columns	49
7.2 Clustering based on logratio distances	50
7.3 Weighted Ward clustering	50
7.4 Isometric logratio versus amalgamation balances	53
8 Problem of zeros, with some solutions	57
8.1 Zero replacement	57
8.2 Sensitivity to zero replacement	58
8.3 Subcompositional incoherence	59
8.4 Correspondence analysis alternative	60
9 Simplifying the task: variable selection	65
9.1 Explaining total logratio variance	65
9.2 Stepwise selection of logratios	66
9.3 Parsimonious variable selection	68
9.4 Amalgamation logratios as variables for selection	70
9.5 Signal and noise in compositional data	70
10 Case study: Fatty acids of marine amphipods	73
10.1 Introduction	73
10.2 Material and methods	74
10.3 Results	75
10.4 Discussion and conclusion	80

A Appendix: Theory of compositional data analysis	81
A.1 Basic notation	81
A.2 Ratios and logratios	82
A.3 Logratio distance	85
A.4 Logratio variance	85
A.5 Logratio analysis (LRA)	86
A.6 Principal component analysis (PCA)	87
A.7 Procrustes analysis	88
A.8 Constrained logratio analysis and redundancy analysis	89
A.9 Permutation tests	89
A.10 Weighted Ward clustering	90
B Appendix: Bibliography of compositional data analysis	91
B.1 Books	91
B.2 Articles	92
B.3 Web resources	95
C Appendix: Computation of compositional data analysis	97
C.1 Simple graphics for compositional data	97
C.2 Logratio transformations	98
C.3 Compositional data modelling	102
C.4 Compositional data analytics	103
D Appendix: Glossary of terms	111
E Appendix: Epilogue	115
Index	119
